Interactive binding mode exploration

Description

Below is the representation of the non-bounded interactions between ligands and residues in the ATP binding site of the selected protein kinase. Each of the 85 residues is represented by eight types of interactions:

- (Column 0) hydrophobic contacts (HYD)
- (Column 1) aromatic face to face (AFF)
- (Column 2) aromatic edge to face (AEF)
- (Column 3) hydrogen bond with protein as hydrogen bond donor (HBD)
- (Column 4) hydrogen bond with protein as hydrogen bond acceptor (HBA)
- (Column 5) salt bridges with positively charged protein (PSB)
- (Column 6) salt bridges with negatively charged protein (NSB)
- (Column 7) salt bridges having an ionic bond with metal ion (ISB)

To display the 680 interactions (85x8), the legend is compressed and does not show all residues and interactions.

Interactions are encoded in two colors:

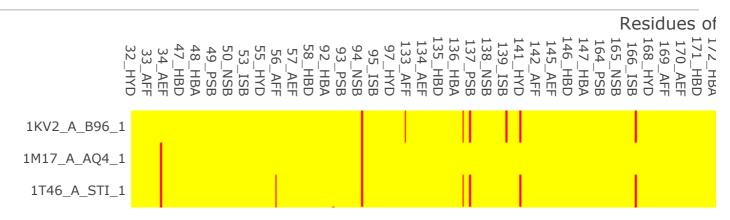
Absence of interaction

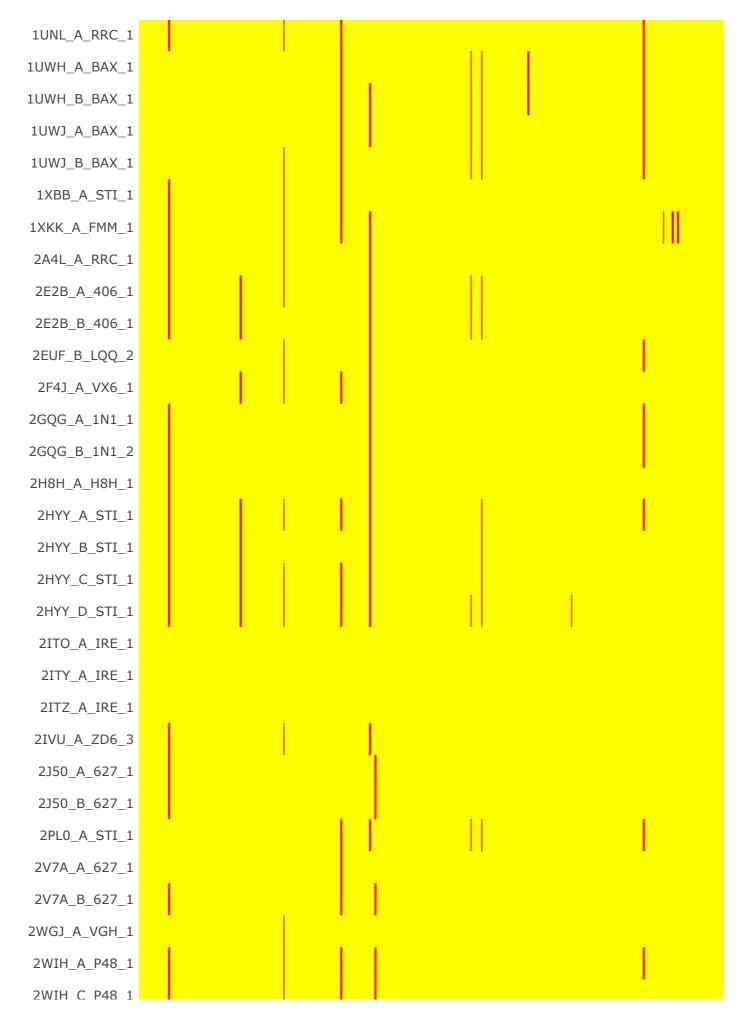
Presence of interaction

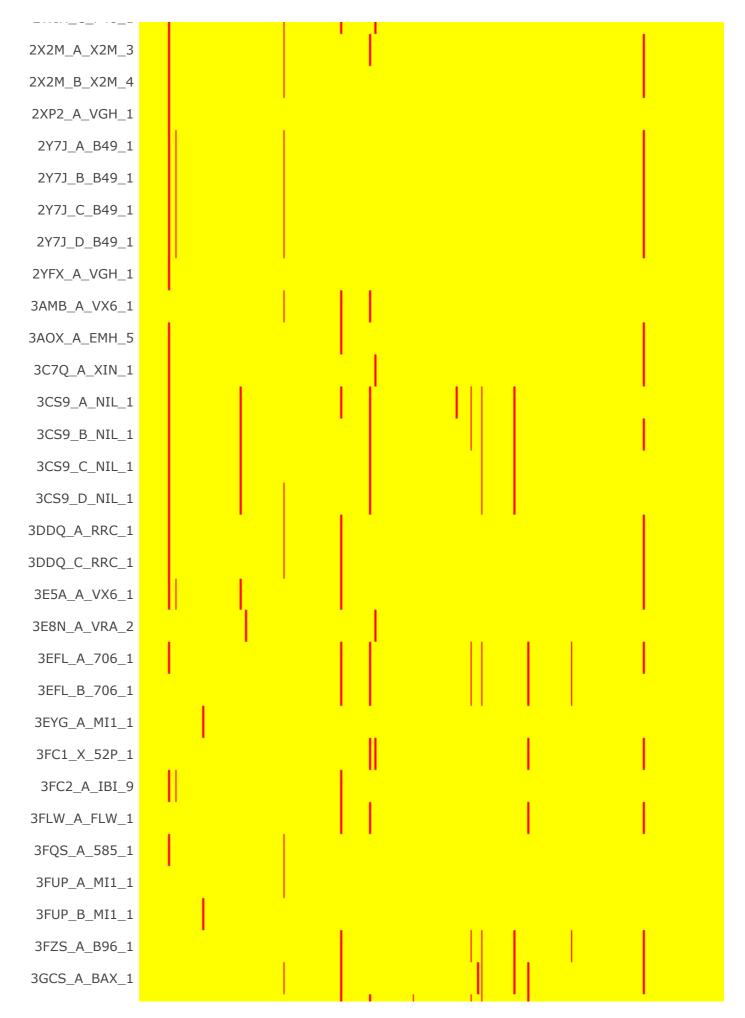
To get all residues, the user can zoom on the heatmap by selecting an area.

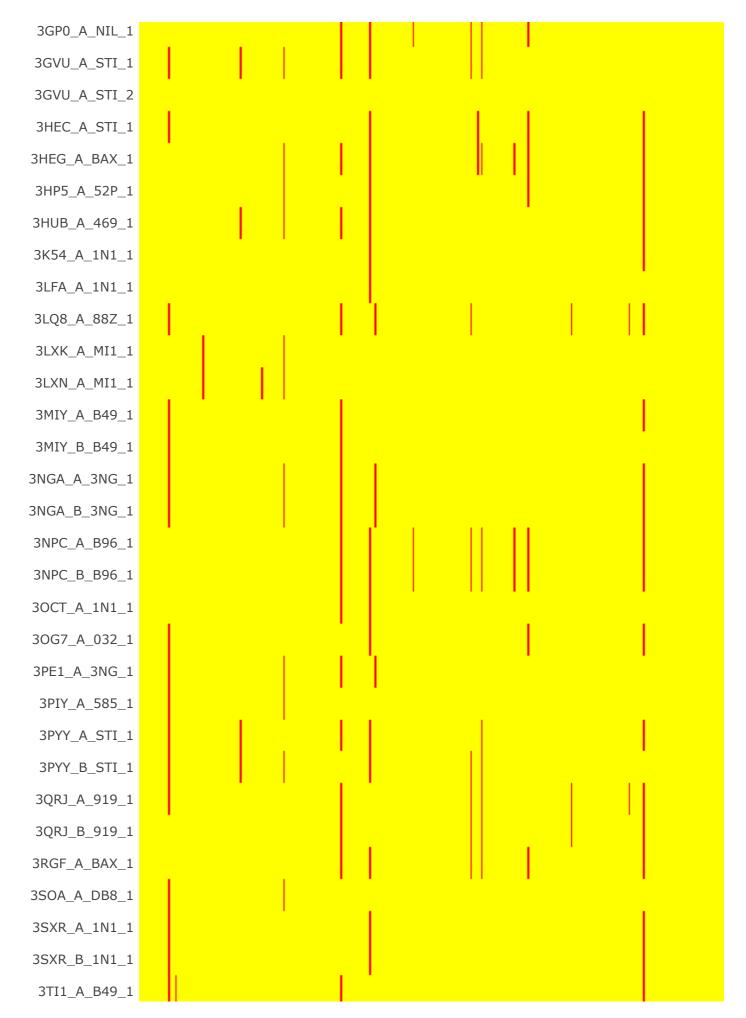
To visualize all information, including bioactivity data on a ligand-target pair, the user can click anywhere on a row of the heatmap.

