

Supplemental Information

1. Synthesis of lysine propionylated and butyrylated peptides

The peptides were synthesized on a Protein Technologies Symphony peptide synthesizer using Fmoc chemistry. All amino acids were purchased from Novabiochem (San Diego, CA) and the solvents were obtained from Fisher Science (Fair Lawn, NJ). Fmoc-Lys(Ac) was used for lysine residues with acetylated side-chains. For lysine residues requiring modification with either butyl or propionyl moieties, an orthogonally-protected Fmoc-Lys(Mtt) reagent was used. At the end of the synthesis, prior to removal of the N-terminal Fmoc protecting group, the methyltrityl (Mtt) side-chain protection was removed with 1% trifluoroacetic acid in dichloromethane. The resin was washed 10x in the acidic solution until the yellow color disappeared. The resin was then treated with 5% diisopropylethylamine to neutralize the TFA salt and the free amino group was reacted with either propionic acid or butyric acid, which had been preactivated with HBTU/HOBt. The coupling efficiency was monitored using a quantitative ninhydrin test. After derivatization the resin was treated with 20% piperidine in NMP to remove the Fmoc group and cleaved with 95% TFA, containing thiol scavengers for 90 mins. The crude peptides were precipitated in diethyl ether and desalted on C-18 RP Sep-Pak columns before lyophilization to a dry powder.

2. Mapping *in vitro* lysine-propionylation and lysine-butyrylation sites in p53, histone H4, p300 and CBP and *in vitro* lysine-acetylation sites in histone H4 by nano-HPLC/mass spectrometry

The substrate of interest was incubated with an acetyltransferase at an enzyme-to-substrate ratio of ~1:10, and a CoA of interest using the reaction conditions described in Experimental Procedures. To determine autopropionylation or autobutyrylation sites, only the enzyme of interest was used for *in vitro* reaction. To determine *in vitro* lysine-acetylation sites in histone H4, CBP was used for reaction. The protein mixture was resolved in SDS-PAGE. The protein of interest was excised and in-gel digested with trypsin. The resulting tryptic peptides were analyzed by nano-HPLC/MS/MS in a LTQ mass spectrometer and protein sequence database search for mapping protein modification sites using a procedure described in Experimental Procedures in the main text.

All the MS/MS raw data regarding the following analysis will be available upon request.

In vitro lysine acetylation sites in histone H4 catalyzed by CBP

gi|28173560 histone H4 [Homo sapiens]

(Note: M1 was removed for position alignment with Fig1B)

K* - acetylated lysine

```
1 SGRGK*GGK*GL GK*GGAK*RHRK VLRDNIQGIT K*PAIRRLARR GGVK*RISGLI
51 YEETRGVLKV FLENVIRDAV TYTEHAK*RK*T VTAMDVVYAL K*RQGRTLYGF
101 GG
```

In vitro lysine propionylation sites in P53 catalyzed by p300

gi|3041867 p53 [Homo sapiens]

K^ - propionylated lysine

```
1 MEEPQSDPSV EPPLSQETFSDLWKLLPENN VLSPLPSQAM DDLMLSPDDI
51 EQWFTEDPGP DEAPRMPEAA PRVAPAPAAP TPAAPAPAPS WPLSSSVPSQ
101 KTYQGSYGFR LGFLHSGTAK SVTCTYSPAL NKMFCQLAKT CPVQLWVDST
151 PPPGTRVRAM AIYKQSQHMT EVVRRCPHHE RCSDSDGLAP PQHLIRVEGN
201 LRVEYLDDRN TFRHSVVVPY EPPEVGS DCT TIHYNMCNS SCMGGMNRNP
251 ILTIITLED SGNLLGRNSF EVRVCACPGR DRRTEENLR KKGEPHHELP
301 PGSTKRALPN NTSSSPQK^K^ KPLDGEYFTL QIRGRERFEM FRELNEALEL
351 KDAQAGKEPG GSRAHSSHLK SKKGQSTSRH KKL MFKTEGP DSD
```

In vitro propionylation sites in histone H4 catalyzed by CBP

gi|28173560 histone H4 [Homo sapiens]

(Note: M1 was removed for position alignment with Fig1B)

K^ - propionylated lysine

```
1 SGRGK^GGK^GL GK^GGAK^RHRK VLRDNIQGIT K^PAIRRLARR GGVK^RISGLI
51 YEETRGVLKV FLENVIRDAV TYTEHAK^RK^T VTAMDVVYAL K^RQGRTLYGF
101 GG
```

In vitro lysine propionylation sites in p300 by autopropionylation

gi|50345997 E1A binding protein p300 [Homo sapiens]

K[^] - propionylated lysine

```
1 MAENVVEPGP PSAKRPKLSS PALSASASDG TDFGSLFDLE HDLPDELINS
51 TELGLTNGGD INQLQTSLGM VQDAASKHK^Q LSELLRSGSS PNLNMGVGGP
101 GOVMASQAQQ SSPGLGLINS MVKSPMTQAG LTSPNMGMGT SGPNOGPTQS
151 TGMMSNPVNO PAMGMNTGMN AGMNPGLAA GNGQGIMPNO VMNGSIGAGR
201 GRQNMQYPNP GMGSAGNLLT EPLQQGSPQM GGQTGLRGPQ PLKMGMMNNP
251 NPYGSPYTQN PGQQIGASGL GLQIQTKTVL SNNLSPFAMD K^KAVPGGGMP
301 NMGQQPAPQV QQPGLVTPVA QGMGSGAHTA DPEKRKLIQQ QLVLLLLHAHK
351 CQRREQANGE VRQCNLPHCR TMK^NVLNHMT HCQSGKSCQV AHCASSRQII
401 SHWKNCTRHD CPVCLPLKNA GDKRNQQPIL TGAPVGLGNP SSLGVGQQSA
451 PNLSTVVSQID PSSIERAYAA LGLPYQVNQM PTQPQVQAKN QQNQQPQOSP
501 QGMRPMSNMA ASPMGVNGGV GVQTPSLLSD SMLHSAINSQ NPMMSENASV
551 PSLGPMPTAA QPSTTGIRKQ WHEDITQDLR NHLVHKLVAQ IFPTPDPAAL
601 K^DRRMENTLVA YARK^VEGDMY ESANNRAEYY HLLAEKIYKI QKELEEKRRT
651 RLQKQNMLPN AAGMVPVSMN PGPNMGQPQP GMTSNGPLPD PSMIRGSVPN
701 QMMPRITPQS GLNQFGQMSM AQPPIVPRQT PPLQHHGQLA QPGALNPPMG
751 YGPRMQPSN QGQFLPQTQF PSQGMNVTNI PLAPSSGQAP VSQAQMSSSS
801 CPVNSPIMPP GSQGSHIHCP QLPQPALHQN SPSVPVSRTP TPHHTPPSIG
851 AQQPATTIP APVPTPPAMP PGPQSQUALHP PPRQTPTPPT TQLPQQVQPS
901 LPAAPSADQP QQQPRSQQST AASVPTPTAP LLPPQPATPL SQPAVSIEGQ
951 VSNPPSTSST EVNSQAIIEK QPSQEVKMEA KMEVDQPEPA DTQPEDISES
1001 KVEDCKMEST ETEERSTELK TEIKEEEDQP STSATQSSPA PGQSK^K^KIFK
1051 PEELRQALMP TLEALYRQDP ESLPFRQVVD PQLLGIPDYF DIVKSPMDLS
1101 TIKRKLDTGQ YQEPWQYVDD IWLMFNNAWL YNRKTSRVYK YCSKLSEVFE
1151 QEIDPVMQSL GYCCGRKLEF SPQTLCCYGK QLCTIPRDAT YYSYQNRHYF
1201 CEKCFNEIQG ESVSLGDDPS QPQTTINKEQ FSKRKNNDTLD PELFVECTEC
1251 GRKMHQICVL HHEIWPAGF VCDGCLKKSA RTRKENKFSA KRLPSTRLGT
1301 FLENRVNDFL RRQNHPESEGE VTRVVVHASD KTVEVKPGMK ARFVDSGEMA
1351 ESFPYRTKAL FAFEEIDGVD LCFFGMHVQE YGSDCPPPNQ RRVYISYLDL
1401 VHFFRPKCLR TAVYHEILIG YLEYVKKLGY TTGHIWACPP SEGDDYIFHC
1451 HPPDQKIPKP KRLQEWYKMK LDKAVSERIV HDYKDIFKQA TEDRLTSAKE
1501 LPYFEGDFWP NVLEESIKEL EQEEEEERKRE ENTSNESTDV TK^GDSK^NAK^K^
1551 K^NNK^K^TSK^NK^ SSLSRGNK^K^K^ PGMPNVSNL SQKLYATMEK HKEVFFVIRL
1601 IAGPAANSLP PIVDPDLIP CDLMDGRDAF LTLARDKHLE FSSLRRAQWS
1651 TMCMLVELHT QSQDRFVYTC NECKHHVETR WHCTVCEDYD LCITCYNTKN
1701 HDHKMEK^LGL GLDDESNNQQ AAATQSPGDS RRLSIQRCIQ SLVHACQCRN
1751 ANCSLPSCQK MKRVVQHTK^G CK^RKTNGGCP ICKQLIALCC YHAKHCQENK
1801 CPVPFCLNIK QKLRQQQLQH RLQQAQMLRR RMASMORTGV VGQQQGLPSP
1851 TPATPTTPTG QQPTTPQTPQ PTSQPQPTPP NSMPPYLPRT QAAGPVSQGK
1901 AAGQVTPPTP PQTAPPLPG PPPAAVEMAM QIQRAAETQR QMAHVQIFQR
1951 PIQHQMPPMT PMAPMGMNPP PMTRGPGSGL EPGMGPTGMQ QQPWSQGG
2001 PQQPQLQSGM PRPAMMSVAQ HGQPLNMAPQ PGLGQVGISP LKPGTVSQA
2051 LQNLRLTLRS PSSPLQQQV LSILHANPQL LAAFIKQRAA KYANSNPQPI
2101 PGQPGMPQGQ PGLQPPTMPG QQGVHNSPAM QNMNPMQAGV QRAGLPQQQP
2151 QQQLQPPMGG MSPQAQMMNM NHNTMPSQFR DILRRQMMQ QQQQGGAGPG
2201 IGPGMANHNQ FQQPQGVGY PQQQQRMQHH MQQMQQGNMG QIGQLPQALG
2251 AEAGASLQAY QQRLLQQMG SPVQPNPMSP QQHMLPNQAQ SPHLQGGQIP
2301 NSLSNQVRSP QPVPSRPQS QPPHSSPSR MQPQPSPHHV SPQTSSPHPG
2351 LVAAQANPME QGHFASPDQN SMLSQLASNP GMANLHGASA TDLGLSTDNS
2401 DLNSNLSQST LDIH
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In vitro propionylation sites in CBP by autopropionylation

gi|4321116 CREB-binding protein [Homo sapiens]

K[^] - propionylated lysine

