



## Supporting Information

for

# Design of Tetra-peptide Ligands of Antibody Fc Regions Using *In Silico* Combinatorial Library Screening

Marko Jukič<sup>1,2,3,\*</sup>, Sebastjan Kralj<sup>1</sup>, Anja Kolarič<sup>1,3</sup> and Urban Bren<sup>1,2,3\*</sup>

<sup>1</sup>Laboratory of Physical Chemistry and Chemical Thermodynamics, Faculty of Chemistry and Chemical Engineering, University of Maribor, Smetanova ulica 17, SI-2000 Maribor, Slovenia

<sup>2</sup>Faculty of Mathematics, Natural Sciences and Information Technologies, University of Primorska, Glagoljaška ulica 8, SI-6000 Koper, Slovenia

<sup>3</sup>Institute of Environmental Protection and Sensors, Beloruska ulica 7, SI-2000 Maribor, Slovenia

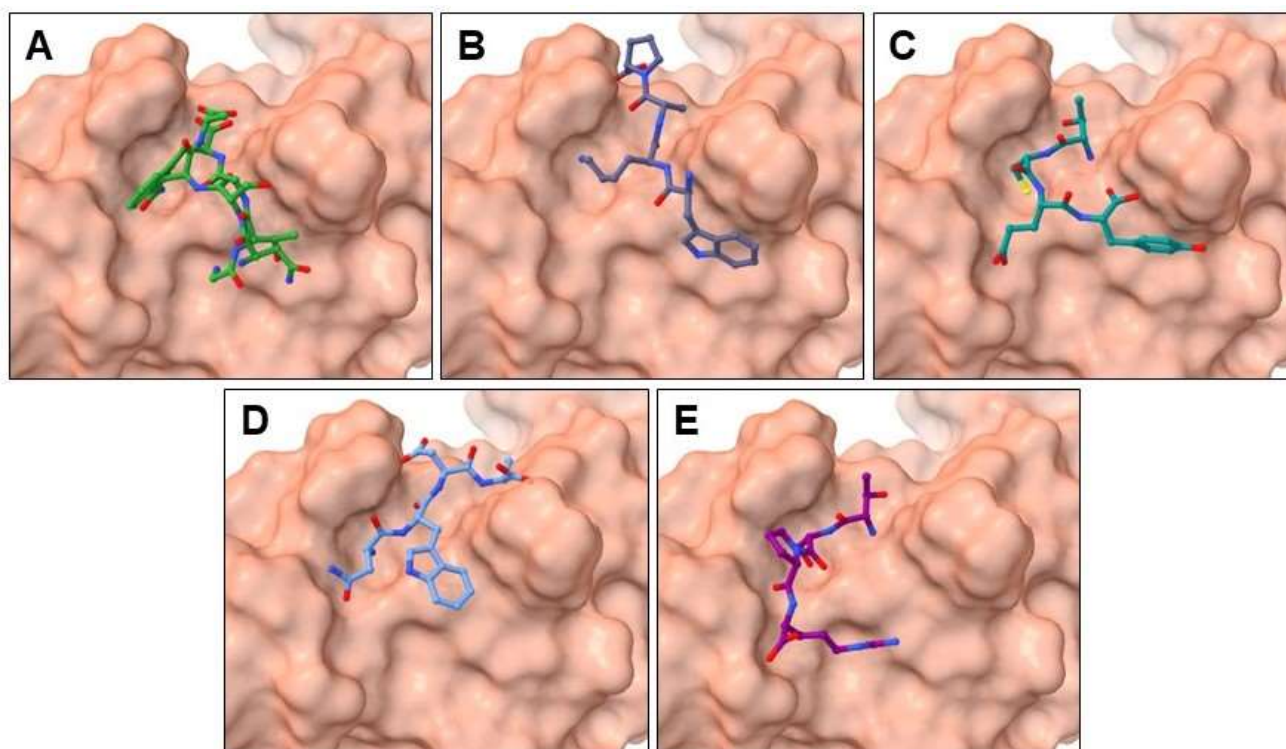
