Drug development is an expensive and time consuming endeavor reflected in the rising cost of novel pharmaceuticals. Computational screening of large molecule libraries can reduce cost associated with exploratory assays of novel drug targets. MTH1 is a novel cancer target involved in maintenance of reactive oxygen species produced in rapidly dividing cancer cells. By inhibiting the molecular function of this enzyme we can selectively target cancer cells while minimizing negative side effects to the patient. A machine-learning algorithm will be trained on molecule fragment screening results and developed to score libraries of small molecules for the inhibition of MTH1.

(*[1-4](#_ENREF_1" \o "Dimitri, 2017 #1)*)

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