

## Supplemental Material

### STRUCTURAL ANALYSIS OF THE MECHANISM OF INHIBITION AND ALLOSTERIC ACTIVATION OF THE KINASE DOMAIN OF HER2

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Running Head: Crystal structure of HER2 kinase domain

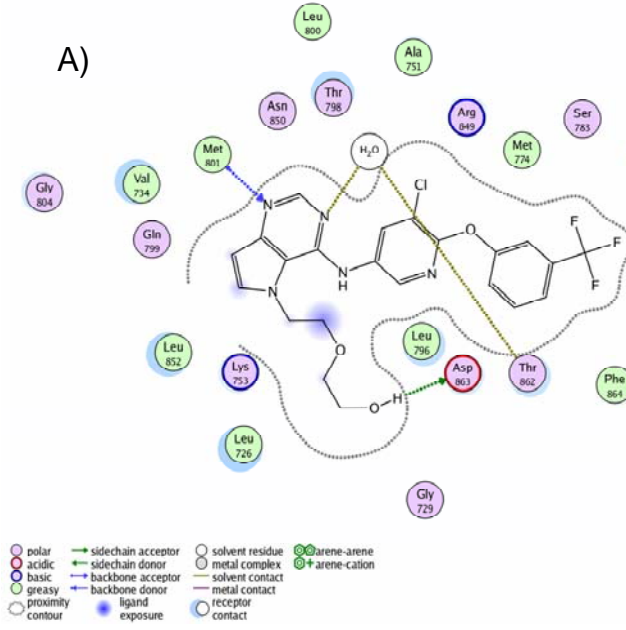
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**Figure S1. Inhibitor interactions between (A) HER2-KD/SYR127063 and (B) EGFR-KD/TAK-285.**

The compounds are shown in a 2D representation at the center of each panel. The legend for types of interactions is shown at the bottom of each panel. Complex water networks that span more than one water molecule or where water acts as both a donor and acceptor are not included. The figure was made with the computer program MOE (<http://www.chemcomp.com/software.htm>).

Figure S1

HER2-KD SYR127063



EGFR-KD TAK-285

