DPQIR(ADP-Ribosyl)DLLTPPTDKPGQDNRS(Phospho)KLR$^{+4}$

Max Intensity: 19310
Num Matched: 16/47 (66.0% unmatched) Matched Intensity: 43.2% Matched Series Intensity: 43.2%

Elemental Composition: C132 H221 N43 O55 P3

| MH$^1$(av) | MH$^1$(mono) | MH$^{+2}$(av) | MH$^{+2}$(mono) | MH$^{+3}$(av) | MH$^{+3}$(mono) | MH$^{+4}$(av) | MH$^{+4}$(mono) |
|------------|--------------|---------------|----------------|---------------|----------------|---------------|---------------|
| 3383.4042  | 3381.5026    | 1692.2058     | 1691.2549      | 1127.8390     | 846.6066       | 846.1311      |

[+] Additional Sequences
- Max Charge: 4
- Count Basic AA: 1
- Max Losses: 1
- Multi Z Internal: 0
- Max Internal Len: 200
- Max MSMS Pks: 200
- Frag Tol (Da): 0.1
- Cal Tol (Da): 0.1
- Cal

[+] Ion Types
- MS-Product
- Output: HTML
### [-] Main Sequence Ions

| b-H₃PO₄ | b-H₃PO₄²⁺ | b | b² | y | y² | γ⁻H₃PO₄ | γ-H₃PO₄²⁺ |
|---------|-----------|---|----|---|----|---------|-----------|
| ...     | ...       | ...| ...| 1 | D  | 24      | ...       |
| ...     | ...       | ...| ...| 2 | P  | 23      | 5265.756 | 1633.7414 |
| ...     | ...       | ...| ...| 3 | Q  | 22      | 1169.4232 | 1585.2151 |
| ...     | ...       | ...| ...| 4 | I  | 21      | 3041.3643 | 1521.1858 |
| ...     | ...       | ...| ...| 5 | (ADP-Ribosyl) | 20 | 2928.2802 | 1446.6437 |
| ...     | ...       | ...| ...| 6 | D  | 19      | 2231.1380 | 1116.0626 |
| ...     | ...       | ...| ...| 7 | L  | 18      | 2116.0910 | 1058.5492 |
| ...     | ...       | ...| ...| 8 | T  | 17      | 1889.9229 | 945.4651  |
| ...     | ...       | ...| ...| 9 | P  | 15      | 1788.8752 | 894.9413  |
| ...     | ...       | ...| ...| 10| P  | 14      | 1691.8225 | 846.4149  |
| ...     | ...       | ...| ...| 12| T  | 13      | 1594.7697 | 797.8885  |
| ...     | ...       | ...| ...| 13| D  | 12      | 1493.7220 | 747.3647  |
| ...     | ...       | ...| ...| 14| K  | 11      | 1378.6951 | 689.8512  |
| ...     | ...       | ...| ...| 15| P  | 10      | 1250.6001 | 625.8037  |
| ...     | ...       | ...| ...| 16| G  | 9       | 1153.5474 | 577.2773  |
| ...     | ...       | ...| ...| 17| Q  | 8       | 1096.5259 | 548.7666  |
| ...     | ...       | ...| ...| 18| D  | 7       | 968.6673  | 484.7373  |
| ...     | ...       | ...| ...| 19| N  | 6       | 853.4044  | 427.2328  |
| ...     | ...       | ...| ...| 20| R  | 5       | 739.3974  | 370.2024  |
| ...     | ...       | ...| ...| 21| 2506.2503 | 1434.6211 |
| ...     | ...       | ...| ...| 22| S(Phospho) | 4  | 583.2963 | 292.1518 |
| ...     | ...       | ...| ...| 23| 1483.6096 | 2966.2119 |
| ...     | ...       | ...| ...| 24| 243.1634  | 845.3194 |
| ...     | ...       | ...| ...| 25| 296.6868  | 3094.3068 |
| ...     | ...       | ...| ...| 26| 604.8627  | 1262.7182 |
| ...     | ...       | ...| ...| 27| 576.8153  | 1152.6232 |
| ...     | ...       | ...| ...| 28| 101.0709  | 408.2241  |
| ...     | ...       | ...| ...| 29| 483.1634  | 1438.6211 |
| ...     | ...       | ...| ...| 30| 243.1634  | 845.3194 |
| ...     | ...       | ...| ...| 31| 243.1634  | 845.3194 |

