

## SUPPLEMENTARY MATERIALS

### Small molecule binding to Inhibitor of nuclear factor kappa-B kinase subunit beta in an ATP non-competitive manner

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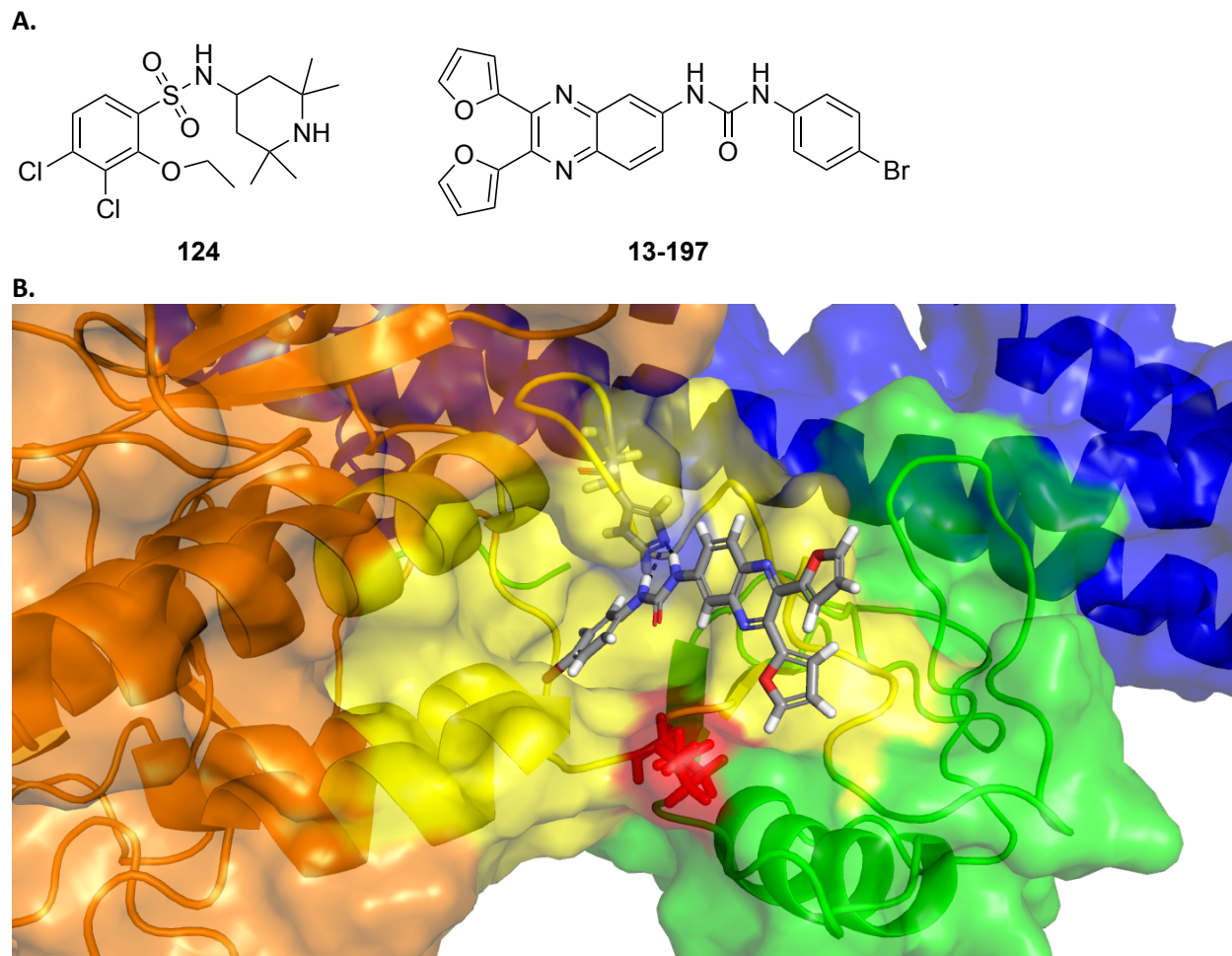
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**Figure S1.** A) Chemical structures of analogue 124 and 13-197. B) Docked structure of 13-197 (sticks) in the allosteric binding site (yellow) at the interface of kinase domain (orange), ubiquitin like domain (green) and scaffold dimerization domain (blue). The urea NH in 13-197 is within hydrogen bonding distance (dashed lines) of the histidine<sup>380</sup> side chain and the lysine<sup>310</sup> that is associated with crosslinking 37-290 is shown as red sticks.

## Methods

### *Kinase assays:*

#### Materials and reagents:

10 mM stock of 13-197, PS-1145, BMS-345541, ML-120B and staurosporine in DMSO was used.

Kinase reaction buffer: 20 mM HEPES-HCl, pH 7.5, 10 mM MgCl<sub>2</sub>, 1 mM EGTA, 0.02% Brij35, 0.1 mM Na<sub>3</sub>VO<sub>4</sub>, 0.02 mg/ml BSA, 2 mM DTT, and 1% DMSO (final is 2% in the reaction).

IKKβ/IKBKB: Recombinant Human full-length IKKβ (Accession# NP\_001547) with N-terminal GST-tagged was expressed in insect cells. MW = 114 kDa.

#### IKKβ Substrate:

IKKtide [KKKKERLLDDRHDSGLDSMKDEE]

#### Reaction conditions:

3 nM IKKβ, 20 μM IKKtide, varied compound conc. and varied ATP conc.

#### Experimental Procedures:

The kinase assays were performed at room temperature. Compounds were added 10-dose IC<sub>50</sub> mode into Enzyme/substrate mixture using acoustic technology with 20 min compound pre-incubation. Then the 5 concentrations of ATP for ATP competition studies or constant ATP for substrate competition studies were added to initiate the reaction. The activity was monitored every 5-15 min for a time course study. The ATP, substrate, and compound concentrations tested:

#### ATP competition assay with IKKβ

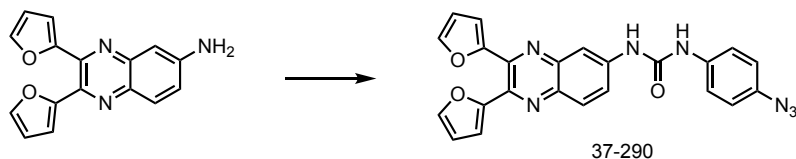
ATP concentrations tested: 3.3, 10, 30, 90, and 270 μM ATP

Substrate concentration: constant at 20 μM

Compound concentrations tested: 10-dose IC<sub>50</sub> with 3-fold serial dilution started at 100 μM.

Time points measured: 0, 5, 10, 15, 20, 30, 45, 60, 75, 90, 105, and 120 min

### *Synthesis of 37-290*



#### **1-(4-azidophenyl)-3-(2,3-di(furan-2-yl)quinoxalin-6-yl)urea (37-290):**

To a stirred solution of 6-aminoquinoxaline (Ref 14) (100 mg, 0.36 mmol) in anhydrous dichloromethane (1 mL) was added pyridine (0.058 mL, 0.72 mmol), followed by slow addition of phenyl chloroformate (0.05 mL, 0.40 mmol) at 0 °C. The reaction mixture was stirred under nitrogen atmosphere for 30 min and slowly brought to rt and further stirred for next 90 minutes. After completion of reaction, the reaction mixture was quenched with water and extracted with dichloromethane. The combined organic layers were evaporated to dryness under reduced pressure and the residue was dissolved in anhydrous

dichloromethane (1 mL). To this solution were added 4-azidoaniline hydrochloride (68 mg, 0.4 mmol) and triethyl amine (0.1 mL, 0.72 mmol) and mixture was stirred for 72 h under nitrogen atmosphere. The organic solvent was evaporated to dryness under reduced pressure and crude was purified using silica gel column chromatography to get 37-290 as a pale yellow solid; Yield = 55%;  $^1\text{H}$  NMR (500 MHz, DMSO)  $\delta$  9.95 (s, 1H), 9.61 (s, 1H), 8.35 (d,  $J$  = 2.3 Hz, 1H), 7.97 (d,  $J$  = 9.6 Hz, 1H), 7.94 – 7.81 (m, 3H), 7.62 (d,  $J$  = 8.4 Hz, 2H), 7.05 (d,  $J$  = 8.3 Hz, 2H), 6.73 – 6.62 (m, 4H) ppm. HRMS (ESI) exact mass calculated for  $\text{C}_{23}\text{H}_{16}\text{N}_7\text{O}_3$   $[\text{M}+\text{H}]^+$  438.1315, found  $[\text{M}+\text{H}]^+$  438.1355.

#### *UV cross linking studies to identify the binding site of 13-197:*

In two eppendorf tubes 20 $\mu\text{g}$  of recombinant IKK $\beta$  was incubated with 10 $\mu\text{M}$  of 37-290 each for 5 min. One of the tubes was subjected to UV cross linking (ref 22) while the other was not. The samples were then desalted using zeba spin columns (Thermo Fisher). Samples were then reduced with 10 mM DTT and alkylated with 50 mM iodoacetamide. Reduced and alkylated sample were subjected two enzyme digestions using Asp-N (promega) 1:50 ratio of protease:protein concentration overnight and MS-grade trypsin (Pierce) at 1:25 of protease:protein concentration, with high temperature denaturation for one hour in between. These peptides cleaned with PepClean C18 spin columns (Thermo) were re-suspended in 2% acetonitrile (ACN) and 0.1% formic acid (FA) and 1  $\mu\text{g}$  of each sample was loaded onto trap column Acclaim PepMap 100 75 $\mu\text{m}$  x 2 cm C18 LC Columns (Thermo Scientific™) at flow rate of 4  $\mu\text{l}/\text{min}$  then separated with a Thermo RSLC Ultimate 3000 (Thermo Scientific™) on a Thermo Easy-Spray PepMap RSLC C18 75 $\mu\text{m}$  x 50cm C-18 2  $\mu\text{m}$  column (Thermo Scientific™) with a step gradient of 4–25% solvent B (0.1% FA in 80 % ACN) from 10-57 min and 25–45% solvent B for 57–62 min at 300 nL/min and 50°C with a 90 min total run time. Eluted peptides were analyzed by a Thermo Orbitrap Fusion Lumos Tribrid (Thermo Scientific™) mass spectrometer in a data dependent acquisition mode. A survey full scan MS (from  $m/z$  350–1800) was acquired in the Orbitrap with a resolution of 120,000. The AGC target for MS1 was set as  $4 \times 10^5$  and ion filling time set as 100 ms. The most intense ions with charge state 2-6 were isolated in 3 s cycle and fragmented using HCD fragmentation with 40 % normalized collision energy and detected at a mass resolution of 30,000 at 200  $m/z$ . The AGC target for MS/MS was set as  $5 \times 10^4$  and ion filling time set 60 ms dynamic exclusion was set for 30 s with a 10 ppm mass window. Protein identification was performed by searching MS/MS data against the swiss-prot human protein database downloaded on Aug 20, 2018. The search was set up for full tryptic peptides with a maximum of two missed cleavage sites. Acetylation of protein N-terminus and oxidized methionine were included as variable modifications and carbamidomethylation of cysteine was set as fixed modification. The precursor mass tolerance threshold was set 10 ppm for and maximum fragment mass error was 0.02 Da. Qualitative analysis was performed using PEAKS 8.5 software. The significance threshold of the ion score was calculated based on a false discovery rate of  $\leq 1\%$ .

