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Supporting Information

Structural Basis for the Inhibition of Cyclin G-Associated Kinase by Gefitinib

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Table S1. Data collection and refinement statistics.

	GAK_1	GAK_2
Data collection		
X-ray source	BL32XU, SPring-8	BL32XU, SPring-8
Wavelength (Å)	1.0	1.0
Space group	$P2_1\ 2_1\ 2_1$	$P2_1\ 2_1\ 2_1$
Cell dimensions		
a, *b*, *c* (Å)	76.4, 85.5, 149.0	70.3, 73.9, 95.3
Resolution (Å)	50.0–2.80 (2.87–2.80)[1]	47.7–2.50 (2.60–2.50)
R_{merge}	0.286 (0.923)	0.148 (0.547)
$I / \sigma(I)$	5.3 (1.46)	11.4 (4.3)
Completeness (%)	97.0 (98.6)	100.0 (100.0)
Redundancy	3.3 (3.0)	9.3 (9.9)
Refinement		
Resolution (Å)	45.3–2.8	44.9–2.5
No. reflections	23789	17740
R_{work} / R_{free}	0.233/0.288	0.230/0.282
No. atoms		
Protein	6898	3410
Ligand/SO_4	62/25	62/0
Water	9	60
B-factors		
Protein	32.4	46.8
Ligand/SO_4	39.0/48.0	44.7/-
Water	19.8	43.4
R.m.s. deviations		
Bond lengths (Å)	0.004	0.005
Bond angles (°)	1.044	1.094
Ramachandran plot		
Favored (%)	97.1	97.4
Allowed (%)	2.9	2.6
Outliers (%)	0.0	0.0
PDB ID	5Y7Z	5Y80

[1]Highest resolution shell is shown in parentheses.

