

iCar-PseCp: Identify carbonylation sites in proteins by Monto Carlo sampling and incorporating sequence coupled effects into general PseAAC

Supplementary Materials

Supporting Information S1: The benchmark dataset $S_{\xi=7}(K)$ used to train and test the model for predicting the possibility of carbonylation at Lys site. It contains 300 positive samples and 1,949 negative samples. None of the sequences included has $\geq 30\%$ pairwise sequence identity with any other in a same subset. See the main text for further explanation.

(1) List of the 300 peptide samples in the positive subset $S_{\xi=7}^+(K)$

SAPAKGRKKSCKMGFQ
 ENSLAEDKDGRKGGK
 VTTGIRDKKGVTVKT
 QCRLKLLKLERIKDY
 NIGYGSNKKTKHMLP
 VTGGAASKLSKIRVV
 QTTWRKYKLLKTDLKR
 RKLLMLKKEKLEKVV
 QKKWKIMKKAALLIQ
 GIGRLILKEEMKARS
 DKLTTADKLLGELQE
 KLQVLPQKASERLQF
 GITNLGYKVLIQPSN
 LAEKVFAKVLREEDS
 SERSGTPKKRKAPPP
 AAKEMEEKISNLKEH
 ADAGRDKKEKVFEKH
 SSAINILKEKKKREK
 GPRLGDAKLKEKFKD
 VSGEHKQKGKVKRKL
 QQEVVRMKLRLQHSI
 DLQEQMNKNKMMPVL
 GQQDTIKKALNYSTA
 SKVTYLGKELLRYVS
 DEKMKAMKRSRTWGQ
 KRQLQTPKEKAQALE
 KEPVGEGKGTAKFKQ
 EADRTSSKKTQTQEI
 QRVLDILKSSHAVE
 HKKPIDLKAIGKLP
 VKQTVQSKILTTGEN
 KRLGRRFKLLDLKKS
 IPVQLVFNKIKLYW
 SQEIKDTKECVQNK
 TRFLEEIKNQDKLNK

CNHIREVKSLEELS
DCSQDLLKKREHHIE
KTLFSCWKESENEKLL
SPPAAACEKGKEQHSQ
AKEHKEPKQKDGAKK
YRIELLRKVREQVLK
RKFVEHVKSQGHKDK
KTLNDSLKKVENKVS
RQICVTQKLLPAKRS
TEKEMIQKLDKLELQ
KQIEKELKQMELIKD
YDASVRNKQQELHLE
KHLKTLSTVFSETW
RSIIGFVKLRSNKVK
NKVKRSQKLVYMGKL
YTKKDTKKNACKSSD
CNKLLAAKNINLRLF
SGYEEALKIFQIKD
PIKQVEEKPQRAQNI
EPTEPLKGIQSRLR
EPAPKKQKLSASVKK
DKLRISTKKLEEYET
LQIIPGAKHGNIQVG
RKLVERRKQVKQLMK
FKLGNKVKSEVNKLY
IEEKDLEKLDLVIKY
ECREEILKFLCIFLE
GLFAGPCKVINAKDV
MASLRRPKRIIRGH
KVPADLLKRAFVRMS
GNGGVVFKVSHKPSG
IPEQILGKVSIAVIK
DSRSLAQKIVATYRL
NIPPLTMKRIRERFI
ISGLGGEKDRWTEAA
RNIYQGVKKKQYDIL
LKLESKLIKADKLYLQ
EVQEVKDKAQKIVDE
KVLMPKLIKAKPIRTA
LLNRLNRKMEIKPLQ
HFRSLRTKLLLMSRN
VIQEIVDKSGVVRVR
GRNQEKLKFMIRIG
KKRIKKRKGEAMALN
TKEKAGPKGSKVSEE
ERIFTGNKFTKDTTK
KILKKINKAIVSKKN
VANAVFVKNASEIEV
CIVILTGKDPLGETF
TEKLAGVKQEVIKES
EREAELKKLQEARER
KKYLEDVKLQARGQL
AECVKQAKGVRQQAV
SISQKKVKIELDKSA
PLAGKKAKKPAKAAA
AAKARVTKPKTAKPK
FQQATKIKKLRAGKL
SVRGPRIKHVCRRAA
RFQLPLDKGNGKHKH

MASQRQAKIQRYKQK
VFDKVSEKLGDKRLF
QGKENLWKENLRKEE
SGKLYKTKSNKELHG
DRKTIPIKYPLKEIV
ASFQAERKFNAAR
GSLGSMKLRKSESK
ESPHFYRKGTTPPRS
KKKYEKEKEKNKILR
IQYVVRLKKENVRLA
TANIQDLKEEYSRKK
ERLKRLOKSADLYKD
DILQALQKLSKDNL
KHLQQKLEKDRELE
GEDDERSKRIWLDYP
PDLRVVQKYPLLKEP
TNDFTKIKGWRGKFH
TLAPVVAKLGNSGAS
AKEADQLKQDLQEAR
AKKPAALPKVPKKE
PGTTKTTKSSAVPPG
IDIYLLKSRVIFQQ
INRALDAKLSRQFFI
NKLMTNLKSTAPHFV
HKLEGNLKNRESME
LEVKSDSKEDENLVI
KLSLEESKKKGYDLR
KETYEKQKGHYLAGK
SQMQSGKEYRKDYE
LLSVKQEKEIQMKMI
IISFAVQKETQFHTE
GEKYLQSKEDLRLML
LMLIELKKKQEAGFA
VTGREGAKDIDISSP
IPKMKMPKFSMPSLK
KLKGPKLKMPMHFK
EMHFKTPKISMPDYN
NLKGPKMKGDVDVSL
EKAKSPVKEEVKSPE
APKKEAPKPKVEEKK
KARLERFKLRRMKAN
LQSQEETKERRHSHT
ADAKKKKKKSWVYEL
ISLKKAKKPLPPSR
IEIKSKNKVRPGSLF
LAAMDATKLEYERAS
KEEKKKKIKTIKSE
GLGVMPPKAGQTITV
GLEAAQIKELEELRQ
ELKAWQEKFFQKEQA
RKVEEVTKVCEGRRK
TLVPAGIKSLGLAVS
REVSQSRKPSASERL
RGGGSPEKPPSRRRP
KKFLPVLKEILDRDP
IHVIQQGKTGNTEKF
KIIKSSSKVHSFGKR
ERMKRHQKALVRERK
EMKKQTLKSLIILS
PPPIKSFKEMKFPAA

QKATTGLKPVDSGCV
IHKDLIKKPTISTAV
CRGIIGGKSQRVNGL
QLDRLLPKLARGSL
SIVRIIGKMLPLEPC
KEKELENKLEELKKQ
KDLQEQNKKNEERMF
EGKDEDAKKSLRTME
EMSAKRAKKDVLHSS
LLRMLEKRQMDRAE
LESMIPIKMNFPQK
SIEKTSKDLAPTSK
VLAKPTPKAETTTKG
MPRVRKPKTTPR
KEERVSLKVLAKNFG
KNPKEEKPKKEKKK
SRTVRLKELRRALG
ARVTEVMKALKCNVR
LLLAPSSKKGKARLS
DMLRLANKDSIGFFI
GDRIQVRKVPPLKIP
TLADIKAKAQLVKAQ
KSIRAFKAGFLAEEK
QMYEEQIKNLEKENY
AVLLKTKKKGQKKSG
HGVCSVLKGSEFMFE
AMPGAAYKAKKAKGD
RLLDEATKRSNRDSL
TEHPYKSKKAVWHKL
LLSVRMGKEEEKLMI
MVTSLFCKLGVLVRH
HFLPLMEKLLKKAAT
EDGEKEEKAKEDKGG
VIPVLQTKTRTNVPT
PEPKKIKKAASPSQ
TQNSYRAKEPILALR
DCENLLKLLVLPNI
LLAYKIKYPENFFL
ERKSPEDKKSMLS
MYLMLDNKRKEVVHK
WSQRGKGKVFPLRK
RGKAAILKAQVAARG
AYPRLVVKLMPNGLR
VPAAYVKKLDPAQSA
KKFDDFQKDLKANES
MAASRAKLNESHRL
VEHWKELQLAAARG
TELIRQEKLEQLAAR
LKQSGQKKSITLVR
KYDAIKFKINQLSEL
DELKSSVTKDKKII
GRIRLPRKATKTKKN
RRKKRAPKADISKSL
ALMEVMMKEMKGSIR
SKKIPEEKVPVPVQK
EKPKAPPKGPEISEK
PIKGVPKKTPSPIEA
VVRSEGKVHTLTLR
PKIKVDVKFKDVTIL
LKVTEITKDSVSITW

LDGGSKIKNYIVEKR
ESSVLRAKEVTWYKD
VQEEISQKALRSEEI
IGAARTTKKRIPNTK
GRNVKSRKLLKEIFNK
PRPPSLKKKQTTKKP
GAVKGLCKLFCLTLH
LSSLGGFKLAHGLLE
HGLLEELKTVLSSHK
RLIGNESKGEHVPGF
KAADALGKLISIIHK
IGSINLKKNEPPLTC
FEALKYPKFSKAIVI
LTKQDKLKSFPKFS
RKMEVGFKARGQPKS
FAKNIPVSKNIRVV
SKKPDKEKPIKEKDK
EKLKEILKERELKIY
KKLALSAKKASTLWR
VNEQEPCKFLLDVAF
VFKTRILKIIDEGLK
LQLSKKLKTVLDQAR
KKKLTSSKPPGELLV
GLTVGFDDKDMMDIK
QQLNGVQKQHICGR
DDVALVSKALQAEEM
TGDFESKKNELPDGL
AARRRFLKLQQDQQE
SKAKPSYKQKRQRNR
ETRESETKCLKELPGV
ANRLFGDKSLTFNET
LKLEDTPKINSRFFG
FFGEGTKKMGLAFES
EKLIKDLKSKEVPEA
EKLTALTKKYRITEN
KFLDMLIKKLSFDY
SYNETKIKFDKYKAE
IDLLKIKKITAHTQ
VSEHEATKCQSFRDH
YLAPNNLKPVVAEFY
YAVAVVKKDSGFQMN
MNQLRGKKSCHTGLG
LFSSPHGKDLLFKDS
LSHHERLKCDEWSVN
EGCAPGSKKDSSLCK
VPQNTGGKNPDPWAK
LCLDGTRKPVEEYAN
AVVTRKDKEACVHKI
YLGEYVKA VG NLRK
TVKVPMMKRLGMFNI
RSVQLTEKRMDKV GK
SNTKVDK KVEPKSCD
LHTLFGDKLCTVATL
NECFLQHKDDNP NLP
LFFAKRYKAAFTECC
AEFAEVSKLVTDLTK
LLVRYTKKVPQVSTP
PVSDRVTKCTESLV
CFAEEGKKLVAASQA
SEVAHRFKDLGEENF

KAACLLPKLDELRDE
SSAKQRLKCASLQKF
DSISSKLKECCEKPL
VLLLRLAKTYETTL
CCKHPEAKRMPCAED
SEKERQIKKQ TALVE
KHKPKATKEQLKAVM
DNEETFLKKYLYEIA
WLNKTFKCKVNSGA
VATALAHKYHXXXXX
VHLTDAEKA AVNGLX
GMYELLLKVRPEQLV
EVERTRNKFLFLKAD
LTAFTNLKIKHPTYC
DICTLPDKEKQIKKQ
AADKTNIKNCWGKIG
KVADALAKAADHVED
KAGQYTDKGLRKCCE
MSAKEKGFEDMAKA
DDSPDLPKLKPDNT
KGACLLPKIETMREK
VGTRCCTKPESERMP
EKTPVSEKVTKCCTE
LVELLKHKPKATEEQ
XXXXX MVK VGVNGFG
TVDGPSGKLWRDGRG

(2) List of the 1,949 peptide samples in the negative subset $\mathbb{S}_\xi^-(K)$

SIAVQMMKRIHSLLE
SPHEQEIKFFAKILL
FGEQLIQSEPLDAV
MASFSFLKDNSTDVC
HSRALLVKTTLNISF
IKVLSSSKVLSEEIS
ETWRLWQKFLDDYSR
RINEYVGKAATRLSI
EKQKSEAKDRKVLEI
EYRLDWAKWKAKIQS
PGEHV FVKGYEKGP
GILDRSSKSQSSASL
ARLEADEKKQLCVLQ
QNLQDAAKDMKKFEA
FVILRDEKWGGNKTY
RQHPDTLKYSTLMDS
PTTLIPAKAPEIIDV
QIQALEDKKEKEMSA
THFVARLKSWRGNEP
WYNLLSYKYLKKQSR
AQPAAPAKVPSPGQQ
SPQPESFKTSRSSKQ
AARVTGMKKWPRTPK
ECLVSAQKVLEGSEL
VTSNEQVKGYGTHLM
NRGWFCEKVVILCPF
RILAAGGKSNHLHLW
NEMASTEKLTDVARY
GSKDREP KPRKREP
QWQFLVQKSAEKSQK
HAPQFPEKEFNITVQ

KMALEVYKLSLEIEQ
RNTRILRKCIEKVAK
KAVMTSIKQLSSEEL
IRMSARQKQIMEIEE
HLSSPPTKFFVSTPS
LENSSGTKSAFVTVR
EELRDYVKARLKVFY
IRVCALNKVGLGEAT
VINYIVEKQDTRKDT
KCSKTSFKVENLTEG
FSQPIINKVKPQLLK
YRVEAAWKLSQWDLV
KARKLFYKAIVRGKE
NAEMHKNKLQYFMEQ
PRLPKLQEEQREL
ALEVDFEKMKKERDQ
YSAVNPEKDIHGLI
SSVNSLRKAAHEALQ
RNTILWVKENKVPCL
HTLVESLKLSITDQQ
ALDEFATKLIQNNHY
EVL MVWYKQIEQVLI
NWCSQMDKGMLHFGS
EKAPATPKTEKKDS
AIPLLAAKANTKNTS
ESIHNSPKSCPTPEV
KEVYQRNKSNTIEP
KREPKEPKEPRKAKE
VFSIENSKFFEQYEV
ALLADSEKPSHKSF
KLVVTGLKEGAFYKF
FESHQNYKDVQDPSV
PLQQFCSKKLSIPE
REPAGDGKSIRTFKE
RYLYTLEKVCQPLYN
NDVLEHVKHVFVINLI
QALEDIKKFASVPE
KGPALSRKRKKEVDA
VFLTLYEKVFEDTYT
TKVPEVSKKIVPQKP
TEFQNHEKQESQDLR
QEWFLGAKAAAKESS
YGALAPFKPSEPGAN
TTILQHWKCDSSWWA
CRGLLLPKVVEDRGV
GDYVDRGKQSLETIC
NVLQYCRKSGLQTDY
PKPPSKVSSSKESS
GRPLVASKKYRISFK
MQLPYRAKKFSLYCT
DLSGADIKAICTEAG
SKADAPVKWFKDGKE
DGFVDQKKKLXXXXX
DVQFYQLKLPMTVA
LVNPAGEKAVFVNVR
KEGLLQMKLPEPVKL
RVNAWQAKANNNKQW
ITGQLGVKPTGNSI
GCFWVIKGCSPFLD
AISDVETKETYSSG