```
1 MAENLLDGPP NPKRAKLSSP GFSANDSTDF GSLFDLENDL PDELIPNGGE
51 LGLLNSGNLV PDAASKHKQL SELLRGGSGS SINPGIGNVS ASSPVQQQLG
101 GQAQGPNSA NMAASLSAMGK SPLSQGDSSA PSLPKQAASST SGPTPAASQA
151 LNPQAQKQVG LATSSPATSQ TGPVICMNAN FNQTHPGLLN SNSGHSLINQ
201 ASQQAQVMN GSLGAAGRGR GAGMPYPTPA MQGASSSVLA ETLTQVSPQM
251 TGHAGLNTAQ AGGMAKMGIT GNTSPFGQPF SQAGGQPMGA TGVNPQLASK
301 QSMVNSLPTF PTDIKNTSVT NVPNMSQMOT SVGIVPTQAI ATGPTADPEK
351 RKLIIQQQLVL LLHAHKCQRR EQANGEVRAC SLPHCRTMKN VLNHMTHCQA
401 GKACQVAHCA SSRQIISHWK NCTRHDPCVC LPLKNASDKR NQQTILGSPA
451 SGIQNTIGSV GTGQQNATSL SNPNIIDPSS MQRAYAALGL PYMNQPQTQL
501 QPQVPGQPPA QPQTHQQMRT LNPLGNNPMN IPAGGITTDQ QPPNLISESA
551 LPTSLGATNP LMNDGSNSGN IGTLLSTIPTA APPSSTGVRK GWHEHVTQDL
601 RSHLVHKLTV AIFPTPDPAAL LKDRRMENTLV AYAKK^VEGDM YESANSRDEY
651 YHLLAEKIYK IQK^ELEEKRR SRLHKQGILG NQPALPAPGA QPPVIPQAQP
701 VRPPNGPLSL PVNRMQVSQG MNSFNPMSLG NVQLPQAPMG PRAASPMNHS
751 VQMNSMGSVP GMAISPSRMP QPPNMMGAHT NNMMAQAPAQ SQFLPQNQFP
801 SSSGAMSVGM GQPPAQTGVS QGQVPGAALP NPLNMLGPQA SQLPCPPVTQ
851 SPLHPTPPPA STAAGMPSLQ HTTPPGMTTP QPAAPTQPST PVSSSGQTPT
901 PTPGSVPSAT QTQSTPTVQA AAQAQVTPQP QTPVQPPSVA TPQSSQQQPT
951 PVHAQPPGTP LSQAAASIDN RVPTPSSVAS AETNSQQPGP DVPVLEMKTE
1001 TQAEDETPDP GESKGEPRSE MMEEDLOGAS QVKEETDIAE QKSEPMEVDE
1051 KKPEVKVEVK EEEEESSNGT ASQSTSPSQP RKKIFKPEEL RQALMPTLEA
1101 LYRQDPESLP FRQPVDPQLL GIPDYFDIVK NPMDLSTIKR KLDTGQYQEP
1151 WQYVDDVWLM FNNAWLYNRK TSVYKFCFSK LAEVFEQEID PVMQSLGYCC
1201 GRKYEFSPQT LCCYGKQLCT IPRDAAYYSY QNRYHFCEKC FTEIQGENVT
1251 LGDDPSQPQT TISKDQFEKK KNDTLDPEPF VDCKECCRKM HQICVLHYDI
1301 IWPSGFVCDN CLKKTGRPRK^ ENK^FSAK^RLQ TTRLGNHLED RVNKFRRQN
1351 HPEAGEVFVR VVASSDKTVE VKPGMKSFRV DSGEMSEFP YRTKALFAFE
1401 EIDGVDVCFE GMHVQEYGS CPPPNTRRVY ISYLDSEHFF RPRCLRTAVY
1451 HEILIGLEY VKKLGVTGH IWACPPSEG DDIYFCHPPD QKIPKPKRLQ
1501 EWYKMLDK^A FAERIIHDYK DIFKQATEDR LTSAKELPYF EGDWFNVLE
1551 ESIKELEQEE EERKKEESTA ASETTEGSQG DSKNAKKNN K^KTNKNK^SSI
1601 SRANK^K^KPSM PNVSNDLSQK LYATMEKHKE VFFVIHLHAG PVINTLPPIV
1651 DPDLLSCDL MDGRDAFLTL ARDKHWEFSS LRRSKWSTLC MLVELHTQGQ
1701 DRFVYTCNEC KHHVETRWHC TVCEDYDLCI NCYNTKSHAH KMKVWGLGLD
1751 DEGSSQGEPO SKSPQESRRL SIQRCIQSLV HACQCRNANC SLPSCQKMKR
1801 VVQHTK^GCK^R KTNGGCPVCK QLIALCCYHA KHCQENKCPV PFCLNIKHL
1851 RQQQIQHRLQ QAQLMRRRMA TMNTRNVPQQ SLPSPTSAPP GTPTQQPSTP
1901 QTPQPPAQPO PSPVSMSPAG FPSVARTQPP TTVSTGKPTS QVPAPPPPAQ
1951 PPPAAVEAAR QIEREAQQQQ HLYRVNINNS MPPGRTGMGT PGSQMAPVSL
2001 NVPRPNQVSG PVMPSMPPGQ WQQAPLPQQQ PMPGLPRPVI SMQAQAAVAG
2051 PRMPVQPPR SISPSALQDL LRTLKSPSSP QQQQQVLNIL KSNPQLMAAF
2101 IKQRTAKYVA NQPGMQPQPQ LQSQPGMQPQ PGMHQQPSLQ NLNAMQAGVP
2151 RPGVPPQQQA MGGLNPQGQA LNIMNPGHNP NMASMNPPQYR EMLRRQLLQ
2201 QQQQQQQQQQ QQQQQQGSAG MAGGMAGHGQ FQQPQGGGY PPAMQQQRM
2251 QQHPLPLQSS MGQMAAQMGQ LGQMGQPGLG ADSTPNIQQA LQQRILQQQ
2301 MKQQIGSPGQ PNPMSPPQHM LSGQPQASHL PGQQIATSLS NQVRSAPVQ
2351 SPRPQSQPPH SSPSPRIQPQ PSPHHVSPQT GSPHPGLAVT MASSIDQGH
2401 GNPEQSAML PQLNTPRSAL SSELSLVGDT TGDITLEKFVE GL
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In vitro lysine butyrylation sites in p53 catalyzed by p300

gi|3041867 p53 [Homo sapiens]

K - butyrylated lysine

```
1 MEEPQSDPSV EPPLSQETFSDLWKLLPENN VLSPLPSQAM DDLMLSPDDI
51 EQWFTEDPGP DEAPRMPEAA PRVAPAPAAP TPAAPAPAPS WPLSSSVPSQ
101 KTYQGSYGFR LGFLHSGTAK SVTCTYSPAL NKMFCQLAKT CPVQLWVDST
151 PPPGTRVRAM AIYKQSQHMT EVVRRCPHHE RCSDSDGLAP PQHLIRVEGN
201 LRVEYLDDRN TFRHSVVVPY EPPEVGS DCT TIHYNMNCNS SCMGGMNRNP
251 ILTIITLEDSDGNLLGRNSF EVRVCACPGRRRTEENLR KKGEPPHEL
301 PGSTKRALPN NTSSSPQKK KPLDGEYFTL QIRGRERFEM FRELNEALEL
351 KDAQAGKEPG GSRAHSSHLK SKKGQSTSRH KKLMPKTEGP DSD
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In vitro lysine butyrylation sites in Histone H4 catalyzed by CBP

gi|28173560 histone H4 [Homo sapiens]

(Note: M1 was removed for position alignment with Fig1B)

K - butyrylated lysine

```
1 SGRGKGGKGL GKGGAKRHRK VLRDNIQGIT KPAIRRLARR GGVKRISGLI
51 YEETRGVLKV FLENVIRDAV TYTEHAKRKT VTAMDVVYAL KRQGRTLYGF
101 GG
```

In vitro lysine butyrylation sites in p300 by autobutyrylation

gi|50345997 E1A binding protein p300 [Homo sapiens]

K - butyrylated lysine

```
1 MAENVVEPGP PSAKRPKLSS PALSASASDG TDFGSLFDLE HDLPDELINS
51 TELGLTNGGD INQLQTSLGM VQDAASKHKQ LSELLRSGSS PNLNMGVGGP
101 GQVMASQAQQ SSPGLGLINS MVKSPMTQAG LTSPNMGMGMT SGPNGQPTQS
151 TGMMNSPVNQ PAMGMNTGMN AGMNPGLAA GNGQGIMPNO VMNGSIGAGR
201 GRQNMQYPNP GMGSAGNLLT EPLQQGSPQM GGQTGLRGPQ PLKMGMMNNP
251 NPYGSPYTQN PGQQIGASGL GLQIQTKTVL SNNLSPFAMD KKAVPGGGMP
301 NMQQPAPQV QQPGLVTPVA QGMGSGAHTA DPEKRKLIQQ QLVLLLHAHK
351 CQRREQANGE VRQCNLPHCR TMKNVLNHMT HCQSGKSCQV AHCASSRQII
401 SHWKNCTRHD CPVCLPLKNA GDKRNQQPIL TGAPVGLGNP SSLGVGQOSA
451 PNLSTVSQID PSSIERAYAA LGLPYQVNQM PTQPQVQAKN QQNQPGQSP
501 QGMRPMSNMS ASPMGVNGGV GVQTPSLLSD SMLHSAINSQ NPMMSNASV
551 PSLGPMPTAA QPSTTGIRKQ WHEDITQDLR NHLVHKLQVA IFPTPDPAAL
601 KDRRMENTLVA YARKVEGDMY ESANNRAEYY HLLAEKIYKI QKELEEKRR
651 RLQKQNMPLN AAGMVPVSMN PGPNMGGPQP GMTSNGPLPD PSMIRGSVPN
701 QMMPRITPQS GLNQFGQMSM AQPPIVPRQT PPLQHHGQLA QPGALNPPMG
751 YGPRMQQPSN QGQFLPQTQF PSQGMNVTNI PLAPSSGQAP VSQAQMSSSS
801 CPVNSPIMPP GSQGSIHCP QLPQPALHQN SPSPVPSRTP TPHHTPPSIG
851 AQQPATTIP APVPTPPAMP PGPQSALHP PPRQTPTPT TQLPQQVQPS
901 LPAAPSADQP QQQPRSQQST AASVPTPTAP LLPPQPATPL SQPAVSIEGQ
951 VSNPPSTSST EVNSQAIAEK QPSQEVKMEA KMEVDQPEPA DTQPEDISES
1001 KVEDCKMEST ETEERSTELK TEIKEEEDQP STSATQSSPA PGQSKKKIFK
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1051 PEELRQALMP TLEALYRQDP ESLPFRQPV D PQLLGIPDYF DIVKSPMDLS
 1101 TIKRKLDTGQ YQEPWQYVDD IWLMFNNAWL YNRKTSRVYK YCSKLSEVFE
 1151 QEIDPVMQSL GYCCGRKLEF SPQTLCCYGK QLCTIPRDAT YYSYQNRHYF
 1201 CEKCFNEIQG ESVSLGDDPS QPQTTINKEQ FSKRKNDTLD PELFVECTEC
 1251 GRKMHQICVL HHEIIPAGF VCDGCLKKSA RTRKENKFS KRLPSTRLGT
 1301 FLENRVNDFL RRQNHPESEGE VTVRVVHASD KTVEVKPGMK ARFVDSGEMA
 1351 ESFPYRTKAL FAFEEIDGVD LCFFGMHVQE YGSDCPPPNQ RRVYISYLDL
 1401 VHFFRPKCLR TAVYHEILIG YLEYVKKLGY TTGHIWACPP SEGDDYIFHC
 1451 HPPDQKIPKP KRLQEWYKMM LDKAVSERIV HDYKDIFKQA TEDRLTSAKE
 1501 LPYFEGDFWP NVLEESIKEL EQEEEEERKRE ENTSNESTDV TKGDSK"NAK"K"
 1551 K"NNK"K"TSK"NK" SLSRGNK"KK PGMPNVSNDL SQKLYATMEK HKEVFFVIRL
 1601 IAGPAANSLP PIVDPDLIP CDLMDGRDAF LTLARDKHLE FSSLRAQWS
 1651 TMCMLVELHT QSQDRFVYTC NECKHHVETR WHCTVCEDYD LCITCYNTKN
 1701 HDHKMEKLG LGLDDESNNQ AAATQSPGDS RRLSIQRCIQ SLVHACQCRN
 1751 ANCSLPSCQK MKRVVQHTK"G CKRKTNGGCP ICKQLIALCC YHAKHCQENK
 1801 CPVPFCLNIK QKLRQQQLQH RLQQAQMLRR RMASMORTGV VGQQQGLPSP
 1851 TPATPTTPTG QQPTTPQTPQ PTSQPQPTPP NSMPPYLPRT QAAGPVSQGK
 1901 AAGQVTPPTP PQTAQPPLPG PPPAAVEMAM QIQRAAETQR QMAHVQIFQR
 1951 PIQHQMPPMT PMAPMGMNPP PMTRGPGSGL EPGMGPTGMQ QPPWVSQGL
 2001 PQPQQQLQSGM PRPAMMSVAQ HGQPLNMAPQ PGLGQVGISP LKPGTVSQQA
 2051 LQNLRLTLRS PSSPLQQQV LSILHANPQL LAAFIKQRAA KYANSNPQPI
 2101 PGQPMPQGG PGLQPPTMPG QQGVHNSPAM QNMNPMQAGV QRAGLPQQQP
 2151 QQQLQPPMGG MSPQAQQMMN NHNTMPSQFR DILRRQQMMQ QQQQQGAGPG
 2201 IGPGMANHNQ FQPPQGVGYP PQQQQRMQHH MQQMQQGNMG QIGQLPQALG
 2251 AEAGASLQAY QRLLQQQMG SPVQPNPMSP QQHMLPNQAQ SPHLQGGQIP
 2301 NSLSNQVRSP QPVPSPRPQS QPPHSSPSR MQPQPSPHHV SPQTSSPHPG
 2351 LVAAQANPME QGHFASPDQN SMLSQLASNP GMANLHGASA TDLGLSTDNS
 2401 DLNSNLSQST LDIH