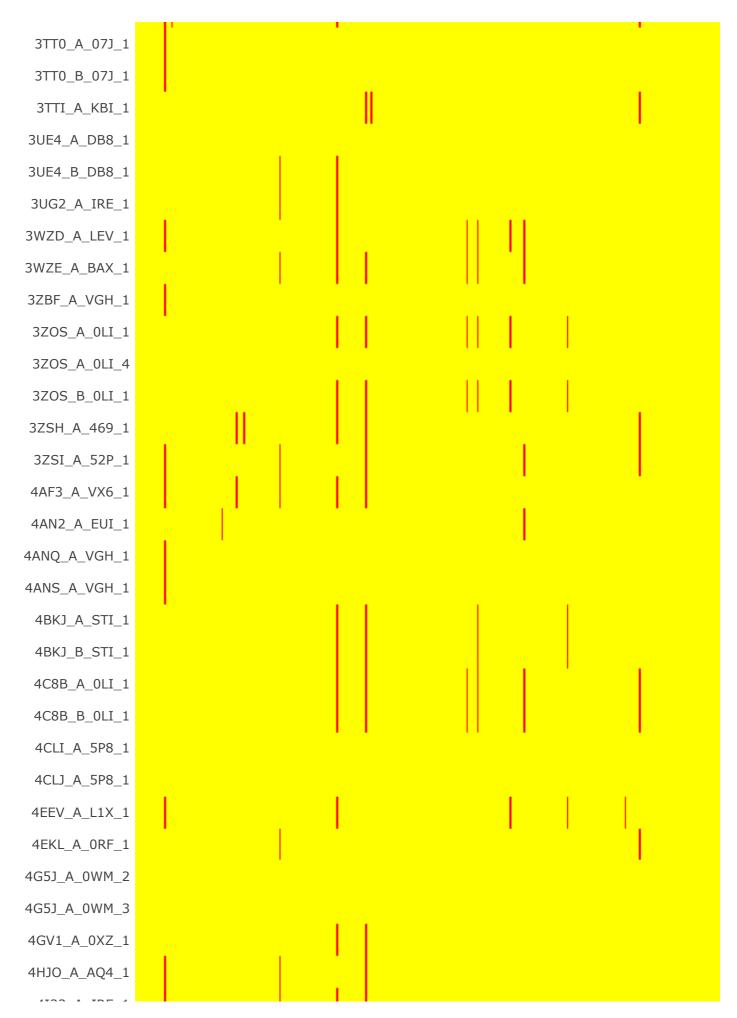
(see User Guide (/user_guide) for complete information about non-bounded interaction in KinoMine).

