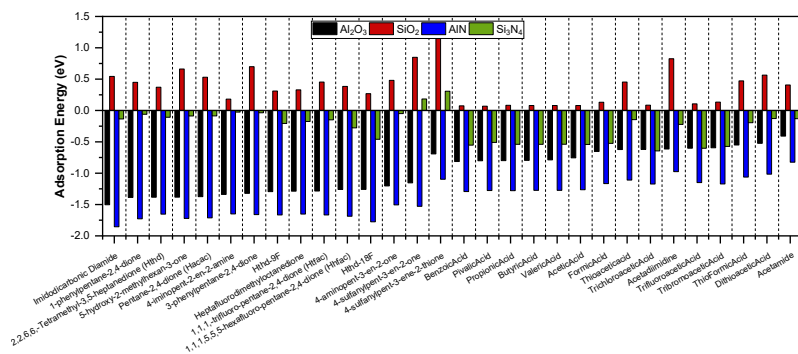a)

b)

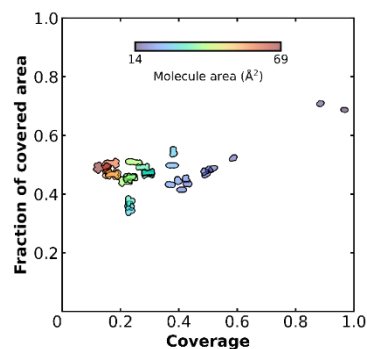*Figure 1: a) The adsorption energy of the candidate SMIs on small clusters. Adsorption strength follows the trend AlN > Al2O3 > Si3N4 > SiO2. b) The coverage and fraction of covered area of the SMI candidates using their 2D footprint, resulting from RSA simulations. Coverage is defined as the amount of consumed sites divided by the total amount of sites, and fraction of covered area is defined as the area covered by all SMIs divided by the total surface area. The markers for the molecules correspond to the footprints, and the marker size color scales with the footprint area. A good inhibitor has high coverage and fraction of covered area, so the best candidates are found in the top right.*
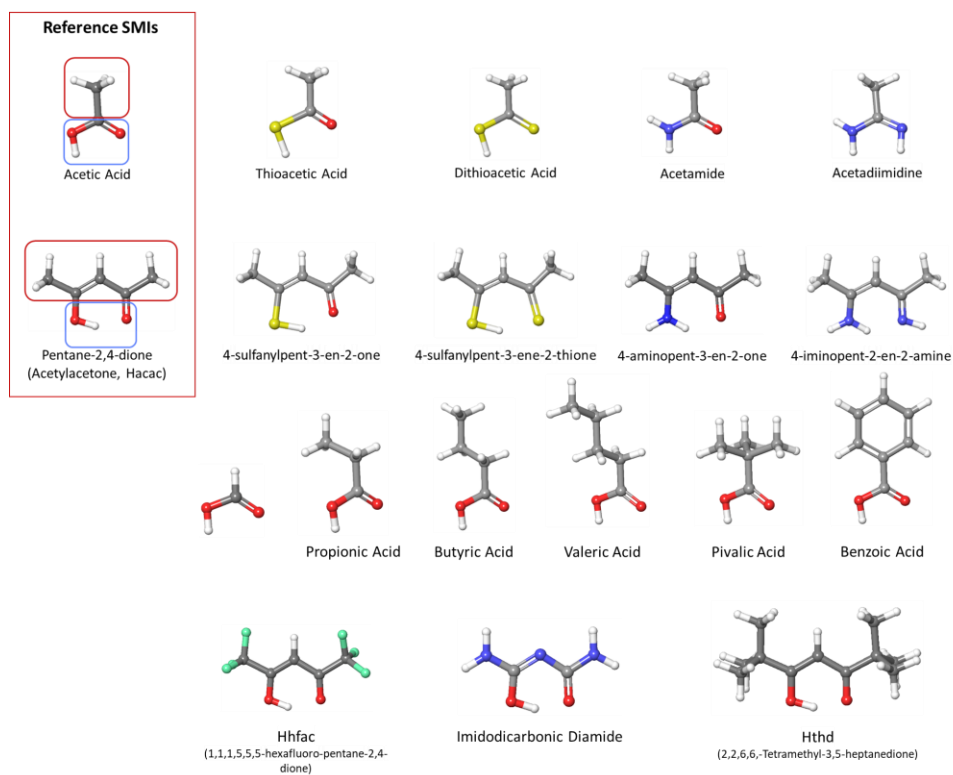

Figure 2: A selection of the SMI candidates. The candidates are chosen based on their reactive group and their inert group, using Hacac and HAc as starting points.