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Supporting information for article:

The structure of a DYRK1A–PKC412 complex reveals disulfide-bridge formation with the anomalous catalytic loop HRD(HCD) cysteine

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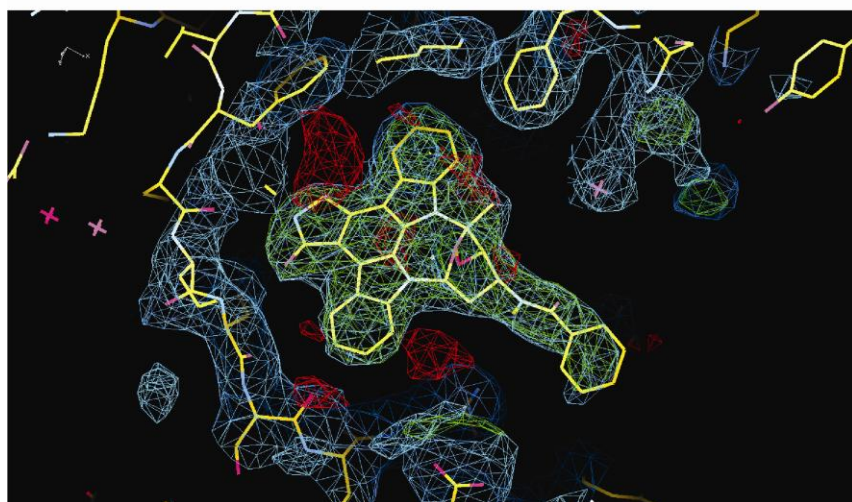
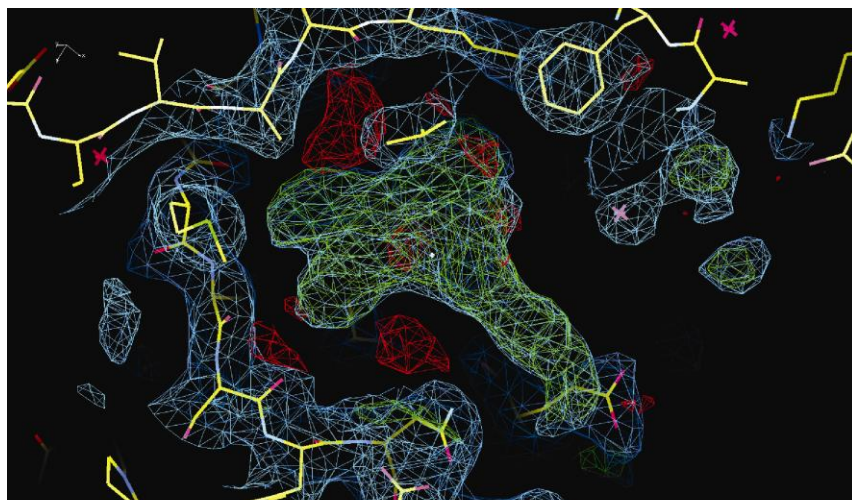


Figure S1 Difference density omit maps (omitting PKC412) after simulated annealing. Electron density contours in blue are calculated at 1σ , difference density contours in green are at 3σ . The lower picture shows in addition the PKC412 molecule after final refinement.

