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## **APPENDICES**

## General characteristic of *Kaempferia parviflora*

**Rhizome** dark purple, with several succulent roots in a fascicle.

**Leaves** 1 to several ; blades ovate or elliptic, slightly unequal sided, 7-11 \* 4-6 cm, apex acute or mucronate, base subcordate, upper surface glabrous, under surface hairy; leaf-sheaths ca 6 cm long, margin membranous, red-tinted; bladeless sheaths greenish, purple-tinted; ligule broadly triangular, ca 2 mm long, membranous, caducous.

**Inflorescence** enclosed by the two innermost leaf-sheaths or by the leaf-sheath and the bladeless sheath, usually elongate; peduncle 5-6 cm long.

**Flowers** few; bracts oblong ca 1.7-2.3\*0.6 cm, glabrous, apex rounded.

Calyx 1.8-2.2 cm long, finely hairy, apex bifid.

**Corolla-tube** 3-3.2 cm long, lobes linear; dorsal lobe ca 1.2\*0.25 cm. Apex hooded, aristate; laterallobes slightly smaller, apex rounded.

**Staminodes** white, oblong, 1-1.3\*0.3 cm, apex acute or rounded.

**Labellum** purple, darker at the middle, obvate, 1.2-1.5 \* 0.8-0.9 cm, apex emarginate.

**Stamen** with very short filament, ca 1 mm long; anther ca 2 mm long, anther-crest suborbicular, entire or emarginate, 1-1.5\*2 mm.

**Ovary** ca 2\*1 mm, hairy; stylodes filiform 8-9 mm long.

Thailand -- Northern : Tak ; South-Western : Kanchanaburi

Distribution -- India, Burma (type, Wallich 6587, Bank of the River Attran.)

Ecology -- Scattered in moist soil, shaded bamboo or deciduous forest, 75-500 m alt.

Vernacular -- Krachai dam (กระชายดำ)

**Table A1** Crystal data and structure refinement for compound 1.

Empirical formula	C <sub>18</sub> H <sub>16</sub> O <sub>5</sub>	
Formula weight	312.31	
Temperature	293 (2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Monoclinic, P21/n	
Unit cell dimensions	A = 7.53630 (10) Å	alpha = 90 deg.
	B = 18.66430 (10) Å	beta = 108.8880 (10) deg.
	C = 11.50920 (10) Å	gamma = 90 deg.
Volume	1531.71 (3) Å <sup>3</sup>	
Z, Calculated density	4, 1.354 Mg / m <sup>3</sup>	
Absorption coefficient	0.099 mm <sup>-1</sup>	
F ( 000 )	656	
Theta range for data collection	2.17 to 30.44 deg.	
Index ranges	-10<=h<=10, -22<=k<=25, -8<=l<=16	
Reflections collected / unique	11160 / 4340 [ R (int) = 0.0200 ]	
Completeness to 2 theta = 30.44	93.30%	
Refinement method	Full – matrix least - squares on F <sup>2</sup>	
Data / restraints / parameters	4340 / 0 / 272	
Goodness - of - fit on F <sup>2</sup>	1.019	
Final R indices [ I > 2sigma (I) ]	R1 = 0.0444, wR2 = 0.1149	
R indices ( all data )	R1 = 0.0608, wR2 = 0.1267	
Largest diff. peak and hole	0.178 and -0.285 e.Å <sup>3</sup>	

**Table A2** Atomic coordinates ( x 10<sup>4</sup> ) and equivalent isotropic displacement parameters ( Å<sup>2</sup> \* 10<sup>3</sup> ) for compound 1.

	X	Y	Z	U(eq)*
C (1)	3601 (3)	-1871 (1)	8632 (2)	72 (1)
C (2)	-276 (3)	1168 (1)	5626 (2)	62 (1)
C (3)	5503 (3)	-62 (1)	13527 (1)	59 (1)

C (4)	-2126 (2)	3379 (1)	8804 (1)	52 (1)
C (5)	-3145 (2)	2892 (1)	7939 (1)	53 (1)
C (6)	-2438 (2)	2213 (1)	7866 (1)	46 (1)
C (7)	-676 (2)	2012 (1)	8659 (1)	36 (1)
C (8)	82 (2)	1284 (1)	8626 (1)	35 (1)
C (9)	-172 (2)	852 (1)	7638 (1)	39 (1)
C (10)	558 (2)	115 (1)	7750 (1)	39 (1)
C (11)	1776 (2)	-81 (1)	8987 (1)	35 (1)
C (12)	2780 (2)	-744 (1)	9303 (1)	40 (1)
C (13)	3895 (2)	-880 (1)	10489 (1)	42 (1)
C (14)	4066 (2)	-371 (1)	11423 (1)	39 (1)
C (15)	3105 (2)	275 (1)	11169 (1)	37 (1)
C (16)	2006 (1)	403 (1)	9955 (1)	34 (1)
C (18)	345 (2)	2508 (1)	9531 (1)	48 (1)
C (19)	-378 (2)	3188 (1)	9594 (1)	58 (1)
O (1)	2590 (1)	-1208 (1)	8355 (1)	55 (1)
O (2)	-1272 (1)	1083 (1)	6496 (1)	52 (1)
O (3)	123 (2)	-286 (1)	6849 (1)	56 (1)
O (4)	5233 (1)	-568 (1)	12551 (1)	52 (1)
O (5)	1142 (1)	1061 (1)	9780 (1)	37 (1)

$U(\text{eq})^*$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

**Table A3** Bond distances (A) for compound 1.

Bond Distances	( A )	Bond Distances	( A )
C (1) - O (1)	1.4058 (13)	C (10) - O (3)	1.2345 (14)
C (2) - O (2)	1.4410 (19)	C (10) - C (11)	1.4685 (17)
C (3) - O (4)	1.4306 (19)	C (11) - C (16)	1.4002 (5)
C (4) - C (5)	1.383 (2)	C (11) - C (12)	1.4353 (16)
C (4) - C (19)	1.383 (2)	C (12) - O (1)	1.3644 (14)
C (5) - C (6)	1.3882 (18)	C (12) - C (13)	1.3751 (18)
C (6) - C (7)	1.3971 (16)	C (13) - C (14)	1.4077 (18)

C (7) - C (18)	1.3979 (17)	C (14) - O (4)	1.3614 (15)
C (7) - C (8)	1.4792 (15)	C (14) - C (15)	1.3880 (15)
C (8) - C (9)	1.3565 (16)	C (15) - C (16)	1.3953 (16)
C (8) - O (5)	1.3749 (13)	C (16) - O (5)	1.3743 (12)
C (9) - O (2)	1.3771 (14)	C (18) - C (19)	1.3928 (18)
C (9) - C (10)	1.4700 (16)		

**Table A4** Bond angles (deg.) for compound 1.

Angles	(deg.)	Angles	(deg.)
C (5) - C (4) - C (19)	119.53 (12)	O (1) - C (12) - C (13)	123.27 (11)
C (4) - C (5) - C (6)	120.60 (12)	O (1) - C (12) - C (11)	115.79 (11)
C (5) - C (6) - C (7)	120.50 (12)	C (13) - C (12) - C (11)	120.92 (10)
C (6) - C (7) - C (18)	118.52 (11)	C (12) - C (13) - C (14)	120.56 (11)
C (6) - C (7) - C (8)	121.49 (10)	O (4) - C (14) - C (15)	124.47 (11)
C (18) - C (7) - C (8)	119.94 (10)	O (4) - C (14) - C (13)	114.69 (10)
C (9) - C (8) - O (5)	120.64 (10)	C (15) - C (14) - C (13)	120.84 (11)
C (9) - C (8) - C (7)	128.17 (10)	C (14) - C (15) - C (16)	117.39 (11)
O (5) - C (8) - C (7)	111.19 (9)	O (5) - C (16) - C (15)	113.58 (9)
C (8) - C (9) - O (2)	119.40 (11)	O (5) - C (16) - C (11)	121.90 (10)
C (8) - C (9) - C (10)	122.39 (10)	C (15) - C (16) - C (11)	124.52 (10)
O (2) - C (9) - C (10)	118.02 (10)	C (19) - C (18) - C (7)	120.47 (12)
O (3) - C (10) - C (11)	125.22 (11)	C (4) - C (19) - C (18)	120.38 (13)
O (3) - C (10) - C (9)	120.17 (11)	C (12) - O (1) - C (1)	117.40 (13)
C (11) - C (10) - C (9)	114.61 (10)	C (9) - O (2) - C (2)	114.20 (11)
C (16) - C (11) - C (12)	115.76 (10)	C (14) - O (4) - C (3)	117.11 (10)
C (16) - C (11) - C (10)	119.26 (10)	C (16) - O (5) - C (8)	120.80 (9)
C (12) - C (11) - C (10)	124.99 (10)		

Symmetry transformations used to generate equivalent atoms:

**Table A5** Anisotropic displacement parameters ( $\text{Å}^2 \cdot 10^3$ ). The anisotropic displacement factor exponent takes the form:  $-2 \pi^2 [ h^2 a^{*2} U_{11} + \dots + 2hka^*b^*U_{12} ]$ .

	$U_{11}$	$U_{22}$	$U_{33}$	$U_{23}$	$U_{13}$	$U_{12}$
C (1)	79 (1)	46 (1)	89 (1)	-16 (1)	25 (1)	16 (1)
C (2)	79 (1)	64 (1)	42 (1)	4 (1)	20 (1)	5 (1)
C (3)	68 (1)	63 (1)	42 (1)	9 (1)	14 (1)	14 (1)

C (4)	62 (1)	38 (1)	54 (1)	6 (1)	16 (1)	14 (1)
C (5)	45 (1)	50 (1)	56 (1)	9 (1)	7 (1)	12 (1)
C (6)	41 (1)	44 (1)	47 (1)	-1 (1)	4 (1)	2 (1)
C (7)	38 (1)	35 (1)	34 (1)	3 (1)	12 (1)	2 (1)
C (8)	33 (1)	35 (1)	35 (1)	1(1)	10 (1)	-1 (1)
C (9)	35 (1)	43 (1)	37 (1)	-3 (1)	10 (1)	-1 (1)
C (10)	38 (1)	39 (1)	43 (1)	-8 (1)	16 (1)	-8 (1)
C (11)	33 (1)	32 (1)	44 (1)	-3 (1)	17 (1)	-5 (1)
C (12)	39 (1)	33 (1)	53 (1)	-5 (1)	22 (1)	-4 (1)
C (13)	42 (1)	33 (1)	57 (1)	5 (1)	23 (1)	4 (1)
C (14)	39 (1)	39 (1)	45 (1)	8 (1)	19 (1)	2 (1)
C (15)	40 (1)	35 (1)	39 (1)	2 (1)	17 (1)	1 (1)
C (16)	33 (1)	29 (1)	42 (1)	2 (1)	16 (1)	-1 (1)
C (18)	48 (1)	40 (1)	47 (1)	-3 (1)	1 (1)	6 (1)
C (19)	67 (1)	39 (1)	55 (1)	-7 (1)	2(1)	8 (1)
O (1)	62 (1)	38 (1)	64 (1)	-13 (1)	20 (1)	5 (1)
O (2)	50 (1)	66 (1)	35 (1)	-3 (1)	5 (1)	11 (1)
O (3)	70 (1)	46 (1)	48 (1)	-16 (1)	14 (1)	-8 (1)
O (4)	59 (1)	48 (1)	47 (1)	11(1)	16 (1)	14 (1)
O (5)	44 (1)	33 (1)	35 (1)	1(1)	10 (1)	5 (1)

**Table A6** Crystal data and structure refinement for compound 2.

Empirical formula	$C_{17}H_{14}O_4$
Formula weight	282
Temperature	293 (2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P21/n
Unit cell dimensions	A = 7.53630 (10) Å    alpha = 90 deg. B = 18.66430 (10) Å    beta = 108.8880 (10) deg. C = 11.50920 (10) Å    gamma = 90 deg.
Volume	1531.71 (3) Å <sup>3</sup>
Z, Calculated density	4, 1.354 Mg / m <sup>3</sup>
Absorption coefficient	0.099 mm <sup>-1</sup>
F ( 000 )	656
Theta range for data collection	2.17 to 30.44 deg.
Index ranges	-.10<=h<=10, -22<=k<=25, -8<=l<=16
Reflections collected / unique	11160 / 4340 [ R (int) = 0.0200 ]



Completeness to 2 theta = 30.44	93.30%
Refinement method	Full - matrix least - squares on F <sup>2</sup>
Data / restraints / parameters	4340 / 0 / 272
Goodness - of - fit on F <sup>2</sup>	1.019
Final R indices [ I > 2sigma (I) ]	R1 = 0.0444, wR2 = 0.1149
R indices ( all data )	R1 = 0.0608, wR2 = 0.1267
Largest diff. peak and hole	0.178 and -0.285 e.A <sup>3</sup>

**Table A7** Atomic coordinates ( x 10<sup>4</sup>) and equivalent isotropic displacement parameters ( A<sup>2</sup> \* 10<sup>3</sup>) for compound 2.

	X	Y	Z	U(eq)*
C (1)	3601 (3)	-1871 (1)	8632 (2)	72 (1)
C (2)	-276 (3)	1168 (1)	5626 (2)	62 (1)
C (3)	5503 (3)	-62 (1)	13527 (1)	59 (1)
C (4)	-2126 (2)	3379 (1)	8804 (1)	52 (1)
C (5)	-3145 (2)	2892 (1)	7939 (1)	53 (1)
C (6)	-2438 (2)	2213 (1)	7866 (1)	46 (1)
C (7)	-676 (2)	2012 (1)	8659 (1)	36 (1)
C (8)	82 (2)	1284 (1)	8626 (1)	35 (1)
C (9)	-172 (2)	852 (1)	7638 (1)	39 (1)
C (10)	558 (2)	115 (1)	7750 (1)	39 (1)
C (11)	1776 (2)	-81 (1)	8987 (1)	35 (1)
C (12)	2780 (2)	-744 (1)	9303 (1)	40 (1)
C (13)	3895 (2)	-880 (1)	10489 (1)	42 (1)
C (14)	4066 (2)	-371 (1)	11423 (1)	39 (1)
C (15)	3105 (2)	275 (1)	11169 (1)	37 (1)
C (16)	2006 (1)	403 (1)	9955 (1)	34 (1)
C (19)	-378 (2)	3188 (1)	9594 (1)	58 (1)
O (1)	2590 (1)	-1208 (1)	8355 (1)	55 (1)
O (2)	-1272 (1)	1083 (1)	6496 (1)	52 (1)
O (3)	123 (2)	-286 (1)	6849 (1)	56 (1)
O (4)	5233 (1)	-568 (1)	12551 (1)	52 (1)
O (5)	1142 (1)	1061 (1)	9780 (1)	37 (1)

**Table A8** Bond distances (A) for compound 2.

Bond Distances	( A )	Bond Distances	( A )
C (1) - C (6)	1.367 (4)	C (10) - C (11)	1.375 (3)
C (1) - C (2)	1.383 (4)	C (11) - O (3)	1.359 (2)
C (2) - C (3)	1.384 (3)	C (11) - C (12)	1.398 (3)
C (3) - C (4)	1.377 (3)	C (12) - C (13)	1.376 (3)
C (4) - C (5)	1.392 (3)	C (13) - O (2)	1.357 (2)
C (4) - C (7)	1.511 (3)	C (13) - C (14)	1.427 (3)
C (5) - C (6)	1.390 (3)	C (14) - C (15)	1.475 (2)
C (7) - O (4)	1.446 (2)	C (15) - O (1)	1.214 (2)
C (7) - C (16)	1.517 (3)	C (15) - C (16)	1.511 (3)
C (9) - O (4)	1.36 (2)	C (17) - O (3)	1.439 (3)
C (9) - C (10)	1.387 (3)	C (18) - O (2)	1.434 (3)
C (9) - C (14)	1.406 (3)		

**Table A9** Bond angles (deg.) for compound 2.

Angles	(deg.)	Angles	(deg.)
C (6) - C (1) - C (2)	119.5 (2)	O (3) - C (11) - C (12)	115.26 (17)
C (1) - C (2) - C (3)	120.3 (3)	C (10) - C (11) - C (12)	121.13 (17)
C (4) - C (3) - C (2)	120.5 (2)	C (13) - C (12) - C (11)	119.98 (17)
C (3) - C (4) - C (5)	119.2 (2)	O (2) - C (13) - C (12)	122.81 (17)
C (3) - C (4) - C (7)	121.81 (18)	O (2) - C (13) - C (14)	116.27 (16)
C (5) - C (4) - C (7)	119.0 (2)	C (12) - C (13) - C (14)	120.91 (16)
C (6) - C (5) - C (4)	119.8 (2)	C (9) - C (14) - C (13)	116.56 (16)
C (1) - C (6) - C (5)	120.7 (2)	C (9) - C (14) - C (15)	118.95 (17)
O (4) - C (7) - C (4)	107.48 (15)	C (13) - C (14) - C (15)	124.44 (16)
O (4) - C (7) - C (16)	108.39 (15)	O (1) - C (15) - C (14)	124.72 (19)
C (4) - C (7) - C (16)	115.55 (16)	O (1) - C (15) - C (16)	120.08 (18)
O (4) - C (9) - C (10)	114.65 (16)	C (14) - C (15) - C (16)	115.20 (16)
O (4) - C (9) - C (14)	122.64 (16)	C (15) - C (16) - C (7)	110.71 (16)
C (10) - C (9) - C (14)	122.70 (17)	C (13) - O (2) - C (18)	117.90 (16)
C (11) - C (10) - C (9)	118.70 (17)	C (11) - O (3) - C (17)	117.58 (17)
O (3) - C (11) - C (10)	123.60 (17)	C (9) - O (4) - C (7)	114.71 (14)

**Table A10** Anisotropic displacement parameters ( $\text{\AA}^2 \cdot 10^3$ ). The anisotropic displacement factor exponent takes the form:  $-2 \pi^2 [ h^2 a^{*2} U_{11} + \dots + 2hka^*b^*U_{12} ]$ .

	$U_{11}$	$U_{22}$	$U_{33}$	$U_{23}$	$U_{13}$	$U_{12}$
C (1)	79 (1)	46 (1)	89 (1)	-16 (1)	25 (1)	16 (1)
C (2)	79 (1)	64 (1)	42 (1)	4 (1)	20 (1)	5 (1)
C (3)	68 (1)	63 (1)	42 (1)	9 (1)	14 (1)	14 (1)
C (4)	62 (1)	38 (1)	54 (1)	6 (1)	16 (1)	14 (1)
C (5)	45 (1)	50 (1)	56 (1)	9 (1)	7 (1)	12 (1)
C (6)	41 (1)	44 (1)	47 (1)	-1 (1)	4 (1)	2 (1)
C (7)	38 (1)	35 (1)	34 (1)	3 (1)	12 (1)	2 (1)
C (8)	33 (1)	35 (1)	35 (1)	1(1)	10 (1)	-1 (1)
C (9)	35 (1)	43 (1)	37 (1)	-3 (1)	10 (1)	-1 (1)
C (10)	38 (1)	39 (1)	43 (1)	-8 (1)	16 (1)	-8 (1)
C (11)	33 (1)	32 (1)	44 (1)	-3 (1)	17 (1)	-5 (1)
C (12)	39 (1)	33 (1)	53 (1)	-5 (1)	22 (1)	-4 (1)
C (13)	42 (1)	33 (1)	57 (1)	5 (1)	23 (1)	4 (1)
C (14)	39 (1)	39 (1)	45 (1)	8 (1)	19 (1)	2 (1)
C (15)	40 (1)	35 (1)	39 (1)	2 (1)	17 (1)	1 (1)
C (16)	33 (1)	29 (1)	42 (1)	2 (1)	16 (1)	-1 (1)
C (18)	48 (1)	40 (1)	47 (1)	-3 (1)	1 (1)	6 (1)
C (19)	67 (1)	39 (1)	55 (1)	-7 (1)	2(1)	8 (1)
O (1)	62 (1)	38 (1)	64 (1)	-13 (1)	20 (1)	5 (1)
O (2)	50 (1)	66 (1)	35 (1)	-3 (1)	5 (1)	11 (1)
O (3)	70 (1)	46 (1)	48 (1)	-16 (1)	14 (1)	-8 (1)
O (4)	59 (1)	48 (1)	47 (1)	11(1)	16 (1)	14 (1)

**Table A11** Crystal data and structure refinement for compound 6.

Empirical formula	$\text{C}_{19}\text{H}_{16}\text{O}_5$	
Formula weight	340.89	
Temperature	293 (2) K	
Wavelength	0.71073 \text{\AA}	
Crystal system, space group	Monoclinic, P21/c	
Unit cell dimensions	$A = 20.2460 (11) \text{\AA}$	$\alpha = 90 \text{ deg.}$
	$b = 7.2651 (4) \text{\AA}$	$\beta = 114.5490 (10) \text{ deg.}$
	$C = 20.8990 (12) \text{\AA}$	$\gamma = 90 \text{ deg}$
Volume	$2796.1 (3) \text{\AA}^3$	

Z, Calculated density	7, 1.417 Mg/m <sup>3</sup>
Absorption coefficient	0.105 mm <sup>-1</sup>
F ( 000 )	1248
Theta range for data collection	1.96 to 30.55 deg.
Index ranges	-.27<=h<=26, -10<=k<=9, -29<=l<=29
Reflections collected / unique	19549 / 8003 [ R ( int ) = 0.0534 ]
Completeness to 2 theta = 30.44	93.30%
Refinement method	Full - matrix least - squares on F <sup>2</sup>
Data / restraints / parameters	8003 / 0 /493
Goodness - of - fit on F <sup>2</sup>	1.033
Final R indices [ I > 2sigma (I) ]	R1 = 0.0729, wR2 = 0.1241
R indices ( all data )	R1 = 0.1760, wR2 = 0.1625
Largest diff. peak and hole	0.205 and -0.219 e.A <sup>-3</sup>

**Table 12** Atomic coordinates ( x 10<sup>4</sup> ) and equivalent isotropic displacement parameters ( A<sup>2</sup> \* 10<sup>3</sup> ) for compound 6.

