

~6x10⁶ compounds

<u>Step</u>

750% - Siological Compounds (C,H,N,O,P,S) yes (C&H only) no

~3x106 compounds

Precursor lon MIMW Matching removed (±10ppm)

~272 compounds

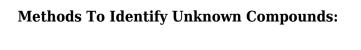
3. ~90% Computational MIMW removed Fragment Matching (±10ppm)

~27 compounds

Additional V LogP, retention time, isotopic
Filter Options V abundance, ionization
Possible V mode (+, -, +/-)

Methods To Identify Unknown Compounds

Damia Barcelo, Yolanda Pico



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