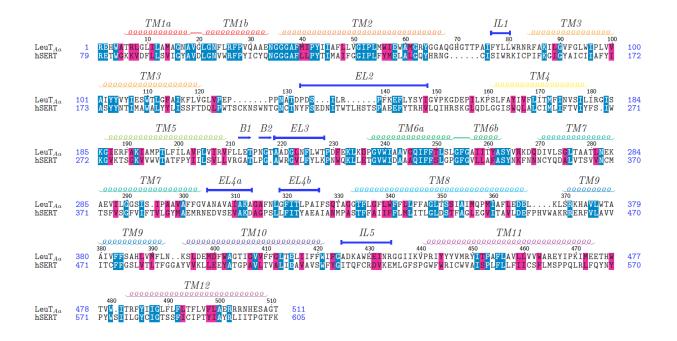


**Supplementary Figure A.** Virtual screening hits MI-11 through MI-20. Affinity dG docking score is indicated below each structure; as the value decreases, predicted binding affinity for the MAT target increases.



**Supplementary Figure B.** Sequence alignment of hSERT and  $\text{LeuT}_{Aa}$ . Identical residues are highlighted in blue; similar residues are highlighted in pink. Membrane topology and residue numbers are indicated above the sequences. Gaps are represented by dots within the sequence.