In vitro lysine butyrylation sites in CBP by autobutyrylation

gi|4321116 CREB-binding protein [Homo sapiens]

K" - butyrylated lysine

1 MAENLLDGPP NPKRAKLSSP GFSANDSTDF GSLFDLENDL PDELIPNGGE
 51 LGLLNSGNLV PDAASKHKQL SELLRGGSGS SINPGIGNVS ASSPVQQGLG
 101 GQAQQPNSA NMAASLQAMGK SPLSQGDSSA PSLPKQAASG SGPTPAASQA
 151 LNPQAQKQVG LATSSPATSQ TGPICMNAN FNQTHPGLLN SNSGHSLINQ
 201 ASQQAQVMN GSLGAAGRGR GAGMPYPTPA MQGASSSVLA ETLTQVSPQM
 251 TGHAGLNTAQ AGGMAKMGIT GNTSPFGQPF SQAGGQPMGA TGVNPQLASK
 301 QSMVNSLPTF PTDIKNTSVT NVPNMSQMQT SVGIVPTQAI ATGPTADPEK
 351 RKLIQQQLVL LLHAHKCQRR EQANGEVRAC SLPHCRTMKN VLNHMTHCQA
 401 GKACQVAHCA SSRQIISHWK NCTRHDPCVC LPLKNASDKR NQQTILGSPA
 451 SGIQNTIGSV GTGQQNATSL SNPNPIDPSS MQRAYAALGL PYMNQPQTQL
 501 QPQVPGQQA QPQTHQQMRT LNPLGNNPMN IPAGGITTDQ QPPNLI SESA
 551 LPTSLGATNP LMNDGSNSGN IGTLSIPTA APPSSTGVRK GWHEHVTQDL
 601 RSHLVHKLQV AIFPTPDPA LKDRRMENLV AYAKK"VEGDM YESANSRDEY
 651 YHLLAEKIYK IQK"ELEEKRR SRLHKQGILG NQPALPAPGA QPPVIPQAQP
 701 VRPPNGPLSL PVNRMQVSQG MNSFNPMSLG NVQLPQAPMG PRAASPMNHS
 751 VQMNMSGVSVP GMAISPSRMP QPPNMMGAHT NNMMAQAPAQ SQFLPQNQFP
 801 SSSGAMSVGM GQPPAQTGVS QGQVPGAALP NPLNMLGPQA SQLPCPPVTQ
 851 SPLHPTPPPA STAAGMPSLQ HTTPPGMTPP QPAAPTQPT PVSSSGQPT
 901 PTPGSVPSAT QTQSTPTVQA AAQAQVTPQP QTPVQPPSVA TPQSSQQPT
 951 PVHAQPPGTP LSQAAASIDN RVPTPSSVAS AETNSQQPGP DVPVLEMKTE

1001 TQAEDTEPDP GESKGEPRSE MMEEDLQAS QVKEETDIAE QKSEPMEVDE
 1051 KKPEVKVEVK EEEEESSNGT ASQSTSPSQP RKKIFKPEEL RQALMPTLEA
 1101 LYRQDPESLP FRQPVDPQLL GIPDYFDIVK NPMDLSTIKR KLDTGQYQEP
 1151 WQYVDDVWLM FNNAWLYNRK TSRVYKFCSE LAEVFEQEID PVMQSLGYCC
 1201 GRKYEFSPQT LCYGYKQLCT IPRDAAYSY QNRYHFCEKC FTEIQGENVT
 1251 LGDDPSQPQT TISKDQFEKK KNDTLDPEPF VDCKECGRKM HQICVLHYDI
 1301 IWPSGFVCDN CLKKTGRPRK ENKFSAKRLQ TTRLGNHLED RVNKFLLRRQN
 1351 HPEAGEVFVVR VVASSDKTVE VKPGMKSFRV DSGEMSESFY YRTKALFAFE
 1401 EIDGVDVCFE GMHVQEYGS DPPPNTRRVY ISYLDSEHFF RPRCLRTAVY
 1451 HEILIGYLEY VKKLGVTGH IWACPPSEG DDIYFHCHPPD QKIPKPKRLQ
 1501 EWYKKMLDK^A FAERIIHDYK DIFKQATEDR LTSAKELPYF EGDWPNVLE
 1551 ESIKELEQEE EERKKEESTA ASETTEGSQG DSKNAKKNN **K**^AKTNKNK^ASSI
 1601 SRANKKPSM PNVSNDSLQK LYATMEKHKE VFFVIHLHAG PVINTLPPIV
 1651 DPDLLSCDL MDGRDAFLTL ARDKHWEFSS LRRSKWSTLC MLVELHTQGQ
 1701 DRFVYTCNEC KHHVETRWHC TVCEDYDLCI NCYNTKSHAH KMKVWGLGLD
 1751 DEGSSQGEPO SKSPQESRRL SIQRCIQSLV HACQCRNANC SLPSCQKMKR
 1801 VVQHT**K**^A**GCK**^AR KTNGGCPVCK QLIALCCYHA KHCQENKCPV PFCLNIKHKL
 1851 RQQQIQHRLQ QAQLMRRRMA TMNTRNVPQQ SLPSPTSAPP GTPTQQPSTP
 1901 QTPQPPAQPO PSPVSMSPAG FPSVARTQPP TTVSTGKPTS QVPAPPPPAQ
 1951 PPPAAVEAAR QIEREAQQQQ HLYRVNINNS MPPGRTGMGT PGSQMAPVSL
 2001 NVPRPNQVSG PVMPSMPPGQ WQQAPLPQQQ PMPGLPRPVI SMQAQAAVAG
 2051 PRMPVQPPR SISPSALQDL LRTLKSPSSP QQQQVNLIL KSNPQLMAAF
 2101 IKQRTAKYVA NQPGMQPQPG LQSQPGMQPQ PGMHQPSLQ NLNAMQAGVP
 2151 RPGVPPQQA MGGLNPQQA LNIMNPGHNP NMASMNPPYR EMLRRQLLQ
 2201 QQQQQQQQQQ QQQQQQGSAG MAGGMAGHGQ FQQPQGGGY PPAMQQQRM
 2251 QQHLPLQGSS MGQMAAQMGO LGQMGPGLG ADSTPNIQA LQQRILQQQ
 2301 MKQQIGSPGQ PNPMSPOQHM LSGQPQASHL PGQIATSLS NQVRSPAPVQ
 2351 SPRPQSOPPH SSPSPRIQPO PSPHHVSPQT GSPHPGLAVT MASSIDQHL
 2401 GNPEQSAMPL QLNTPSRSAL SSELSLVGDT TGDITLEKFVE GL

Supplemental Figure Captions:

F1. MS/MS analysis of individual synthetic peptide.

- (A) The fragmentation spectrum of the synthetic Peptide 1
(GK_{Prop}GGK_{Ac}GLGK_{Prop}GGAK_{Ac}R) containing acetylated and propionylated lysines;
- (B) The fragmentation spectrum of the synthetic Peptide 12
(GK_{Butyl}GGK_{Ac}GLGK_{Ac}GGAK_{Ac}R) containing acetylated and butyrylated lysines;
- (C) The fragmentation spectrum of the synthetic Peptide 13
(GK_{Ac}GGK_{Ac}GLGK_{Butyl}GGAK_{Ac}R) containing acetylated and butyrylated lysines;
- (D) The fragmentation spectrum of the synthetic Peptide 2
(GGK_{Prop}GLGK_{Ac}GGAK_{Ac}R) containing acetylated and propionylated lysines;
- (E) The fragmentation spectrum of the synthetic Peptide 3
(GGK_{Ac}GLGK_{Prop}GGAK_{Ac}R) containing acetylated and propionylated lysines.

F2. Annotation of the MS/MS spectrum in Fig. 2A for identification of Peptide 1, 12, and 13.

- (A) Peak assignment in spectrum Fig. 2A for identification of lysine-propionylated and -acetylated Peptide 1 ($\text{GK}_{\text{Prop}}\text{GGK}_{\text{Ac}}\text{GLGK}_{\text{Prop}}\text{GGAK}_{\text{Ac}}\text{R}$);
- (B) Peak assignment in spectrum Fig.2A for identification of lysine-butyrylated and -acetylated Peptide 12 ($\text{GK}_{\text{Butyl}}\text{GGK}_{\text{Ac}}\text{GLGK}_{\text{Ac}}\text{GGAK}_{\text{Ac}}\text{R}$). The square labels show the fragment ions specific to Peptide 12 as compared to Peptide 1;
- (C) Peak assignment in spectrum Fig.2A for identification of lysine-butyrylated and -acetylated Peptide 13 ($\text{GK}_{\text{Ac}}\text{GGK}_{\text{Ac}}\text{GLGK}_{\text{Butyl}}\text{GGAK}_{\text{Ac}}\text{R}$). The circle labels show the fragment ions specific to Peptide 13 as compared to Peptide 1.
- (D) Peak annotation including all three peptides: Peptide 1, Peptide 12 and Peptide 13 (peptide sequences are shown above) in the same spectrum, similar to Fig. 2A. For each b- or y-ion label, the numbers at the upper right corner show the peptide assignment of this fragment ion. For example, $y_1^{1,12,13}$ means the fragment ion can be assigned as y_1 of either Peptide 1, Peptide 12 or Peptide 13.

F3. Annotation of the MS/MS spectrum in Fig. 2C for identification of Peptide 2 and 3.

- (A) Peak assignment in Spectrum Fig. 2C for identification of lysine propionylated and -acetylated Peptide 2 ($\text{GGK}_{\text{Prop}}\text{GLGK}_{\text{Ac}}\text{GGAK}_{\text{Ac}}\text{R}$);
- (B) Peak assignment in spectrum Fig.2C for identification of lysine- propionylated and -acetylated Peptide 3 ($\text{GGK}_{\text{Ac}}\text{GLGK}_{\text{Prop}}\text{GGAK}_{\text{Ac}}\text{R}$). The triangle labels show the fragment ions specific to Peptide 3 as compared to Peptide 2.
- (C) Peak annotation including two peptides: Peptide 2 and Peptide 3 (peptide sequences are shown above) in the same spectrum, similar to Fig. 2C. For each b- or y-ion label, the numbers at the upper right corner show the peptide assignment of this fragment ion. For example, $y_1^{2,3}$ means the fragment ion can be assigned as y_1 of either Peptide 2 or Peptide 3.

F4. Identification of lysine-modified peptides (listed in Table) and annotation of their corresponding fragmentation ions. Peak m/z table for each peptide was generated by Mascot software.