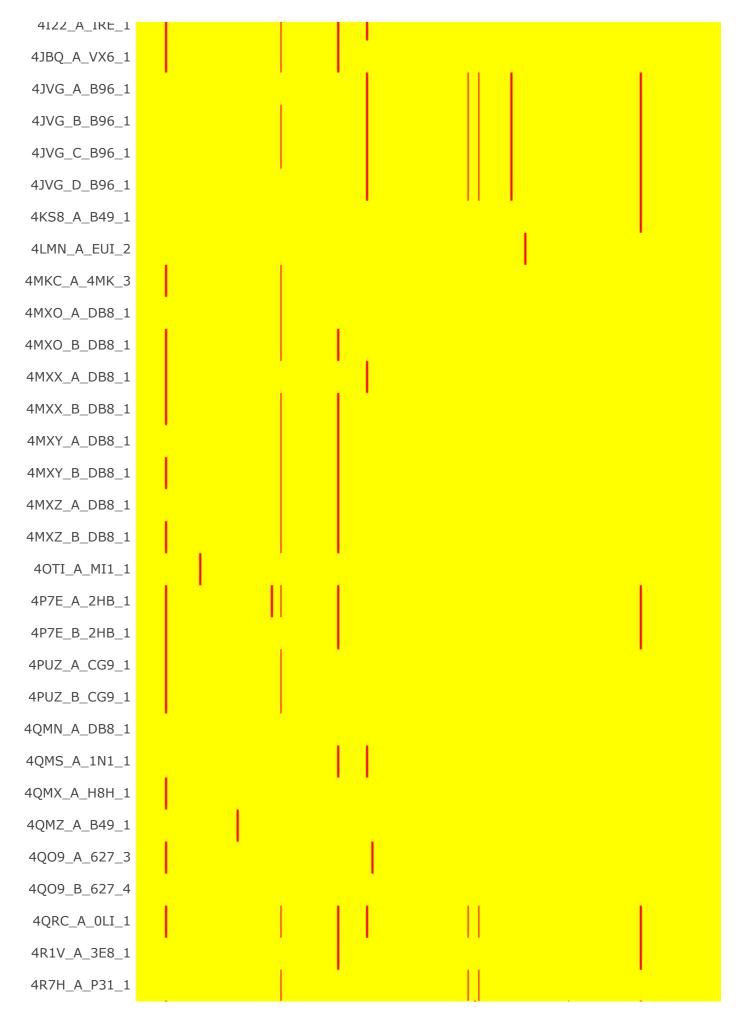


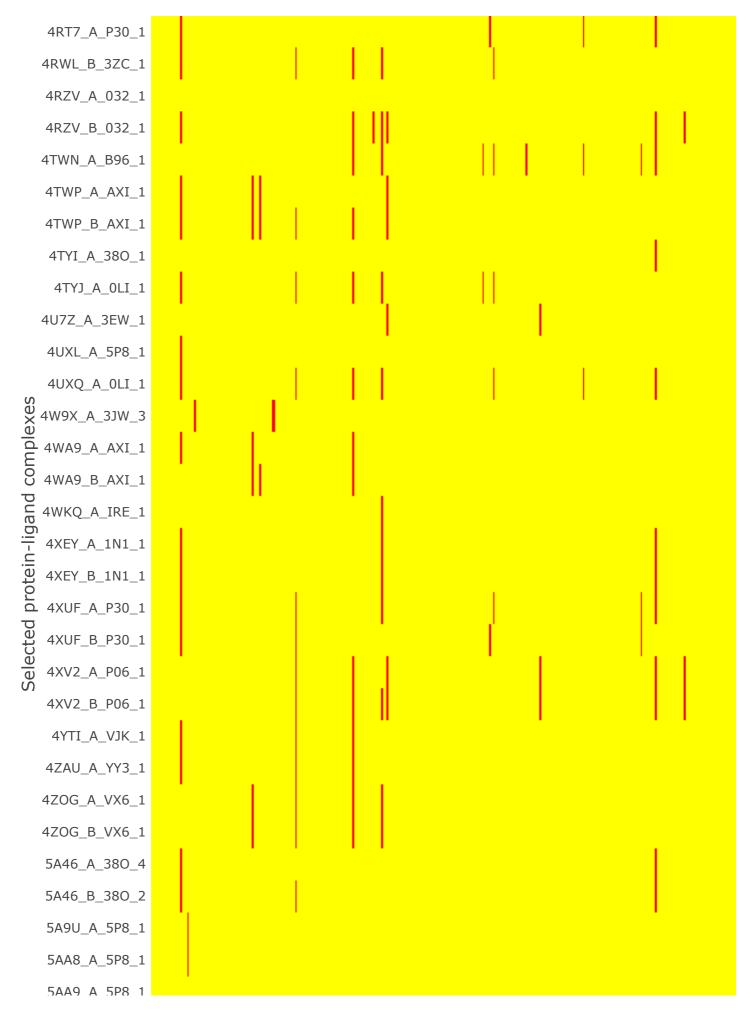


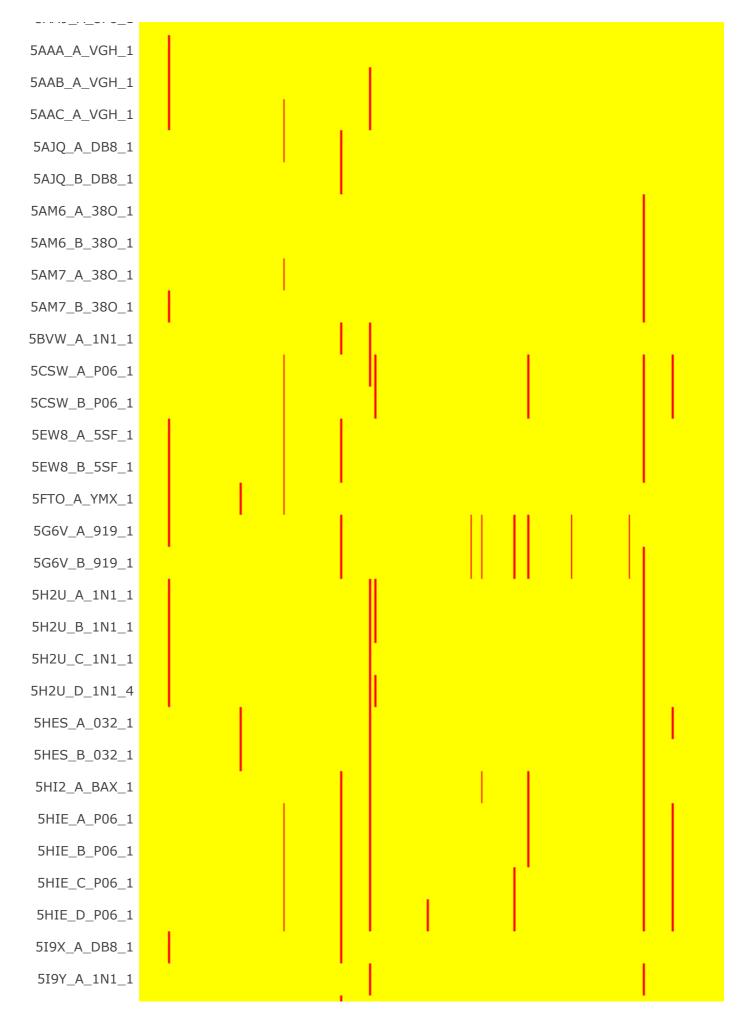


