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FDR-controlled metabolite annotation for high-resolution imaging mass spectrometry

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Abstract

© 2017 Nature America, Inc., part of Springer Nature. All rights reserved. High-mass-resolution imaging mass spectrometry promises to localize hundreds of metabolites in tissues, cell cultures, and agar plates with cellular resolution, but it is hampered by the lack of bioinformatics tools for automated metabolite identification. We report pySM, a framework for false discovery rate (FDR)-controlled metabolite annotation at the level of the molecular sum formula, for high-mass-resolution imaging mass spectrometry (<https://github.com/alexandrovteam/pySM>). We introduce a metabolite-signal match score and a target-decoy FDR estimate for spatial metabolomics.

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