References

Machine learning model for ionization efficiency prediction

Quantification for non-targeted LC/MS screening without standard substances.
Jaanus Liigand, Tingting Wang, Joshua Kellogg, Jørn Smedsgaard, Nadja Cech, Anneli Kruve, *Sci. Rep* **2020**, *10*, 5808. https://doi.org/10.1038/s41598-020-62573-z

Bypassing the Identification: MS2Quant for Concentration Estimations of Chemicals Detected with Nontarget LC-HRMS from MS2 Data.
Helen Sepman, Louise Malm, Pilleriin Peets, Matthew MacLeod, Jonathan Martin, Magnus Breitholtz, and Anneli Kruve, *Anal. Chem.* **2023**, *95* (33), 12329-12338. DOI: 10.1021/acs.analchem.3c01744

Methods for analysis of glyphosate

Glyphosate detection: methods, needs and challenges.
A. L. Valle, Fernanda C. C. Mello, Renata P. Alves-Balvedi, Luciano Rodrigues, Luiz R. Goulart, *Environ. Chem. Lett.* **2019**, *17,* 291–317. https://doi.org/10.1007/s10311-018-0789-5

Novel liquid chromatography/mass spectrometry-based approaches for the determination of glyphosate and related compounds: A review.
Priscilla Rocío-Bautista, David Moreno-González, Ana B. Martínez-Piernas, Juan F. García-Reyes, Antonio Molina-Díaz, *Trends in Environmental Analytical Chemistry,* **2022**, *Volume 36, e00186,* https://doi.org/10.1016/j.teac.2022.e00186

Synthetic Accessibility Score

Estimation of synthetic accessibility score of drug-like molecules based on molecular complexity and fragment contributions.
Peter Ertl, Ansgar Schuffenhauer, *J. Cheminform.* 2009, *1,* 1-8.
https://doi.org/10.1186/1758-2946-1-8

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.
DOI:10.1126/science.aat2663

Generative Models as an Emerging Paradigm in the Chemical Sciences.
Dylan M. Anstine, Olexandr Isayev, *J. Am. Chem. Soc.* **2023**, *145* (16), 8736-8750. DOI: 10.1021/jacs.2c13467