### [-] All Sequence Ions

#### MH

| Low Mass | 88.0393 | 70.0651 | 126.0550 | 84.0444 | 101.0709 | 129.0659 | 78.0917 | 100.0869 | 112.0869 |
|----------|---------|---------|----------|---------|---------|---------|---------|---------|---------|
| 70.0651  | 126.0550 | 84.0444 | 101.0709 | 129.0659 | 78.0917 | 100.0869 | 112.0869 |

#### MH₃PO₄

| Low Mass | 1381.9826 | 1691.2549 | 1127.8390 | 846.1311 |
|----------|-----------|-----------|-----------|---------|

#### MH₂O

| Low Mass | 3283.5257 | 1642.2665 | 1095.1801 | 821.6369 |
|----------|-----------|-----------|-----------|---------|

#### MH₃N₃

| Low Mass | 3364.4760 | 1682.7416 | 1122.1635 | 841.8687 |
|----------|-----------|-----------|-----------|---------|

#### N-terminal

| a-NH₃⁺ | ... | ... | 296.124 | 409.2082 | 1106.3704 | 1221.3937 | 1334.4814 | 1447.5655 | 1548.6131 | 1645.6659 | 1742.7187 | 1843.7663 | 1958.7933 | 2086.8882 | 2183.9410 | 2240.9625 | 2369.0210 | 2484.0480 | 2589.0909 | 2754.1920 | 2921.1904 | 3049.2854 | 3162.3694 | ... |
| a-NH₃⁺² | ... | ... | ... | 553.6888 | 611.2023 | 677.7443 | 724.2864 | 781.8302 | 823.3366 | 871.8630 | 922.3868 | 979.9003 | 1043.9478 | 1092.4741 | 1120.9849 | 1155.0142 | 1242.5276 | 1299.5417 | 1377.5997 | 1461.0988 | 1525.1463 | 1581.6883 | ... |
| a-NH₃⁺² | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... |
| a-NH₃⁺² | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... |
| a-NH₃⁺² | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... |

