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

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Supporting Information

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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

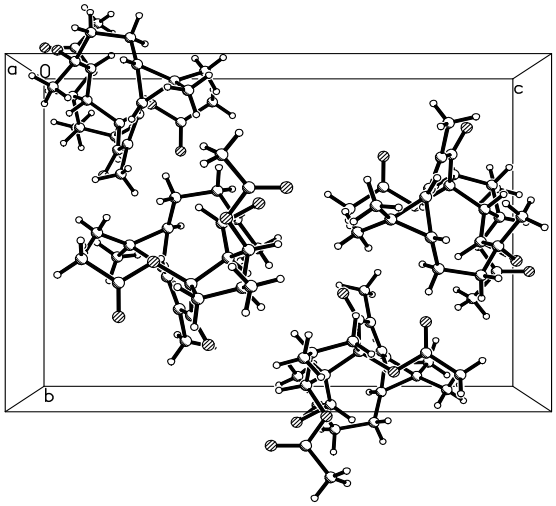

Figure S1. Crystal Cell Diagram for **1.**

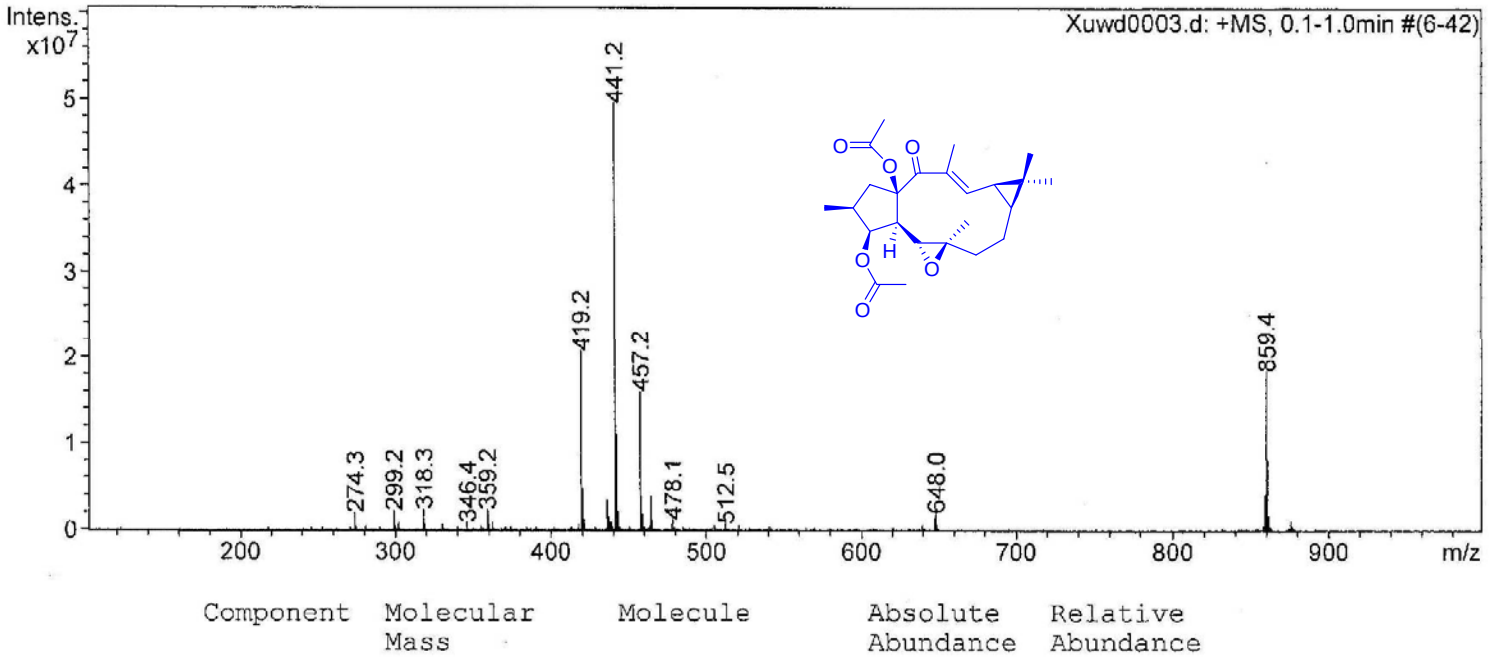

Figure S2. (+)-ESIMS Spectrum of 1.

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[...

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

Charge number:1
Tolerance:5.00(mmu)
Unsaturation Number:-1.5 .. 20.0 (Fraction:Both)
Element:^{12}C:0 .. 100, ^{1}H:0 .. 200, ^{23}Na:1 .. 1, ^{16}O:0 .. 10

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.

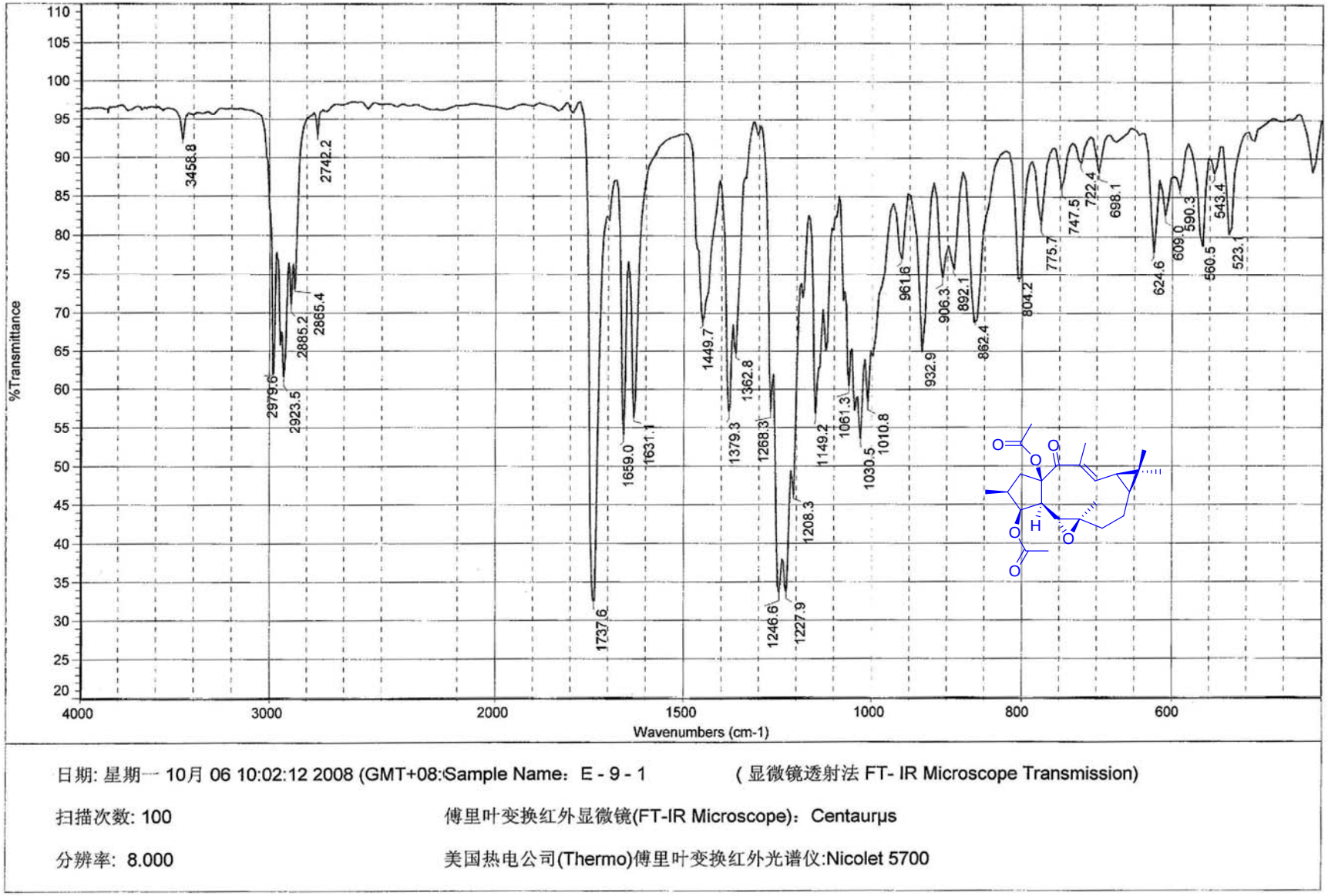

Figure S3. The IR Spectrum of 1.

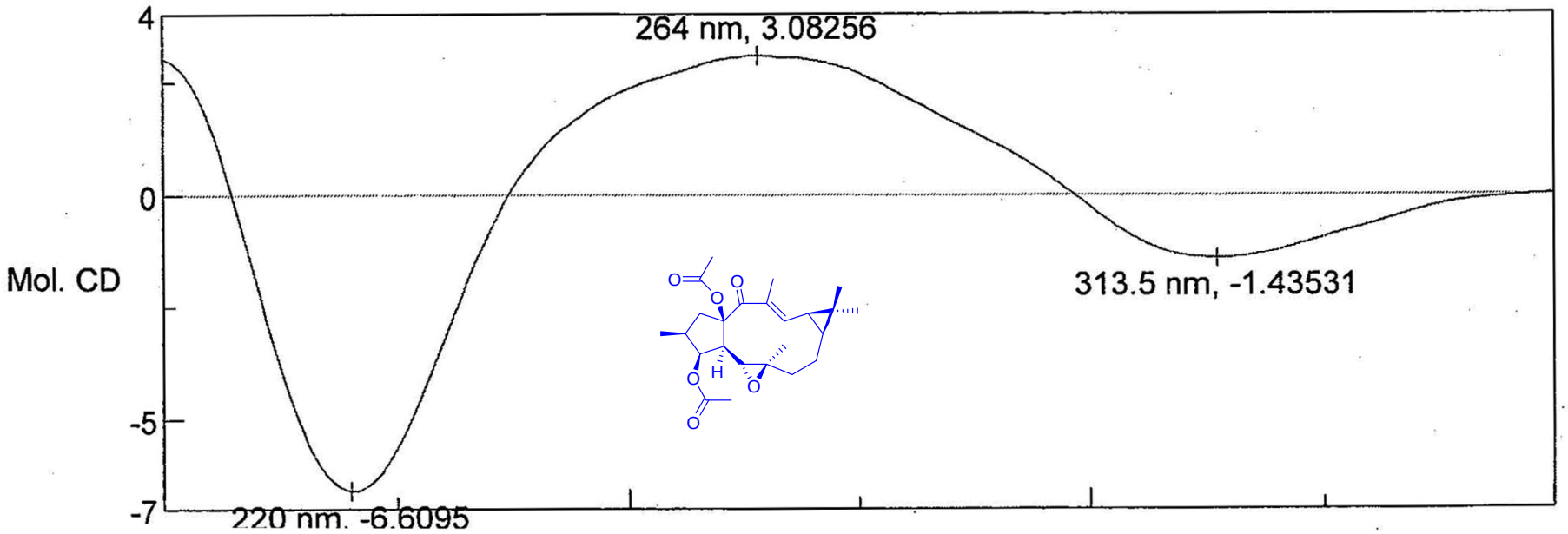

Figure S4. The CD Spectrum of 1.

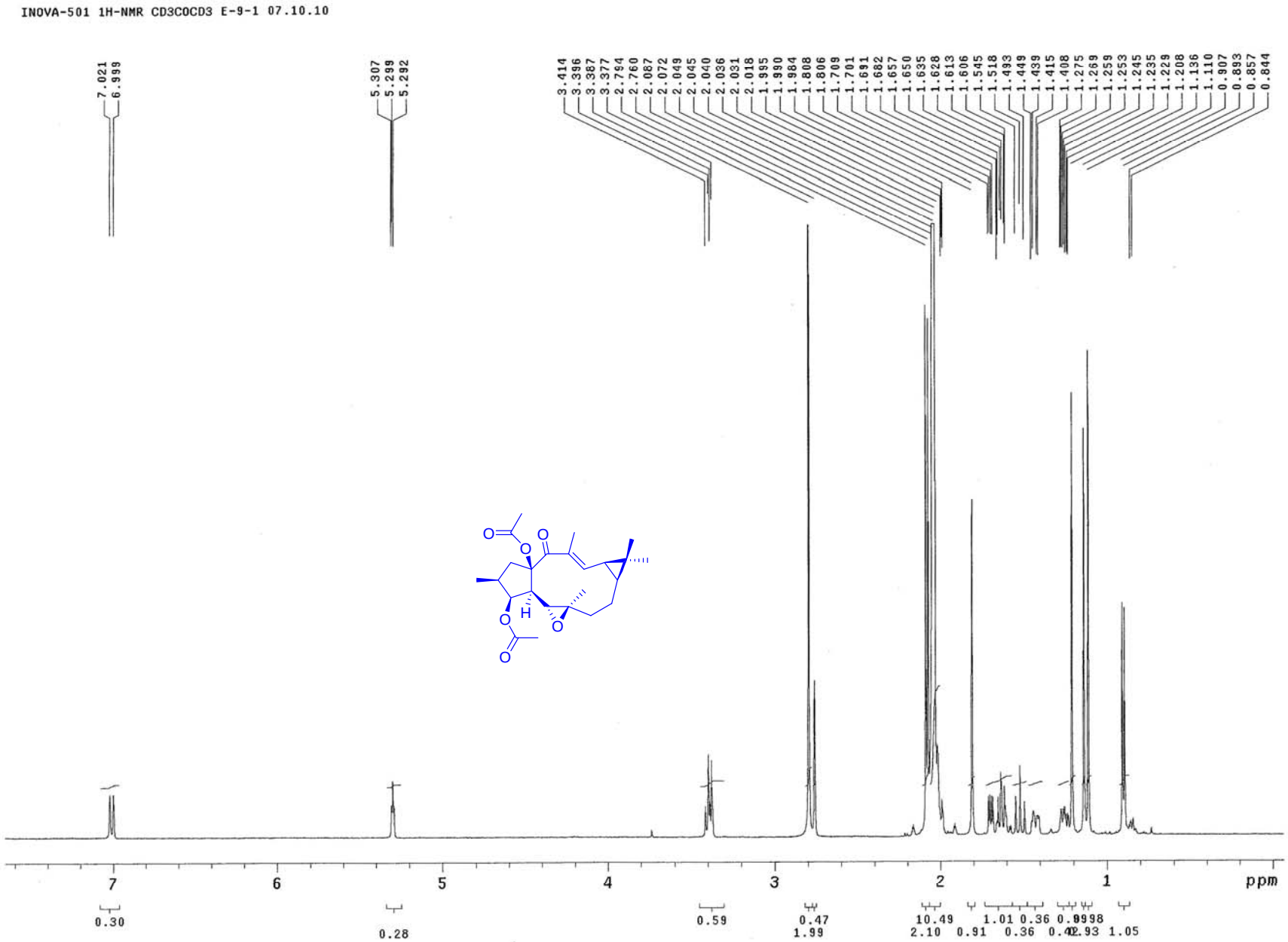

Figure S5. The ^{1}H NMR Spectrum of 1 in CD_3COCD_3 (500 MHz).

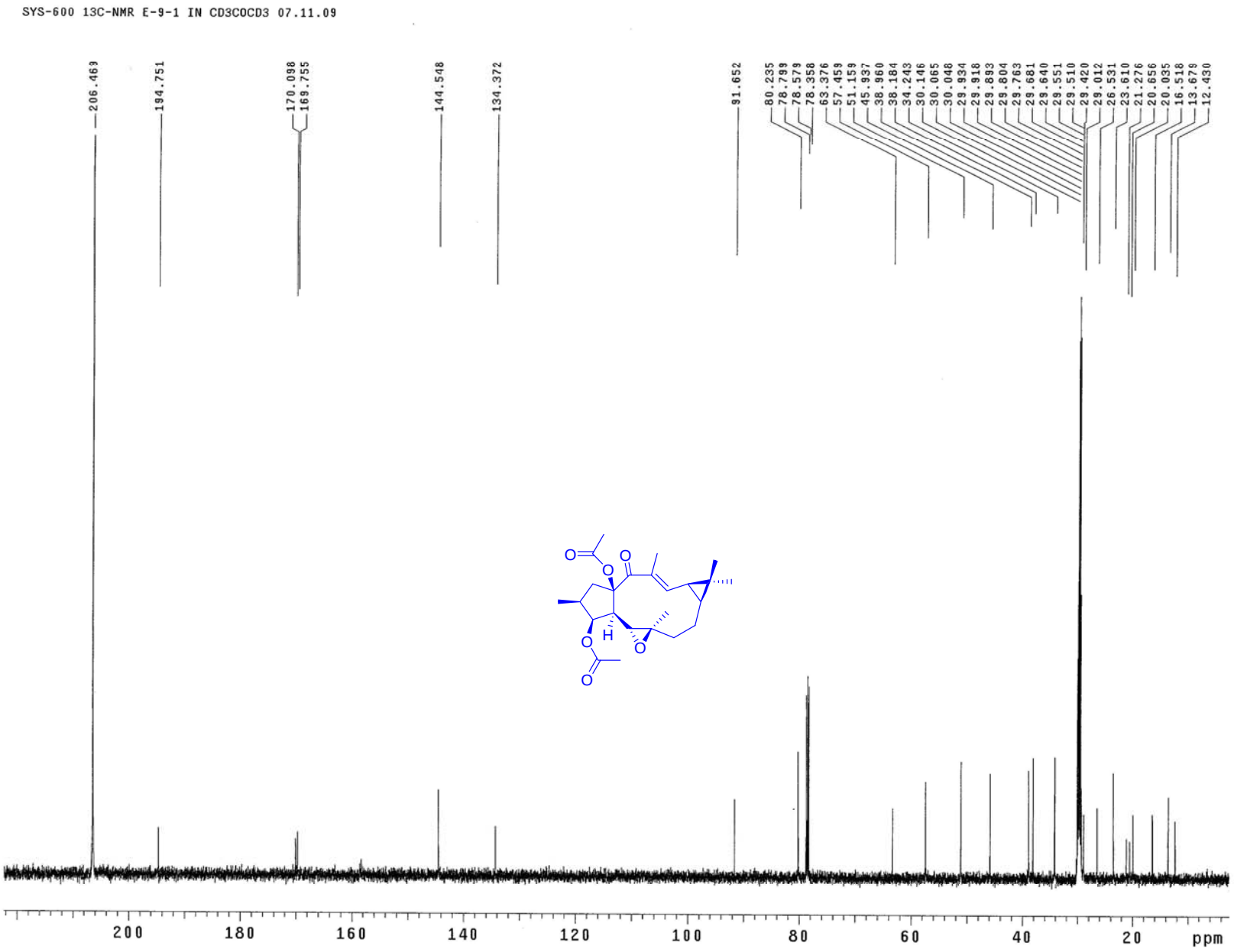

Figure S6. The ^{13}C NMR Spectrum of 1 in CD_3COCD_3 (150 MHz).

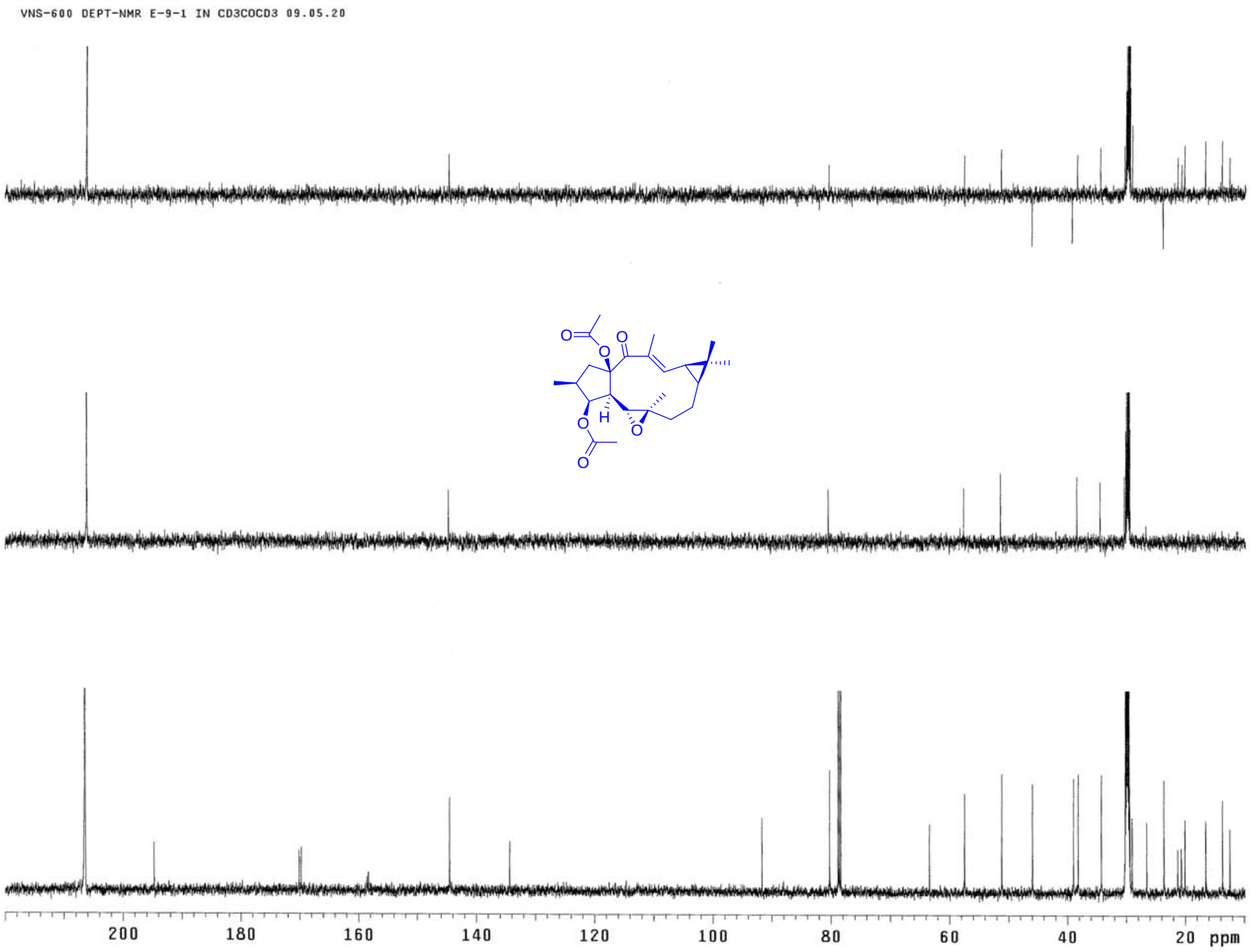

Figure S7. The DEPT Spectrum of 1 in CD_3COCD_3 (150 MHz).

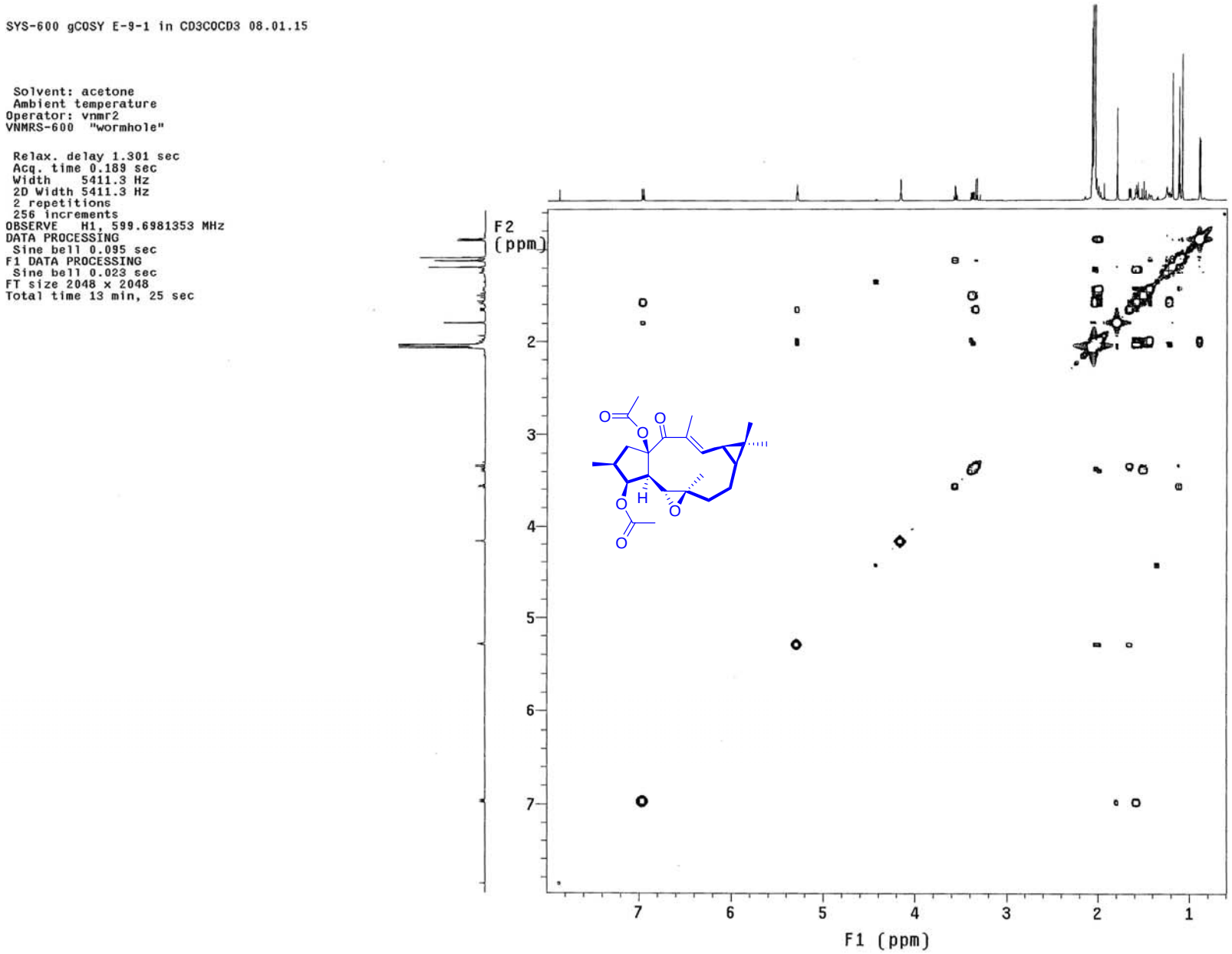

Figure S8. The ^{1}H-^{1}H gCOSY Spectrum of 1 in CD_3COCD_3 (600 MHz).

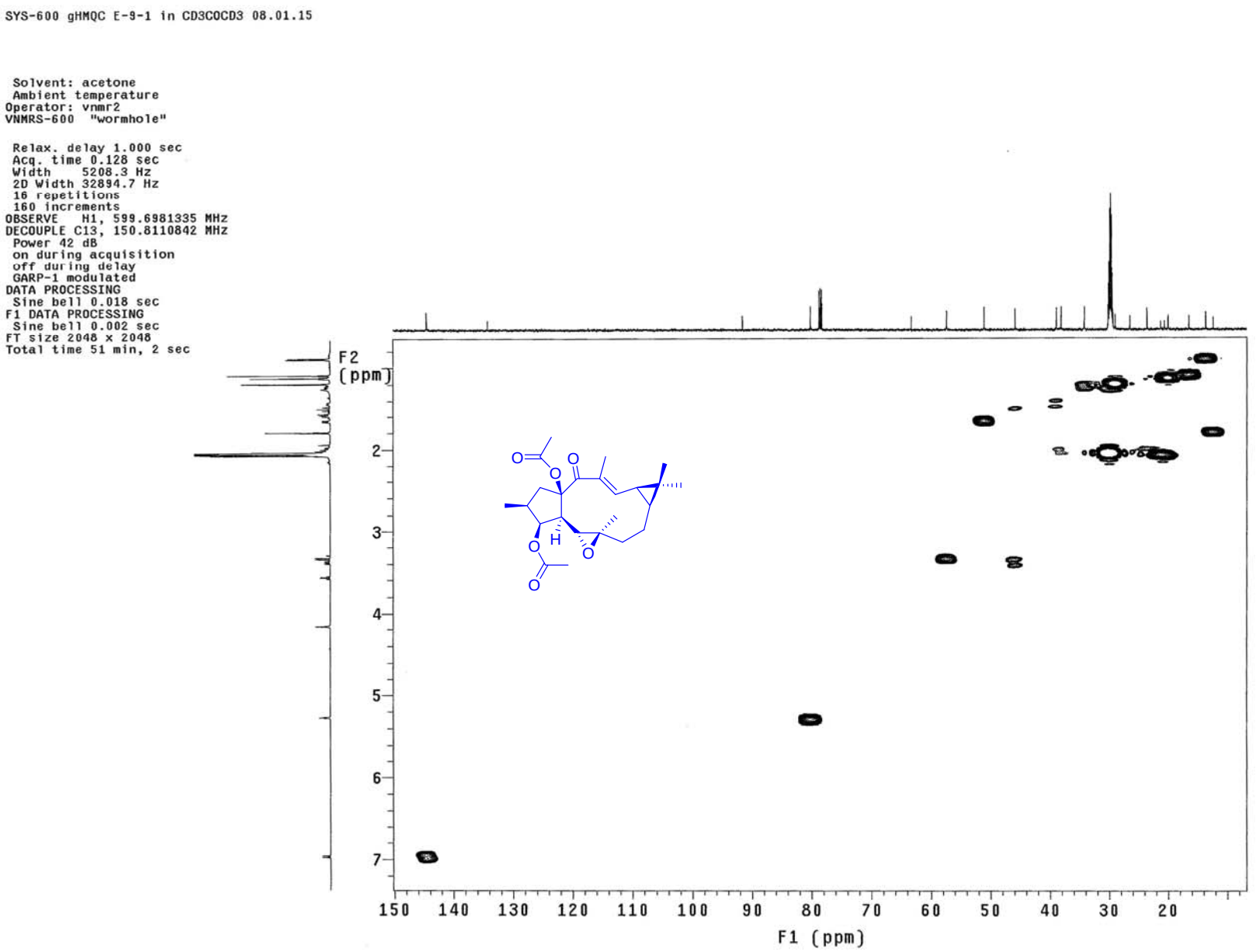

Figure S9. The gHSQC Spectrum of 1 in CD_3COCD_3 (600MHz for ^1H NMR).

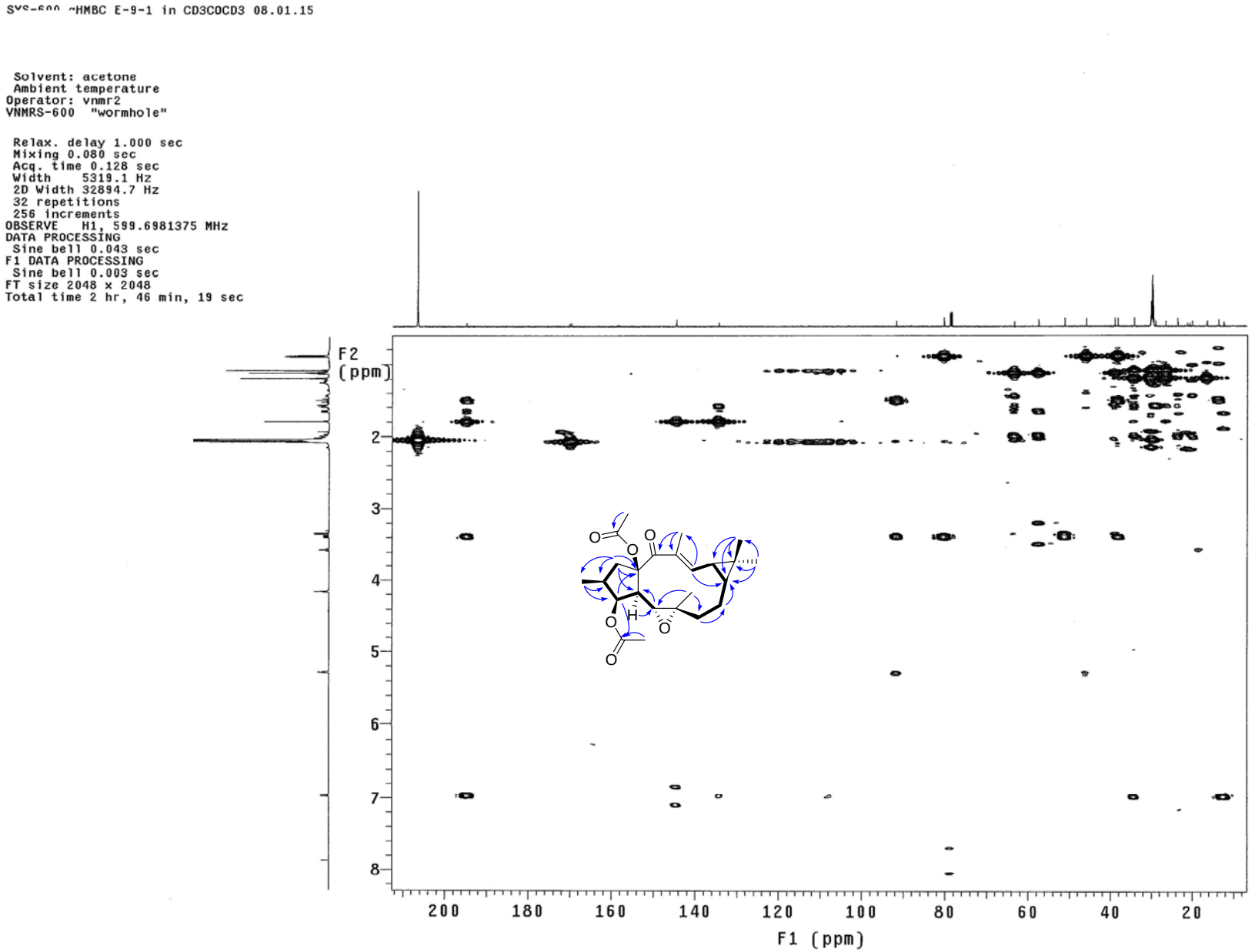

Figure S10. The gHMBC Spectrum of 1 in CD_3COCD_3 (600MHz for ^1H NMR).

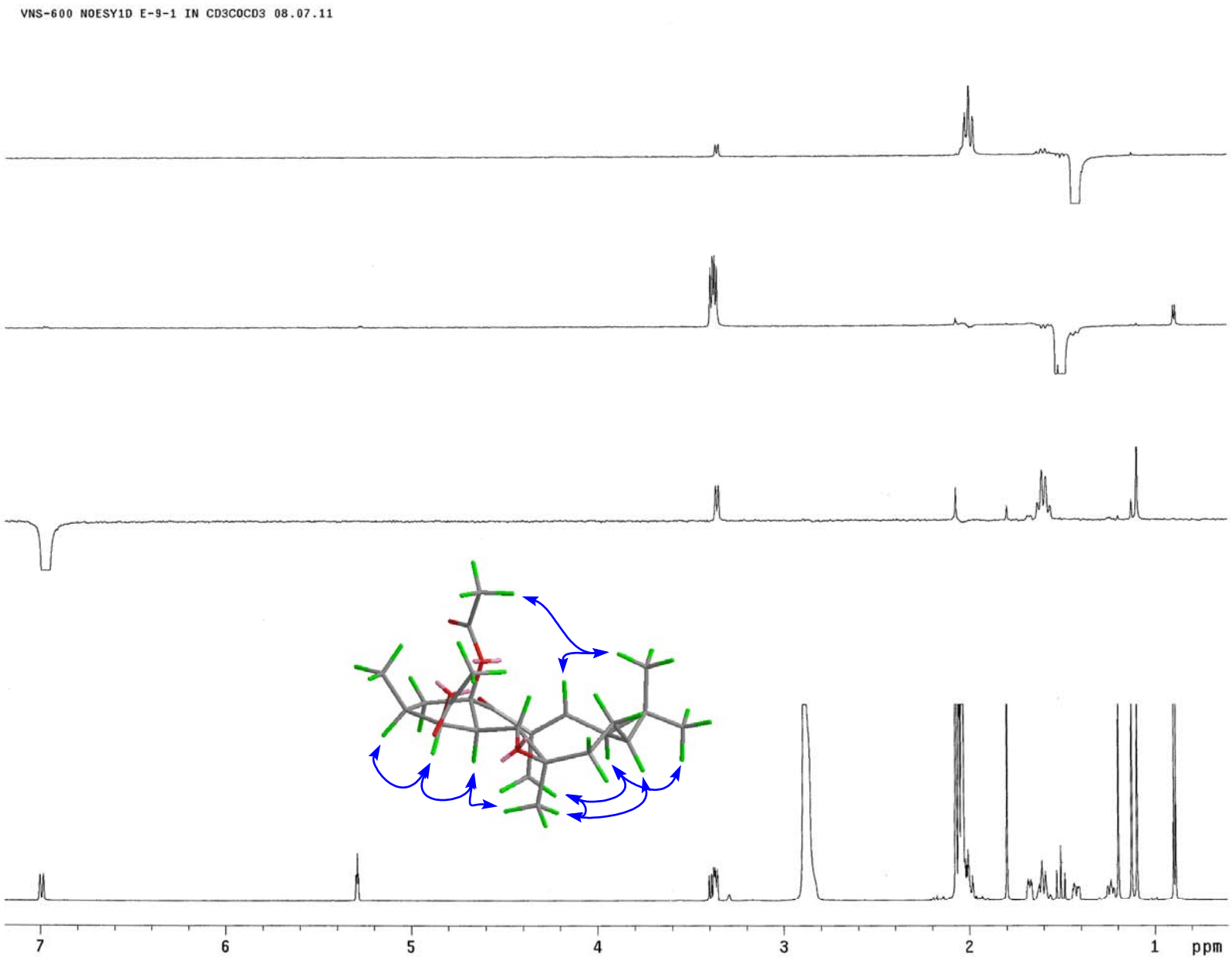

Figure S11. The NOE Difference Spectrum 1 of 1 in CD_3COCD_3 (600 MHz).

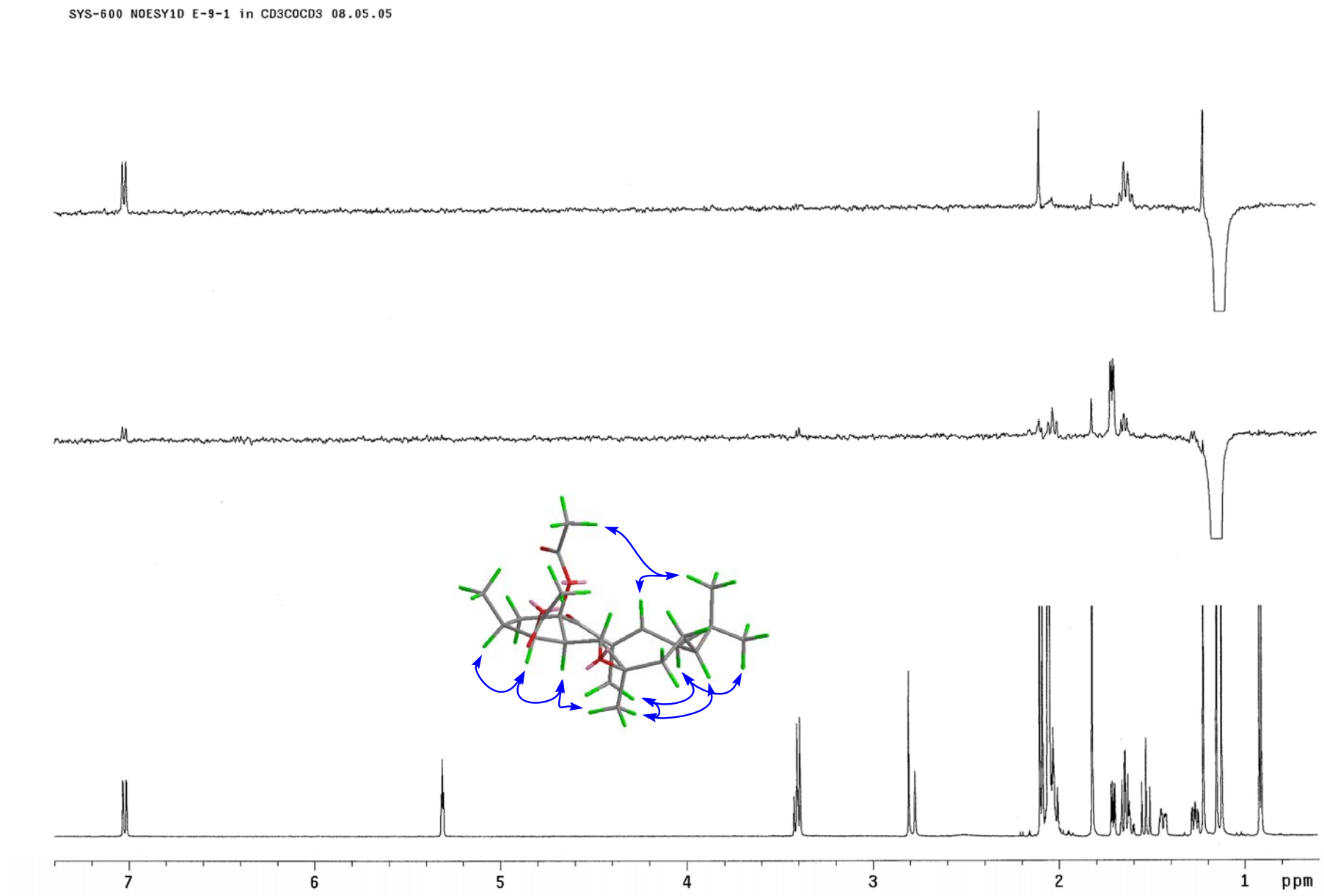

Figure S12. The NOE Difference Spectrum 2 of 1 in CD_3COCD_3 (600 MHz).

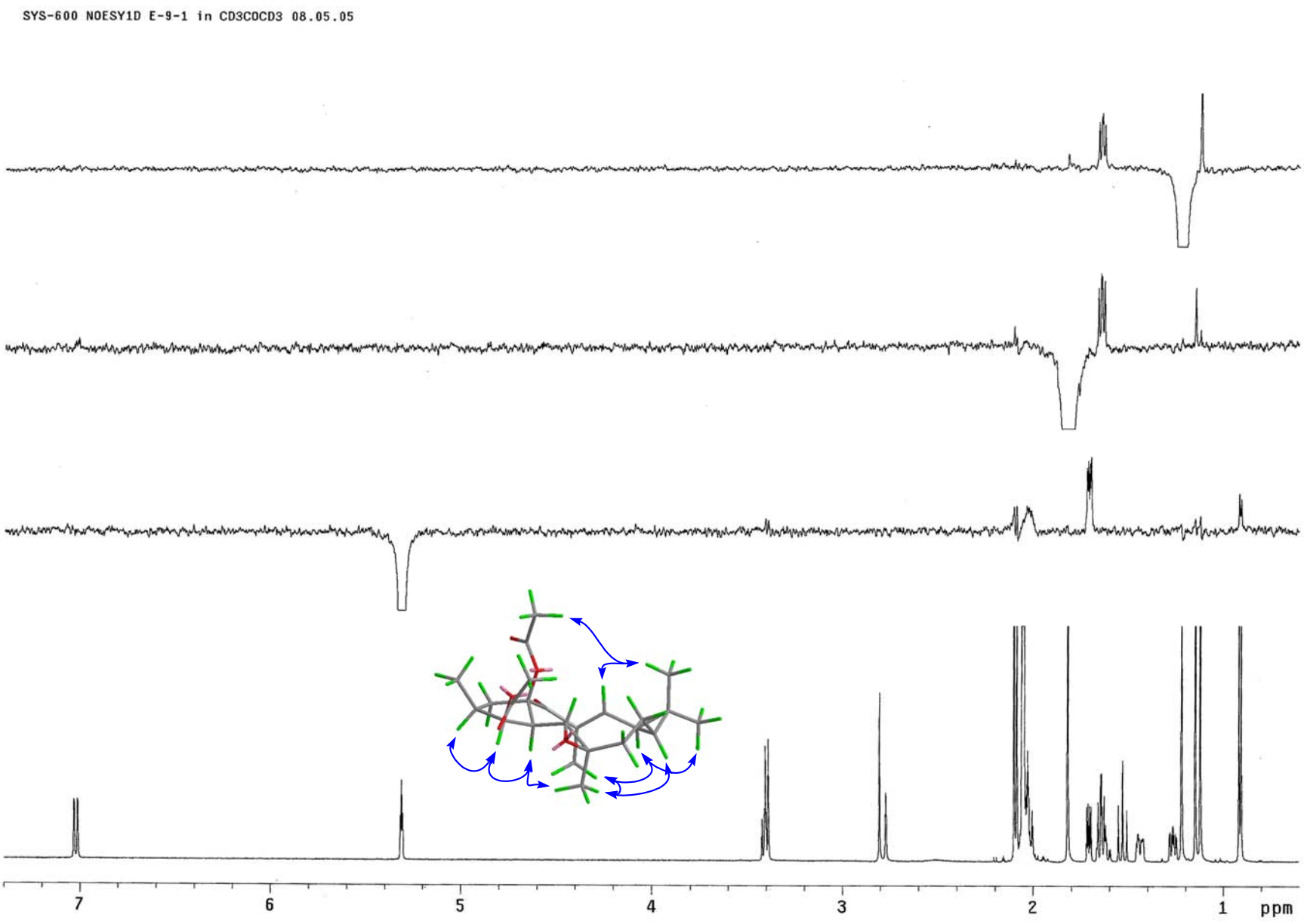

Figure S13. The NOE Difference Spectrum 3 of 1 in CD_3COCD_3 (600 MHz).

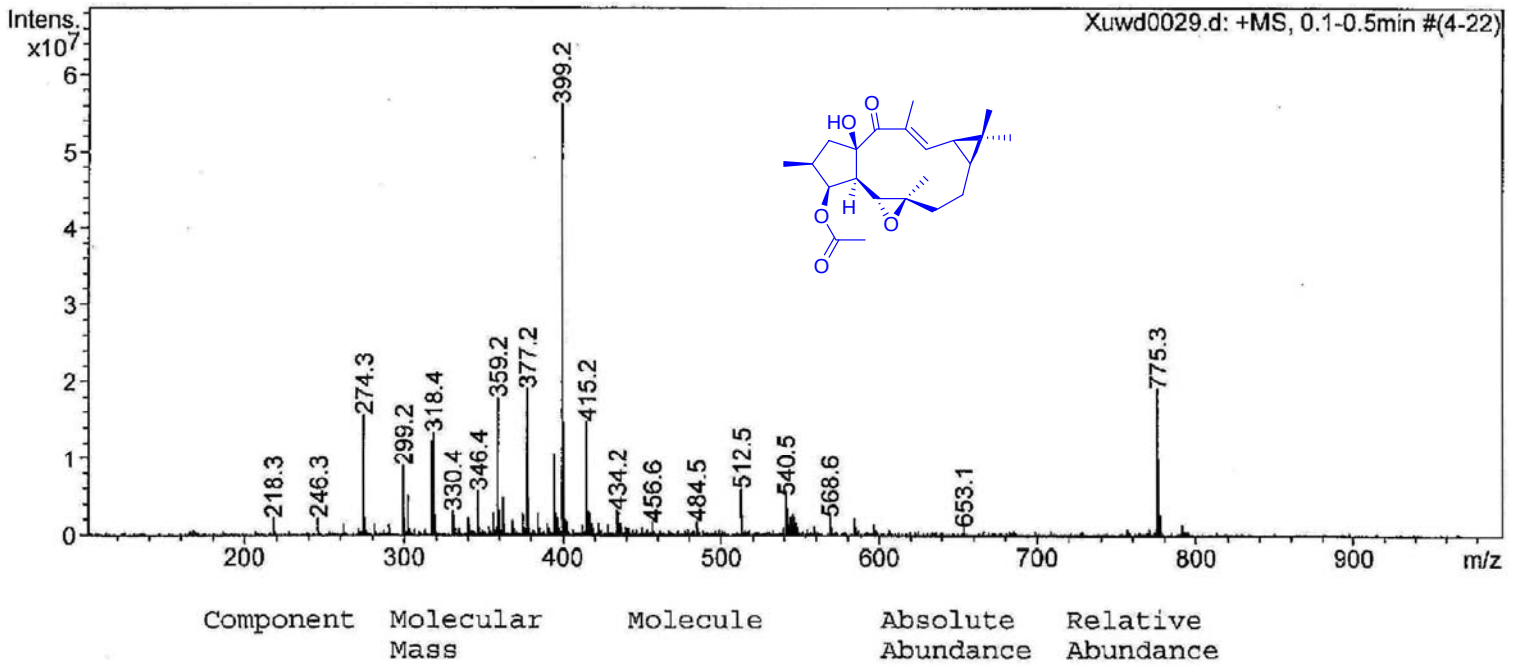

Figure S14. (+)-ESIMS Spectrum of 2.

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

Tolerance:5.00(mmu)

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

Mass	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	^{12}C	^{1}H	^{39}K	^{16}O	Unsaturation Number
415.10331	415.18868	4.63	11.14	22	32	1	5	6.5

(+)-HRESIMS Data of 2.

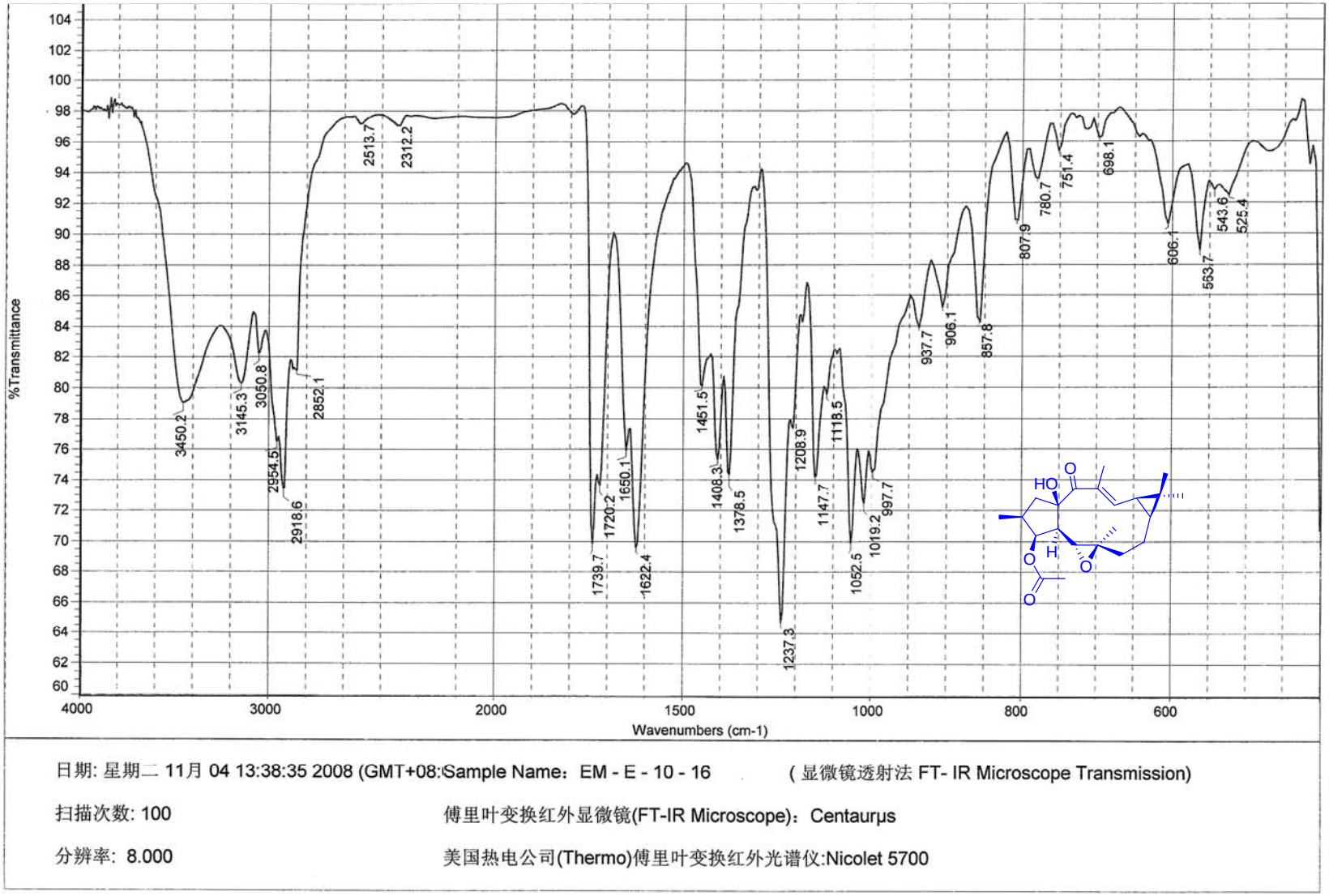

Figure S15. The IR Spectrum of 2.

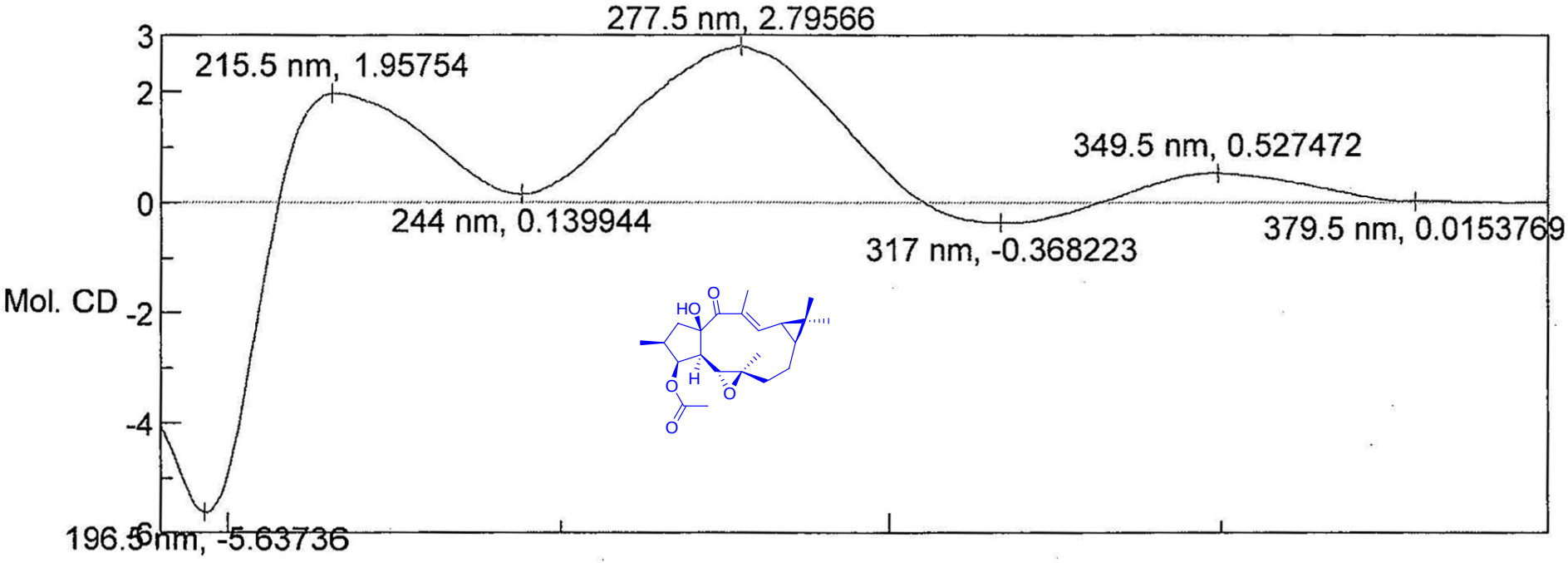

Figure S16. The CD Spectrum of 2.

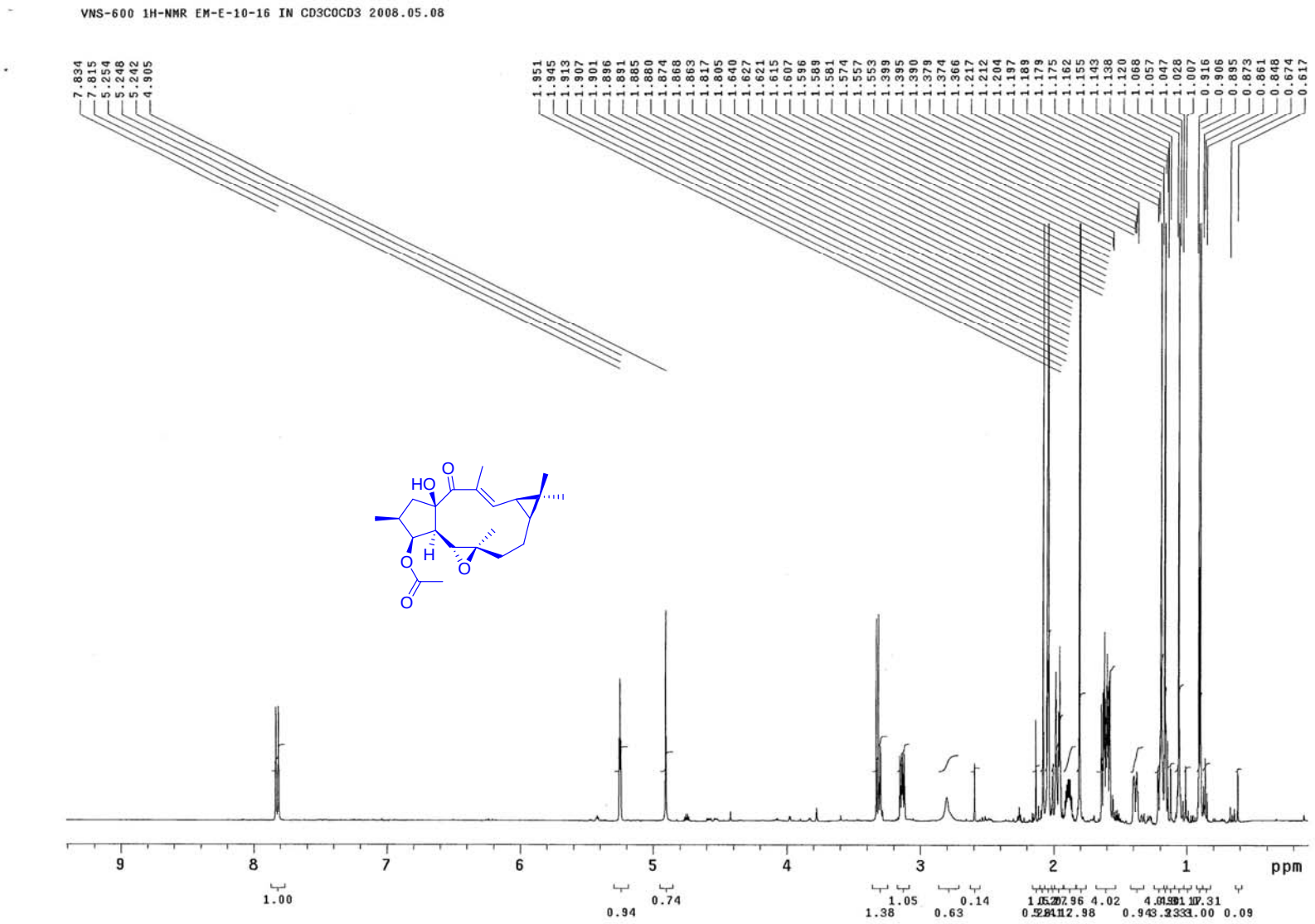

Figure S17. The ^{1}H NMR Spectrum of 2 in CD_3COCD_3 (600 MHz).

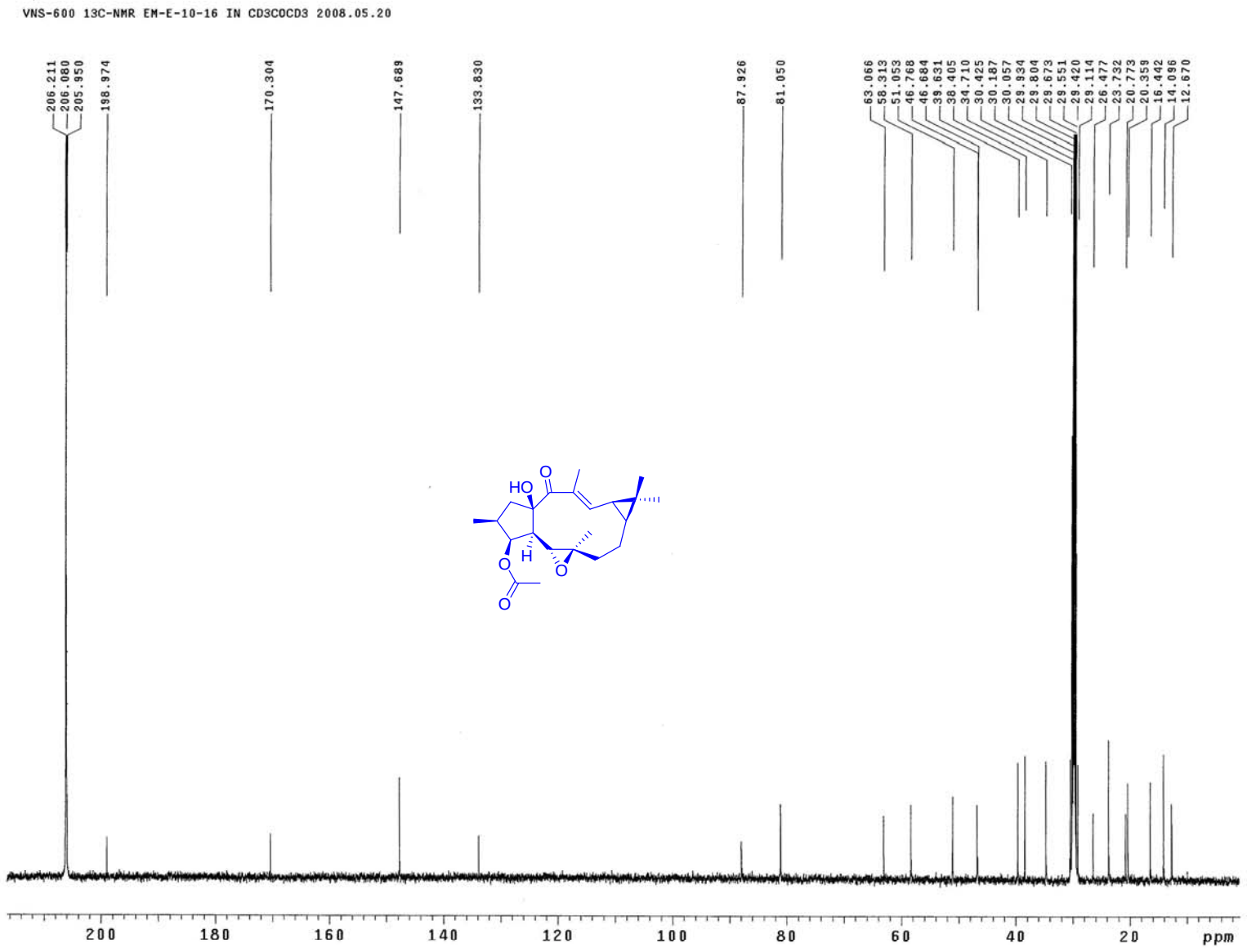

Figure S18. The ^{13}C NMR Spectrum of 2 in CD_3COCD_3 (150 MHz).

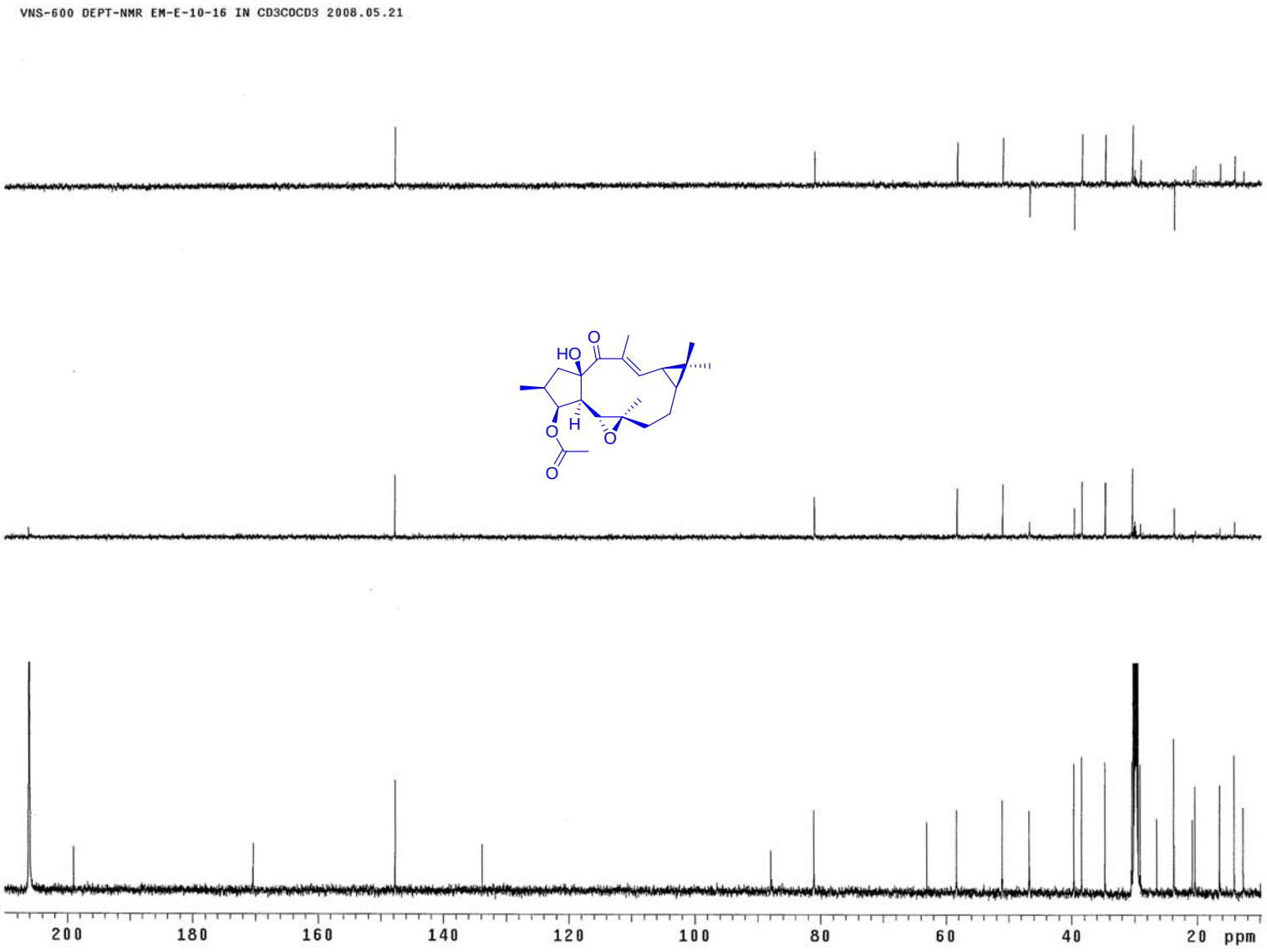

Figure S19. The DEPT Spectrum of 2 in CD_3COCD_3 (150 MHz).

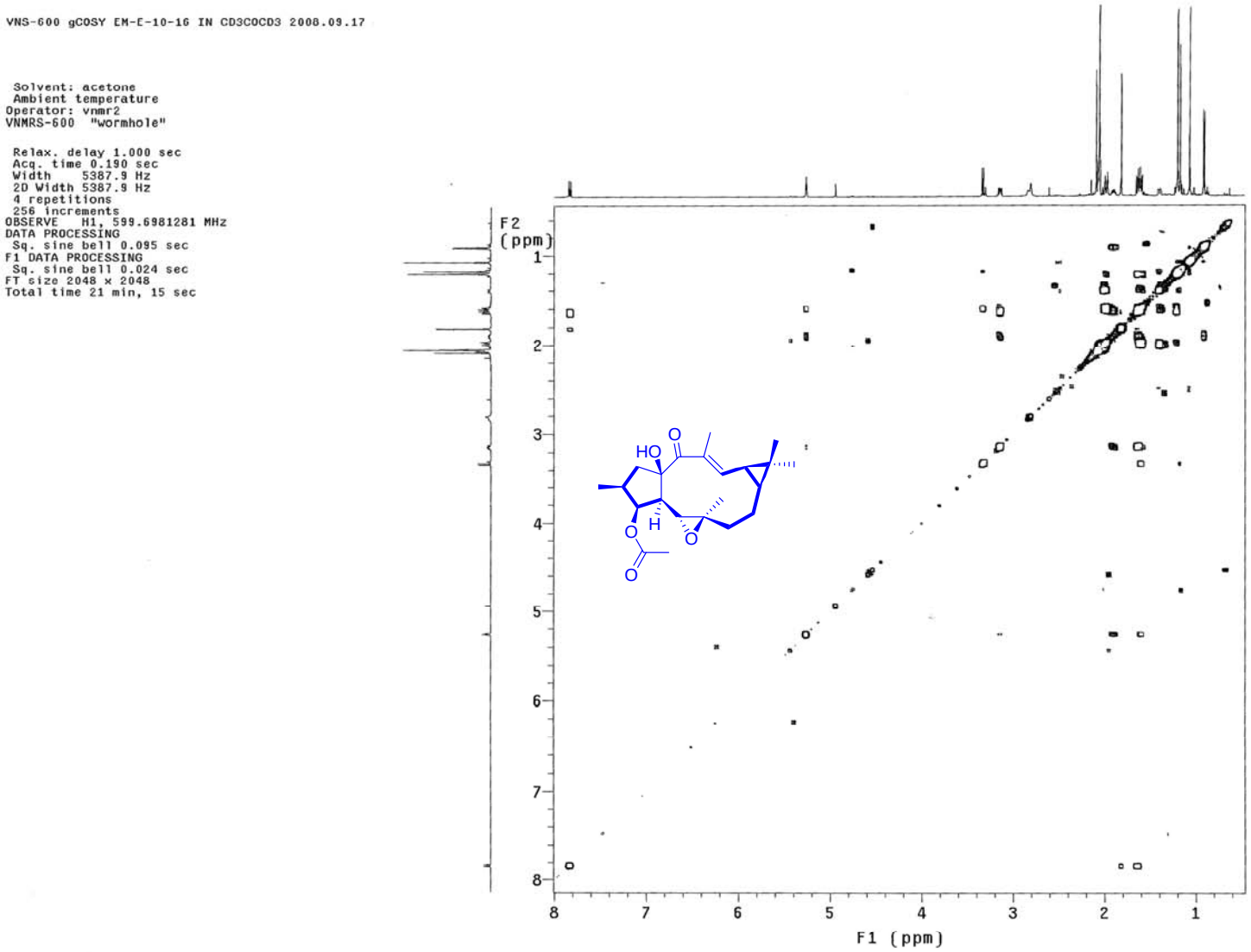

Figure S20. The ^{1}H-^{1}H gCOSY Spectrum of 2 in CD_3COCD_3 (600 MHz).

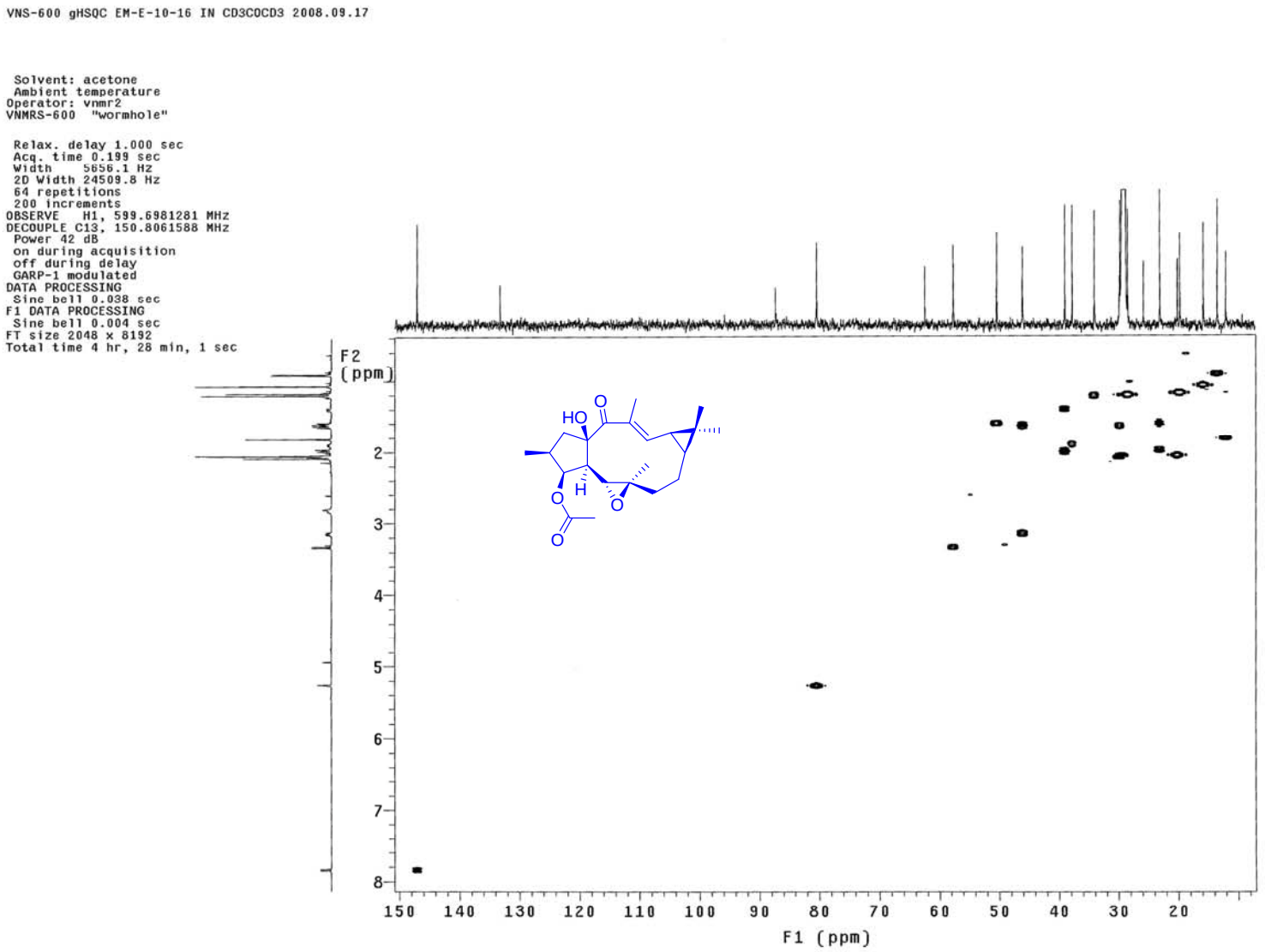

Figure S21. The gHSQC Spectrum of 2 in CD_3COCD_3 (600MHz for ^1H NMR).

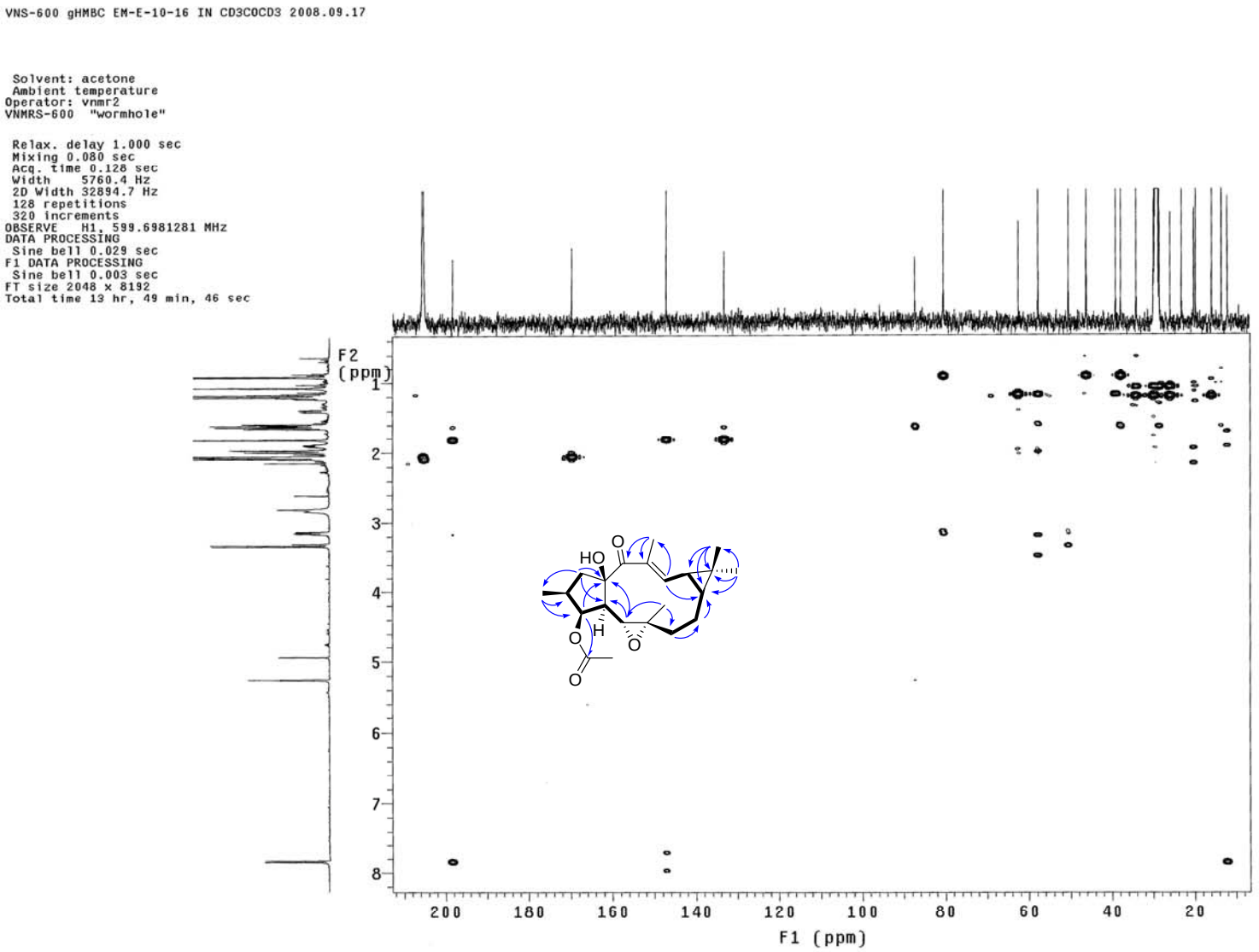

Figure S22. The gHMBC Spectrum of 2 in CD_3COCD_3 (600MHz for ^1H NMR).

