Xyloccensins O and P, Unique 8, 9, 30-Phragmalin Orthoesters from *Xylocarpus granatum*

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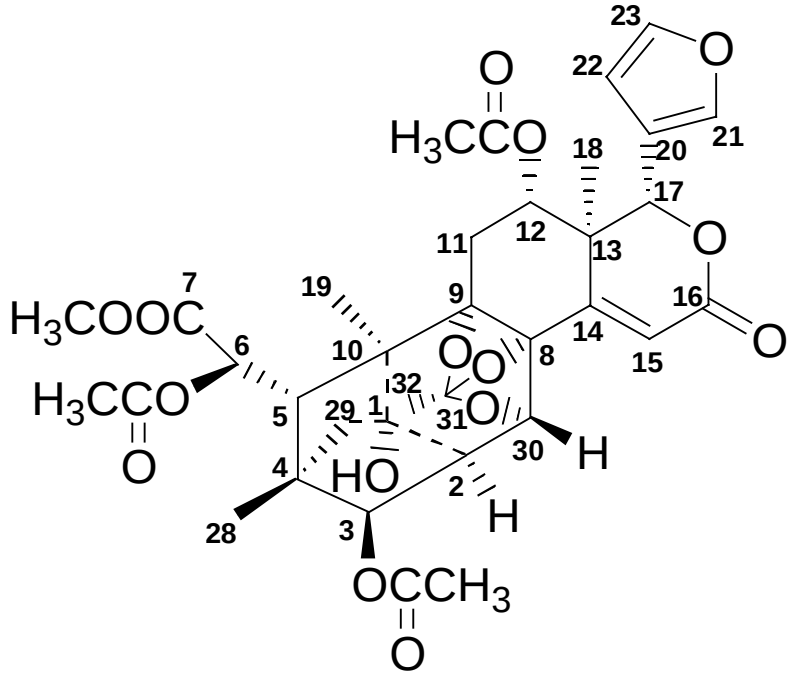
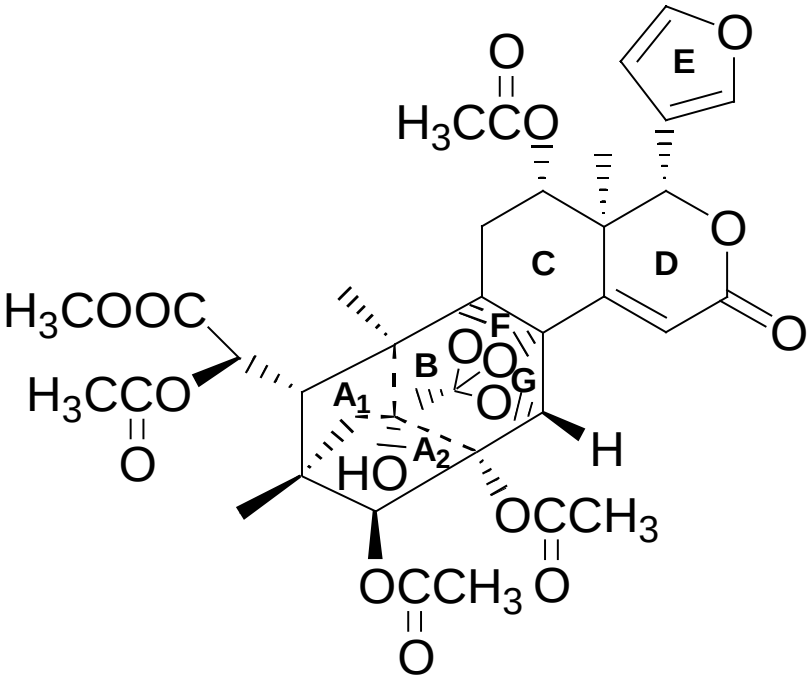
Supporting Information: Copies of Crystal data of xyloccensin O (1), MS, 1D and 2D NMR spectra of xyloccensin O (1), P (2)

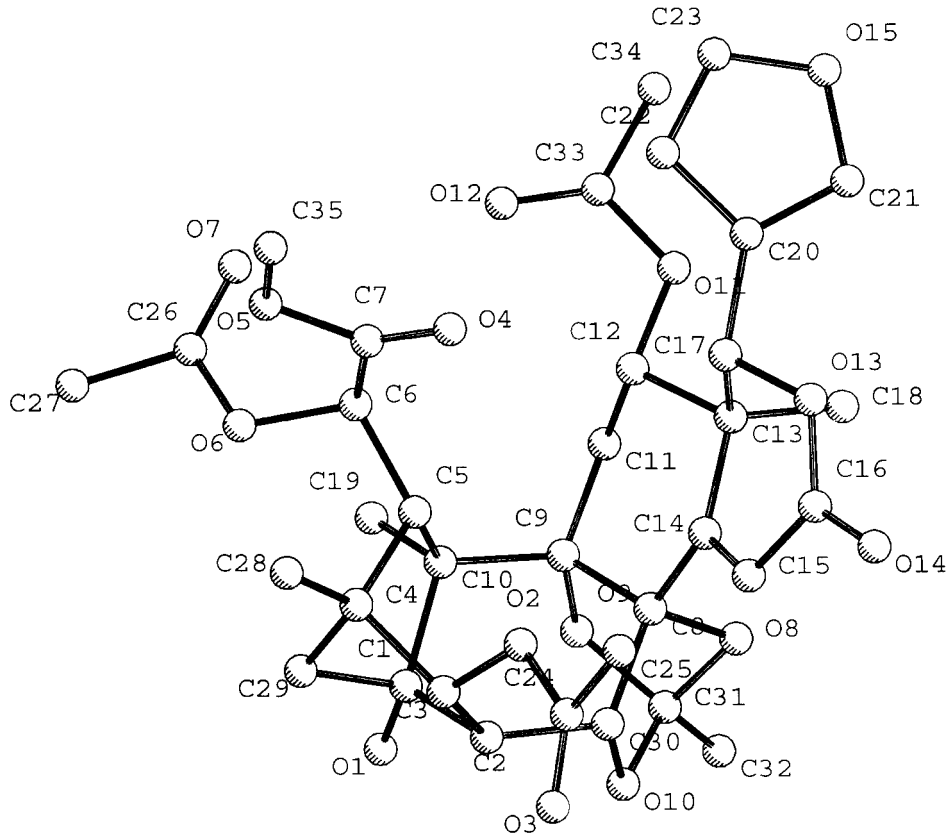


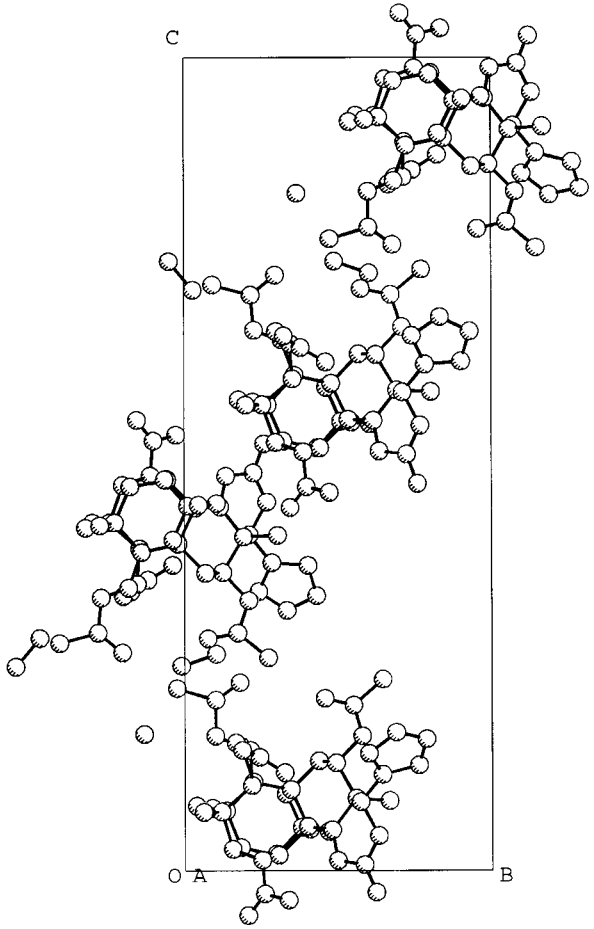
Xyloccensin O (**1**)



Xyloccensin P (**2**)

Structures of xyloccensins O (**1**) and P (**2**)





X-ray structure of xyloccensin O (1)

Table 1.Crystal data and structure refinement for xyloccensin O (1)

Identification code	Xyloccensin O (1)
Empirical formula	$(C_{35}H_{40}O_{15})_2 \cdot [(CH_3OH)_{0.5}]_2 \cdot (H_2O)_{0.5}$
Formula weight	1442.44
Temperature	296K
Wavelength	0.71073Å
Crystal system	Monoclinic
Space group	$P2_1$
Unit cell parameters	a=10.692(1)Å ,b=11.727(1)Å ,c=31.535(3) Å,β=80.79(1)°
Volume, z	3903.0(5)$Å^3$, 2
Density (calculated)	1.232g/cm^3
Absorption coefficient	0.08mm^{-1}
F(000)	1526
Crystal size	0.15×0.20×0.30mm
θ range for data collection	0.0 to 25.0 °
Limiting indices	-10≤h≤10,0≤k≤11,0≤l≤30
Reflections collected	11833
Independent reflections	7680
Max. and min. transmission	no
Refinement method	Full least-square
Data / restrains /parameters	5379/2301/972
Goodness-of-fit on F^2	2.814
Final R indices[I>2σ(I)]	0.064
R indices (all data)	0.036
Absolute structure parameter	no
Largest diff. peak and hole	0.260 and -0.220 e/ $Å^{-3}$

Table 2. Atomic Parameters x,y,z and Biso.

	x	y	z	Biso
O 1	.3675(7)	.2233(7)	.5755(2)	4.2(4)
O 2	.7767(7)	.3880(7)	.5142(2)	3.8(4)
O 3	.7823(12)	.3446(10)	.4462(3)	9.2(7)
O 4	.8924(8)	.4612(8)	.6243(3)	6.3(5)
O 5	.9162(8)	.2993(8)	.6619(3)	5.8(5)
O 6	.6851(7)	.2275(7)	.6636(2)	4.0(4)
O 7	.6482(9)	.2964(8)	.7313(3)	6.3(6)
O 8	.4025(6)	.6046(7)	.5485(2)	3.9(4)
O 9	.3261(7)	.4619(7)	.5934(2)	3.9(4)
O10	.3698(7)	.4345(7)	.5193(2)	4.1(4)
O11	.5738(7)	.7094(7)	.6676(2)	3.8(4)
O12	.6148(9)	.5758(8)	.7145(3)	6.4(5)
O13	.8278(7)	.7686(7)	.5468(2)	4.3(4)
O14	.8518(7)	.7597(7)	.4755(2)	4.4(4)
O15	.8661(11)	.9302(10)	.6621(3)	8.5(6)
C 1	.4924(11)	.2715(10)	.5718(4)	3.8(6)
C 2	.5494(10)	.3222(11)	.5276(3)	3.6(6)
C 3	.6909(11)	.2974(11)	.5259(4)	3.9(6)
C 4	.7013(10)	.2548(10)	.5720(3)	3.7(6)
C 5	.6629(10)	.3530(11)	.6039(3)	3.7(6)
C 6	.7072(11)	.3450(11)	.6471(4)	4.2(6)
C 7	.8504(11)	.3799(11)	.6422(3)	4.3(6)
C 8	.5125(9)	.5345(10)	.5541(3)	3.0(5)
C 9	.4660(10)	.4788(10)	.5983(3)	3.4(6)
C10	.5134(10)	.3590(10)	.6083(3)	3.6(6)
C11	.4615(10)	.5682(11)	.6343(4)	3.9(6)
C12	.5919(10)	.6245(10)	.6334(3)	3.4(6)
C13	.6360(10)	.6928(9)	.5899(3)	3.3(6)
C14	.6218(9)	.6161(10)	.5529(3)	3.1(5)
C15	.6966(10)	.6351(10)	.5152(4)	3.3(6)
C16	.7975(10)	.7247(11)	.5113(4)	4.0(6)

C17	.7798(11)	.7110(10)	.5874(3)	3.8(6)	C15'	.7989(10)	.9977(9)	.9874(3)	3.3(6)
C18	.5631(11)	.8036(10)	.5880(4)	4.0(6)	C16'	.7037(10)	1.0848(10)	.9927(3)	3.4(5)
C19	.4347(11)	.3173(11)	.6519(4)	4.2(6)	C17'	.7131(11)	1.0723(10)	.9159(3)	3.9(6)
C20	.8222(12)	.7845(12)	.6215(4)	4.6(6)	C18'	.9339(11)	1.1669(11)	.9147(4)	3.9(6)
C21	.8170(15)	.9024(14)	.6251(5)	7.1(9)	C19'	1.0547(12)	.6839(10)	.8480(4)	4.3(6)
C22	.8766(16)	.7415(13)	.6568(5)	7.6(9)	C20'	.6656(11)	1.1443(12)	.8827(4)	5.0(7)
C23	.9064(18)	.8335(15)	.6798(6)	9.5(11)	C21'	.5847(14)	1.1001(15)	.8568(4)	6.7(8)
C24	.8204(12)	.3982(13)	.4717(4)	5.7(7)	C22'	.6836(14)	1.2627(13)	.8711(4)	5.8(8)
C25	.9369(12)	.4724(13)	.4647(5)	6.6(8)	C23'	.6161(13)	1.2876(13)	.8390(5)	6.4(8)
C26	.6530(11)	.2169(12)	.7069(4)	4.4(6)	C24'	.6679(13)	.7598(11)	1.0285(4)	5.5(7)
C27	.6235(13)	.0918(12)	.7195(4)	5.6(7)	C25'	.5588(11)	.8376(12)	1.0361(5)	5.8(7)
C28	.8327(11)	.1995(11)	.5718(4)	4.4(6)	C26'	.8347(12)	.6009(13)	.7904(4)	5.4(7)
C29	.5870(11)	.1767(10)	.5783(4)	3.9(6)	C27'	.8471(14)	.4742(13)	.7760(5)	6.3(8)
C30	.5068(9)	.4426(10)	.5193(3)	3.4(6)	C28'	.6655(12)	.5613(11)	.9283(4)	4.7(6)
C31	.3136(12)	.5104(13)	.5518(4)	5.5(7)	C29'	.9112(11)	.5384(10)	.9207(4)	3.8(6)
C32	.1800(10)	.5453(11)	.5506(4)	4.6(7)	C30'	.9924(10)	.8055(10)	.9810(3)	3.4(6)
C33	.5901(12)	.6731(12)	.7076(4)	5.0(7)	C31'	1.1811(12)	.8801(11)	.9467(4)	4.7(7)
C34	.5785(14)	.7726(13)	.7383(4)	6.3(8)	C32'	1.3172(11)	.9071(12)	.9490(4)	5.0(7)
C35	1.0536(13)	.3245(19)	.6565(6)	9.3(12)	C33'	.8882(13)	1.0498(13)	.7970(4)	5.6(7)
O 1'	1.1327(7)	.5898(7)	.9234(2)	4.0(4)	C34'	.9120(13)	1.1450(13)	.7650(4)	6.3(8)
O 2'	.7204(7)	.7517(7)	.9869(2)	4.1(4)	C35'	.4311(13)	.6872(18)	.8526(5)	8.1(11)
O 3'	.7148(12)	.7053(10)	1.0550(3)	9.3(7)	OM	.2401(23)	.4890(30)	.7482(7)	16.5(29)
O 4'	.5987(8)	.8255(8)	.8802(3)	5.5(5)	CM	.2100(30)	.6030(30)	.7338(11)	13.3(30)
O 5'	.5693(7)	.6665(8)	.8436(2)	5.2(5)	OM'	.2400(30)	-.0500(30)	.7484(11)	19.8(35)
O 6'	.8027(7)	.5998(7)	.8349(2)	4.2(4)	CM'	.2660(30)	.0280(30)	.7131(9)	11.4(25)
O 7'	.8541(10)	.6793(9)	.7689(3)	7.0(6)	OW	.1830(40)	.3673(20)	.8325(16)	19.7(38)
O 8'	1.0947(6)	.9684	.9519(2)	3.5(4)	HO1	.300	.290	.571	5.3
O 9'	1.1708(7)	.8286(7)	.9062(2)	4.1(4)	H 2	.517	.267	.504	4.7
O10'	1.1317(7)	.7990(7)	.9791(2)	3.8(4)	H 3	.715	.225	.504	4.8
O11'	.9187(7)	1.0781(7)	.8349(2)	3.8(4)	H 5	.702	.433	.588	4.7
O12'	.8533(12)	.9560(10)	.7885(3)	8.5(7)	H 6	.650	.404	.669	5.4
O13'	.6671(7)	1.1317(7)	.9569(2)	4.3(4)	H11A	.432	.528	.666	4.6
O14'	.6514(7)	1.1225(7)	1.0267(2)	4.4(4)	H11B	.392	.635	.631	4.6

