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Isolation and Structure determination of new anthraquinone from the flowers of *Tagetes erecta*

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Abstract

***Tagetes erecta* belongs to family asteraceae is found plentifully in most of the places of India, either cultivated in gardens or wild. The villagers use this plant in bronchial asthma, anusthans, different ceremony. The pastes of flowers were often applied on wound and cuts and leaves juice dropped in otalgia. *Tagetes erecta* are richest source of yellow dyes in ancient arts of Rajasthan and Orrisa. The present communication deals with the isolation and structure elucidation of a new anthraquinone together with quercitin and loganic acid. The structure of compound was described with the help of spectral data and chemical studies.**

Introduction

The family asteraceae is one of the largest family of plant kingdom, which includes about 1100 genera and 30,000 species. About 157 genera and 900 species are reported in India. *Tagetes erecta*(Gainda), is an annual, sparingly-branched, aromatic herb. Branches angular, ribbed. Leaves pinnate, oblong, acute, base decurrent. Flowers yellow or orange. Flowering throughout the year. It is most commonly cultivated in gardens in major parts of India. The pastes of flowers were often applied on wound and cuts and leaves juice dropped in otalgia (Gaur, 1999)

Most of the species of Tagetes were analysed for their essential oil compositions (Chawdhury, 2001). *Tagetes patula* is widely distributed in montane and sub montane Himalayan zone,Its leaves powder is used as an insect repellent and paste used in skin ailments.Flowers of *Tagetes erecta* are richest source of yellow dyes in ancient arts of Rajasthan and Orrisa (Lemmens and Wulijarni 1991).

Principle constituents isolated from flowers of *T. minuta* are anthocyanins and it derivatives (Putlano 2000). Some long chain fatty acids, aromatic hydrocarbons and phenyl acetaldehydes are extracted from floral extract of *T. erecta*. The present study describe the isolation and structure elucidation of a new anthraquinone glycoside together with quercitin and loganic acid.

Material and Methods

Collection of plant material

The flowers of *Tagetes erecta* was collected from the Pasulok Barrage Rishikesh of District, Dehradun, (Garhwal) in the month of August. The identity of the plant was confirmed by Dr. P.K. Uniyal, Department of Botany, H.N.B. Garhwal University Campus, Badshahithaul, Tehri Garhwal (U.A.) and the voucher specimen is available in the herbarium of Plant Identification Laboratory of Botany Department.

Extraction and isolation

The air-dried and coarsely powered flowers of the plant were defatted with light petroleum in a soxhlet. The defatted mass was exhaustively extracted repeatedly with 90 % aqueous EtOH, until the extractive became colourless. All the extracts were mixed and concentrated under reduced pressure using rotatory vacuum

evaporator.

The concentrated extract was adsorbed on Silica gel and fractionated through column chromatography using the solvent system of chloroform-methanol (95:5). The polarity of solvent was gradually increased by addition of methanol. Repeated column chromatography afforded compounds MT-1 (1.5 gm), MT-2 (0.5 gm),and MT-3 (0.7gm), with some other inseparable compounds.Compound MT-2 and MT-3 were identified as quercetin and loganic acid by their reported data ,mmp co TLC with an authentic sample.

M.P.were uncorrected.UV spectra were taken in MeOH.1H-NMR spectra were taken using TMS as internal standard and CDCl3 and CD3OD as solvent,all the signals are expressed as values downfield from TMS .CC was carried out on silica gel(60-120 mesh,Merck ,eluting solvent $CHCl_3$: MeOH).

Results and Discussion

The ethanolic extract of flowers of *Tagetes erecta* on repeated column chromatography over silica gel afforded compounds MT-1,MT-2 and MT-3.Compounds MT-2 and MT-3 were identified as quercetin and loganic acid by comparison with authentic sample and reported data (Potter and Thomas,1995).

Compound MT-1

It was crystallized from methanol as yellow powder.

Melting point	:	177-178°C
Molecular formula	:	$C_{15}H_{10}O_4$
Molecular weight	:	254 amu
U.V (max MeOH) nm	:	242(sh), 279, 310, 414.
I.R (maxKBr) cm-1	:	3240, 3040, 1895, 1660, 1625, 1450, 1250, 1190, 915
EI-MS (m/z)	:	255[M+H]+254[M]+,236[M-H2O]+, 226[M-CO]+,225[M-CHO]+152, 141,115.
1H-NMR (CDCl3 , ppm)	:	

13.19-8.27(1H,s),8.22-8.30(2H,m),7.74-7.80(2H,m),7.27(1H,s),2.23 (3H,s).

13C-NMR (CDCl3, ? ppm)

142.2(C-1), 142.8(C-2), 124.2(C-3), 124.1(C-4), 112.7(C-5), 151.3(C-6), 123.2(C-7), 158.2(C-8), 180.2(C-9), 179.2(C-10), 138.8(C-11), 113.3(C-12), 114.1(C-13), 139.8 (C-14), 29.8(CH3).

Compound MT-1 was crystallized from methanol as yellow powder.Its UV spectrum showed absorption bands at 242,279,310 and 414 nm,and IR spectrum displayed characteristic peaks for carbonyl group at 1625 cm^{-1}. Its IR spectrum also showed a bands at 3450, 1662 and 1630cm^{-1} for free hydroxyl, unchelated and chelated carbonyl groups, respectively. The EI mass spectrum of compound displayed the peak at m/z 254 [M]+ ,calculated for molecular formula $C_{15}H_{10}O_4$.The 1H-NMR spectrum of compound showed a peri hydroxyl group at 13.19 and two meta -coupled protons at 8.22 (2H,m) and 7.27(2H,m),and a singlets for methyl group at 2.23 (3H,s).

The 13C-NMR data of the compound indicate the presence of fifteen carbon atoms. The downfield signals in 13C-NMR appeared at 142.2, 142.8 and 153.16 were assigned for substituted C-1, C-3 and C-2 carbons respectively. Thus on the basis of above spectral findings the compound MT-1 was identified as 1, 3-dihydroxy-2-methyl anthraquinone (Figure-1) It was further confirmed by comparison of its data with that of reported compound (Thomson, 1971 and Wijnsma and Ver poorte, 1986).

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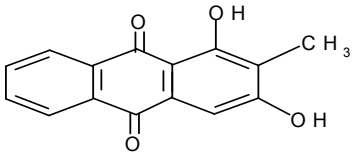
Figure 1:



Compound MT- 1