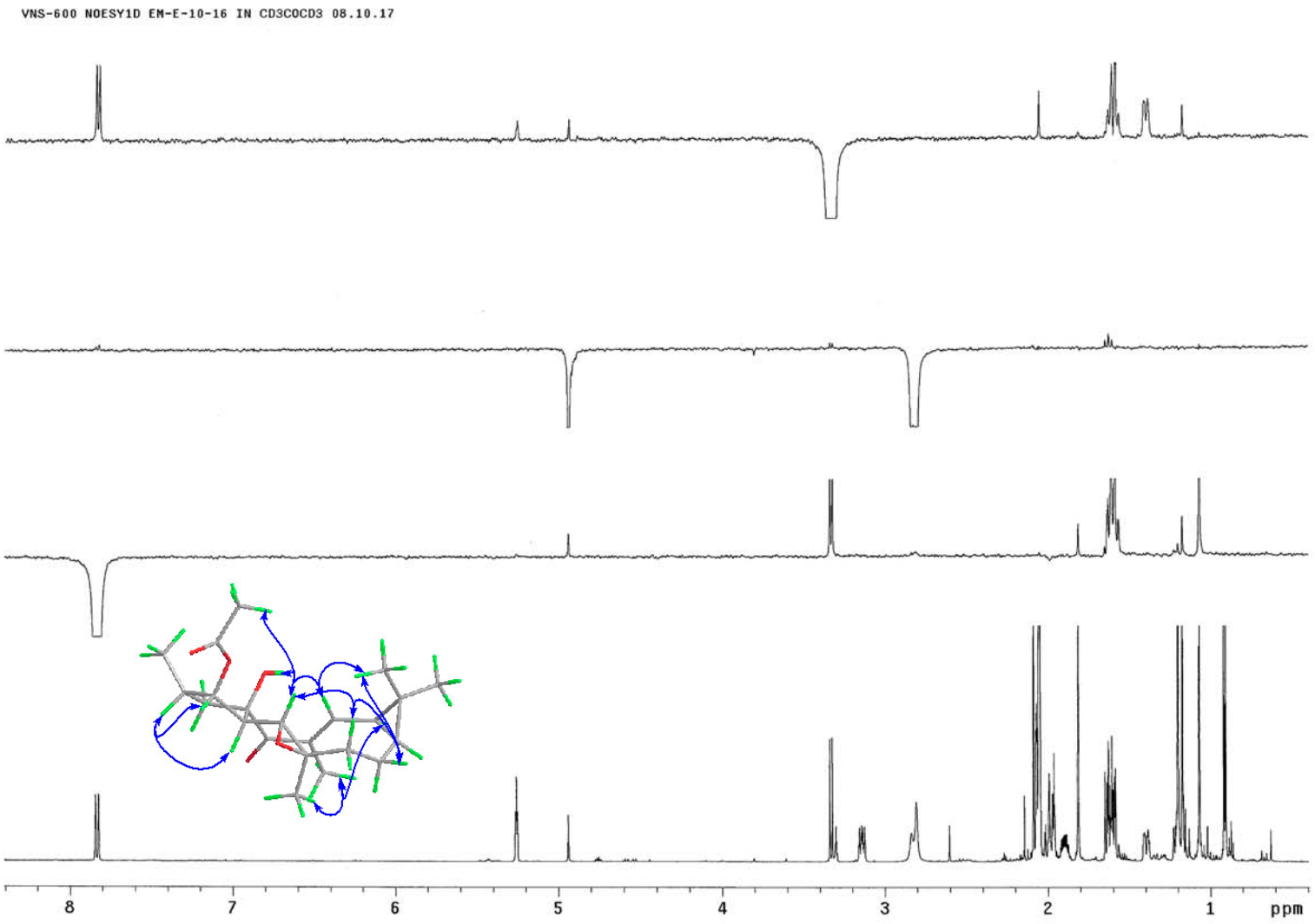

Figure S23. The NOE Difference Spectrum 1 of 2 in CD3COCD3 (600 MHz).

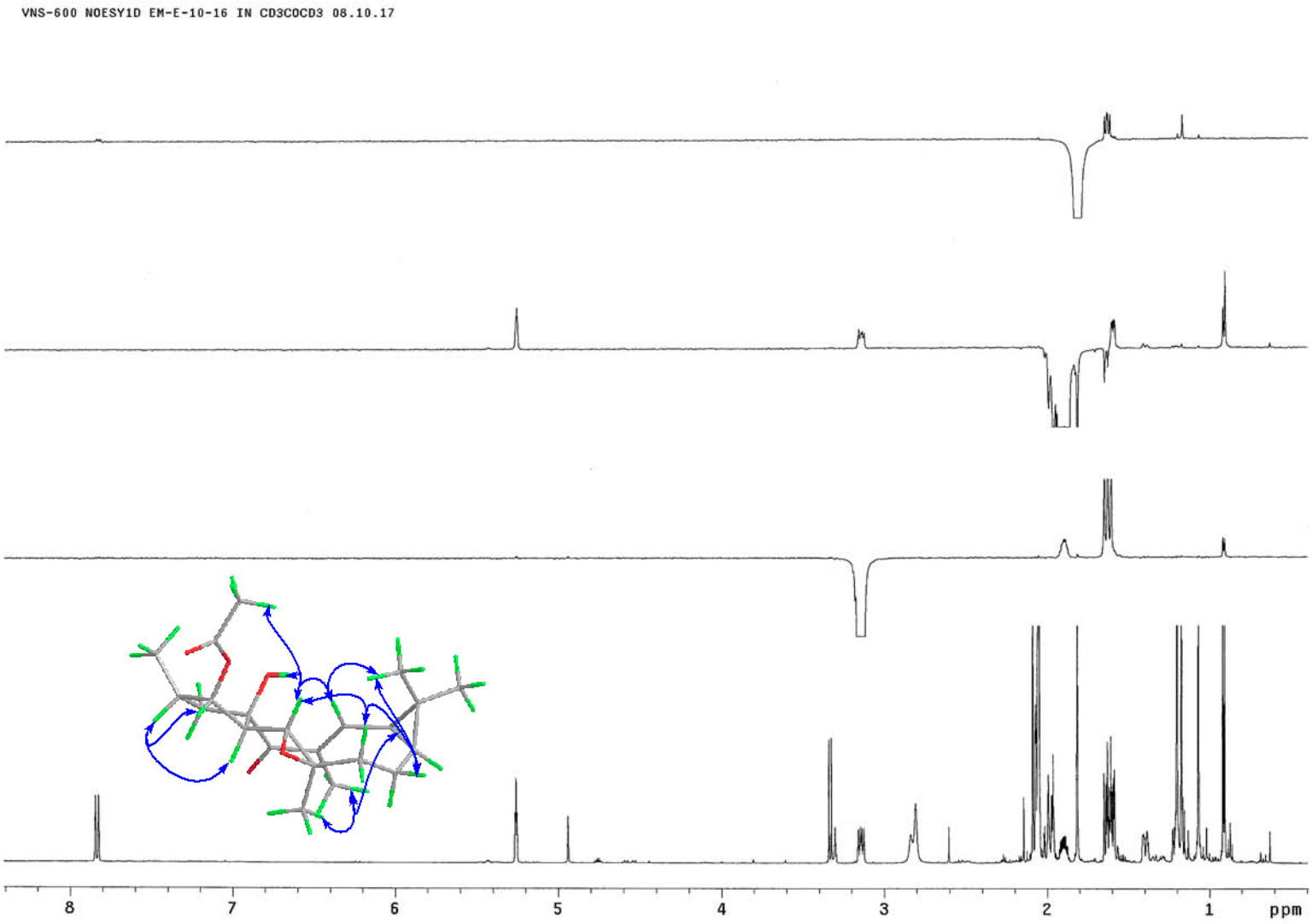

Figure S24. The NOE Difference Spectrum 2 of 2 in CD3COCD3 (600 MHz).

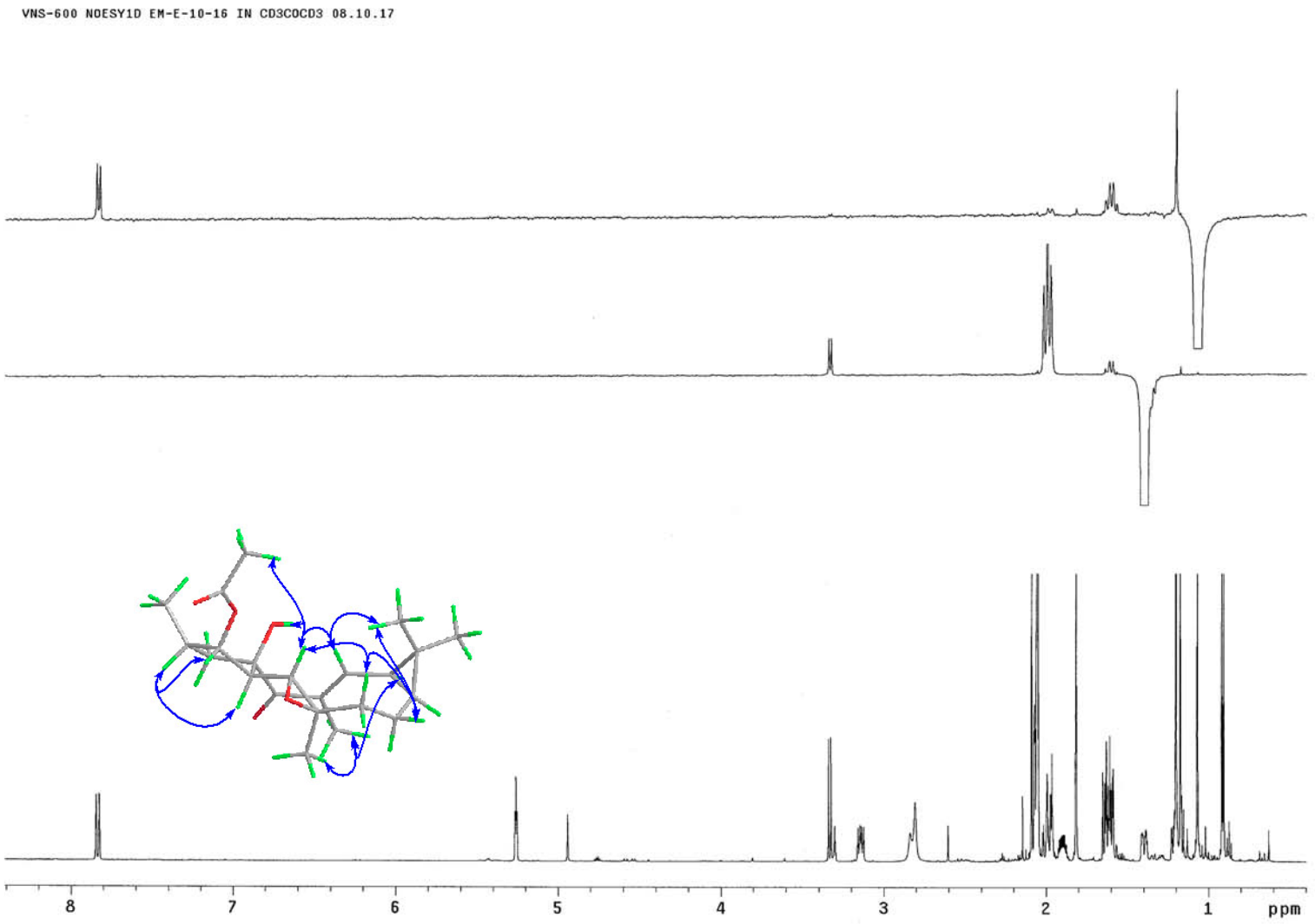

Figure S25. The NOE Difference Spectrum 3 of 2 in CD3COCD3 (600 MHz).

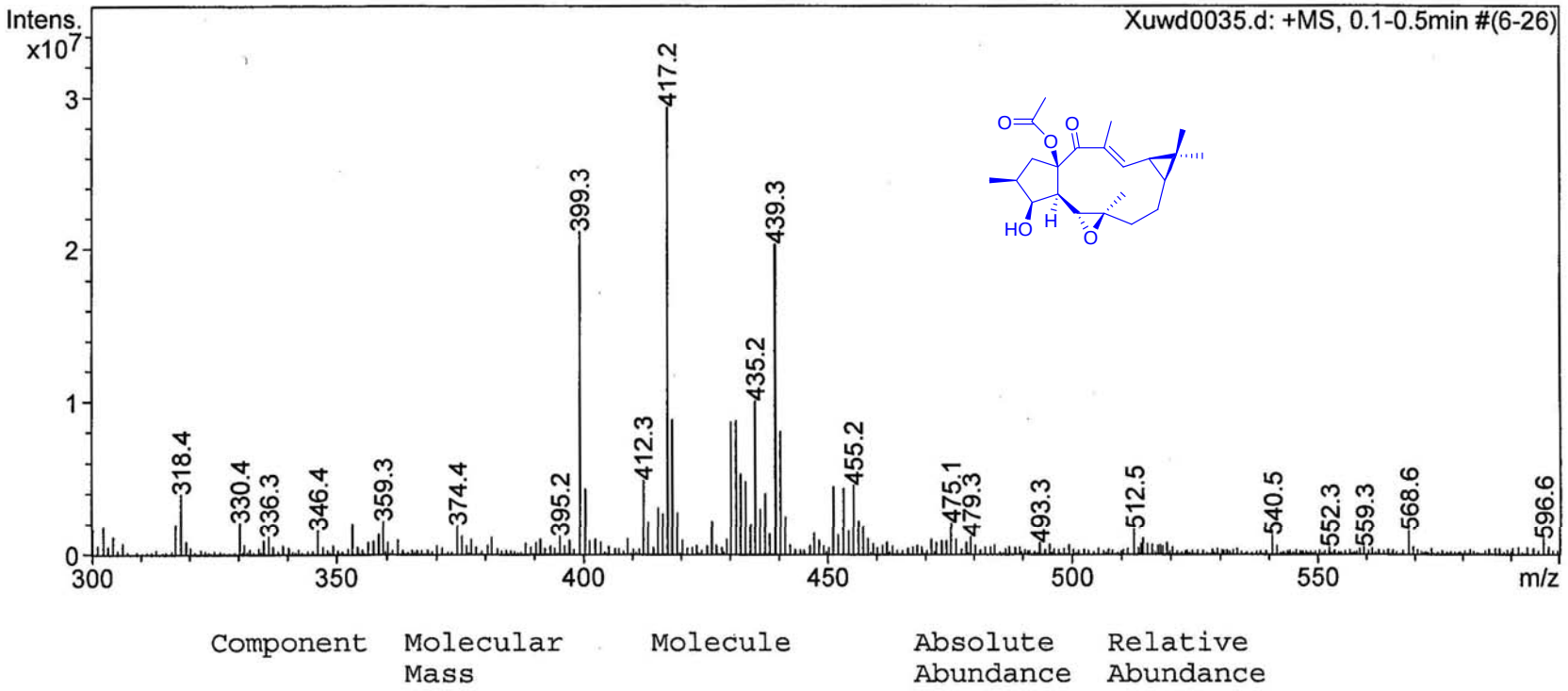

Figure S26. (+)-ESIMS Spectrum of 3.

Peak List

m/z	z	Abund	Formula	Ion
317.21096		28446		
377.23272		59921		
399.21513	1	280189	C22 H32 Na O5	(M+Na)+
400.21858	1	61003	C22 H32 Na O5	(M+Na)+
415.18890		51884		
481.21796		18752		
775.43996	1	103704		
776.44317	1	46486		

(+)-HRESIMS Data of 3.

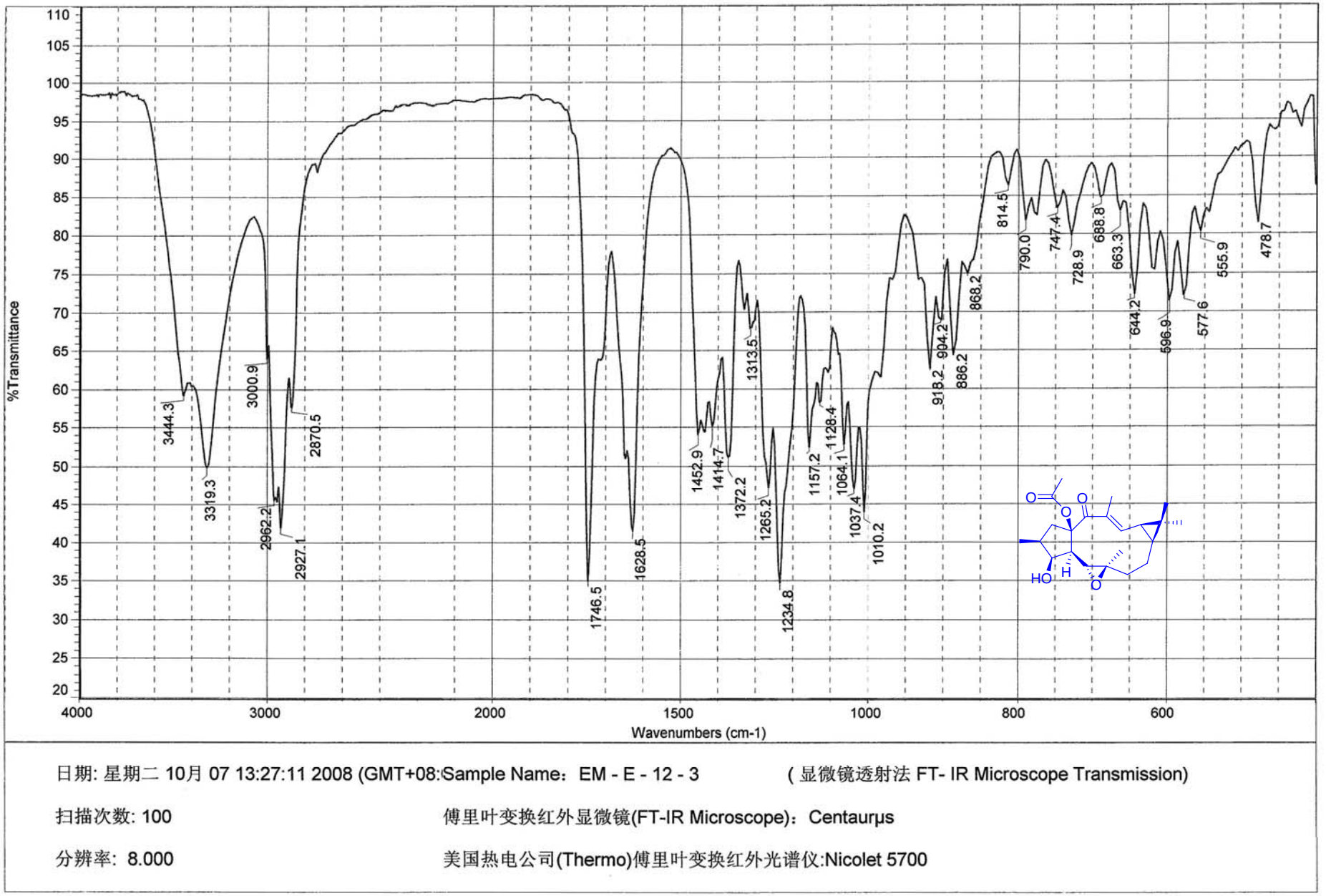

Figure S27. The IR Spectrum of 3.

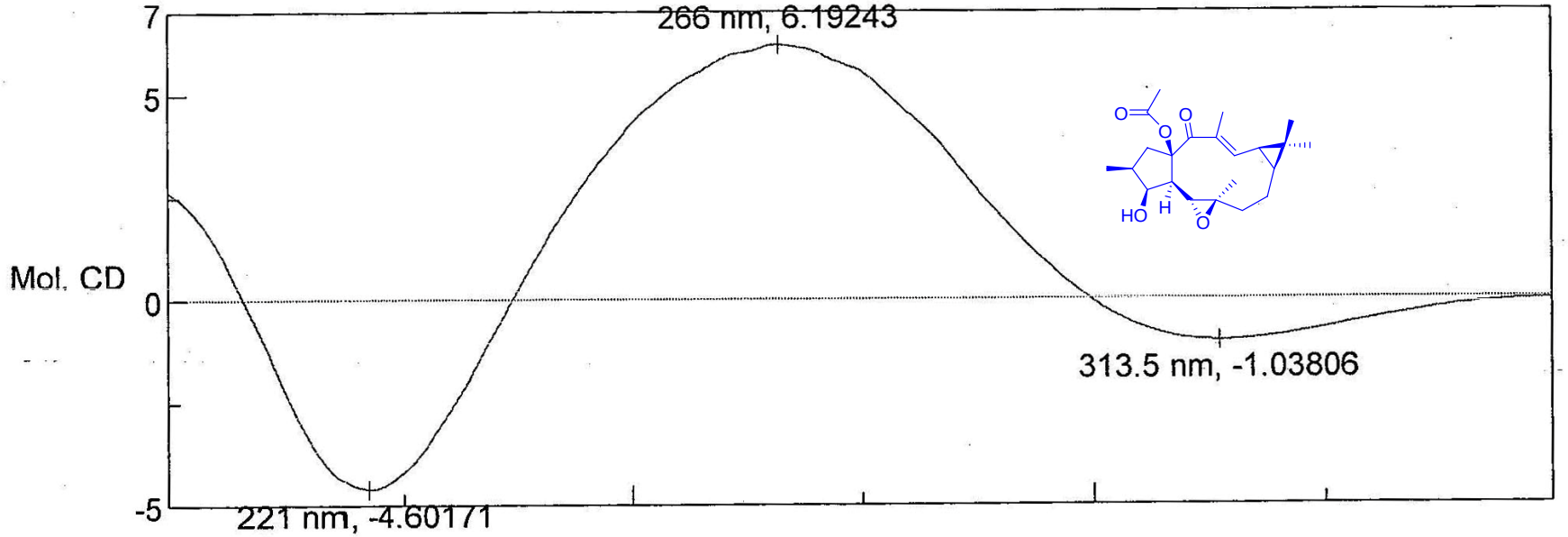

Figure S28. The CD Spectrum of 3.

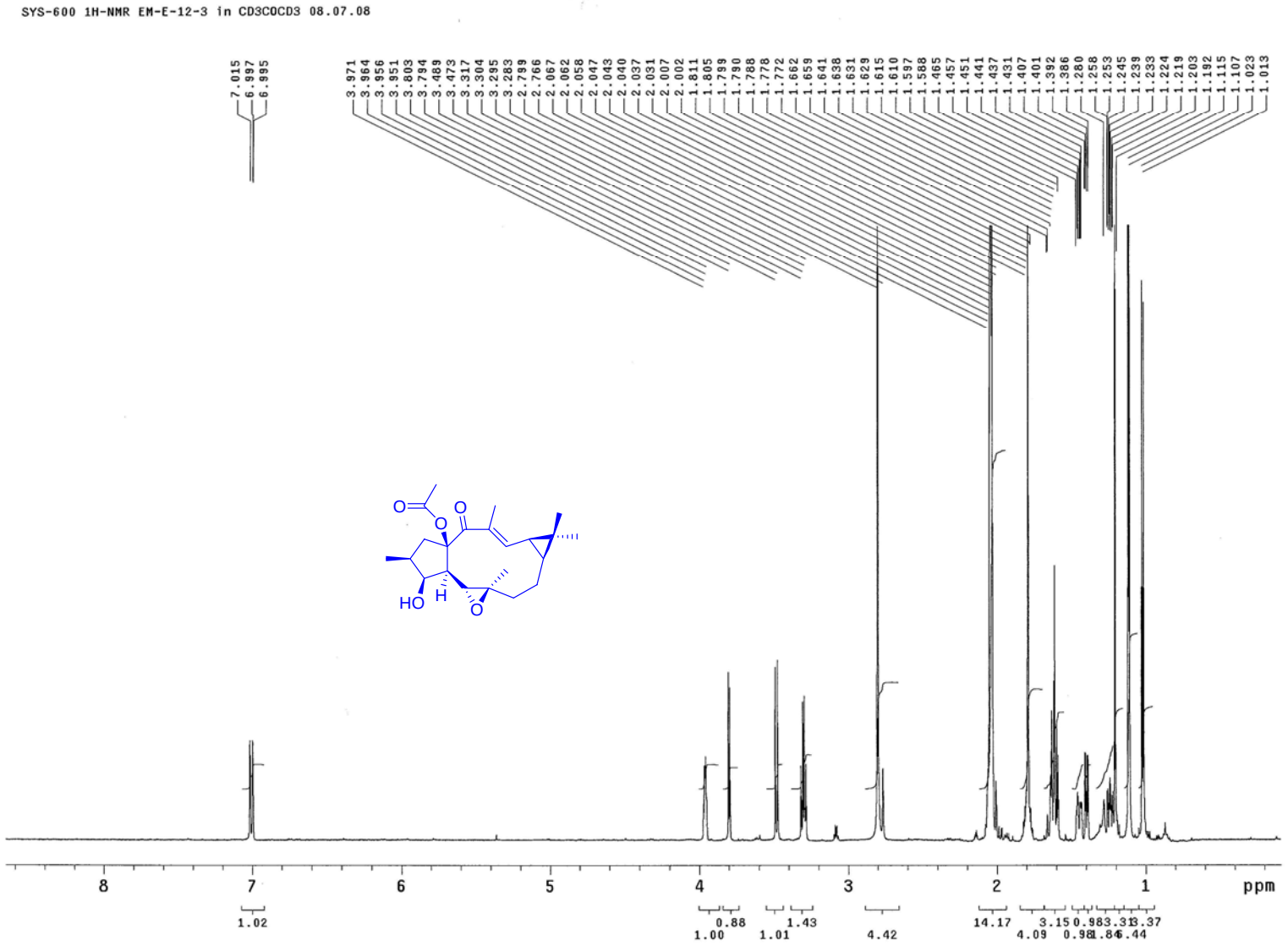

Figure S29. The ^{1}H NMR Spectrum of 3 in CD_3COCD_3 (600 MHz).

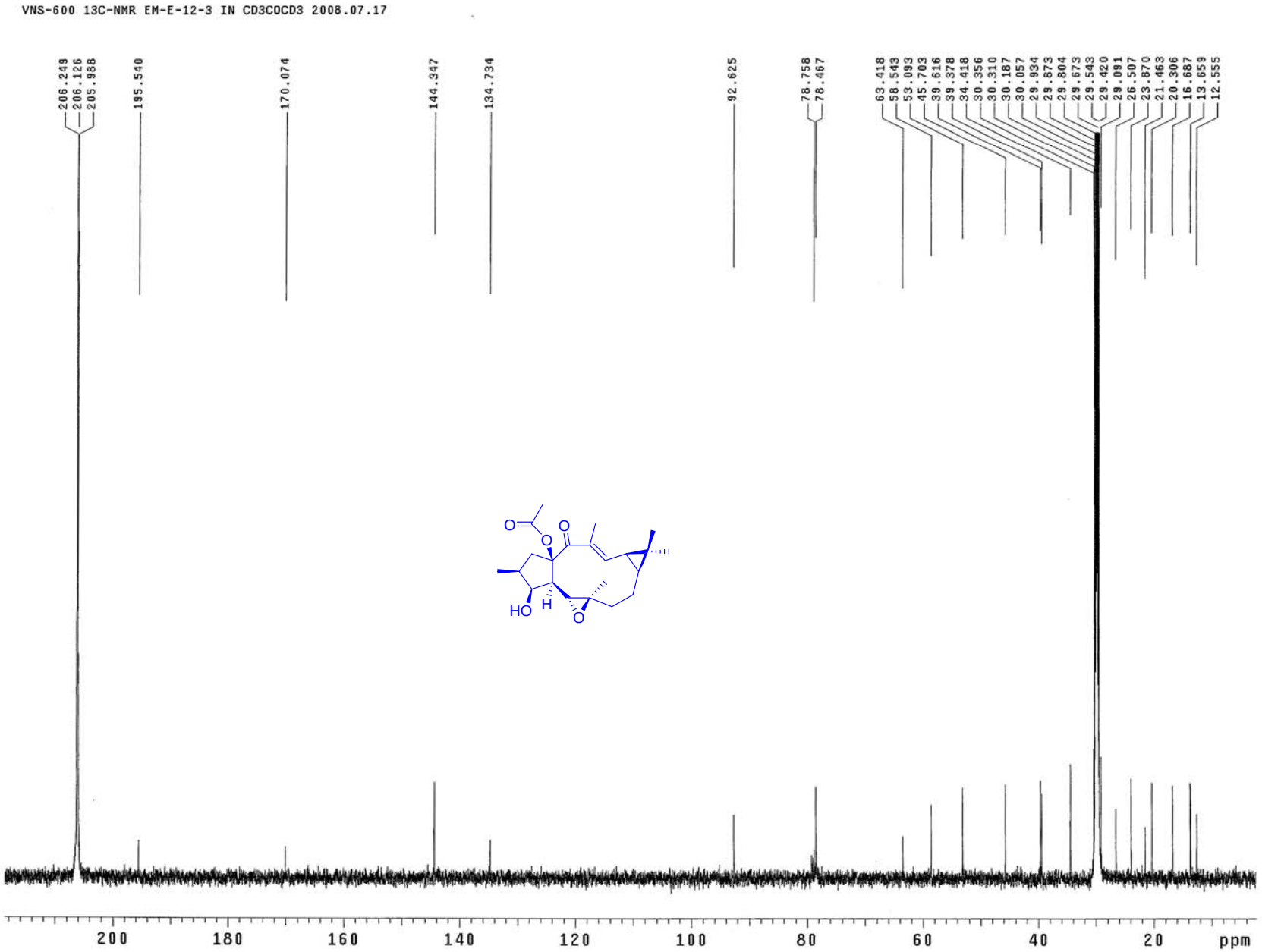

Figure S30. The ^{13}C NMR Spectrum of 3 in CD_3COCD_3 (150 MHz).

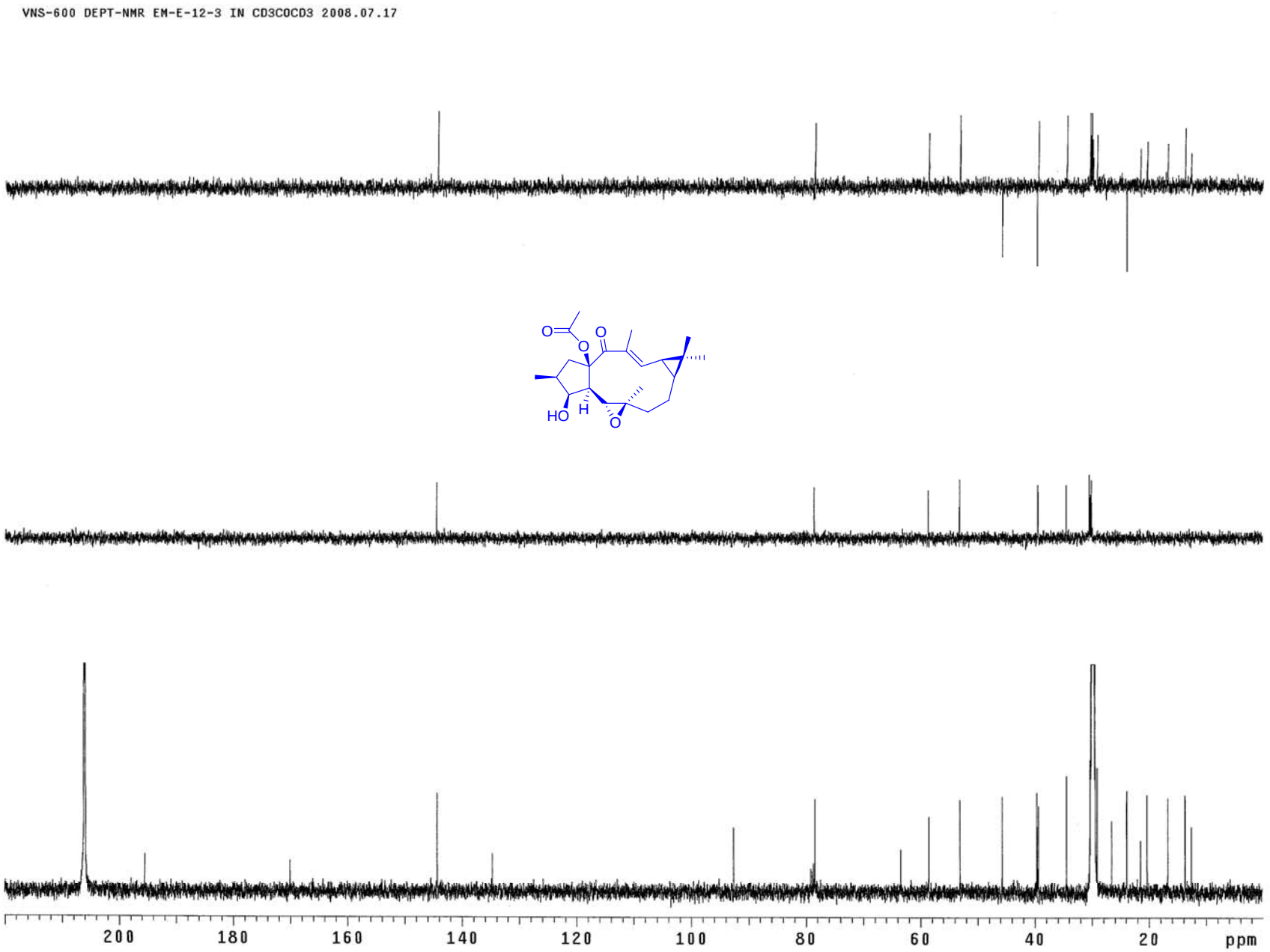

Figure S31. The DEPT Spectrum of 3 in CD_3COCD_3 (150 MHz).

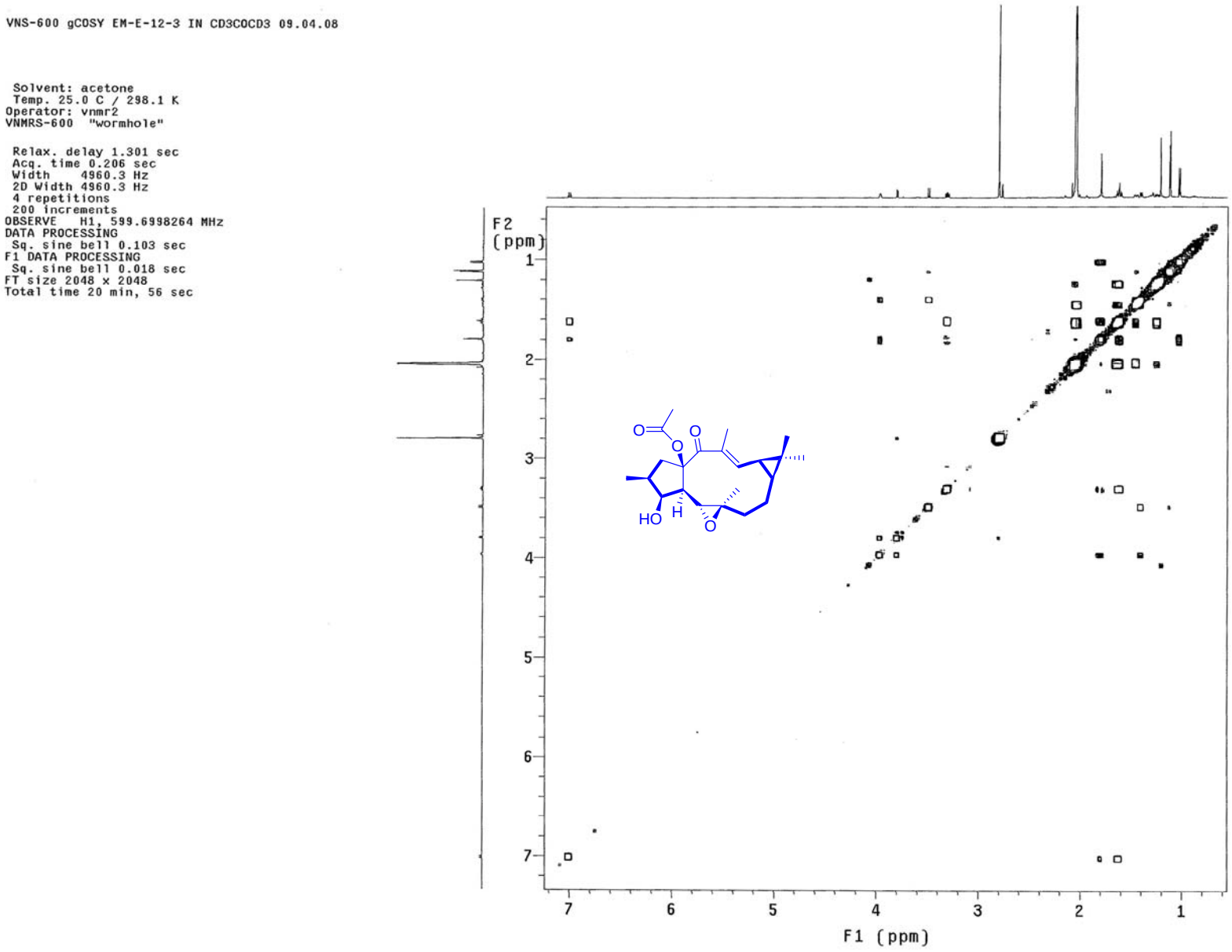

Figure S32. The ^{1}H-^{1}H gCOSY Spectrum of 3 in CD_3COCD_3 (600 MHz).

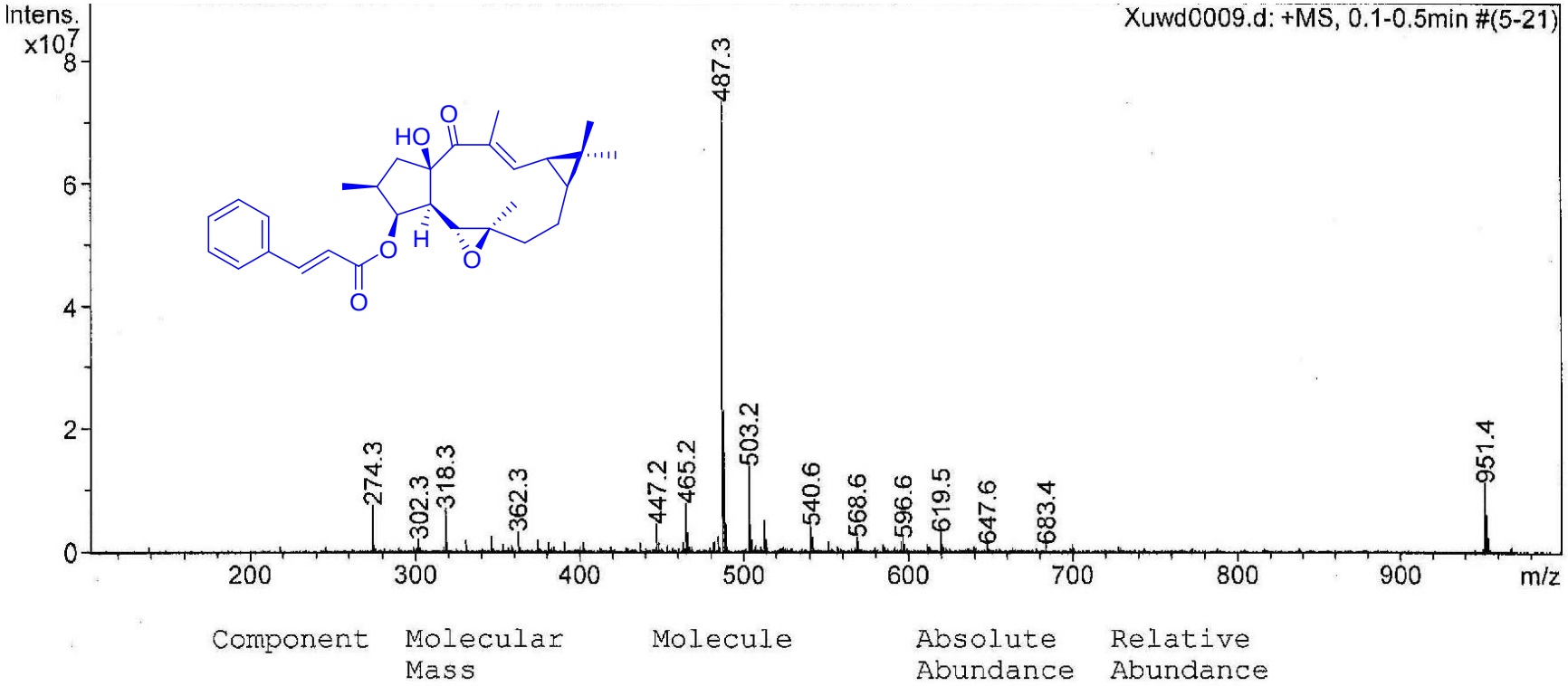

Figure S33. (+)-ESIMS Spectrum of 4.

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:^{12}C:0 .. 100, ^{1}H:0 .. 200, ^{23}Na:1 .. 1, ^{16}O: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.

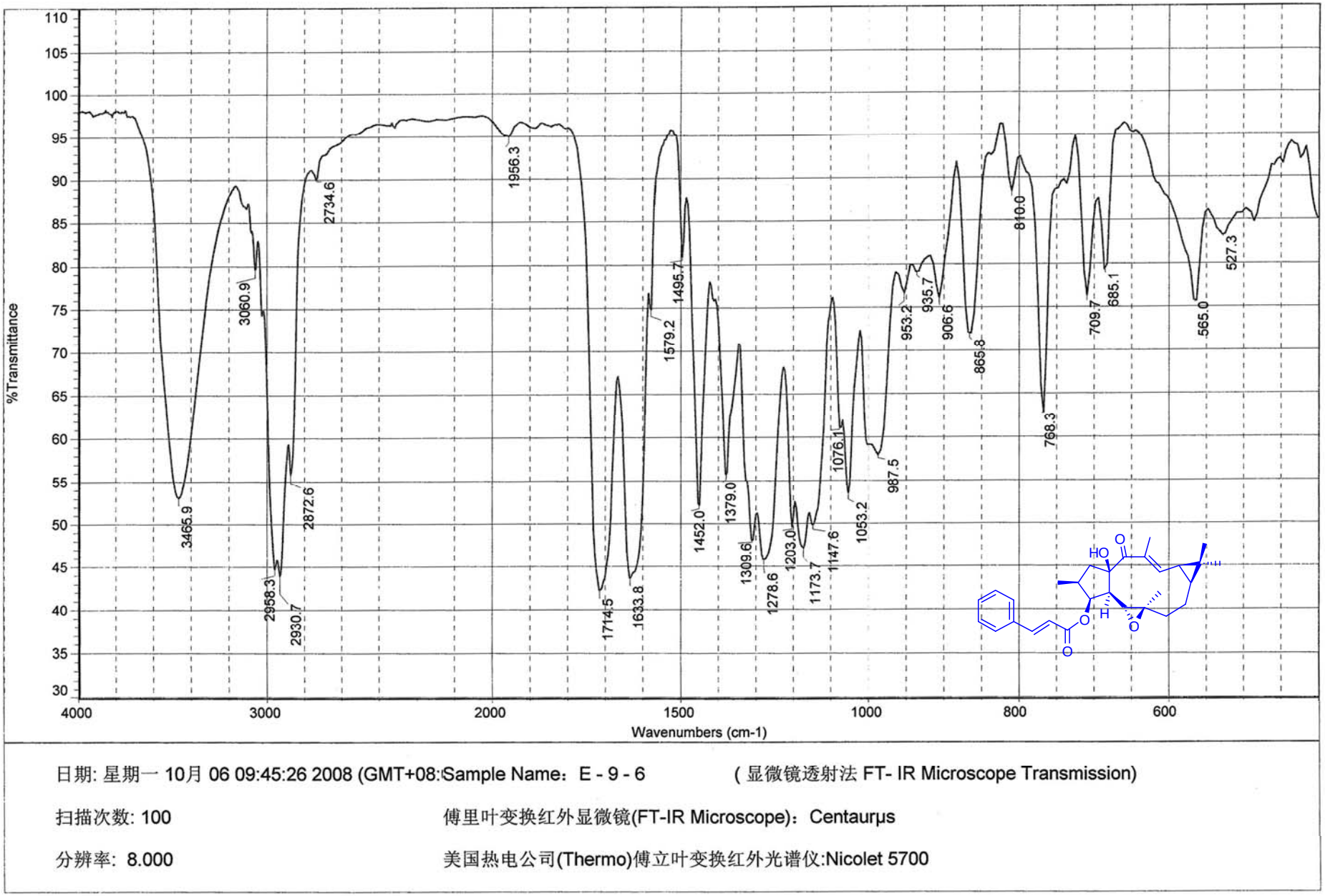

Figure S34. The IR Spectrum of 4.

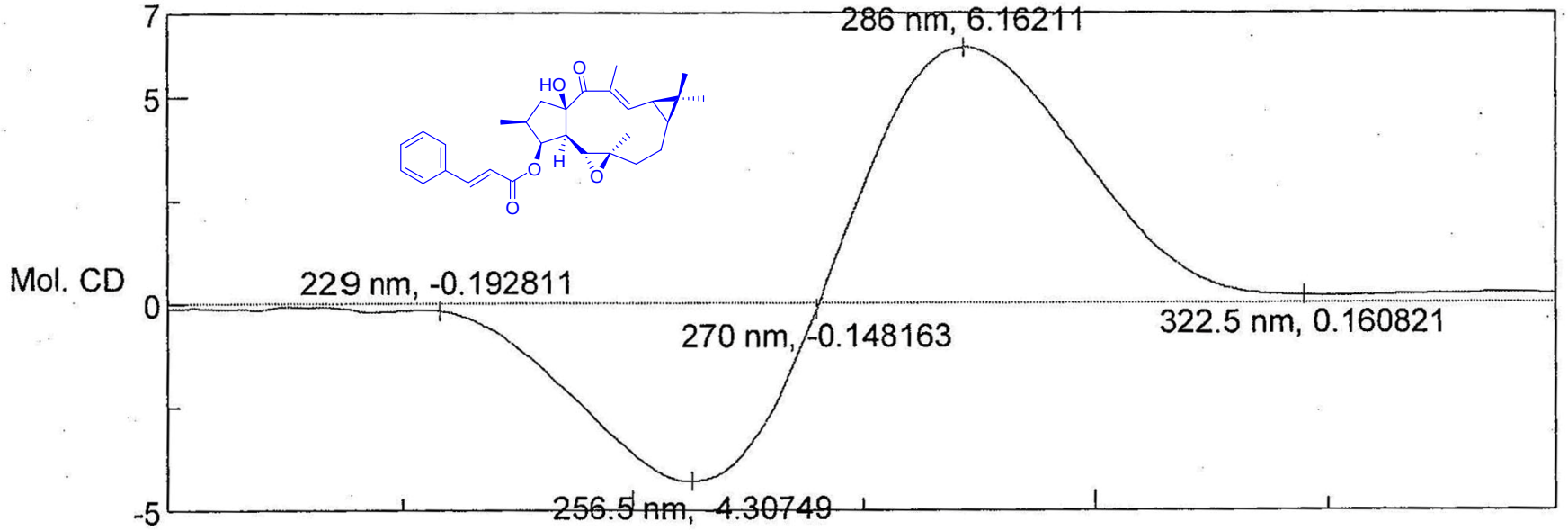

Figure S35 The CD Spectrum of 4.

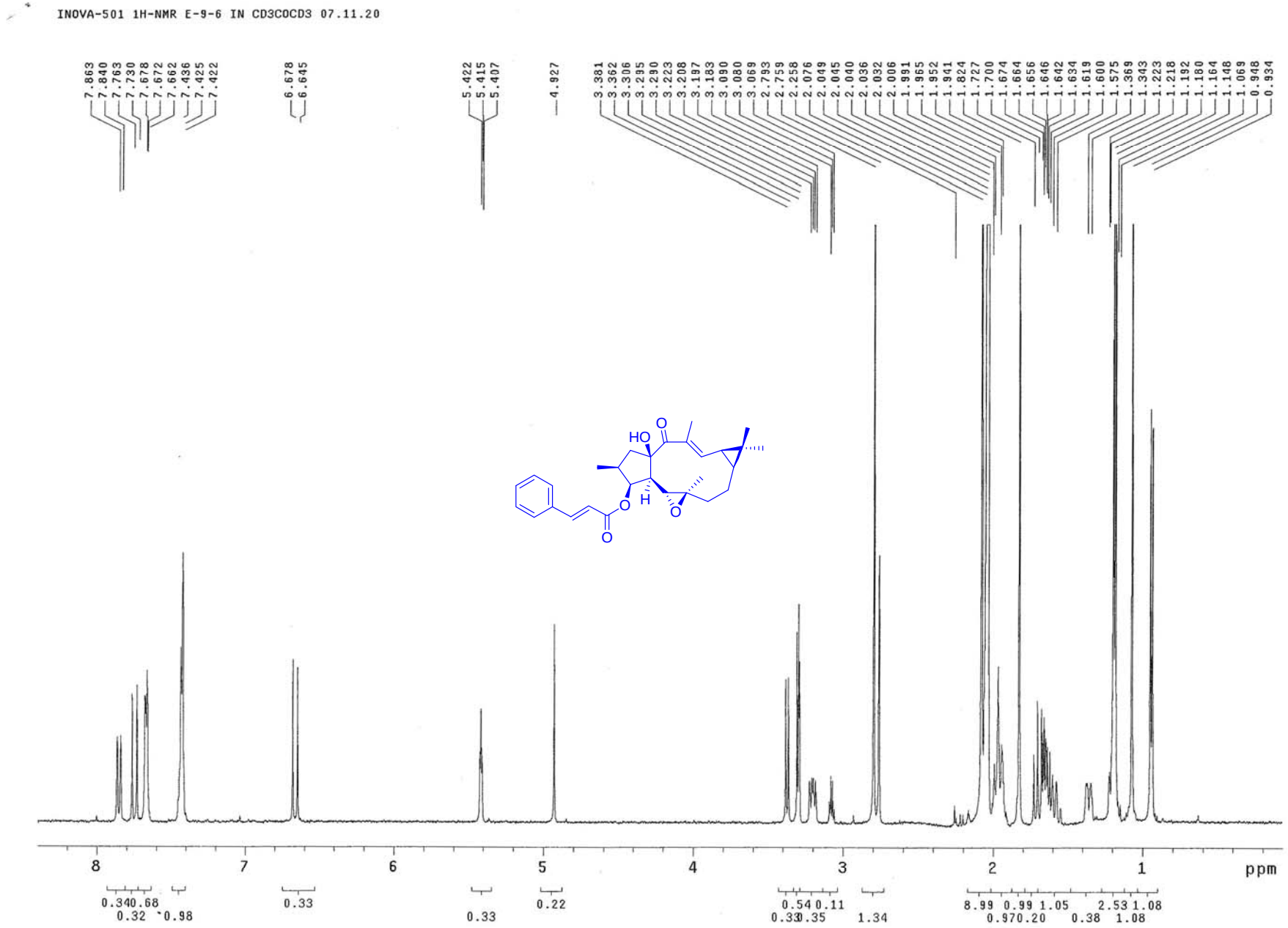

Figure S36. The ^{1}H NMR Spectrum of 4 in CD_3COCD_3 (500 MHz).

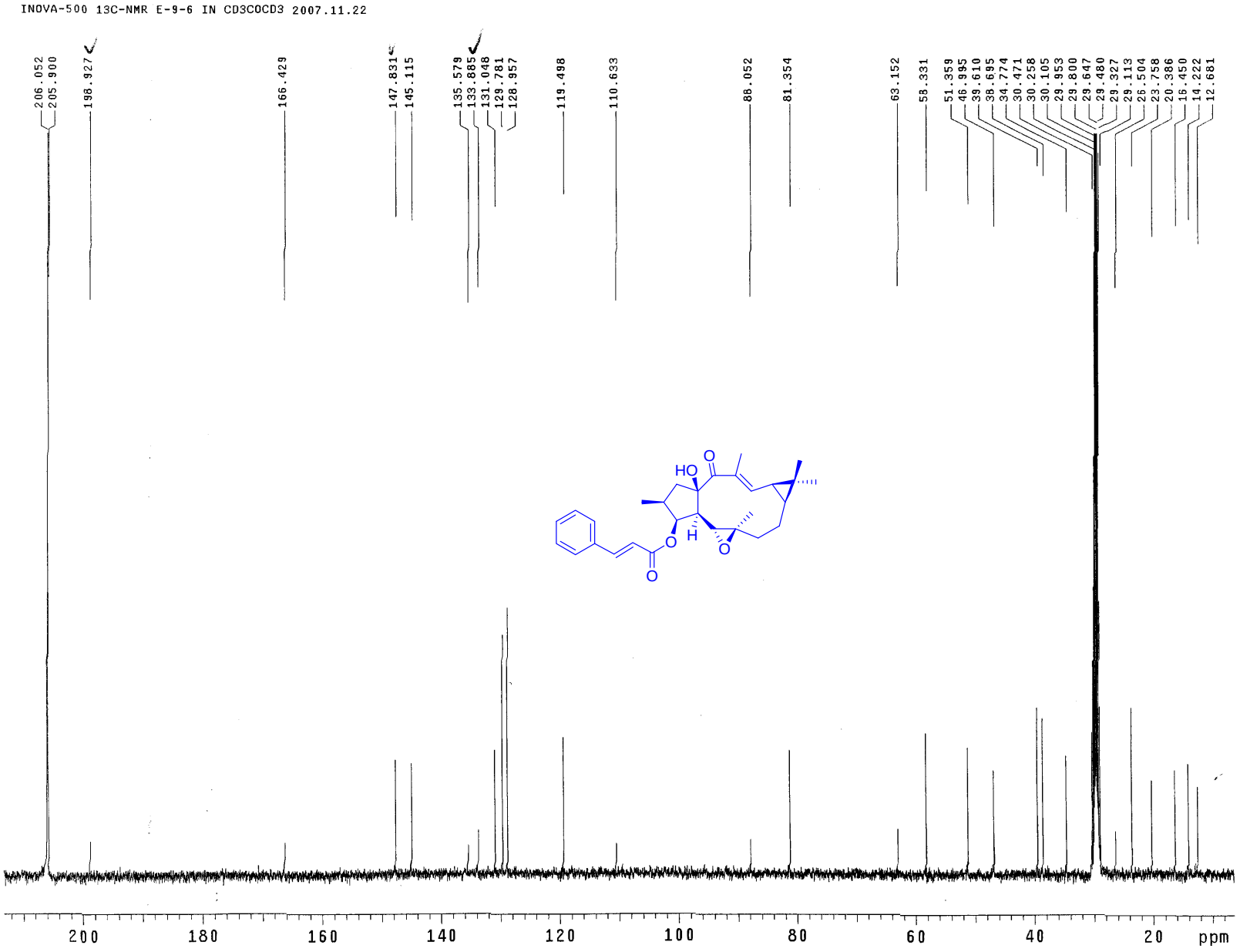

Figure S37. The ^{13}C NMR Spectrum of 4 in CD_3COCD_3 (125 MHz).

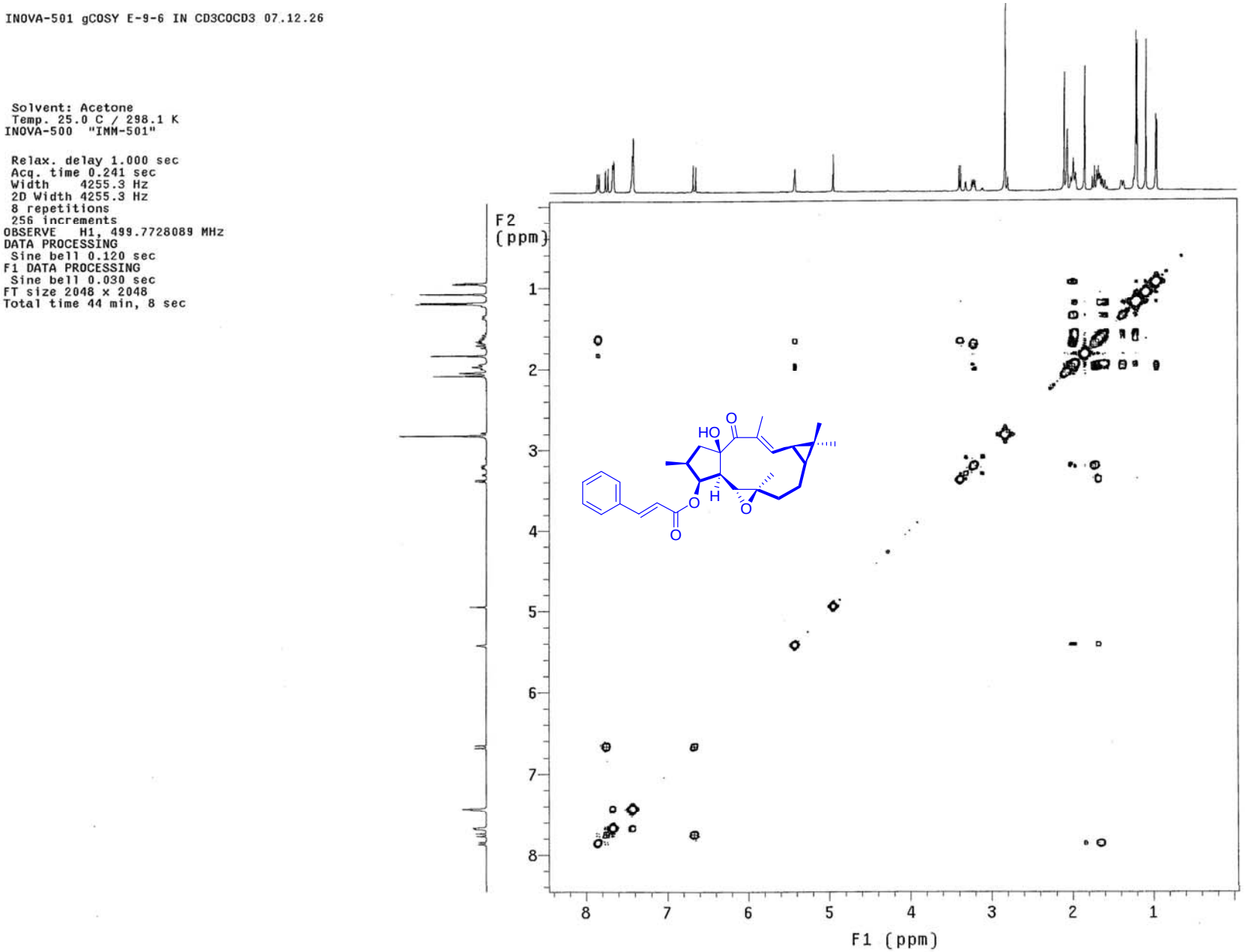

Figure S38. The ^{1}H-^{1}H gCOSY Spectrum of 4 in CD_3COCD_3 (500 MHz).

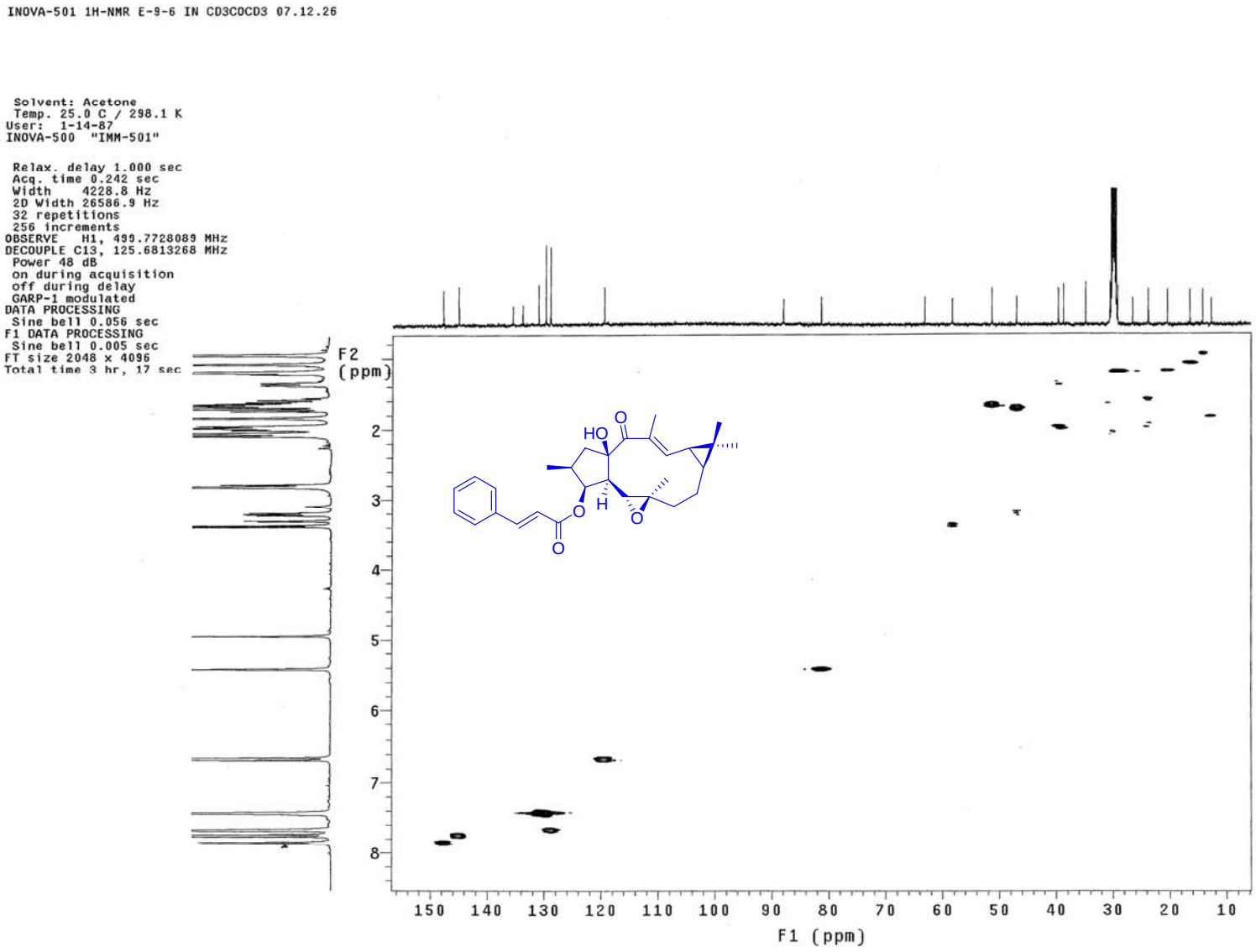

Figure S39. The gHSQC Spectrum of 4 in CD_3COCD_3 (500MHz for ^1H NMR).

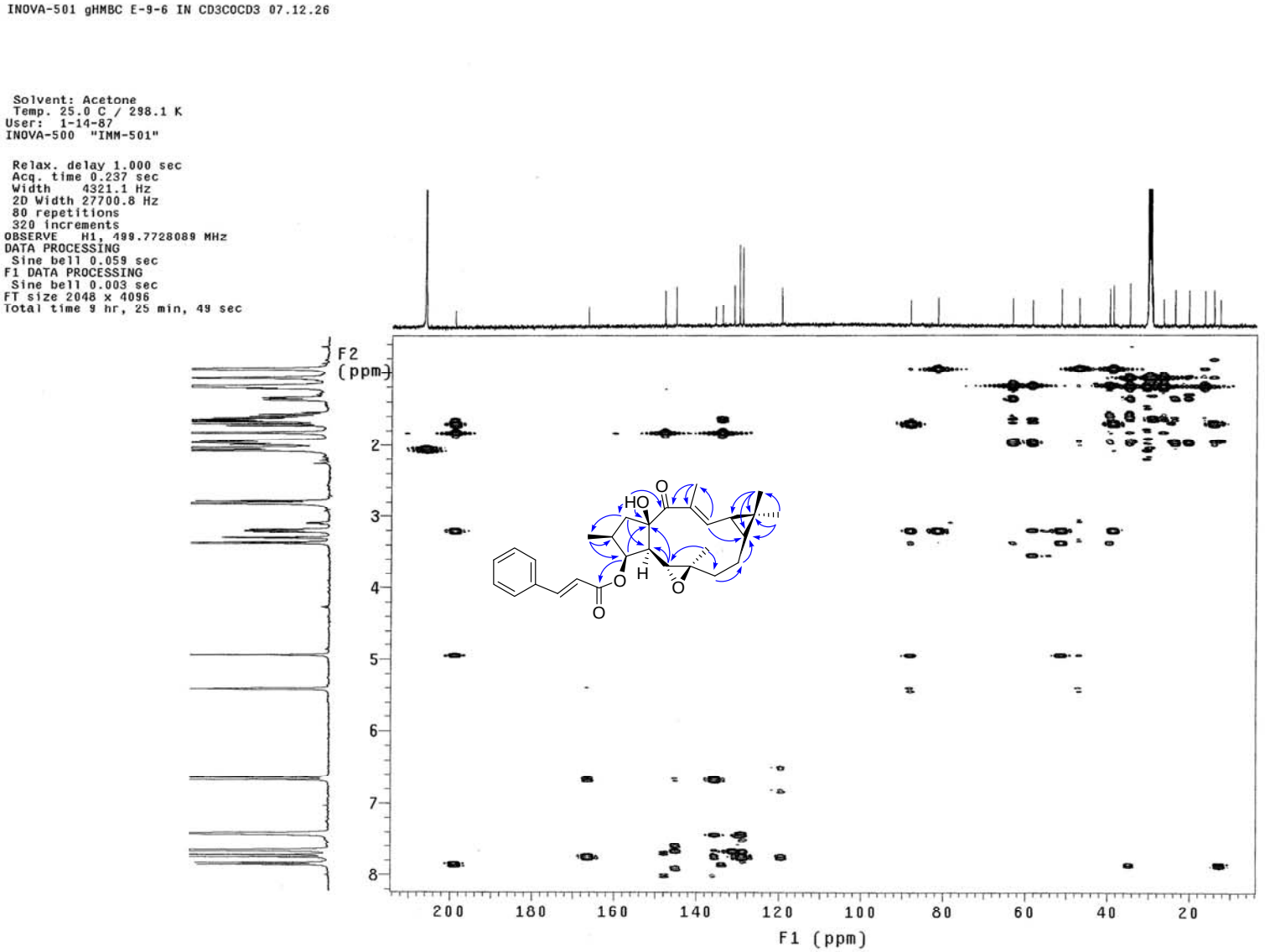

Figure S40. The gHMBC Spectrum of 4 in CD_3COCD_3 (500MHz for ^1H NMR).

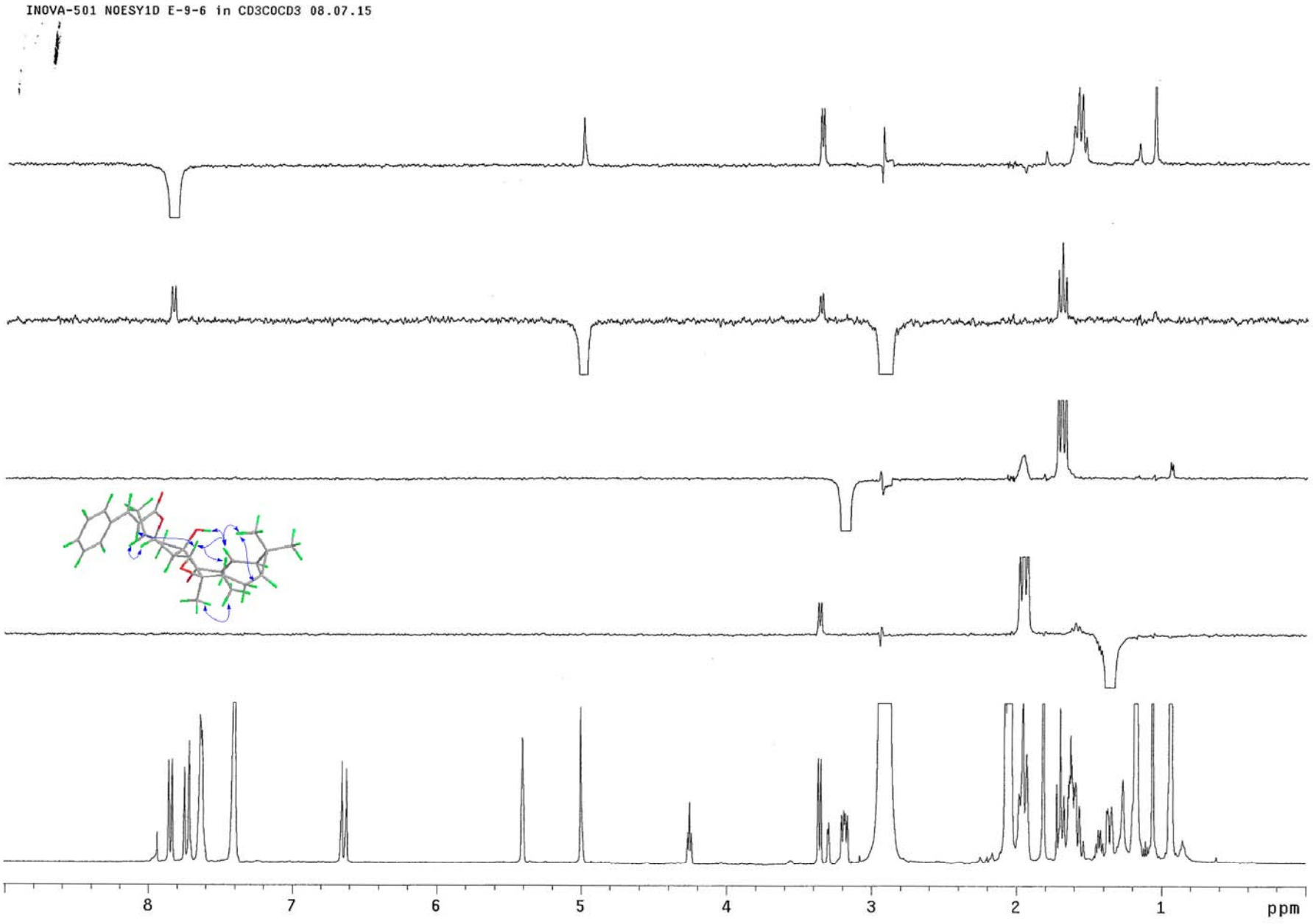

Figure S41. The NOE Difference Spectrum 1 of 4 in CD_3COCD_3 (500 MHz).

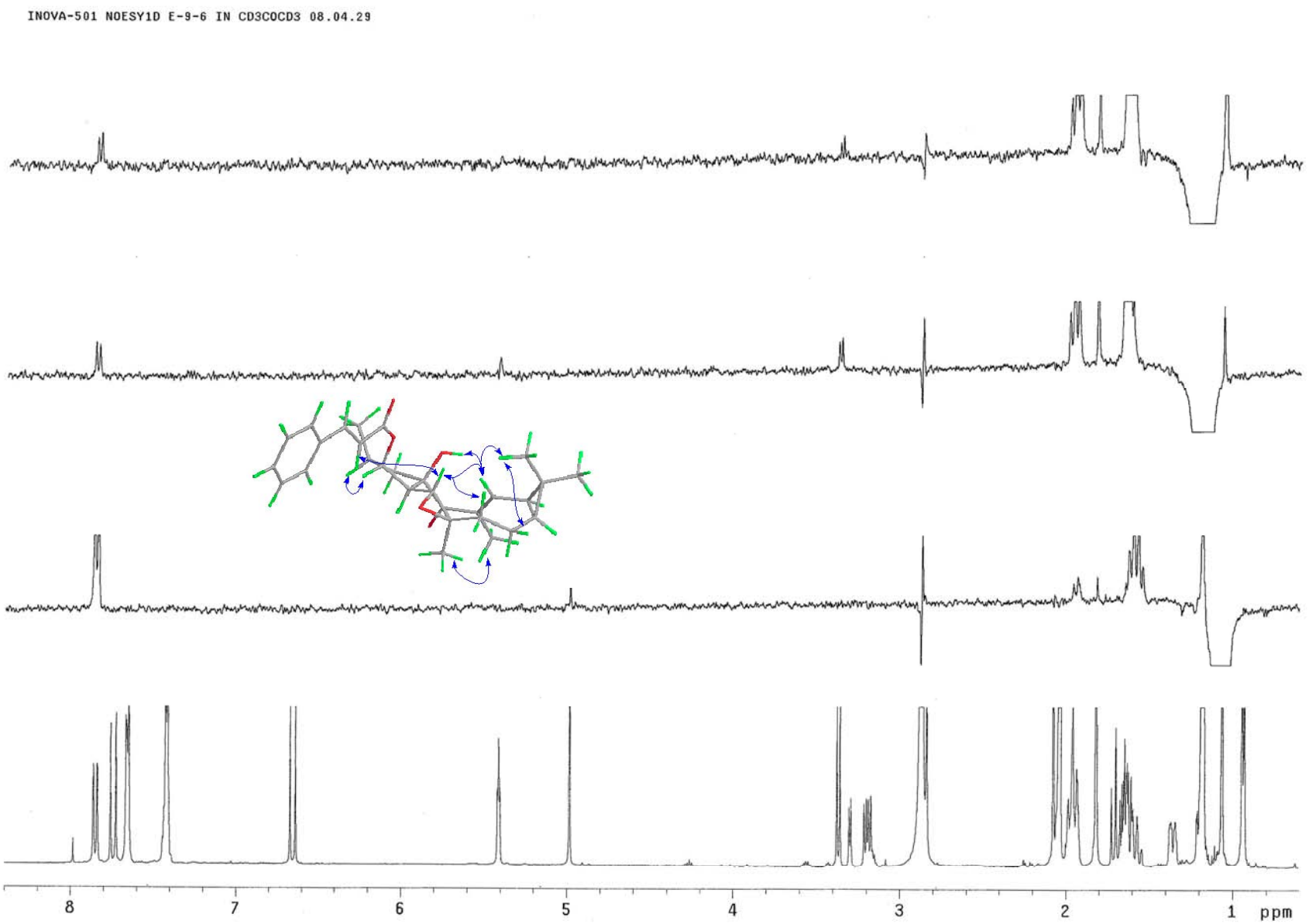

Figure S42. The NOE Difference Spectrum 2 of 4 in CD_3COCD_3 (500 MHz).

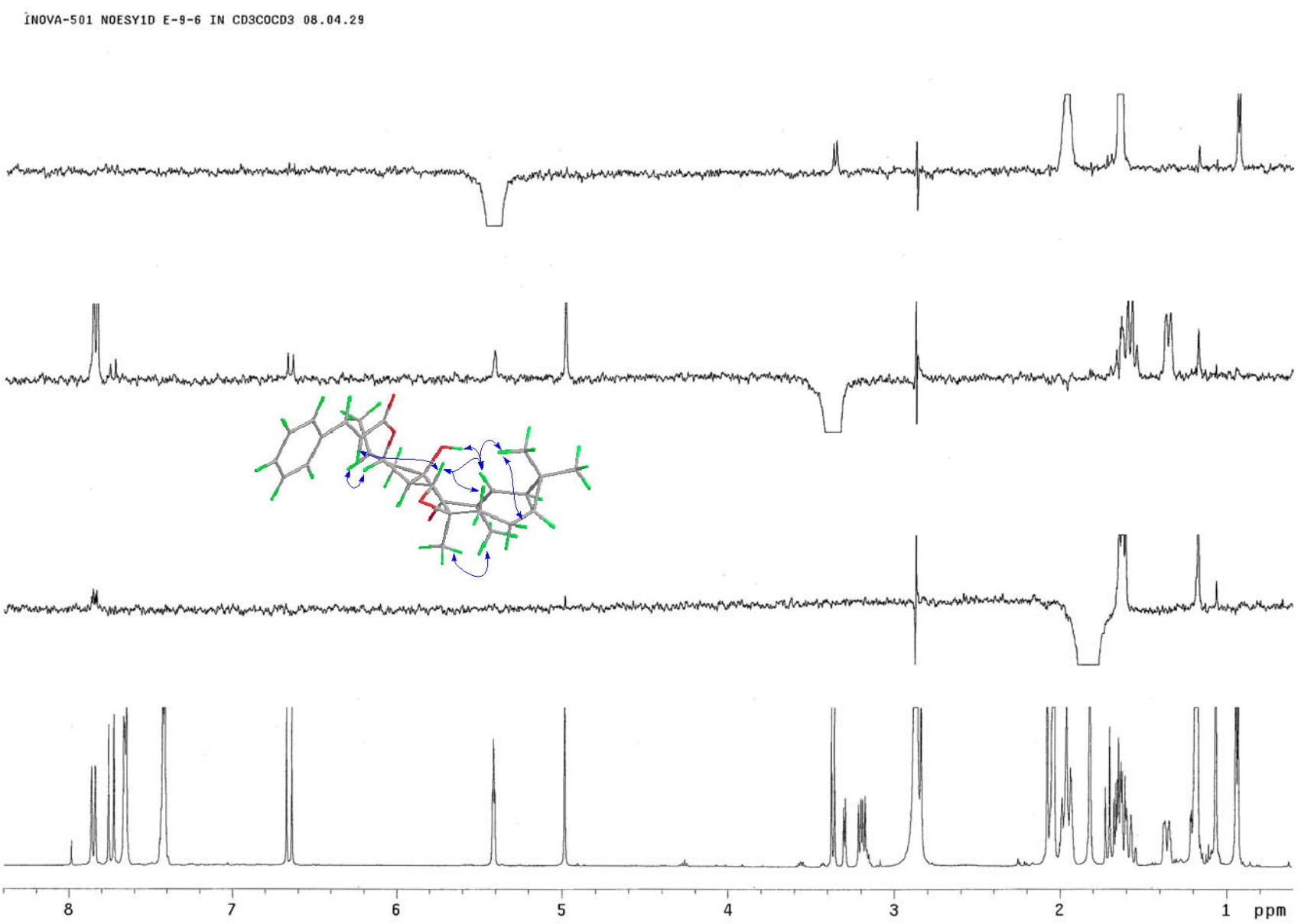

Figure S43. The NOE Difference Spectrum 3 of 4 in CD_3COCD_3 (500 MHz).

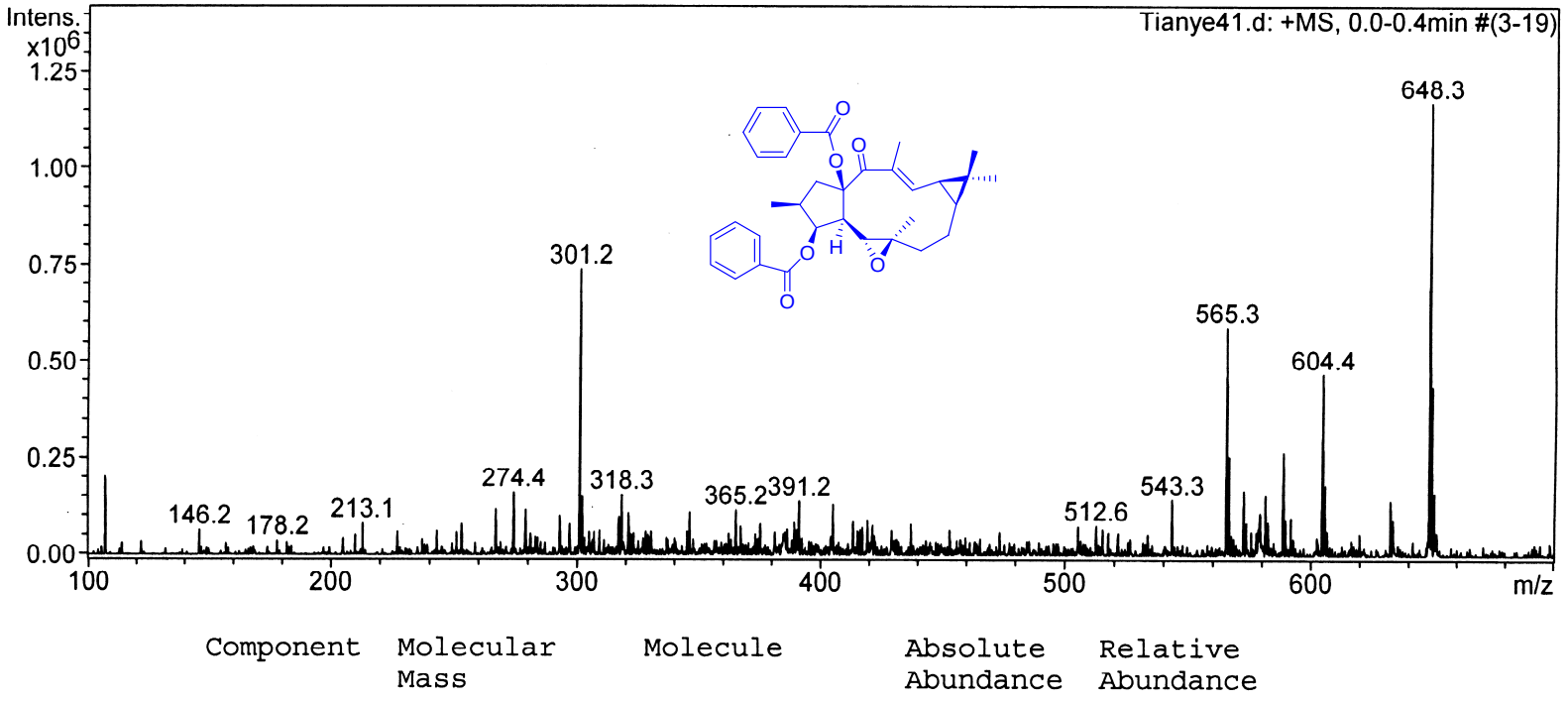

Figure S44. The (+)-ESIMS Spectrum of 5.