H12	.663	.559	.638	4.3	HO1'	1.164	.559	.891	4.9
H15	.684	.584	.486	4.4	H 2'	.986	.628	.995	4.7
H17	.825	.627	.588	4.7	H 3'	.783	.582	.995	5.0
H18A	.463	.787	.590	5.0	H 5'	.795	.798	.912	4.2
H18B	.598	.849	.559	5.0	H 6'	.835	.777	.831	4.8
H18C	.575	.857	.616	5.0	H11'A	1.099	1.000	.869	4.5
H19A	.462	.233	.660	5.4	H11'B	1.053	.895	.835	4.5
H19B	.334	.317	.650	5.4	H12'	.832	.929	.864	4.6
H19C	.449	.376	.678	5.4	H15'	.811	.944	1.015	4.1
H21	.780	.962	.602	8.4	H17'	.669	.986	.916	4.8
H22	.887	.652	.664	8.3	H18'A	.923	1.224	.889	5.0
H23	.968	.828	.705	9.8	H18'B	1.033	1.146	.913	5.0
H25A	.949	.516	.494	7.3	H18'C	.901	1.209	.945	5.0
H25B	.926	.538	.440	7.3	H19'A	1.024	.601	.840	5.4
H25C	1.019	.423	.453	7.3	H19'B	1.155	.686	.848	5.4
H27A	.636	.035	.691	6.3	H19'C	1.034	.744	.823	5.4
H27B	.530	.079	.737	6.3	H21'	.549	1.011	.857	7.9
H27C	.692	.060	.740	6.3	H22'	.746	1.322	.886	7.0
H28A	.905	.266	.567	5.7	H23'	.615	1.373	.822	7.4
H28B	.853	.139	.546	5.7	H25'A	.543	.877	1.007	6.5
H28C	.837	.158	.602	5.7	H25'B	.575	.906	1.059	6.5
H29A	.568	.139	.611	5.0	H25'C	.474	.792	1.050	6.5
H29B	.592	.109	.555	5.0	H27'A	.824	.419	.803	7.0
H30	.556	.473	.487	4.2	H27'B	.945	.456	.761	7.0
H32A	.146	.604	.577	5.6	H27'C	.785	.456	.753	7.0
H32B	.117	.472	.554	5.6	H28'A	.654	.493	.951	5.9
H32C	.172	.589	.521	5.6	H28'B	.659	.527	.897	5.9
H34A	.589	.744	.770	7.1	H28'C	.590	.623	.937	5.9
H34B	.486	.814	.740	7.1	H29'A	.926	.499	.889	5.0
H34C	.651	.836	.728	7.1	H29'B	.905	.470	.944	5.0
H35A	1.104	.265	.674	9.8	H30'	.944	.834	1.013	4.2
H35B	1.066	.411	.673	9.8	H32'A	1.375	.828	.943	6.1
H35C	1.096	.333	.624	9.8	H32'B	1.330	.941	.980	6.1

H32'C	1.358	.967	.924	6.1
H34'A	.942	1.220	.781	7.1
H34'B	.827	1.164	.752	7.1
H34'C	.986	1.120	.739	7.1
H35'A	.380	.624	.837	9.4
H35'B	.409	.772	.840	9.4
H35'C	.396	.688	.887	9.4
HOM	.335	.466	.733	3.2
HCMA	.110	.633	.749	14.9
HCMB	.272	.671	.739	14.9
HCMC	.204	.598	.698	14.9
HOM'	.166	-.015	.772	3.2
HCM'A	.340	-.011	.690	12.2
HCM'B	.302	.105	.726	12.2
HCM'C	.179	.041	.701	12.2

Biso is the Mean of the Principal Axes of the Thermal Ellipsoid

Table 3. Bond Lengths

O(1)-C(1)	1.437(13)	O(4')-C(7')	1.179(17)
O(1)-Ho(1)	1.090(40)	O(5')-C(7')	1.361(14)
O(2)-C(3)	1.414(14)	O(5')-C(35')	1.479(16)
O(2)-C(24)	1.354(15)	O(6')-C(6')	1.447(14)
O(3)-C(24)	1.146(17)	O(6')-C(26')	1.392(14)
O(4)-C(7)	1.160(16)	O(7')-C(26')	1.142(18)
O(5)-C(7)	1.384(14)	O(8')-C(8')	1.472(11)
O(5)-C(35)	1.482(16)	O(8')-C(31')	1.381(14)
O(6)-C(6)	1.479(15)	O(9')-C(9')	1.554(13)
O(6)-C(26)	1.358(14)	O(9')-C(31')	1.431(14)
O(7)-C(26)	1.205(16)	O(10')-C(30')	1.483(13)
O(8)-C(8)	1.469(12)	O(10')-C(31')	1.434(14)
O(8)-C(31)	1.451(15)	O(11')-C(12')	1.447(13)
O(9)-C(9)	1.541(12)	O(11')-C(33')	1.332(14)
O(9)-C(31)	1.457(14)	O(12')-C(33')	1.205(19)
O(10)-C(30)	1.469(12)	O(13')-C(16')	1.365(13)
O(10)-C(31)	1.415(17)	O(13')-C(17')	1.484(13)
O(11)-C(12)	1.459(13)	O(14')-C(16')	1.214(13)
O(11)-C(33)	1.367(14)	O(15')-C(21')	1.409(18)
O(12)-C(33)	1.200(17)	O(15')-C(23')	1.392(20)
O(13)-C(16)	1.323(13)	C(1')-C(2')	1.551(15)
O(13)-C(17)	1.464(13)	C(1')-C(10')	1.574(16)
O(14)-C(16)	1.251(14)	C(1')-C(29')	1.563(17)
O(15)-C(21)	1.391(17)	C(2')-C(3')	1.565(15)
O(15)-C(23)	1.364(22)	C(2')-C(30')	1.550(16)
C(1)-C(2)	1.548(16)	C(2')-H(2')	1.090(50)
C(1)-C(10)	1.586(16)	C(3')-C(4')	1.515(16)
C(1)-C(29)	1.539(16)	C(3')-H(3')	1.110(40)
C(2)-C(3)	1.534(16)	C(4')-C(5')	1.546(17)
C(2)-C(30)	1.519(17)	C(4')-C(28')	1.563(16)
C(2)-H(2)	1.090(50)	C(4')-C(29')	1.539(16)
C(3)-C(4)	1.558(16)	C(5')-C(6')	1.538(15)
C(3)-H(3)	1.100(30)	C(5')-C(10')	1.603(14)

C(4)-C(5)	1.542(17)	C(5')-H(5')	1.100(30)	C(20)-C(21)	1.388(21)	C(23')-H(23')	1.110(40)
C(4)-C(28)	1.546(16)	C(6')-C(7')	1.545(17)	C(20)-C(22)	1.428(19)	C(24')-C(25')	1.471(19)
C(4)-C(29)	1.514(17)	C(6')-H(6')	1.100(40)	C(21)-H(21)	1.110(50)	C(25')-H(25'A)	1.080(50)
C(5)-C(6)	1.512(16)	C(8')-C(9')	1.562(15)	C(22)-C(23)	1.365(23)	C(25')-H(25'B)	1.100(40)
C(5)-C(10)	1.584(15)	C(8')-C(14')	1.478(15)	C(22)-H(22)	1.090(30)	C(25')-H(25'C)	1.080(40)
C(5)-H(5)	1.110(30)	C(8')-C(30')	1.587(15)	C(23)-H(23)	1.110(60)	C(26')-C(27')	1.552(21)
C(6)-C(7)	1.568(17)	C(9')-C(10')	1.553(17)	C(24)-C(25)	1.505(19)	C(27')-H(27'A)	1.080(40)
C(6)-H(6)	1.090(30)	C(9')-C(11')	1.537(16)	C(25)-H(25A)	1.070(50)	C(27')-H(27'B)	1.100(40)
C(8)-C(9)	1.546(15)	C(10')-C(19')	1.537(15)	C(25)-H(25B)	1.110(50)	C(27')-H(27'C)	1.080(60)
C(8)-C(14)	1.505(15)	C(11')-C(12')	1.490(16)	C(25)-H(25C)	1.070(40)	C(28')-H(28'A)	1.070(40)
C(8)-C(30)	1.547(16)	C(11')-H(11'A)	1.070(40)	C(26)-C(27)	1.539(19)	C(28')-H(28'B)	1.090(50)
C(9)-C(10)	1.543(17)	C(11')-H(11'B)	1.090(40)	C(27)-H(27A)	1.100(40)	C(28')-H(28'C)	1.080(40)
C(9)-C(11)	1.541(16)	C(12')-C(13')	1.567(15)	C(27)-H(27B)	1.070(40)	C(29')-H(29'A)	1.100(50)
C(10)-C(19)	1.568(16)	C(12')-H(12')	1.090(40)	C(27)-H(27C)	1.110(60)	C(29')-H(29'B)	1.080(40)
C(11)-C(12)	1.539(16)	C(13')-C(14')	1.562(15)	C(28)-H(28A)	1.090(40)	C(30')-H(30')	1.110(40)
C(11)-H(11A)	1.100(40)	C(13')-C(17')	1.533(15)	C(28)-H(28B)	1.080(40)	C(31')-C(32')	1.502(17)
C(11)-H(11B)	1.090(40)	C(13')-C(18')	1.524(16)	C(28)-H(28C)	1.080(50)	C(32')-H(32'A)	1.110(30)
C(12)-C(13)	1.593(16)	C(14')-C(15')	1.337(15)	C(29)-H(29A)	1.100(50)	C(32')-H(32'B)	1.070(50)
C(12)-H(12)	1.110(40)	C(15')-C(16')	1.433(16)	C(29)-H(29B)	1.080(40)	C(32')-H(32'C)	1.090(40)
C(13)-C(14)	1.502(15)	C(15')-H(15')	1.100(50)	C(30)-H(30)	1.110(40)	C(33')-C(34')	1.499(19)
C(13)-C(17)	1.541(16)	C(17')-C(20')	1.495(17)	C(31)-C(32)	1.492(17)	C(34')-H(34'A)	1.080(40)
C(13)-C(18)	1.521(16)	C(17')-H(17')	1.110(30)	C(32)-H(32A)	1.100(40)	C(34')-H(34'B)	1.080(60)
C(14)-C(15)	1.339(14)	C(18')-H(18'A)	1.080(50)	C(32)-H(32B)	1.080(40)	C(34')-H(34'C)	1.080(40)
C(15)-C(16)	1.497(16)	C(18')-H(18'B)	1.080(50)	C(32)-H(32C)	1.090(50)	C(35')-H(35'A)	1.080(50)
C(15)-H(15)	1.110(50)	C(18')-H(18'C)	1.090(40)	C(33)-C(34)	1.507(19)	C(35')-H(35'B)	1.110(40)
C(17)-C(20)	1.503(16)	C(19')-H(19'A)	1.070(30)	C(34)-H(34A)	1.080(50)	C(35')-H(35'C)	1.080(50)
C(17)-H(17)	1.110(30)	C(19')-H(19'B)	1.070(50)	C(34)-H(34B)	1.100(50)	Om-Cm	1.460(50)
C(18)-H(18A)	1.080(50)	C(19')-H(19'C)	1.110(50)	C(34)-H(34C)	1.090(40)	Om-Hom	1.080(20)
C(18)-H(18B)	1.070(40)	C(20')-C(21')	1.382(20)	C(35)-H(35A)	1.080(50)	Cm-Hcma	1.110(50)
C(18)-H(18C)	1.100(50)	C(20')-C(22')	1.440(20)	C(35)-H(35B)	1.110(40)	Cm-Hcmb	1.070(50)
C(19)-H(19A)	1.080(30)	C(21')-H(21')	1.110(30)	C(35)-H(35C)	1.050(50)	Cm-Hcmc	1.110(70)
C(19)-H(19B)	1.090(50)	C(22')-C(23')	1.367(19)	O(1')-C(1')	1.416(14)	Om(')-Cm(')	1.430(50)
C(19)-H(19C)	1.100(50)	C(22')-H(22')	1.110(50)	O(1')-Ho(1')	1.090(40)	Om(')-Hom(')	1.080(30)

O(2')-C(3')	1.479(14)	Cm(')-Hcm('A)	1.080(30)
O(2')-C(24')	1.343(15)	Cm(')-Hcm('B)	1.080(30)
O(3')-C(24')	1.222(17)	Cm(')-Hcm('C)	1.080(40)