#### *Western blot analyses*

HPNE cells (normal pancreatic hTERT immortalized cell line) were maintained in DMEM plus 10% FBS at 37°C / 5%  $\text{CO}_2$ . TNF $\alpha$  was used at 20 ng/ml for activation of the NF $\kappa$ B pathway. In Figure 4A, 13-197 inhibitor was used at 20  $\mu\text{M}$ . To collect cell extracts, cells were washed twice with 1  $\times$  PBS then lysed using 50 mM Tris-base (pH 7.5), 150 mM sodium chloride, 0.5% NP40, 1 mM EDTA, 0.1% SDS, 1 mM sodium orthovanadate, 25 mM sodium fluoride,  $\beta$ -glycerophosphate, and 1 mmol/l PMSF. Samples were incubated on ice for 30 minutes, centrifuged at 14,000 rpm for 20 minutes at 4°C, and cleared supernatants were collected. Protein quantification was performed using BCA Protein Assay (Pierce;

#23225). 30  $\mu$ g protein extracts were fractionated on 4-15% Mini-PROTEAN TGX precast protein gels (Bio-Rad; #4561085), then transferred to a polyvinylidene difluoride sheets. Membranes were saturated using 5% fat-free milk diluted in 1  $\times$  Tris-buffered saline with 0.1% Tween 20 for 1 hour at room temperature. Primary antibodies were diluted in 5% milk in 1  $\times$  Tris-buffered saline / 0.1% Tween 20 and applied to membranes overnight at room temperature. After 3  $\times$  10 minutes washes with 1  $\times$  Tris-buffered saline / 0.1% Tween 20, horseradish peroxidase-conjugated secondary antibody was applied for 1 hour at room temperature. Finally, after 3  $\times$  10 minutes washes with 1  $\times$  Tris-buffered saline / 0.1% Tween 20, ECL Prime (GE Healthcare; #RPB2236) was used to detect proteins expression profile by standard autoradiography. The primary antibodies used are p-I $\kappa$ B $\alpha$  (S32/36) (Cell Signaling #9246S), I $\kappa$ B $\alpha$  (Cell Signaling #4812S), IKK $\alpha$  (Santa Cruz Biotechnology #sc-52932), IKK $\beta$  (Cell Signaling #8943S), NF $\kappa$ B (p65) (Santa Cruz Biotechnology #sc-372), and I $\kappa$ B $\beta$  (Cell Signaling #8635S).

## Supplementary Table 1

Protein = IKK $\beta$

Found by = PEAKS DB

Carbamidomethylation = CBM

IKK $\beta$  + 39-290 + UV

| Peptide   | m/z       | Area No_UV | PTM                      |
|---|-----------|------------|--------------------------|
| R.LGTGGFGNVIRWHNQETGEQIAIKQC(+57.02)R.Q                                       | 1023.8535 | 122000000  | CBM                      |
| M.KERLGTGGFGNVIRWHNQETGEQIAIKQC(+57.02)R.Q                                    | 697.3631  | 571000000  | CBM                      |
| R.LGTGGFGNVIRWHNQETGEQIAIKQC(+57.02)RQELSPR.N                                 | 945.7335  | 515000000  | CBM                      |
| M.VTGTIHTYPVTEDESLQSLKAR.I  | 815.7596  | 487000000  |                          |
| R.LGTGGFGNVIRWHNQETGEQIAIKQC(+57.02)RQELSPRNRER.W                             | 867.8469  | 384000000  | CBM                      |
| M.GRKQGGTLDDLEEQARELYRRLREKPR.D   | 545.7993  | 266000000  |                          |
| R.EGAILTLLSDIASALRYLHENRIIHRD.L   | 773.1782  | 173000000  |                          |
| M.EQAVELC(+57.02)GRENEVKLLVER.M   | 757.731   | 157000000  | CBM                      |
| M.GRKQGGTLDDLEEQARELYRRLREKPRD.Q  | 564.9706  | 153000000  |                          |
| M.KERLGTGGFGNVIRWHNQETGEQIAIKQC(+57.02)RQELSPR.N                              | 839.4375  | 129000000  | CBM                      |
| M.GRKQGGTLDDLEEQARELYRRLREKPRDQRTEGD.S  | 679.3541  | 110000000  |                          |
| M.NEDEKTVVRLQEKRQKELWNLLKIAC(+57.02)SKVRGPVSGSPD.S                            | 630.4867  | 107000000  | CBM                      |
| M.VTGTIHTYPVTEDESLQSLKARIQQDTGIPEEDQELLQEAGLALIPDKPATQC(+57.02)ISDG.K         | 1244.627  | 102000000  | CBM                      |
| M.KERLGTGGFGNVIRWHNQETGEQIAIKQC(+57.02)RQELSPRNRER.W                          | 594.4375  | 927000000  | CBM                      |
| R.EGAILTLLSDIASALRYLHEN(+.98)RIIHRD.L.K                                       | 641.553   | 924000000  | Deamidation (NQ)         |
| M.VTGTIHTYPVTEDESLQSLKARIQQD.T  | 733.129   | 854000000  |                          |
| M.VRLLLQAIQSFEEK.V  | 558.3423  | 854000000  |                          |
| R.EGAILTLLSDIASALRYLHENRIIHR.D  | 595.7384  | 801000000  |                          |
| T.YGPNGCFKALDDILN(+.98)LK(+411.13)LVHILNMVTGTIHTYPVTEDESLQSLKAR.I             | 924.145   | 720000000  | Deamidation (NQ); 37-290 |
| D.PTYGPNGC(+57.02)FKALDDILNLKLVHILNMVTGTIHTYPVTEDESLQSLKARIQ(+.98)QDTG.I      | 1005.1855 | 702000000  | CBM; Deamidation (NQ)    |
| M.KERLGTGGFGNVIRWHNQETGEQIAIKQCRQELSPR.N.R                                    | 608.0319  | 541000000  |                          |
| D.LKPENIVLQQGEQRLIHKIIDLGYAKELD.Q   | 563.1544  | 519000000  |                          |
| R.LGTGGFGNVIRWHNQETGEQIAIKQC(+57.02)RQELSPRNR.E                               | 675.8514  | 500000000  | CBM                      |
| D.TGIPEEDQELLQEAGLALIPD.K   | 1126.0718 | 481000000  |                          |
| R.LGTGGFGNVIRWHNQETGEQIAIKQC(+57.02)RQELSPRNRERWCLEIQ(+.98)IMRRLTHPNVVAARDV.P | 771.7348  | 456000000  | CBM; Deamidation (NQ)    |
| M.EYC(+57.02)QGGDLRKYLNQFENC(+57.02)C(+57.02)GLREGAILTLLSDIASALRYLHENRIIHRD.L | 732.2449  | 424000000  | CBM                      |
| T.YGPN(+.98)GCFKALDDILNLK(+411.13)LVHILNMVTGTIHTYPVTEDESLQSLKAR.I             | 924.145   | 401000000  | Deamidation (NQ); 37-290 |
| E.DEKTVVRLQEKRQKELWNLLKIAC(+57.02)SKVRGPVSGSPD.S                              | 595.7603  | 397000000  | CBM                      |
| R.LGTGGFGNVIRWHNQETGEQ(+.98)IAIKQC(+57.02)R.Q                                 | 614.9129  | 394000000  | Deamidation (NQ); CBM    |
| D.DLEEQARELYRRLREKPR.D  | 590.0767  | 391000000  |                          |
| M.VRLLLQAIQSFEEK.K  | 515.644   | 377000000  |                          |
| D.PTYGPNGC(+57.02)FKALD.D   | 720.3354  | 371000000  | CBM                      |
| M.VTGTIHTYPVTEDESLQSLKARIQQDTGIPEE.D  | 1185.9331 | 369000000  |                          |
| M.VTGTIHTYPVTE.D  | 659.3383  | 369000000  |                          |
| K.VRVITYTQLSKTVVC(+57.02)KQKALELLPK.V   | 563.7393  | 366000000  | CBM                      |
| M.KERLGTGGFGNVIRWHNQETGEQIAIKQC(+57.02)RQELSPRNR.E                            | 744.723   | 337000000  | CBM                      |
| M.VTGTIHTYPVTEDESLQSLKARIQQ.D   | 704.3719  | 335000000  |                          |
| T.YGPNGCFKALDDILN(+.98)LK(+411.13)LVHILN(+.98)MVTGTIHTYPVTEDESLQSLKAR.I       | 792.4105  | 310000000  | Deamidation (NQ); 37-290 |
| T.YGPNGCFKALDDILNLK(+411.13)LVHILN(+.98)MVTGTIHTYPVTEDESLQSLKAR.I             | 792.269   | 294000000  | 37-290; Deamidation (NQ) |
| E.DQELLQEAGLALIPD.K   | 812.9275  | 280000000  |                          |
| D.NSKITYETQISPRPQPEVSC(+57.02)ILQEPKRNLAFFQLR.K                               | 855.8542  | 273000000  | CBM                      |
| D.LNGTVKFSSSLPYPNNLNSVLAERLEK.W   | 997.5381  | 269000000  |                          |
| R.IQQDTGIPEEDQELLQEAGLALIPD.K   | 912.4609  | 268000000  |                          |