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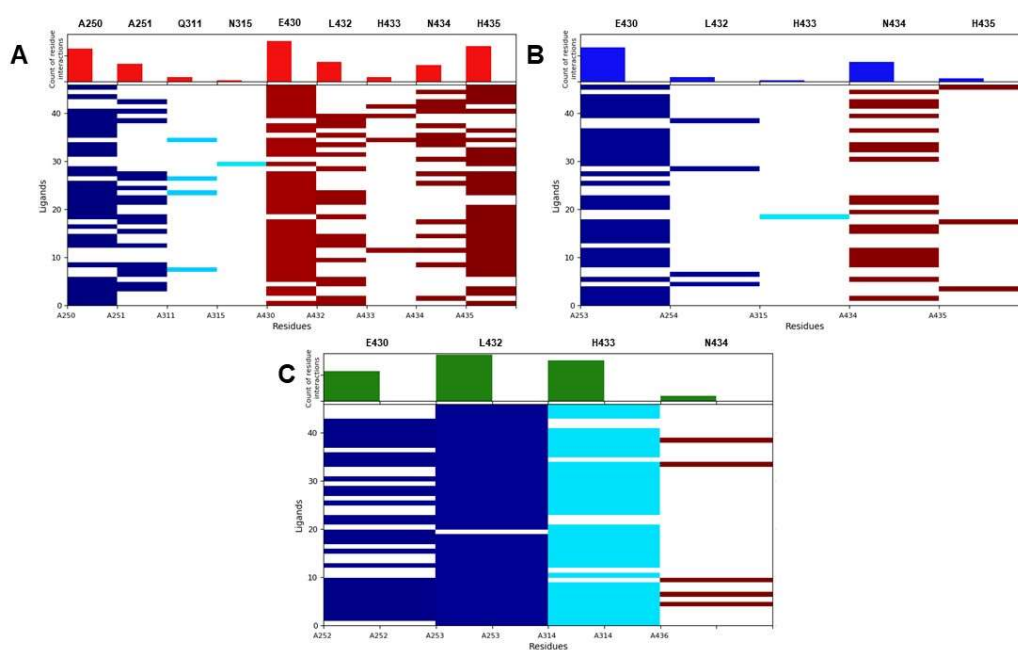
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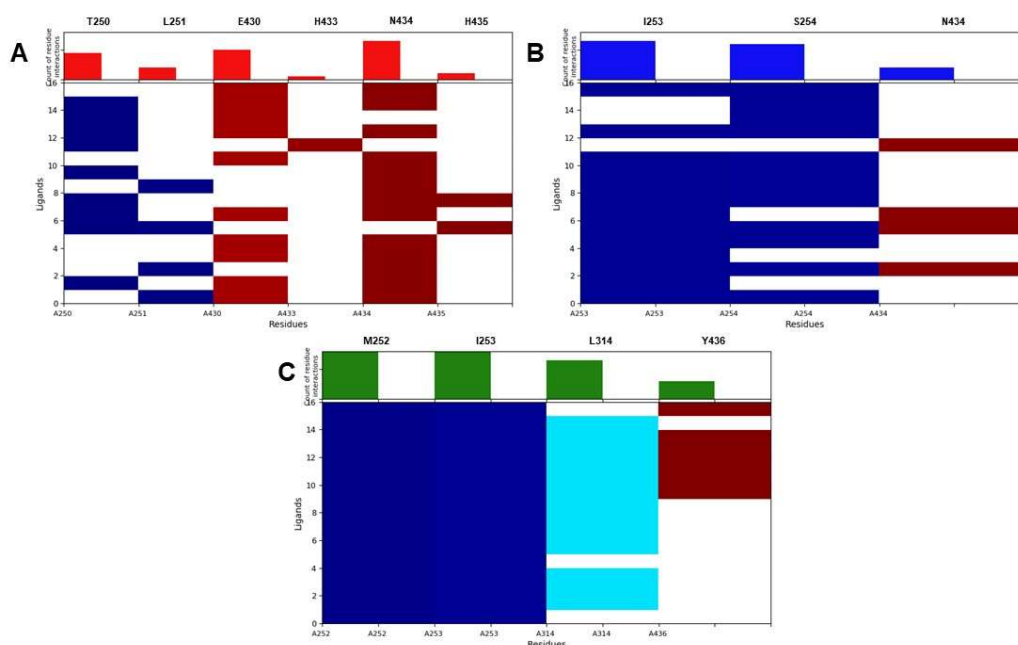
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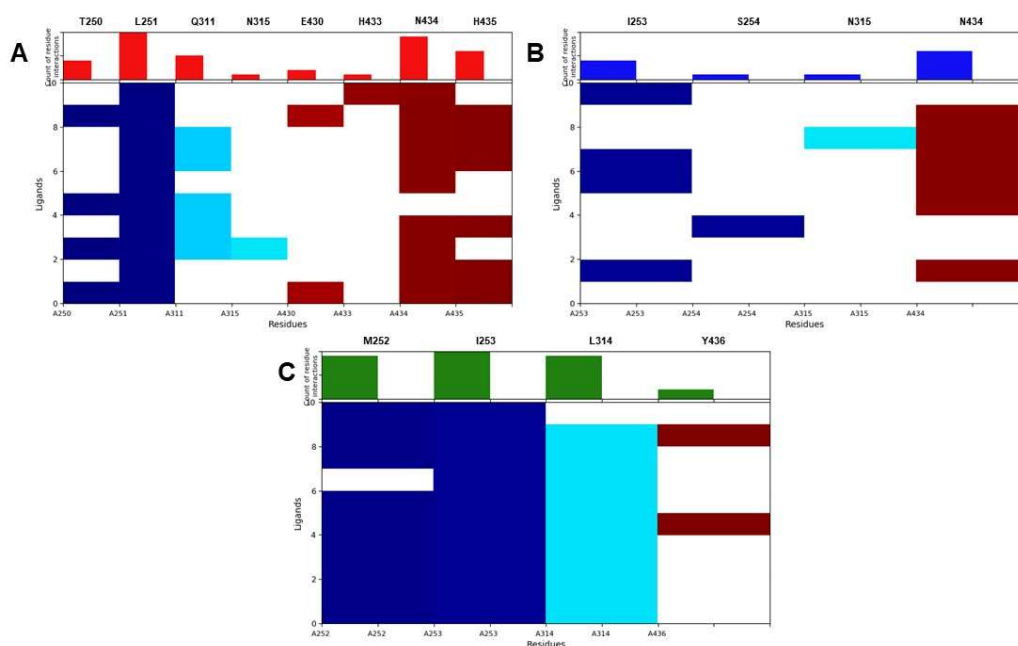
**Figure S1.** Showing a representative compound with its binding pose for each of 5 clusters. **(A)** NSNA and GTGW (in green), representatives of cluster 1. **(B)** WKAP (in dark blue), representative of cluster 2. **(C)** TCEY (in dark green), representative of cluster 3. **(D)** NWDA (in light blue), representative of cluster 4. **(E)** TSPR (in violet), representative of cluster 5. Ligands are shown in ball and stick representation, while the Fc region of the antibody is represented as light brown surface.



