





# 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**  
( $\pm 10$ ppm)  
 $\sim 99.99\%$  removed  
 $\sim 272$  compounds
3.  **Experimental vs  
Computational MIMW  
Fragment Matching** ( $\pm 10$ ppm)  
 $\sim 90\%$  removed  

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

# Methods To Identify Unknown Compounds

**D Siedentop**



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