**Application of molecular data science to study phthalate plasticizers**

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Plasticizers are additives applied in most plastic products to enhance their performance. However, the most used plasticizer – phthalate – raise concerns regarding its negative environmental and health impacts. In addition, phthalate is a downstream product from petroleum industry and subjective to future supply chain insecurity. Although both industry and academia are both actively looking for non-toxic and renewable alternatives since 2000, phthalates remain dominant in the industry. Data science may hold the key to the dilemma, by extracting knowledge and insights from accumulated data and generating new chemical structures with minimal human intervention. Sponsored by Cargill, our team utilize data science method to design plasticizers that are non-toxic and renewable. SMILES strings are used to represent chemical structures, so that they are readable to machine learning models and used to construct latent space that enable the generate new plasticizer structures.