	X	Y	Z	U (eq)*
O (10)	1420 (1)	6740 (2)	4656 (1)	48 (1)
O (4)	3192 (1)	6381 (3)	4632 (1)	58 (1)
C (15)	2005 (1)	6069 (4)	3672 (1)	46 (1)
C (14)	1235 (1)	6032 (3)	3475 (1)	43 (1)
O (3)	969 (1)	5284 (3)	2279 (1)	64 (1)
O (2)	-959 (1)	5834 (3)	3024 (1)	61 (1)
C (10)	232 (1)	6301 (4)	3822 (1)	47 (1)
O (1)	2270 (1)	5759 (3)	3236 (1)	60 (1)
C (6)	2524 (1)	7183 (3)	5630 (1)	43 (1)
C (12)	-.5 (2)	5558 (4)	2613 (1)	52 (1)
C (16)	2454 (1)	6488 (4)	4403 (1)	45 (1)
C (7)	2158 (1)	6805 (3)	4869 (1)	42 (1)
C (9)	957 (1)	6350 (3)	3975 (1)	42 (1)
C (11)	.-250 (1)	5897 (4)	3134 (1)	47 (1)
C (13)	728 (1)	5625 (4)	2785 (1)	47 (1)
C (5)	2127 (2)	7050 (4)	6036 (2)	55 (1)
C (18)	.-1503 (2)	5744 (7)	2316 (2)	69 (1)
C (3)	3172 (2)	7875 (4)	7074 (2)	63 (1)
C (1)	3250 (2)	7678 (4)	5967 (2)	55 (1)
C (2)	3570 (2)	8024 (4)	6683 (2)	62 (1)

C (17)	3515 (2)	7744 (5)	4348 (2)	77 (1)
C (4)	2453 (2)	7395 (5)	6755 (2)	67 (1)

$U(\text{eq})^*$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

**Table A13** Bond distances (A) for compound 6.

Bond Distances	( A )	Bond Distances	( A )
O (10) - C (9)	1.370 (3)	C (10) - C (9)	1.368 (3)
O (10) - C (7)	1.371 (3)	C (10) - C (11)	1.393 (3)
O (4) - C (16)	1.369 (3)	C (6) - C (1)	1.387 (4)
O (4) - C (17)	1.442 (3)	C (6) - C (5)	1.394 (4)
C (15) - O (1)	1.255 (3)	C (6) - C (7)	1.476 (3)
C (15) - C (14)	1.438 (3)	C (12) - C (13)	1.376 (4)
C (15) - C (16)	1.448 (3)	C (12) - C (11)	1.393 (3)
C (14) - C (9)	1.395 (3)	C (16) - C (7)	1.358 (3)
C (14) - C (13)	1.412 (3)	C (5) - C (4)	1.390 (4)
O (3) - C (13)	1.357 (3)	C (3) - C (2)	1.369 (4)
O (2) - C (11)	1.357 (3)	C (3) - C (4)	1.372 (4)
O (2) - C (18)	1.433 (4)	C (1) - C (2)	1.385 (4)

**Table A14** Bond angles (deg.) for compound 6.

Angles	(deg.)	Angles	(deg.)
C (9) - O (10) - C (7)	121.79 (18)	C (16) - C (7) - O (10)	120.5 (2)
C (16) - O (4) - C (17)	115.6 (2)	C (16) - C (7) - C (6)	129.1 (2)
O (1) - C (15) - C (14)	121.9 (2)	O (10) - C (7) - C (6)	110.3 (2)
O (1) - C (15) - C (16)	122.2 (2)	C (10) - C (9) - O (10)	116.9 (2)
C (14) - C (15) - C (16)	115.9 (2)	C (10) - C (9) - O (14)	123.3 (2)
C (9) - C (14) - C (13)	116.9 (2)	O (10) - C (9) - C (14)	119.8 (2)
C (9) - C (14) - C (15)	120.6 (2)	O (2) - C (11) - C (10)	114.8 (2)
C (13) - C (14) - C (15)	122.5 (2)	O (2) - C (11) - C (12)	123.8 (2)
C (11) - O (2) - C (18)	118.8 (2)	C (10) - C (11) - C (12)	121.4 (2)
C (9) - C (10) - C (11)	117.9 (2)	O (3) - C (13) - C (12)	119.2 (2)
C (1) - C (6) - C (5)	117.9 (3)	O (3) - C (13) - C (14)	119.4 (2)
C (1) - C (6) - C (7)	123.1 (2)	C (12) - C (13) - C (14)	121.4 (2)
C (5) - C (6) - C (7)	119.0 (2)	C (4) - C (5) - C (6)	120.6 (3)
C (13) - C (12) - C (11)	119.0 (3)	C (2) - C (3) - C (4)	119.9 (3)
C (7) - C (16) - O (4)	120.2 (2)	C (2) - C (1) - C (6)	121.1 (3)
C (7) - C (16) - C (15)	121.4 (2)	C (3) - C (2) - C (1)	120.2 (3)
O (4) - C (16) - C (15)	118.2 (2)	C (3) - C (4) - C (5)	120.2 (3)

Symmetry transformations used to generate equivalent atoms:

**Table A15** Anisotropic displacement parameters ( $\text{\AA}^2 * 10^3$ ). The anisotropic displacement factor exponent takes the form:  $-2 \pi^2 [ h^2 a^{*2} U_{11} + \dots + 2hka^*b^*U_{12} ]$ .

	<i>U</i> <sub>11</sub>	<i>U</i> <sub>22</sub>	<i>U</i> <sub>33</sub>	<i>U</i> <sub>23</sub>	<i>U</i> <sub>13</sub>	<i>U</i> <sub>12</sub>
O (10)	42 (1)	61 (1)	39 (1)	-6 (1)	16 (1)	1 (1)
O (4)	43 (1)	71 (1)	60 (1)	-1 (1)	22 (1)	5 (1)
C (15)	52 (2)	44 (2)	47 (2)	6 (1)	26 (1)	10 (1)
C (14)	47 (2)	39 (1)	39 (1)	4 (1)	20 (1)	7 (1)
O (3)	65 (1)	91 (2)	39 (1)	-5 (1)	24 (1)	11 (1)
O (2)	42 (1)	86 (2)	49 (1)	-5 (1)	14 (1)	-1 (1)
C (10)	46 (2)	56 (2)	41 (2)	-3 (1)	20 (1)	2 (1)
O (1)	55 (1)	82 (2)	51 (1)	0 (1)	29 (1)	12 (1)
C (6)	49 (2)	36 (1)	43 (2)	0 (1)	18 (1)	6 (1)
C (12)	56 (2)	56 (2)	38 (2)	1 (1)	14 (1)	5 (1)
C (16)	43 (2)	46 (2)	47 (2)	3 (1)	19 (1)	5 (1)
C (7)	39 (1)	40 (2)	45 (2)	3 (1)	16 (1)	3 (1)
C (9)	43 (2)	44 (2)	38 (1)	0 (1)	14 (1)	2 (1)
C (11)	42 (2)	48 (2)	48 (2)	2 (1)	17 (1)	2 (1)
C (13)	54 (2)	49 (2)	40 (2)	2 (1)	22 (1)	10 (1)
C (5)	50 (2)	69 (2)	47 (2)	-8 (1)	20 (1)	0 (2)
C (18)	51 (2)	85 (3)	58 (2)	-16 (2)	10 (2)	-1 (2)
C (3)	69 (2)	62 (2)	44 (2)	-8 (1)	9 (2)	8 (2)
C (1)	52 (2)	58 (2)	50 (2)	0 (1)	17 (2)	-2 (1)
C (2)	58 (2)	63 (2)	54 (2)	-3 (2)	12 (2)	-2 (2)
C (17)	63 (2)	88 (3)	96 (3)	-9 (2)	49 (2)	-17 (2)
C (4)	73 (2)	81 (2)	49 (2)	-8 (2)	28 (2)	3 (2)

**Table A16** Hydrogen bonds for compound 6 [  $\text{\AA}$  and deg.].

D-H...A	d (D-H)	d (H...A)	d (D...A)	$\angle$ (DHA)
O (3) - H (31).....O (1)	1.05 (4)	1.61 (4)	2.584 (3)	154 (3)
O (3A) - H (32).....O (1A)	0.92 (4)	1.75 (4)	2.606 (3)	155 (3)

Symmetry transformations used to generate equivalent atoms:

**Table A17** Crystal data and structure refinement for compound 7.

Empirical formula	$\text{C}_{16}\text{H}_{12}\text{O}_4$
Formula weight	268
Temperature	293 (2) K

Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P21/c
Unit cell dimensions	A = 20.2460 (11) Å      alpha = 90 deg. B = 7.2651 (4) Å      beta = 114.5490 (10) deg. C = 20.8990 (12) Å      gamma = 90 deg
Volume	2796.1 (3) Å <sup>3</sup>
Z, Calculated density	7, 1.417 Mg/m <sup>3</sup>
Absorption coefficient	0.105 mm <sup>-1</sup>
F ( 000 )	1248
Theta range for data collection	1.96 to 30.55 deg.
Index ranges	-.27<=h<=26, -10<=k<=9, -29<=l<=29
Reflections collected / unique	19549 / 8003 [ R ( int ) = 0.0534 ]
Completeness to 2 theta = 30.44	93.30%
Refinement method	Full - matrix least - squares on F <sup>2</sup>
Data / restraints / parameters	8003 / 0 / 493
Goodness - of - fit on F <sup>2</sup>	1.033
Final R indices [ I > 2sigma (I) ]	R1 = 0.0729, wR2 = 0.1241
R indices ( all data )	R1 = 0.1760, wR2 = 0.1625
Largest diff. Peak and hole	0.205 and -0.219 e.Å <sup>-3</sup>

**Table A18** Atomic coordinates ( x 10<sup>4</sup> ) and equivalent isotropic displacement parameters ( Å<sup>2</sup> \* 10<sup>3</sup> ) for compound 7.

	X	Y	Z	U(eq)*
C (1)	3195 (4)	7054 (2)	2176 (2)	39 (1)
C (2)	948 (4)	7421 (2)	1513 (2)	39 (1)
C (3)	768 (4)	8675 (2)	1592 (2)	38 (1)
C (4)	-1360 (4)	9165 (2)	1025 (2)	41 (1)
C (5)	-1513 (5)	10370 (2)	1130 (2)	45 (1)
C (6)	469 (4)	11105 (2)	1801 (2)	44 (1)
C (7)	2586 (4)	10660 (2)	2382 (2)	44 (1)
C (8)	2656 (4)	9456 (2)	2270 (2)	38 (1)
C (10)	4933 (4)	7855 (2)	2841 (2)	37 (1)
C (11)	7149 (4)	7642 (2)	3645 (2)	36 (1)
C (12)	7967 (5)	8465 (2)	4554 (2)	45 (1)
C (13)	10009 (5)	8306 (2)	5321 (2)	48 (1)

C (14)	11333 (4)	7314 (2)	5216 (2)	40 (1)
C (15)	10573 (4)	6493 (2)	4320 (2)	40 (1)
C (16)	8503 (4)	6662 (2)	3550 (2)	39 (1)
O (1)	528 (4)	12305 (2)	1957 (2)	60 (1)
O (2)	13328 (3)	7241 (2)	6029 (1)	53 (1)
O (3)	-3279 (3)	8441 (2)	374 (1)	59 (1)
O (4)	-750 (3)	6686 (2)	933 (1)	54 (1)

**Table A19** Bond distances (A) for compound 7.

Bond Distances	( A )	Bond Distances	( A )
O (10) - C (9)	1.370 (3)	C (10) - C (9)	1.368 (3)
O (10) - C (7)	1.371 (3)	C (10) - C (11)	1.393 (3)
O (4) - C (16)	1.369 (3)	C (6) - C (1)	1.387 (4)
O (4) - C (17)	1.442 (3)	C (6) - C (5)	1.394 (4)
C (15) - O (1)	1.255 (3)	C (6) - C (7)	1.476 (3)
C (15) - C (14)	1.438 (3)	C (12) - C (13)	1.376 (4)
C (15) - C (16)	1.448 (3)	C (12) - C (11)	1.393 (3)
C (14) - C (9)	1.395 (3)	C (16) - C (7)	1.358 (3)
C (14) - C (13)	1.412 (3)	C (5) - C (4)	1.390 (4)
O (3) - C (13)	1.357 (3)	C (3) - C (2)	1.369 (4)
O (2) - C (11)	1.357 (3)	C (3) - C (4)	1.372 (4)
O (2) - C (17)	1.433 (4)	C (1) - C (2)	1.385 (4)

**Table A20** Bond angles (deg.) for compound 7.

Angles	(deg.)	Angles	(deg.)
C (10) - C (1) - O (5)	119.83 (19)	C (7) - C (8) - C (3)	123.21 (19)
C (10) - C (1) - O (2)	121.08 (19)	C (1) - C (10) - O (6)	121.42 (19)
O (5) - C (1) - C (2)	118.37 (18)	C (1) - C (10) - C (11)	128.62 (19)
O (4) - C (2) - C (3)	122.4 (2)	O (6) - C (10) - C (11)	109.88 (17)
O (4) - C (2) - C (1)	121.9 (2)	C (16) - C (11) - C (12)	117.52 (19)
C (3) - C (2) - C (1)	115.65 (19)	C (16) - C (11) - C (10)	123.26 (18)
C (8) - C (3) - C (4)	117.2 (2)	C (12) - C (11) - C (10)	119.21 (19)
C (8) - C (3) - C (2)	120.52 (19)	C (13) - C (12) - C (11)	121.4 (2)
C (4) - C (3) - C (2)	122.25 (19)	C (12) - C (13) - C (14)	120.3 (2)
O (3) - C (4) - C (5)	119.3 (2)	O (2) - C (14) - C (13)	115.40 (19)
O (3) - C (4) - C (3)	119.5 (2)	O (2) - C (14) - C (15)	125.2 (2)
C (5) - C (4) - C (3)	121.1 (2)	C (13) - C (14) - C (15)	119.4 (2)
C (4) - C (5) - C (6)	118.8 (2)	C (16) - C (15) - C (14)	119.8 (2)
O (1) - C (6) - C (5)	123.8 (2)	C (15) - C (16) - C (11)	121.6 (2)



O (1) - C (6) - C (7)	114.3 (2)	C (6) - O (1) - C (19)	118.6 (2)
C (5) - C (6) - C (7)	121.9 (2)	C (14) - O (2) - C (16)	118.34 (18)
C (8) - C (7) - C (6)	117.7 (2)	C (1) - O (5) - C (17)	114.61 (19)
O (6) - C (8) - C (7)	116.18 (19)	C (8) - O (6) - C (10)	120.64 (17)
O (6) - C (8) - C (3)	120.60 (19)		

**Table A21** Anisotropic displacement parameters ( $\text{Å}^2 \cdot 10^3$ ). The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2hka^*b^*U_{12}]$ .

	$U_{11}$	$U_{22}$	$U_{33}$	$U_{23}$	$U_{13}$	$U_{12}$
O (10)	42 (1)	61 (1)	39 (1)	-6 (1)	16 (1)	1 (1)
O (4)	43 (1)	71 (1)	60 (1)	-1 (1)	22 (1)	5 (1)
C (15)	52 (2)	44 (2)	47 (2)	6 (1)	26 (1)	10 (1)
C (14)	47 (2)	39 (1)	39 (1)	4 (1)	20 (1)	7 (1)
O (3)	65 (1)	91 (2)	39 (1)	-5 (1)	24 (1)	11 (1)
O (2)	42 (1)	86 (2)	49 (1)	-5 (1)	14 (1)	-1 (1)
C (10)	46 (2)	56 (2)	41 (2)	-3 (1)	20 (1)	2 (1)
O (1)	55 (1)	82 (2)	51 (1)	0 (1)	29 (1)	12 (1)
C (6)	49 (2)	36 (1)	43 (2)	0 (1)	18 (1)	6 (1)
C (12)	56 (2)	56 (2)	38 (2)	1 (1)	14 (1)	5 (1)
C (16)	43 (2)	46 (2)	47 (2)	3 (1)	19 (1)	5 (1)
C (7)	39 (1)	40 (2)	45 (2)	3 (1)	16 (1)	3 (1)
C (9)	43 (2)	44 (2)	38 (1)	0 (1)	14 (1)	2 (1)
C (11)	42 (2)	48 (2)	48 (2)	2 (1)	17 (1)	2 (1)
C (13)	54 (2)	49 (2)	40 (2)	2 (1)	22 (1)	10 (1)
C (5)	50 (2)	69 (2)	47 (2)	-8 (1)	20 (1)	0 (2)
C (18)	51 (2)	85 (3)	58 (2)	-16 (2)	10 (2)	-1 (2)
C (3)	69 (2)	62 (2)	44 (2)	-8 (1)	9 (2)	8 (2)
C (1)	52 (2)	58 (2)	50 (2)	0 (1)	17 (2)	-2 (1)
C (2)	58 (2)	63 (2)	54 (2)	-3 (2)	12 (2)	-2 (2)
C (17)	63 (2)	88 (3)	96 (3)	-9 (2)	49 (2)	-17 (2)
C (4)	73 (2)	81 (2)	49 (2)	-8 (2)	28 (2)	3 (2)

**Table A22** Hydrogen bonds for compound 7 [ Å and deg.].

D-H...A	d (D-H)	d (H...A)	d (D.....A)	< (DHA)
O (3) - H (31).....O (1)	1.05 (4)	1.61 (4)	2.584 (3)	154 (3)
O (3A) - H (32).....O (1A)	0.92 (4)	1.75 (4)	2.606 (3)	155 (3)

**Table A23** Crystal data and structure refinement for compound 8.

Empirical formula	C <sub>18</sub> H <sub>17</sub> O <sub>6</sub>	
Formula weight	329.32	
Temperature	293 (2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Triclinic, P(-1)	
Unit cell dimensions	a = 5.3069 (5) Å	alpha = 95.845 (2) deg.
	b = 11.4472 (10) Å	beta = 100.490 (2) deg.
	c = 20.9516 (11) Å	gamma = 94.957 (2) deg
Volume	765.18 (12) Å <sup>3</sup>	
Z, Calculated density	2, 1.429 Mg / m <sup>3</sup>	
Absorption coefficient	0.108 mm <sup>-1</sup>	
F ( 000 )	346	
Theta range for data collection	1.80 to 30.43 deg	
Index ranges	-7<=h<=7, -14<=k<=15, -18<=l<=14	
Reflections collected / unique	5645 / 4124 [ R (int) = 0.0205 ]	
Completeness to 2 theta = 30.44	88.70%	
Refinement method	Full - matrix least - squares on F <sup>2</sup>	
Data / restraints / parameters	4124 / 0 / 285	
Goodness - of - fit on F <sup>2</sup>	1.014	
Final R indices [ I > 2sigma (I) ]	R1 = 0.0644, wR2 = 0.1509	
R indices ( all data )	R1 = 0.1128, wR2 = 0.1853	
Largest diff. peak and hole	0.202 and -0.262 e.Å <sup>-3</sup>	

**Table A24** Atomic coordinates ( x 10<sup>4</sup> ) and equivalent isotropic displacement parameters ( Å<sup>2</sup> \* 10<sup>3</sup> ) for compound 8.

	X	Y	Z	U(eq)*
C (1)	3195 (4)	7054 (2)	2176 (2)	39 (1)
C (2)	948 (4)	7421 (2)	1513 (2)	39 (1)
C (3)	768 (4)	8675 (2)	1592 (2)	38 (1)
C (4)	-1360 (4)	9165 (2)	1025 (2)	41 (1)
C (5)	-1513 (5)	10370 (2)	1130 (2)	45 (1)

C (6)	469 (4)	11105 (2)	1801 (2)	44 (1)
C (7)	2586 (4)	10660 (2)	2382 (2)	44 (1)
C (8)	2656 (4)	9456 (2)	2270 (2)	38 (1)
C (10)	4933 (4)	7855 (2)	2841 (2)	37 (1)
C (11)	7149 (4)	7642 (2)	3645 (2)	36 (1)
C (12)	7967 (5)	8465 (2)	4554 (2)	45 (1)
C (13)	10009 (5)	8306 (2)	5321 (2)	48 (1)
C (14)	11333 (4)	7314 (2)	5216 (2)	40 (1)
C (15)	10573 (4)	6493 (2)	4320 (2)	40 (1)
C (16)	8503 (4)	6662 (2)	3550 (2)	39 (1)
C (17)	3683 (6)	5197 (3)	1271 (2)	56 (1)
C (18)	14842 (6)	6271 (2)	5950 (2)	55 (1)
C (19)	-1668 (6)	12838 (3)	1480 (3)	61 (1)
O (1)	528 (4)	12305 (2)	1957 (2)	60 (1)
O (2)	13328 (3)	7241 (2)	6029 (1)	53 (1)
O (3)	-3279 (3)	8441 (2)	374 (1)	59 (1)
O (4)	-750 (3)	6686 (2)	933 (1)	54 (1)
O (5)	3320 (3)	5864 (1)	2234 (1)	47 (1)
O (6)	4722 (3)	9045 (1)	2876 (1)	42 (1)

$U(\text{eq})^*$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

**Table A25** Bond distances (A) for compound 8.

Bond Distances	( A )	Bond Distances	( A )
C (1) - C (10)	1.356 (3)	C (8) - O (6)	1.375 (2)
C (1) - O (5)	1.379 (3)	C (10) - O (6)	1.373 (3)
C (1) - C (2)	1.457 (3)	C (10) - C (11)	1.476 (3)
C (2) - O (4)	1.256 (3)	C (11) - C (16)	1.391 (3)
C (2) - C (3)	1.441 (3)	C (11) - C (12)	1.407 (3)
C (3) - C (8)	1.393 (3)	C (12) - C (13)	1.369 (3)
C (3) - C (4)	1.422 (3)	C (13) - C (14)	1.394 (3)
C (4) - O (3)	1.355 (3)	C (14) - O (2)	1.366 (3)
C (4) - C (5)	1.383 (3)	C (14) - C (15)	1.391 (3)
C (5) - C (6)	1.391 (3)	C (15) - C (16)	1.385 (3)
C (6) - O (1)	1.365 (3)	C (17) - O (5)	1.447 (3)
C (6) - C (7)	1.399 (3)	C (18) - O (2)	1.432 (3)
C (7) - C (8)	1.375 (3)	C (19) - O (1)	1.431 (3)

**Table 26** Bond angles (deg.) for compound 8.

Angles	(deg.)	Angles	(deg.)
C (10) - C (1) - O (5)	119.83 (19)	C (7) - C (8) - C (3)	123.21 (19)
C (10) - C (1) - O (2)	121.08 (19)	C (1) - C (10) - O (6)	121.42 (19)
O (5) - C (1) - C (2)	118.37 (18)	C (1) - C (10) - C (11)	128.62 (19)
O (4) - C (2) - C (3)	122.4 (2)	O (6) - C (10) - C (11)	109.88 (17)
O (4) - C (2) - C (1)	121.9 (2)	C (16) - C (11) - C (12)	117.52 (19)
C (3) - C (2) - C (1)	115.65 (19)	C (16) - C (11) - C (10)	123.26 (18)
C (8) - C (3) - C (4)	117.2 (2)	C (12) - C (11) - C (10)	119.21 (19)
C (8) - C (3) - C (2)	120.52 (19)	C (13) - C (12) - C (11)	121.4 (2)
C (4) - C (3) - C (2)	122.25 (19)	C (12) - C (13) - C (14)	120.3 (2)
O (3) - C (4) - C (5)	119.3 (2)	O (2) - C (14) - C (13)	115.40 (19)
O (3) - C (4) - C (3)	119.5 (2)	O (2) - C (14) - C (15)	125.2 (2)
C (5) - C (4) - C (3)	121.1 (2)	C (13) - C (14) - C (15)	119.4 (2)
C (4) - C (5) - C (6)	118.8 (2)	C (16) - C (15) - C (14)	119.8 (2)
O (1) - C (6) - C (5)	123.8 (2)	C (15) - C (16) - C (11)	121.6 (2)
O (1) - C (6) - C (7)	114.3 (2)	C (6) - O (1) - C (19)	118.6 (2)
C (5) - C (6) - C (7)	121.9 (2)	C (14) - O (2) - C (18)	118.34 (18)
C (8) - C (7) - C (6)	117.7 (2)	C (1) - O (5) - C (17)	114.61 (19)
O (6) - C (8) - C (7)	116.18 (19)	C (8) - O (6) - C (10)	120.64 (17)
O (6) - C (8) - C (3)	120.60 (19)		

Symmetry transformations used to generate equivalent atoms:

**Table A27** Anisotropic displacement parameters ( $\text{Å}^2 \cdot 10^3$ ). The anisotropic displacement factor exponent takes the form:  $-2 \pi^2 [ h^2 a^{*2} U_{11} + \dots + 2hka^*b^*U_{12} ]$ .

