BIOLOGICAL CRYSTALLOGRAPHY

Volume 71 (2015)

Supporting information for article:

Combining `dry' co-crystallization and *in situ* diffraction to facilitate ligand screening by X-ray crystallography

Muriel Gelin, Vanessa Delfosse, Frédéric Allemand, François Hoh, Yoann Sallaz-Damaz, Michel Pirocchi, William Bourguet, Jean-Luc Ferrer, Gilles Labesse and Jean-François Guichou

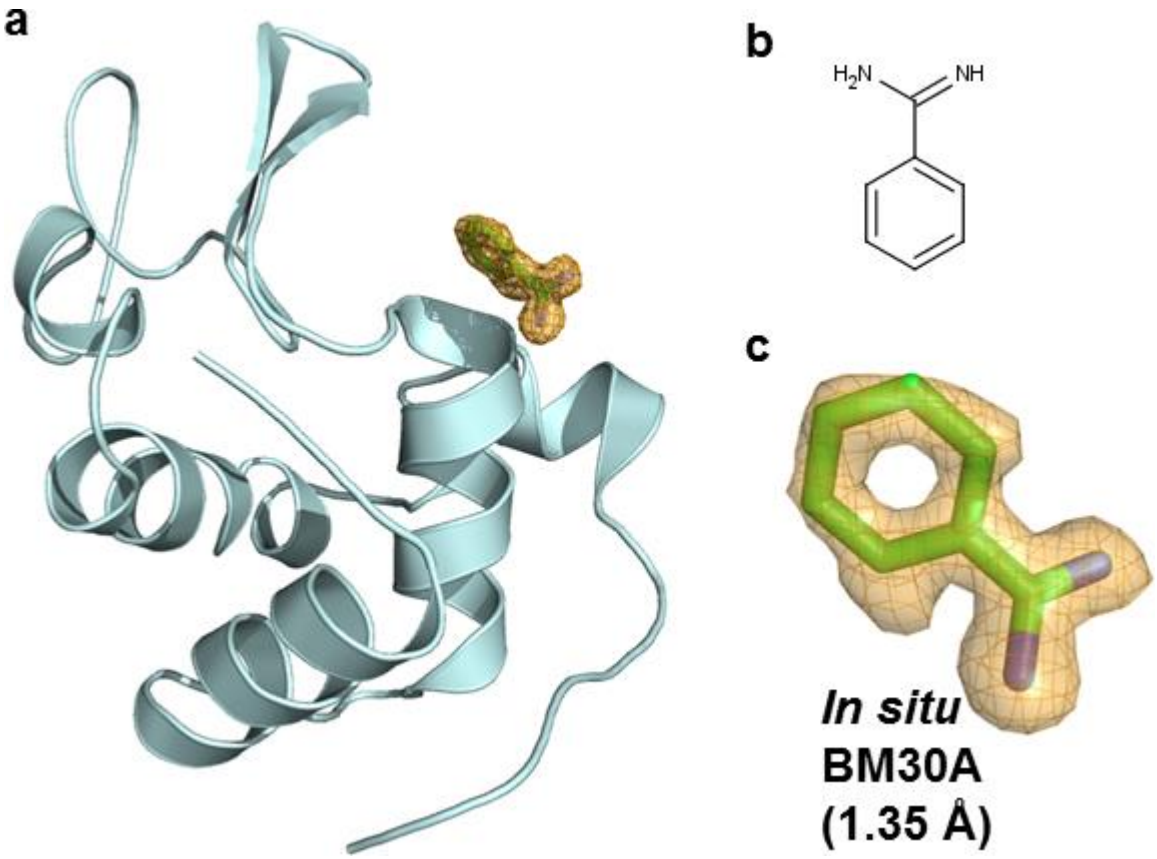

Figure S1 Crystal structures of the hen-egg lysozyme in complex with benzamidine. (A) The overall structure of lysozyme shown as cartoon representation. (B) Chemical structure of benzamidine. (C) Structure solved at high resolution at RT using data collected on the synchrotron beamline BM30A (ESRF). The 2*F*o−*F*c electron density map (contoured at 1σ) was computed with the ligand molecule omitted in the Fourier synthesis.

