# Supporting Information

# Pyrazolylamine derivatives reveal the conformational switching between type-I and type-II binding modes of anaplastic lymphoma kinase (ALK)

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## Contents

**Figure S1.** SPR single-cycle kinetic analysis was used to evaluate the binding kinetics of (A) **5a**, (B) **4**, and (C) crizotinib with ALK. The insertion figure was the steady-state analysis.

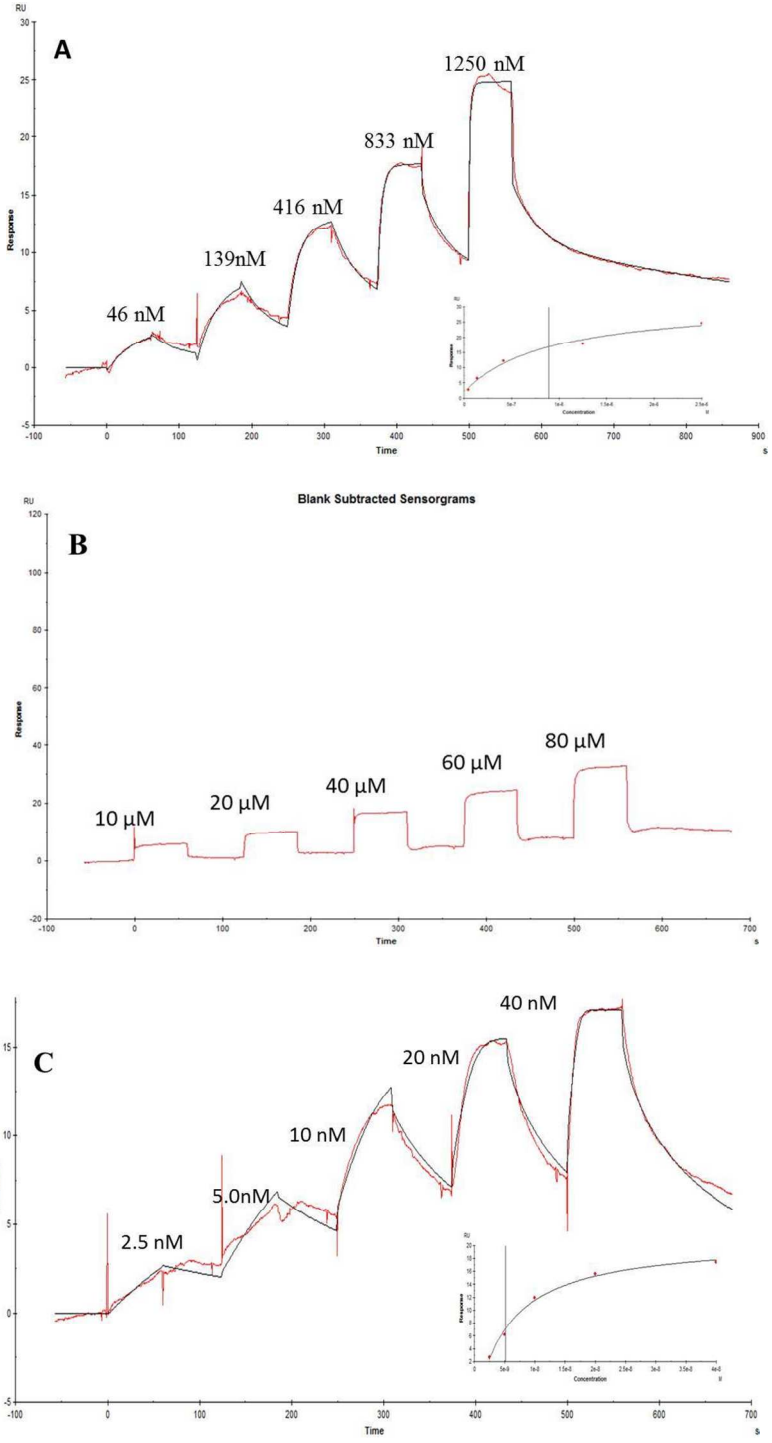
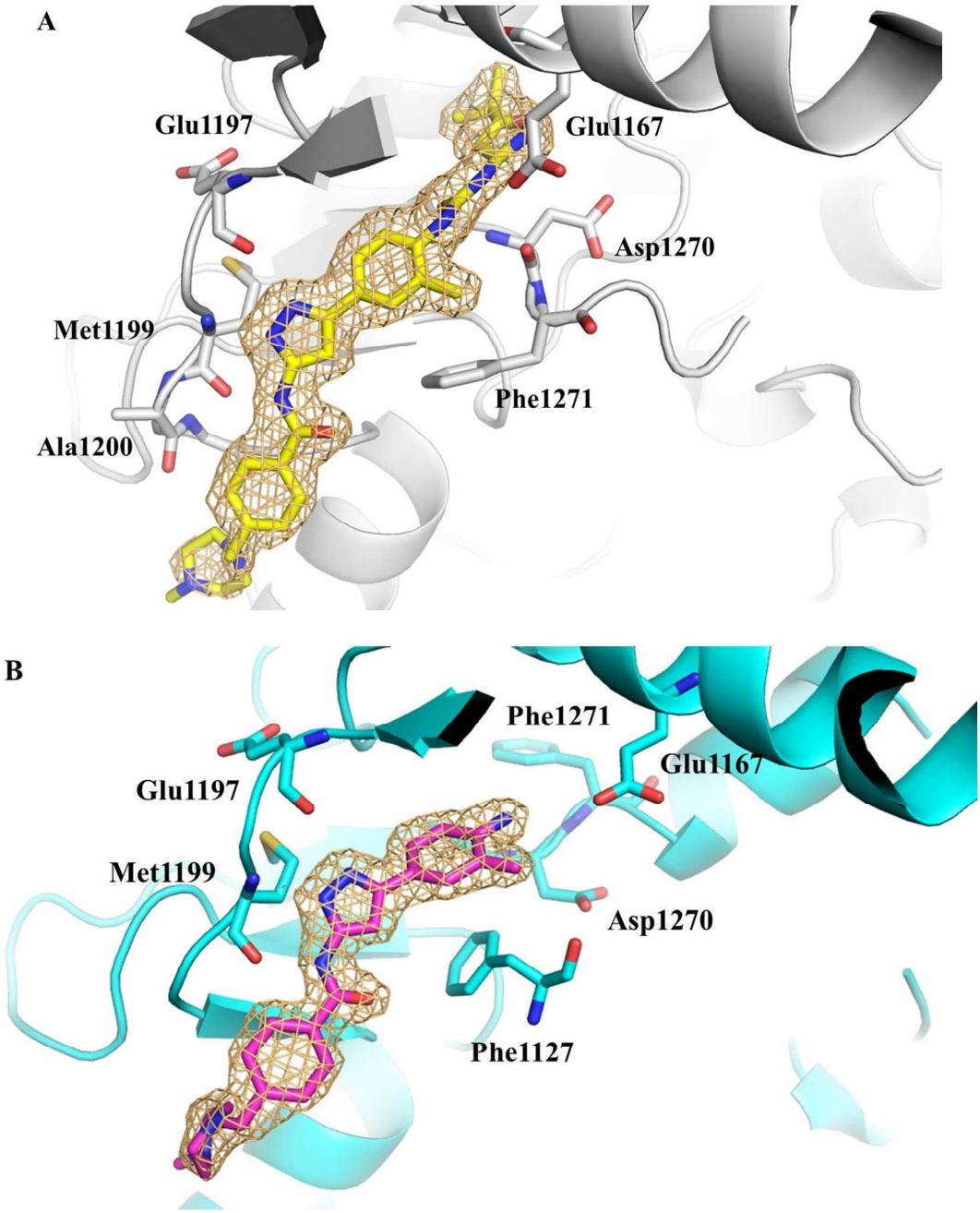