#### a-H₂O

| Low Mass | 187.0113 | 295.1401 | 408.2214 | 1105.3864 | 1220.4133 | 1333.4974 | 1446.5814 | 1547.6291 | 1644.6819 | 1741.7346 | 1842.7823 | 1957.8093 | 2085.9042 | 2182.9570 | 2239.9785 | 2368.0370 | 2483.0860 | 2597.1069 | 2753.2080 | 2920.2064 | 3048.3013 | 3161.3854 | ... |
|     |      |      |      |      |      |
|-----|------|------|------|------|------|
| KPGQ | 411.2350 | 383.2401 | 394.2085 | —     |      |
| GQDN | 415.3725 | 387.1623 | 399.1306 | 397.4666 |      |
| LLTP | 425.2755 | 397.2809 | —     | 407.2653 |      |
| NRS(Phospho) | 438.1497 | 410.1548 | 421.2131 | 420.1391 |      |
| TDKP | 442.2296 | 414.2347 | 425.2031 | 424.2191 |      |
| PTDK | 442.2296 | 414.2347 | 425.2031 | 424.2191 |      |
| DLLT | 443.2500 | 415.2551 | —     | 425.2395 |      |
| RS(Phospho)K | 452.2017 | 424.2068 | 435.1752 | 434.1911 |      |
| TDKPQ | 499.2511 | 472.2562 | 482.2245 | 481.2405 |      |
| LTPTP | 510.2922 | 482.2973 | —     | 492.2817 |      |
| PGQDN | 512.2100 | 484.2150 | 495.1834 | 494.1994 |      |
| TPFDTD | 512.2351 | 484.2402 | —     | 494.2245 |      |
| QDNR | 514.2368 | 486.2419 | 497.2103 | 496.2263 |      |
| LLTPP | 522.3286 | 494.3337 | —     | 504.3180 |      |
| KPGQDN | 526.2620 | 498.2671 | 509.2354 | 508.2514 |      |
| DKPGQ | 526.2620 | 498.2671 | 509.2354 | 508.2514 |      |
| PTDKP | 539.2824 | 511.2875 | 522.2558 | 521.2718 |      |
| PPTDK | 539.2824 | 511.2875 | 522.2558 | 521.2718 |      |
| DLLTP | 540.3028 | 512.3079 | —     | 522.3022 |      |
| DNRS(Phospho) | 553.1766 | 525.1817 | 536.1501 | 535.1661 |      |
| RS(Phospho)KL | 565.2858 | 537.2909 | 548.2592 | 547.2752 |      |
| NRS(Phospho)K | 566.2446 | 538.2497 | 549.2181 | 548.2341 |      |
| GQDNK | 571.2583 | 543.2634 | 554.2318 | 553.2477 |      |
| PTDKPG | 596.3039 | 568.3089 | 579.2737 | 578.2933 |      |
| LTPTPT | 623.7363 | 595.3814 | —     | 605.3657 |      |
| LTPPTD | 625.3192 | 597.3243 | —     | 607.3086 |      |
| TDKPGQ | 627.3079 | 599.3148 | 610.2831 | 609.2991 |      |
| PPTDKP | 636.3352 | 608.3402 | 619.3086 | 618.3246 |      |
| DLLTPP | 637.3556 | 609.3666 | —     | 619.3450 |      |
| KPGQDN | 640.3049 | 612.3100 | 623.2784 | 622.2944 |      |
| TPTDKP | 640.3301 | 612.3352 | 623.3035 | 622.3195 |      |
| DKPGQDN | 641.2889 | 613.2940 | 624.2624 | 623.2784 |      |
| PGQDNR | 668.3111 | 640.3161 | 651.2843 | 650.3005 |      |
| NRS(Phospho)KL | 679.3237 | 651.3338 | 662.3022 | 661.3181 |      |
| QDNRS(Phospho) | 681.2352 | 653.2400 | 664.2086 | 663.2246 |      |
| DNRS(Phospho)K | 681.2716 | 653.2490 | 664.2459 | 663.2610 |      |
| PPTDKPG | 693.3566 | 665.3617 | 676.3501 | 675.3661 |      |
| FTDKPGQ | 724.3624 | 696.3675 | 707.3539 | 706.3591 |      |
| TPTTDKP | 737.3828 | 709.3879 | 720.3653 | 719.3723 |      |
| GQDNRS(Phospho) | 738.2567 | 710.2617 | 721.2301 | 720.2461 |      |
| DLLTPT | 738.4032 | 710.4083 | —     | 720.3927 |      |
| LTPPTTD | 738.4032 | 710.4083 | —     | 720.3927 |      |
| TDKPGQD | 742.3366 | 714.3417 | 725.3101 | 724.3260 |      |
| DLLTPD | 753.4141 | 725.4192 | 736.3876 | 735.4036 |      |
| TKPGQDN | 755.3319 | 727.3369 | 738.3053 | 737.3213 |      |
| DNRS(Phospho)KL | 758.3556 | 766.3607 | 777.3291 | 776.3451 |      |
| TPTDKPG | 794.4043 | 766.4094 | 777.3777 | 776.3937 |      |
| KPGQDNR | 796.4060 | 768.4111 | 779.3795 | 778.3955 |      |
| QDNRS(Phospho)K | 809.3302 | 781.3352 | 792.3036 | 791.3196 |      |
| IR(ADP-Ribosyl) | 815.2356 | 783.2586 | 794.2287 | —     |      |
| RADF-RibosylI | 815.2356 | 783.2586 | 794.2287 | —     |      |
| PFDKPGQ | 821.4172 | 793.4205 | 804.3886 | 803.4086 |      |