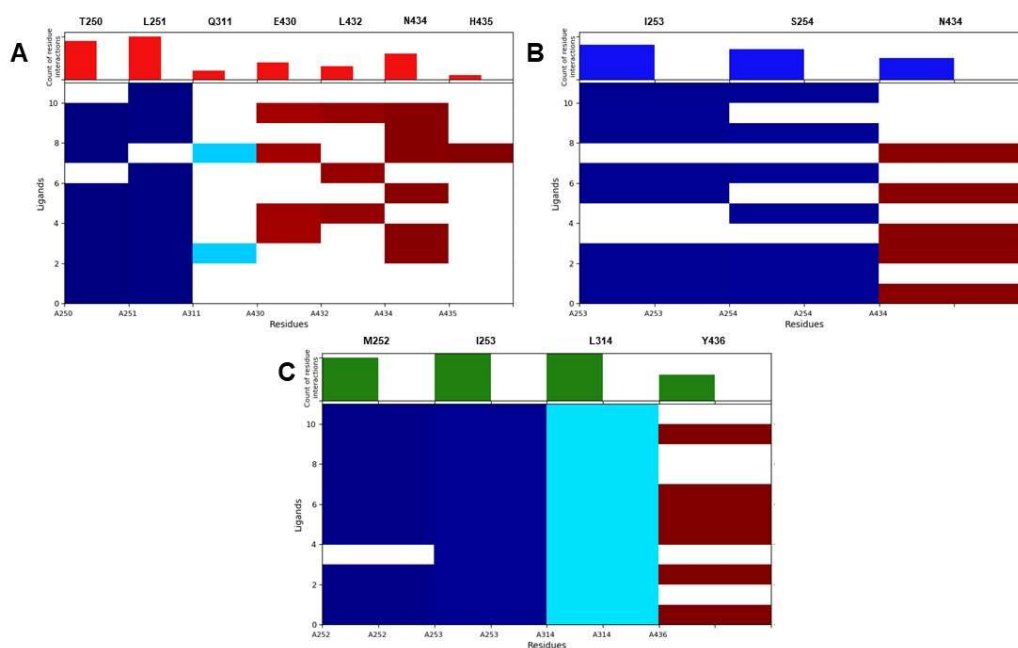
**Figure S2.** Interaction fingerprints of hydrogen bond acceptor (A) hydrogen bond donor (B) and hydrophobic residues (C), showing the residues that showed maximum number of interactions with peptide ligands in cluster 1.