SKPPGNLKECSPWMS
LRWTRVNKDYVVYDT
PVAAPEPKKETESEA
LGTNGTVKYSISAGD
EETARREKQQLLDVQ
HQSADRAKSEMATMK
EPPPSTVKTYHYLVD
ENYRPLAKTRQQNIS
LTMEINPKVPVNLLR
DGPLSPGKMEDISPV
EMDTDQLKLYEEPLS
LYRSVYEKNMKIHI
TEFLALMKKVSXSPL
DNAPQFLKSKYFTPV
KPEELVSKELSTWKE
EKKNEVHKVEMFLGE
RGPQVDVKGPFVEAE
EMLTPEEKALLYEAI
ITLGPPSKPKGPIRF
IEKSKSLKQTDQPKA
RNYLPALKVEYNTSA
KRGAAVKTSGSPRS
LCNQCRGKKAKNPKE
EVCRAGSKHSRPIPL
QKELVLSKPCKFEEK
SRTRDVVKSALGFIK
STDWSGVKKPIYLSK
TGASGSFKLNKKASS
KKAKKPAKAAAASKK
GSELELAKMTMLLLY
YYSALSGKSISDGHS
KGSLEEEKRRAADAL
GSLEQIMKDRWMNVG
GETTHTDKVPGGEDK
PLLPSLLKCLKMDTD
SLESISTKVIVTQTT
TSKMDLEKPNYIVPD
QAHPVMRKCLQSLCD
FHLVRDVKQGNLPPG
IMEAPLLKHKDDIED
TGPPQVGKTGSYLQF
EEDWEINKDSAVEMA
RVLQALMKRFYLPGT
LSFINGYKNIYAEKV
PLQEAESKVSMALIE
VNRETDTKRPDARLA
EHSEIHTKLYFLQWL
ETADQFLKRSLEMRE
RGHEELRKLESTLDG
REHPFLVKGGEDLRQ
TLENGNKQHQLGVW
ERSAEESKPRSLQEL
KYQALLSKMRAIDLQ
NFSPNQTKFTVQRTD
LVFCERGLQPPRKA
AFSASARKVVNRDSC
EKPPPVNKQENAGTL
LLETGQEKMAGDQKI
SLLIGVFKHGYERYN
DITLTNDKPATAIGV

EVSEIHIKVKPTTKS
CFPEGLVKSCSETLL
TAFVQEPKVGETAPG
PFSSADVPKVEDLD
DLLSLSGKTLCVTAG
SIEEPEGKLGPKFK
INQVNTIKNEAEVIN
YQPLRRSKRRWVITT
TAAVQLLKPEGVLVY
NTSLLSQKKKLEADV
ESTPLANKPGKQSGH
SCQLSREKANVKWYR
DIAEQLLKANPPGKD
DLTTILTKLAKTDN
RVMGFPEKSDIFDVD
EDTATSSKRRPRTRA
YSIQDWAKRMKALVE
NSFISIPKMEVKSYSY
AGAQALEKLEAAESL
MTTQLICKLLRSREA
LRLLEPVKRAQEMDA
XXXMAKRKEENFSSP
IEIGLEGKGFEPTE
RSVDSSAKREKPVVR
MESICIMKGMKPERK
EISESVGKNQFTSES
APVPRGRKGKTKNQ
QSPAVLDKADGQKPV
KLNMMMLSKGELLSTL
YTTQSTIKPXXXXXX
HTQAGWRKEGNLGH
AGTERWMKVVTLKPT
KEAYEHTKAYGYTLG
WYRLRLLKPQNIIP
EEFVTSYKALKSRIS
WNLRLDVKKNPVQDK
TSLAIAQKLMELKLG
KVEDLPLKLTIIYSEA
VTACNPYKPPGPPST
RGQVDYSKIMNGNLS
GVIYTVAKEELKFFE
TWSKDGQKLPPGKDY
LANSAARKKKLLEAQ
HPVSGVRKEQGGGCH
IFTDSEIKDEAFLEY
GEVQLTAKDFKTHAN
SPTSPFYKACDTVFK
SHDNIRVKWFKNDQR
HMYKMPEKILPKILG
KEKQEANKQKVPNPS
ISFDDSSKTQSHSDA
GAGEEEAKGGKRPKE
GEEVPAKKTKTIVS
VFLDSGRKTRSARRR
NMVLPDEKGAGALPF
SSEKLFVKYDLILTS
TNLTDDLKALYKVAG
FNEGPCSKILIQCKA
VVPGASIKYDAVKEE
MLQVTQAKKSQAIAS

KLLKELHKESKTRDD
IEAHEQGKDIDLNV
EVREAAAKTFEQLHS
PIPPDAKELELMFG
TVWRQADKHNIPRIC
PRIQQAKTSLQEEM
QSLAPGKFSPAGVE
IDFRLFAKLNAFCVI
TSTDILKVPKPEPI
ELYSPVQKANPGTLA
GATCNNKLSLSNAI
EELPEISKTKEAATT
QDPACSDKAPGMEGT
QTLAGTQKFSIRPSP
GKGSTFAKASFVAGS
IIPHISTKTIDSWMS
ITSEERTKHDRQFDN
CIDDALRKNDFKPLK
NRFEDCQKEEETKQQ
HESTSVAKDKSSTAS
AAHTQSFKQPSCTHI
IQNVHASKRILFSIV
ETTTAAPKMTKETAT
QHTLNYWKEQSLNVS
YKADTVAKVQGVFES
DFEEQFLKEKRFHDQ
IVALIAQKGNFSKTS
LKIEAENKYDAIKFK
QNEYNAVKEREHFNQ
IETLRLAKNYIWALS
GAWEQQIKQLEAELS
WAEMCSIKAVTAIEK
PVDNHRYKWNGRWWE
ILLNLEKIPGKNAI
FAQVFLSKFTMVKNK
FLAGCQAKVEQAVET
RIEEALQAAEKGTH
LRDGQTYKFRVLAVN
TLWFPPKDDGGSKI
DATRLTDKLELCNK
ENQTEINKPKAKRCL
NQTVTEFKQLISKAI
PEAKTPAKEEARSPA
SSSIFCLKMHKEMIF
YRCWRAHKEYLAILK
KKEEKEPKKEIKKLP
HTSVTLLKCTCTISM
QLWHHWCKKDKELYH
VSSPVIGKLNISETA
DYHKTAKINIPADM
GHTFLLEKPPVPPKP
QVTMPGIKVGSGVN
GVSVADQKGKSTVAS
FLAQADCKLLECRNV
ALHPNAFKRLGASLA
SSCIDMGKELLARSH
NASKEERKRWQATLD
DSGTYTCKVSNVAGG
TQILEELKTKMDNL
TVEARLIKVEKPLYG

TSTTQHNVSTSPKI
MSLDFYTKVLKSCRS
PSPVGALKGSDVILQ
DAMTHLIKISRIIRT
GENMTSGKLTVAGGA
ENRFGVSKPLESAPI
GTRPGDVKEEAPQEM
ARPAFNLKKPSKYCN
HIFFDAAKNLVWKER
VRYENNLKPVLKHVK
KYEGAKVKVLEERQR
FISDGVKSLKVVPE
GIPPPTLKWEKDGQP
QELEQENKLFKDDME
QDNLGLQQLDLQRE
SEAGVEVKKEVGVSI
AAAEENSKMEQSNLE
LAMAVIRKKHGMXXX
ELLETLQKFKAVDKE
WYQETHEKQQDLNIM
RSVLESLKRYRFGKD
LSSHSSKRDWSKSD
VQVITHVKEKLFHMD
ECPDAKLGPKFKMP
DVETQSGKTVIRLPS
IDYNPFAKGFRDDGL
LNELTQLKQLVDAQK
QLSDLNYKVEGEKLL
WQEKFFQKEQALSTL
VVSITCLKHKSGGHA
SASLAHMKAKFRET
EEKQTSWKEIDNDFT
TDEDTFKEFLKLA
SCTLLSEKDESSSP
EKASQLEKTGNDASK
FSFPASPKVFGGRLY
CTKPITCKDELAPPT
KVFERASKDTFQLEA
MSPDQADKLPQLQGE
EVLGDGVEKMKSMSQL
LLEFHYYKCLVLGLV
DLSAAPAKQFNLEII
GFVLRGAKAETPIEE
ESFFSNCKSLPEAPL
QLDRETKEKRFVLM
LRYRQAAKPPDLNPE
HLNEVSLKPLSDVA
LRIVVPLKDTRVKEQ
SAATQALKRNGAQIA
DSASIMVKAINIAGE
NTFSFAEKNFEVNYQ
ASLENCMKLSQMAVQ
IQLPVVSKQHCKIEI
RQSWSVCKQVFPGLN
MDWGAQQKKANRSSE
SGILDREKEERVSLK
LSLQSEHKILHDQHC
PYIAHSQKMQDLFSP
LTSEETAKMMVKIEA
RPEEEEPKVEPKKLE

DMMATLAKSQVTTVK
EGKEEWEKGGKDEVR
AAVSEDGKSDELLES
QKELAEQKSVETAKR
AYEDLSQKYKAAQEK
NEEIDISKAAQTIE
KGDKGRYKIVLQNKH
PFLVMIKNLKKYFT
SHVILGDKVTKNSSG
TQEWDNSKSILGVQC
TPHLRILKVGKGDSG
HLLQYFLKFVPAGYE
TSNGLVTKALEHAFQ
RADQRKAKLGDSHDL
RGGSGFLKSGGEMLK
PDKEKPIKEKDKGQW
LLFGQRAKTIKNTVC
GEELVSLKEKSKSPK
EDDCLAFKVHQYFNV
FHLEFGEKSNKIKD
YFTTQSWKTAQQHLR
EILQDLQKRLESSEA
AETEIVCKVVESSSI
LDLKINLKASYIIVP
VQAASSSKERGGVSL
RAEVHLRKSADFDMFN
FLCIFLEKMGQKIAP
PKKTRNLKKITREQR
IQIVYLHKFLMSLLN
GLDTPCFKTSVNDSQ
KREVELEKNTKEEED
SDVWVETKPKKKARW
DLSSQLLKVLGTRKL
GQSQDNEKELAALFQ
LILKEEMKARSSSYA
VANLEEGKSYFFRVF
VFFQSCAKAVMWQKM
LSSDDYTKKKKKGKK
TARFLYGKKVEGTAF
DGAKKARKPREASGT
FTVQLSNKLIMDIRR
EKEQLRSKLEEMYEE
QDLCSIGKEHVFSLE
VEEGLTYKFHAAWSS
LSSHDSIKMEIVDHA
GFIDDAVKKLNELSF
SSQDVESKRSDKTDF
QDLEDLIKAKEKEVE
DPMAGLLKFADDLGM
PPGQLQVKAQPQARM
EYDVTMPKVESEIKV
FTEPAIAKNPYDPPG
GHRKRASKSPRKTAS
ESTIGHLKDVVGRIA
QAEFADLKKLQDLTL
LPYQNMDKTKTDYTR
QKEIYQVKQQRLELA
KNDFKPLKTLLQIDI
EFDVNLSKANVDISA
PYMVKMLKXXXXXXXX

RLYRKANKSSKLVSA
STGTLVSKREVELEK
TRVVHAAKAALAAFN
ADEMDRMKKEYTDCV
YYWGMESKIPVEDNK
DSFTSAPKQTPDSGK
FHKSVEIKPSDKHRL
ETQIIPGKGQEKPLQ
RENFDKKEKGKTPKYN
TQQCVQCKESVGSGL
KVASLLGKKGASATK
IFENLANKADRQYE
LQDQLLQKEQENAKL
CSALLSVKEPATITE
EGEEEGDKNGDGGCG
GRSEERDKEELEDLK
EEGLRSQKSDERQGV
VKKLEASKIVKAGDS
ERYLENYKCYRKMEE
EEKAKEDKGKQKLRQ
XXXMDDDKPFQPKNI
SLPGSITKAGDFLEA
ENLAGPGKPSKSTEP
SSHRSNFKDPLQVAN
HLCRIIEKKHVSLNK
GDRVNYIKRSLQSLD
DEVPPTIKLRLSVRG
AALDNLRKVVP CYSK
LSGVPLYKGDVPTQD
IIPTFQDKSLSFPQH
IGLHLVEKEIDIEKQ
GTDYQLSKEYTLDVY
KRRPQTPKEEAQALE
NDSQEIFKLAKDVLI
EEPWLEIKHLHESLL
VNTATCDKNPSASKN
TVVERLVKVTLYGSQ
TQDTTTPFKITTLKTT
VVMASFMTMQNAKN
VTKNVRHKLTSRNER
AIITQGCKSLSEMY
AFAICDQKSVHGTF
VSTSQAGKLPTRITV
LKAMIMCKGCGAFCH
ILSLNQRKEDLLVDL
VYVYVAPAKSLVGQVA
VSISAVKSAPEENS
LPYFIRNKLCKVIVD
DELALFDKSINEFWN
YKDGKRLKNYNMPWG
LDDISQIKAQVKELS
IFDDWARKVQQRNLG
KAARGEKDKETKNA
AESD TDVKLSIFCEQ
DRTRV PNKFRYPFYY
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KSTRSSVKLQGTSKI
GTDCLEAKEKVHVIG
VFQREQTKQVEELSK
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PCGRWLAKNEDDGS
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SEPSEFYKAADPIDP
GNQTTALKHAKDVKD
RGPGRPRKRTHAPSA
VTDEPLLKMLLTKAD
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DFLDFMTKINGLEVQ
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HTISVRVKAAPYWLD
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KSALGFIKVAVTVMD
IKVKSEEKIKVVEKS
RTWAEAAKTVLEKYP
TVLHG NRKD NELIRV
VKQAEKAKDSVYKRS
TNGEHTSKATLELSP
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VGPDGLMKLN GSALN
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STYHIPTKAEASTSY
VTMDSAPKPF TDVSI
LVSDNNLKDYFERGR

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DCQRIELKQGYTFVI
TDTVSDVKYKEDLTW
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MEEIENLKKQHDLK
LQYMTMAKLQKEFGP
FRRLQFNKHGVL RVE
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WRESSLLKNLWVSQK
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KNNGQFVKASASLKG
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FKIFRETKENEIQDL
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DPLVTVMKVEKAPQE
PELPLQTKDAADGEA
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VETICHRKEGGSLI
KKETTVKKAVVVPAR
VFEYFNAKSKHSWRK
PSVENRPKIAAFLPA
CLYQTNSKLYESLTY
QKLVYMGKLEKESF
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ALRAEVSKLEQQCQK
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FDTSAAYKSILRKKV
DELTTEIKELKETLE
EILMSLQKVL SGLGG
KHGFSVLKGQAELQM

NRVNHIVKKIETENE
TYVAQFLKHYPDIHN
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GFNTSQGKLLRILF
PIETERSKCDITGLL
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FTLQYLNKLSMKPEP
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EIMEHRFKTYQQFRR
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FHKLNIPKLD FSSQA
DAGLYTCKVSN DAGS
QTEETLTKVSATPGP
EDSEQELKGYACRHC
LNINPDRKEHNCREE
NFILLFYKVSTSSVV
LLDVNLAKFLAQDVP
FSTALYGKLLKLPTC
LDPESQRKRTVQNVL