	$U_{11}$	$U_{22}$	$U_{33}$	$U_{23}$	$U_{13}$	$U_{12}$
C (1)	41 (1)	36 (1)	38 (1)	4 (1)	6 (1)	3 (1)
C (2)	39 (1)	43 (1)	33 (1)	2 (1)	4 (1)	-.1 (1)
C (3)	37 (1)	41 (1)	35 (1)	5 (1)	4 (1)	2 (1)
C (4)	35 (1)	50 (1)	37 (1)	9 (1)	0 (1)	2 (1)
C (5)	37 (1)	53 (1)	44 (1)	10 (1)	0 (1)	10 (1)
C (6)	43 (1)	42 (1)	45 (1)	7 (1)	4 (1)	9 (1)
C (7)	40 (1)	43 (1)	44 (1)	3 (1)	-.3 (1)	4(1)
C (8)	34 (1)	40 (1)	37 (1)	6 (1)	2 (1)	4(1)
C (10)	39 (1)	34 (1)	37 (1)	4 (1)	6 (1)	4(1)
C (11)	36 (1)	36 (1)	36 (1)	7 (1)	5 (1)	2 (1)
C (12)	50 (1)	36 (1)	48 (1)	0 (1)	2 (1)	12 (1)
C (13)	53 (1)	42 (1)	42 (1)	-.4 (1)	-.2 (1)	8 (1)
C (14)	40 (1)	40 (1)	38 (1)	8 (1)	3 (1)	3 (1)
C (15)	42 (1)	38 (1)	39 (1)	3 (1)	5 (1)	7 (1)

C (16)	41 (1)	38 (1)	36 (1)	-.1 (1)	4 (1)	5 (1)
C (17)	60 (2)	47 (2)	58 (2)	-.9 (1)	8 (1)	6 (1)
C (18)	53 (2)	45 (1)	61 (2)	8 (1)	-.7 (1)	10 (1)
C (19)	56 (2)	55 (2)	71 (2)	15 (2)	3 (2)	20 (1)
O (1)	59 (1)	42 (1)	73 (1)	5 (1)	-.11 (1)	15 (1)
O (2)	52 (1)	54 (1)	47 (1)	-.2 (1)	-.10 (1)	14 (1)
O (3)	47 (1)	57 (1)	61 (1)	5 (1)	-.15 (1)	0 (1)
O (4)	48 (1)	47 (1)	56 (1)	-.2 (1)	-.7 (1)	-.5 (1)
O (5)	56 (1)	35 (1)	47 (1)	3 (1)	4 (1)	2 (1)
O (6)	40 (1)	35 (1)	46 (1)	5 (1)	-.5 (1)	4 (1)

**Table A28** Hydrogen bonds for compound 8 [ A and deg.].

D-H...A	d (D-H)	d (H...A)	d (D...A)	< (DHA)
O (3) - H (30).....O (4)	0.95 (4)	1.71 (4)	2.601 (2)	155 (4)

Symmetry transformations used to generate equivalent atoms:

**Table A29** Crystal data and structure refinement for compound 10.

Empirical formula	C <sub>22</sub> H <sub>21</sub> O <sub>5</sub>	
Formula weight	379.06	
Temperature	293 (2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Orthorhombic, P2(1) 2(1) 2(1)	
Unit cell dimensions	a = 5.51390 (10) Å	alpha = 90 deg.
	b = 8.9049 (2) Å	beta = 90 deg.
	c = 28.9882 (2) Å	gamma = 90 deg.
Volume	1423.34 (4) Å <sup>3</sup>	
Z, Calculated density	3, 1.327 Mg / m <sup>3</sup>	
Absorption coefficient	0.094 mm <sup>-1</sup>	
F ( 000 )	600	
Theta range for data collection	2.39 to 30.46 deg	
Index ranges	-.7<=h<=7, -12<=k<=10, -35<=l<=40	
Reflections collected / unique	10566 / 4030 [ R (int) = 0.0278 ]	

Completeness to 2 theta = 30.44	96.50%
Refinement method	Full - matrix least - squares on F <sup>2</sup>
Data / restraints / parameters	4030 / 0 / 218
Goodness - of - fit on F <sup>2</sup>	1.058
Final R indices [ I > 2sigma (I) ]	R1 = 0.0526, wR2 = 0.1110
R indices ( all data )	R1 = 0.0795, wR2 = 0.1250
Absolute structure parameter	0.2 (12)
Largest diff. peak and hole	0.136 and -0.171 e.A <sup>-3</sup>

**Table A30** Atomic coordinates ( x 10<sup>4</sup> ) and equivalent isotropic displacement parameters ( A<sup>2</sup> \* 10<sup>3</sup> ) for compound 10.

	X	Y	Z	U (eq)*
C (1)	1017 (5)	7851 (3)	7077 (1)	71 (1)
C (2)	483 (5)	7345 (3)	7516 (1)	68 (1)
C (3)	1959 (4)	7728 (3)	7884 (1)	56 (1)
C (4)	3969 (4)	8620 (2)	7818 (1)	44 (1)
C (5)	4509 (5)	9124 (3)	7375 (1)	57 (1)
C (6)	3021 (5)	8726 (3)	7008 (1)	71 (1)
C (7)	5626 (4)	9049 (2)	8212 (1)	44 (1)
C (9)	7673 (3)	7894 (2)	8836 (1)	42 (1)
C (10)	8941 (4)	6615 (2)	8964 (1)	47 (1)
C (11)	10628 (4)	6722 (2)	9312 (1)	45 (1)
C (12)	11034 (4)	8080 (2)	9541 (1)	47 (1)
C (13)	9748 (4)	9342 (2)	9417 (1)	43 (1)
C (14)	7988 (4)	9287 (2)	9056 (1)	40 (1)
C (15)	6448 (4)	10563 (2)	8917 (1)	47 (1)
C (16)	4637 (4)	10226 (2)	8540 (1)	50 (1)
C (17)	11901 (5)	4182 (2)	9193 (1)	72 (1)
C (18)	11914 (5)	10811 (3)	9971 (1)	59 (1)
O (1)	6545 (4)	11810 (2)	9085 (1)	73 (1)
O (2)	10098 (3)	10700 (1)	9618 (1)	54 (1)
O (3)	12037 (3)	5556 (2)	9452 (1)	63 (1)
O (4)	6130 (3)	7700 (1)	8472 (1)	51 (1)

U(eq)\* is defined as one third of the trace of the orthogonalized U<sub>ij</sub> tensor.

**Table A31** Bond distances (A) for compound 10.

Bond Distances	( A )	Bond Distances	( A )
C (1) - C (6)	1.367 (4)	C (10) - C (11)	1.375 (3)
C (1) - C (2)	1.383 (4)	C (11) - O (3)	1.359 (2)
C (2) - C (3)	1.384 (3)	C (11) - C (12)	1.398 (3)
C (3) - C (4)	1.377 (3)	C (12) - C (13)	1.376 (3)
C (4) - C (5)	1.392 (3)	C (13) - O (2)	1.357 (2)
C (4) - C (7)	1.511 (3)	C (13) - C (14)	1.427 (3)
C (5) - C (6)	1.390 (3)	C (14) - C (15)	1.475 (2)
C (7) - O (4)	1.446 (2)	C (15) - O (1)	1.214 (2)
C (7) - C (16)	1.517 (3)	C (15) - C (16)	1.511 (3)
C (9) - O (4)	1.36 (2)	C (17) - O (3)	1.439 (3)
C (9) - C (10)	1.387 (3)	C (18) - O (2)	1.434 (3)
C (9) - C (14)	1.406 (3)		

**Table A32** Bond angles (deg.) for compound 10.

Angles	(deg.)	Angles	(deg.)
C (6) - C (1) - C (2)	119.5 (2)	O (3) - C (11) - C (12)	115.26 (17)
C (1) - C (2) - C (3)	120.3 (3)	C (10) - C (11) - C (12)	121.13 (17)
C (4) - C (3) - C (2)	120.5 (2)	C (13) - C (12) - C (11)	119.98 (17)
C (3) - C (4) - C (5)	119.2 (2)	O (2) - C (13) - C (12)	122.81 (17)
C (3) - C (4) - C (7)	121.81 (18)	O (2) - C (13) - C (14)	116.27 (16)
C (5) - C (4) - C (7)	119.0 (2)	C (12) - C (13) - C (14)	120.91 (16)
C (6) - C (5) - C (4)	119.8 (2)	C (9) - C (14) - C (13)	116.56 (16)
C (1) - C (6) - C (5)	120.7 (2)	C (9) - C (14) - C (15)	118.95 (17)
O (4) - C (7) - C (4)	107.48 (15)	C (13) - C (14) - C (15)	124.44 (16)
O (4) - C (7) - C (16)	108.39 (15)	O (1) - C (15) - C (14)	124.72 (19)
C (4) - C (7) - C (16)	115.55 (16)	O (1) - C (15) - C (16)	120.08 (18)
O (4) - C (9) - C (10)	114.65 (16)	C (14) - C (15) - C (16)	115.20 (16)
O (4) - C (9) - C (14)	122.64 (16)	C (15) - C (16) - C (7)	110.71 (16)
C (10) - C (9) - C (14)	122.70 (17)	C (13) - O (2) - C (18)	117.90 (16)
C (11) - C (10) - C (9)	118.70 (17)	C (11) - O (3) - C (17)	117.58 (17)
O (3) - C (11) - C (10)	123.60 (17)	C (9) - O (4) - C (7)	114.71 (14)

Symmetry transformations used to generate equivalent atoms:

**Table A33** Anisotropic displacement parameters ( $\text{Å}^2 \cdot 10^3$ ). The anisotropic displacement factor exponent takes the form:  $-2 \pi^2 [ h^2 a^{*2} U_{11} + \dots + 2hka^*b^*U_{12} ]$

	<i>U</i> <sub>11</sub>	<i>U</i> <sub>22</sub>	<i>U</i> <sub>33</sub>	<i>U</i> <sub>23</sub>	<i>U</i> <sub>13</sub>	<i>U</i> <sub>12</sub>
C (1)	63 (2)	81 (2)	68 (2)	-10 (1)	-20 (1)	12 (1)
C (2)	45 (1)	67 (2)	92 (2)	-6 (1)	-7 (1)	-3 (1)
C (3)	44 (1)	64 (1)	60 (1)	5 (1)	4 (1)	1 (1)
C (4)	43 (1)	42 (1)	46 (1)	1 (1)	-1 (1)	11 (1)
C (5)	58 (1)	59 (1)	55 (1)	12 (1)	-5 (1)	2 (1)
C (6)	80 (2)	82 (2)	50 (1)	10 (1)	-11 (1)	11 (2)
C (7)	43 (1)	44 (1)	43 (1)	4 (1)	-1 (1)	7 (1)
C (9)	47 (1)	40 (1)	39 (1)	1 (1)	0 (1)	6 (1)
C (10)	59 (1)	34 (1)	48 (1)	-1 (1)	-2 (1)	6 (1)
C (11)	51 (1)	40 (1)	45 (1)	6 (1)	-1 (1)	10 (1)
C (12)	52 (1)	47 (1)	42 (1)	3 (1)	-7 (1)	3 (1)
C (13)	50 (1)	40 (1)	39 (1)	1 (1)	2 (1)	3 (1)
C (14)	46 (1)	36 (1)	39 (1)	1 (1)	3 (1)	7 (1)
C (15)	54 (1)	42 (1)	44 (1)	-3 (1)	3 (1)	13 (1)
C (16)	47 (1)	49 (1)	53 (1)	-3 (1)	-2 (1)	14 (1)
C (17)	83 (2)	47 (1)	88 (2)	-2 (1)	-15 (1)	26 (1)
C (18)	71 (1)	56 (1)	50 (1)	-6 (1)	-10 (1)	-6 (1)
O (1)	96 (1)	49 (1)	75 (1)	-19 (1)	-20 (1)	32 (1)
O (2)	71 (1)	41 (1)	51 (1)	-5 (1)	-11 (1)	3 (1)
O (3)	74 (1)	44 (1)	70 (1)	2 (1)	-19 (1)	19 (1)
O (4)	63 (1)	39 (1)	50 (1)	-1 (1)	-14 (1)	8 (1)



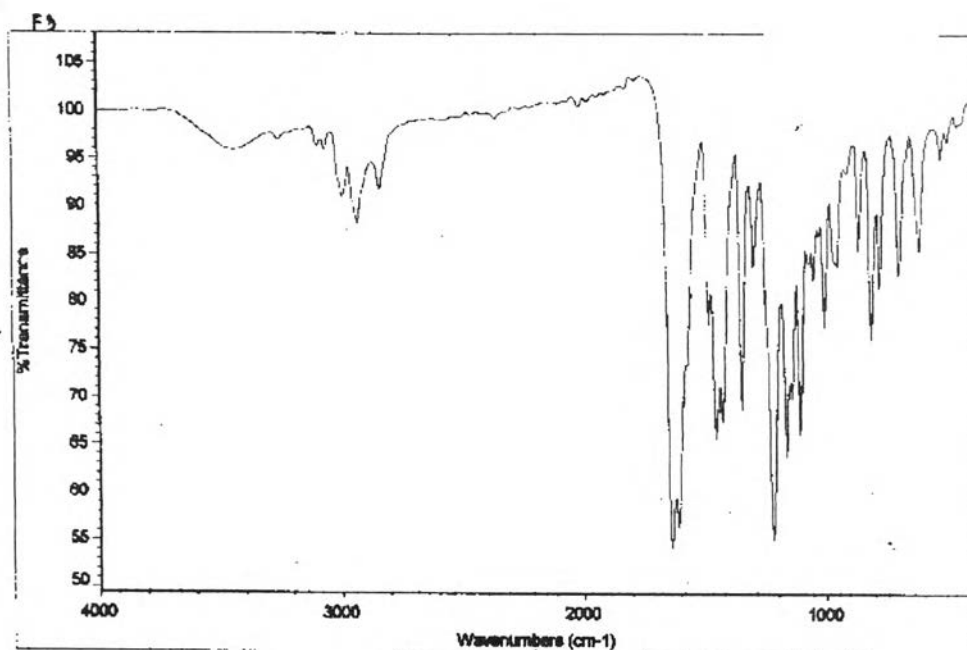


Figure A1 The IR spectrum of Compound 1.(3,5,7-trimethoxyflavone)

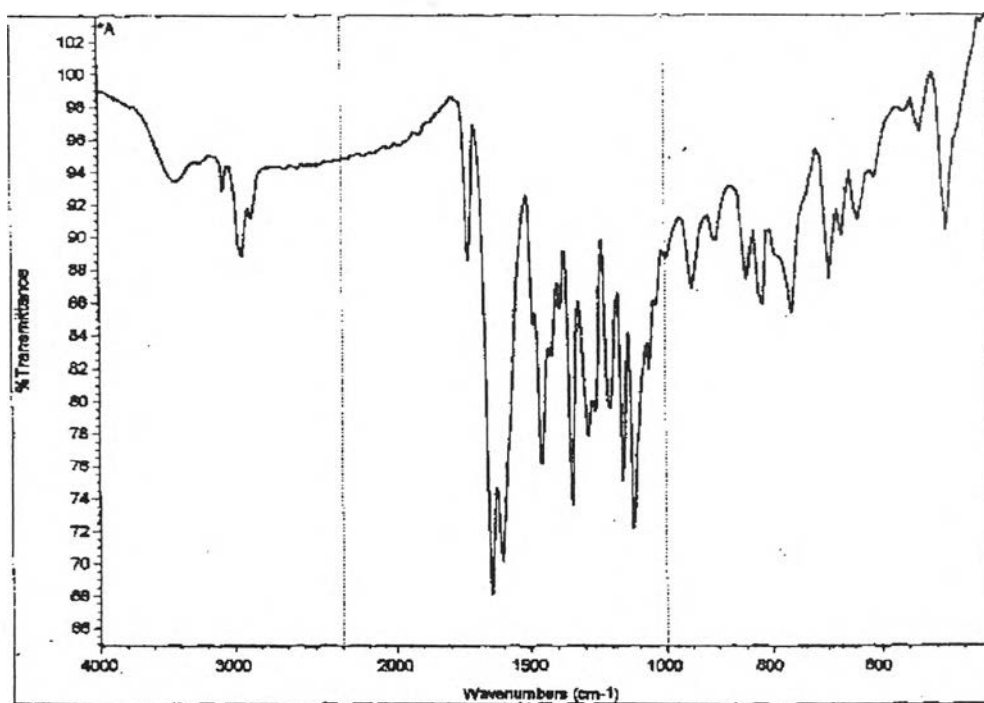


Figure A2 The IR spectrum of Compound 2.(5,7-dimethoxyflavone)

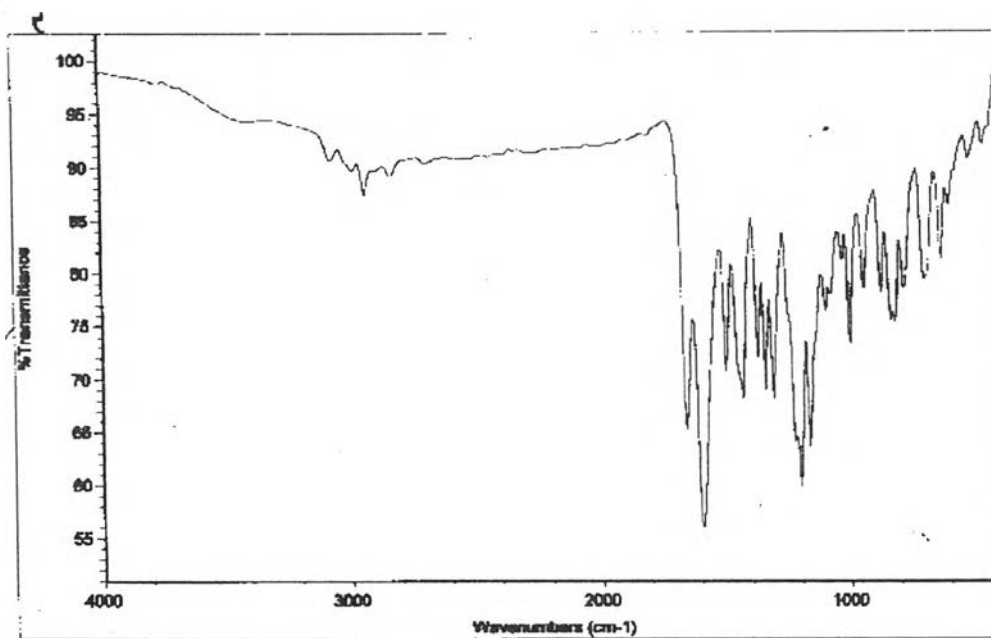


Figure A3 The IR spectrum of Compound 3.(5,7,4'-trimethoxyflavone)

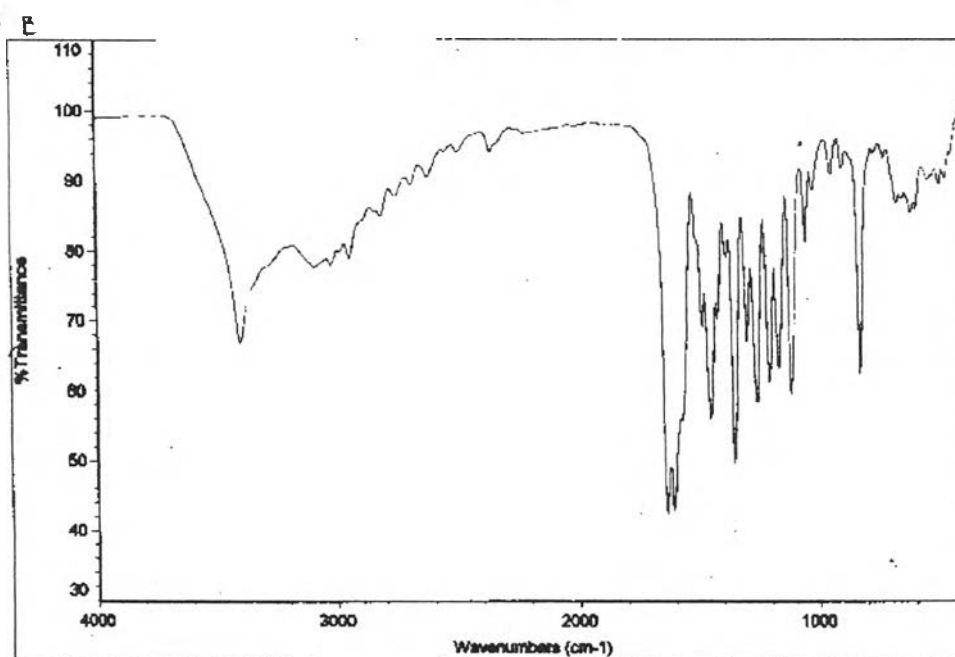


Figure A4 The IR spectrum of Compound 4.(4'-hydroxy-5,7-dimethoxyflavone)

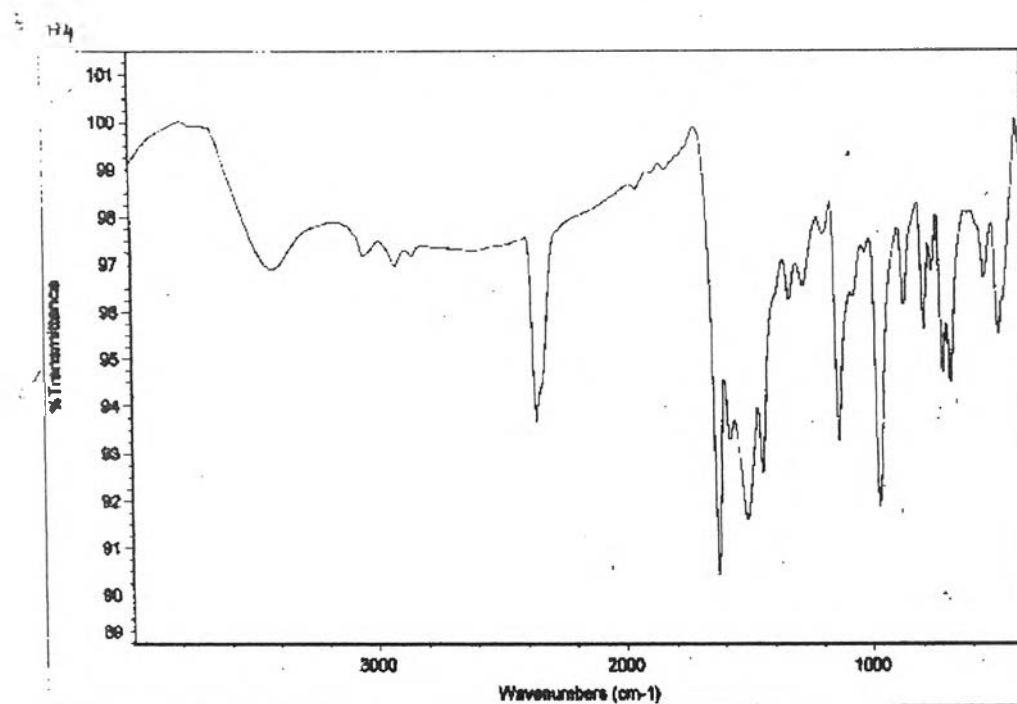


Figure A5 The IR spectrum of Compound 5.(dicinnamylmethane)