Table 4. Bond Angles

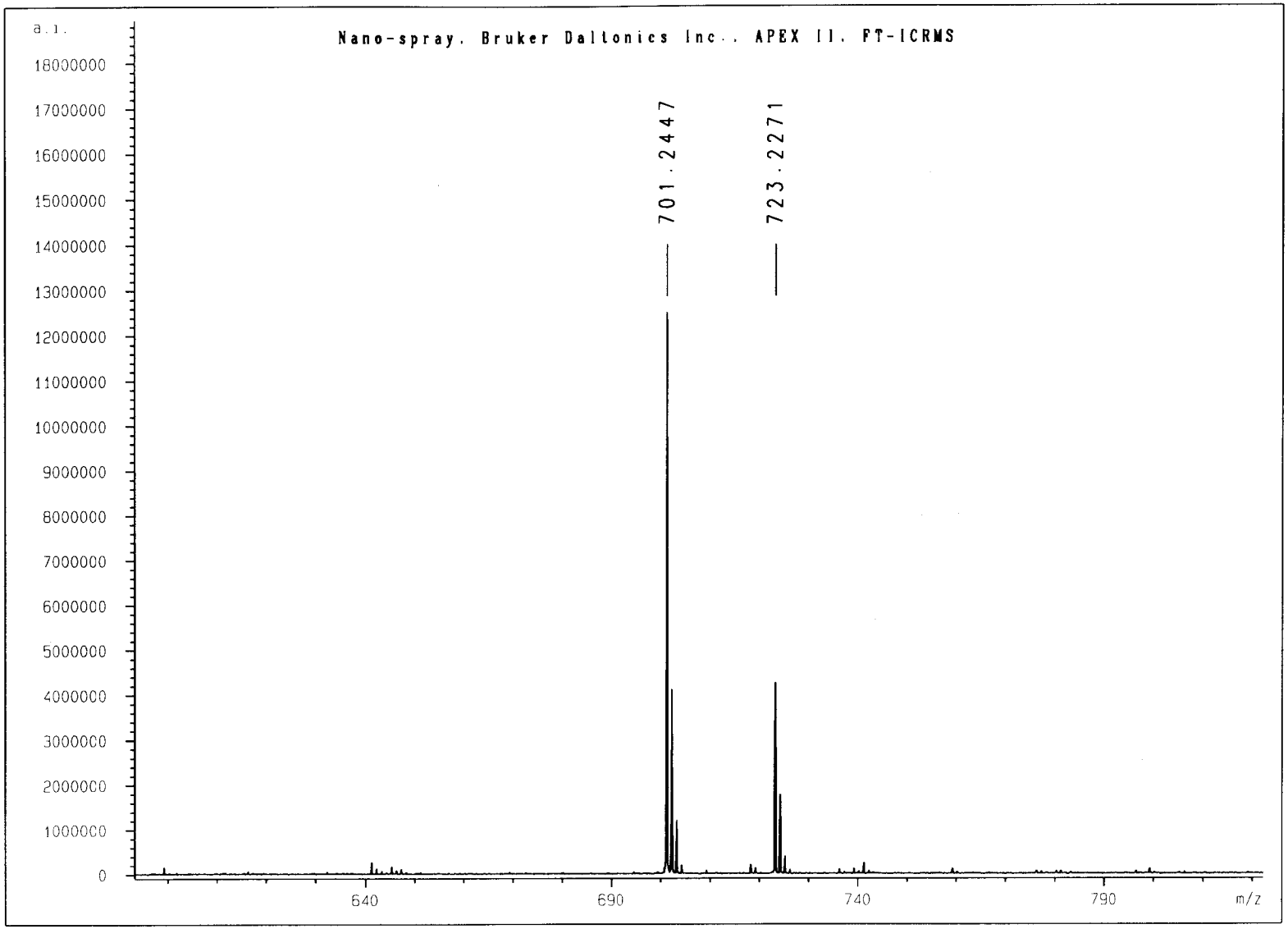
C(1)-O(1)-Ho(1)	109.1(21)	C(12')-O(11')-C(33')	117.9(10)
C(3)-O(2)-C(24)	115.5(9)	C(16')-O(13')-C(17')	115.6(8)
C(7)-O(5)-C(35)	112.2(11)	C(21')-O(15')-C(23')	109.1(10)
C(6)-O(6)-C(26)	116.2(9)	O(1')-C(1')-C(2')	115.1(9)
C(8)-O(8)-C(31)	95.4(9)	O(1')-C(1')-C(10')	117.4(9)
C(9)-O(9)-C(31)	105.7(8)	O(1')-C(1')-C(29')	111.1(10)
C(30)-O(10)-C(31)	105.5(8)	C(2')-C(1')-C(10')	107.8(9)
C(12)-O(11)-C(33)	116.6(9)	C(2')-C(1')-C(29')	101.4(9)
C(16)-O(13)-C(17)	117.6(9)	C(10')-C(1')-C(29')	102.1(9)
C(21)-O(15)-C(23)	109.6(12)	C(1')-C(2')-C(3')	101.9(9)
O(1)-C(1)-C(2)	116.8(9)	C(1')-C(2')-C(30')	116.0(9)
O(1)-C(1)-C(10)	115.6(9)	C(1')-C(2')-H(2')	106.2(20)
O(1)-C(1)-C(29)	109.1(9)	C(3')-C(2')-C(30')	119.1(9)
C(2)-C(1)-C(10)	109.0(9)	C(3')-C(2')-H(2')	106.5(24)
C(2)-C(1)-C(29)	103.0(9)	C(30')-C(2')-H(2')	106.2(23)
C(10)-C(1)-C(29)	101.4(9)	O(2')-C(3')-C(2')	115.4(9)
C(1)-C(2)-C(3)	101.7(9)	O(2')-C(3')-C(4')	110.2(9)
C(1)-C(2)-C(30)	115.2(9)	O(2')-C(3')-H(3')	109.9(19)
C(1)-C(2)-H(2)	106.0(21)	C(2')-C(3')-C(4')	103.6(8)
C(3)-C(2)-C(30)	119.4(10)	C(2')-C(3')-H(3')	108.0(30)
C(3)-C(2)-H(2)	106.7(23)	C(4')-C(3')-H(3')	109.0(30)
C(30)-C(2)-H(2)	106.9(23)	C(3')-C(4')-C(5')	111.3(9)
O(2)-C(3)-C(2)	117.5(10)	C(3')-C(4')-C(28')	108.5(9)
O(2)-C(3)-C(4)	110.1(9)	C(3')-C(4')-C(29')	97.8(9)
O(2)-C(3)-H(3)	109.6(20)	C(5')-C(4')-C(28')	117.4(9)
C(2)-C(3)-C(4)	104.2(9)	C(5')-C(4')-C(29')	105.3(9)
C(2)-C(3)-H(3)	107.0(30)	C(28')-C(4')-C(29')	114.8(10)
C(4)-C(3)-H(3)	107.0(30)	C(4')-C(5')-C(6')	117.7(9)
C(3)-C(4)-C(5)	108.6(9)	C(4')-C(5')-C(10')	102.8(9)
C(3)-C(4)-C(28)	109.3(9)	C(4')-C(5')-H(5')	107.1(22)
C(3)-C(4)-C(29)	98.0(9)	C(6')-C(5')-C(10')	114.4(8)
C(5)-C(4)-C(28)	117.6(9)	C(6')-C(5')-H(5')	107.0(30)
C(5)-C(4)-C(29)	104.0(9)	C(10')-C(5')-H(5')	107.0(30)

C(28)-C(4)-C(29)	117.5(10)	O(6')-C(6')-C(5')	109.3(9)	C(9)-C(10)-C(19)	108.4(9)	O(11')-C(12')-C(11')	105.4(8)
C(4)-C(5)-C(6)	116.9(10)	O(6')-C(6')-C(7')	111.0(9)	C(9)-C(11)-C(12)	110.9(9)	O(11')-C(12')-C(13')	106.0(9)
C(4)-C(5)-C(10)	104.5(9)	O(6')-C(6')-H(6')	110.6(19)	C(9)-C(11)-H(11A)	110.0(20)	O(11')-C(12')-H(12')	111.0(30)
C(4)-C(5)-H(5)	107.3(21)	C(5')-C(6')-C(7')	107.5(8)	C(9)-C(11)-H(11B)	110.0(30)	C(11')-C(12')-C(13')	114.8(9)
C(6)-C(5)-C(10)	112.4(9)	C(5')-C(6')-H(6')	108.0(30)	C(12)-C(11)-H(11A)	109.0(30)	C(11')-C(12')-H(12')	109.8(21)
C(6)-C(5)-H(5)	107.0(30)	C(7')-C(6')-H(6')	110.0(30)	C(12)-C(11)-H(11B)	108.8(23)	C(13')-C(12')-H(12')	109.0(22)
C(10)-C(5)-H(5)	107.0(30)	O(4')-C(7')-O(5')	123.8(11)	H(11A)-C(11)-H(11B)	106.0(30)	C(12')-C(13')-C(14')	108.6(9)
O(6)-C(6)-C(5)	108.7(10)	O(4')-C(7')-C(6')	124.1(10)	O(11)-C(12)-C(11)	105.5(8)	C(12')-C(13')-C(17')	107.5(8)
O(6)-C(6)-C(7)	112.1(9)	O(5')-C(7')-C(6')	112.0(11)	O(11)-C(12)-C(13)	106.3(9)	C(12')-C(13')-C(18')	111.8(9)
O(6)-C(6)-H(6)	109.1(19)	O(8')-C(8')-C(9')	101.2(8)	O(11)-C(12)-H(12)	113.0(30)	C(14')-C(13')-C(17')	103.4(8)
C(5)-C(6)-C(7)	109.7(9)	O(8')-C(8')-C(14')	107.0(8)	C(11)-C(12)-C(13)	112.0(8)	C(14')-C(13')-C(18')	108.2(8)
C(5)-C(6)-H(6)	107.0(30)	O(8')-C(8')-C(30')	98.4(7)	C(11)-C(12)-H(12)	110.0(22)	C(17')-C(13')-C(18')	116.7(10)
C(7)-C(6)-H(6)	109.0(30)	C(9')-C(8')-C(14')	118.1(9)	C(13)-C(12)-H(12)	109.8(22)	C(8')-C(14')-C(13')	119.5(9)
O(4)-C(7)-O(5)	126.5(11)	C(9')-C(8')-C(30')	107.5(9)	C(12)-C(13)-C(14)	108.4(9)	C(8')-C(14')-C(15')	122.3(10)
O(4)-C(7)-C(6)	123.9(10)	C(14')-C(8')-C(30')	120.9(9)	C(12)-C(13)-C(17)	105.6(8)	C(13')-C(14')-C(15')	117.5(10)
O(5)-C(7)-C(6)	109.6(10)	O(9')-C(9')-C(8')	97.4(7)	C(12)-C(13)-C(18)	112.3(9)	C(14')-C(15')-C(16')	122.2(10)
O(8)-C(8)-C(9)	101.3(7)	O(9')-C(9')-C(10')	104.2(9)	C(14)-C(13)-C(17)	105.5(9)	C(14')-C(15')-H(15')	118.9(20)
O(8)-C(8)-C(14)	105.9(9)	O(9')-C(9')-C(11')	106.6(8)	C(14)-C(13)-C(18)	111.4(9)	C(16')-C(15')-H(15')	118.8(20)
O(8)-C(8)-C(30)	100.5(8)	C(8')-C(9')-C(10')	118.8(9)	C(17)-C(13)-C(18)	113.1(9)	O(13')-C(16')-O(14')	115.6(10)
C(9)-C(8)-C(14)	115.4(9)	C(8')-C(9')-C(11')	109.1(9)	C(8)-C(14)-C(13)	122.3(9)	O(13')-C(16')-C(15')	119.0(9)
C(9)-C(8)-C(30)	107.6(9)	C(10')-C(9')-C(11')	117.8(9)	C(8)-C(14)-C(15)	118.7(10)	O(14')-C(16')-C(15')	125.5(10)
C(14)-C(8)-C(30)	122.8(8)	C(1')-C(10')-C(5')	101.4(8)	C(13)-C(14)-C(15)	117.9(10)	O(13')-C(17')-C(13')	108.5(8)
O(9)-C(9)-C(8)	98.2(7)	C(1')-C(10')-C(9')	112.9(9)	C(14)-C(15)-C(16)	120.8(10)	O(13')-C(17')-C(20')	104.1(9)
O(9)-C(9)-C(10)	105.0(8)	C(1')-C(10')-C(19')	107.9(9)	C(14)-C(15)-H(15)	120.2(21)	O(13')-C(17')-H(17')	110.0(22)
O(9)-C(9)-C(11)	104.2(8)	C(5')-C(10')-C(9')	111.6(9)	C(16)-C(15)-H(15)	119.1(20)	C(13')-C(17')-C(20')	116.4(10)
C(8)-C(9)-C(10)	120.0(9)	C(5')-C(10')-C(19')	114.2(9)	O(13)-C(16)-O(14)	119.7(11)	C(13')-C(17')-H(17')	108.5(24)
C(8)-C(9)-C(11)	110.1(9)	C(9')-C(10')-C(19')	108.8(9)	O(13)-C(16)-C(15)	118.2(10)	C(20')-C(17')-H(17')	109.0(30)
C(10)-C(9)-C(11)	116.1(9)	C(9')-C(11')-C(12')	112.1(9)	O(14)-C(16)-C(15)	122.0(10)	C(13')-C(18')-H(18'A)	110.0(30)
C(1)-C(10)-C(5)	99.5(8)	C(9')-C(11')-H(11'A)	109.0(30)	O(13)-C(17)-C(13)	108.4(9)	C(13')-C(18')-H(18'B)	109.9(18)
C(1)-C(10)-C(9)	110.5(9)	C(9')-C(11')-H(11'B)	107.9(20)	O(13)-C(17)-C(20)	104.9(9)	C(13')-C(18')-H(18'C)	109.4(20)
C(1)-C(10)-C(19)	108.4(9)	C(12')-C(11')-H(11'A)	109.4(22)	O(13)-C(17)-H(17)	109.9(23)	H(18'A)-C(18')-H(18'B)	109.0(30)
C(5)-C(10)-C(9)	112.5(9)	C(12')-C(11')-H(11'B)	108.0(30)	C(13)-C(17)-C(20)	117.1(10)	H(18'A)-C(18')-H(18'C)	108.0(30)
C(5)-C(10)-C(19)	117.1(9)	H(11'A)-C(11')-H(11'B)	109.0(30)	C(13)-C(17)-H(17)	108.4(25)	H(18'B)-C(18')-H(18'C)	108.0(40)