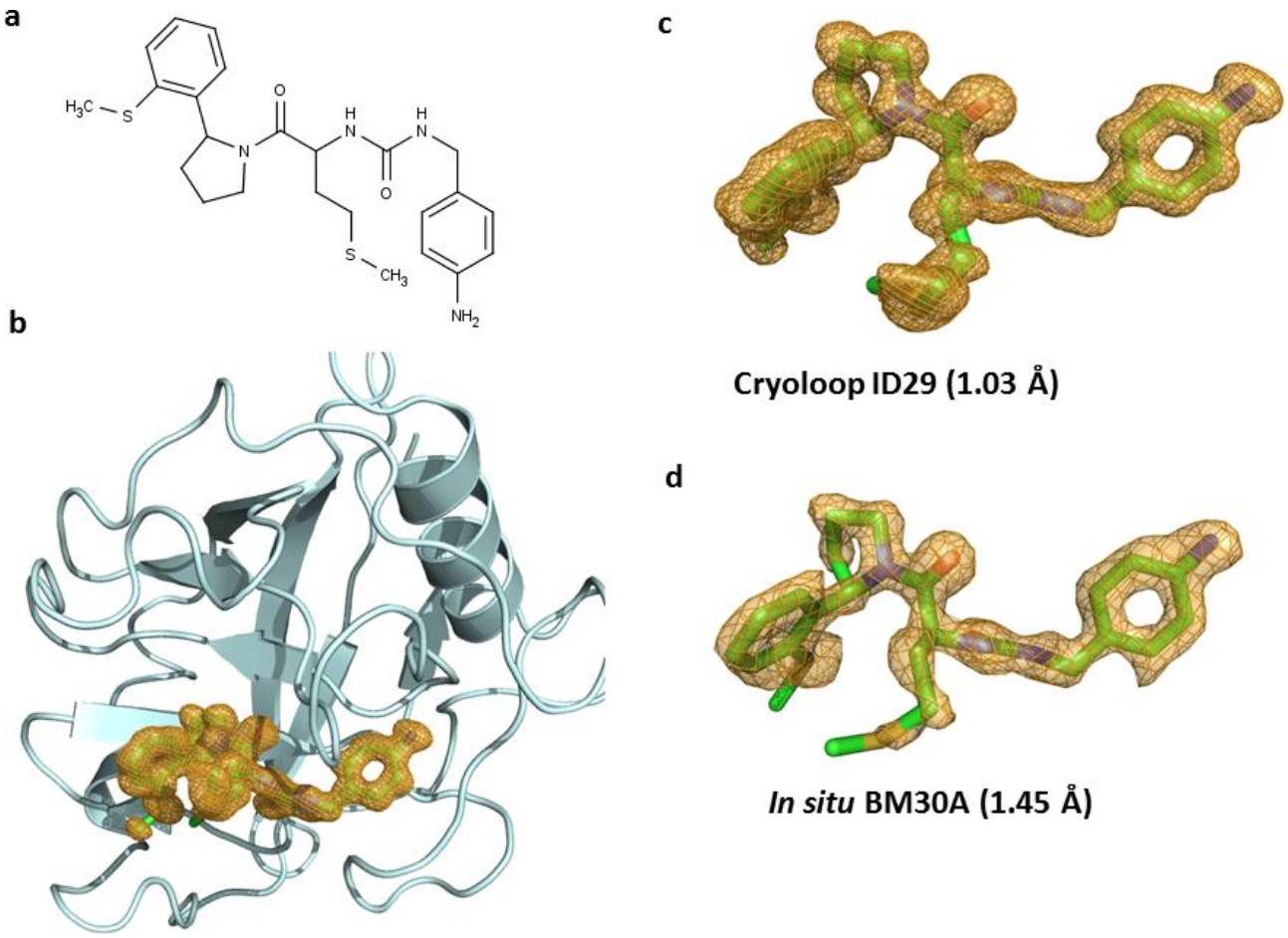

Figure S2 Crystal structures of the human prolyl-isomerase cyclophilin D in complex 1-(4-aminobenzyl)-3-(4-methyl-1-(2-(2-(methylthio)phenyl)pyrrolidin-1-yl)-1-oxopentan-2-yl)urea. (A) Chemical structure of 1-(4-aminobenzyl)-3-(4-methyl-1-(2-(2-(methylthio)phenyl)pyrrolidin-1-yl)-1-oxopentan-2-yl)urea. (B) The overall structure of cyclophilin D shown as cartoon representation. (C) Structure solved at high resolution at 100 K. (D) Same structure at RT using data collected on the synchrotron beamline BM30A (ESRF). In all panels, the 2*F*o−*F*c electron density map (contoured at 1σ) was computed with the ligand molecule omitted in the Fourier synthesis.