|   |           |          |                          |
|---|-----------|----------|--------------------------|
| M.GRKQGGTLDDLEEARELYRRLREKPRDQR.T   | 459.4994  | 26400000 |                          |
| D.LKPENIVLQQGEQRLIHKIID.L   | 621.8643  | 25500000 |                          |
| T.DPTYGPNCGFKALDDILNLKLVHILNMVGTIHTYPTVEDESLQSLKARIQQD.T                    | 847.2991  | 25200000 |                          |
| M.VTGTIHTYPTVED.E   | 716.8518  | 24500000 |                          |
| M.EYC(+57.02)QGGDLRKYLNQFENC(+57.02)C(+57.02)GLREGAILTLLSDIASALRYLHENRIHR.D | 956.8212  | 22500000 | CBM                      |
| M.VTGTIHTYPTVEDESLQSLKARIQQDTGIPEED.Q                                       | 1224.278  | 21800000 |                          |
| D.LRKYLN(+.98)QFENC(+57.02)C(+57.02)GLREGAILTLLSDIASALRYLHENRIHR.D.L        | 841.2817  | 21600000 | Deamidation (NQ); CBM    |
| M.SQQLKAKLDFFKTSIQID.L  | 528.2943  | 20800000 |                          |
| E.DESLQSLKARIQQDTGIPEE.D  | 1129.071  | 19900000 |                          |
| M.KERLGTGGFGNVIRWHNQETGEQIAIKQ.C  | 634.1368  | 19500000 |                          |
| M.GRKQGGTLDDLEEARELYRRLREKPRDQRTEG.D  | 660.1829  | 18000000 |                          |
| T.YGPNGC(+411.13)FKALDDILN(+.98)LKLVHILN(+.98)MVTGTIHTYPTVEDESLQSLKAR.I     | 792.4105  | 18000000 | 37-290; Deamidation (NQ) |
| M.VTGTIHTYPTVEDESLQ(+.98)SLKARI.Q   | 640.5828  | 17800000 | Deamidation (NQ)         |
| D.Q(-17.03)ELLQEAGLALIPD.K  | 746.8992  | 16500000 | Pyro-glu from Q          |
| M.E(-18.01)QAVELC(+57.02)GRENEVKLLVER.M                                     | 751.728   | 16200000 | Pyro-glu from E; CBM     |
| M.VTGTIHTYPTVEDESLQSLKARIQQDTGIPEEDQELLQ(+.98)EAGLALIPDKPATQC(+57.02)ISD.G  | 1541.5276 | 15500000 | Deamidation (NQ); CBM    |
| P.RN(+.98)RERWCLEIQIMRRLTHPNVVAAR.D   | 520.6129  | 14600000 | Deamidation (NQ)         |
| D.DLEEARELYRRLREKPRDQRTEGD.S  | 790.4071  | 14300000 |                          |
| E.DLNGTVKFSSSLPYPNNLNSVLAERLEK.W  | 777.1614  | 14000000 |                          |
| D.DLEEARELYRRLR.E   | 616.3347  | 13300000 |                          |
| D.LEEARELYRRLREKPRDQRTEGD.S   | 609.5223  | 12900000 |                          |
| M.EYC(+57.02)QGGDLRKYLNQFENC(+57.02)C(+57.02)GLR.E                          | 695.8149  | 12800000 | CBM                      |
| D.ESLQSLKARIQQD.T   | 758.4106  | 12700000 |                          |
| R.LGTGGFGNVIRWHNQETGEQIAIKQCRQELSPRN.R                                      | 640.3288  | 12400000 |                          |
| D.LNGTVKFSSSLPYPNNLNSVLAER.L  | 874.13    | 12300000 |                          |
| P.RNRERWCLEIQ(+.98)IMRRLTHPNVVAAR.D   | 520.6127  | 12300000 | Deamidation (NQ)         |
| D.DLEEARELYRRLREKPRD.Q  | 495.2677  | 12300000 |                          |
| D.LEEARELYRRLREKPR.D  | 561.3194  | 11600000 |                          |
| D.LRKYLNQFENC(+57.02)C(+57.02)GLR.E   | 657.6615  | 11400000 | CBM                      |
| M.GRKQGGTLDDLEEARE.E  | 591.6345  | 11300000 |                          |
| M.ALQTDIVDLQR.S   | 636.3518  | 10900000 |                          |
| D.LKPENIVLQQGEQRLIHKIIDLGYAKEL.D  | 543.9833  | 10700000 |                          |
| M.GRKQGGTLDDLEEARELYRRL   | 498.8625  | 10400000 |                          |
| R.E(-18.01)GAILTLLSDIASALRYLHENRIHRD.L                                      | 615.142   | 9960000  | Pyro-glu from E          |
| M.KERLGTGGFGNVIRWHNQ(+.98)ETGEQIAIKQC(+57.02)R.Q                            | 697.5613  | 9680000  | Deamidation (NQ); CBM    |
| D.LEKYSEQTEFGITSDKLLLAWR.E  | 657.5999  | 8760000  |                          |
| D.Q(-17.03)ELLQEAGLALIPDKPATQC(+57.02)ISD.G                                 | 1247.1343 | 8490000  | Pyro-glu from Q; CBM     |
| K.VRVYITQLSKTVVC(+57.02)KQK.A   | 410.8427  | 8260000  | CBM                      |
| M.GRKQGGTLDDLEEARELYR.R   | 584.3007  | 7800000  |                          |
| D.PTYGPNGC(+57.02)FKALDD.I  | 777.8489  | 7780000  | CBM                      |
| D.LEEARELYRRLREKPRD.Q   | 472.262   | 7570000  |                          |
| R.DLKPENIVLQQGEQRLIHK.I   | 565.3209  | 7340000  |                          |
| R.ERWC(+57.02)LEIQIM(+15.99)RRLTHPNVVAAR.D                                  | 553.6989  | 7250000  | CBM; Oxidation (M)       |
| R.NRERWC(+57.02)LEIQIMRRLTHPNVVAAR.D  | 503.9421  | 6540000  | CBM                      |
| D.EKTVVRLQEKRQKELWNLKAC(+57.02)SKVRGPVSGSPD.S                               | 810.6556  | 6260000  | CBM                      |
| M.VTGTIHTYPTVEDESLQSLK.A  | 740.0474  | 5940000  |                          |
| L.Q(+.98)RSPMGRKQGGTLDDLEEARELYRRLREKPR.D                                   | 553.7197  | 5790000  | Deamidation (NQ)         |
| D.LEEARELYRRLR.E  | 433.746   | 5770000  |                          |
| R.DLKPENIVLQQGEQRLIHKIIDLGYAK.E   | 783.6968  | 5680000  |                          |
| R.ERWC(+57.02)LEIQIMRRLTHPNVVAAR.D  | 550.4996  | 5640000  | CBM                      |
| R.LGTGGFGNVIRWHNQETGEQ(+.98)IAIKQC(+57.02)RQELSPRN.RER.W                    | 542.9053  | 5630000  | Deamidation (NQ); CBM    |
| R.LGTGGFGNVIRWHNQETGEQIAIKQ(+.98)C(+57.02)RQELSPRN.RER.W                    | 542.9053  | 5630000  | Deamidation (NQ); CBM    |
| L.Q(-17.03)QGEQRLIHKIIDLGYAKEL.D  | 584.5759  | 5420000  | Pyro-glu from Q          |
| R.LGTGGFGNVIRWHNQ(+.98)ETGEQIAIKQC(+57.02)RQELSPRN.RER.W                    | 723.5382  | 5350000  | Deamidation (NQ); CBM    |
| D.LKPENIVLQQGEQRLIHK.I  | 536.5643  | 5280000  |                          |

|  |           |         |                                 |
|--|-----------|---------|---------------------------------|
| D.NSKITYETQ(+.98)ISPRQPESVSC(+57.02)ILQEPKRNLAFFQLRKVWGQVWHSIQTLKED.C                        | 1036.0469 | 5250000 | Deamidation (NQ); CBM           |
| D.NSKITYETQISPRQPESVSC(+57.02)ILQEPKRNLAFFQLRKVWGQ(+.98)VWHSIQTLKED.C                        | 1036.0469 | 5250000 | CBM; Deamidation (NQ)           |
| D.ESLQSLKARIQQDTGIPEED.Q   | 1129.0715 | 5070000 |                                 |
| M.KERLGTGGFGNVIRWHNQETGEQ(+.98)IAIKQC(+57.02)R.Q   | 697.5613  | 4880000 | Deamidation (NQ); CBM           |
| D.ILNLKLVHILNMVGTIHTYPVTEDESLQSLKARIQQDT.G   | 887.2825  | 4880000 |                                 |
| R.LGTGGFGNVIRWHN(+.98)QETGEQIAIKQC(+57.02)R.Q  | 614.9125  | 4840000 | Deamidation (NQ); CBM           |
| R.LGTGGFGN(+.98)VIRWHNQETGEQIAIKQC(+57.02)R.Q  | 614.9125  | 4840000 | Deamidation (NQ); CBM           |
| D.EKTVVRLQEKRQKELWNLLK.I   | 508.504   | 4800000 |                                 |
| E.DEKTVVRLQEKRQKELWNLLK.I  | 531.5093  | 4600000 |                                 |
| M.KERLGTGGFGNVIRWHNQ(+.98)ETGEQIAIKQ(+.98)C(+57.02)RQELSPNRERWCLEIQIMRRLTHPNVVAARDV.P        | 817.7622  | 4530000 | Deamidation (NQ); CBM           |
| M.KERLGTGGFGNVIRWHNQ(+.98)ETGEQIAIKQC(+57.02)RQELSPRN(+.98)RERWCLEIQIMRRLTHPNVVAARDV.P       | 817.7622  | 4530000 | Deamidation (NQ); CBM           |
| M.KERLGTGGFGNVIRWHNQETGEQIAIKQCRQELSPNRERWC(+411.13)LEIQIM(+15.99)RRLTHPNVVAARDV.P.E         | 869.4525  | 4280000 | 37-290; Oxidation (M)           |
| M.KERLGTGGFGNVIRWHNQETGEQIAIK(+411.13)QCRQELSPNRERWCLEIQIM(+15.99)RRLTHPNVVAARDV.P.E         | 869.4525  | 4280000 | 37-290; Oxidation (M)           |
| D.IASALRYLHENRIIHRD.L  | 416.2346  | 4190000 |                                 |
| D.ESLQSLKARIQQ.D   | 467.6003  | 4080000 |                                 |
| E.DESLQSLKARIQQD.T   | 544.2847  | 4010000 |                                 |
| D.PTYGPNGC(+57.02)FKAL.D   | 662.8221  | 3970000 | CBM                             |
| P.RNRERWC(+57.02)LEIQ(+.98)IMRRLTHPNVVAAR.D  | 530.1161  | 3830000 | CBM; Deamidation (NQ)           |
| K.FSSSLPYPNNLNSVLAERLEK.W  | 793.4177  | 3750000 |                                 |
| S.DIASALRYLHENRIIHR.D  | 416.2342  | 3690000 |                                 |
| M.KERLGTGGFGNVIRWHNQETGEQIAIKQC(+57.02).R  | 666.1423  | 3500000 | CBM                             |
| D.PTYGPNGC(+57.02)FKALDDILNLKLVHILNM.V   | 1478.7667 | 3400000 | CBM                             |
| D.NSKITYETQISPRQPESVSC(+57.02)ILQEPK.R   | 783.1531  | 3350000 | CBM                             |
| F.DNSKITYETQISPRQPESVSC(+57.02)ILQ(+.98)EPKRNLAFFQ(+.98)LRKVWGQVWHSIQTLKED.C                 | 1055.3861 | 3260000 | CBM; Deamidation (NQ)           |
| L.GTGGFGNVIRWHNQETGEQIAIKQC(+57.02)R.Q   | 739.8716  | 3240000 | CBM                             |
| R.LGTGGFGNVIR.W  | 545.8042  | 3190000 |                                 |
| E.DESLQSLKARIQQDTGIPEED.Q  | 791.3917  | 3150000 |                                 |
| D.LKPENIVLQQGEQR.L   | 551.3094  | 3090000 |                                 |
| M.KERLGTGGFGNVIR.W   | 501.9515  | 3010000 |                                 |
| R.LGTGGFGNVIRWHNQ(+.98)ETGEQIAIKQC(+57.02)R.Q  | 768.3896  | 2980000 | Deamidation (NQ); CBM           |
| M.KERLGTGGFGNVIRWHNQETGEQ(+.98)IAIKQC(+57.02)RQELSPR.N                                       | 699.8655  | 2960000 | Deamidation (NQ); CBM           |
| K.IIDLGYAKEL.D   | 567.8245  | 2950000 |                                 |
| N.RERWCLEIQ(+.98)IMRRLTHPNVVAAR.D  | 570.5054  | 2950000 | Deamidation (NQ)                |
| D.ESLQSLKARIQQDTGIPEE.D  | 1071.5559 | 2910000 |                                 |
| E.DLNGTVKFS.S  | 490.7563  | 2880000 |                                 |
| M.KERLGTGGFGNVIRWHNQETGEQIAIK.Q  | 760.4038  | 2800000 |                                 |
| R.DLKPENIVLQQGEQRILHIIID.L   | 650.6202  | 2770000 |                                 |
| S.KVRQKSEVDIVVSE.D   | 404.731   | 2720000 |                                 |
| P.RNRERWCLEIQ(+.98)IMRRLTHPNVVAARD.V   | 539.7855  | 2710000 | Deamidation (NQ)                |
| S.SSLPYPNNLNSVLAER.L   | 887.4623  | 2690000 |                                 |
| M.KERLGTGGFGNVIRWHNQETGEQIAIKQC(+57.02)RQELSPNRERWC(+411.13)LEIQIM(+15.99)RRLTHPNVVAARDV.P.E | 875.7881  | 2680000 | CBM; 37-290; Oxidation (M)      |
| M.VGTIHTYPVTEDESLQSLKARIQ.Q  | 672.3566  | 2600000 |                                 |
| D.DLEEARELYRRLREKPRDQR.T   | 552.0994  | 2590000 |                                 |
| D.LEEQARELYRRLREKPRDQR.T   | 529.0942  | 2450000 |                                 |
| M.VRLLQAIQSFEEKVR.V  | 482.8011  | 2380000 |                                 |
| N.GTVKFSSSLPYPNNLNSVLAER.L   | 798.4215  | 2340000 |                                 |
| D.KPATQC(+57.02)ISDGKLNIGHTLD.M  | 695.3418  | 2320000 | CBM                             |
| D.E(-18.01)KTVVRLQEKRQKELWNLLKIAC(+57.02)SKVRGPVSGSPD.S                                      | 672.7142  | 2320000 | Pyro-glu from E; CBM            |
| D.FFKTSIQID.L  | 549.7953  | 2280000 |                                 |
| S.SSLPYPNNLNSVLAERLEK.W  | 715.3841  | 2260000 |                                 |
| D.IPTTENLYFQGAMDPEFM(+15.99)SWSPSLTTQ(+.98)TCGAWEM(+15.99)KE.R                               | 1387.2722 | 2250000 | Oxidation (M); Deamidation (NQ) |
| D.IPTTENLYFQGAM(+15.99)DPEFMSPSWSPSLTTQ(+.98)TCGAWEM(+15.99)KE.R                             | 1387.2722 | 2250000 | Oxidation (M); Deamidation (NQ) |
| R.LGTGGFGNVIRWHNQETGEQIAIKQ(+.98)C(+57.02)RQELSPR.N  | 756.9879  | 2240000 | Deamidation (NQ); CBM           |
| R.LGTGGFGN(+.98)VIRWHNQETGEQIAIKQC(+57.02)RQELSPR.N  | 756.9879  | 2240000 | Deamidation (NQ); CBM           |
| D.IVVEDLNGTVK.F  | 637.354   | 2170000 |                                 |



