



KALEIDOSCOPE

Webinar on

“Quantitative Structure Activity Relationship (QSAR) & Artificial Intelligence”

- ❖ **Academic Year** : 2023– 2024
- ❖ **Program Title** : “Quantitative Structure Activity Relationship (QSAR) & Artificial Intelligence”
- ❖ **Organized By** : PG Pharmaceutical Chemistry & SAVANT Club
- ❖ **Mode** : Online Through GOOGLE MEET
<https://meet.google.com/nxp-ipuk-etd>
- ❖ **Date & Time** : Saturday, 13th April 2024, 11:00 AM onwards
- ❖ **Target Audience** : M. Pharm students and other institute’s participants
- ❖ **Total Participations** : 30+
- ❖ **Event Coordinator** : Dr. Gaurav Gopal Naik
- ❖ **Program Advisor** : Dr. Vijay A. Jagtap

PROGRAM INTRODUCTION:

Quantitative structure-activity relationship (QSAR) is a computational modeling method for revealing relationships between structural properties of chemical compounds and biological activities. Artificial Intelligence (AI) is an evolving technology that tries to simulate human intelligence using machines. To know the latest updates of Quantitative structure-activity relationship (QSAR) and Artificial Intelligence, PG Pharmaceutical Chemistry department & SAVANT Club of Yashwantrao Bhonsale College of Pharmacy, Sawantwadi has organized a Webinar on “**Quantitative Structure Activity Relationship (QSAR) & Artificial Intelligence**” by an expert resource person **Mr. Ravi Singh, Data Scientist at Syensqo**, on Saturday, 13th April 2024, 11:00 AM onwards for Institute students and other participants.

PROGRAM OBJECTIVES:

- 1. To be aware of Quantitative Structure Activity Relationship (QSAR) & Artificial Intelligence**
- 2. To know the future strategies to conduct QSAR**

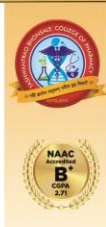
ABOUT THE PROGRAM:

Like all other events, to make this event a blessed one, a virtual lamp lightning ceremony was conducted. The welcome address was given by Hon’ble Dr. Rohan Barse. Later the program was put forward to Mr. Purushottam Kaloji who gave a brief introduction of Guest Speaker and requested her to start the session. In this webinar, Mr. Ravi Singh discussed about usage of Artificial Intelligence in drug discovery. Mr. Singh also explained about different algorithms and principle of QSAR. Applications of QSAR employing BCA1 inhibitors data set were also demonstrated. About 30+ participants in hybrid mode along with the faculty members participated in this webinar.

PROGRAM PARTICIPANTS & AUDIENCE:

Sr. No.	Participants Category	No. of Participants
1.	Student Present Online	25
2.	Faculty Members	5
Total		30

EVENT FLYER



PG Department of Pharmaceutical Chemistry & SAVANT Club of

YASHWANTRAO BHONSALE COLLEGE OF PHARMACY

Sawantwadi, Sindhudurg, Maharashtra

Organizes

Expert Webinar on

“Quantitative Structure Activity Relationship (QSAR) & Artificial Intelligence”



Mr. Ravi Singh,
Data Scientist

» 5+ years of experience in
Artificial Intelligence & Drug Discovery



Saturday, 13th April 2024, 11:00 AM onwards



Dr. Gaurav G. Naik
PG HOD Pharmaceutical Chemistry
SAVANT Club Coordinator



Dr. Vijay A. Jagtap
Convener & Principal



**BHONSALE
KNOWLEDGE
CITY**

Charhe, Vazarwadi,
Sawantwadi, Dist.Sindhudurg, 416 510
Phone : 02363-273535/273456