KNSNGIPKLKYIPLK
SSAPSSPKLQHGSTE
KLEYIYAKQQALEAQ
DQLKLEKDIQMWKV
RRVAQAQKALSDVAY
KESARDPKPEASRAS
DRMTEESKVEAELHA
FIRTRLEKEGIVFKS
YSSVSQRKYYSTKHF
KALLLEAKQKVPPVL
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KEETNIVKLEKQYQ
CNSVHLCKQLVESGA
LITPEDRKYGTTNLH
LLDYQDHKGADSHAG
TECHARFKTPEDAQA
ATVNIQLKGTNEYVP
KNLDHVNKILKAKKL
ANQGCVRKVYLKDTA
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QEEVIEVKVPAVHTK
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LISLQEAKDICEEQV
LRNLVHSHKHKMIAMG
IVCSSEIKRQVVETM
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AETLNQSKERNRFSL
SEPSELIKVLGEKPE
VAGGAISKPLTDQTV
AFKNIASKIANELKL
PVLQEEIKESQDPQH
RSLVEQHKRERKELE
VPGPDAQKTETPSVS
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MGLKGPLKTPIAAGH
VVYCEELKCWCRAIV
SSEEPTEKEPPGQLQ
HLRTRVQKVQVKEEP
GRIETDTKVLEILYE
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EPIRNSVKERESERN
SVTRSTFKFTRLTEG

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RAENLRFKEEGVRDV
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IENIDFNKSGSSTAS
LEDEAARKAKQGKEN
LVAEFPEKEAQLSLV
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QSLKDLEKEFVDFWE
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SELHESWKYNMSFIN
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GLGKVGSKGREAPLM
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ERFDVGPKEKPLEEP
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HLTEETLKVTAIPEP
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ISSLTPKHLQAGMQ
EFSDDIVKIIQAAN
YLDSTFTKRDPGEY
IVSNEAGKASCTHL
NDNAPIFKEDPFISE
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PVLPEPKIRAVSPH
DRVQAIVKGTKQRLV
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PGVQGDVKGPQVALK
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SVHSREAKESSAAQA
ERNIEAGKDDGLTDA
CSISQELKLSFTYE
SPQRLCSKHMPQLHS
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ALKMSPYKDILETHL
VSRYGELKSVPTTQC
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AKDLEQHKKIQEEIL
RTLTYTAKPVGIGG
LKKLEEEKAEAAEAA
MDAENMRKELAELES
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NVSSRGGKKFLPVLK
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QEERAFKVDPELVV
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KEVMAAYKGKRRSEA
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LPCLSLRKLPPRSEI
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DLGEENFKALVLIAF
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DNEETFLKKYLYEIA
PELLFFAKRYKAAFT
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LKCASLQKFGERAFFK
RLSQRFPKAEFAEVS
KLVTDLTKVHTECCH
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VLLLRLAKTYETTL
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EEPQNLIKQNCLEFE
FEQLGEYKFQNALLV
ALLVRYTKKVPQVST
EVSRLGKVGSKCCK
QLCVLHEKTPVSDRV
VDETYVPKEFNAETF
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DFAAFVEKCKADDK

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PQLSEYCKMPLKMWL
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KVSTEHNKECLINIS
MHLIQTGKGEAIRIR
QELISLAKSRYSCRD
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VFANMQMKLSQSRPI
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VVGYYCLKVPLVVK
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AEGSPQYKKWYFELI
GIISIPKLPKSLNKE
KQLRKIVKHEIMSVK
DGFAESTKRKAAVWP
LYPMLFNKLNKNTISK
TRHMEAVKTQFLEQA
VVAASEAKEDSPAQT
ATAPEDDKAPAEPE
NNLHLQEKSDDPVK
EENGMAWKEILNLLY
QHSPGLDKENVELSP
TALAELVKHKPKATE
TVRKQVTKSYKMADE
EFWANLEKETDWLRN
DVAVWFSKRLPTFVN
RFAGPFSKQTQIPDY
CAIYTYGKPVPGHVK
DLVPGSFKSQLQEGP
AAVRQRMKCSSMQR
GELLITNKSELIFA
WLTAYVVKVFLAAN
ARYEREMKTYIPPKG
LSGFIPLKPTVKKLE
SVSRVELKPGDNLNV
RVTAILDKLITMTIN
NMVIADV KMLSGFIP
KCCAADDKEACFAVE
ISCADAEKEIMRLGT
ANHVLFKTEEHMRPF
SVRFVCQKGFVLRGS
VSREINLDYEGQQK
QMLFYICKLTS HQM
FPNNYWDKFVKKRVI
GGLVEGAKNIRVTKI
SSPCSSDKQNVXXXX

LEPDLEKVVTYLAG
RYNMPLEKQQPAFAL
QYDSTHGKFGHTVKA
KEYDPDGKGIISRKE
NLLQMTEKFFHAIIS
DLLVHCGKLCALVYK
PSFSSETKSACKEED
LMVCNHEKVGLQIRT
VERSYAVKSGKWYFE
YAVYSLSKSYIYLDT
MVLSAADKTNKNCW
LLKETAFKFKALKKV
GMRDIPMKYSCORRA
AVINSLEKAFWNWVE
GMGVPEIKYGDSVCF
FAYKFLRKILKYVDS
NSLDFDQKNNKDSNS
RGNFLEIKNKFLARR
SLSHSPGKXXXXXXXX
NAFERQNKAEGLGMV
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SVLGMPDKVEDMCPD
TVKAENGKLVINGKA
LFIVSISKTLANEP
LQMISASKGEMSPMV
PPVEPNTKVFPVAVFL
DQTEQWEKFGLEKRQ
EIPLQILKTKALSML
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FQVELPRKAFITNFS
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QAELLPSKSVSLIIL
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PTLSQQRKSQNEQDT
YINVDCAKLRLLKE
SLLNGNSKYMVLVPS
EAMQAYPKQDRPLPS
TNVEMILKFFDMFLK
LLALLLLKDFDSVPP
VTVQDFLKKQVLTSE
MSFSAGVKNWVDHMM
GVELMEAKSQLFLKY
ALLDERTKKSNRDSL
ESHQHLSKESMAGNK
SPEALVGKSLYVSVT
MAPSLTFKEKVTSLK
PMTVICQKDLSWSML
KVTSLKFKEKPTDLE
EILKSLDKEAIREDN
VTYPGLSKRRLKPEA
LQLSGPDKVTISLLS
VAFNFFRKFYNKSED
VIPELNGKLTGMAFR
VDESNINKKLFLDSL
TVYVDAVKDSGRDYV
RWPSHFQKEAFVKPG
VREDMETKCFICIG

Supporting Information S2: The benchmark dataset $S_{\xi}(P)$ used to train and test the model for predicting the possibility of carbonylation at Pro site. It contains 126 positive samples and 792 negative samples. None of the sequences included has $\geq 30\%$ pairwise sequence identity with any other in a same subset. See the main text for further explanation.

(1) List of the 126 peptide samples in the positive subset $S_{\xi}^{+}(P)$

GKWELYIPPKQNKSV
PLPRKRPPVTQAAGA
QRPARRGPPPLARAV
ASKLQVLPQKASERL
GYKVLIQPSNRRAIH
KVSAAPGPADQKTET
PASKDTRPKEKRLVN
GRKSTEFPRKIREQE
KQRAKKKPNPVEEEP
YYYWKKTPEAASSRA
QRNRETAPRTIFQRV
KSLQAKFPSNLKVSI
NSRTMLLPLLRFP
EPQKQVQPQVQPQAH
IAKQSLRPFCTVCNR
ERKQNLRPMPKKYHS
SPVQKANPGTLAAEI
PTLPKRVPRAGEARN
VVRLSCLPAFKDLIA
KERKMAVPMPKRRS
LKKAGRIPEQILGKV
ASLKRLKPHVPLGRN
STKEKAGPKGSKVSE
VGIPDKIPFKRPCTY
YQDLGLPCIVILT
KTVMGAAPELKVRL
AGRLFLIPATIQDKL
AKARVTKPKTAKPKK
PNSRFSAPSCGSSEK
VFKLLECPHLNVRKA
CSGKKVEPSALACRS
KEKQPTMPILKNEIK
RLKNEKEPMVLKLD
STIPLSHPKIPRCQE
VAKAVECPPRRTAR
GSETPDGPLSPGKME
KQATDVKPKAAKEKT
KKEEKEKPKKEVAKK
EVKKETPPKEVKKEV
KKPAALKPKVPKKEE
KESLKVGPLDSVTYL
LFNRIGDPSVDEDAQ
LGGKLGPDVKLPDM
KIPKMKMPKFSMPSL
VDLHLKGPKVKGDAD
NMPKISMPEIDLNLK
KSKIKMPKFNFSKP
PKGRPDRPRDLELTD
DSKKEEAPKKEAPK
KEEKAKKPEEKPKTE
ADGRGMLPKRAKAPG

VVRPEEIPPVENRF
RKRVSLEPHQPGTP
KKATSCFPRPMTPRD
FPENKKQPYYPFD
STLERVLPRVRFTRH
VVERRRRPRDSPTLS
YKPKRGRPKSKEMPQ
IPREKKPPRPPKKKY
KIHRNRYPVCTKPYA
ERSPGGRPIHKRKRQ
KGSDEKKPFKEKGKT
RALGVQTPSIRKSLV
ELIEELHPIIKEALE
NPKEEKKPKEKKKKG
MDPSAPQPRAETSGK
ILDLC AAPGGKTTHI
KHTFSVLPGDCQQRL
RVPRRASPLRTSRSR
KKKGRDPYAYIPLN
LLKTHFLPLMEKLLK
KIKKAASPSQSVRR
KKAKSPTSPSPPRN
KKLLVLNPIKRGSL
RRRAPPPPKRAPSTT
LPGPEKLPGLRKG
PDMLKNAPMLKSMKN
LMEKEVEPEGSKRTD
KLTRCLKPFENSRLR
SYRTVEKPPKFTEKG
EEIRSHRPTLDALRE
KVSRTVSPKSFACAF
KSTLAIDPATSKEIP
KEPFKAAPHTIHPPC
KVPIKQVPGGVKQLE
PAKVPEAPKKIVPEK
PEEKVPVPIPKLKP
PEVKPKVPVPAPVPE
RPIKPPGPPINPKLK
PFVVPDAPKAPEVTT
TQEGRQQVPAPQQK
ARKALCDPLEEVREA
LRLKPKQNIPTVK
KKPLKKKPTVLLPQ
VIRSLKRPPPADAPT
PRKRTHAPSALSPPR
KQDKLKS PFKFSDSA
GNGHISSPLTGKRQD
IREATAAPHGKRKRK
LLVNEQEPCKFLDA
KTLGIKLPFLVMIK
ESKKNELPDGLNKKR
LKLYRLLPMRAAKRP
ASQRCDPPSNPVAA
RRAHTANPLHRCRCG
AVETEPEPELRQQTE
VYDAYLAPNNLKPVV
GLLYCDLPEPRKPLE
CLDNTRKPVDEYKDC
EFQLFSSPHGKDLLF
FFSEGCAPGSKKDSS

QNTGGKNPDPWAKNL
KTPKYFKPGMPFDLM
RNGQWSEPPKCLHPC
EFLRACTPGASLRKG
SHFRHGIPFFVKVRL
ENVGTPCPVSAFPSS
LSHKDDSPDLPLKLP
DKGACLLPKIETMRE
ARLSQKFPKAEFVEV
KVPQVSTPTLVEVSR
GTRCCTKPESERMP
CVLHEKTPVSEKVTK
ESLVNRRPCFSALTP
VELLKHKPKATEEQL
KRVIISAPSADAPMF

(2) List of the 792 peptide samples in the negative subset $\mathbb{S}_{\xi}^{-}(\mathbf{P})$

LCGMLSLPWIYSHSD
SGGSYVYPPVQEFPL
YIVPDYMPVVYDKLP
TTAGATQPAAPTPTA
QMANNFTPPSATPQG
KGSETYSPNTAYGVD
STNMGILPSVTMYNF
GKSTDFAPIKEDFGQ
HSWQEQAPNQPPGPT
REKLKAKPLLLQLPI
SSFIKRQPLVIARLA
VLGEYYTPALKCEVN
LRRVAGTPCGVFGQR
ALEHEYEPYSRLKSD
VIINQLQPFAEICND
KSDDPVVPSLFKQKT
SDFDFSAPKINLEIE
VGGTIKSPKNNEKNF
TGRQIFQPLHALRNA
YLSTEDVPLARMLVP
PEKEAKSPVKEEAKS
SHGEKELPQWLREDE
SPTASQAPNQPPAPT
LEKQFVKPDGENRAR
RFMEIESPHINENYI
RSLWRLEPLRISWSG
EEYIALYPYSSVEPG
DALKSREPQAKPQLD
AIIALFTPTTDPEAE
SSALGEKPITFYRQA
PIPKKLPKPPPKVPE
SLSSAGRPGPSEGGD
RLCNDLPPGTVKLX
AELEIANPPELQKHL
NIVGIGKPSKVSECY
RDIPAMLPAARLPTT
VMTLKWTPNQLMNGS
KPSKSTEPILIKDPI
AELLANMPDPTQDEV
IKLNYALPPPLHQTE
VQGLGVMPPKAGQTI
ISQNESRPHFLIELF

PLVDHTSPSSDILLF
SSTVNGVPSRSPRLV
TPEDQDLPPCPEDIA
RCISSALPRRRPPVS
SSISDHTPWLMPPTI
SLSHSACPTPNPLSR
MVVCWGHPDSDGGSE
SESSFGKPXXXXXXX
RQFDNLKPSGGYITG
TVLDANDPPIFTLNI
SWSRISNPSAFSIVP
SSIALGDPHIPTSPE
FNQSLKSPSRLGCPG
PPLLASMPAQLPPRD
IAQDPKQPPDPPVDV
ECHISGYPSPTVTWY
KASVVTLPVYLNFR
NTSSDCRPSESELL
WVKENKVPCLCNYK
SWLKDGLPLKESEFV
EEVDCMDPTCSGRGV
AESPEVLPHIEKELS
SCRSEGTPAWYMHGE
VAFQLHLPLSQRACS
DRFCLSSPTEALKMG
QVRVVAQPSLPAVPQ
WIRDALRPPLQNINS
HKESFLAPVFTKDEQ
AAVQKAIPMYKIATK
WGMESKIPVEDNKRF
AQNPVDAPGRPEVTD
SEDSVQVPRNLVGKV
YPDIGWNPCCGERYL
IGSKAGVPSKSSGSA
SLEPHQGPPTPESKK
LWGCHSAPHGPGLIY
EIGDGFLPVCSLPGG
GAETLTFPCDRWLAT
LKASVCKPFLFLLKK
ESGKIQEPFSAMSKS
GTQVSQRPGAQALKV
KEQQKDSPVFCRFFH
QSRPTGVPTPTSCLS
EMFGVWEPLLEPLEI
YTEVANIPVARPGRR
SRLDLPLPGCAEPP
YLNKKGNPKKFAFLA
AIESLVKPQAKKKAG
ENIDGILPLHDAVAN
GKLYIEAPTFDLQGS
VQIKKMEDPEQLRND
KRKKKKRPEDTAASA
SERLQRAPLKSVGPD
DPRQLGVPVIARDIE
ELLSTTHPANKASLT
SVTVTTIPASQAMNP
LSAHTILPGSKTREP
ALKISVAPGLADQKT
DRGEIIDPFVEVEII
HKDLIKKPTISTAVG

