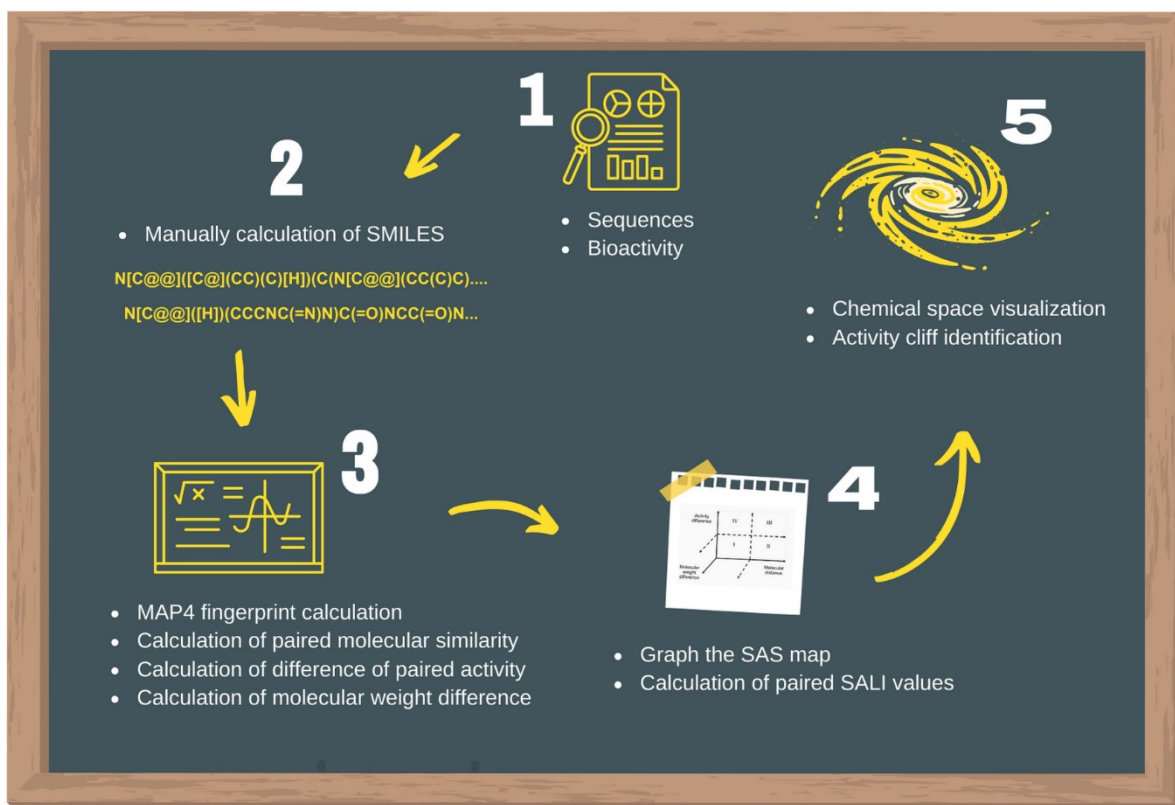
