NDnano Summer Undergraduate Research
2026 Project Summary

1. Student name & home university: Yashkumar Shailesh Dodiya, Indian Institute of Technology Indore, India

2. ND faculty name & department: Prof. Jennifer Schaefer & Prof. Nosang Myung, Department of Chemical and Biomolecular Engineering

3. Summer project title: Electrochemical Sensing of dissolved species in water

4. Briefly describe new skills you acquired during your summer research:

Developed Python-based data processing pipelines and an interactive Streamlit application for sensor calibration analysis. Gained experience in electrochemical sensor calibration, feature engineering, machine learning model development, automated data visualization, and evaluation techniques that prevent data leakage. Improved scientific programming, data analysis, and research communication skills.

5. Briefly share a practical application/end use of your research:

This work enables rapid and reproducible calibration of solid-contact ion-selective electrodes used for water quality monitoring. The automated workflow significantly reduces manual analysis time while improving consistency. The generated datasets also support machine learning models capable of predicting ion concentration, paving the way for automated and real-time chemical sensing systems.

6. 50- to 75-word abstract of your project:

This project automated the processing and analysis of calibration data for solid-contact ion-selective electrodes using a Python and Streamlit application. The workflow automatically detects concentration transitions, extracts stable sensor responses, generates calibration curves, and tracks sensor performance over time. The processed data were used to train machine learning models for ion concentration prediction, with the Extra Trees model achieving the highest prediction accuracy on unseen electrodes and experimental runs.

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One-page project summary that describes problem, project goal, and your research activities / results:

Solid-contact ion-selective electrodes (SC-ISEs) are widely used for measuring ion concentrations in applications such as water quality monitoring and environmental analysis. Before they can be used reliably, these sensors require calibration to establish the relationship between electrode potential and ion concentration. Traditionally, calibration data are processed manually by identifying concentration transitions, extracting stable sensor responses, and generating calibration curves. This workflow is repetitive, time-consuming, and prone to user-to-user variability, particularly when analyzing data from multiple electrodes.

The objective of this project was to automate the calibration workflow and develop a user-friendly tool that performs data processing, calibration analysis, and long-term sensor evaluation. Using Python and Streamlit, I developed an application consisting of two automated analysis pipelines. The first pipeline performs date-wise calibration analysis by cleaning raw potentiometric data, automatically detecting concentration transition points, allowing user verification of detected windows, extracting stable sensor responses, and generating calibration curves with parameters such as slope, intercept, coefficient of determination (R^2), and limit of detection. The second pipeline reorganizes multiple calibration experiments into sensor-wise histories, enabling the visualization and analysis of sensor stability, reproducibility, and drift over time.

The automated workflow was evaluated using calcium ion calibration experiments conducted between December 2025 and June 2026. The application successfully processed calibration data from **44 electrodes** across a concentration range of **10^{-8} M to 10^{-1} M**, reducing analysis time from several hours of manual processing to only a few minutes while producing consistent and reproducible results.

The processed calibration data were also used to develop machine learning models for predicting ion concentration directly from electrode responses. Six regression algorithms were trained using sixteen statistical and signal-based features extracted from each concentration window. To ensure realistic evaluation, one entire electrode and one experimental run were excluded during testing. Among the evaluated models, the **Extra Trees Regressor** achieved the best performance, obtaining an **R^2 score of 0.938** for unseen electrodes and **0.875** for unseen experimental runs.

This work demonstrates that automation can significantly improve the efficiency and reproducibility of electrochemical sensor calibration while creating high-quality datasets for machine learning. Future work will focus on expanding the dataset, extending the framework to additional ion types, and integrating the workflow with automated sensing platforms for real-time concentration prediction.