

PROTON MAGNETIC RESONANCE SPECTRA OF PHYTOXANTHONES

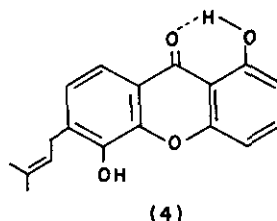
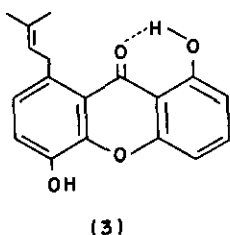
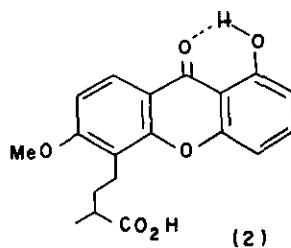
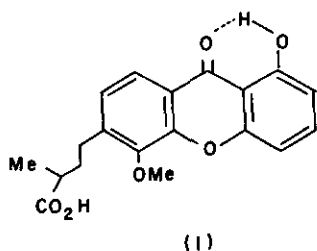
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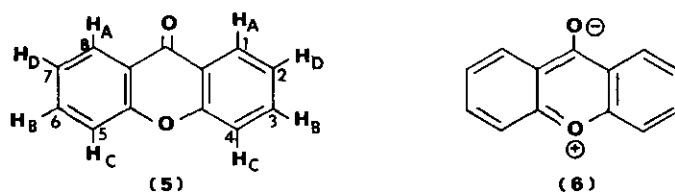
Proton magnetic resonance spectra of phytoxanthones with particular reference to structural elucidation has been discussed.

Pmr and cmr spectroscopy has been of immense use in determining the structure of natural xan-
thones. Substitution patterns are usually determined on the basis of chemical shift and spin
coupling data for the aromatic protons¹. Thus in structures (1) and (2) for scriblitifolic
acid, a metabolite of Callophyllum scriblitifolium Hend & Wyatt Smith, the chemical shifts of
aromatic protons favoured structure (1) for this compound, although the position of aromatic
protons in (1) and (2) remain unchanged. Also in guanandin (4) and isoguanandin (3), where
the oxygenation pattern is the same, differentiation between the two metabolites has been made
by careful interpretation of the chemical shifts of the aromatic protons².



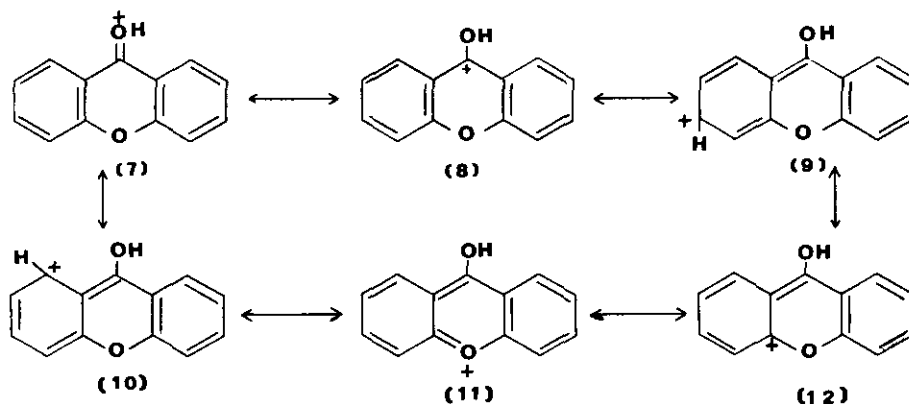
In order to predict the substitution and oxygenation pattern of xanthenes, it is now possible to calculate the chemical shifts of the aromatic protons of any xanthone containing hydroxy, alkoxy, alkyl and even fused ring substituents. This has been made possible by finding out the fundamental parameters for xanthone itself³.

Martin et al⁴ have reported that the protons at the C-1 and C-8 positions of xanthone skeleton (5) are deshielded by the anisotropic effect of the ortho carbonyl group. These



workers have assigned chemical shifts to the other six protons. Scheinmann and co-workers³ have reaffirmed the chemical shifts of H-1 and H-8 in xanthone nucleus. These workers have also measured the chemical shifts of xanthone, in different solvents and were able to assign the other six protons along with protons at C-1 and C-8, by collecting the data obtained through first order analysis of spectra at 60,100 and 220 MHz instruments.

From a graphical correlation of chemical shifts of H-1, H-2, H-3 and H-4 in various solvents (Fig.1), H-1 appeared anomalous, but H-2, H-3 and H-4 the signals were deshielded with increasing dielectric constants of the solvent⁵. The anomaly for H-1 has been explained in terms of solvation in deuterioacetone and deuteriodimethyl sulphoxide, which favours separation of charge typified by canonical form (6), resulting in diminished diamagnetic anisotropy of the carbonyl group. This results in shielding of H-1 as compared with measurements in deuteriochloroform. A similar effect has been demonstrated when trifluoroacetic acid is used as solvent, in which relative deshielding of hydrogen is maximum at C-1 and C-3 and minimum at C-2 and C-4. Use of pentadeuterio pyridine (dielectric constant 12.5) as solvent, has also been suggested to make solvent - solute collision complex⁶ at the ring carbonyl group, thus resulting in deshielding at C-1 and shielding at other positions when compared with corresponding measurements in deuteriochloroform.



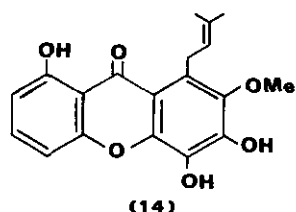
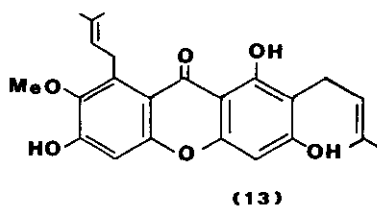
(Fig. 1)

Coupling constants are also suggested to be solvent dependent. It has been observed that ortho-coupling increases with increasing dielectric constant of the solvent and regular changes occur with meta- and para-coupling constants.

The fundamental parameters of the A, B, C and D protons of xanthone (5) in various solvents have been measured by Schienmann and co-workers and the effect of oxygen substituent on these parameters has also been measured in these solvents. The magnitude of increments on chemical shift of the protons at C-1, C-2, C-3 and C-4, caused by ortho-, meta- and para-hydroxy- or alkoxy- substituent has been calculated by subtracting the spectrum of xanthone from the spectrum of reference compounds with a mono-oxygenated ring. The additive shielding parameters for various aromatic protons in mono- and dioxygenated xanthenes are in good agreement with the experimental values. Although the diamagnetic effect of hydroxy- and alkoxy groups on neighbouring aromatic protons is reported⁷ to be identical, irrespective of the relative location of the oxygenated site and the proton. Scheinmann *et al*³ have shown that a slight but consistent paramagnetic shift of the proton signal occurs upon methylation of ortho and para-hydroxy groups in xanthenes. This effect is specially pronounced for the signal due to H-4 upon methylation of a 1-hydroxy group.

The effect of a variety of C-substituents on the chemical shift of the protons on the xanthone nucleus has been shown to be less significant. The variations around the mean calculated values have been attributed to purely steric effects. The chemical shifts of the methylene groups adjacent to the xanthone nucleus in mangostin⁸ (13) a metabolite of mangosteen tree,

Garcinia mangostana, and celebixanthone (14) have been suggested⁹ to depend whether the side chain was attached to an electron poor site (C-1 or C-3) or to a relatively electron rich site (C-2). Whereas Scheinmann et al¹⁰ have shown that the chemical shifts of the benzylic methylene group in 5-allyl-1,6-dihydroxy and 6-allyl-1,5-dihydroxyxanthone derivatives are the same, if the side chain was para - or meta- to the xanthone carbonyl group. Thus these workers have suggested that the low chemical shift of the methylene group attached to C-1 or C-8 in mangostin (13) and celebixanthone (14) was because of the close proximity of the xanthone carbonyl group which causes deshielding largely by anisotropic effect¹¹ in preference to electrostatic effects¹².