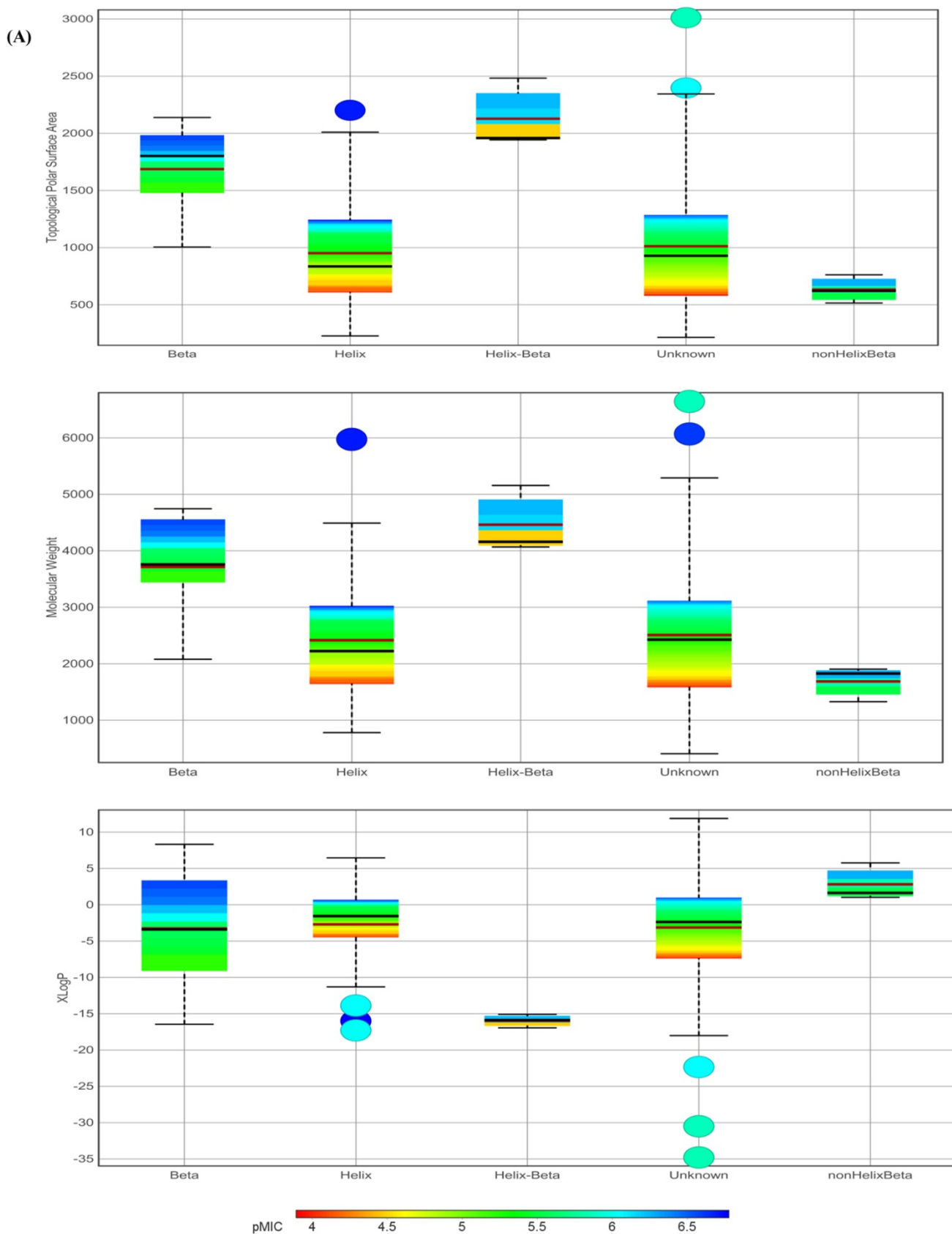