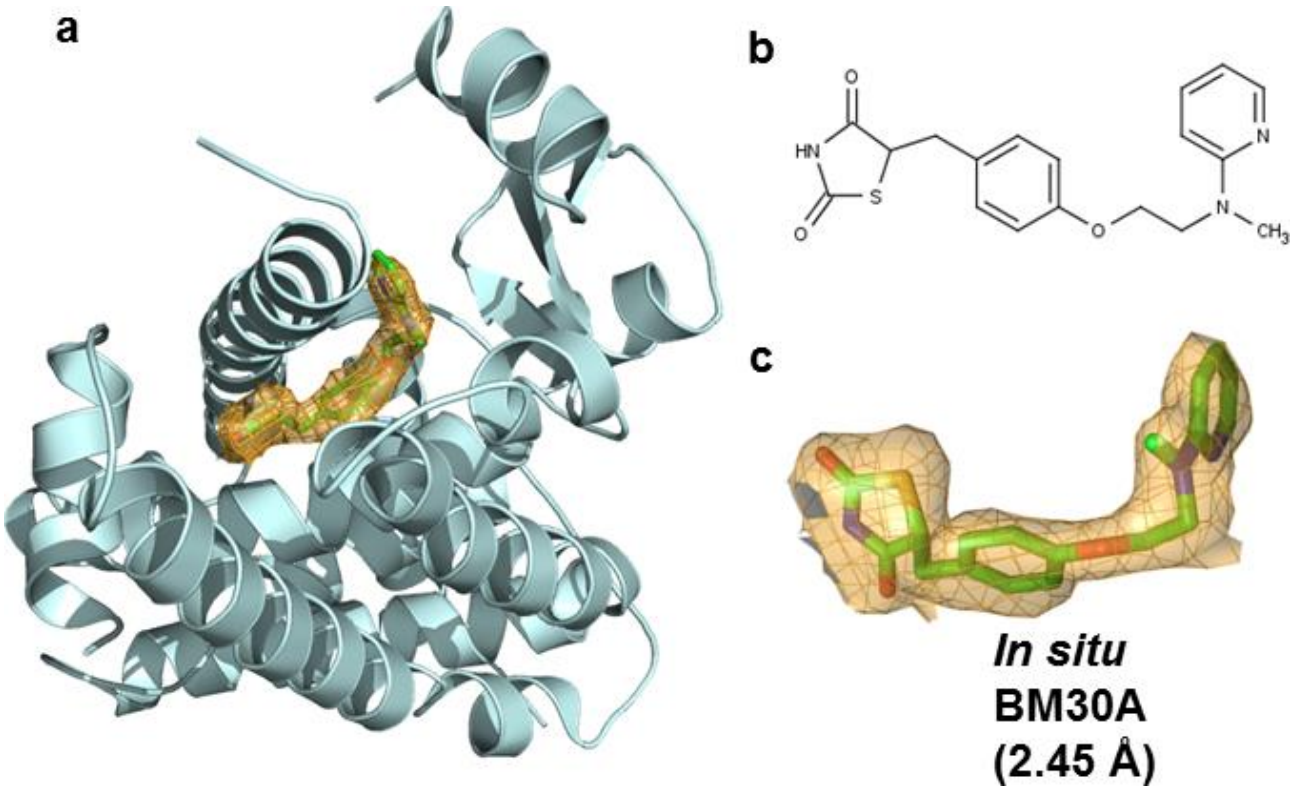

Figure S3 Crystal structures of the human nuclear receptor PPARγ in complex with rosiglitazone. (A) The overall structure of PPARγ shown as cartoon representation. (B) Chemical structure of rosiglitazone. (C) Structure solved at high resolution at RT using data collected on the synchrotron beamline BM30A (ESRF). The 2*F*o−*F*c electron density map (contoured at 1σ) was computed with the ligand molecule omitted in the Fourier synthesis.