|  |           |         |                       |
|--|-----------|---------|-----------------------|
| R.LGTGGFGNVIRWHNQ(+.98)ETGEQIAIKQC(+57.02)RQELSPRNR.E                                  | 676.0137  | 1950000 | Deamidation (NQ); CBM |
| D.IASALRYLHENRIHR.D  | 393.2291  | 1940000 |                       |
| M.RRLTHPNVVAARDVPEG.M  | 472.5138  | 1830000 |                       |
| R.E(-18.01)GAILTLLSDIASALRYLHENRIHR.D  | 592.1364  | 1670000 | Pyro-glu from E       |
| D.DLEEQARELYRR.L   | 526.6061  | 1620000 |                       |
| R.LGTGGFGNVIRWHNQETGEQIAIKQC(+57.02)RQELSPRNR.R  | 779.5983  | 1510000 | CBM                   |
| D.Q(-17.03)ELLQEAGLALIP.D  | 689.3855  | 1500000 | Pyro-glu from Q       |
| D.NSKITYETQISPRPQPESVS.C   | 754.3855  | 1490000 |                       |
| R.KGGGLDDLEEQAR.E  | 520.5936  | 1480000 |                       |
| R.EGAILTLLSDIASALRYLHENR.I   | 819.1166  | 1470000 |                       |
| R.NRERWC(+57.02)LEIQIM(+15.99)RRLTHPNVVAAR.D   | 506.6059  | 1450000 | CBM; Oxidation (M)    |
| R.LGTGGFGNVIRWHNQETGEQIAIKQC(+57.02)RQEL.S   | 860.6871  | 1420000 | CBM                   |
| R.LLLQAIQSFEEK.V   | 473.2858  | 1330000 |                       |
| R.LGTGGFGNVIRWHNQETGEQ(+.98)IAIKQC(+57.02)RQELSPRNR.E                                  | 579.5851  | 1320000 | Deamidation (NQ); CBM |
| F.DNSKITYETQISPRPQPESVSC(+57.02)IL.Q   | 921.4617  | 1300000 | CBM                   |
| D.IPTTENLYFQ.G   | 613.3093  | 1200000 |                       |
| M.EQAVELC(+57.02)GRENEVK.L   | 554.2704  | 1160000 | CBM                   |
| M.KERLGTGGFGNVIRWHNQETGEQIAIKQ(+.98)C(+57.02)RQELSPR.N                                 | 699.8621  | 1150000 | Deamidation (NQ); CBM |
| V.TGTIHTYPVTEDESLQSLKAR.I  | 782.7369  | 1140000 |                       |
| G.TGGFGNVIRWHNQETGEQIAIKQC(+57.02)R.Q  | 725.616   | 1100000 | CBM                   |
| M.NEDEKTVVRLQEKRQKELWNLLKIA.C  | 616.9505  | 1090000 |                       |
| M.KERLGTGGFGNVIRWHNQETGEQIAIKQ(+.98)C(+57.02)RQELSPRN(+.98)RERWCLEIQIMRRLTHPNVVAARDV.P | 919.8556  | 1080000 | Deamidation (NQ); CBM |
| F.DNSKITYETQISPRPQPESVSC(+57.02)ILQEPKRNLAFFQLR.K                                      | 878.8601  | 1060000 | CBM                   |
| R.WC(+57.02)LEIQIMRRLTHPNVVAAR.D   | 493.4707  | 1010000 | CBM                   |
| F.DNSKITYETQISPRPQPESVS.C  | 792.7281  | 962000  |                       |
| R.IQQDTGIPEE.D   | 565.2723  | 962000  |                       |
| K.QGGTLDDLEEQAR.E  | 716.3394  | 855000  |                       |
| D.E(-18.01)SLQSLKAR.I  | 507.2909  | 840000  | Pyro-glu from E       |
| M.GRKQ(+.98)GGTLDDLEEQ(+.98)ARELYRRLREKPR.D  | 546.1302  | 822000  | Deamidation (NQ)      |
| R.ERWC(+57.02)LEIQIMRRLTHPNVVAARD.V  | 573.5057  | 818000  | CBM                   |
| M.VTGTIHTYPVTEDESLQSL.K  | 1045.5205 | 814000  |                       |
| L.DDLEEQARELYRRLR.E  | 491.2595  | 814000  |                       |
| T.GTIHTYPVTEDESLQSLKAR.I   | 749.054   | 810000  |                       |
| R.IQQDTGIPEED.Q  | 622.7861  | 787000  |                       |
| D.LKPENIVLQQGEQRLIHKIIDLG.Y  | 664.3898  | 776000  |                       |
| M.RRLTHPNVVAARDVPEGM(+15.99)QNLAPND.L  | 697.3588  | 775000  | Oxidation (M)         |
| Y.PVTEDESLQSLKAR.I   | 524.9498  | 767000  |                       |
| E.DQELLQ(+.98)EAGLALIPD.K  | 813.4198  | 760000  | Deamidation (NQ)      |
| R.LGTGGFGNVIRWHNQETGEQIAIKQC(+57.02)RQE.L  | 832.4169  | 743000  | CBM                   |
| Q.Q(-17.03)GEQRLIHKIIDLGYAKEL.D  | 552.5604  | 706000  | Pyro-glu from Q       |
| R.LGTGGFGNVIRWHNQETGEQIAIKQC(+57.02)RQ.E   | 800.1569  | 682000  | CBM                   |
| M.ALQTDIVDLQRSP.M  | 728.3945  | 680000  |                       |
| M.VTGTIHTYPVTEDE.S   | 781.3732  | 641000  |                       |
| L.GTGGFGN(+.98)VIRWHNQETGEQIAIKQC(+57.02)RQELSPRNRER.W                                 | 704.6937  | 618000  | Deamidation (NQ); CBM |
| M.KERLGTGGFGNVIRWHNQETGE.Q   | 622.0646  | 614000  |                       |
| D.LRKLYLNQFEN.C  | 442.2388  | 572000  |                       |
| M.GRKQGGTLDDLEEQ(+.98)ARELYRRLR.E  | 460.915   | 556000  | Deamidation (NQ)      |
| R.ENEVLLVER.M  | 614.8484  | 555000  |                       |
| L.Q(-17.03)QGEQRLIHKIIDLGYAK.E   | 524.0432  | 553000  | Pyro-glu from Q       |
| R.QKELWNLLK.I  | 391.2332  | 551000  |                       |
| D.EKTVVRLQEKRQKELWNLLKIAC(+57.02)SK.V  | 517.1343  | 540000  | CBM                   |
| G.GFGNVIRWHNQETGEQIAIKQC(+57.02)R.Q  | 549.0798  | 535000  | CBM                   |
| R.VIYQLSKTVVC(+57.02)KQKALELLPK.V  | 640.6298  | 505000  | CBM                   |
| D.NSKITYETQISPRPQPESVSC(+57.02)ILQEPKRNLAFFQLRKVWGVVHSIQLTKEDC(+57.02)NRLQQGQRAAMM.N   | 970.2554  | 497000  | CBM                   |
| P.RNRERWC(+57.02)LEIQ(+.98)IMRRLTHPN(+.98)VVAAR.D                                      | 530.2817  | 490000  | CBM; Deamidation (NQ) |