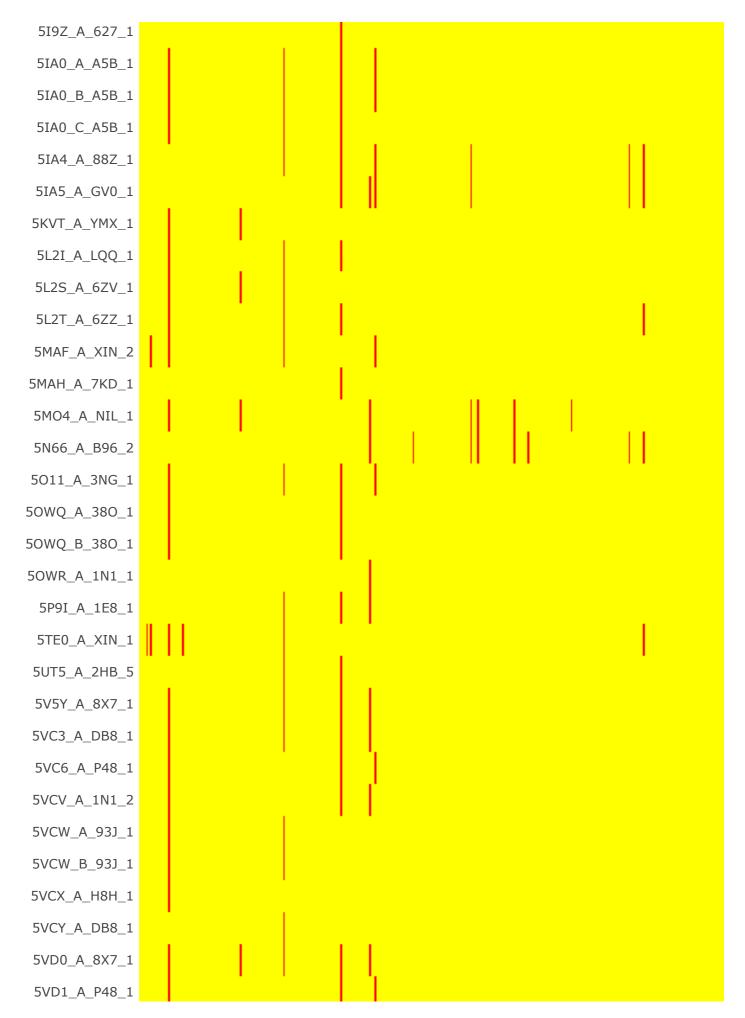


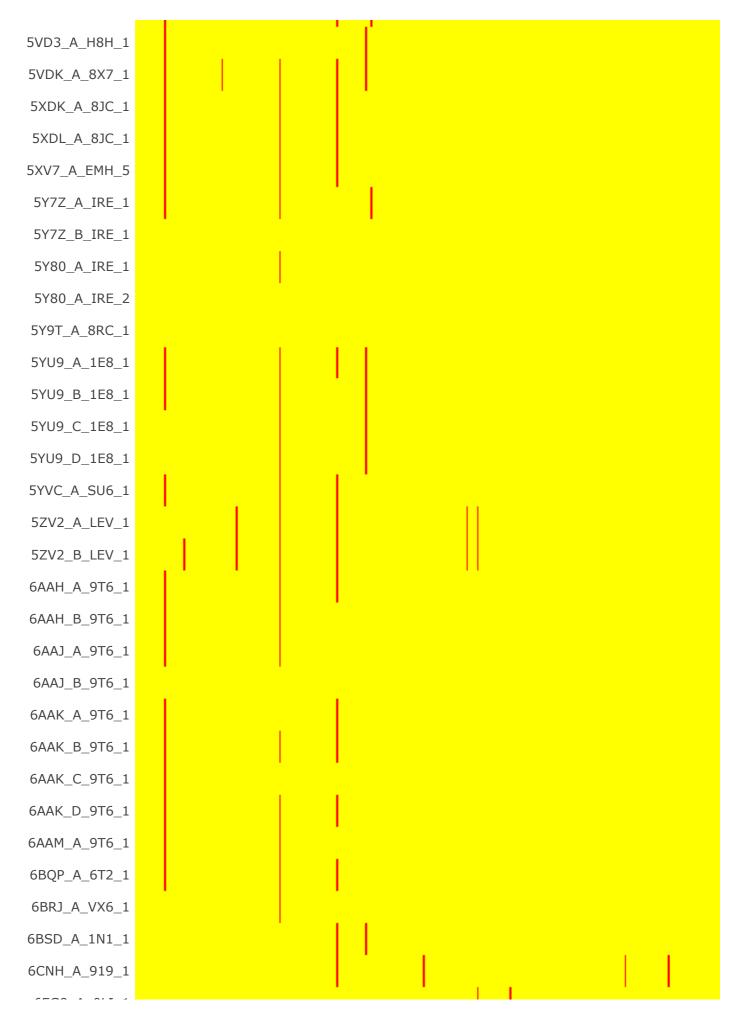


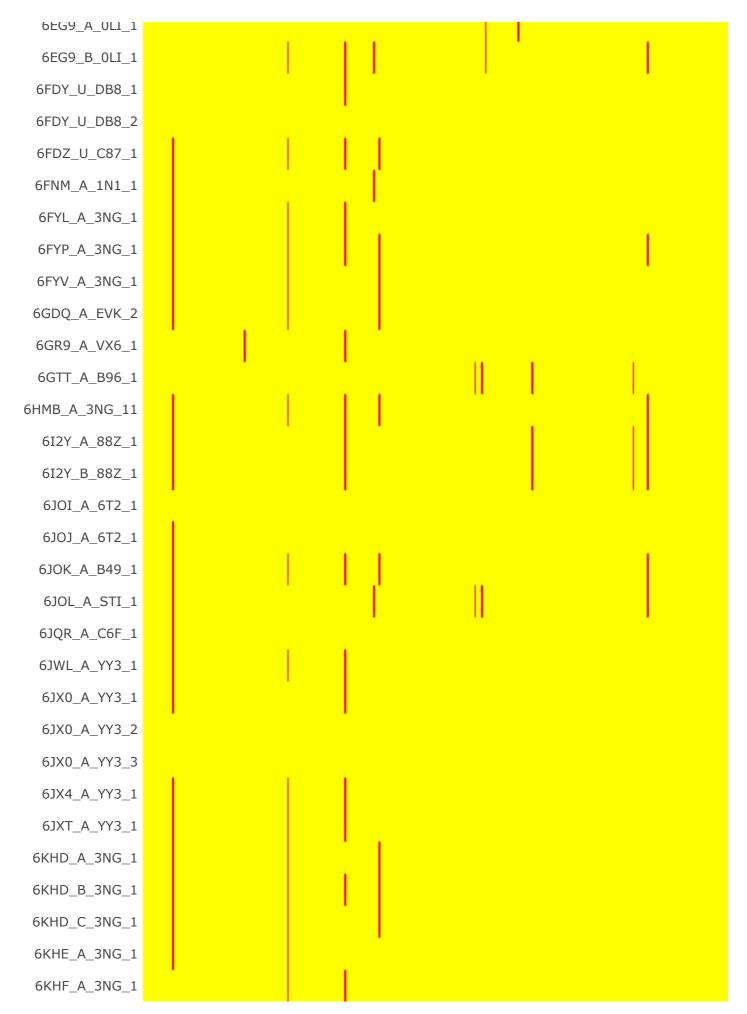


