**Table S1:** Ovalbumin hydrolysate peptides and their SMILES

|  |  |  |
| --- | --- | --- |
| **SN** | **Hydrolysate peptides (Ligands)** | **SMILES notation** |
| 1 | GSI**GAA**SM | NCC(=O)N[C@@]([H])(CO)C(=O)N[C@@]([H])([C@]([H])(CC)C)C(=O)NCC(=O)N[C@@]([H])(C)C(=O)N[C@@]([H])(C)C(=O)N[C@@]([H])(CO)C(=O)N[C@@]([H])(CCSC)C(=O)O |
| 2 | DVF | N[C@@]([H])(CC(=O)O)C(=O)N[C@@]([H])(C(C)C)C(=O)N[C@@]([H])(Cc1ccccc1)C(=O)O |
| 3 | CPIAIM | N[C@@]([H])(CS)C(=O)N1[C@@]([H])(CCC1)C(=O)N[C@@]([H])([C@]([H])(CC)C)C(=O)N[C@@]([H])(C)C(=O)N[C@@]([H])([C@]([H])(CC)C)C(=O)N[C@@]([H])(CCSC)C(=O)O |
| 4 | SAL | N[C@@]([H])(CO)C(=O)N[C@@]([H])(C)C(=O)N[C@@]([H])(CC(C)C)C(=O)O |
| 5 | GAK | NCC(=O)N[C@@]([H])(C)C(=O)N[C@@]([H])(CCCCN)C(=O)O |
| 6 | DSTR | N[C@@]([H])(CC(=O)O)C(=O)N[C@@]([H])(CO)C(=O)N[C@@]([H])([C@]([H])(O)C)C(=O)N[C@@]([H])(CCCNC(=N)N)C(=O)O |
| 7 | TQIN | N[C@@]([H])([C@]([H])(O)C)C(=O)N[C@@]([H])(CCC(=O)N)C(=O)N[C@@]([H])([C@]([H])(CC)C)C(=O)N[C@@]([H])(CC(=O)N)C(=O)O |
| 8 | **VVR** | **N[C@@]([H])(C(C)C)C(=O)N[C@@]([H])(C(C)C)C(=O)N[C@@]([H])(CCCNC(=N)N)C(=O)O** |
| 9 | PGF | N1[C@@]([H])(CCC1)C(=O)NCC(=O)N[C@@]([H])(Cc1ccccc1)C(=O)O |
| 10 | GDSIEAQCGTSVN | NCC(=O)N[C@@]([H])(CC(=O)O)C(=O)N[C@@]([H])(CO)C(=O)N[C@@]([H])([C@]([H])(CC)C)C(=O)N[C@@]([H])(CCC(=O)O)C(=O)N[C@@]([H])(C)C(=O)N[C@@]([H])(CCC(=O)N)C(=O)N[C@@]([H])(CS)C(=O)NCC(=O)N[C@@]([H])([C@]([H])(O)C)C(=O)N[C@@]([H])(CO)C(=O)N[C@@]([H])(C(C)C)C(=O)N[C@@]([H])(CC(=O)N)C(=O)O |
| 11 | SSL | N[C@@]([H])(CO)C(=O)N[C@@]([H])(CO)C(=O)N[C@@]([H])(CC(C)C)C(=O)O |
| 12 | DIL | N[C@@]([H])(CC(=O)O)C(=O)N[C@@]([H])([C@]([H])(CC)C)C(=O)N[C@@]([H])(CC(C)C)C(=O)O |
| 13 | QITK | N[C@@]([H])(CCC(=O)N)C(=O)N[C@@]([H])([C@]([H])(CC)C)C(=O)N[C@@]([H])([C@]([H])(O)C)C(=O)N[C@@]([H])(CCCCN)C(=O)O |
| 14 | DVY | N[C@@]([H])(CC(=O)O)C(=O)N[C@@]([H])(C(C)C)C(=O)N[C@@]([H])(Cc1ccc(O)cc1)C(=O)O |
| 15 | ASR | N[C@@]([H])(C)C(=O)N[C@@]([H])(CO)C(=O)N[C@@]([H])(CCCNC(=N)N)C(=O)O |
| 16 | AEER | N[C@@]([H])(C)C(=O)N[C@@]([H])(CCC(=O)O)C(=O)N[C@@]([H])(CCC(=O)O)C(=O)N[C@@]([H])(CCCNC(=N)N)C(=O)O |
| 17 | PIL | N1[C@@]([H])(CCC1)C(=O)N[C@@]([H])([C@]([H])(CC)C)C(=O)N[C@@]([H])(CC(C)C)C(=O)O |