Similarly the position of side chain and oxygenation pattern of a large number of natural xanthones has been established with the help of proton magnetic resonance spectroscopy.

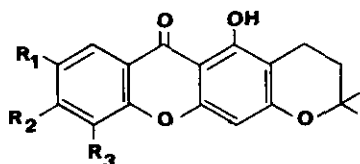
Arends and Helboe^{13,14} have described a supplementary method based upon measurement of the chemical shifts in DMSO- d_6 of the hydroxyl protons of oxygenated xanthones, for structure elucidation. These workers have established the substitution pattern on xanthone nucleus by measuring the chemical shift of the hydroxyl protons present, either isolated or in conjunction with other hydroxy/prenyl groups in the same ring of xanthone nucleus.

Benzene induced solvent shifts for isolated OMe groups have been particularly useful in establishing the positions of these groups. It has been shown¹⁵⁻¹⁷ that isolated OMe groups are selectively solvated in benzene relative to chloroform or carbon tetrachloride. The resonances of such OMe groups suffer a 20-40 H_z upfield shift in benzene relative to comparatively "inert" solvent, such as carbon tetrachloride or deuteriochloroform¹⁸⁻²⁰. The potential of such solvent shifts for structure elucidation in the coumarin and flavones has also been emphasised^{20,21}. Use of this techniques has been made by Scheinmann et al for structure elucidation of xanthones. Thus the solvent induced shifts (Δ) in hexadeuteriobenzene relative to deuteriochloroform have been recorded according to the definition^{21,22}.

$$\Delta \text{ (p.p.m.)} = \tau_{C_6D_6} - \tau_{CDCl_3}$$

The Δ -values for C-2 protons vary from -0.30 to 0.12 p.p.m. depending upon the nature of the other substituents and for C-4 protons, the values vary from -0.15 to +0.30 p.p.m. These workers have further suggested that this spread of the values for the 2- and 4- protons resulting from variation in xanthone substitution pattern indicates a collision complex of hexadeuteriobenzene not only with ring carbonyl but also with certain ring substituents. These workers have recorded benzene induced solvent shifts for a number of substituted xanthenes. Dreyer²³ has made use of this technique for structure elucidation of four natural xanthenes.

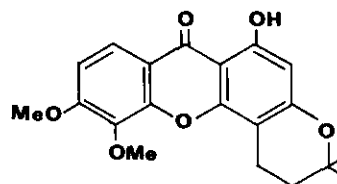
Scheinmann and co-workers^{24,25} have also examined dimethyl ethers of dihydrojacareubin and dihydroisojacareubin, to establish Δ - values for linear and angular isomers (15) and (16) respectively. Under identical conditions, the benzylic methylene group in (15) had a lower Δ -value (0.07 p.p.m.) than that in the angular isomer (16), (0.22 p.p.m.).



(15) $R_2 = R_3 = OMe$; $R_1 = H$

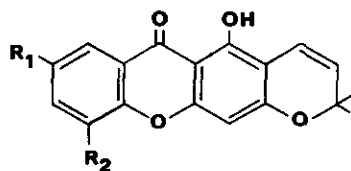
(17) $R_2 = R_3 = H$; $R_1 = OMe$

(18) $R_1 = R_2 = H$; $R_3 = OMe$



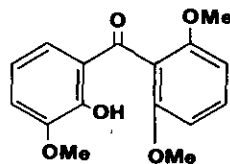
(16)

The Δ -values, for the benzylic methylenes in the monomethyl ethers of dihydro-osajaxanthone (17) ($\Delta = 0.08$ p.p.m.) and dihydro-6-deoxyjacareubin (18) ($\Delta = 0.09$ p.p.m.), have supported²⁶ the linear pyranoxanthone structures for osajaxanthone (19) and 6-deoxyjacareubin (20), metabolites of *Calophyllum scriblitifolium* Hend & Wyatt-Smith.



(19) $R_1 = OH$; $R_2 = H$

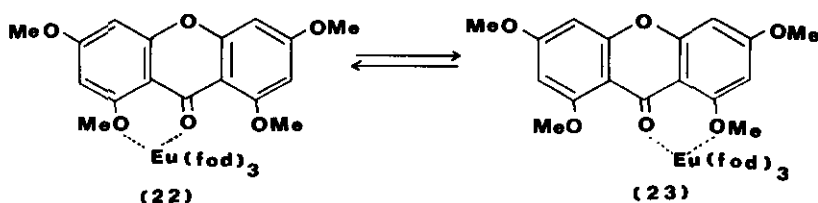
(20) $R_1 = H$; $R_2 = OH$



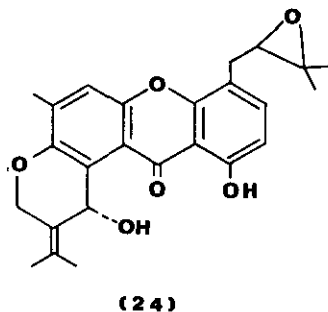
(21)

Structure (21) for 2-hydroxy-2',3-6'-trimethoxybenzophenone, an intermediate in the synthesis of 1,5-dihydroxy and 5-hydroxy-1-methoxyxanthenes was proved²⁷ by benzene induced shifts. Thus the n.m.r. spectra of (21) in deuteriochloroform and in hexadeuteriobenzene were shifted by about 0.5 p.p.m. in aromatic solvent^{5,16}.

The effects of $\text{Eu}(\text{fod})_3$, tris(1,1,1,2,2,3,3-heptafluoro-7,7-dimethyloctane-4,6-dionato europium III), on the Pmr spectra of xanthenes has also been studied^{28,29}. The shifts of protons attached to C-2 of the xanthenes are shown to be greater than those attached to C-4, indicating that the Eu^{3+} atom coordinates with the carbonyl oxygen and the methoxyl oxygen of the 1- and 8- methoxyxanthenes. However, in the case of 1,8-dimethoxyxanthenes the ΔEu values of the H-2 are shown³⁰ to be much smaller than those of 1-methoxyxanthenes indicating that the Eu^{3+} co-ordinates to both the carbonyl oxygen atom and the neighbouring methoxy-oxygens (22,23) in which the co-ordination number³¹ of Eu^{3+} is 8



¹³C Nuclear magnetic resonance spectroscopy has also been used for structural elucidation of naturally occurring complex xanthenes³². Thus valuable structural information has been obtained by using ¹³C n.m.r. in case of tajixanthone (24) and other metabolites of *Aspergillus variegator*³³. The ¹³C n.m.r. has also been recorded for arugosin A,B,C, the metabolites of *Aspergillus rugulosus*³⁴. The reported proton magnetic resonance spectra of the phyto-xanthenes are reproduced in the forthcoming tables.