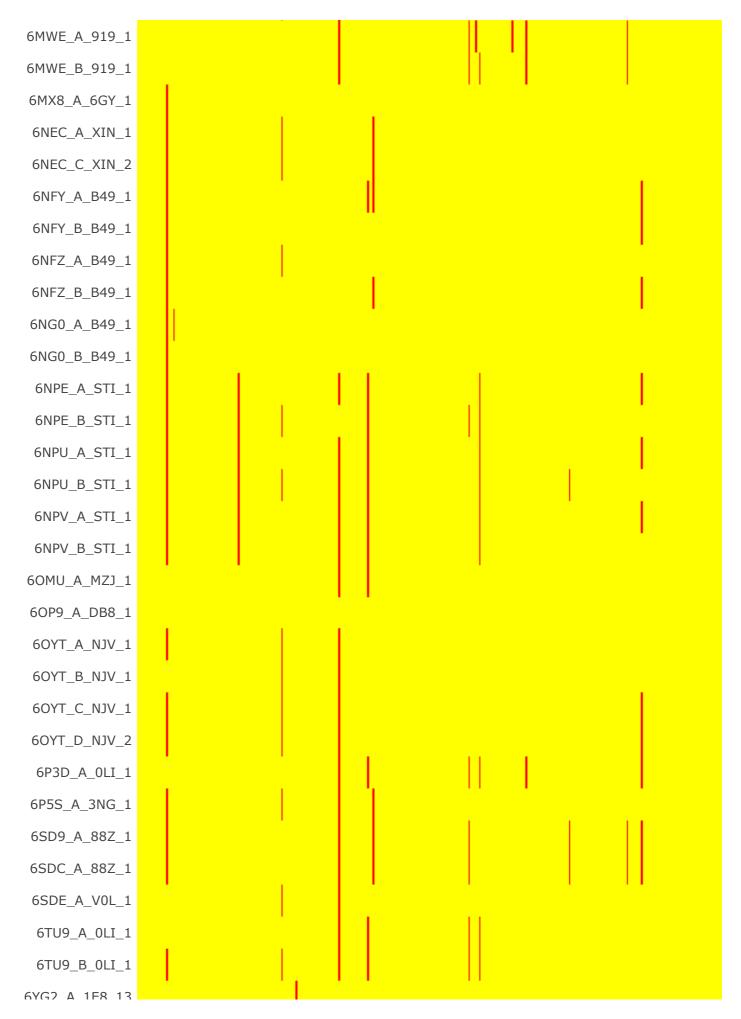


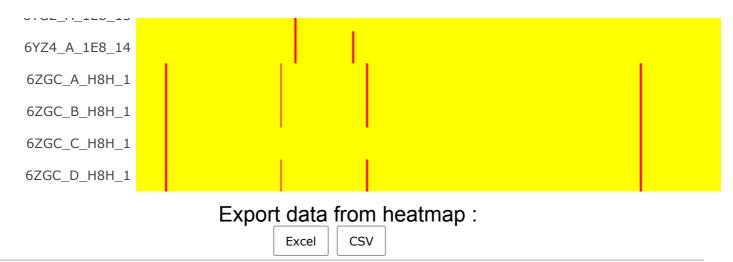












This heatmap has been generated thanks to Plotly (https://plot.ly).

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