| 18 | PEY | N1[C@@]([H])(CCC1)C(=O)N[C@@]([H])(CCC(=O)O)C(=O)N[C@@]([H])(Cc1ccc(O)cc1)C(=O)O |
| 19 | QCVK | N[C@@]([H])(CCC(=O)N)C(=O)N[C@@]([H])(CS)C(=O)N[C@@]([H])(C(C)C)C(=O)N[C@@]([H])(CCCCN)C(=O)O |
| 20 | GGL | NCC(=O)NCC(=O)N[C@@]([H])(CC(C)C)C(=O)O |
| 21 | EPIN | N[C@@]([H])(CCC(=O)O)C(=O)N1[C@@]([H])(CCC1)C(=O)N[C@@]([H])([C@]([H])(CC)C)C(=O)N[C@@]([H])(CC(=O)N)C(=O)O |
| 22 | QTAADQAR | N[C@@]([H])(CCC(=O)N)C(=O)N[C@@]([H])([C@]([H])(O)C)C(=O)N[C@@]([H])(C)C(=O)N[C@@]([H])(C)C(=O)N[C@@]([H])(CC(=O)O)C(=O)N[C@@]([H])(CCC(=O)N)C(=O)N[C@@]([H])(C)C(=O)N[C@@]([H])(CCCNC(=N)N)C(=O)O |
| 23 | VESQTN | N[C@@]([H])(C(C)C)C(=O)N[C@@]([H])(CCC(=O)O)C(=O)N[C@@]([H])(CO)C(=O)N[C@@]([H])(CCC(=O)N)C(=O)N[C@@]([H])([C@]([H])(O)C)C(=O)N[C@@]([H])(CC(=O)N)C(=O)O |
| 24 | GIIR | NCC(=O)N[C@@]([H])([C@]([H])(CC)C)C(=O)N[C@@]([H])([C@]([H])(CC)C)C(=O)N[C@@]([H])(CCCNC(=N)N)C(=O)O |
| 25 | QPSSVDSQTAM | N[C@@]([H])(CCC(=O)N)C(=O)N1[C@@]([H])(CCC1)C(=O)N[C@@]([H])(CO)C(=O)N[C@@]([H])(CO)C(=O)N[C@@]([H])(C(C)C)C(=O)N[C@@]([H])(CC(=O)O)C(=O)N[C@@]([H])(CO)C(=O)N[C@@]([H])(CCC(=O)N)C(=O)N[C@@]([H])([C@]([H])(O)C)C(=O)N[C@@]([H])(C)C(=O)N[C@@]([H])(CCSC)C(=O)O |
| 26 | AIVF | N[C@@]([H])(C)C(=O)N[C@@]([H])([C@]([H])(CC)C)C(=O)N[C@@]([H])(C(C)C)C(=O)N[C@@]([H])(Cc1ccccc1)C(=O)O |
| 27 | DEDTQAM | N[C@@]([H])(CC(=O)O)C(=O)N[C@@]([H])(CCC(=O)O)C(=O)N[C@@]([H])(CC(=O)O)C(=O)N[C@@]([H])([C@]([H])(O)C)C(=O)N[C@@]([H])(CCC(=O)N)C(=O)N[C@@]([H])(C)C(=O)N[C@@]([H])(CCSC)C(=O)O |
| 28 | VTEQESK | N[C@@]([H])(C(C)C)C(=O)N[C@@]([H])([C@]([H])(O)C)C(=O)N[C@@]([H])(CCC(=O)O)C(=O)N[C@@]([H])(CCC(=O)N)C(=O)N[C@@]([H])(CCC(=O)O)C(=O)N[C@@]([H])(CO)C(=O)N[C@@]([H])(CCCCN)C(=O)O |
| 29 | PVQM | N1[C@@]([H])(CCC1)C(=O)N[C@@]([H])(C(C)C)C(=O)N[C@@]([H])(CCC(=O)N)C(=O)N[C@@]([H])(CCSC)C(=O)O |
| 30 | QIGL | N[C@@]([H])(CCC(=O)N)C(=O)N[C@@]([H])([C@]([H])(CC)C)C(=O)NCC(=O)N[C@@]([H])(CC(C)C)C(=O)O |
| 31 | VASM | N[C@@]([H])(C(C)C)C(=O)N[C@@]([H])(C)C(=O)N[C@@]([H])(CO)C(=O)N[C@@]([H])(CCSC)C(=O)O |
| 32 | ASEK | N[C@@]([H])(C)C(=O)N[C@@]([H])(CO)C(=O)N[C@@]([H])(CCC(=O)O)C(=O)N[C@@]([H])(CCCCN)C(=O)O |
| 33 | ASGTM | N[C@@]([H])(C)C(=O)N[C@@]([H])(CO)C(=O)NCC(=O)N[C@@]([H])([C@]([H])(O)C)C(=O)N[C@@]([H])(CCSC)C(=O)O |