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.

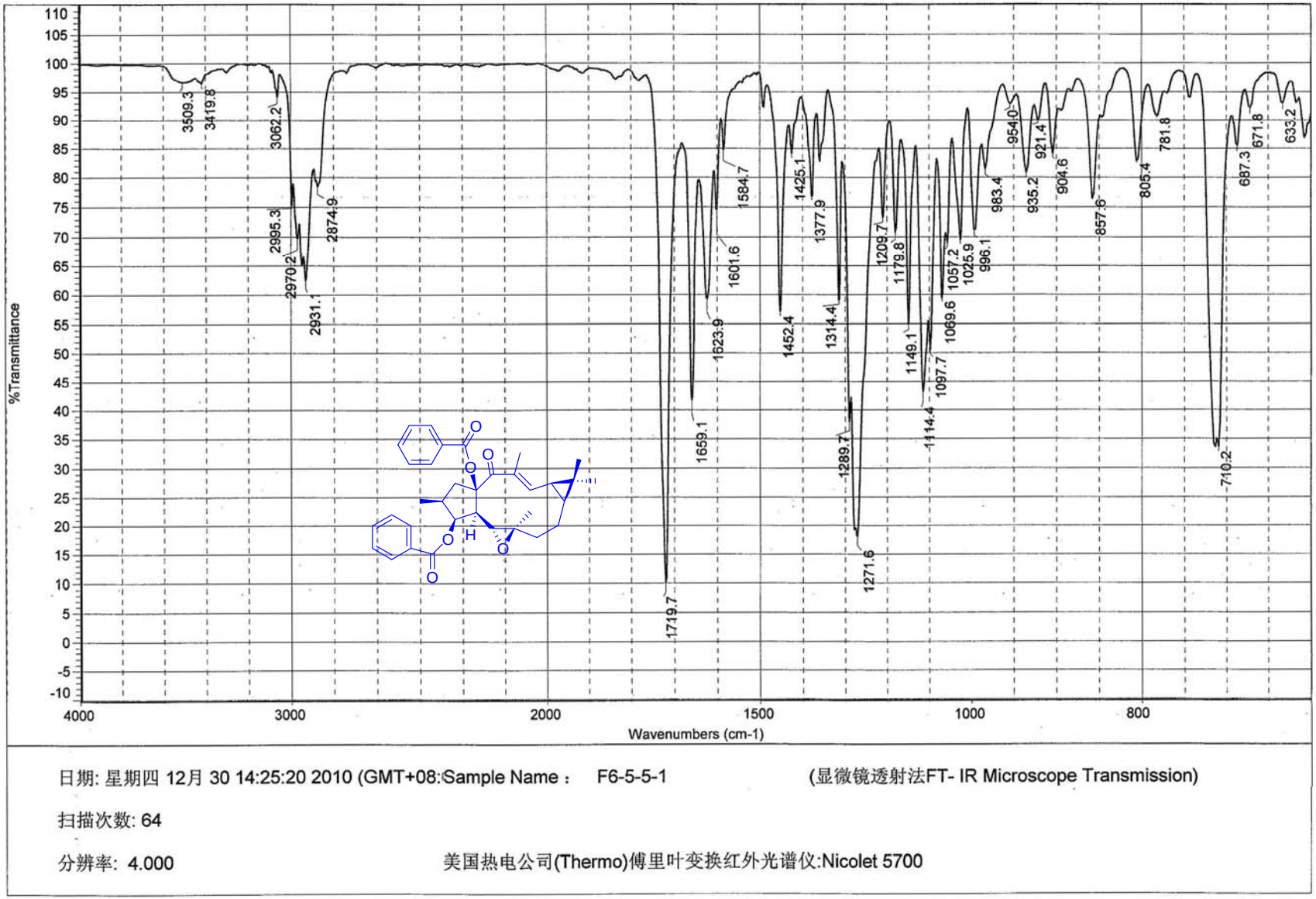

Figure S45. The IR Spectrum of 5.

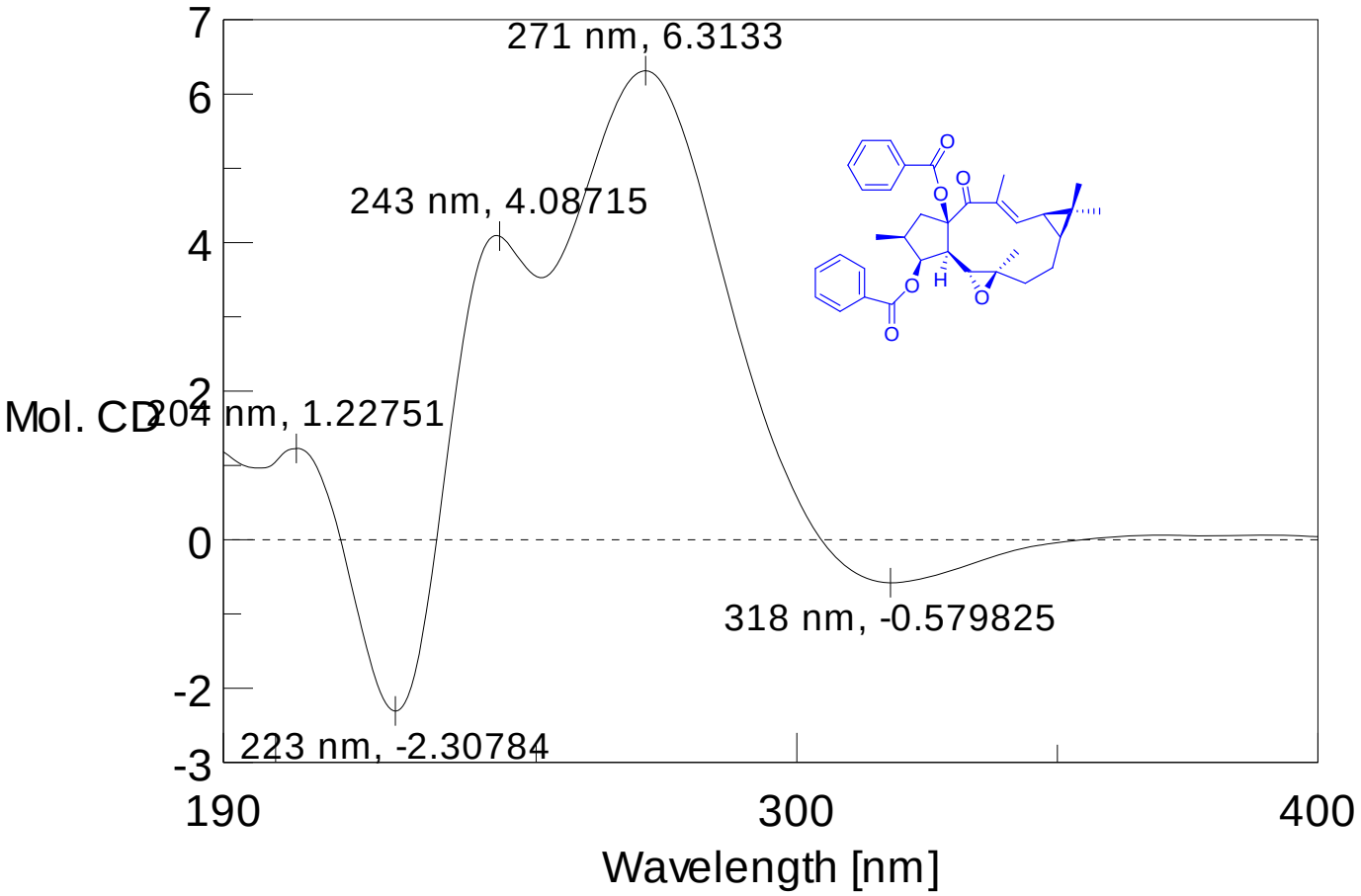

Figure S46. The CD Spectrum 5.

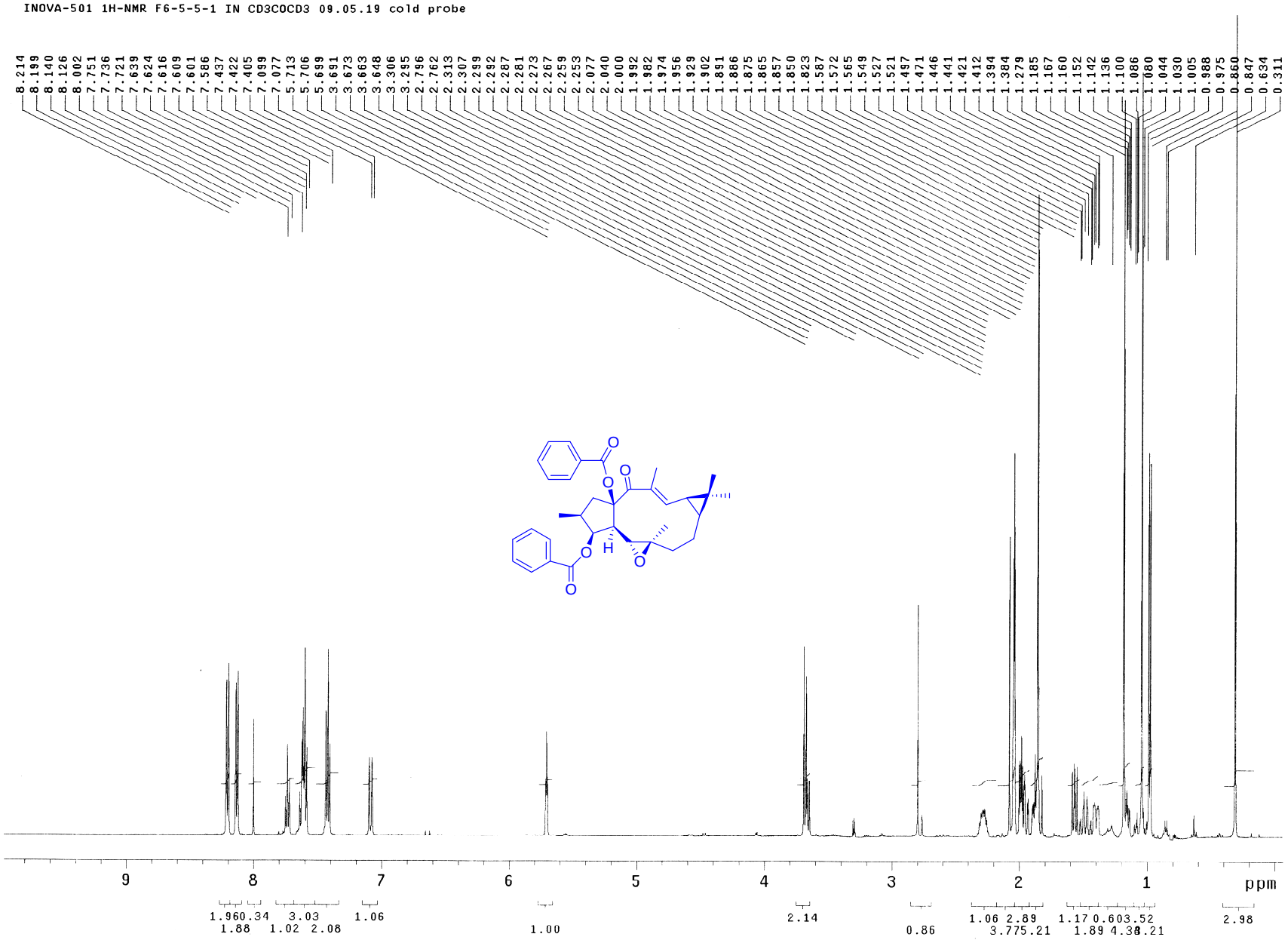

Figure S47. The ^{1}H NMR Spectrum of 5 in CD_3COCD_3 (500 MHz).

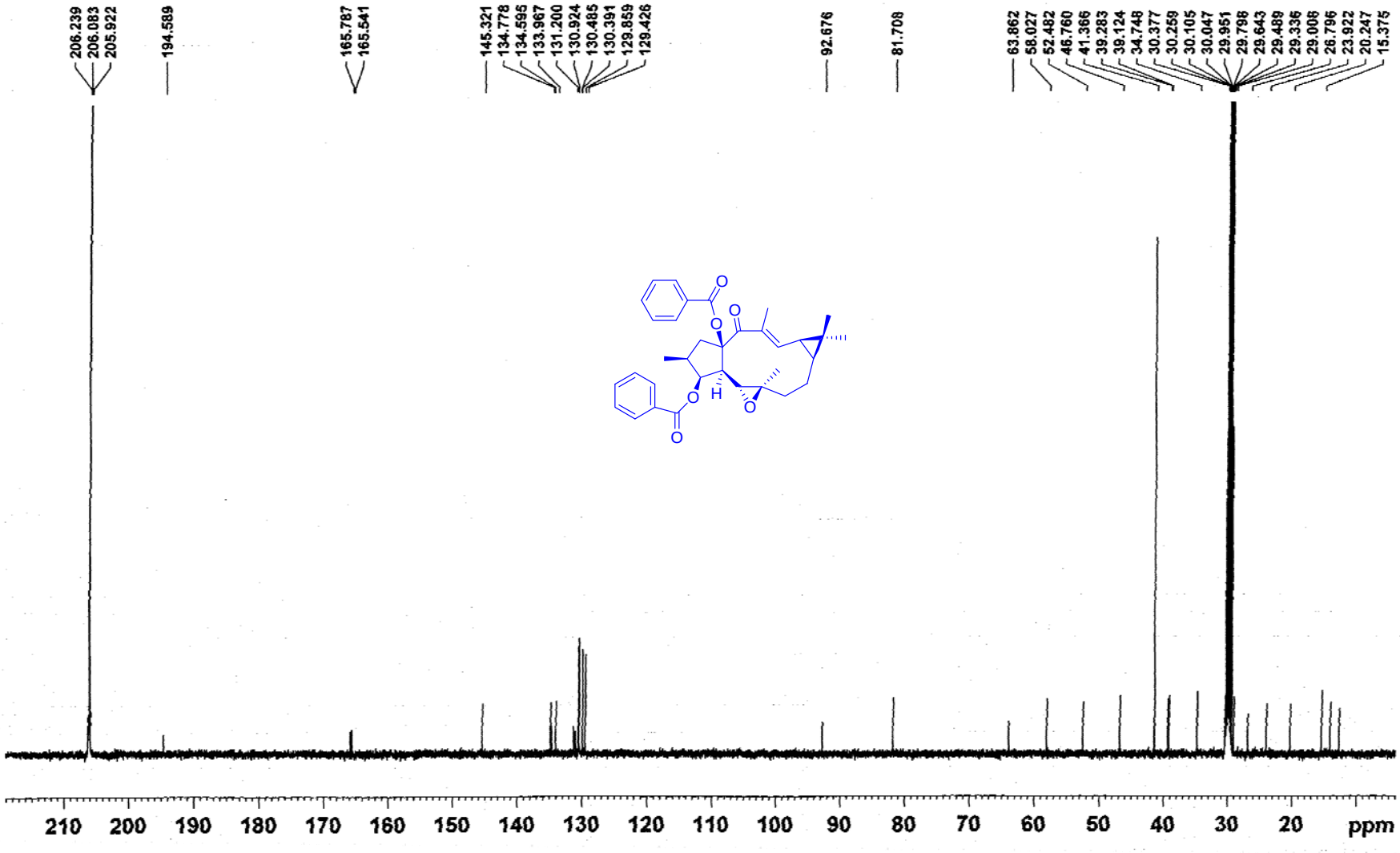

Figure S48. The ^{13}C NMR Spectrum of 5 in CD_3COCD_3 (125 MHz).

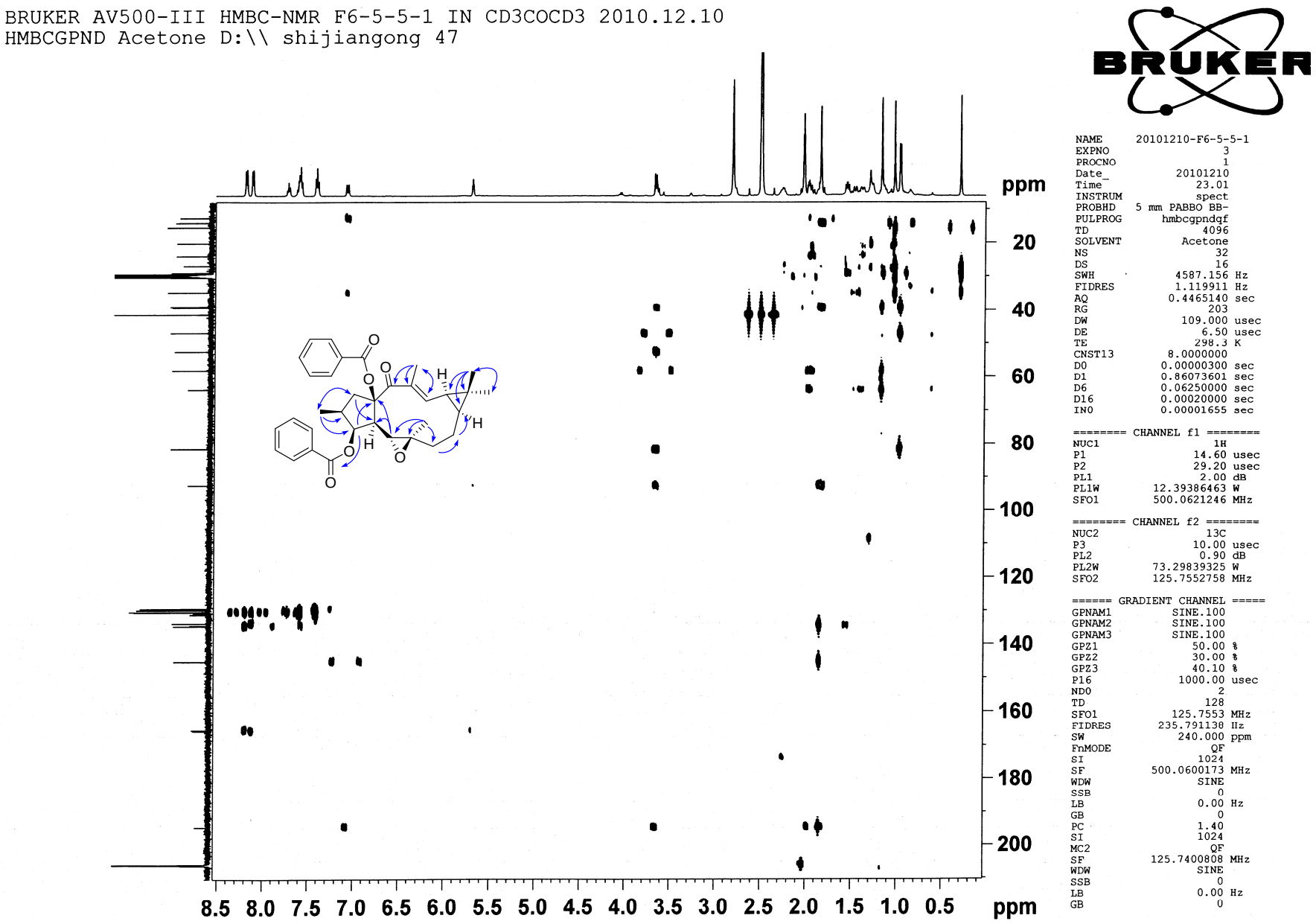

Figure S49. The gHMBC Spectrum of 5 in CD_3COCD_3 (500 MHz for ^1H NMR).

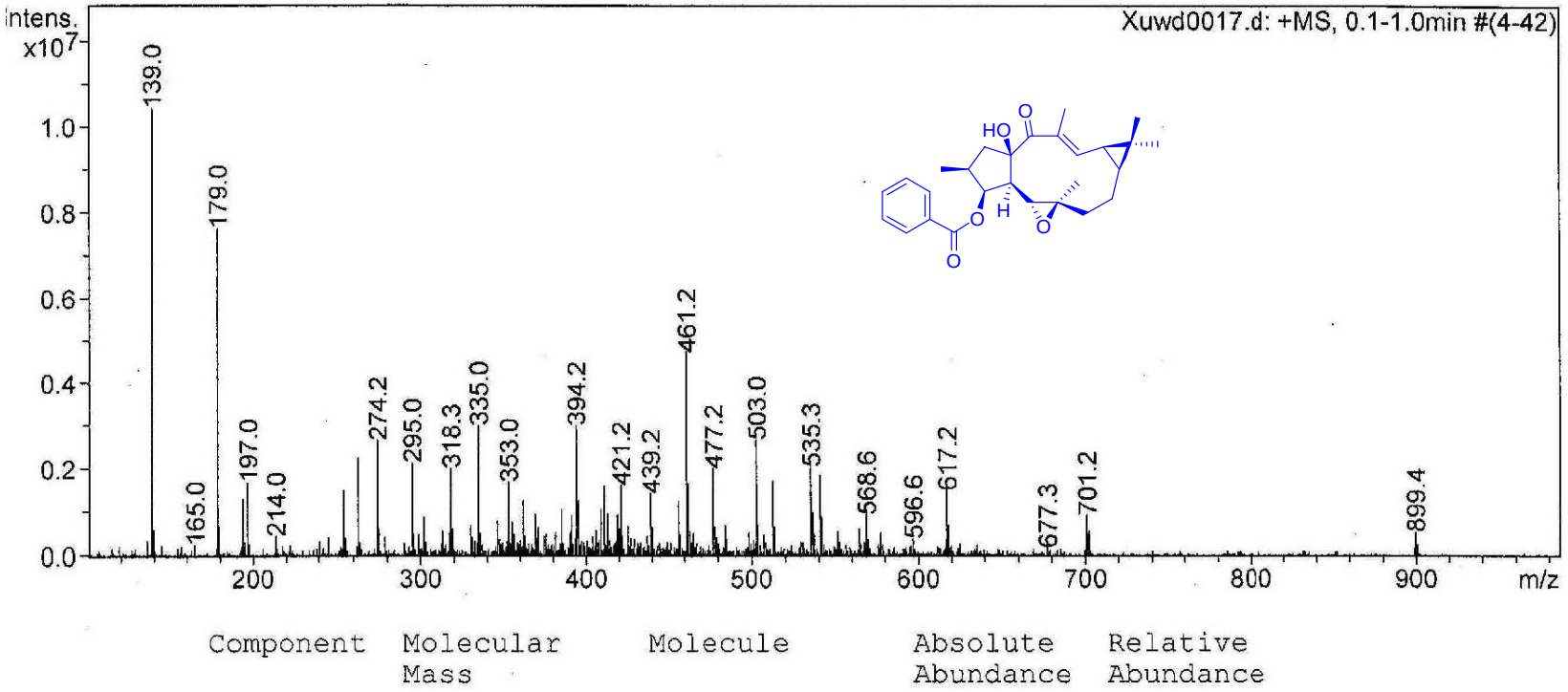

Figure S50. (+)-ESIMS Spectrum of 6.

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:^{12}C:0 .. 100, ^{1}H:0 .. 200, ^{23}Na:1 .. 1, ^{16}O: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.

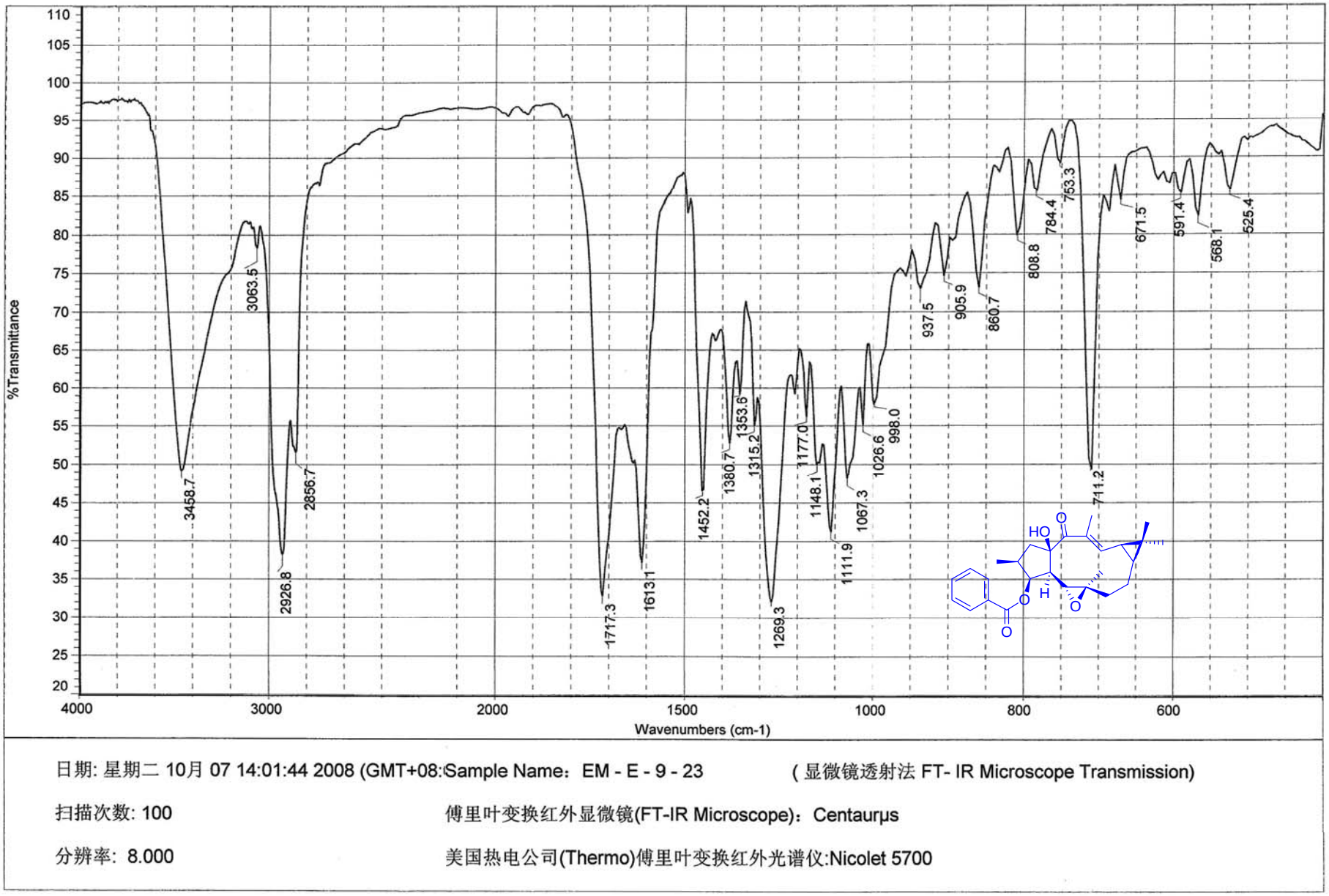

Figure S51. The IR Spectrum of 6.

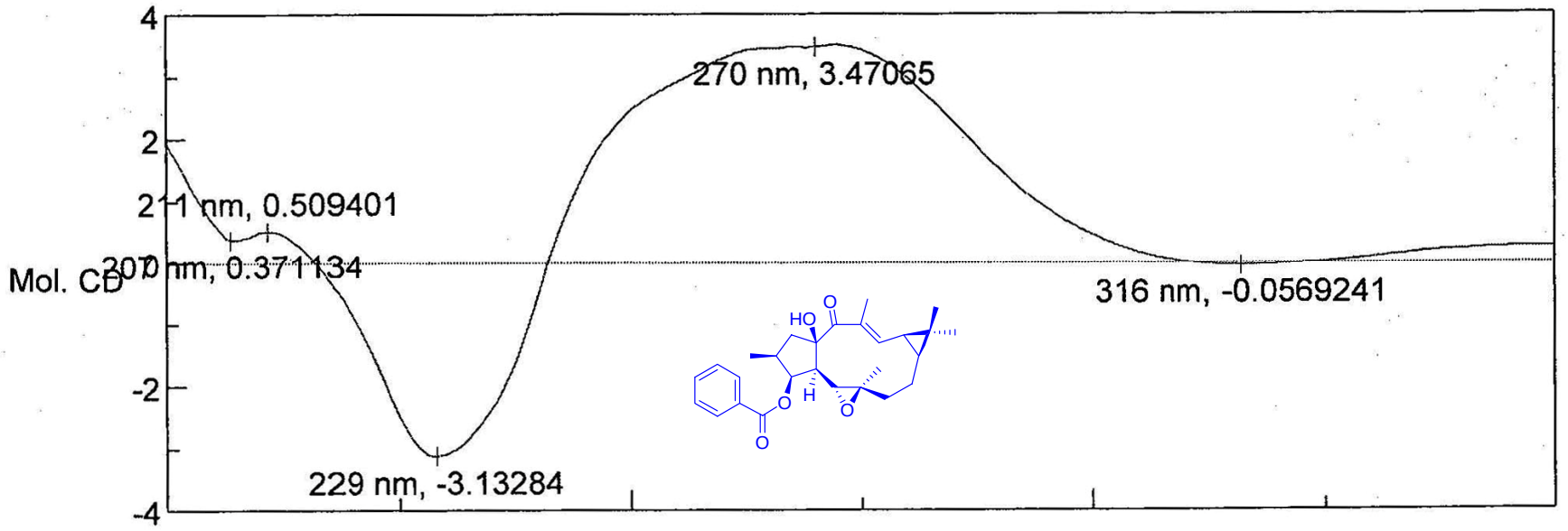

Figure S52. The CD Spectrum of 6.

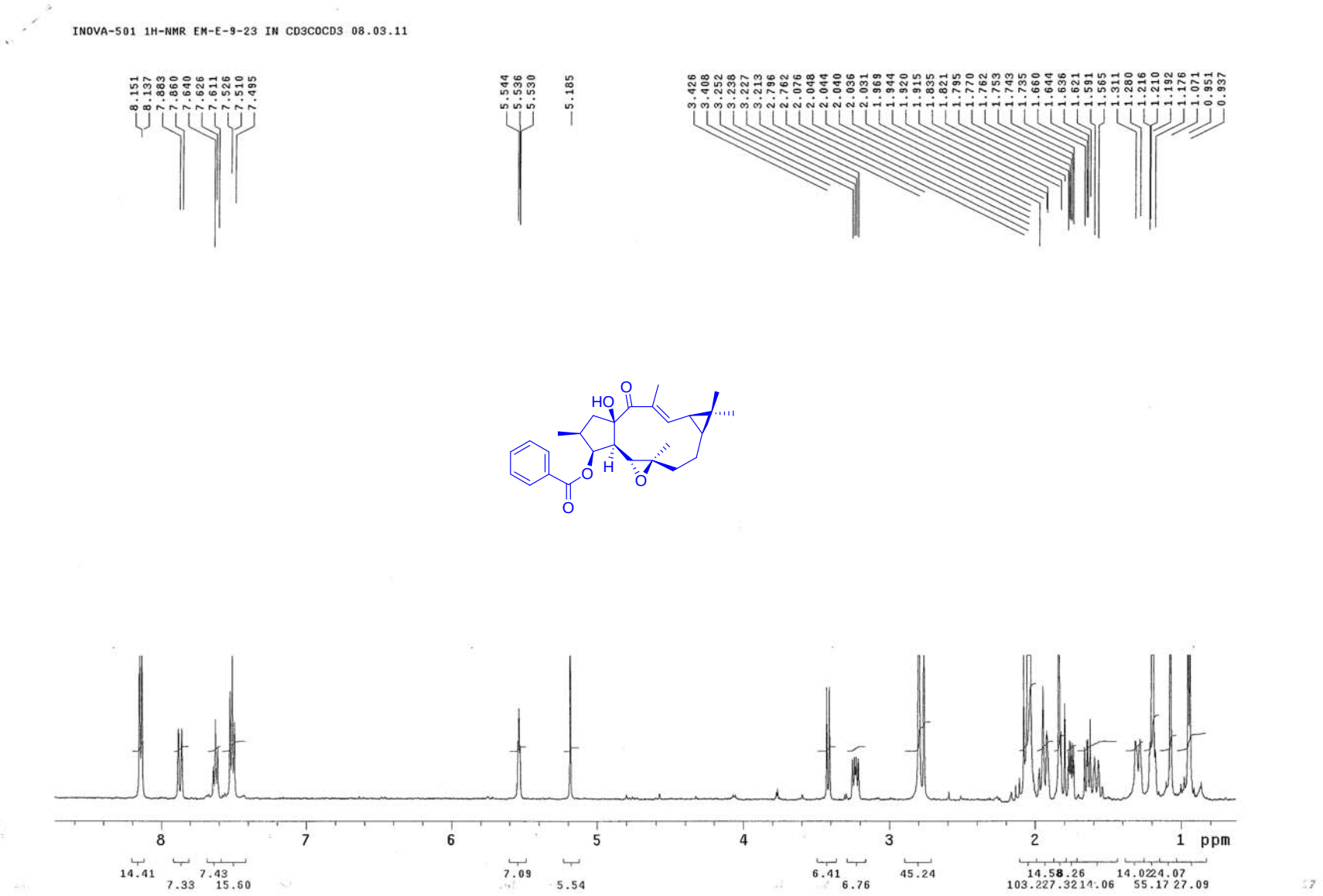

Figure S53. The ^{1}H NMR Spectrum of 6 in CD_3COCD_3 (500 MHz).

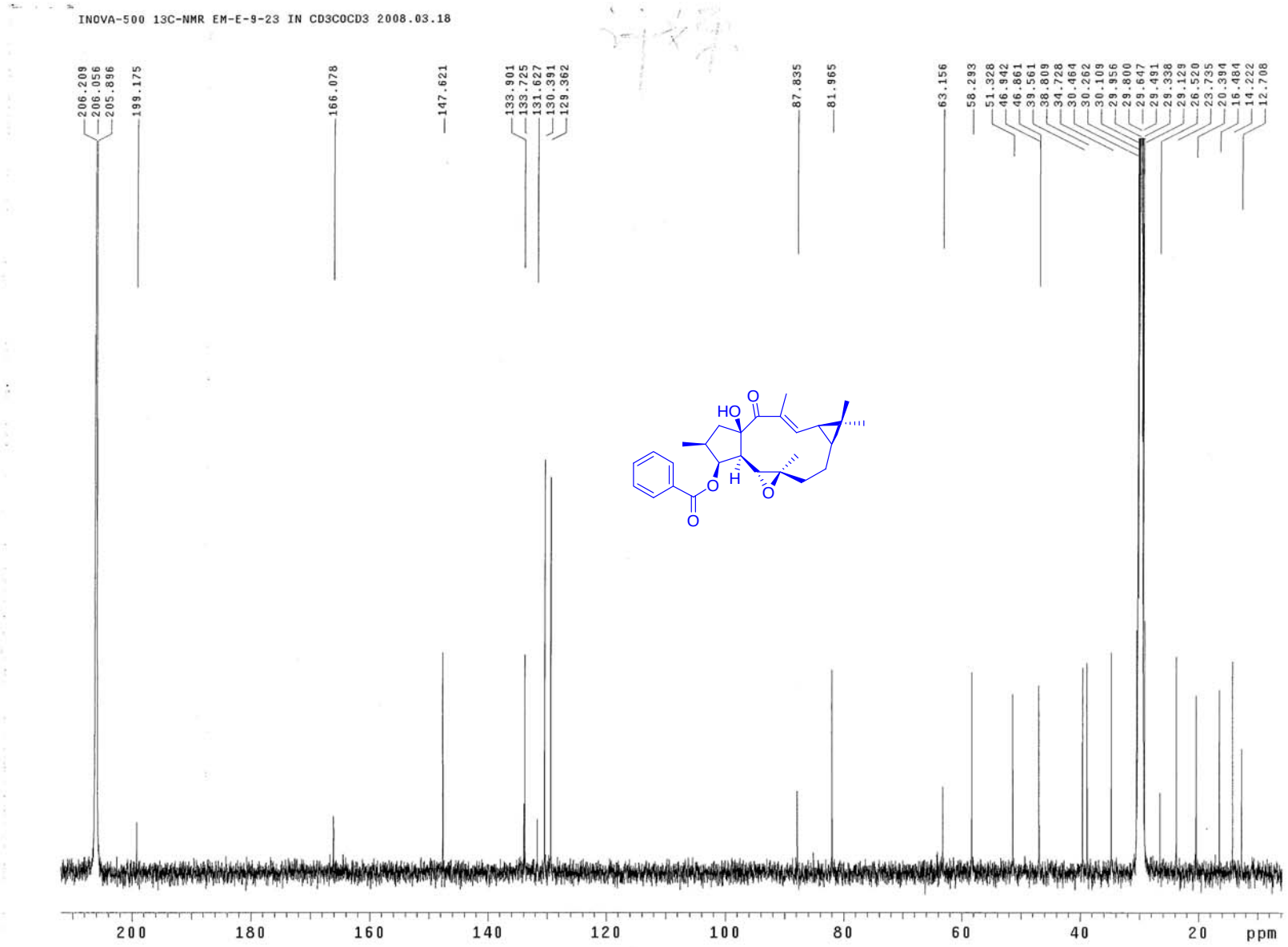

Figure S54. The ^{13}C NMR Spectrum of 6 in CD_3COCD_3 (125 MHz).

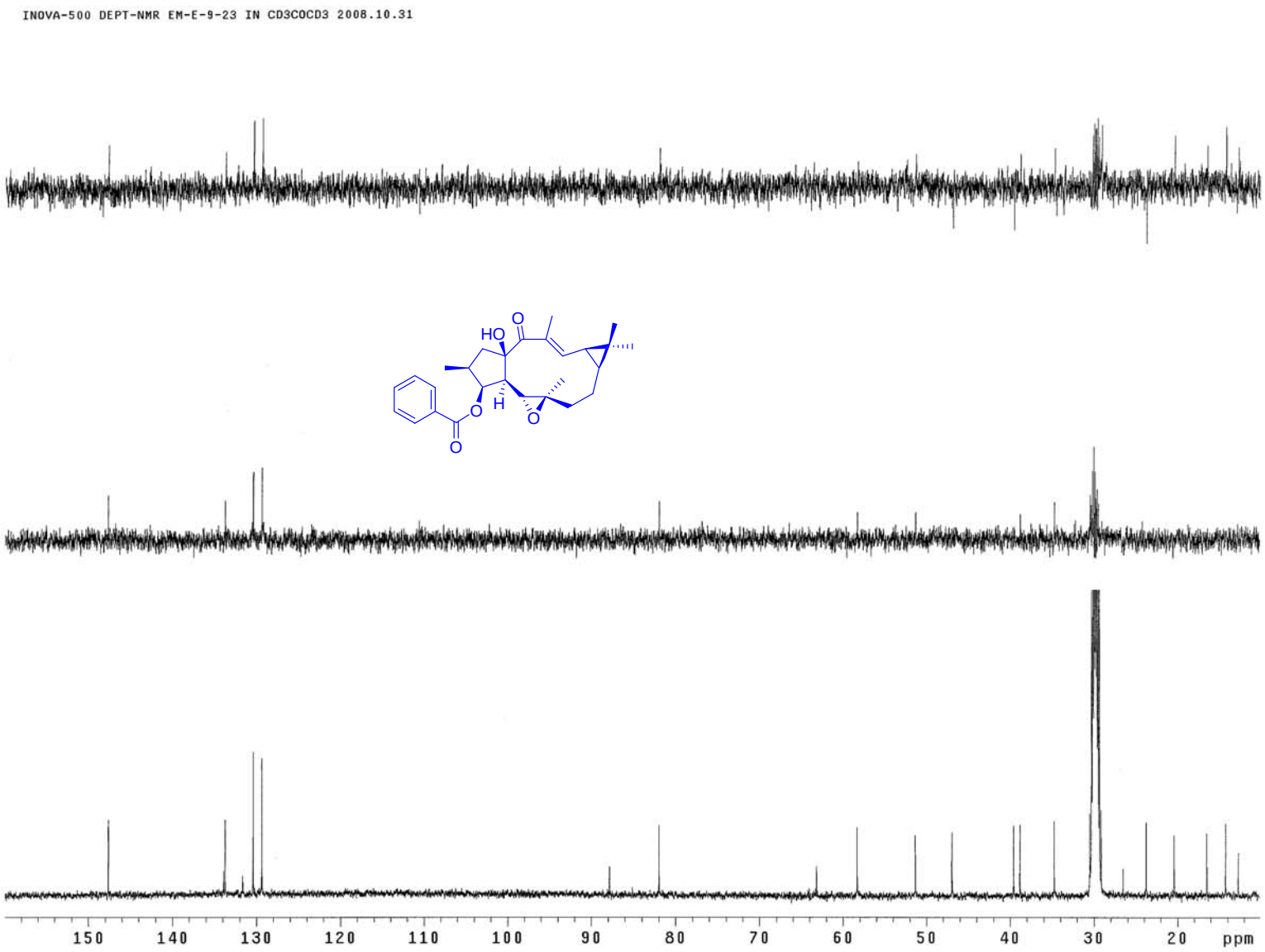

Figure S55. The DEPT Spectrum of 6 in CD_3COCD_3 (125 MHz).

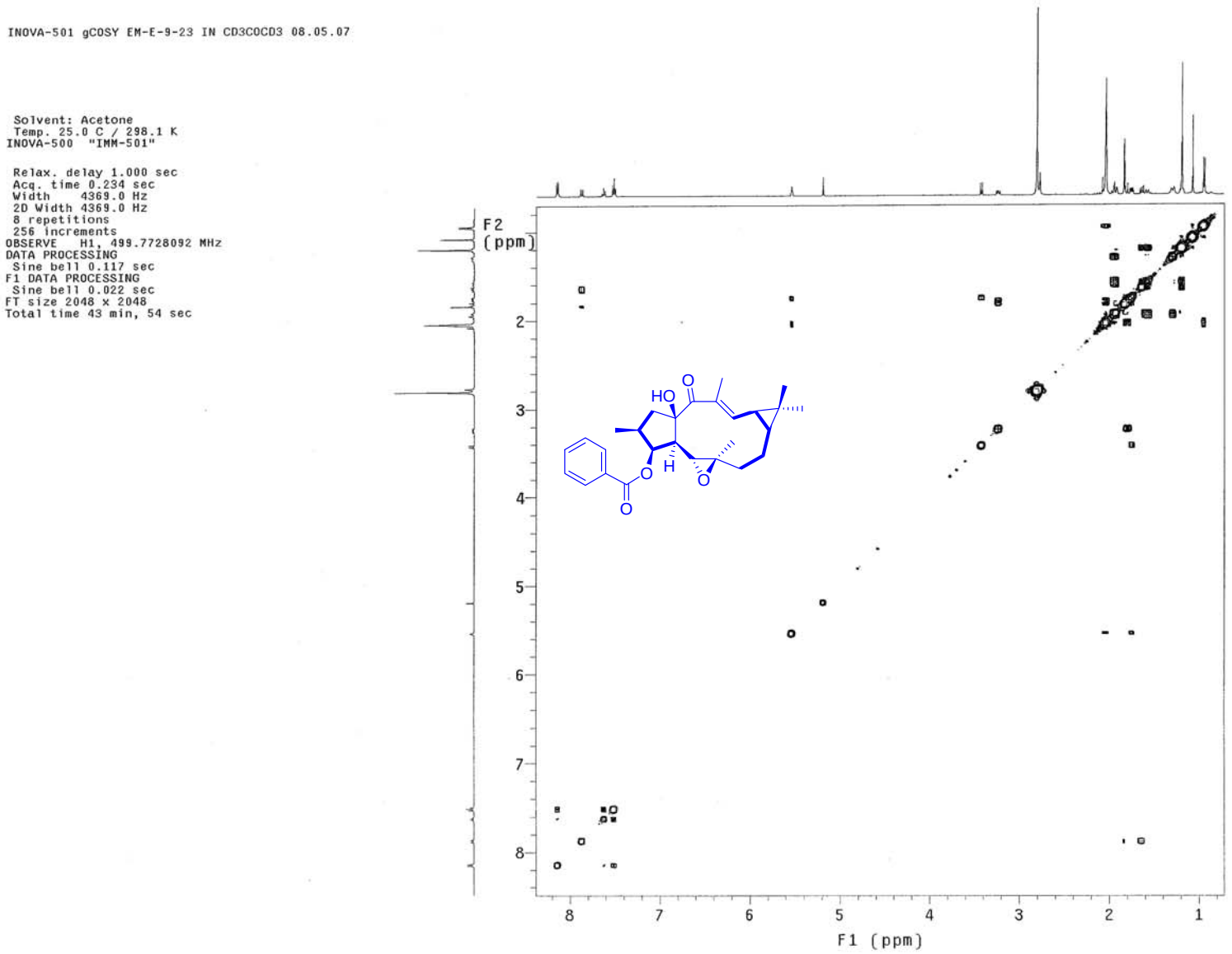

Figure S56. The ^{1}H-^{1}H gCOSY Spectrum of 6 in CD_3COCD_3 (500 MHz).

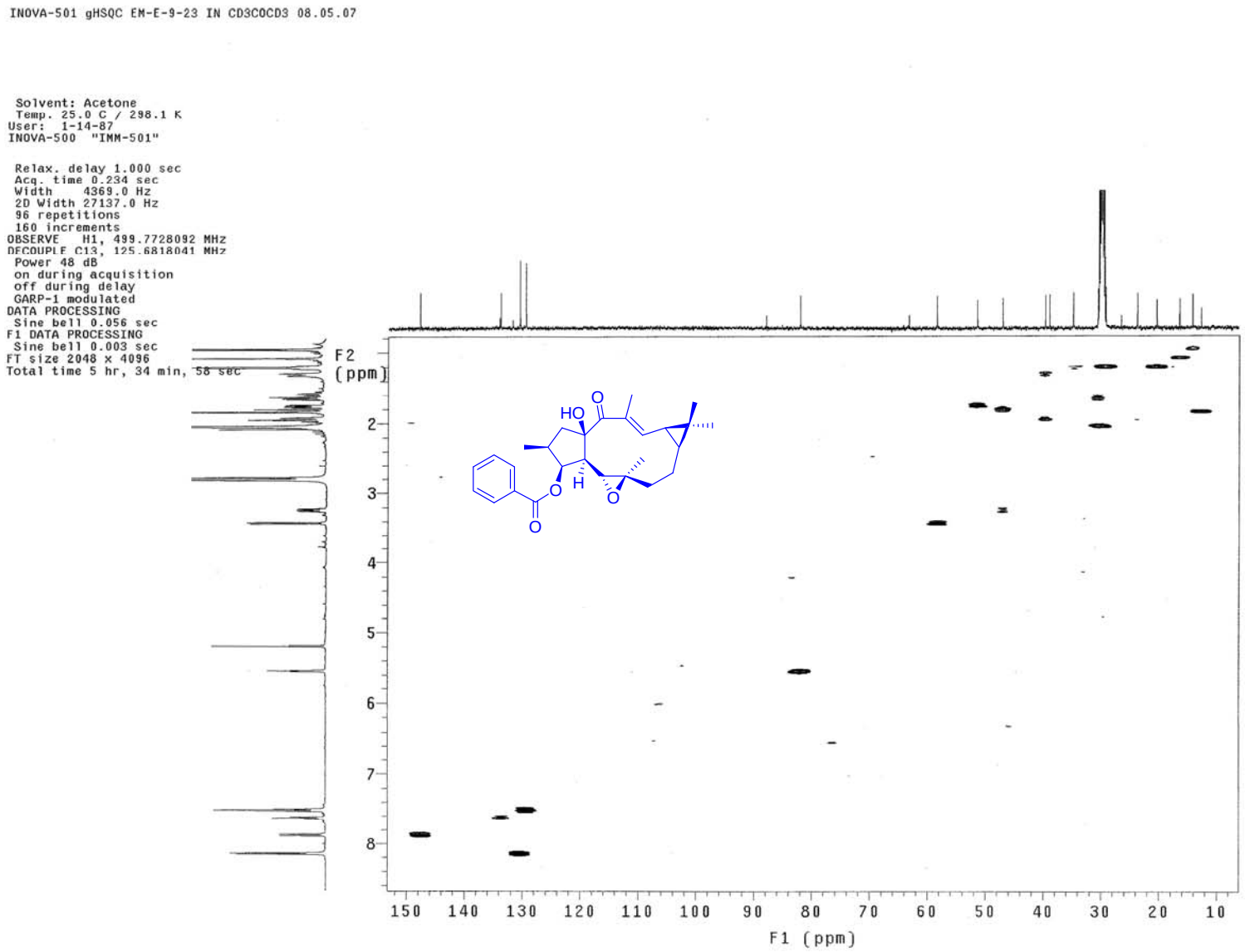

Figure S57. The gHSQC Spectrum of 6 in CD_3COCD_3 (500 MHz for ^1H NMR).

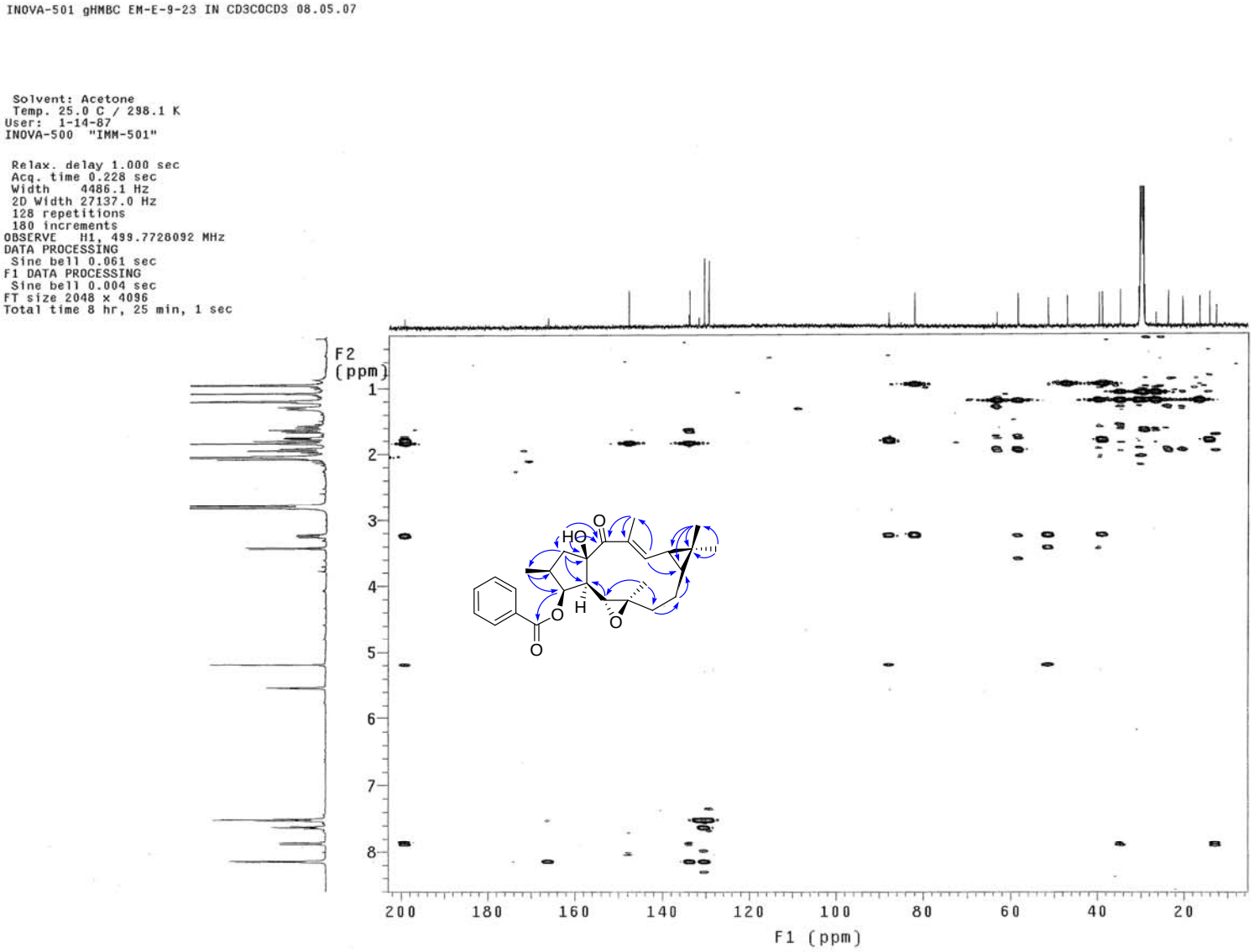

Figure S58. The gHMBC Spectrum of 6 in CD_3COCD_3 (500 MHz for ^1H NMR).

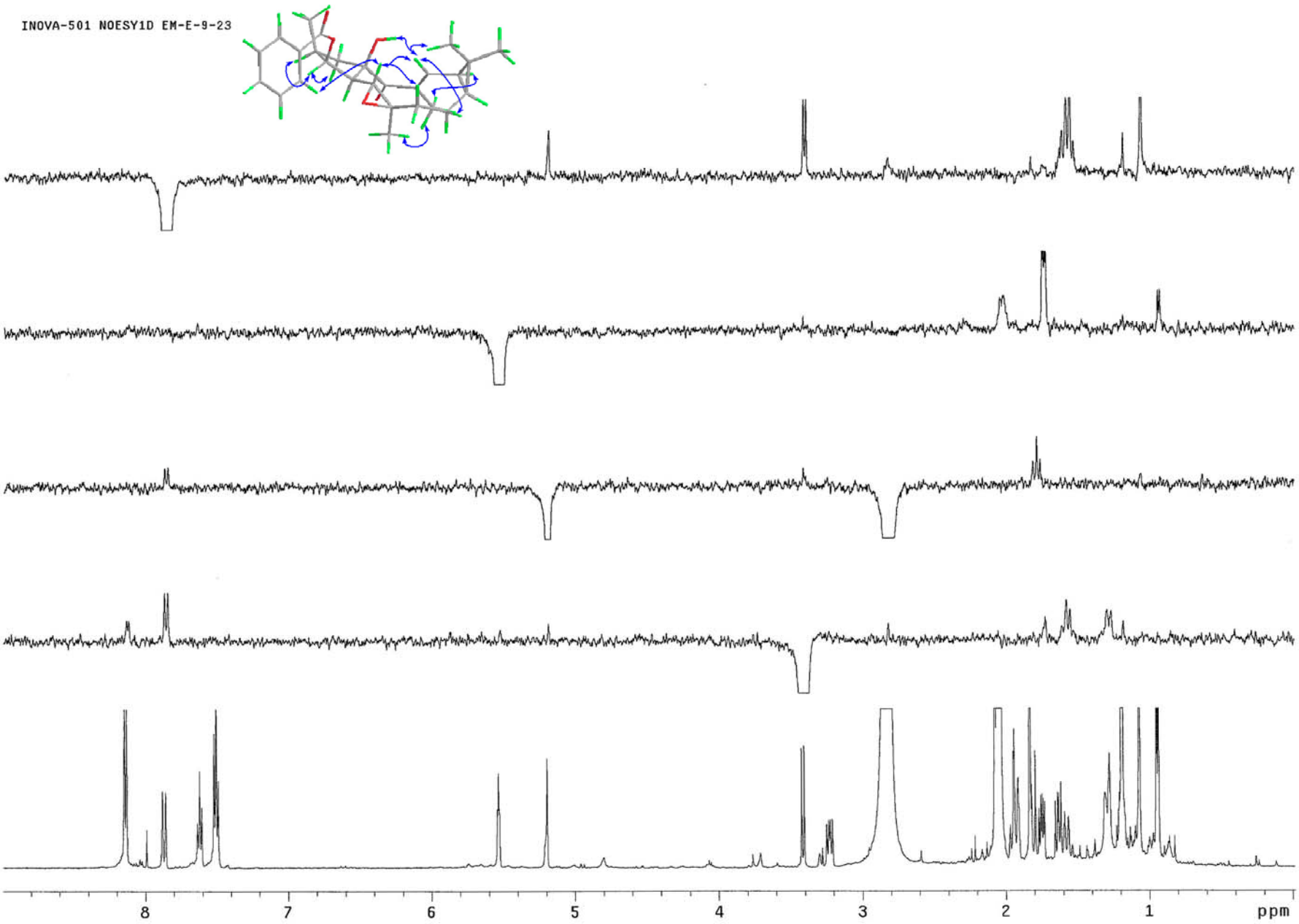

Figure S59. The NOE Difference Spectrum 1 of 6 in CD_3COCD_3 (500 MHz).

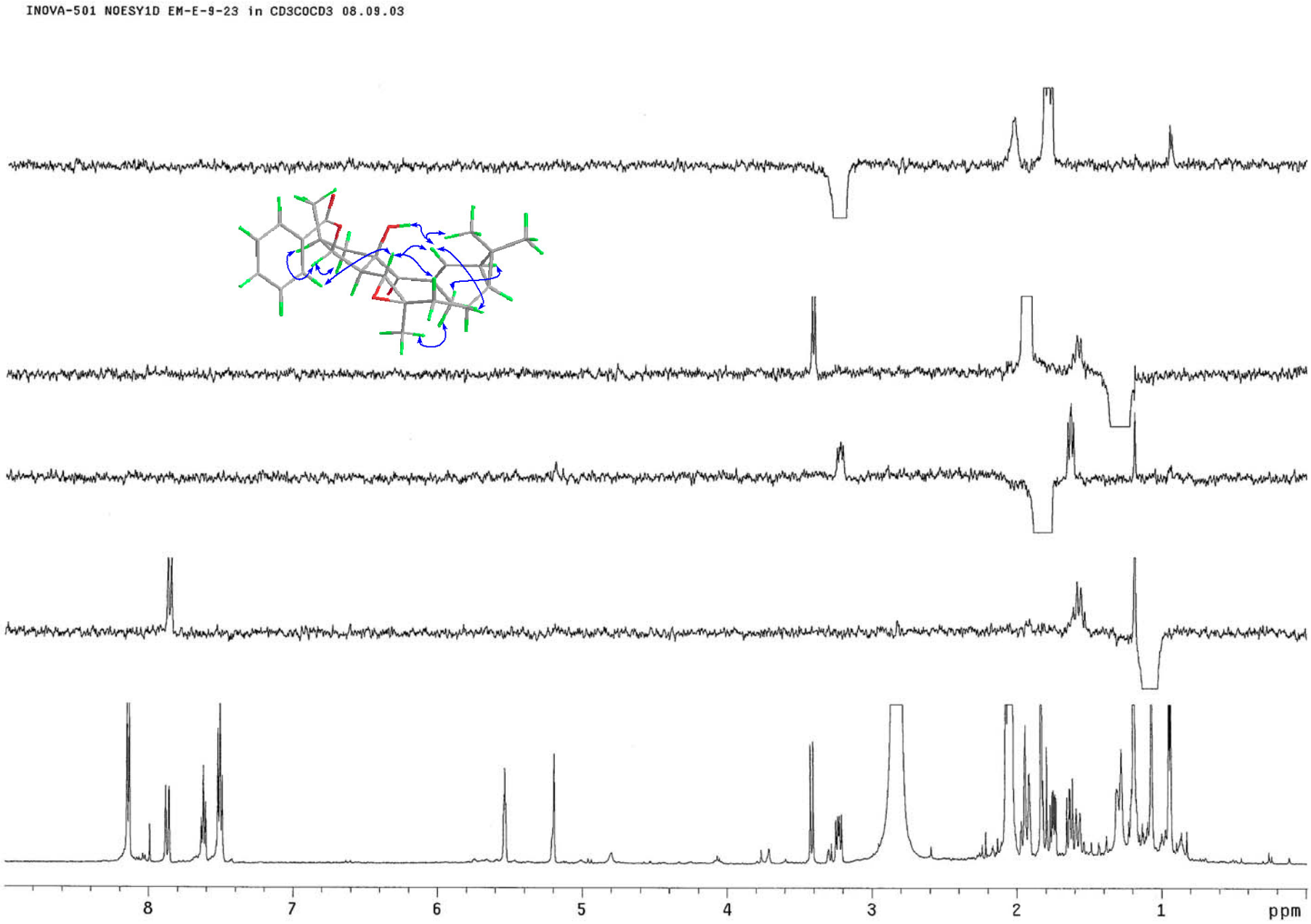

Figure S60. The NOE Difference Spectrum 2 of 6 in CD_3COCD_3 (500 MHz).

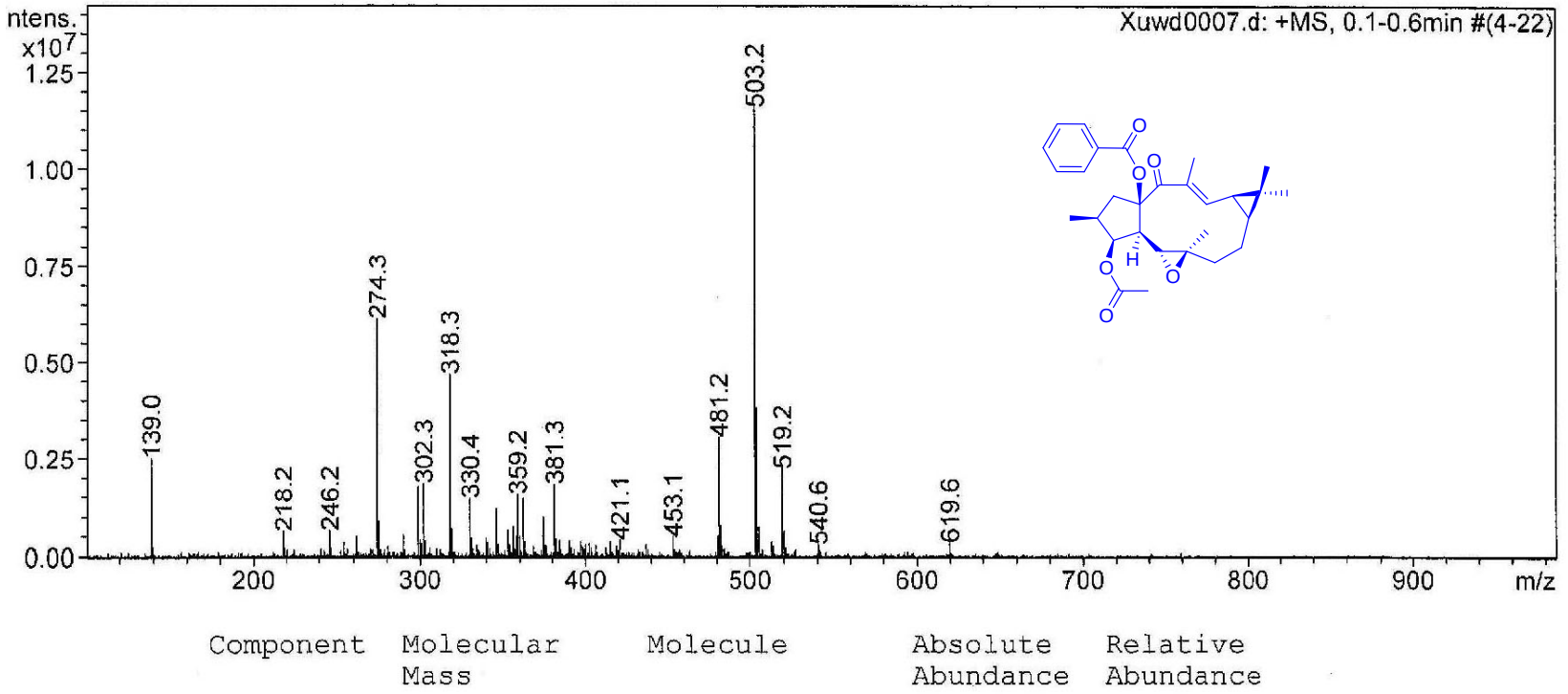

Figure S61. (+)-ESIMS Spectrum of 7.

MS Formula Results: + Scan (9.276 min) Sub (200905202.d)

m/z	Ion	Formula	Abundance
481.25734	(M+H)+	C29 H37 O6	222290.2

Best	Formula (M)	Ion Formula	Score	Cr	Calc m/z	Diff (ppm)	Mass Ma	Abund M	Spacing	DBE
☑	C29 H36 O6	C29 H37 O6	96.4		481.25847	2.37	94.28	97.75	99.05	12

m/z	Ion	Formula	Abundance
503.23957	(M+Na)+	C29 H36 Na O6	531147.5

Best	Formula (M)	Ion Formula	Score	Cr	Calc m/z	Diff (ppm)	Mass Ma	Abund M	Spacing	DBE
☑	C29 H36 O6	C29 H36 Na O6	97.69		503.24041	1.78	96.92	98.05	98.8	12

(+)-HRESIMS Data of 7.

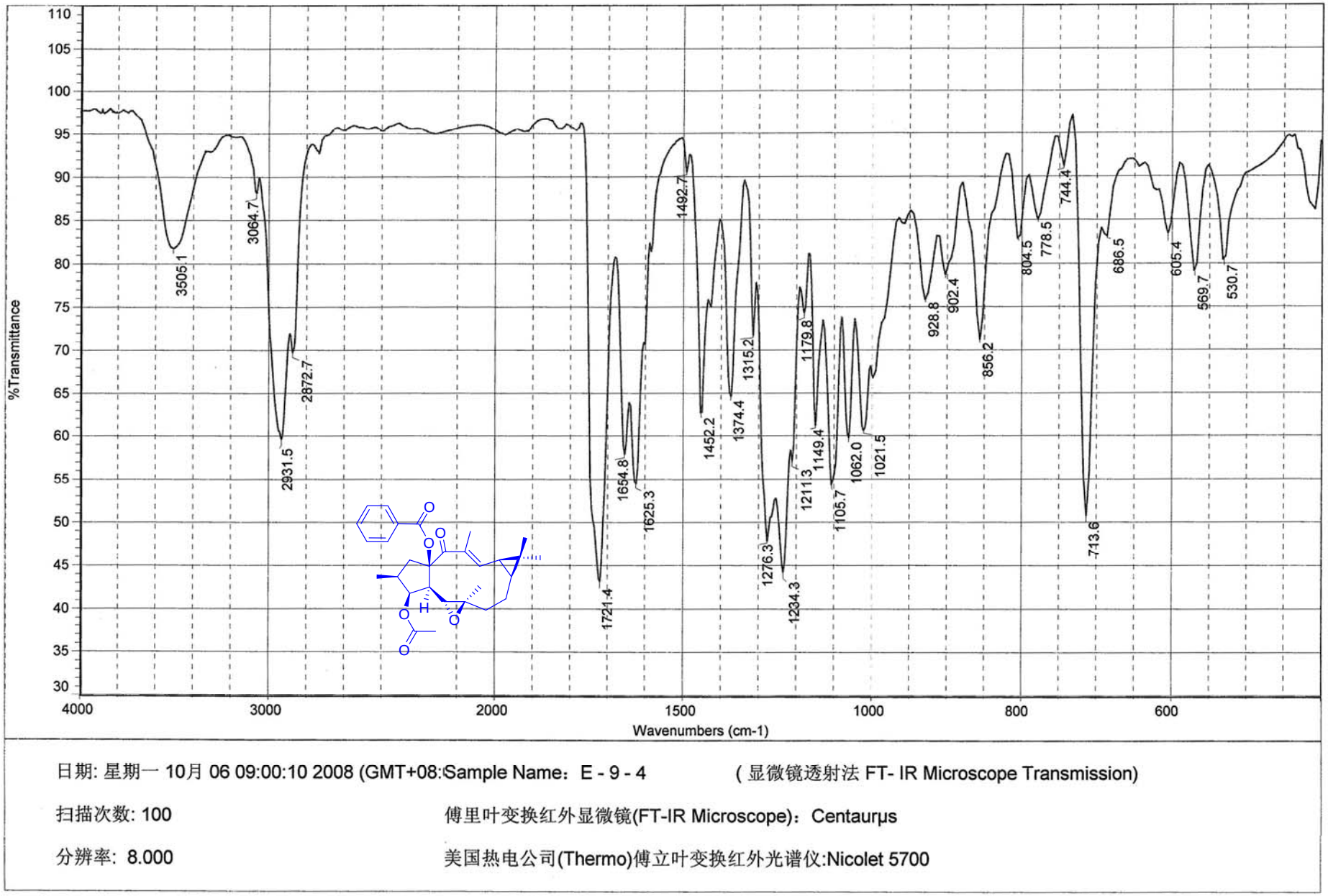

Figure S62. The IR Spectrum of 7.

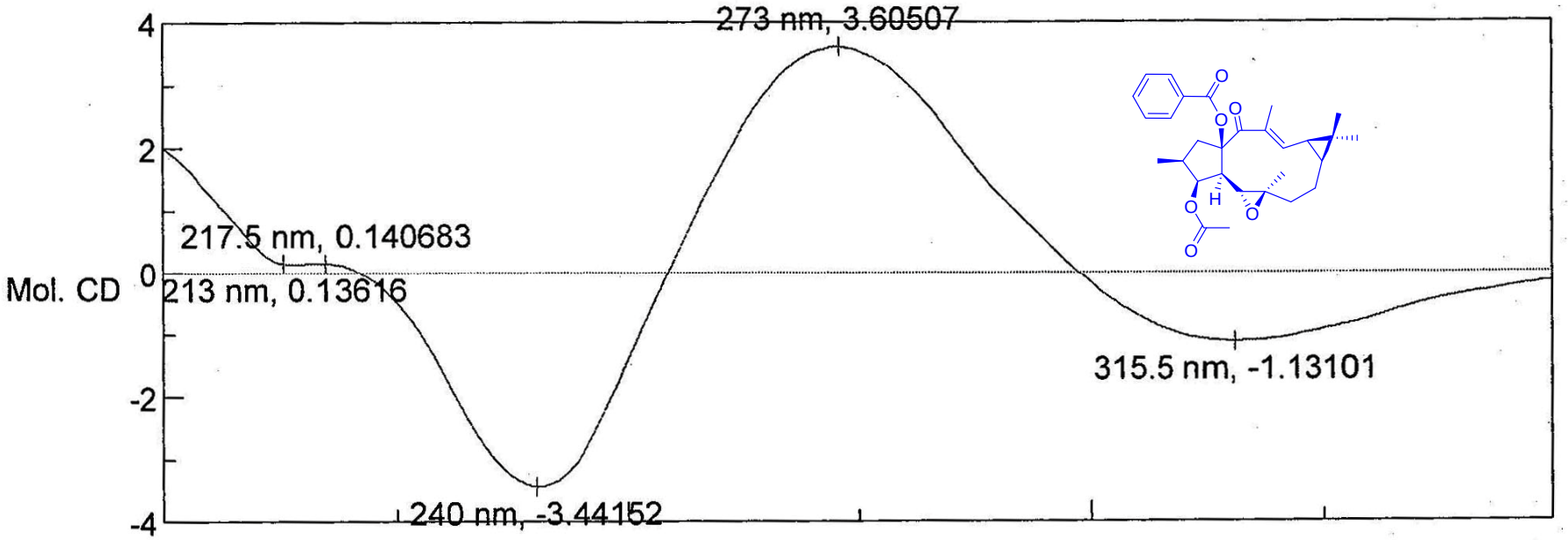

Figure S63. The CD Spectrum of 7.

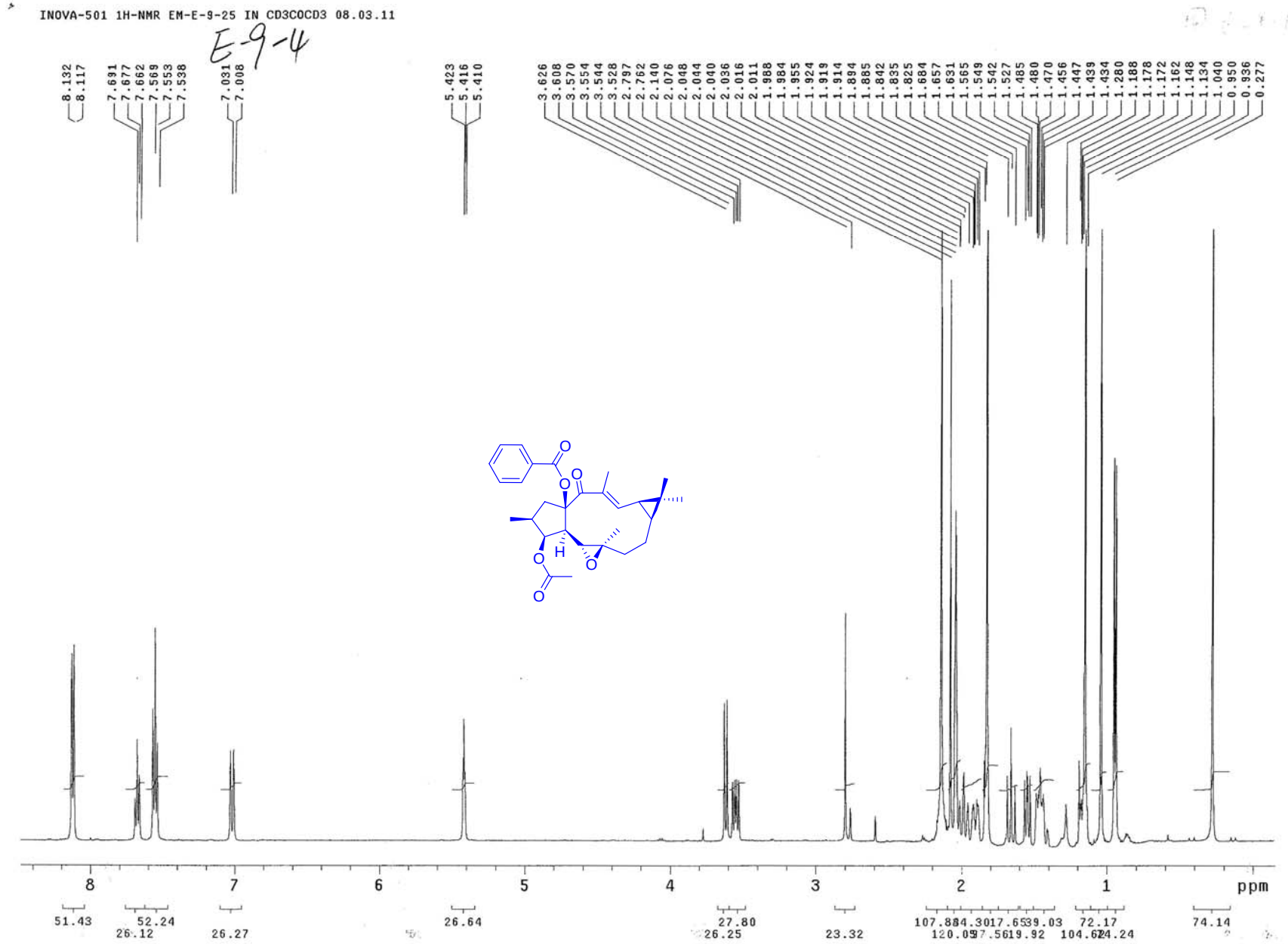

Figure S64. The ^{1}H NMR Spectrum of 7 in CD_3COCD_3 (500 MHz).

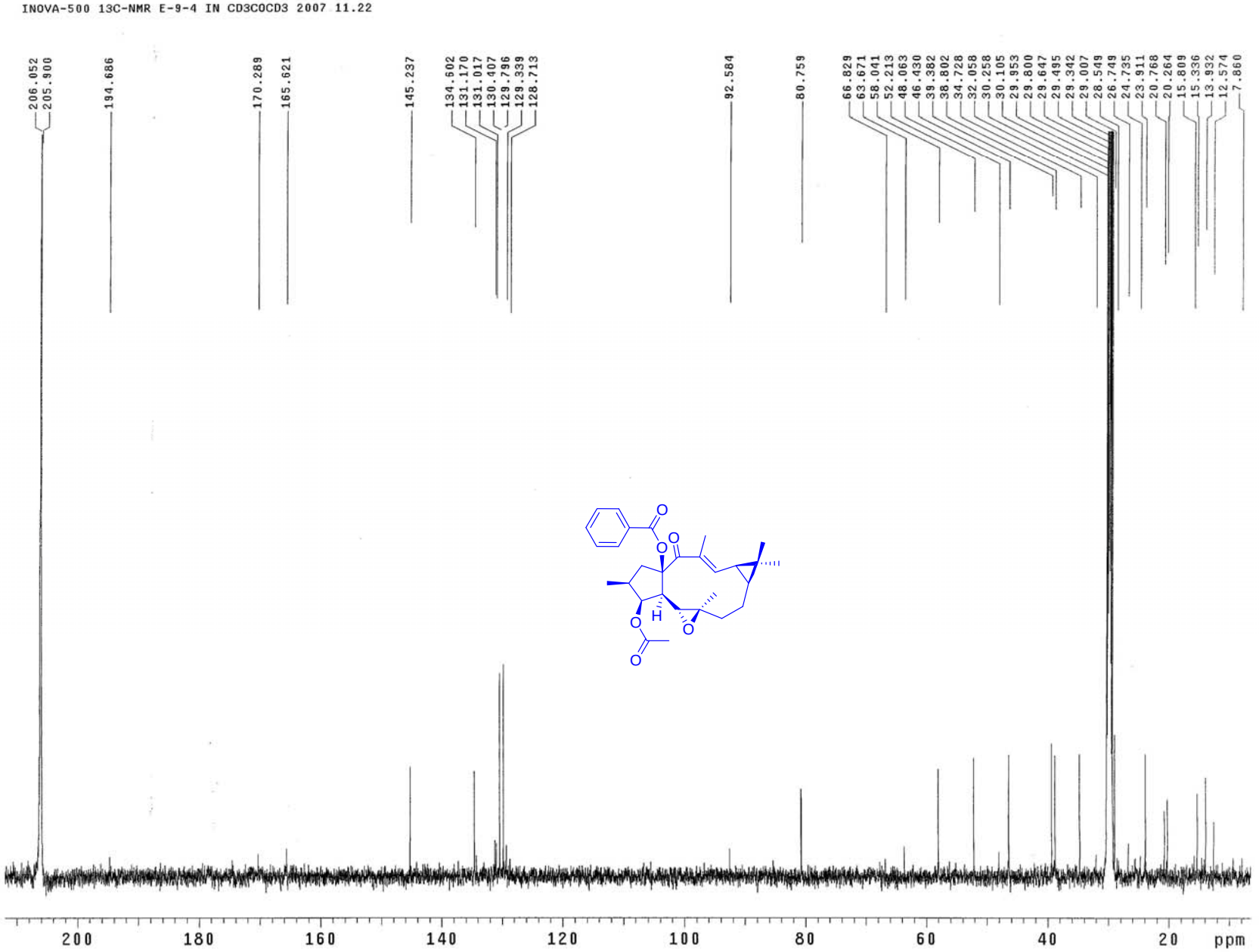

Figure S65. The ^{13}C NMR Spectrum of 7 in CD_3COCD_3 (125 MHz).

