Inophyllum F, a new coumarin from Calophyllum inophyllum grown in French Polynesia

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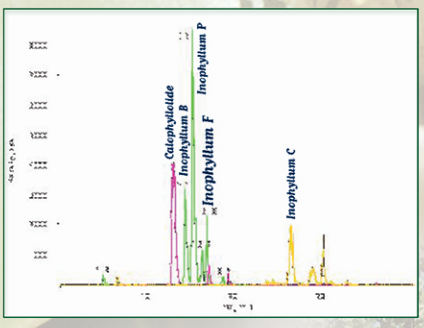
1 • Introduction

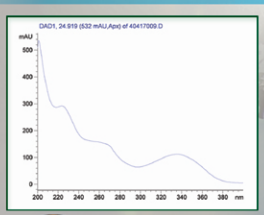
Calophyllum inophyllum, locally called "Tamanu" had been widely used in Polynesian traditional medicine for many centuries (1). Different parts of this plant contain bioactive secondary metabolites such as coumarins (2).

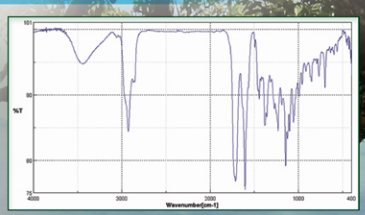
A new compound, named Inophyllum F, had been isolated from Calophyllum Inophyllum grown in French Polynesia as a minor component with regard to inophyllums B, P and C obtained from the same source. This compound was detected by normal-phase liquid chromatography – tandem mass spectrometry using a special electrospray source configuration and isolated from leaf extracts by preparative HPLC using UV detection (3). The structure was determined from 1D and 2D NMR techniques, HR-ESI-MS and tandem mass spectrometry, and cristallography.

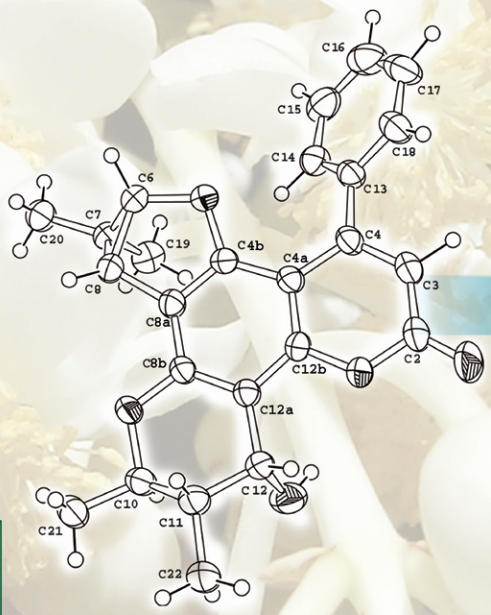
2 • Leaf extract chromatogram



3 • UV spectra - IR spectra







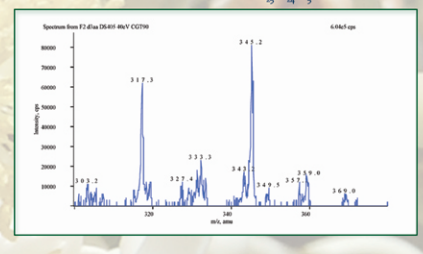
Inophyllum F

4 • NMR data

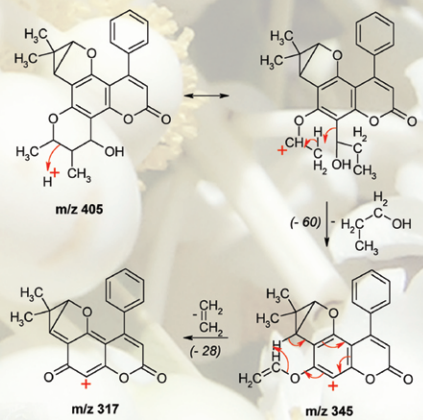
Position n°	Inophyllum F ^{1}H (δ, ppm)	Inophyllum G2 ^{1}H littrature (δ, ppm)
2	---	---
3	5.97, s	6.02, s
4	---	---
4a	---	---
4b	---	---
6	4.26, d, J=5.7 Hz	4.21, d, J=5.7 Hz
7	---	---
8	2.48, d, J=5.7 Hz	2.42, d, J=5.7 Hz
8a	---	---
8b	---	---
10	4.26, dq, J=6.2, 10.8 Hz	4.40, ddq, J=0.8, 3.3, 6.8 Hz
11	1.76, ddq, J=3.0, 6.8, 10.8 Hz	2.33, ddq, J=3.3, 5.3, 7.1 Hz
12	4.94, d, J=3.0 Hz	5.18, dd, J=5.3, 0.8 Hz
12a	---	---
12b	---	---
13	---	---
14, 18	7.34, m	7.32, m
15, 17	7.40, m	7.42, m
16	7.40, m	7.42, m
19	1.03, s	1.05, s
20	0.68, s	0.73, s
21	1.45, d, J=6.2 Hz	1.45, d, J=6.8 Hz
22	1.15, d, J=6.8 Hz	1.18, d, J=7.1 Hz

5 • MS-MS spectra

HR - ESI - MS : obsvd 404.1641 (M^+) for $C_{25}H_{24}O_5$ (calcd 404.1624)



6 • fragmentations



7 • Conclusion

Inophyllum F contains a fused dimethyl-cyclopropyldihydrofuran ring as well as the rare inophyllums G1 and G2, and in addition a chromanol ring having the three sequential (R, S, R) stereochemistries at the 10, 11 and 12 positions. This (10R, 11S) inophyllum stereoisomer may show an antiviral activity such as anti-HIV-1 but bioassays will be carried on to confirm its activity (4,5).

References :

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