| 34 | PD**EVSGL** | N1[C@@]([H])(CCC1)C(=O)N[C@@]([H])(CC(=O)O)C(=O)N[C@@]([H])(CCC(=O)O)C(=O)N[C@@]([H])(C(C)C)C(=O)N[C@@]([H])(CO)C(=O)NCC(=O)N[C@@]([H])(CC(C)C)C(=O)O |
| 35 | EQL | N[C@@]([H])(CCC(=O)O)C(=O)N[C@@]([H])(CCC(=O)N)C(=O)N[C@@]([H])(CC(C)C)C(=O)O |
| 36 | ESIIN | N[C@@]([H])(CCC(=O)O)C(=O)N[C@@]([H])(CO)C(=O)N[C@@]([H])([C@]([H])(CC)C)C(=O)N[C@@]([H])([C@]([H])(CC)C)C(=O)N[C@@]([H])(CC(=O)N)C(=O)O |
| 37 | TEW | N[C@@]([H])([C@]([H])(O)C)C(=O)N[C@@]([H])(CCC(=O)O)C(=O)N[C@@]([H])(CC(=CN2)C1=C2C=CC=C1)C(=O)O |
| 38 | TSSN | N[C@@]([H])([C@]([H])(O)C)C(=O)N[C@@]([H])(CO)C(=O)N[C@@]([H])(CO)C(=O)N[C@@]([H])(CC(=O)N)C(=O)O |
| 39 | EER | N[C@@]([H])(CCC(=O)O)C(=O)N[C@@]([H])(CCC(=O)O)C(=O)N[C@@]([H])(CCCNC(=N)N)C(=O)O |
| 40 | EEK | N[C@@]([H])(CCC(=O)O)C(=O)N[C@@]([H])(CCC(=O)O)C(=O)N[C@@]([H])(CCCCN)C(=O)O |
| 41 | T**SVL** | N[C@@]([H])([C@]([H])(O)C)C(=O)N[C@@]([H])(CO)C(=O)N[C@@]([H])(C(C)C)C(=O)N[C@@]([H])(CC(C)C)C(=O)O |
| 42 | GITDVF | NCC(=O)N[C@@]([H])([C@]([H])(CC)C)C(=O)N[C@@]([H])([C@]([H])(O)C)C(=O)N[C@@]([H])(CC(=O)O)C(=O)N[C@@]([H])(C(C)C)C(=O)N[C@@]([H])(Cc1ccccc1)C(=O)O |
| 43 | **SSS**AN | **N[C@@]([H])(CO)C(=O)N[C@@]([H])(CO)C(=O)N[C@@]([H])(CO)C(=O)N[C@@]([H])(C)C(=O)N[C@@]([H])(CC(=O)N)C(=O)O** |
| 44 | SGISSAESL | N[C@@]([H])(CO)C(=O)NCC(=O)N[C@@]([H])([C@]([H])(CC)C)C(=O)N[C@@]([H])(CO)C(=O)N[C@@]([H])(CO)C(=O)N[C@@]([H])(C)C(=O)N[C@@]([H])(CCC(=O)O)C(=O)N[C@@]([H])(CO)C(=O)N[C@@]([H])(CC(C)C)C(=O)O |
| 45 | I**SQAVH** | N[C@@]([H])([C@]([H])(CC)C)C(=O)N[C@@]([H])(CO)C(=O)N[C@@]([H])(CCC(=O)N)C(=O)N[C@@]([H])(C)C(=O)N[C@@]([H])(C(C)C)C(=O)N[C@@]([H])(CC1=CN=C-N1)C(=O)O |
| 46 | AAH | N[C@@]([H])(C)C(=O)N[C@@]([H])(C)C(=O)N[C@@]([H])(CC1=CN=C-N1)C(=O)O |
| 47 | AEIN | N[C@@]([H])(C)C(=O)N[C@@]([H])(CCC(=O)O)C(=O)N[C@@]([H])([C@]([H])(CC)C)C(=O)N[C@@]([H])(CC(=O)N)C(=O)O |
| 48 | EAGR | N[C@@]([H])(CCC(=O)O)C(=O)N[C@@]([H])(C)C(=O)NCC(=O)N[C@@]([H])(CCCNC(=N)N)C(=O)O |
| 49 | EVVGS**AEAGVD**AASVSEEF | N[C@@]([H])(CCC(=O)O)C(=O)N[C@@]([H])(C(C)C)C(=O)N[C@@]([H])(C(C)C)C(=O)NCC(=O)N[C@@]([H])(CO)C(=O)N[C@@]([H])(C)C(=O)N[C@@]([H])(CCC(=O)O)C(=O)N[C@@]([H])(C)C(=O)NCC(=O)N[C@@]([H])(C(C)C)C(=O)N[C@@]([H])(CC(=O)O)C(=O)N[C@@]([H])(C)C(=O)N[C@@]([H])(C)C(=O)N[C@@]([H])(CO)C(=O)N[C@@]([H])(C(C)C)C(=O)N[C@@]([H])(CO)C(=O)N[C@@]([H])(CCC(=O)O)C(=O)N[C@@]([H])(CCC(=O)O)C(=O)N[C@@]([H])(Cc1ccccc1)C(=O)O |