- (A) Peak assignment for the identification of lysine-propionylated and -acetylated Peptide 1 in Table 1 ($\text{GK}_{\text{Prop}}\text{GGK}_{\text{Ac}}\text{GLGK}_{\text{Prop}}\text{GGAK}_{\text{Ac}}\text{R}$);
- (B) Peak assignment for the identification of lysine-propionylated and -acetylated Peptide 2 in Table 1 ($\text{GGK}_{\text{Prop}}\text{GLGK}_{\text{Ac}}\text{GGAK}_{\text{Ac}}\text{R}$);
- (C) Peak assignment for the identification of lysine-propionylated and -acetylated Peptide 3 in Table 1 ($\text{GGK}_{\text{Ac}}\text{GLGK}_{\text{Prop}}\text{GGAK}_{\text{Ac}}\text{R}$);
- (D) Peak assignment for the identification of lysine-propionylated and -acetylated Peptide 4 in Table 1 ($\text{GK}_{\text{Prop}}\text{GGK}_{\text{Ac}}\text{GLGK}_{\text{Ac}}\text{GGAK}_{\text{Ac}}\text{R}$);
- (E) Peak assignment for the identification of lysine-propionylated and -acetylated Peptide 5 in Table 1 ($\text{GK}_{\text{Ac}}\text{GGK}_{\text{Prop}}\text{GLGK}_{\text{Ac}}\text{GGAK}_{\text{Ac}}\text{R}$);

- (F) Peak assignment for the identification of lysine-propionylated and -acetylated Peptide 6 in Table 1 ($\text{GK}_{\text{Ac}}\text{GGK}_{\text{Ac}}\text{GLGK}_{\text{Prop}}\text{GGAK}_{\text{Ac}}\text{R}$);
- (G) Peak assignment for the identification of lysine-propionylated and -acetylated Peptide 7 in Table 1 ($\text{GK}_{\text{Prop}}\text{GGK}_{\text{Ac}}\text{GLGK}_{\text{Ac}}\text{GGAK}$);
- (H) Peak assignment for the identification of lysine-propionylated and -acetylated Peptide 8 in Table 1 ($\text{GK}_{\text{Ac}}\text{GGK}_{\text{Prop}}\text{GLGK}_{\text{Ac}}\text{GGAK}$);
- (I) Peak assignment for the identification of lysine-propionylated and -acetylated Peptide 9 in Table 1 ($\text{GK}_{\text{Ac}}\text{GGK}_{\text{Ac}}\text{GLGK}_{\text{Prop}}\text{GGAK}$);
- (J) Peak assignment for the identification of lysine-propionylated and -acetylated Peptide 10 in Table 1 ($\text{GGK}_{\text{Ac}}\text{GLGK}_{\text{Prop}}\text{GGAK}$);
- (K) Peak assignment for the identification of lysine-propionylated and -acetylated Peptide 11 in Table 1 ($\text{GGK}_{\text{Prop}}\text{GLGK}_{\text{Ac}}\text{GGAK}$);
- (L) Peak assignment for the identification of lysine-propionylated and -acetylated Peptide 12 in Table 1 ($\text{GK}_{\text{Butyl}}\text{GGK}_{\text{Ac}}\text{GLGK}_{\text{Ac}}\text{GGAK}_{\text{Ac}}\text{R}$);
- (M) Peak assignment for the identification of lysine-propionylated and -acetylated Peptide 13 in Table 1 ($\text{GK}_{\text{Ac}}\text{GGK}_{\text{Ac}}\text{GLGK}_{\text{Butyl}}\text{GGAK}_{\text{Ac}}\text{R}$);

Figure F1

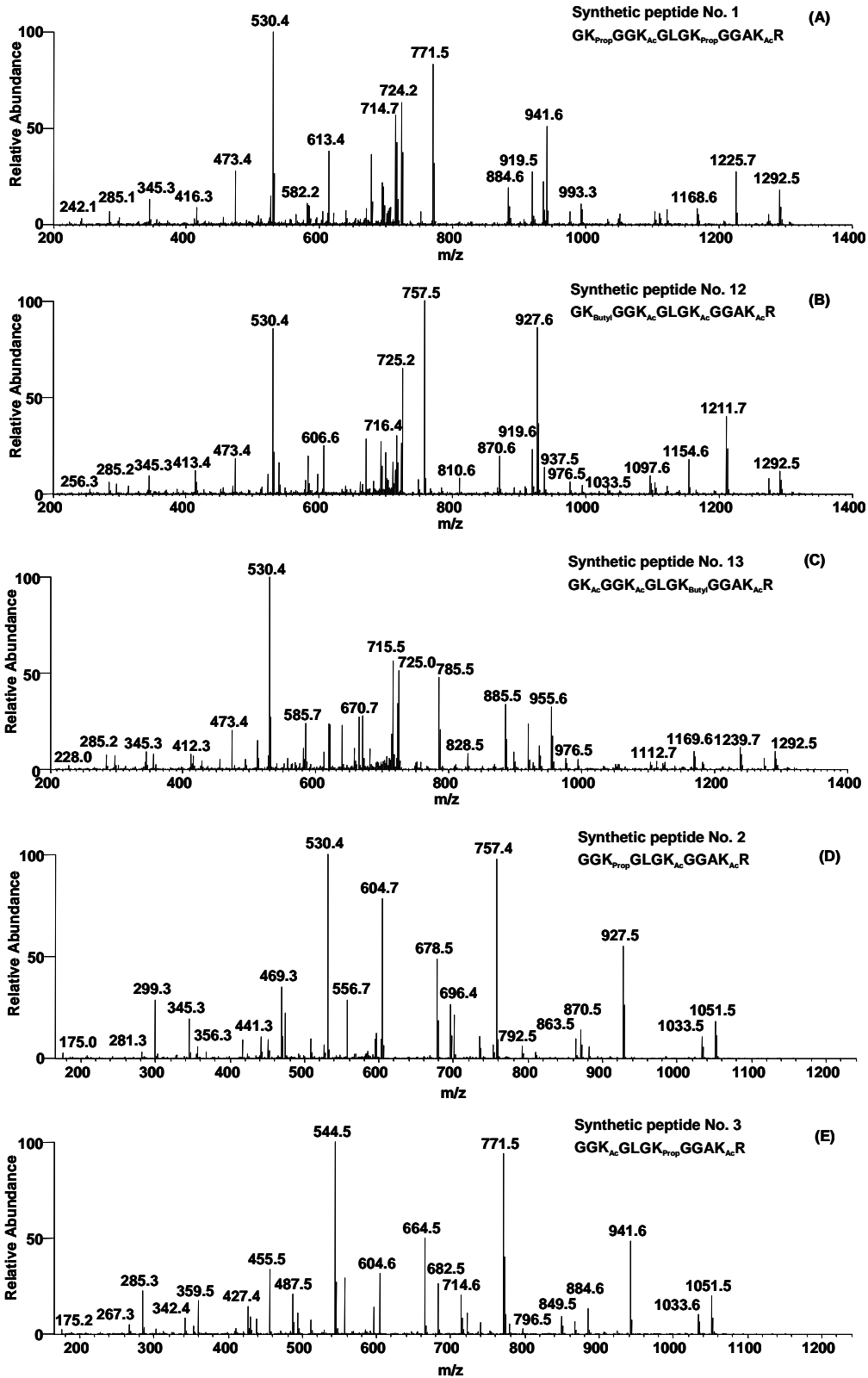


Figure F2

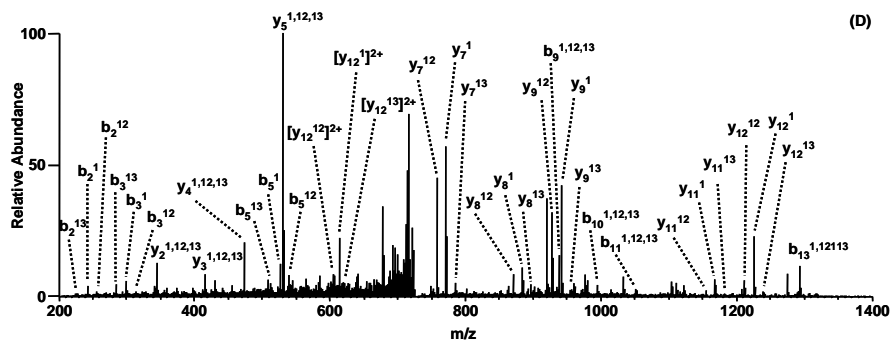
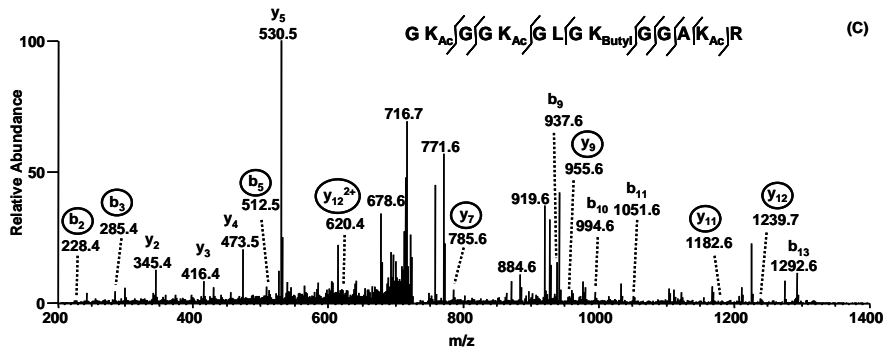
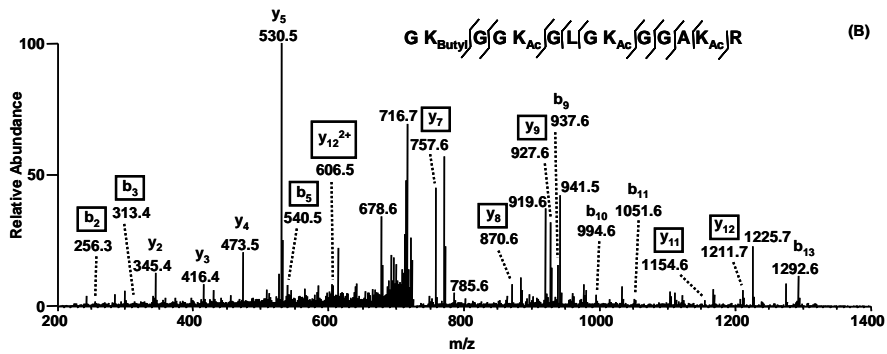
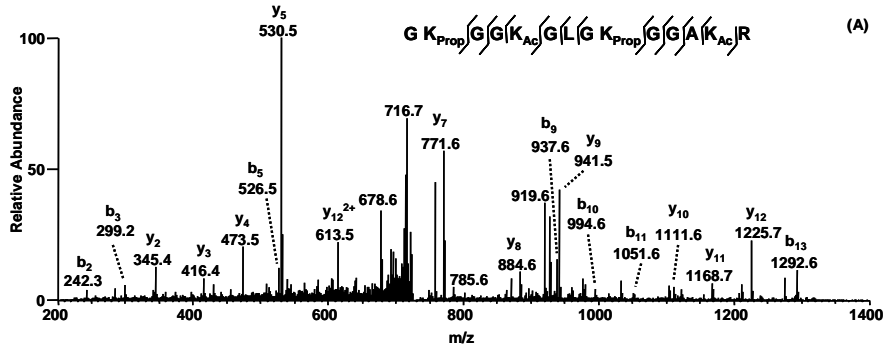


