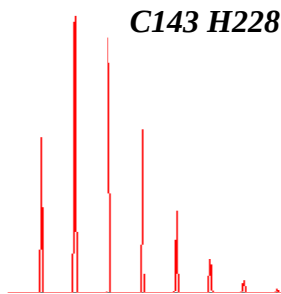


C143 H228 N39 O43 S1



$$\frac{\sum (I_{\text{theoretical}} - I_{\text{observed}})^2}{\sum I_{\text{theoretical}}^2} < I_{\text{threshold}} ??$$