|  |           |        |                                 |  |
|--|-----------|--------|---------------------------------|--|
| D.KPATQC(+57.02)ISDGKLNIGHTL.D                         | 656.9991  | 483000 | CBM                             |  |
| M.GRKQGGTLDLLEEARELYRRLRE.K                            | 482.258   | 475000 |                                 |  |
| M.GRKQGGTLDLLEEQ(+.98)AR.E                             | 591.9625  | 467000 | Deamidation (NQ)                |  |
| M.SQQLKAKLDFFK.T                                       | 484.9453  | 455000 |                                 |  |
| M.ALQTDIVDLQ(+.98)R.S                                  | 636.8438  | 455000 | Deamidation (NQ)                |  |
| E.DESLQSLKARIQ(+.98)Q.D                                | 506.2708  | 433000 | Deamidation (NQ)                |  |
| Y.DIPTTENLY.F  | 533.2588  | 406000 |                                 |  |
| E.DLNGTVKF.S   | 447.2399  | 401000 |                                 |  |
| G.DLRKYLNQFENC(+57.02)C(+57.02)GLR.E                   | 522.2546  | 397000 | CBM                             |  |
| D.QELLQEAGLALIP.D                                      | 697.8996  | 381000 |                                 |  |
| D.NSKITYETQISPRPQPE.S                                  | 663.3421  | 378000 |                                 |  |
| K.YLNQFENC(+57.02)C(+57.02)GLR.E                       | 787.3489  | 374000 | CBM                             |  |
| C.RQELSPRNRERWC(+57.02)LEIQ(+.98)IMRRLTHPNVVAARD.V     | 572.4419  | 368000 | CBM; Deamidation (NQ)           |  |
| D.LRKYLNQFENC(+57.02).C                                | 495.5822  | 359000 | CBM                             |  |
| M.EQAVELC(+57.02)GREN(+.98)EVKLLVER.M                  | 568.799   | 359000 | CBM; Deamidation (NQ)           |  |
| M.E(-18.01)QAVELC(+57.02)GRENEVK.L                     | 821.8971  | 351000 | Pyro-glu from E; CBM            |  |
| K.VRVYITQLSK.T   | 402.9119  | 345000 |                                 |  |
| G.GTLDLLEEARELYRRLREKPR.D                              | 549.498   | 333000 |                                 |  |
| M.RRLTHPNVVAARDVPE.G                                   | 458.2582  | 332000 |                                 |  |
| R.LGTGGFGNVIRWHN(+.98).Q                               | 510.2602  | 326000 | Deamidation (NQ)                |  |
| K.IIDLGYAK.E   | 446.761   | 317000 |                                 |  |
| M.N(+.98)EDEKTVVRLQEKRQKELWNLLKIAC(+57.02)SKVR.G       | 531.157   | 310000 | Deamidation (NQ); CBM           |  |
| L.QAIQSFEKK.V  | 539.7983  | 302000 |                                 |  |
| M.VTGTIHTYPVTEDESLQ.S                                  | 945.4604  | 292000 |                                 |  |
| D.LEEQARELYRRLREKPRDQRTEG.D                            | 488.9316  | 286000 |                                 |  |
| M.SQQLKAKLDFFKT.S                                      | 389.2227  | 284000 |                                 |  |
| M.GRKQ(+.98)GGTLDLLEEARELYRRLRE.K                      | 482.4252  | 271000 | Deamidation (NQ)                |  |
| D.E(-18.01)SLQSLKARIQQDTGIPEE.D                        | 1062.5503 | 262000 | Pyro-glu from E                 |  |
| M.ALQTDIVD.L   | 437.7294  | 253000 |                                 |  |
| R.LIHKIIDLGYAK.E                                       | 461.9502  | 248000 |                                 |  |
| E.DESLQSLKARIQ.Q                                       | 463.2564  | 236000 |                                 |  |
| Q.AVELC(+57.02)GRENEVKLLVER.M                          | 672.0311  | 227000 | CBM                             |  |
| F.GNVIRWHNQETGEQIAIKQC(+57.02)R.Q                      | 635.0757  | 223000 | CBM                             |  |
| S.KVRQKSEVDIVSED.L                                     | 577.6481  | 215000 |                                 |  |
| M.SQQLKAKLDFFKTSIQI.D                                  | 499.5377  | 211000 |                                 |  |
| D.LGYAKELDQG.E   | 547.28    | 196000 |                                 |  |
| M.KERLGTGGFGNVIRWHNQETGEQIAIKQC(+57.02)RQ(+.98)ELSPR.N | 839.6346  | 193000 | CBM; Deamidation (NQ)           |  |
| K.ARIQQDTGIPEE.D                                       | 678.8414  | 188000 |                                 |  |
| D.NSKITYETQISPRPQPEVSC(+57.02)ILQEPKR.N                | 657.9445  | 186000 | CBM                             |  |
| M.KERLGTGGFGNVIRWHNQ(+.98)ETGEQIAIKQC(+57.02)RQE.L     | 624.3218  | 176000 | Deamidation (NQ); CBM           |  |
| E.NIVLQQGEQRLIHK.I                                     | 559.3251  | 175000 |                                 |  |
| M.EYC(+57.02)QGGDLRKYLNQFENC(+57.02)C(+57.02)GLRE.G    | 728.0761  | 173000 | CBM                             |  |
| K.KVRVIYITQLSKTVVC(+57.02)KQK.A                        | 545.3256  | 171000 | CBM                             |  |
| N.Q(-17.03)ETGEQIAIKQC(+57.02)RQELSPRNRER.W            | 562.6887  | 168000 | Pyro-glu from Q; CBM            |  |
| G.TGGFGN(+.98)VIRWHNQETGEQIAIKQC(+57.02)RQELSPRNRER.W  | 695.1901  | 164000 | Deamidation (NQ); CBM           |  |
| K.VRVYITQLSKTVVC(+57.02)KQKAL.E                        | 559.332   | 164000 | CBM                             |  |
| D.VPEGM(+15.99)QNLAPND.L                               | 650.7962  | 151000 | Oxidation (M)                   |  |
| M.KERLGTGGFGNVIRWHNQETGEQIAIK(+411.13)QC(+57.02)R.Q    | 779.5879  | 138000 | 37-290; CBM                     |  |
| D.LEKYSQTEFGITSD.K                                     | 873.9073  | 128000 |                                 |  |
| R.QELSPRN(+.98)RERWCLEIQ(+.98)IM(+15.99)RRLTHPNVVAAR.D | 615.8246  | 127000 | Deamidation (NQ); Oxidation (M) |  |
| M.WHPRQRGTDPTYGPNGC(+57.02)FKALD.D                     | 644.0582  | 126000 | CBM                             |  |
| R.LGTGGFGNVIRWHN(+.98)QETGEQIAIKQCRQ(+.98)ELSPR.N      | 768.5917  | 120000 | Deamidation (NQ)                |  |
| R.WHNQETGEQIAIKQC(+57.02)R.Q                           | 500.2463  | 118000 | CBM                             |  |
| W.GQVWHSIQTLKED.C                                      | 514.2642  | 115000 |                                 |  |
| W.SPSTTTQTC(+57.02)GAWEM(+15.99)KER.L                  | 666.6401  | 114000 | CBM; Oxidation (M)              |  |

|   |          |        |                                 |
|---|----------|--------|---------------------------------|
| M.GRKQ(+.98)GGTDDLEEQ(+.98)ARELYRRLR.E                | 461.0818 | 112000 | Deamidation (NQ)                |
| M.GRKQ(+.98)GGTDDLEEQAR.E                             | 444.2241 | 105000 | Deamidation (NQ)                |
| M.RRLTHPNVVAARDVPEGM(+15.99)QNLAPN(+.98).D            | 668.8483 | 105000 | Oxidation (M); Deamidation (NQ) |
| R.LGTGGFGNVIRWHN.Q                                    | 509.9321 | 96500  |                                 |
| C.RQ(+.98)ELSPRN(+.98)RERWCLEIQ(+.98)IMRRLTHPNVVAAR.D | 548.1489 | 87100  | Deamidation (NQ)                |
| K.RNLAFFQLR.K   | 388.8927 | 73000  |                                 |
| M.NASRLSQPGQLM(+15.99)SQPS.T                          | 858.9216 | 72500  | Oxidation (M)                   |
| D.DLEEQARELYR.R                                       | 711.356  | 62900  |                                 |
| H.SKVRQKSEVDIVVSE.D                                   | 568.3164 | 58300  |                                 |
| E.E(-18.01)QARELYRRLREKPR.D                           | 397.2294 | 56900  | Pyro-glu from E                 |
| C.ILQEPKRNLAFFQLR.K                                   | 469.0264 | 54200  |                                 |
| D.LKPENIVLQQGEQRL.I                                   | 589.0042 | 47400  |                                 |
| K.RNLAFFQLRK.V  | 431.5912 | 42700  |                                 |
| M.Q(-17.03)NLPNDLPL.L                                 | 539.2836 | 41400  | Pyro-glu from Q                 |
| C.GRENEVKLLVER.M                                      | 481.2762 | 34400  |                                 |
| Q.E(-18.01)LLQEAGLALIPD.K                             | 682.3773 | 28900  | Pyro-glu from E                 |
| R.LGTGGFGNVIRWHN.N                                    | 471.9184 | 28400  |                                 |
| R.KYLNQFENC(+57.02)C(+57.02)GLR.E                     | 567.9335 | 23400  | CBM                             |
| D.VPEGM(+15.99)QNLAPN(+.98).D                         | 593.7745 | 23100  | Oxidation (M); Deamidation (NQ) |
| H.NQETGEQIAIKQC(+57.02)RQELSPR.N                      | 597.0543 | 23000  | CBM                             |
| E.LC(+57.02)GRENEVKLLVER.M                            | 572.3146 | 22400  | CBM                             |
| A.SRLSQPGQL.M   | 493.2719 | 2750   |                                 |