**Figure S2.** Compounds **5a, 4** and **5d** with density maps. (A) The 2fo-fc map of compound **5a** contoured at 0.8 σ (B) The 2fo-fc map of compound **4** contoured at 1.0 σ (C) The 2fo-fc map of compound **5d** contoured at 1.0 σ.



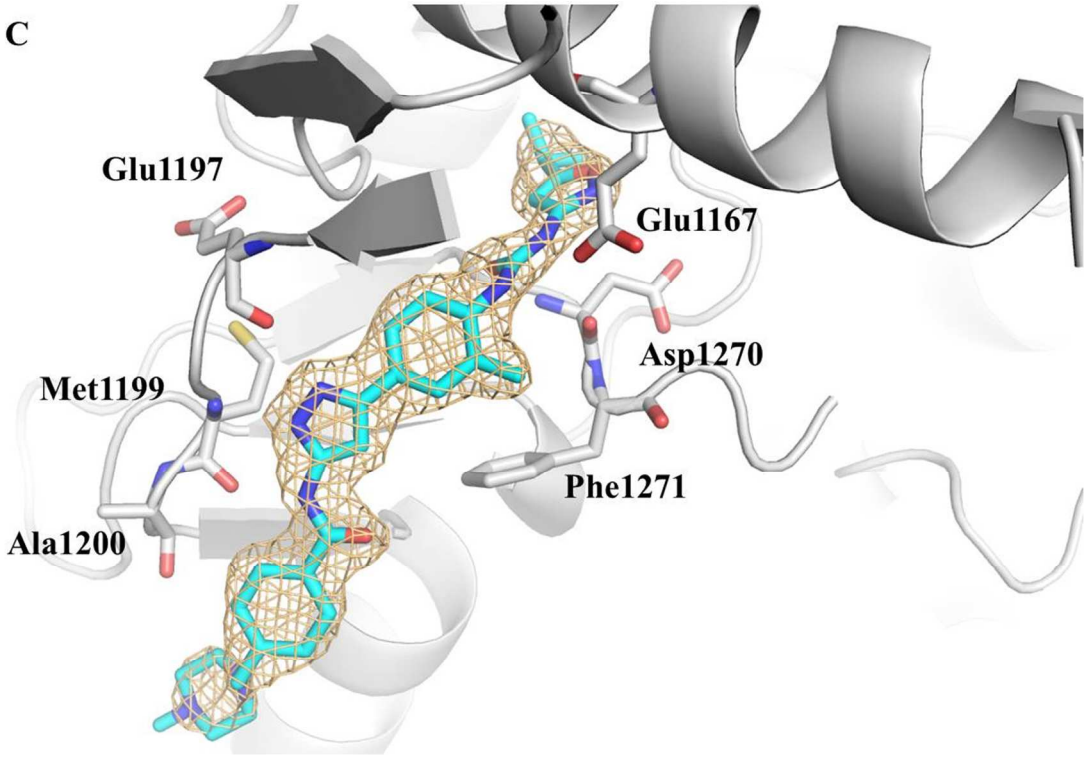

C
Glu1197
Glu1167
Asp1270
Met1199
Phe1271
Ala1200

**Figure S3.** (A) The structure of **5a** bound to ALK (B) The docking position of the designed ALK inhibitor in the binding site of ALK. Hydrogen bond and charge-charge interaction are shown with red and green dashed lines, respectively. Docking study was performed by GOLD Suite v5.2.