Figure F3

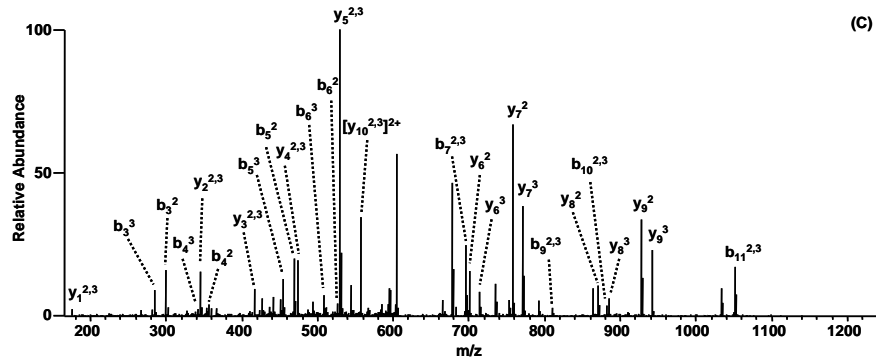
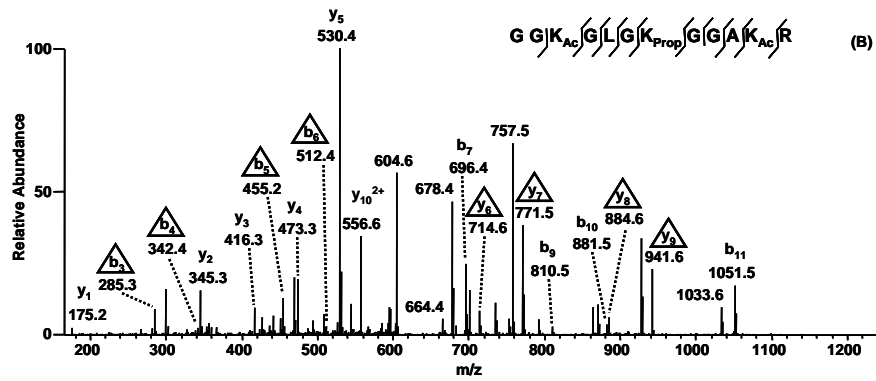
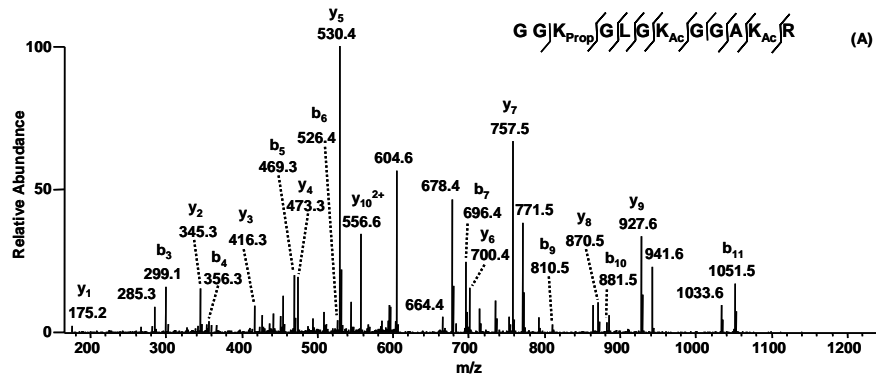
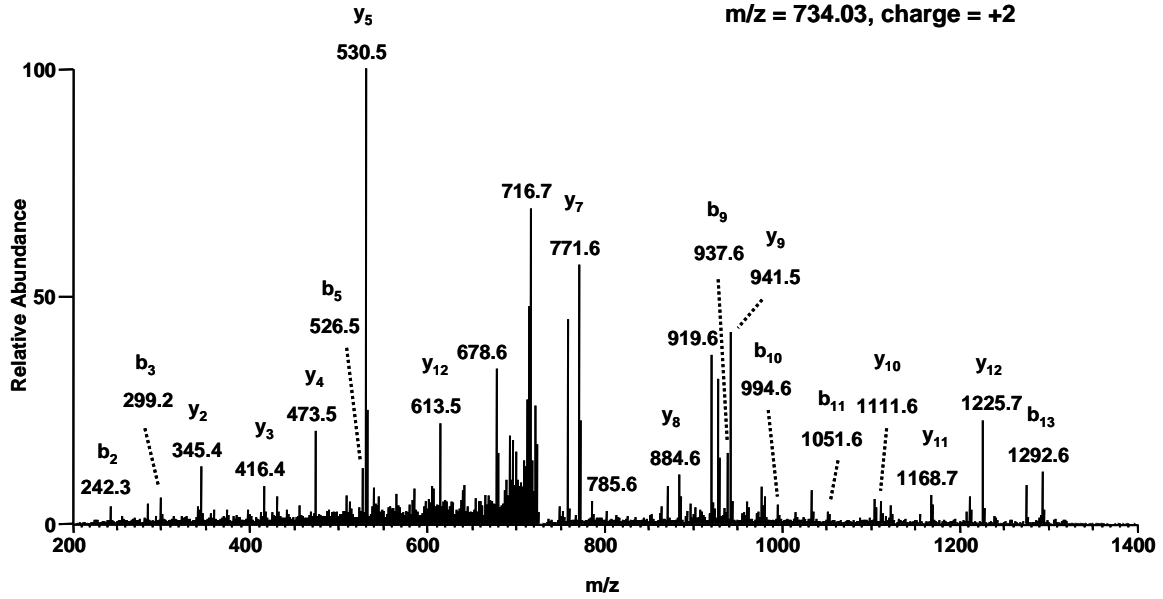


Figure F4

(A) Peptide 1

GK_{Prop}GGK_{Ac}GLGK_{Prop}GGAK_{Ac}R

m/z = 734.03, charge = +2



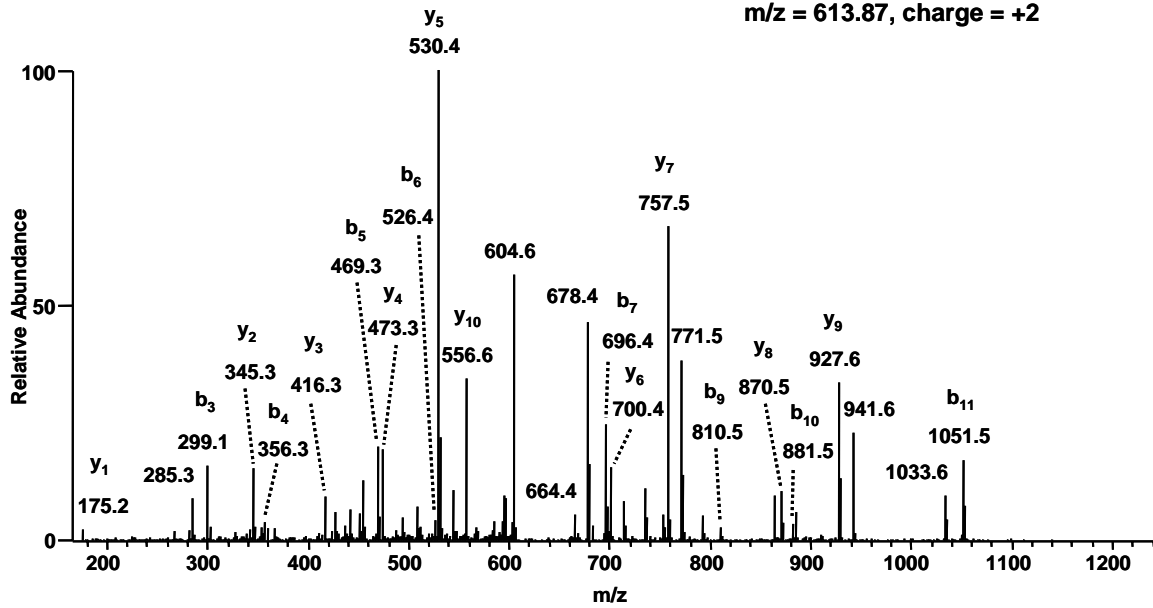
#	b	b ⁺⁺	b [*]	b ⁺⁺⁺	Seq.	y	y ⁺⁺	y [*]	y ⁺⁺⁺	#
1	58.03	29.52			G					14
2	242.15	121.58	225.12	113.07	K	1409.82	705.41	1392.8	696.9	13
3	299.17	150.09	282.14	141.58	G	1225.7	613.35	1208.67	604.84	12
4	356.19	178.6	339.17	170.09	G	1168.68	584.84	1151.65	576.33	11
5	526.3	263.65	509.27	255.14	K	1111.66	556.33	1094.63	547.82	10
6	583.32	292.16	566.29	283.65	G	941.55	471.28	924.53	462.77	9
7	696.4	348.71	679.38	340.19	L	884.53	442.77	867.5	434.26	8
8	753.43	377.22	736.4	368.7	G	771.45	386.23	754.42	377.71	7
9	937.55	469.28	920.52	460.76	K	714.43	357.72	697.4	349.2	6
10	994.57	497.79	977.54	489.27	G	530.3	265.66	513.28	257.14	5
11	1051.59	526.3	1034.56	517.79	G	473.28	237.15	456.26	228.63	4
12	1122.63	561.82	1105.6	553.3	A	416.26	208.63	399.24	200.12	3
13	1292.73	646.87	1275.71	638.36	K	345.22	173.12	328.2	164.6	2
14					R	175.12	88.06	158.09	79.55	1

Figure F4

(B) Peptide 2

GGK_{Prop}GLGK_{Ac}GGAK_{Ac}R

m/z = 613.87, charge = +2



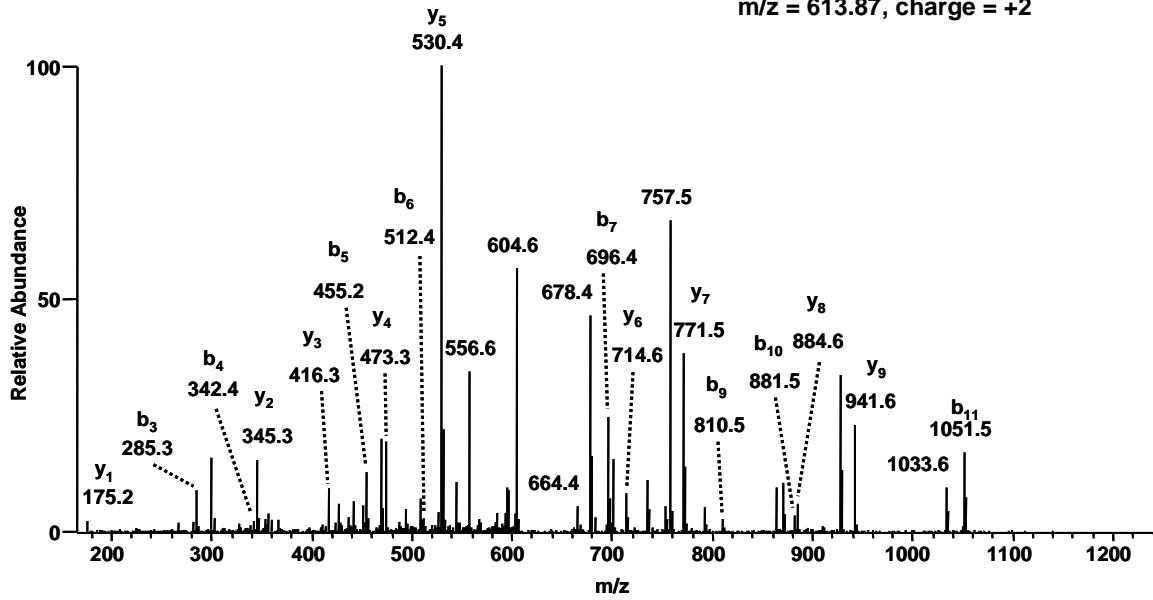
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1	58.03	29.52			G					12
2	115.05	58.03			G	1168.68	584.84	1151.65	576.33	11
3	299.17	150.09	282.14	141.58	K	1111.66	556.33	1094.63	547.82	10
4	356.19	178.6	339.17	170.09	G	927.54	464.27	910.51	455.76	9
5	469.28	235.14	452.25	226.63	L	870.52	435.76	853.49	427.25	8
6	526.3	263.65	509.27	255.14	G	757.43	379.22	740.4	370.71	7
7	696.4	348.71	679.38	340.19	K	700.41	350.71	683.38	342.2	6
8	753.43	377.22	736.4	368.7	G	530.3	265.66	513.28	257.14	5
9	810.45	405.73	793.42	397.21	G	473.28	237.15	456.26	228.63	4
10	881.48	441.25	864.46	432.73	A	416.26	208.63	399.24	200.12	3
11	1051.59	526.3	1034.56	517.79	K	345.22	173.12	328.2	164.6	2
12					R	175.12	88.06	158.09	79.55	1