Protein = IKK $\beta$   
Found by = PEAKS DB  
Carbamidomethylation = CBM  
IKK $\beta$  + 39-290

| Peptide   | m/z       | Area No UV | PTM                                    |
|---|-----------|------------|--|
| R.LGTGGFGNVIRWHNQETGEQIAIKQC(+57.02)RQELSPRNRER.W                             | 723.3738  | 245000000  | CBM                                    |
| R.LGTGGFGNVIRWHNQETGEQIAIKQC(+57.02)RQELSPR.N                                 | 756.7905  | 219000000  | CBM                                    |
| M.KERLGTGGFGNVIRWHNQETGEQIAIKQC(+57.02)R.Q                                    | 697.3629  | 176000000  | CBM                                    |
| M.VTGTIHTYPVTEDESLQSLKAR.I  | 815.7598  | 118000000  |  |
| R.EGAILTLLSDIASALRYLHENRIIHRD.L   | 618.7435  | 91600000   |  |
| R.LGTGGFGNVIRWHNQETGEQIAIKQC(+57.02)RQELSPRNR.E                               | 675.8501  | 83100000   | CBM                                    |
| R.EGAILTLLSDIASALRYLHEN(+.98)RIIHRD.L.K                                       | 641.5525  | 75200000   | Deamidation (NQ)                       |
| R.EGAILTLLSDIASALRYLHENRIIHR.D  | 595.7377  | 65600000   |  |
| M.VTGTIHTYPVTEDESLQSLKARIQQD.T  | 977.1691  | 65500000   |  |
| M.GRKQGGTDDLEEQARELYRRLR.E  | 552.7003  | 62300000   |  |
| M.KERLGTGGFGNVIRWHNQETGEQIAIKQC(+57.02)RQELSPR.N                              | 699.6987  | 57700000   | CBM                                    |
| M.KERLGTGGFGNVIRWHNQETGEQIAIKQC(+57.02)RQELSPRNRER.W                          | 679.2125  | 56600000   | CBM                                    |
| M.GRKQGGTDDLEEQARELYRRLREKPRD.Q   | 564.9705  | 53700000   |  |
| M.VRLLQLAIQSFEKK.V  | 558.3422  | 51300000   |  |
| M.GRKQGGTDDLEEQARELYRRLREKPR.D  | 467.9717  | 51300000   |  |
| T.YGPNGC(+57.02)FKALDDILN(+.98)LK(+411.13)LVHILNMVTGTIHTYPVTEDESLQSLKAR.I     | 933.649   | 42700000   | CBM; Deamidation (NQ); 37-290          |
| M.VTGTIHTYPVTEDESLQSLKARIQQDTGIPEEDQELLQEAGLALIPDKPATQC(+57.02)ISDG.K         | 1244.6274 | 38000000   | CBM                                    |
| M.EYC(+57.02)QGGDLRKYLNQFENC(+57.02)C(+57.02)GLREGAILTLLSDIASALRYLHENRIIHRD.L | 732.2454  | 35300000   | CBM                                    |
| M.VTGTIHTYPVTE.D  | 659.3383  | 29900000   |  |
| D.LTYGPNGC(+57.02)FKALDDILNKLVLHILNMVTGTIHTYPVTEDESLQSLKARIQQDT.G             | 1194.418  | 28400000   | CBM                                    |
| R.LGTGGFGNVIRWHNQETGEQ(+.98)IAIKQC(+57.02)R.Q                                 | 614.9131  | 27200000   | Deamidation (NQ); CBM                  |
| M.E(-18.01)YC(+57.02)QGGDLRKYLNQ(+.98)FENCCGLREGAILTLLSDIASALRYLHENRIIHRD.L.K | 972.99    | 25800000   | Pyro-glu from E; CBM; Deamidation (NQ) |
| M.GRKQGGTDDLEEQARELYRRLREKPRDQRTEGD.S   | 679.3538  | 24900000   |  |
| D.LRKYLNQFENC(+57.02)C(+57.02)GLREGAILTLLSDIASALRYLHENRIIHRD.L                | 721.098   | 23800000   | CBM                                    |

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|---|-----------|----------|-----------------------------------|
| M.EQAVELC(+57.02)GRENEVKLLVER.M   | 757.731   | 23700000 | CBM                               |
| D.LNGTVKFSSSLYPNNLNSVLAERLEK.W  | 748.4052  | 23500000 |                                   |
| R.LGTGGFGNVIRWHNQETGEQIAIKQCRQELSPRN.R                                      | 640.3286  | 23300000 |                                   |
| D.LKPENIVLQQGEQRLIHKIIDLGYAKELD.Q   | 563.1541  | 22800000 |                                   |
| P.RNRERWCLEIQ(+.98)IMRRLTHPNVVAAR.D   | 624.5332  | 21200000 | Deamidation (NQ)                  |
| M.EYC(+57.02)QGGDLRKYLNQFENC(+57.02)C(+57.02)GLREGAILLLSDIASALRYLHENRIIHR.D | 717.8664  | 20600000 | CBM                               |
| M.KERLGTGGFGNVIRWHNQETGEQIAIKQC(+57.02)RQELSPRN.R.E                         | 638.4775  | 18900000 | CBM                               |
| D.TGIPEEDQELLQEAGLALIPD.K   | 1126.0715 | 17100000 |                                   |
| M.NEDEKTVVRLQEKRQKELWNLLKIAC(+57.02)SKVRGPVSGSPD.S                          | 735.3999  | 17100000 | CBM                               |
| E.DEKTVVRLQEKRQKELWNLLKIAC(+57.02)SKVRGPVSGSPD.S                            | 694.8849  | 15700000 | CBM                               |
| N.RERWCLEIQ(+.98)IMRRLTHPNVVAAR.D   | 570.5051  | 15400000 | Deamidation (NQ)                  |
| M.VTGTIHTYPVTED.E   | 716.8516  | 14800000 |                                   |
| N.SM(+15.99)ASMSQQLKAKLDFFKTSIQID.L   | 527.4777  | 14600000 | Oxidation (M)                     |
| M.VTGTIHTYPVTEDESLQSLKARIQQDTGIPEE.D  | 889.7025  | 14200000 |                                   |
| P.RN(+.98)RERWCLEIQIMRRLTHPNVVAAR.D   | 520.6126  | 14100000 | Deamidation (NQ)                  |
| D.LKPENIVLQQGEQRLIHKIIDLGYAKEL.D  | 543.9827  | 14000000 |                                   |
| L.DDLEEQARELYRRLREKPR.D   | 618.8326  | 13100000 |                                   |
| D.NSKITYETQISPRQPESVSC(+57.02)ILQEPKRNLAFFQLR.K                             | 855.8538  | 13000000 | CBM                               |
| R.DLKPENIVLQQGEQRLIHKIIDLGYAKEL.D   | 675.5835  | 12400000 |                                   |
| M.KERLGTGGFGNVIRWHNQETGEQIAIKQCRQELSPRN.R                                   | 709.2023  | 12100000 |                                   |
| E.DLNGTVKFSSSLYPNNLNSVLAERLEK.W   | 777.1619  | 12100000 |                                   |
| M.GRKQGGTLDDLEEQARELYRRLREKPRDQR.T  | 524.9986  | 11900000 |                                   |
| D.PTYGPNGC(+57.02)FKALD.D   | 720.3357  | 11100000 | CBM                               |
| M.KERLGTGGFGNVIRWHNQETGEQIAIKQ.C  | 634.1366  | 10600000 |                                   |
| E.DESLQSLKARIQQDTGIPEEDQELLQEAGLALIPD.K                                     | 1288.3259 | 10500000 |                                   |
| M.SQQLKAKLDFFKTSIQID.L  | 528.2944  | 9700000  |                                   |
| D.DLEEQARELYRRLR.E  | 462.503   | 9640000  |                                   |
| M.GRKQGGTLDDLEEQARELYRRLREKPRDQRTEG.D                                       | 495.3895  | 9570000  |                                   |
| D.Q(-17.03)ELLQEAGLALIPD.K  | 746.8989  | 9150000  | Pyro-glu from Q                   |
| D.LKPENIVLQQGEQRLIHKIIDLGYAK.E  | 604.153   | 9130000  |                                   |
| R.E(-18.01)GAILTLLSDIASALRYLHEN(+.98)RIIHRDL.K                              | 637.9537  | 8950000  | Pyro-glu from E; Deamidation (NQ) |
| E.DESLQSLKARIQQ.D   | 505.9424  | 8320000  |                                   |
| E.DESLQSLKARIQQDTGIPEE.D  | 1129.0701 | 8080000  |                                   |
| M.EYC(+57.02)QGGDLRKYLNQFENC(+57.02)C(+57.02)GLR.E                          | 927.4183  | 7870000  | CBM                               |
| R.ERWC(+57.02)LEIQIMRRLTHPNVVAAR.D  | 550.4996  | 7420000  | CBM                               |
| M.GRKQGGTLDDLEEQAR.E  | 591.6343  | 7170000  |                                   |
| E.DQELLQEAGLALIP.D  | 755.4125  | 7000000  |                                   |
| E.DEKTVVRLQEKRQKELWNLLK.I   | 531.5089  | 6340000  |                                   |
| M.VTGTIHTYPVTEDESLQSLKARIQQ.D   | 938.8273  | 6180000  |                                   |
| K.VRVIYTQLSKTVVC(+57.02)KQKALELLPK.V  | 563.7392  | 6130000  | CBM                               |
| D.LKPENIVLQQGEQRLIHKIID.L   | 621.8638  | 5900000  |                                   |
| M.GRKQGGTLDDLEEQARELYRR.L   | 498.8627  | 5890000  |                                   |
| M.GRKQGGTLDDLEEQARELYR.R  | 584.3008  | 5880000  |                                   |
| D.EKTVVRLQEKRQKELWNLLKIAC(+57.02)SKVRGPVSGSPD.S                             | 810.6561  | 5690000  | CBM                               |
| D.LEEQARELYRRLREKPR.D   | 449.2562  | 5670000  |                                   |
| D.ESLQSLKARIQQD.T   | 758.4099  | 5590000  |                                   |
| R.LGTGGFGNVIRWHNQETGEQIAIKQC(+57.02)RQELSPRN.R                              | 779.5978  | 5250000  | CBM                               |
| T.DPTYGPNGC(+57.02)FKALDDILNLKLVHILNMVTGTIHTYPVTEDESLQSLKAR.I               | 786.2707  | 5160000  | CBM                               |
| S.PRN(+.98)RERWCLEIQ(+.98)IM(+15.99)RRLTHPNVVAAR.D                          | 539.6193  | 5070000  | Deamidation (NQ); Oxidation (M)   |
| K.VRVIYTQLSKTVVC(+57.02)KQK.A   | 513.3015  | 4290000  | CBM                               |
| M.VTGTIHTYPVTEDESLQ(+.98)SLKARI.Q   | 640.5822  | 4130000  | Deamidation (NQ)                  |
| D.Q(-17.03)ELLQEAGLALIPDKPATQC(+57.02)IS.D                                  | 1189.6157 | 4000000  | Pyro-glu from Q; CBM              |
| D.DLEEQARELYRRLREKPRD.Q   | 495.2674  | 3930000  |                                   |
| D.LRKYLNQFENC(+57.02)C(+57.02)GLR.E   | 493.4979  | 3870000  | CBM                               |
| E.DLNGTVKFS.S   | 490.756   | 3830000  |                                   |

