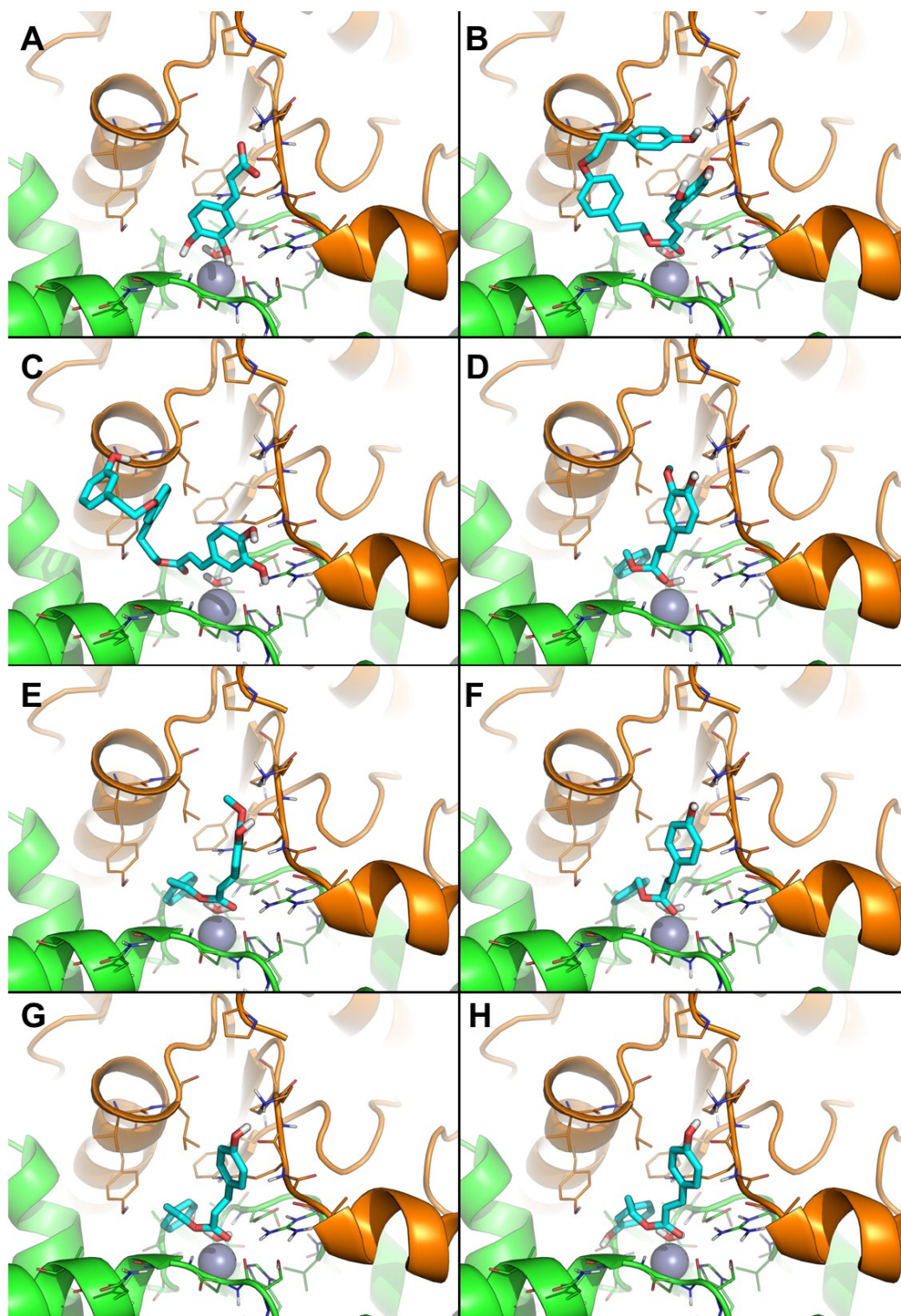
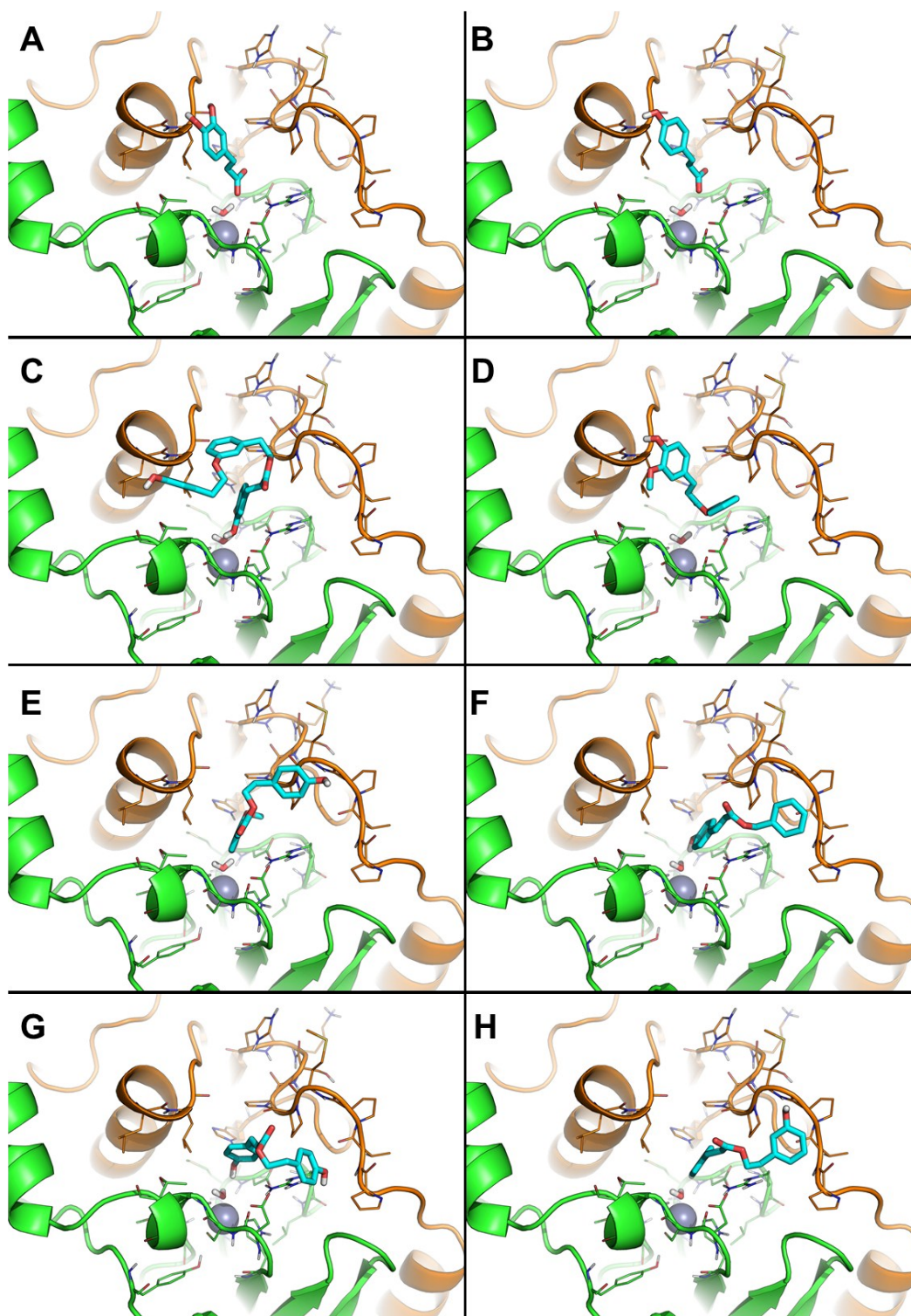