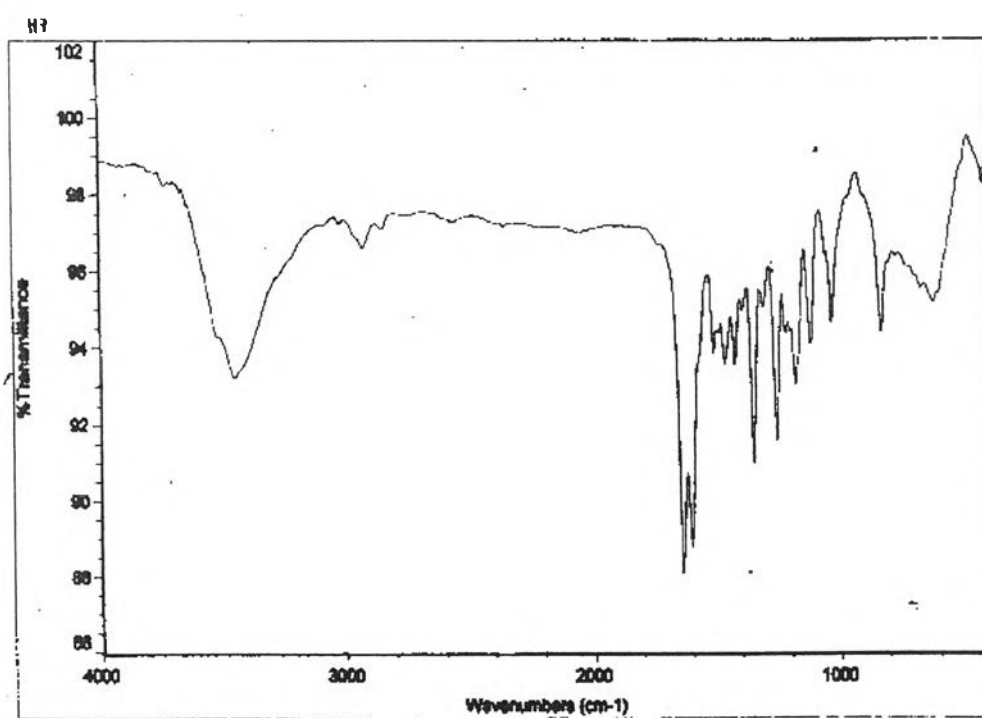


Figure A6 The IR spectrum of Compound 6.(5-hydroxy-3,7-dimethoxyflavone)

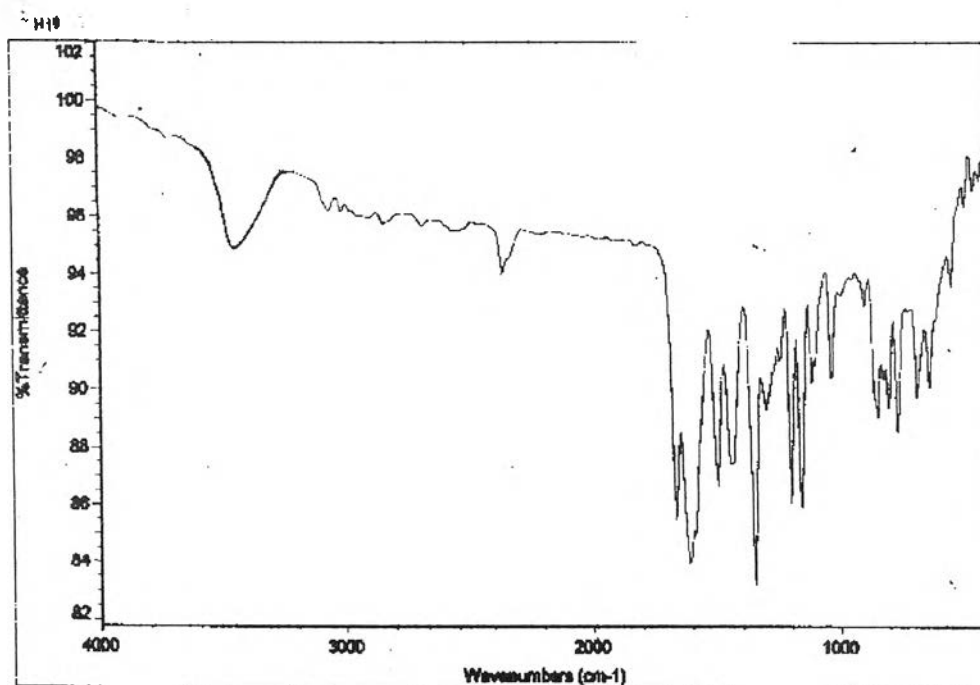


Figure A7 The IR spectrum of Compound 7.(5-hydroxy-7-methoxyflavone)

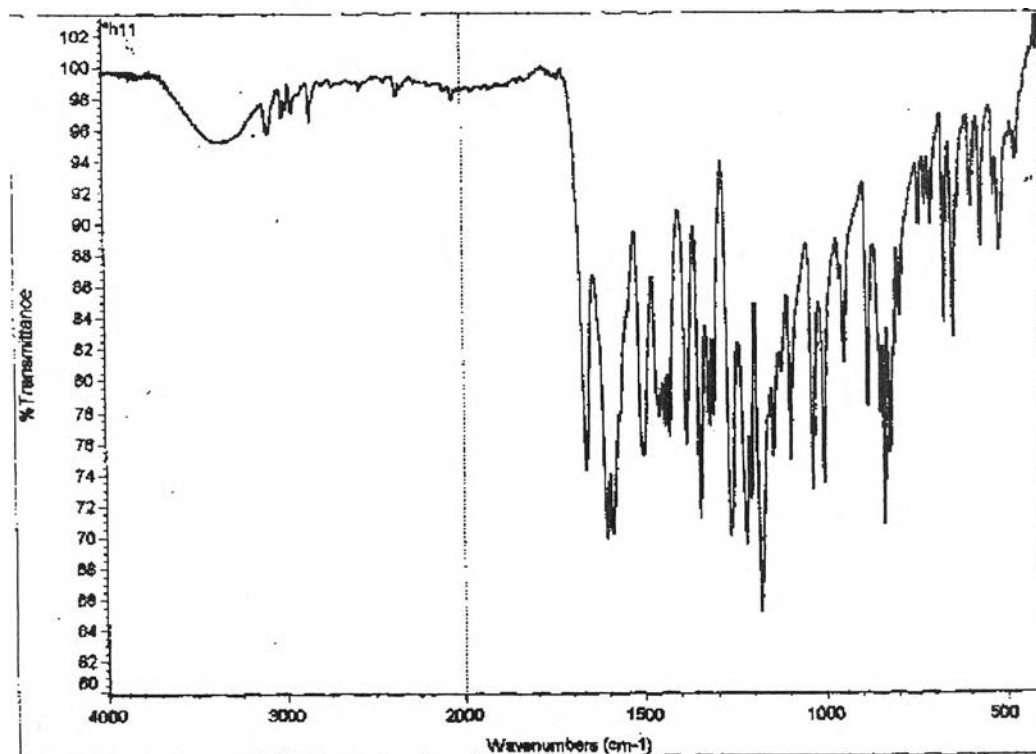


Figure A8 The IR spectrum of Compound 8.(5-hydroxy-3,7,4'-trimethoxyflavone)

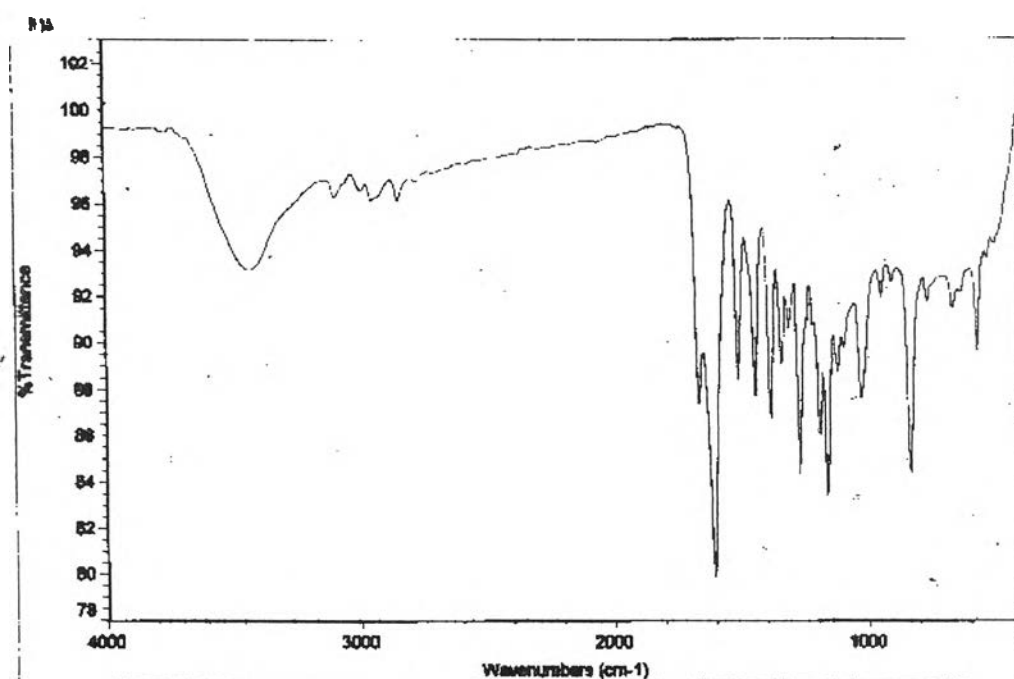


Figure A9 The IR spectrum of Compound 9.(5-hydroxy-7,4'-dimethoxyflavone)

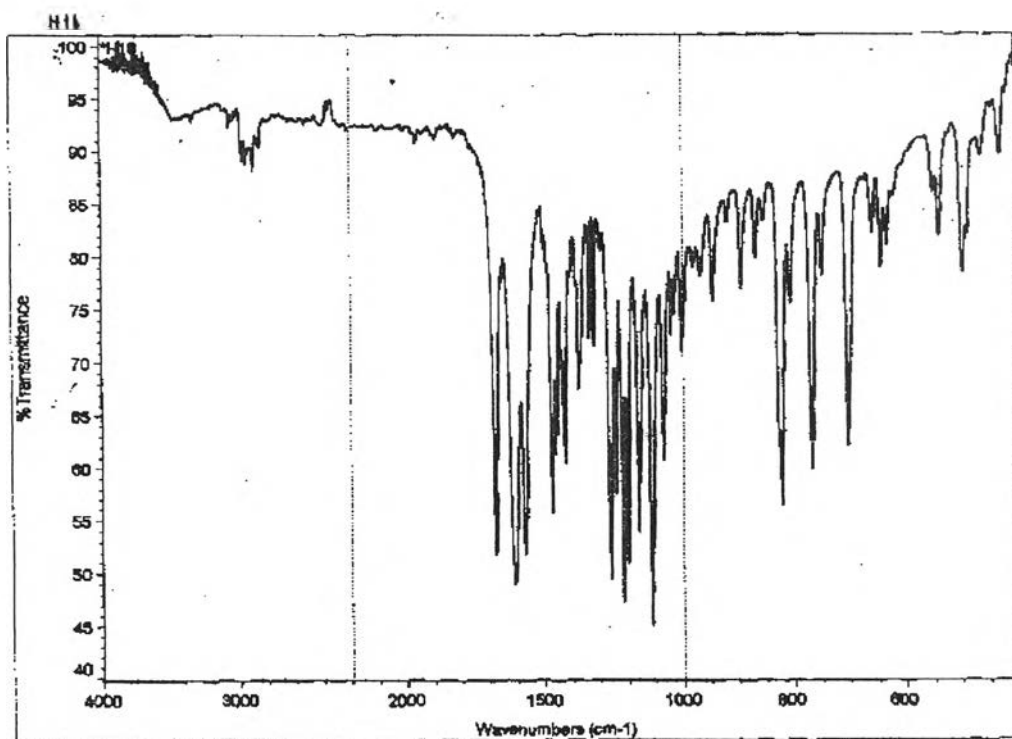


Figure A10 The IR spectrum of Compound 10.(5,7-dimethoxyflavanone)

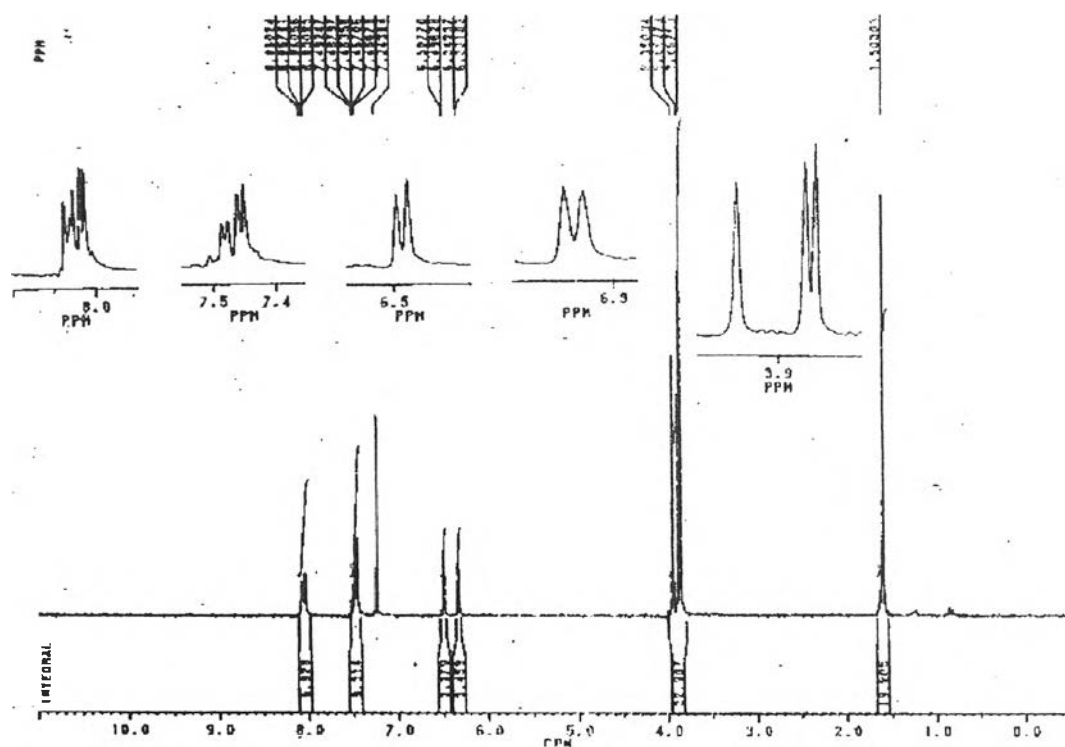


Figure A11 The  $^1\text{H-NMR}$  spectrum of Compound 1.(3,5,7-trimethoxyflavone)

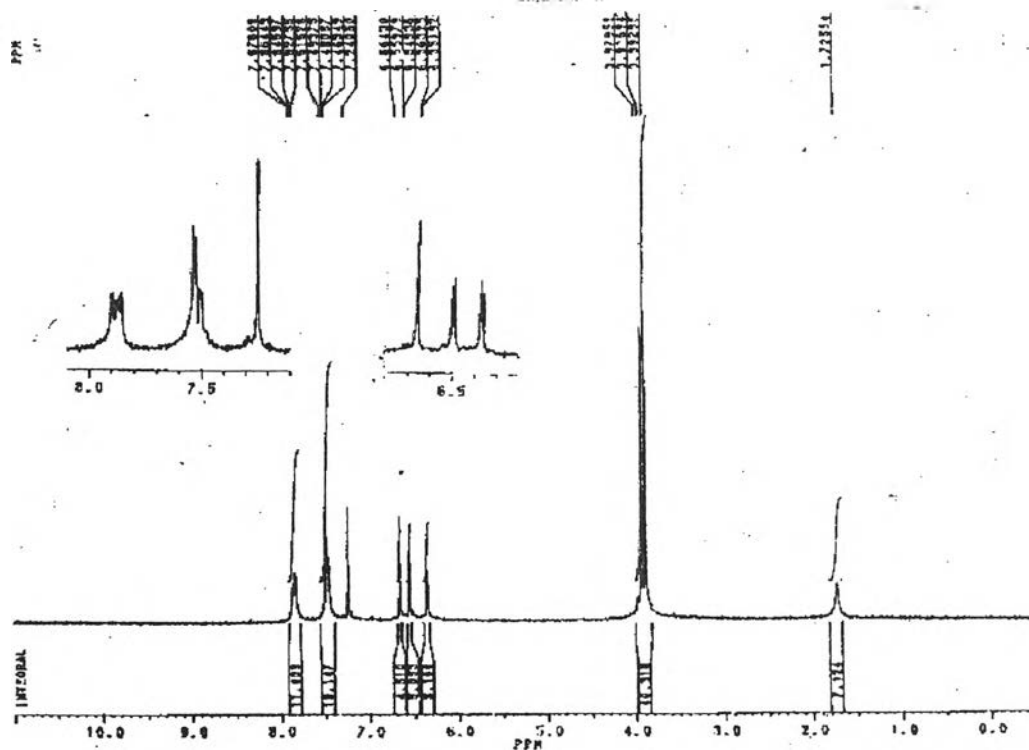


Figure A12 The  $^1\text{H-NMR}$  spectrum of Compound 2.(5,7-dimethoxyflavone)

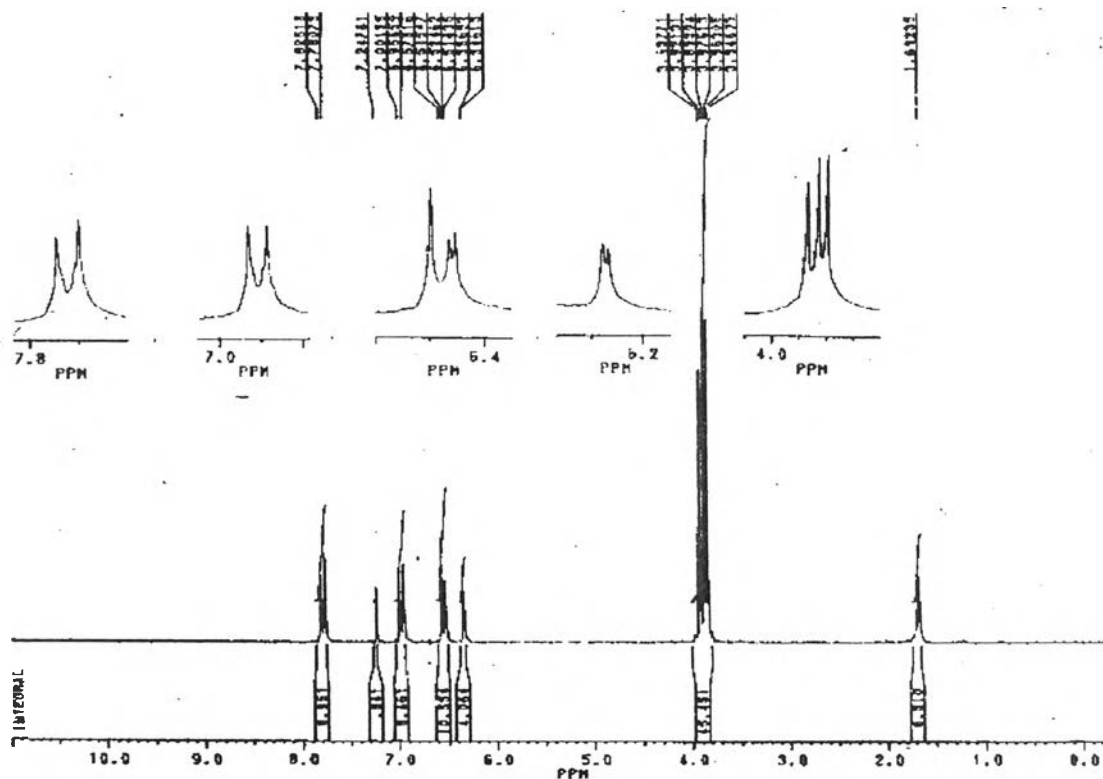


Figure A13 The  $^1\text{H-NMR}$  spectrum of Compound 3 (5,7,4'-trimethoxyflavone)

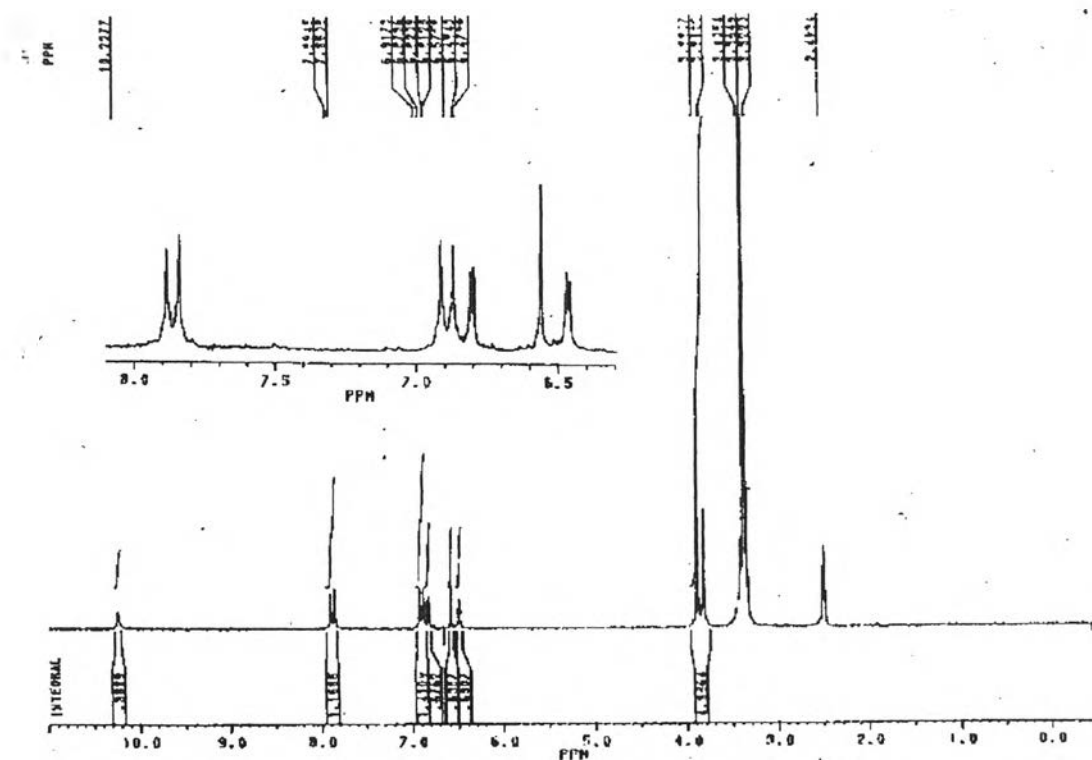


Figure A14 The  $^1\text{H-NMR}$  spectrum of Compound 4 (4'-hydroxy-5,7-dimethoxyflavone)