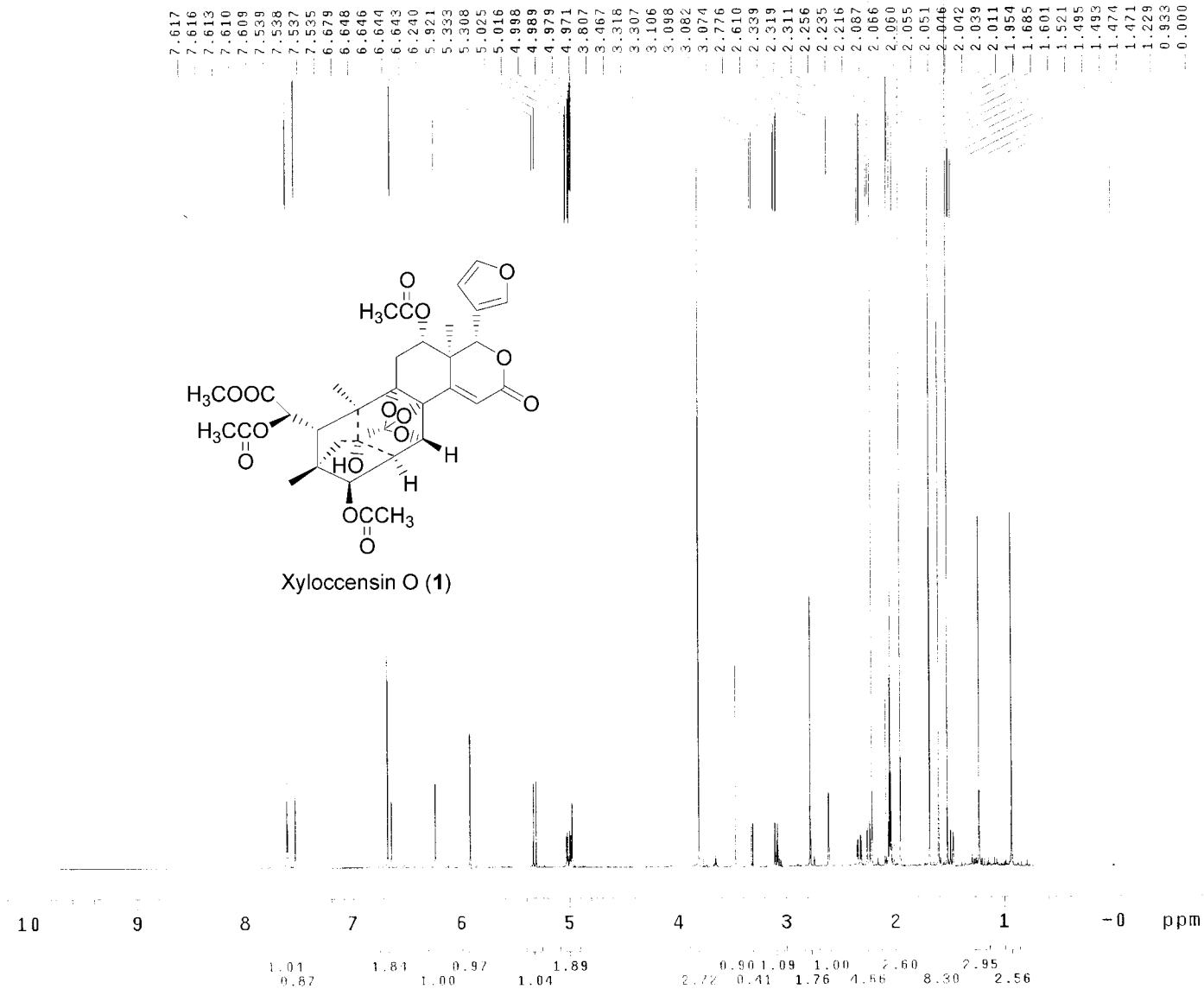
C(20)-C(17)-H(17)	108.0(30)	C(10')-C(19')-H(19'A)	111.3(23)	H(25B)-C(25)-H(25C)	107.0(30)	H(27'A)-C(27')-H(27'B)	108.0(30)
C(13)-C(18)-H(18A)	110.5(17)	C(10')-C(19')-H(19'B)	110.0(30)	O(6)-C(26)-O(7)	123.3(12)	H(27'A)-C(27')-H(27'C)	109.0(40)
C(13)-C(18)-H(18B)	110.5(20)	C(10')-C(19')-H(19'C)	108.8(20)	O(6)-C(26)-C(27)	110.8(10)	H(27'B)-C(27')-H(27'C)	107.0(40)
C(13)-C(18)-H(18C)	109.1(25)	H(19'A)-C(19')-H(19'B)	111.0(30)	O(7)-C(26)-C(27)	125.9(11)	C(4')-C(28')-H(28'A)	109.0(30)
H(18A)-C(18)-H(18B)	109.0(40)	H(19'A)-C(19')-H(19'C)	107.0(40)	C(26)-C(27)-H(27A)	112.2(20)	C(4')-C(28')-H(28'B)	110.1(23)
H(18A)-C(18)-H(18C)	107.0(30)	H(19'B)-C(19')-H(19'C)	107.0(30)	C(26)-C(27)-H(27B)	113.8(18)	C(4')-C(28')-H(28'C)	109.7(24)
H(18B)-C(18)-H(18C)	108.0(30)	C(17')-C(20')-C(21')	121.0(13)	C(26)-C(27)-H(27C)	110.0(19)	H(28'A)-C(28')-H(28'B)	109.0(30)
C(10)-C(19)-H(19A)	112.1(22)	C(17')-C(20')-C(22')	132.5(12)	H(27A)-C(27)-H(27B)	108.0(30)	H(28'A)-C(28')-H(28'C)	109.0(30)
C(10)-C(19)-H(19B)	110.0(30)	C(21')-C(20')-C(22')	106.4(12)	H(27A)-C(27)-H(27C)	104.0(30)	H(28'B)-C(28')-H(28'C)	108.0(40)
C(10)-C(19)-H(19C)	109.9(20)	O(15')-C(21')-C(20')	107.9(14)	H(27B)-C(27)-H(27C)	107.0(40)	C(1')-C(29')-C(4')	93.6(9)
H(19A)-C(19)-H(19B)	108.0(30)	O(15')-C(21')-H(21')	124.0(30)	C(4)-C(28)-H(28A)	109.0(23)	C(1')-C(29')-H(29'A)	114.3(21)
H(19A)-C(19)-H(19C)	107.0(40)	C(20')-C(21')-H(21')	127.0(30)	C(4)-C(28)-H(28B)	110.0(30)	C(1')-C(29')-H(29'B)	115.0(30)
H(19B)-C(19)-H(19C)	107.0(30)	C(20')-C(22')-C(23')	109.2(13)	C(4)-C(28)-H(28C)	110.9(23)	C(4')-C(29')-H(29'A)	112.0(30)
C(17)-C(20)-C(21)	128.1(11)	C(20')-C(22')-H(22')	123.6(24)	H(28A)-C(28)-H(28B)	108.0(30)	C(4')-C(29')-H(29'B)	113.2(22)
C(17)-C(20)-C(22)	124.3(12)	C(23')-C(22')-H(22')	127.0(30)	H(28A)-C(28)-H(28C)	108.0(40)	H(29'A)-C(29')-H(29'B)	107.0(30)
C(21)-C(20)-C(22)	107.7(12)	O(15')-C(23')-C(22')	107.3(12)	H(28B)-C(28)-H(28C)	109.0(30)	O(10')-C(30')-C(2')	104.9(8)
O(15)-C(21)-C(20)	106.7(13)	O(15')-C(23')-H(23')	126.0(30)	C(1)-C(29)-C(4)	94.6(9)	O(10')-C(30')-C(8')	100.4(8)
O(15)-C(21)-H(21)	128.3(25)	C(22')-C(23')-H(23')	125.0(30)	C(1)-C(29)-H(29A)	112.8(21)	O(10')-C(30')-H(30')	111.0(30)
C(20)-C(21)-H(21)	125.0(23)	O(2')-C(24')-O(3')	118.6(12)	C(1)-C(29)-H(29B)	113.0(30)	C(2')-C(30')-C(8')	117.4(8)
C(20)-C(22)-C(23)	107.1(14)	O(2')-C(24')-C(25')	113.6(11)	C(4)-C(29)-H(29A)	113.0(30)	C(2')-C(30')-H(30')	110.9(18)
C(20)-C(22)-H(22)	124.0(30)	O(3')-C(24')-C(25')	127.8(12)	C(4)-C(29)-H(29B)	113.9(23)	C(8')-C(30')-H(30')	110.7(21)
C(23)-C(22)-H(22)	128.0(30)	C(24')-C(25')-H(25'A)	110.7(21)	H(29A)-C(29)-H(29B)	108.0(30)	O(8')-C(31')-O(9')	106.2(9)
O(15)-C(23)-C(22)	108.9(13)	C(24')-C(25')-H(25'B)	110.0(30)	O(10)-C(30)-C(2)	105.4(9)	O(8')-C(31')-O(10')	104.4(9)
O(15)-C(23)-H(23)	126.9(19)	C(24')-C(25')-H(25'C)	110.6(21)	O(10)-C(30)-C(8)	101.4(8)	O(8')-C(31')-C(32')	118.1(10)
C(22)-C(23)-H(23)	123.5(21)	H(25'A)-C(25')-H(25'B)	108.0(30)	O(10)-C(30)-H(30)	110.0(30)	O(9')-C(31')-O(10')	106.4(9)
O(2)-C(24)-O(3)	122.8(13)	H(25'A)-C(25')-H(25'C)	109.0(40)	C(2)-C(30)-C(8)	118.7(9)	O(9')-C(31')-C(32')	110.2(10)
O(2)-C(24)-C(25)	110.0(11)	H(25'B)-C(25')-H(25'C)	107.0(30)	C(2)-C(30)-H(30)	109.7(17)	O(10')-C(31')-C(32')	110.8(10)
O(3)-C(24)-C(25)	126.4(13)	O(6')-C(26')-O(7')	126.7(13)	C(8)-C(30)-H(30)	110.9(21)	C(31')-C(32')-H(32'A)	109.0(30)
C(24)-C(25)-H(25A)	111.2(22)	O(6')-C(26')-C(27')	106.4(12)	O(8)-C(31)-O(9)	101.9(9)	C(31')-C(32')-H(32'B)	112.6(25)
C(24)-C(25)-H(25B)	109.0(30)	O(7')-C(26')-C(27')	126.7(11)	O(8)-C(31)-O(10)	103.4(9)	C(31')-C(32')-H(32'C)	112.0(30)
C(24)-C(25)-H(25C)	110.7(23)	C(26')-C(27')-H(27'A)	110.5(21)	O(8)-C(31)-C(32)	114.1(12)	H(32'A)-C(32')-H(32'B)	107.0(40)
H(25A)-C(25)-H(25B)	107.0(30)	C(26')-C(27')-H(27'B)	110.4(19)	O(9)-C(31)-O(10)	108.5(11)	H(32'A)-C(32')-H(32'C)	106.0(30)
H(25A)-C(25)-H(25C)	110.0(40)	C(26')-C(27')-H(27'C)	110.7(19)	O(9)-C(31)-C(32)	110.9(10)	H(32'B)-C(32')-H(32'C)	108.0(30)

O(10)-C(31)-C(32)	116.9(10)	O(11')-C(33')-O(12')	123.8(12)
C(31)-C(32)-H(32A)	110.0(30)	O(11')-C(33')-C(34')	112.3(13)
C(31)-C(32)-H(32B)	111.0(30)	O(12')-C(33')-C(34')	123.7(11)
C(31)-C(32)-H(32C)	111.1(24)	C(33')-C(34')-H(34'A)	109.0(30)
H(32A)-C(32)-H(32B)	107.0(30)	C(33')-C(34')-H(34'B)	110.3(21)
H(32A)-C(32)-H(32C)	107.0(30)	C(33')-C(34')-H(34'C)	109.6(22)
H(32B)-C(32)-H(32C)	108.0(40)	H(34'A)-C(34')-H(34'B)	109.0(30)
O(11)-C(33)-O(12)	121.9(11)	H(34'A)-C(34')-H(34'C)	109.0(30)
O(11)-C(33)-C(34)	109.9(11)	H(34'B)-C(34')-H(34'C)	109.0(40)
O(12)-C(33)-C(34)	128.2(11)	O(5')-C(35')-H(35'A)	111.4(24)
C(33)-C(34)-H(34A)	110.4(19)	O(5')-C(35')-H(35'B)	109.0(30)
C(33)-C(34)-H(34B)	110.0(30)	O(5')-C(35')-H(35'C)	111.0(30)
C(33)-C(34)-H(34C)	110.4(23)	H(35'A)-C(35')-H(35'B)	107.0(40)
H(34A)-C(34)-H(34B)	108.0(30)	H(35'A)-C(35')-H(35'C)	109.0(30)
H(34A)-C(34)-H(34C)	108.0(40)	H(35'B)-C(35')-H(35'C)	107.0(30)
H(34B)-C(34)-H(34C)	107.0(30)	Cm-Om-Hom	109.5(25)
O(5)-C(35)-H(35A)	112.0(30)	Om-Cm-Hcma	113.0(30)
O(5)-C(35)-H(35B)	107.0(30)	Om-Cm-Hcmb	117.0(50)
O(5)-C(35)-H(35C)	113.0(30)	Om-Cm-Hcmc	108.0(30)
H(35A)-C(35)-H(35B)	104.0(40)	Hcma-Cm-Hcmb	105.0(40)
H(35A)-C(35)-H(35C)	112.0(30)	Hcma-Cm-Hcmc	103.0(50)
H(35B)-C(35)-H(35C)	106.0(30)	Hcmb-Cm-Hcmc	108.0(40)
C(1')-O(1')-Ho(1')	108.0(30)	Cm(')-Om(')-Hom(')	109.0(40)
C(3')-O(2')-C(24')	118.7(9)	Om(')-Cm(')-Hcm('A)	106.0(30)
C(7')-O(5')-C(35')	114.8(11)	Om(')-Cm(')-Hcm('B)	106.0(30)
C(6')-O(6')-C(26')	112.3(10)	Om(')-Cm(')-Hcm('C)	107.3(25)
C(8')-O(8')-C(31')	96.7(7)	Hcm('A)-Cm(')-Hcm('B)	109.5(24)
C(9')-O(9')-C(31')	104.9(8)	Hcm('A)-Cm(')-Hcm('C)	113.0(30)
C(30')-O(10')-C(31')	104.4(8)	Hcm('B)-Cm(')-Hcm('C)	113.0(30)

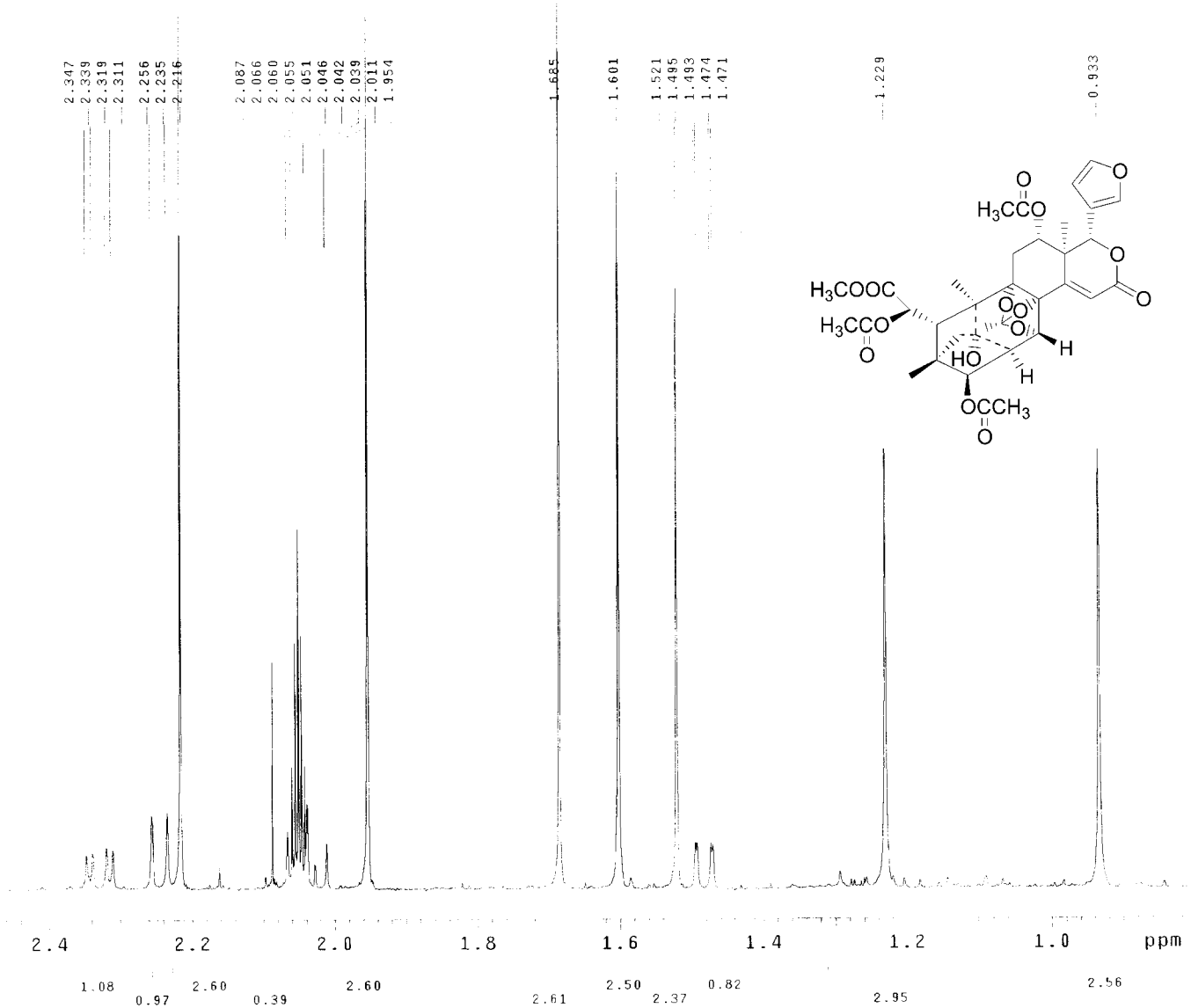
HR-ESIMS of xyloccensin O (**1**)



