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Data article

Synthesis of pyrazole fused pyran analogues: Antimicrobial, antioxidant and molecular docking studies

Pavithra Gurunanjappa[a], Mylarappa B Ningappa[b], Ajay Kumar Kariyappa[a,*]

[a] Department of Chemistry, Yuvaraja College, University of Mysore, Mysore, India
[b] Transplant Surgery, Rangos Research Center, University of Pittsburgh, PA 15201, USA

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ABSTRACT

A series of six new pyrazole fused pyrans were synthesized by intramolecular cyclisation reaction of 3-(1-hydroxynaphthalen-2-yl)-1-aryl-1*H*-pyrazole-4-carbaldehydes with ethyl alcohol in the presence of conc. sulphuric acid under reflux conditions. The synthesized compounds were characterized by ^{1}H NMR, ^{13}C NMR, MS studies and elemental analysis, and were evaluated *in vitro* for their antimicrobial and antioxidant susceptibilities against different strains of bacteria, fungi, and DPPH and hydroxyl free radicals. Molecular docking of these compounds studied for their antimicrobial and antioxidant activities.

Specifications table

Subject area	*Bioorganic chemistry*
Compound	*Six fused pyran analogues*
Data category	*Spectral, biological data*
Data acquisition format	*Spectral*
Data type	*Analyzed*
Procedure	*A series of six new fused pyrans were synthesized from formylpyrazoles. The synthesized compounds were characterized by spectral studies and evaluated for their biological potency. Molecular docking studies were carried out.*

* Corresponding author. Fax: +918212419239.
E-mail addresses: ajaykkchem@gmail.com, ajaykumar@ycm.uni-mysore.ac.in (A.K. Kariyappa).

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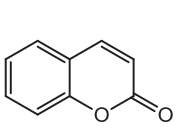
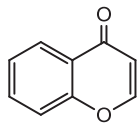
1. Rationale

The emergence of new infectious diseases and increasing resistance of microorganisms is the major cause of morbidity and mortality [1]. Excessive ROS produced by the human bodies result in the damage to various cell constituents that leads to serious health problems, which was overcome by antioxidants [2]. Chromenes form elite classes of naturally occurring and synthesized compounds, which comprises of two types of structural skeletons, *viz.*, coumarin (i), and chromene (ii). Compounds containing these skeletons have known for their enormous applications. Naturally occurring Warfarin (iii) is used to prevent clotting of blood in the veins, lungs or heart. Ningalin B (iv) and Lamellarin D (v) derived from the marine alkaloids exhibit HIV-1 integrace inhibition, immunomodulatory activity and cytotoxicity. (+)-Calanolide A (vi) isolated from *Calophyllum lanigerum* is a non-nucleoside reverse transcriptase inhibitor with potent activity against HIV-1. (+)-Inophyllum B (vii) isolated from *C. inophyllum* was found to be most active against HIV-reverse transcriptase [3].


(i)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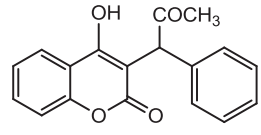
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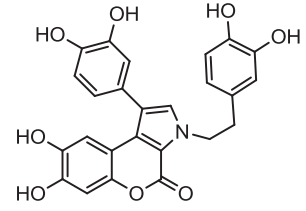
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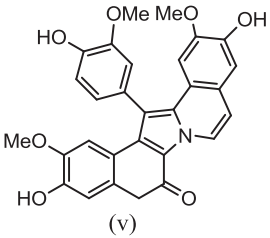
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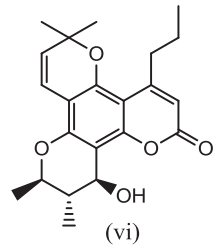
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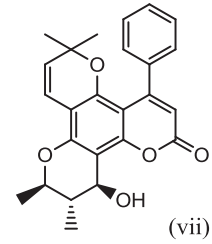
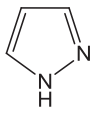

(vii)

Among the nitrogen heterocycles, pyrazole core (viii) occupies prime position in bioorganic chemistry for their bioactive nature. Pyrazole derivatives have played a crucial role in the field of pharmaceutical chemistry and have been extensively used as important pharmacores in drug designing. Designed series of pyrazoles exhibited broad spectrum of biological activities, few to mention that, selective monoamine oxidases, swine kidney diamine oxidase and bovine serum amine oxidase inhibition (ix); kinesin spindle protein inhibition (x); neuronal nitric oxide synthase (nNOS) inhibition (xi); anticancer and anti-inflammatory activities (xii); anti-tubercular activities (xiii) and antiproliferative activities (xiv) [4].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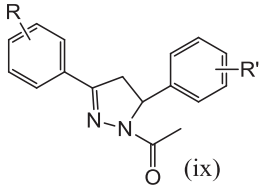
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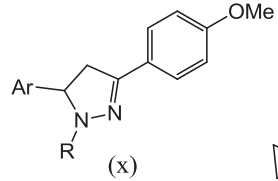
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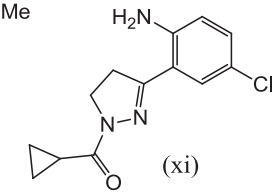
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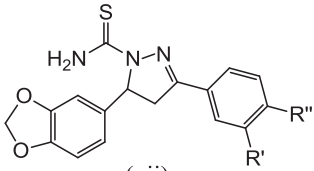
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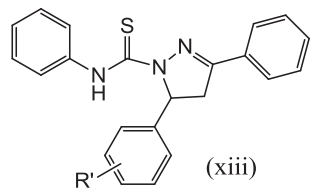
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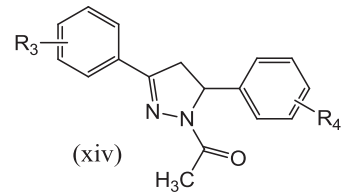
(xiv)