Our project uses a small dataset trained machine learning model to predict reaction reactivity and interpret the reaction mechanism. As we all know, the machine learning model needs to screen a large number of existing databases from the literature report. However, those existing databases are only reported from successful reactions. For those, unsuccessful reactions are rarely used for building a machine learning model. Moreover, reactivity prediction took a large amount of time on manual experiments to check the feasibility among starting materials. Therefore, we developed a machine learning model that used successful and unsuccessful reactions to build a flow chart to guide a substrate reactivity and outcome. The N-sulfonylimines are chosen to be our model substrate since N-sulfonylimines is a good electrophile.

Furthermore, the oxadiazole scaffold plays a crucial role in organic synthesis and medicinal chemistry due to its broad-spectrum of bioactivity as an anticancer, antimicrobial, and antifungal pharmacological agent, especially for the 1,3,4-oxadiazole.

Among reported synthesis of 1,3,4-oxadiazole, one strategy is using four building blocks (secondary amine, aldehyde, carboxylic acid, and N-isocyanoimino triphenylphosporane) to get 1,3,4-oxadiazole in a one-pot manner utilizing multicomponent reaction approach as reported by Ramazani *et al* and Yudin *et al.* This traditional approaches of multicomponent synthesis of 1,3,4-oxadiazole scaffold have a few limitations such as multistep synthesis, limited substrate scope or use of harsh reaction conditions. Multicomponent reactions are highly sensitive to the reactivity of starting material. To create a better multicomponent reaction of 1,3,4-oxadiazole, we used the ML model to suggest a type of starting material. In this way, we reduce the wastage of valuable reagents, time, and efforts.

When we set up the optimization study, we first selected moderate nucleophile benzoic acid to prepare future experiment of a diverse range of benzoic acid derivatives., This benzoic acid reacts with the most reactive acyclic N-sulfonylimine, which is selected from density functional theory. The amount of time needed for acyclic *N*-sulfonylimine and benzoic acid to convert into the desired product at -10 Celsius degree was 10 mins. Such a short time curious us to understand the mechanism behind the reaction. We found out the first intermediate is formed by the nucleophilic attack from the +1 nitrogen in triphenylphosphine (PINC).

The nucleophilic attack forms the second intermediate from benzoic acid.

The third intermediate is a formation of a 5-member ring between the oxygen from benzoic acid and nitrogen from the PINC.

The fourth intermediate contained a five-member ring and four-member ring attached together.

This restrained ring structure eliminated the formation of the transition state between intermediate three and intermediate four.

To better understand the reactivity, we compared our result with cyclic N-sulfonylimine. And we found out the cyclic *N*-sulfonylimine is more reactive than acyclic *N*-sulfonylimine because the cyclic *N*-sulfonylimine also reacts with the *para*-position of carboxylic acid. To test the validity of the machine learning model's prediction, we generated other substrate reaction that was predicted from the flow chat. And the result has highly matched the prediction from the flow chat. Therefore, we conclude that *Para*-methyl substitution in benzoic acid increase reactivity, and para-hydroxy substitution decrease the reactivity.