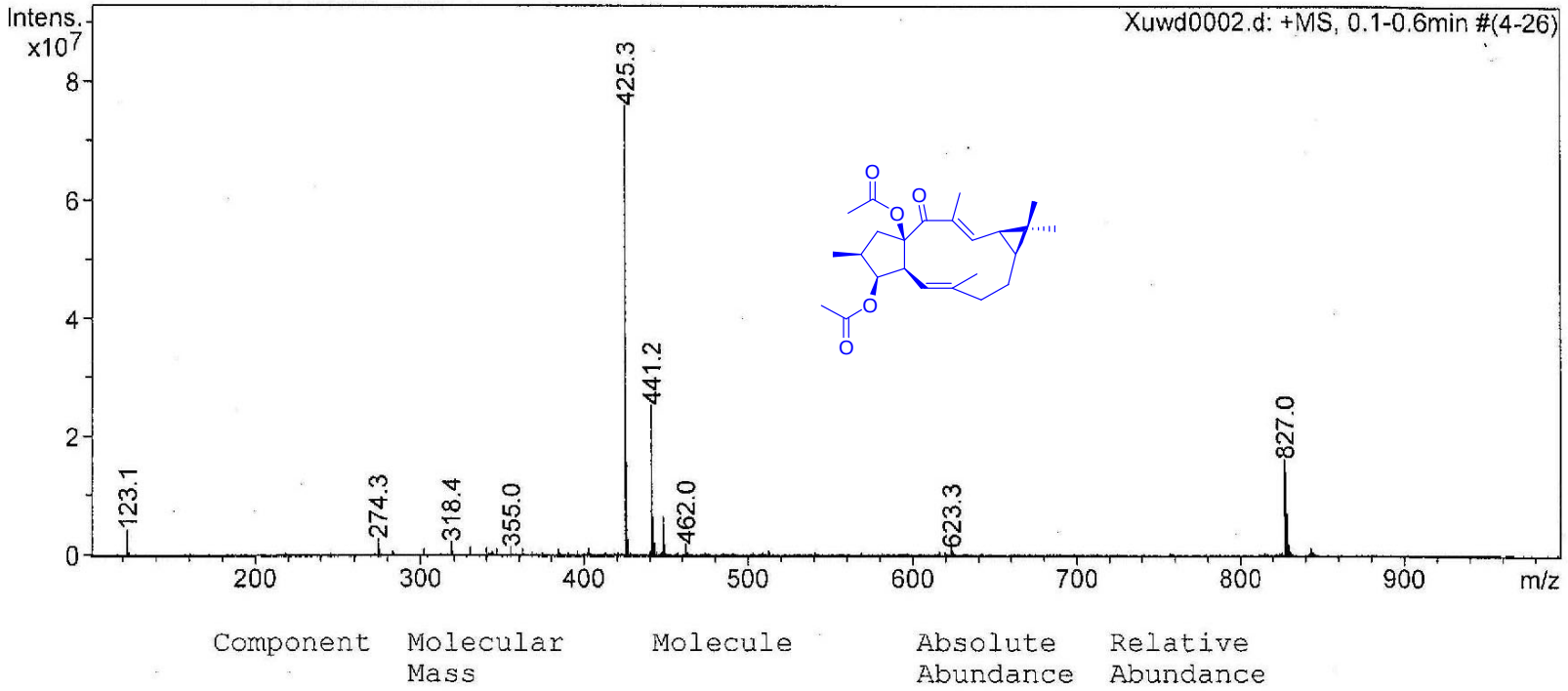

Figure S66. (+)-ESIMS Spectrum of 8.

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:^{12}C:0 .. 100, ^{1}H:0 .. 200, ^{23}Na:1 .. 1, ^{16}O: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.

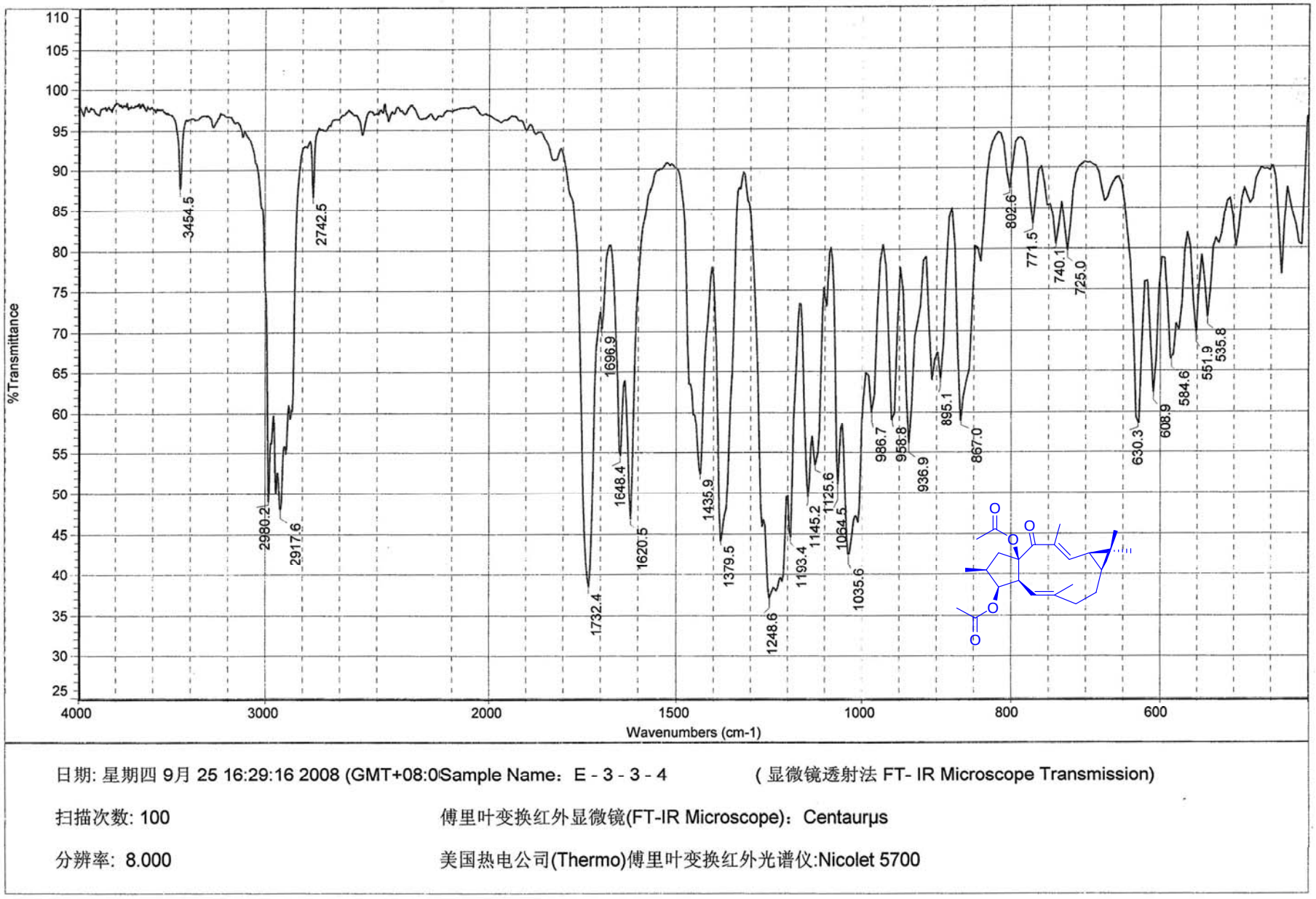

Figure S67. The IR Spectrum of 8.

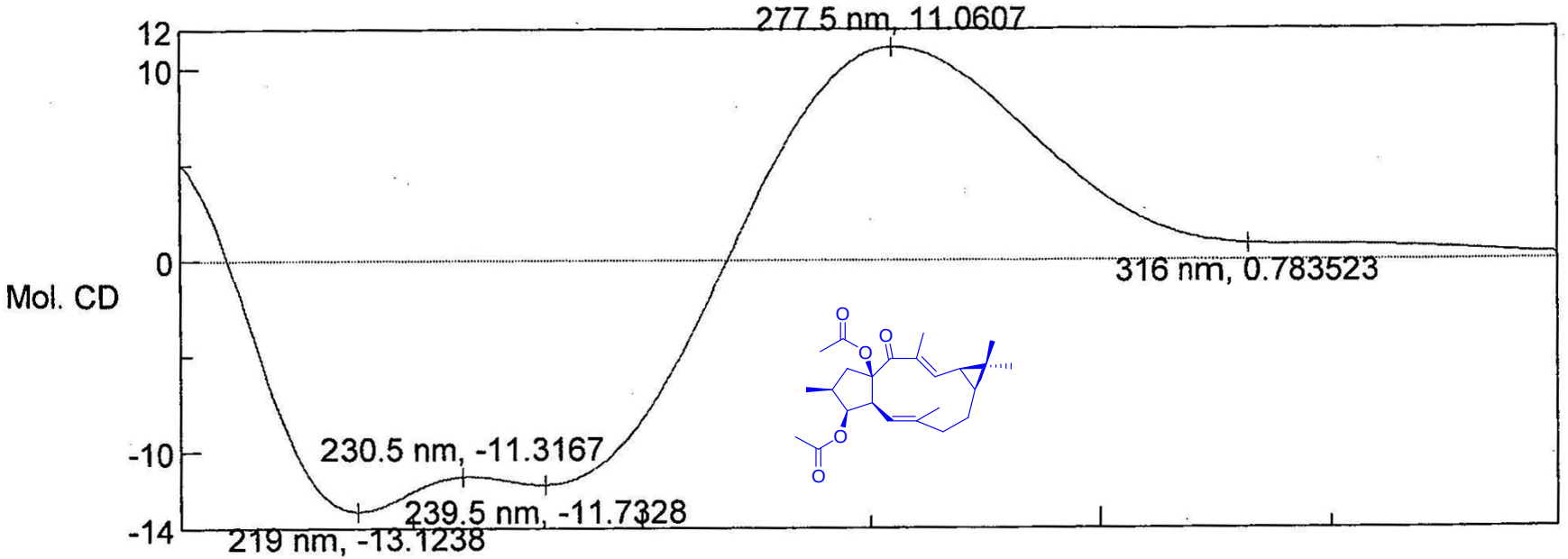

Figure S68. The CD Spectrum of 8.

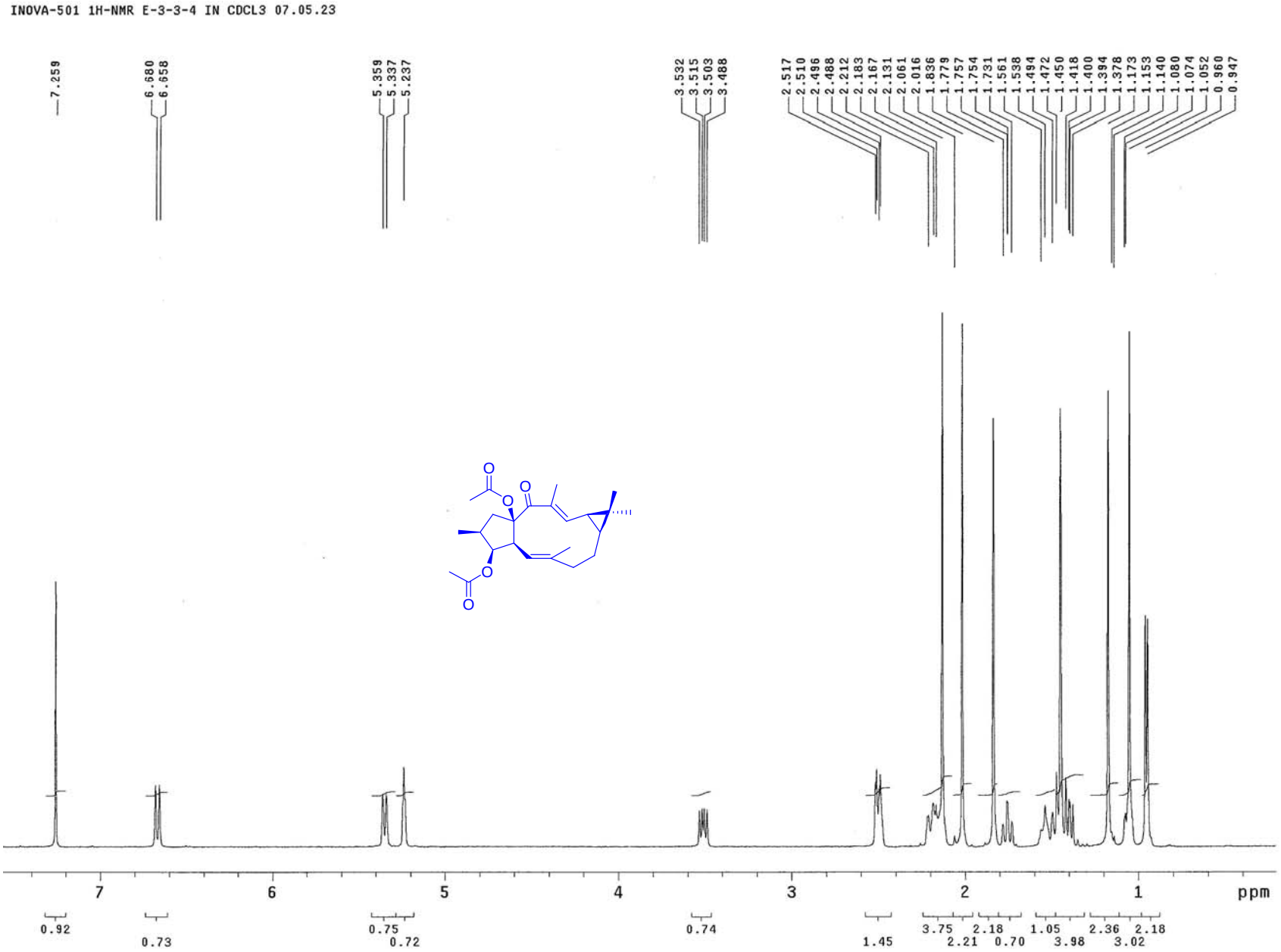

Figure S69. The ^{1}H NMR Spectrum of 8 in $CDCl_3$ (500 MHz).

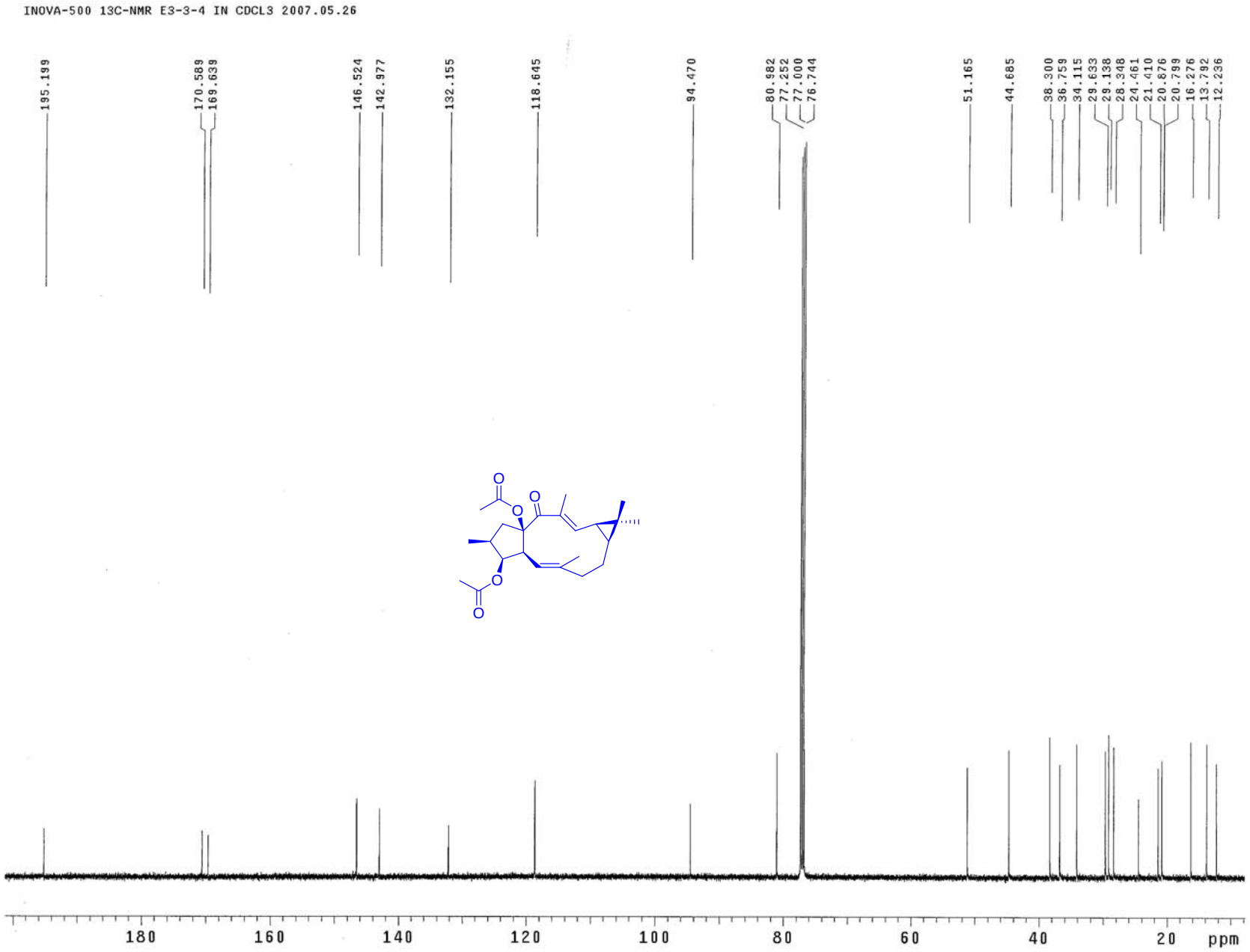

Figure S70. The ^{13}C NMR Spectrum of 8 in $CDCl_3$ (125 MHz).

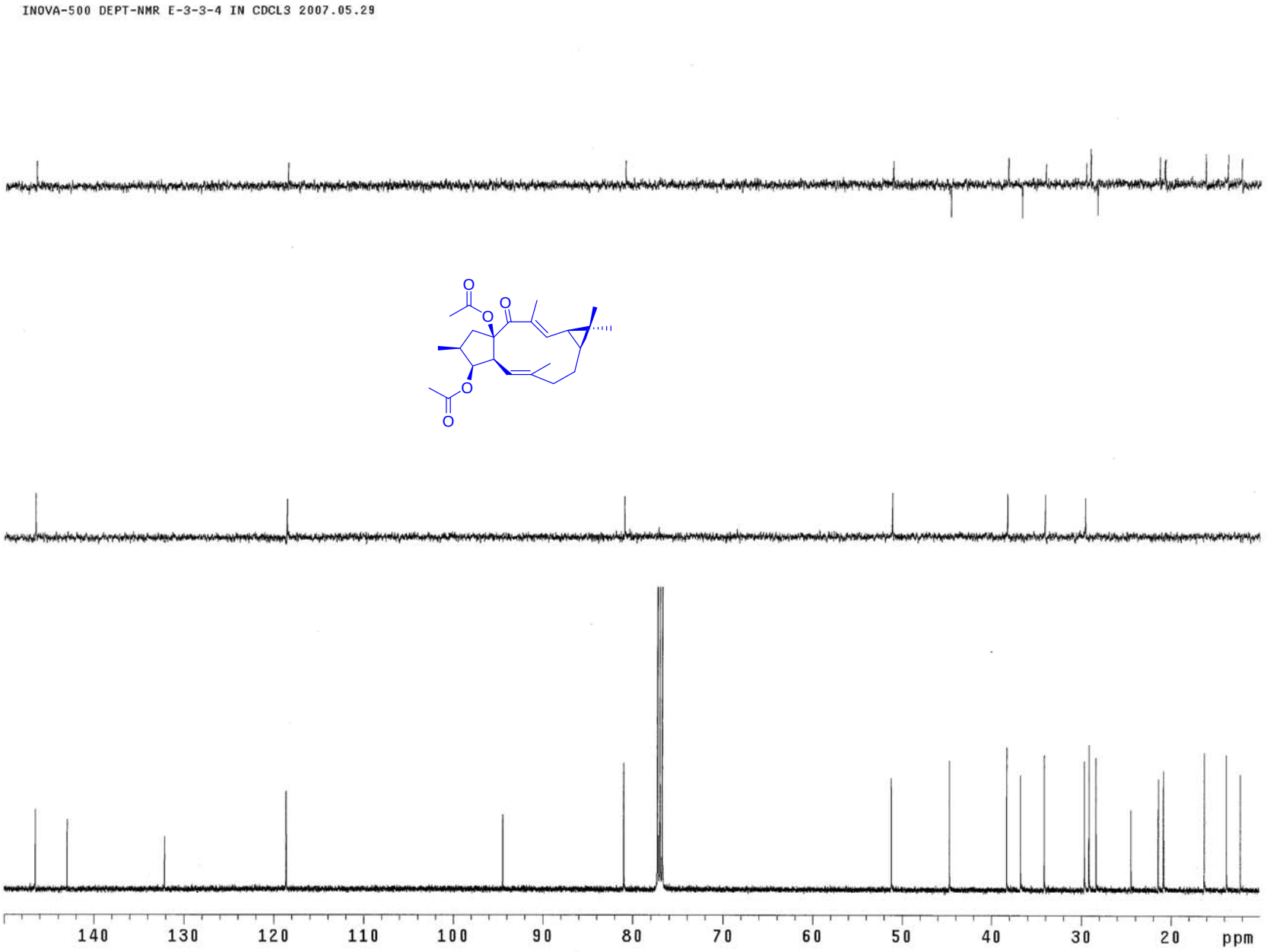

Figure S71. The DEPT Spectrum of 8 in $CDCl_3$ (125 MHz).

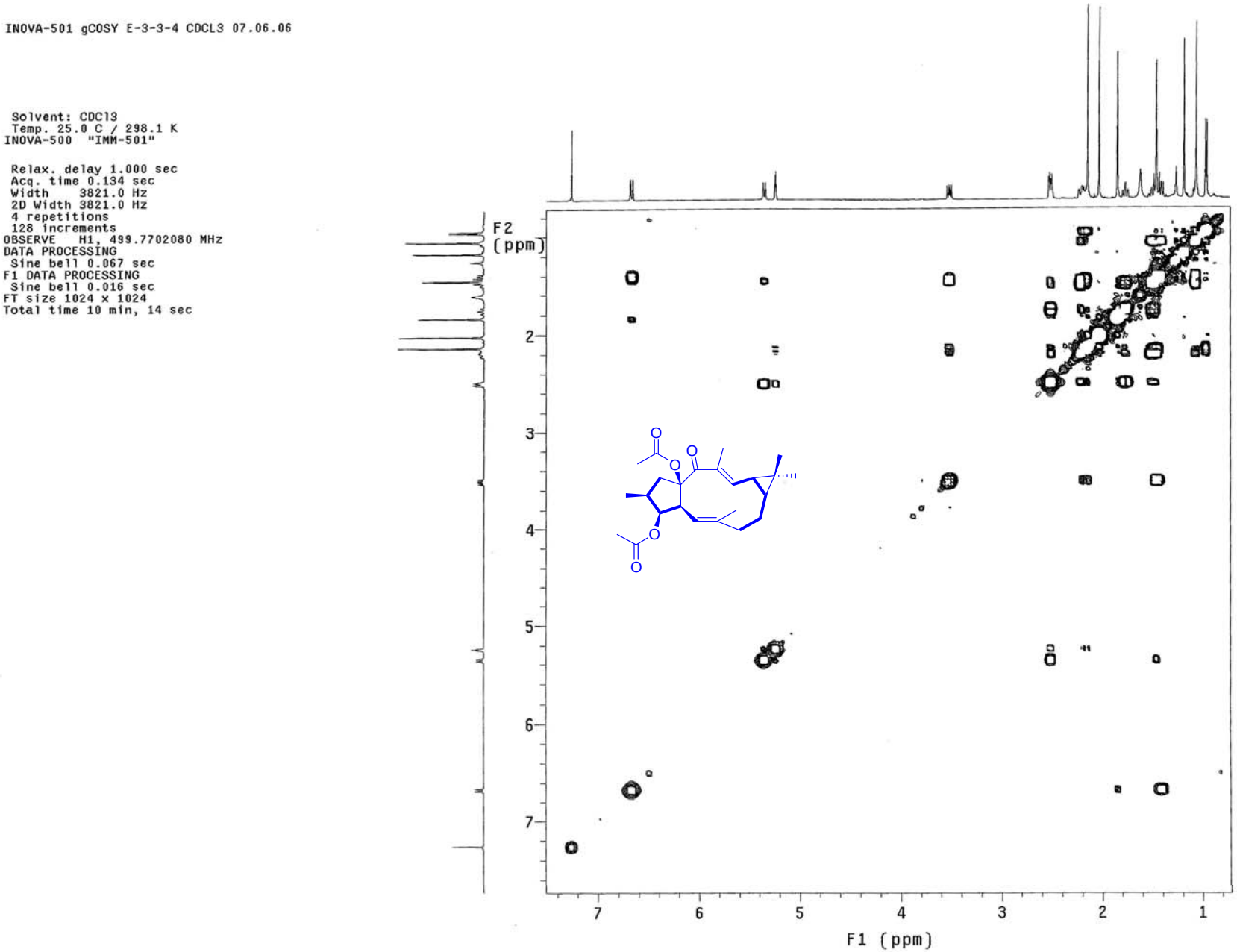

Figure S72. The ^{1}H-^{1}H gCOSY Spectrum of 8 in $CDCl_3$ (500 MHz).

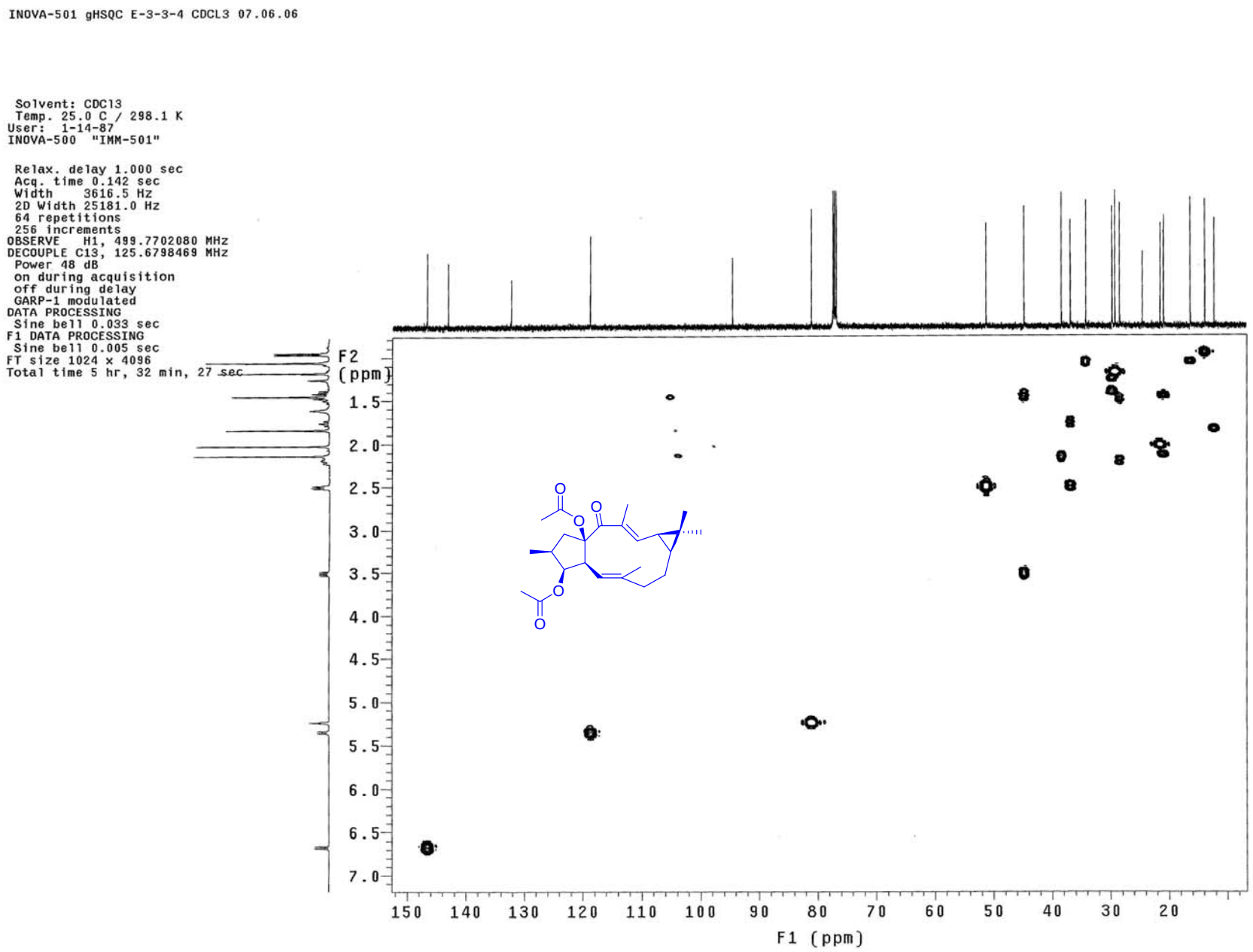

Figure S73. The gHSQC Spectrum of 8 in $CDCl_3$ (500MHz for ^1H NMR).

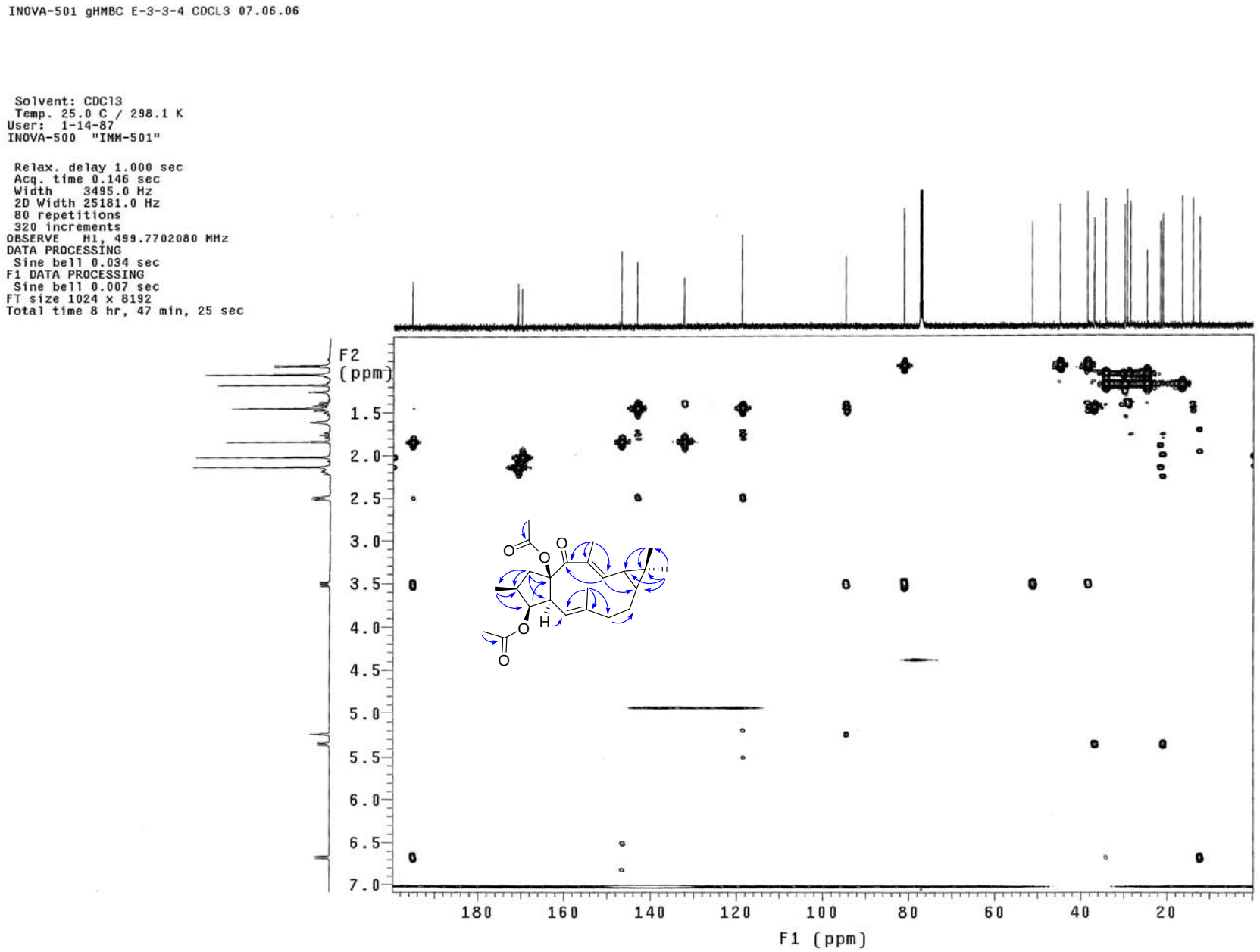

Figure S74. The gHMBC Spectrum of 8 in $CDCl_3$ (500MHz for ^1H NMR).

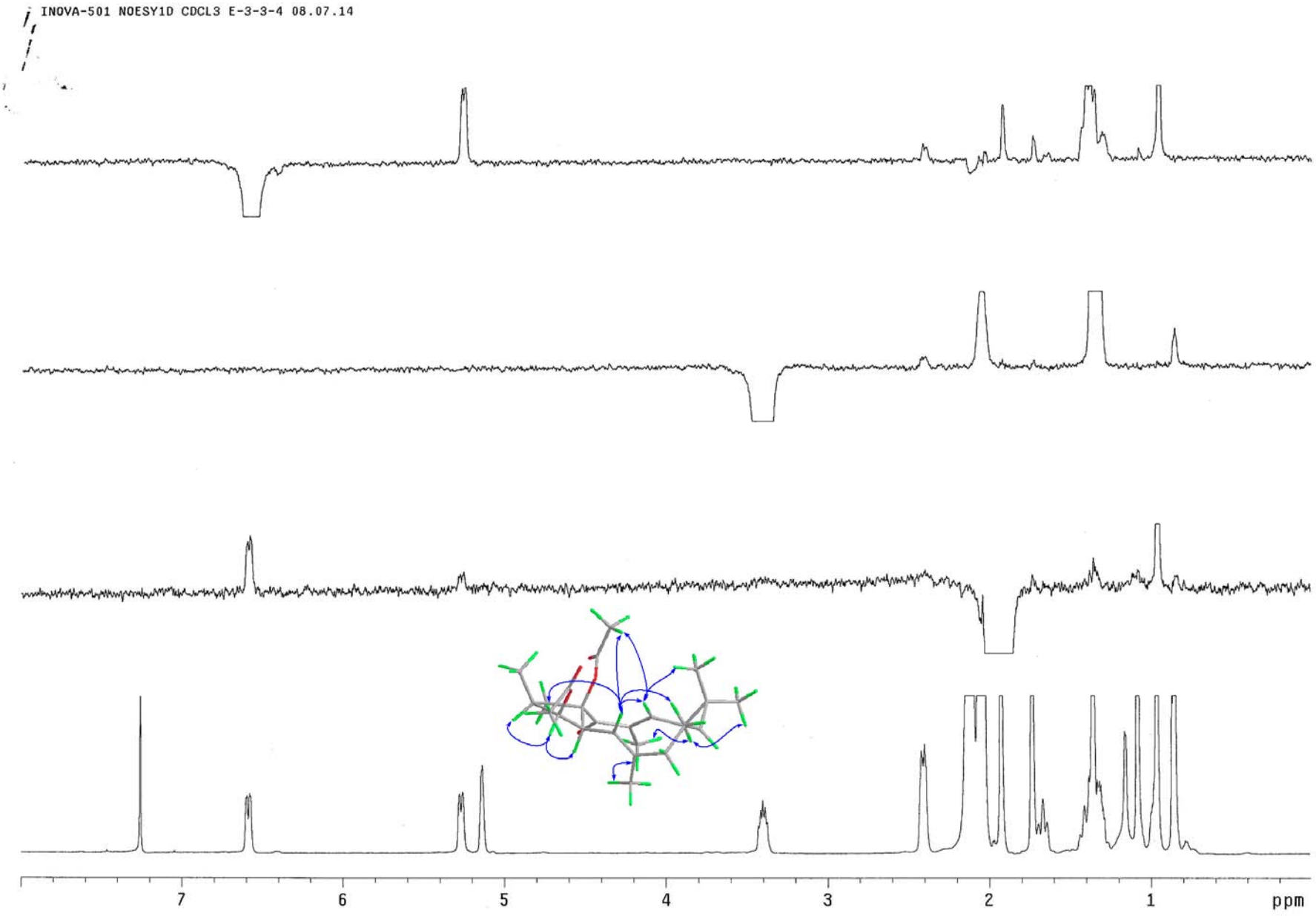

Figure S75. The NOE Difference Spectrum 1 of 8 in $CDCl_3$ (500 MHz).

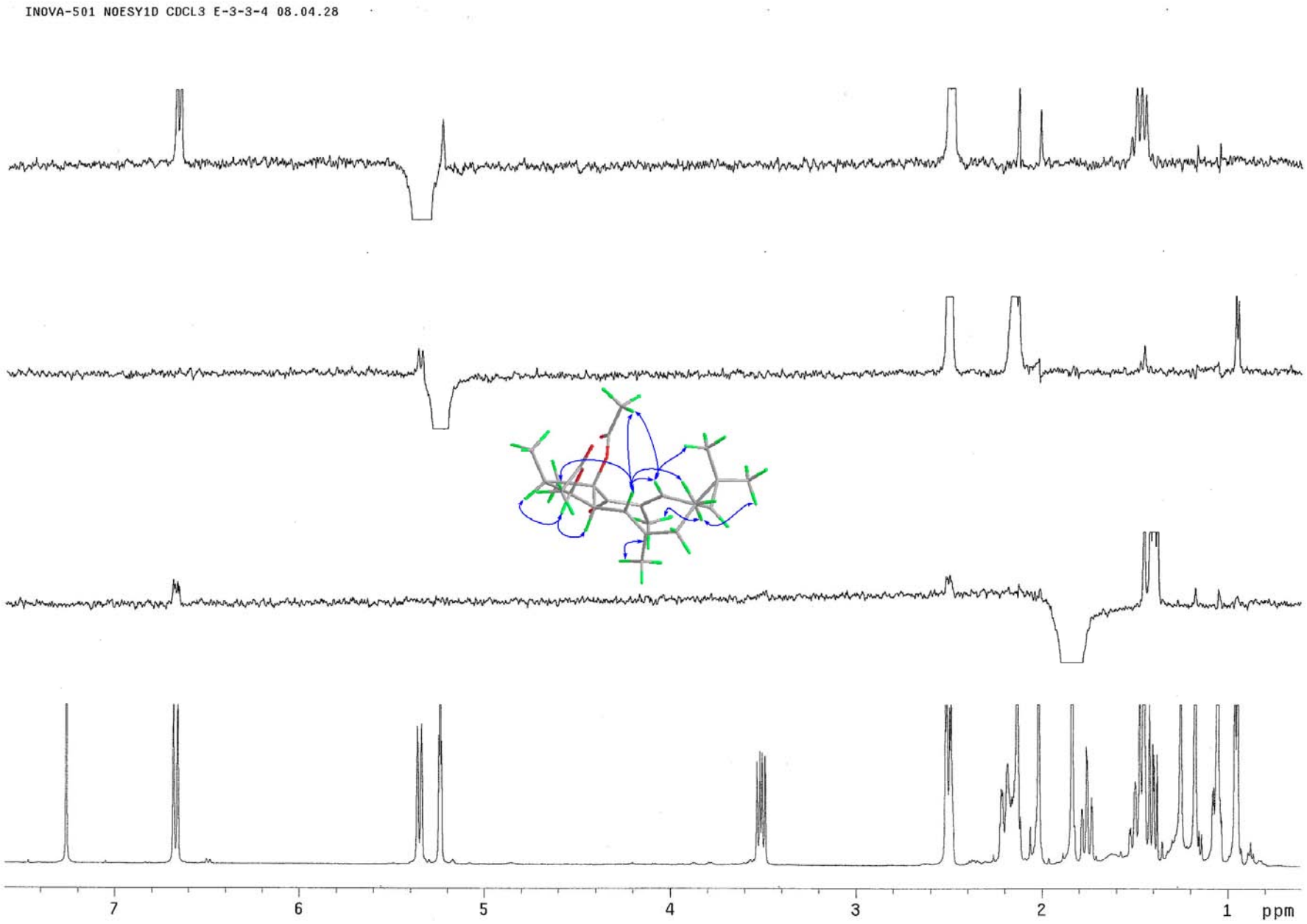

Figure S76. The NOE Difference Spectrum 2 of 8 in $CDCl_3$ (500 MHz).

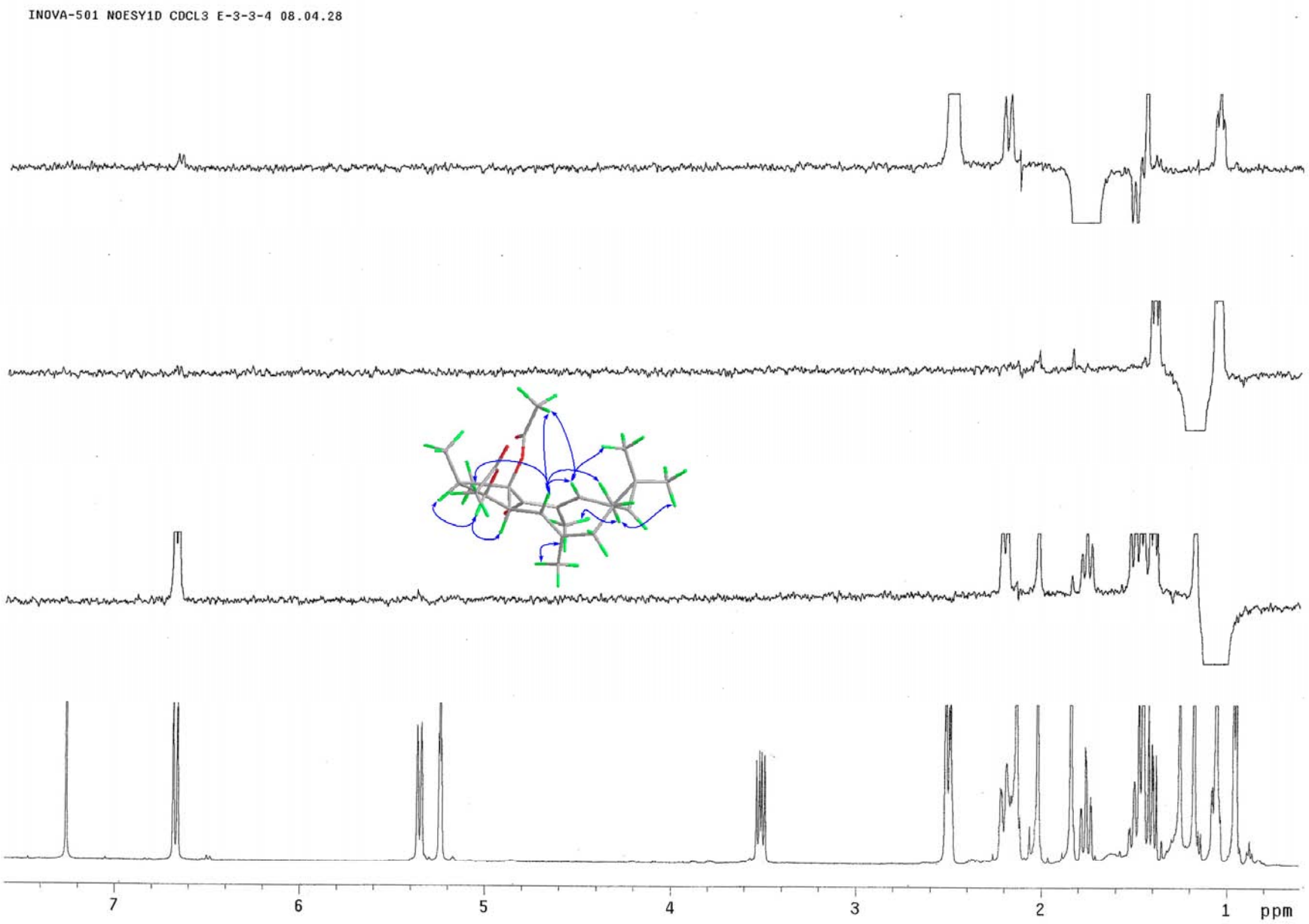

Figure S77. The NOE Difference Spectrum 3 of 8 in $CDCl_3$ (500 MHz).

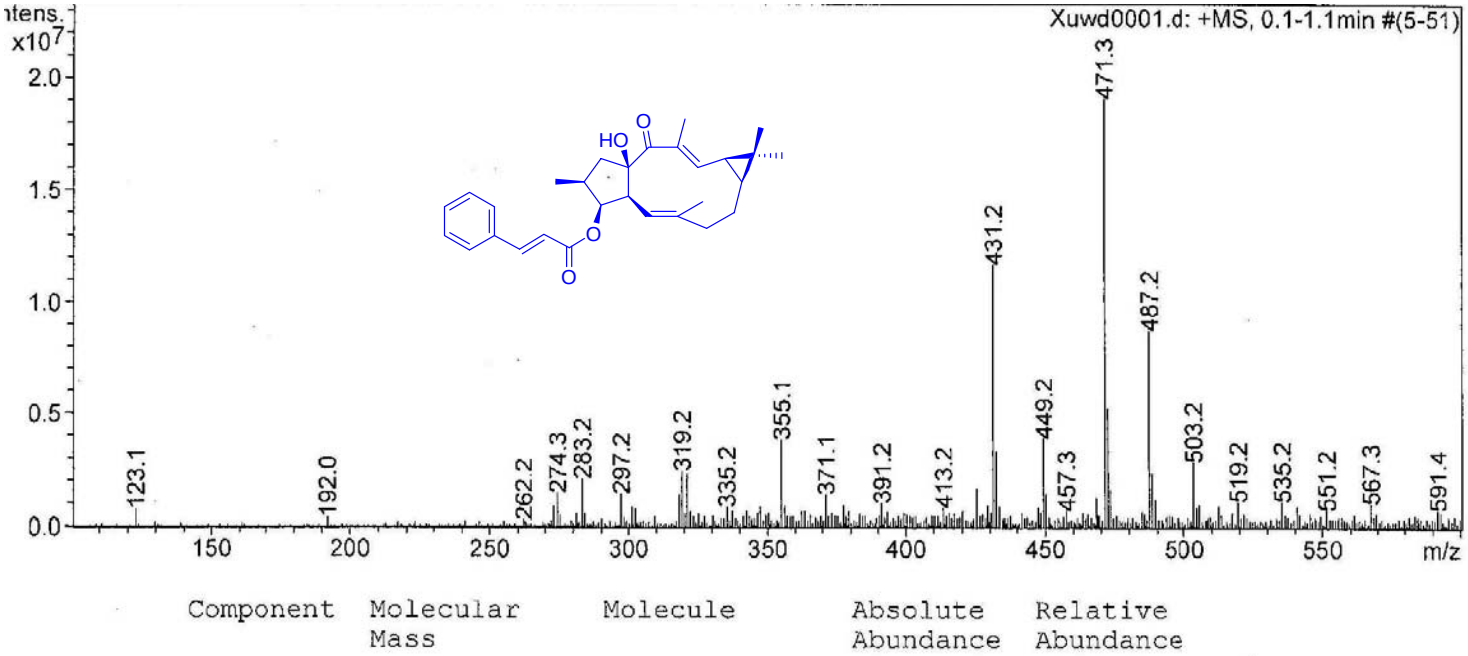

Figure S78. (+)-ESIMS Spectrum of 9.

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:^{12}C:0 .. 100, ^{1}H:0 .. 200, ^{23}Na:1 .. 1, ^{16}O: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.

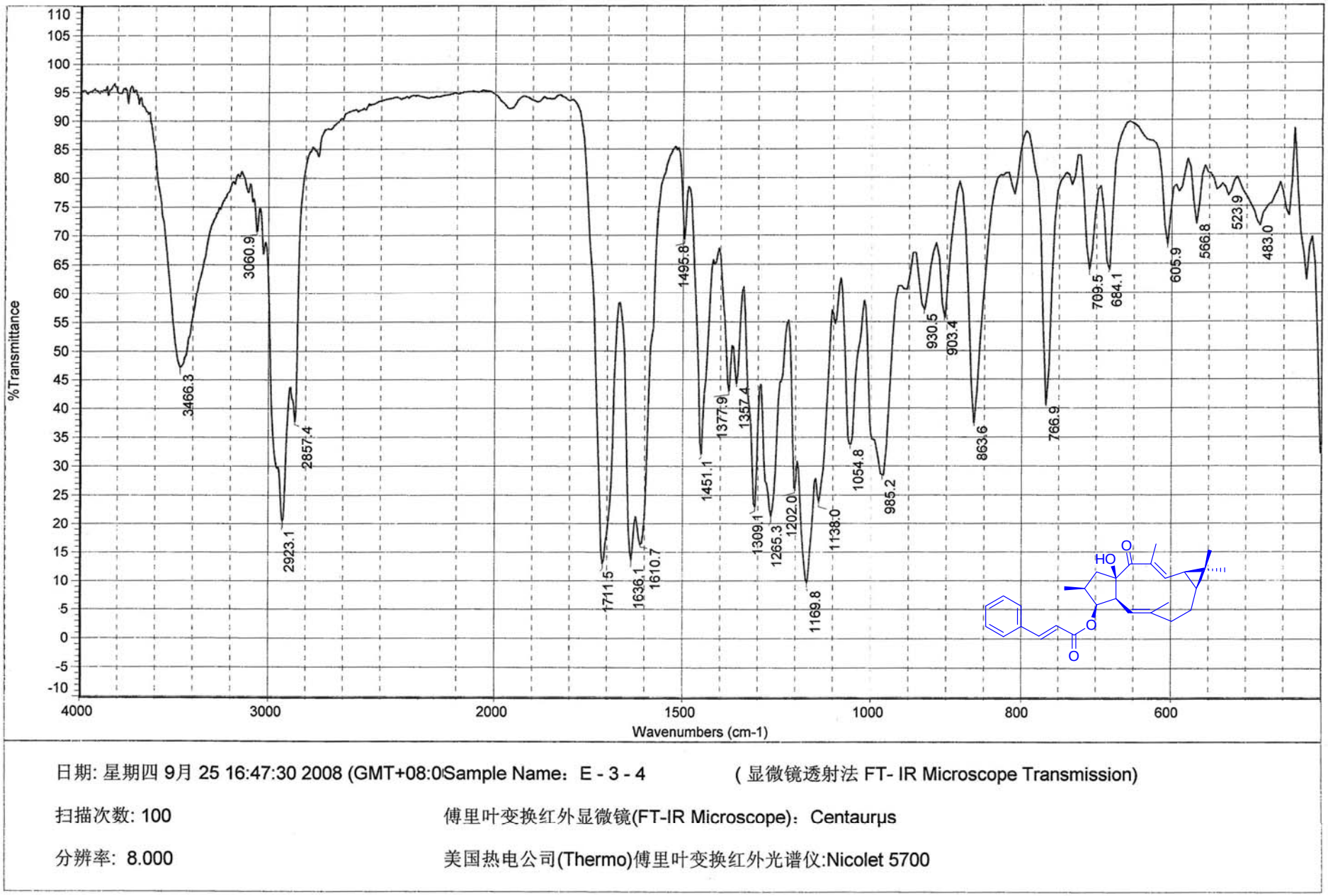

Figure S79. The IR Spectrum of 9.

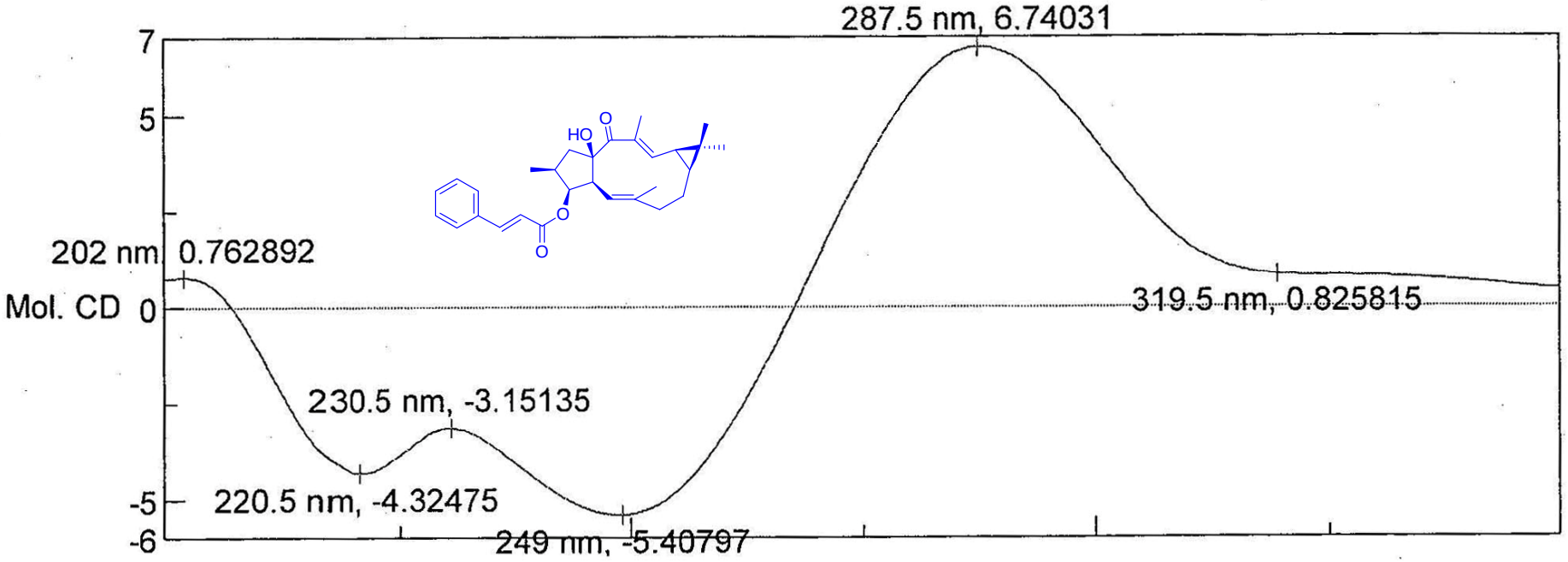

Figure S80. The CD Spectrum of 9.

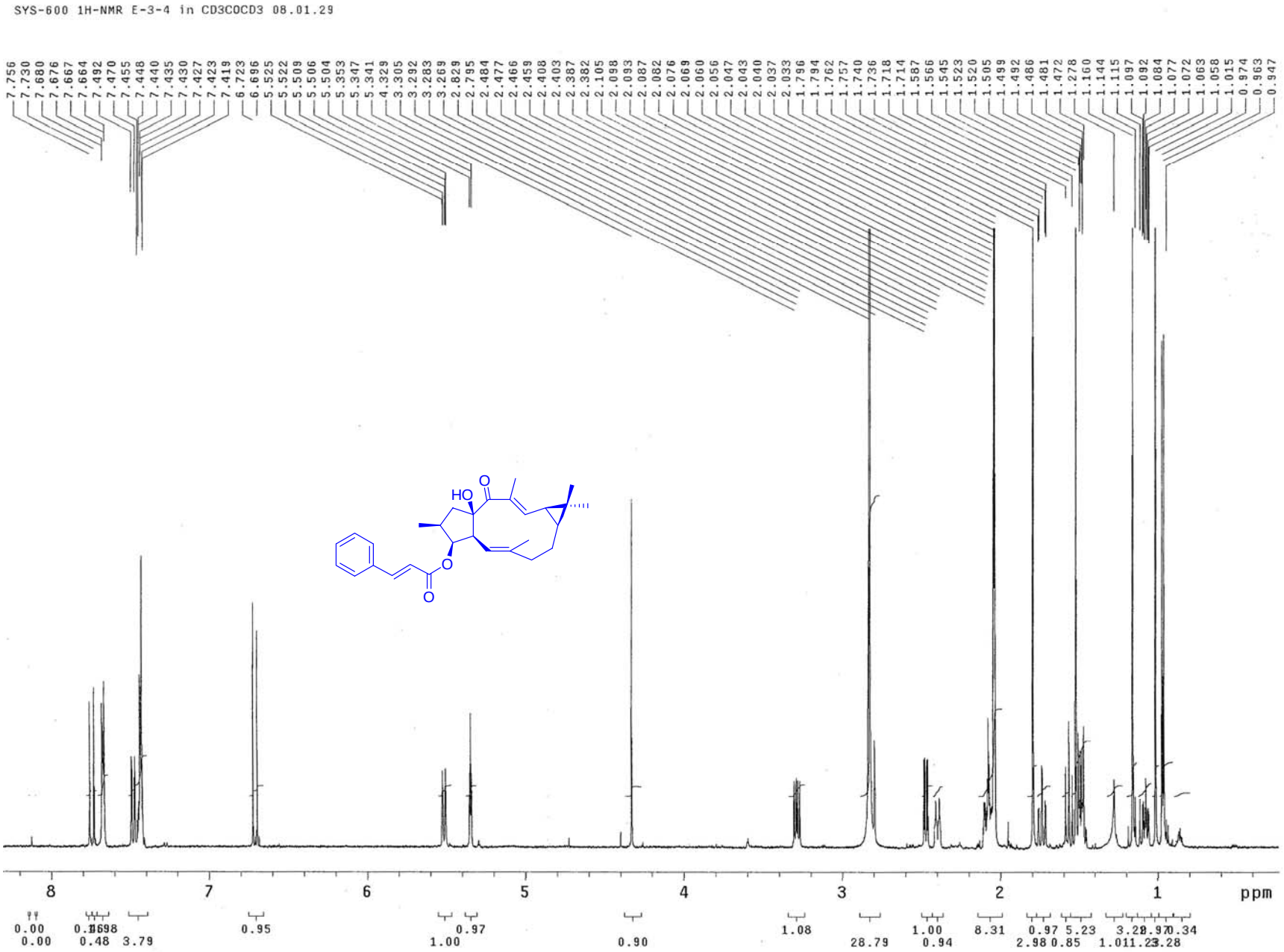

Figure S81. The ^{1}H NMR Spectrum of 9 in CD_3COCD_3 (600 MHz).

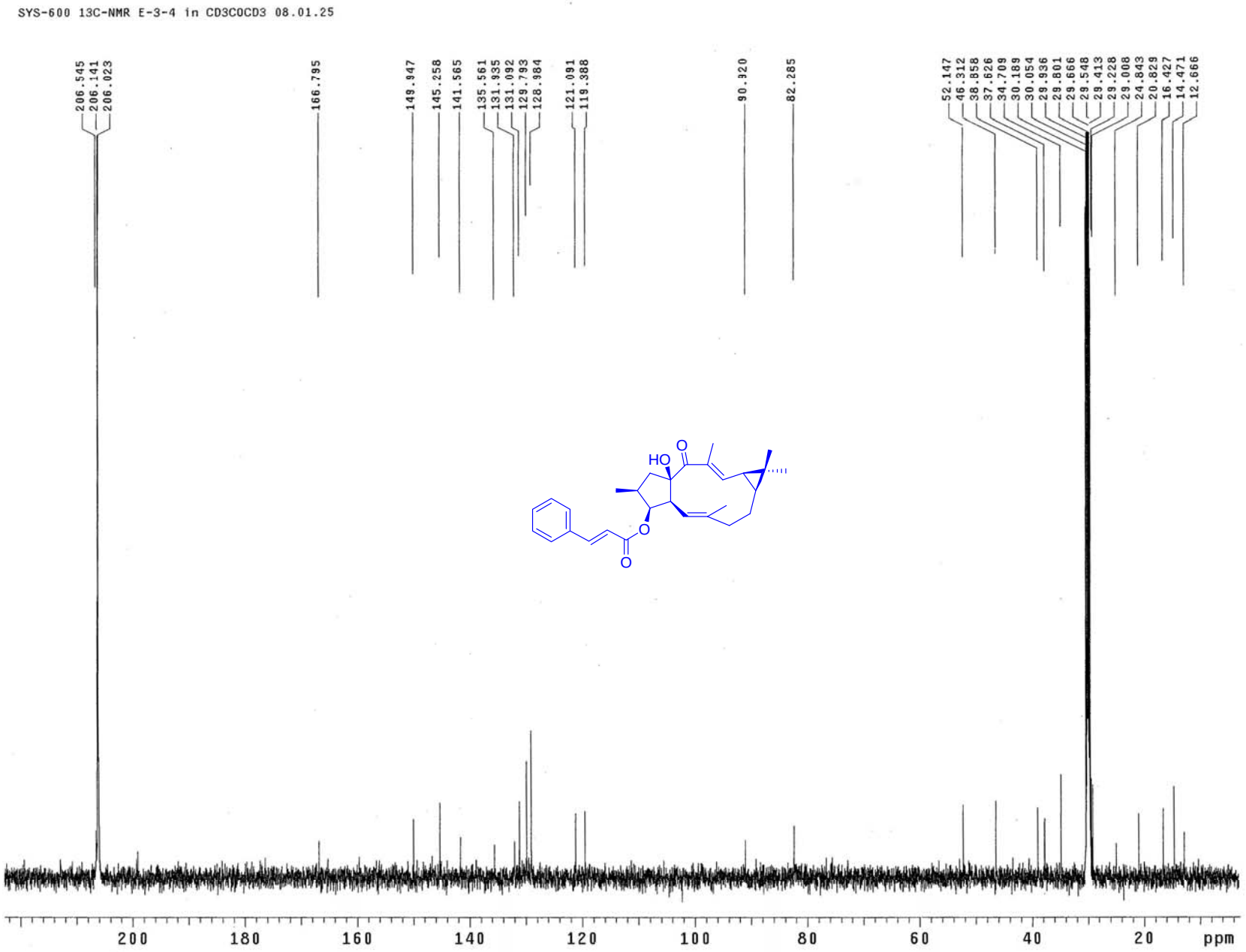

Figure S82. The ^{13}C NMR Spectrum of 9 in CD_3COCD_3 (150 MHz).

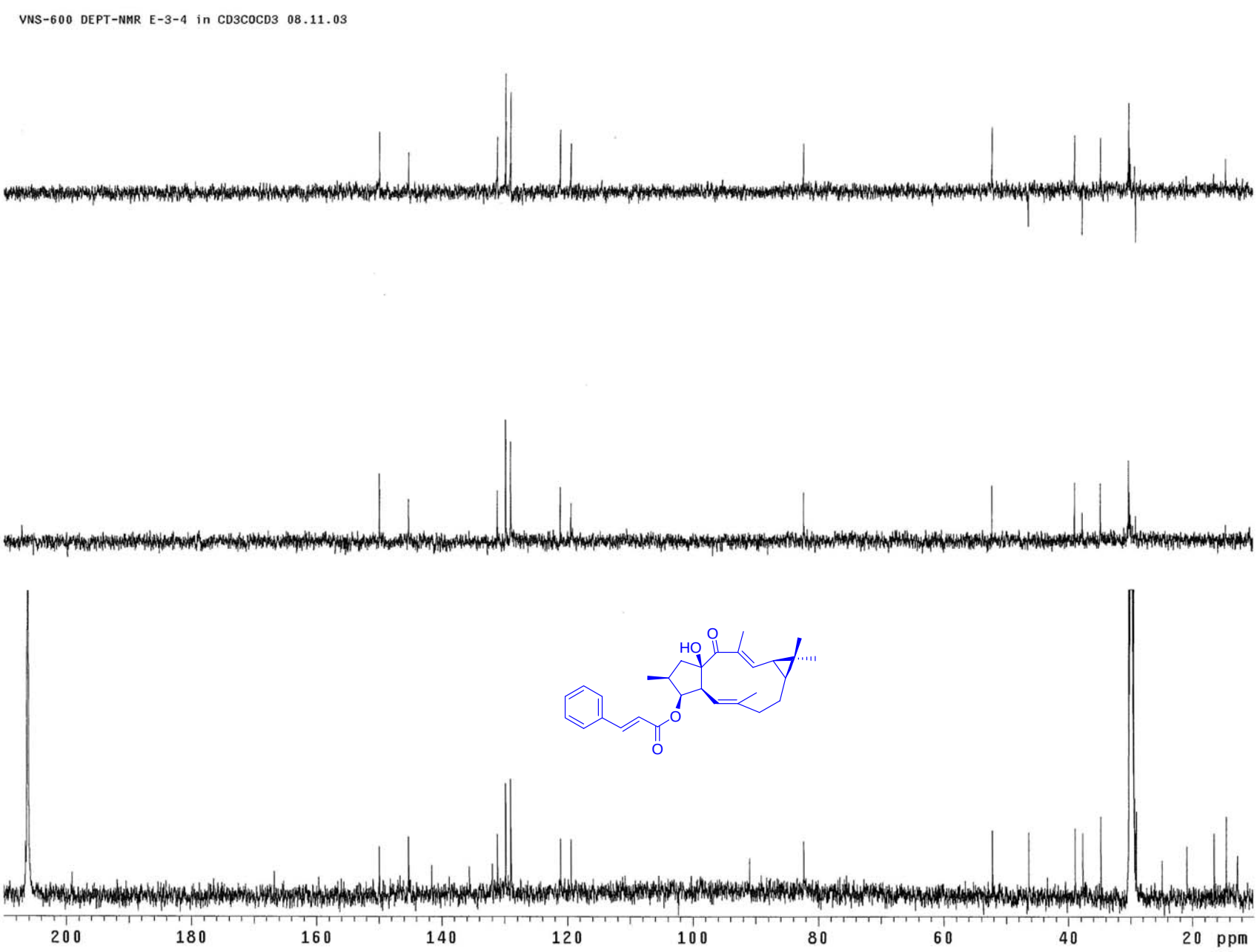

Figure S83. The DEPT Spectrum of 9 in CD_3COCD_3 (150 MHz).

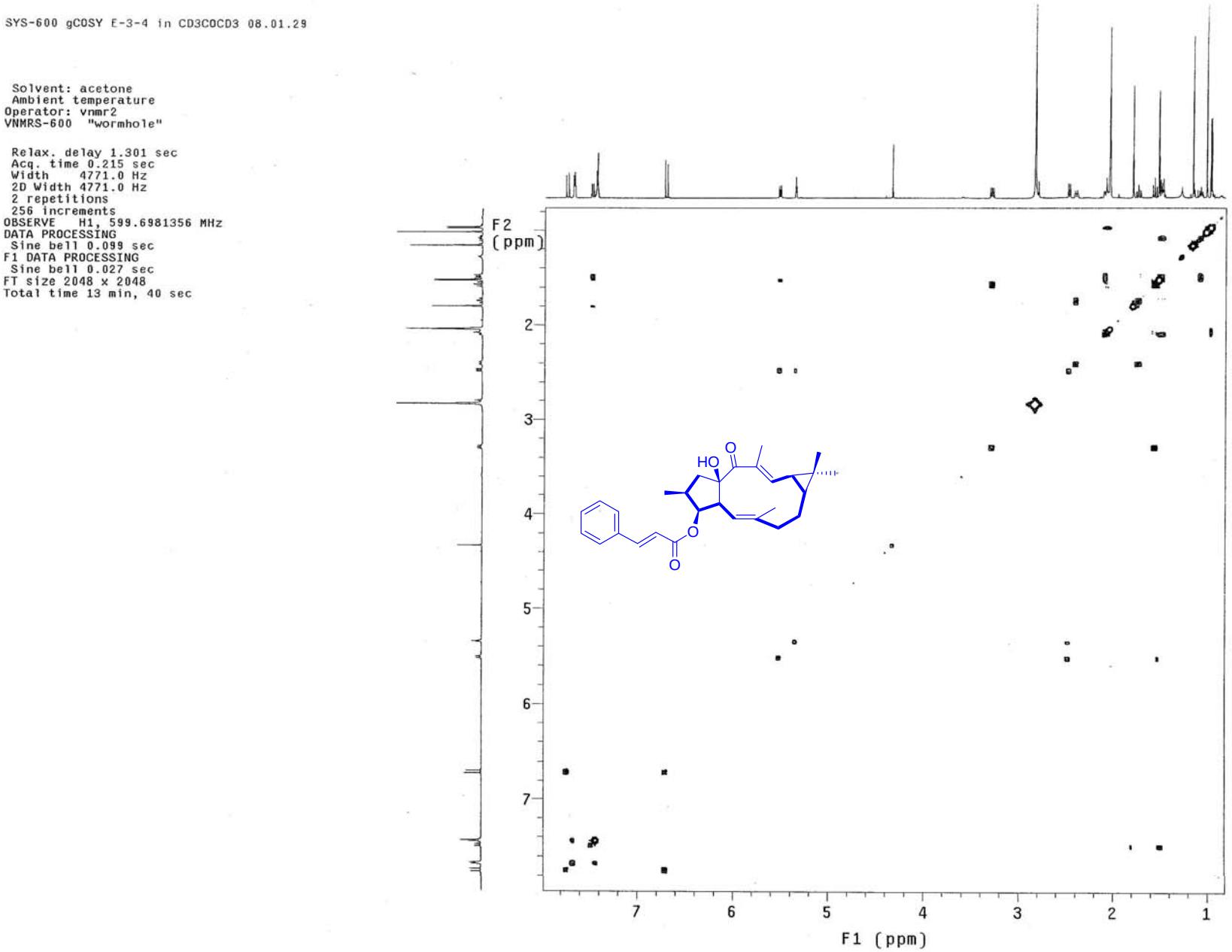

Figure S84. The ^{1}H-^{1}H gCOSY Spectrum of 9 in CD_3COCD_3 (600 MHz).

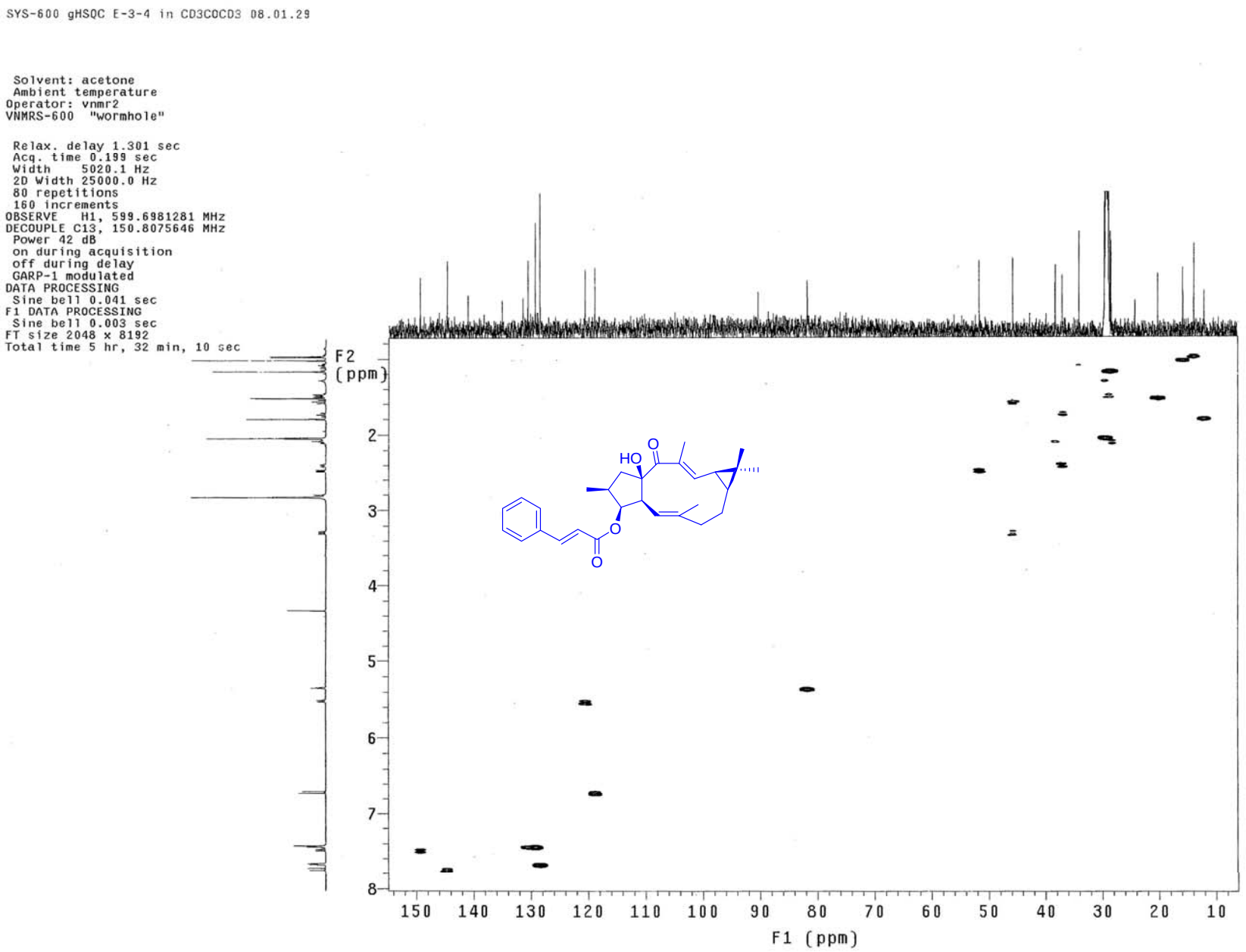

Figure S85. The gHSQC Spectrum of 9 in CD_3COCD_3 (600MHz for ^1H NMR).

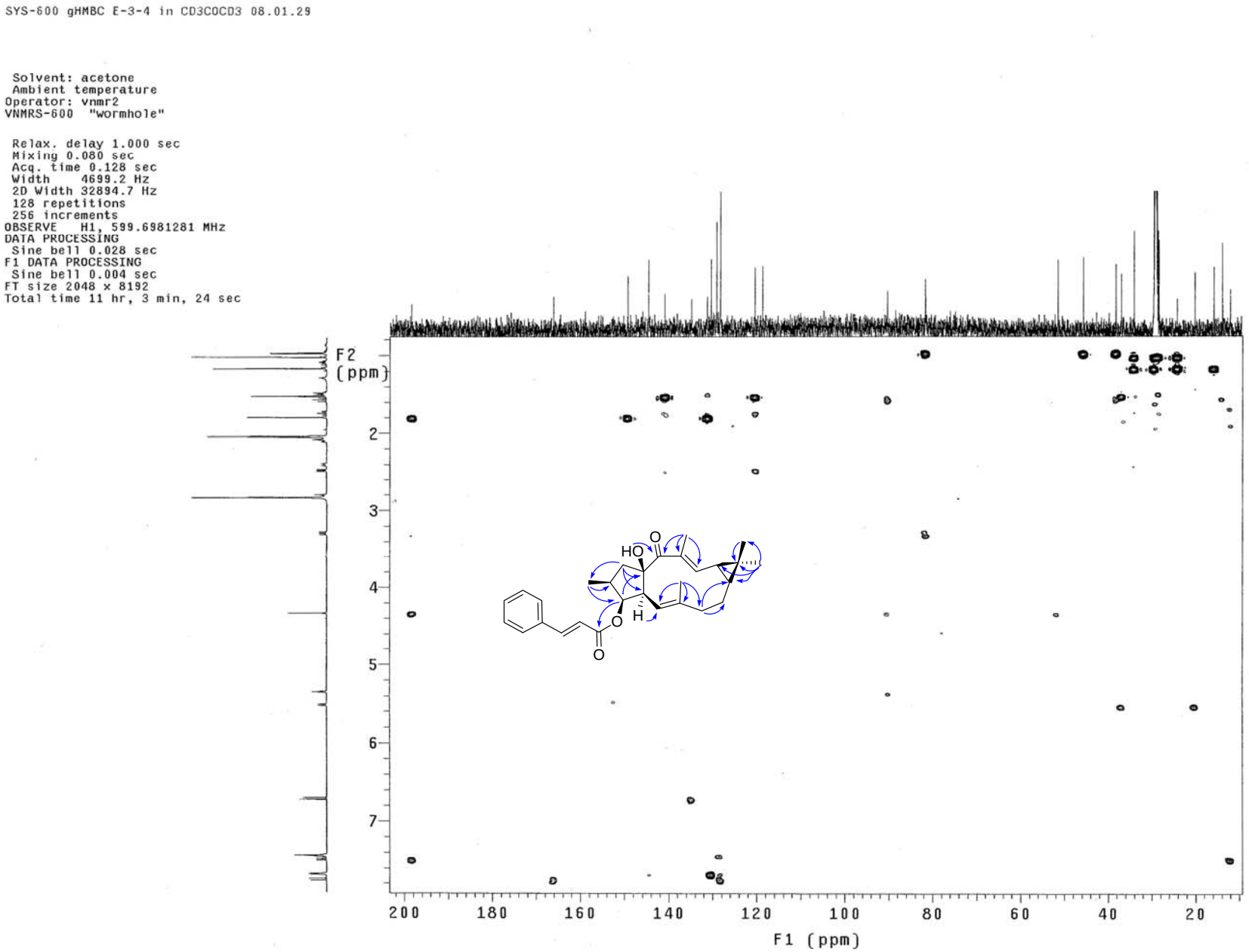

Figure S86. The gHMBC Spectrum of 9 in CD_3COCD_3 (600MHz for ^1H NMR).

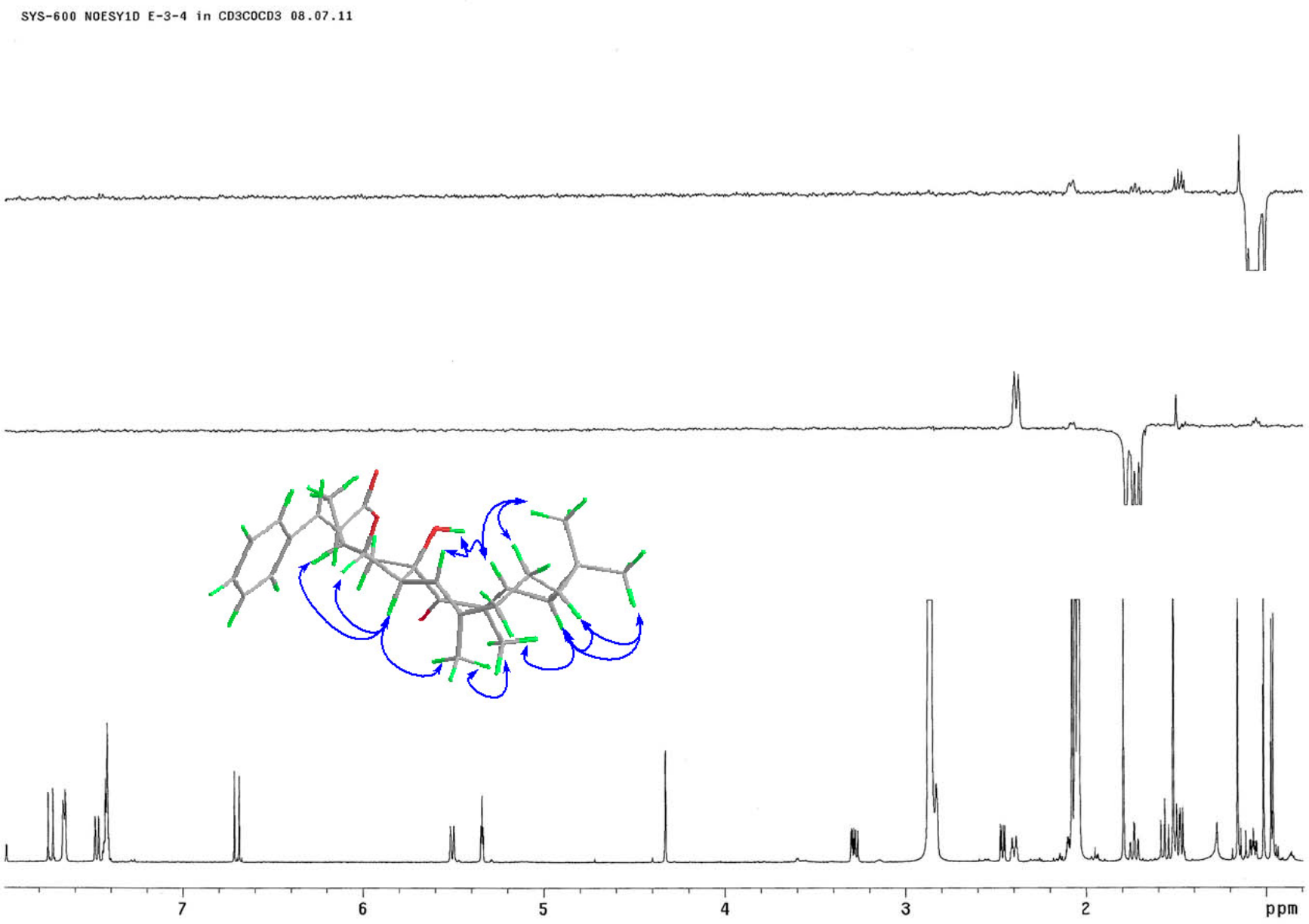

Figure S87. The NOE Difference Spectrum 1 of 9 in CD_3COCD_3 (600 MHz).

