**Supporting Information:**

# Identification and Mechanistic Characterization of Pancreatic Lipase-Inhibitory Peptides from Pea Protein Hydrolysates by Peptidomics, Molecular Docking, and Molecular Dynamics Simulation

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Table S1. Hydrolysis conditions of different enzymes.

| Type | pH | Temperature（℃） |
|---|---|---|
| Trypsin | 8 | 37 |
| Pepsin | 2.5 | 37 |
| Papain | 7 | 50 |
| Alkaline protease | 7 | 50 |
| Neutral protease | 10 | 50 |

Table S2. Factor levels for the response surface design.

| Std | Run | A | B | C | D | Inhibition |
|---|---|---|---|---|---|---|
| 23 | 1 | 10.5 | 45 | 3 | 3000 | 27.9897 |
| 9 | 2 | 10 | 40 | 2 | 6000 | 26.4875 |
| 3 | 3 | 10 | 50 | 2 | 4000 | 24.0074 |
| 11 | 4 | 10 | 50 | 2 | 6000 | 21.1431 |
| 12 | 5 | 11 | 50 | 2 | 6000 | 28.2613 |
| 14 | 6 | 11 | 40 | 4 | 6000 | 27.4194 |
| 15 | 7 | 10 | 50 | 4 | 6000 | 32.4584 |
| 24 | 8 | 10.5 | 45 | 3 | 7000 | 31.2683 |
| 28 | 9 | 10.5 | 45 | 3 | 5000 | 43.8836 |
| 16 | 10 | 11 | 50 | 4 | 6000 | 25.0993 |
| 18 | 11 | 11.5 | 45 | 3 | 5000 | 23.5716 |
| 6 | 12 | 11 | 40 | 4 | 4000 | 22.8122 |
| 25 | 13 | 10.5 | 45 | 3 | 5000 | 43.4882 |
| 8 | 14 | 11 | 50 | 4 | 4000 | 24.2052 |
| 13 | 15 | 10 | 40 | 4 | 6000 | 32.9649 |
| 22 | 16 | 10.5 | 45 | 5 | 5000 | 30.4585 |
| 26 | 17 | 10.5 | 45 | 3 | 5000 | 41.1969 |
| 29 | 18 | 10.5 | 45 | 3 | 5000 | 41.495 |
| 4 | 19 | 11 | 50 | 2 | 4000 | 26.6224 |
| 17 | 20 | 9.5 | 45 | 3 | 5000 | 26.4585 |
| 5 | 21 | 10 | 40 | 4 | 4000 | 32.8089 |
| 19 | 22 | 10.5 | 35 | 3 | 5000 | 33.9971 |
| 30 | 23 | 10.5 | 45 | 3 | 5000 | 42.5323 |
| 1 | 24 | 10 | 40 | 2 | 4000 | 27.8925 |
| 21 | 25 | 10.5 | 45 | 1 | 5000 | 29.1127 |
| 2 | 26 | 11 | 40 | 2 | 4000 | 32.5883 |
| 7 | 27 | 10 | 50 | 4 | 4000 | 31.1621 |
| 20 | 28 | 10.5 | 55 | 3 | 5000 | 25.5618 |
| 10 | 29 | 11 | 40 | 2 | 6000 | 33.497 |
| 27 | 30 | 10.5 | 45 | 3 | 5000 | 41.1796 |

Table S3. ANOVA results for the RSM model.

| Source | Degree of Freedom | Sum of squares | Mean of squares | *F* value | *P* value |
|---|---|---|---|---|---|
| FO(A, B, C, D) | 4 | 87.2859 | 21.8215 | 19.2739 | 0.0000 |
| TWI(A, B, C, D) | 6 | 196.0741 | 32.6790 | 28.8638 | 0.0000 |
| PQ(A, B, C, D) | 4 | 981.2339 | 245.3085 | 216.6695 | 0.0000 |
| Lack of fit | 10 | 9.8890 | 0.9889 | 0.6970 | 0.7073 |
| Pure error | 5 | 7.0936 | 1.4187 | | |
| Residuals | 15 | 16.9827 | 1.1322 | | |

FO: first order; TWI: two-way interactions; PQ: pure quadratic

Table S4. Peptide sequences identified in PPH.