Figure F4

(C) Peptide 3

GGK_{Ac}GLGK_{Prop}GGAK_{Ac}R

m/z = 613.87, charge = +2



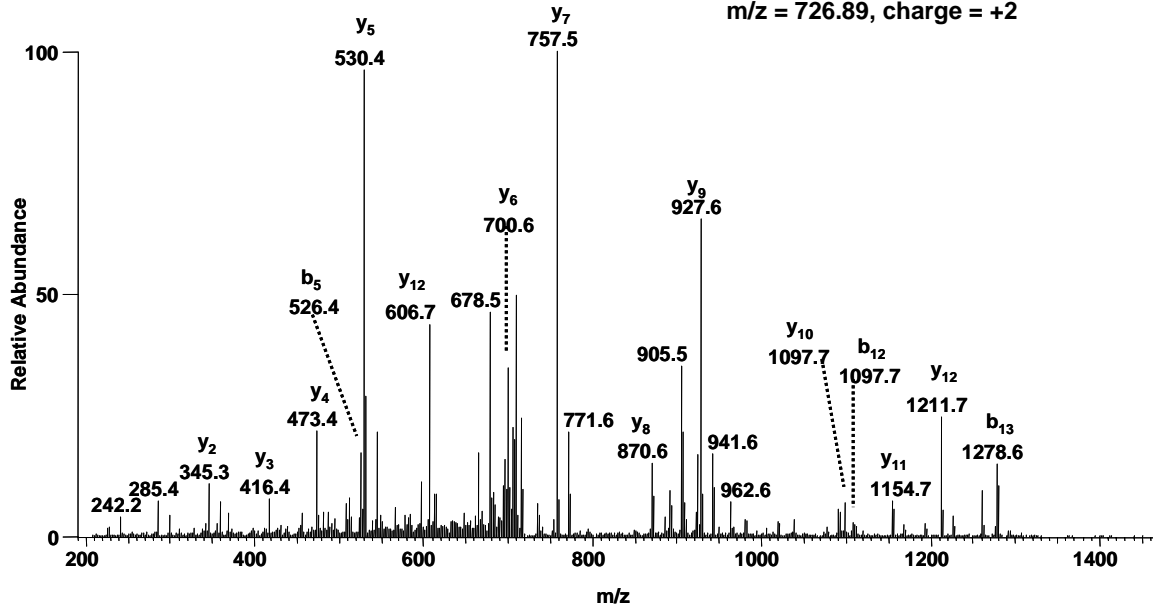
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1	58.03	29.52			G					12
2	115.05	58.03			G	1168.68	584.84	1151.65	576.33	11
3	285.16	143.08	268.13	134.57	K	1111.66	556.33	1094.63	547.82	10
4	342.18	171.59	325.15	163.08	G	941.55	471.28	924.53	462.77	9
5	455.26	228.13	438.23	219.62	L	884.53	442.77	867.5	434.26	8
6	512.28	256.64	495.26	248.13	G	771.45	386.23	754.42	377.71	7
7	696.4	348.71	679.38	340.19	K	714.43	357.72	697.4	349.2	6
8	753.43	377.22	736.4	368.7	G	530.3	265.66	513.28	257.14	5
9	810.45	405.73	793.42	397.21	G	473.28	237.15	456.26	228.63	4
10	881.48	441.25	864.46	432.73	A	416.26	208.63	399.24	200.12	3
11	1051.59	526.3	1034.56	517.79	K	345.22	173.12	328.2	164.6	2
12					R	175.12	88.06	158.09	79.55	1

Figure F4

(D) Peptide 4

GK_{Prop}GGK_{Ac}GLGK_{Ac}GGAK_{Ac}R

m/z = 726.89, charge = +2



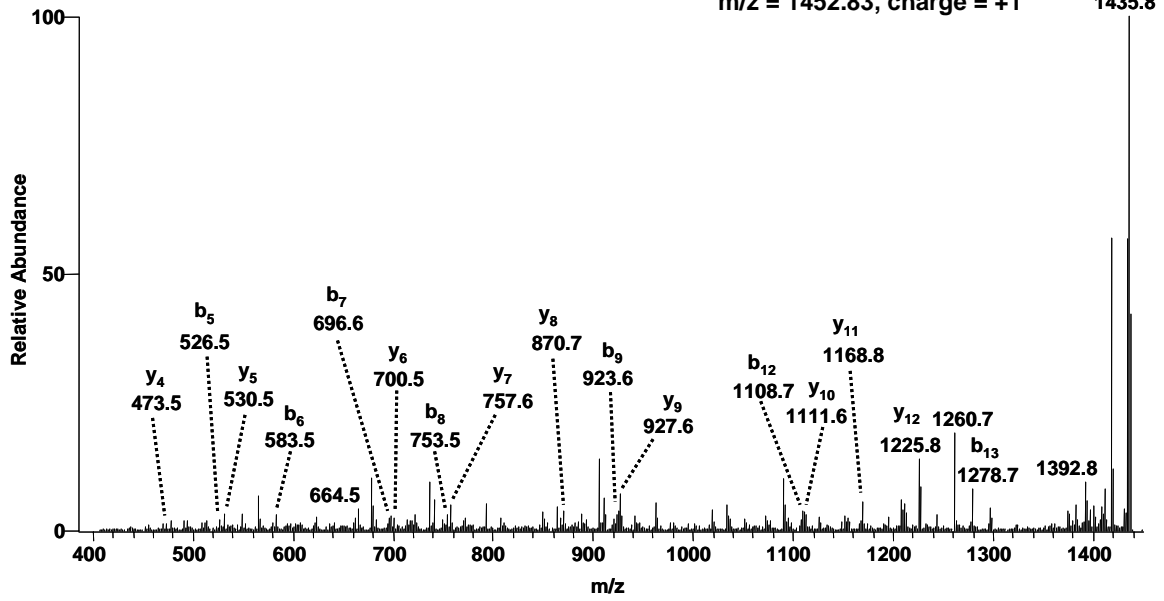
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1	58.03	29.52			G					14
2	242.15	121.58	225.12	113.07	K	1395.81	698.41	1378.78	689.89	13
3	299.17	150.09	282.14	141.58	G	1211.69	606.35	1194.66	597.83	12
4	356.19	178.6	339.17	170.09	G	1154.66	577.84	1137.64	569.32	11
5	526.3	263.65	509.27	255.14	K	1097.64	549.32	1080.62	540.81	10
6	583.32	292.16	566.29	283.65	G	927.54	464.27	910.51	455.76	9
7	696.4	348.71	679.38	340.19	L	870.52	435.76	853.49	427.25	8
8	753.43	377.22	736.4	368.7	G	757.43	379.22	740.4	370.71	7
9	923.53	462.27	906.5	453.76	K	700.41	350.71	683.38	342.2	6
10	980.55	490.78	963.53	482.27	G	530.3	265.66	513.28	257.14	5
11	1037.57	519.29	1020.55	510.78	G	473.28	237.15	456.26	228.63	4
12	1108.61	554.81	1091.58	546.3	A	416.26	208.63	399.24	200.12	3
13	1278.72	639.86	1261.69	631.35	K	345.22	173.12	328.2	164.6	2
14					R	175.12	88.06	158.09	79.55	1

Figure F4

(E) Peptide 5

GK_{Ac}GGK_{Prop}GLGK_{Ac}GGAK_{Ac}R

m/z = 1452.83, charge = +1



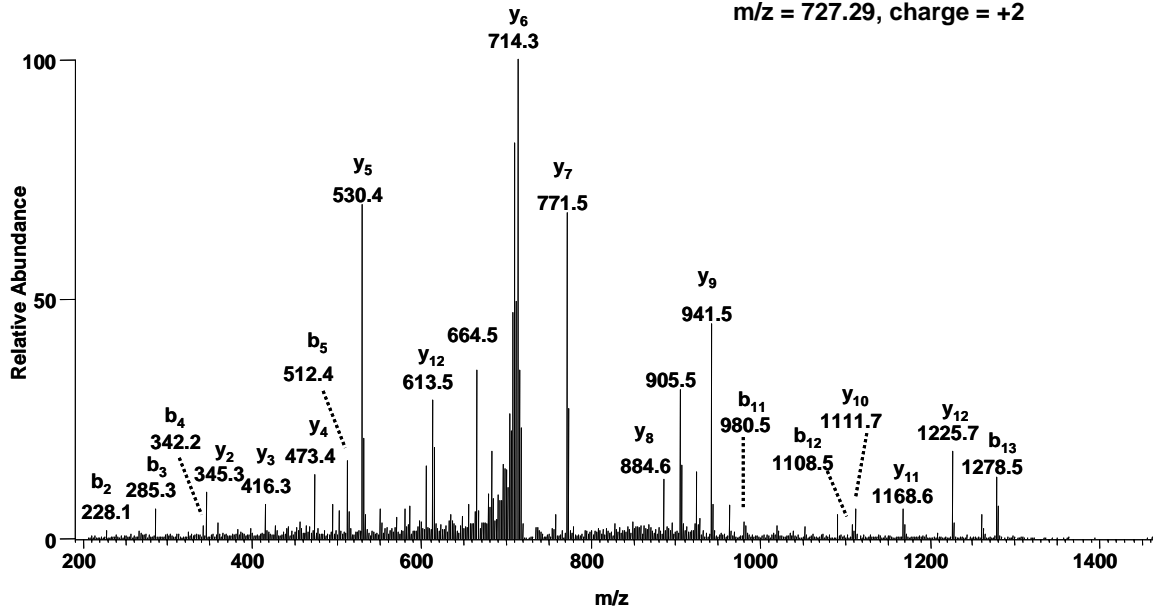
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3	285.16	268.13	G	1225.7	1208.67	12
4	342.18	325.15	G	1168.68	1151.65	11
5	526.3	509.27	K	1111.66	1094.63	10
6	583.32	566.29	G	927.54	910.51	9
7	696.4	679.38	L	870.52	853.49	8
8	753.43	736.4	G	757.43	740.4	7
9	923.53	906.5	K	700.41	683.38	6
10	980.55	963.53	G	530.3	513.28	5
11	1037.57	1020.55	G	473.28	456.26	4
12	1108.61	1091.58	A	416.26	399.24	3
13	1278.72	1261.69	K	345.22	328.2	2
14			R	175.12	158.09	1