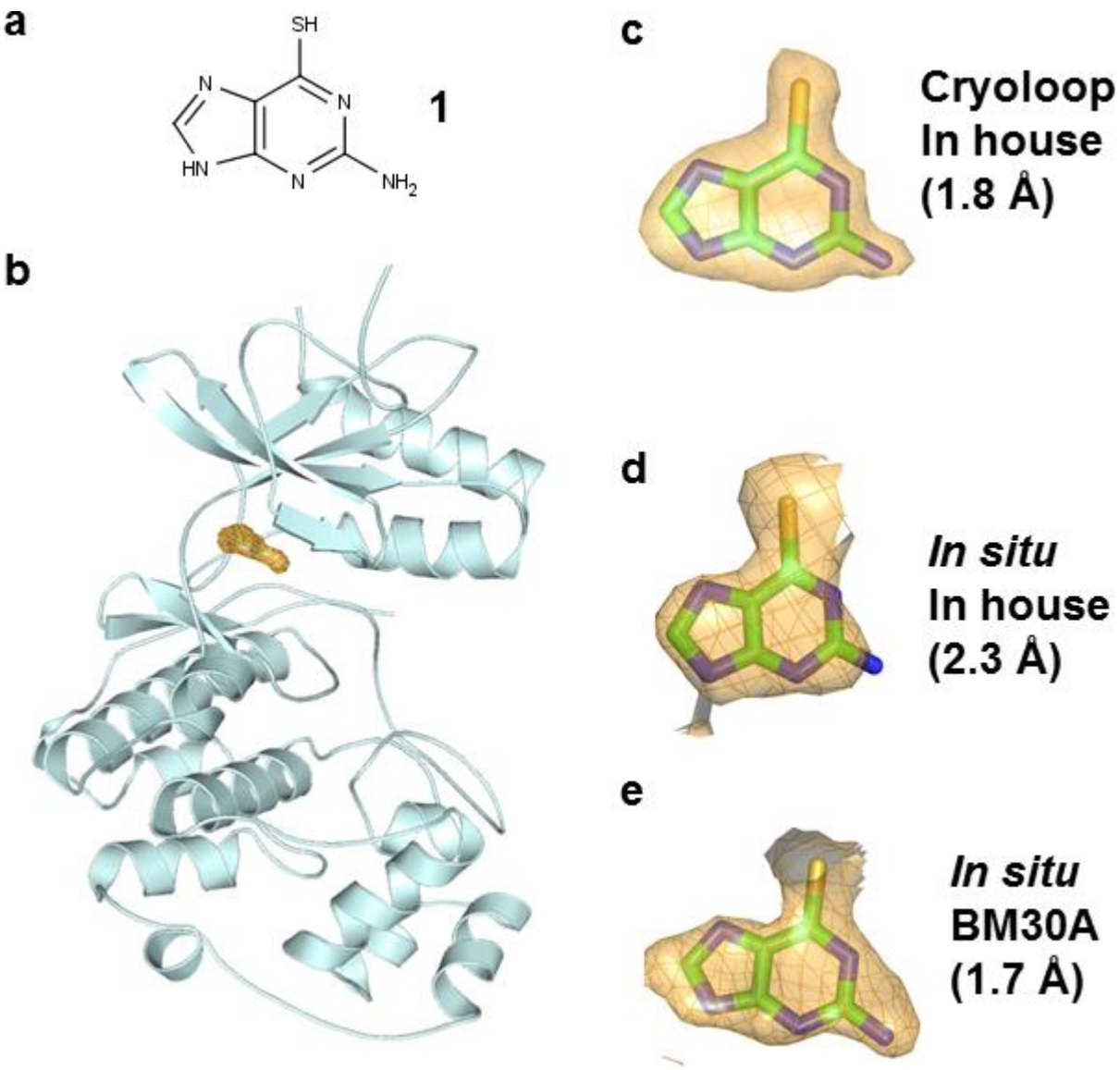

Figure S4 Crystal structures of the protein-kinase Erk-2 in complex with 2-amino-6-thio-purine (**1**). (A) Chemical structure of compound **1**. (B) The overall structure of Erk-2 shown as cartoon representation. (C) Structure solved at high resolution at 100 K. (D) Same structure at RT using data collected on a lab anode. (E) Same structure at RT using data collected on the synchrotron beamline BM30A (ESRF). In all panels, the 2*F*o−*F*c electron density map (contoured at 1σ) was computed with the ligand molecule omitted in the Fourier synthesis.