Compound	Solv	PMR Values	Ref.
<u>Mono-oxygenated Xanthenes</u>			
2-Hydroxy	a	1.48, br.d (J 7.OH ₂), 8-H; 1.76-2.75, m, 1, 3-7H	30,35-42
2-Methoxy	b	1.76, q, 8-H; 2.4, d, 1-H; 2.4, t, 3 & 6-H; 2.6-2.9,m, 4-, 5- & 7-H; 6.20, s, OMe.	42-45,74
<u>Dioxygenated Xanthenes</u>			
3-Hydroxy-2-methoxy	a	1.98, s, 1-H; 1.28, br.d (J 7H ₂), 8-H; 1.48-2.28, m, 5-, 6-, & 7-H;2.50, s, 4-H; 5.76, s, OMe.	35
3-Hydroxy-4-methoxy	c	1.86, q(J 8 & 1H ₂), 8-H; 2.19,t(J 8 & 8H ₂), 6-H; 2.21, d(J 8H ₂), 1-H; 2.35, q(J 8 & 1H ₂), 5-H; 2.57, t(J 8 & 8H ₂), 7-H; 3.01, d(J 8H ₂), 2-H; 6.08, s, OMe.	42,46
1,5-Dihydroxy	c	-2.40, -0.24 exchangeable with D ₂ O; 2.19-3.49, m; 6H.	30,36,40, 42,47-52
5-Hydroxy-1-methoxy	c	0.0, br. s, 5-OH (exchangeable), 2.1-2.1, m, Ar-H; 6.03, s, OMe.	27,51,53
1-Hydroxy-5-methoxy	b	-2.79, s, 1-OH; 2.11, q, 8-H; 2.31, t, 3-H; 2.70, m, 7-H; 2.92, d, 4-H; 3.15, d, 2-H; 5.93, s, 5-OMe.	
1,2-Dihydro-6-hydroxy-3,3-dimethylpyrano-(2,3- α) xanthene-12(3H)-one. (Cardato-oblongu-xanthone)	c	1.85, q(J 8 & 1H ₂), 8-H; 2.31, t(J 8 & 8H ₂) 6-H; 2.32, s, 3-H; 2.46, t(J 8 & 8H ₂), 7-H; 2.87, q(J 8 & 1H ₂), 5-H; 6.24, t(J 7 & 7H ₂), Ar-CH ₂ ; 8.0, -CH ₂ -; 8.60 and 8.67, 2s, Me ₂ .	46
6-(3,3-Dimethylallyl)-1,5-dihydroxy, (Guanandin; calophyllin B)	d	3.23, q(J 8.5 & 1.OH ₂), 2-H; 2.32, t(J 8.5H ₂), 3-H; 2.97,q(J 8.5 & 1.OH ₂), 4-H; 2.78, d(J 8.5H ₂), 7-H; 2.33, d(J 8.5H ₂), 8-H; 4.58,	2,27,47, 54-58

Compound	Solv	PMR Values (τ)	Ref.
Dehydrocycloguanandin	b	t(J 7.0H ₂), :CH-; 6.45, d(J 7H ₂), -CH ₂ -; 8.23, s, Me ₂ 3.22, q(J 8.3 & 1.1H ₂), 2-H; 2.4, t(J 8.3H ₂), 3-H; 2.73, q(J 8.3 & 1.1H ₂), 4-H; 3.0, d(J 8H ₂), 7-H; 2.24, d(J 8.0H ₂), 8-H; 3.56, d(J 9.8H ₂), :CH-; 4.17, d(J 9.8H ₂), :CH-; 8.44, s, Me ₂ .	2,27,59
6-(4-Hydroxy-3-methylbutanyl)- 1,5-dihydroxy	b	-2.62, 1-OH; 2.06, d(J 8.5H ₂), 8-H; 2.83, d(J 8.5H ₂), 7-H; 3.22, q(J 8.5 & 1.5H ₂), 2-H; 3.03, q(J 8.5 & 1.5H ₂), 4-H; 2.43, t(J 8.5H ₂), 3-H; 6.45, d(J 6.0H ₂), 4'-CH ₂ ; 7.18, t(J 7.0 & 2.0H ₂), 1'-CH ₂ ; 8.3, m, 2'- CH ₂ - & 3'-CH; 8.4, br., 4'OH; 8.97, d(J 6.0H ₂), 3'OMe.	54
Scriblitifolic acid	b	-2.61, br., s, 1-OH; 3.20, md, 2-H; 2.40, t, 3-H; 3.02, md, 4-H; 2.79, d, 7-H; 2.04, d, 8-H; 6.02, s, OMe; 7.20, t, 1'- CH ₂ -; 8.12, m, 2'-CH ₂ -; 8.75, d, 3'-Me; 7.5, m, 3'-CH-.	15,46,55, 57
4,8-Dihydroxy-1-(3',3'-di- methylallyl) (Isoguanandin)	d	3.25, q(J 8.3 & 1.1H ₂), 2-H; 2.33, t(J 8.3H ₂), 3-H; 3.01, q(J 8.3 & 1.1H ₂), 4-H; 2.70, d(J 8.3H ₂), 6-H; 2.9, d(J 8.3H ₂), 7-H; 4.58, t(J 7.0H ₂), :CH-; 6.01, d(J 7.0H ₂), -CH ₂ -; 8.25, s, 2Me; 1.14, 5-OH; -2.97, s, 1-OH.	2,27,58
1,7-Dihydroxy (Euxanthone)	d	-2.41, 1-OH; 1.05, 7-OH; 2.1-3.19, complex Ar-H.	30,38,40, 47,49,50,55 60-79
1-Hydroxy-7-methoxy	b	-2.41, 1-OH; 2.39-3.50, A-H; 6.20, s, OMe.	38,42,44, 49,66
<u>Trihydroxyxanthenes</u>			
1-Methoxy-2,3-dihydroxy	b	-1.41, s, 3-OH; 1.77, octet (J 8.5 & 2.0H ₂), 8-H; 2.80-2.25, m, 5-, 6- & 7-H; 3.40, br., 2-OH; 3.51, s, 4-H; 5.98, s, OMe.	80-82
3-Hydroxy-1,2-dimethoxy	a	1.43, octet (J 7.5 & 1.8H ₂), 8-H; 1.74, m(J 8.5 6.5 & 1.8H ₂), 6-H; 2.06, q(J 8.5 & 1.5H ₂), 5-H;	80,81,83, 84

Compound	Solv	PMR Values (τ)	Ref.
2,3,4-Trihydroxy	d	2.16, m(J 7.5, 6.5 & 1.5H ₂), 7-H; 2.66, s, 4-H; 5.39, s, 1-OMe; 5.85, s, 2-OMe.	25,35
3,4-Dihydroxy-2-methoxy	d	1.71, q, 8-H; 2.15-2.65, m, 5-, 6-, & 7-H; 2.7, s, 1-H; 6.02, s, OMe.	25,43,44
4-Hydroxy-2,3-dimethoxy	a	1.80, octet, 8-H; 1.95-2.75, m, 5-, 6- & 7-H; 2.82, s, 1-H; 5.81, s, 3-OMe; 6.03, s, 2-OMe	25,36,37, 43,44,80, 81,84,85
3-Hydroxy-2,4-dimethoxy	b	1.53, d, 8-H; 2.15-2.60, m, 5-, 6- & 7-H; 2.40, s, 1-H; 3.48, br., 3-OH; 5.85 & 5.95, 2s, OMe	25,36,37, 80,82,86, 87
4-Methoxy-2,3-methylenedioxy	a	2.59, s, 1-H; 1.80-2.55, m, 5-, 6-, & 7-H; 1.62, octet, 8-H; 5.67, 4-OMe; 3.76, s, -O-CH ₂ -O-	43,44,64, 84,86,87
Globuxanthone	b	-2.62, s, 1-OH; 1.0-2.0, br., OH; 2.51, s, 3-H; 2.65-2.92, m, 6-, & 7-H; 2.17, q, 8-H; 3.73, q, :CH-; 4.82, t, :CH ₂ ; 8.51, s, 2xMe.	88,89
2,8-Dihydroxy-1-methoxy	a	2.30, t(J 8.0H ₂), 6-H; 2.41, d(J 10.0H ₂), 3-H; 2.60, d(J 9.5H ₂), 4-H; 2.91, q(J 8.0 & 1.0H ₂), 5-H; 3.08, q(J 8.0 & 1.0H ₂), 7-H; 5.90, s, OMe.	38,55,61, 85,90,91
1,2-Dimethoxy-8-hydroxy	a	2.30, t(J 8.5H ₂), 6-H; 2.36, d(J 9.5H ₂), 3-H; 2.62, d(J 10.0H ₂), 4-H; 3.0, q(J 8.5 & 1.0H ₂), 5-H; 5.81 & 5.96, 2s, 2xOMe.	90,91
2-Hydroxy-1,8-dimethoxy	c	1.58, s, 2-OH; 2.31, t(J 8.4H ₂), 6-H; 2.68, d(J 8.4H ₂), 3-H; 2.80, d(J 8.4H ₂), 4-H; 2.98, d(J 8.4H ₂), 7-H; 3.08, d(J 8.4H ₂), 5-H; 6.15, s, 2xOMe	55