http://msviewer.ucsf.edu/prospector/cgi-bin/mssearch.cgi?search_name=msproduct&output_ty...
| Peptide Sequence | m/z | m/z | m/z | m/z |
|------------------|-----|-----|-----|-----|
| LTPPTDKPGQDN     | 2046.6180 | 2366.6219 | 247.5903 | 2346.6962 |
| PTDKPGQDNRS(Phospho) | 2366.5318 | 238.5340 | 259.5052 | 258.5212 |
| QRR(ADP-Ribosyl)DLL | 258.5072 | 252.5123 | 263.4807 | 262.4966 |
| TDKPGQDNRS(Phospho)K | 262.5740 | 279.5791 | 290.5474 | 289.5634 |
| TPPTDKPGQDN      | 289.6339 | 279.6389 | 290.6073 | 289.6235 |
| DKGQDNRS(Phospho)KL | 302.6140 | 301.6183 | 302.5838 | 301.5998 |
| R(ADP-Ribosyl)DLLTPPT | 301.5857 | 306.5229 | 317.5412 | 316.5472 |
| R(ADP-Ribosyl)DLLTP | 316.5472 | 312.5542 | 323.5225 | 322.5385 |
| PPTDKPGQDNRS     | 315.5745 | 314.5789 | 315.5580 | 314.5744 |
| L(ADP-Ribosyl)DLLT | 314.5744 | 313.5788 | 314.5580 | 313.5744 |
| TPDKPGQDN        | 313.5818 | 312.5861 | 313.5657 | 312.5818 |
| TPDKPGQDNRS(K)   | 312.5818 | 311.5861 | 312.5657 | 311.5818 |
| R(ADP-Ribosyl)DLLTPPTD | 311.5345 | 316.5807 | 315.5580 | 314.5744 |
| R(ADP-Ribosyl)DLLTPPT | 314.5744 | 313.5788 | 314.5580 | 313.5744 |
| L(ADP-Ribosyl)DLLT | 313.5818 | 312.5861 | 313.5657 | 312.5818 |
| TPDKPGQDN        | 312.5818 | 311.5861 | 312.5657 | 311.5818 |
| TPDKPGQDNRS(K)   | 311.5818 | 310.5861 | 311.5657 | 310.5818 |
| R(ADP-Ribosyl)DLLTPPTD | 310.5345 | 315.5807 | 314.5580 | 313.5744 |
| R(ADP-Ribosyl)DLLTPPT | 313.5744 | 312.5788 | 313.5580 | 312.5744 |
| L(ADP-Ribosyl)DLLT | 312.5818 | 311.5861 | 312.5657 | 311.5818 |
| TPDKPGQDN        | 311.5818 | 310.5861 | 311.5657 | 310.5818 |
| TPDKPGQDNRS(K)   | 310.5818 | 309.5861 | 310.5657 | 309.5818 |
| R(ADP-Ribosyl)DLLTPPTD | 309.5345 | 314.5807 | 313.5580 | 312.5744 |
| R(ADP-Ribosyl)DLLTPPT | 313.5744 | 312.5788 | 313.5580 | 312.5744 |
| L(ADP-Ribosyl)DLLT | 312.5818 | 311.5861 | 312.5657 | 311.5818 |
| TPDKPGQDN        | 311.5818 | 310.5861 | 311.5657 | 310.5818 |
| TPDKPGQDNRS(K)   | 310.5818 | 309.5861 | 310.5657 | 309.5818 |
| R(ADP-Ribosyl)DLLTPPTD | 309.5345 | 314.5807 | 313.5580 | 312.5744 |
| R(ADP-Ribosyl)DLLTPPT | 313.5744 | 312.5788 | 313.5580 | 312.5744 |
| L(ADP-Ribosyl)DLLT | 312.5818 | 311.5861 | 312.5657 | 311.5818 |
| TPDKPGQDN        | 311.5818 | 310.5861 | 311.5657 | 310.5818 |
| TPDKPGQDNRS(K)   | 310.5818 | 309.5861 | 310.5657 | 309.5818 |
| Peak Table |
|------------|