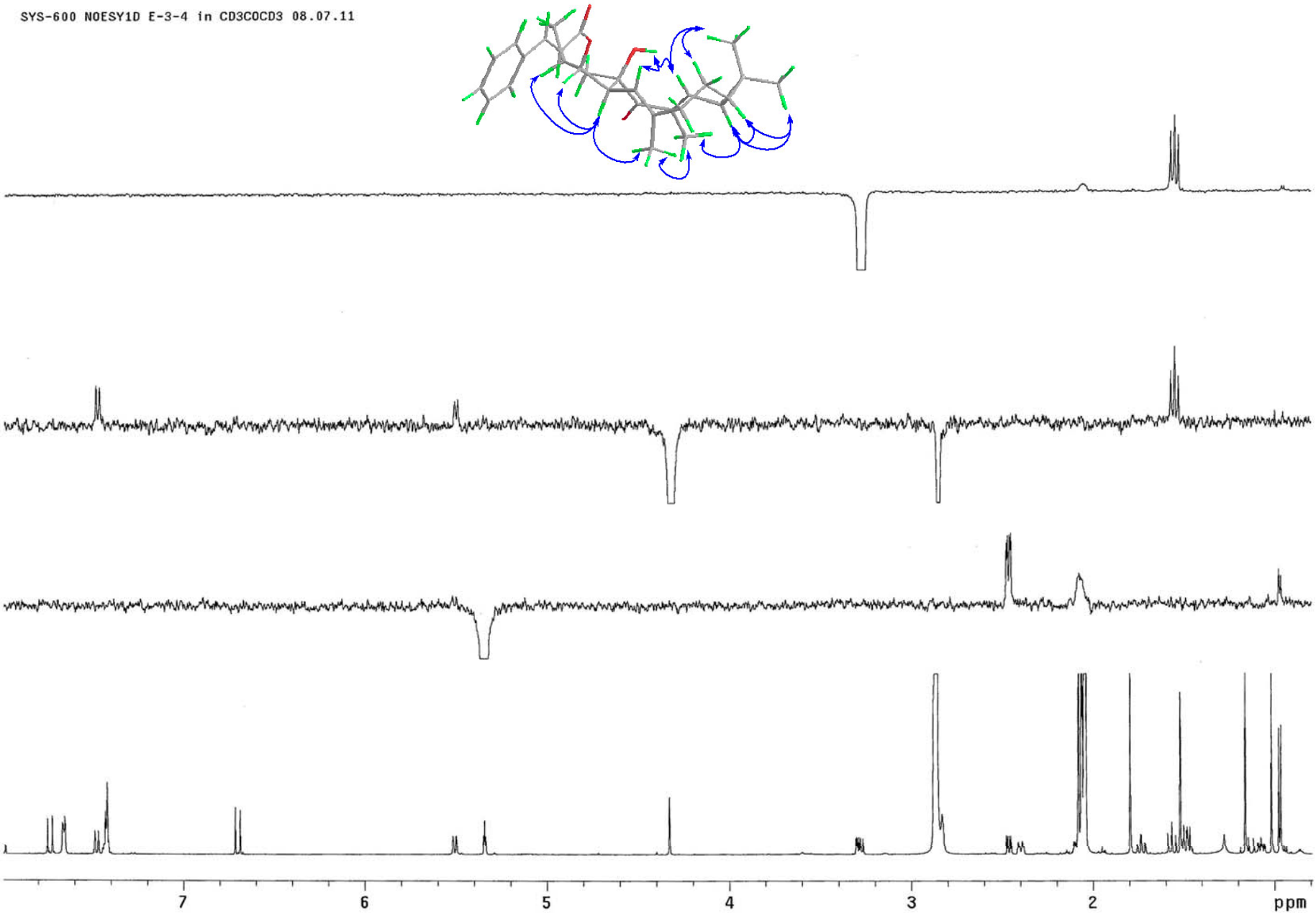

Figure S88. The NOE Difference Spectrum 2 of 9 in CD_3COCD_3 (600 MHz).

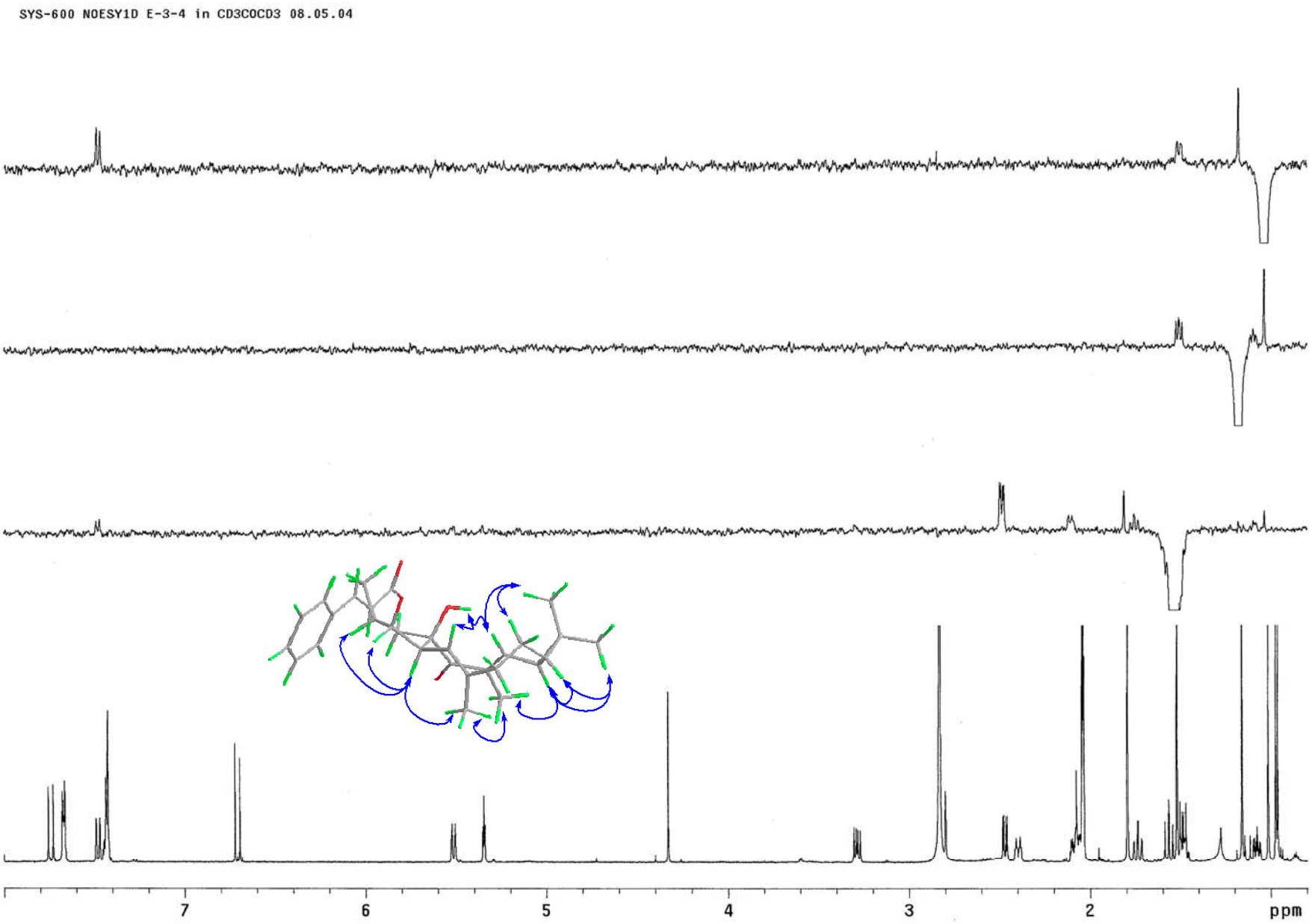

Figure S89. The NOE Difference Spectrum 3 of 9 in CD_3COCD_3 (600 MHz).

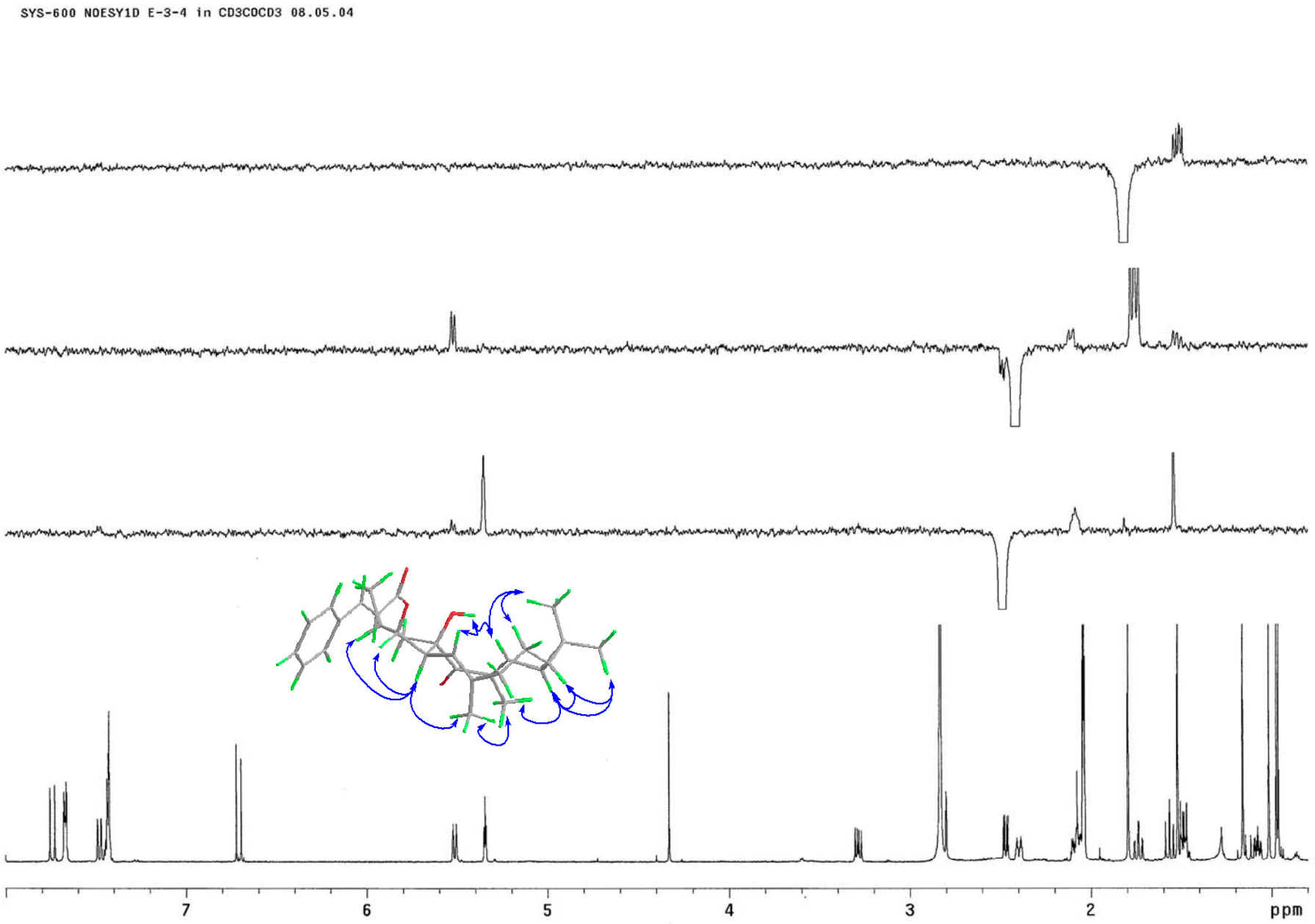

Figure S90. The NOE Difference Spectrum 4 of 9 in CD_3COCD_3 (600 MHz).

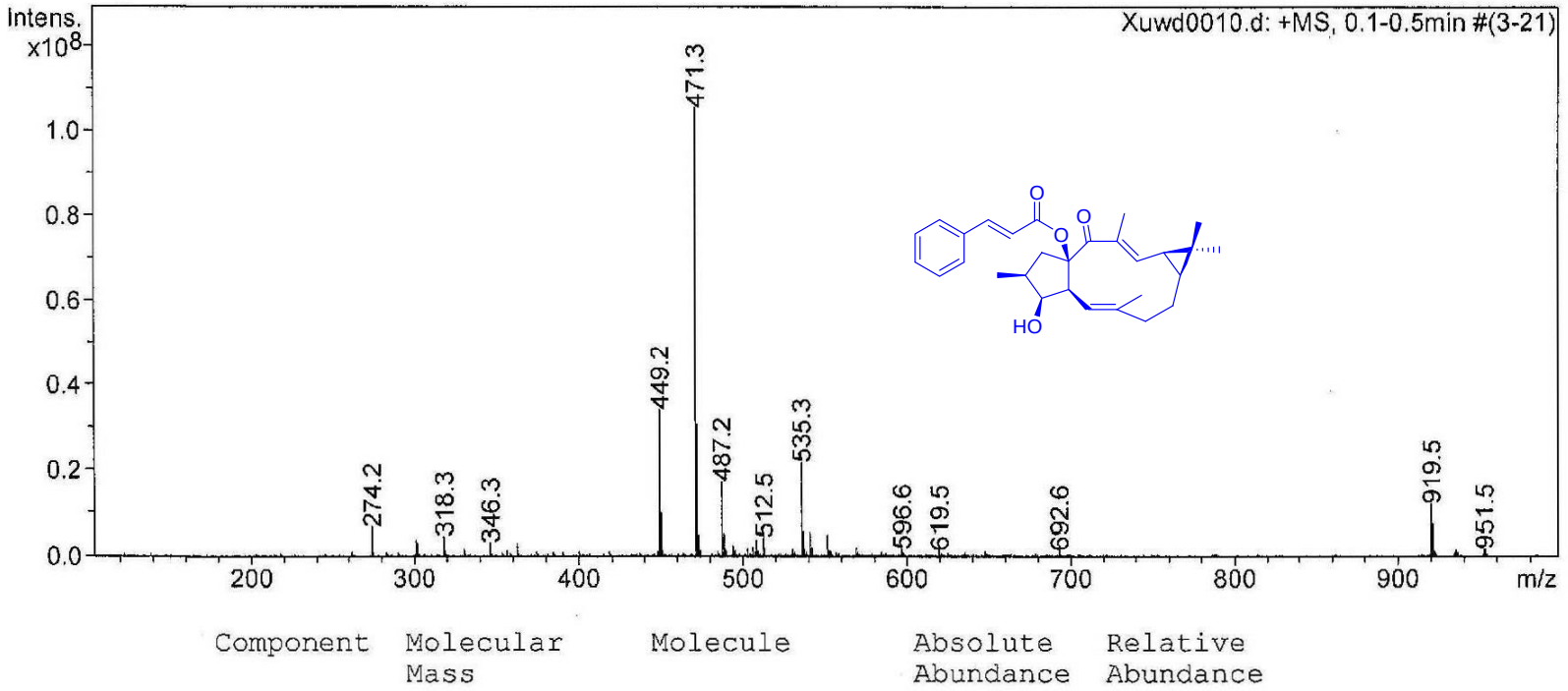

Figure S91. (+)-ESIMS Spectrum of 10.

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.

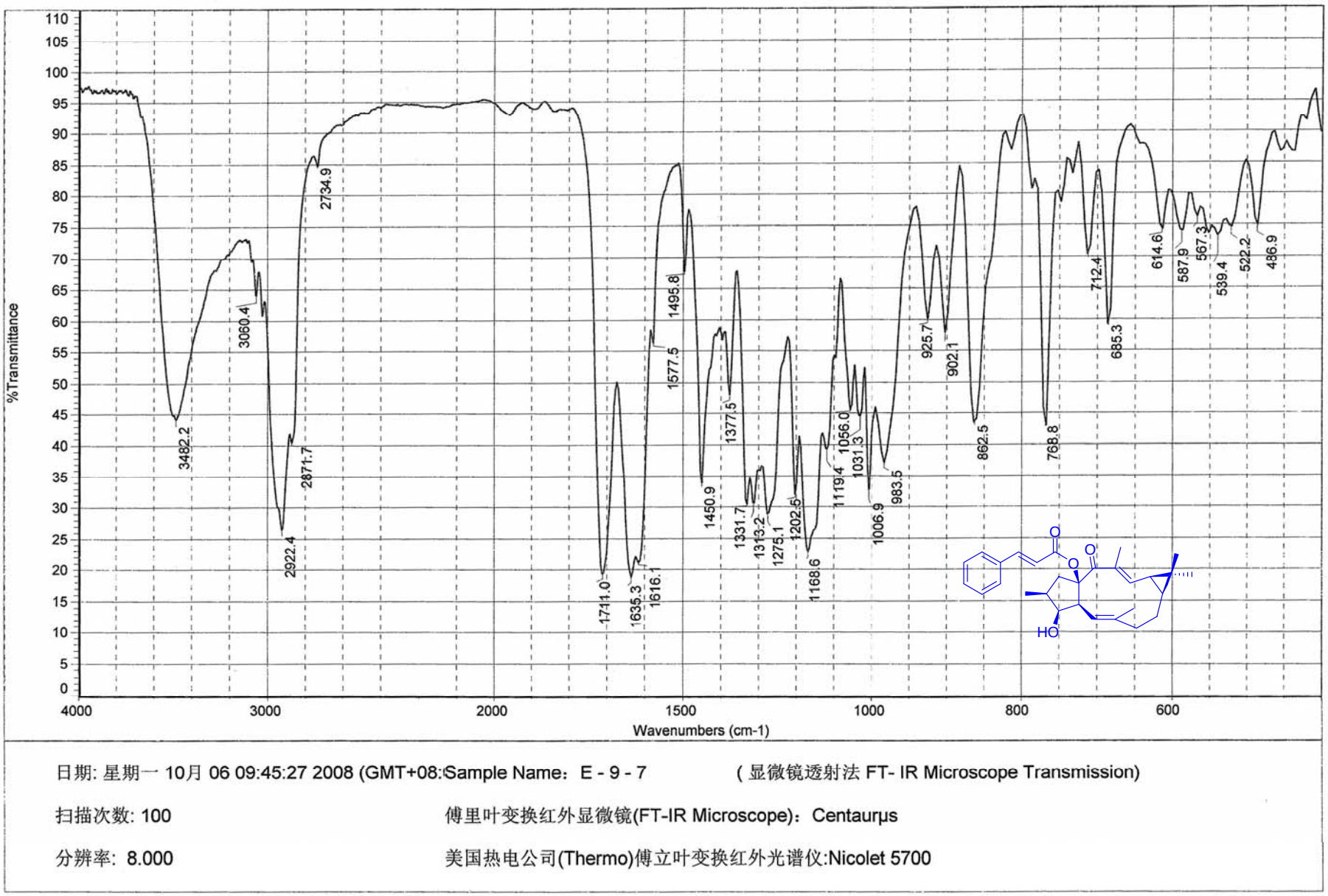

Figure S92. The IR Spectrum of 10.

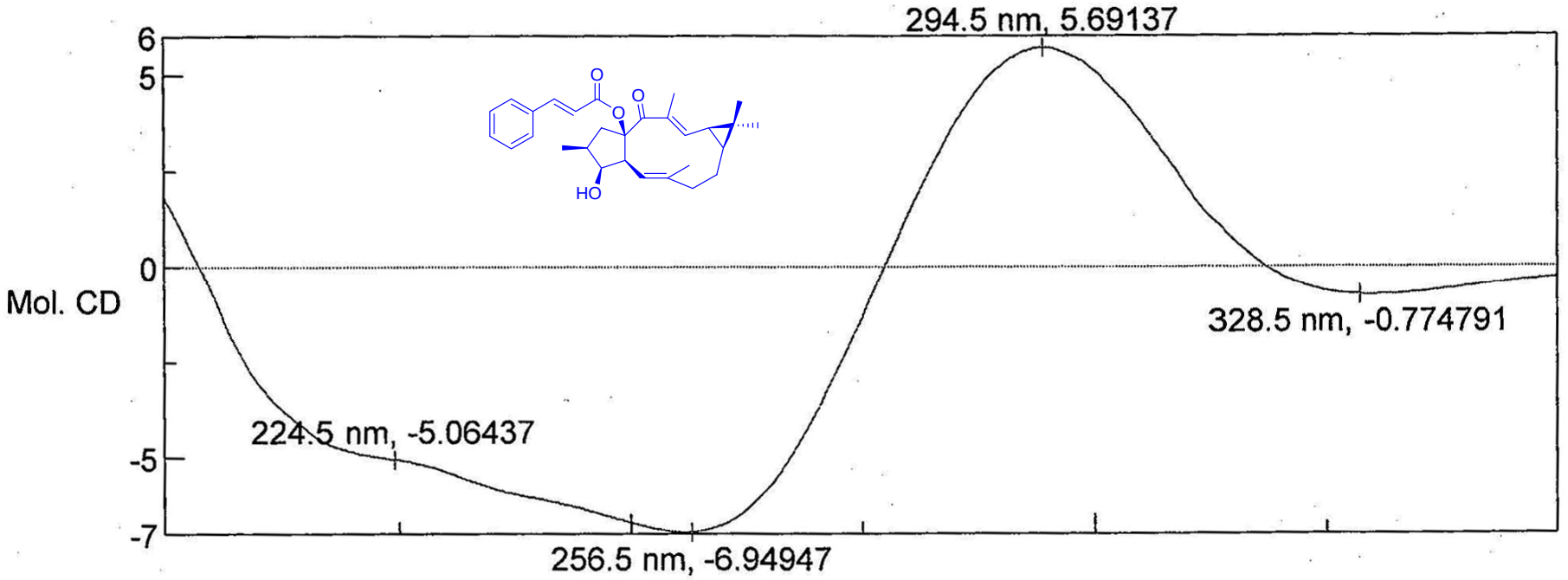

Figure S93. The CD Spectrum of 10.

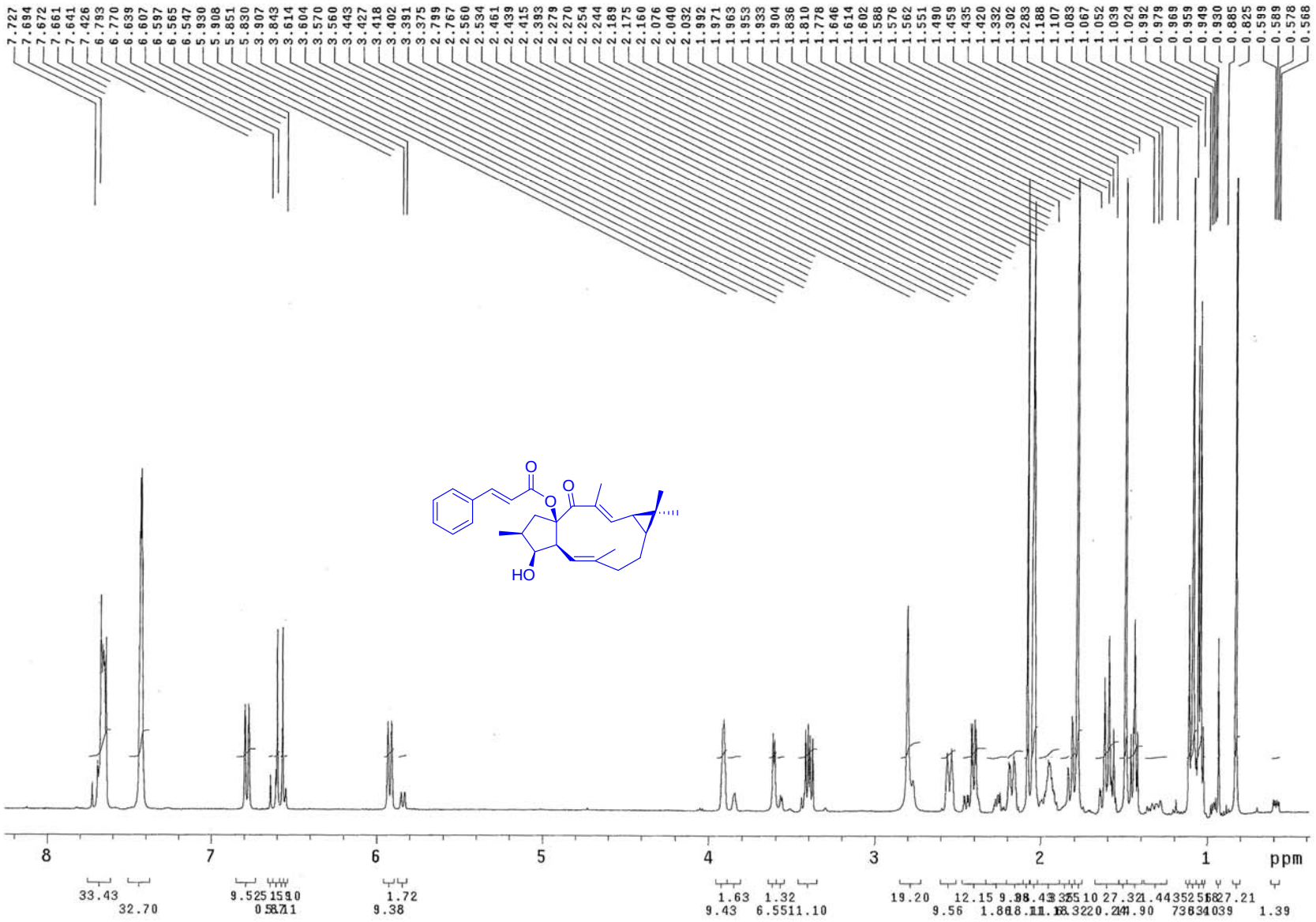

Figure S94. The ^{1}H NMR Spectrum of 10 in CD_3COCD_3 (500 MHz).

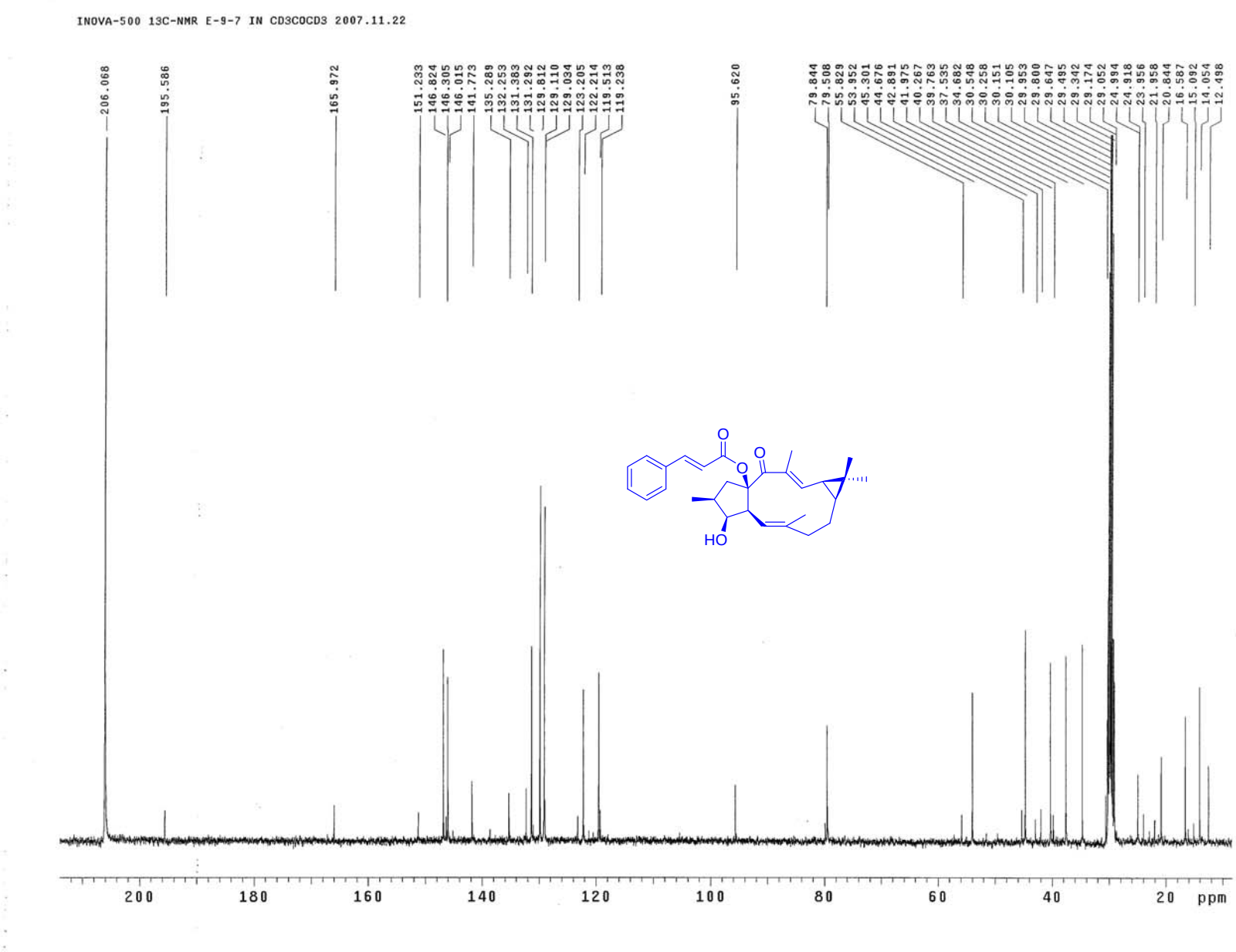

Figure S95. The ^{13}C NMR Spectrum of 10 in CD_3COCD_3 (125 MHz).

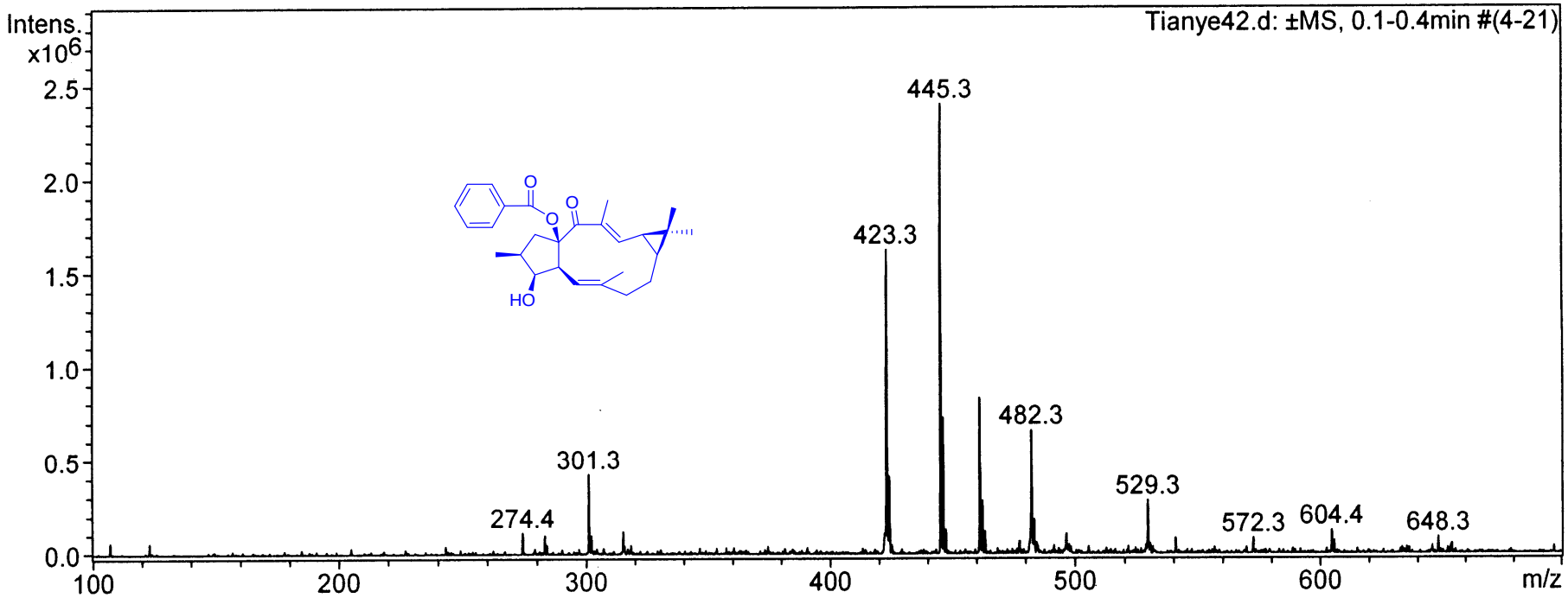

Figure S96. The (+)-ESIMS Spectrum of 11.

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

m/z	Ion	Formula	Abundance
423.2527	(M+H)+	C27 H35 O4	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
☑	C27 H34 O4	C27 H35 O4	423.253	99.92		422.2454	422.2457	0.74	0.74	99.77	99.99	99.98	423.2527	11
☐	C22 H34 N2 O6	C22 H35 N2 O6	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)+	C27 H34 Na O4	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
☑	C27 H34 O4	C27 H34 Na O4	445.2349	99.82		422.2448	422.2457	2.05	2.05	99.62	99.95	99.87	445.234	11
☐	C22 H34 N2 O6	C22 H34 N2 Na O6	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.

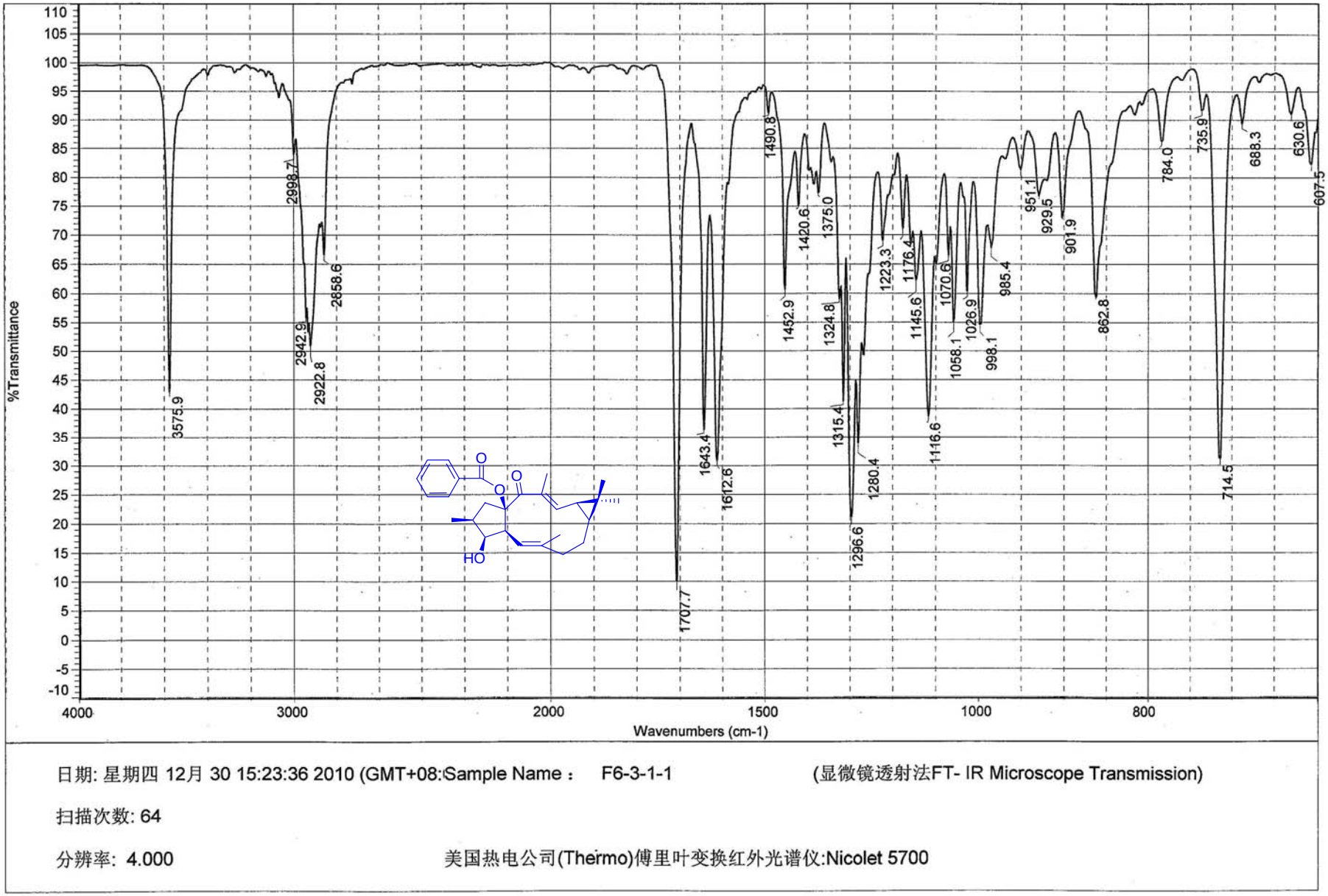

Figure S97. The IR Spectrum of 11.

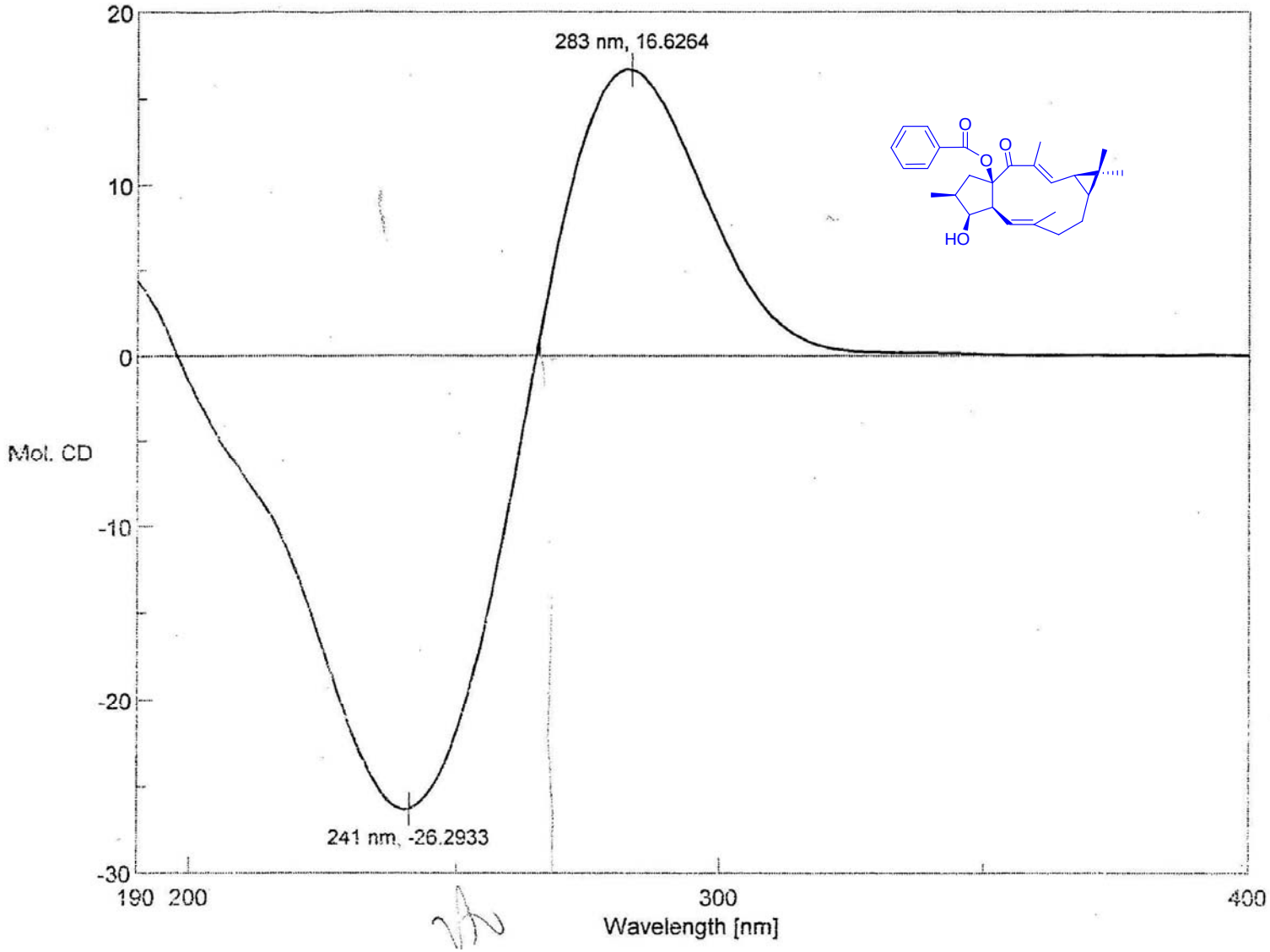

Figure S98. The CD Spectrum of 11.

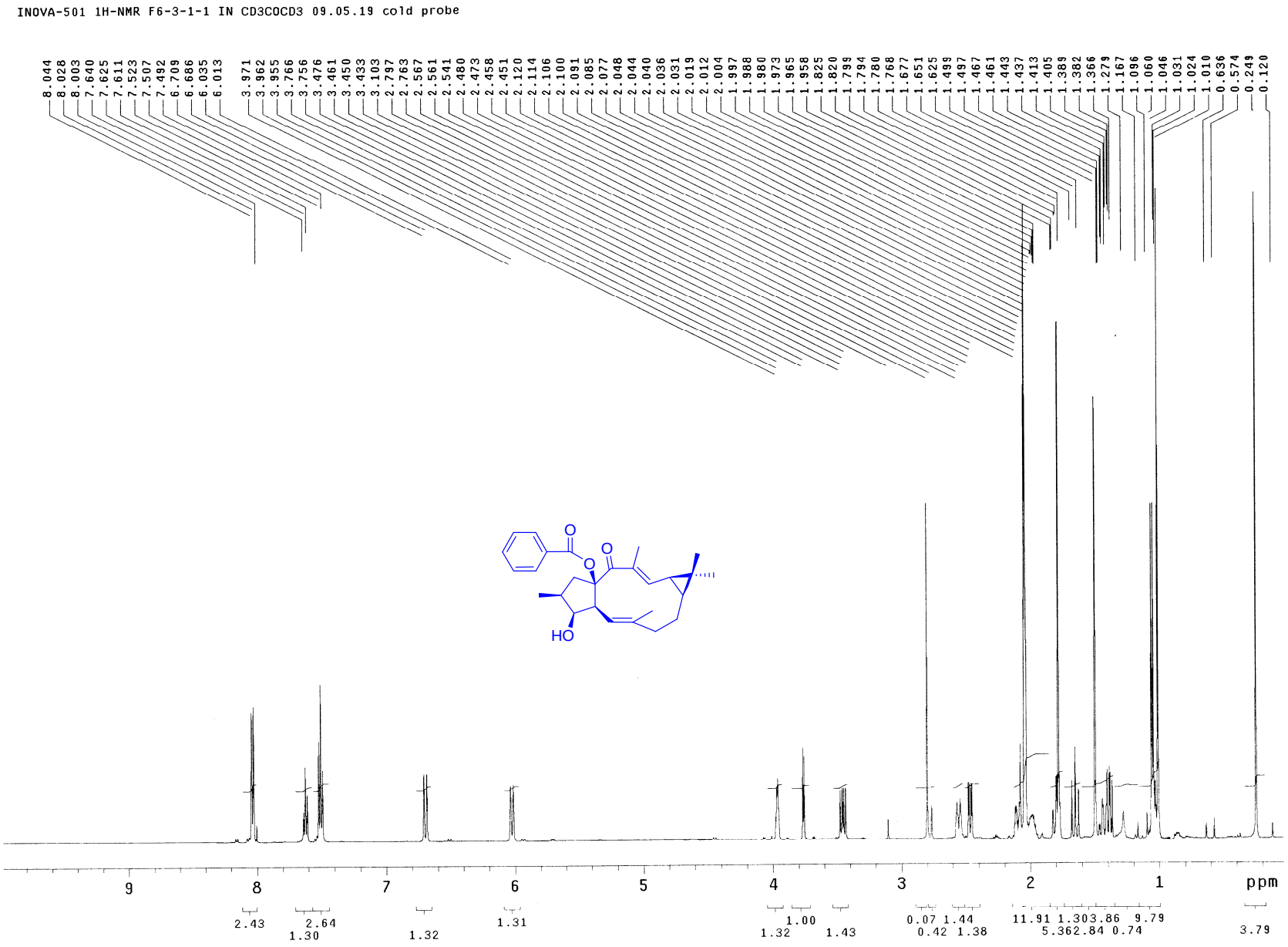

Figure S99. The ^{1}H NMR Spectrum of 11 in CD_3COCD_3 (500 MHz).

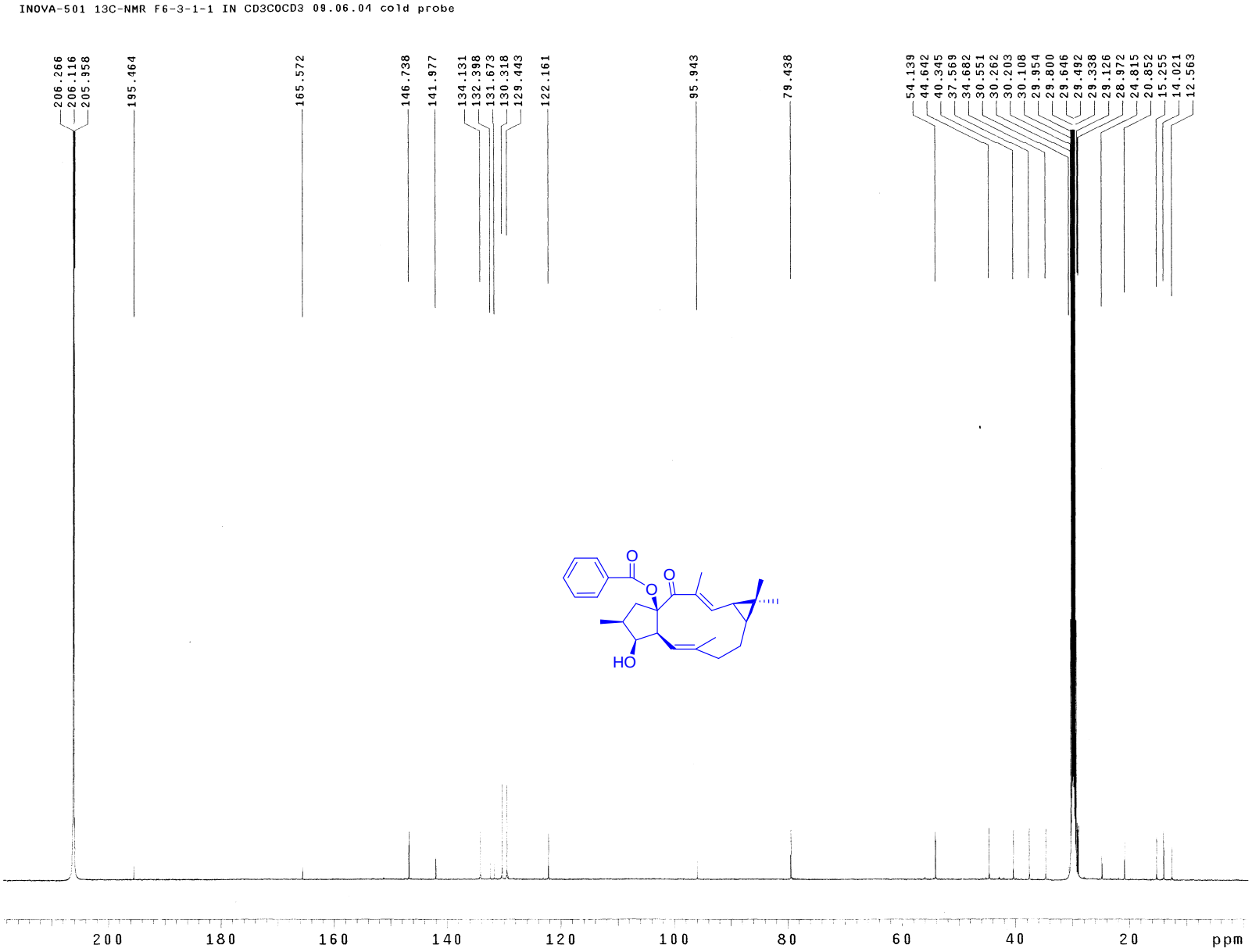

Figure S100. The ^{13}C NMR Spectrum of 11 in CD_3COCD_3 (125 MHz).

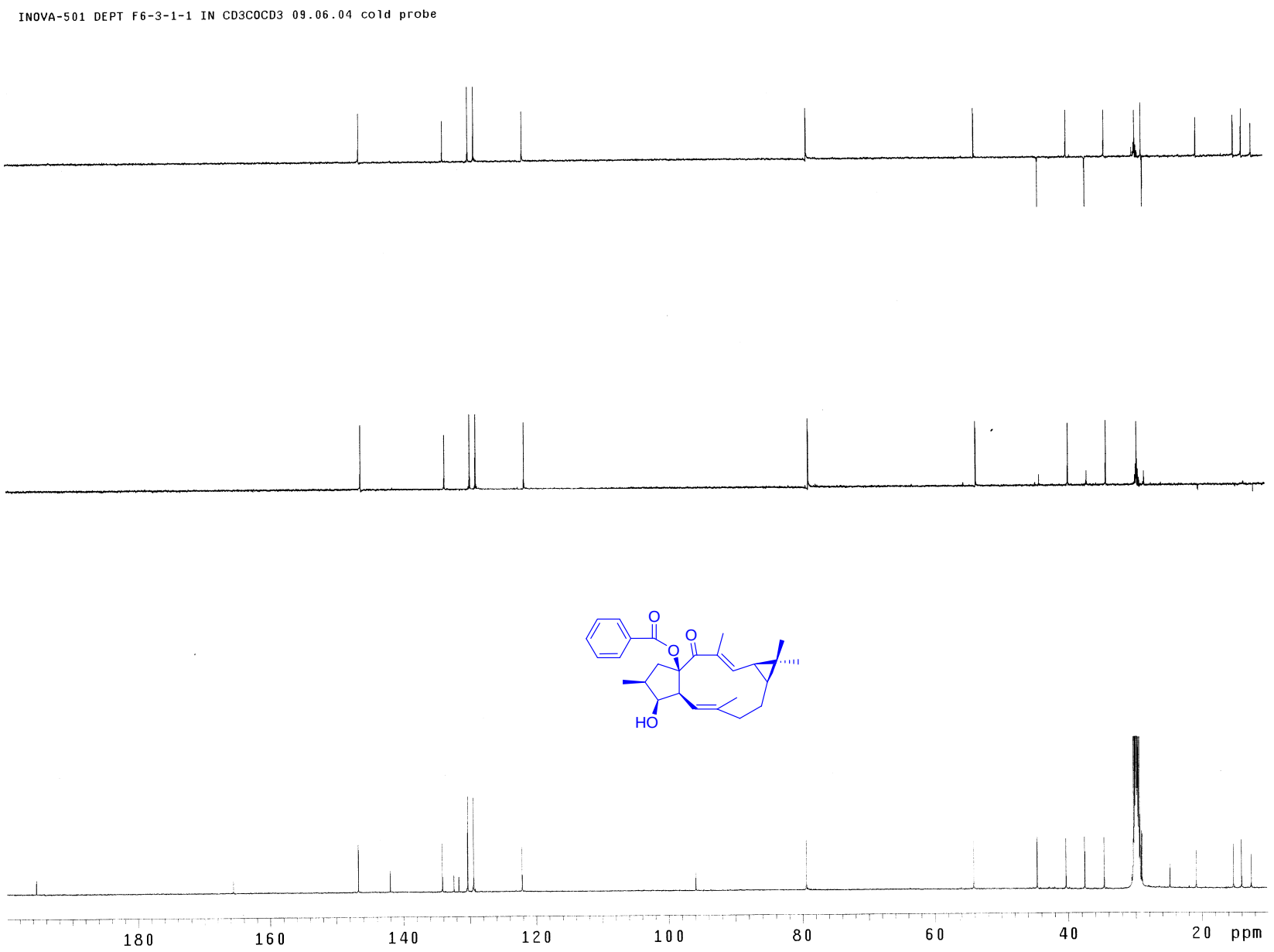

Figure S101. The DEPT Spectrum of 11 in CD_3COCD_3 (125 MHz).

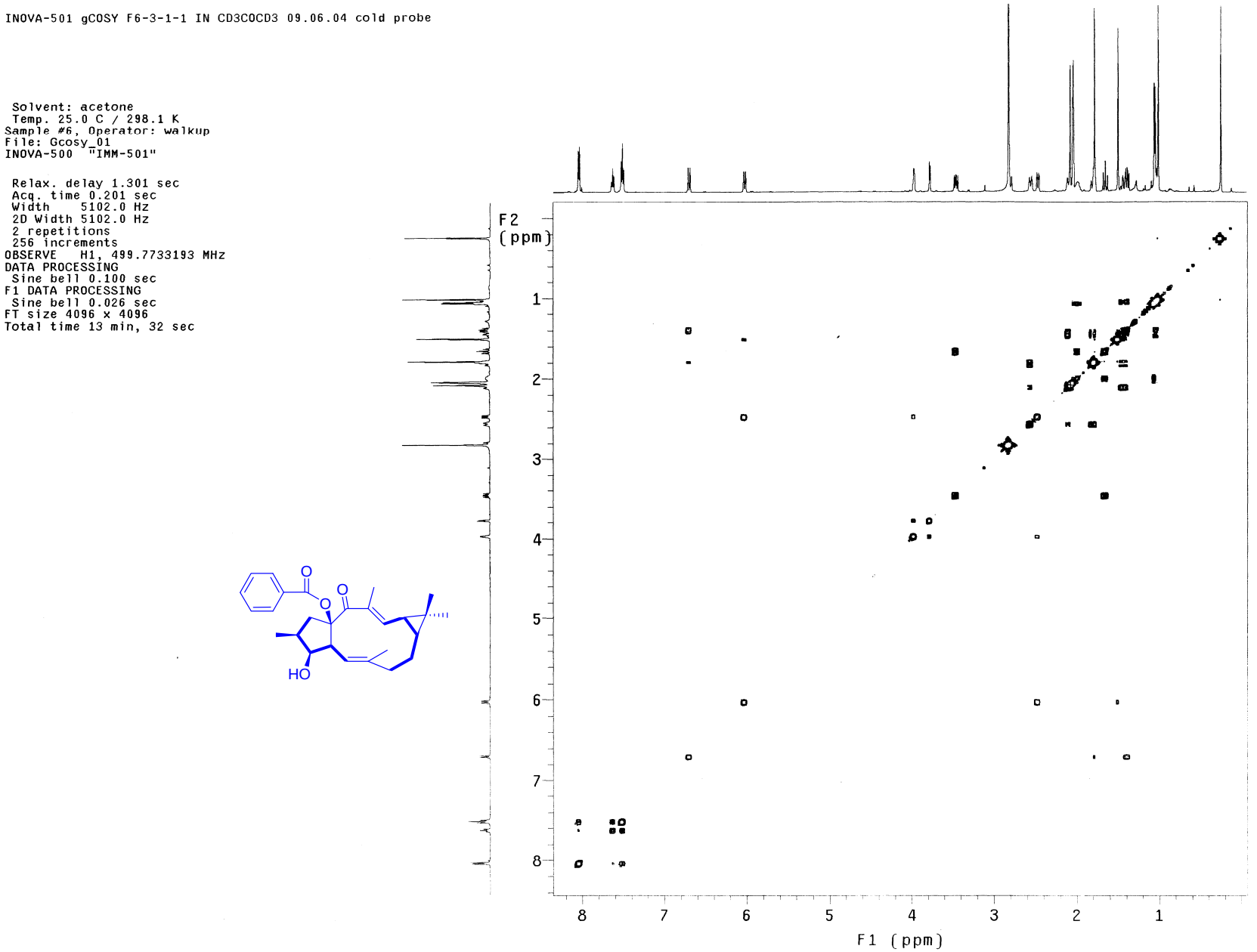

Figure S102. The ^{1}H-^{1}H gCOSY Spectrum of 11 in CD_3COCD_3 (500 MHz).

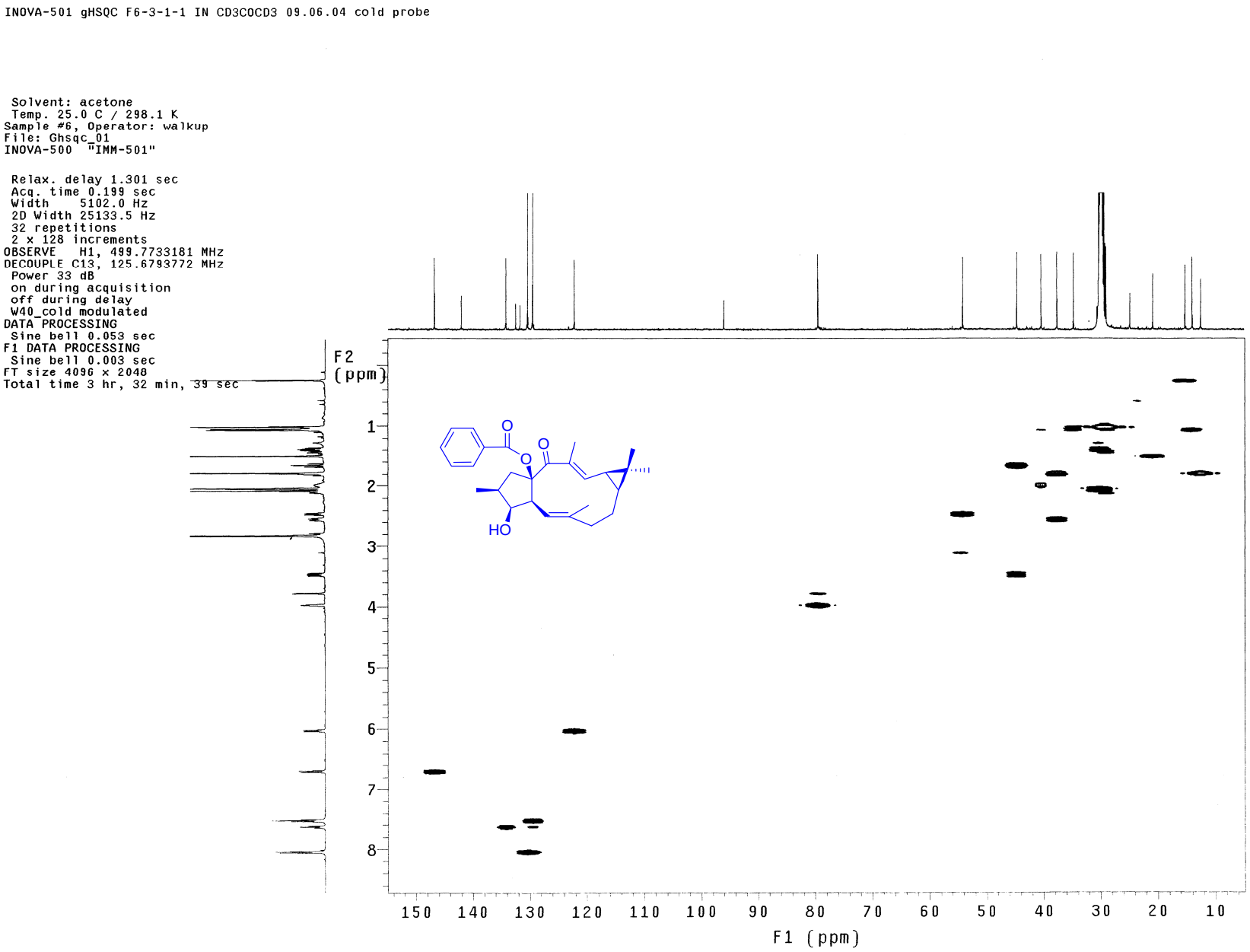

Figure S103. The gHSQC Spectrum of 11 in CD_3COCD_3 (500 MHz for ^1H NMR).

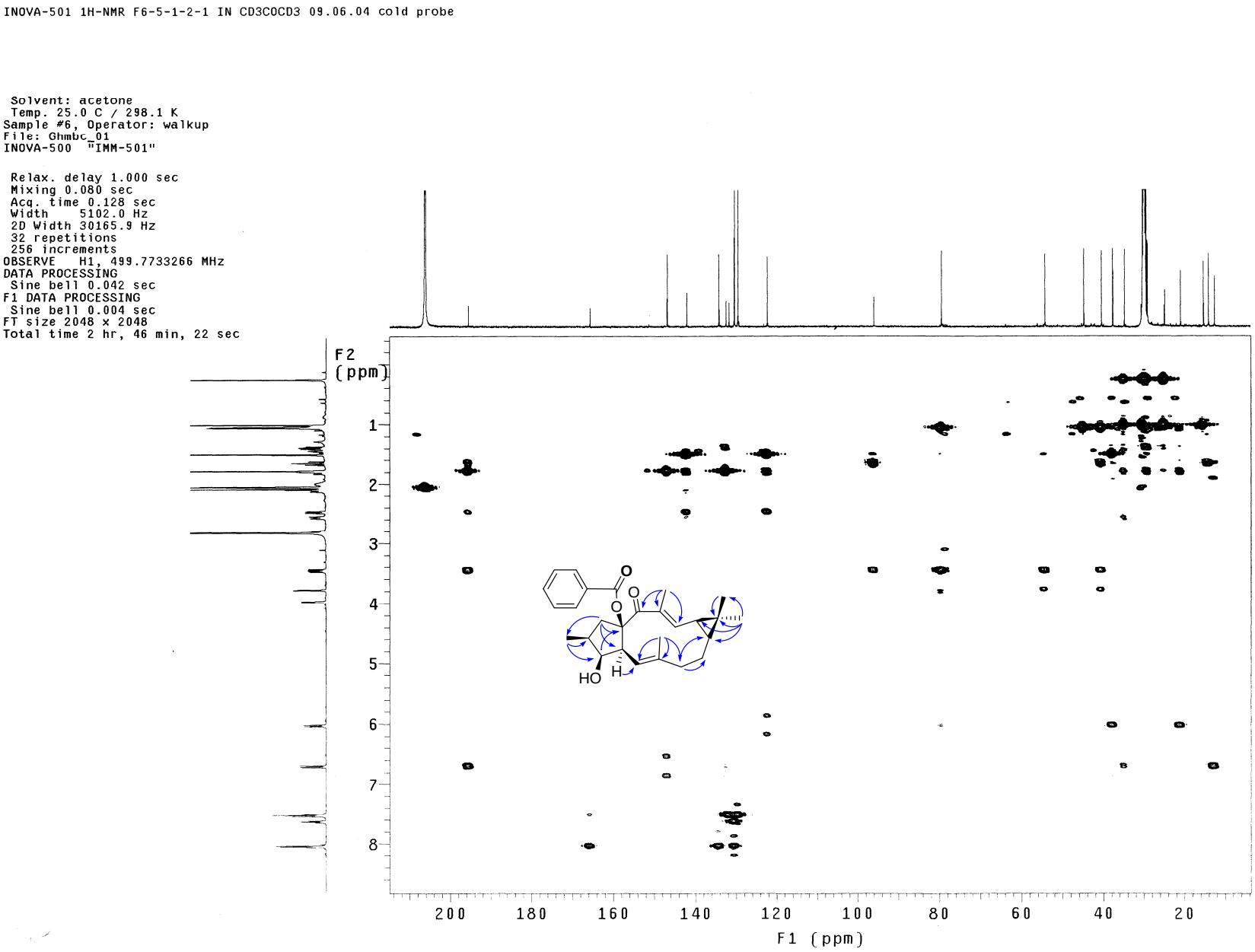

Figure S104. The gHMBC Spectrum of 11 in CD_3COCD_3 (500 MHz for ^1H NMR).

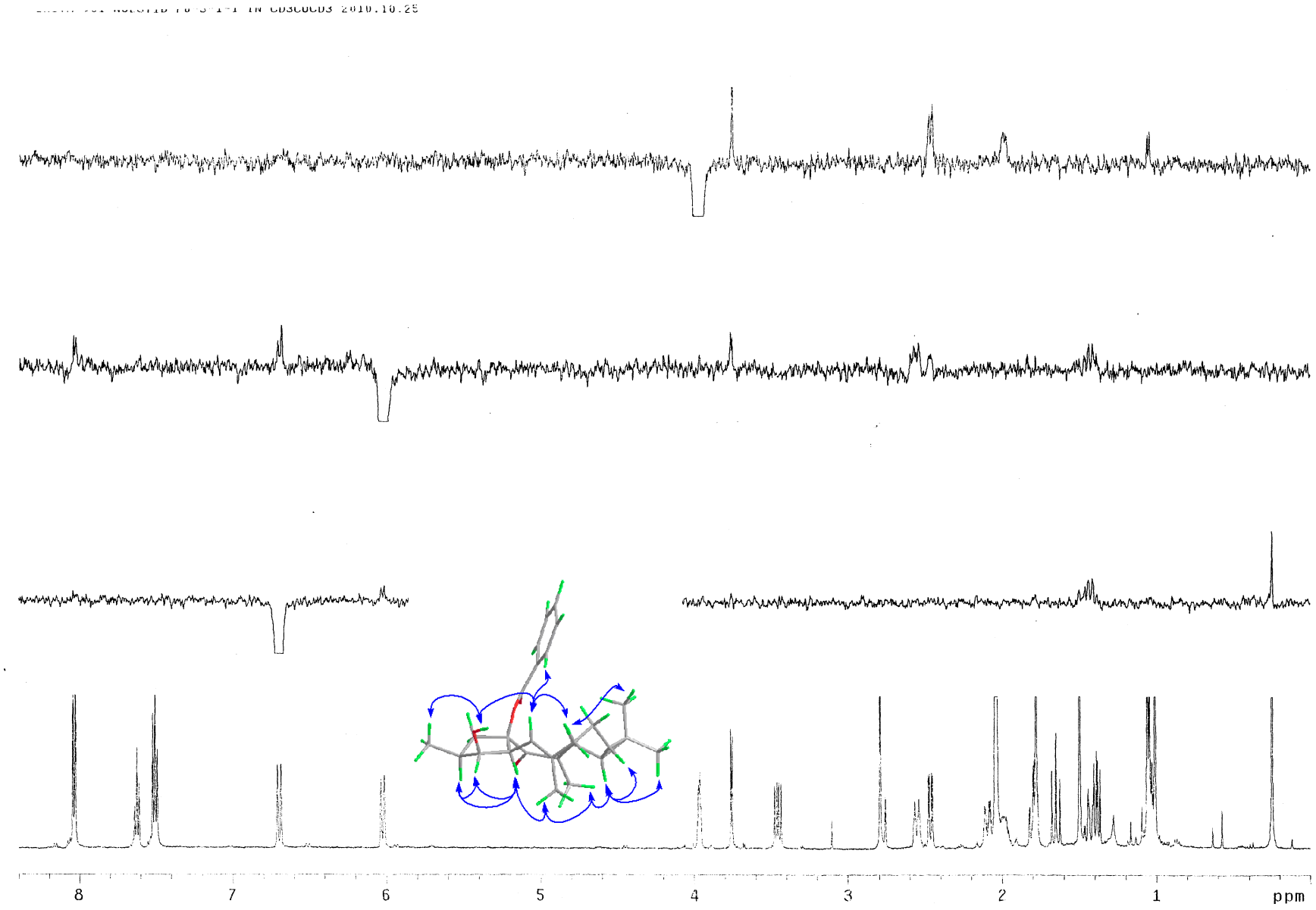

Figure S105. The NOE Difference Spectrum 1 of 11 in CD_3COCD_3 (500 MHz).

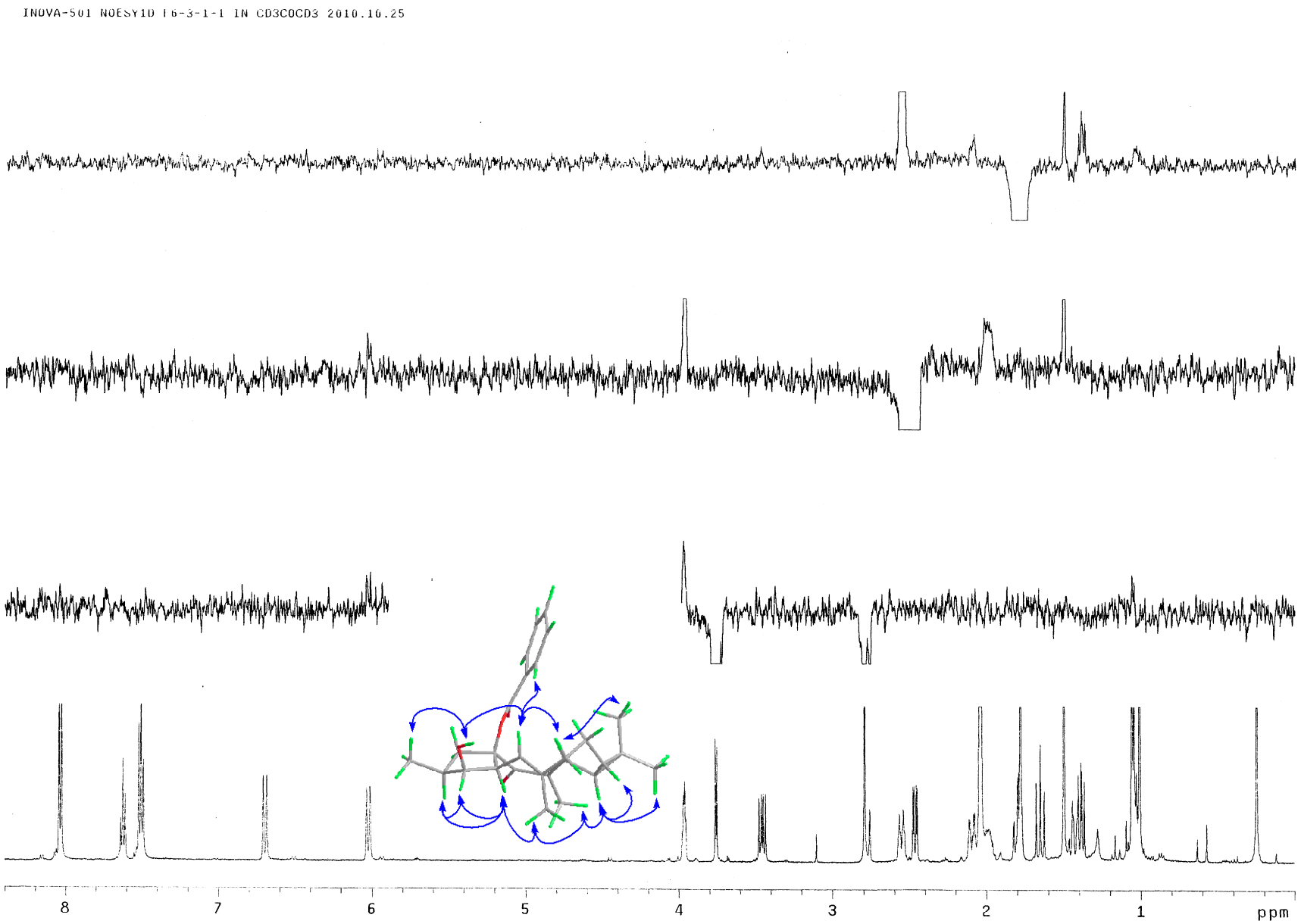

Figure S106. The NOE Difference Spectrum 2 of 11 in CD_3COCD_3 (500 MHz).

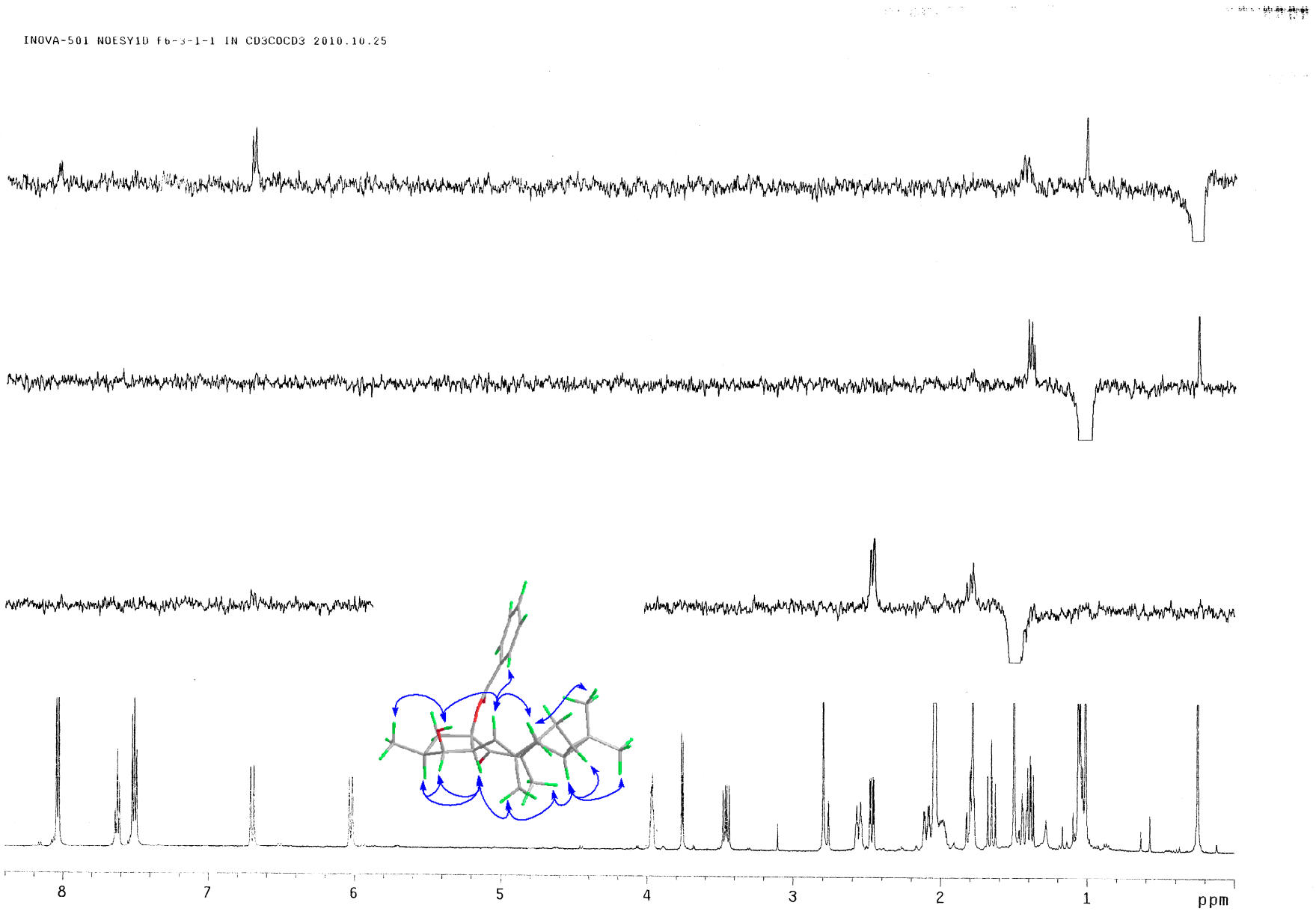

Figure S107. The NOE Difference Spectrum 3 of 11 in CD_3COCD_3 (500 MHz).

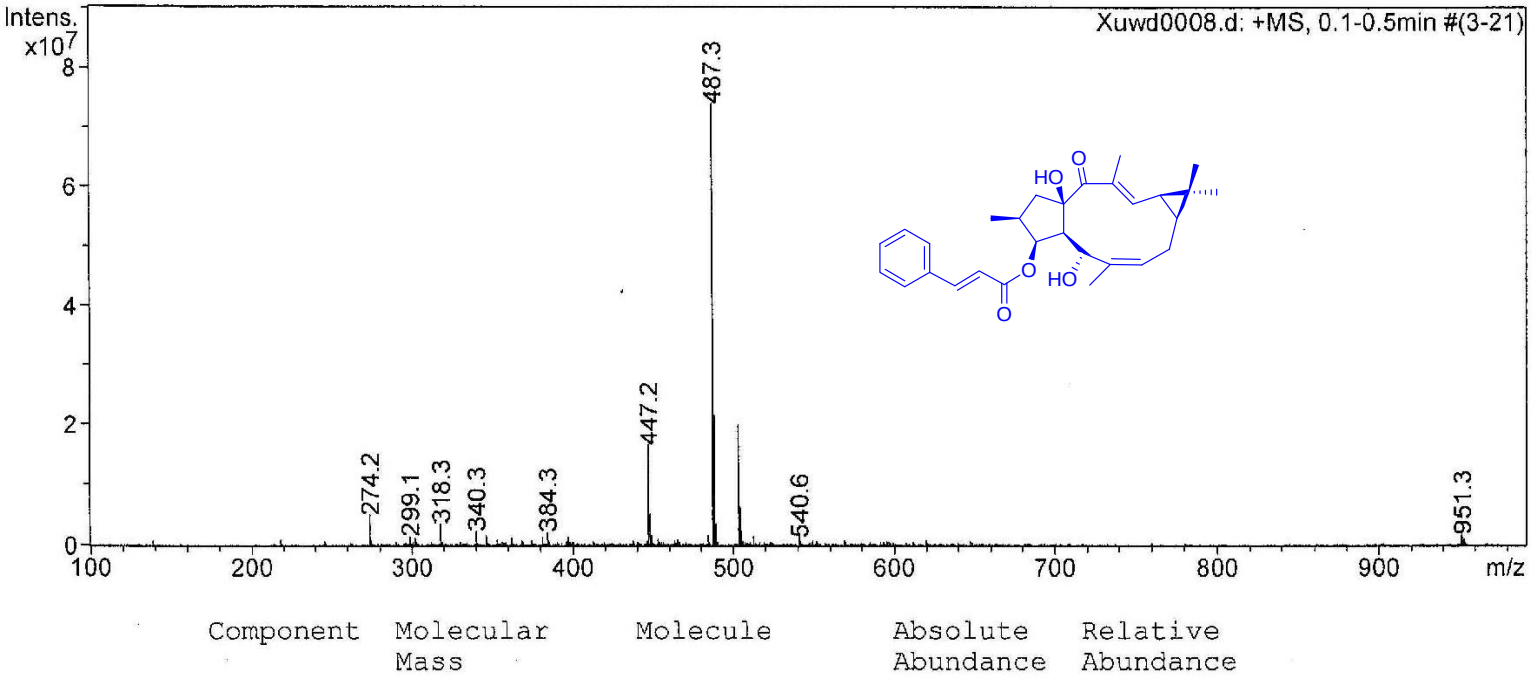

Figure S108. (+)-ESIMS Spectrum of 12.

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

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
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.

