



607/E2

Citriquinone: a potentially new anticancer active 1,4-benzoquinone from *Penicillium citrinum*

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Fungal metabolites are an obvious choice for drug discovery today. As an initiation of research in this area, chemical investigation of *P. citrinum* was done and herein we report an isolation of a new fungal metabolite, citriquinone (1) having an inhibition activity on the human cancer cell line HEP2, when subject to the scratch wound assay. The fungus isolated from a soil sample collected from the garden of the Department of Botany, University of Sri Jayewardenepura, showed significant antibacterial activity against gram positive bacteria. The fungus was identified as *Penicillium citrinum* by studying its molecular characteristics. The MeOH extract of the fungal culture grown on Potato dextrose agar (PDA), was concentrated and subject to a series of solvent-solvent partitioning using EtOAc, hexane and CH₂Cl₂. The CH₂Cl₂ fraction having antibacterial activity was subjected to silica gel column chromatography followed by prep. TLC, and yielded citriquinone (1) as a yellow solid. Structure of 1 was established as 3-(5-hydroxy-2-methyl-3,6-dioxo-4-(5-oxohexyl) cyclohexa-1,4-dienyl) butan-2-yl formate by HRESI(+)-MS data (*m/z* 337.1646 [M+H]⁺ C₁₈H₂₅O₆ requires 337.1644) and 1D and 2D NMR experiments (Table 1). ¹³C assignments were made with the help of both gHSQC and gHMBC experiments.

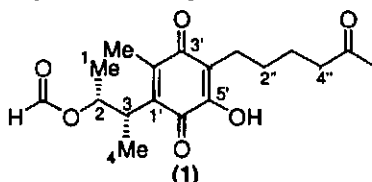


Table 1: NMR (600MHz, CDCl₃) data of Citriquinone (1)

#	δ_H (m, J (Hz))	δ_C	gCOSY (δ_H)	gHMBC
1	1.34 (3H, d, 6.0)	19.02		4, 3, 2
2	5.46 (1H, m)	72.83	1.34	4, 3, 1', 2-OCHO
3	3.04 (1H, m)	40.04	1.23, 5.46	2, 6'
4	1.23 (3H, d, 7.2)	15.42	3.04	1, 3, 2, 1'
2-OCHO	7.84 (1H, s)	160.19		
2'-Me	2.07 (3H, s)	12.53		2, 3, 4, 1', 2', 3', 6'
5'-OH	7.05 (1H, s)			
1''	2.39 (2H, t, 7.8)	22.60	1.43	3'' 2'', 5', 4', 3'
2''	1.43 (2H, m)	27.51	2.39, 1.57	1'', 4'', 5'
3''	1.57 (2H, m)	23.58	2.43	1'' 2'', 4'', 5''
4''	2.43 (2H, t, 7.8)	43.36		1'', 2'', 5''
6''	2.11 (3H, s)	29.91		3'', 4'', 5''

Acknowledgement: Financial assistance from NSF research grant RG/2005/HS/11

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