

## Accepted Manuscript

Microwave Synthesis, Biological Screening and Computational Studies of Pyrimidine Based Novel Coumarin Scaffolds

Soniya D. Naik , K.M. Hosamani , Shyam Kumar Vootla

PII: S2405-8300(18)30102-2  
DOI: [10.1016/j.cdc.2018.06.002](https://doi.org/10.1016/j.cdc.2018.06.002)  
Reference: CDC 118



To appear in: *Chemical Data Collections*

Received date: 18 May 2018  
Revised date: 5 June 2018  
Accepted date: 7 June 2018

Please cite this article as: Soniya D. Naik , K.M. Hosamani , Shyam Kumar Vootla , Microwave Synthesis, Biological Screening and Computational Studies of Pyrimidine Based Novel Coumarin Scaffolds, *Chemical Data Collections* (2018), doi: [10.1016/j.cdc.2018.06.002](https://doi.org/10.1016/j.cdc.2018.06.002)

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

# Microwave Synthesis, Biological Screening and Computational Studies of Pyrimidine Based Novel Coumarin Scaffolds

Soniya D. Naik<sup>a</sup>, K. M. Hosamani<sup>a\*</sup> and Shyam Kumar Vootla<sup>b</sup>

<sup>a</sup> Department of studies in Chemistry, Karnatak University, Dharwad-580003, Karnataka, India.

Corresponding Author E-mail: [dr\\_hosamani@yahoo.com](mailto:dr_hosamani@yahoo.com)

<sup>b</sup> Department of studies in Biotechnology and Microbiology, Karnatak University, Dharwad-580003, Karnataka, India.

<sup>a\*</sup> Corresponding author address:

Dr. Kallappa M. Hosamani.

Department of Studies in Chemistry,  
Karnatak University, Pavate Nagar,  
Dharwad - 580003, Karnataka State, INDIA.

E-mail: [dr\\_hosamani@yahoo.com](mailto:dr_hosamani@yahoo.com)

Tel.: +91-836-2215286; fax: +91-836-2771275 & +91-836-2747884.

## ABSTRACT

A series of new coumarin linked with pyrimidine derivatives have been synthesized *via* microwave irradiation. Structures of the synthesized compounds were characterized by IR, <sup>1</sup>H NMR, <sup>13</sup>C NMR, GC-MS and CHN analysis techniques. All newly synthesized compounds screened for their *in-vitro* anti-microbial and anti-cancer activities (Hela and A549 Cell lines). Further DNA cleavage studied and reports revealed that most of the synthesized compounds inhibit the growth of the pathogenic organism by genome cleavage as no traces of DNA were found. The present investigation points out that the synthesized coumarin-pyrimidine analogs are promising in targeted drug delivery systems, can be used for cancer therapy. Docking results also supported the studies. A good pharmacokinetic profile is suggested by theoretical calculation of ADME properties. Insights into enzyme inhibitor interactions provided by docking stimulations and permitted us to rationalize the observed SARs.

Download English Version:

<https://daneshyari.com/en/article/7561674>

Download Persian Version:

<https://daneshyari.com/article/7561674>

[Daneshyari.com](https://daneshyari.com)