|  |  |  |
| --- | --- | --- |
| **Amino acid residues in CTII that interact with PC** | **Interactive residues in CTII that are shared between the phospholipid head group binding sites of PS and PC (shown are CT residues docked with PS)**  | **Interactive residues in CTII that are shared between the phospholipid head group binding sites of CL and PC** **(shown are CT residues docked with CL)** |
| №  |  Affinity (kcal/mol) | Interactive residues | № | Affinity(kcal/mol) | Interactive residues | № | Affinity(kcal/mol) | Interactive residues |
| 1 | ‒2.8 | **K+23** | 1 | -3.3 | **K+23** | 8 | -3.5 | **K+23** |
| 2 | ‒2.6 | **K+44**, **S45**(OH σ+), **S45**(NHpbσ+) | 3 | -3.2 | **K+44**, **S45**(OH σ+), **S45**(NHpbσ+) | NA | NA | **no match** |
| 3 | ‒2.5 | **K+44**, **S45**(OH σ+), **S45**(NHpbσ+), **K+50** | 3 | -3.2 | **K+44**, **S45**(OH σ+), **S45**(NHpbσ+), **K+50** | NA | NA | **no match** |
| 4 | ‒2.4 | **K+44**, **S45**(OH σ+), **S45**(NHpbσ+) | 3 | -3.2 | **K+44**, **S45**(OH σ+), **S45**(NHpbσ+) | NA | NA | **no match** |
| 5 | ‒2.3 | **K+5**, **K+18**, **Y22**(OH σ+) | 9 | -2.8 | **K+5**, **K+18**, **Y22**(OH σ+) | 6 | -3.6 | **K+5**, **K+18**, **Y22**(OH σ+) |
| 6 | ‒2.3 | **K+18**, **Y22**(OH σ+), **K+35** | 9 | -2.8 | **K+18**, **Y22**(OH σ+), **K+35** | 6 | -3.6 | **K+18**, **Y22**(OH σ+), **K+35** |
| 7 | ‒2.3 | **K+44**, **S45**(OH σ+), **S45**(NHpbσ+) | 3 | -3.2 | **K+44**, **S45**(OH σ+), **S45**(NHpbσ+) | NA | NA | **no match** |
| 8 | ‒2.3 | **P33**(C=Opb σ−), **K+35**, **R+36** | 9 | -2.8 | **K+35** | 6 | -3.6 | **K+35** |
| 9 | ‒2.2 | **G17**(NHpb σ+), **N19**(NH2 σ+), **N19**(C=Opb σ−) | NA | NA | **no match** | 9 | -3.9 | **no match** |

**S3 Table. Summary of amino acid residues in CTII that are shared among lipid binding sites.**

Amino acid residues on the molecular surface of CTII that bind to the phospholipid head group of CL, PC, and PS based on a total of nine top ranking docked conformations as determined by AutoDock. In addition, the table also shows the total number of amino acids that interact with either PS or CL and that are shared with PC binding sites. For the complete list of amino acid residues that interact with CTII refer to Tables S9 and S11. Numbers in columns (№) correspond to the binding site number in the order by which it was ranked by AutoDock. Energies of binding affinities are expressed in kcal/mol. Subscript pb denotes peptide bonds. NA: Not applicable