### Electronic Supplementary information

The predicted binding mode of inhibitors **1**, **4–7**, **9–11** towards the catalytic site of Rv3588  $\beta$ -CA, and inhibitors **1**, **3**, **5–7**, **9–11** towards the catalytic site of Rv1248  $\beta$ -CA is shown in Figure S1 and S2, respectively.



**Figure S1.** The predicted binding mode of **1** (panel A), **4** (panel B), **5** (panel C), **6** (panel D), **7** (panel E), **9** (panel F), **10** (panel G), and **11** (panel H) towards the catalytic active site of the Rv3588  $\beta$ -CA is shown as cyan sticks; the catalytic Zn(II) ion is shown as a grey sphere; the protein monomer A is colored green, the monomer B is colored orange. Residues within 5 Å from the Zn(II) ion and those contacted by the inhibitors are shown as lines. The water molecule coordinated to the Zn(II) ion is shown as sticks.



**Figure S2.** The predicted binding mode of **1** (panel A), **3** (panel B), **5** (panel C), **6** (panel D), **7** (panel E), **9** (panel F), **10** (panel G), and **11** (panel H) towards the catalytic active site of the Rv1248  $\beta$ -CA is shown as cyan sticks; the catalytic Zn(II) ion is shown as a grey sphere; the protein monomer A is colored green, the monomer B is colored orange. Residues within 5 Å from the Zn(II) ion and those contacted by the inhibitors are shown as lines. The water molecule coordinated to the Zn(II) ion is shown as sticks.