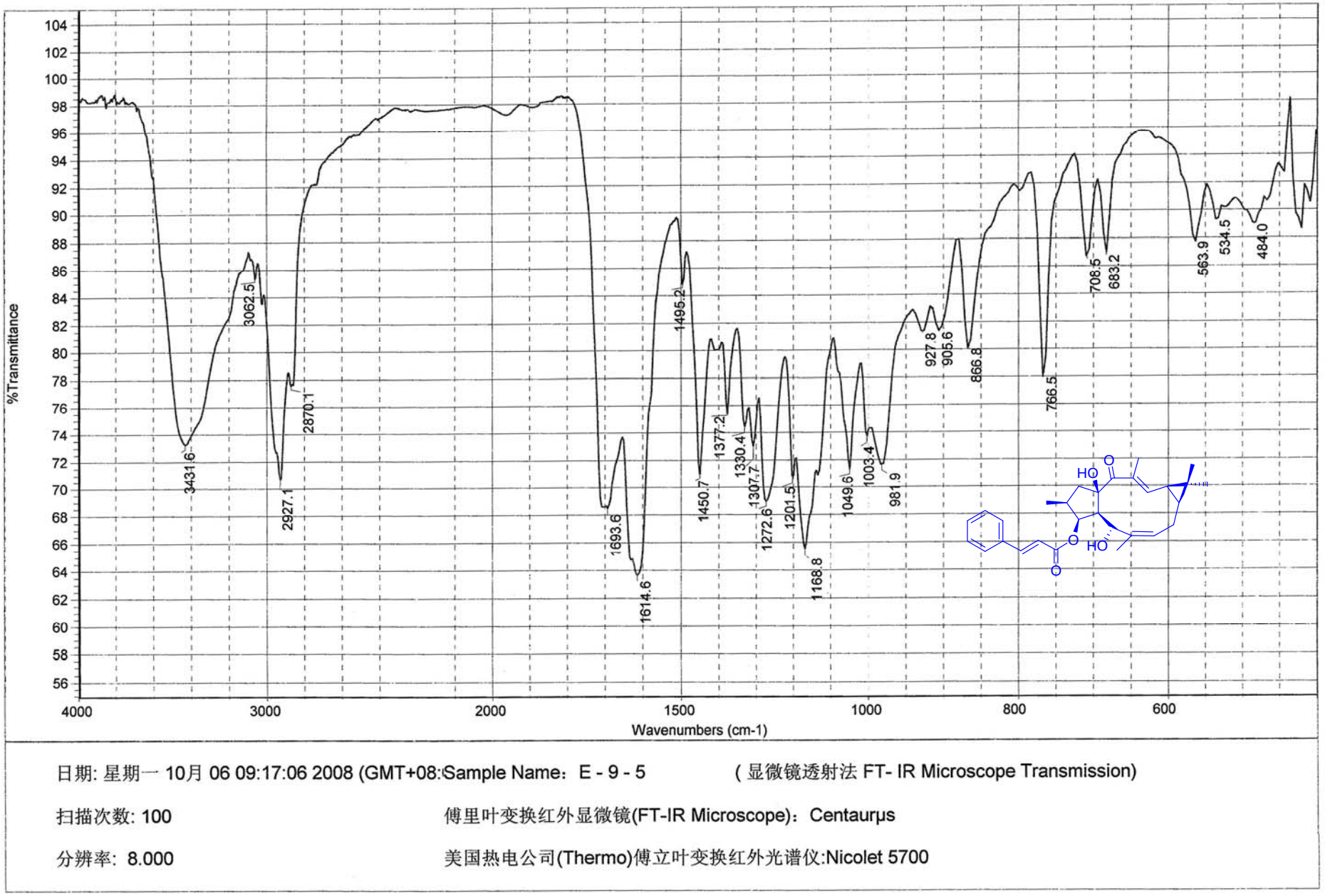

Figure S109. The IR Spectrum of 12.

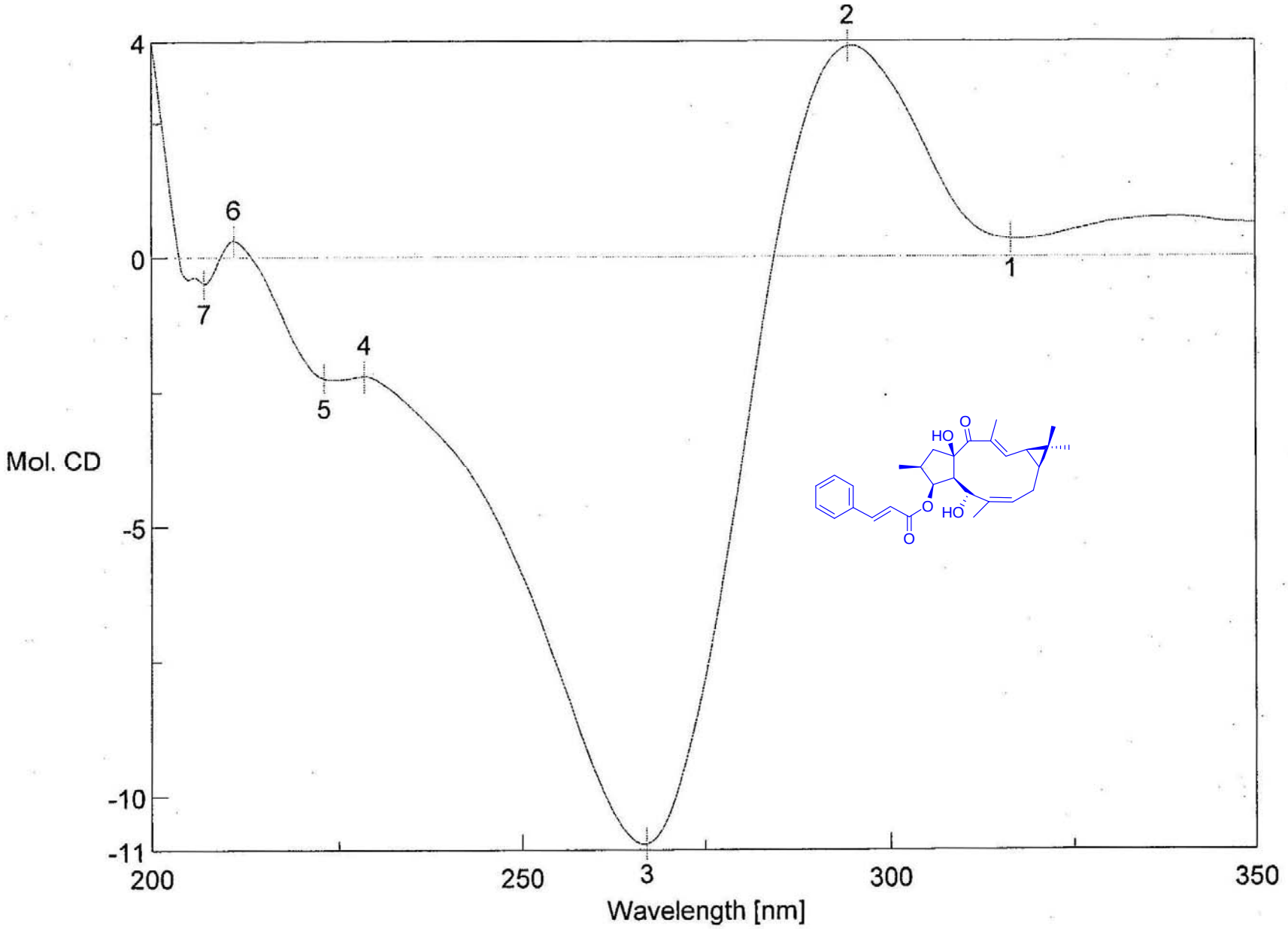

Figure S110. The CD Spectrum of 12.

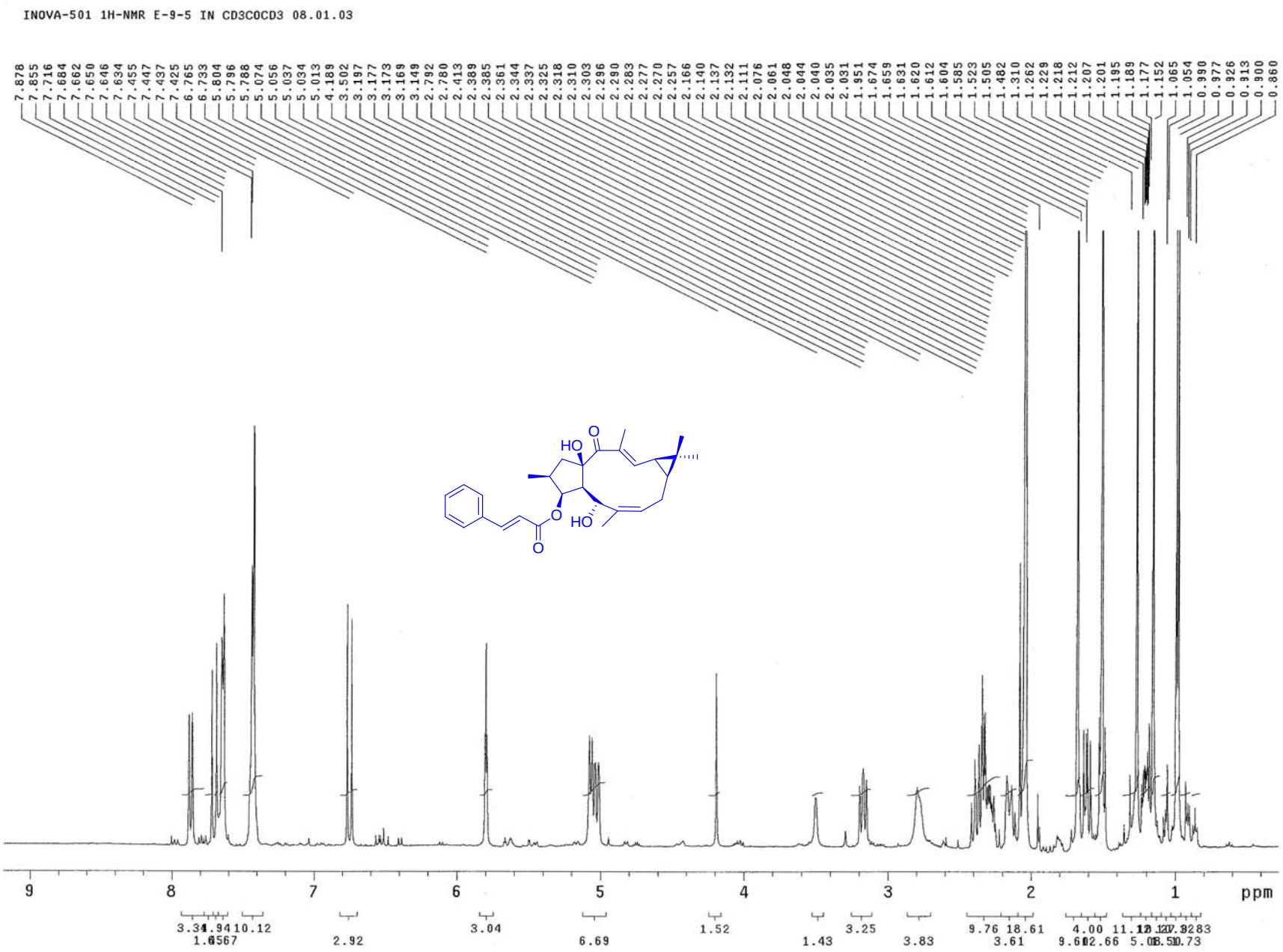

Figure S111. The ^{1}H NMR Spectrum of 12 in CD_3COCD_3 (500 MHz).

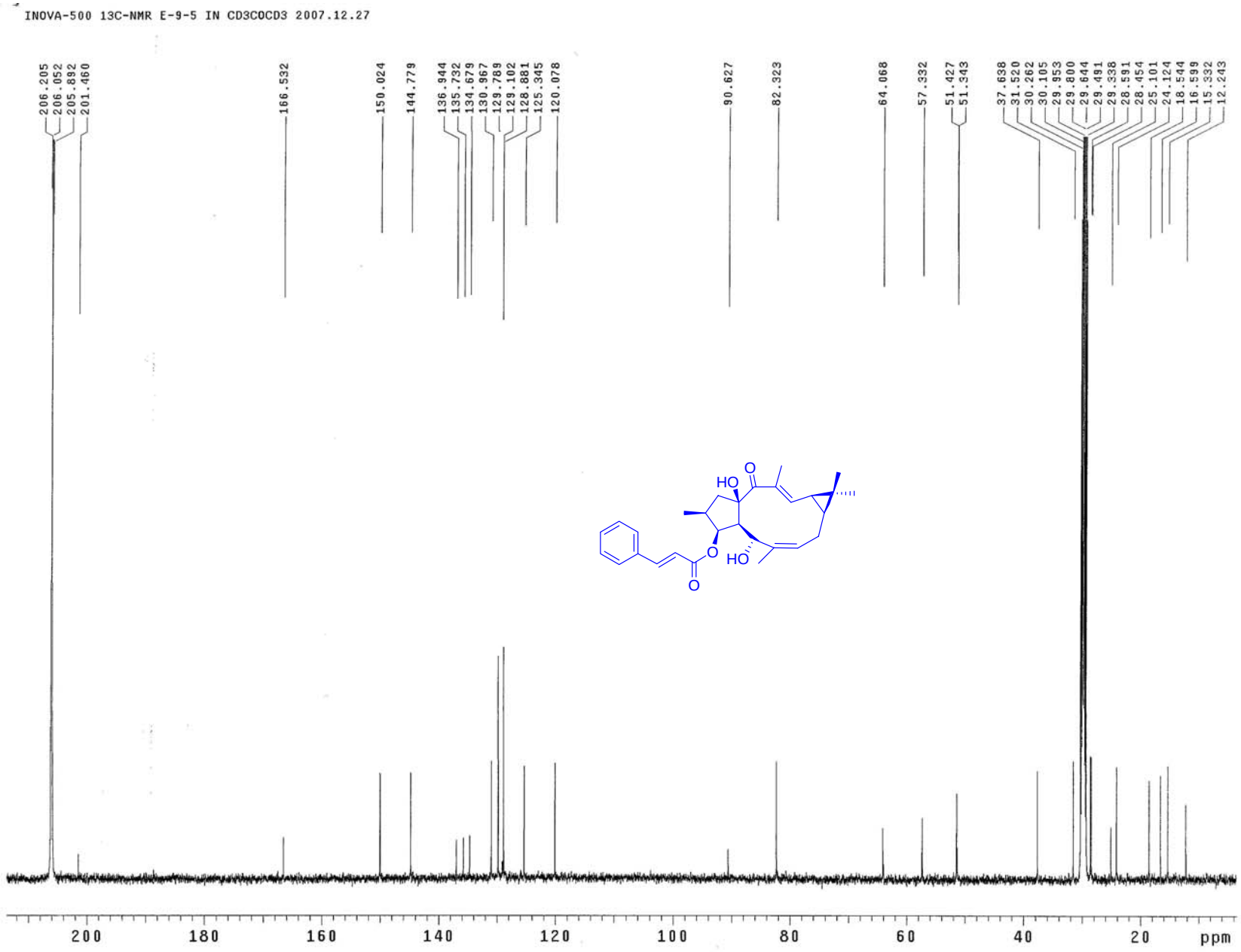

Figure S112. The ^{13}C NMR Spectrum of 12 in CD_3COCD_3 (125 MHz).

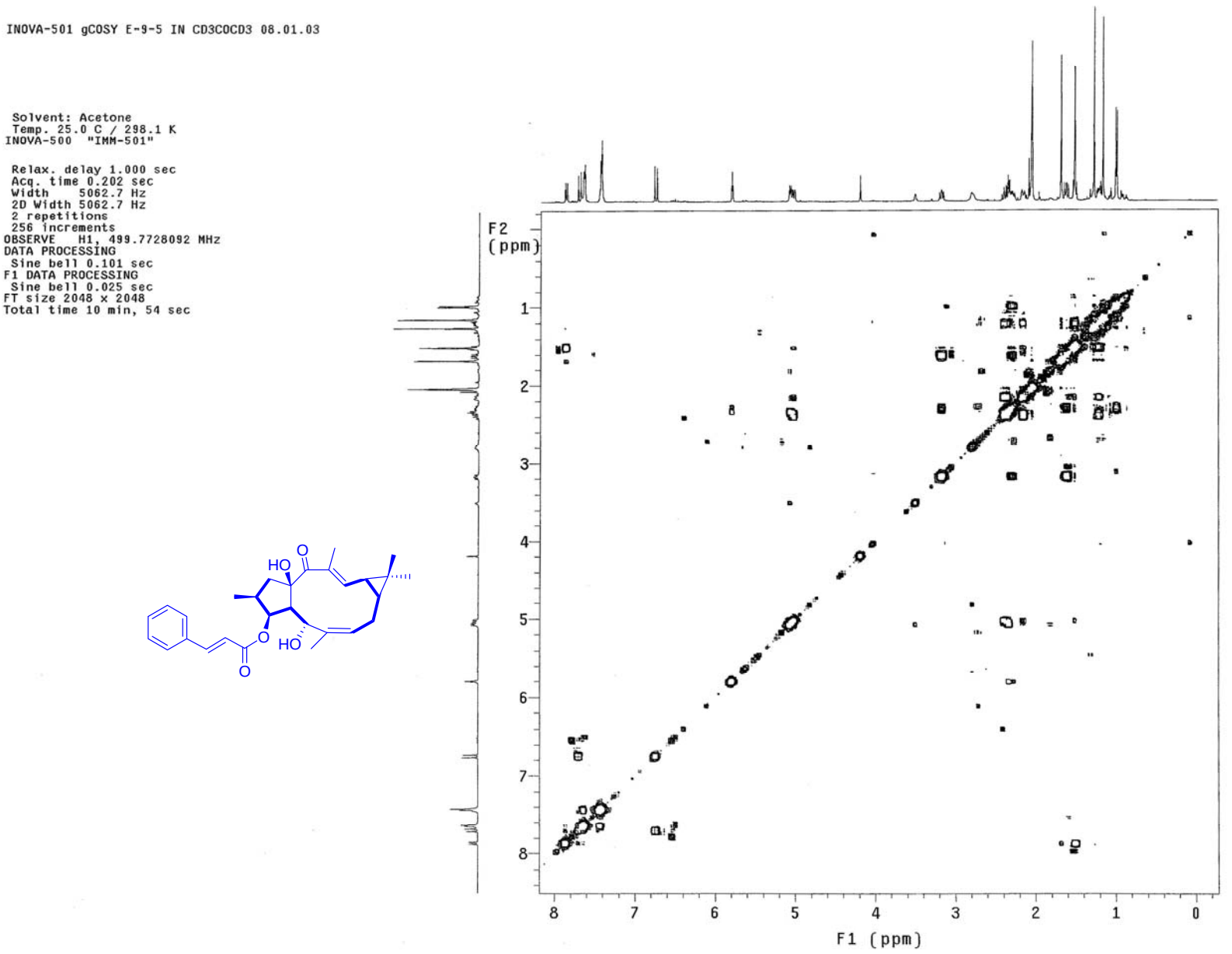

Figure S113. The ^{1}H-^{1}H gCOSY Spectrum of 12 in CD_3COCD_3 (500 MHz).

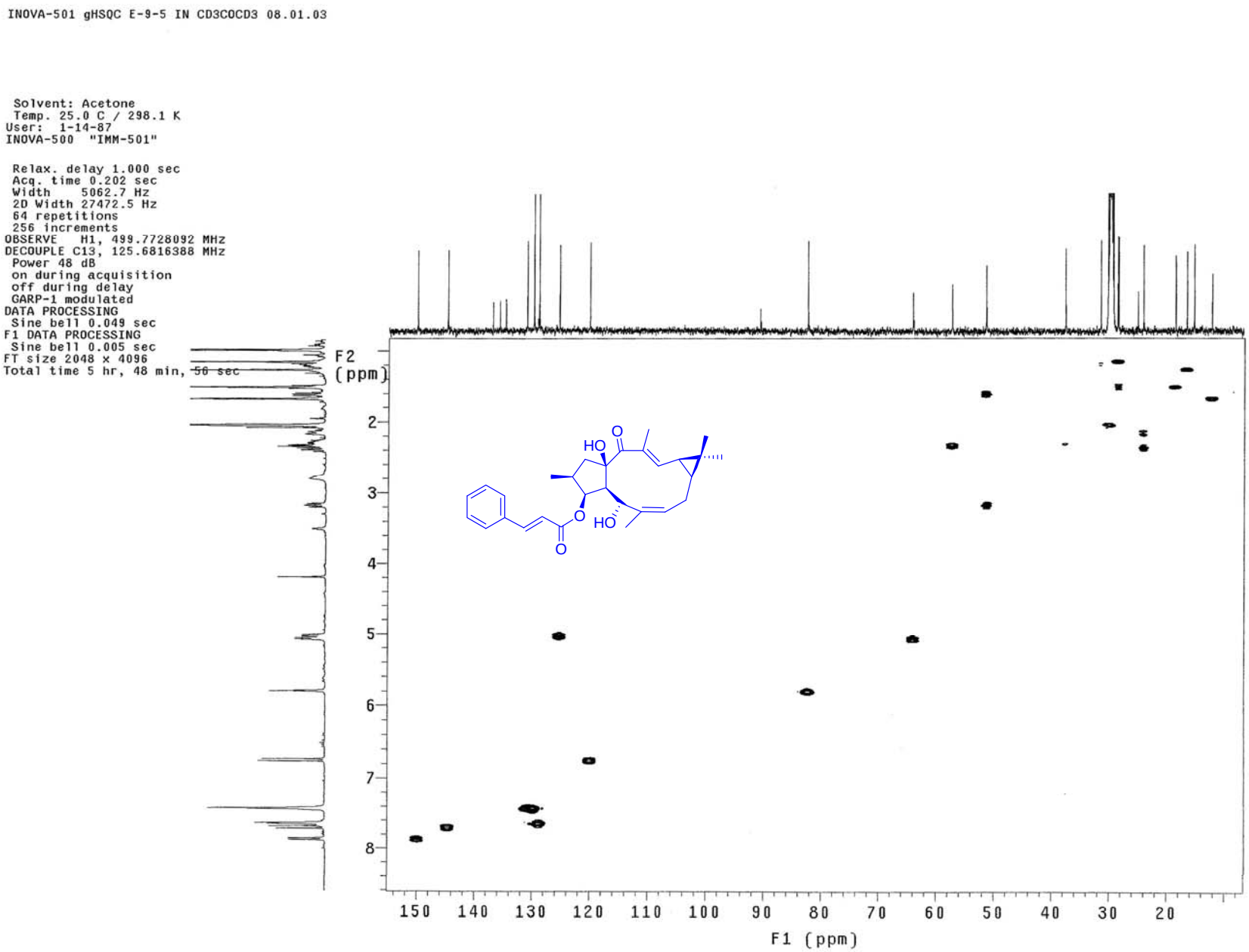

Figure S114. The gHSQC Spectrum of 12 in CD_3COCD_3 (500MHz for ^1H NMR).

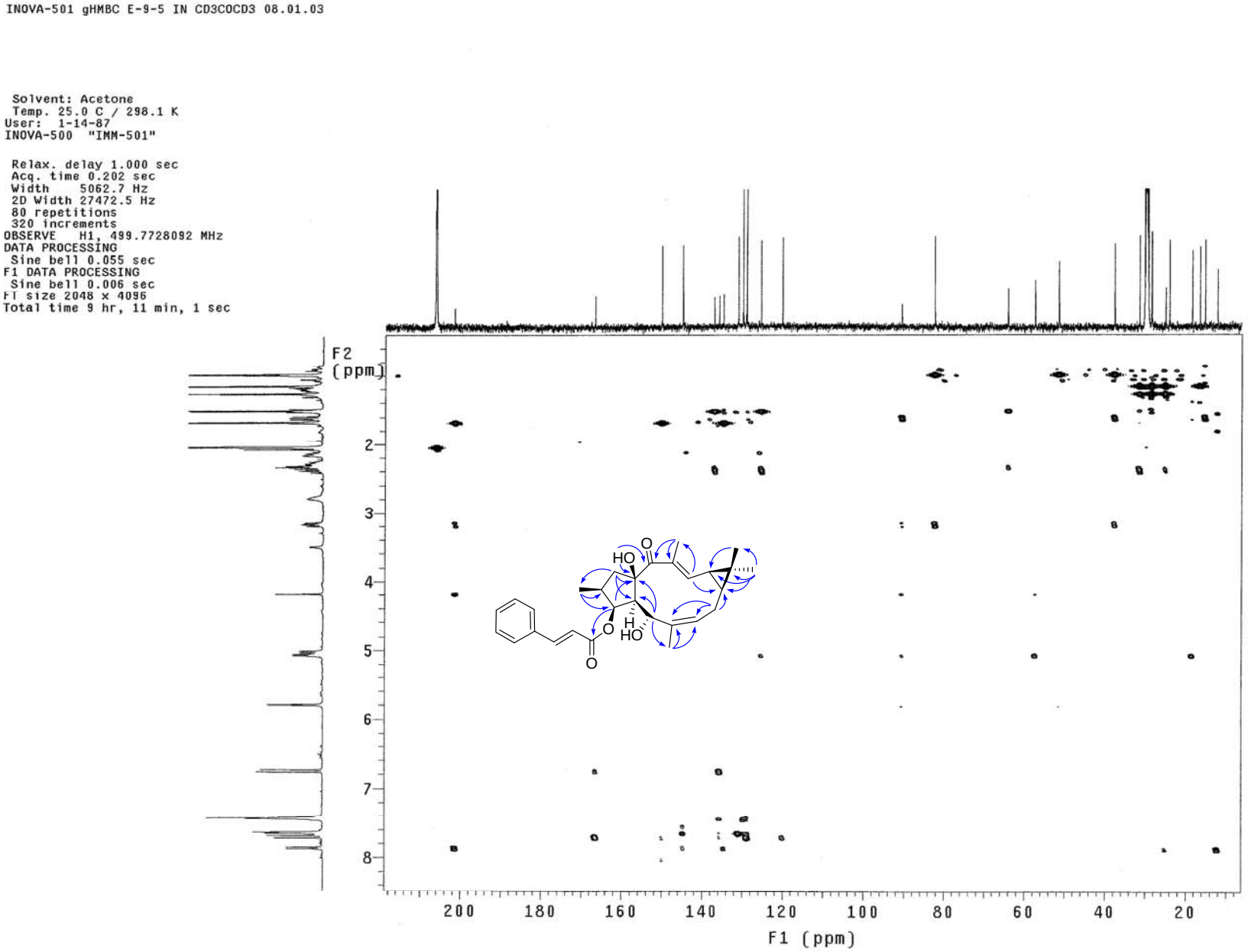

Figure S115. The gHMBC Spectrum of 12 in CD_3COCD_3 (500MHz for ^1H NMR).

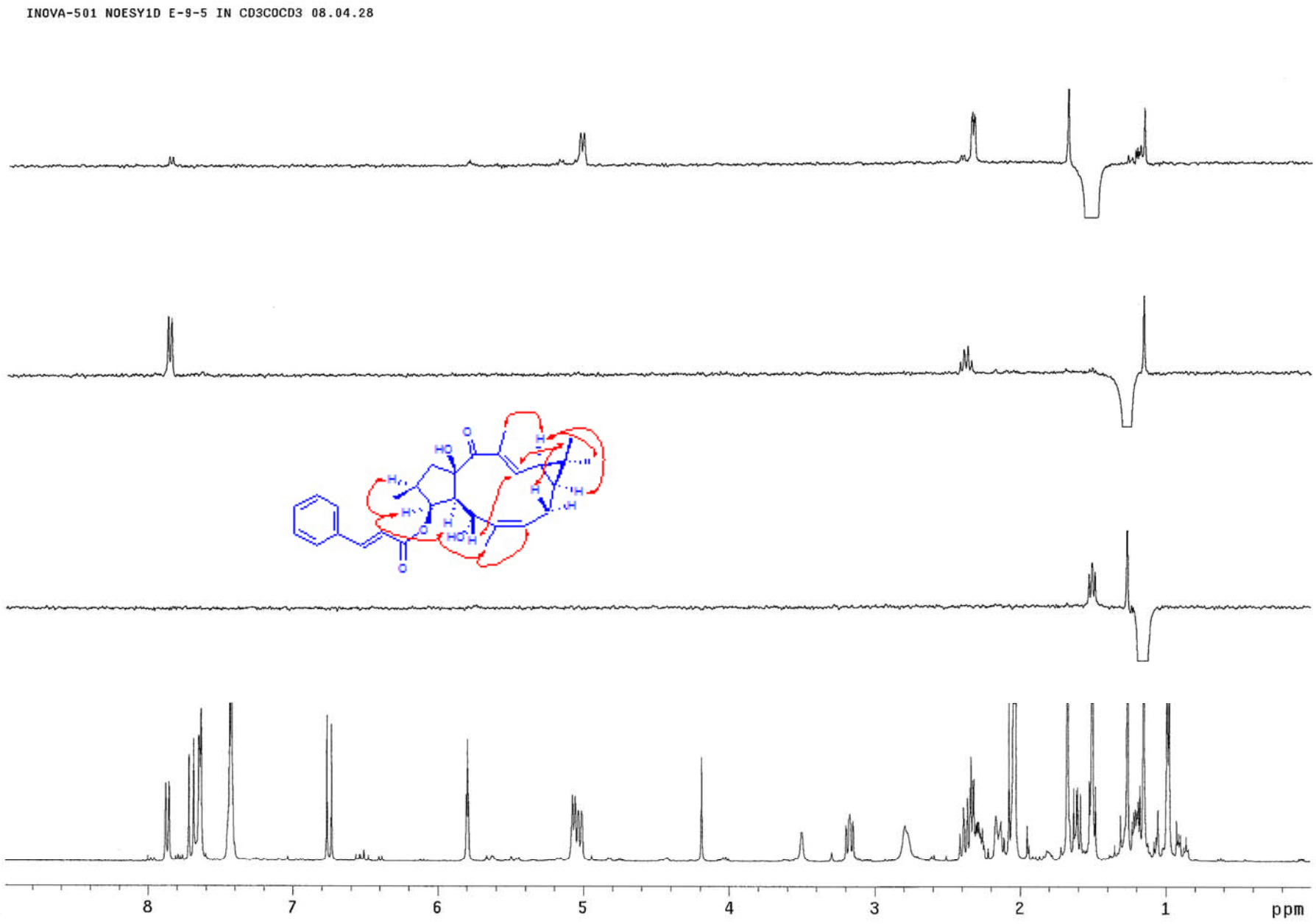

Figure S116. The NOE Difference Spectrum 1 of 12 in CD_3COCD_3 (500 MHz).

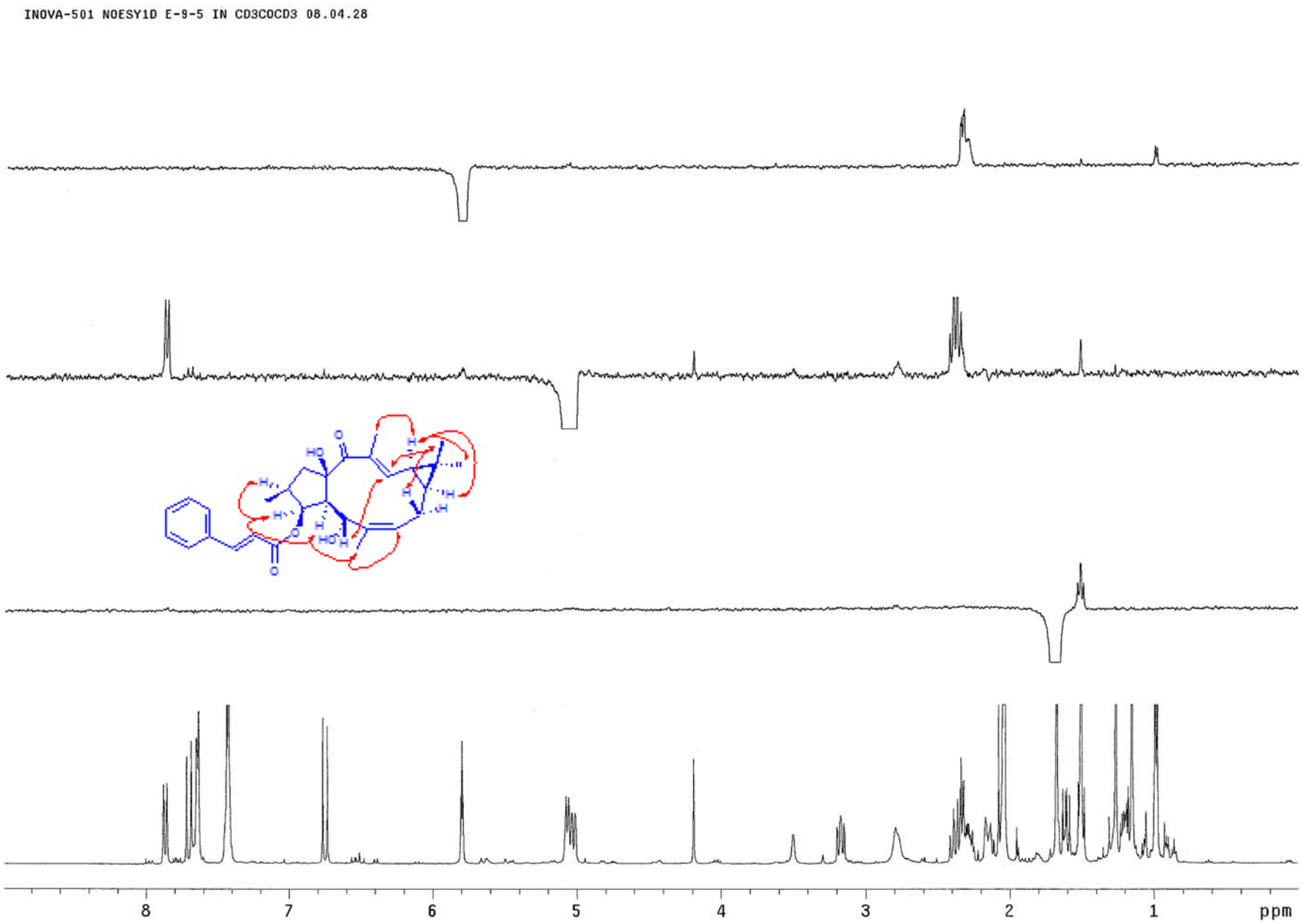

Figure S117. The NOE Difference Spectrum 2 of 12 in CD_3COCD_3 (500 MHz).

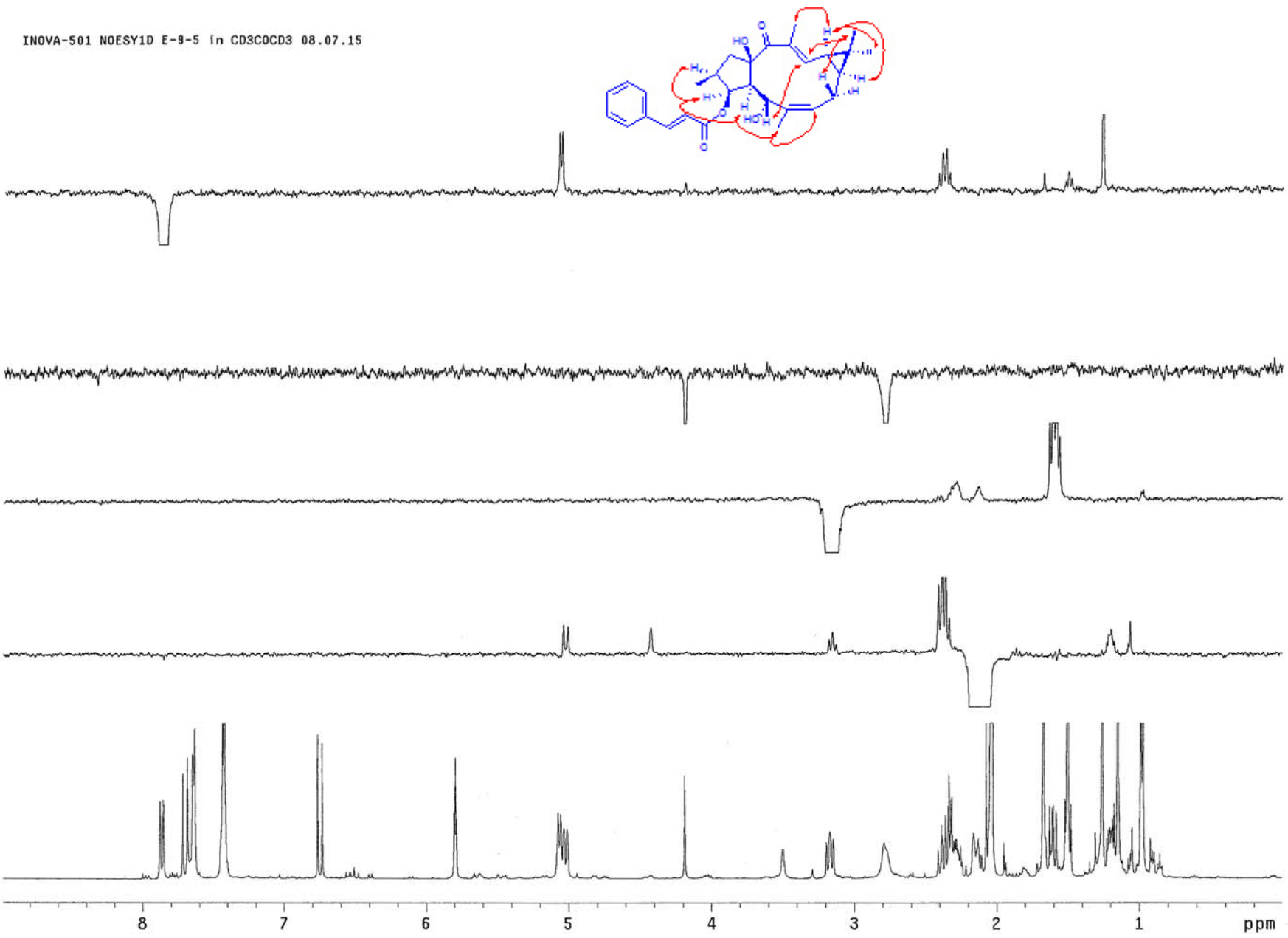

Figure S118. The NOE Difference Spectrum 3 of 12 in CD_3COCD_3 (500 MHz).

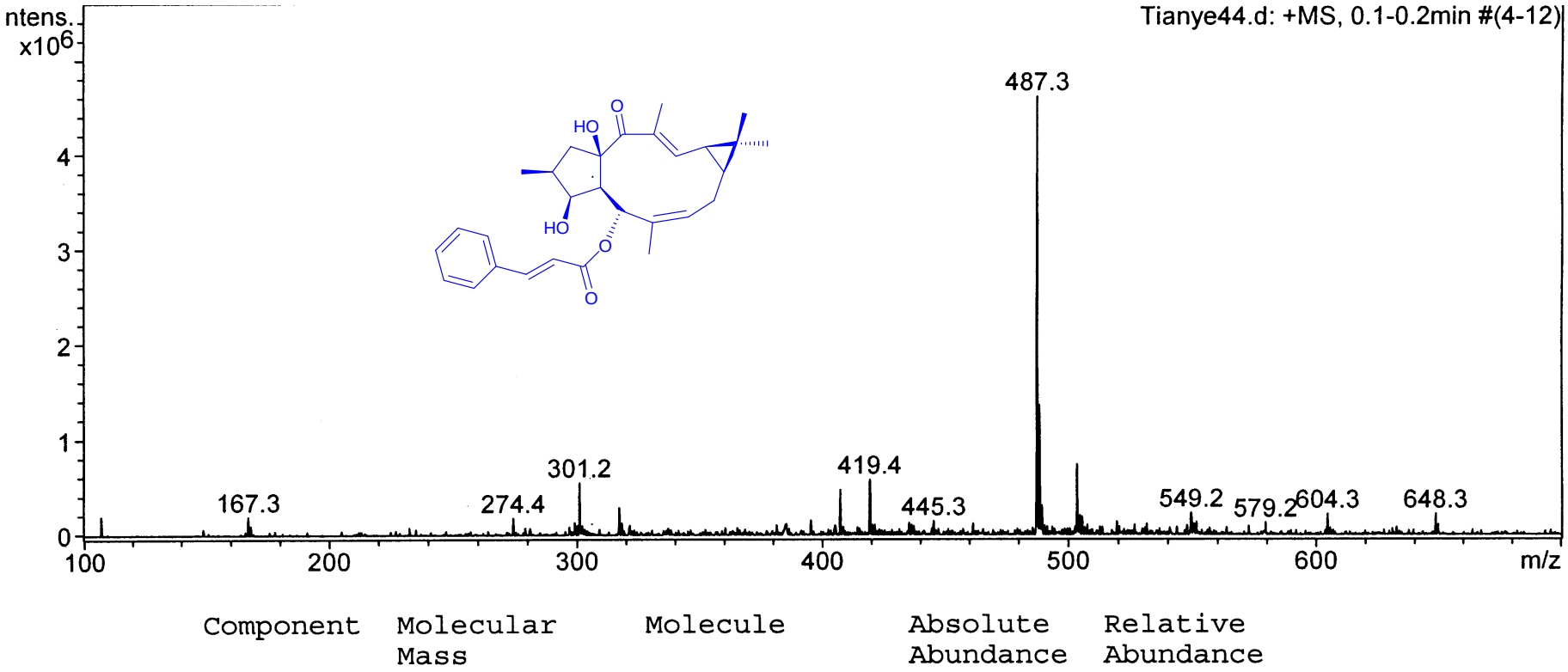

Figure S119. The (+)-ESIMS Spectrum of 13.

MS Formula Results: + Scan (8.713 min) Sub (201011154.d)

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

(+)-HRESIMS Data of 13.

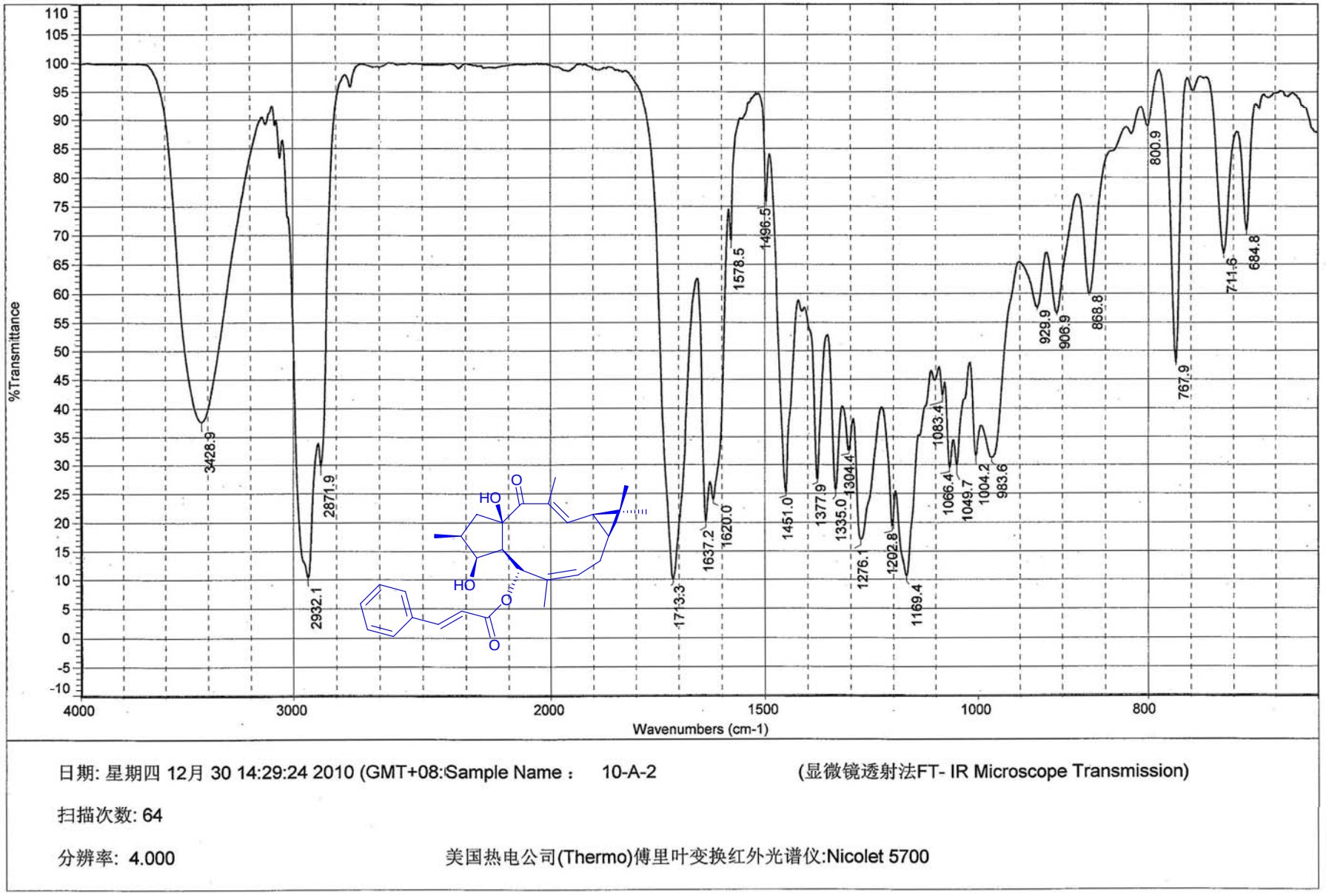

Figure S120. The IR Spectrum of 13.

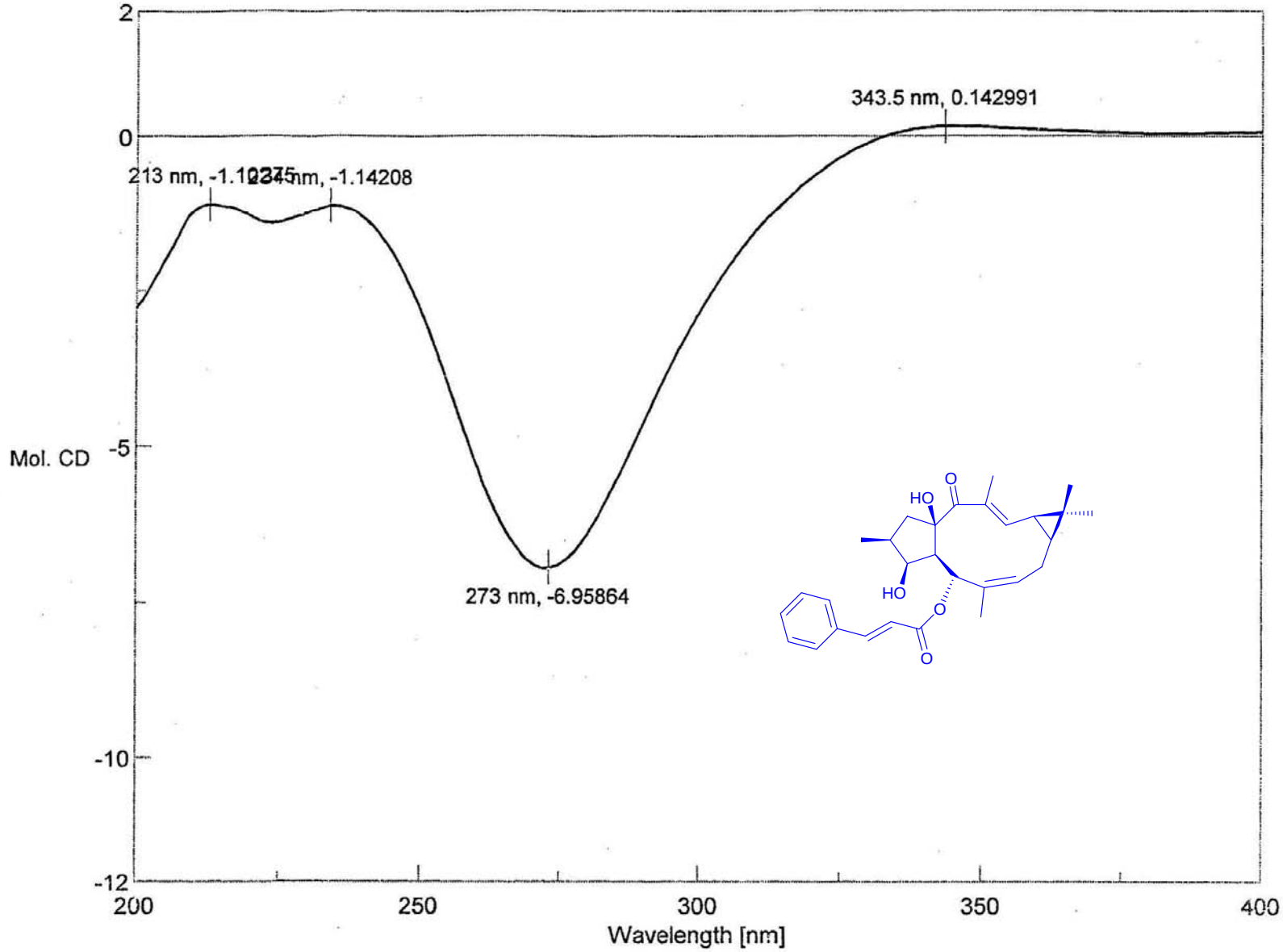

Figure S121. The CD Spectrum of 13.

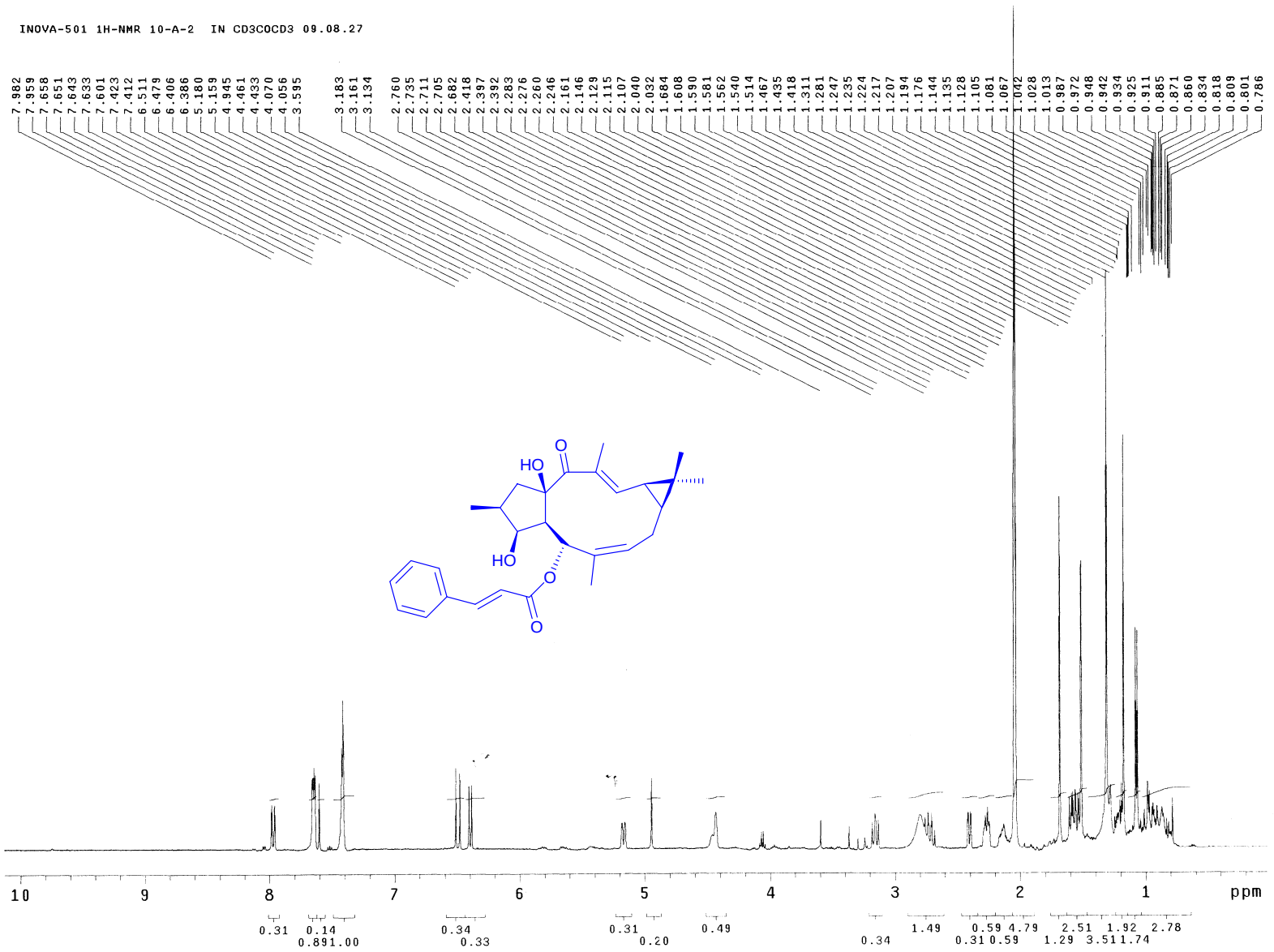

Figure S122. The ^{1}H NMR Spectrum of 13 in CD_3COCD_3 (500 MHz).

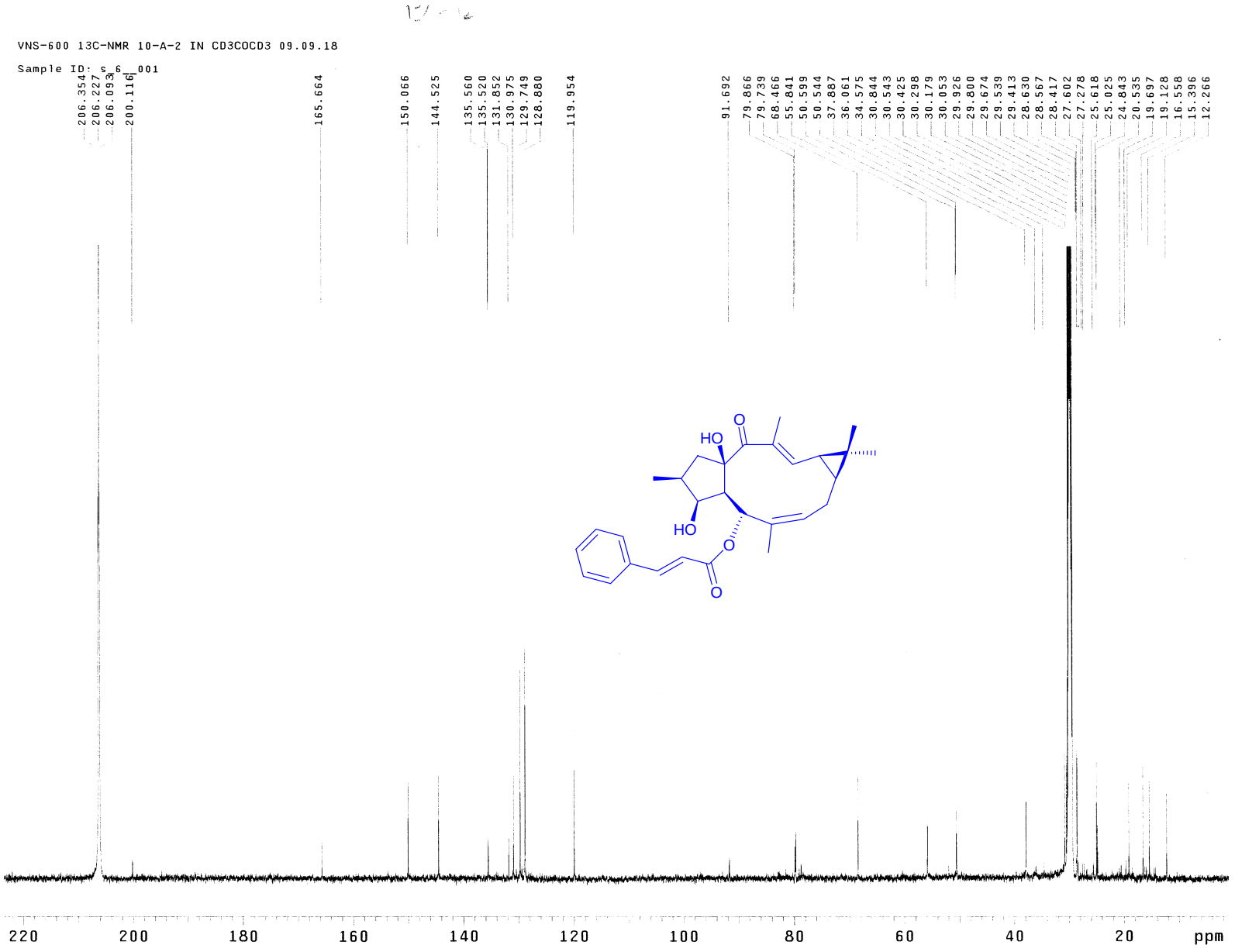

Figure S123. The ^{13}C NMR Spectrum of 13 in CD_3COCD_3 (150 MHz).

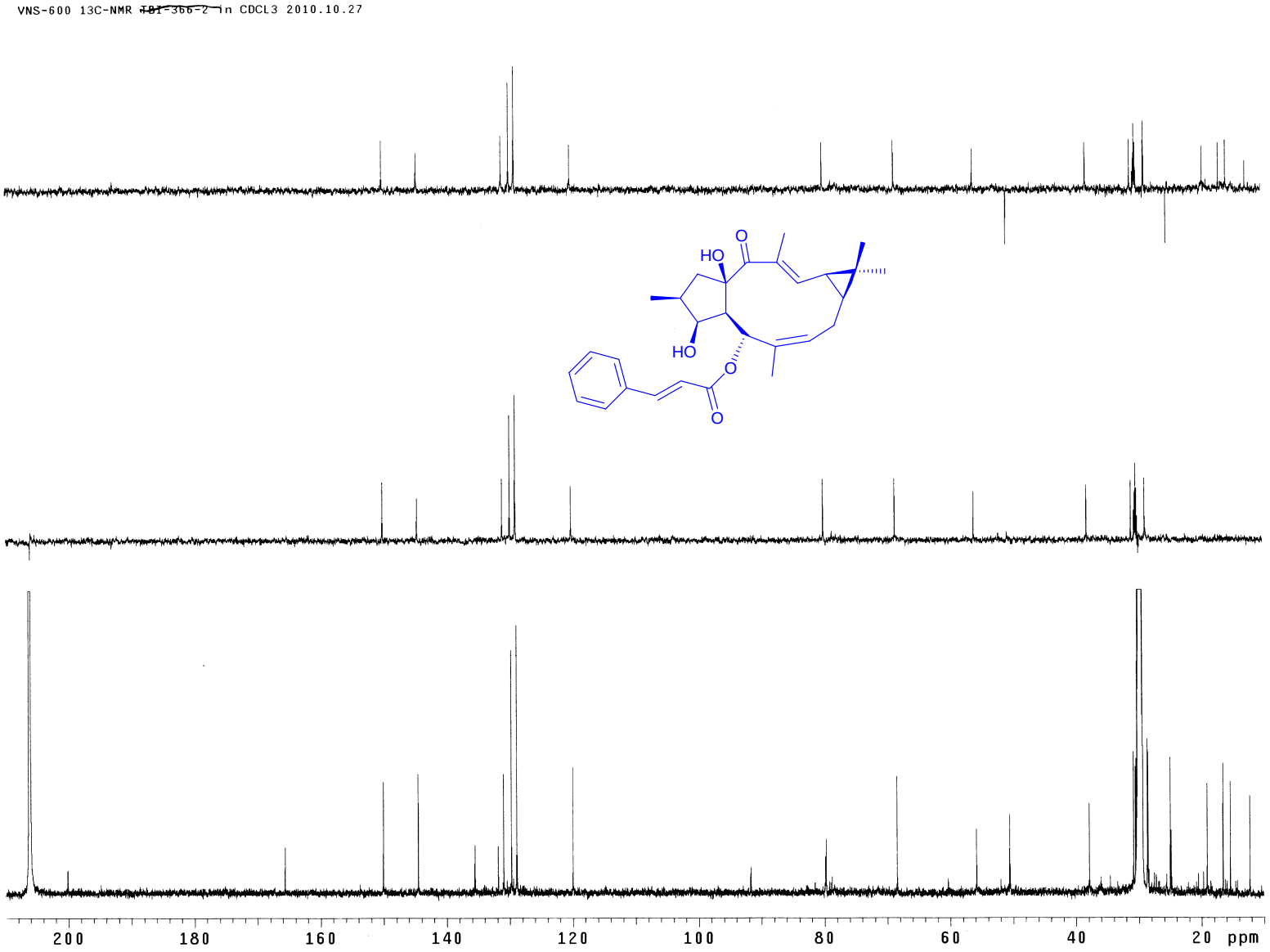

Figure S124. The DEPT Spectrum of 13 in CD_3COCD_3 (150 MHz).

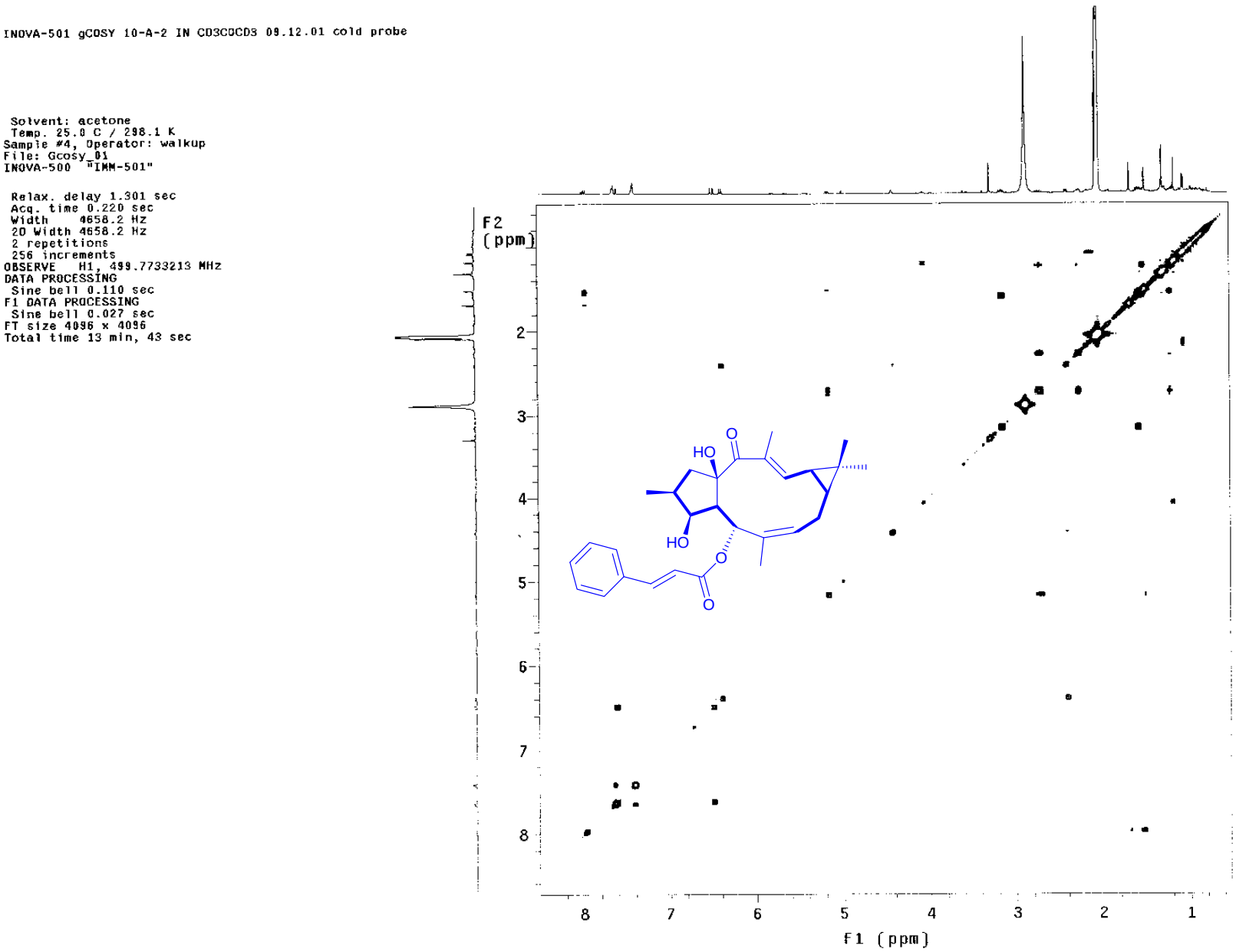

Figure S125. The ^{1}H-^{1}H gCOSY Spectrum of 13 in CD_3COCD_3 (500 MHz).

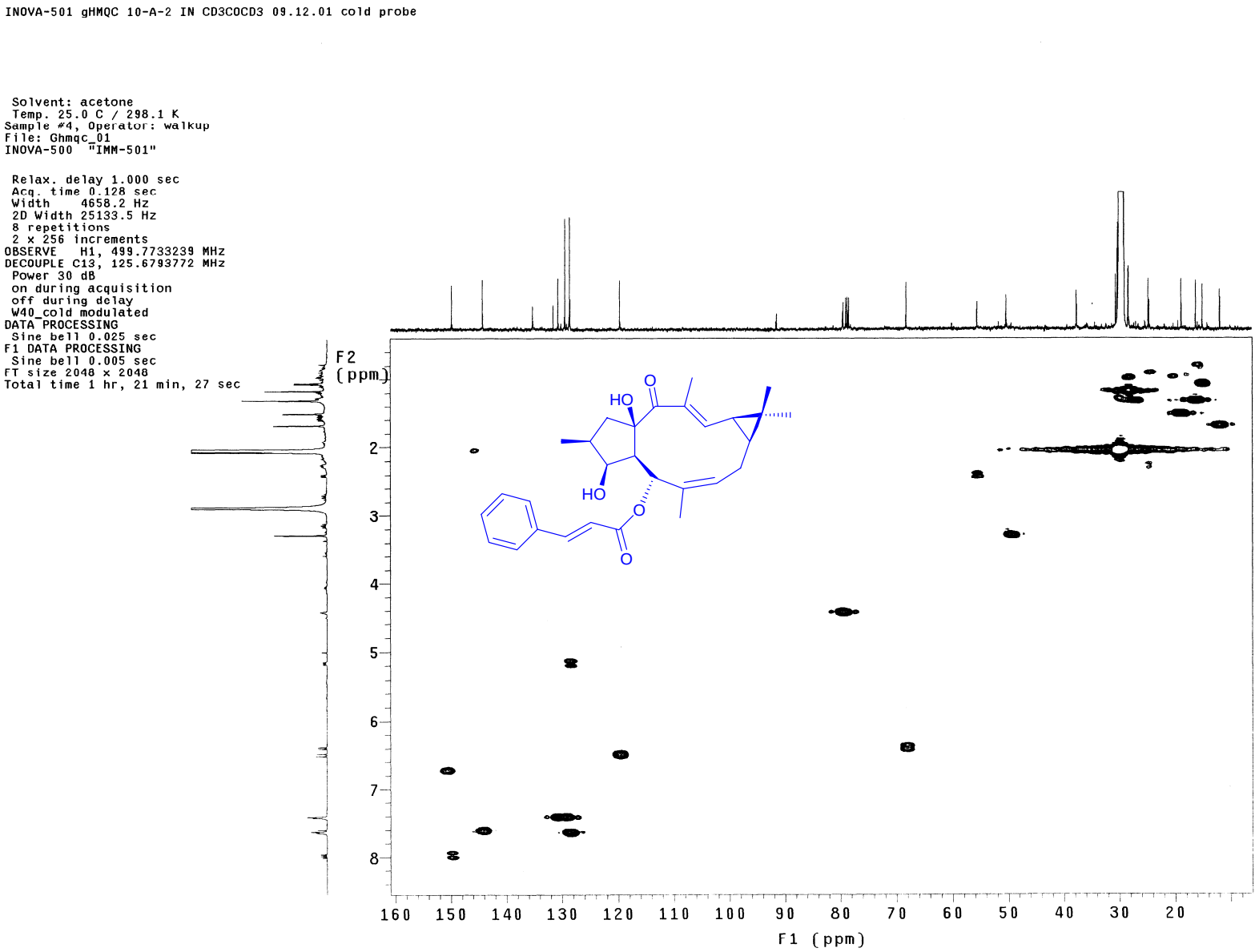

Figure S126. The gHSQC Spectrum of 13 in CD_3COCD_3 (500 MHz for ^1H NMR).

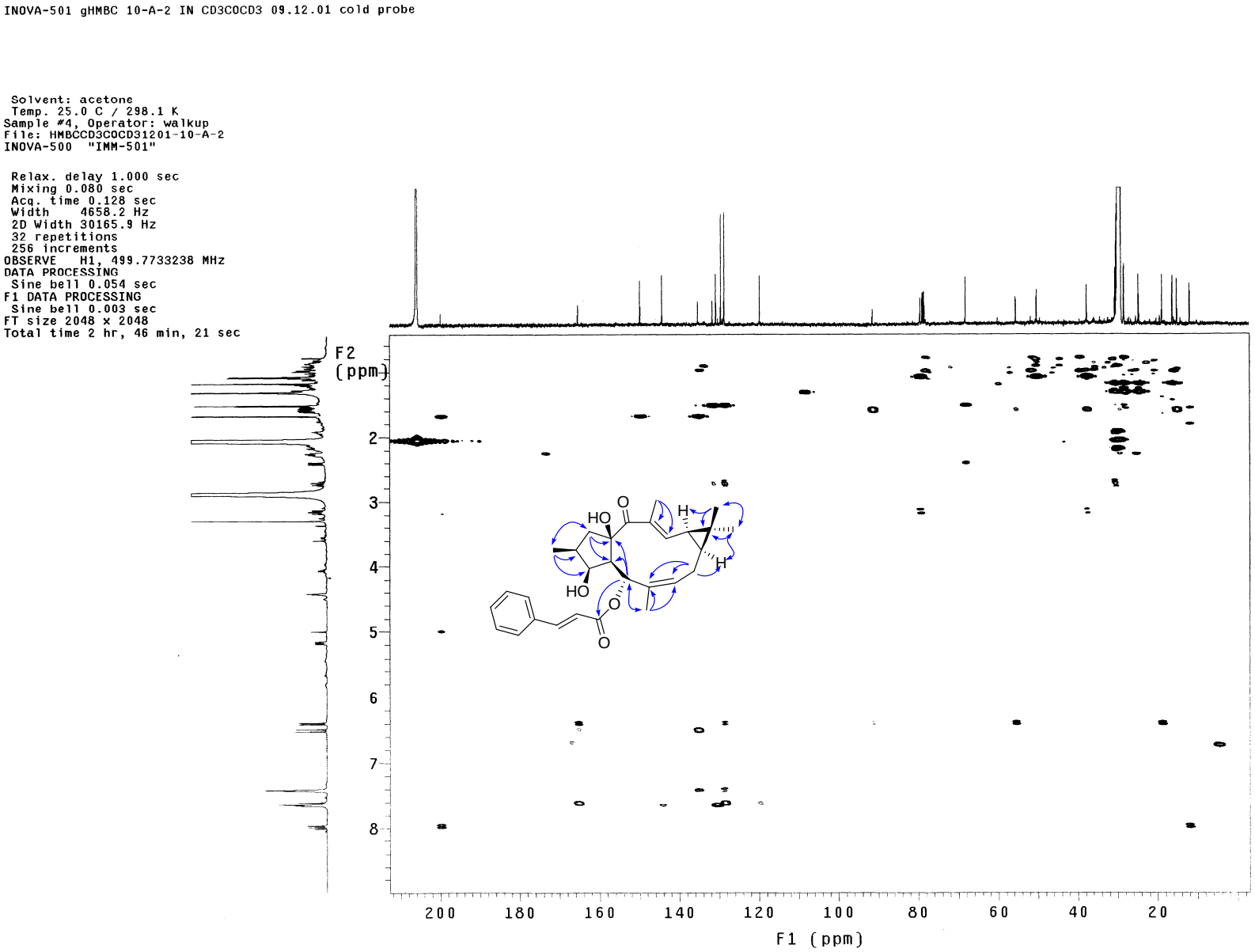

Figure S127. The gHMBC Spectrum of 13 in CD_3COCD_3 (500 MHz for ^1H NMR).

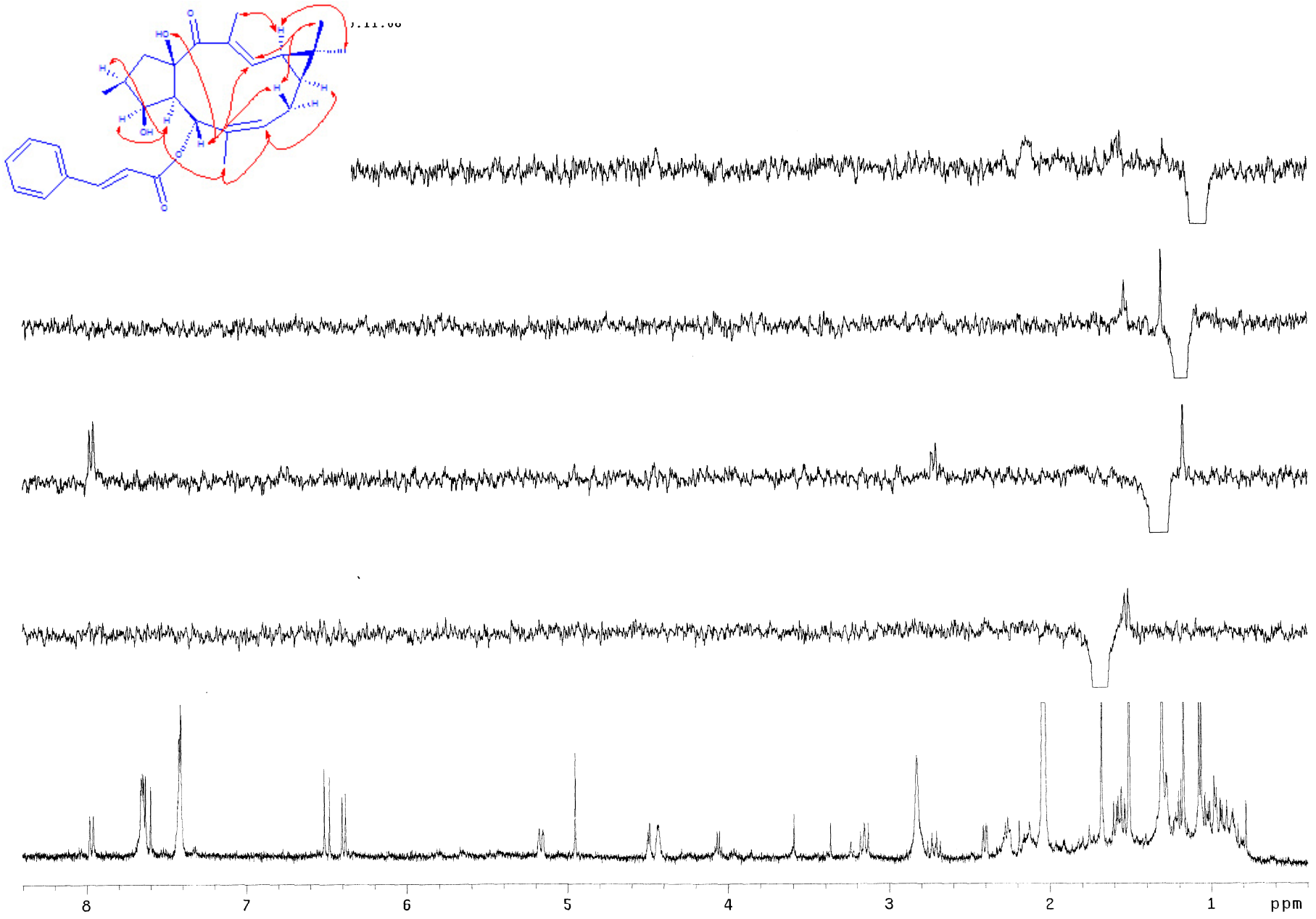

Figure S128. The NOE Difference Spectrum 1 of 13 in CD_3COCD_3 (500 MHz).

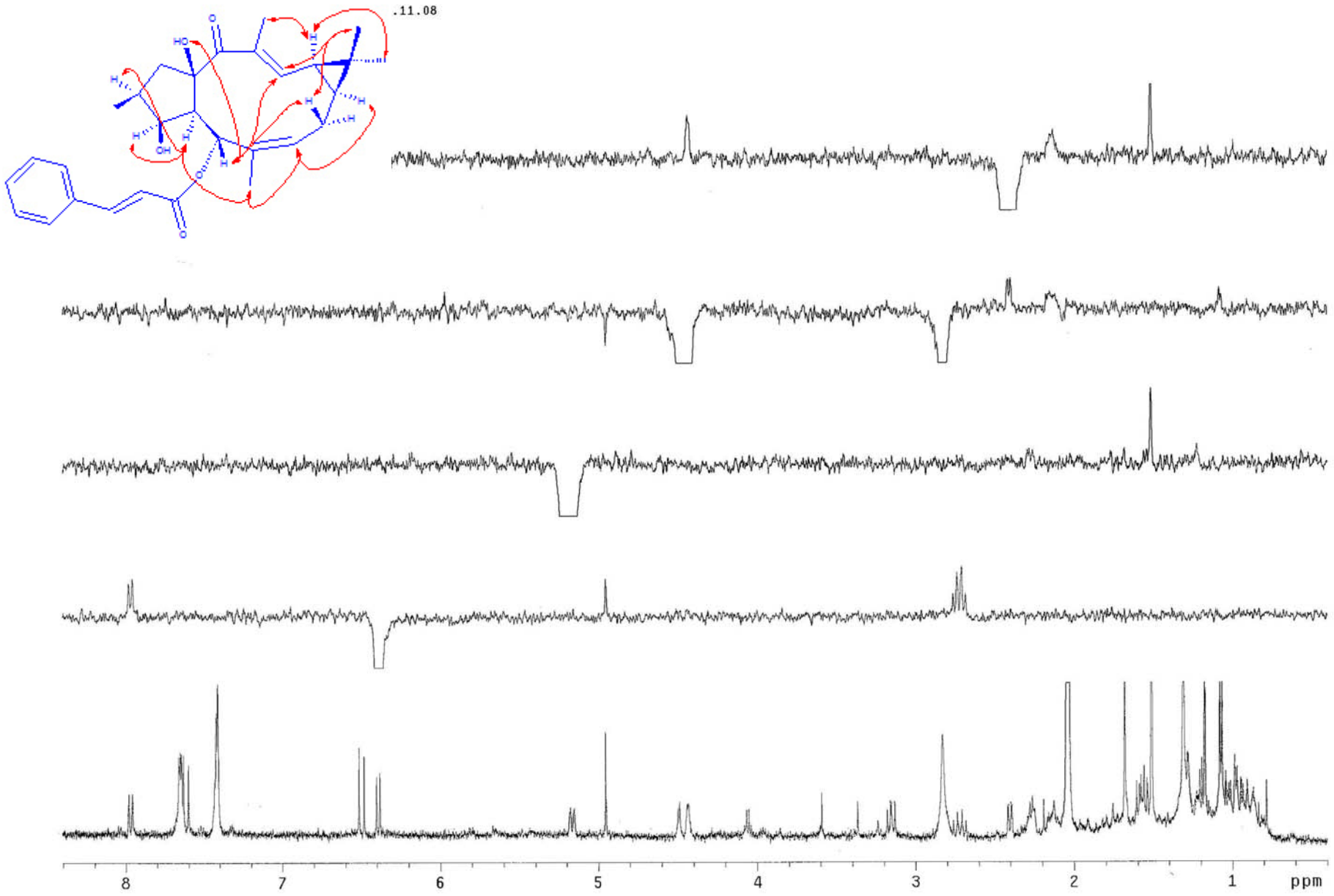

Figure S129. The NOE Difference Spectrum 2 of 13 in CD_3COCD_3 (500 MHz).

