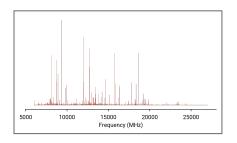
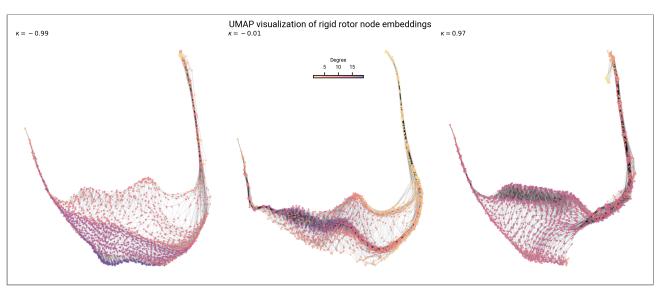
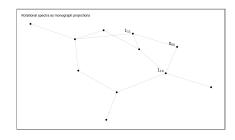
Applying machine learning to molecular spectra







Use graph representations of rotational spectra

Graph/node embeddings successfully capture spectroscopic intuition

