



ISSN : 0973-7057

Isolation of a new flavone from *Nigella sativum*

Kumari Shikha* and Syed Mumtazuddin

Department of Chemistry, B.R.A. Bihar University, Muzaffarpur, Bihar, India

Received : 17th April, 2017; Revised : 20th May, 2017

Abstract : The plants produce a lot of organic compounds but some compounds like alkaloids, terpenoids, phenolics, flavonoids, chromines and other minor chemicals have some medicinal use. A new flavonoid from *Nigella sativum* has been isolated and on the basis of U.V., NMR spectra and microanalysis the new flavone tephrorianin is characterized as {2'' 3'' dihydro - 5-methoxy-3'' 2''- acetoxy 2''- methyl propylidene)- 2''-Oxo furyl (4'' 5'' 7,8. flavones)

Keywords : Plants, isolation, flavones, *Nigella sativum*

INTRODUCTION

The plants produce a lot of organic compounds but their essential components which metabolite are called primary compounds.

The primary compounds like carbohydrate lipids, nucleotides and peptides are shared by all living organism and are central to life processes. The secondary compound is also derived from essential components, but is not central to metabolism.

Secondary compounds include alkaloids terpenoids, phenolics, flavonoids, chromines and other minor chemicals. The so called secondary compounds, which have no known function in photo synthesis, growth or other aspects of plant physiology but help in protection against diseases, herbivores and environment stress. A lot of study has been done on the role of natural products from plants for the control of insect pests.^{1,2}

Accordingly, chemical investigation of seeds *Nigella sativum* was taken up that resulted in the isolation of new flavone tephrorianin characterized as {2'' 3'' di hydro - 5

Methoxy-3'' (2'' acetoxy 2'' -methylpropylidene) - 2''- Oxofuryl 4'' 5'' 7,8- flavone)

EXPERIMENTAL

Mps (uncorrected) were recorded on electro thermal apparatus. U.V. spectra were recorded on syfronics U.V. visible spectrophotometer 119. ¹H NMR spectra were recorded in CDCl₃ on a Bruker WM400 MHz spectrometer. Using Me₄Si as an internal reference. Mass spectra were measured on Jeol JMSD-300 spectrometer at 70 eV. Micro analysis were performed by RSIC at CDIR Lucknow. Silica gel used for column chromatography was 60-120 mesh.

EXTRACTION

Oven dried *Nigella sativum* seeds (0.75Kg.) were extracted with hot CHCl₃; and concentrated extract (4.5 gm) on column chromatography yield among other unidentified compounds tephrorianin (10mg) in CHCl₃ - EtOAc (80:20).

Elemental Analysis

Required for the	found experimentally
Molecular formula C ₂₄ H ₂₀ O ₇	
C, 68.57%.	C, 68.51%

*Corresponding author :

Phone:

E-mail : snjvkmr1995@gmail.com

Biospectra : Vol. 12(2), September, 2017

An International Biannual Refereed Journal of Life Sciences

H,4.76%. H,4.82%
O,26.66%. O,26.62%
Colure crystals from methanol (10mg)
M.P.-228.300
U.V.CHCl₃/nm:266,341
I.R(KBr)/cm-1:1796,1727,1651,1599 and 1496
1HNMR(400 MHzCDCl₃):1.90(1H,S,Gen-Me₂),
2.12(3H,S,OCOCH₃);4.05(3H,OCH₃)6.65 (1H,S,H6)
6.68 (1H, S, H₃); 7.50-7.60 (3H,M. H-3.H-4' and H-5');
7.80 - 7.84 (2H,m,H-2' and H-6');7.85 (1H.S.H-1")
Mass (70ev) m/z 419 ([M-1]⁺, 4.8(7.1); 376 (5.2);
360 (5-7); 359 (11.2); 358 (34.8);301 (5-1)
213 (100);156 (11.4) 102 (5.0)

DISCUSSION

Tephrorinin exhibited UV absorption maxima at 266 and 341 nm. The I.R. spectrum showed the presence of chromone carbonyl absorption at 1615 cm⁻¹: actoxyl carbonyl absorption at 1727 cm⁻¹ and lactone carbonyl absorption at 1796 cm⁻¹

The 1HNMR spectrum of tephorianin revealed the presence of an unsubstituted phenyl ring (7.50, 7.84 & m, 5H), a gem-dimethyl group (1.90) and one methoxyl group (4.05). The C-3 Proton appeared as a singlet at 6.68. The spectrum further revealed two more singlets at 6.65 and 7.85 each integrating to one proton. The presence of lactones carbonyl group as indicated by I.R. together with an acetoxyl group, gem-dimethyl group and one

proton singlet at 7.85 suggested the presence of an additional five member lactone ring system with an acetoxyl-2 methyl propylidene substituent. Thus additional ring system was placed at the C-7 and C-8 position on biogenetic grounds and the methoxyl group at C-5 position the singlet at 7.85 was assigned to C-1" proton and 2-acetoxyl- 2 methyl propylidene substituent³ and the singlet at 6.65 was assigned to C-6 proton. Thus the structure of tephrorianin was established as [2", 3". di hydro-5 methoxy 3"(2" 'actoxy 2" methyl propylidene) 2"-Oxofuryl-(4" 5" 7.8) flavones). The mass spectrum of tephrorianin exhibited [M-1] + peak corresponding to 419. Flavones having either C-5 or C-8 methoxyl group normally exhibit [M -1] +Peak.^{4,5}

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