Compound	Solv.	PMR Values (τ)	Ref.
1,5,6- Trihydroxy (Mesuaxanthone B)	d	-2.71, 1-OH, 2.04, d(J 9.OH ₂), 8-H; 2.54, t(J 9H ₂), 3-H; 2.72, d(J 9H ₂), 4-H; 3.19, d(J 9.OH ₂), 7-H; 3.19, d(J 9.OH ₂), 2-H; 4.58, br., 5- & 6-OH.	25,62,35, 42,46,50- 52,55,56, 61,64,69, 70,71,182.
1,6-Dihydroxy-5-methoxy (Buchanaxanthone)	c	-2.84, 1-OH; 2.18, d(J 9H ₂), 8-H; 2.33, t, 3-H; 2.99, d(J 9H ₂), 7-H; 2.99, md, 4-H; 3.23, md, 2-H; 6.04, s, OMe.	46,52,55, 61,62
1,6,7-Trihydroxy	c	2.45, t(J 9H ₂), 3-H; 2.53, s, 8-H, 3.12, md(J 9 & 3H ₂), 4-H; 3.10, s, 5-H; 3.33, md(J 9 & 3H ₂), 2-H; 4.1, br., 6- & 7-OH.	63,64,68, 93
Tovoxanthone	b	-3.1, s, 1-OH; 2.05, d(J 10.OH ₂), 4'-H; 2.55, t(J 8.OH ₂), 3-H; 3.20, s, 5-H; 3.23, dd(J 1.0 & 8.OH ₂), 4-H; 3.33, dd(J 1.5 & 8.OH ₂), 2-H; 4.22, d(J 10.OH ₂), 5'-H; 8.51, s, 2xMe.	94,95
6-Deoxyjacareubin		2.35, q(J 7 & 3H ₂), 8-H; 2.7, m, 6- & 7-H; 3.61, s, 4-H; 3.33, d(J 9.OH ₂) and 4.27, d(J 9.OH ₂), CH:CH (chromen); 8.54, s, 2xMe.	2,15,48, 55,57,58, 61,85,97- 100,102, 103.
1,5-Dihydroxy-3-methoxy (Mesuaxanthone A)	a	3.20, d(J 2.5H ₂), 2-H; 2.92, d(J 2.5H ₂) 4-H; 2.20-2.60, m, 6- & 7-H; 2.02, q(J 6.5 & 3.5H ₂), 8-H; 5.70, s, 1-OMe; 5.90, s, 3-OMe.	36,43,44, 69,81,84, 101,104
1,5,6-Trihydroxy (Mesuxanthone)	d	-2.71, 1-OH; 2.04, d(J 9H ₂), 8-H; 2.54, t(J 9H ₂), 3-H; 2.72, d(J 9H ₂), 4-H; 3.19, d(J 9H ₂), 7-H; 3.19, d(J 9H ₂), 2-H; 4.58, br., 5- & 6-H.	15,25,35, 42,46,50, 52,56,61, 62,64,69- 71,182

Compound	Solv.	PMR Values (τ)	Ref.
1,3,5-Trihydroxy-4-(3-methylbut-2-enyl) xanthene-9-one.	d	-3.02, 1-OH; 3.53, d(J 2.5H ₂), 7- & 8-H; 2.74, m, 6-H; 3.63, s, 2-H; 4.80, t, :CH-; 6.71, d, -CH ₂ -; 8.26, s, Me; 8.38, s, Me.	53
6,11-Dihydroxy-3,3-dimethyl-pyrano-(2,3-c) xanthene-7-(3H)-one.	d	-2.95, s, 6-OH; 2.43, q, 8-H; 2.8, m, 9- & 10-H; 3.92, s, 5-H; 3.06, d(J 10H ₂), 1-H; 4.35, d(J 10H ₂), 2-H; 8.58, s, 2xMe.	105
8-Deoxygartanin	b	-3.16, 1H, s; 0.25, 1H, s; 0.95, 1H, s; 2.42, 1H, q; 2.7-2.95, 2H, m; 4.76, 2H, br; 6.40-6.60, 4H, br; 8.18 & 8.34, 12H, S's.	96,106, 107
5,10-Dihydroxy-2,2-dimethyl-12-(3-methylbut-2-enyl)-pyrano(3,2-b)-xanthene-6(2H)-one (Trapezifolixanthone)	b	2.25, q(J 8 & 3H ₂), 7-H; 2.61, m, 8- & 9-H; 3.24, d(J 10H ₂), 4-H; 3.60-4.00, m, 10-OH; 4.38, d(J 10H ₂), 3-H; 4.73, m, :CH; 6.51, d(J 7H ₂), Ar-CH ₂ ; 8.12 & 8.27, s, :CMe ₂ ; 8.51, s, CMe ₂ -3.25, s, 5-OH.	99,107, 108
Morellin		-2.77, s, 1-OH; 0.37, s, -CHO; 2.4, d(J 7H ₂), 8-H; 3.35, d(J 10H ₂), 14-H; 4.43, d(J 10H ₂), 15-H; 3.9, t(J 8H ₂), 30-H; 4.75, t, (J 7.5H ₂), 20-H; 6.4, 7-H; 6.6-6.7, d, 19- & 29-H; 7.35, q, 24-H; 7.7, d(J 4.5H ₂), 25-H; 8.2, 23-Me; 8.25, 33-Me; 8.3, 22-Me; 8.47, 17- & 18-Me; 8.5, 27-Me; 8.67, 28-Me.	109-111
Gambogic acid	e	-0.92, br.s, -CO ₂ H; -2.55, s, 1-OH; 1.35, m, <u>o</u> -H pyr; 2.25, m, <u>p</u> -H pyr; 2.62, m, <u>m</u> -H pyr; 2.42, d(J 7H ₂), 8-H; 3.37, d(J 10.2H ₂), 14-H; 3.88, t(J 7.3H ₂), 30-H; 4.61, d(J 10.2H ₂), 15-H; 4.89, t(J 7H ₂), 35 & 20-H; 6.53, q(J 7.3 & 4.6H ₂), 7-H; 6.72, d(J 7H ₂), 19-H; 6.95, d (J 7.2H ₂), 29-H; 8.27, s, 33-H; 8.28, s, 22- & 37-H; 8.34, s, 23- & 38-H; 8.44, s, 18-H; 8.64, s, 27-H; 8.71, s, 28-H.	6,112-125