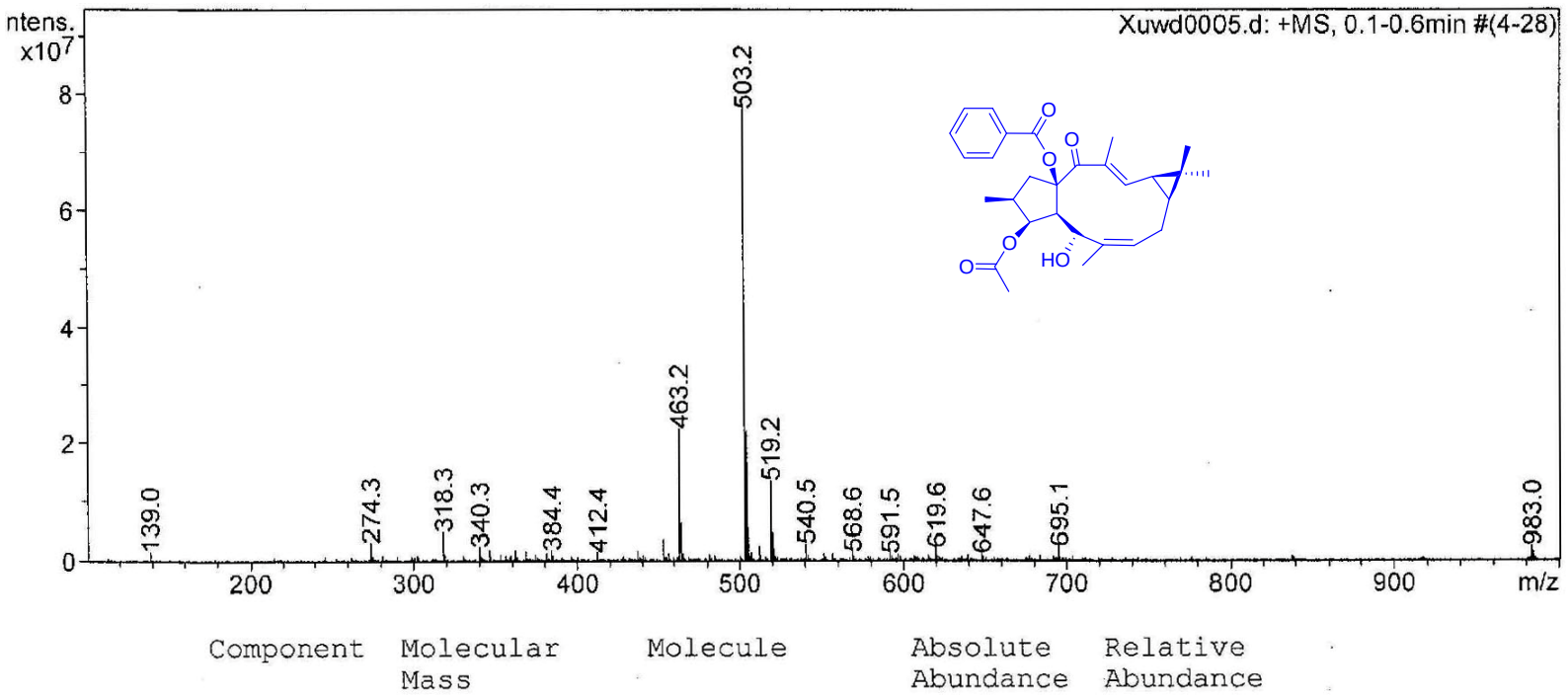

Figure S130. (+)-ESIMS Spectrum of 14.

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

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*
503.24136	0.40	0.80	29	36	1	6	11.5

(+)-HRESIMS Data of 14.

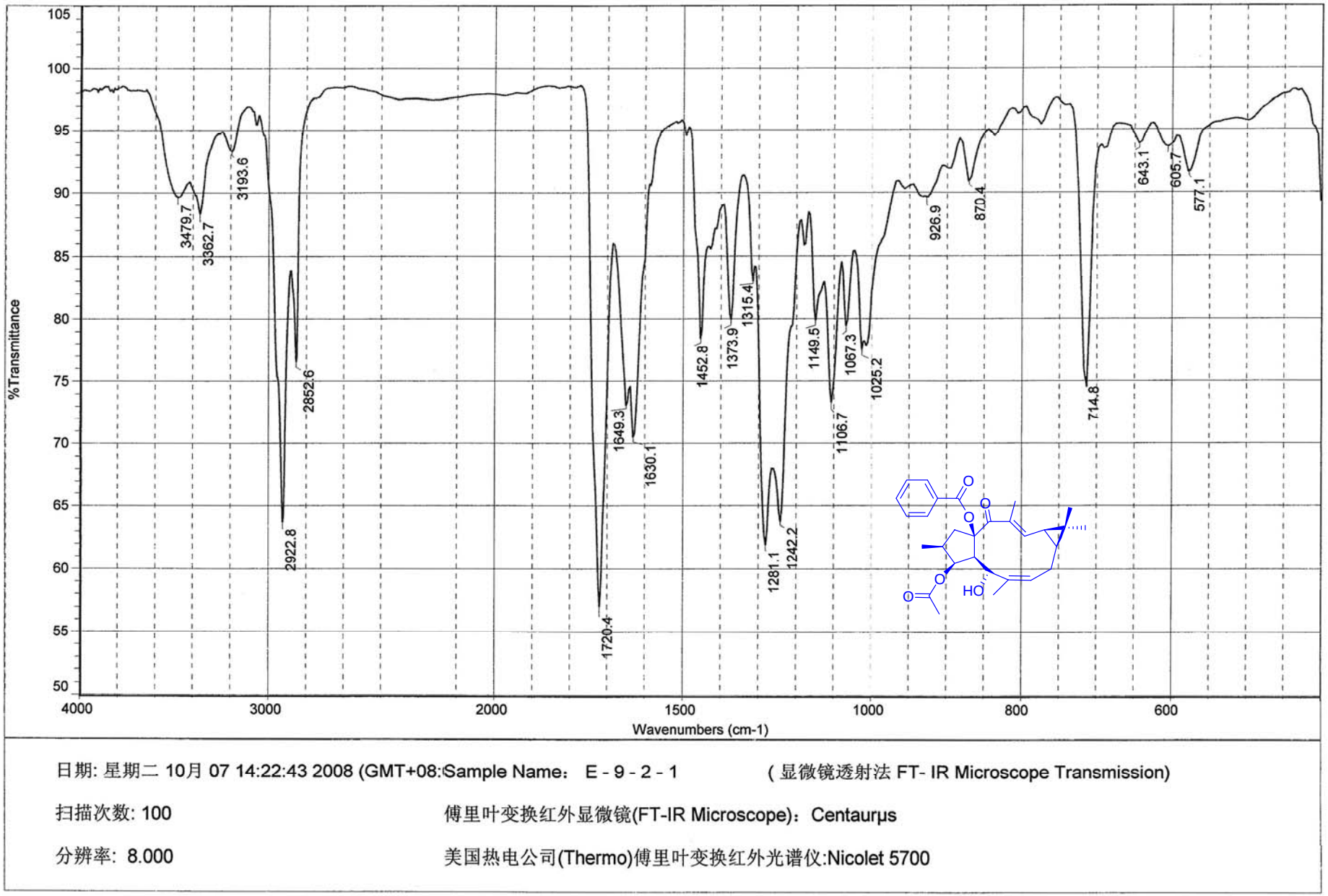

Figure S131. The IR Spectrum of 14.

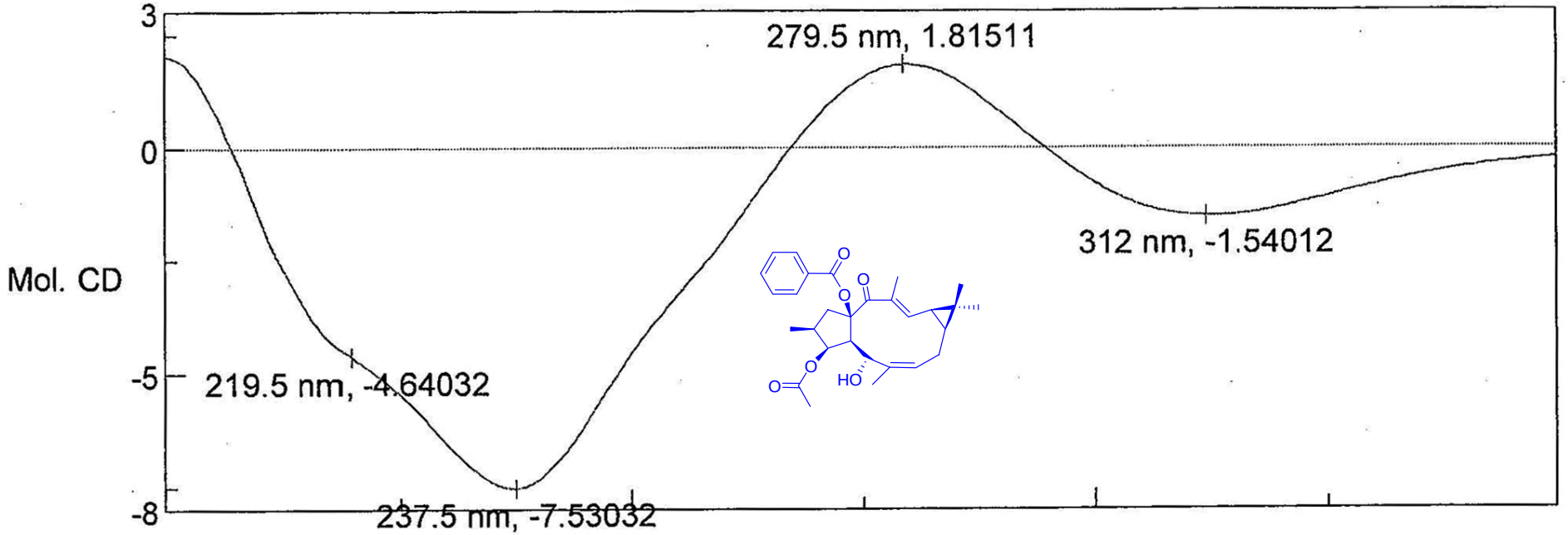

Figure S132. The CD Spectrum of 14.

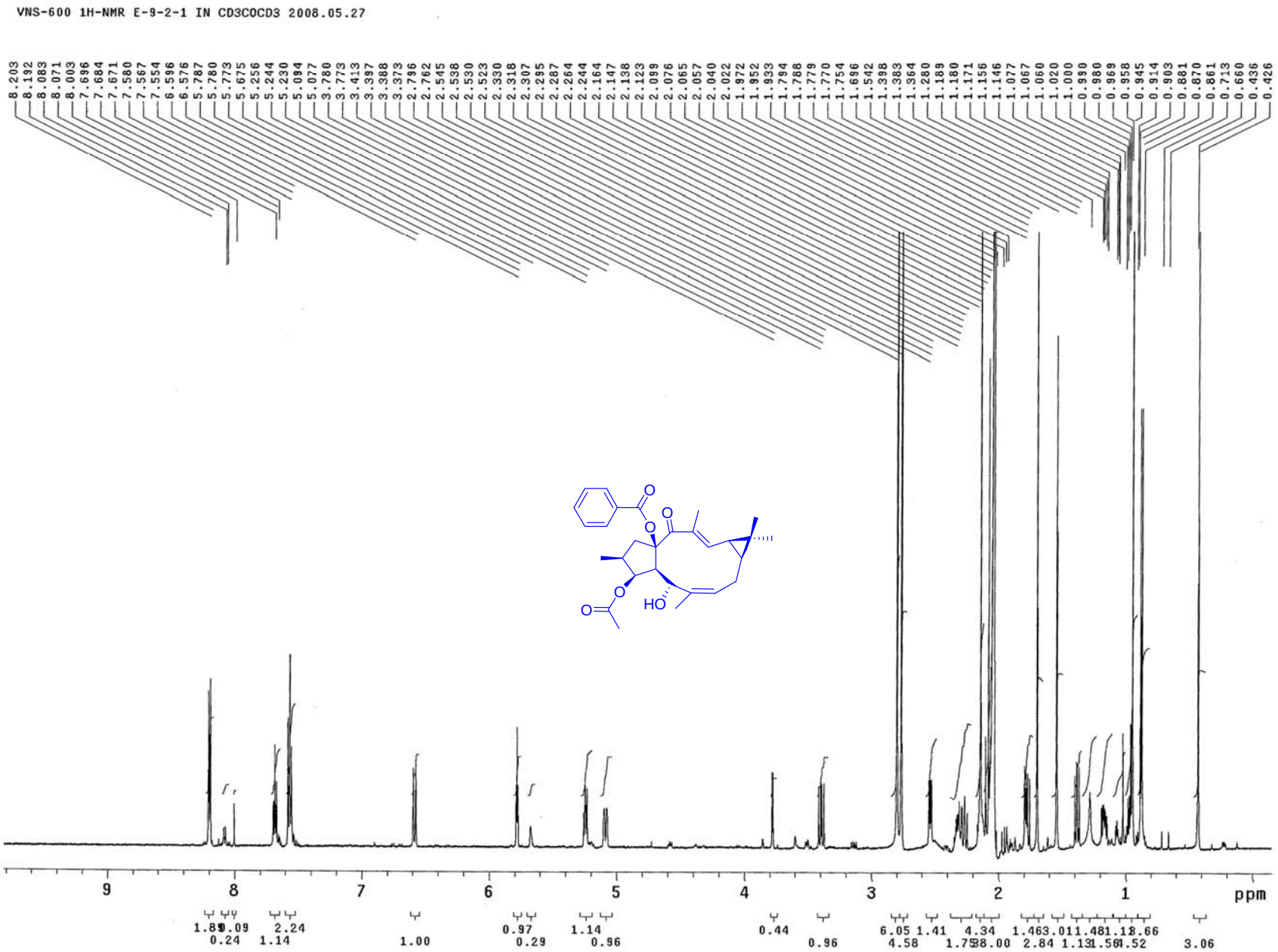

Figure S133. The ^{1}H NMR Spectrum of 14 in CD_3COCD_3 (600 MHz).

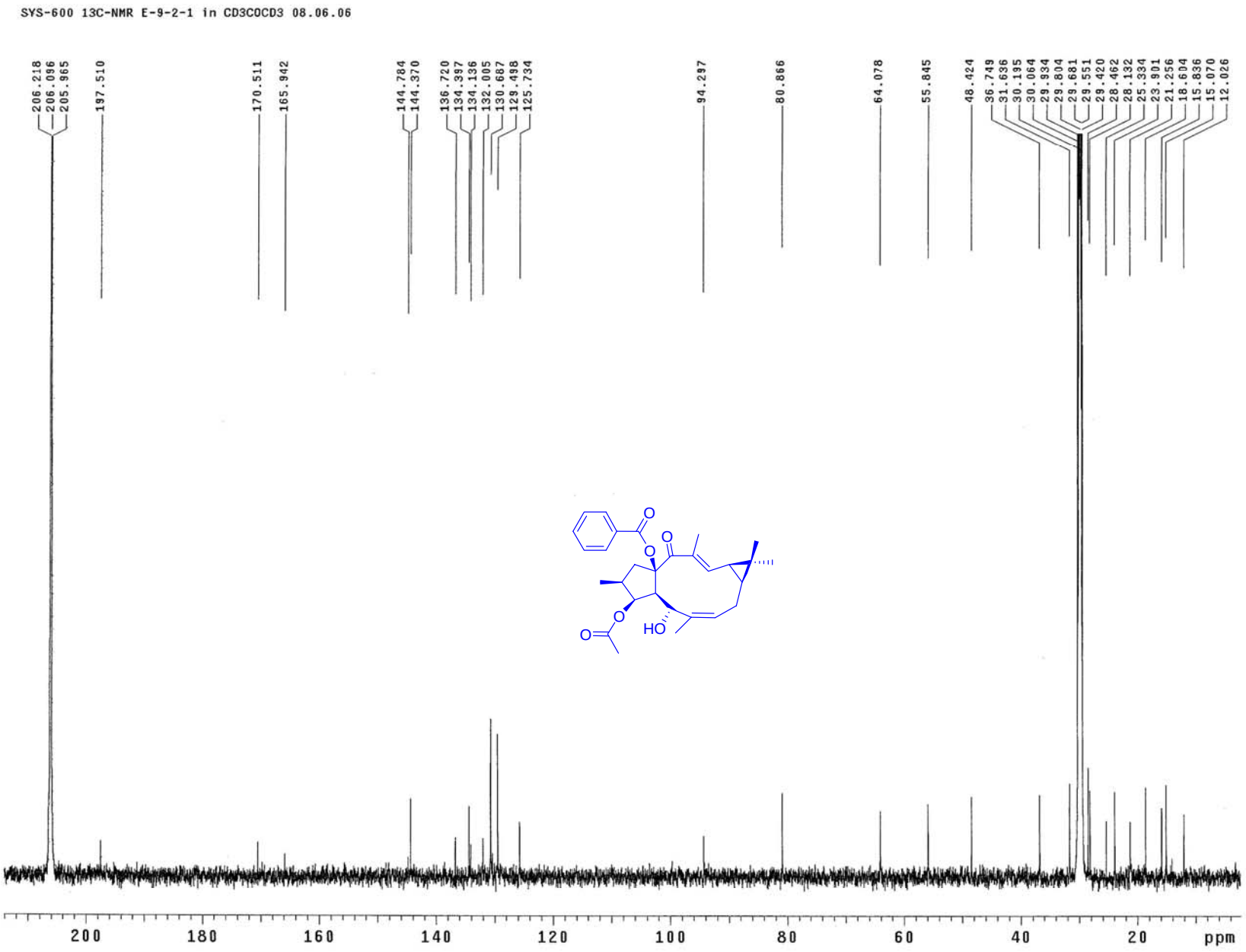

Figure S134. The ^{13}C NMR Spectrum of 14 in CD_3COCD_3 (150 MHz).

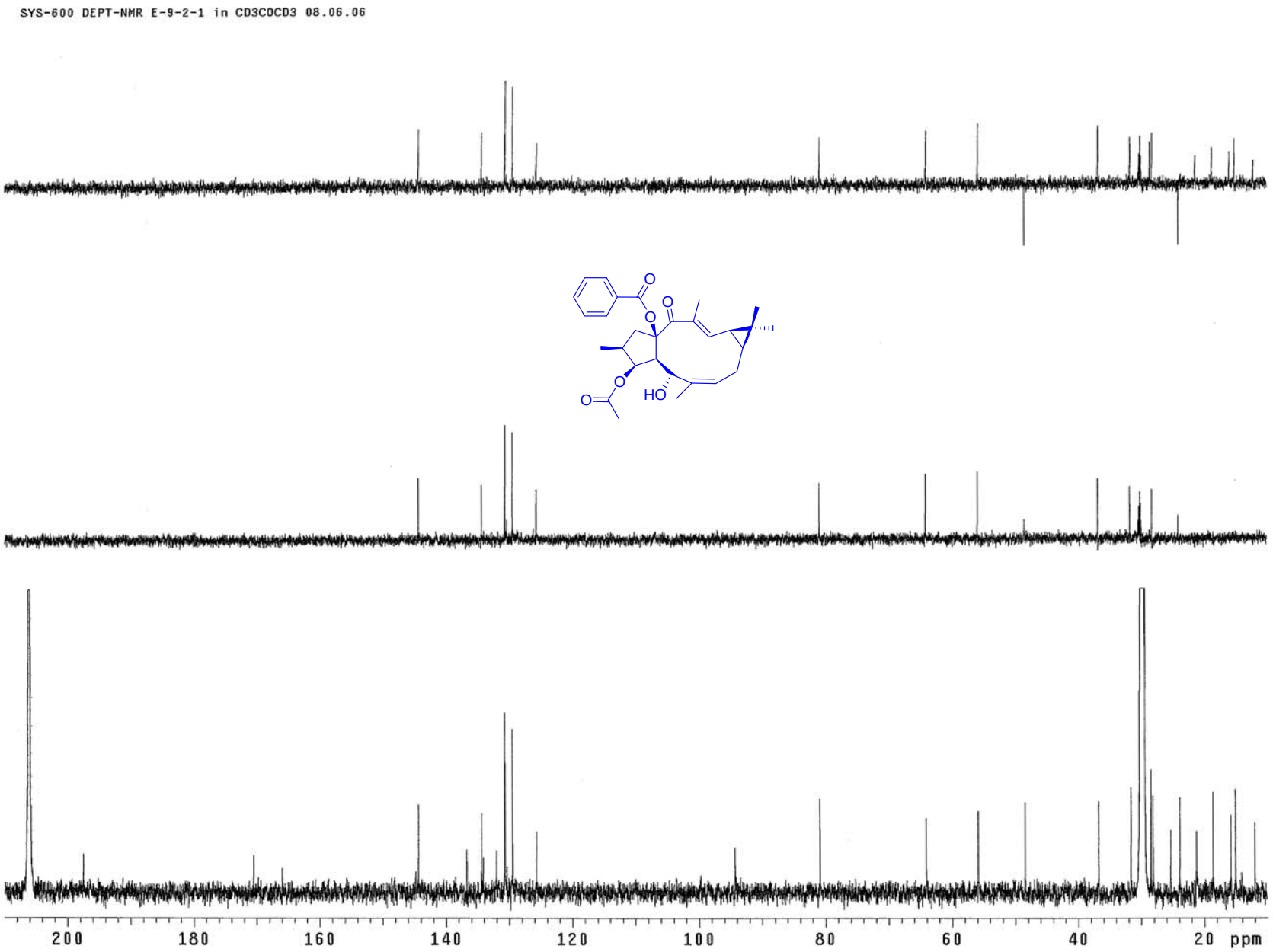

Figure S135. The DEPT Spectrum of 14 in CD_3COCD_3 (150 MHz).

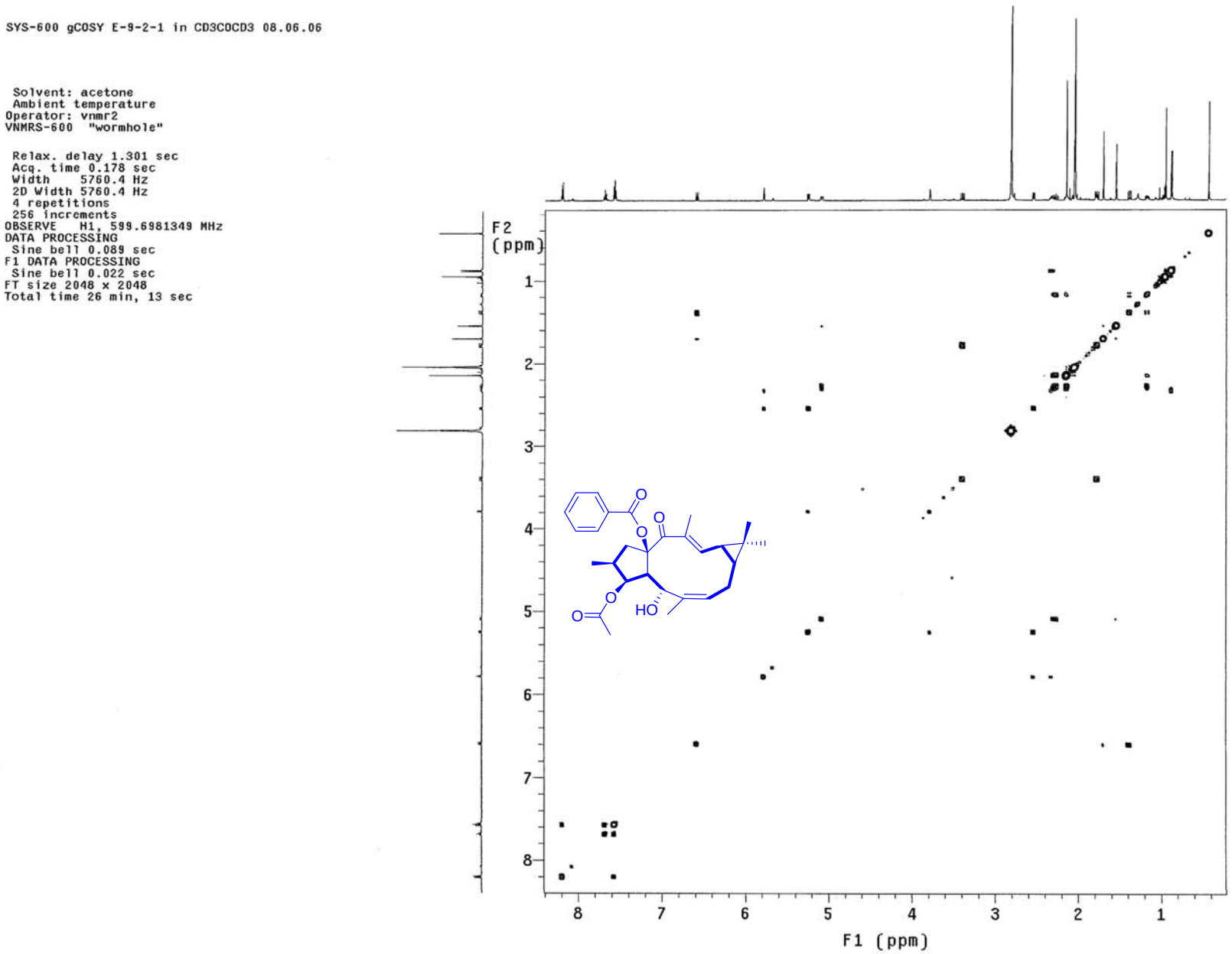

Figure S136. The ^{1}H-^{1}H gCOSY Spectrum of 14 in CD_3COCD_3 (600 MHz).

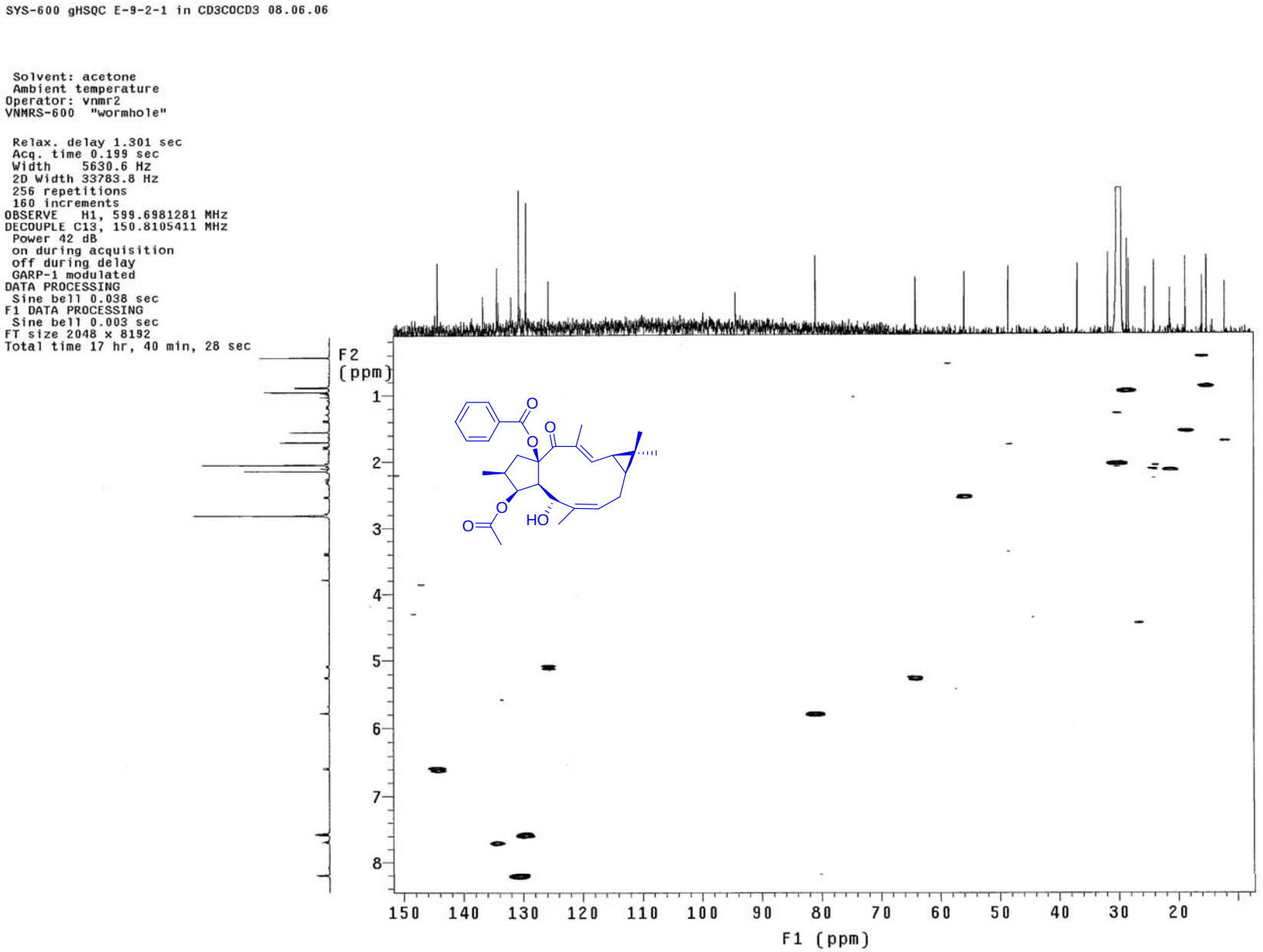

Figure S137. The gHSQC Spectrum of 14 in CD_3COCD_3 (600MHz for ^1H NMR).

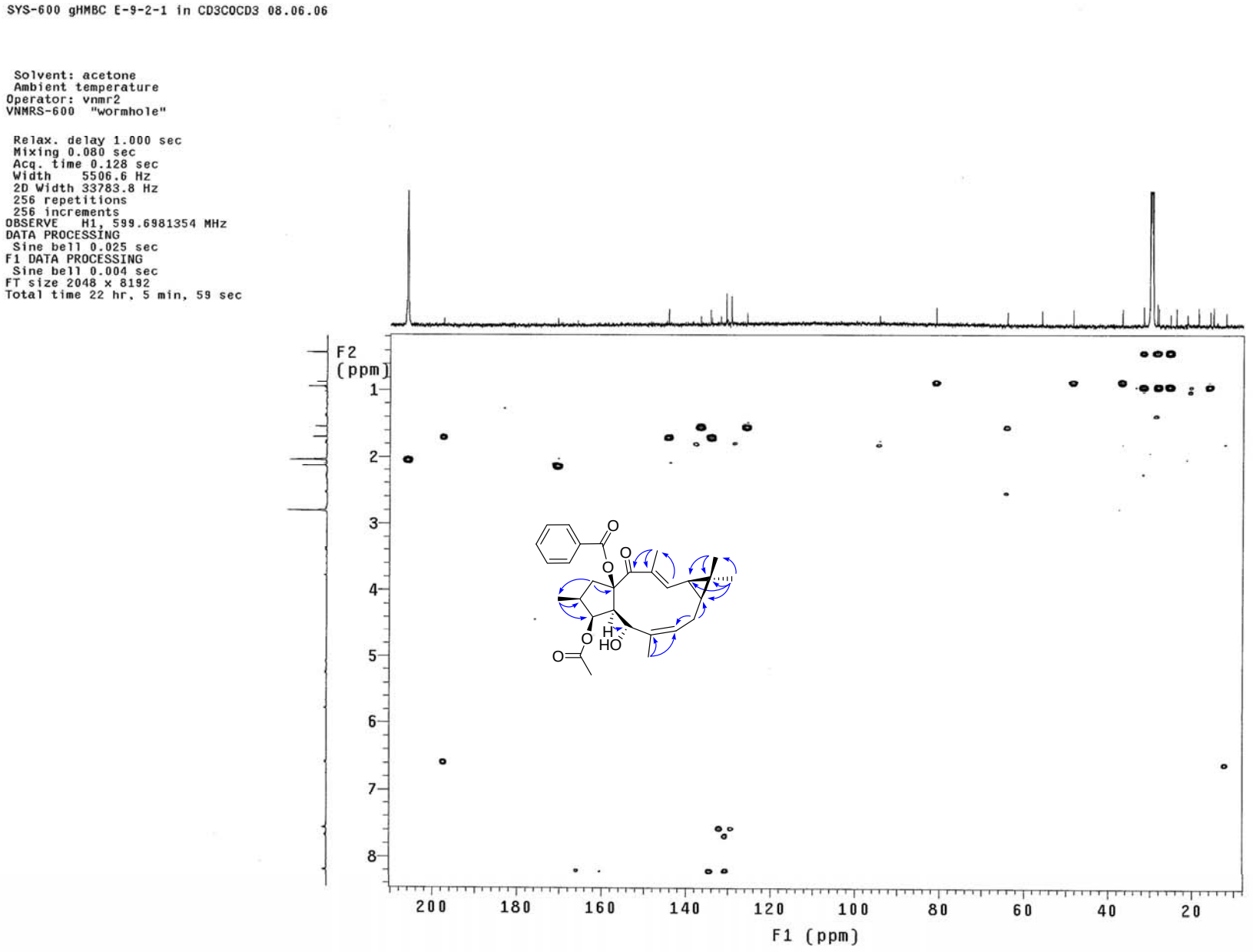

Figure S138. The gHMBC Spectrum of 14 in CD_3COCD_3 (600MHz for ^1H NMR).

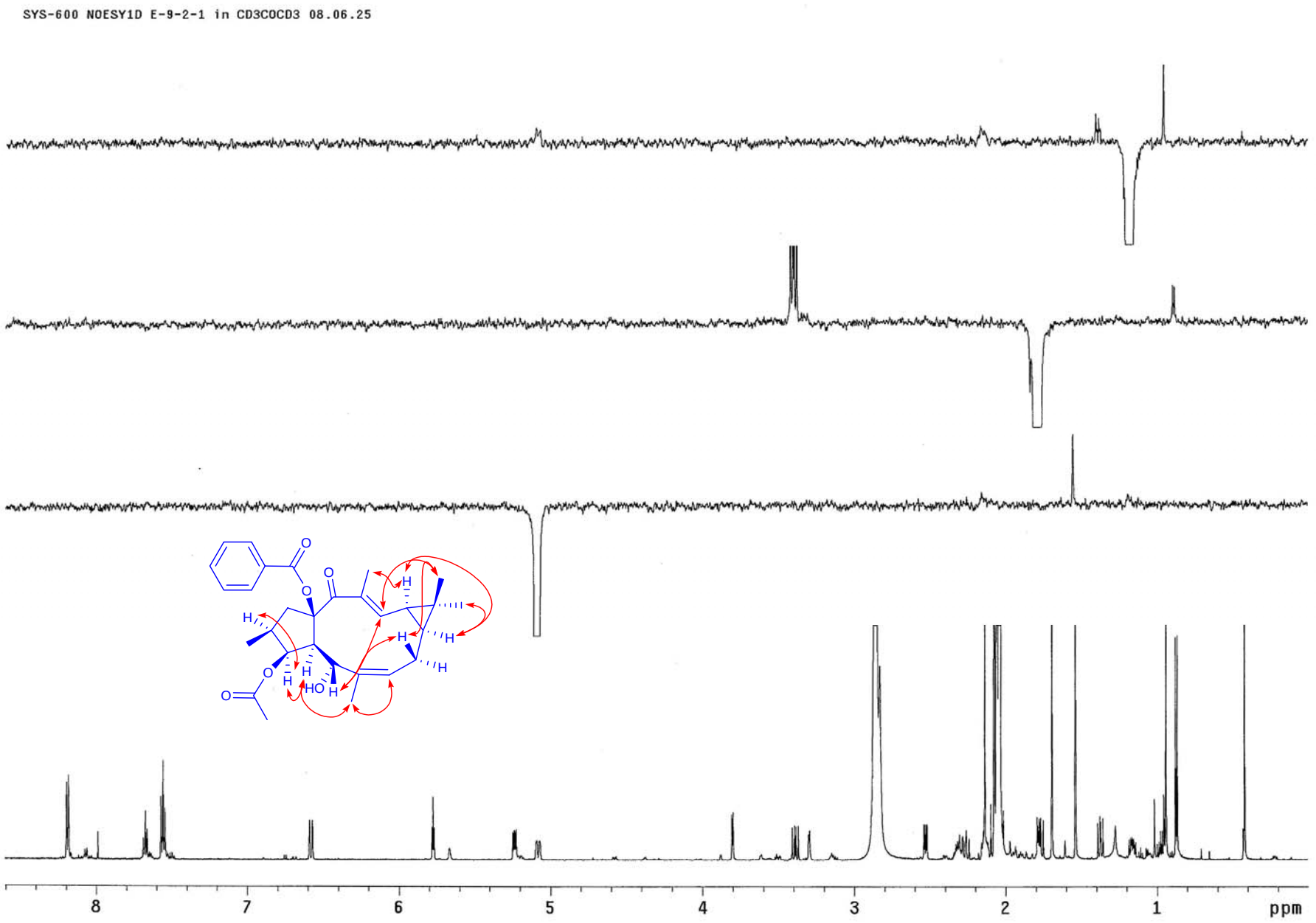

Figure S139. The NOE Difference Spectrum 1 of 14 in CD_3COCD_3 (600 MHz).

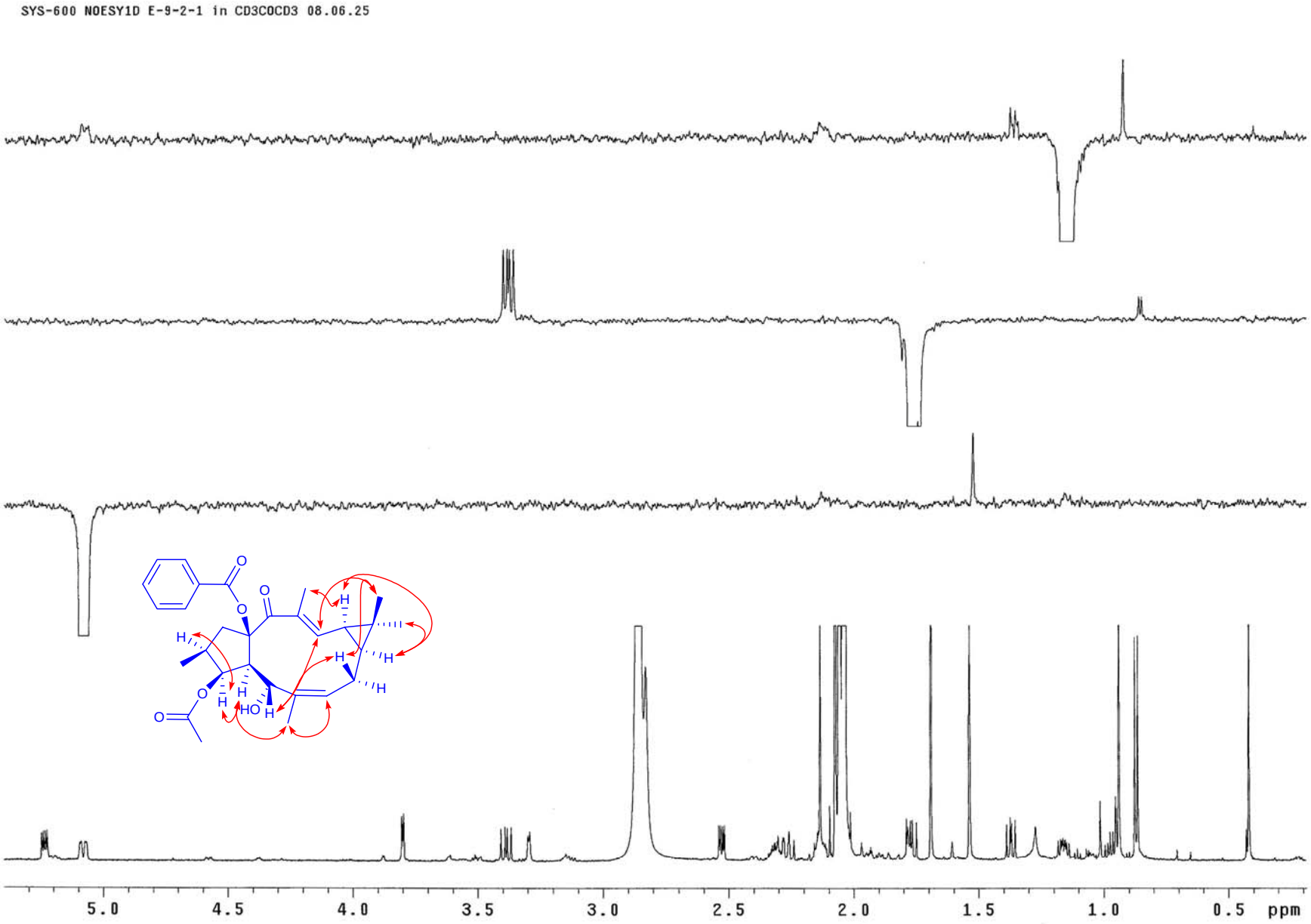

Figure S140. The NOE Difference Spectrum 2 of 14 in CD_3COCD_3 (600 MHz).

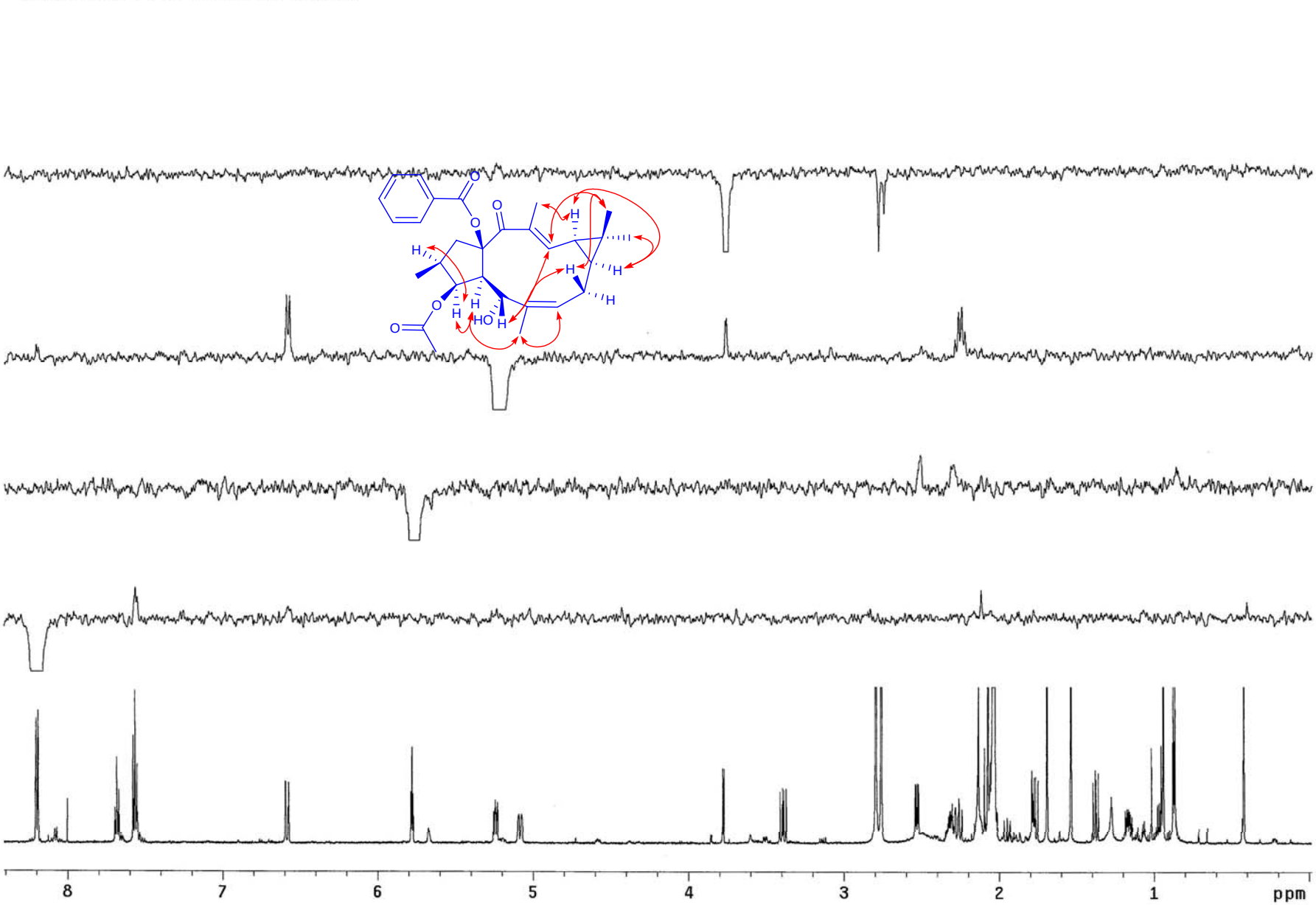

Figure S141. The NOE Difference Spectrum 3 of 14 in CD_3COCD_3 (600 MHz).

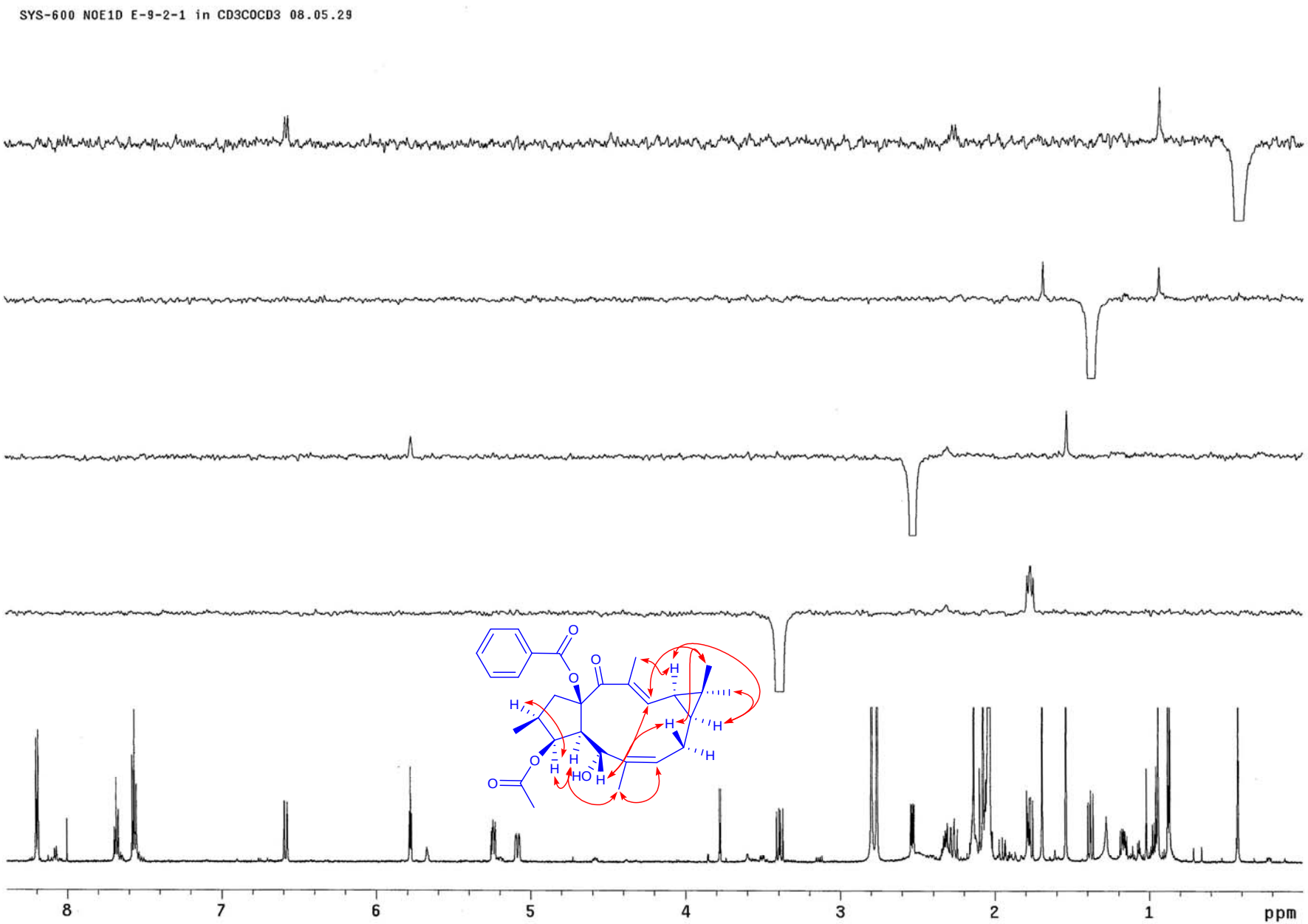

Figure S142. The NOE Difference Spectrum 4 of 14 in CD_3COCD_3 (600 MHz).

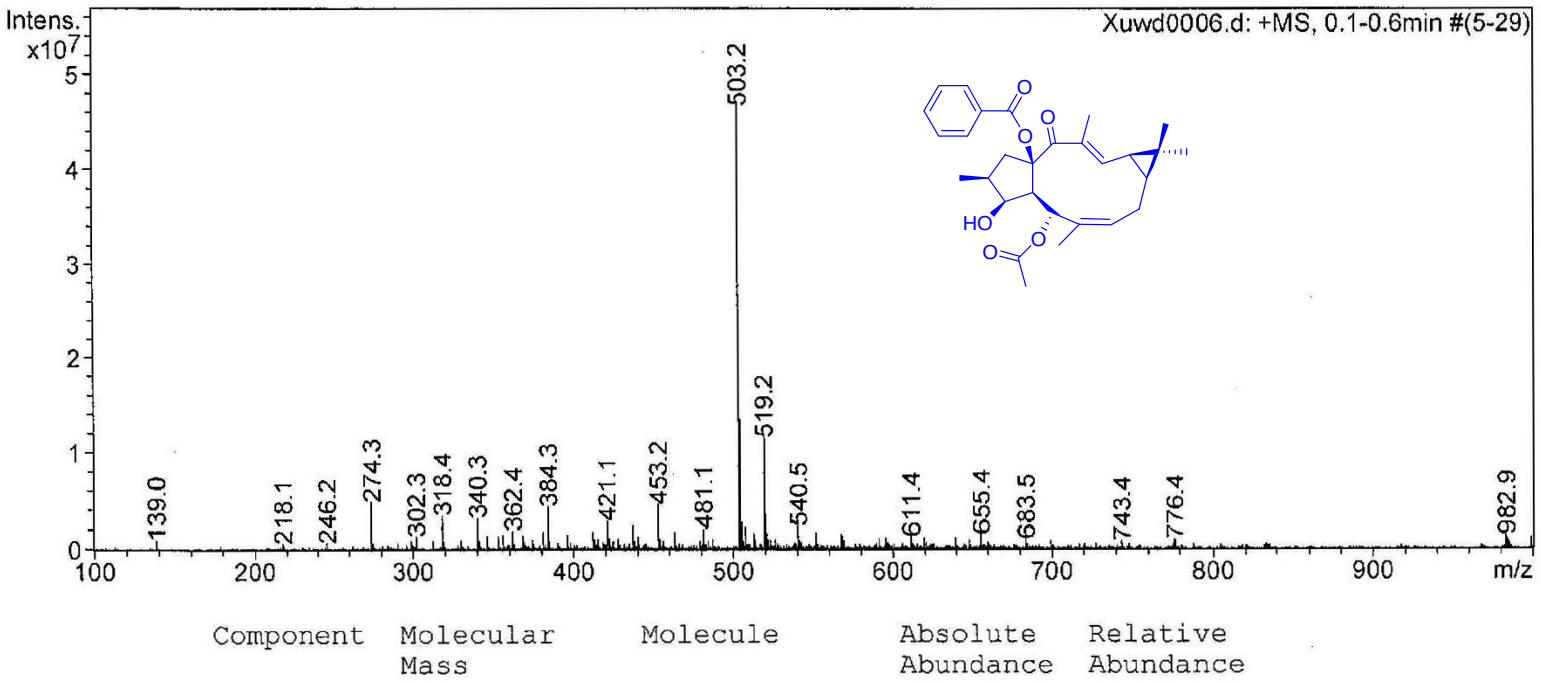

Figure S143. (+)-ESIMS Spectrum of 15.

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

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

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.

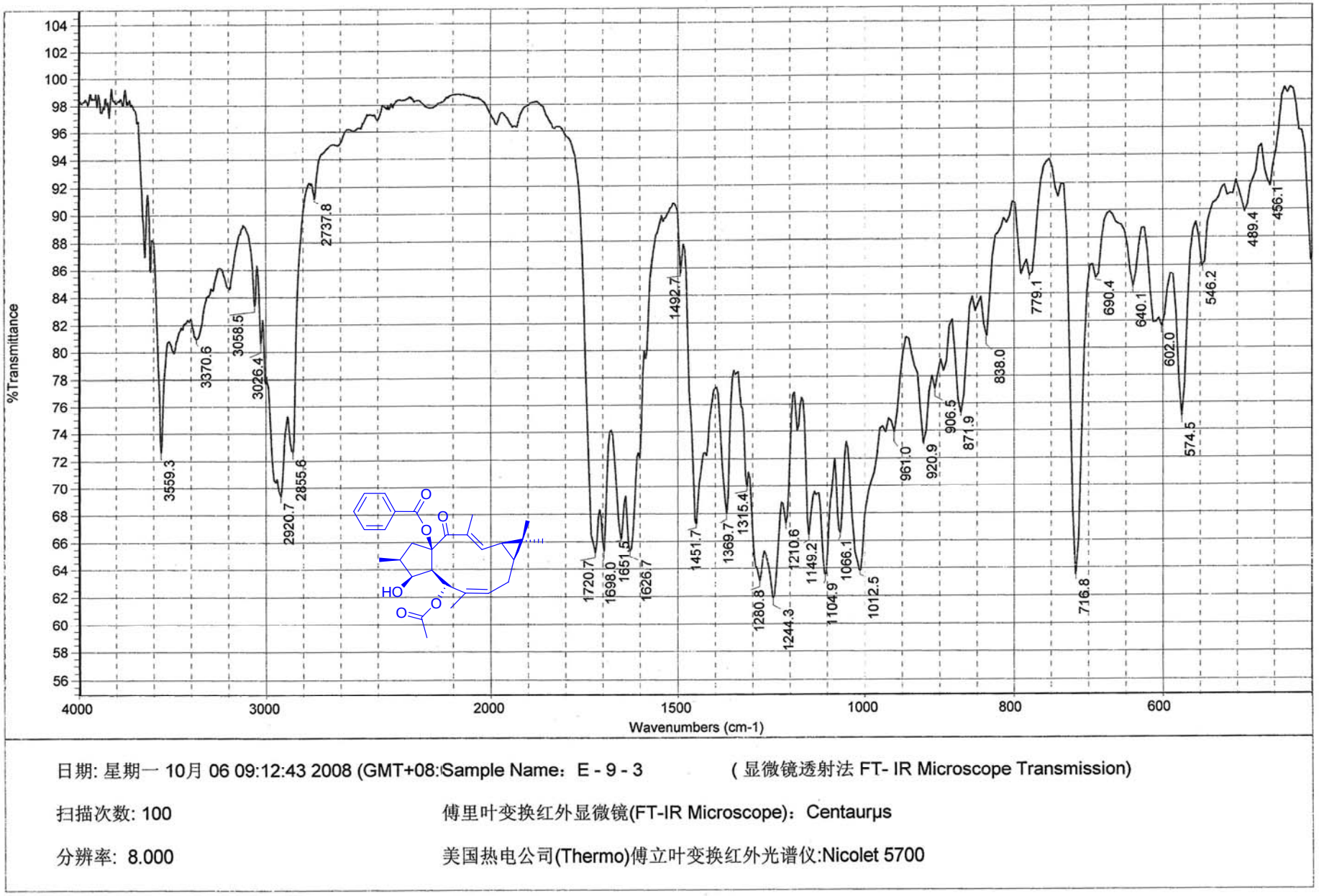

Figure S144. The IR Spectrum of 15.

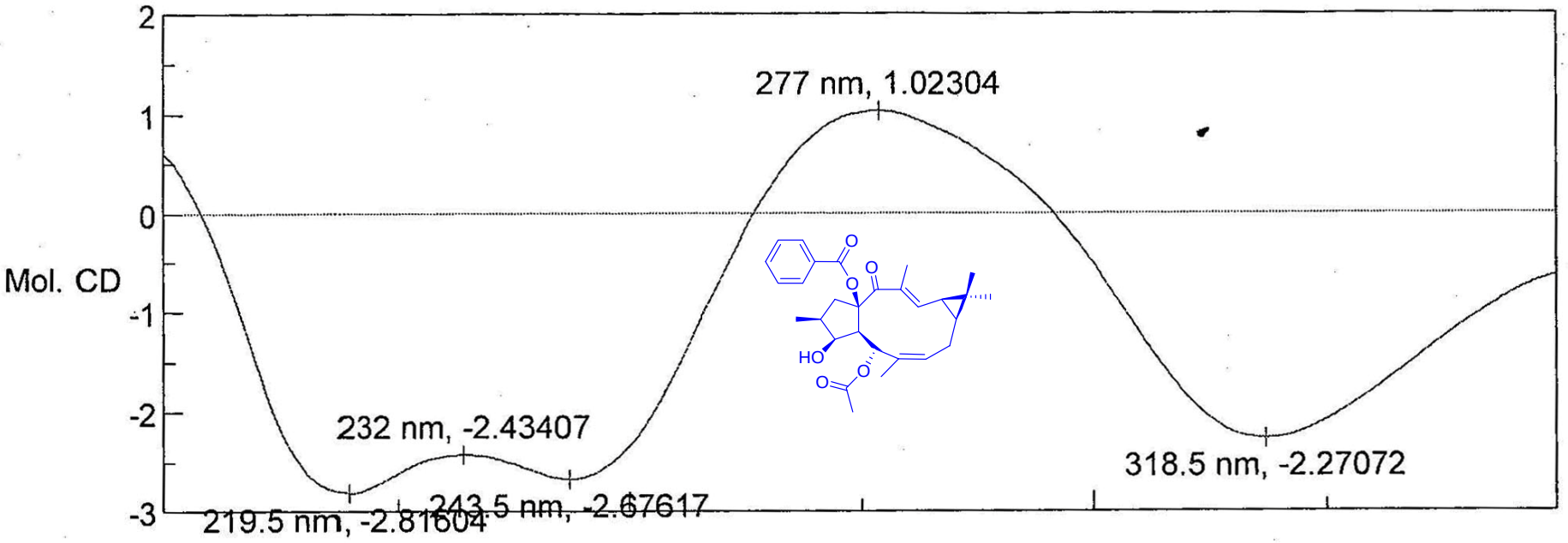

Figure S145. The CD Spectrum of 15.

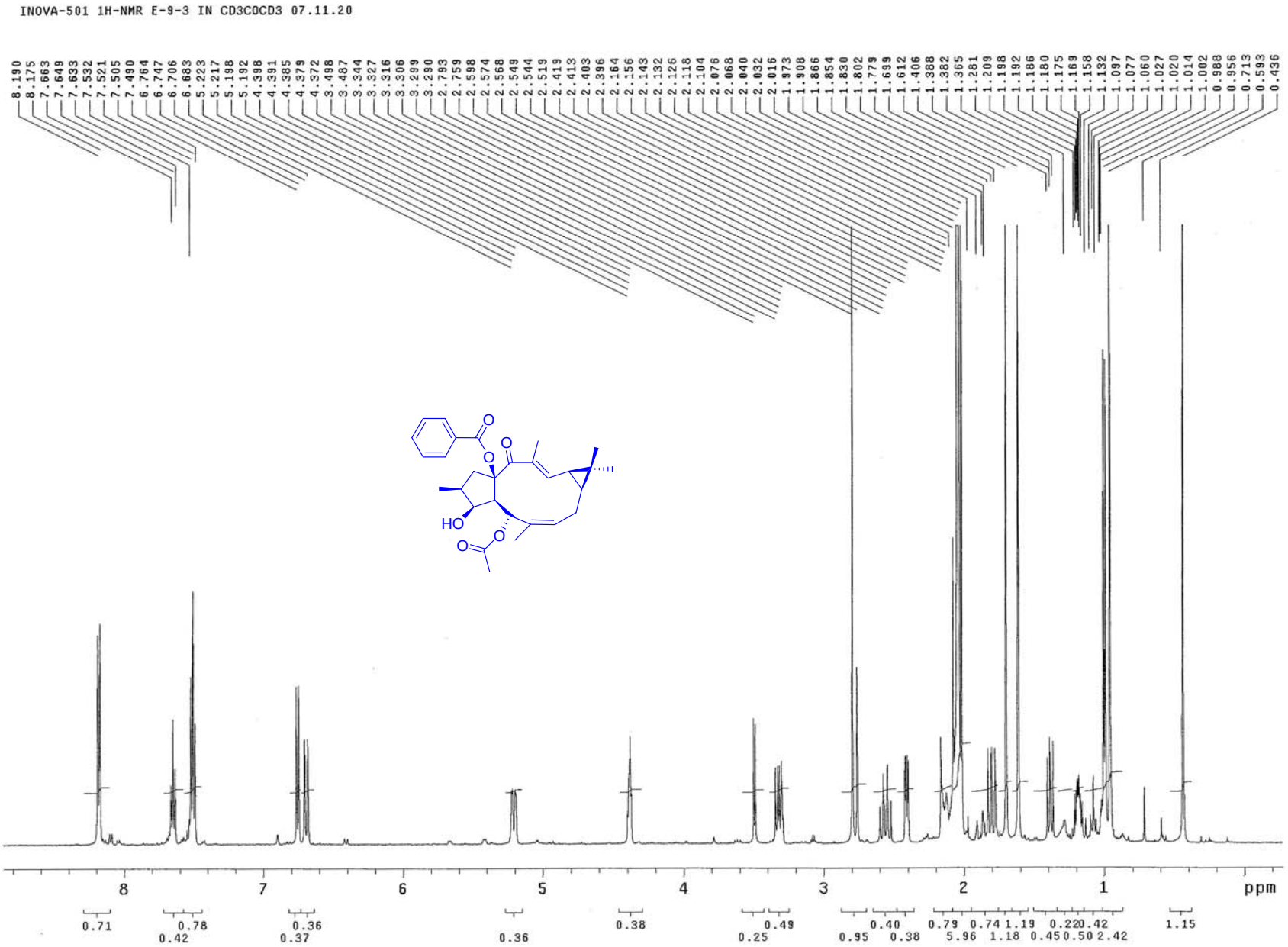

Figure S146. The ^{1}H NMR Spectrum of 15 in CD_3COCD_3 (500 MHz).

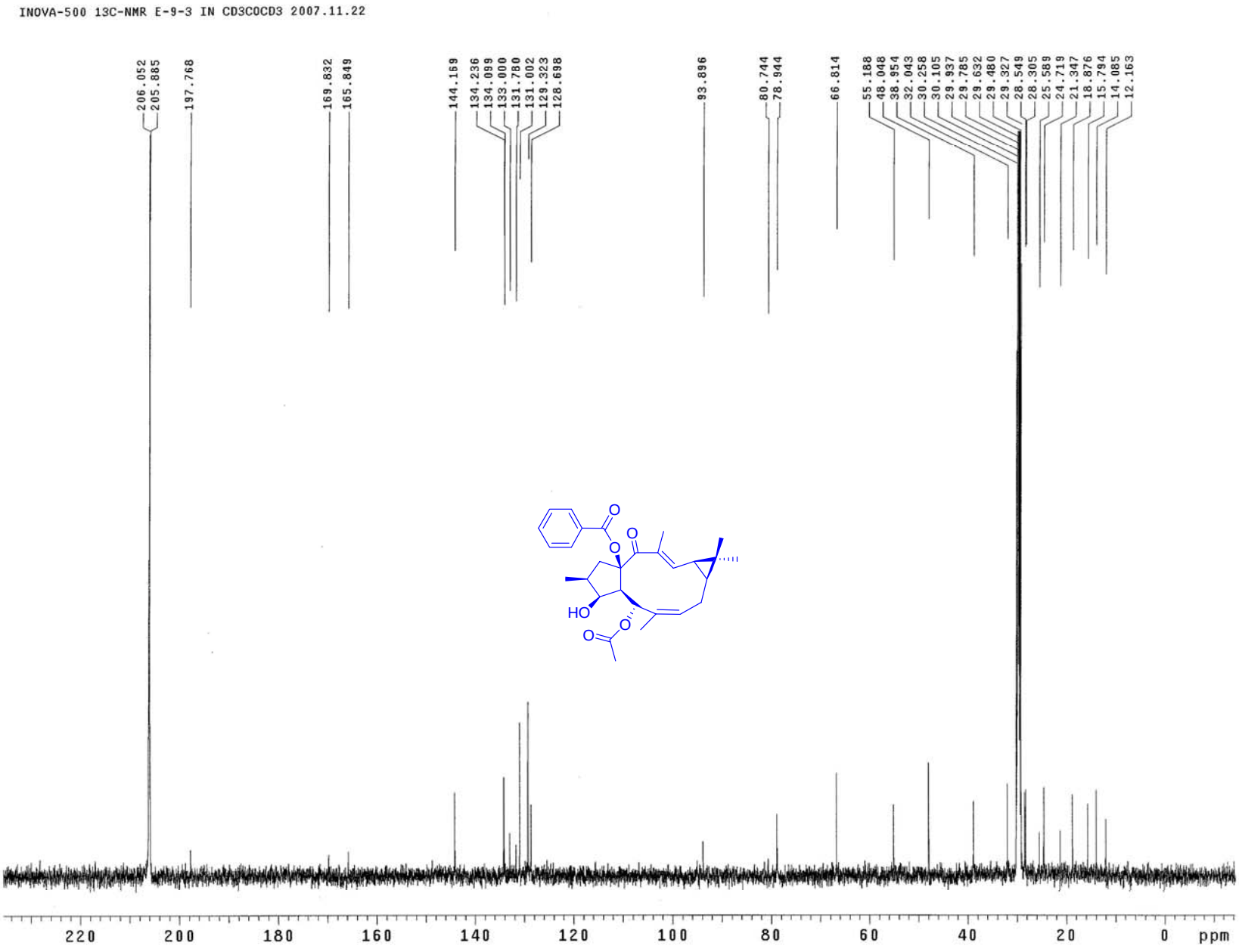

Figure S147. The ^{13}C NMR Spectrum of 15 in CD_3COCD_3 (125 MHz).

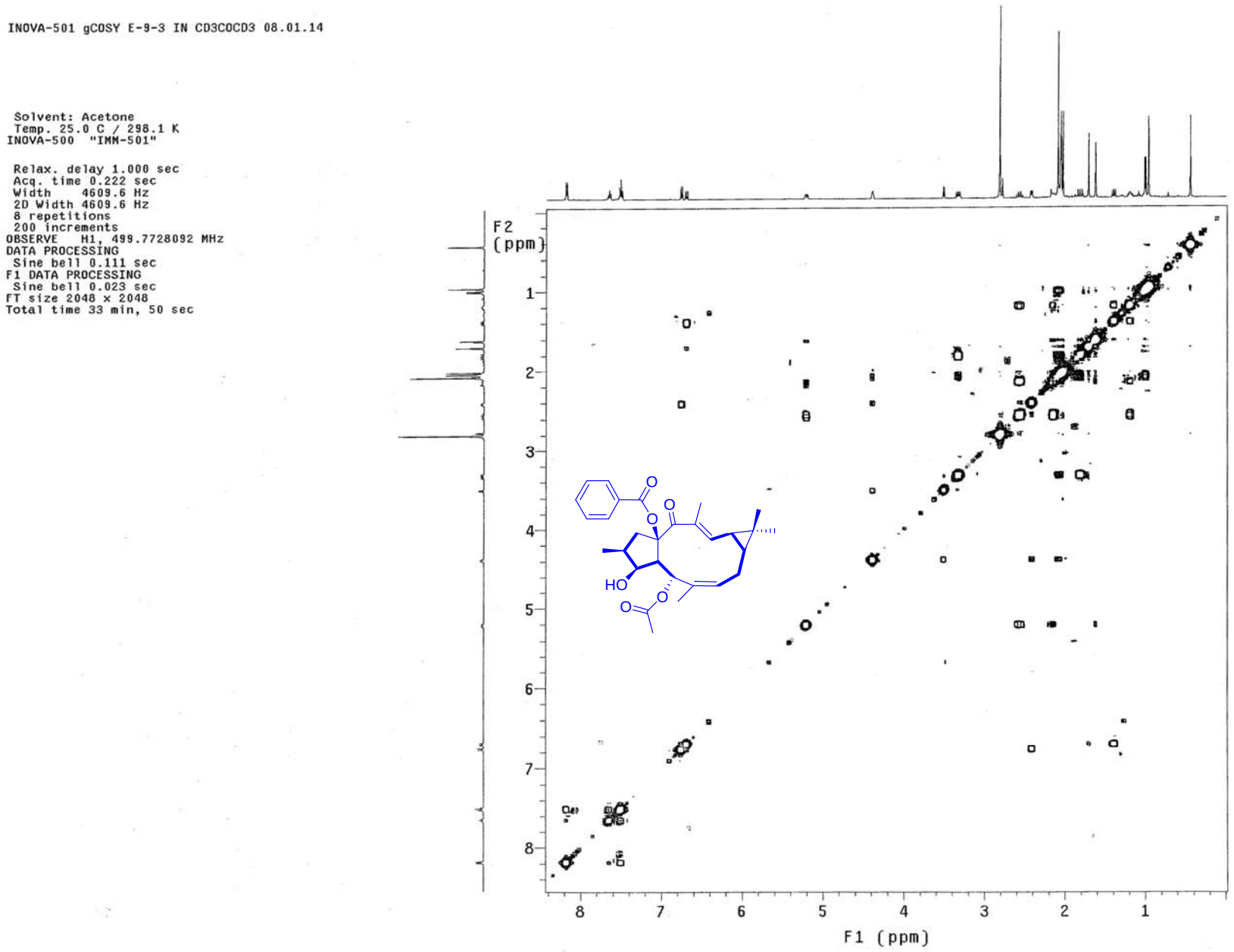

Figure S148. The ^{1}H-^{1}H gCOSY Spectrum of 15 in CD_3COCD_3 (500 MHz).

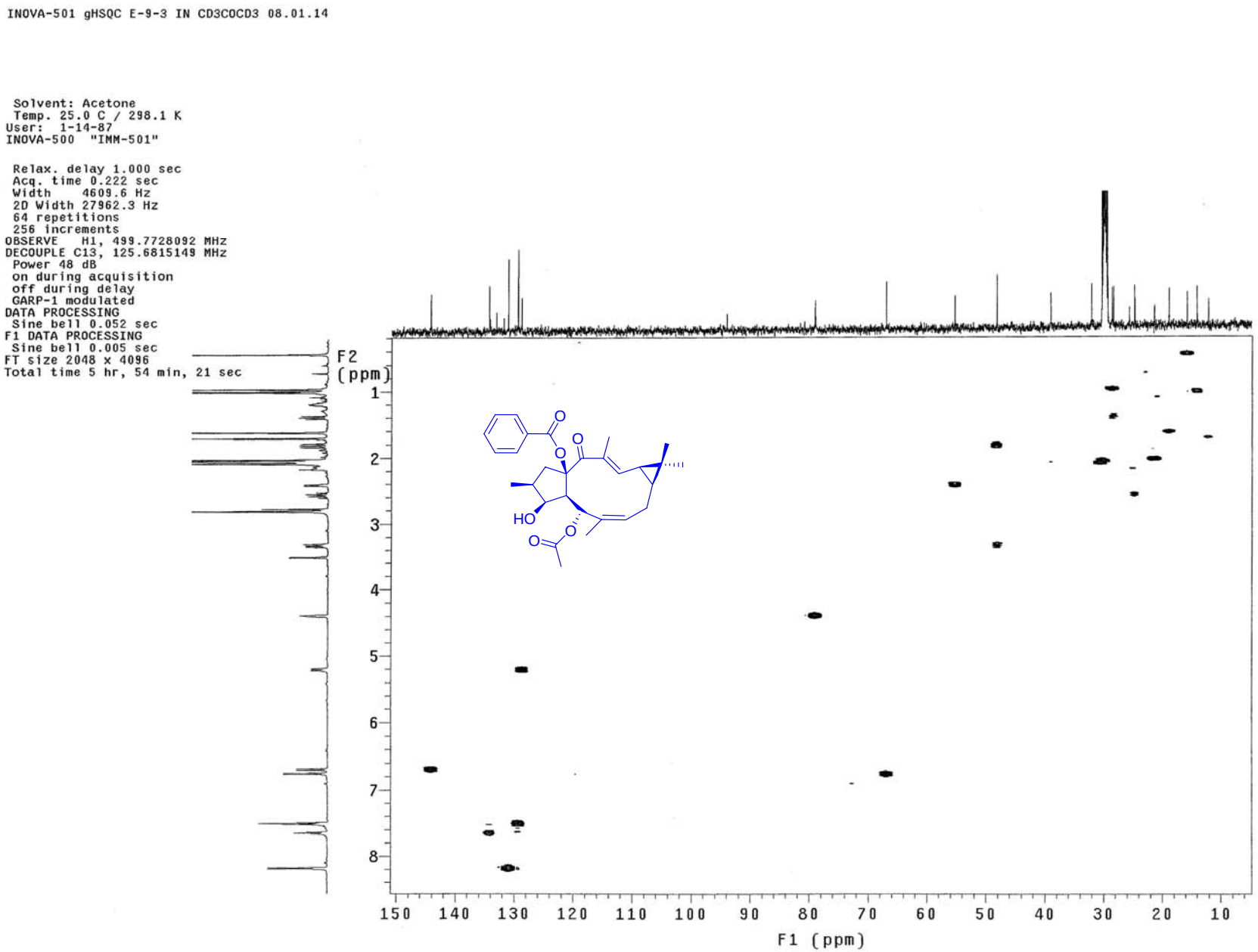

Figure S149. The gHSQC Spectrum of 15 in CD_3COCD_3 (500MHz for ^1H NMR).

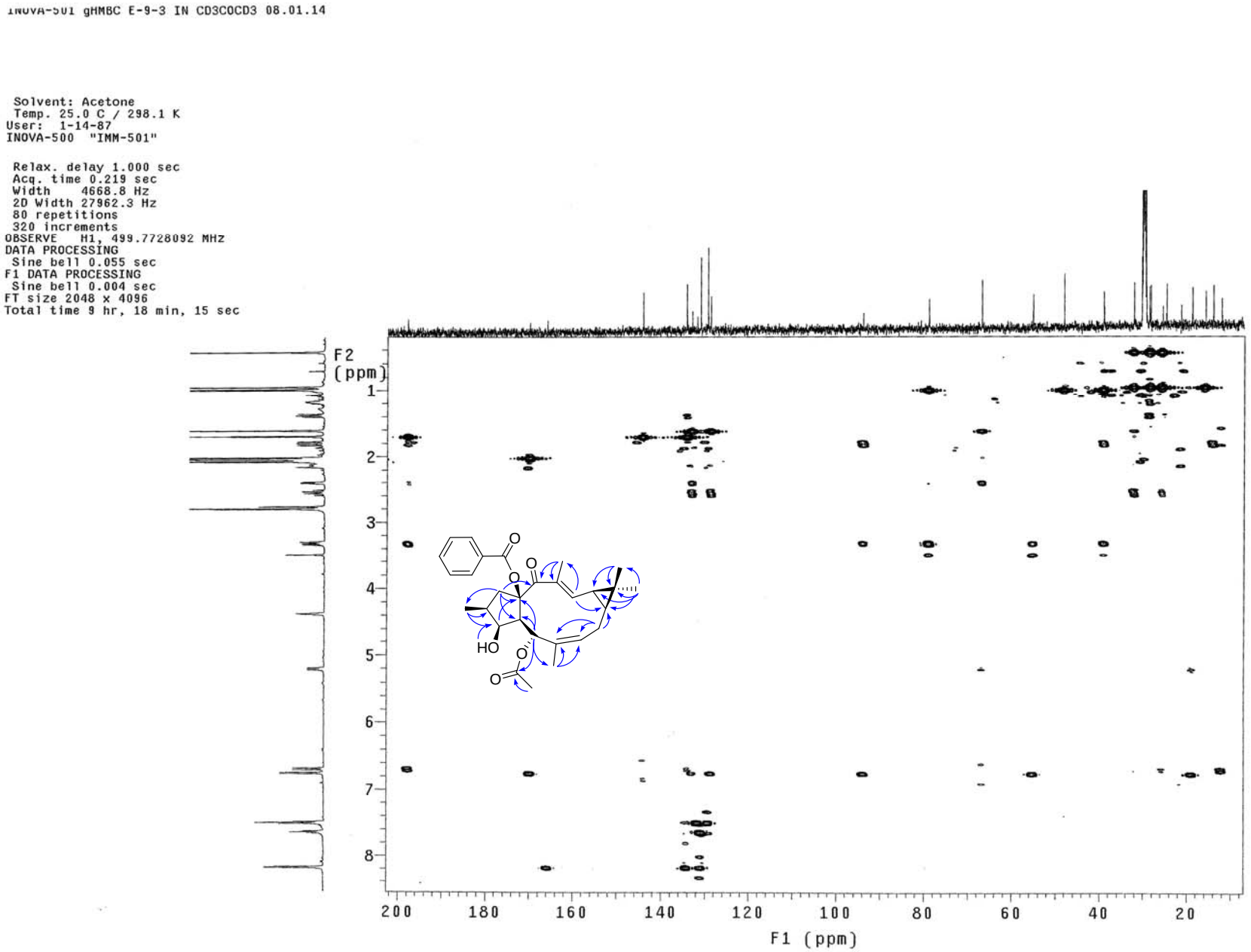

Figure S150. The gHMBC Spectrum of 15 in CD_3COCD_3 (500MHz for ^1H NMR).

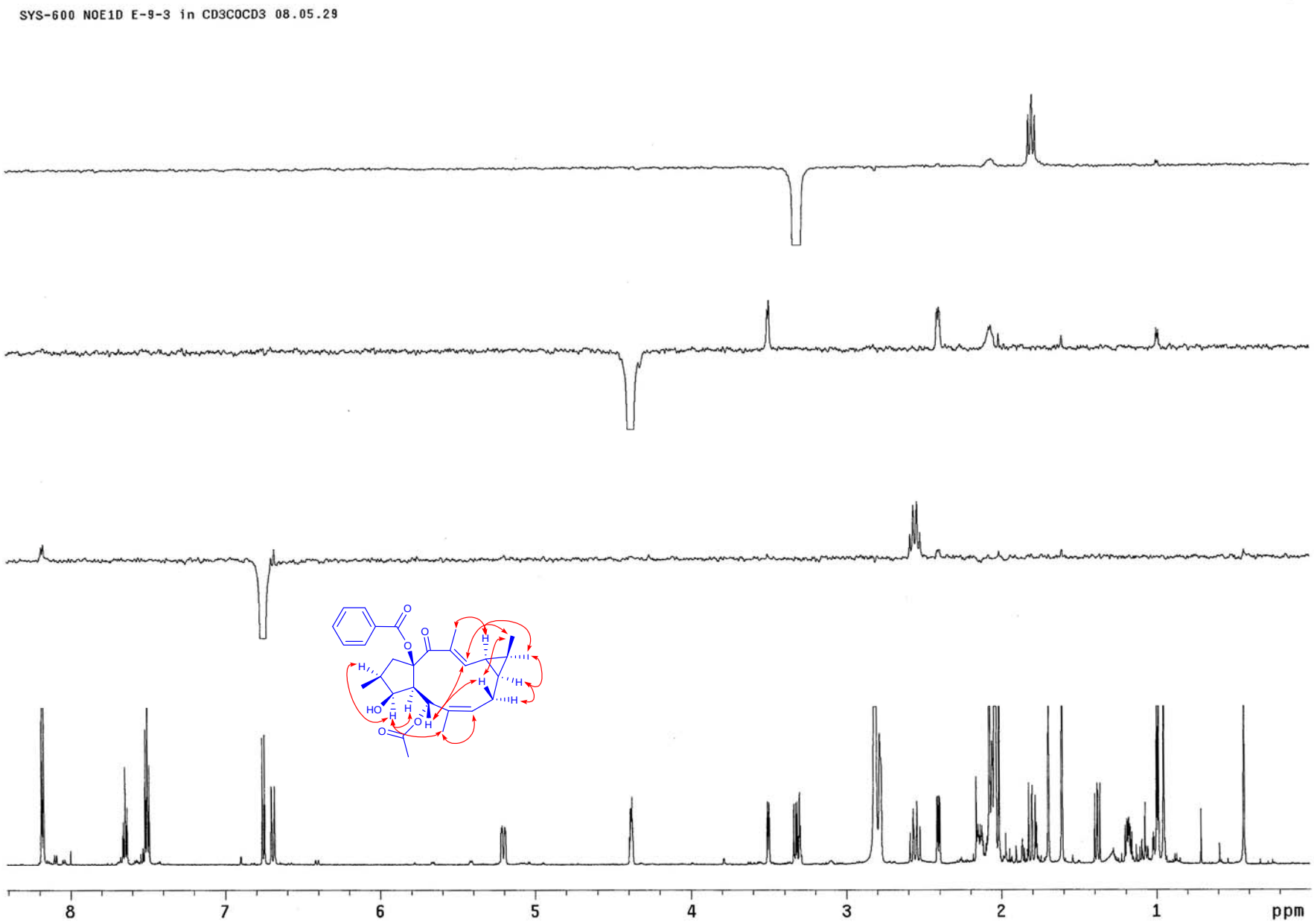

Figure S151. The NOE Difference Spectrum 1 of 15 in CD_3COCD_3 (600 MHz).