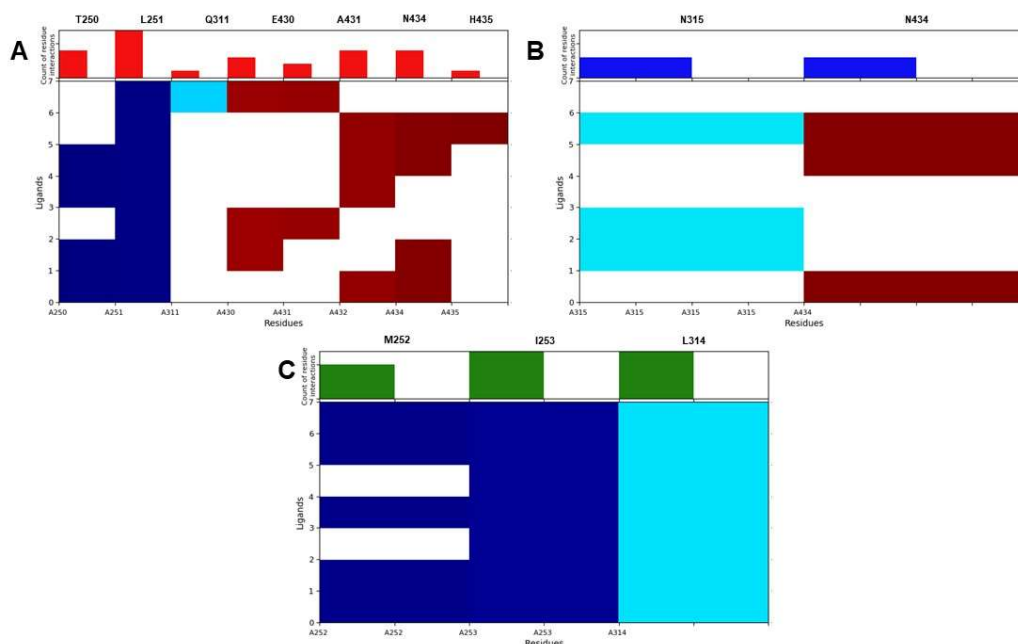
**Figure S3.** Interaction fingerprints of hydrogen bond acceptor (A) hydrogen bond donor (B) and hydrophobic residues (C), showing the residues that showed maximum number of interactions with peptide ligands in cluster 2.



**Figure S4.** Interaction fingerprints of hydrogen bond acceptor (A) hydrogen bond donor (B) and hydrophobic residues (C), showing the residues that showed maximum number of interactions with peptide ligands in cluster 3.



**Figure S5.** Interaction fingerprints of hydrogen bond acceptor (A) hydrogen bond donor (B) and hydrophobic residues (C), showing the residues that showed maximum number of interactions with peptide ligands in cluster 4.



**Figure S6.** Interaction fingerprints of hydrogen bond acceptor (A) hydrogen bond donor (B) and hydrophobic residues (C), showing the residues that showed maximum number of interactions with peptide ligands in cluster 5.