DRETILDPNLQATLX
DGAVPAAPASADAAR
VLAERKSPEISERIV
SPHPPLQPLTGSAGQ
FLPASTAPMQGKRKS
LNNSSSSPQRSVDQR
KNALENYPNFRSVVD
ERLALAGPQLRPEMS
LKSQTQHPWEKLLNL
NANQNASPNVPGKRG
SLEMGILPREIRKLV
EATPTAAPPTLPPTT
EKHTHHAPLSPRTFH
QYRKVLMKPKLAKPI
ALSELDVFPKVKAGQ
DAEVYNVPLDSQSDD
DKLTLKIPWKNLYGE
LSPTLNTPAPVAMPA
TRSLGEEPVGGLGSL
EEQVNSLPGSITKAG
KVVIGFVPLAEIMGY
TYIELMRPVSELIRS
PDVEAHGPEWNLKMP
YFPNRKFPSSSVAFK
EGSRLSLPRLIDMSA
PRLTPVRPAAASPIV
PQPGLVVPVPTVRPL
LLVTAMGPPGGGRND
KIEKELKPYGSSAIN
ENLELTNPQEFGSSW
AVDKRFLPDDHGKNA
PSAFSIVPRRAAKSS
RLLSLSKIPILPQQDN
IKRQCVWPFIVMMDD
ANLHPAKPKDFSAFI
TQITTESPEKTLFSS
SDCCGQKPTGPGGPL
ACVTACEPPKTCQDG
TMATRTSPRLAAQKL
ALTALTTPIQTAALQ
KLQSILKPMMLRRLK
RKKMNLKPIRMNGN
EKAFEGSPARELDVP
GSSGAGVPGGAAAAS
SKQKKVAPRPSIPVK
LPGSVLSPPPPPPLP
GDSGGLIPGKSLVFA
NKEEGARPGTLLGTF
RRTEGQYPSICPRLE
HEAILKPEAIEMYI
HPFASFHPGLNPLER
PDGLKLYPTLVIRGT
PQRPASEPHVVPKAV
EIPKKKVPEERKPVP
RLFNDSSPVVLEESW
GDRSGIFPSNYVKPK
QAIIQIPKASNRT
EKRDYREFFRKKDR
FTNTSLHPQRMKALA
PQFSSLQPPCFPPVQ

ACRCSIFPDLSFVTF
LMDYADLPYQIEDIF
FIDDINMPVINEWGD
GTLVLCLPQIKIISA
ISTSEAAPYAPPSGL
TPSWLGLPNNAERVL
DLEDESTPIVKLGDA
EDVVASLPLCHAALR
RTHTGERPFQCHSCG
GNLHLLSPGNSARLT
EAIIDVRPASTRFLP
EMSDSNSPPIPYSQK
DSVGVMSPPLSRSSV
PRSVSRSPIRMSPAR
NMVNGMGPMGTEGLF
TNTSVLGPMGGGLTL
TQGSEKCPQKTTRRD
EESQHQQPDDSNIA
FAGTEIDPENEELML
KVTIKDKPAVAPATK
NHDESLLPESLESMM
QHLPSVSPSVSDAFL
LNRDLSTPGLEKDSG
CEELRAAPRQGPAPA
PSKEEPSVKAEVAE
NSSRQERPPVKPFIL
GTEEKKKPSDFKKKV
GGESSASPGEPQRTL
QADRKILPFTSMRHQ
RARTDEVPAAGSRSE
RFEMEGLPVDES DSC
LLSQLGQPSIFDTQK
FDAEDGEPQTCKSMK
AASLAELPLTPPPA
ISDTLLPDLSQISP
NRFTMEVPKKLTEWF
TPESSLPVALQTPT
ITESQSSPPPVIDLI
PLLPSSEPPPAPPLD
EMVSGFGPIYNYKDT
VQVLKYEPFLDCALS
LGRASVVPLPYERLL
KKTGKGNPNSHPEPA
ARNLFSVPGAPDKPT
AKVMELLPTHAFSTL
HAWAWGTPGFLTVML
TTSQDEAPREELAVQ
SYQEAQLPALPESVP
IVEREMAPDFELDAE
ATLEEGNPTDEVPST
LLKPEADPRPCERAP
PKKVAKSPAKAKAVK
SRRRPRAPKEKAQPL
IPMLYVVPRPGKAAF
PMNPIPAPLPPDIPS
GNDSDEEPPAAAPT
DKVVIQDPYRLPGPP
FAKSDNQPSTEKAME
IAKEKRTPAPEPEPC
SAKITSLPPPPPTLF

LHLQRINPTTVKMKS
LDIKAKAPKVKMPDV
ESGDAPRPPPAATPP
VDLHRFHPEPYGLED
RRMQQAAPTDPLPP
KAVSSADPRAPGESP
TIELEWEPPAFNGGG
XXMNTSIPYQQNPYN
GALMTLGPSVVRYHL
VTFKANRPFLVFIRE
VKVAQRSPVDSGTL
PMKPLLLQPEVLS
NLVLKRVSPVLIKK
MDDLISPGKNKSGR
PRESACLPEKLKEKE
RAWGCAGPCGRAVFL
NWRQPELPEVIAMLG
MDRDCRMPMGLSTGI
TVENASKPDFTKNSQ
RTDLYFMPLAGSKLA
DRGLQLVPVWDIILS
NALNSCDPWVQAKCY
TNMGIIIPDFARSGV
SKTIYTAPLDMLQVT
RTPPRRMPPPPRHRR
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YYRQSEVPDSVYQHL
EKDDSVRPNMTLKAM
ECLGAAVPARLRKVA
RSLQKDFPIQILSID
VSDVAKPNQACIST
SLKKAKKPPPLPSRT
EKFRIELPDLGRFYK
AARISTSPIRSVRSP
AFPDGHLPEEALKVS
ETYTEEDPEGAMSVV
ALDDAEEPESPPPPP
ECTTIEHPFCMYDAD
GAAGSMSPSRVEANV
EDVQVLIPFKGRPPP
EKVSEVLPIQKNDEE
LKFSSMAPDLRLNE
HPQRPPSPHPPPHPS
NRLCFLEPTSNAQNV
TDEILLNPNNKWFKP
GKLSNWEPKDDAMSE
GSGTDMEPSLYRCSN
FKSDGIIPFAHAIWH
DMLKRVEPLRNELQK
FGYIKIIPFYILNAT
GESKQHIPEKKNEVH
ATLSVLEPATIVEKP
LQGGNKSPVTLTAYI
DIIQVTVDPSPSTSE
ALGNQSTPAPPTGEV
FTNFMRSACDIFNP
PDVSMVDPEALAIEQ
TSLFSNKPFLKLGAV
LLCGSDLPLHKMAIQ
CTVLTLEPNSQVQQR

YNGKLTGPAAVELKR
GDASIAAPFTSKLSS
IRDWLVKPIRDQHVK
SQVFIDHPVHLKFNV
AEDVSGMPALCSPIS
NHARLRTPPPPLSHA
LSHTLGDPIKIRAWQ
FQELSQTPGHTEELA
LGRPPSAPADKDGSK
GFLSYLGPFNQIFRN
ESQGEVQPNFSTSSE
LMLTAGLPELTSVKD
RPGPHSVPSQAPRLE
ILDEFYGPEKSLQPI
KIINFKTPEDARWIL
DREDQEAPDSDAEVD
KQNGIPHRGSTAIF
AGQVAVLPEVQVTQN
LAELLRGPCGSFDVR
KAKKRRLPRGFPPSA
LQRAFPAPAACQCHC
VTRQLYEPLVMQLIH
EWFLRTFPDPTSWYS
NPKAITAPQMFGRLD
KLNQHDSPRIKALEK
MMLCSECPTVFVDAE
ILKKYGIPFSRITQE
EKTAAPSPSLLYKST
AECWRSRPEERPTFE
TLTYTAKPVGGIGGG
VTSSQVQPVTIQQQV
CQTSTVFPLKKKVISI
RTVKDSTPSSLDSDP
QVTDANDPPAFHPQS
LADTDLSPMDGISTC
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KKIIEQPQPSGKQE
DCFSEEAPDATKHKL
SGQRSASPSVPGPTK
KTVKLKSPVLSNTTT
QKSLSLSPGKXXXXXX
FVASGMGPSASSHGS
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QWIRNLVPEFGVSSS
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DRSLESNPEQLQAMR
VASSEAKPAATIRIV
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FLRMSKVPTDLAVEE
DFLKRRLPKLSKSTA
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VLKFSCKPGFTIVGP
RLEVELYPSEVVEIQ
TTKSSAVPPGLPVYL
QLYDDSFPMERQYL
KKDTKKYPESTDTES
SHGDVIRPLRKQVEL
ESGLMGEPQPQGPPS

GHETEEFPDEEQLRR
GDSRGPSPSYLGGPR
ESRYQTLPGRGLSGS
DNANSRLPEDTTSVL
KAAYLSDPRAPPCEY
IGFLDNWPLLEQWFS
LFQKKIDPVTMDPEK
SVAQTGGPPEADGLV
EMEVCKLPRLSLNGV
SVQSSHFPSGSYSVR
ITEVWGIPSPIDTVF
SAQDMHVPVPKQLAH
SKDIPLSPPAQKNDP
YRGVKVMPFSTACNT
YQEKLYRPPPVLDAL
PAGPTESPASKGVTA
WVRCNKMPVKDTTYR
EKECAPTPAPVTRAK
RHAVKGDQPSPGRHW
TASLLAIPHTPESSS
VEAFFYEPYQGAIQG
FMAVKNWPWMRLFFK
ENYVQETPLVLSRCS
MTISWHEPLSDGGSP
SAEKNQRPRKQTSAP
FAASSTVPHCEQSCR
VATPQVSPNTVKRAG
EEDLLDDPSLEGMCG
ASYESES PENQTEKE
WQMWTL LPGFCTRPT
RQLDRLLPKLARGSL
GKKVRKMPVSYLGSK
ICHEISEPRLQNYDE
IVDVLDPGPVGT
PFKKS RFWEPNKVSSNS
QRFCIGHPTQEMTFG
RARSLKFPGLISGCT
LIKEQLEPPEIDMKN
HSDSGYEPSFGKSSR
GLAWARAPQPKAWVS
ASSVETKPGASKVAT
LIRICKP VVLPKGP
AKKEDKTPIKKEEK
PKASIKDPHFLNFK
MTMMSHIPSVMKAHG
ISELTGTPFDVESDS
DYALLTLPAEFSSQL
GATAPPAPAEPTPPP
EYGGKWSPLILNPSY
EGKSLRFPLALEEKQ
NRFGVSKPLESAPII
PQLSVCNPHSGKEYF
SNRKGETPLKVANSP
YGIWKLIPNGQYEF
RGGAEERPGTPELAP
APLNVPPEVPSEEL
ELVQAMFPKLNNQER
GTELSLNPTCAV
FITKVFEEAKPNSEL
CCKVTS AISLPNIRK
PDG

CDEDHQTPRDGETSH
VNYCECNPCFNNGSC
AFYQQTLPNSHLTEE
VYIESRRPNTPYFIC
YLAQQIHPVVARICE
VEDKSDPPEGSEEEAA
XXXMTAEPMSSEKLN
KSVHLQKPKPKKKKF
ADSVSLLPAAPEGSR
GCEGSSKPFYNRQD
RRREQRDPTVHDDVL
LDGEEEEPEEETTLG
SGIRAGYPLSERQQV
MKRESQNPDKDETN
NKVGASDPSDSSDPQ
MKVVTLKPTVLEHTV
ITPKSDVPIQAPHFK
ENLKIDRPEDAGEKE
ISDHSETPNMELSCR
SCSENQEPGYCTVSN
SFIKQNNPKFSAVQD
PEDDGGSPITNYVIE
TLVSGSLPFDGQNLK
LARYSYNPFEGPNEN
PASTRFLPQGTRIAA
LHEIYFLPDHPELKK
LNRMTFPEELDMST
GRIFVFEPPIGVKAN
QSKLYHLPPPTVGPH
IKNSNGIPKLKYIPL
FLEVDEYPEHIKNLV
QETAEGIPPGSQDSS
XXXXMSEPGGGGGED
VYCLALVPANTLPKT
RCFLEADPYIDIDQN
ASLEVEVPAKIHLPK
KKVPAPVPKKEKVP
QVFKPFLPSIALCM
YSVYGTEPYIRLGVL
MSPARMSPARMSPGR
PVPEEKEPASSPWAS
KKTFFVGEPQRLGSET
KDMVKMFLLVEKLR
LGAMSAAPSQPNSQI
TDRLVITPLTDRCYI
SLRQNETPQAAQRS
LSKDLLKPIQDVNSL
TASPSSRPVSPGAI
KSQVRDYPKHNGQIS
GKDVLRRLPPSSITD
GLETYLGPLQVAYRE
REYQEYNPYEVLNLD
RVELLHNPAFCSLAT
SVVSITGPLIRILGD
PEQNQDMPPHLPTAS
RLTPIGDPTMVVEWL
TCRDEYAPPKAELDA
GDEDIKIPENPLEPL
GEIRSVRPLDREKVS
LSPPPTEPTDGEQAG

KKELKVGPYANTTRY
GKDELSKPSSDAESR
ATLVDQSPESLKRKS
KLKVLDPGPPASVK
CTDSMGVPRALGETW
ANGDSGSPSYMSSLS
LGRVFIHPESPSTGH
SLKTAHSPNVFLQQG
DKIQMNPPEFEMIE
ALLKDQQPGTFLLRF
AVGTSAAPVPSDNHX
EVKISHFPAADLGFS
CVDGCYCPNGLIFED
EGVLLTLPRQSGGSG
ESMENSQPQVTEVTA
SSSGAVDPSVQRSFT
XXMMAQFPTAMNGGP
EEVRVRSPTRSPSVK
CLEENERPLEDQLEN
SSSSGISPDNRDFYQ
ATSTSSEPLSSNQPA
TTCNCKKPDDDTRKG
MLTGESVPQMKEPIE
VPGGSVKPKIMSPEK
ILTTLQEPHDKHLLD
TNVEDVCPNIPSLEK
RLEYLEGPTVTSSYR
QSPTKAKPKVEDEAP
PPPSTQAPSVNGVCT
HGDACFLPEECPCTW
EVSIGSAPLAKQQSY
NILVELDPDGCPWL
DDTERRSPTPERTRP
GSFGYKKPPPATGTA
XXXXXMAPVHGDDSL
APQQEELPLSSDMVE
KKLRSDEPLIDPKPV
AFTRTVSPGSVSPH
QLELADPLKDELNL
TPNPLERPIKMGWLK
FKELFQTPGHTEELV
EASKEYSPCVAPCGR
KSFATGRPKKTKKRS
HPYVTHIPSPTLPGS
DAWLQTDPEIQSPF
SEIKISNPTEFQNH
HNIENASPATVSRMG
SLESSFPLPKQYLD
TGQLGVKQGTGNSIP
CSPLMADPLLAGDAF
FVYKDIKGRKRKKH
TSANEVSPVSSSGVT
FQRSRSESPDAPES
ADSDGWTPLHCAASC
VEENNASPHFEPDLH
NQIGCLPELSELKK
ETQAEDHPPRLYGCS
FKISFGTPAPGFSSM
GVCTDGEPSPQLLGQ
LSPDSHYPLEEEKTD