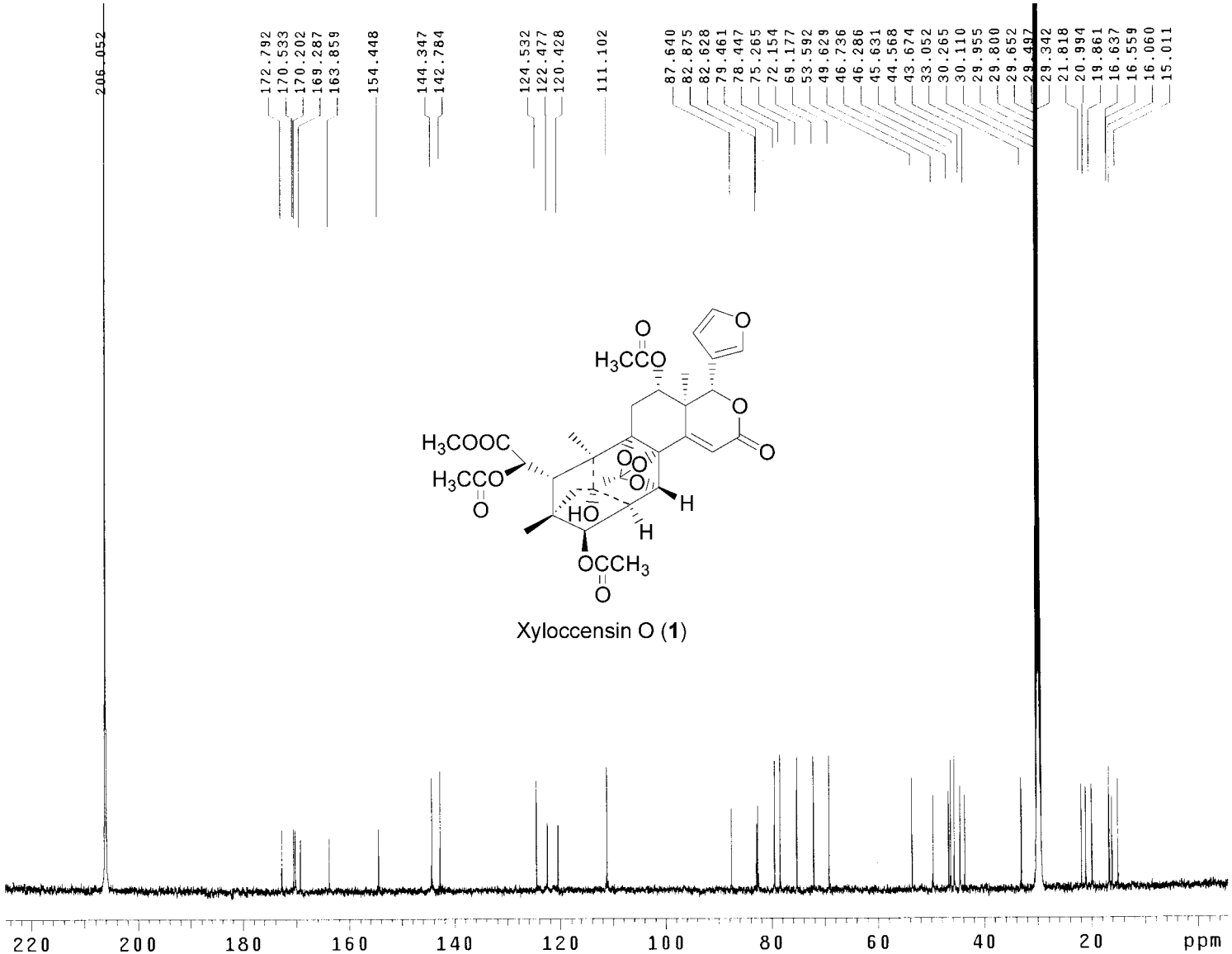
^{1}H NMR (500 MHz) of xyloccensin O (**1**) in acetone-d_6



^{1}H NMR (500 MHz) of xyloccensin O (**1**) in acetone-d_6

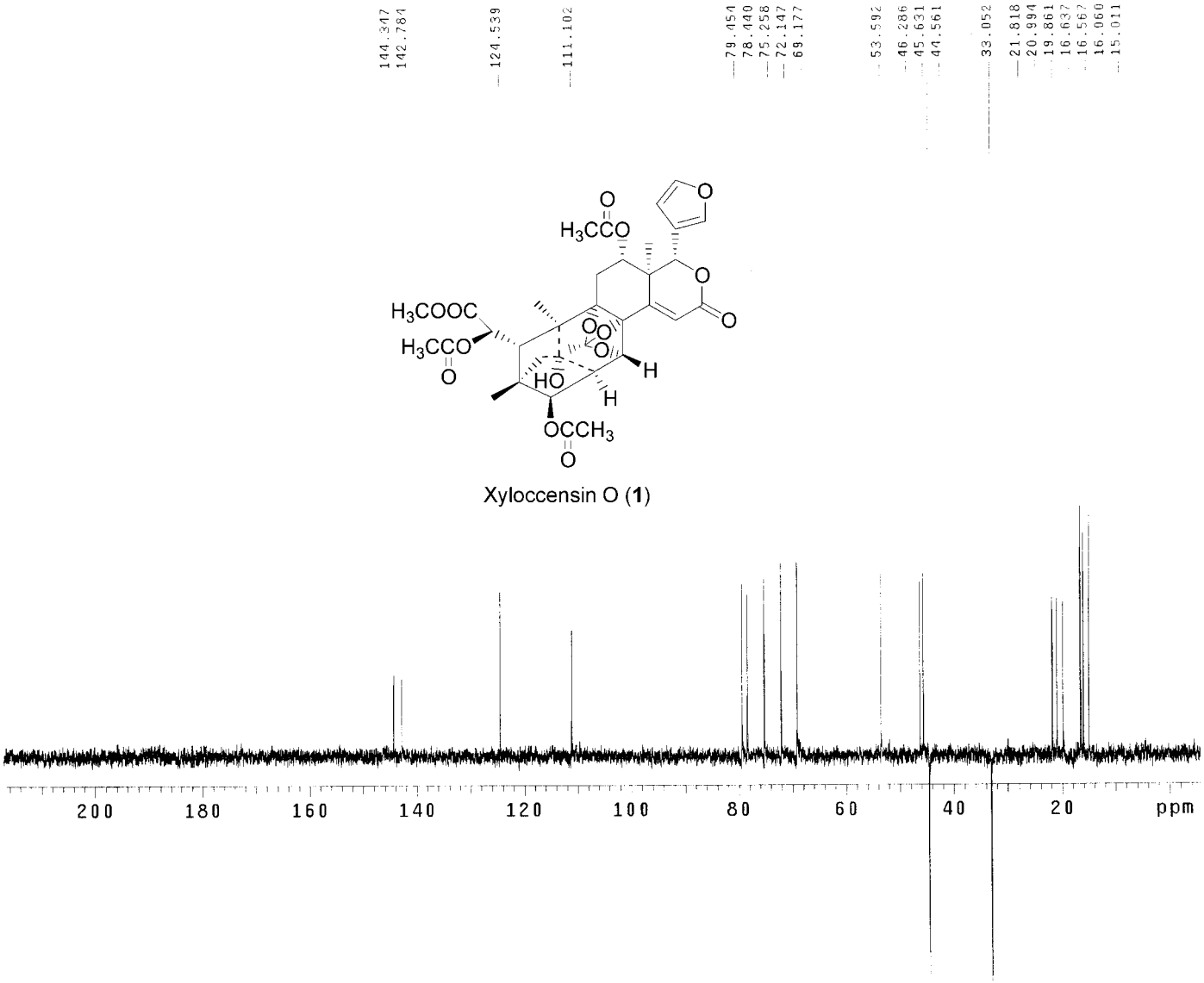


^{13}C NMR (125 MHz) of xyloccensin O (**1**) in acetone-d_6

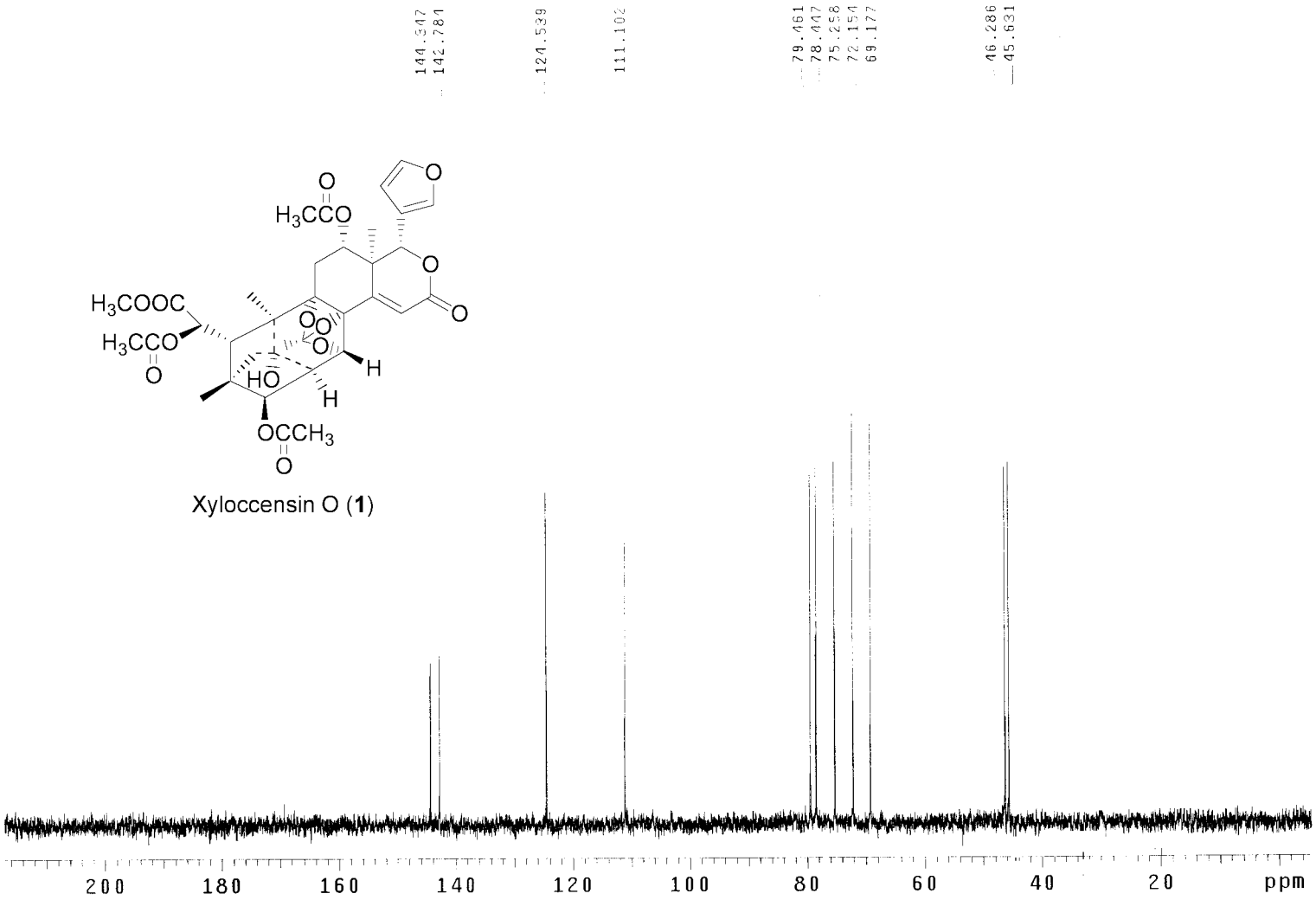


Xyloccensin O (**1**)

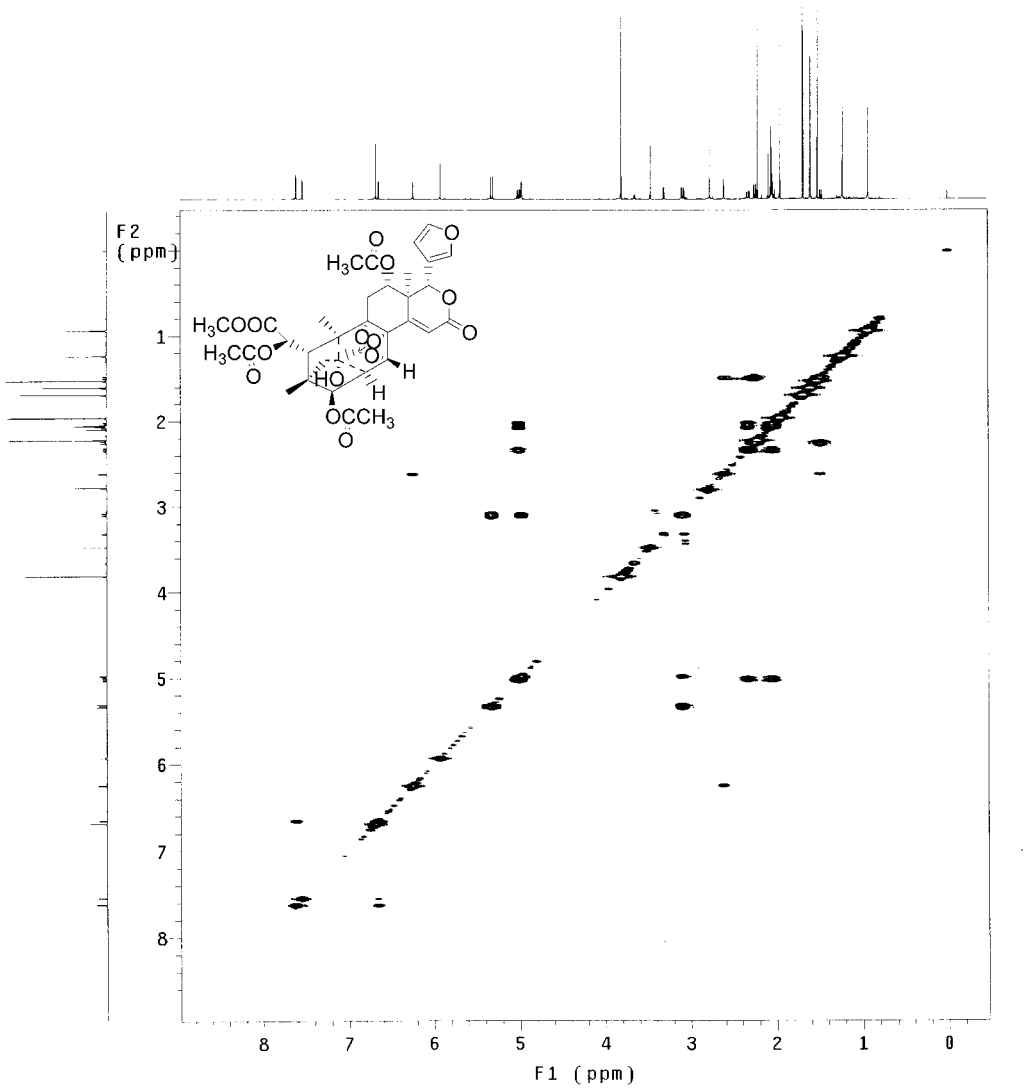
DEPT 135° experiment of xyloccensin O (1) in acetone-d_6



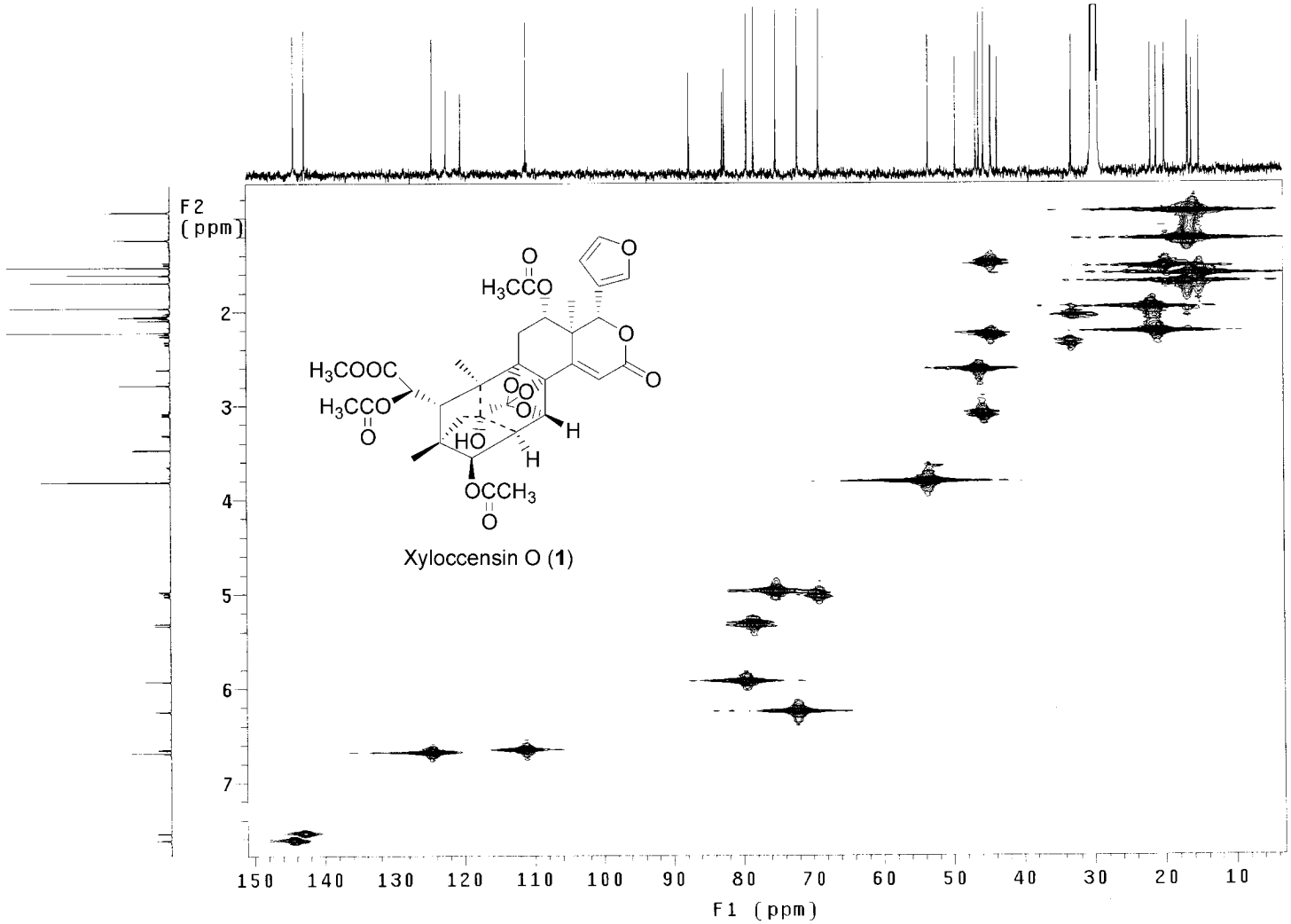
DEPT 90° experiment of xyloccensin O (1) in acetone-d_6



