

## 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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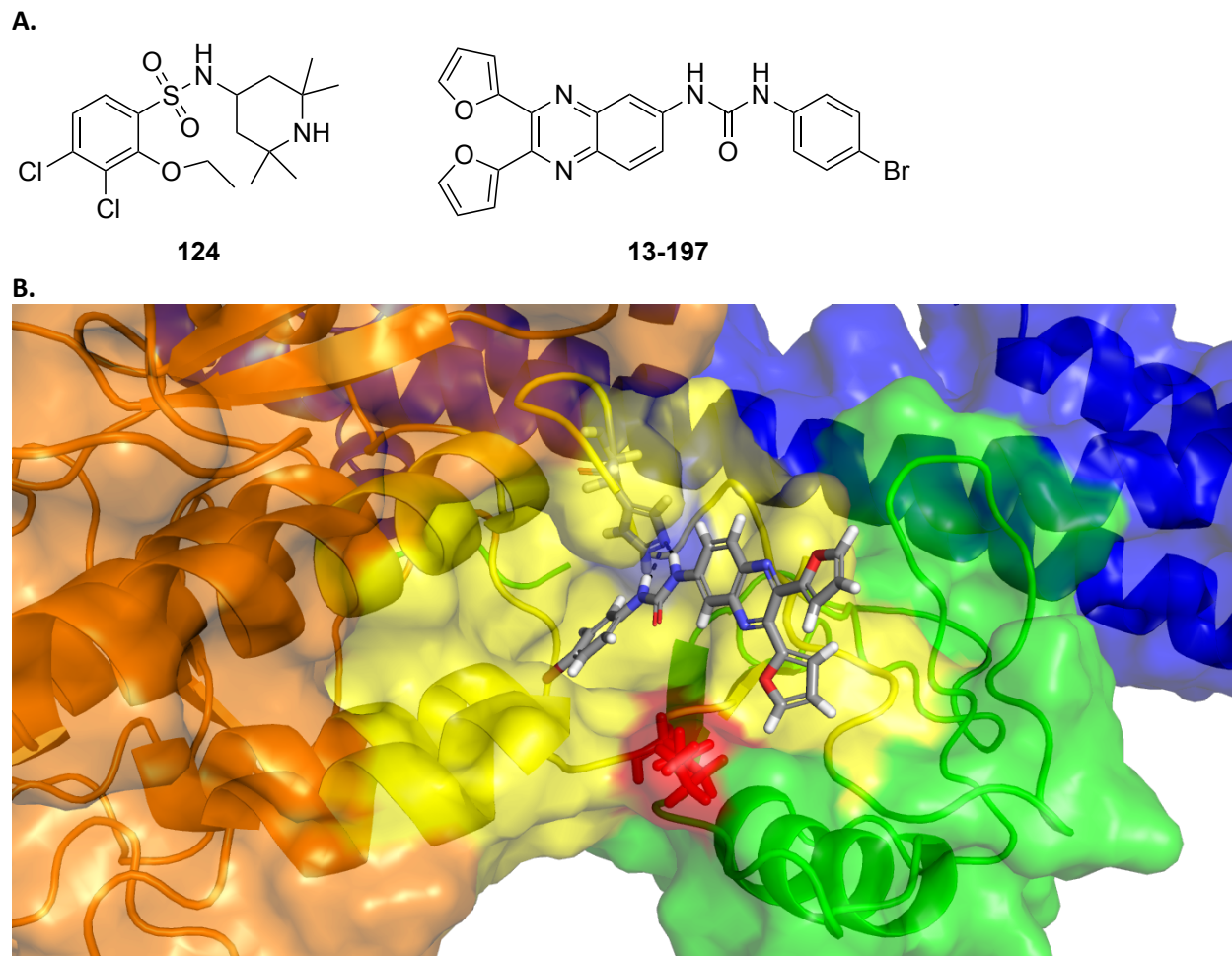
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Electronic Supplementary Information (ESI) available: [details of any supplementary information available should be included here]. See DOI: 10.1039/x0xx00000x



**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

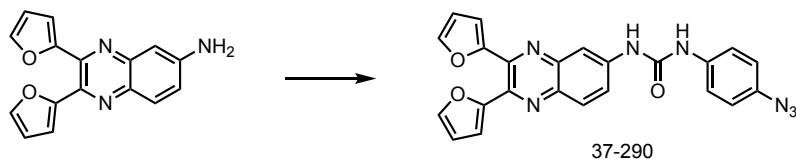
ATP concentrations tested: 3.3, 10, 30, 90, and 270 μM ATP

