

$$U_{\text{ML/MM}}(X_P, X_L)$$

=

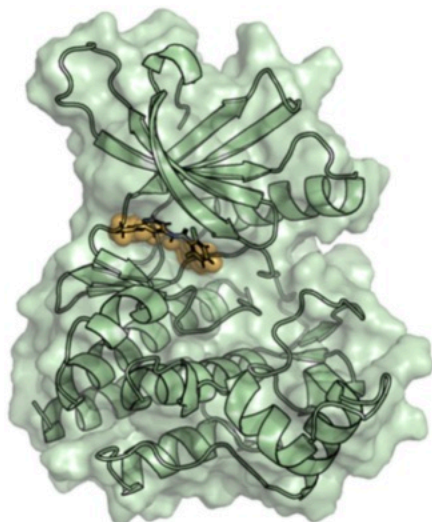
$$U_{\text{MM}}(X_P, X_L)$$

-

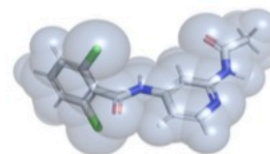
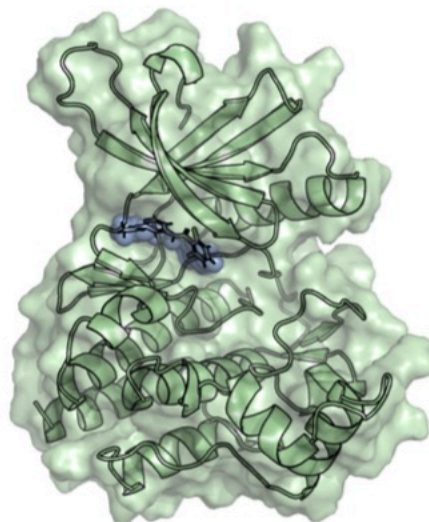
$$U_{\text{MM}}^{\text{vacuum}}(X_L)$$

+

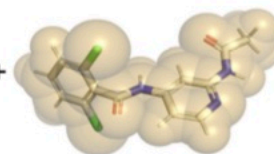
$$U_{\text{ML}}^{\text{vacuum}}(X_L)$$



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MM

openff-1.0.0

ML

ANI-2x