SPISQRLPPKVESLE
AAEFISKQNLEILE
NKCLIKNPAERADLK
ELVAAVWPYRRLALL
RQTVAQMPPQLVELP
NPALTLWPMFLQGKD
QDIAKDFPRGEESLE
VTLKWAKPEYTGDFK
QHVFSAGPVSDEVLP
LYPPGRSPLHHAQQL
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QLAPDPGPAGHTLFQ
GLCAALEPILSAKTK
PADVTGLPMPKIEWS
QKFRFNHPAEAAVLR
SAMEMNEPQAPAPSL
FHKVKALPLVSWRR
AFKRANDPVNYLESK
VRATRASDPDPRAYVP
KVIKMEEPLPAKVTE
QQVTAEIPVDLNTRE
GKVIGEFPGVVHCLD
MIKKQDQPTFDNSGN
SASDGYCPREHMLPC
LKHSPEDPEKYSCFA
LIKHLPLWWDGCI
SSSLGKKPSLTSESS
GILKRRYPNSLPALI
SKRQLQTPKEKAQAL
VYVDYPGPASLTQIY
AEEDLTDPVRCNSLE
NSAGRSAPRESRPVI
FQEFLLKRPDHLKQDFV
QAESQVEPSYSEQAD
LTAKQKLPSYILENN
RSTEGIVPQYDGSSS
LSLSLAQPLRSERSG
EMKEIERPFETYKEN
NATSAFGPNLRYIVK
VDQKIEHPLQPQGL
HRRTSAIPRAFTRE
GDFKVTTPDTSTTQH
VISRTGVPQPTQAQS
RGKKAKNPKEEKPK
YTLKKDVPDGVKELS
GNNDVKQPEGTMID
VESEIKVPDVELKSA
KLGVQVRPENWCSQM
SWLKDDEPLYIGNRM
PAYDGGSPIIGYLVE
LAKILQNPITHSLQV
KLSSQALPSFGYIKI
PPARQLGPRSPRVGR
SKVWYNCPPXXXXXX
GKDFERKPLEMNDP
GQAVTLLPFFTSLTG
KLAHQEPWTTDAKI
PGGKEEAEPPDGGD
QMHSTSDPSHRSSSP
LKNKGIQPLLDVMTM

SNIDIRIPTGQLTMI
CDEFHETPSGSYWDH
IDKNTKIPCKSPPE
NAWERRAPLAPKHIK
TDWEKTKPVTGNLRP
CYHFGLSPDLPICKE
EALVIREPITVPERP
GDMGDTTTPAEPPTPE
FVRPDLGPKMYNAYG
DQKYRQHPSNFQFKK
QMSFSQSPFLSIKAS
FSALRALPDMEVVGL
TSPEGVAPTSGHDRR
GSHVNQGPLHLGGIY
GRITDVIPSEAINEL
VAEYEVTPDDKRKAC
LVRDPLSPAVRQKET
GNICVYCPGGPDSDF
RLLERYIPKHQKCLT
PLTTALNPPVTATEE
FLTYHMMWPLTFLSPS
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LRISLTHPTIPFNLK
ENSIEGTPSKCYCRL
NESKKTAPRQEAIPD
INPSTSLPLIGSPPV
QHRTFIKPKLEGLP
RVRVVGKPDPECEWY
LQALDLLPLLIQTVE
WAQQIHSPLTCEQLT
ITVITLGPPSKPKGP
AWDSGQGPRLPSSVA
STIGLNQPSTPTHAA
GEYDVTMPKVESEIK
FKTSIFSPMKKEVKT
DEREFSGPSTPTGTL
GDEGADEPRGAGRKA
STSKNTSPMRNSFAH
LRPHVFMPEVTPDMD
VDLSLGSPKLGDIK
LLVGAKSPNLPEHIL
ILDGLYGPIAFKDFI
ARHRCQTPHLLAAXX
AAAARTEPYCAICTL
LFHILVTPLFLLSTV
AQILILEPPYFVKQL
PPPGQLDPEDQDSEE
CLVKDYFPEPVTVSW
TPELSAETPKALEN
TAALAVAPGPRFLVT
GRPAEPQPEPEEPAE
DLRTDAIPIRAATAA
AGIAAIGPAKELEAE
EEITDNYPQAIVYPF
APPGLQPPAEDEARA
LVIPPQPPTTGPPRK
SRGTDGQPLLLPYKP
KVDALHCPPAAVVTV
TMKMRILPDQFSPLN

QVTTVKVPMMKRLGM
KKACMFEPLPIKLSK
RQONTRDPDTMVPLT
EEALKVSPVSIPAEQ
IWWANKDPLPPLDPQ
ELKLESEPEPGRSPE
MMGLDLQPDLCSLLI
TRLFVKEPAAFLKRL
FDMHKRSPLLRAPRF
ALGRTYHPKCFVCSL
QESARAVPEKSTAPL
VVLCNLKPQKMRGVE
DASSSWGPMQMSASVH
AGVSSGAPPGRNSFY
PSASERLPDEKVELF
TVSQFTLPKSVSDGI
TNSKATTPKPQKPTK
KESKVEEPRKRETVS
ALSSVGSPKAKEALN
EGQTQRQPGSPMYRR
KKPKTVKPKKVAKSP
AAVRGSEPISVTWMK
QFPFADTPDTYKSEA
LAQADKLPMTDKRVA
XXXXXMDPPRPALLA
PEVRSTEPVAPPEQL
EDEAPPRPPLPELYS
EKPVDPPPFMFKPVK
IQTDVVLPSCKKKAP
ALSLFTVPEDCPIGQ
SQPRDGWPMMLRIPE
EGGGRSLPRSSLEHG
TLSISVQPGEGNKAA
TKSNDTLPSSHREIP
ASAEGREPSQCGGS
SGGEWKGPQVSSALN
YTHIQMPRGNHFTI
PGQHLLAPEDVISCC
SLCVNEVPSFYVPMV
KGVTSILPVLREGVL
EQQAQFTPLADPPDI
IPLLLPTPEEKKPPP
PPTLSRTPEVQSRVP
TDQKDSKPPEKATED
EAMGLGTPSEAIEIT
IKTLSDVPAPRRLAE
TLLELLPWALLINE
RIEEGERPDRAKGYD
WARVTKDPIHPYTKF
KLLVNFDPKILEVVR
ESKQATTPASRKSSK
LVKMKFLPVDDNFSL
NIETSNFPKLLLALF
HLDFLKQPLATQKDL
LNKLSMKPEPLFRSV
KDKIHHTTPDTPEIRQ
DAAHGYSRAIDMSN
KTKEKAQPLEDLAGL
ECQITGTPKIRVSWY
FGTLEVMPQNESETQ

ESEKSDFPPTVAEV
FVNKADFPKVRAKEQ
SGQLVVIPSDHLPHF
ATGRPWLPLHTLSVS
ADLGVSGPKVDIDVP
WKQVHNYPMFNLLMD
PPCLQQNPGTMQGVY
GSAGPVHPLVDPLTA
AHLFSWIPLSASITP
LKWNFTTPRDEYIEQ
VKKTDSQPTSVMLLD
EGCANRLPNGHVNFE
RGGKKFLPVLKEILD
STCSSTFPEELSPPS
RSKLEDDPLYTSYSS
SVVSQRFQNSIGAV
SLLALGSPMYSIITP
ASKGEMSPMVVETLK
HCLSFTIPRLPSSEE
IDKTCLSPTPTLEQH
TIFQERDPANIKWGD
NTDGLFFPVMSFSAG
KADIGCTPGSGKNYA
MTSTSLSPQGISTLE
KTVGVWSPSPPTCER
PRERSMWPLRKCPWK
VDYASKIPAQGGTNI
NRLCFLEPTSEAKKI
ETERCLQPLQMMALH
AVRMKIRPLVGQXXX
TLVVKGDPRDNRQPA
LLRRIEHPTAGNIEA
HVLLTLKPYAKPYE
DEEVLTDPKIQALLL
LISDTKAPKRQEMES
SSVTFEYPSNAVEDV
TSSWLVTPKSLGNVN
KVYDRYIPDLCVCN
CWYSQWTPAAPQCKA
SNGYKPAPLDLSDVK
LGVAEGSPQYKKWYF
IALTKLQPLLNKDSP
DTWVEHWPEAEQCQD
GYLAATYPAVGQTSP
GGEFEMMPLGVNKSP
LSAEAACPMFNFSIR
YLCSAVLPLLTRCAP
MDVSLHLPSRSSPTV
TIEELKEPEKNGIST
AIDRFNAPGAQQFCF
GGFQVLLPLVDQYFT
ILLTDGEPTVGETNP
KMLSGFIPLKPTVKK
EELTYSPYGREKDV
SLKFKEKPTDLETRS
DLGQGLMPVLEAWKA
SRLANRAPEPPPQQV
RTKKEGIPDARQATR
GCKEICCPVPDPKSV
FSHIDVSPGSAQVKA

IILLILCPEIIQDIS
KAHIQFKPTLSQQRK
MGNCGHKPEPTEVE
EKASKEAPVKGLLQT
LKNLLFNPSKPFSSRG
RGGKGISPPSFSSYL
SRTQWEKPQVKESKR
NSALDWWPKIDAVYC
GVQREDVPAADLSDQ
YRDRSFSPGSYERET
KVNSGAFPAPIEKSI
AIMRYGMPPQDAFTT
KEVKSTAPEATVECA
SEGNIDSPVSRFMDR
TLGEKAKPALDDLQ
GAAFSQKQPQSNALIG
SNQAELLPSKSVSLI
LRNDKDKPLPPLAR
EKSLSHSPGKXXXXX
GYYCLKVPLVVKRE
FYQEVANPLLSSVTF
ALLESLPDTDPVVS
EKCLAGQPKDTMRLD
GTSKAGNPIFYVAR
YSRIKYDPLFRMAL
TQKTVDGPGSKLWRD
EAERSGIPVTSPYQ
TNLKIKHPTYCYEMN
YAAFNNRPPSTWLTA
ICLAQNSPSTFHYVL

Supporting Information S3: The benchmark dataset used $\mathbb{S}_\xi(\mathbf{R})$ to train and test the model for predicting the possibility of carbonylation at Arg site. It contains 136 positive samples and 847 negative samples. None of the sequences included has pairwise $\geq 30\%$ sequence identity with any other in a same subset. See the main text for further explanation.

(1) List of the 136 peptide samples in the positive subset $\mathbb{S}_\xi^+(\mathbf{R})$

ASKLSKIRVVRKSIA
IIIQSYRMHVQKK
HCKAFKIRKHYLHLR
IHLELRNRTPAAVRE
LEELDRERCFLNEI
YEMHKMTRDPLNLAL
RPPVSGLRRRKPRAT
KTQRSPVRIPFMQRP
KQFFKDWRDKDQSDG
KSEYKSYRLRAQLYK
KSRDEGPRLGDAKLL
SLRKLPPRSEISSEK
RKSTEFPRKIREQEP
GSVTGTKRLRCMPAP
ELQDMAARQQQIEN
RKLANAPRPLKKRSS
ASSRAHRRHRRQAVF
RALLTAPRSLRRSSC
TMLLPLLRFPQVR
SIDSLKQRLNAVKE

EADEEKERILAQLRE
VADLEKQRDCSQDLL
EEEEELRLHQKEQ
IELLRKVREQVLKCP
LLAEVERRIRRGHAR
PDGENRARFLPGKDL
WERKQNLRPMPKKYH
RVLSGRWRLPLRALP
VSWGKLRKRVKGWAP
TLPKRVPRAGEARNL
EGGHFKLRVTISSNN
TLVEKEMRVTLAKLL
GDSRLKMRAELGEYI
REQEPTERPLKGIQS
ALAKHKERKMAVPMP
KDLGLHPRAVSTSG
CLEVVLCRVEGMTEL
IKGLTYLREKHKIMH
MQKLNQKRAELKLVV
RIPQLWKRVSWDSST
GYKRKVMRMLKRQVS
ALVPPWTRVYRVQRD
KCSEETFRFELGGGV
GAGSGLGRLLALQFA
SQDKMEIRSCLPKLL
VDKSGVVRVVEGDN
KERLQEVDRKGLQY
YVGKAATRLSILSLL
RSVFTVMRRQLEQA
QRGLTEKREELLSVP
RKQLIPRHTKTREK
LLEAEKERNKLSLQ
STEPLPGRKQVRDTL
RQLAIETRKTAAQT
LSHPKIPRCQERLLR
RDRPGDPRRKRSSDG
FKDITDMKRLSMEIEK
LKRSLMRERVLGPD
DRGHEELRKLESTLD
SGILRQLRQTVEATN
TAEDLRTRKSKLQEL
KAAAADGRGMLPKRA
PPSAASSRYSMRNRI
SRSYTRSRLASSHS
HIAQKLFRDGHFNPE
ETSLNKAREHLLRS
HVTKTRRRCKTVRVD
RLSSVFLRVRTNVGV
GQDGSRRGPQKRGV
PRVFPPRRPHTPAER
APYVTLRRGLNAESS
TSQGKLLRTILFGVK
IYKPKRGRPKSKEMP
ENELTFLRSQIAAIV
IANVFQNRDYQCDTV
LMEFITSRKRGPLWN
VVRPKDRRVGTSPSQ
RRSVRMKRPSSVKSL
PKTMPRVKPKTTPT
HFHTVIARRAGMAAS

RIKNPKARVTEVMKA
LFTQELARRLKGSGV
WDATEDLRISRTDSF
ELIRLTQRLRFHKVK
LPLVSWRRLEFQGE
FLQVETRRAGERLGW
LSYRSLRRRVRLRR
VGLGLPNRLRFFRQS
GLAARLQRQFVVRAW
SLRKGIPRTKSVGED
ETRQLLRTVKKEVK
AIVRQRERESHAAAL
ASPWKSARLMVHTVA
LGKRADQRKAKLGDS
IKSMAASRRAKLNES
QRMKALARALPLQPR
SASKASVRSISVEDK
EEELLNVRRELMVSF
AQLNIKERLIPPSFT
SDPIKACRPIKPPGP
HHVVSGLRENEYFF
VVESVLRAKEVTWY
LKRTKKPRPPSLKKK
KESLLQDRRQEEDQR
QEERLEQRLKREEVE
PEKENAVRDNKVYCK
EKLHLITRNLQEVLG
HGKQPSLRAAKEHAM
NCILDDKRPHVKKAT
NRRTLLVRPISKQDP
QADNPLGRSVLRKDI
GPPTGAGRGPQLQA
KVLKNNIRFMNHMKH
SRLSRHRRAVHGPPE
LAPLNDTRVVHAAKA
YCDLPEPRKPLEKAV
CALSHHERLKCDEWS
VKVPMMKRLGMFNIQ
YQLEGNKRITCRNGQ
HKSEVAHRFKDLGEE
LPKLDELDEGKASS
SLQKFGERAFKAWAV
EKTPVSDRVTKCCTE
CTLSEKERQIKKQTA
PLPKEPPRKDPPPKD
XXXXXXERIDGGITG
RGGEGNARTHGTPDL
VLGNDGHREVVEV
RGADYSLRAVRMKIR
QQARLHERGAAEMVL
LPKIETMREKVLTS
CTKPESERMPCTEDY
YLSLILNRLCVLHEK
TESLVNRRPCFSALT
VGVNGFGRIGRLVTR
AITIFQERDPANIKW

(2) List of the 847 peptide samples in the negative subset $\mathbb{S}_{\xi}^{-}(\mathbf{R})$

