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Data-Driven Retrosynthetic Predictions for Energetic Materials MICHAEL FORTUNATO, CONNOR COLEY, MIT, BRIAN BARNES, ARL, IGOR SCHWEIGERT, NRL, ARIANA BESTE, ARL, KLAVS JENSEN, MIT — We present recent work in computer-aided synthesis planning strategies of interest to synthetic chemists, and demonstrate the utility of a new neural network for predicting synthetic pathways to energetic material precursors. These data-driven machine learning techniques have shown great promise in the pharmaceutical industry, and are poised to have a dramatic impact on the research and development process for novel materials. This work expands on previously developed techniques by addressing the "rare template" problem. Although there is an abundance of computationally accessible reaction data, a significant data imbalance can make models less inclined to recommend energetically relevant reaction templates. A data augmentation strategy leveraging cheminformatics toolkits and high performance computing was used to train a deep neural network to restore fidelity to the rare, energetically relevant templates. The performance of this new neural network is compared to the previous one to highlight its enhanced predictive power for new synthetic routes for energetic materials. A web application created for transitioning this new model to synthetic chemists for everyday use will also be demonstrated.

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