| Sequence | Length | Sequence | Length | Sequence | Length | Sequence | Length |
|---|---|---|---|---|---|---|---|
| LLF | 3 | LNF | 3 | LFLQ | 4 | LLSL | 4 |
| WRL | 3 | VAW | 3 | VEFL | 4 | FDLL | 4 |
| VVF | 3 | LVY | 3 | KLLL | 4 | DLLR | 4 |
| FEK | 3 | LVR | 3 | LLGF | 4 | LKLF | 4 |
| LYL | 3 | MVL | 3 | VLLV | 4 | LLAL | 4 |
| FVF | 3 | QYL | 3 | PLLR | 4 | YLEL | 4 |
| SLL | 3 | NPR | 3 | VVAL | 4 | TFVL | 4 |
| LLL | 3 | ALW | 3 | LEVL | 4 | LLVQ | 4 |
| QLL | 3 | SLW | 3 | DLRL | 4 | LANL | 4 |
| LFL | 3 | FML | 3 | VTLR | 4 | YDAL | 4 |
| YLF | 3 | WKS | 3 | VGSL | 4 | FLLR | 4 |
| FAL | 3 | PKL | 3 | DFTF | 4 | VVLE | 4 |
| DLL | 3 | YML | 3 | LNRF | 4 | NYGL | 4 |
| TLF | 3 | FRL | 3 | LEKL | 4 | VTEL | 4 |
| YSF | 3 | GLR | 3 | LYRF | 4 | PLRL | 4 |
| VRL | 3 | PVL | 3 | LEFL | 4 | YKLL | 4 |
| GLL | 3 | LPH | 3 | FDPF | 4 | FNLR | 4 |
| NLF | 3 | DLR | 3 | KLFL | 4 | VTAL | 4 |
| SYL | 3 | KGF | 3 | LRLL | 4 | HLLL | 4 |
| LFE | 3 | VSW | 3 | VALL | 4 | LAPL | 4 |
| LSF | 3 | ELL | 3 | RNPF | 4 | YLFK | 4 |
| LRL | 3 | WLR | 3 | SGLL | 4 | DLGL | 4 |
| YVL | 3 | FGF | 3 | YLFR | 4 | VEKL | 4 |
| ELF | 3 | LFW | 3 | LVKL | 4 | LHML | 4 |
| LKL | 3 | VLW | 3 | KFLL | 4 | LFLK | 4 |
| FFK | 3 | WLE | 3 | LLLL | 4 | VVFK | 4 |
| EFL | 3 | WFE | 3 | LLLR | 4 | LKPF | 4 |
| VDL | 3 | VMF | 3 | FLVR | 4 | LAAL | 4 |
| LQL | 3 | VFK | 3 | VRGL | 4 | AVAL | 4 |
| VKL | 3 | LKF | 3 | LVLL | 4 | FLGR | 4 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| LVF | 3 | VHP | 3 | FFSN | 4 | LFLE | 4 |
| VLR | 3 | ELY | 3 | LHVL | 4 | NLFF | 4 |
| VFW | 3 | LDF | 3 | FLLF | 4 | RLLY | 4 |
| VYL | 3 | MGF | 3 | VLTL | 4 | LLKF | 4 |
| LWL | 3 | LPF | 3 | LLRL | 4 | VLVK | 4 |
| YLL | 3 | LWR | 3 | LFSY | 4 | FSLR | 4 |
| VDF | 3 | QLK | 3 | TALL | 4 | LDRQ | 4 |
| LDL | 3 | FSL | 3 | VLLQ | 4 | FLVM | 4 |
| LNL | 3 | HGL | 3 | LYPL | 4 | LKLY | 4 |
| WAL | 3 | LQY | 3 | VKLL | 4 | VGHS | 4 |
| LHL | 3 | LPR | 3 | VLKL | 4 | KLLR | 4 |
| YAL | 3 | LSY | 3 | LHPG | 4 | EFLR | 4 |
| LGR | 3 | LKA | 3 | LKVL | 4 | RKRL | 4 |
| VAR | 3 | LAW | 3 | LLEY | 4 | VFKK | 4 |
| FLM | 3 | PNK | 3 | SPPL | 4 | PATL | 4 |
| TFL | 3 | YLM | 3 | GRLF | 4 | LRDLL | 5 |
| FRF | 3 | YPL | 3 | GKLF | 4 | LALTL | 5 |
| VVK | 3 | PLY | 3 | LLFL | 4 | KDLLL | 5 |
| DRL | 3 | LEY | 3 | LEAL | 4 | DLRLL | 5 |
| FLK | 3 | LMY | 3 | SSLL | 4 | LFLQL | 5 |
| FLY | 3 | GEL | 3 | YLPF | 4 | RKFLL | 5 |
| LLR | 3 | TLP | 3 | LKYL | 4 | EFDLR | 5 |
| KFL | 3 | QNL | 3 | LLNL | 4 | VGSLL | 5 |
| FLA | 3 | KFT | 3 | YALL | 4 | TLLFL | 5 |
| GWL | 3 | ELK | 3 | GFSL | 4 | VRDLL | 5 |
| LQF | 3 | FSK | 3 | VHLF | 4 | VADLL | 5 |
| LLK | 3 | NHV | 3 | LKFL | 4 | LAVFK | 5 |
| WLL | 3 | NKE | 3 | VAWR | 4 | LVKLL | 5 |
| RVL | 3 | TFR | 3 | TLFE | 4 | KLLRL | 5 |
| SKW | 3 | LFR | 3 | VADL | 4 | LLRNL | 5 |
| KPF | 3 | RLL | 3 | NFPF | 4 | LLRLL | 5 |
| KLL | 3 | LKW | 3 | LRLV | 4 | LFSLF | 5 |
| FKF | 3 | PNR | 3 | SKVV | 4 | FKKLF | 5 |
| YMF | 3 | LALF | 4 | FDLR | 4 | LKFLT | 5 |