VTPHTQCRLKLLKLE

VLSFSETRAHQVVQQ
ELSKANSRFATTFYQ
EEAAGSDRASDLDSV
GSNGVDHRSYRIIRG
HSGASQHRIARPSRQ
DSLLGKNRKALAKGL
IVDEVHERDVNTDFL
SDVEAHFRAAHENTK
ELFVKGVREVDYDYC
HASCYGIRPELVNEG
ASPATVSRMGMVYIS
RVQRLGERVVDSGRS
RSLSRFERSARFDIF
PNTYDIHRLEKILKA
EKPGGKERGSSASHP
VTEASPWRATNPFLN
KKKKKKGRMKKEDNI
GEPKDVIRKDVRAIL
PHQLLLQRLQEEKDR
LSLSHFCSRPFCLFG
TTEAPVKRASLLGDM
QEECGYLRRHHQEEV
VSNTLESRLDLIAQQ
KKKMTKARLERFKLR
VYTTKSPRERAILGL
PASPISQRLPPKVES
GAQMEAARPLVQENP
TKDNEHKRSLTKTPA
LHVTDAGRKHIAIAW
INYVLESRLIGTEKF
SSASLIWRSEAEASV
KFTTEEKRFVESRDV
EGEQYLFRIRAQNEK
PPIYTAAREQTPFRH
IRGNEAGRFRDLITL
EWDKDVARKLGSTTV
TDDSGTYRAVCTNYK
ESKGPMTRRLLLHEV
LDLKETLRLRILSED
DELLRHHRDEQKPAT
ALNMLTWRAEQEGGM
PSSGLKKRPISRLQT
CVIQSYWRMRQDRVR
DVWIDVQRRWVYLEG
WLLAHCGRPQTECRH
AACVMPSRLKALGTL
HKQTKKRILIPSDI
SIQDWAKRMKALVEQ
QENCILLRLDNELGG
SQFNLSGRNPQKQAR
KSMSIVLRENHQKPE
LPEEIALRASDGPQL
EIEKLEFRVRELEQA
EKQVELYRNGQRILLE
AKKPAATRKSSKNPK
EGQEYSFRVRAVNKA
SISGCKMRLSYLSSR
RFRTLMMRRRFLSLK
TYDSYYSRSRSRSRS
EKETLLQRLTEVEQE

HWGQQQIRPIKSVIP
AVPPAKGRTVLEEKV
DLSTIQERMEELKGQ
SECGFCLRQFPRSLL
TPSEAHSRIFESVTL
RIQVFLARYSYNPF
KREKEVARKLEFDGL
PLKTDIPRHPMPFAA
CYIFPGGRGDSALFA
RDMEKVERQAVPQAN
LDLDELKRGIVVRA
SNQSVLHRWERKQNL
ECSKTSFRVANLEEG
MSTIEPHRQVAWKRA
YKDKRELRSKGYKI
LEAQLPRFQPRVLQ
SPQPPLSRAEAIKQV
ELEAHLCRMMKHSMD
EKKLEDARARCEGQE
TYSSAEERMQSEQIR
GLELSIDRFRLRKKT
SEIRITHRSHHFIPR
CSKDELERALHYLKN
HFIPITIGRLRKRAGK
KQLPQVPRPLQLFSA
CEPLSNKRNSNSVTN
HVHEASSRSHAFIT
KNPASSKRRLKTSLG
GPKLEALRAEVSKLE
WICKCVRCKSCGST
NCVSGQERGLGVL
KLNEMERQRTEIAR
NYSESLYRQAMEEAK
LAMLAKERLQEVDRK
EEKQEEERSKVDDL
SEPGANMRHIRKPI
HVEAVYSRRCVSFIL
QNQVGIGRPAELKEA
IHYLMLPRVREELID
YGLITHQRIHTGKPK
TGLETPDRKGGKTTE
KVVPPSMRRIRAQKG
RRELLELRRKGREEK
PLGLILNRFSADTNI
GNLSILSRQESSFFT
IQGKDVLRRLPSSIT
LNTSIDLRTNVLNDA
EKTINQQRIHARIGQ
KAKEQETRISEEITK
VLIPFKGRPPPTVTW
MALEETLRQYQAAKS
PGFKGEGREVDVNLP
RDLLLQTRLVNHVSS
DNKKKKQRTSSKKKA
WDDIITNRCFFLSKI
RKTRSARRRTQIIN
YIRISPTRAYNRPTL
LEEELPKRVRSRLSL
QLKSFPARLRQYASY
STGLLPGRGPGTSAP

VKAGDSSRLECKIAG
ATEISTERDLGQCDR
CREVGLQRRSVQLFC
EFKQKLCRAEQAFQA
KVNGCLGRNCKLPIT
HQAAAATREASSED
GAQMLAMRGEQLGVV
TEGMDDFRYACQSPE
IKKANMKRENKAYSF
FSCQRRTRFISLGEA
NSIEASLRCSVVPR
ALTDEESRKNWEEFG
EEKPEEERSAEESKP
SQELDVKRREAIYND
EKKSkkIRDKTSKKK
DVFLDSGRKTRSARR
KIDHELHRLQALLKH
LCPEGVHRFQWIRNL
QDQKVNIRVAVLPCS
GATTSTIRSSCLVGC
APMTPAARPEDYEA
KNLVQKEREELEEQEK
QFGGIDQRKIFTFAE
QERDRKFRLEEQKVR
VVLPLDERAFEKTLT
ALAVEGKRIGKVLDH
EFLELKYRLLSLLVL
AKWFKDGRELSADSK
RVRPLSKRETKEGGR
IDVNVIARPSAPKEL
EAYITATRQYVAQAN
AQSEAAGRTEPTGPK
CYFHSGPRGTHDLWD
VNLVSVGRVLWQWTK
ALHTEITRNKDSTLE
LQVNDHVRKVTDQIS
VTLQSAYRGMKVRKR
IVTEEHLRRAIGNIE
CPGMMLWRYPEPRVL
EDVHIKGRIIDTVAQ
ELVPPSFRGGKQIDS
KLQTAIHRVTLAQTA
VHSPDIYRVVVEGER
DIANVMQRLQDEQEI
KFVGDATRLTDKLE
GLTNPSLRSPEESTE
KGNEIVLRQDIMPTT
RSRSGKGRGLPKKGG
SGAGCSSRDPGPPEP
LEKIKAKRSDSGKYC
KFSSKYLRTHEGSEM
SKSIEKKRGRPPTFP
RKVFSPIRSEPRSPS
WYNVENWRTAVTSPD
HRLIAKSRELYEKTE
GLLFYSLRTLTTMAP
ESDSFCLRNIMEAPL
VKEVAAWRERYEDSQ
KLGKVNDRWQHLLDL
LGYWLEKREVNSTHW

ERDYLLERRDLAVDF
IIDEGLKRFIIEITF
AEAAHNQRAGAPGIQ
TSVPTTTPRATPILQP
PLDQTLPRQGPGQSL
IKALADEREAVQKKT
LINGGSERKSCFWKL
VADLGNIRIRFIRKN
AKISDLHRESVDHLT
EDVTFNKRRMKLEED
KKQQQCRPSISISS
PKVLQDYRKLKNTAE
IKKLEPSRIVKQDEF
GKPKVLARTKGSMLV
AWIPVPARREAEKVP
SLDWLISRLEAS
RLKAQEHRAEMEEKG
DEAKTSARDAALAYH
PTRRSSARRSQAGVS
LYYYNFTRTVISSGG
DTQTIWARTGYLGFL
NELAYFKRENQELMI
ETQIDETRMGYKPA
ALFPKGSRSVVPRDT
EVFTYSVRGLYENHK
PRARPRERDPGRRPH
NAALDNLKVVPCYS
ESTSQIERPLSQEPA
YDGPKNVRSDISDQE
PFTPVPPRGEPVTVY
MKKFEESRAELEKVL
GTIDGEVRLTGELDR
SETKDPLRVQPHLKK
LMVHVDKRITLAAFK
FFAKLNCRLYRKANK
QKVAEQERTAQQLRA
SEILSNIRSCRLQCF
PLPTVNERDTENHTS
EQEQLYLRSGVVSSA
AVVDVSDRAVPPSFT
LEYCEVQRPYSNYG
EDISKLNRAAKVVQE
QGETNKNRTKGGWQQ
EFITSRKRGPLWNHE
DMSMLEERIKRSKR
AKQFRAVRTTEGEEE
VKERESERNQC�FKP
DKINKTYRSQLSSEE
EGVKYQFRAMAINAA
GPPASNLRKQKSLTN
DVLLGASRTLSLALD
EEVMHTPRTPSCSAD
PGLPVEVRGSNGAFY
PGSTVLYRIFTVNHK
AQGALPERDASRGGL
PVWAAKQRVLCALNH
LEKRQMDRAEHKGEL
ITESDAQRTMYPGSC
ETPSYAKRRRLAGPS
EDEVQFLRTDDEVVL

AVVLTSYRSTAERKL
RSEGEKVRVGDDLIL
LHNSLLQRKSKLQSL
GWWVRNTRILRKIE
LLANAPERVVERRRR
RNGPAQTRVSSSSSH
SVQLTEKRMDKVGKY
EDTWKLGRNWGQSVE
SWIWWQLRTGLARDG
HCFHMCDRMVYFFI
STPSLTSRKIHGLSH
QSVAKMFRAVEEGLT
LSVKDAVRVDSGNYI
KIYNIEDRTRVPNKF
DADLEALRRKLANAP
NFLASKHRQPPEYNP
CEPNCYSRVINIDGQ
PPEPVDKRAKAPKAR
NKPIPALRVVEEKKK
SKLLKNWRDLARIT
IRNGVTKRGETLSWL
YTMESTDRNQTFSE
CNGQNTLRNIVHLSK
PLPIDLYRYDDVSGK
LRGLLSRGAWEQQI
EDELQLPRLPELFET
FKHIKDTRYMSSYFK
QRAAAMARTKVEIAN
QNSSVLDRLPQPAES
TSKSSDNRETPRNHS
KDTLMISRTPEVTCV
QLKNLKIRTNRIQRF
HQWIQETRTYLLDGS
QALLSKMRAIDLQIK
KKTWAKVRTAKFFIL
MSFKDAERGDDTSCE
VEEIMYLRQIYKQQL
TTAATVQRPGPGQTG
VGLWSMCRNTNRGTVG
XXXXMSARTPLPTVN
PHPSPEARAPLASAS
DTPPSALRGSQSVSL
HCSLDALREFFSTIV
STSYMHQSPGGPTK
LLIQYYRAYSIGRE
ESESNDHRSSSDFFE
ARFDIFSRYESMKAA
TNYILEKRETMSKRW
KAPSESARGPPGPTD
RKKKSKDRPSKLEKK
KVELSQLRVAKVTGG
VTSQFTTRDDILRDW
GHDEDNTRISSAGCL
SGSFVSSRARREKKS
HLFYKIHRNRYPVCT
GLCIEFFVRCRNDVAI
SLEKNLDRMKLDWVN
MTCLSIDRFIAVVHP
AETVPEERARGDPDS
NEHCPSKRDPKLYK

LQQEQLRALQGRQA
RLPTLPKRVPRAGEA
PDSMFGDRGEIIDPF
EGQEYYEREDEGYDEG
EVNAAWQRLKGLALQ
TFQTLPRASDAKNQ
FLALILQRTFLQASY
EHQMYEFRVKAVNEI
QVWETWPRAQELCPE
IVNLLKMRQGEEVFQ
QIHMQRRDAMAHR
SLSEEIQRRLATGM
VYTTAEQRPNAYIPE
RRVRETQRHISTVKY
AFYEKMGRMLGSAFP
PGAKVTIRASLGPLQ
TKLLKALVRKKTGG
ITLMDVTRNSVLSW
LVAVLLSRTWHVRRQ
YLTVTLQRPTKELHG
AAMFQSERKNPAPQC
QDHFQVARQNHFPQR
SPRRRKSRSRSPRRR
SSEKTQRMSLMRHH
KHKGTEKRESPSPAP
FLDVFLPRVTELALT
HFFPKSRIVRSLMP
AVQKTTFRVTRLHEG
GYTEVQFRPYRTDDF
DPVEHGQRHTATKRE
HEYEPYSRLKSDIKD
TKFQKLHRDMEEATL
PSAMPQSRSTESAHA
VWEPLIERVEGKRQW
PNVDYQFRVCARGDG
SWIADCARHHCSTP
VLESTTGRENDSQHY
ELSLNKQRKLNKSES
AWYMHGERAHYSHTM
SATLKNFRYHISLKT
YIKSELDRELQDRYV
LGLDEHNRVKVYRFX
LDTYNVKREAAEQWL
KAWKKHCRGEGKISK
VFKHGYERYNAMRAD
QLSEEQGRNLELQVL
IKVLEKKRAMFECEV
GTPVFADRLPEKMKT
DPSAPQPRATSGKD
KSLLDWLRQQADYSL
KAAQQHWRHELASAQ
LNKHTALRGEMSGRL
TCMKFYARVCRSGSG
PKKVEMQRSLPGSLL
AKCQVTPRRNVLQKR
FVELGVTRVGHMNI
IMEEAVTRKRVHEDS
EPIQFTKRIQNIVVS
LVIQKYWRRVLAQRK
LEAKQKARKKEERQS

LLEEALLRLLPAELP
YQTMLKGRCPSVSAP
LTKEKVSRLDRIVAE
KELADLARLHPTSCA
FNELEALRAESVATK
YLVLQQLRCNGVLEG
QMVTPPPRLVVGTYD
VPYFEQCRRDACRCG
EQEIVQKRTFTKWIN
KNQGLFHRVLRREEIS
AACCGSCRNVSCLFT
SLAKFAGRKLKDCGE
CSSLSPQRLCSKHMP
DAAAAGDRRPAPDTW
LDINVVIRQVYHLME
DDQEIQKRLAEQQDL
RYIRSALRQEKALSA
LEKAAAQRKAKLDEN
SGEAPGIRKEMKDVT
REEAEKQRVASENLR
VLQKCSHRLQELEKN
MEFAVNGRPLEPSQA
AREHSLLRSDRPAYV
SNYQSTTRVKPFICT
AVASAASRPDSTH MV
LKYQSLLRMFLSYCI
NSQVTFPRIQVTSLS
DALTDPSRKTQKCLQ
EVLFLSSRSKVFERA
DTIAHLERTRENMEQ
AEQKSLLRSVASRGE
TSAEQDNRF SNKQKK
PANAGNMRYSHSTGK
MVAVLVSRTVGPQR
NHHMEVLRELCEELP
LVNKDSTRRDSGAYT
AMVFMDVRMPKFKIY
LVSHVTLRLLKPECV
EKFGLEKRQGALELI
EGCEYEYRVYAENAA
YACGVEDRKSARLF
QPDVTGIRLLSLGAG
EELHKEIRLIGNESK
SFLKLTTRAQLGAKS
LRVIEMEREGKGRIS
QIYGQKGRTEILLN
IYNTKSSRERAALS
VELLFNTRYAKAIGI
YGGSYGGRGRGRRTG
EDTQYQFRVYAVNKI
NSQPVAVRGGGGKQV
TPSPPPRRRSPSPRR
LEFDGGSRGKGEHFP
YLMGGTYRCTYTRKR
MAVGMGERPEVLHLT
EGGKGEKRKRETDDE
ITMWLSKRLPQFLQV
NIVWKYQRYHFIMAY
LTASPSSRPVASPGA
XXXXMAVRQALGRGL