| 50 | ADH | N[C@@]([H])(C)C(=O)N[C@@]([H])(CC(=O)O)C(=O)N[C@@]([H])(CC1=CN=C-N1)C(=O)O |
| 51 | CIK | N[C@@]([H])(CS)C(=O)N[C@@]([H])([C@]([H])(CC)C)C(=O)N[C@@]([H])(CCCCN)C(=O)O |
| 52 | IATN | N[C@@]([H])([C@]([H])(CC)C)C(=O)N[C@@]([H])(C)C(=O)N[C@@]([H])([C@]([H])(O)C)C(=O)N[C@@]([H])(CC(=O)N)C(=O)O |
| 53 | **AVL** | **N[C@@]([H])(C)C(=O)N[C@@]([H])(C(C)C)C(=O)N[C@@]([H])(CC(C)C)C(=O)O** |
| 54 | C**VSP** | N[C@@]([H])(CS)C(=O)N[C@@]([H])(C(C)C)C(=O)N[C@@]([H])(CO)C(=O)N1[C@@]([H])(CCC1)C(=O)O |
| 55 | VY | N[C@@]([H])(C(C)C)C(=O)N[C@@]([H])(Cc1ccc(O)cc1)C(=O)O |
| 56 | PR | N1[C@@]([H])(CCC1)C(=O)N[C@@]([H])(CCCNC(=N)N)C(=O)O |
| 57 | AF | N[C@@]([H])(C)C(=O)N[C@@]([H])(Cc1ccccc1)C(=O)O |
| 58 | SF | N[C@@]([H])(CO)C(=O)N[C@@]([H])(Cc1ccccc1)C(=O)O |
| 59 | EK | N[C@@]([H])(CCC(=O)O)C(=O)N[C@@]([H])(CCCCN)C(=O)O |
| 60 | IL | N[C@@]([H])([C@]([H])(CC)C)C(=O)N[C@@]([H])(CC(C)C)C(=O)O |
| 61 | VM | N[C@@]([H])(C(C)C)C(=O)N[C@@]([H])(CCSC)C(=O)O |
| 62 | EF | N[C@@]([H])(CCC(=O)O)C(=O)N[C@@]([H])(Cc1ccccc1)C(=O)O |
| 63 | SL | N[C@@]([H])(CO)C(=O)N[C@@]([H])(CC(C)C)C(=O)O |
| 64 | PF | N1[C@@]([H])(CCC1)C(=O)N[C@@]([H])(Cc1ccccc1)C(=O)O |
| 65 | GL | NCC(=O)N[C@@]([H])(CC(C)C)C(=O)O |
| 66 | **YNL** | **N[C@@]([H])(Cc1ccc(O)cc1)C(=O)N[C@@]([H])(CC(=O)N)C(=O)N[C@@]([H])(CC(C)C)C(=O)O** |
| 67 | **YLG** | **N[C@@]([H])(Cc1ccc(O)cc1)C(=O)N[C@@]([H])(CC(C)C)C(=O)NCC(=O)O** |
| 68 | **LPF** | **N[C@@]([H])(CC(C)C)C(=O)N1[C@@]([H])(CCC1)C(=O)N[C@@]([H])(Cc1ccccc1)C(=O)O** |
| 69 | **QIGLF** | **N[C@@]([H])(CCC(=O)N)C(=O)N[C@@]([H])([C@]([H])(CC)C)C(=O)NCC(=O)N[C@@]([H])(CC(C)C)C(=O)N[C@@]([H])(Cc1ccccc1)C(=O)O** |
| 70 | **VSP** | **N[C@@]([H])(C(C)C)C(=O)N[C@@]([H])(CO)C(=O)N1[C@@]([H])(CCC1)C(=O)O** |
| 71 | **LWE** | **N[C@@]([H])(CC(C)C)C(=O)N[C@@]([H])(CC(=CN2)C1=C2C=CC=C1)C(=O)N[C@@]([H])(CCC(=O)O)C(=O)O** |

Serial number (SN) 1-65 were peptides from enzymatic hydrolyzed protein, and SN 66-71 were most active peptides from the unhydrolyzed screening.