

PubChem Data Base

~6x10⁶ compounds

Step

1. ~50% removed  Biological Compounds
(C,H,N,O,P,S) yes
(C&H only) no
~3x10⁶ compounds
2. ~99.99% removed  Precursor Ion
MIMW Matching
(±10ppm)
~272 compounds
3. ~90% removed  Experimental vs
Computational MIMW
Fragment Matching (±10ppm)

~27 compounds
4. Additional Filter Options Possible  LogP, retention time, isotopic
abundance, ionization
mode (+, -, +/-)

Methods To Identify Unknown Compounds

Damia Barcelo, Yolanda Pico



Methods To Identify Unknown Compounds:

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