





PubChem Data Base

$\sim 6 \times 10^6$ compounds

Step

1.  **Biological Compounds**
(C,H,N,O,P,S) yes
(C&H only) no
 $\sim 50\%$ removed
 $\sim 3 \times 10^6$ compounds
2.  **Precursor Ion
MIMW Matching**
(± 10 ppm)
 $\sim 99.99\%$ removed
 ~ 272 compounds
3.  **Experimental vs
Computational MIMW
Fragment Matching** (± 10 ppm)
 $\sim 90\%$ removed

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

Methods To Identify Unknown Compounds

Annelies Wilder-Smith



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