

Proceedings of  
**2<sup>nd</sup> International Conference on  
AI - Driven Research and Innovations in  
Pharmaceutical Analysis:  
Global Perspectives and Future Trends**



*Organized by*

**Department of Pharmaceutical Analysis  
K.G.R.L College of Pharmacy  
Bhimavaram**

**in Association with  
Indian Pharmaceutical Association (IPA) Education Division  
IPA State Branch & IPA Local Branch (Bhimavaram)**

ISBN:978-93-5717-708-5

# **PROCEEDINGS of**

## **2<sup>nd</sup> International Conference on AI - Driven Research and Innovations in Pharmaceutical Analysis: Global Perspectives and Future Trends**

**28<sup>th</sup> February 2026**

© No part of the book or parts thereof may be reproduced, stored in a retrieval system or transmitted in any language or by any means, electronic, mechanical, photocopying, recording or otherwise without the prior written permission of the publishers.

**Editors**

Dr. Kavala Nageswara Rao

Dr. D. Raghava

Mr. G. Edward Raju

**Associate Editors**

Bh. Sriswetha

Md. Kathiza Begum

**Co-Associate Editors**

N.B.V.S Sumanasri

P. Naga Sravani

D. Mohana Rupa

Printed at: Renu Graphics

D.No: TF6, Anjanadri Towers

Vijayawada – 521108

6309385400

ISBN:978-93-5717-708-5

**Published by Conference Team**

Department of Pharmaceutical Analysis

K.G.R.L College of Pharmacy, Bhimavaram

The author(s) are responsible for their contributed research papers / articles regarding any existing copyright or other intellectual property rights issues if any person in any manner whatsoever. The publishers / Editors of the book are not responsible for errors in the contents or any consequences arising from the use of information contained in it. The quality of the language of papers is under the authors responsibility.

# Machine Learning Approach In Solubility Enhancement Of Dextromethorphan Syrup Using Molecular Descriptor

Dr.S.Uma Devi<sup>\*1</sup>, Jayasuriya G<sup>2</sup>

<sup>1</sup>Professor, School of Pharmaceutical Sciences, VELS Institute of Science Technology and Advanced Studies, Chennai -600 117

<sup>2</sup>PG Scholar, School of Pharmaceutical Sciences, VELS Institute of Science Technology and Advanced Studies, Chennai - 600 117

**Corresponding author E-mail:** [umdevi.sps@vistas.ac.in](mailto:umdevi.sps@vistas.ac.in)

## ABSTRACT

Dextromethorphan is a commonly prescribed antitussive agent; however, its therapeutic effectiveness can be limited by physicochemical constraints such as moderate aqueous solubility and inconsistent dissolution behaviour. Enhancing its solubility is therefore essential to improve bioavailability and formulation performance. The present study focuses on improving the solubility profile of dextromethorphan using a molecular descriptor based computational approach integrated with Machine Learning (ML) tools. A comprehensive set of molecular descriptors—including topological indices, hydrogen bond donor and acceptor counts, logP, polar surface area, molecular flexibility, and relevant electronic parameters were generated to characterize the molecule. These descriptors served as input variables for building predictive ML models. An Artificial Neural Network (ANN) model was developed to establish quantitative relationships between molecular features and solubility outcomes. The optimized ANN model demonstrated high predictive performance and successfully identified critical structural attributes influencing solubility enhancement. This ML-guided strategy minimized the need for extensive experimental screening and facilitated rational, targeted formulation development aimed at improving aqueous solubility and dissolution rate. Overall, the study underscores the potential of data-driven molecular modelling and artificial intelligence tools in modern pharmaceutical formulation design and offers a scalable approach for addressing solubility challenges of poorly water-soluble drugs.

Keywords - Dextromethorphan, Solubility Enhancement, Molecular Descriptors, Artificial Neural Network, Machine Learning.

