



 $openff_unconstrained - 2 \textit{d}p \textbf{0} nff_unconstraine \textbf{d}p \textbf{2} \textbf{2} \textit{f} \textbf{1} \underline{\textbf{1}} \underline{\textbf{1}} \underline{\textbf{1}} unconstrained - 2.2.1 - s data$