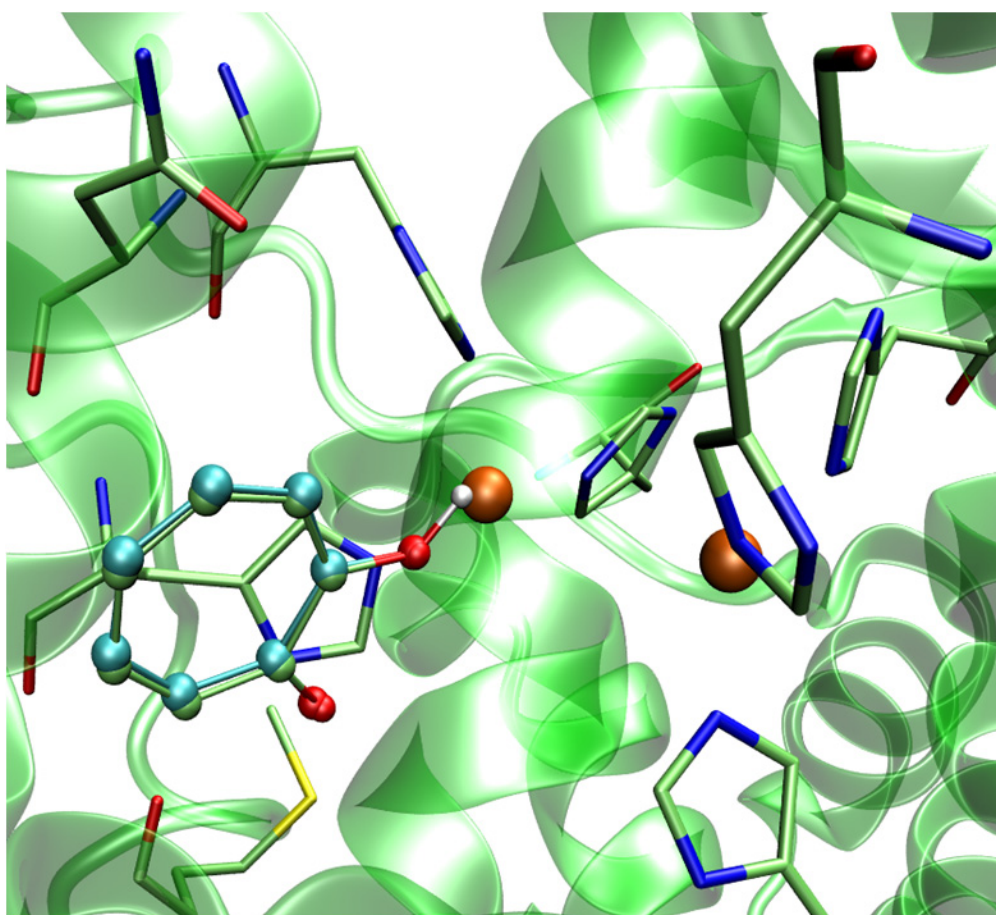


## Supporting Information

**Table S1.** Root mean square deviation (RMSD) obtained by MD simulations for all inhibitors. The standard deviations are in parenthesis.

<b>Inhibitor</b>	<b>RMSD (Å)</b>
Tropolone	1.02 (0.18)
KA	0.67 (0.27)
INH1	0.91 (0.23)
INH2	1.28 (0.13)
INH3	1.87 (0.36)
INH4	0.74 (0.37)

**Figure S1.** Re-docking result of crystal inhibitor obtained by MVD software.



**Figure S2.** Docking results of Kojic Acid and its analogous obtained by MVD software.