| 60.0444 | S | C12 H16 N1 O1 | 736.6023 | H₂₃₋₂₅P₂O₄²⁻ | 1318.254551 N39 O45 P2 | 258.05797 | C50 H18 N16 O24 P2 |
| 70.0651 | P | C4 H8 N1 | 737.3213 | DKPGQDN⁻⁻H₂O | C30 H45 N10 O12 | 253.660000 | C51 H87 N16 O23 P2 |
| 70.0651 | R | C4 H8 N1 | 737.3282 | TPTTDKP | C33 H53 N8 O11 | 255.576000 | C55 H84 N18 O22 P1 |
| 74.0600 | T | C13 H18 N1 | 737.6555 | H₂₅₋₂₆P₂O₃ | C90 H142 N25 O36 P2 | 256.550000 | C55 H83 N17 O23 P3 |
| 79.5498⁻² | 1₁₋₁₃H₁²⁺ | C6 H12 N3 O2 | 737.7918 | β₃₋₄H₂O⁻⁻ | C57 H90 N17 O25 P2 | 259.549400 | C55 H85 N16 O22 P2 |
| 84.0444 | Q | C14 H8 N1 O1 | 737.8058 | H₂₅₋₂₆P₂O₃ | C90 H141 N24 O37 P2 | 256.533400 | C55 H84 N18 O23 P2 |
| 84.0808 | K | C5 H10 N1 | 738.9385 | H₂₅₋₂₆P₂O₃ | C90 H140 N23 O37 P2 | 256.533400 | C55 H84 N18 O23 P2 |
| 86.0964 | I | C13 H18 N1 | 738.5185 | H₂₅₋₂₆P₂O₃ | C114 H181 N35 O51 P3 | 259.674300 | C60 H91 N17 O23 P3 |
| 86.0964 | L | C3 H2 N1 | 738.2565 | GQDNRS(Phospho) | C24 H41 N11 O14 P1 | 256.674300 | C55 H84 N18 O23 P2 |
| 87.0533 | N | C3 H7 N2 O1 | 738.2838 | H₂₅₋₂₆H₂O⁺⁻ | C57 H89 N16 O26 P2 | 256.682500 | C55 H85 N19 O19 P1 |
| 87.0917 | R | C4 H11 N2 | 738.3053 | DKPGQDN⁻⁻H₂O | C40 H34 N9 O13 | 261.492300 | C51 H78 N16 O24 P2 |
199.0713
189.6213
189.4281
186.0873
185.0921
181.3482
181.0972
171.1128
169.0609
167.1128
165.1106
164.4247
163.0815
161.1790
160.0924
158.9242
157.1190
156.0972
154.3472
153.4824
152.0870
151.2481
150.6213
149.0764
148.1063
147.1128
146.8281
145.0870
144.2481
143.6213
142.0764
141.1063
140.0870
139.1790
138.1106
137.0815
136.0870
135.1190
134.0870
133.0592
132.0815
131.1128
130.0870
129.0222
128.0505
127.0866
126.0959
125.0913
124.6213
123.1128
122.0870
121.0764
120.0815
119.1190
118.0870
117.1790
116.0815
115.0924
114.0924
113.0972
112.0972
111.1190
110.1790
109.0870
108.2481
107.6213
106.0764
105.0870
104.1190
103.0870
102.1128
101.0870
100.0869
99.0839

http://msviewer.ucsf.edu/prospector/cgi-bin/mssearch.cgi?search_name=msproduct&output_ty...
| 735.3971 | $\text{LTPDK}$ | C133 H184 N36 O30 P3 | E449.7060 | $\text{LLTPPTDKPGQDN-CO}$ | C59 H97 N16 O20 | 363.4920 | MH-H$_2$O | C132 H219 N43 O54 P3 |
| 735.4036 | LTPPTDK-H$_2$O | C34 H55 N8 O10 | E350.5491 | $\text{IR(ADP-Ribosyl)DLLTP}$ | C52 H86 N15 O23 P2 | 364.4760 | MH-NH$_3$ | C132 H218 N42 O55 P3 |
| 736.3876 | LTPPTDK-NH$_3$ | C34 H54 N7 O11 | E350.6960 | DLLTPPTDKPGQD-CO | C59 H96 N15 O21 | 381.5026 | MH | C132 H221 N43 O55 P3 |