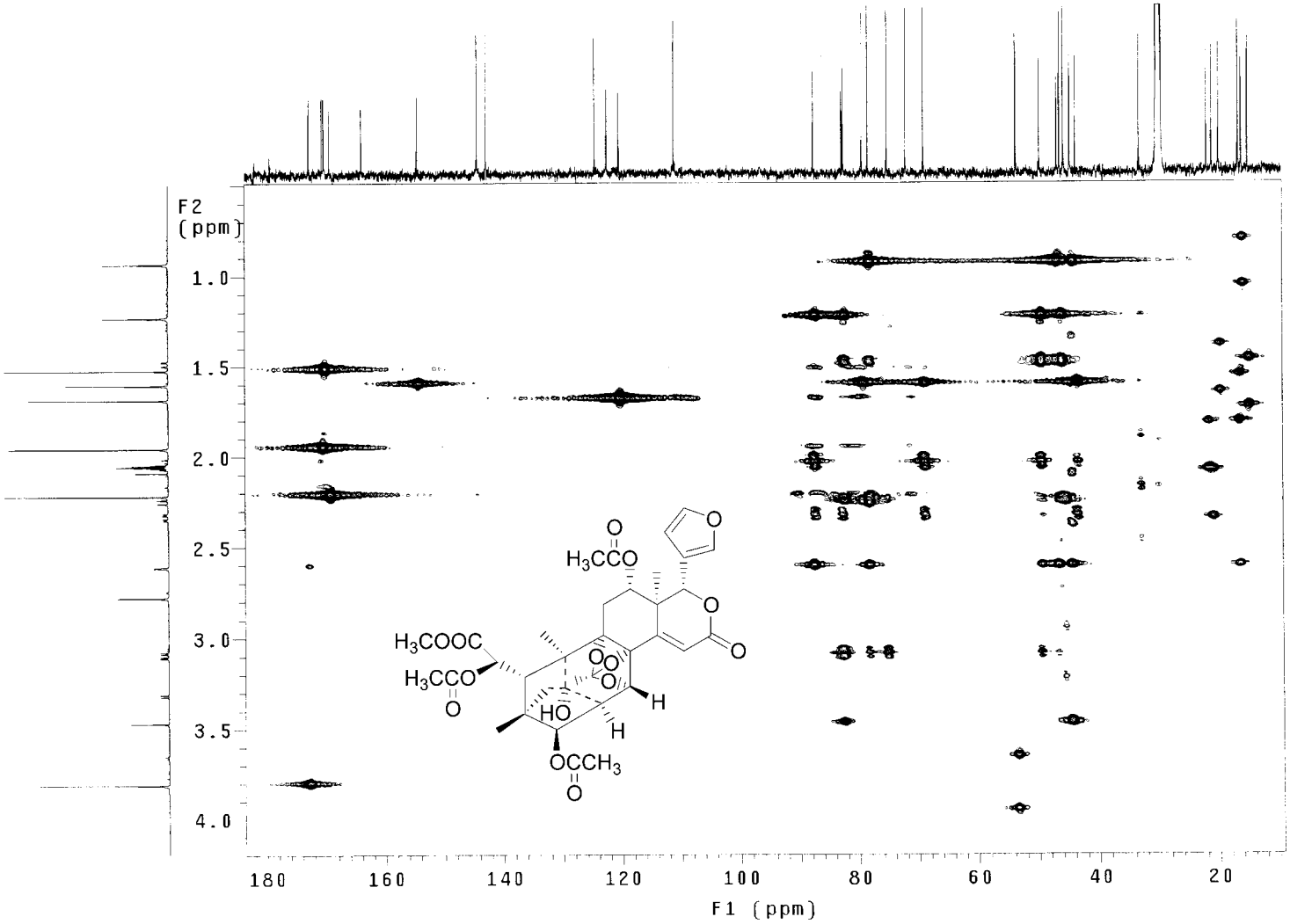
^{1}H-^{1}H COSY of xyloccensin O (**1**) in acetone-d_6



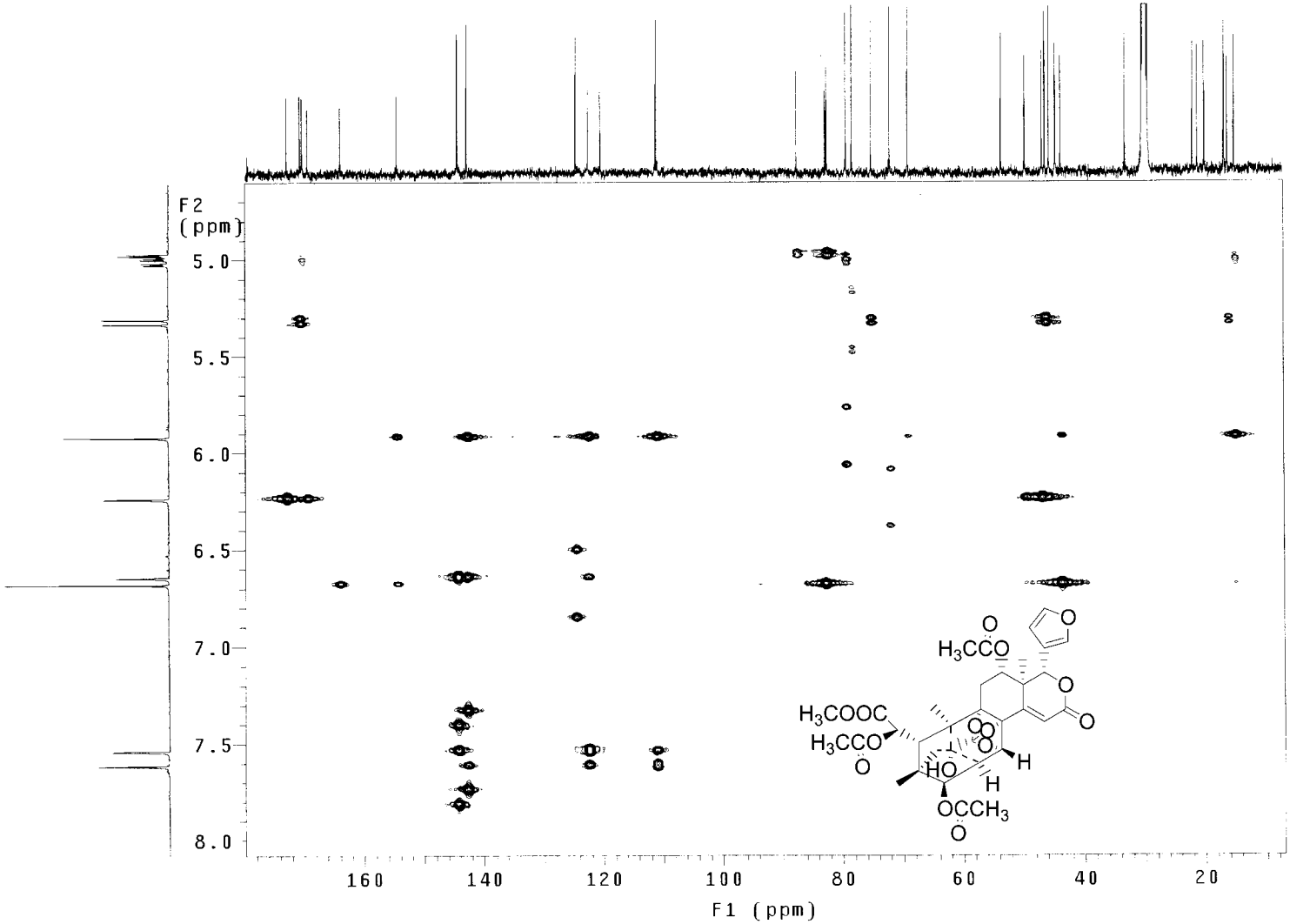
HMQC of xyloccensin O (**1**) in acetone-d_6



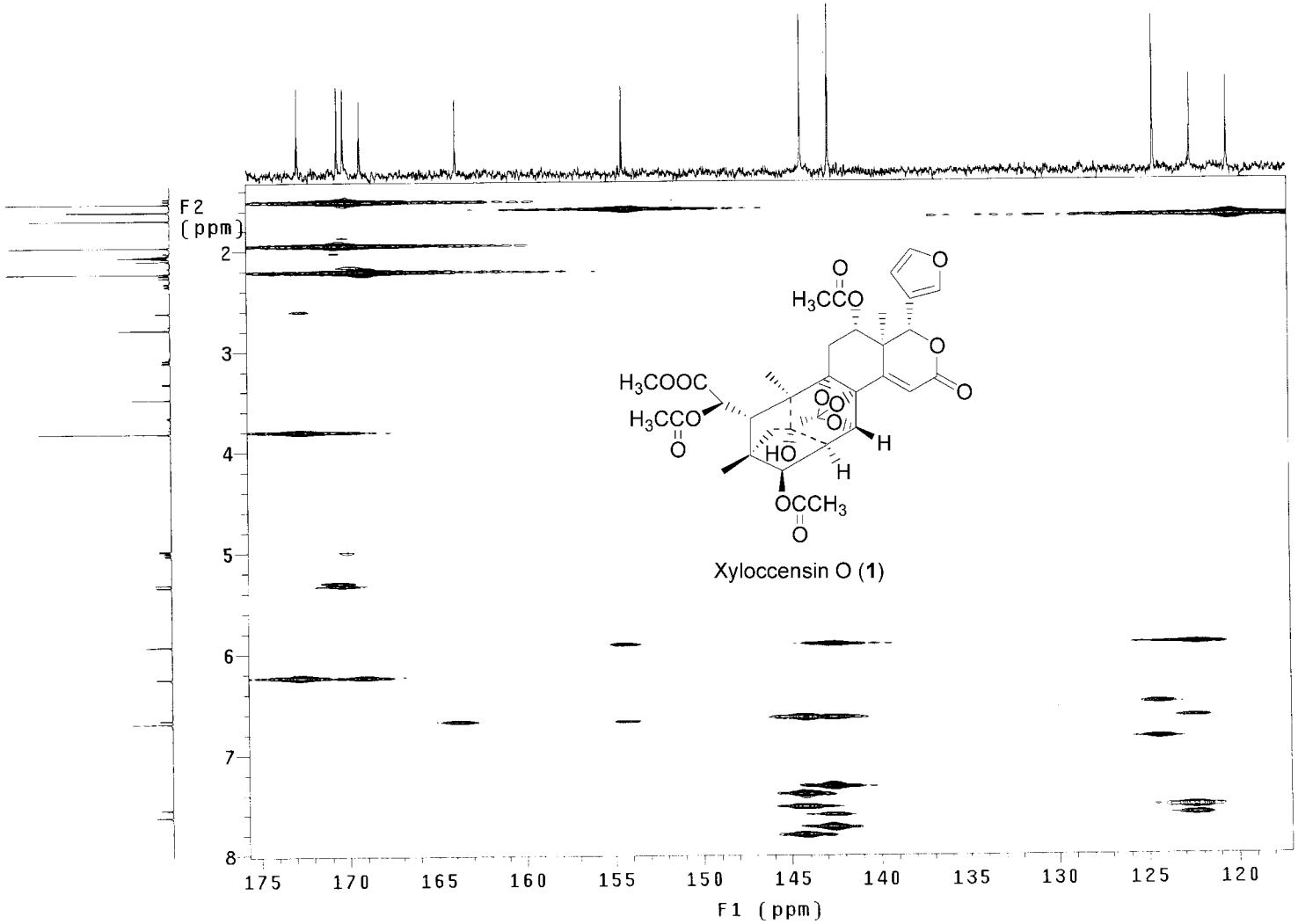
A segment of HMBC of xyloccensin O (**1**) in acetone-d_6



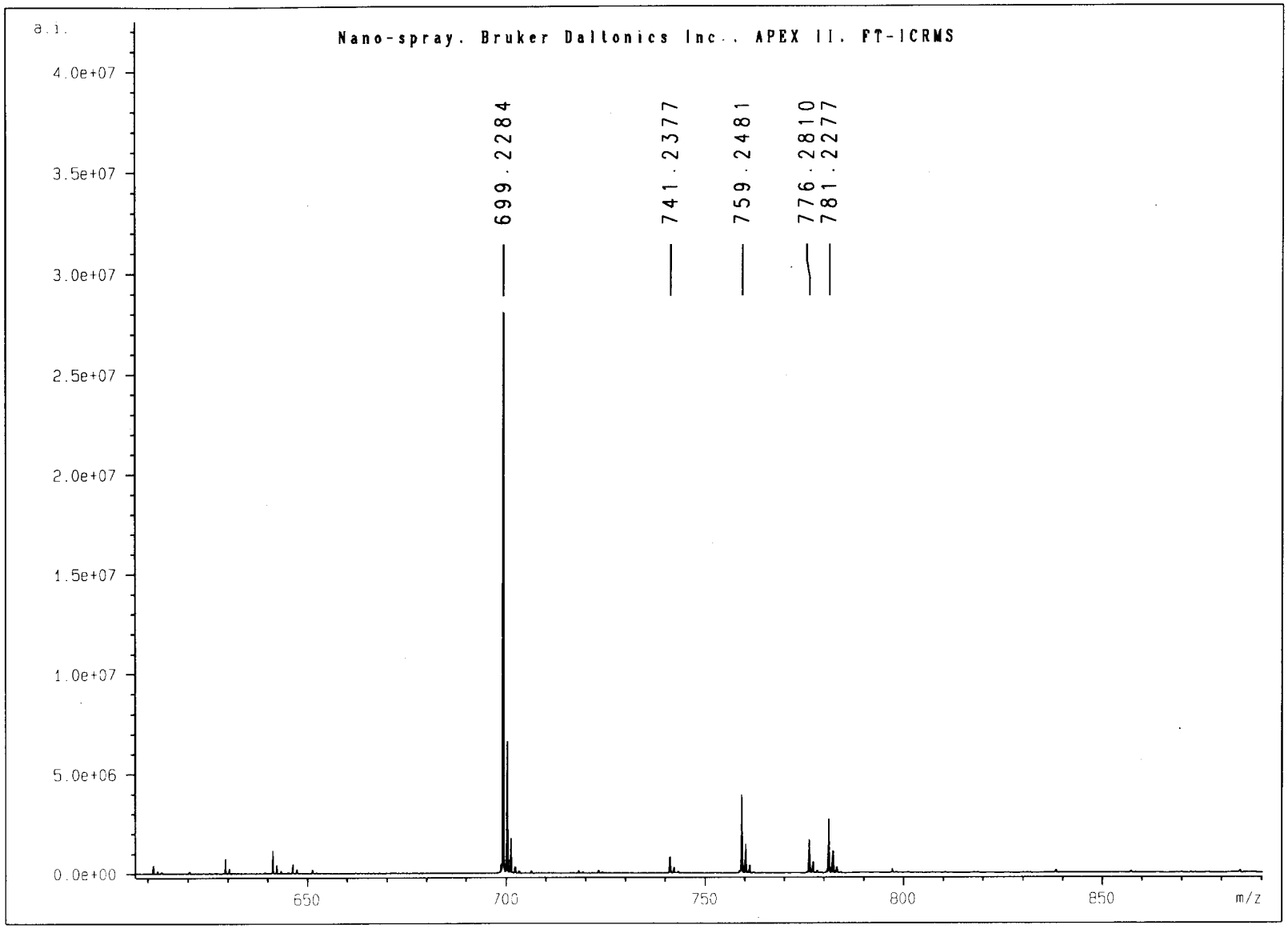
A segment of HMBC of xyloccensin O (**1**) in acetone-d_6