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| M.VRLLQAIQSFEEKVR.V                                      | 482.8007  | 3780000 |                                      |
| D.PTYGPNGC(+57.02)FKALDD.I                               | 777.849   | 3770000 | CBM                                  |
| M.VTGTIHTYPVTEDESLQSLK.A                                 | 740.0474  | 3730000 |                                      |
| M.KERLGTGGFGNVIRWHNQETGEQIAIKQ(+.98)CRQ(+.98).E          | 593.4729  | 3670000 | Deamidation (NQ)                     |
| D.IPTTENLYFQGA.M   | 677.3392  | 3660000 |                                      |
| R.DLKPENIVLQQGEQRLIHKIIDLGYAK.E                          | 627.1578  | 3660000 |                                      |
| M.VRLLQAIQSFEEK  | 515.6439  | 3460000 |                                      |
| D.ESLQSLKARIQQDTGIPEE.D                                  | 1071.5564 | 3420000 |                                      |
| D.EKTVVRLQEKRQKELWNLLK.I                                 | 508.5034  | 3390000 |                                      |
| T.DPTYGPNGCFKALDDILNLKLVHILNMVGTIHTYPVTEDESLQSLKARIQQD.T | 988.3492  | 3370000 |                                      |
| R.LGTGGFGNVIR.W  | 545.8043  | 3260000 |                                      |
| R.ERWC(+57.02)LEIQIMRRLTHPNVVAARDV.P                     | 593.3134  | 3220000 | CBM                                  |
| M.NEDEKTVVRLQEKRQKELWNLLK.I                              | 483.6063  | 2870000 |                                      |
| R.LGTGGFGNVIRWHNQETGEQIAIKQC(+57.02).R                   | 729.1182  | 2790000 | CBM                                  |
| R.DLKPENIVLQQGEQRLIHKIID.L                               | 650.6199  | 2770000 |                                      |
| D.DLEEQARELYRRLREKPRDQRTEG.D                             | 609.5223  | 2760000 |                                      |
| D.ESLQSLKARIQQ.D   | 467.6002  | 2550000 |                                      |
| E.DESLQSLKARIQQD.T                                       | 544.2852  | 2440000 |                                      |
| R.NRERWC(+57.02)LEIQIMRRLTHPNVVAAR.D                     | 503.9416  | 2380000 | CBM                                  |
| D.IVISEDLNVTYK.F   | 637.3538  | 2370000 |                                      |
| R.LGTGGFGNVIRWHNQETGEQIAIKQ(+.98)C(+57.02)RQELSPR.N      | 630.99    | 2350000 | Deamidation (NQ); CBM                |
| R.LGTGGFGNVIRWHNQ(+.98)ETGEQIAIKQC(+57.02)R.Q            | 614.9122  | 2340000 | Deamidation (NQ); CBM                |
| D.LEEQARELYRRLREKPRD.Q                                   | 590.076   | 2340000 |                                      |
| M.KERLGTGGFGNVIRWHNQETGEQIAIK.Q                          | 608.5251  | 2300000 |                                      |
| N.RERWCLEIQ(+.98)IMRRLTHPNVVAARD.V                       | 593.5104  | 2230000 | Deamidation (NQ)                     |
| R.LGTGGFGN(+.98)VIRWHNQETGEQ(+.98)IAIKQC(+57.02)R.Q      | 768.6398  | 2130000 | Deamidation (NQ); CBM                |
| D.LEEQARELYRRLREKPRDQRTEG.D.S                            | 609.5223  | 2050000 |                                      |
| M.KERLGTGGFGNVIR.W                                       | 501.9513  | 2000000 |                                      |
| D.ESLQSLKARIQQDTGIPEED.Q                                 | 753.0497  | 1850000 |                                      |
| R.DLKPENIVLQQGEQRLIHK.I                                  | 452.4584  | 1830000 |                                      |
| R.LGTGGFGNVIRWHNQETGEQ(+.98)IAIKQC(+57.02)RQELSPR.N      | 630.9911  | 1790000 | Deamidation (NQ); CBM                |
| T.DPTYGPNGCFKALDDILNLKLVHILNMVGTIHTYPVTEDESLQSLKAR.I     | 1088.9709 | 1770000 |                                      |
| K.FSSSLPYPNNLNSVLAERLEK.W                                | 793.4182  | 1720000 |                                      |
| M.KERLGTGGFGNVIRWHN(+.98)QETGEQ(+.98)IAIKQC(+57.02)R.Q   | 697.7615  | 1690000 | Deamidation (NQ); CBM                |
| M.KERLGTGGFGNVIRWHN(+.98)Q(+.98)ETGEQIAIKQC(+57.02)R.Q   | 697.7615  | 1690000 | Deamidation (NQ); CBM                |
| D.DILNLKLVHILN(+.98)MVTGTIHTYPVTE.D                      | 945.8575  | 1600000 | Deamidation (NQ)                     |
| R.ERWC(+57.02)LEIQIM(+15.99)RRLTHPNVVAAR.D               | 553.6987  | 1530000 | CBM; Oxidation (M)                   |
| D.NSKITYETQISPRPQPEVSC(+57.02)ILQEPK.R                   | 783.1512  | 1510000 | CBM                                  |
| S.SSLPYPNNLN(+.98)SVLAERLEKWLQ(+.98)LMLM(+15.99)W.H      | 1088.5498 | 1500000 | Deamidation (NQ); Oxidation (M)      |
| S.SSLPYPNN(+.98)LNSVLAERLEKWLQ(+.98)LMLM(+15.99)W.H      | 1088.5498 | 1500000 | Deamidation (NQ); Oxidation (M)      |
| L.DDLEEQARELYRRLR.E                                      | 491.2599  | 1490000 |                                      |
| E.DESLQSLKARIQQDTGIPEED.Q                                | 791.3951  | 1480000 |                                      |
| D.IASALRYLHENRIIHRD.L                                    | 416.2344  | 1480000 |                                      |
| D.DLEEQARELYRRL  | 526.6061  | 1480000 |                                      |
| M.KERLGTGGFGNVIRWHNQETGEQIAIKQC(+57.02).R                | 666.1428  | 1470000 | CBM                                  |
| R.QELSPRNRRERWC(+57.02)LEIQIMRRLTHPNVVAAR.D              | 533.5757  | 1380000 | CBM                                  |
| R.ERWC(+57.02)LEIQIM(+15.99)RRLTHPN(+.98)VVAAR.D         | 553.8988  | 1380000 | CBM; Oxidation (M); Deamidation (NQ) |
| R.ERWC(+57.02)LEIQ(+.98)IM(+15.99)RRLTHPNVVAAR.D         | 553.8988  | 1380000 | CBM; Deamidation (NQ); Oxidation (M) |
| S.KVRQKSEVDIVVSE.D                                       | 539.3058  | 1370000 |                                      |
| R.DLKPENIVLQQGEQRLIHKII.D                                | 621.8634  | 1360000 |                                      |
| D.LEEQARELYRRLR.E  | 433.7462  | 1360000 |                                      |
| D.DLEEQARELYRRLREKPRDQR.T                                | 552.0995  | 1340000 |                                      |
| D.LKPENIVLQQGEQRLIHK.I                                   | 536.5643  | 1290000 |                                      |
| M.RRLTHPNVVAARDVPEG.M                                    | 472.5134  | 1260000 |                                      |
| D.PTYGPNGC(+57.02)FKAL.D                                 | 662.8219  | 1220000 | CBM                                  |

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| D.NSKITYETQISPRQPESVSC(+57.02)ILQE.P   | 968.8204 | 1220000 | CBM                             |
| F.DNSKITYETQISPRQPESVSC(+57.02)IL.Q  | 921.4619 | 1200000 | CBM                             |
| N.RERWCLEIQ(+.98)IM(+15.99)RRLTHPNVVAAR.D  | 573.7051 | 1180000 | Deamidation (NQ); Oxidation (M) |
| D.IASALRYLHENRIHR.D  | 393.2289 | 1130000 |                                 |
| D.LKPENIVLQQGEQR.L   | 551.3093 | 1100000 |                                 |
| K.IIDLGYAKEL.D   | 567.8246 | 1080000 |                                 |
| P.RNRERWCLEIQ(+.98)IM(+15.99)RRLTHPNVVAAR.D  | 523.2798 | 1070000 | Deamidation (NQ); Oxidation (M) |
| M.GRKQGGTLDDLEEQARELYRRLRE.K   | 482.2581 | 1050000 |                                 |
| D.E(-18.01)KTVVRLQEKQRQKELWNLLKIAC(+57.02)SKVRGPVSGSPD.S                               | 576.7545 | 1040000 | Pyro-glu from E; CBM            |
| K.ERLGTGGFGNVIRWHNQETGEQIAIKQC(+57.02)R.Q  | 671.745  | 1020000 | CBM                             |
| F.DNSKITYETQISPRQPESVSC(+57.02)ILQEPKRNLAFFQLR.K                                       | 878.8597 | 994000  | CBM                             |
| D.E(-18.01)SLQSLKAR.I  | 507.2905 | 993000  | Pyro-glu from E                 |
| R.E(-18.01)GAILTLLSDIASALRYLHENRIHRD.L   | 768.6778 | 983000  | Pyro-glu from E                 |
| M.VTGTIHTYPVTEDESLQ(+.98)SLKAR.I   | 816.0905 | 940000  | Deamidation (NQ)                |
| D.E(-18.01)KTVVRLQEKQRQKELWNLLK.I  | 504.9016 | 882000  | Pyro-glu from E                 |
| R.WC(+57.02)LEIQ(+.98)IMRRLTHPNVVAARDV.P   | 536.4821 | 861000  | CBM; Deamidation (NQ)           |
| K.FSSSLPYPNNLNSVLAER.L   | 1004.51  | 859000  |                                 |
| D.Q(-17.03)ELLQEAGLALIP.D  | 689.3851 | 856000  | Pyro-glu from Q                 |
| R.EGAILTLLSDIASALRYLHENR.I   | 614.5891 | 839000  |                                 |
| D.FFKTSIQID.L  | 549.7956 | 834000  |                                 |
| M.VTGTIHTYPVTEDESLQSLKARIQ.Q   | 672.3575 | 821000  |                                 |
| K.VRVYITQLSK.T   | 402.9117 | 811000  |                                 |
| S.SSLPYPNNLNSVLAER.L   | 887.4608 | 799000  |                                 |
| D.LEKYSEQTEFGITSDKLLLAWR.E   | 657.5988 | 794000  |                                 |
| R.LGTGGFGNVIRWHNQETGEQIAIKQC(+57.02)RQEL.S   | 860.6887 | 743000  | CBM                             |
| R.NRERWC(+57.02)LEIQIM(+15.99)RRLTHPNVVAAR.D   | 506.6072 | 742000  | CBM; Oxidation (M)              |
| L.Q(+.98)RSPM(+15.99)GRKQGGTLDDLEEQARELYRRLR.E   | 563.4668 | 701000  | Deamidation (NQ); Oxidation (M) |
| R.ENEVLLVER.M  | 614.8485 | 681000  |                                 |
| M.KERLGTGGFGNVIRWHNQ(+.98)ETGEQIAIKQC(+57.02)RQELSPRN(+.98)RERWCLEIQIMRRLTHPNVVAARDV.P | 817.7626 | 636000  | Deamidation (NQ); CBM           |
| D.NSKITYETQISPRQPESVS.C  | 754.3855 | 631000  |                                 |
| R.LGTGGFGNVIRWHNQETGEQIAIKQC(+57.02)RQE.L  | 666.1358 | 617000  | CBM                             |
| F.DNSKITYETQISPRQPESVS.C   | 792.7282 | 605000  |                                 |
| M.KERLGTGGFGNVIRWHNQETGEQ(+.98)IAIKQC(+57.02)RQELSPRN(+.98)RERWCLEIQIMRRLTHPNVVAARDV.P | 817.7648 | 554000  | Deamidation (NQ); CBM           |
| D.SQEMVRLLLQAIQSFEKK.V   | 537.8018 | 540000  |                                 |
| D.LEEQARELYRRLREKPRDQR.T   | 529.0934 | 463000  |                                 |
| D.IPTTENLYFQ.G   | 613.3096 | 461000  |                                 |
| E.RWCLEIQIM(+15.99)RRLTHPNVVAAR.D  | 516.4803 | 452000  | Oxidation (M)                   |
| M.NEDEKTVVRLQEKQRQKELWNLLKIAC(+57.02)SK.V  | 691.9824 | 441000  | CBM                             |
| M.EQAVELC(+57.02)GRENEVK.L   | 554.2706 | 428000  | CBM                             |
| V.TGTIHTYPVTEDESLQSLKAR.I  | 782.7369 | 410000  |                                 |
| L.Q(-17.03)QGEQRLIHKIIDLGYAKEL.D   | 584.5757 | 402000  | Pyro-glu from Q                 |
| R.KQGGTLDDLEEQAR.E   | 520.5933 | 388000  |                                 |
| G.TGGFGNVIRWHNQETGEQIAIKQC(+57.02)R.Q  | 725.6156 | 383000  | CBM                             |
| R.LGTGGFGNVIRWHNQETGEQIAIK.Q   | 875.7909 | 356000  |                                 |
| M.KERLGTGGFGNVIRWHNQE.T  | 550.2865 | 349000  |                                 |
| D.KPATQC(+57.02)ISDGKLNEGHTLD.M  | 695.3411 | 335000  | CBM                             |
| E.DLNGTVKF.S   | 447.2404 | 329000  |                                 |
| D.LRKYLNQFEN.C   | 442.2387 | 313000  |                                 |
| K.QGGTLDDLEEQARELYRRLR.E   | 484.4558 | 311000  |                                 |
| E.DESLQSLKARIQQ(+.98).D  | 506.2709 | 306000  | Deamidation (NQ)                |
| R.IQQDTGIPEE.D   | 565.2721 | 303000  |                                 |
| Q.Q(-17.03)GEQRLIHKIIDLGYAKEL.D  | 552.5605 | 297000  | Pyro-glu from Q                 |
| D.KLLLAWR.E  | 450.2953 | 281000  |                                 |
| M.SQQLKAKLDFFK.T   | 363.9609 | 277000  |                                 |
| R.WC(+57.02)LEIQIMRRLTHPNVVAAR.D   | 616.5859 | 270000  | CBM                             |