## Mapping the structure-activity landscape of non-canonical peptides with MAP4 fingerprinting

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**Figure S1.** Overview step by step of the protocol implemented in this work.



(B)

Descriptors	1	2	3	4
MW	1	0.981	-0.642	0.346
TPSA	2	0.981	-0.733	0.327
XLogP	3	-0.642	-0.733	-0.0817
pMIC	4	0.346	0.327	-0.0817

**Figure S2.** Property diversity of the anti-MRSA peptide dataset used in this work. Properties calculated with KNIME-CDK node. The red and black lines denote the mean and median distributions, respectively. The data points outside of the boxes indicate outliers.



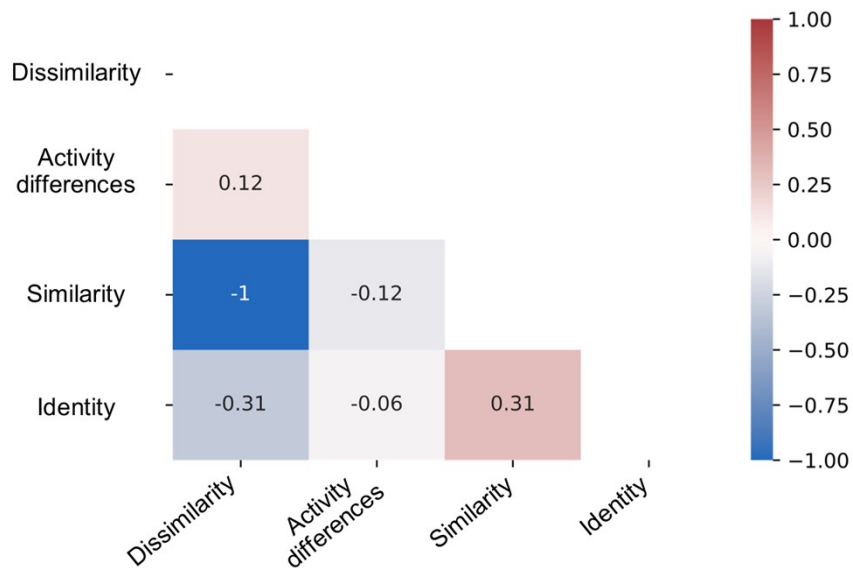


Figure S4. Correlations of identity values and fingerprint-based similarity values.

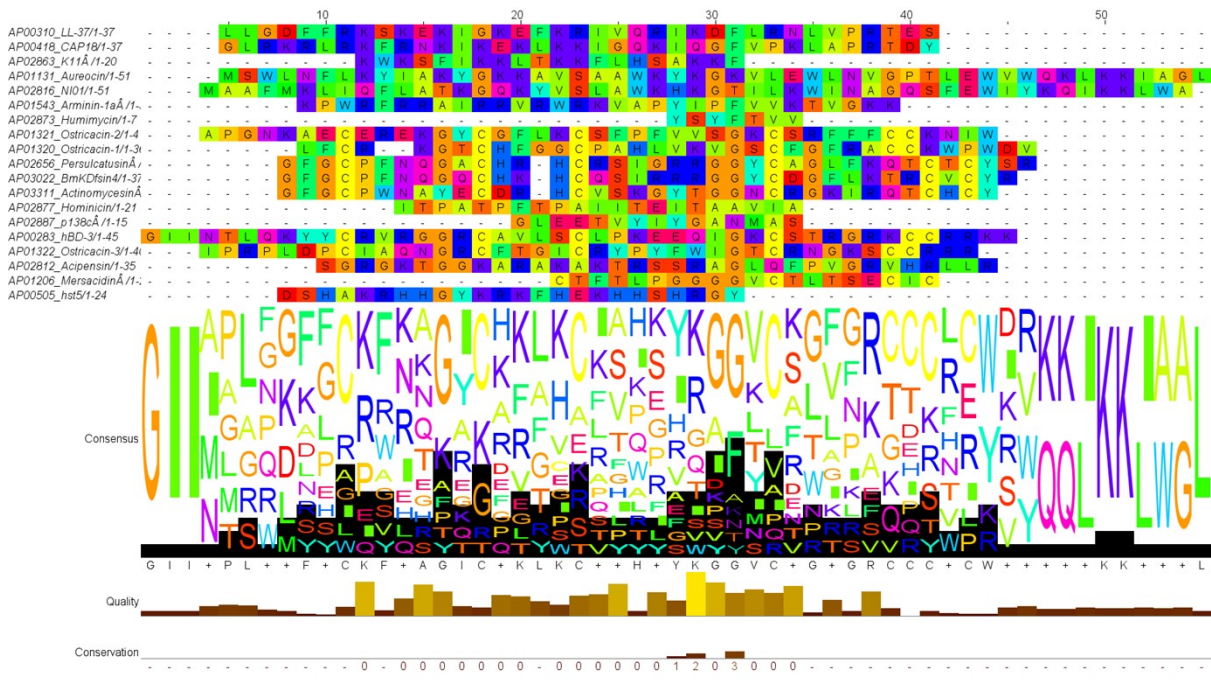


Figure S5. Alignment analysis of the 20 most potent anti-MRSA peptides.