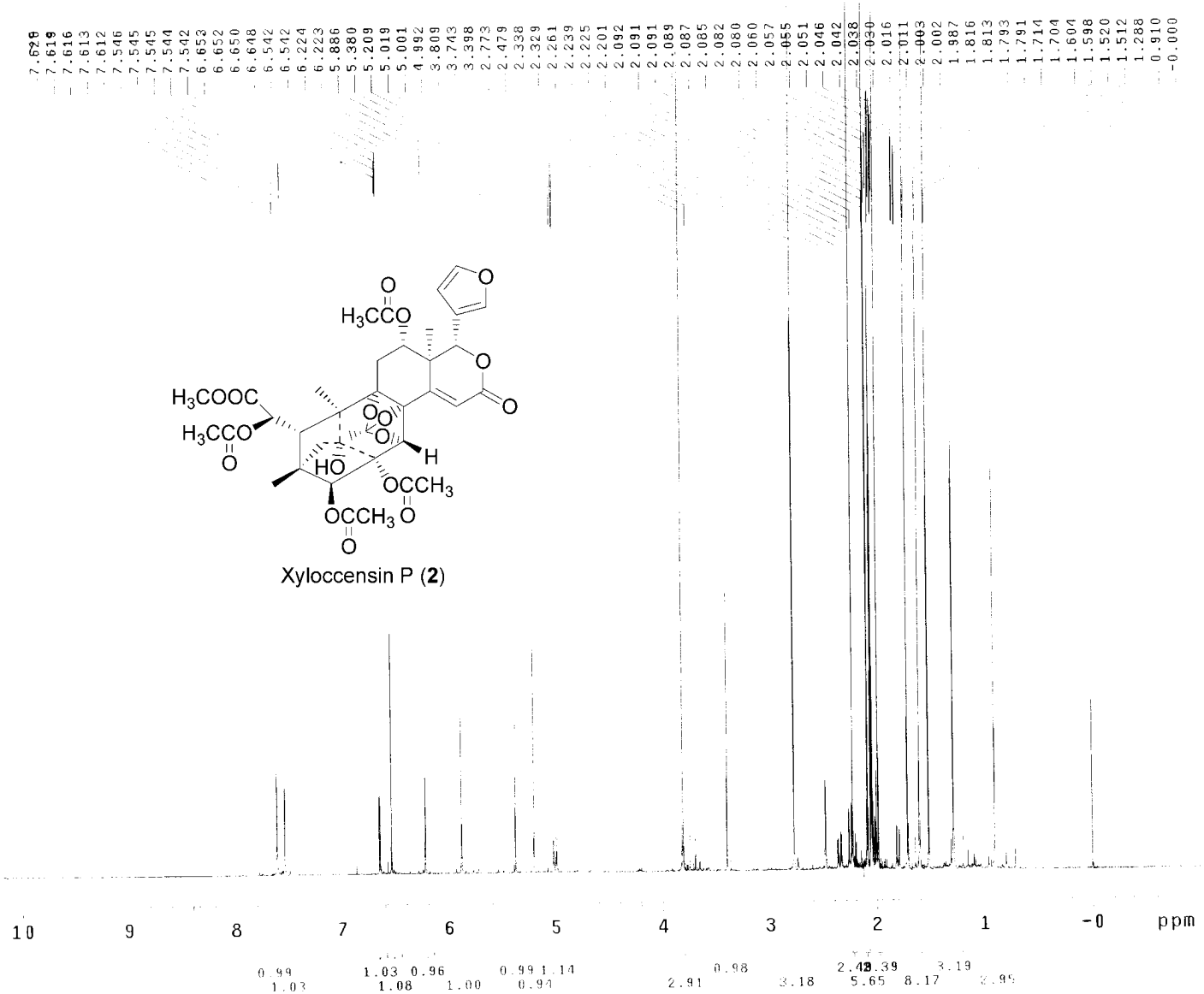
A segment of HMBC of xyloccensin O (**1**) in acetone-d_6



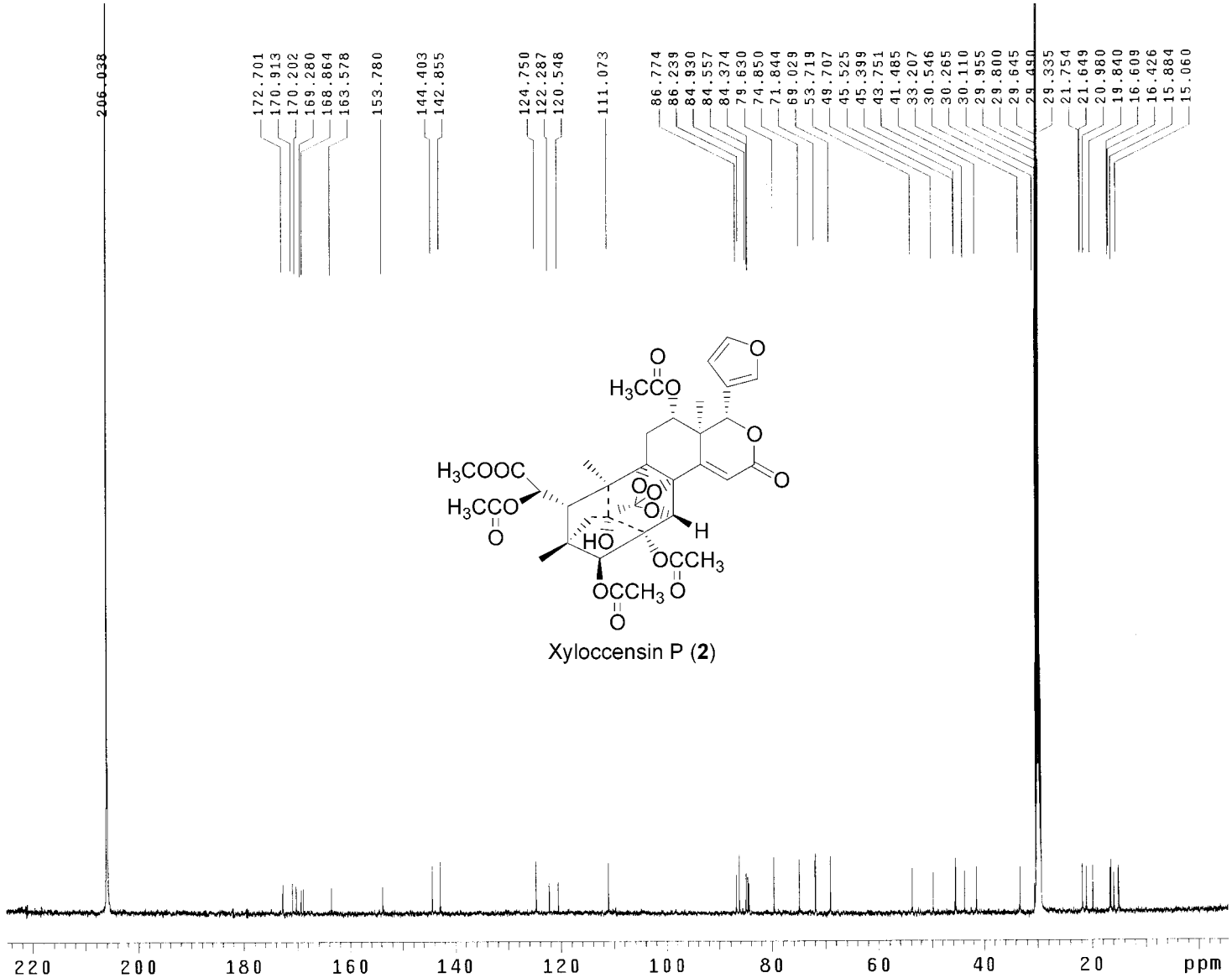
HR-ESIMS of xyloccensin P (**2**)



^{1}H NMR (500 MHz) of xyloccensin P (**2**) in acetone-d_6

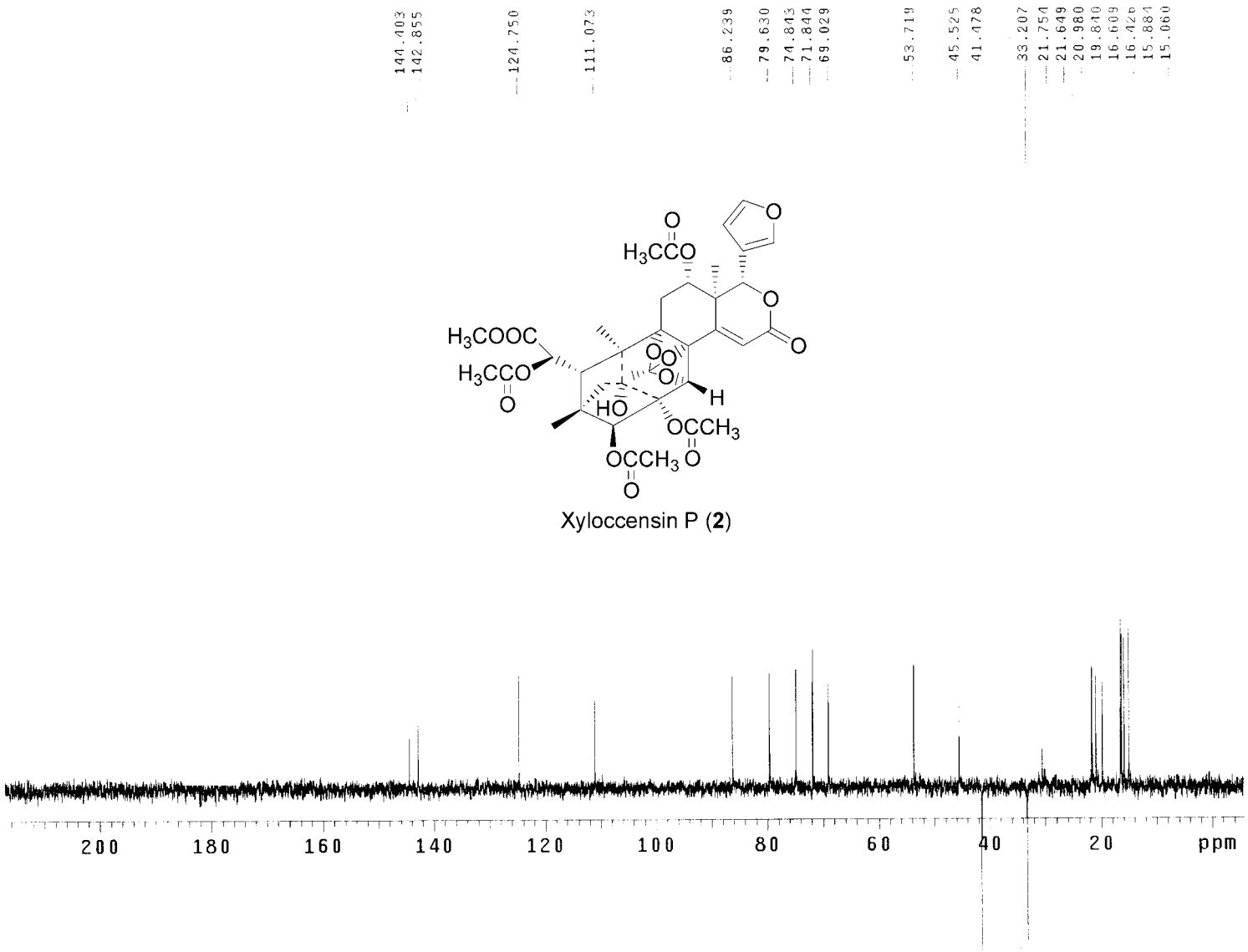


^{13}C NMR (125 MHz) of xyloccensin P (**2**) in acetone-d_6



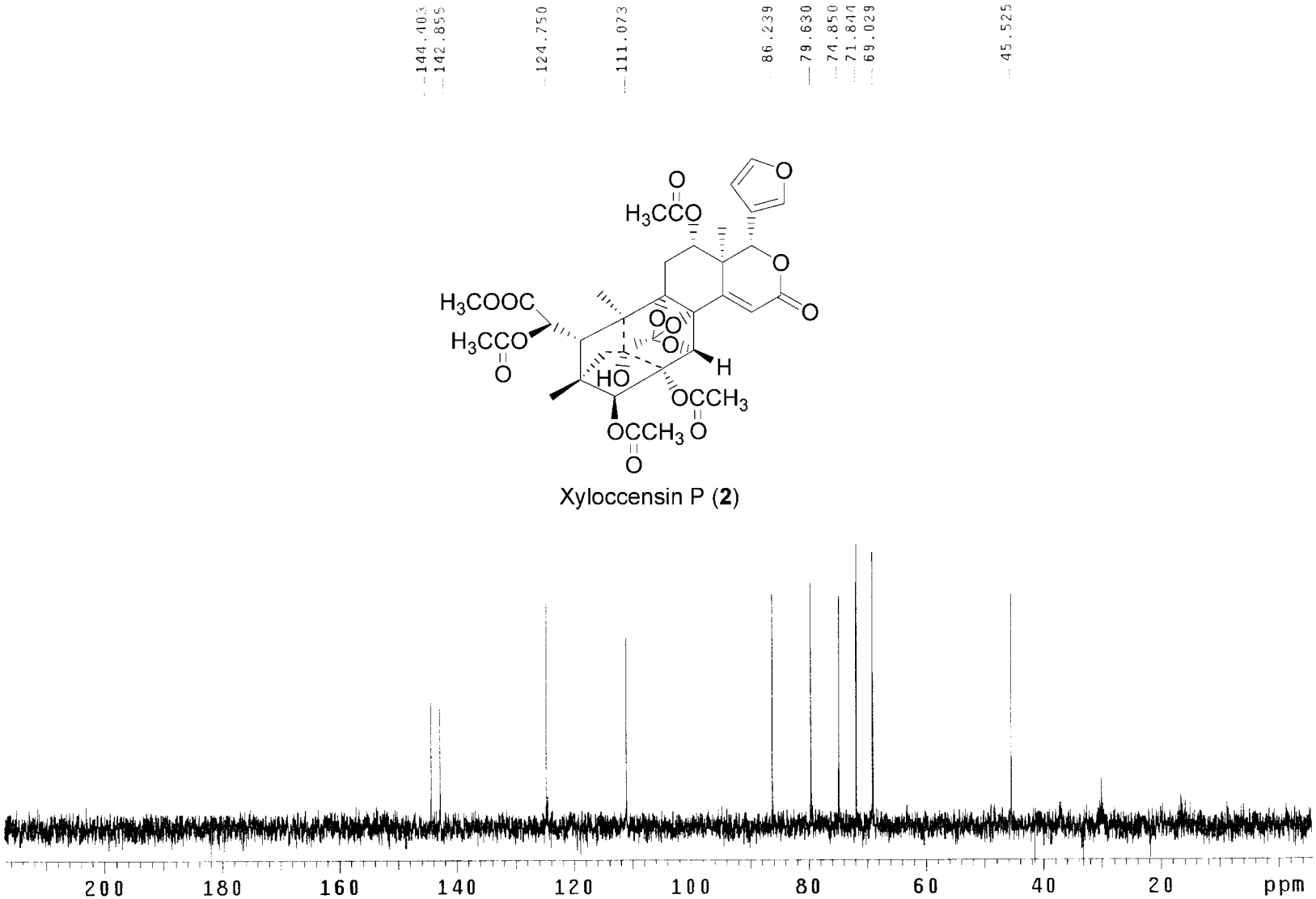
Xyloccensin P (**2**)

