Supporting Information: Evaluating the Performance of a Transformer-based Organic Reaction Prediction Model

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Incorrect and High Confidence Forward Predictions

Reaction Number	Literature Reaction	Predicted Reaction
11		
12		
15		
16		
18		
19		
25		Failure
27		Failure
40		
43		
50		
71		

Figure 1: Reactions for All Incorrect and High Confidence Forward Predictions

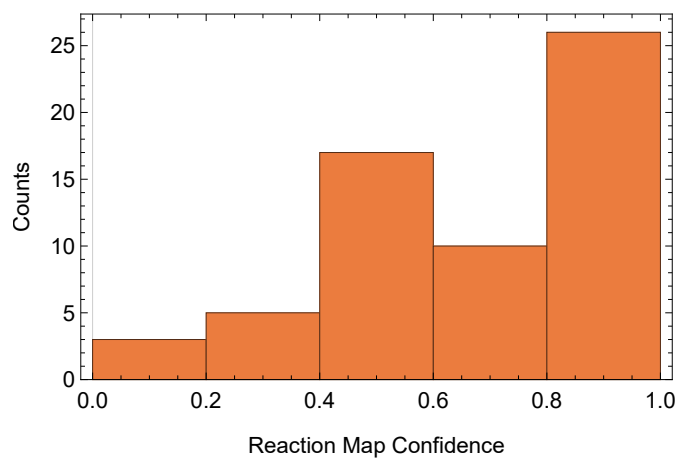# RXNMapper Map Confidence Distributions

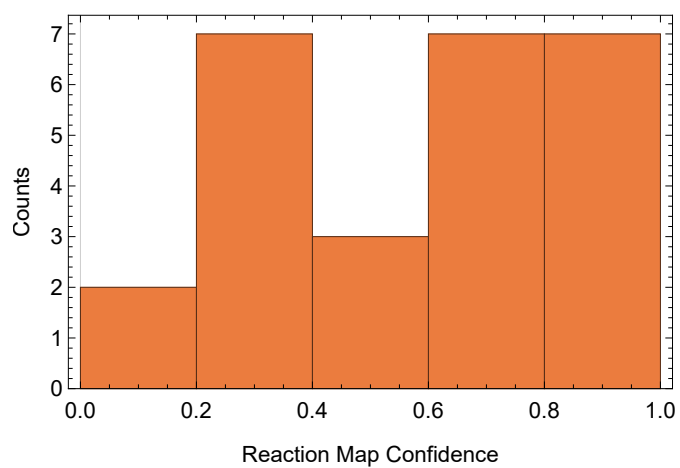Figure 2: RXNMapper Map Confidences for Top-1 Correct Predictions

Figure 3: RXNMapper Map Confidences for Top-1 Incorrect Predictions