Figure F4

(F) Peptide 6

GK_{Ac}GGK_{Ac}GLGK_{Prop}GGAK_{Ac}R

m/z = 727.29, charge = +2



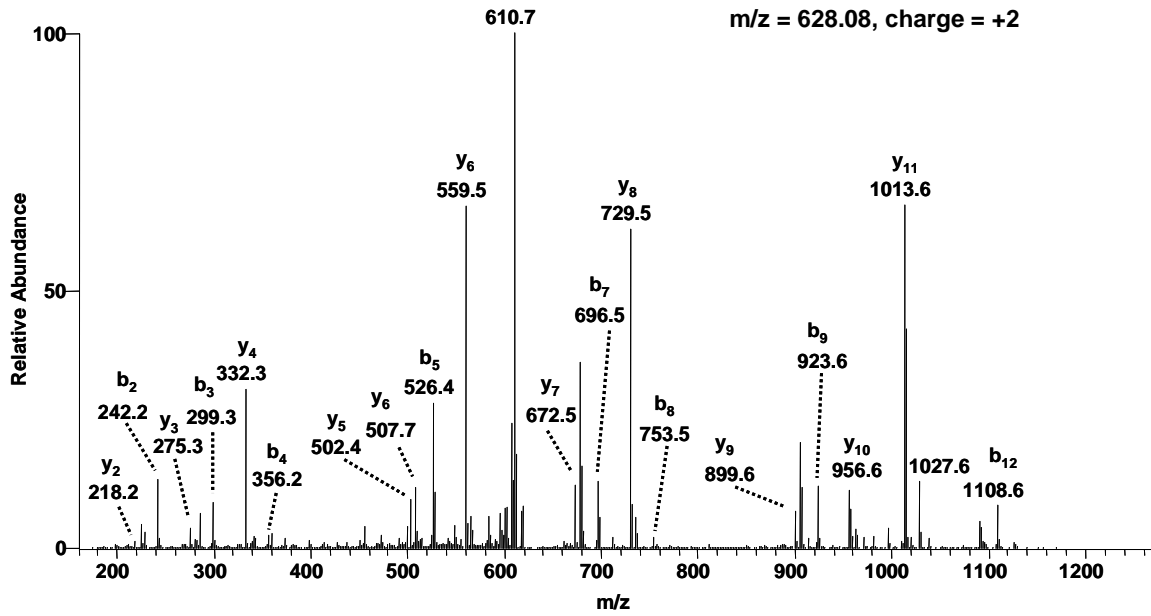
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2	228.13	114.57	211.11	106.06	K	1395.81	698.41	1378.78	689.89	13
3	285.16	143.08	268.13	134.57	G	1225.7	613.35	1208.67	604.84	12
4	342.18	171.59	325.15	163.08	G	1168.68	584.84	1151.65	576.33	11
5	512.28	256.65	495.26	248.13	K	1111.66	556.33	1094.63	547.82	10
6	569.3	285.16	552.28	276.64	G	941.55	471.28	924.53	462.77	9
7	682.39	341.7	665.36	333.18	L	884.53	442.77	867.5	434.26	8
8	739.41	370.21	722.38	361.7	G	771.45	386.23	754.42	377.71	7
9	923.53	462.27	906.5	453.76	K	714.43	357.72	697.4	349.2	6
10	980.55	490.78	963.53	482.27	G	530.3	265.66	513.28	257.14	5
11	1037.57	519.29	1020.55	510.78	G	473.28	237.15	456.26	228.63	4
12	1108.61	554.81	1091.58	546.3	A	416.26	208.63	399.24	200.12	3
13	1278.72	639.86	1261.69	631.35	K	345.22	173.12	328.2	164.6	2
14					R	175.12	88.06	158.09	79.55	1

Figure F4

(G) Peptide 7

GK_{Prop}GGK_{Ac}GLGK_{Ac}GGAK

m/z = 628.08, charge = +2



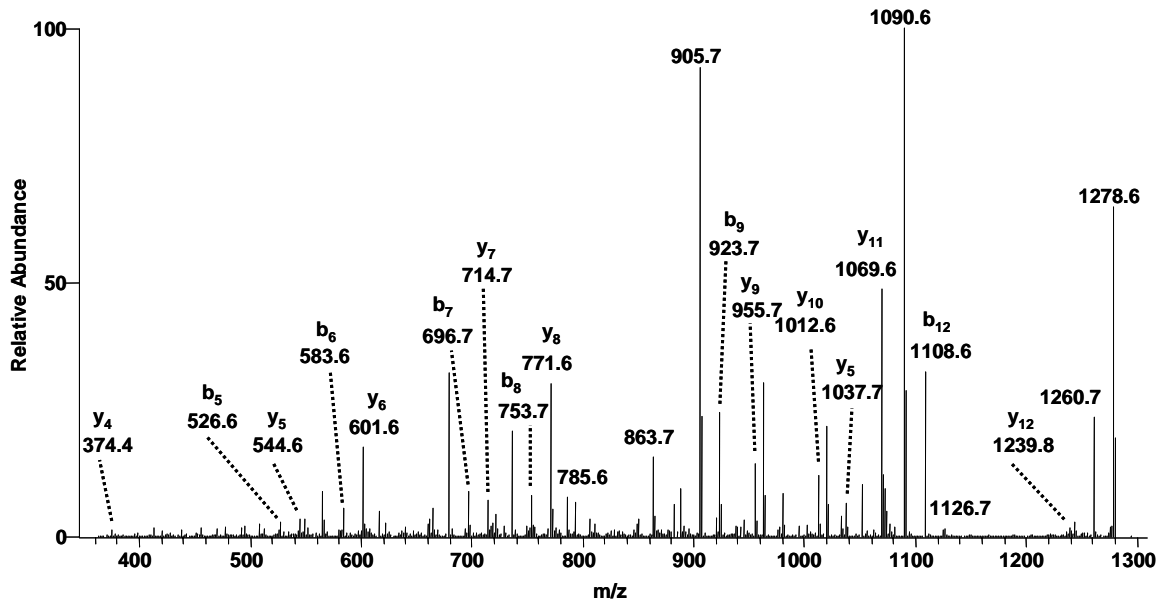
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2	242.15	121.58	225.12	113.07	K	1197.69	599.35	1180.67	590.84	12
3	299.17	150.09	282.14	141.58	G	1013.57	507.29	996.55	498.78	11
4	356.19	178.6	339.17	170.09	G	956.55	478.78	939.53	470.27	10
5	526.3	263.65	509.27	255.14	K	899.53	450.27	882.5	441.76	9
6	583.32	292.16	566.29	283.65	G	729.43	365.22	712.4	356.7	8
7	696.4	348.71	679.38	340.19	L	672.4	336.71	655.38	328.19	7
8	753.43	377.22	736.4	368.7	G	559.32	280.16	542.29	271.65	6
9	923.53	462.27	906.5	453.76	K	502.3	251.65	485.27	243.14	5
10	980.55	490.78	963.53	482.27	G	332.19	166.6	315.17	158.09	4
11	1037.57	519.29	1020.55	510.78	G	275.17	138.09	258.14	129.58	3
12	1108.61	554.81	1091.58	546.3	A	218.15	109.58	201.12	101.07	2
13					K	147.11	74.06	130.09	65.55	1

Figure F4

(H) Peptide 8

GK_{Ac}GGK_{Prop}GLGK_{Ac}GGAK

m/z = 1296.67, charge = +1



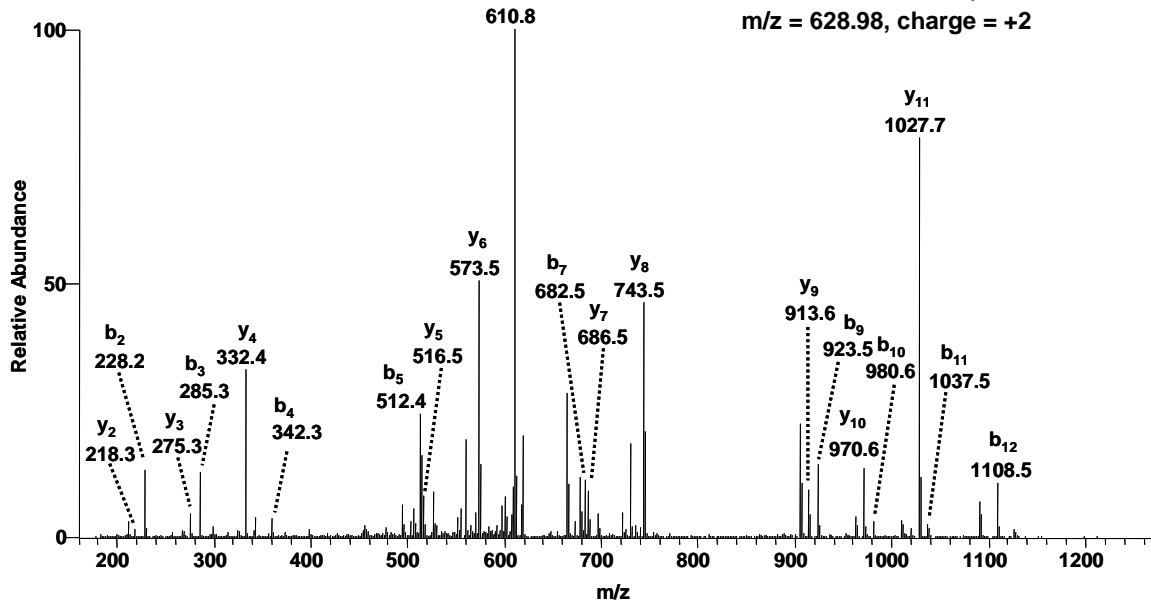
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2	228.13	211.11	K	1239.71	1222.68	12
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4	342.18	325.15	G	1012.58	995.55	10
5	526.3	509.27	K	955.56	938.53	9
6	583.32	566.29	G	771.44	754.41	8
7	696.4	679.38	L	714.41	697.39	7
8	753.43	736.4	G	601.33	584.3	6
9	923.53	906.5	K	544.31	527.28	5
10	980.55	963.53	G	374.2	357.18	4
11	1037.57	1020.55	G	317.18	300.16	3
12	1108.61	1091.58	A	260.16	243.13	2
13			K	189.12	172.1	1

Figure F4

(I) Peptide 9

GK_{Ac}GGK_{Ac}GLGK_{Prop}GGAK

m/z = 628.98, charge = +2



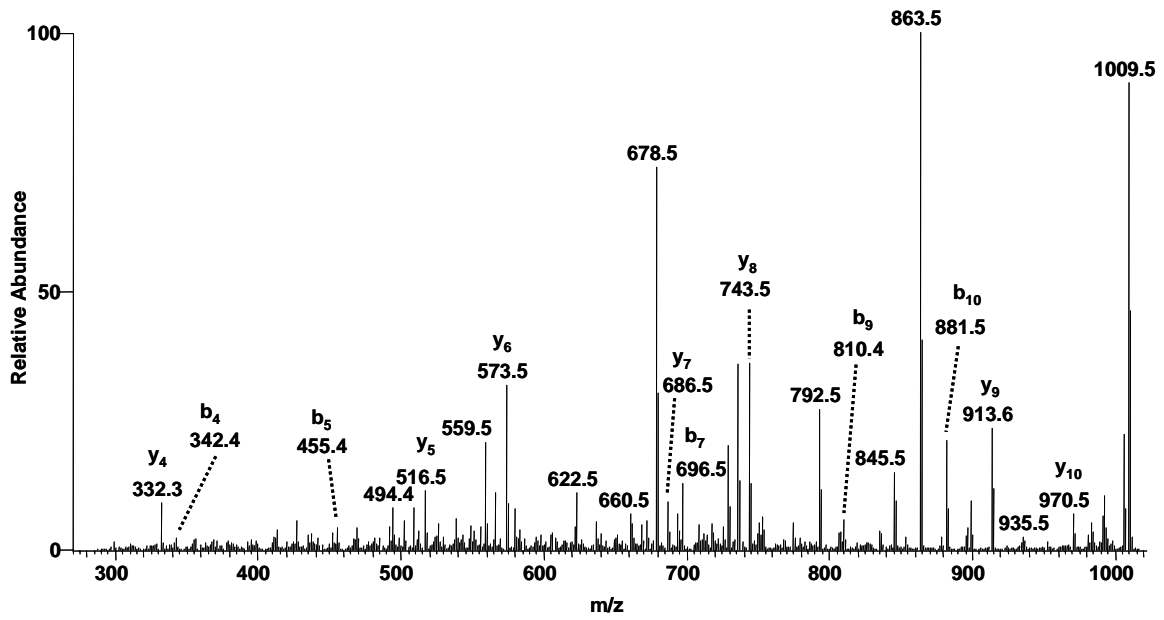
#	b	b ⁺⁺	b ⁺	b ⁺⁺⁺	Seq.	y	y ⁺⁺	y ⁺	y ⁺⁺⁺	#
1	58.03	29.52			G					13
2	228.13	114.57	211.11	106.06	K	1197.69	599.35	1180.67	590.84	12
3	285.16	143.08	268.13	134.57	G	1027.59	514.3	1010.56	505.79	11
4	342.18	171.59	325.15	163.08	G	970.57	485.79	953.54	477.27	10
5	512.28	256.65	495.26	248.13	K	913.55	457.28	896.52	448.76	9
6	569.3	285.16	552.28	276.64	G	743.44	372.22	726.41	363.71	8
7	682.39	341.7	665.36	333.18	L	686.42	343.71	669.39	335.2	7
8	739.41	370.21	722.38	361.7	G	573.34	287.17	556.31	278.66	6
9	923.53	462.27	906.5	453.76	K	516.31	258.66	499.29	250.15	5
10	980.55	490.78	963.53	482.27	G	332.19	166.6	315.17	158.09	4
11	1037.57	519.29	1020.55	510.78	G	275.17	138.09	258.14	129.58	3
12	1108.61	554.81	1091.58	546.3	A	218.15	109.58	201.12	101.07	2
13					K	147.11	74.06	130.09	65.55	1