QAMPYNCRNNLAFPA
LFGKMIARAGRAGNL
LIVCFIKRSRGGKYP
AHEKRKERLQMLQTN
ASLQPKGRRDPPLLP
LQRQHLYLRQRHSAVI
ELKALAQRGIGYHHS
QDEWEIPRQSLRLVR
AALESLNRAVLAAMD
QFLEEEGRTLEDVAR
KDDIKSTRKLIKESLI
YVRVKTERKNFLAVQ
VNSTHWSRVNKSLLN
VDTKYQIRIQIQEKL
AGLSTDNRNVCLWDT
PRRASPLRTSRSRPH
MPSKFSCRQLREAGQ
GENQLLERRRLYHCA
TTIDDGSRCCFFTKSK
AAKVFGLRSRKLKLF
ERLKEPTRQALQQRL
VIFYDFLRGLEASWI
DEEASYLRFNRSIWK
PKNDGGSRIKGYIVE
LQVITTLRTAAKEME
SGEGDLRHLGLLGL
NDQLEEQRQEALQR
QEGSLARWPVAGQI
RQILRLLLRCTEND
DPVDSTLRDFCGRCI
PVYKTSARRGTLSTT
KTIGSPKRIQSPLNN
TNSVTAVRIQPLEDI
LIPVIGPRKNIKKQQ
ILVNTNLRALINKHT
WGTATVGRPRGPPKA
WLEAQEERLKTLOKP
GETPEACRQARSYLE
LRQCLAPRLPHSVTC
ADEIYELRVTGRTQD
NAEKYYGRKSPVGRD
LELESQKRLYEKNLT
KSEAKLSRKQVDSEH
SSLSSAGRPGPSEGG
KVFAKVLREEDSKDA
FIAKAFKRIKDSEFE
QHHRLESRYSSSSGG
LAVGKFTRTSGETTH
VKMCVGSRRMVDVMD
QRPSGEDRWQEKDQD
GSKKVTIRSPVQIRN
TSENTLKRVSLLAGF
QPGTFLLRFSESSRE
TDFWKTLRYLSLLYP
AEPGEGTRPATVGDS
PLSPPQHRYSEGERT
GCFLFISRSKPLKTL
VFLHQKPRLPKLFKQ
HSYSVLERFVEECFQ
TNDLTAKRLLHVKGR

KSLKAKFRKSDTNEW
LNELEILRNSAVSQE
EWKFKLFRVRSFEKT
KASAAMVRLRLYDIL
EYNAVKEREFHNQYR
MVTMGFARDEINDAL
INIDQFVRKYRAALG
DISALTLRISELESQ
SCFKDGVRRQPIESI
PWAKYVVREGDNVNY
LSFLDAYRNYAQHKR
SESEDEQRPRTRSAK
IGSDSQGRATAANNK
EEPGSSSRESVSKAG
GPIFTTARQLVHALA
GQSPFQQRKKKIKRE
DALEEQQRCISELKA
YKTLHDTRTHFLKTK
HSSEHAGRNGRNAAD
AAIGATPRAK GKAKH
SKRKVLGRRDSDDDH
INKEAQKRWTRREQA
SFMSLQLRELVIKSL
EHKTMASRAKVMADW
VKQKELSRIEEALQK
QYSFNSQRFAELLST
SLHYALARKGGAGGT
AHTKPLNRRSVLEKN
SLDAANARLMSALTQ
SGLDIFERINTSAFE
AVDSPAGRQQLLQRG
LVFHSITRSHAENLE
AEYTVVARNKYGEDS
NAQILSQRIEKAKCL
EDKGEPKRRGYLQVN
YGQIESVRFRLIPA
ENQQCLLREETWLAS
HQVESFIRKKLESLL
MKFKQKPREEQLEAD
ASAADTSRSLWGIQ
LPKVTLSRDGVPLKA
ETLGVLARAVGEMPR
EPRRLSSRRSVLTSP
SVVWLKDRGEVIRE
ILTLAWDRVDIAKNH
VYNENSNRQKLEHVK
FKIAGDMRATCPAFN
PSHGLADRVINCREV
AQQEELERRKRLEQQ
MEDKIYDRQVTKQSL
EEQPTSQRDRLSQVL
TNYVIELRDKTSIRW
QKKSASFTRTVSPGSV
EVLNEVNRRSLKCLA
QTAGVIDRWELLQAQ
RSKVDDLGRTPMSVG
REGITTKREQVQITQ
EASTSALRESCQAEH
PANGFLVRYLRRKLV
NNTDEMARLIRSVMQ

ASERKLNRRGSMSYL
YSASTPVRKPRPGQQ
EMDISADRVKVEGEL
WDLSKCLRIPASRL
SLALKNIRCRRGIHK
ALQAALARVVPSYMQ
GMYSEPLRQFRDSSV
MDGAAWDRRNGKLME
GSYLQFLRILFRMLI
LKHFIGQREEFETAR
LVSKDLIRKAGVGSV
GFKSHLIRLIGNLCY
AHEDISQRVAAENQD
EIEEDKARRILELSG
SMLQHLLRRLVFDVP
ISPPSPDRPPHSQTS
RSRGKEQRKLARQRS
EEAEAAARALARFAQ
TLTIQKARVTEKAVT
EFTQDLFRFLQLLCE
GAHKATLRIGQDGIS
ANLKMELRDALCAII
ENSLETLRFSISNLS
MFKWLVARINRALDA
HKFLTIPRLEELYNT
RYNERKGRSELIVVE
SVDVKSVRMGSIQRK
KGGSKLLRMKLSDFN
TGTPSDPRRRLRSYE
PEVFKYNRFLNPDGS
ESVKASERPLPPGKI
AYPICEWRYDACASP
PETIDTARLHYRNSW
RSALFALRYNILTLM
EPLKELFRQQEAVRG
GDEEQKLRFAFSIYD
YLMLDNKRKEVVHKI
RLDPVSGRLSTISSL
KPQDYIPRAPTFMLN
NSHHECIRKLLQSKC
TSSLSPQRSKLRIMS
QGLKIHQRFHFASAL
SSKPIKIRGPSHCAG
HANNVTIRESMQNDV
PGHFVGPRGPHPSQF
GLDPTQFRVHHYHKD
PSTNTESRKDVITIS
IDAIGTKRYDSNSGG
AESNSNMRCTCRIIE
VEVAATERTLLGFFL
YDYVHSVRGKVAPTT
SRALSHDRQLISQDA
GLPNNAERVLLTTQG
FDFPDLNRFLTRTLQ
GGKPVQNRELQGYES
LSLQVVNREIREENK
KAFVTLERFDQLYGS
EAVKYSERSLTKCIG
FGKKAANRSWQNVYC
TLRMRSHRVPCGQNT

QVSETLKRFBAGKVT
EAVNVCGRATAVVEV
EKALRSMRKAQVSPQ
EKVLSPLRSPPLIGS
LDLVSHPRATQTHVE
LISQINKRYKTKDDI
SSEKVAERKETEFFF
TAKPINPRPSLPPNS
EAKAELERKLSEKDE
ITKVGEEKGPLPKS
LVEETEERLVERISF
QIYSTGLRKGNLHNV
KHFPNIDREKAMSRP
SMSKGGKRKDSVWGS
WADPTGTRKLTWTYA
AQIADGFIRVDLAS
LRDWNLIRDAATLIL
AEAADNQREEAADNQ
VYQIKVHRKYTGEDF
ARLETLVRKAGEQQE
DASPGDKRLAAYLML
LSSYATARLMMNNEY
KLPVDFERSFQEEKP
GPLPYPERQKRARM
DSAKELQRSVEFDRE
TGTLVSKREVELEKN
GLFNKNPRHSSSENN
FNVPDEERCSFATVN
EREREREREERA
QQLNKDTRSLGEEPV
FSPLISARFGMGSM
KTKTDYTRIKSLSIN
SSPSSGQRSASPSVP
QHTTMATRSPALPPE
VQQVTFSRGTDGQPL
KKKGGLFRRGSLLS
GNFTDAERRKCEEEI
FLNPDPLRADGISDL
WFETQEKRLKQQHRI
QGYIIEKRRHDKPDF
SLWSNTVRCYLIYTD
FDFQAMGRIFVGLCQ
TPGGTISRARDLLK
DTDMDSLREARREDM
KKLRLKFRDVKCIDP
EPSFEATRSRNRYSV
SSGKSVARTSLQAED
VMLADSPREESNKRQ
LSCLTTSRSMTDKLA
KNYVIDKRESTRKAY
VWGGIWPRHRFSLQV
GRREAGSRAHPLRL
YIQLEVPREATISYI
DSVSEATRQDGVLR
NQLAEKVRLRLRYEE
ILKPMMLRRLKDDVE
VSPFPKGRGRPKRQM
ATDQEKSRKLHELV
MVLVSLPRIQSQRVQ
XXXXXXMRGAMELEP

FREEEQLRQEREEQQ
QNLPVQDRNLMLPDG
DEFTTLARDLYAFYP
DMAAHEERVNEVNQF
TAEDIQERRQQVLDR
KMAEESERRAKEADQ
ALHQKTLRVDVCTTD
LAAERHARLND SYRL
RLDDEIGRKVYMRDR
IKIQAMWRRYRAKKY
ESLHQNSRATLLYGK
QSKALTERLKLNSKR
PSLEGDLRGPDKLE
TFYVTKSRDALTETA
AVSSADPRAPGESPC
PISDGGSRVIGYHLE
PHQIGGIRFLYDNLV
GNMELEKRRQALMEQ
EEQQESARAVPEKST
PDLEKVVRYLAGCGL
EMEPLVPRVKEVKS
YNINTYARFCKCCRE
EKIDLEVRSLTCMY
LAKMFLNRINYWHLE
TILDMVERECGTIIE
KLAYYEIRYQFYKRD
VPTVTWLRKGQVLST
DMNKVKLRAIERSPG
LLDSPYARVHIAEDQ
GKMPLEERIQKIKEI
KLKPVELRELLNPVV
LQVVACTRGGMSRLF
YLQHLCYRNDKVKTD
DEVEVYSRANEQPC
EDFSQLLRNFGWLQ
LLFRGANRDVRNYNS
TKSEKLVRLHQEYQR
GPLASHMRWFIWLMA
QSVQETVRVRKVDVS
SLPCLSLRKLPPRSE
KEVEVAKRNLAQQKI
LSPGNSARLTPLRYD
TVGDSSARPARRVLL
QEEITEYRRQLQART
MPWKTCWRYLTSGGF
IVVEEKVRVPEEPRV
PSFSRQLRDVQETVG
KKFGGPGRMKQSCVL
TSLQKLFREVRIMKI
PPVETIQRTTARDPI
SQLLTSVRRMVLTLT
CKLAALVRHRVSLFG
TLFSNVQRVQGVSER
EVQYEIFRSLMYWMT
IELPDLGRFYKIRVW
AAEELLQRCISSALP
ELSHDNIRVKWFKND
VPDALNDRHPDVRKC
NNAENLFRAFLGELK
VIAMLGFRLLDAVKS

KNMLIHGRAMLLVGR
AQAGAKSRPKKREGV
DFEYKLDREFLKGCK
LDALVMDRVAFVKLL
VSIEAPKREPQPIKE
PIGYQCSRUYWSTTD
SANKENFRILVESVK
HQLTEEDRERLKEEL
EAAQLSERTAQEVRT
ECIQMKARLTQELQQ
AGPGLLPRKPPGLAA
NFPVHLSRIRRLRAE
KVDQFVTRFLLRETV
HYPFENKREFEDAFP
NNLHSGIRKLEDYLT
RNLWQSSRPLICLLD
IQSAPNVRWFQWFKAG
ISSPPACRSPSPVAN
GYPGGKARIIHKESD
DQRLHTTRSVMQDE
APPVTSARFPSWVTF
DKCNDIIRNKDDTAA
IEVPISGRPKPTITW
TEINAKLRNIIVLDS
VRQEQHKRLEDLRRR
ITDASALRLVDKAQV
SILLDFTRGSRGRKN
FHHCEQCRQYMDFTS
EYEMPLYRKYWPNHI
IRPRPPSRRAAQSP
RAARTLYRIELLRKV
VGGSGLPRGRRPPRW
MHHDPLRSMAYWIL
LCTVATLRETYGEMA
CAKQEPERNECFLQH
DDNPNLPRLVRPEVD
KYLVEIARRHPYFYA
ELLFFAKRYKAAFE
KASSAKQRLKCASLQ
FKAWAVARLSQRFPK
LLECADDRADLAKYI
MFLYEYARRHPDYSV
YSVVLLRLAKTYET
FQNALLVRYTKKVPQ
PTLVEVSRNLGKVG
CKHPEAKRMPCAEDY
CTESLVNRRPCFSAL
PIPQCPPRLDVQTIQ
WNPIEGERYLSFLRF
QFLEQAQRELAELLD
LNFTMNRHTGPAWN
CDCELQHRVEAIVAF
FCQEMKFRNKMVEYL
QEEQAARIIRNTTA
LVIEEQLRRAAYLNM
DDIKCLTRDLQASM
DMKADVTRLPATIAR
YLHLLTLRGSVLRVE
MKCSSMQRFGERAFK
GKNIIYVERQRPALGE

SKPEGTPRGPQVYTM
KLTGMAFRVPTPNVS
SLGKVGTRCCTKPES
GPLSLASRNRSQDSG
LKNVNNMRIFGEAAE
CQKGFVLRGSGVIHC
VVVKLLIRRPECFGP
CAKQEPERNECFLQH
TCKKFDLRVTIKPAP
KATLKNLRKQYRNVK
LVEVMMARRDDLFC
TENAIGSRKFLSLGL
YHKDLQTRATFMEVL
ANIHKEQRKFCLAAE
CSGSLVERRPCFSAL
YDDKAIERLLDRNQD
EHMPNDSRLKCLLDP
VLVFEQVRLLMKSYS
TEILKWLREILICRN
SFEVDPTRLEPSESL
NMGQWKIRAFYEHAP
FSKKCSGRWKTMSAK
EIMEACMRDIPTCKW
VNGILVSRGVKDMEL
TLGSTVGRLQEQLGP
GLAESGARYTEMPHV
PLPPLLARVGGNIEV
TYPGLSKRRLKPEAI
STLQTIYRLSKGRSL
YPVGTVLRVYICRPGY
GGITGNMRQEADR
EKETDWLRNEMNKDL
ANQDFTNRINKLKNS
KYLPGLLRSGFYDLL
GVVWVPFRGADYSLR
RIPPVAVRLQMSERN
LFLHGYQRFWIETEA
LAFDVGLREHATGYL
VCALGNSRVASALCS
ENAQTGGRKRGMSRR
VSLHLPSRSSPTVFR
LHKTIVKRRMSHVSG
YELLLKVRPEQLVKH
PMKYSCQRRARLITQ
VLVNSLHRIITNSAL
DTTVKKTRRRGQKAE
EKADMEDREKEDKIK
SCRSVSREINLKDY
WLISKLDRELESSGI
PAVNGTLRTSSYEEH
WVQAVVSRFDEQLPI
VPLVVFKEKEIARK
DLSWSMLRGCKEICC
KGDPPKPRGKMSSYT
NPDGSPARRVPVVTQ
IPITSSSTRNIRLYPD
MLQQLLRRLLVFDVPQ

IQQLEQRISASGAE
TSFSNYYRTWNVVVH
EAGGAGTRARSLWRV
GQPKDTMRLDETMLV
DDIAILARYMLMSF
FQNAILVRYTQKAPQ
AHTVVTSRVVNRADT
GDLYGAERIAELLGL
QTLWLWARPRAGGAW

Supporting Information S4: The benchmark dataset $\mathbb{S}_\xi(\mathbb{T})$ used to train and test the model for predicting the possibility of carbonylation at Thr site. It contains 121 positive samples and 732 negative samples. None of the sequences included has $\geq 30\%$ pairwise sequence identity with any other in a same subset. See the main text for further explanation.

