

BEYOND THE MACHINE: AUTOMATING SPECTRA GENERATION AND ANALYSIS FROM MACHINE LEARNING RESULTS

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Almost 300 molecules have been detected in the interstellar medium, with an exponential explosion in recent years thanks to rapid innovation in technology and technique. However, detections alone only offer tantalizing hints to future chemistry; we generally have been unable to make reliable predictions of the chemical species that will be subsequently detected. Prior work in the McGuire group was able to use Machine Learning approaches to accurately reproduce the inventories of 87 known species in TMC-1. The model went on to make over 1500 predictions of potential targets. Not only is this more than can efficiently be pursued, but these predictions provided only column densities and did not account for other key factors of detectability such as how many spectral lines fall within the range of our astronomical observations and the intensities of those lines. My work takes the results of this machine learning model, and others like it, and further narrows the list of candidates for detection by applying detectability metrics. Through automation, this workflow leads to extended usability of ML inventory predictions.