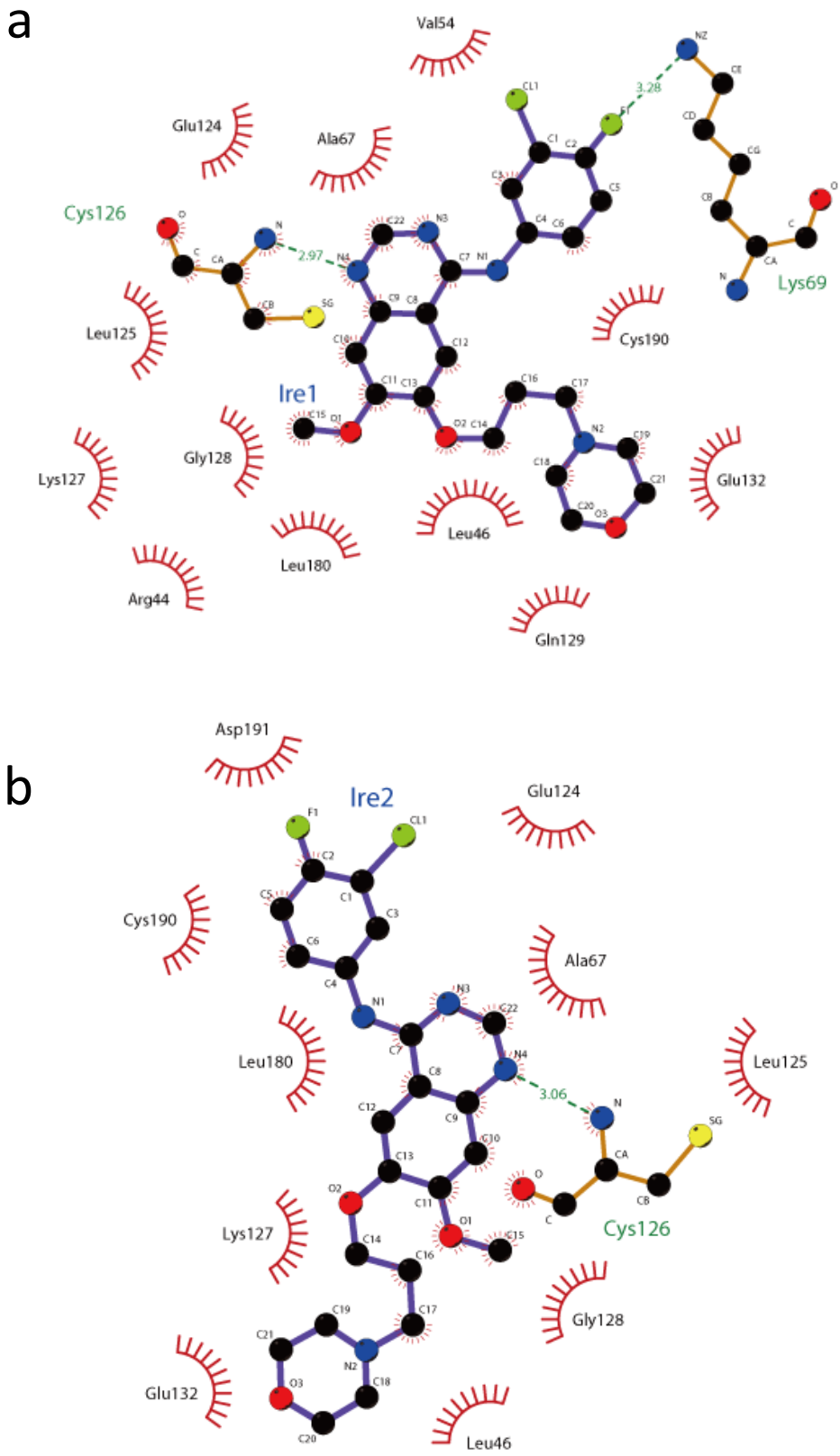

Figure S1. Two-dimensional schematic illustration of the gefitinib•GAK interactions at the ATP binding pocket in the GAK_1 structure. Hydrogen bonds are represented as green dashed lines. Ire1 and Ire2 indicate gefitinib at each site, respectively. The figure is depicted by using LigPlot+[1]. (a) interactions in chain A. (b) interactions in chain B.

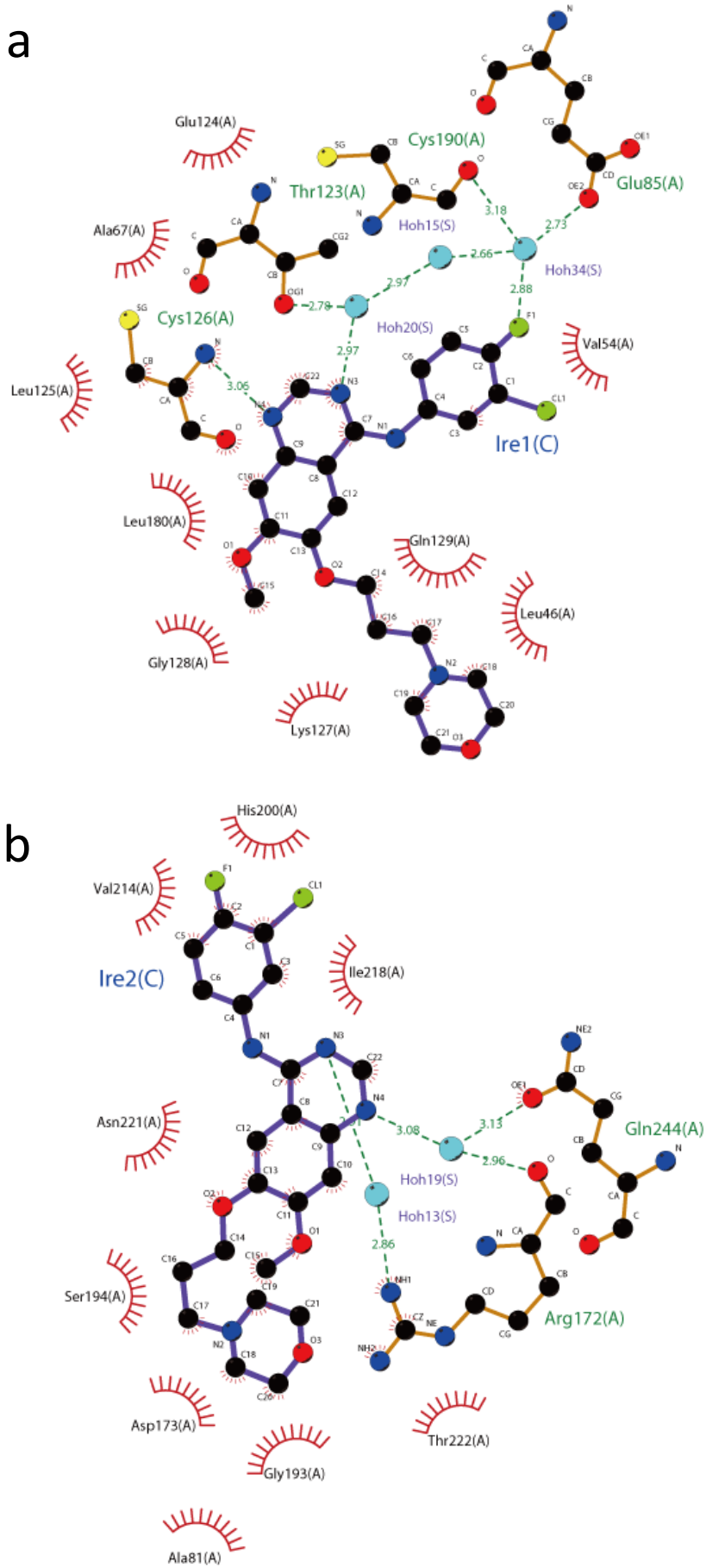

Figure S2. Two-dimensional schematic illustration of the gefitinib•GAK interactions in the GAK_2 structure. Hydrogen bonds are represented as green dashed lines. Ire1 and Ire2 indicate gefinitib. The figure is depicted by using LigPlot+[1]. (a) interactions at the ATP binding pocket. (b) interactions at the second binding site.

Reference

1. R. A. Laskowski,M. B. Swindells, LigPlot+: multiple ligand-protein interaction diagrams for drug discovery. *J. Chem. Inf. Model*. **2011**, *51*, 2778-2786.