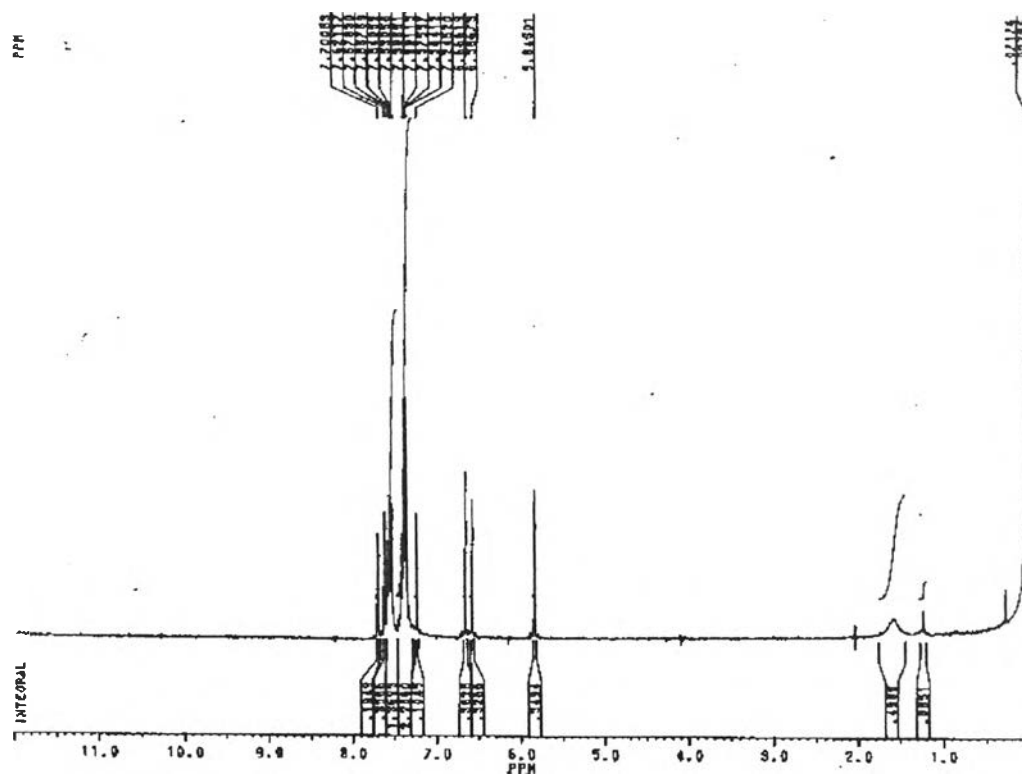


Figure A15 The  $^1\text{H-NMR}$  spectrum of Compound 5.(dicinnamoylmethane)

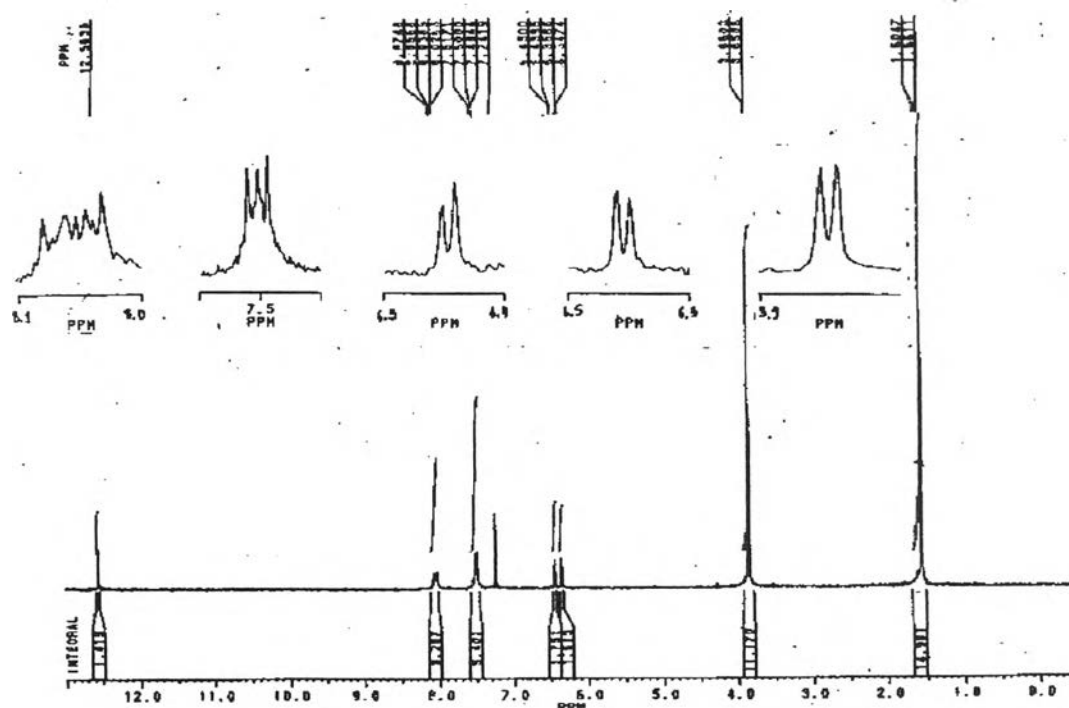


Figure A16 The  $^1\text{H-NMR}$  spectrum of Compound 6.(5-hydroxy-3,7-dimethoxyflavone)



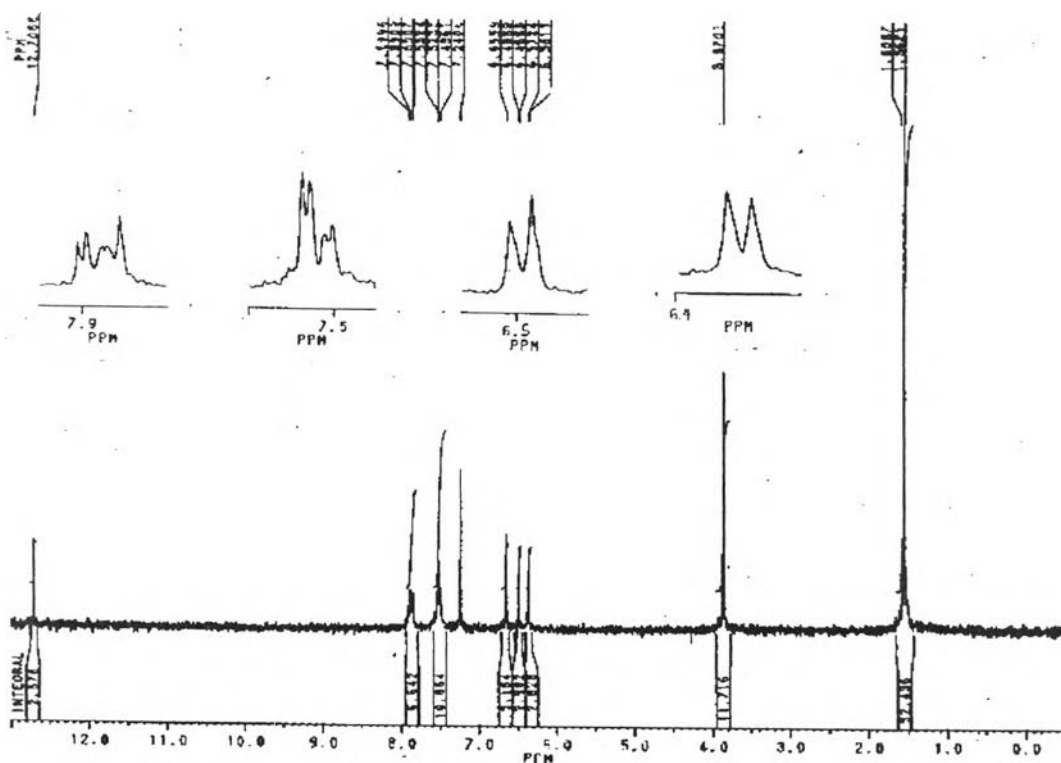


Figure A17 The  $^1\text{H-NMR}$  spectrum of Compound 7.(5-hydroxy-7-methoxyflavone)

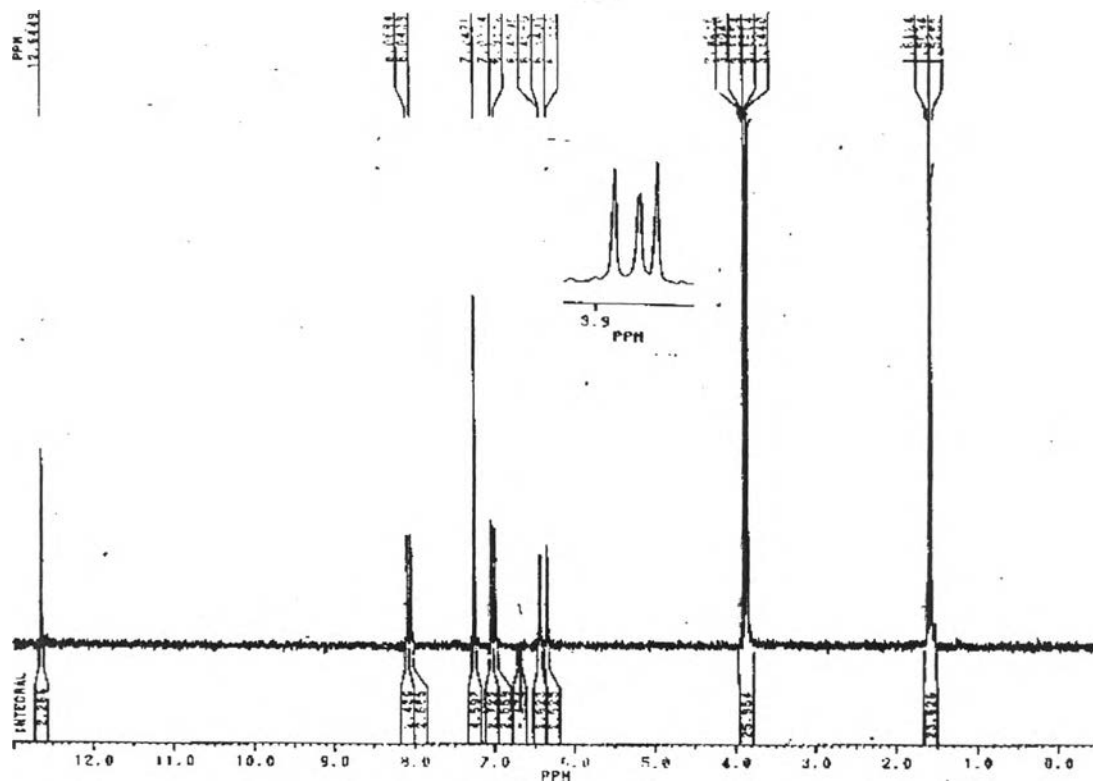


Figure A18 The  $^1\text{H-NMR}$  spectrum of Compound 8.(5-hydroxy-3,7,4'-trimethoxyflavone)

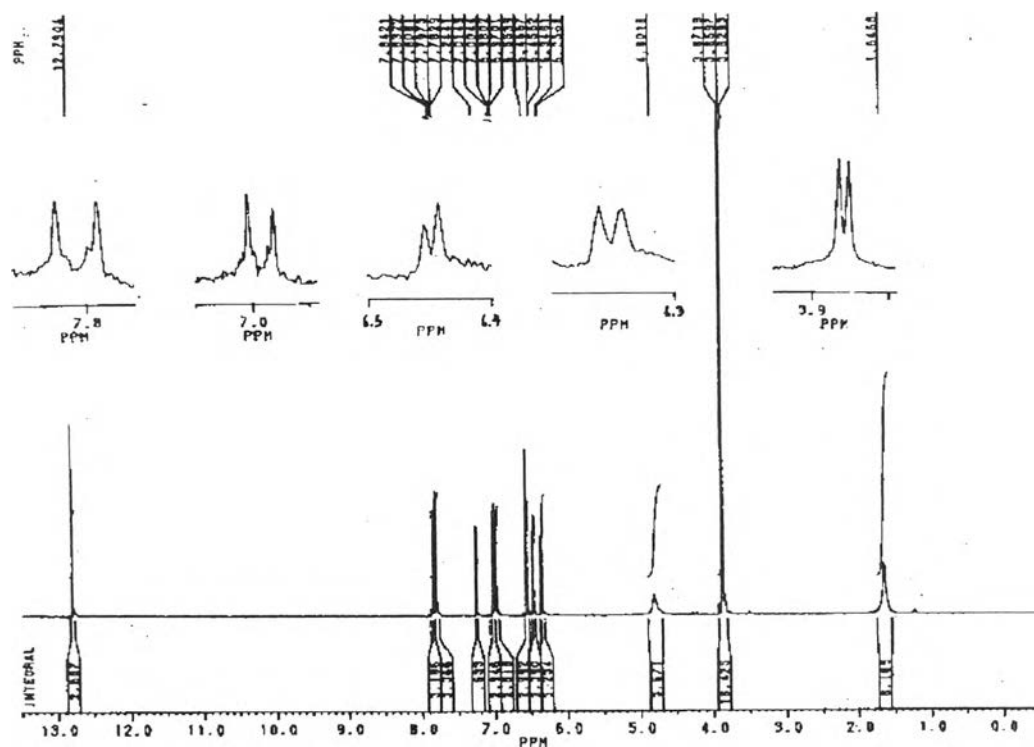


Figure A19 The  $^1\text{H-NMR}$  spectrum of Compound 9.(5-hydroxy-7,4'-dimethoxyflavone)

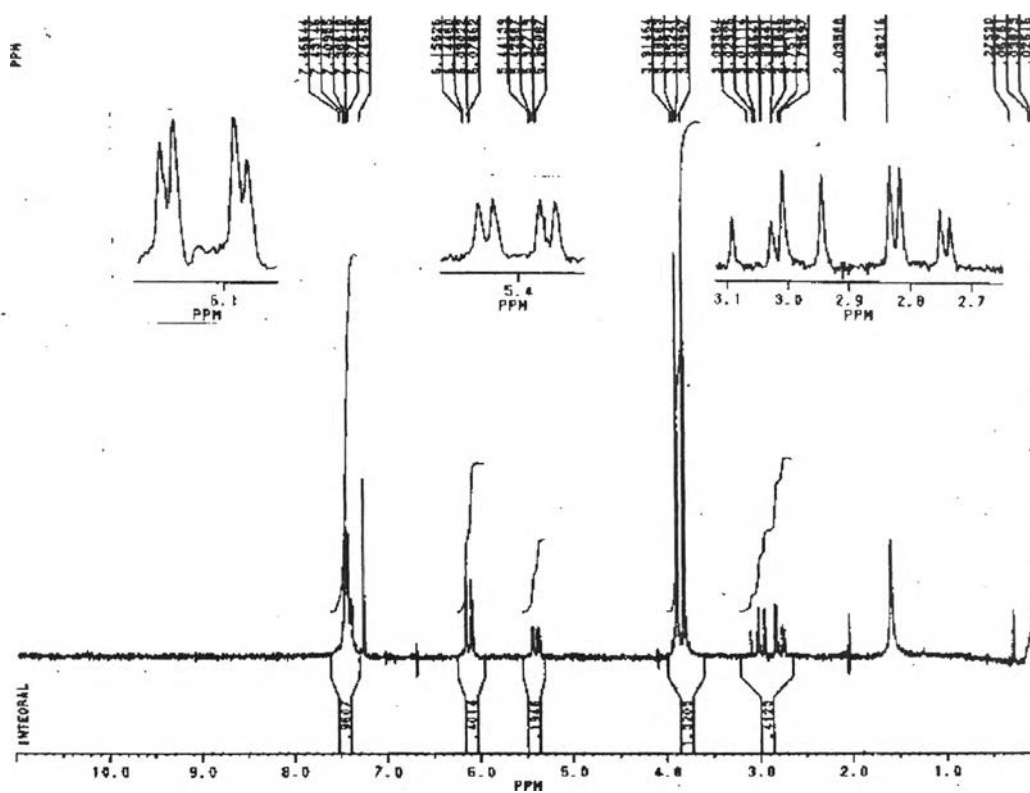


Figure A20 The  $^1\text{H-NMR}$  spectrum of Compound 10.(5,7-dimethoxyflavanone)

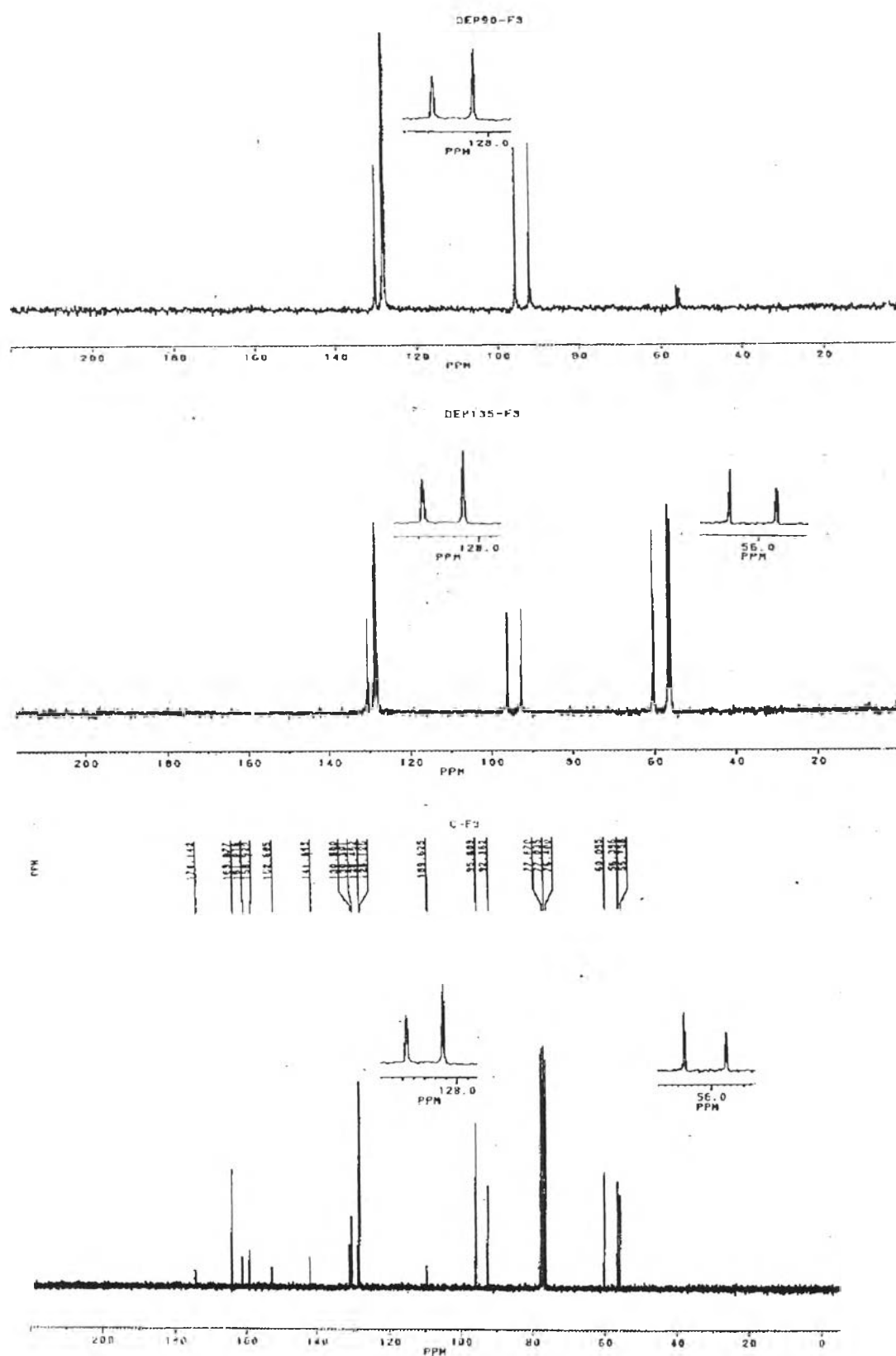


Figure A21 DEPT90, DEPT135 and  $^{13}\text{C}$ -NMR spectra of Compound 1 (3,5,7-trimethoxyflavone)

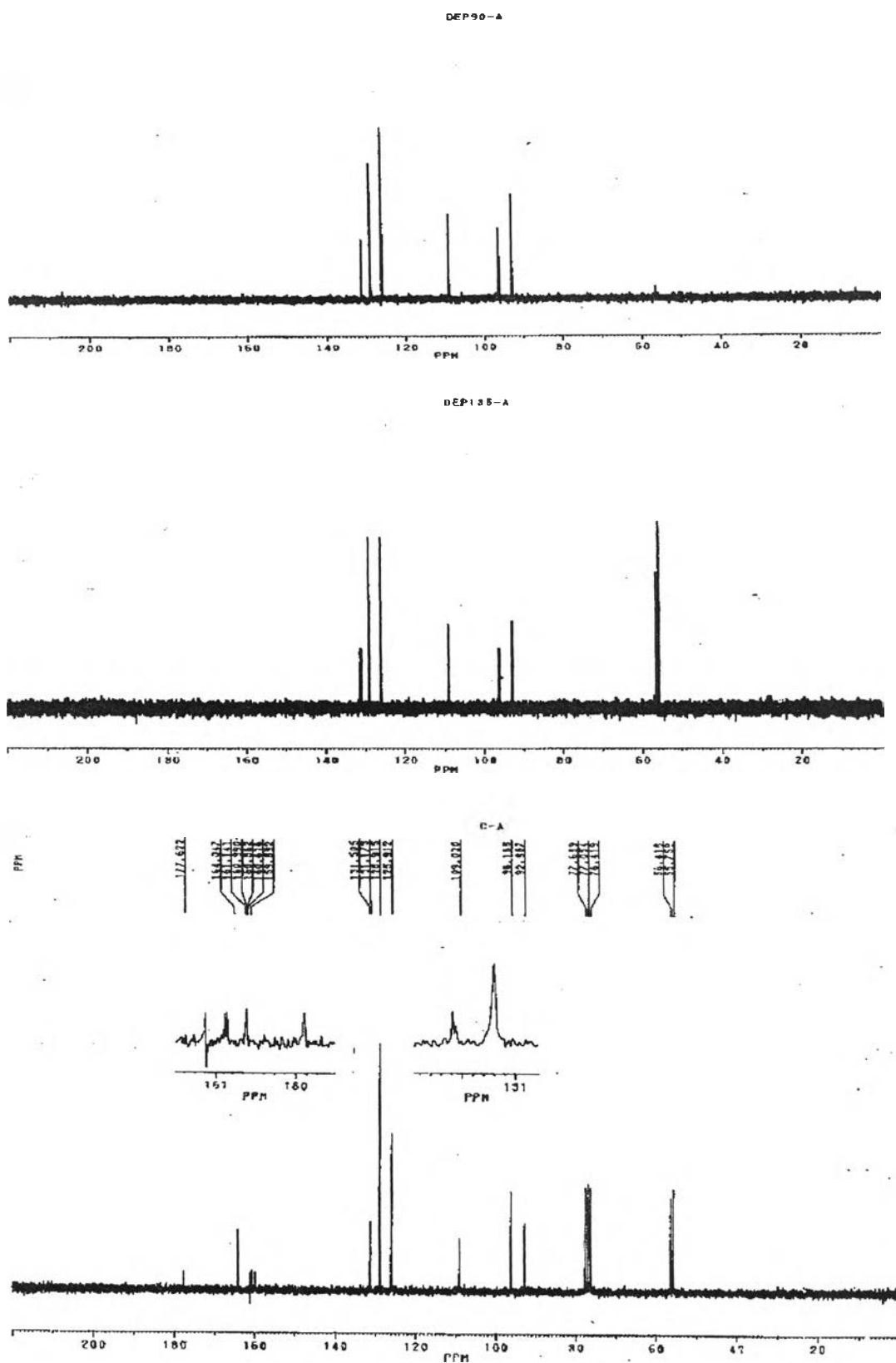


Figure A22 DEPT90, DEPT135 and  $^{13}\text{C}$ -NMR spectra of Compound 2.(5,7-dimethoxyflavone)

