SWAYAM Plus+

IITM PRAVARTAK CATALYSING INNOVATION

Course Outline

AI in Chemistry

Brief about the course

No.	Module Name	Topics Covered	Hands-on activity	Dataset used
1	Introduction to AI and its role in Chemistry	- Basics of AI and ML - AI Applications in physical, organic, analytical and materials chemistry - Tools and platforms (Python, RDKit, scikit-learn, TensorFlow, Chemprop)	Install Anaconda, set up Jupyter Notebook	N/A (Introductory Module)
2	Molecular Descriptors and Fingerprints	- SMILES notation, InChI, and molecular representations - Feature extraction using RDKit - Morgan fingerprints, MACCS keys	Generate fingerprints and visualize molecules	ZINC Database, PubChem
3	Supervised Learning in Chemistry	- Regression and classification models - QSAR/QSPR models - Cross-validation and model evaluation	Predict solubility or boiling points	ESOL dataset, AqSolDB
4	Deep Learning for Molecular Properties	- Neural networks in chemistry - Molecular graph neural networks (GNNs) - Use of Chemprop and DeepChem	Build a GNN to predict molecular bioactivity	MoleculeNet, especially Tox21 or BACE datasets
5	Reaction Prediction and Retrosynthesis	- Sequence-to-sequence models for chemical reactions - Transformer models (e.g., RXN for Chemistry)	Reaction outcome prediction	USPTO Reaction Dataset, Pistachio (free subset)
6	Materials Discovery with AI	- High-throughput screening - Predicting material properties	Predict properties of organic semiconductors or polymers	Materials Project, Open Quantum Materials Database (OQMD)
7	AI in Drug Discovery	- Virtual screening - ADMET prediction	Predict toxicity or drug-likeness	ChEMBL, DrugBank

8	Ethical AI and Future Trends	- Bias in chemical datasets - Interpretability and explainability - Future of AI in chemistry	Critical analysis of a research paper	N/A
Capstone Project		- Choose a problem (e.g., predict bioactivity, synthesize molecules, optimize materials) - Use a real dataset and deploy an AI model. - Final Preparation		

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