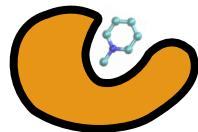
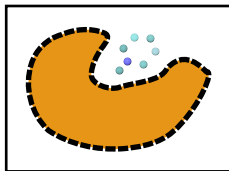


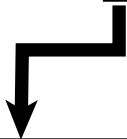
Initial Structure

All-atom MD

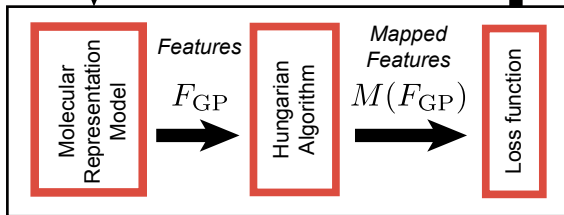
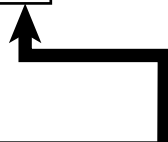
Final Structure



Positions and attributes  
 $X_{GP}, A_{GP}$



Forces  
 $-\nabla L(M(F_{GP}), F_T)$



MLForce