DEPT 135° experiment of xyloccensin P (**2**) in acetone-d_6



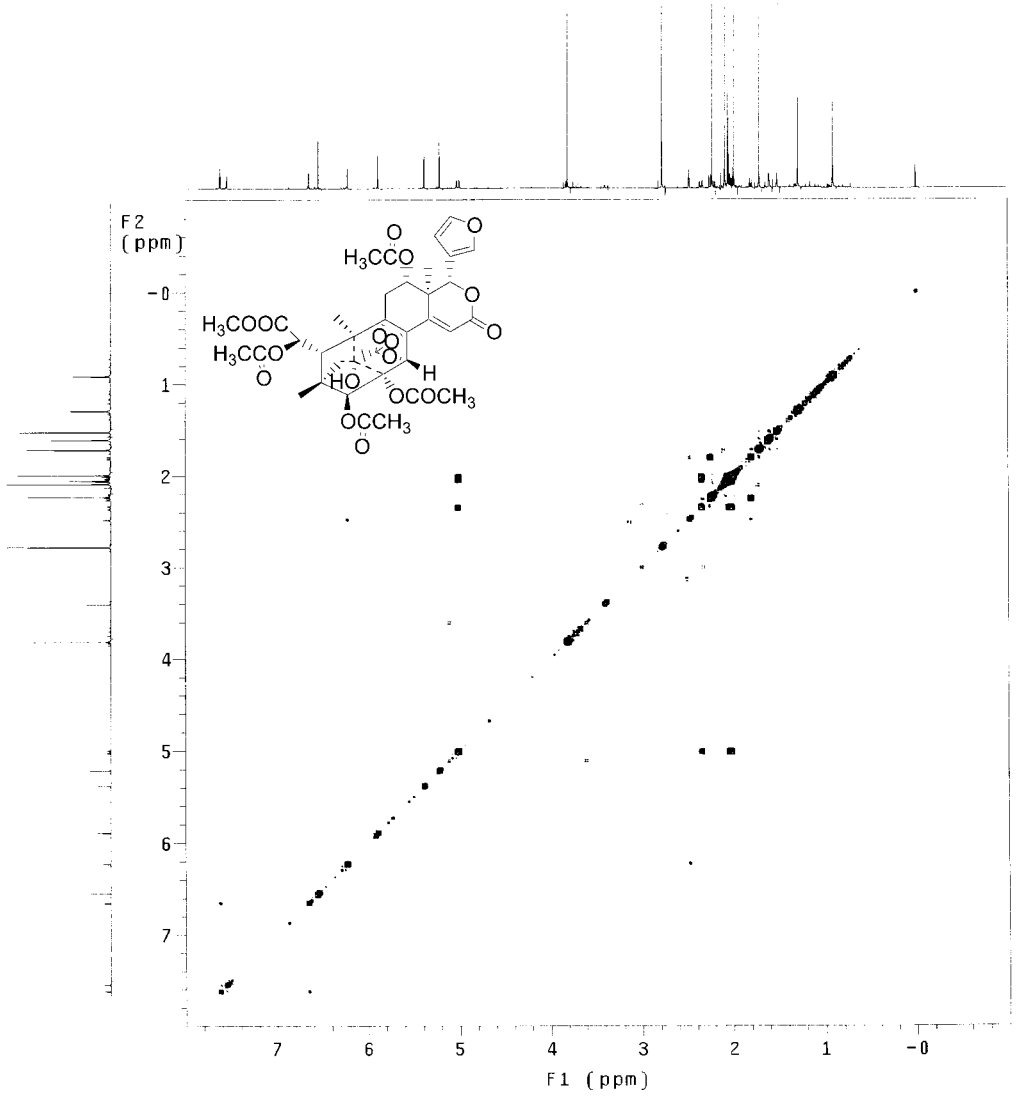
Xyloccensin P (**2**)

DEPT 90° experiment of xyloccensin P (**2**) in acetone-d_6

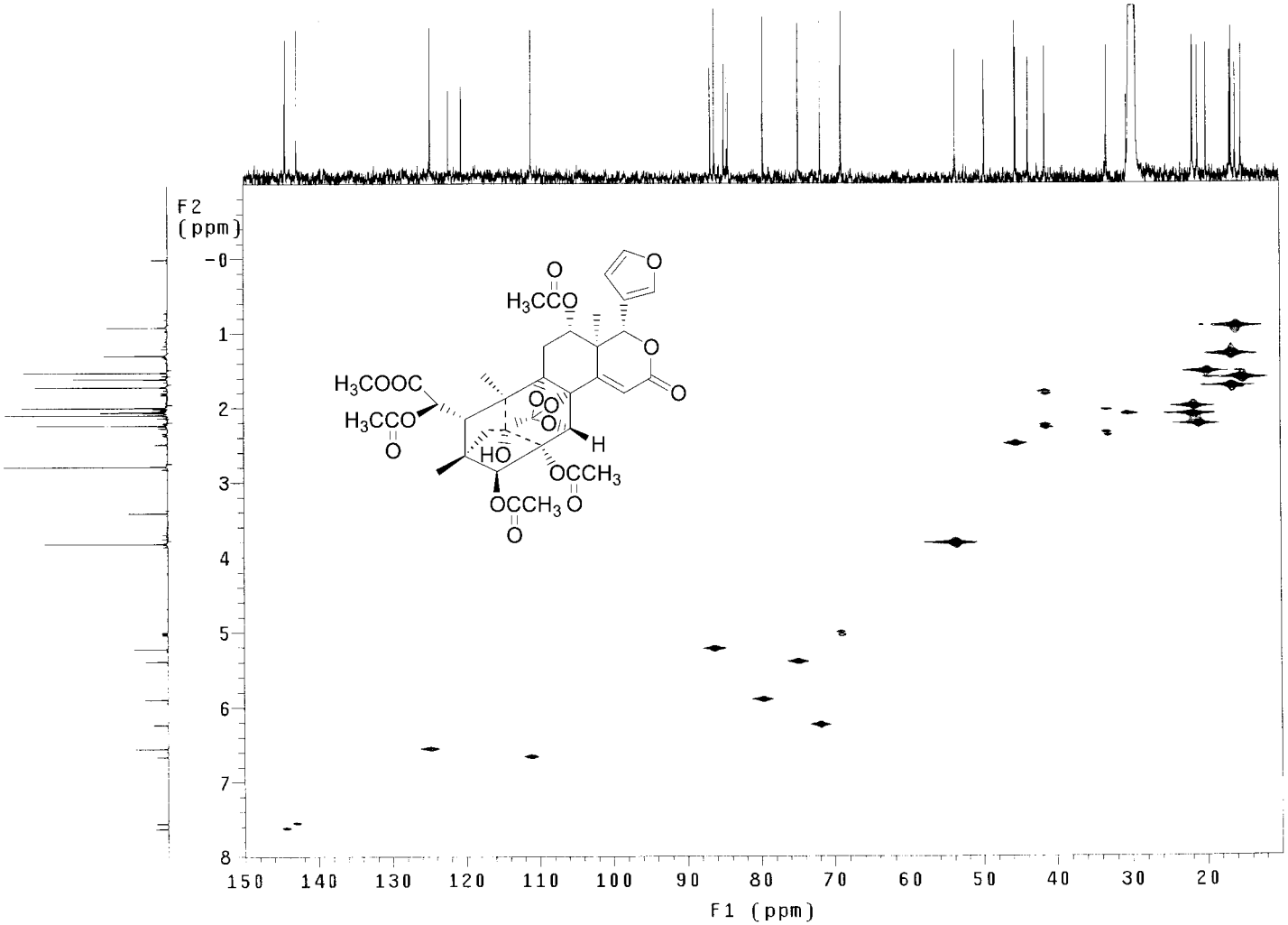


Xyloccensin P (**2**)

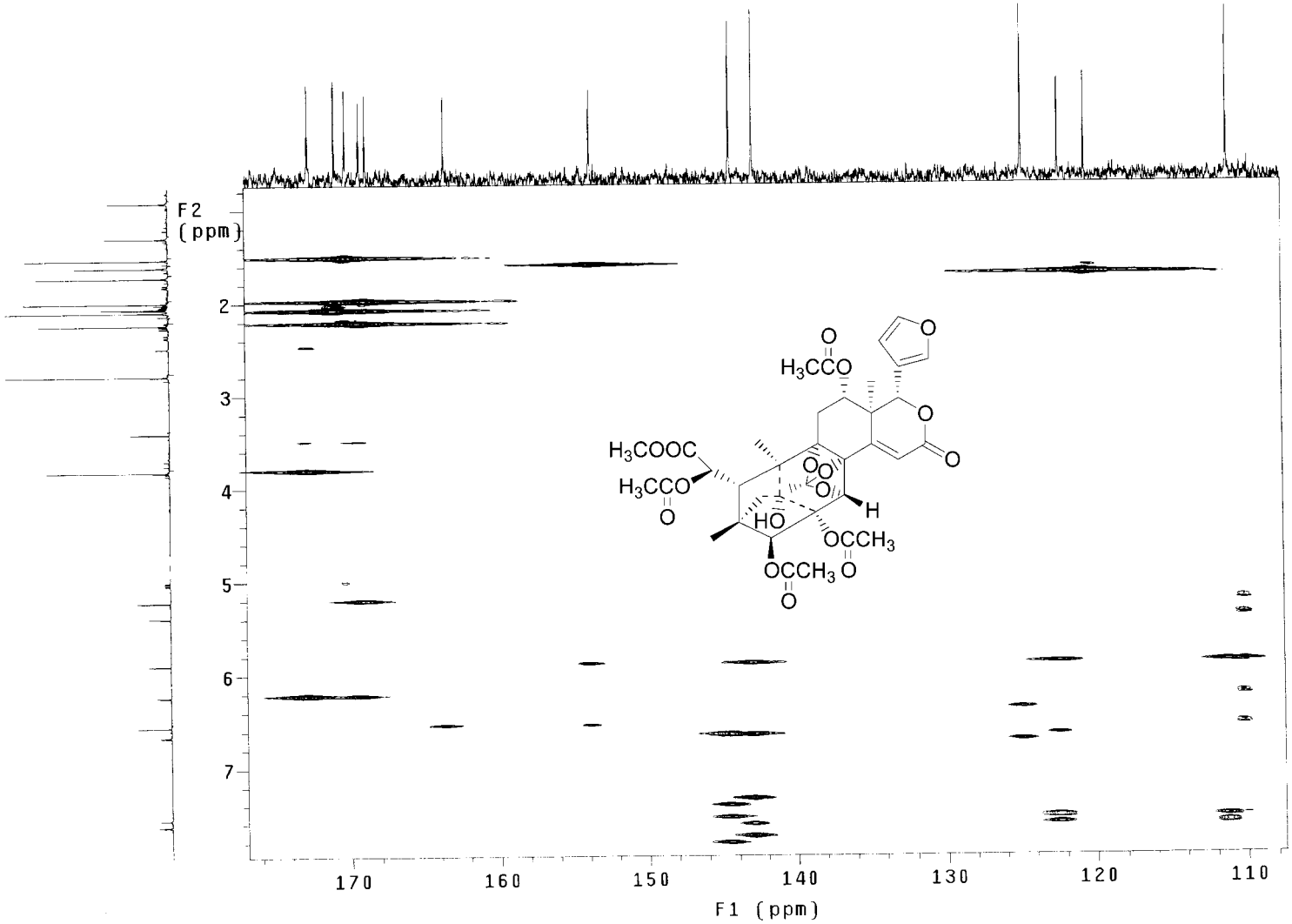
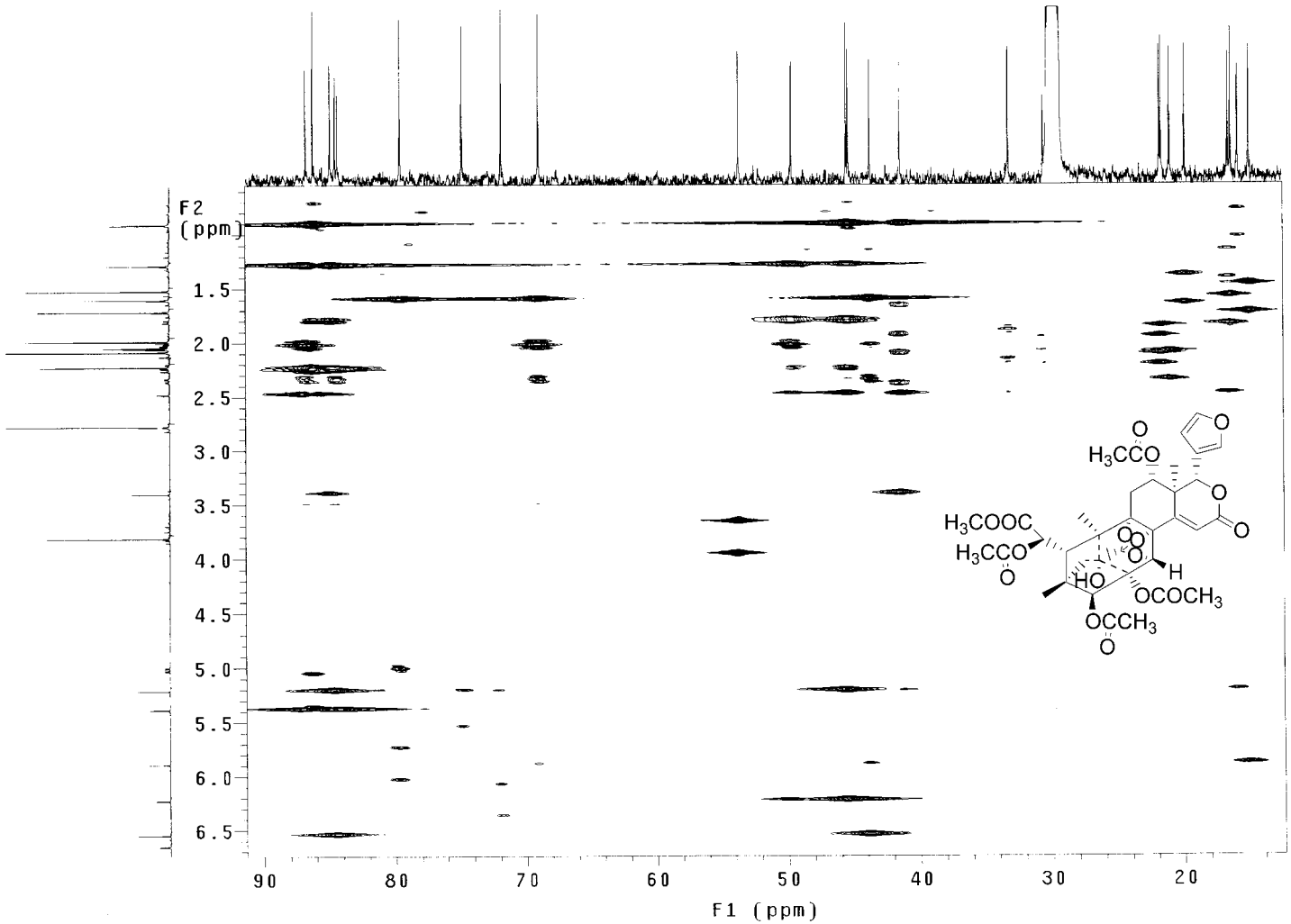
^{1}H-^{1}H COSY of xyloccensin P (**2**) in acetone-d_6



HMQC of xyloccensin P (**2**) in acetone-d_6



A segment of HMBC of xyloccensin P (**2**) in acetone-d_6



A segment of HMBC of xyloccensin P (**2**) in acetone-d_6