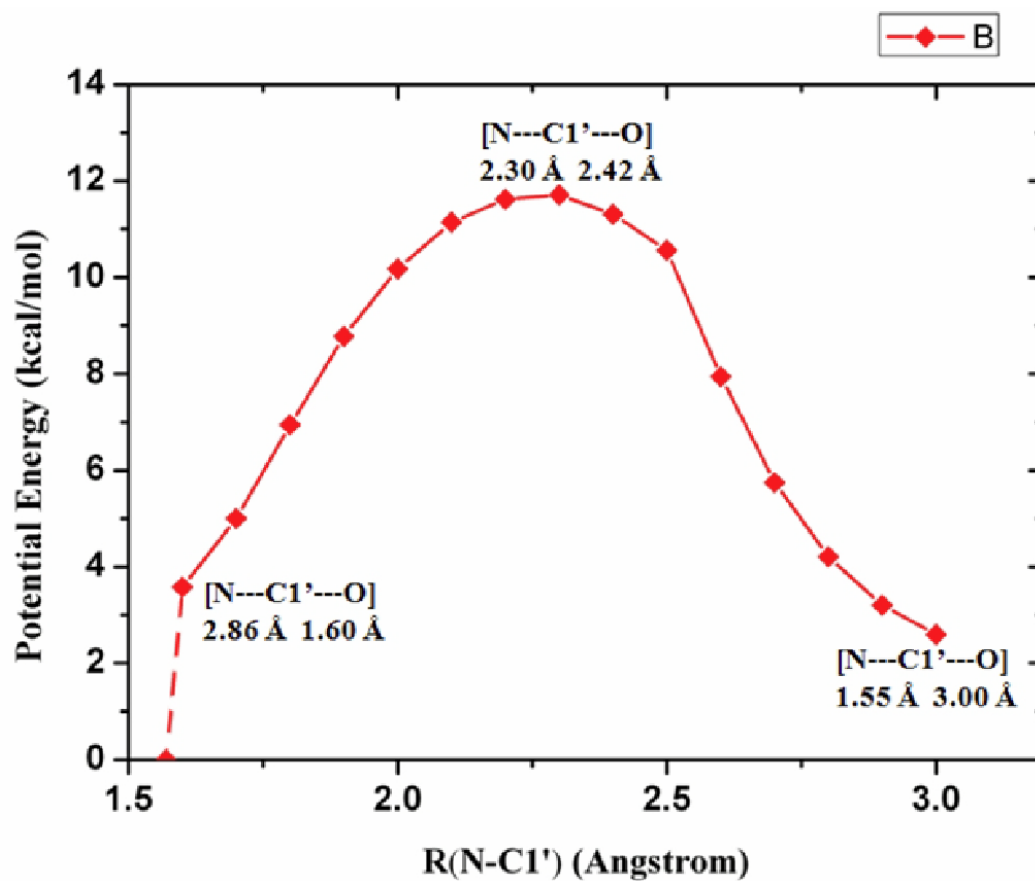


Supporting Information



Potential energy for the yHst2-ALY-NAD<sup>+</sup> system catalyzed nicotinamide cleavage reaction determined at the ONIOM (B3LYP/6-31G\*:AMBER) level. The bond lengths of N\_C1' and C1'\_O at different states are labeled in the Figure.