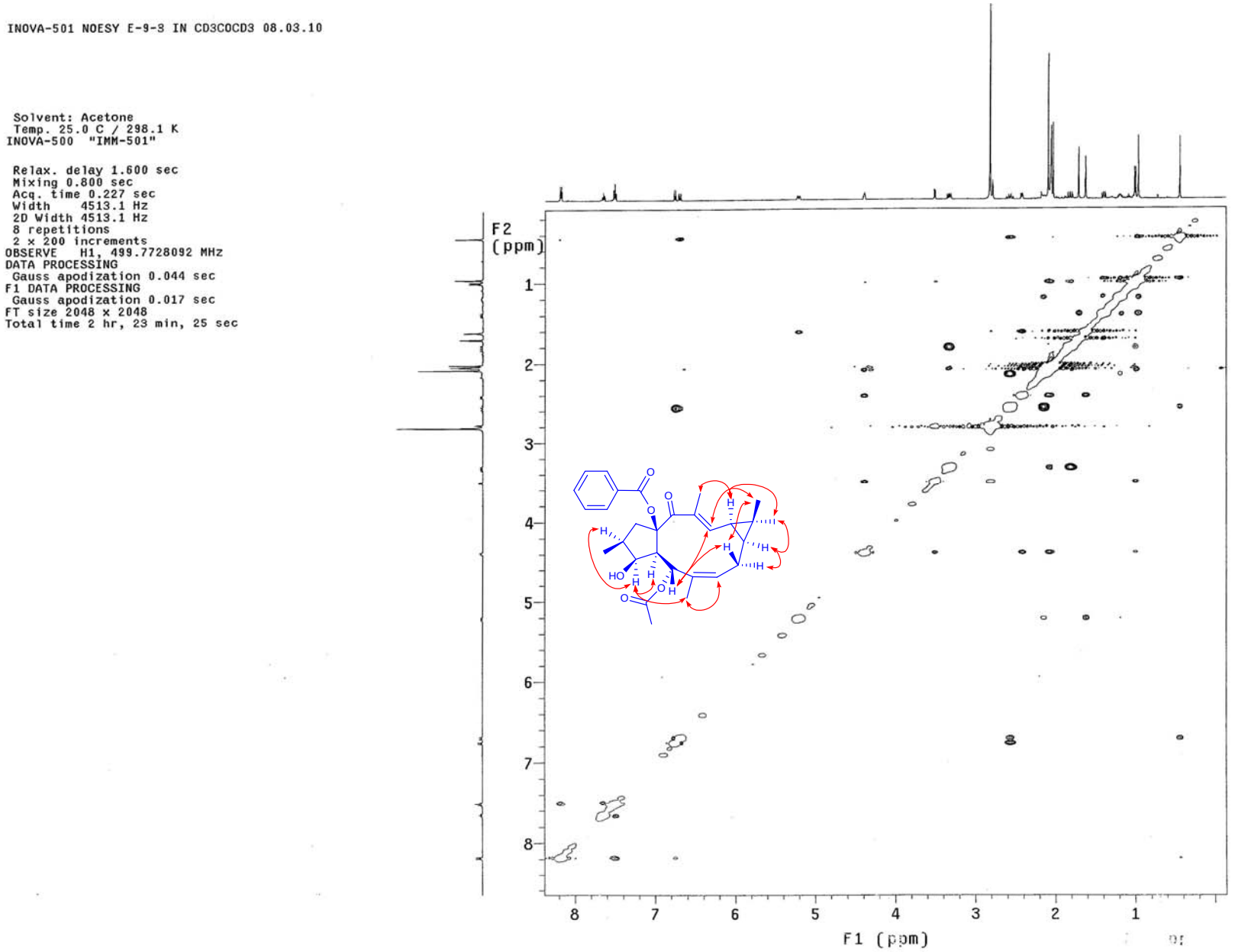

Figure S152. The NOESY Spectrum of 15 in CD_3COCD_3 (500 MHz).

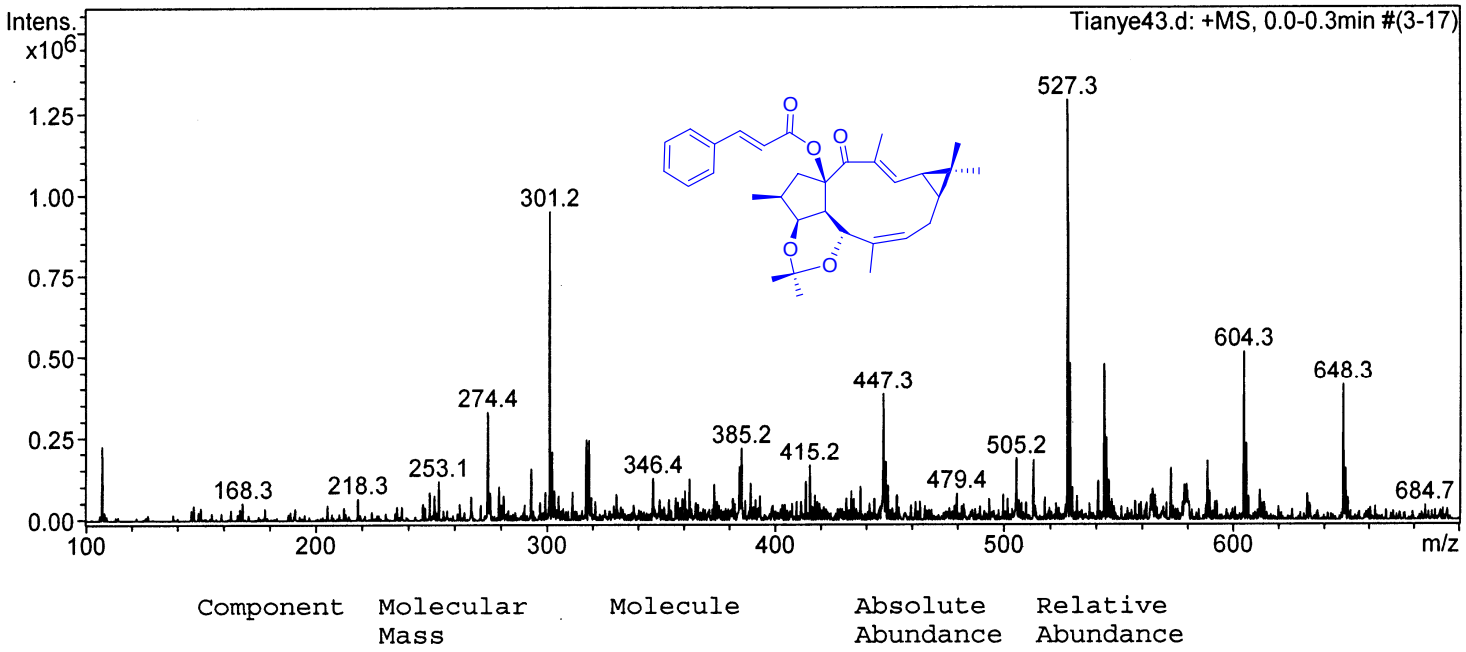

Figure S153. The (+)-ESIMS Spectrum of 16.

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.

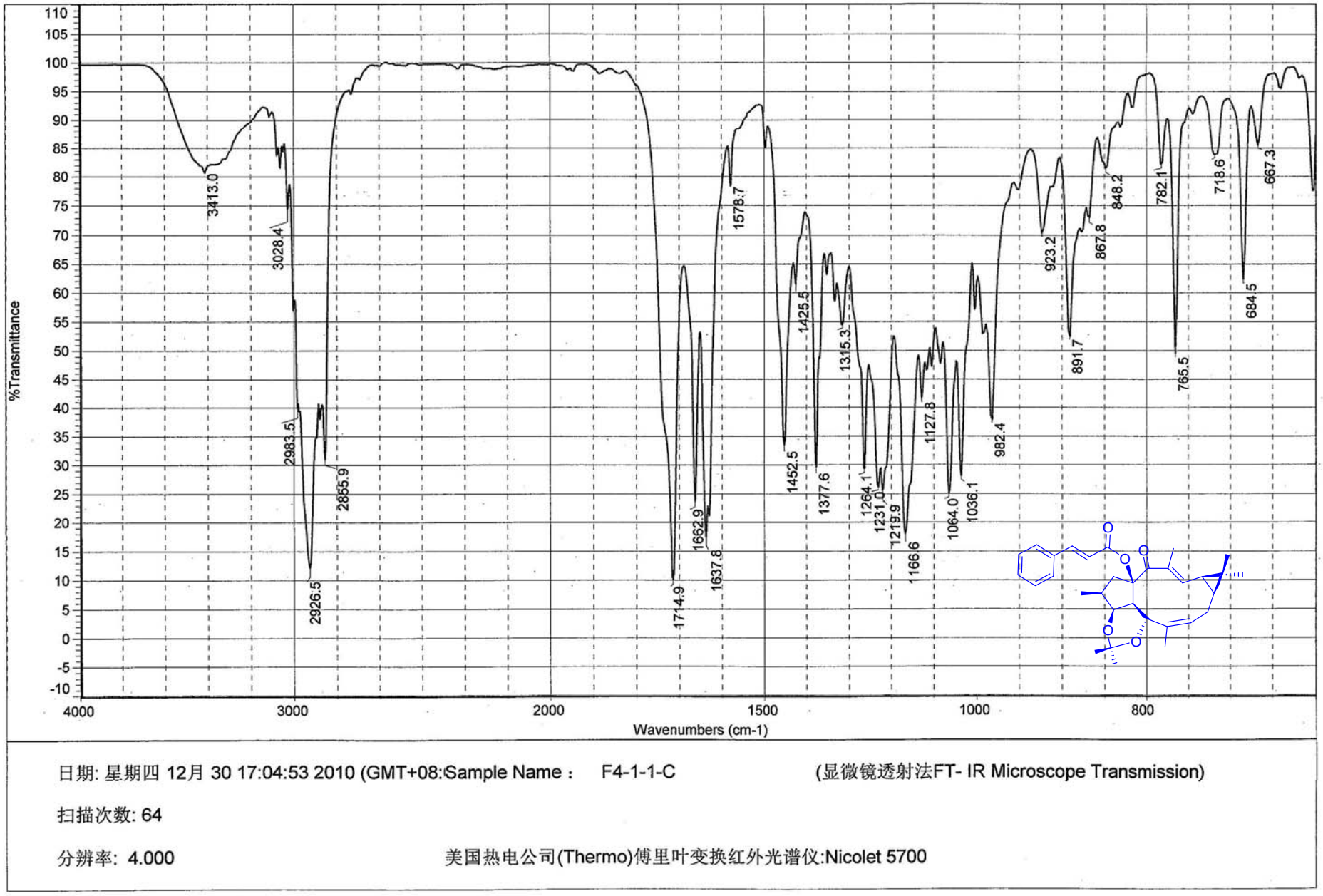

Figure S154. The IR Spectrum of 16.

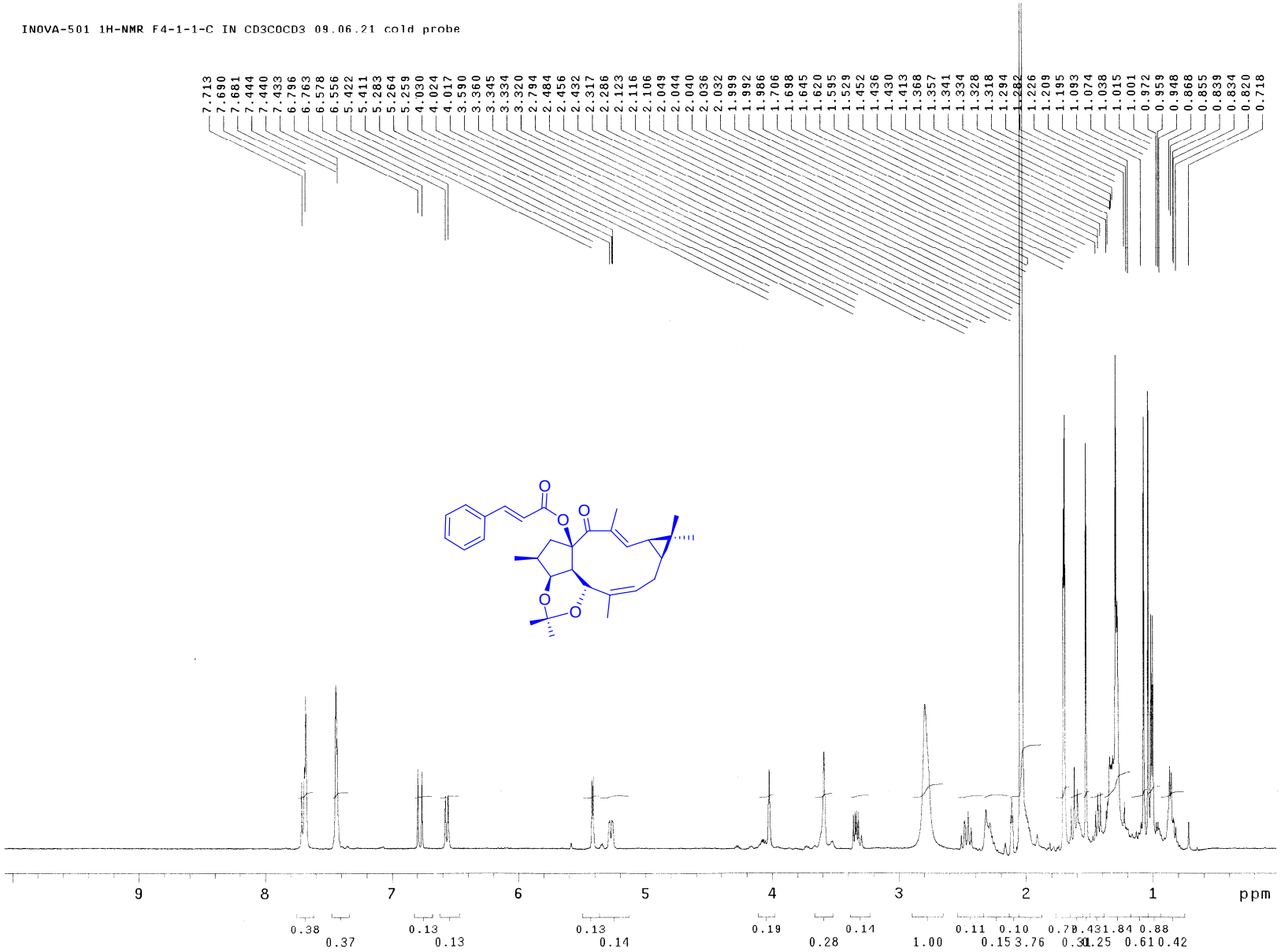

Figure S155. The ^{1}H NMR Spectrum of 16 in CD_3COCD_3 (500 MHz).

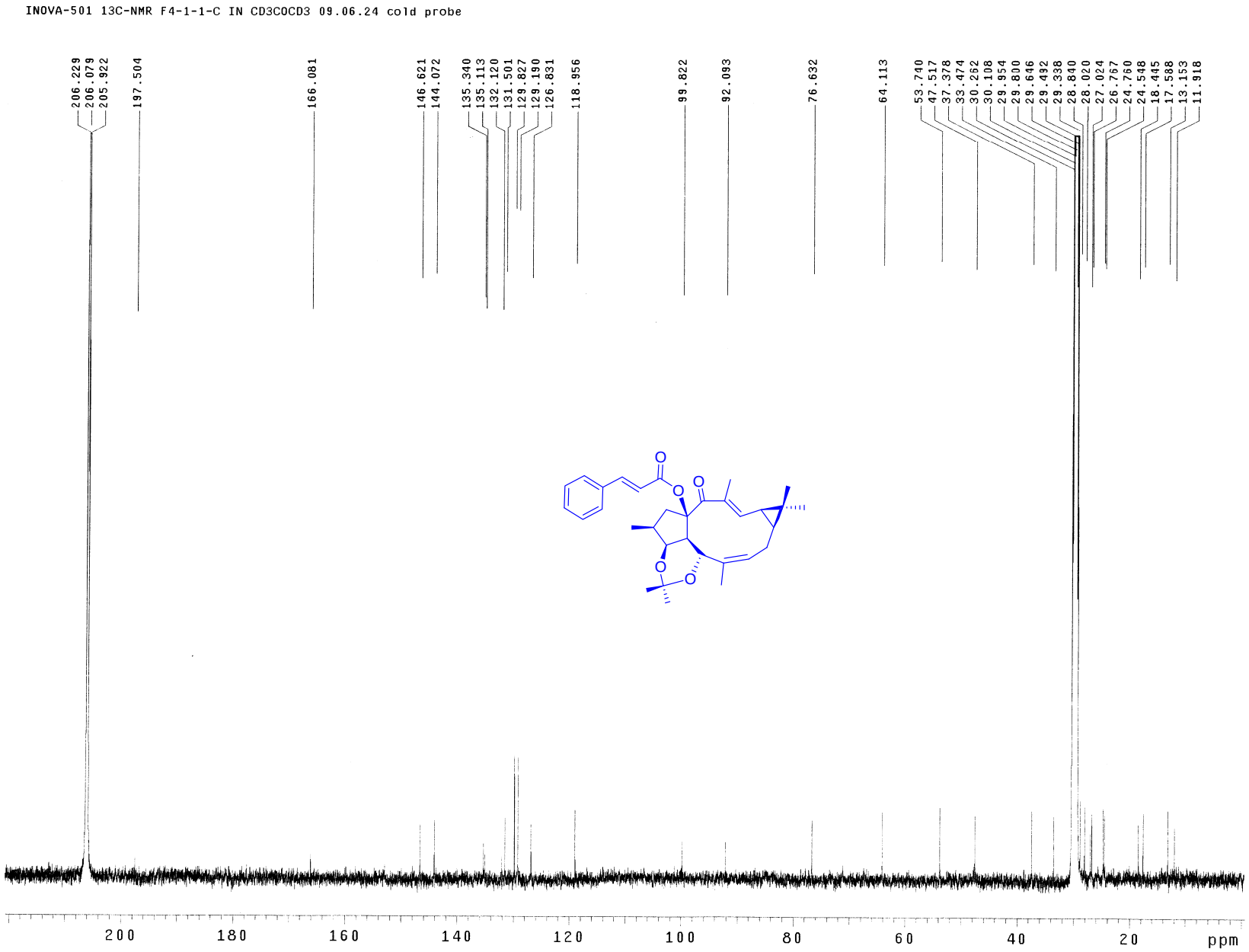

Figure S156. The ^{13}C NMR Spectrum of 16 in CD_3COCD_3 (125 MHz).

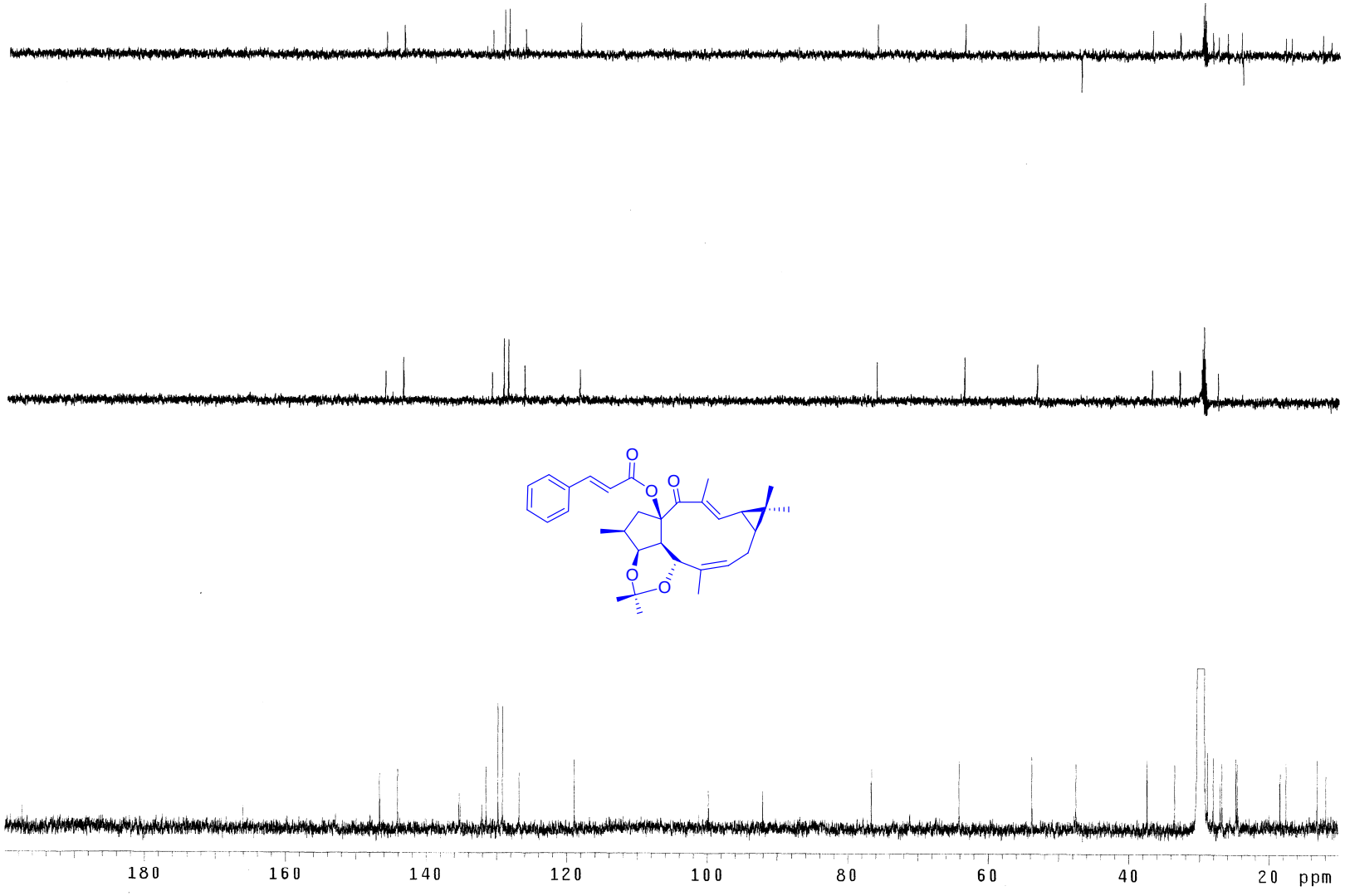

Figure S157. The DEPT Spectrum of 16 in CD_3COCD_3 (125 MHz).

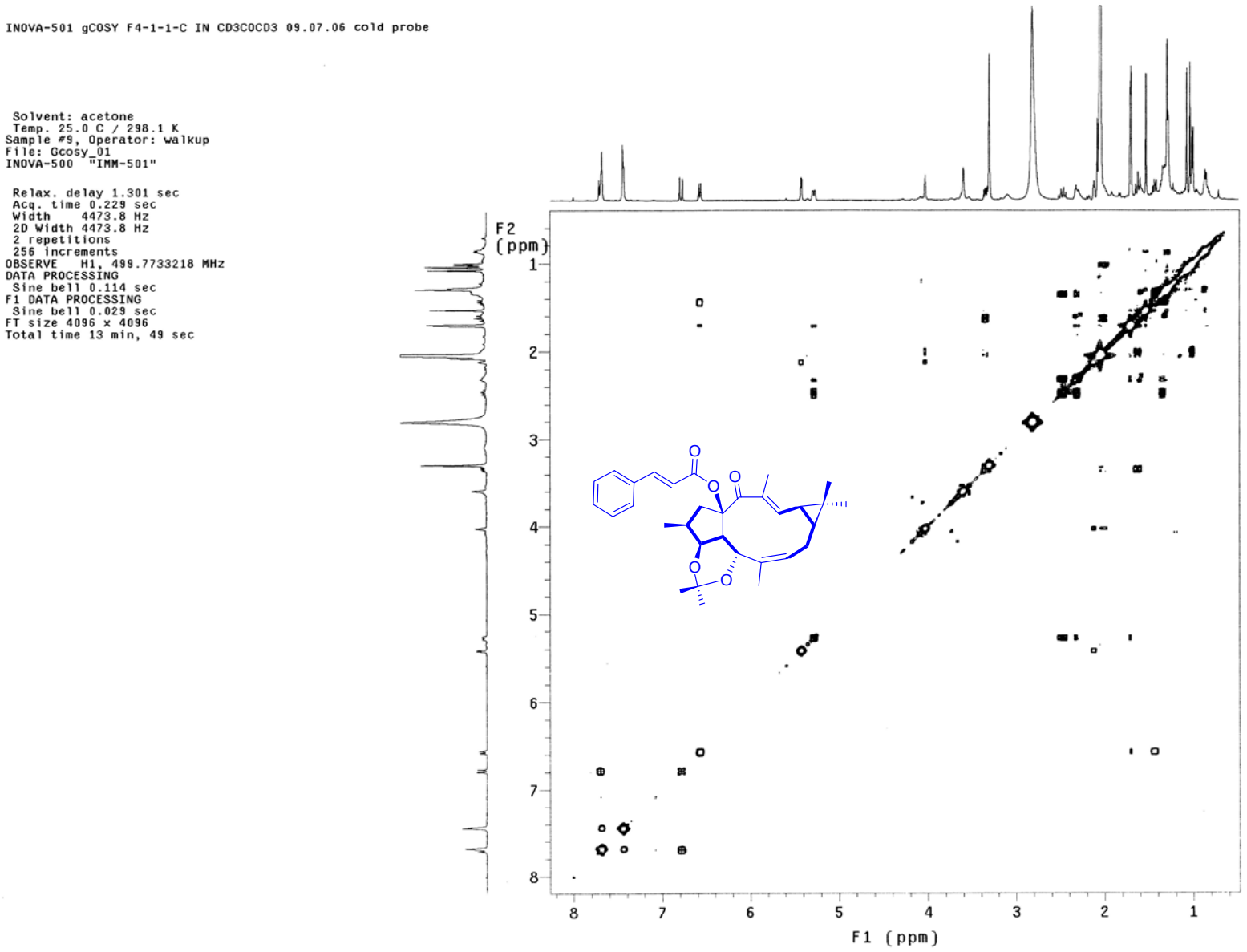

Figure S158. The ^{1}H-^{1}H gCOSY Spectrum of 16 in CD_3COCD_3 (500 MHz).

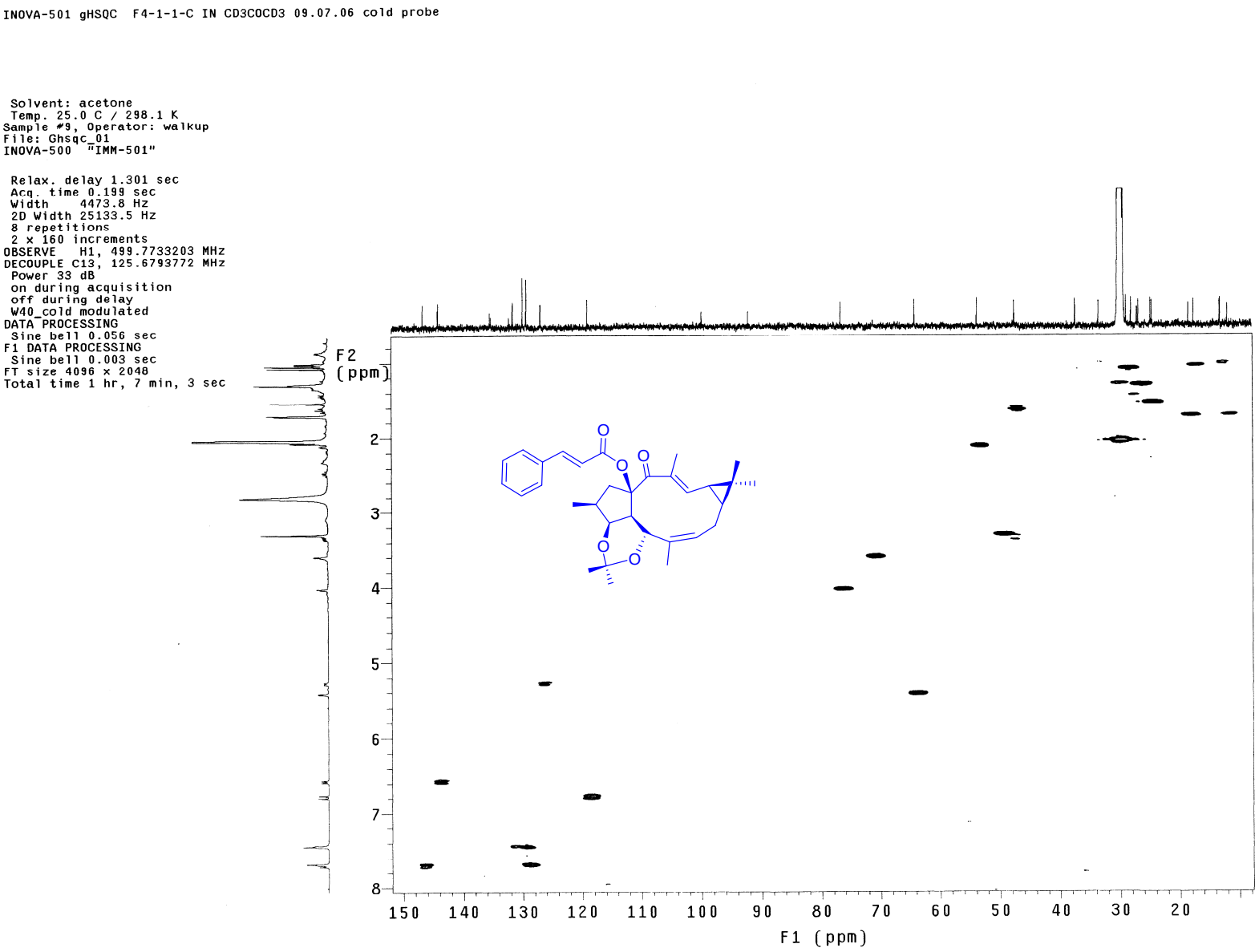

Figure S159. The gHSQC Spectrum of 16 in CD_3COCD_3 (500 MHz for ^1H NMR).

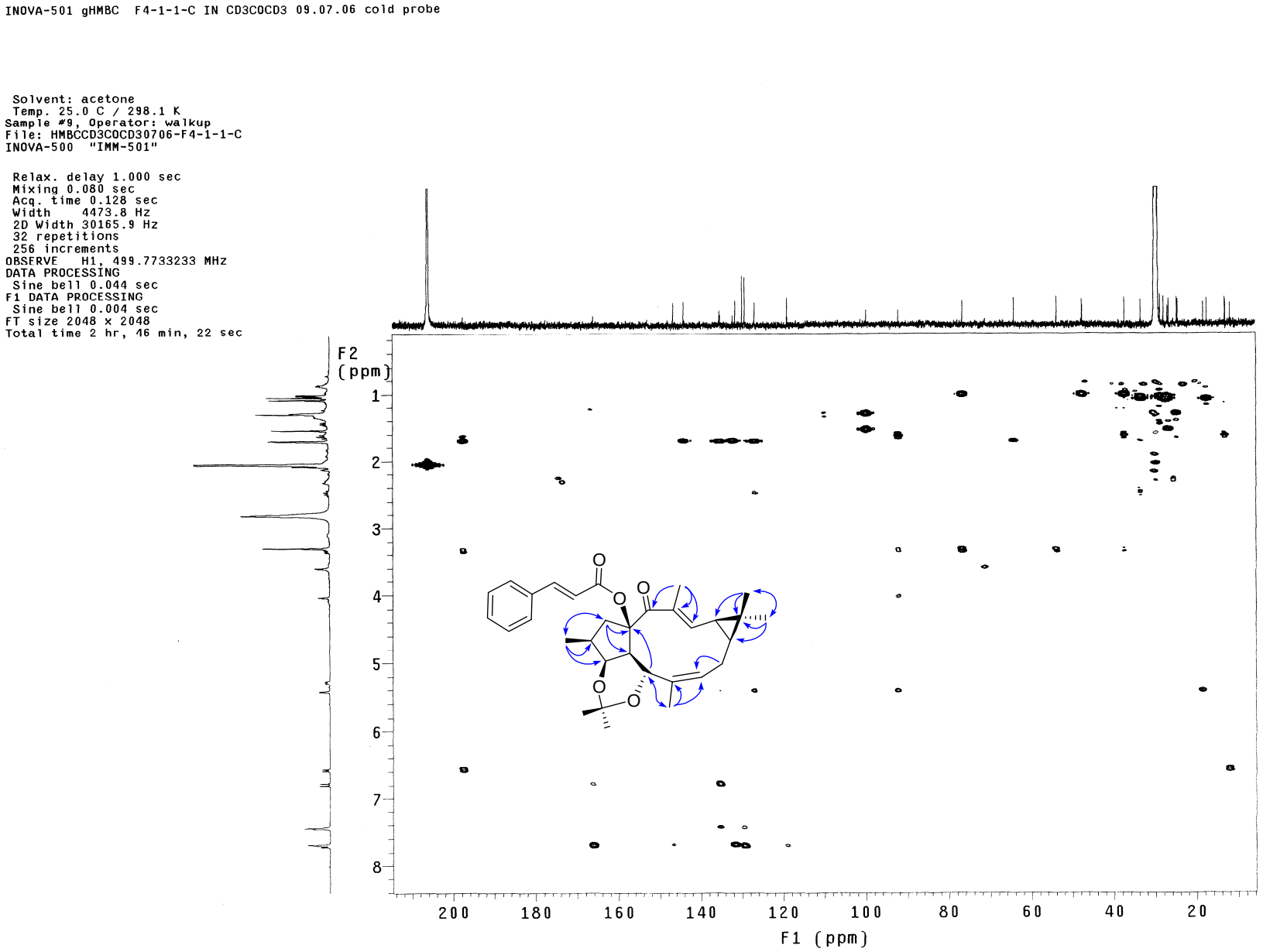

Figure S160. The gHMBC Spectrum of 16 in CD_3COCD_3 (500 MHz for ^1H NMR).

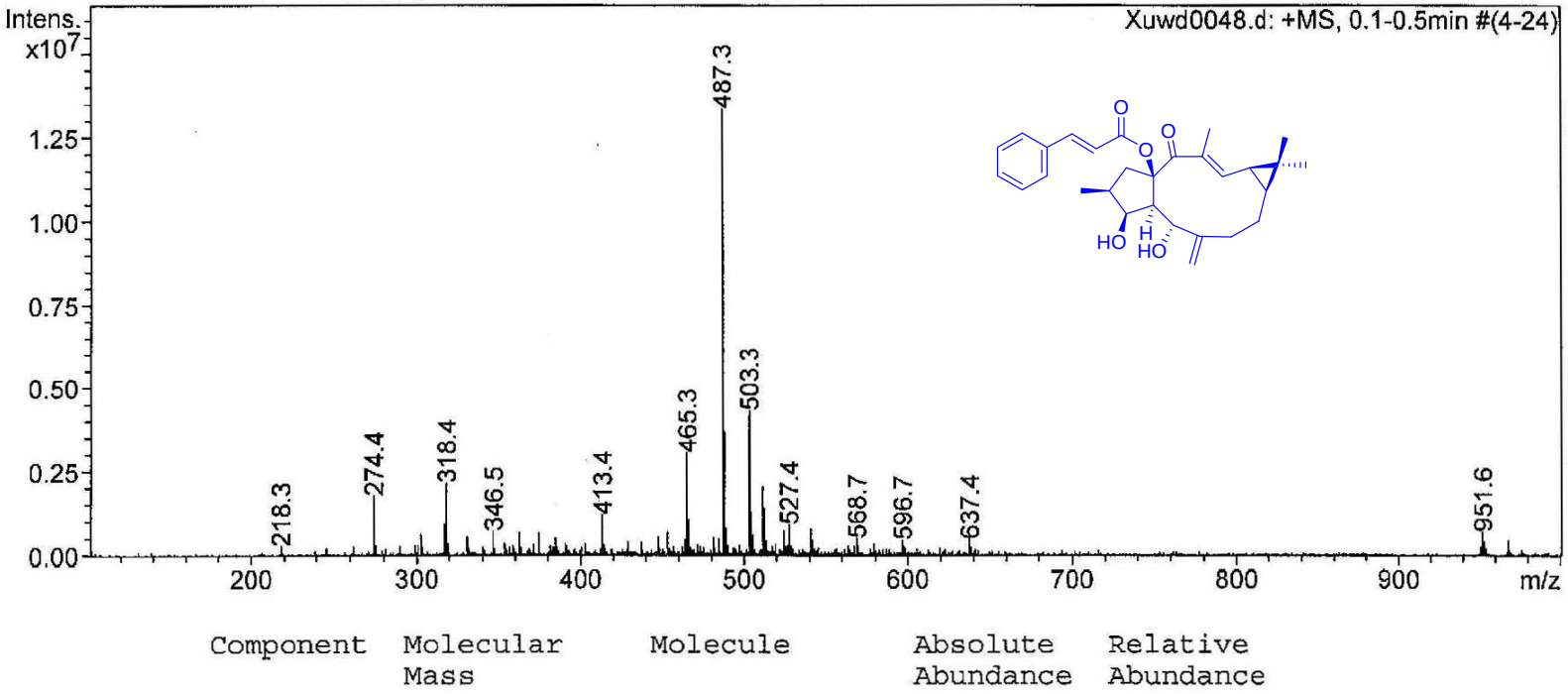

Figure S161. (+)-ESIMS Spectrum of 17.

MS Formula Results: + Scan (9.180 min) Sub (200904164.d)

m/z	Ion	Formula	Abundance
465.26535	(M+H)+	C29 H37 O5	568767

Best	Formula (M)	Ion Formula	Score	Cr	Calc m/z	Diff (ppm)	Mass Ma	Abund M	Spacing	DBE
	C22 H40 O10	C22 H41 O10	67.88		465.26942	8.8	45.56	78.91	99.29	3
☑	C29 H36 O5	C29 H37 O5	92.71		465.26355	-3.86	85.97	98.43	99.3	12

m/z	Ion	Formula	Abundance
487.24806	(M+Na)+	C29 H36 Na O5	1622477.5

Best	Formula (M)	Ion Formula	Score	Cr	Calc m/z	Diff (ppm)	Mass Ma	Abund M	Spacing	DBE
	C22 H40 O10	C22 H40 Na O10	71.3		487.25137	7.17	60.91	65.74	98.76	3
☑	C29 H36 O5	C29 H36 Na O5	87.2		487.2455	-5.48	74.86	98.5	98.32	12

(+)-HRESIMS Data of 17.

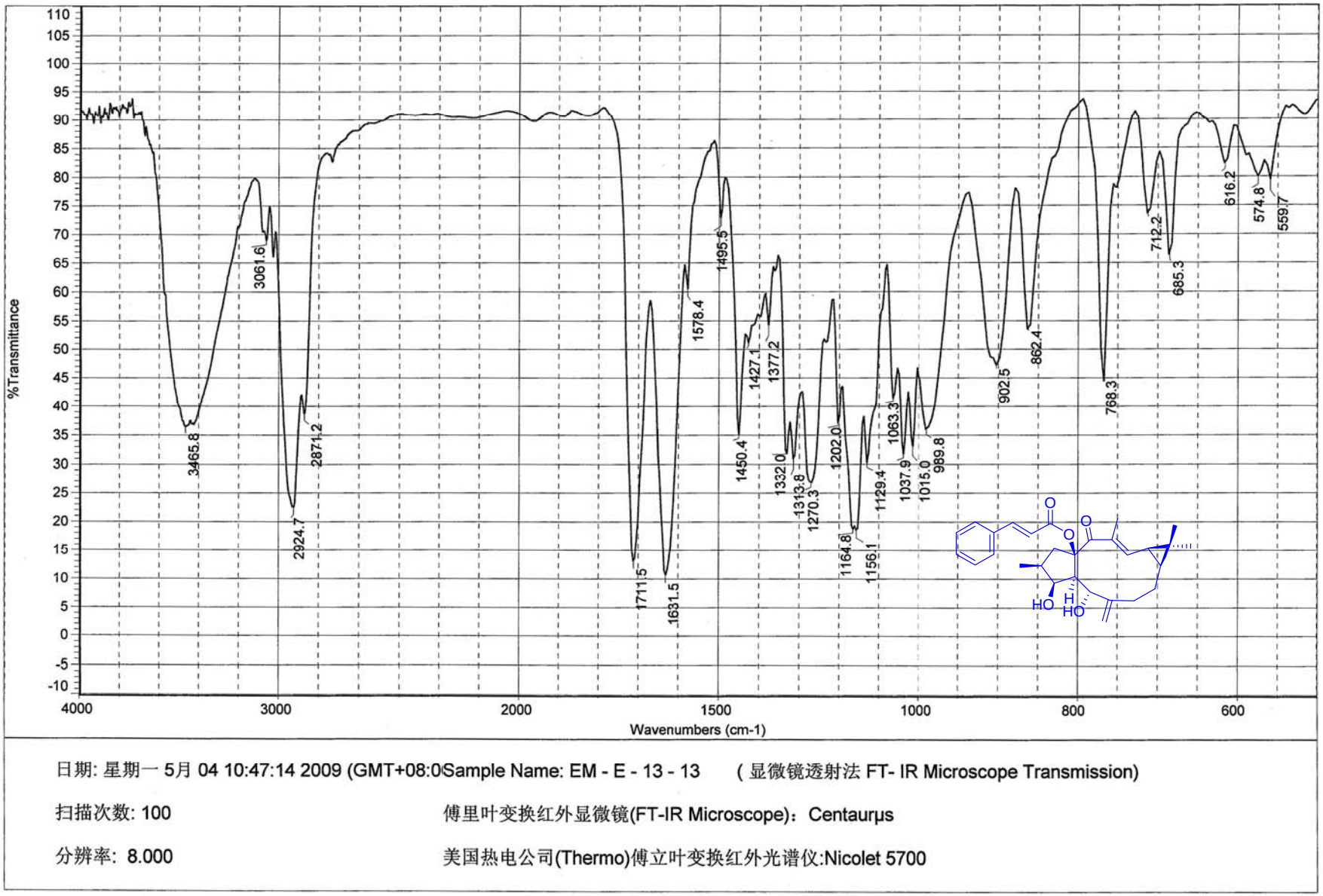

Figure S162. The IR Spectrum of 17.

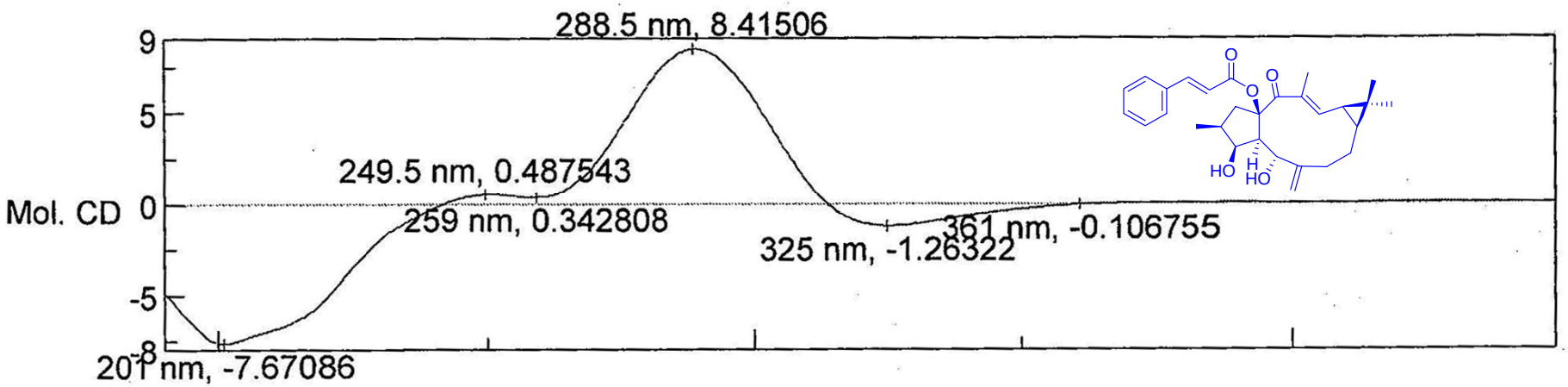

Figure S163. The CD Spectrum of 17.

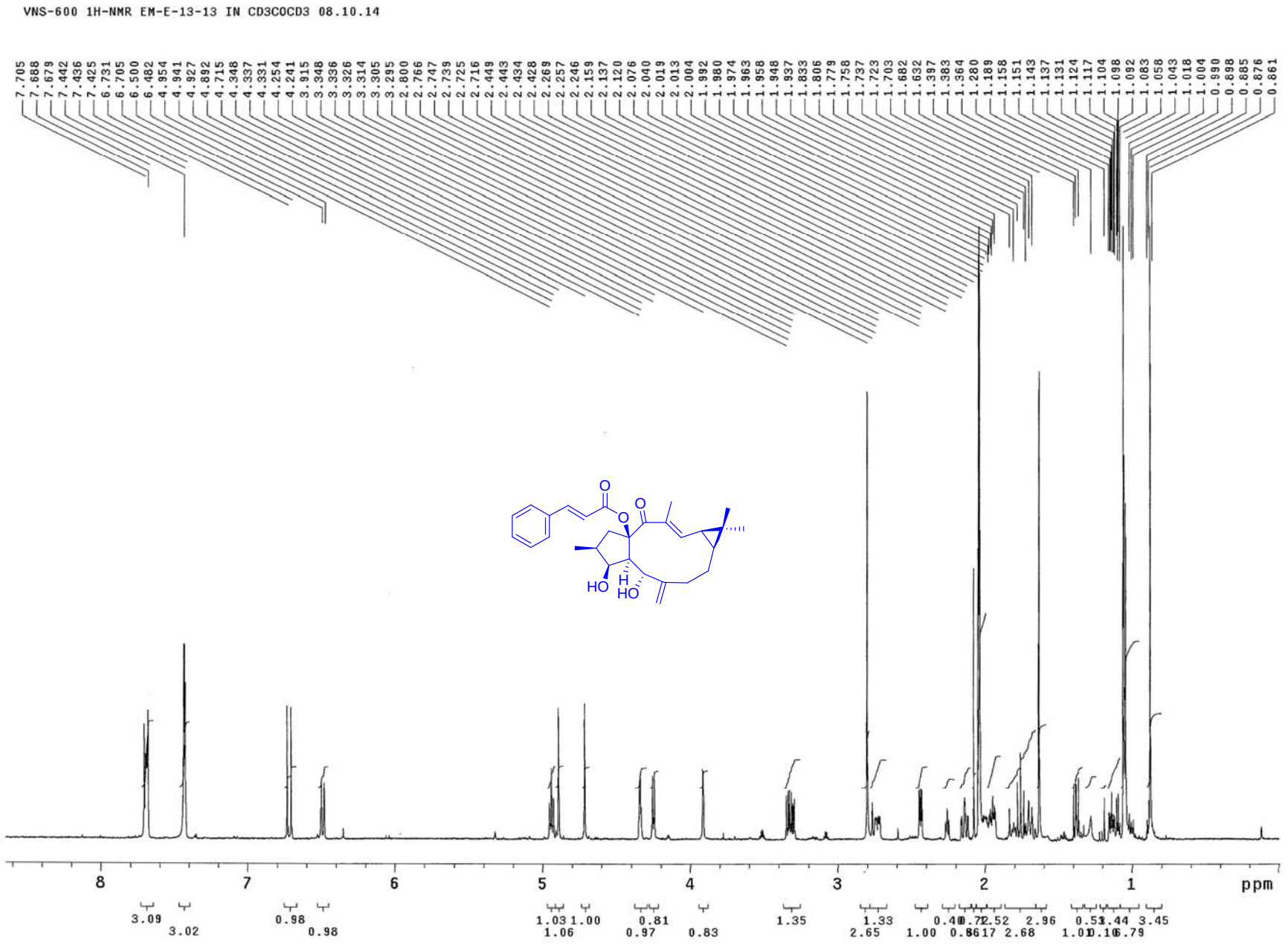

Figure S164. The ^{1}H NMR Spectrum of 17 in CD_3COCD_3 (600 MHz).

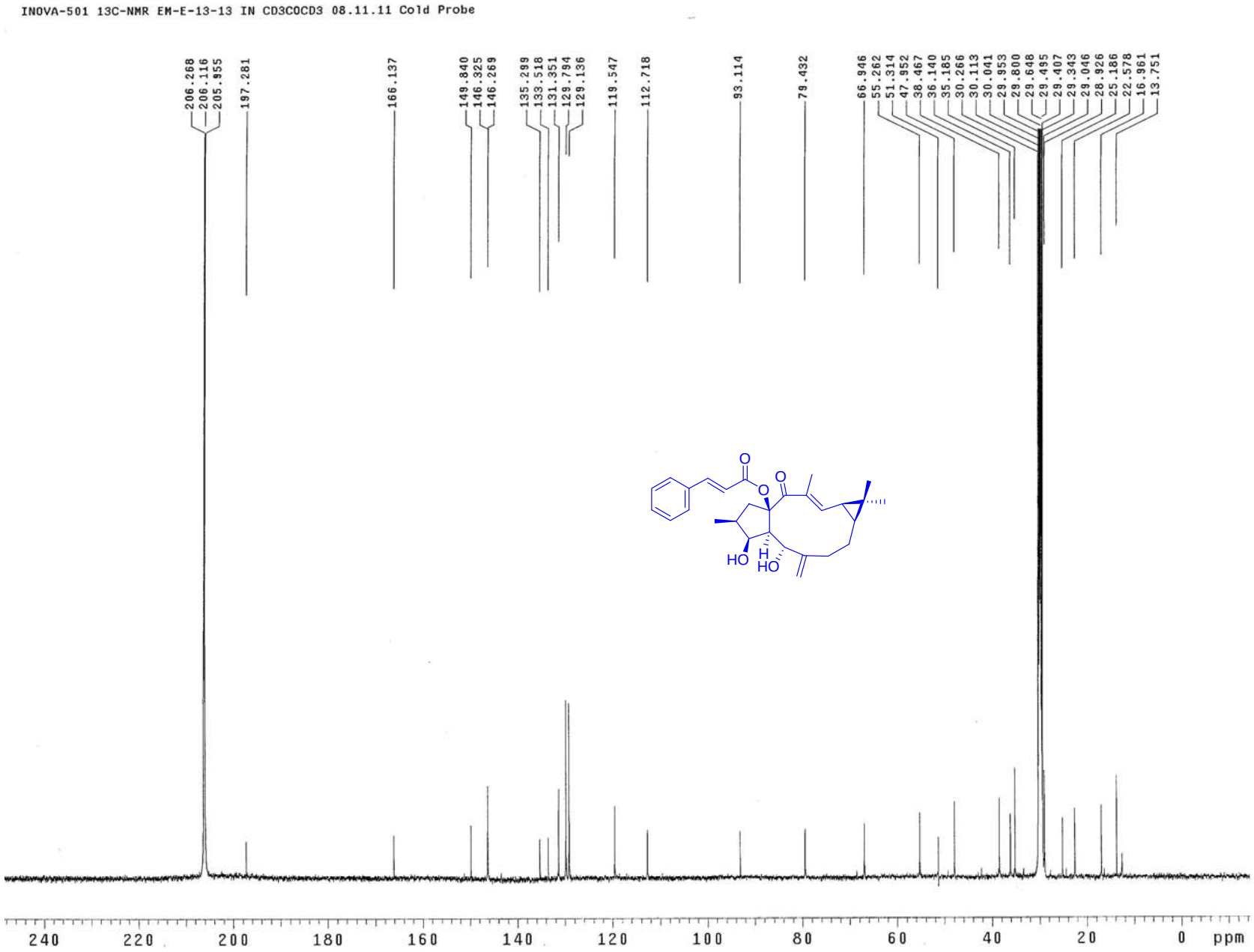

Figure S165. The ^{13}C NMR Spectrum of 17 in CD_3COCD_3 (125 MHz).

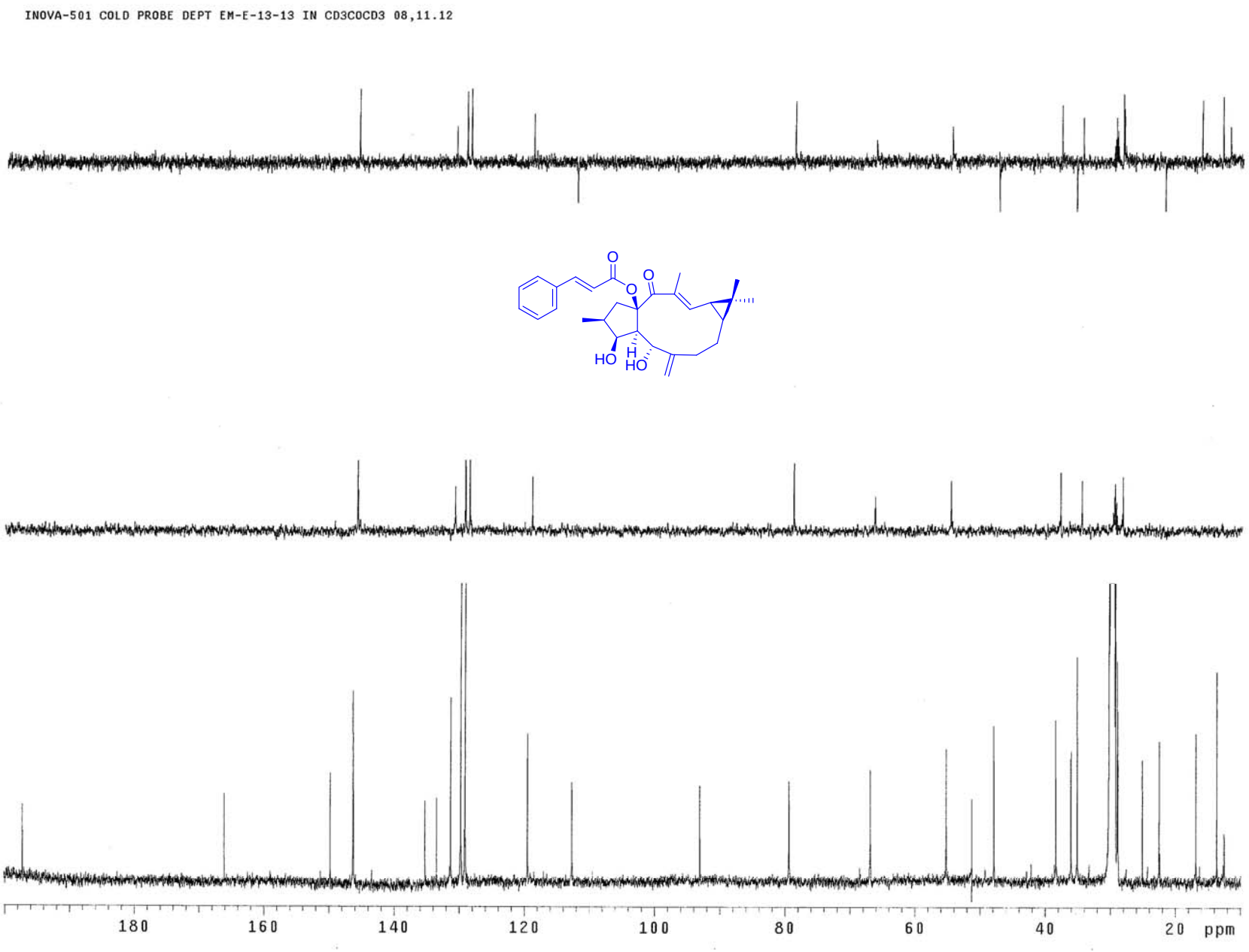

Figure S166. The DEPT Spectrum of 17 in CD_3COCD_3 (125 MHz).

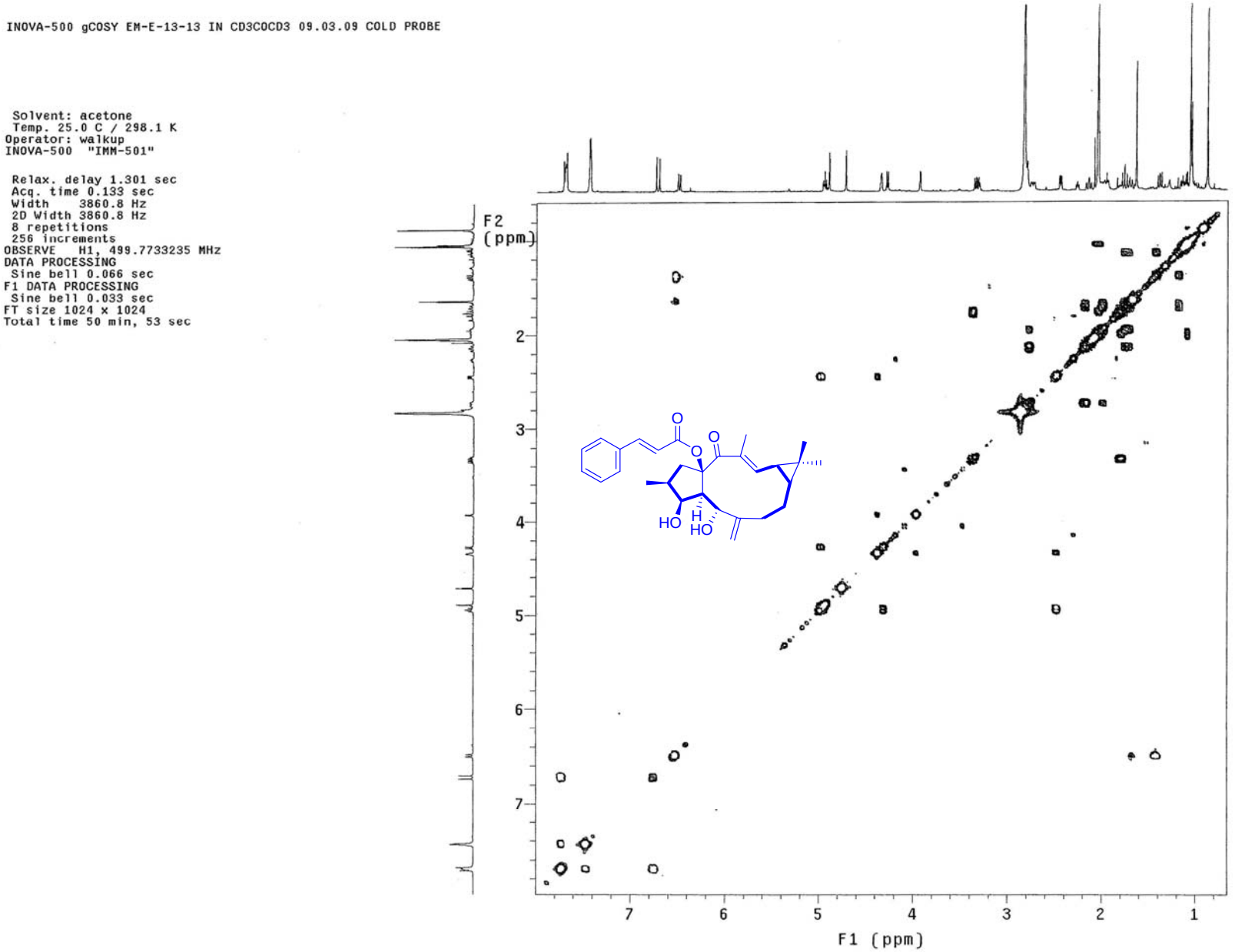

Figure S167. The ^{1}H-^{1}H gCOSY Spectrum of 17 in CD_3COCD_3 (500 MHz).

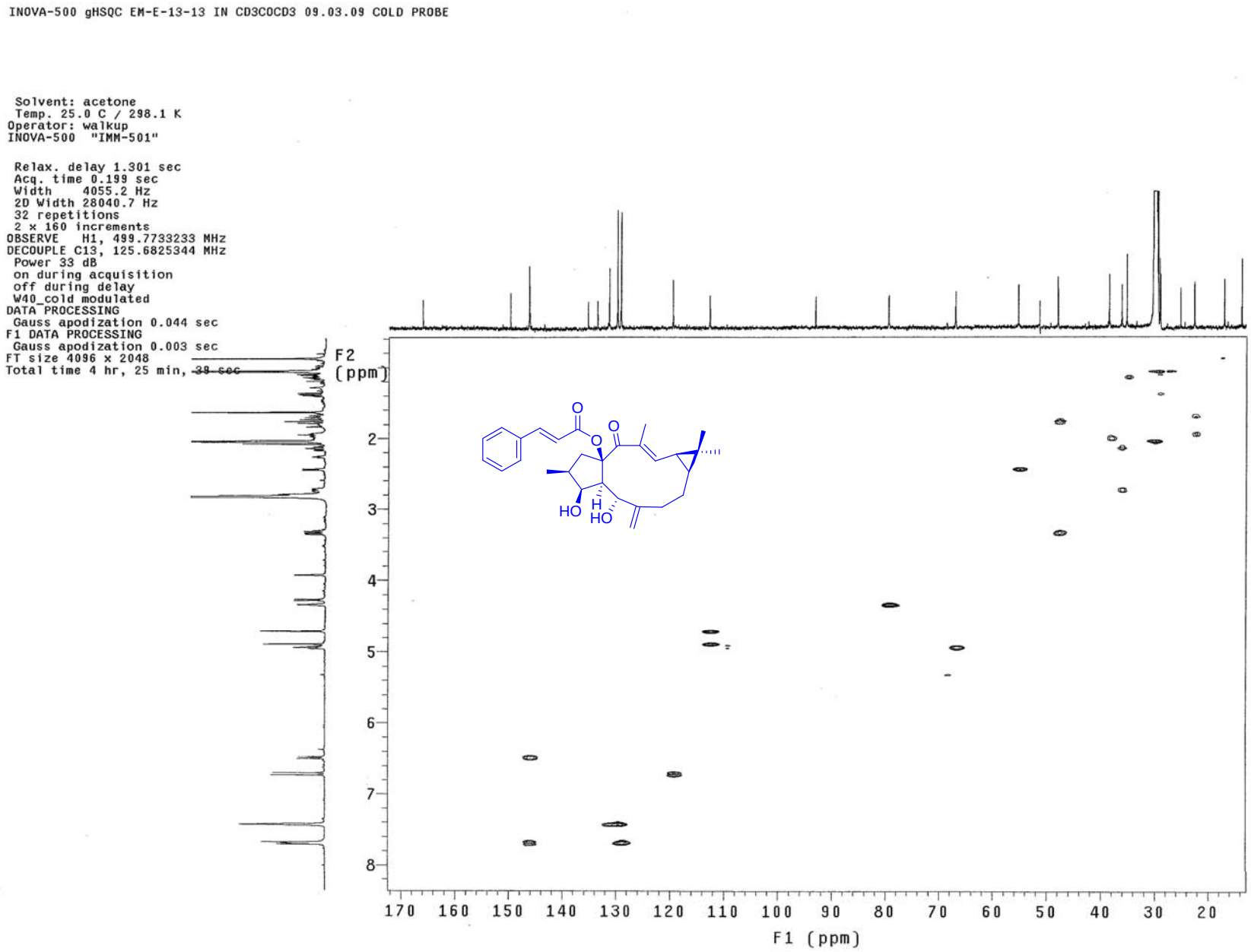

Figure S168. The gHSQC Spectrum of 17 in CD_3COCD_3 (500MHz for ^1H NMR).

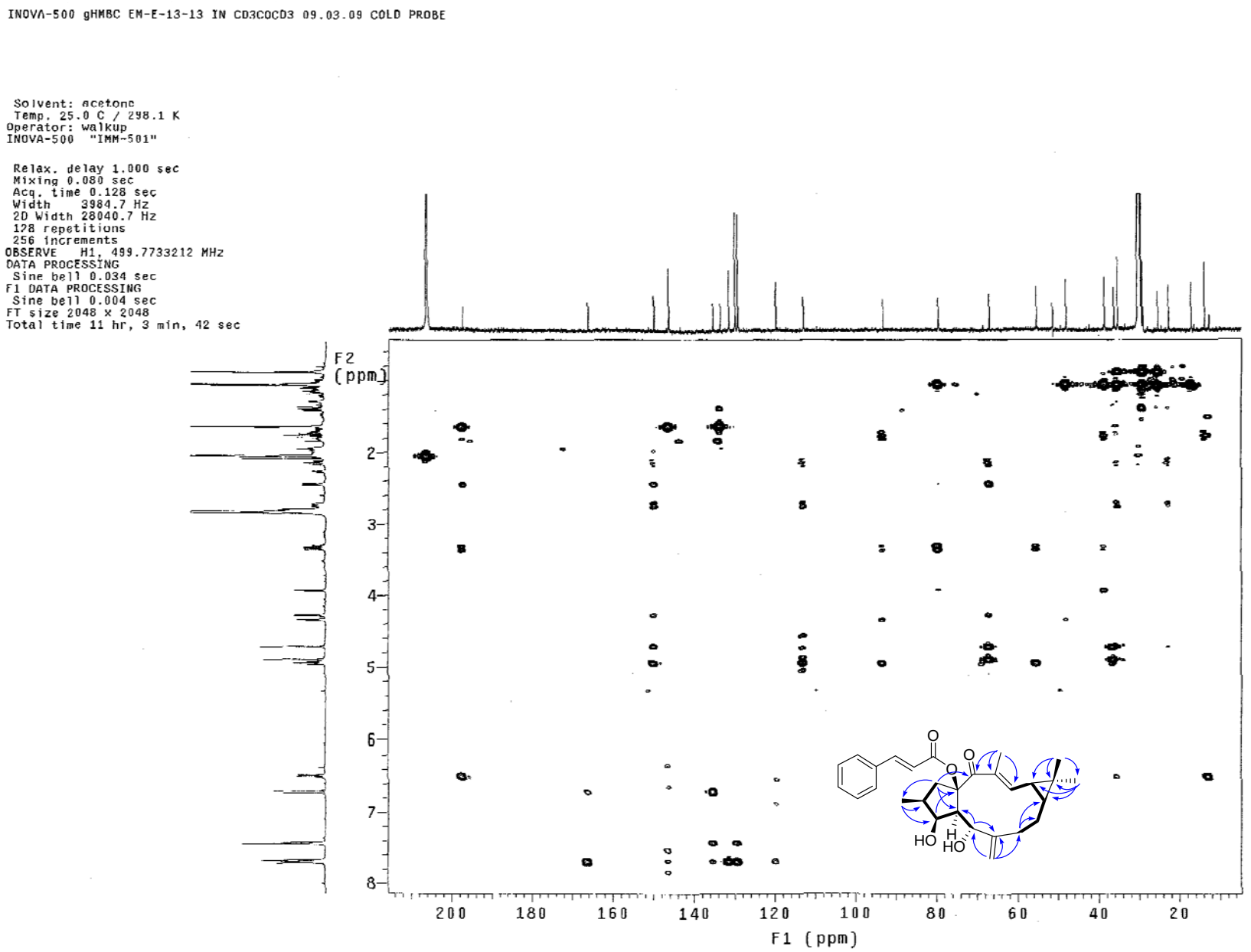

Figure S169. The gHMBC Spectrum of 17 in CD_3COCD_3 (500MHz for ^1H NMR).

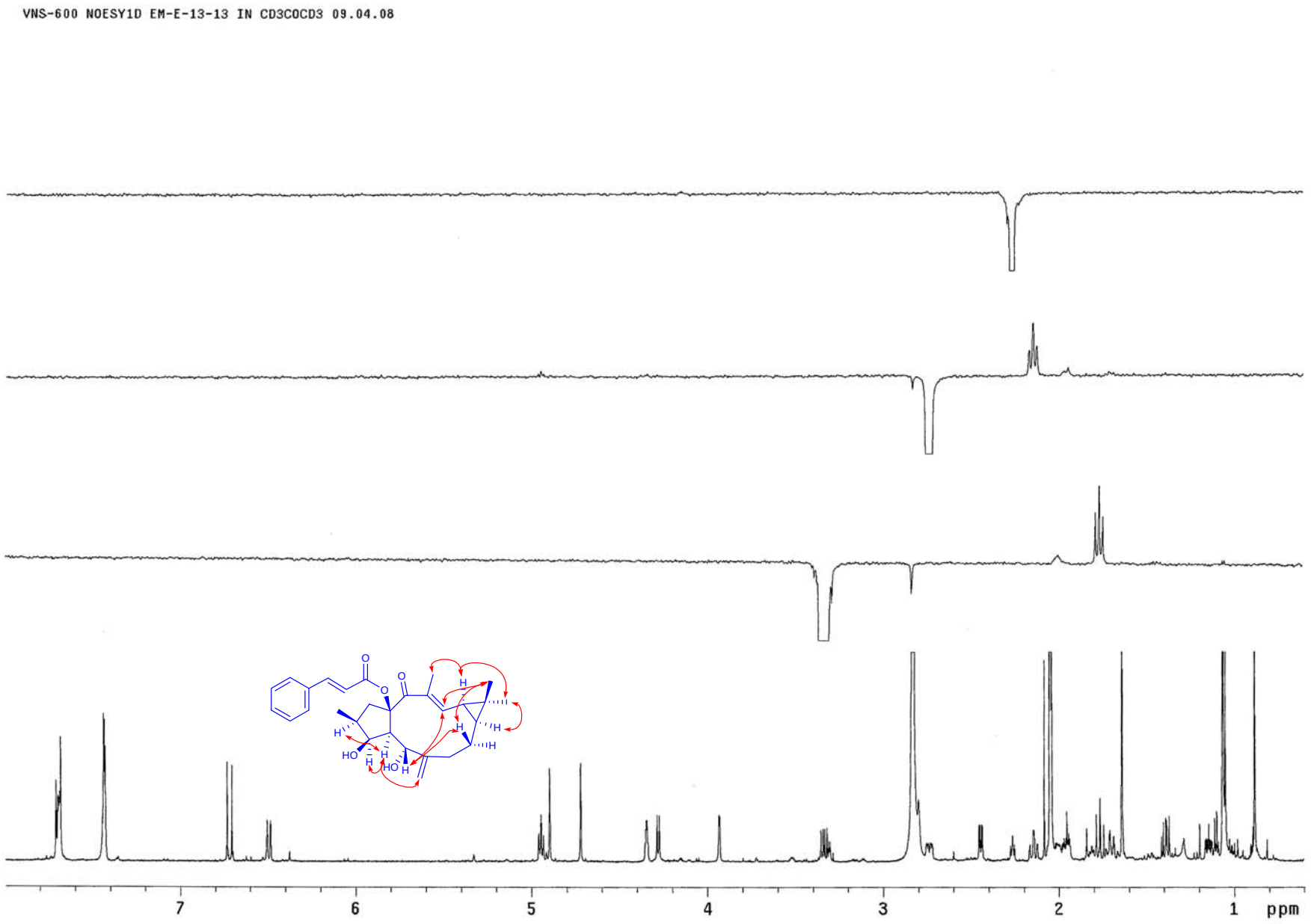

Figure S170. The NOE Difference Spectrum 1 of 17 in CD_3COCD_3 (600 MHz).

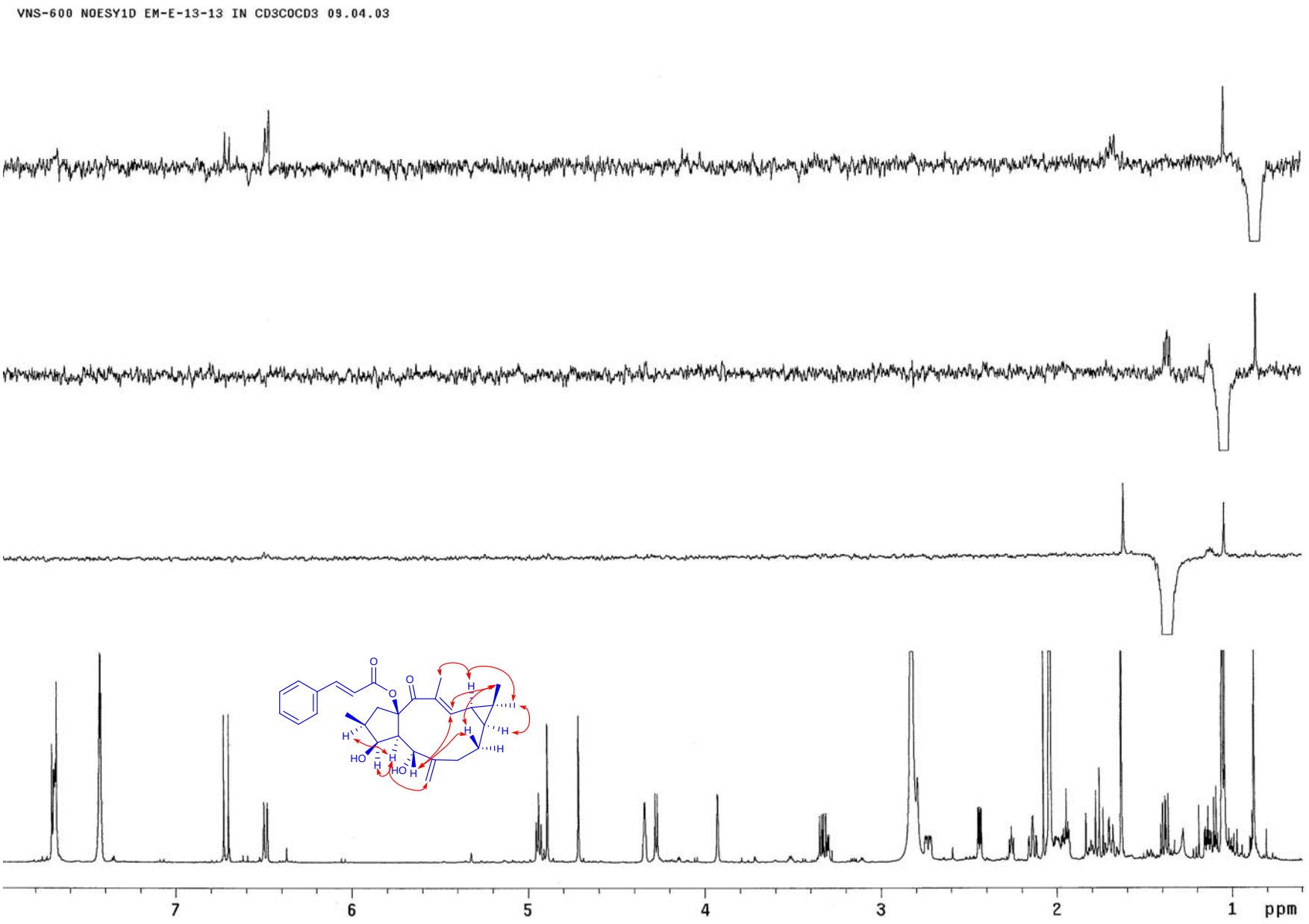

Figure S171. The NOE Difference Spectrum 2 of 17 in CD_3COCD_3 (600 MHz).

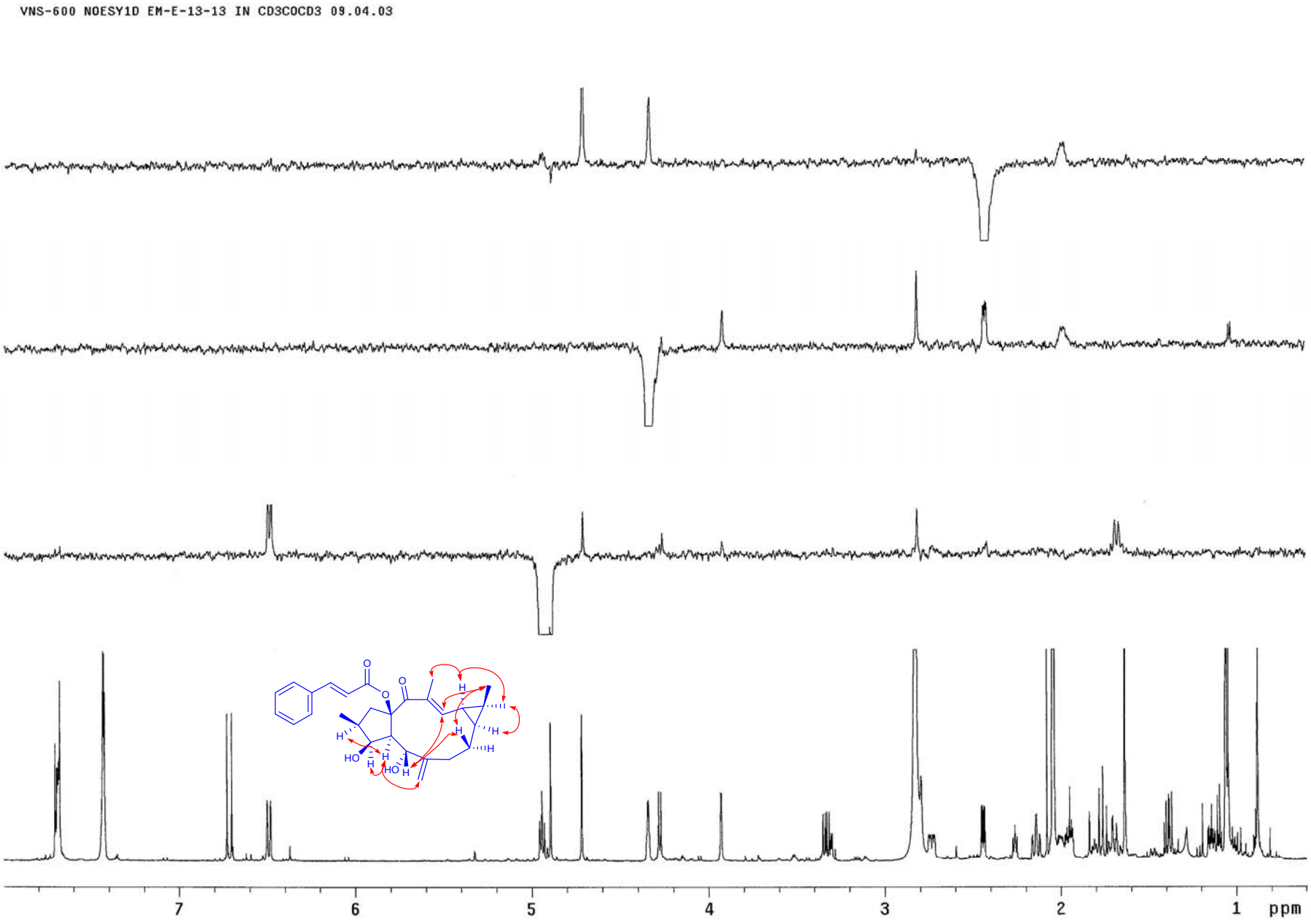

Figure S172. The NOE Difference Spectrum 3 of 17 in CD_3COCD_3 (600 MHz).