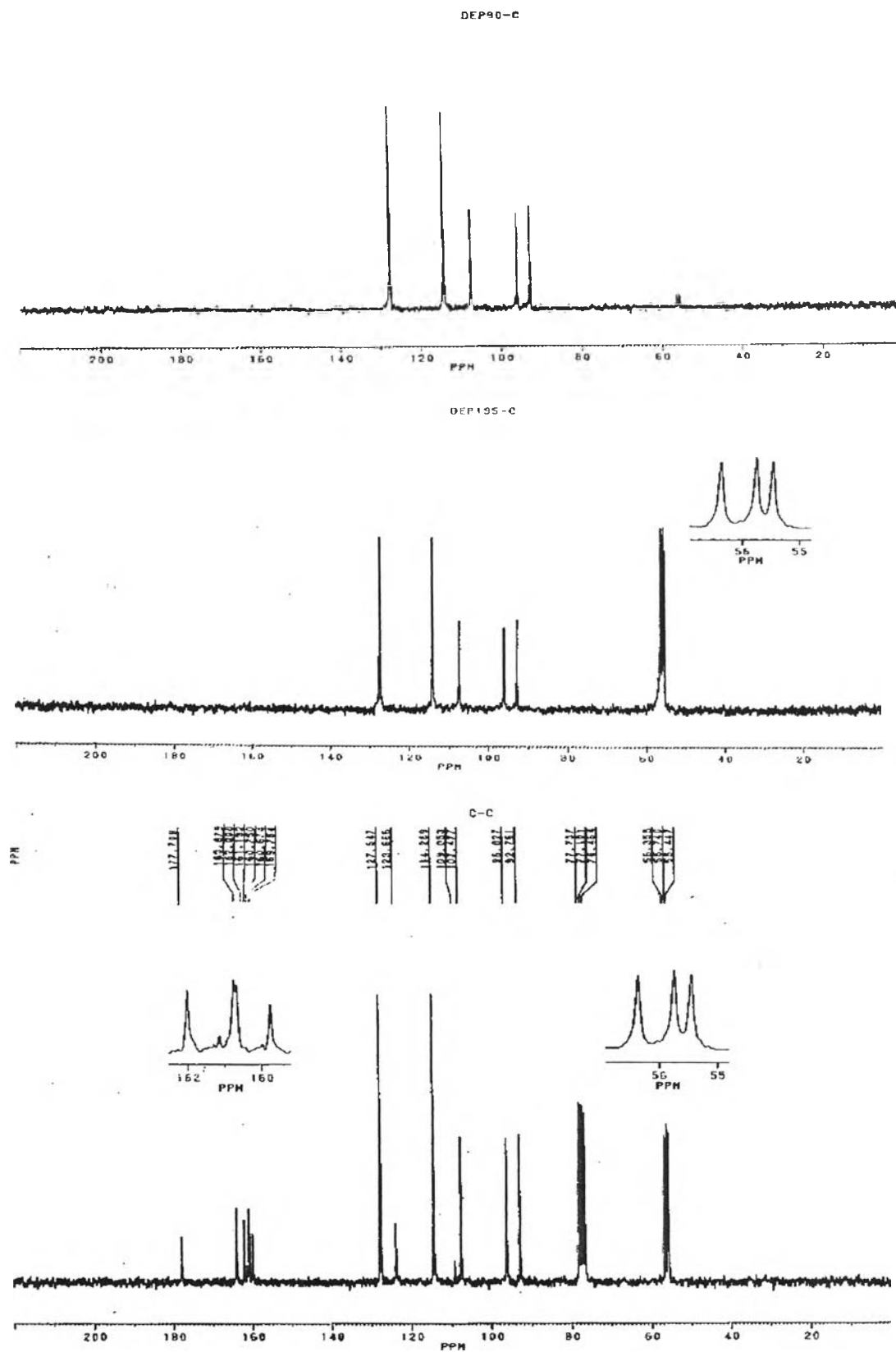


Figure A23 DEPT90, DEPT135 and  $^{13}\text{C}$ -NMR spectra of Compound 3. (5,7,4'-trimethoxyflavone)

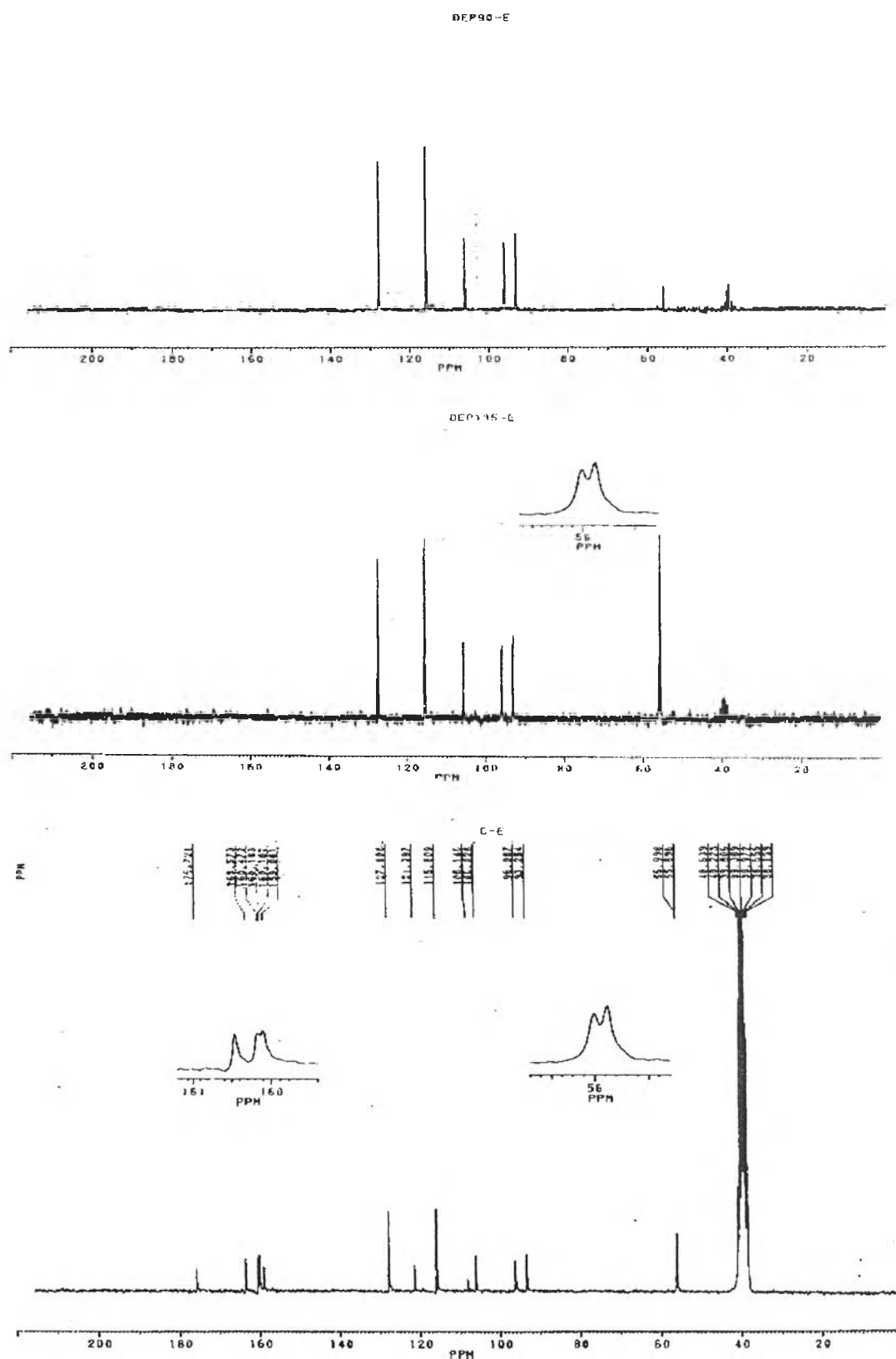


Figure A24 DEPT90, DEPT135 and  $^{13}\text{C}$ -NMR spectra of Compound 4.  
(4'-hydroxy-5,7-dimethoxyflavone)

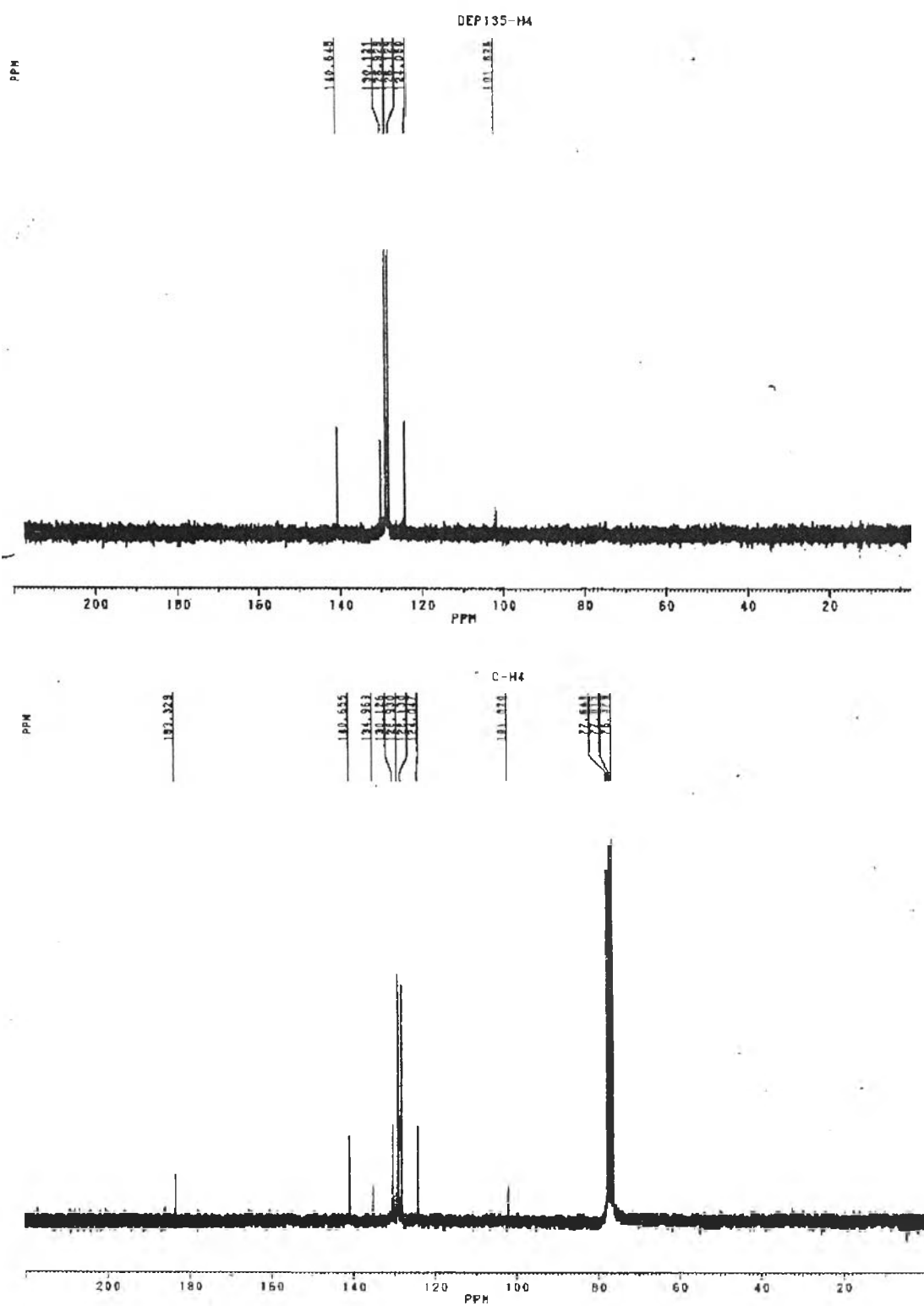


Figure A25 DEPT90, DEPT135 and  $^{13}\text{C}$ -NMR spectra of Compound 5.(dicinnamylmethane)

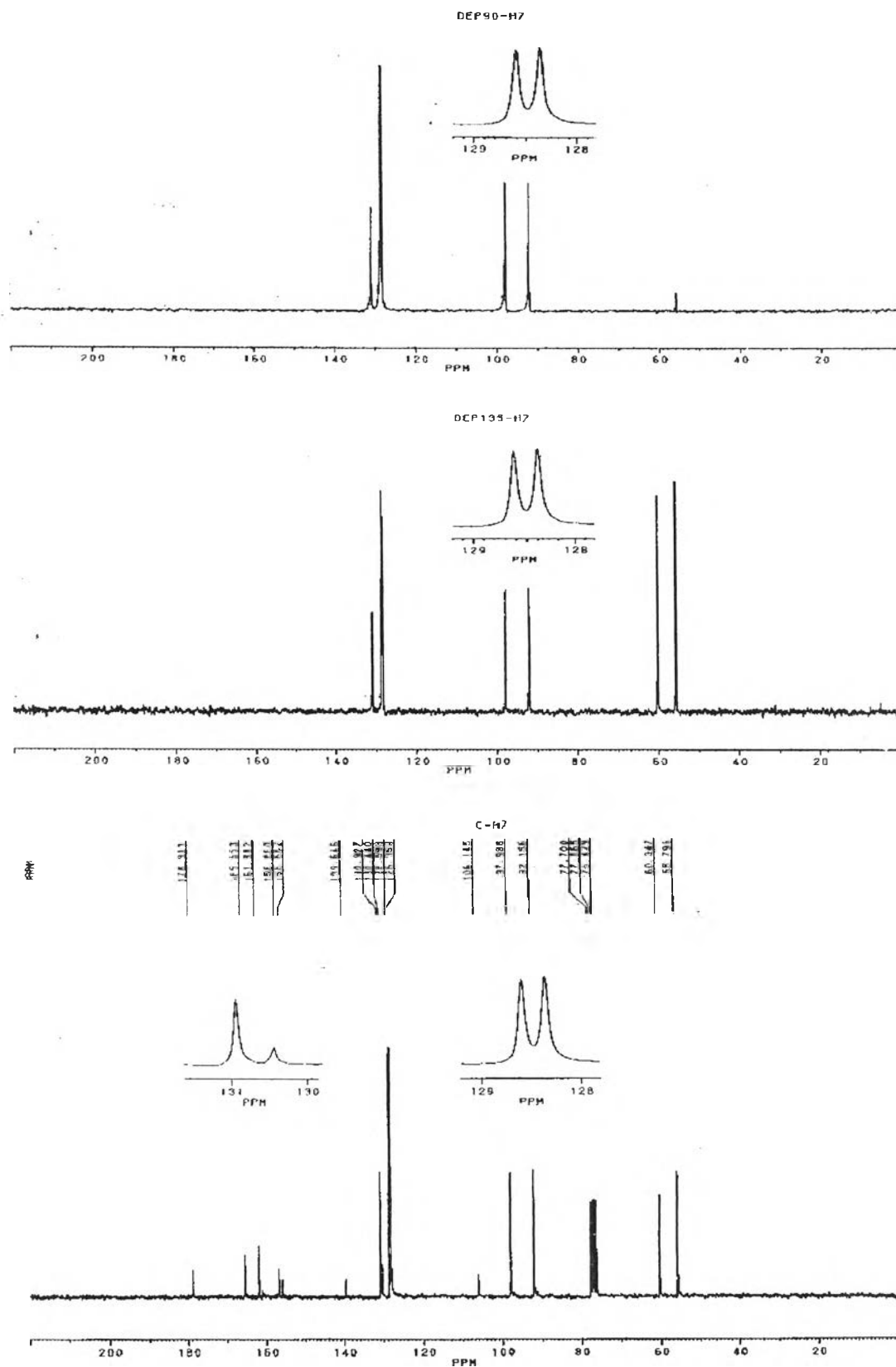


Figure A26 DEPT90, DEPT135 and  $^{13}\text{C}$ -NMR spectra of Compound 6.  
(5-hydroxy-3,7-dimethoxyflavone)



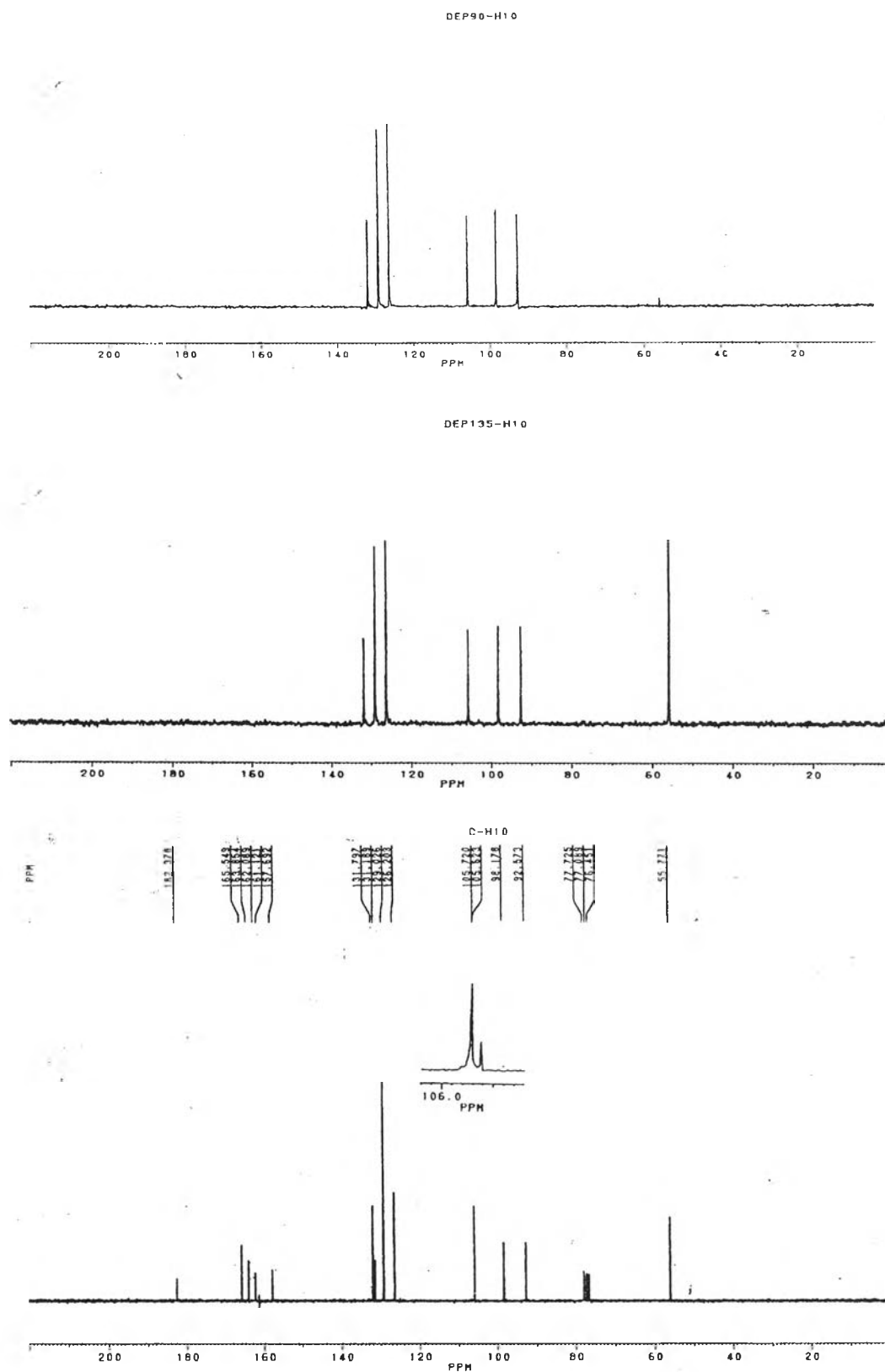
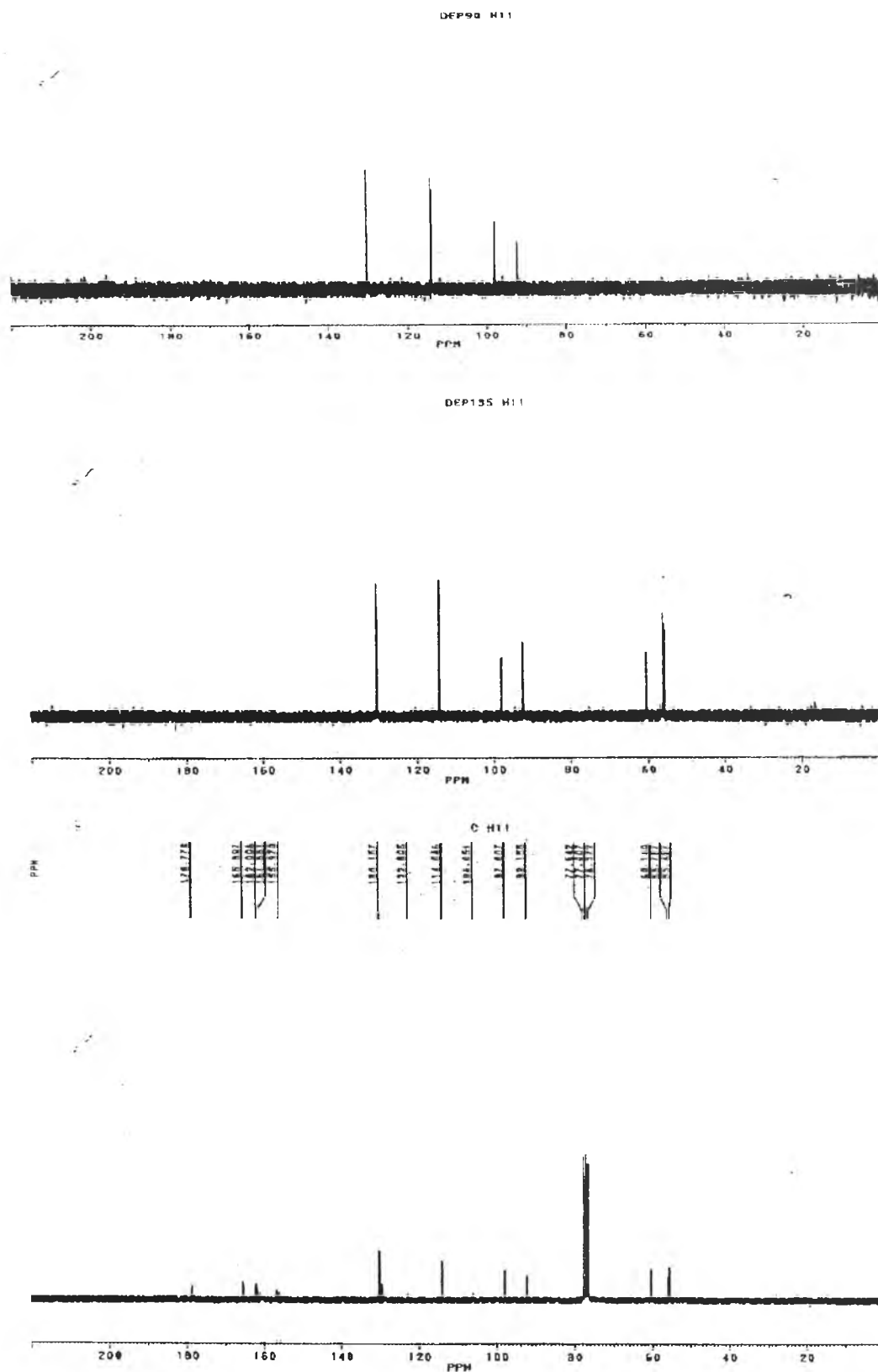