Compound	Solv	PMR Values (τ)	Ref.
1,7-Dihydroxy-3-methoxy (Gentisin)	c	2.35-2.65, m, 5-, 6- & 8-H; 3.40, d(J 3H ₂), 4-H; 3.62, d(J 3H ₂), 2-H; 6.09, s, OMe.	36,49,58, 64,126-133
1-Hydroxy-3,7-dimethoxy (Methylgentisin)	b	-2.94, 1-OH; 3.58, d(J 2.5H ₂), 4-H; 3.70, d(J 2.5H ₂), 2-H; 2.41, q, 8-H; 2.68, m, 5- & 6-H; 6.08, s, 3-OMe; 6.11, s, 7-OMe.	1,128
2-(3,3-Dimethylallyl)-1,3,7- trihydroxy	b	-3.33, 1-OH; 0.82, br; 3- & 7-OH; 3.48, s, 4-H; 2.34, m, 8-H; 2.54, m, 5- & 6-H; 4.65, br. t, :CH-; 6.58, d, CH ₂ ; 8.28 & 8.33, 2xMe.	15,73,134, 135
Mbarraxanthone (as it's dimethylether)	b	-2.50, s, 1-OH; 2.43, d(J 2.4H ₂), 8-H; 2.65- 2.80, m, 5- & 6-H; 3.45, s, 2-H; 4.47, t, :CH-; 6.0, s, 2xOMe; 6.45, d, Ar-CH ₂ ; 8.13, s, & 8.32, s, & 8.32, s,:CMe ₂ .	11,88,89
Calabaxanthone	b	-3.70, s, 5-OH; 2.75, s, 9- & 10-H, 3.25, d(J 9.6H ₂), 4-H; 4.34, d(J 9.6H ₂), 3-H; 3.75, s, 12-H; 4.76, t, :CH-; 5.85, d, -CH ₂ -; 6.12, s, 8-OMe, 8.15 & 8.34, s, :CMe ₂ ; 8.54, s, CMe ₂ .	47,55,99, 136
Thwaitesixantnone	b	-3.53, s, 13-OH; 1.98, d(J 10.2H ₂), 1-H; 2.83, s, 5- & 6-H; 3.26, d, (J 10.2H ₂), 12-H; 4.19, d(J 10.2H ₂), 2-H; 4.41, d(J 10.2H ₂), 11-H; 3.72, s, 8-H; 8.52 & 8.52, s, 3- & 10-Me ₂ .	47
1-Methoxy-3,5-dihydroxy	c	2.48, q(J 6 & 4H ₂), 8-H; 2.8, m, 6- & 7-H; 3.45, d(J 3H ₂), 4-H; 3.6, d(J 3H ₂), 2-H; 6.12, s, OMe	26
3-O-Rutinosyl-1-methoxy-5- hydroxy	c	2.42, q, 8-H; 2.78, m, 6- & 7-H; 3.46, d(J 3H ₂), 4-H; 3.62, d(J 3H ₂), 2-H; 5.0, br., glucosyl 1-H; 5.78, d, (J 2H ₂), rhamnosyl 1-H; 6.12, s, OMe; 6.4, rhamnoglucosyl-H; 9.15, m, rhamnosyl- Me.	26
1,3-Dihydroxy-7-methoxy (Iso- gentisin)		-1.56, 1-OH; -0.22, 3-OH; 5.90, 7-OMe	60,128,137, 169

Compound	Solv	PMR Values (τ)	Ref.
1,3,7-Trimethoxy		6.06, 1-OMe; 6.13, 3- & 7-OMe.	1,60,25,128 137
<u>Tetraoxygenated Xanthenes</u>			
1,3,6,7-Tetrahydroxy (Norathyriol)	c	-3.3, s, 1-OH; 1.03(-0.28), br, 3-, 6-, & 7-OH; 3.0, s, 5-H; 3.55, d(J 2H ₂), 4-H; 3.73, d(J 2H ₂), 2-H; 2.65, s, 8-H	25,35,51, 53,65,70, 73,76,143- 152,92
1,7-Dihydroxy-3,6-dimethoxy	c	-3.07, s, 1-OH; 2.63, s, 8-H; 3.14, s, 5-H; 3.51, & 3.72, 2 d(J 2H ₂), 2- & 4-H; 6.14 & 6.17, s, 2xOMe.	57
6,7-Dihydroxy-1-methoxypyrano- (2',3':3,4) xanthone (Lorostemin)	d	2.06, s, 8-H; 2.33, s, 5-H; 3.35, s, 2-H; 3.17, d(J 10.3H ₂), 4'-H; 4.10, d(J 10.3 H ₂), 5'-H; 6.0, s, OMe; 8.41, s, 2xMe.	153
Normangostin (γ - Mangostin)	b+c	-3.92, 1H, s; 3.25, 1H, s; 3.65, 1H, s; 4.75, 2H, br; 5.92, 2H, br; 6.75, 2H, br; 8.25, 8.35, 12H, s.	106,154
β - Mangostin	b	-3.38, 1H, s; 3.26, 1H, s; 3.63, 1H, br; 3.76, 1H, s; 4.8, 2H, m; 5.95, 2H, d(J 7H ₂); 6.16, 3H, s; 6.24, 3H, s; 6.68, 2H, d(J 7H ₂); 8.20, 8.22, 6H; 8.34, 6H.	
Tovopyrifolin-A 6-O-methyl ether	b	-3.33, s, 1-OH; 2.46, s, 8-H; 3.24, d(J 10H ₂), 4'-H; 3.36, s, 4-H; 4.40, d(J 10 H ₂), 5'-H; 4.80, t(J 7.5 H ₂), :CH; 6.01, s, 2xOMe; 6.39, d(J 7.5H ₂), 5-CH ₂ ; 8.11, s, Me; 8.31, s, Me; 8.51, s, 2xMe.	155
Tovophyllin-A	b	-3.33, s, 1-OH; 1.95, d(J 10H ₂), 4'-H; 3.68, s, 4-H; 4.25, d(J 10H ₂), 5'-H; 4.78, t(J 7.5H ₂), 2x:CH; 6.02, s, OMe; 6.05, s, OMe; 6.40, d(J 7.5H ₂), 5-CH ₂ ; 6.62, d(J 7.5H ₂), 2-CH ₂ ; 8.10, s,	155,156