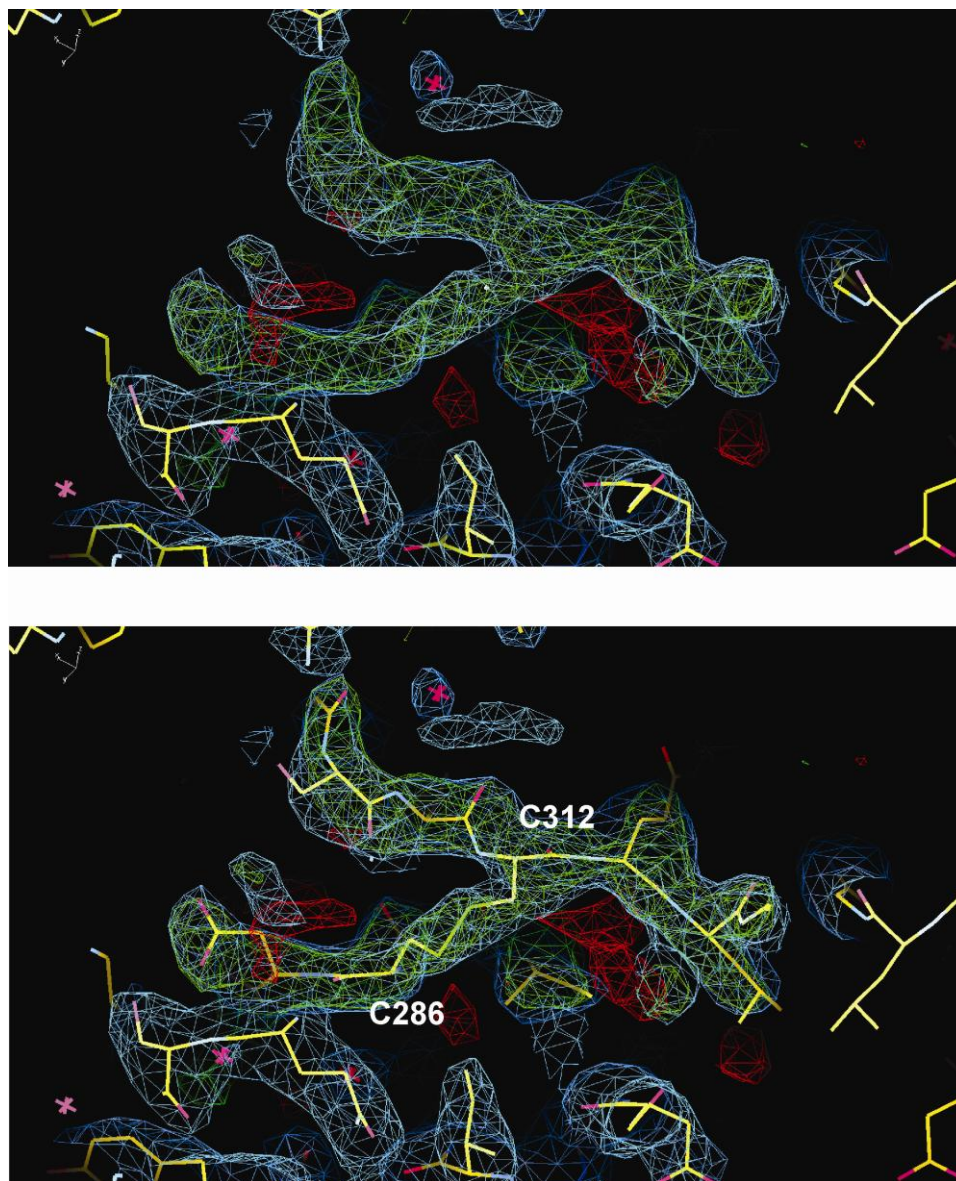


Figure S2 Difference density omit maps (omitting the disulfide bridge and the adjacent residues) after simulated annealing. Electron density contours in blue are calculated at 1σ , difference density contours in green are at 3σ . The lower picture shows in addition the disulfide bridge after final refinement.

