|  |  |  |  |
| --- | --- | --- | --- |
| Binding site # | *PS polar groups* | *CTI amino acid residues & PS* | *Bond type and orientation* |
| **Binding site 1**Affinity (kcal/mol)‒3.3 | **PO4–** | **K+23**(N+H3) | ionic |
| **COO–** | **NA** | into solution |
| **2C=O**σ− | **K+23**(N+H3) | ion-polar |
| **N+H3** | **T56**(Oσ−H) | ion-polar |
| **Binding site 2**Affinity (kcal/mol)‒3.3 | **PO4–** | **K+2**(N+H3) | ionic, into solution |
| **COO–** | **T13**(OH σ+), **T13**(NHpbσ+) | 2 hydrogen |
| **1CO**σ**–C** | **S11**(OHσ+) | hydrogen |
| **1****C=O**σ− | **S11**(OHσ+) | hydrogen |
| **N+H3** | **S11**(Oσ−H), **S11**(C=Opbσ−) | 2 ion-polar |
| **Binding site 3**Affinity (kcal/mol)‒3.2 | **PO4–** | **K+44**(N+H3), **S45**(NHpbσ+), **PS**(N+H3) | 3 ionic |
| **COO–** | **K+50**(N+H3) | ionic |
| **2C=O** σ− | **S45**(OHσ+) | hydrogen |
| **N+H3** | **PS**(PO4–) | ionic, into solution |
| **Binding site 4**Affinity (kcal/mol)‒3.2 | **PO4–** | **S45**(OH σ+), **K+50**(N+H3) | ionic, ion-polar |
| **COO–** | **C53**(NHpb σ+) | ion-hydrogen |
| **2C=O** σ− | **K+50**(N+H3) | ion-polar |
| **N+H3** | **K+44**(N+H3), **P43**(C=Opbσ−) | ionic repulsion, ion-polar, i.s. |
| **Binding site 5**Affinity (kcal/mol)‒3.0 | **PO4–** | **S45**(OH σ+), **S45**(NHpb σ+) | 2 ion-hydrogen |
| **COO–** | **C53**(NHpb σ+) | ion-hydrogen |
| **1CO**σ**–C** | **K+50**(N+H3) | ion-polar |
| **1C=O** σ− | **K+50**(N+H3) | ion-polar |
| **N+H3** | **K+44**(N+H3), **P43**(C=Opbσ−) | ionic repulsion, ion-polar, i.s. |
| **Binding site 6**Affinity (kcal/mol)‒2.9 | **PO4–** | **S45**(NHpb σ+), **PS**(N+H3) | ion-hydrogen, ionic |
| **COO–** | **K+50**(N+H3) | ionic |
| **1CO**σ**–C** | **K+50**(N+H3) | ion-polar |
| **1C=O** σ− | **K+50**(N+H3) | ion-polar |
| **2CO**σ**–C** | **S45**(OH σ+) | hydrogen |
| **N+H3** | **PS**(PO4–) | ionic, into solution |
| **Binding site 7**Affinity (kcal/mol)‒2.8 | **PO4–** | **K+44**(N+H3), **S45**(NHpbσ+), **S45**(OH σ+) | ionic, 2 ion-hydrogen |
| **COO–** | **C53**(NHpb σ+) | ion-hydrogen |
| **1CO**σ**–C** | **K+50**(N+H3) | ion-hydrogen |
| **N+H3** | NA | into solution |
| **Binding site 8**Affinity (kcal/mol)‒2.8 | **PO4–** | **K+23**(N+H3) | ionic |
| **COO–** | NA | into solution |
| **1C=O** σ− | **K+23**(N+H3) | ion-polar |
| **NH3+** | **C59**(C=Opbσ−) | ion-polar |
| **Binding site 9**Affinity (kcal/mol)‒2.8 | **PO4–** | **Y22**(OH σ+) | ion-hydrogen |
| **COO–** | **K+35**(N+H3), **Y22**(OHσ+) | ionic, ion-hydrogen |
| **1CO**σ**–C** | **C38**(NHpb σ+) | hydrogen |
| **1C=O** σ− | **K+5**(N+H3) | ion-polar |
| **2C=O** σ− | **K+18**(N+H3) | ion-polar |
| **N+H3** | **Y22**(Oσ−H) | ion-polar |

**S8 Table. Summary of amino acid residues in CTII that interact with PS**

Hypothetical binding sites in CTII that bind to the phospholipid head group of PS as determined by AutoDock modeling. The table shows a complete list of amino acid residues in CTII that interact with the PS charged and polar groups for various binding sites. Pb in C=Opbσ− or in NHpbσ+ denotes a peptide bond.