Compound	Solv	PMR Values (τ)	Ref.
Tovophyllin-B	b	Me; 8.20, s, Me; 8.30, s, 2xMe; 8.50, s, 6'-2xMe -3.68, s, 1-OH; 1.97, d(J 10H ₂), 4'-H; 3.24, d(J 10H ₂), 4''-H; 3.69, s, 4-H; 4.24, d(J 10H ₂), 5'-H; 4.41, d(J 10H ₂), 5''-H; 4.78, t(J 7.5H ₂), :CH; 6.10, s, OMe; 6.43, d(J 7.5H ₂), CH ₂ ; 8.11, s, Me; 8.35, s, Me; 8.46, s, 2xMe; 8.49, s, 2xMe.	155,156
Pentadesmaxanthone	d	-3.2 to -3.3, 11-OH; 2.0, d(J 10 H ₂), 1-H; 3.74, s, 10-H; 4.16, d(J 10H ₂), 2-H; 4.7, t(J 7.4H ₂), :CH; 6.4, m, Ar-CH ₂ ; 8.22, s, & 8.36, s, :CMe ₂ ; 8.56 & 8.66, s, - (-O)CMe ₂	157,158,
1,3,5,6-Tetrahydroxy	b	-2.8, s, 1-OH; 2.04, d(J 9H ₂), 8-H; 3.01, d(J 9H ₂), 7-H; 3.55, d(J 9H ₂), 4-H; 3.72, d(J 9 H ₂), 2-H	8, 25, 35, 60,71,182, 101,145, 149,159-161
3,5,6-Trihydroxy-1-methoxy	b	-1.00, br, OH; 2.13, d(J 9H ₂), 8-H; 2.89, d(J 9H ₂), 7-H; 3.7, d(J 9H ₂), 4-H; 4.10, d(J 9H ₂), 2-H; 6.48, s, OMe.	25,60,162
3-Hydroxy-1,5,6-trimethoxy	b	3.73, d(J 2.5H ₂), 2-H; 3.63, d(J 2.5H ₂), 4-H; 3.04, d(J 9H ₂), 7-H; 2.02, d(J 9H ₂), 8-H; 5.87, 6.00 & 6.05, s, 3xOMe.	84,162,163
Cudraniaxanthone	c	-4.03, s, 1-OH; 2.45, d(J 10H ₂), 8-H; 3.10, d(J 10H ₂), 7-H; 3.40, s, 4-H; 3.70, m, :CH; 5.15, 5.35, 2d, :CH ₂ ; 8.47, s, 2xMe.	164,165
2-(3,3-Dimethylallyl)-1,3,5,6-tetrahydroxy	d	-3.5, s, 1-OH; 0.97, br., -OH; 2.35, d(J 9H ₂), 8-H; 3.02, d(J 9H ₂), 7-H; 3.47, s, 4-H; 4.69, t, :CH; 6.62, d, > CH ₂ ; 8.21, s, 2xMe.	15,60-63, 97,98,134, 145,92
Jacareubin	d	-3.61, s, 1-OH; 1.2, br., -OH; 2.40, d(J 9H ₂), 8-H; 3.06, d(J 9H ₂), 7-H; 3.70, s, 4-H; 3.38, d, 48,55,58	2,15,46-

Compound	Solv	PMR Values (τ)	Ref.
		:CH; 8.56, s, 2xMe	60-62,85, 97,98,134, 145,157,160 166-170,92
4-(3,3-Dimethylallyl)-1,3,5,6-tetrahydroxy (Ugaxanthone)	b	-2.45, s, 1-OH; 2.01, d(J 8.5H ₂), 8-H; 3.02, d(J 9H ₂), 7-H, 3.61, s, 2-H; 4.70, t, :CH; 6.0, s, 2xOMe; 6.08, s, OMe; 6.45, d(J 9H ₂), CH ₂ ; 8.12, s, Me; 8.31, s, Me.	88,89,165
Macluraxanthone (trimethylether)	b	1.99, d(J 9.4H ₂), 8-H; 3.04, d(J 9.4H ₂), 7-H; 3.21, d(J 10.OH ₂), :CH; 4.30, d(J 10.OH ₂), :CH; 3.54, 5.09 & 5.18, (J _{ax} 17.9, J _{bx} 10.0 & J _{ab} 10.OH ₂), vinyl group; 6.01, 6.06, 6.07, s, 3xOMe; 8.28, s, 2xMe; 8.59, s, 2xMe (chromene)	85,159,162, 171
10-O-Methylmacluraxanthone	b	-3.58, s, 5-H; 2.10, d(J 9H ₂), 7-H; 3.04, d(J 9H ₂), 8-H; 3.26, d(J 10H ₂), 4-H; 3.68, q(J 18 & 10H ₂), X of ABX system, :CH; 4.43, d(J 10H ₂), 3-H; 5.11 & 5.16, 2d(J 18 & 10H ₂), AB of ABX system; 6.06, s, 10-OMe; 8.28, s, 2xMe; 8.54, s, 2xMe (chromene)	172-174
Alvaxanthone (triacetate)	b	-2.45, s, 1-OH; 2.97, s, 7-H; 3.53, s, 4-H; 4.62, t(J 6.6H ₂), :CH; 5.09, 5.13, 3.72, (J _{ax} 10.8 & J _{ab} 1.2H ₂) vinyl group; 5.96, d(J 6.6H ₂), CH ₂ ; 7.62, 7.67, 7.78, s, 3xOAc; 8.25, s, 2xMe; 8.41, s, 2xMe.	160,175
1,3,5,8-Tetrahydroxy-2,4-(3,3-dimethylallyl) (Gartanin)	b	-2.16, 1-H, s; -1.33, 1H, s; 0.67, 1H, s; 2.78, 1H, d(J 9H ₂), 3.48, 1H, d(J 9H ₂); 4.75, 2H, br; 6.35-6.65, 4H, br; 8.20 & 8.30, 12H, s.	96,106,176
1,3,5-Trihydroxy-2-methoxy (Tovopyrifolin)	d	-3.06, s, 1-OH; 2.35, q, 8-H; 2.74, m, 6- & 7-H; 3.49, s, 4-H; 6.12, s, 2-OMe	48,55,157, 172,177

Compound	Solv	PMR Values (τ)	Ref.
1,5-Dihydroxy-2,3-dimethoxy	c	-2.68, s, 1-OH; 2.30-2.98, m, 6-, 7-, & 8-H; 3.22, s, 4-H; 6.03 & 6.22, s, 2- & 3-OMe.	47
Kayeaxanthone	b	2.05, d(J 9H ₂), 6-H; 2.90, d(J 9H ₂), 5-H; 3.46, d(J 10H ₂), 4-H; 3.51, q(J 20 & 12H ₂), X of ABX system, :CH; 4.32, d(J 10H ₂), 3-H; 5.01, q(J 20 & 1.2H ₂), and 5.15, q(J 12 & 1.2H ₂), AB of ABX system, CH ₂ ; 6.00, 6.33, 2s, 8- & 10-OMe; 8.25, s, 2xMe; 8.41, s, 2-Me ₂ .	172
1,2-Dimethoxy-3,8-dihydroxy	c	-3.25, 1-OH; 2.42, t(J 9.OH ₂), 6-H; 3.13, md(J 9.0 & 1.OH ₂), 5-H, 3.33, md(J 9.0 & 1.OH ₂), 7-H; 6.08 & 6.16, s, 2xOMe.	48
1,3,8-Trihydroxy-7-methoxy	c	-1.9 to 1.54, br. s, 1-, 3-, & 8-OH; 2.58, d(J 9.1H ₂), 6-H; 3.72, d(J 2.1H ₂), 4-H; 3.12, d(J 9.1H ₂), 5-H; 3.86, d(J 2.1H ₂), 2-H; 6.23, s, OMe.	80,101
1,4,7-Trihydroxy-3-methoxy	d	- 2.34, s, 1-OH; 1.0, br, 4- & 7-OH; 2.35-2.60, m, 5-, 6- & 8-H; 3.70, s, 2-H; 6.06, s, OMe.	64
1,5-Dihydroxy-6,7-dimethoxy	a	2.13, 5(J 8.5H ₂), 3-H; 2.59, s, 8-H; 2.68, q(J 8.5 & 1.5H ₂), 4-H; 2.94, q(J 8.5 & 1.5H ₂), 2 H; 5.76, s, OMe; 5.93, s, OMe.	25,178
3,4,8-Trihydroxy-1-(3,3-di- methylallyl)-2-methoxy (Celebixanthone)	b	-3.16, s, 8-OH; 1.28, br; 3- & 9, 4-OH; 2.59, t(J 8H ₂), 6-H; 3.25, d(J 8H ₂), 5-H; 3.49, d(J 8H ₂), 7-H; 4.80, t(J 6H ₂), :CH; 6.03, d(J 6H ₂), CH ₂ ; 6.15, s, OMe; 7.1, s, Me; 8.33, s, Me.	9,179-181
4-(1,1-Dimethylallyl)-1,2,5,6- tetrahydroxy (Symphoxanthone)	d	-3.0, s, 1-OH; 1-2, br., OH; 2.63, s, 3-H; 2.95, d(J 9H ₂), 7-H; 2.29, d(J 9H ₂), 8-H; 8.30, s, Me ₂ ; 3.53, q, :CH; 4.89, t, :CH ₂	88,89

