

Description of Additional Supplementary Files

File name: Supplementary Data 1

Description: List of quantified proteins from proteomics data

File name: Supplementary Data 2

Description: Numerical source of data in Figure panel 4E

File name: Supplementary Data 3

Description: Numerical source of data in Figure panel 4F

File name: Supplementary Data 4

Description: The initial and final atom coordinates before and after MD simulation of the imidazopyrazines.

File name: Supplementary Data 5

Description: Copies of spectra and chromatograms.

File name: Supplementary Video 1

Description: MD trajectory of KIRA6 scaffold

File name: Supplementary Video 2

Description: MD trajectory of acalabrutinib scaffold

File name: Supplementary Video 3

Description: MD trajectory of linsitinib scaffold