

## Supplementary Material to “A Kunitz-type peptide from *Dendroaspis polylepis* venom as a simultaneous inhibitor of serine and cysteine proteases”

**Additional file 3:** Sequences found in Peaks analysis (Figure 3B) present in the DPKEN9 peptide.

| Peptide                            | -10lgP | Mass      | Length | ppm  | m/z       | Z | RT    | Accession | PTM                  |
|------------------------------------|--------|-----------|--------|------|-----------|---|-------|-----------|----------------------|
| KQC(+57.02)EGFTWSGC(+57.02)GGNSNR  | 85.37  | 1943.8003 | 17     | -0.1 | 972.9073  | 2 | 18.28 | sp P00979 | Carbamidomethylation |
| KQC(+57.02)EGFTWSGC(+57.02)GGNSNR  | 47.24  | 1943.8003 | 17     | -0.1 | 648.9407  | 3 | 18.28 | sp P00979 | Carbamidomethylation |
| QC(+57.02)EGFTWSGC(+57.02)GGNSNR   | 66.08  | 1815.7053 | 16     | 0.0  | 908.8599  | 2 | 18.82 | sp P00979 | Carbamidomethylation |
| QC(+57.02)EGFTWSGC(+57.02)GGNSNR   | 30.57  | 1815.7053 | 16     | -0.3 | 606.2422  | 3 | 19.02 | sp P00979 | Carbamidomethylation |
| QC(+57.02)EGFTWSGC(+57.02)GGNSNR   | 19.89  | 1815.7053 | 16     | -0.6 | 908.8594  | 2 | 19.55 | sp P00979 | Carbamidomethylation |
| C(+57.02)YQKIPAFYYNQKK             | 63.34  | 1849.9185 | 14     | -0.3 | 617.6466  | 3 | 18.53 | sp P00979 | Carbamidomethylation |
| C(+57.02)YQKIPAFYYNQKK             | 61.35  | 1849.9185 | 14     | 0.4  | 925.9669  | 2 | 18.58 | sp P00979 | Carbamidomethylation |
| KKQC(+57.02)EGFTWSGC(+57.02)GGNSNR | 63.19  | 2071.8953 | 18     | 0.3  | 1036.9552 | 2 | 17.82 | sp P00979 | Carbamidomethylation |
| KKQC(+57.02)EGFTWSGC(+57.02)GGNSNR | 45.57  | 2071.8953 | 18     | -1.0 | 691.6383  | 3 | 17.80 | sp P00979 | Carbamidomethylation |
| C(+57.02)YQKIPAFYYNQK              | 58.74  | 1721.8235 | 13     | 0.6  | 861.9196  | 2 | 19.06 | sp P00979 | Carbamidomethylation |
| C(+57.02)YQKIPAFYYNQK              | 55.41  | 1721.8235 | 13     | -0.6 | 574.9481  | 3 | 19.04 | sp P00979 | Carbamidomethylation |
| IPAFYYNQKK                         | 56.58  | 1270.6709 | 10     | 0.7  | 636.3432  | 2 | 18.55 | sp P00979 |                      |
| IPAFYYNQKK                         | 28.02  | 1270.6709 | 10     | 1.3  | 424.5648  | 3 | 18.55 | sp P00979 |                      |
| IPAFYYNQK                          | 54.77  | 1142.5760 | 9      | 0.8  | 572.2958  | 2 | 19.17 | sp P00979 |                      |
| IPAFYYNQK                          | 54.21  | 1142.5760 | 9      | -0.3 | 572.2951  | 2 | 19.45 | sp P00979 |                      |
| IPAFYYNQK                          | 45.24  | 1142.5760 | 9      | -1.3 | 572.2946  | 2 | 19.72 | sp P00979 |                      |
| IPAFYYNQK                          | 45.15  | 1142.5760 | 9      | 0.2  | 572.2954  | 2 | 21.82 | sp P00979 |                      |
| IPAFYYNQK                          | 43.59  | 1142.5760 | 9      | -1.3 | 572.2946  | 2 | 20.50 | sp P00979 |                      |
| IPAFYYNQK                          | 42.06  | 1142.5760 | 9      | -0.3 | 572.2951  | 2 | 21.02 | sp P00979 |                      |
| IPAFYYNQK                          | 41.78  | 1142.5760 | 9      | -0.6 | 572.2950  | 2 | 19.99 | sp P00979 |                      |
| IPAFYYNQK                          | 41.61  | 1142.5760 | 9      | 0.1  | 572.2953  | 2 | 20.77 | sp P00979 |                      |