Figure F4

(J) Peptide 10

GGK_{Ac}GLGK_{Prop}GGAK

m/z = 1027.63, charge = +1



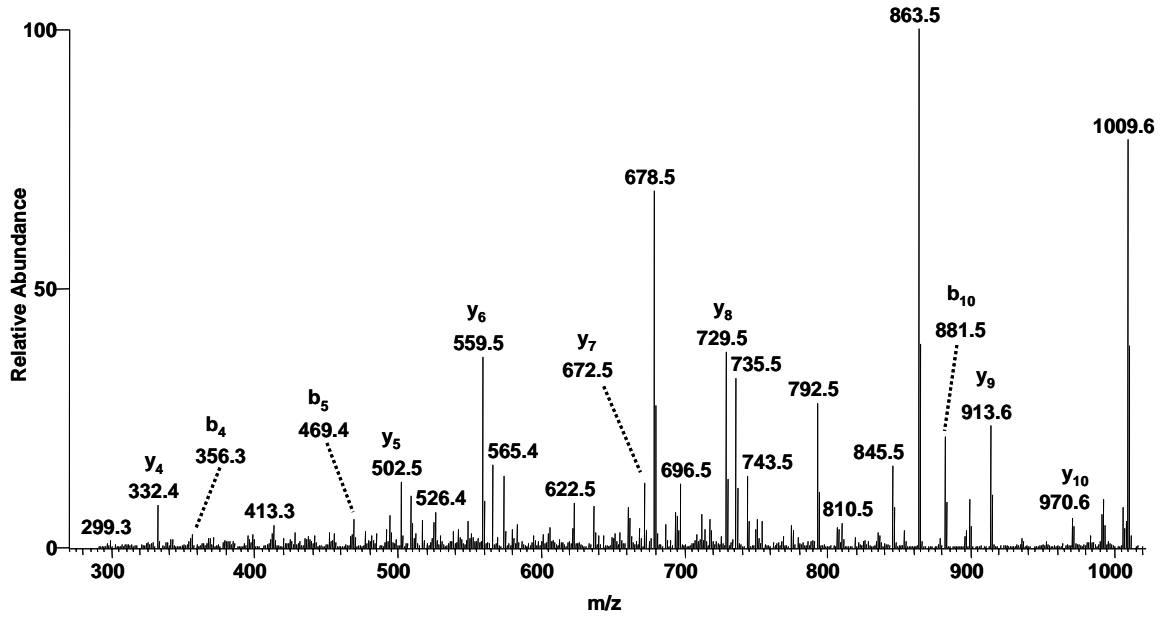
#	b	b*	Seq.	y	y*	#
1	58.03		G			11
2	115.05		G	970.57	953.54	10
3	285.16	268.13	K	913.55	896.52	9
4	342.18	325.15	G	743.44	726.41	8
5	455.26	438.23	L	686.42	669.39	7
6	512.28	495.26	G	573.34	556.31	6
7	696.4	679.38	K	516.31	499.29	5
8	753.43	736.4	G	332.19	315.17	4
9	810.45	793.42	G	275.17	258.14	3
10	881.48	864.46	A	218.15	201.12	2
11			K	147.11	130.09	1

Figure F4

(K) Peptide 11

GGK_{Prop}GLGK_{Ac}GGAK

m/z = 1027.57, charge = +1



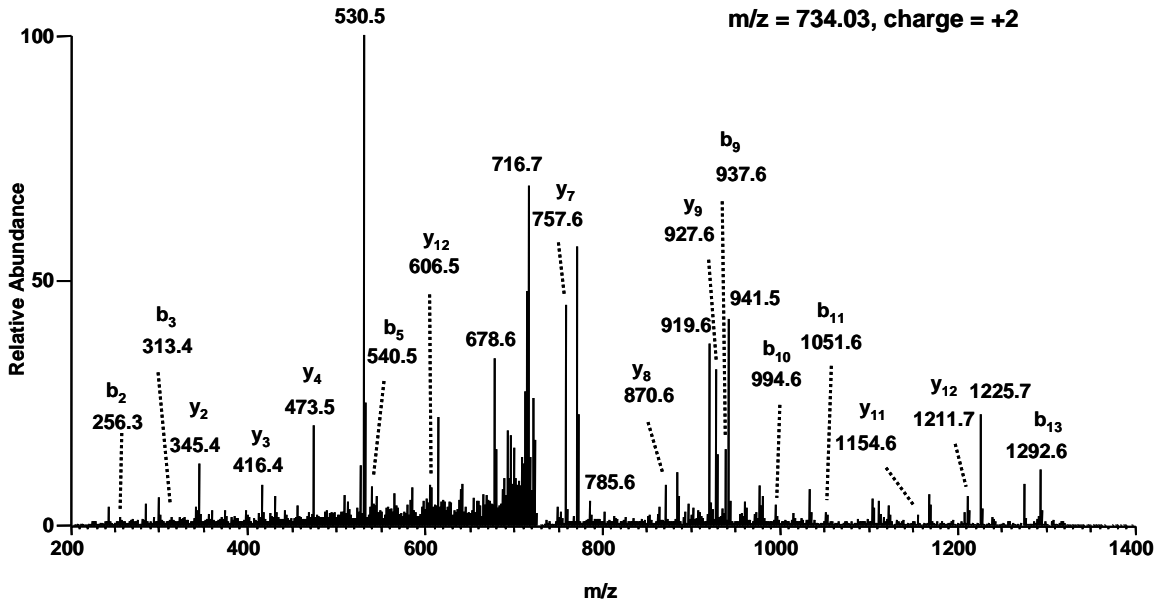
#	b	b*	Seq.	y	y*	#
1	58.03		G			11
2	115.05		G	970.57	953.54	10
3	299.17	282.14	K	913.55	896.52	9
4	356.19	339.17	G	729.43	712.4	8
5	469.28	452.25	L	672.4	655.38	7
6	526.3	509.27	G	559.32	542.29	6
7	696.4	679.38	K	502.3	485.27	5
8	753.43	736.4	G	332.19	315.17	4
9	810.45	793.42	G	275.17	258.14	3
10	881.48	864.46	A	218.15	201.12	2
11			K	147.11	130.09	1

Figure F4

(L) Peptide 12

GK_{Butyl}GGK_{Ac}GLGK_{Ac}GGAK_{Ac}R

m/z = 734.03, charge = +2



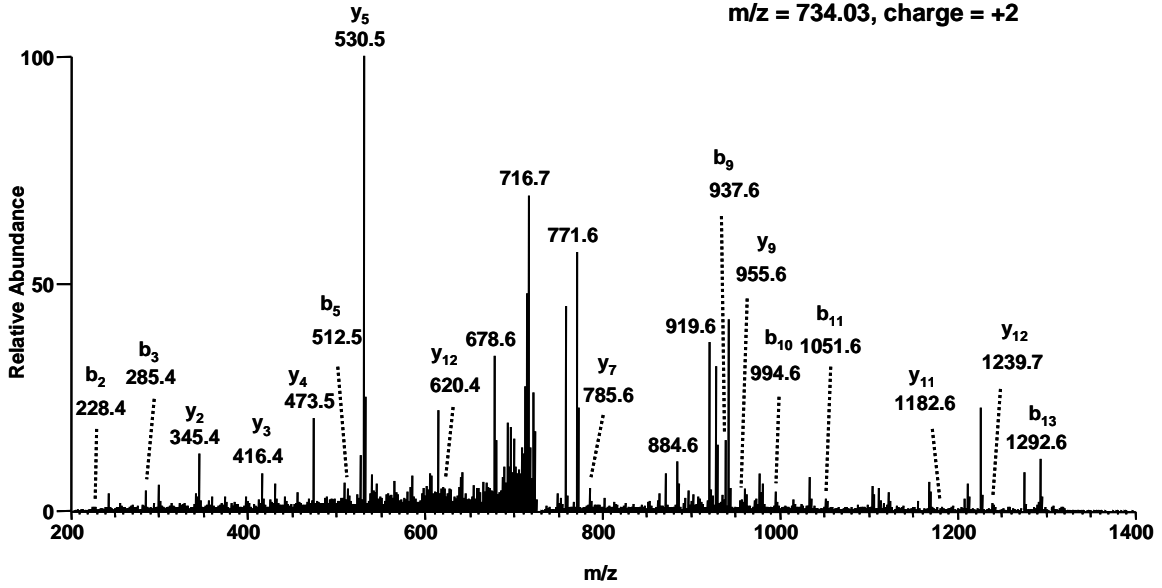
#	b	b ⁺⁺	b ⁺	b ⁺⁺⁺	Seq.	y	y ⁺⁺	y ⁺	y ⁺⁺⁺	#
1	58.03	29.52			G					14
2	256.17	128.59	239.14	120.07	K	1409.82	705.41	1392.8	696.9	13
3	313.19	157.1	296.16	148.58	G	1211.69	606.35	1194.66	597.83	12
4	370.21	185.61	353.18	177.09	G	1154.66	577.84	1137.64	569.32	11
5	540.31	270.66	523.29	262.15	K	1097.64	549.32	1080.62	540.81	10
6	597.34	299.17	580.31	290.66	G	927.54	464.27	910.51	455.76	9
7	710.42	355.71	693.39	347.2	L	870.52	435.76	853.49	427.25	8
8	767.44	384.22	750.41	375.71	G	757.43	379.22	740.4	370.71	7
9	937.55	469.28	920.52	460.76	K	700.41	350.71	683.38	342.2	6
10	994.57	497.79	977.54	489.27	G	530.3	265.66	513.28	257.14	5
11	1051.59	526.3	1034.56	517.79	G	473.28	237.15	456.26	228.63	4
12	1122.63	561.82	1105.6	553.3	A	416.26	208.63	399.24	200.12	3
13	1292.73	646.87	1275.71	638.36	K	345.22	173.12	328.2	164.6	2
14					R	175.12	88.06	158.09	79.55	1

Figure F4

(M) Peptide 13

GK_{Ac}GGK_{Ac}GLGK_{Butyl}GGAK_{Ac}R

m/z = 734.03, charge = +2



#	b	b ⁺⁺	b [*]	b ⁺⁺⁺	Seq.	y	y ⁺⁺	y [*]	y ⁺⁺⁺	#
1	58.03	29.52			G					14
2	228.13	114.57	211.11	106.06	K	1409.82	705.41	1392.8	696.9	13
3	285.16	143.08	268.13	134.57	G	1239.72	620.36	1222.69	611.85	12
4	342.18	171.59	325.15	163.08	G	1182.7	591.85	1165.67	583.34	11
5	512.28	256.65	495.26	248.13	K	1125.67	563.34	1108.65	554.83	10
6	569.3	285.16	552.28	276.64	G	955.57	478.29	938.54	469.77	9
7	682.39	341.7	665.36	333.18	L	898.55	449.78	881.52	441.26	8
8	739.41	370.21	722.38	361.7	G	785.46	393.24	768.44	384.72	7
9	937.55	469.28	920.52	460.76	K	728.44	364.72	711.41	356.21	6
10	994.57	497.79	977.54	489.27	G	530.3	265.66	513.28	257.14	5
11	1051.59	526.3	1034.56	517.79	G	473.28	237.15	456.26	228.63	4
12	1122.63	561.82	1105.6	553.3	A	416.26	208.63	399.24	200.12	3
13	1292.73	646.87	1275.71	638.36	K	345.22	173.12	328.2	164.6	2
14					R	175.12	88.06	158.09	79.55	1