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| C.RQELSPRNRERWC(+57.02)LEIQ(+.98)IMRRLTHPNVVAAR.D                | 556.0099  | 266000 | CBM; Deamidation (NQ)    |
| S.PRNRERWC(+411.13)LEIQ(+.98)IMRRLTHPNVVAAR.D                    | 605.3193  | 260000 | 37-290; Deamidation (NQ) |
| R.DLKPENIVLQQGEQR.L  | 589.6514  | 253000 |                          |
| T.GTIHTYPVTEDESLQSLKAR.I   | 749.0538  | 251000 |                          |
| D.E(-18.01)SLQSLKARIQQD.T  | 749.4048  | 246000 | Pyro-glu from E          |
| D.E(-18.01)SLQSLKARIQQ.D   | 691.892   | 228000 | Pyro-glu from E          |
| D.LRKYLNQFENC(+57.02)C(+57.02)GLREGAILTLLS.D                     | 717.8779  | 226000 | CBM                      |
| R.LGTGGFGNVIRWHNQETGE.Q  | 691.3369  | 217000 |                          |
| D.PTYGPNGC(+57.02)FKALDDILNLK(+411.13)LVHILNMVTGTI.H             | 768.5914  | 208000 | CBM; 37-290              |
| E.DQELLQ(+.98)EAGLALIP.D   | 755.9056  | 206000 | Deamidation (NQ)         |
| K.QGGTLDDLEEQR.E   | 716.3392  | 196000 |                          |
| A.KLDFFK(+411.13)TSIQID.L  | 622.6454  | 195000 | 37-290                   |
| D.FFKTSIQIDLEK.Y   | 490.2732  | 191000 |                          |
| M.VTGTIHTYPVTEDE.S   | 781.3727  | 188000 |                          |
| Y.DIPTTENLY.F  | 533.2594  | 188000 |                          |
| R.IQQDTGIPEED.Q  | 622.786   | 184000 |                          |
| M.KERLGTGGFGNVIRWHNQETGEQ(+.98)IAIKQ.C                           | 634.3339  | 168000 | Deamidation (NQ)         |
| D.NSKITYETQISPRQPE.S   | 663.3412  | 161000 |                          |
| F.DNSKITYETQISPRQPE.S  | 701.684   | 150000 |                          |
| D.LRKYLNQFENC(+57.02).C  | 495.5827  | 150000 | CBM                      |
| S.DIASALRYLHENRIHR.D   | 416.2344  | 143000 |                          |
| M.ALQTDIVDLQ(+.98)R.S  | 636.8417  | 139000 | Deamidation (NQ)         |
| M.SQQLKAKLDFFKT.S  | 518.6278  | 136000 |                          |
| M.E(-18.01)QAVELC(+57.02)GRENEVK.L                               | 821.8973  | 132000 | Pyro-glu from E; CBM     |
| M.SQQLKAKLDFFKTSIQI.D  | 499.5377  | 129000 |                          |
| G.DLRKYLNQFENC(+57.02)C(+57.02)GLR.E                             | 522.2549  | 128000 | CBM                      |
| R.EGAILTLLSDIA.S   | 608.3453  | 119000 |                          |
| F.DNSKITYETQ(+.98)ISPRQPESVSC(+57.02)ILQEPKRNLAFFQLRK.V          | 754.0663  | 113000 | Deamidation (NQ); CBM    |
| E.DESLQSLKARIQ.Q   | 463.2564  | 110000 |                          |
| M.RRLTHPNVVAARDVPE.G   | 458.2581  | 109000 |                          |
| M.GRKQGGTLDDLEEQ(+.98)AR.E                                       | 444.2233  | 106000 | Deamidation (NQ)         |
| K.ALELLPK.V  | 392.2525  | 105000 |                          |
| M.NEDEKTVVRLQEKRQKELWNLKAC(+57.02)SKVR.G                         | 531.0133  | 103000 | CBM                      |
| P.RN(+.98)RERWCLEIQ(+.98)IMRRLTHPNVVAAR.D                        | 624.7343  | 101000 | Deamidation (NQ)         |
| D.LKPENIVLQ.Q  | 527.3192  | 98200  |                          |
| M.KERLGTGGFGNVIRWHNQETGEQ(+.98)IAIKQ(+.98)CRQELSPRN(+.98).R      | 608.4586  | 94000  | Deamidation (NQ)         |
| M.NASRLSQPGQL.M  | 585.8154  | 89300  |                          |
| D.LEEQARELYR.R   | 436.2301  | 88700  |                          |
| D.IPTTENLYFQGAM(+15.99)DPEFM(+15.99)SWSPSLTTQTCGAWEM(+15.99)KE.R | 1044.4598 | 88400  | Oxidation (M)            |
| M.VTGTIHTYPVT.E  | 594.8166  | 79000  |                          |
| R.LIHKIDLGyak.E  | 461.9505  | 70800  |                          |
| D.ESLQSLKARIQ.Q  | 424.9142  | 67400  |                          |
| G.DSQ(+.98)EMVRLLLQAIQSFEK.K                                     | 712.7113  | 66400  | Deamidation (NQ)         |
| D.LGYAKELDQG.E   | 547.2804  | 63800  |                          |
| M.NLLRNNSC(+57.02)L.S  | 552.2853  | 63000  | CBM                      |
| R.LTHPN(+.98)VVAAR.D   | 539.8066  | 61000  | Deamidation (NQ)         |
| G.TGGFGNVIRWHNQ(+.98)ETGEQ(+.98)IAIKQC(+57.02)RQELSPR.N          | 723.1688  | 57300  | Deamidation (NQ); CBM    |
| K.ARIQDTGIPEE.D  | 678.8417  | 53800  |                          |
| M.GRKQGGTLDDLEEQ(+.98)ARELYRRLR.E                                | 460.9153  | 50400  | Deamidation (NQ)         |
| G.NVIRWHNQETGEQIAIKQC(+57.02)R.Q                                 | 620.8197  | 46800  | CBM                      |
| K.AKLDFFKTSIQID.L  | 509.281   | 43900  |                          |
| K.TSIQIDLEK.Y  | 523.7903  | 43900  |                          |
| D.PTYGPNGC(+57.02)FKA.L  | 606.2802  | 43800  | CBM                      |
| L.Q(-17.03)EPKRNLAFFQLR.K  | 543.9674  | 40300  | Pyro-glu from Q          |
| S.KVRQKSEVDIVVSED.L  | 577.6479  | 37900  |                          |

|   |          |       |                                      |  |
|---|----------|-------|--------------------------------------|--|
| D.VPEGM(+15.99)QNLAPND.L                            | 650.7964 | 36200 | Oxidation (M)                        |  |
| P.RNRERWCLEIQ(+.98)IM(+15.99)RRLTHPN(+.98)VVAAR.D   | 523.4459 | 34100 | Deamidation (NQ); Oxidation (M)      |  |
| D.LKPENIVLQQGEQRLIHKII.D                            | 593.1082 | 30300 |                                      |  |
| K.TVVC(+57.02)KQKALELLPK.V                          | 542.9916 | 30100 | CBM                                  |  |
| K.RNLAFFQLR.K                                       | 388.8928 | 25100 |                                      |  |
| P.RN(+.98)RERWC(+57.02)LEIQIM(+15.99)RRLTHPNVVAAR.D | 532.7818 | 23800 | Deamidation (NQ); CBM; Oxidation (M) |  |
| Q.E(-18.01)LLQEAGLALIPD.K                           | 682.3776 | 21600 | Pyro-glu from E                      |  |
| T.E(-18.01)DESLQSLKAR.I                             | 629.3214 | 21400 | Pyro-glu from E                      |  |