/sybespharmacy

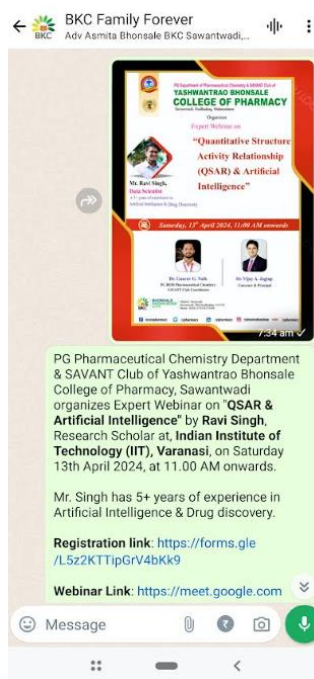
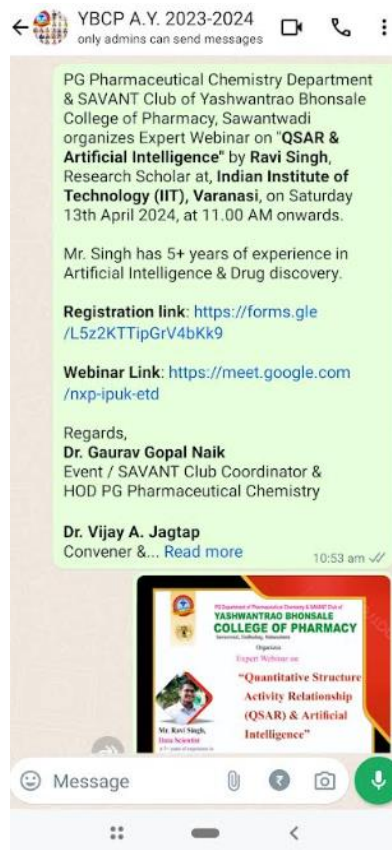
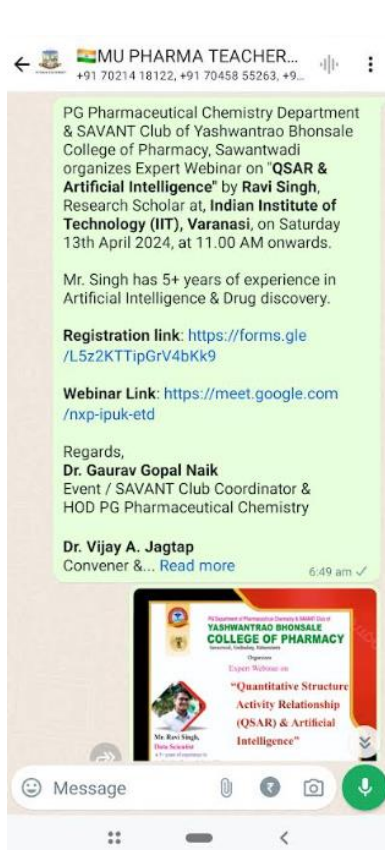
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FLYER-CUM-MESSAGE FOR CIRCULATION



GLIMPSES OF EVENT

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ARC YBCP (You, presenting) Stop presenting

Mr. Ravi Singh, Data Scientist
5+ years of experience in Artificial Intelligence & Drug Discovery

Saturday, 13th April 2024, 11:00 AM onwards

Dr. Gaaran G. Nalk, PG DBM Pharmaceutical Chemistry, SASTY CMA Coordinator
Dr. Vijay A. Jagtap, Professor & Principal

11:07 AM | nxp-ipuk-etd

https://meet.google.com/nxp-ipuk-etd?pli=1&authuser=2

Ravi Singh, IIT BHU Varanasi (Presenting)

Machine learning classification algorithms:

1. Naive Bayesian
2. Support Vector Machine
3. kNN
4. Random Forest
5. XGBoost

Performance Metrics:

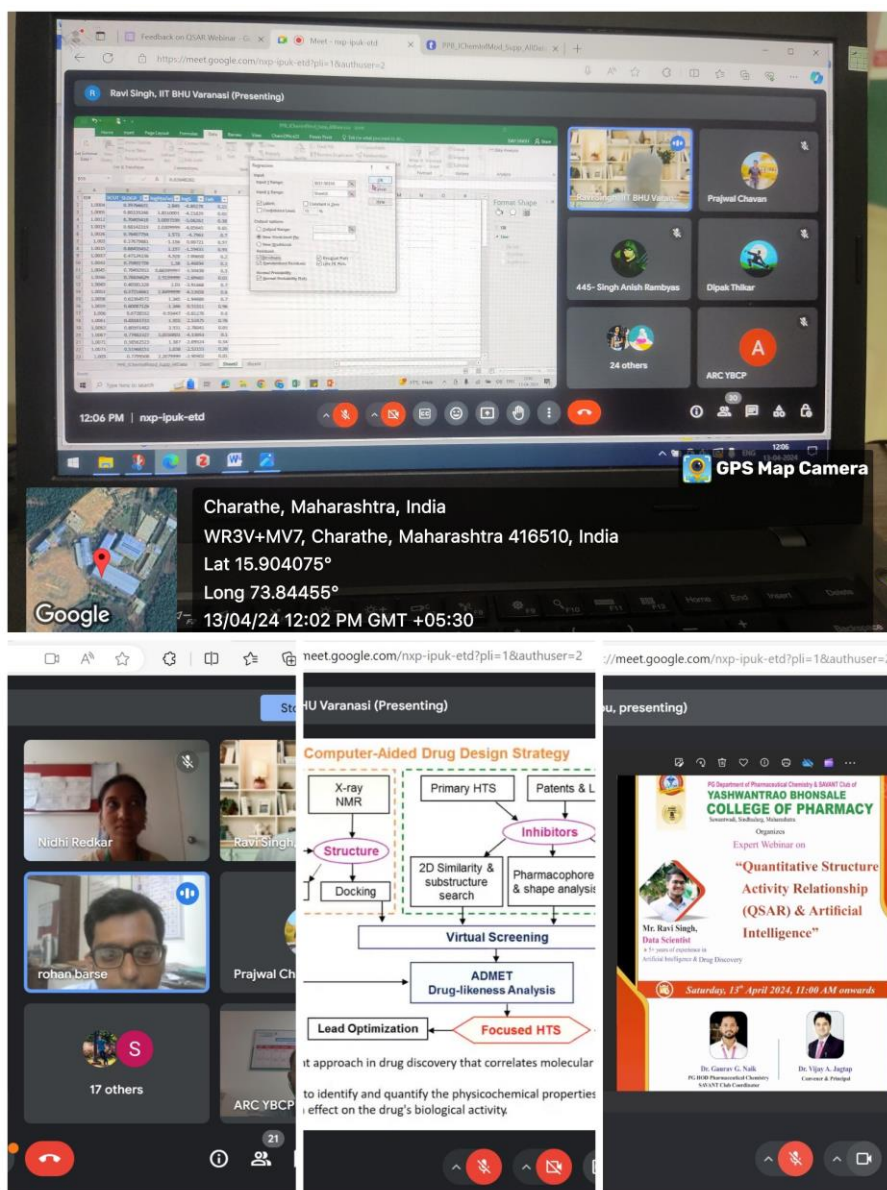
		Predicted Class		
		Positive	Negative	
Actual Class	Positive	True Positive (TP)	False Negative (FN) Type II Error	Sensitivity $\frac{TP}{TP + FN}$
	Negative	False Positive (FP) Type I Error	True Negative (TN)	Specificity $\frac{TN}{TN + FP}$
		Precision $\frac{TP}{TP + FP}$	Negative Predictive Value $\frac{TN}{TN + FN}$	Accuracy $\frac{TP + TN}{TP + TN + FP + FN}$

Recall

$$F1 \text{ Score} = \frac{2 \cdot \text{Precision} \cdot \text{Recall}}{\text{Precision} + \text{Recall}}$$

33

11:57 AM | nxp-ipuk-etd



Felicitation and Welcome of speaker Mr. Ravi Singh was done by Hon'ble Dr. Rohan Barse sir, Anchoring by M.Pharm student Ms. Nidhi Redkar. Introduction of guest by M.Pharm student Mr. Purushottam Kaloji & Vote of thanks given by M.Pharm student Mr. Prajwal Chawan.

Report Prepared & Approved By:

Dr. Gaurav Gopal Naik
Event & SAVANT Club Coordinator

Dr. Vijay A. Jagtap
Convener & Principal