| Peptide                             | -10lgP | Mass      | Length | ppm  | m/z      | Z | RT    | Accession | PTM                  |
|-------------------------------------|--------|-----------|--------|------|----------|---|-------|-----------|----------------------|
| IPAFYYNQK                           | 39.13  | 1142.5760 | 9      | -0.1 | 572.2952 | 2 | 22.77 | sp P00979 |                      |
| IPAFYYNQK                           | 38.83  | 1142.5760 | 9      | -1.0 | 572.2947 | 2 | 20.23 | sp P00979 |                      |
| IPAFYYNQK                           | 38.45  | 1142.5760 | 9      | 0.3  | 572.2955 | 2 | 22.07 | sp P00979 |                      |
| IPAFYYNQK                           | 37.76  | 1142.5760 | 9      | 0.3  | 572.2955 | 2 | 21.56 | sp P00979 |                      |
| IPAFYYNQK                           | 34.10  | 1142.5760 | 9      | -0.3 | 572.2951 | 2 | 22.35 | sp P00979 |                      |
| IPAFYYNQK                           | 33.16  | 1142.5760 | 9      | 0.0  | 572.2953 | 2 | 21.31 | sp P00979 |                      |
| TWSGC(+57.02)GGNSNRFK               | 45.24  | 1469.6470 | 13     | -1.2 | 735.8299 | 2 | 17.36 | sp P00979 | Carbamidomethylation |
| SGC(+57.02)GGNSNRFK                 | 43.79  | 1182.5200 | 11     | -1.6 | 592.2664 | 2 | 15.48 | sp P00979 | Carbamidomethylation |
| KQC(+57.02)EGFTWSGC(+57.02)GGNSNRFK | 39.54  | 2218.9636 | 19     | -0.5 | 740.6614 | 3 | 18.48 | sp P00979 | Carbamidomethylation |
| C(+57.02)YQKIPAFYY                  | 35.00  | 1351.6271 | 10     | -0.3 | 676.8206 | 2 | 20.03 | sp P00979 | Carbamidomethylation |
| FKTIEEC(+57.02)R                    | 33.93  | 1081.5226 | 8      | -0.4 | 541.7684 | 2 | 17.18 | sp P00979 | Carbamidomethylation |
| FKTIEEC(+57.02)R                    | 29.76  | 1081.5226 | 8      | 0.5  | 361.5150 | 3 | 17.19 | sp P00979 | Carbamidomethylation |
| KLC(+57.02)ILHR                     | 32.74  | 938.5484  | 7      | -0.5 | 470.2812 | 2 | 17.57 | sp P00979 | Carbamidomethylation |
| KLC(+57.02)ILHR                     | 29.86  | 938.5484  | 7      | -0.2 | 470.2814 | 2 | 17.85 | sp P00979 | Carbamidomethylation |
| KLC(+57.02)ILHR                     | 18.38  | 938.5484  | 7      | 0.1  | 313.8568 | 3 | 17.57 | sp P00979 | Carbamidomethylation |
| KQC(+57.02)EGFTW                    | 32.69  | 1054.4542 | 8      | -0.6 | 528.2341 | 2 | 19.80 | sp P00979 | Carbamidomethylation |
| QKIPAFYYNQK                         | 31.40  | 1398.7295 | 11     | 0.1  | 700.3721 | 2 | 18.66 | sp P00979 |                      |
| QKIPAFYYNQK                         | 23.73  | 1398.7295 | 11     | -0.6 | 467.2502 | 3 | 18.75 | sp P00979 |                      |
| LC(+57.02)ILHR                      | 29.94  | 810.4534  | 6      | 0.7  | 406.2343 | 2 | 18.10 | sp P00979 | Carbamidomethylation |
| LC(+57.02)ILHR                      | 26.76  | 810.4534  | 6      | 0.1  | 406.2340 | 2 | 18.37 | sp P00979 | Carbamidomethylation |
| LC(+57.02)ILHR                      | 24.91  | 810.4534  | 6      | 0.6  | 406.2342 | 2 | 18.65 | sp P00979 | Carbamidomethylation |
| LC(+57.02)ILHR                      | 19.58  | 810.4534  | 6      | 0.6  | 271.1586 | 3 | 18.10 | sp P00979 | Carbamidomethylation |
| LC(+57.02)ILHR                      | 19.26  | 810.4534  | 6      | 0.0  | 406.2340 | 2 | 19.03 | sp P00979 | Carbamidomethylation |
| TIEEC(+57.02)R                      | 27.76  | 806.3593  | 6      | 0.4  | 404.1871 | 2 | 15.92 | sp P00979 | Carbamidomethylation |
| TIEEC(+57.02)RR                     | 26.30  | 962.4603  | 7      | 0.0  | 482.2375 | 2 | 16.12 | sp P00979 | Carbamidomethylation |
| TIEEC(+57.02)RR                     | 19.79  | 962.4603  | 7      | -0.1 | 482.2374 | 2 | 15.83 | sp P00979 | Carbamidomethylation |
| TIEEC(+57.02)RR                     | 17.67  | 962.4603  | 7      | 0.2  | 482.2375 | 2 | 15.30 | sp P00979 | Carbamidomethylation |
| TIEEC(+57.02)RR                     | 16.66  | 962.4603  | 7      | -0.7 | 482.2371 | 2 | 15.57 | sp P00979 | Carbamidomethylation |
| KKQC(+57.02)EGF                     | 25.96  | 895.4222  | 7      | 0.1  | 448.7184 | 2 | 16.39 | sp P00979 | Carbamidomethylation |
| KKQC(+57.02)EGF                     | 22.74  | 895.4222  | 7      | -0.3 | 448.7182 | 2 | 16.65 | sp P00979 | Carbamidomethylation |