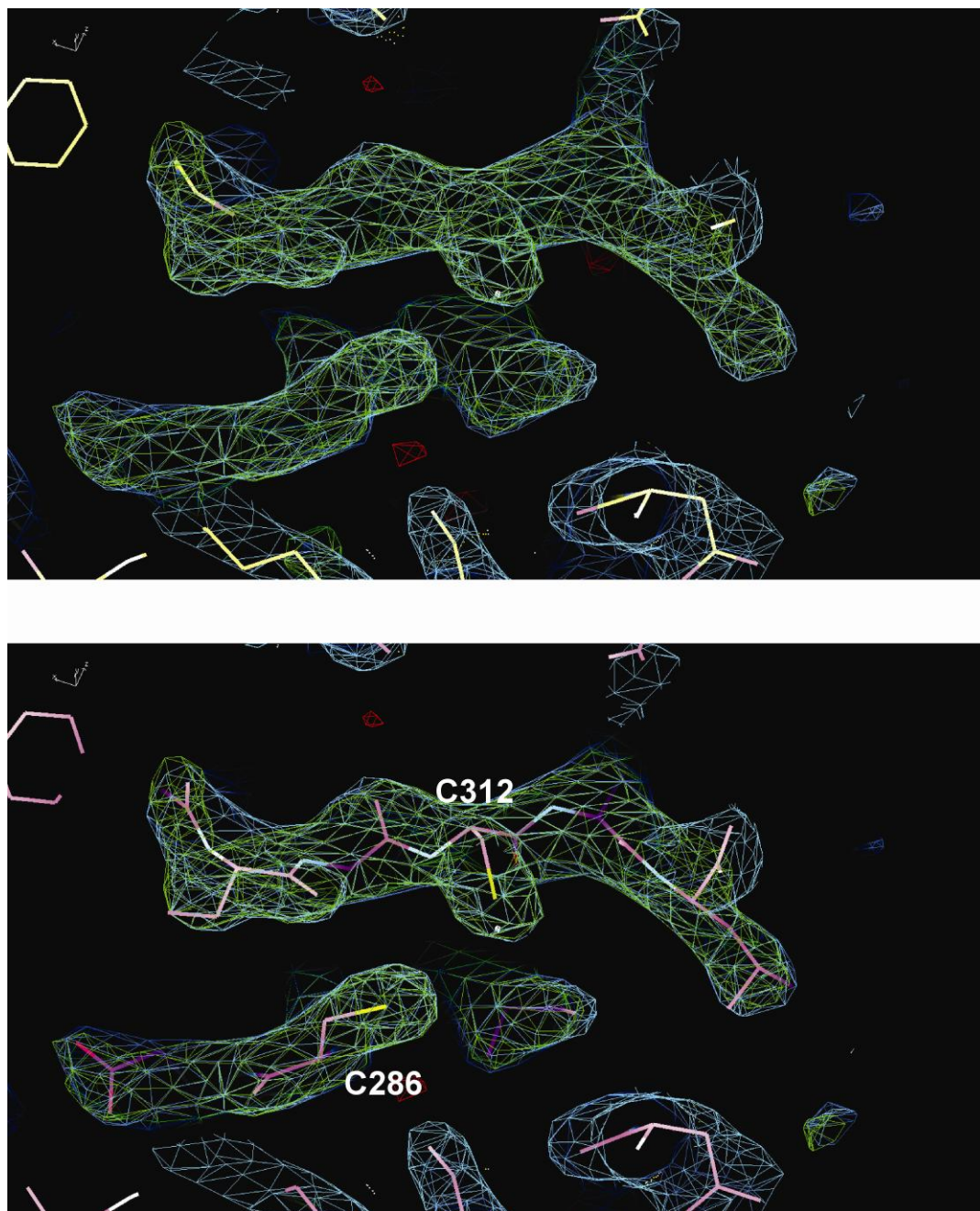


Figure S3 Difference density omit maps (omitting the cysteines C286 and C312 and the adjacent residues) after simulated annealing of the DYRK1A structure with the pdb code 2VX3. Electron density contours in blue are calculated at 1σ , difference density contours in green are at 3σ . The lower picture shows in addition the cysteines in the reduced form (lacking the disulfide bridge) as seen for the DYRK1A structure (4NCT) after final refinement. Calculations were done with the coordinates and structure factors deposited to the pdb.

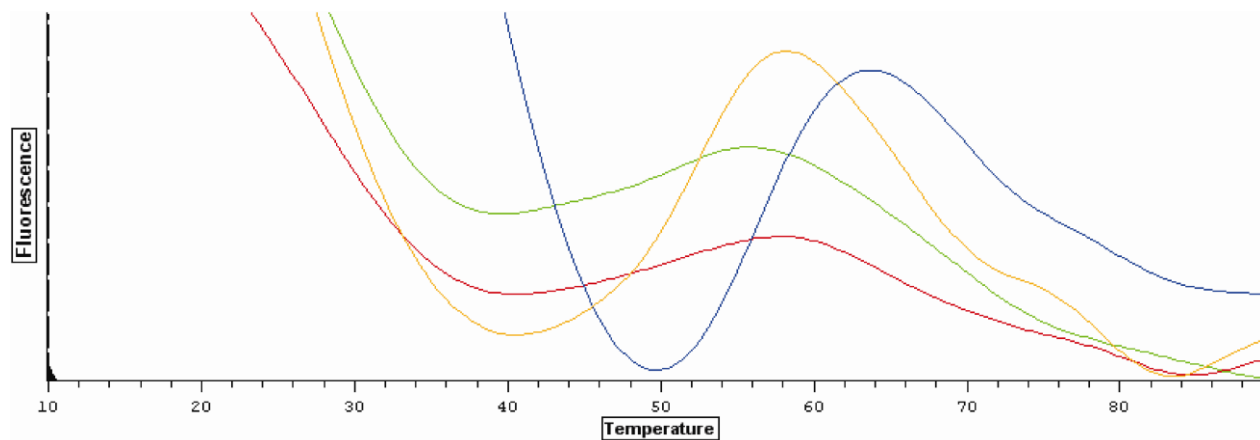


Figure S4 Raw data curves of the thermal shift experiments. For better clarity only one curve of the triplicated experiments is shown for native (red), DMSO (green), PKC412 (orange) and harmine (purple).