Compound	Solv	PMR Values (τ)	Ref.
1-Hydroxy-2,3,5-trimethoxy	f	-2.65, 1H, s; 2.22, 1H, q; 2.74, 2H, m; 3.44, 1H, s; 6.02, 3H, s; 6.06, 3H, s; 6.16, 3H, s.	1,43,138
1-Hydroxy-2,3,7-trimethoxy	f	-2.65, 1H, s; 2.45, 1H, q; 2.73, 2H, m; 3.59, 1H, s; 6.07, 3H, s; 6.12, 3H, s; 6.16, 3H, s.	1,177
1,8-Dihydroxy-3,5-dimethoxy (Methylbellidifolin, Swerchirin)	b	-1.96, -1.33, 1- & 8-OH; 3.16/3.22, 7-H; 2.60/2.76, 6-H; 3.36/3.40, 4-H; 3.58/3.63, 2-H; 6.0/6.05, 2xOMe.	1,139-142, 176,177, 183,14
1,3-Dihydroxy-4,5-dimethoxy	c	2.32, 1H, q; 2.56, 2H, m; 3.70, 1H, s; 6.0, 3H, s; 6.12, 3H, s.	177,183, 184
1,3,4,7-Tetramethoxy	f	2.42, 1H, q; 2.72, 2H, m; 3.61, 1H, s; 6.04, 3H, s; 6.06, 3H, s; 6.15, 6H, s.	25,177
1,3,4,5-Tetramethoxy	f	2.25, 1H, q; 2.80, 2H, m; 3.57, 1H, s; 5.99, 3H, s; 6.01, 3H, s; 6.06, 3H, s, 6.10, 3H, s.	177,215
1-Hydroxy-3,7,8-trimethoxy (Decussatin)	b	-3.30, 1-OH; 2.70, d(J 9.2H ₂), 5-, & 6-H; 3.65, s, 2- & 4-H; 5.99, 6.04, 6.12, s, 3xOMe.	101,142, 183,185 195
1,7-Dihydroxy-3,8-dimethoxy (Gentianacaulin)	b	-3.2, 1-OH; 2.59, 6-H; 2.8, 5-H; 3.61, 2- & 4-H; 5.92, 6.20, s, OMe.	186-188, 194
3,8-Dihydroxy-1,7-dimethoxy (Isogentiacaulin) (diacetate derivative)	b	2.61, 6-H; 2.89, 5-H; 3.30, 2-H; 3.49, 4-H; 6.10, 1-OMe; 6.15, 7-OMe; 7.55, 8-OCOMe; 7.69, 3-OCOMe.	169,186, 190
1,8-Dihydroxy-3,7-dimethoxy (Swertiaperennine, Methyl- swertianin)	c	2.20-2.35, d, 6-H; 2.9-3.05, d, 5-H; 3.4-3.45, d, 4-H; 3.67-3.72, d, 2-H; 6.05, 6.1, s, 2xOMe.	142,186, 191,194,196
1,3,7,8-Tetrahydroxy (Norswertianin) (as tetra- acetate derivative)	b	2.50, 2.69, (J 9.5H ₂), 5- & 6-H; 2.79, 3.22 (J 2.5H ₂), 2- & 4-H; 7.6 & 7.7, 4xOCOMe.	101,142,188 187,191,192 196

Compound	Solv	PMR Values (τ)	Ref.
1,3,5,8-Tetrahydroxy (Desmethylbellidifolin) (as tetraacetate derivative)	b	3.18, d, 2.78, d, (J 2.5H _z), 2- & 4-H; 3.07, d, 2.55, d(J 9.5H _z), 6- & 7-H; 7.67, 7.58, 4XOCOMe.	139,142, 191,192, 197,198
1,5,8-Trihydroxy-3-methoxy (Bellidifolin)	c	-3.5, br., 1- & 8-H; 3.25/3.4, 7-H; 2.62/2.78, 6-H; 3.42/3.46, 4-H; 3.68/3.71, 2-H; 6.1, OMe.	139,142, 196,198,199
1,3,8-Trihydroxy-5-methoxy (Isobellidifolin)	c	-3.45, br., 1-OH; 3.26/3.41, 7-H; 2.67/2.83, 6-H; 3.42/3.45, 4-H; 3.70/3.74, 2-H; 6.0, OMe.	26,141,142, 190,192,14
1-Hydroxy-3,5,8-trimethoxy		-3.33, 1-OH; 3.12/3.28, 7-H; 2.60/2.76, 6-H; 3.35/3.40, 4-H; 3.52/3.57, 2-H; 6.0/6.05, 3xOMe.	139,142, 191
1,3,5-Trihydroxy-6-methoxy	c	2.05/221, d, 8-H; 3.07/3.23, d, 7-H; 3.52/3.58, d, 4-H; 3.68/3.73, d, 2-H; 6.05, OMe.	60,101, 200
1,5,6-Trihydroxy-3-methoxy	c	-3.1, 1-OH; 2.4, d(J 10H _z), 8-H; 3.12, d(J 10H _z), 7-H; 3.5, d(J 3H _z), 4-H; 3.62, d(J 3H _z), 2-H; 6.05, OMe.	149,201
3,7,8-Trimethoxyxanthone-1-O- primeveroside (Decussatin-O- primeveroside)	b	2.82, 2.95, (J 9.5H _z), 5- & 6-H; 3.28, 3.42, (J 2.5H _z), 2- & 4-H; 6.08, 3H; 6.13, 3H; 6.15, 3H, OMe.	187,202- 204
7-Hydroxy-3,8-dimethoxy- xanthone-1-O-primeveroside (Gentiabavaroside) (as acetate derivative)	b	2.72, 2.92 (J 9.5H _z), 5- & 6-H; 3.30, 3.40 (J 2.5H _z), 2- & 4-H; 6.10, 6H, 2xOMe; 7.69, 3H, OCOMe.	187,202
1,8-Dihydroxy-3-methoxy- xanthone-7-O-acetyl-rutinoside (Gentiabavarutinoside)	b	2.59, 2.64 (J 9.5H _z), 5- & 6-H; 3.33, 3.50 (J 2.5H _z), 2- & 4-H; 6.14, 3H, OMe; 7.57, 6H, OCOMe.	187,205
7,8-Dihydroxy-3-methoxy- xanthone-1-O-primeveroside (Isogentiakochianoside) (Diacetate derivative)	b	2.65, 2.76 (J 9.5H _z), 5- & 6-H; 3.37, 3.47 (J 2.0H _z), 2- & 4-H; 6.11, 3H, OMe, 7.52, 7.71, 6H, OCOMe.	187,202

