

## **Description of Additional Supplementary Files**

File Name: Supplementary Movie 1

Description: Molecular dynamics (MD) simulation of wild-type RET kinase domain (KD) in complex with vandetanib. Movie representing a 1  $\mu$ s MD simulation of the wild-type RET KD in complex with vandetanib is shown (see also Supplementary Figure 7f).

File Name: Supplementary Movie 2

Description: Molecular dynamics (MD) simulation of S904F mutant RET kinase domain (KD) in complex with vandetanib. Movie representing a 1  $\mu$ s MD simulation of the S904F mutant RET KD in complex with vandetanib is shown (see also Supplementary Figure 7f).