| Peptide                                   | -10lgP | Mass      | Length | ppm  | m/z      | Z | RT    | Accession | PTM                  |
|---|--------|-----------|--------|------|----------|---|-------|-----------|----------------------|
| <b>FKTIEEC(+57.02)RR</b>                  | 24.27  | 1237.6237 | 9      | 0.1  | 619.8192 | 2 | 16.64 | sp P00979 | Carbamidomethylation |
| <b>TWSGC(+57.02)GGNSNR</b>                | 23.01  | 1194.4836 | 11     | -0.3 | 598.2489 | 2 | 16.43 | sp P00979 | Carbamidomethylation |
| <b>KKQC(+57.02)EGFTW</b>                  | 22.98  | 1182.5492 | 9      | -0.7 | 592.2814 | 2 | 19.33 | sp P00979 | Carbamidomethylation |
| <b>RTC(+57.02)IR</b>                      | 21.83  | 704.3752  | 5      | 0.6  | 353.1951 | 2 | 14.87 | sp P00979 | Carbamidomethylation |
| <b>RTC(+57.02)IR</b>                      | 16.18  | 704.3752  | 5      | 0.2  | 353.1949 | 2 | 14.60 | sp P00979 | Carbamidomethylation |
| <b>QC(+57.02)EGFTWSGC(+57.02)GGNSNRFK</b> | 21.04  | 2090.8687 | 18     | -0.4 | 697.9632 | 3 | 18.99 | sp P00979 | Carbamidomethylation |
| <b>KQC(+57.02)EGF</b>                     | 18.17  | 767.3272  | 6      | -0.7 | 384.6706 | 2 | 17.32 | sp P00979 | Carbamidomethylation |
| <b>TC(+57.02)IRK</b>                      | 17.16  | 676.3690  | 5      | 0.2  | 339.1919 | 2 | 15.70 | sp P00979 | Carbamidomethylation |
| <b>TC(+57.02)IRK</b>                      | 16.63  | 676.3690  | 5      | 0.4  | 339.1919 | 2 | 14.21 | sp P00979 | Carbamidomethylation |

-10logP = peptide score; RT = Retention time; m/z = mass/charge; Z = charge; PTM = Post-translational modification