Auto-deconvolution and molecular networking of gas chromatography–mass spectrometry data

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Resumen

We engineered a machine learning approach, MSHub, to enable auto-deconvolution of gas chromatography–mass spectrometry (GC–MS) data. We then designed workflows to enable the community to store, process, share, annotate, compare and perform molecular networking of GC–MS data within the Global Natural Product Social (GNPS) Molecular Networking analysis platform. MSHub/GNPS performs auto-deconvolution of compound fragmentation patterns via unsupervised non-negative matrix factorization and quantifies the reproducibility of fragmentation patterns across samples.

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