Figure A27 DEPT90, DEPT135 and  $^{13}\text{C}$ -NMR spectra of Compound 7.  
(5-hydroxy-7-methoxyflavone)



**Figure A28** DEPT90, DEPT135 and  $^{13}\text{C}$ -NMR spectra of Compound 8.  
(5-hydroxy -3,7,4'-trimethoxyflavone)

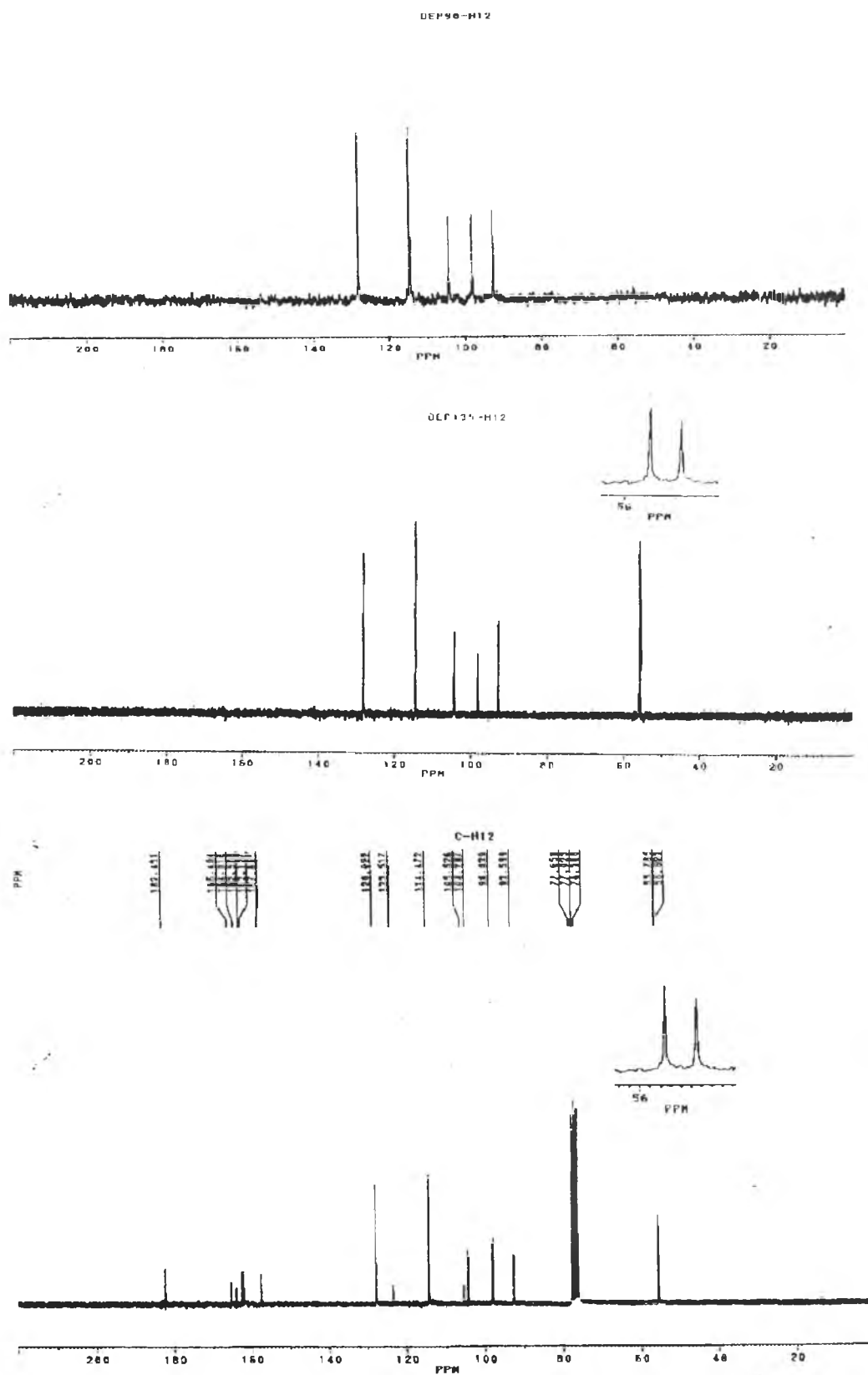
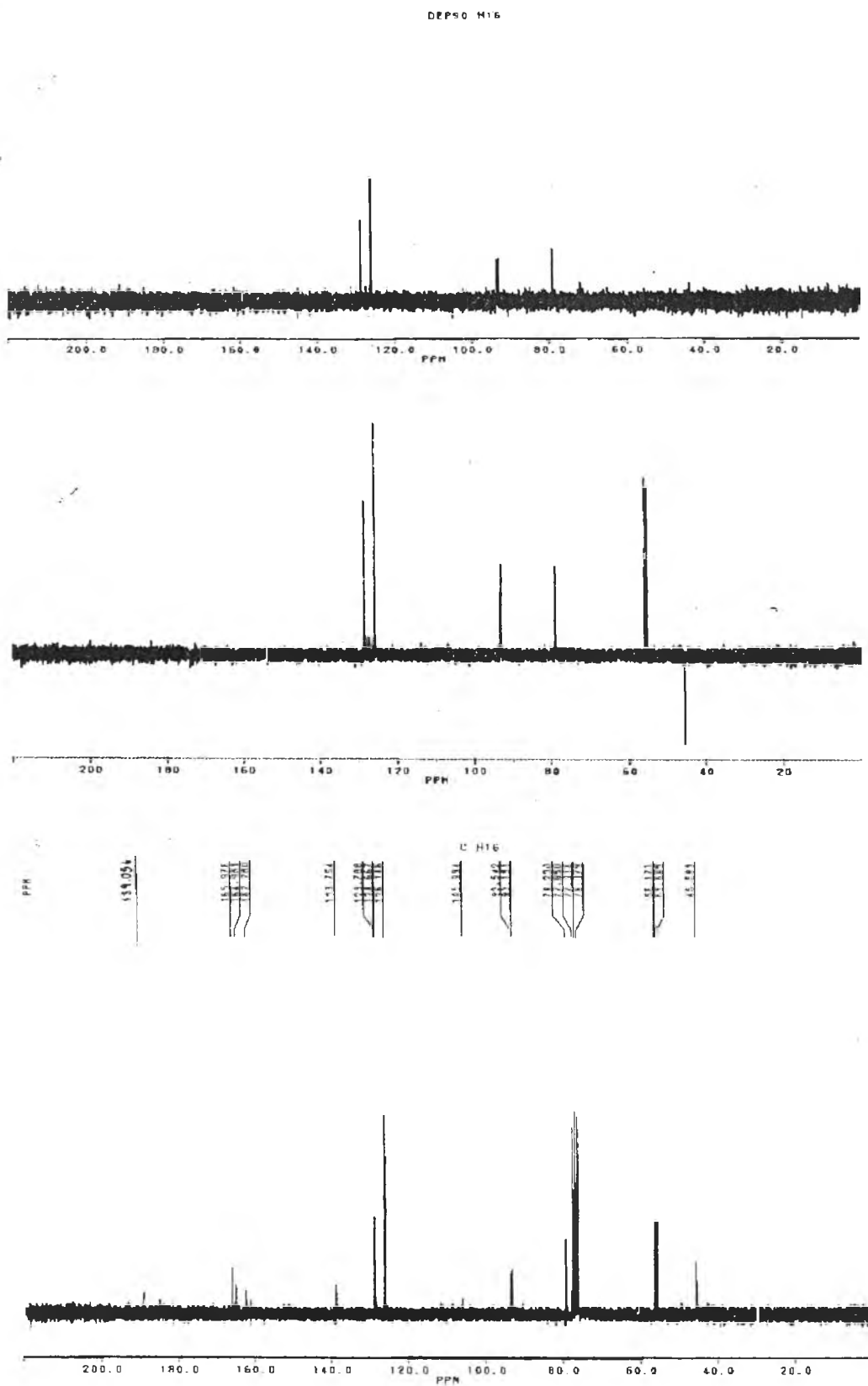


Figure A29 DEPT 90, DEPT 135 and  $^{13}\text{C}$ -NMR spectra of Compound 9.  
(5 - hydroxy -7, 4' -dimethoxyflavone)



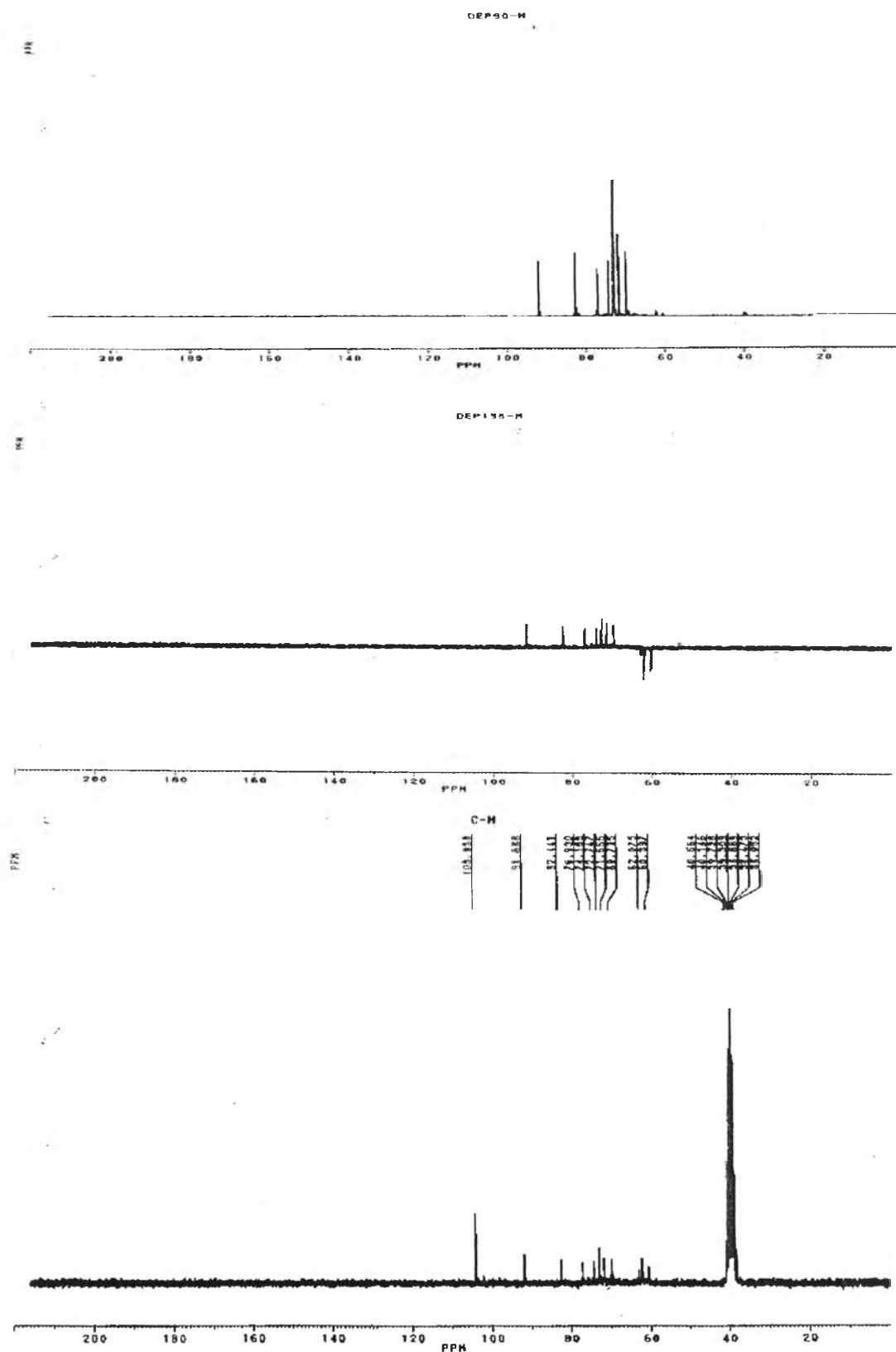


Figure A31 DEPT90, DEPT135 and  $^{13}\text{C}$ -NMR spectra of Compound 11. (Sucrose)

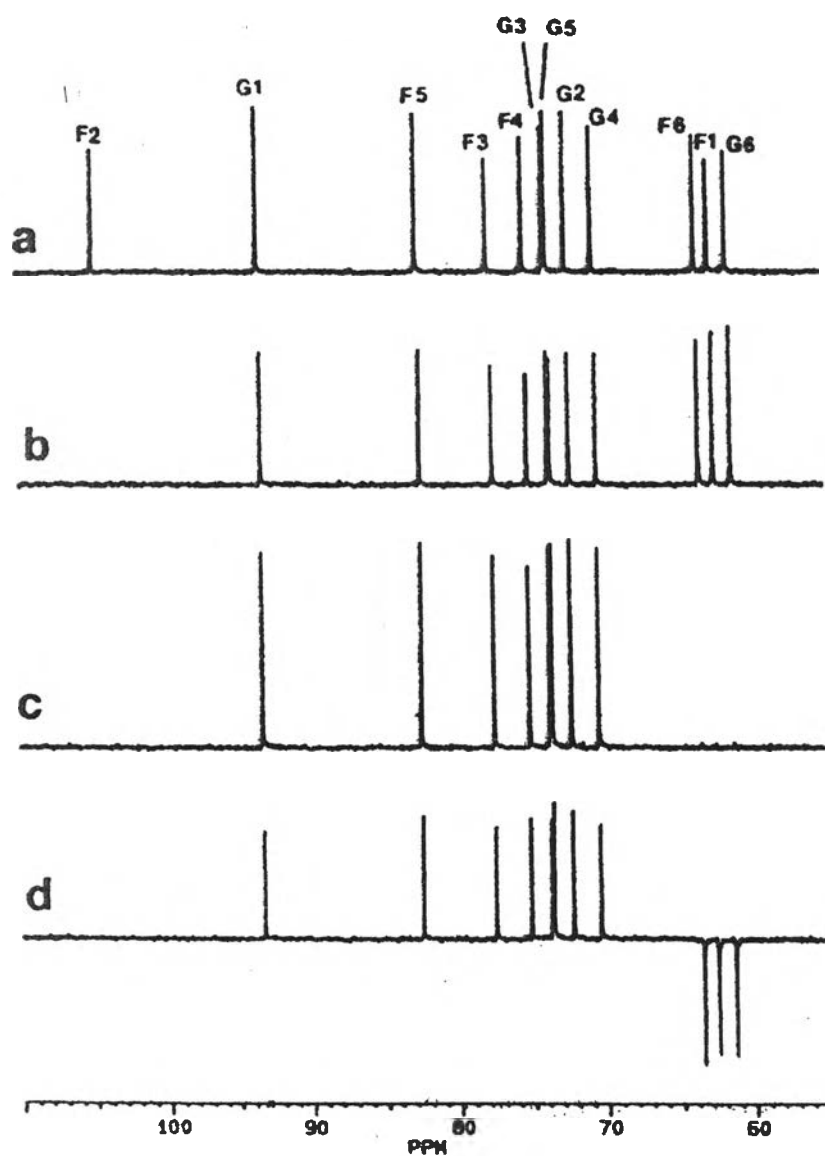


Figure A31a DEPT 90, DEPT 135 AND  $^{13}\text{C}$ -NMR spectra of sucrose ( in  $\text{D}_2\text{O}$  )<sup>(25)</sup>  
 (a) Broadband proton-decoupled  $^{13}\text{C}$ -NMR spectra of a sucrose solution in  $\text{D}_2\text{O}$ .  
 (b) DEPT spectra of the same sucrose solution  $\theta$  45 .  
 (c) DEPT spectra of the same sucrose solution  $\theta$  90.  
 (d) DEPT spectra of the same sucrose solution  $\theta$  135.

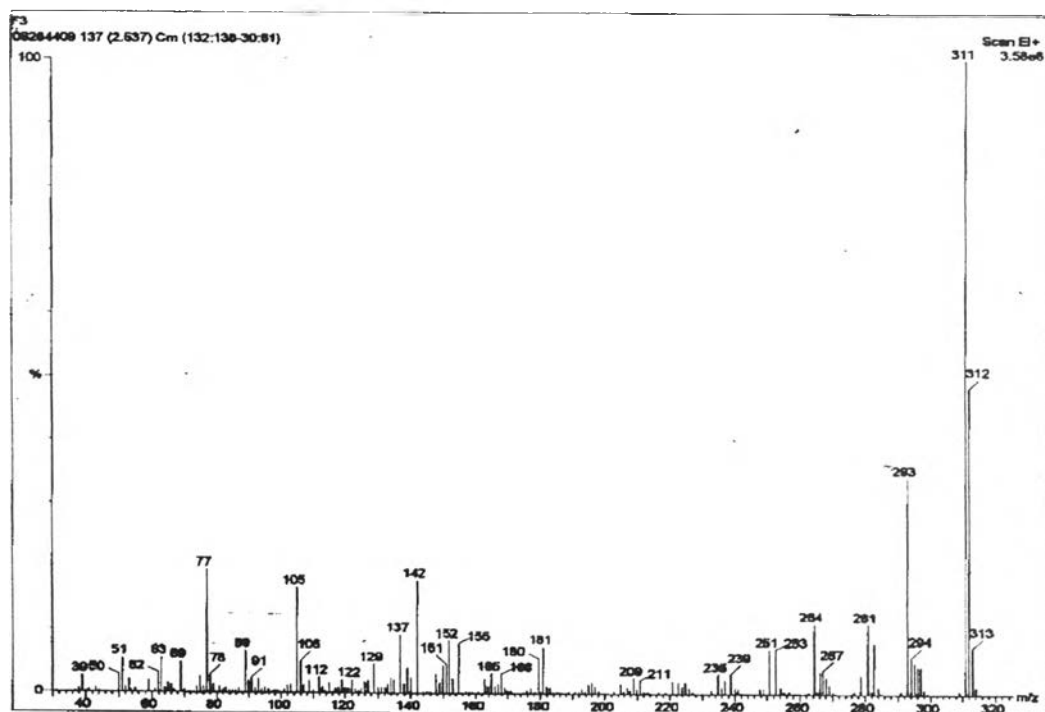


Figure A32 The EI mass spectrum of Compound 1.(3,5,7-trimethoxyflavone)

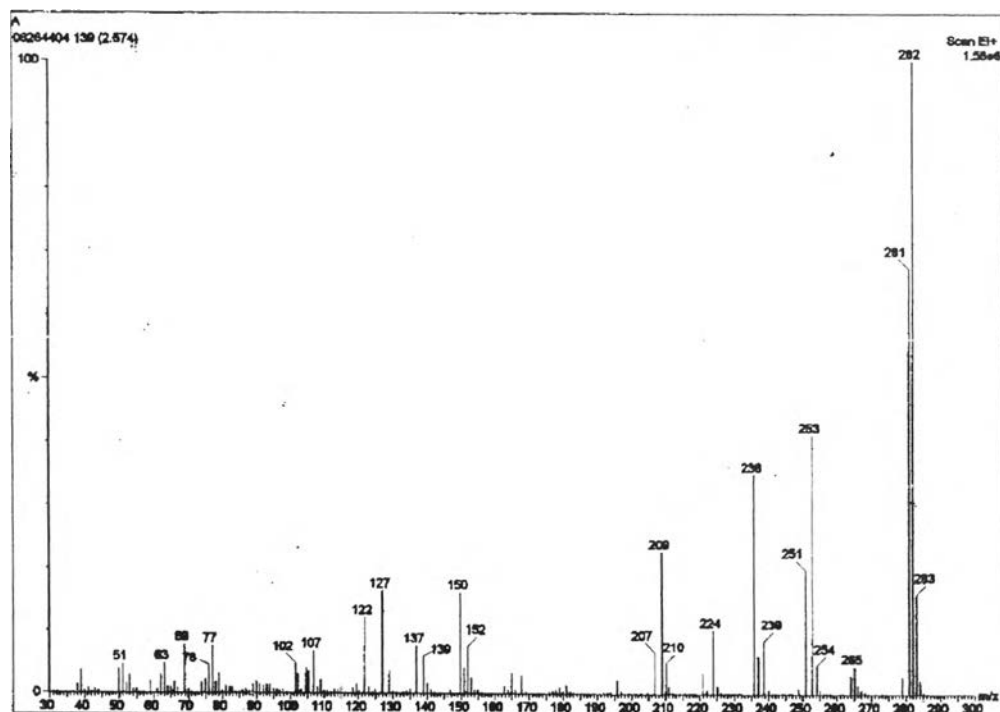


Figure A33 The EI mass spectrum of Compound 2.(5,7-dimethoxyflavone)

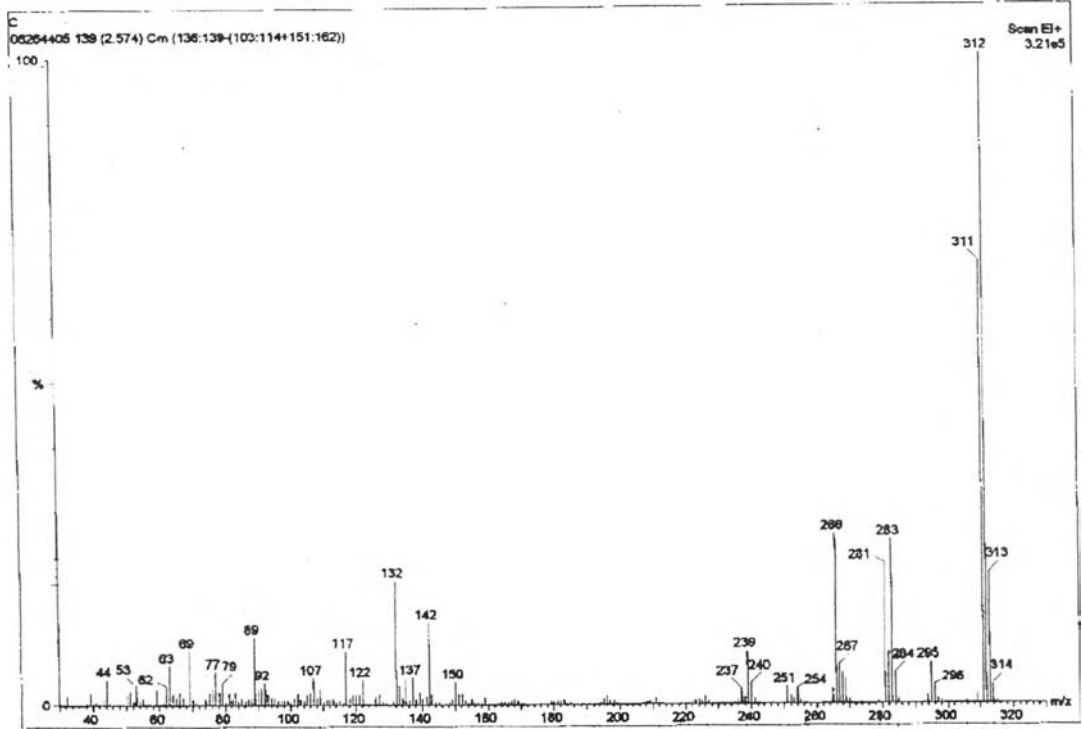


Figure A34 The EI mass spectrum of Compound 3.(5,7,4'-trimethoxyflavone)