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	92400000	Deamidation (NQ)
M.VTGTIHTYPVTEDESLQSLKARIQQD.T	733.129	85400000	
M.VRLLLQAIQSFEEK.V	558.3423	85400000	
R.EGAILTLLSDIASALRYLHENRIIHR.D	595.7384	80100000	
T.YGPNGCFKALDDILN(+.98)LK(+411.13)LVHILNMVTGTIHTYPVTEDESLQSLKAR.I	924.145	72000000	Deamidation (NQ); 37-290
D.PTYGPNGC(+57.02)FKALDDILNLKLVHILNMVTGTIHTYPVTEDESLQSLKARIQ(+.98)QDTG.I	1005.1855	70200000	CBM; Deamidation (NQ)
M.KERLGTGGFGNVIRWHNQETGEQIAIKQCRQELSPR.N.R	608.0319	54100000	
D.LKPENIVLQQGEQRLIHKIIDLGYAKELD.Q	563.1544	51900000	
R.LGTGGFGNVIRWHNQETGEQIAIKQC(+57.02)RQELSPRNR.E	675.8514	50000000	CBM
D.TGIPEEDQELLQEAGLALIPD.K	1126.0718	48100000	
R.LGTGGFGNVIRWHNQETGEQIAIKQC(+57.02)RQELSPRNRERWCLEIQ(+.98)IMRRLTHPNVVAARDV.P	771.7348	45600000	CBM; Deamidation (NQ)
M.EYC(+57.02)QGGDLRKYLNQFENC(+57.02)C(+57.02)GLREGAILTLLSDIASALRYLHENRIIHRD.L	732.2449	42400000	CBM
T.YGPN(+.98)GCFKALDDILNLK(+411.13)LVHILNMVTGTIHTYPVTEDESLQSLKAR.I	924.145	40100000	Deamidation (NQ); 37-290
E.DEKTVVRLQEKRQKELWNLLKIAC(+57.02)SKVRGPVSGSPD.S	595.7603	39700000	CBM
R.LGTGGFGNVIRWHNQETGEQ(+.98)IAIKQC(+57.02)R.Q	614.9129	39400000	Deamidation (NQ); CBM
D.DLEEQARELYRRLREKPR.D	590.0767	39100000	
M.VRLLLQAIQSFEEK.K	515.644	37700000	
D.PTYGPNGC(+57.02)FKALD.D	720.3354	37100000	CBM
M.VTGTIHTYPVTEDESLQSLKARIQQDTGIPEE.D	1185.9331	36900000	
M.VTGTIHTYPVTE.D	659.3383	36900000	
K.VRVITYTQLSKTVVC(+57.02)KQKALELLPK.V	563.7393	36600000	CBM
M.KERLGTGGFGNVIRWHNQETGEQIAIKQC(+57.02)RQELSPRNR.E	744.723	33700000	CBM
M.VTGTIHTYPVTEDESLQSLKARIQQ.D	704.3719	33500000	
T.YGPNGCFKALDDILN(+.98)LK(+411.13)LVHILN(+.98)MVTGTIHTYPVTEDESLQSLKAR.I	792.4105	31000000	Deamidation (NQ); 37-290
T.YGPNGCFKALDDILNLK(+411.13)LVHILN(+.98)MVTGTIHTYPVTEDESLQSLKAR.I	792.269	29400000	37-290; Deamidation (NQ)
E.DQELLQEAGLALIPD.K	812.9275	28000000	
D.NSKITYETQISPRPQPEVSC(+57.02)ILQEPKRNLAFFQLR.K	855.8542	27300000	CBM
D.LNGTVKFSSSLPYPNNLNSVLAERLEK.W	997.5381	26900000	
R.IQQDTGIPEEDQELLQEAGLALIPD.K	912.4609	26800000	

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)ILQEPKRNLAFFQLRKVWGQVWHSIQLTKED.C	1036.0469	5250000	Deamidation (NQ); CBM
D.NSKITYETQISPRQPESVSC(+57.02)ILQEPKRNLAFFQLRKVWGQ(+.98)VWHSIQLTKED.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)LRKVWGQVWHSIQLTKED.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.VTGTIHTYPVTEDESLQSLK.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.GRKQGGTLDLLEEQARELYRRLRE.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.GTLDLLEEQARELYRRLREKPR.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)GGTLDLLEEQARELYRRLRE.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)ELSPRN.R	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)GGTLDLLEEQ(+.98)ARELYRRLR.E	461.0818	112000	Deamidation (NQ)
M.GRKQ(+.98)GGTLDLLEEQAR.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.LGTGGFGNVIRWH.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.GRKQGGTLDLLEEQARELYRRLR.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.GRKQGGTLDLLEEQARELYRRLREKPRD.Q	564.9705	53700000	
M.VRLLQLAIQSFEKK.V	558.3422	51300000	
M.GRKQGGTLDLLEEQARELYRRLREKPR.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.GRKQGGTLDLLEEQARELYRRLREKPRDQRTEGD.S	679.3538	24900000	
D.LRKYLNQFENC(+57.02)C(+57.02)GLREGAILTLLSDIASALRYLHENRIIHRD.L	721.098	23800000	CBM

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.NSKITYETQISPRPQPEVSC(+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.LKPENIVLQQGEQRLIHKIIDL.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		

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

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

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.NEDEKTVVRLQEKRQKELWNLLKIAC(+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.LIHKIIDLGYAK.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	