Compound	Solv	PMR Values (τ)	Ref.
3,6-Dihydroxy-1,7,8-trimethoxy	c	2.96, 5-H; 3.53, 4-H; 3.64, 2-H; 6.16, 7- & 8-OMe; 6.4, 1-OMe.	42
1,2,3,5,8-Pentamethoxy	f	2.93, d(J 9H ₂), 1H; 3.29, s, 1H; 3.37, d(J 9H ₂), 1H; 6.10, s, 3H; 6.12, s, 3H; 6.15, s, 3H; 6.18, s, 3H; 6.21, s, 3H.	177
1,3-Dihydroxy-4,5,8-trimethoxy	b	-2.74, 1-OH; 2.85, d(J 9H ₂), 6-H; 3.22, d(J 9H ₂), 7-H; 3.6, s, 2-H; 5.98-6.05, 3xOMe.	183
1,3,8-Trihydroxy-4,5-dimethoxy (4,5-Di-O-methylcorymbin)	c	-1.6, -1.3, 1- & 8-OH; 2.45, 2.6, 6-H; 3.18, 3.7, 7-H; 3.6, 2-H; 6.06, 6.13, 2xOMe.	176,216
4,7-Dimethoxy-1,3,8-trihydroxy (4,7-Dimethoxybellidin)	c	-2.18, -1.73, 1- & 8-OH; 2.48, 2.6, 6-H; 2.8, 3.0, 5-H; 3.5, 2-H; 6.03, 6.06, 2xOMe.	176
1-Hydroxy-3,4,7,8-tetramethoxy	b	-3.04, 1-OH; 5.98-6.06, 3xOMe; 3.6, s, 2-H; 2.95, d(J 9H ₂), 5-H; 2.72, d(J 9H ₂), 6-H.	191,192
1-Hydroxy-3,5,7,8-tetramethoxy	b	3.60, d(J 1.5H ₂), 2-H; 3.45, d(J 1.5H ₂), 4-H; 2.96, s, 6-H; 5.98, OMe; 6.02, 2xOMe; 6.10, OMe.	199
1-Hydroxy-2,3,4,5-tetramethoxy	b	-2.55, 1H, s, 2.20, 1H; q; 2.62, 2H, m; 5.86, 3H, s; 5.96, 3H, s; 6.00, 3H, s; 6.09, 3H, s.	1,138,177
1,4-Dihydroxy-2,3,4,7-tri- methoxy	b	-2.66, 1-OH; 2.12, q, 8-H; 2.66, m, 6- & 7-H; 5.9-6.08, 4xOMe.	1,177,183
1,4-Dihydroxy-2,3,7-trimethoxy	b	-2.05, 1-OH; 2.37, q, 8-H; 2.54, m, 6- & 7-H; 5.88-5.98, 3xOMe.	183
1-Hydroxy-2,3,4,7-tetramethoxy	f	-2.62, 1H, s; 2.39, 1H, q; 2.55, 2H, m; 5.86, 3H, s; 6.04, 3H, s; 6.09, 6H d.	1,138,177
1,2,3,4,7-Pentamethoxy (Polygalaxanthone B)	g	2.3, d(J 3H ₂), 8-H; 2.5, d(J 9H ₂), 5-H; 2.7, q(J 9 & 3H ₂), 6-H; 5.80, 5.90, 5.95, 5xOMe.	23,217
	h	5.75, 5.91, 6.00, 6.38, 5xOMe.	

Compound	Solv	PMR Values (τ)	Ref.
3,7,8-Trihydroxyxanthone-1-O-glucoside (Norswertianin-1-O-glucoside)(Triacetate derivative)	b	2.6, 2.72 (J 9.5H ₂), 5- & 6-H; 3.04, 3.25 (J 2.5H ₂), 2- & 4-H; 7.51, 7.63, 7.70, 3xOCOMe.	187,206
1,3,5-Trihydroxyxanthone-8-O- β -D-glucopyranoside (Desmethylbellidifolin-8-O-glucoside)(Triacetate derivative)	b	3.22, d, 2.85, d(J 2.5H ₂), 2- & 4-H; 3.04, d, 2.69, d(J 9.5H ₂), 6- & 7-H; 7.70, 7.62, 7.52, 3xOCOMe.	198
1,5-Dihydroxy-3-methoxy-xanthone-8-O- β -D-glucopyranoside. (Bellidifolin-8-O-glucoside; Isoswertianolin)	c	-3.18, br., s, 1-OH; 2.85, d(J 9H ₂), 7-H; 2.67, d(J 9H ₂), 6-H; 3.45, d(J 3H ₂), 4-H; 3.62, d(J 3H ₂), 2-H; 5.02, C ₁ -H of β -glucoside; 6.5, six glucosyl protons & H ₂ O.	101,198, 201,207
5,8-Dihydroxy-3-methoxy-xanthone-1-O-glucoside (Swertianolin)	c	-2.95, br.s, 8-OH; 2.70, d(J 9H ₂), 6-H; 3.32 d(J 9H ₂), 7-H; 3.40, d(J 3H ₂), 4-H; 3.48, d(J 3H ₂), 2-H; 5.0, m, C ₁ -H of β -glucoside, 6.50, six glucosyl protons & H ₂ O	208-210
3,5,8-Trihydroxyxanthone-1-O-glucoside (Norswertianolin)	c	2.72, d(J 9H ₂), 6-H; 3.35, d(J 9H ₂), 7-H; 3.42, d(J 3H ₂), 4-H; 3.56, d(J 3H ₂), 2-H; 5.08, m, C ₁ -H of β -glucoside, 6.5, six glucosyl protons & H ₂ O	142,208, 211-214
<u>Pentaoxygenated Xanthenes</u>			
1,8-Dihydroxy-2,3,7-trimethoxy	d	-3.2, s, 1-OH; -0.3, br.s, 8-OH; 2.55, d(J 9H ₂), 6-H; 2.85, d(J 9H ₂), 5-H; 3.37, s, 4-H; 6.07, 6.15 & 6.25, s, 2-, 3- & 7-OMe.	55
1,7-Dimethoxy-2,3,8-trihydroxy	d	-1.27, s, 1-OH; 2.67, d(J 9H ₂), 6-H; 3.43, d(J 9H ₂), 5-H; 3.55, s, 4-H; 6.18, s, OMe; 6.23, s, OMe.	115
1,3,6-Trihydroxy-7,8-dimethoxy	c	-2.91, 1-OH; 3.82, 2-H; 3.42, 4-H; 2.94, 5-H; 6.14, 7-OMe; 6.12, 8-OMe.	42

Compound	Solv	PMR Values (τ)	Ref.
7-Hydroxy-1,2,3,4-tetramethoxy	a	1.8, s, Ar-H; 5.25, 5.57, 5.67, 4xOMe.	23,177,217
1-Methoxy-2,3,6,7-dimethylene-dioxy	a	2.1, s, 8-H; 2.5, s, 4-H; 2.65, s, 5-H; 3.43, s, -O-CH ₂ -O; 5.2, s, OMe.	23
	b	2.38, s, 8-H; 3.18, s, 4-H; 3.38, s, 5-H; 3.87, 3.92, s, methylenedioxy, 5.8, s, OMe.	
	h	4.52, & 4.72, methylenedioxy, 5.99, OMe.	
1,2,3-Trimethoxy-6,7-methylenedioxy (Polygalaxanthone A)	b	2.17, s, 8-H; 3.15, s, 4-H; 3.25, s, 5-H; 3.85, s, methylenedioxy; 5.90, 5.97, 6.01, OMe.	23,217
	h	5.83, 6.13, 6.67, OMe.	
1,2,3,4,6,7-Hexamethoxy	b	2.5, s, 8-H; 3.3, s, 5-H; 5.78, 5.80, 5.85, 5.88, 5.9, 6xOMe.	23
	h	5.75, 5.93, 6.01, 6.06, 6.42, 6.56, 6xOMe.	

Solvents mentioned in the tables:-

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|--|-------------------------|
| a = Trifluoroacetic acid; | b = Deuteriochloroform; |
| c = Dimethyl sulphoxide - d ₆ | d = Diuterioacetone; |
| e = Pyridine salt | f = Methylene chloride; |
| g = Carbon tetrachloride | h = Benzene |

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