(1) List of the 121 peptide samples in the positive subset $\mathbb{S}_\xi^+(\mathbb{T})$

HLELRNRTPAAVREL
PRKRPPVTQAAGALP
LLAKQHKTQRSPVRI
NEPEAEKTHLFAKQE
RKSLVMHTPPVLKKI
GSKRQLQTPKEKAQA
KDGSVTGKRLRCMP
DTEEADRTSSKKTKT
MPRRLTQTGKRKHGA
GTARRTGTPSDPRRR
NSKHLNGTITAKYTY
GKEMLEQTLQKVTEL
NELLKQKTIELTRAC
LDTMSKKTALDQLS
ASKEQGPTPVEKSKK
DLIQHRRTQDHKIAK
IEEELKTTKRKMNLK
VQKANPGTLAAEIRA
WIWVQLRTGLARDGR
VSAAQTTGTAPGAR
FQASLPLTRIDEEEA
LNDKHLKTLSTVFS
RPLKSQITVTRHDKR
DSKNSKKTNTEFLHT
ERVEQFLTIARRRGR
PDDRTARTLTLIAKV
RDLRFVRTAEILAGK
KDNIPPLTMKRIRER
KGITFIFTDSEIKDE
MHFRSLRTKLLMSR
RQPVTKNTRQYRVL
SEVLVQQTQIRIQS
FVQRRGHTVLKIHP
KAKKPAATRKSSKNP
MAVLEALTGVLRSRG
HSGKLYKTKSNKELH
VQSIKLITEGASKRI
YSAEWKSTVSRLGRW
GAFKAVMTSIKQLSS
RDKLKFTRPKVRVP
VKRGDIFTLEEELPK

QLIPIRHTKTREKVD
NEIVNIRTSLLNLVD
KQELEVELTANIQDLK
PKDEDERTVYVELLP
EKIRLAKTQQASKHI
EDLGRKRRTMLKIAT
EVAEKQATDVKPKAA
EKFKALYTLPRSVDD
ARIKAKLTQIRRYGE
SKGELLSTLLTKEKA
LTKLKAKTDNVVQAK
QWIRATATALERCSE
PLGAEKITGELEEMR
ISNVDVETQSGKTVI
LPDMSVKTPKISMPD
RSIRKSSTSSDNFKA
TPESKKATSCFPRPM
SVFLRVRTNVGVRVL
SVSVEKSTSSNRKNQ
TSPLQSPTKAKPKVE
SQGKLLRTILFGVKR
STAVGLVTKDPGKKP
LGKKGSTVGLVAKD
NYDKILATKKNLDHV
RAALDKATVLLSMSK
LLRAGYLTLYGIEAL
ETKETTTTNKQTSTD
TPKKPAPTPKEPAP
RTARAITTRSGQTLS
KNGKVYFTSDAGIAG
IALTTYETLRLCLDE
SSVGWDATEDLRISR
TEELIRLTQRLRFHK
NHFLQVETRRAGERL
QTSLIVATLKKMLPI
DVKSTAFTFRSSKEK
NKEKEMVTSLFCKLG
LRIHAHFTGLRYLLY
TSSPPRKTRRLSPSA
RLLRIAATPSCHLLH
PPKRAPSTTLTRSK
LRKGIPRTKSVGEDE
EPARWD TTLPTSPK
WKKLLEATELKGIKL
VEKPPKFTEKGNLEV
LRLLNKHTALRGEMS
ATRVRNITKKSSHLP
SYKLSATGSVVSTR
ITKKMDKTIPEGRIR
VARQTLETIRSVGY
DLKTIYQTGCQTSTV
ITKSSTSTIKDKDEL
VRVTGIPTPVVKFYR
IMKETRKTVPKIV
KKLSDISTVVGKEVQ
SSEPKECTYTIPKLL
VDVKFKDTVILKAGE
KILSNNNTSENTLKR
CLQTL DTKFVHFID

KPLKKKPTPVLLPQS
GISSPLTGKRQDSG
VLCIIQDTTNSKTVN
QLSKKLKTVLDQARQ
LEEIKERTATGLTHI
KKTILMVTNRRVLCI
RKIKVSNTLESRLDL
KGFTVKRTLVIHQRT
LLAPLNDTRVVHAAK
NETRESETKCLKELPG
DGTWSPRTPSCGDIC
RDSARQSTLDKELXX
AVSEHEATKCQSFRD
KEGYGYTGAFRCLV
SSLLEACTFRPXXX
LEGNKRITCRNGQWS
QKLEPLGTELHKNAK
CLLPKIETMREKVLT
KVGTRCCTKPESERM
TPVSEKVTKCCTESL
EKQIKKQTALVELLK

(2) List of the 732 peptide samples in the negative subset $\mathbb{S}_{\xi}^{-}(T)$

HGSIFSGTAAPRCEI
SRNKSGRTALMLACE
LPAIFEYTVVGEPA
SIAFQMPTIAKDGNV
YDINQIITAVMTH
GAAGLEGTAATAAAG
AREPPGSTAGLPQEP
KMMHIAATLIQRRFR
CPPGLYQTVPPEEHY
QNIPPSFTKCLKMD
SASAPSSTPTGTTVV
VSPRGMVTRSSPGAG
DEDDNMSTVMRLRTK
ARNGISPTNPTKLQI
RELQARLTLVGKEGP
NLKFQPPTLGPEPAA
SHRVGAATAGRLPAS
PAAASLSTATDGLAA
PKESMLKTTLTAFGF
YPEPRVLTIVRITPV
DSLPSPTIVSGDIP
RVNKVPVTMTRYRST
HLRKAAITIQSSYRR
RLLMASPTRKPEPQV
QYHKMYRTVKAITGR
KSKKRNSTQLKSRVK
KAKEDDKTLSKEPSK
GGGRNDITGRFTRHL
ENHPQWDTAIEGDED
DRWNSAFTRKDEIIT
SEPSDAITCRDDVEA
PRCAEHGTCRDGKCE
NGDGGCGTGGRNC
LCKAFVPTCIEQIHV
DFEVLMTAHGHLVP
IVYHRKVTDDISKIK

RSSRKICTIGIAPWG
VQGDSQGTPTSSQGS
YIVQKRETSRLAWTN
DRKILDDTEDTVVSQ
CRDELVRTTAQYDQA
QEKSPVNTKSLFKRL
IEELLSQTTNPDRFS
ATQPAAPTPTATITS
SKKDDFFTSFKISCQ
EWRRANHTPESCPET
PSAFYQQTLPNSHLT
MREEAERTRDELERR
GHMYMILTPSDIQIQ
SPQREVLTVPEANSE
KLESLVLTHLSRCDS
FSCGADGTMKMRILP
KPESIKVTTGDTCTL
VVKYRAGTSVKLRAG
LKDLLLNTMSQEEKA
SYSSLEETIEVKGAG
PHGGAMDTHFANMRS
KFTSITDTPEQVLAK
AQEERLKTQKPELV
NPYSLLDTSEPEPPV
ICESLEKTKQKISHE
ECGLGHRTVPLLLAE
SFIDGLATFQISGAR
SSAMESLTKHLFAIL
RKLDLSDTKSIRAF
PEAKCACTDSMGVPR
PGPPVNVTVKEISKD
VSPENLHTEEILVCG
VNIQLKGTNEYVPRF
PIAAVLATFVTHAYA
LESHMILTETLFRKI
RLTYTERTKSTITLD
LSRKLRETDSQLKT
GDKRRVFTFPCLSAF
VLDEDEETKEPLVQV
SSQEKVATLTSQLSA
ESVSSLSTNDFSIPW
CFIKLCITLNEGKSI
SICSARVTLREPPSF
KELNALETSSSAMDM
SSTCEPSTVAAVLSR
ILKAALITEENQQLS
NKYHWEHTGLTLREV
MRTQEDLTQGLLLID
DKEGRELTLEKPELK
HQYKCLKETIQKLSNV
QAEAVLKTQELKKL
LDCVLDLTMKIHNS
AKGDRAATLEEGNPT
LKGTQEITGDDRFEL
LVVFNHLTPPPPDEH
VSPLLSRTEFCTAPL
FGQRLDETVAYEQKF
KRLQEEKTQEKIQEE
PTGPELDTSYKGYMK
VTPEVKKTSFHVTNL

NSSNFMNTTNFQSLR
SASKHSPTETEESAK
VEGAKKVTVTELLAG
ENMNRSETEACFFIC
EVCQKSLTGYLEKKR
GLSPGSLTSLAPSTH
GEQLGVVTNWPPSLE
LIGPCCATANLEAKW
AELERLRTQLLSHE
GQTSMPGTLVLCLPQ
TLQRTGQTILPSLNE
VNSSVKRTQIKVTHL
MASFLYSTALPNHAI
TVAKELQTLHNLRLK
IARILKDTAIKSADN
GDGDLMMTSFERMLS
RIFADGKTWSYTYLE
DLRKVYGTVLSRHHH
ALGRDILTKTKQARE
AMMSVDETLMCSFQI
XMSLADLTKTNIDEH
AAGGPKLTKRGLAAP
SPAARISTSPIRSVR
FKGRPPPTVTWRKDE
AALECYNTFIGERTV
MAEILSGTESVPLTQ
LLAPVALTCGSDGSL
YEGWRIDTYLDIPLV
QQMCCVSTSIVSFVR
YEGGAVCTHARSLWR
KFHGVLTLCLEVVV
RMVYCSLTDQKAVY
SQRVNGLTSSKNSQP
CSLRPNQTEEGTTPP
HESQISFTIEGPLTS
AEAKPKSTCELYSSQ
SESPVYPTKFDSEKE
VEKLLDCTVIVDSVF
TVLKSSATFQSTVAG
KQQKEEKTQEAAYAQ
GVCVSEGTILHRRHS
LERQNLETFKDRMTE
IFESVHGTAPDIAGK
LGPADQKTGTPTPTS
KLCYDAFTENMAGEN
KKGASFQTVASLHKE
KDAYKVNTNLDYKKQ
VGKPGIPTGPIKFDE
QKSDDKVTLEERLDK
RDFVGQRTVTFSSLV
LEISEDCTYADV KAL
KNCREAFTADGDQVF
EPLPAKVTERHMQIT
ALMRSEETADLLAEK
IDHKEKSTEINHEIP
STERLKKTNEILKGI
CEESLSQTPPRVTGT
GPSSERATPAFHPVC
GPKQASFTDVRDPSL
KIQQLVNTLKRPKRP

ICELSFETEHILLQH
KKALLPPTVSLSATS
LHNFSIYTLLGKQVT
KDLVNRYTQNGSLDF
KGEDPLATDTRVSVE
LKANQVATGIRYNER
LQSHFIPTIGRLRKR
AFMDISATDLVLRKV
AFLRHKMTLISPIL
YLRNLPITAHPEVFG
LWEGKPRTYITEERA
IRILCCLTFLVKVKS
GYGSNKKTKHMLPSG
EPALVPGTPKAEDRM
GYHVINNTFQSLLGC
XXXXMWPTRRLVTIK
RFRHLKKTSTKEAVGV
KLAQLIATCPPSKSS
LKDSDEITEDDNIRM
GGEVIEDTYGAGGGE
PKAAKEKTVKKETKV
PPEVLDVTKSSVSL
HPSVMMTAGRCHTL
AVPAAISTSEAAPYA
VDRHREKTLRLLWKI
SLKSLILTALQRETE
RVDALERTLEQKNKE
AGGSLKVTLQSSDS
TLTAYIVTSLLGYRK
GKPVDGLTTLRNGTL
TKQSFSLTMSIEMPY
LVSKELSTWKERPAR
GEAGGGSTAAEEASE
IACDNIGTPLAVFSG
RPCDEDKTDSETGKL
RTSAPSPTALKLATV
RGQPRTRTRASVRGF
VENMILLTIQYLVRL
VMADDEFTQDLFRFL
NVSQDLDTIRSNINN
SRSKADYTSHLRSLV
KSRHSDGTEKNKLPS
SVPKVEGTLKGPEVD
KEEVPEPTPEPPKKQ
ADGLQGETQLLVSrk
NKVQLMVTDSLSNQ
ILYGPPGTGKTLLAK
CIEVVFVTKFLYSIL
EQSIWNVTVLPNSKW
GLNMCAPTDQDLITL
SLIKQIATKVHPPGT
HGREAKVTETARVPA
TDGSEIKTDEHYTVE
SFIWELITPTKDGQA
AAMRAFKTVTTKCSK
SDKFYKQTVNLQLQP
EIVFCAVTSNEQVKG
PPHLKPATEKLIVVN
EVKGAGMTEHYVTQL
CLKEIDSTLYKNLFV

SPNPDVWTSEQNPPY
EWPFLIITDLFLKSP
YEAQKRITQVFELEI
KAVVNEDTQGNVSQL
GFTFGTATLASGGTG
PSEAIEITAPEGSFA
AESGIRYTQMPHVME
DALCLVLTLMNGGDL
KSLQAVITNLTQGEE
LQPEPINTPTHTKQQ
GTLVSHVTLRLLKPE
VNVRRDSTGMPLWLV
MFDERIFTGNKFTKD
KVLKWNFTTTPRDEYI
DITENAATVSWTLPK
SSIQEITKANEEFQ
GSMLVSWTPPLDNGG
FLPLFKATINPQDHR
PRAEKEDTAELGVHL
CLSVLSSTSLRLHSN
QSLQLSTCDVESKR
HSADVHHTFRQLDRL
HQQALPGTHIPEEAQ
SAPYLLATSCSDEKV
GLVVKAGTTVRFPAI
ALYSRIGTAEVEKPA
IALSSSETTKHATNT
NRLVDYITKTSCHLA
AEAQPEATAKNLLHS
FFLYSKLTVDKSRWQ
CVSSIFWTQEVSQAL
ALQPSVLTCMNGGAG
YKDSRGLTPLYHSAL
EPKECTYTIPKLLEG
EALIKKLTQDNLAL
AIQIASATMPALSLN
QKEVEQQTGLSVFLP
LEEKAAMTDAMVPRS
NVIRSIQTDKREKYY
AGGHPLDTPHLPQEL
KVQIHHNTWLHFPGH
KAEPLAFTFSHDYKG
KLYIEAPTFDLQGSY
DCNKAAVTIQSKYRA
TILEPLFTESESKIF
RHLKESQTESTNAIL
GDGFYLPTAGAPGSL
LSLSVELTEAKLHHG
PSQFPSETAFLEEFQ
RVASNPYTWFTMEAL
PSPFDCSTDQEEKIE
TSESSIHTITPSVVN
AELENIATLCFKALE
EQVAWALTKFPCLQL
KNYSLKYTKYTKKDT
QHPAASPTHPSAIRG
QNAQVCQTNPEPPAT
IPVNEKDTLTYFIYS
XXXMAAATVGRDTLP
IILGNPATELSVATH

KDNSRDETFHFQCDC
YLDGNEITAIQKHGI
LFGDVGDTGERLLYN
KKAEAVATVVAVDQ
NLELRNLTVELEQKI
VEDNKRFTRIPLVQL
EALHELRTAEFEKTE
QDLRVLPTIDLSTMP
LADDLKKTVTIRAGA
AVNNYHKTNPQTQE
INKFAEYTHEKWAFD
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