

## **References for the Poster *In silico generated reagents for detection of pesticides using mass spectrometry: An out-of-distribution task***

### ***Machine learning model for ionization efficiency prediction***

*Quantification for non-targeted LC/MS screening without standard substances.*

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*Bypassing the Identification: MS2Quant for Concentration Estimations of Chemicals Detected with Nontarget LC-HRMS from MS2 Data.*

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### ***Myopic common edge subgraph distance***

*Small molecule machine learning: All models are wrong, some may not even be useful.*

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### ***Out-of-distribution learning in chemistry***

*A systematic study of key elements underlying molecular property prediction.*

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## **Synthetic Accessibility Score**

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## **Review articles on generative models and inverse design**

*Inverse molecular design using machine learning: Generative models for matter engineering.*

Benjamin Sanchez-Lengeling, Alán Aspuru-Guzik, *Science* **2018**, *361*, 360-365.

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