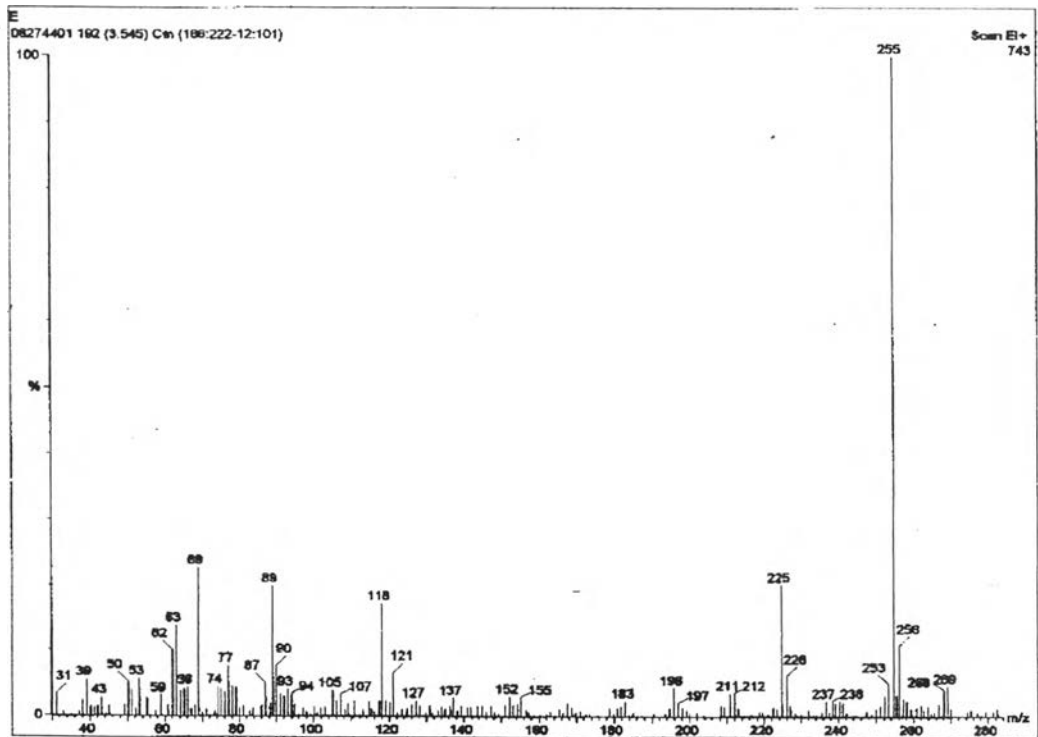


Figure A35 The EI mass spectrum of Compound 4.(4'-hydroxy-5,7-dimethoxyflavone)



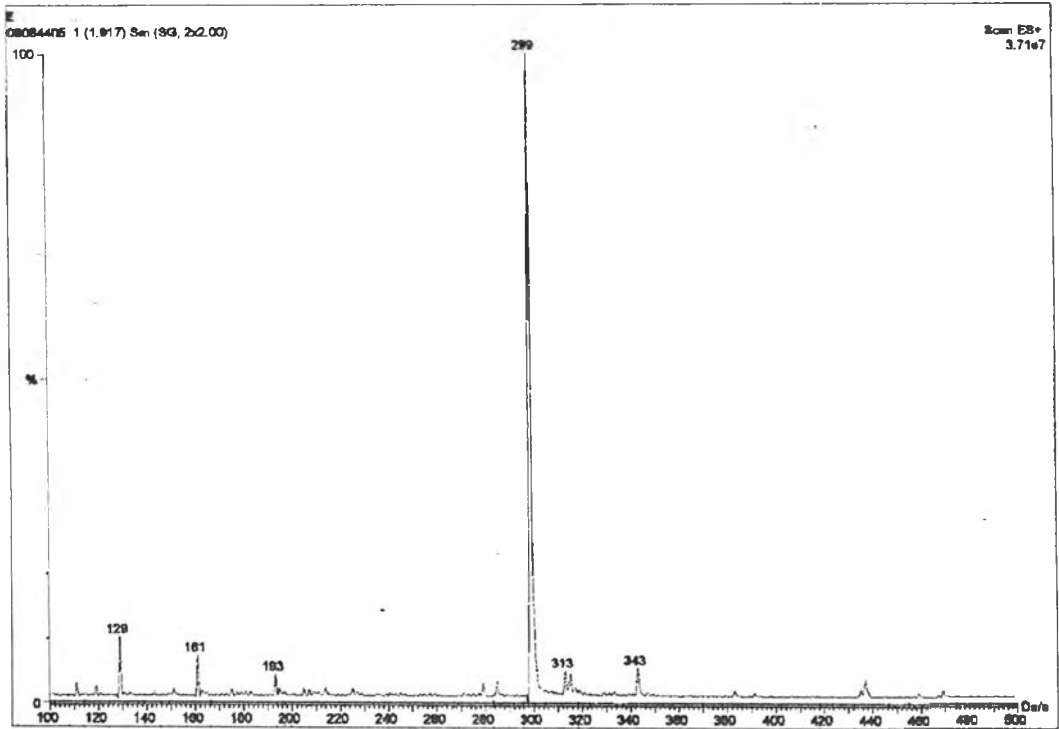


Figure A36 The LC mass spectrum of Compound 4.(4'-hydroxy -5,7-dimethoxyflavone)

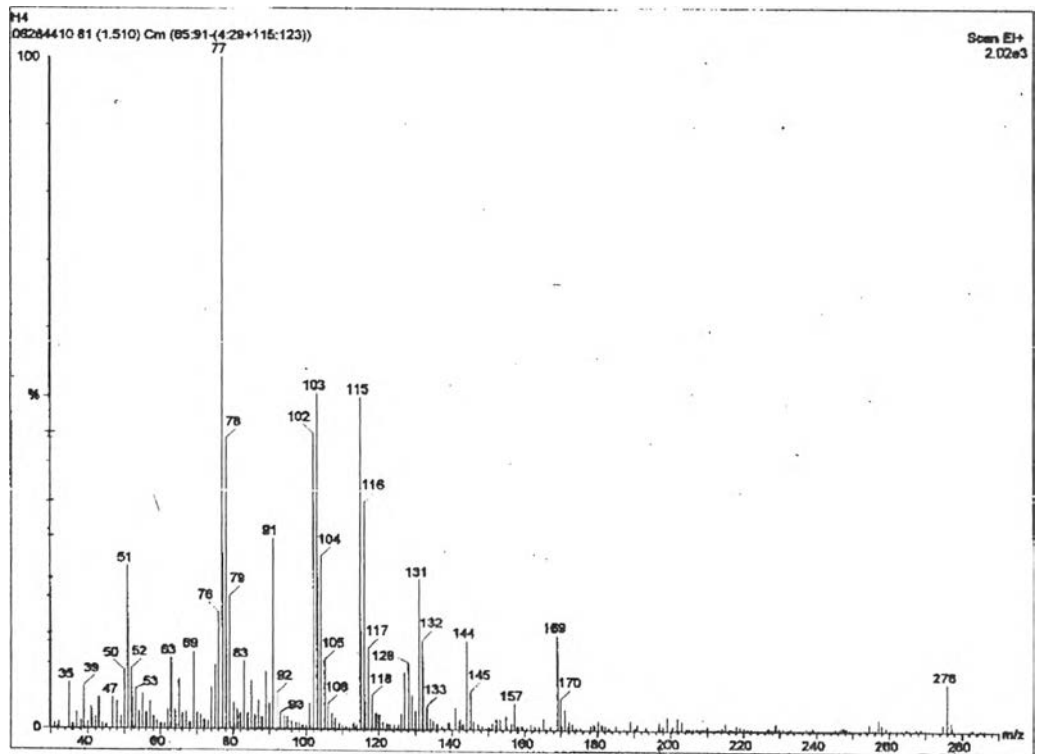


Figure A37 The EI mass spectrum of Compound 5.(dicinnamylmethane)

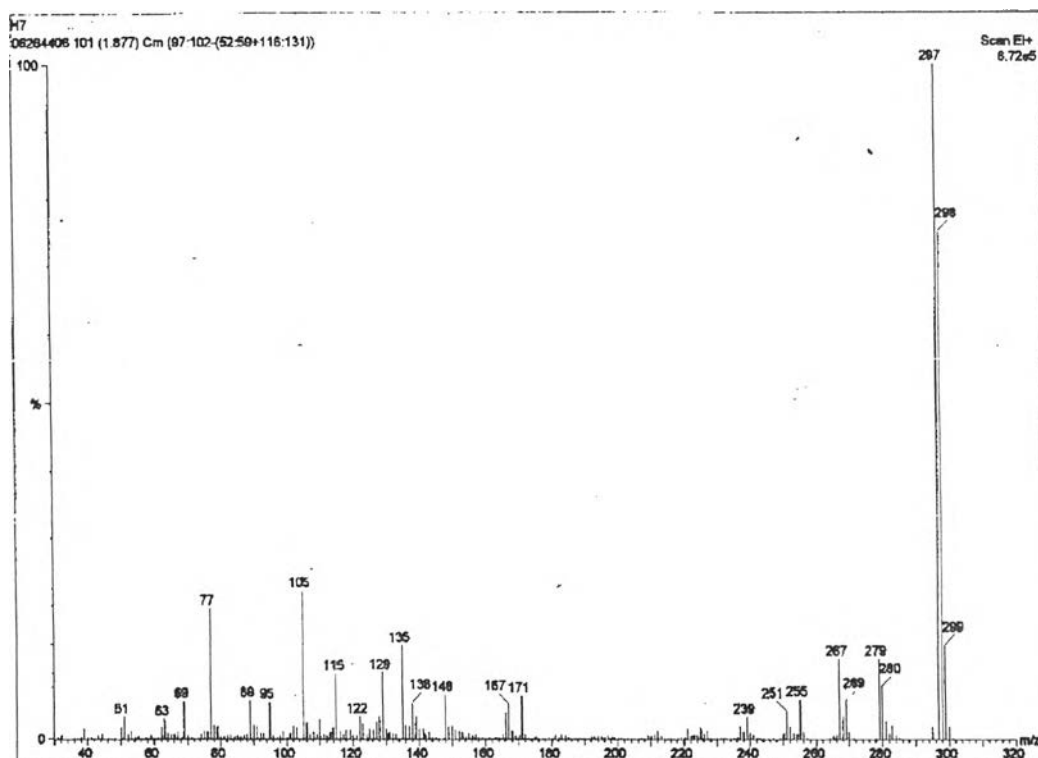


Figure A38 The EI mass spectrum of Compound 6.(5-hydroxy -3,7-dimethoxyflavone)

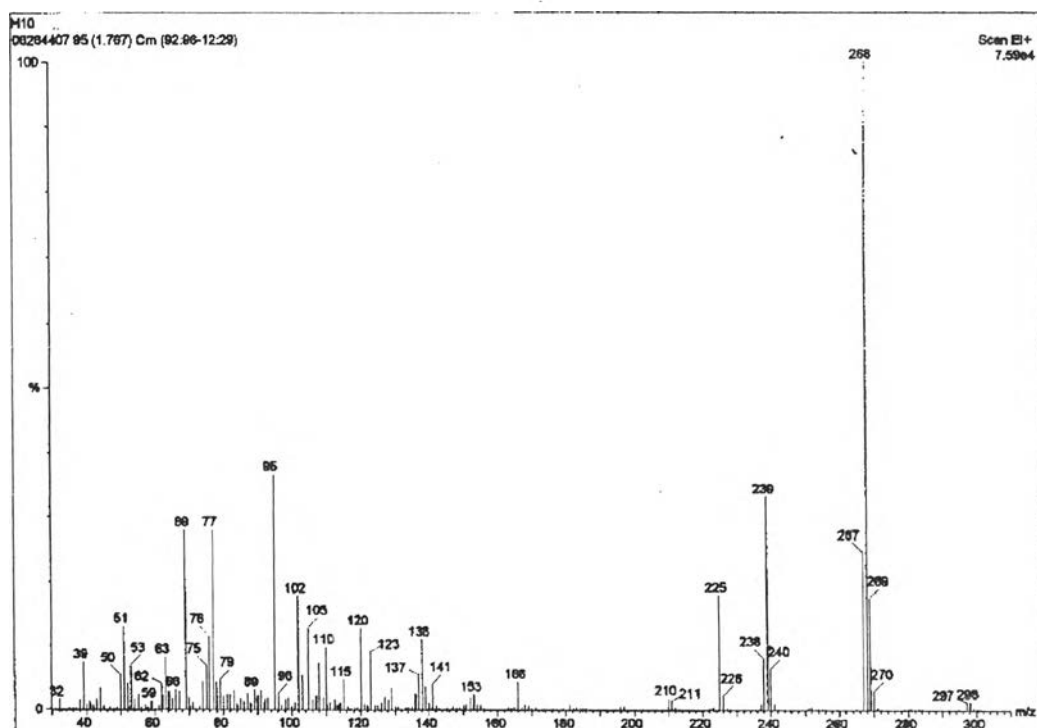


Figure A39 The EI mass spectrum of Compound 7.(5-hydroxy-7-methoxyflavone)

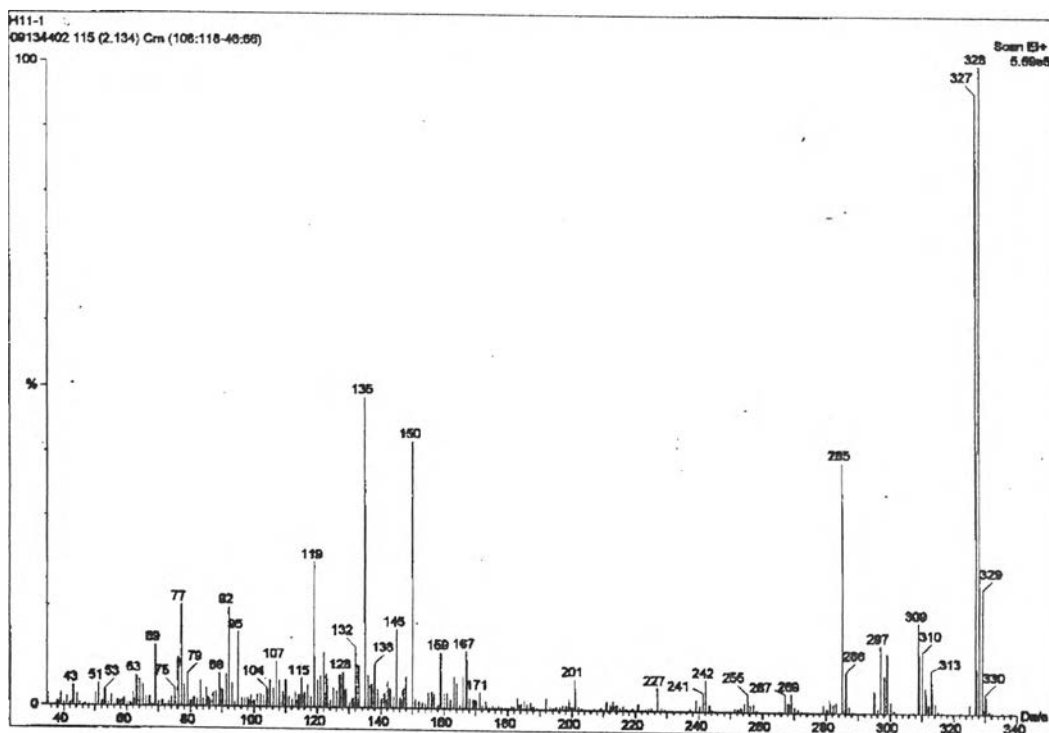


Figure A40 The EI mass spectrum of Compound 8. (5-hydroxy-3,7,4'-trimethoxyflavone)

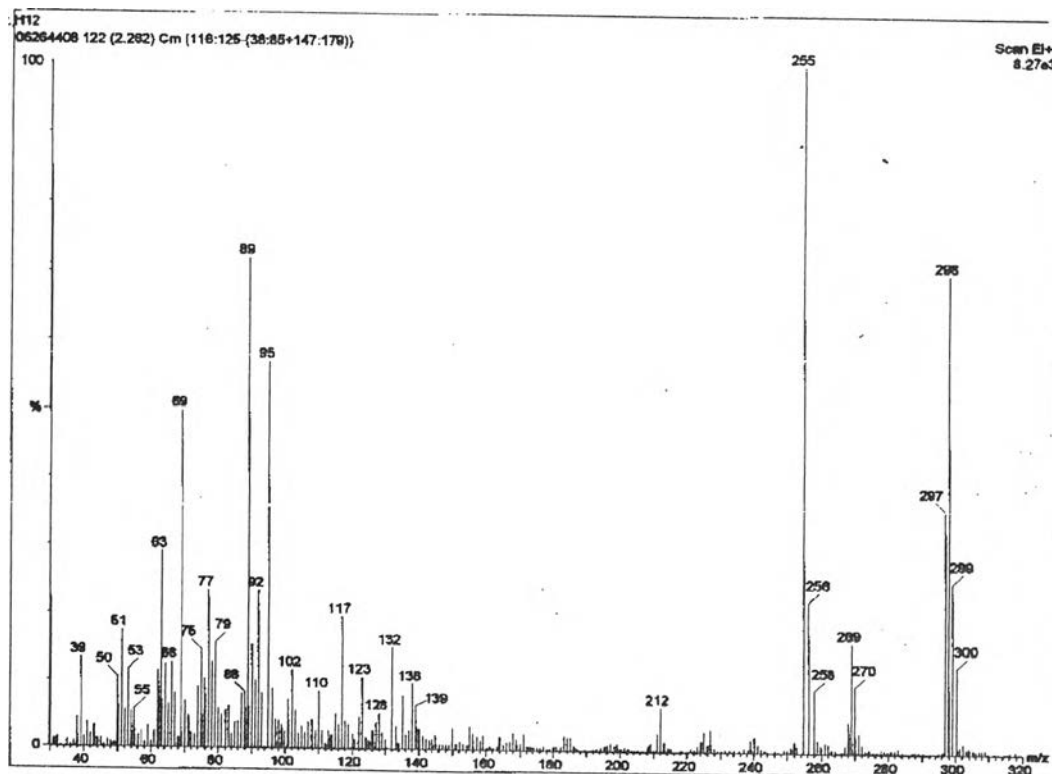
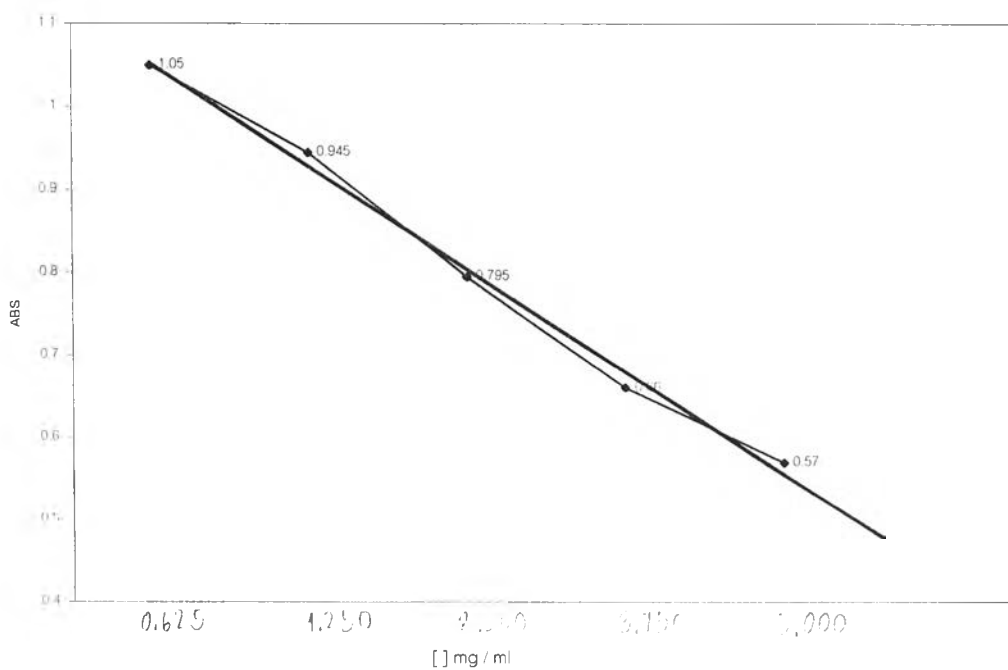
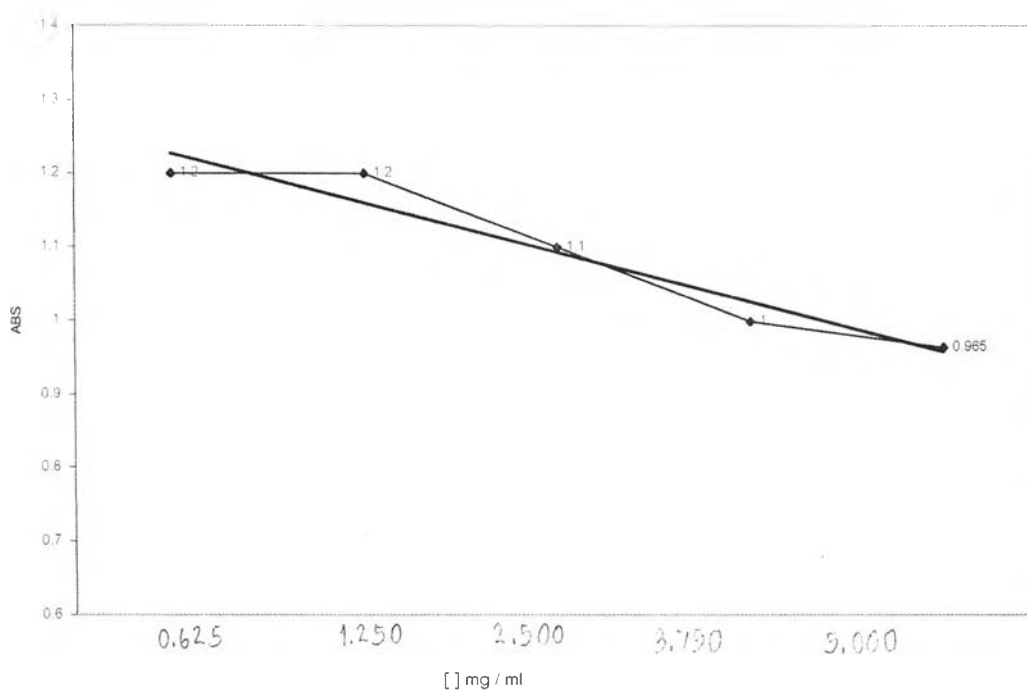


Figure A41 The EI mass spectrum of Compound 9. (5-hydroxy-7,4'-dimethoxyflavone)



$IC_{50} = 16 \text{ mM}$

**Figure A44**  $IC_{50}$  values of dicinnamoylmethane by DPPH method.



$IC_{50} > 14 \text{ mM}$

**Figure A45**  $IC_{50}$  values of sucrose by DPPH method.

## VITA

Miss Supana Deachodomphan was born on February 16, 1974 in Bangkok, Thailand. She graduated primary school at Assumption Convent and high school at Mahaphurtaram. She graduated with a Bachelor Degree of Science, Faculty Agro-industry field of study Biotechnology from Kasetsart University in March 1996. In 1999, she was admitted into a Master Degree program in Biotechnology at Chulalongkorn University.

