Anticipated Use Cases:

1. A user may discover new correlations between a molecules’ chemical properties and its effectiveness (or lack thereof) as a plasticizer. These correlations may be between individual properties or linear combinations of groups of properties decomposed to a lower dimensionality.
2. A user may discover new information on the relative importance of certain chemical properties within a single class of plasticizers (e.g. phthalates).
3. A user may search for new molecules that have been optimized for a user-defined property or set of properties (those that have been identified as having the highest correlation with good plasticizing behavior).
4. A user may assess the synthesizability of newly discovered molecules with high plasticizing likelihood.
5. A user may take data gathered on the highest likelihood candidate molecules and make iterative improvements to the model through an adaptive learning & design framework.