

**Table S3.** Selection of potential DPPIV-inhibitory peptides as a function of PepSite *P* value, structure-activity relationship (SAR) modelling and *in silico* gastro-intestinal digestion (GID) stability. Selected peptides were reported in bold red.

| Sequence     | PepSite <i>P</i> value for DPPIV (pdb: 1NU6) | SAR  | GID   |
|--------------|--|--|---|
| PPF          | 1.63E-05                                     | /  | /   |
| PNP          | 2.64E-05                                     | /  | /   |
| <b>IPP</b>   | 4.26E-05                                     | I at the N-terminus and P in second position | Stable  |
| QGP          | 1.02E-04                                     | /  | /   |
| PFP          | 1.11E-04                                     | /  | /   |
| PIP          | 1.18E-04                                     | /  | /   |
| VPP          | 1.59E-04                                     | /  | /   |
| <b>LPPT</b>  | 4.76E-04                                     | L at the N-terminus and P in second position | Stable  |
| PFPE         | 5.59E-04                                     | /  | /   |
| QTPVVVPPFL   | 6.76E-04                                     | /  | /   |
| PGPI         | 7.04E-04                                     | /  | /   |
| KIHPF        | 7.71E-04                                     | /  | /   |
| RFFVAPFPE    | 8.09E-04                                     | /  | /   |
| FALPQ        | 8.71E-04                                     | F at the N-terminus and A in second position | Unstable. Potential cleavage sites: F-A chymotrypsin and pepsin; L-P pepsin |
| FVAPFPE      | 9.62E-04                                     | /  | /   |
| FVAPFP       | 1.02E-03                                     | /  | /   |
| PFL          | 1.13E-03                                     | /  | /   |
| GIPIN        | 1.20E-03                                     | /  | /   |
| <b>APFPE</b> | 1.26E-03                                     | A at the N-terminus and P in second position | Stable  |
| VAPFPEVFGK   | 1.31E-03                                     | /  | /   |
| VMF          | 1.33E-03                                     | /  | /   |
| PNPIG        | 1.47E-03                                     | /  | /   |
| PGPIP        | 1.59E-03                                     | /  | /   |

|           |          |  |  |
|-----------|----------|--|--|
| IPPL*     | 1.68E-03 | I at the N-terminus<br>and P in second<br>position | Stable   |
| VPPFL     | 1.84E-03 | /  | /  |
| VVPPF     | 1.84E-03 | /  | /  |
| LVYFPFPGP | 1.86E-03 | /  | /  |
| FGK       | 2.02E-03 | /  | /  |
| PGIPN     | 2.07E-03 | /  | /  |
| IPPLT     | 2.20E-03 | I at the N-terminus<br>and P in second<br>position | Unstable. Potential<br>cleavage sites: L-T<br>chymotrypsin |
| FRQFYQL   | 2.46E-03 | /  | /  |
| WIQPK*    | 2.48E-03 | /  | /  |
| VAPFP     | 2.64E-03 | /  | /  |
| FVAPFPEVF | 2.83E-03 | /  | /  |
| LHLPLP    | 2.89E-03 | /  | /  |
| DKIHPF    | 2.91E-03 | /  | /  |
| FFVAP     | 2.96E-03 | /  | /  |
| EPF       | 3.45E-03 | /  | /  |
| PFPI      | 3.47E-03 | /  | /  |
| VAPFPEVF  | 3.61E-03 | /  | /  |
| PIPN      | 3.62E-03 | /  | /  |
| IHPF      | 3.80E-03 | /  | /  |
| NIPPL     | 3.84E-03 | /  | /  |
| PLW       | 4.31E-03 | /  | /  |
| EMPFPK    | 4.91E-03 | /  | /  |
| FFV       | 4.98E-03 | /  | /  |
| TPVVVPPFL | 5.22E-03 | /  | /  |
| WDQ       | 5.28E-03 | /  | /  |
| KFQ       | 5.37E-03 | /  | /  |
| VFG       | 5.47E-03 | /  | /  |
| FVAP      | 5.54E-03 | /  | /  |

|        |          |  |  |
|--------|----------|--|--|
| LPLP   | 6.04E-03 | L at the N-terminus<br>and P in second<br>position | Unstable. Potential<br>cleavage sites: L-P<br>pepsin |
| LVYPFP | 6.28E-03 | /  | /  |

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\* Previously identified as DPPIV-inhibitor

Threshold was set at 0.01. Peptides with *P*-value below the threshold are not shown