

1 Independent test dataset
2 The positive dataset contains 50 malonyllysine peptides while the negative dataset contains
3 450 non-malonyllysine peptides. None of them has been existed in the training dataset.
4
5 Positive dataset

AC	Position	Fragments
Q9DD20	155	SVQSPRKVLQEVQRVL
P56480	133	DSGAPIKIPVGPETLG
Q8R0Y6	757	HEAHLRKLVEYCCQRGV
Q91Y97	14	LTPEQKKELSEIAQRI
Q91V64	285	EIQNLIKASAPESGLL
Q93092	286	QTSDESEKIHLDEKAFR
Q8CHT0	98	KFCYADKALLNRAIDA
Q91XE8	122	ALQSIEKERGLGTEVP
P00329	227	IADVINKDKFAKAKEL
Q91Y97	243	GHACTKKYTPEQVAMA
Q8R0Y6	767	YQQRGVKEGATLVCGG
Q91ZJ5	291	KTRADVKKGGTLTQYEG
F8VFN3	108	TEWLDGKHVVFQKVKKE
B1AXW4	93	WINTPKKQGGGLGPMNI
E0CZH6	63	LFGLDIKGRDCGDEVA
P06801	337	IWLVDKGLIVKGRAS
Q3UEJ6	330	IVALFPKDISRMRMS
P10639	94	EFSGANKEKLEASITE
Q8R0Y6	205	TYEGIQKKETAMINWD
P40142	314	SYKVGDKIATRKAYGL
P12710	90	KLEGDNKMVTTFKGIK
Q3UEJ6	639	KKGYEAKYEALPEL
A8DUK4	96	SELHCDKLHVDPENFR
P55096	260	MTIMEQKYEGEYRYVN
H3BKL5	261	QGLAKLKPAPFKDGGST
O35490	93	GNVVAEKISGQKVNEA
Q99J08	230	WKEVLLKHISPDQLPV
F2Z459	194	RAEHAQKAGHFDKEIV
P07758	292	SKELISKFLLNRRRRL
D3YXP9	107	GRADLKYIEACARRI
D3YVY3	58	TNDQVTKDAAEAIKKY
H3BJZ9	302	TLNLNELKRRGRRAYGV
P16858	261	DIKKVVKQASEGPLKG
Q8R0Y6	298	IQLEDGKMPASQFFK
P55096	289	NGNKREKQTIHSVFRK
E9PZJ8	573	GDMQLSKSEILRTQML
P08228	92	GNVTAGKDGVANVSI E
B1AU25	239	VRGNMVKLNDGSQITF
Q6P2B2	49	NFRVGGKIGCGNFGEL
Q91ZJ5	91	SIQPYEKIKARGLPDN
Q9DBP5	43	LLRDERKNPDSQYGEL
Q91Y97	108	GIVVGIKLDQGGAPLA
Q9EQ20	364	LITPQAKERVCNLIDS
D3YYI5	195	VDGPGSKLWRDSRGAA
D3Z041	644	DLLKLGKEAGLKPFEQ
A2AIT6	178	TPSVAKKIAAVLTDSF
P62082	90	EKKFSGKHVVFIAQRR
P09041	131	HVEEEGKGDSSGKKI
Q8CGC7	300	TPAEQMKAEEREQRTE
H3BJZ9	205	DDKGDKKTITVSQDEG

57
58
59 Negative dataset

AC	Position	Fragments
Q8VC30	148	AFTVLKKAGRRGLCGT
P38060	137	SELFTRKNANCSIEES
P63038	180	ISANGDKDIGNIISDA
E9Q133	153	FEENGRKEIDIKKYAR
O35129	97	SSPTGSKDLQMVNISL
Q99J08	321	GFGIFLKTGMGERQRA
D3Z041	357	LLMDDLKVLQPTIFPV
Q9DBP5	173	EEMGKVKKIDASKSVD
Q9D0F9	219	SGPNRLKIRIDAMHGV
O88451	153	MLPLVRKARGRVVNIS
P61358	107	FRDPALKRKARREAKV
Q8VCW8	349	EAI SREKGTLLYGTPT
F6SAC3	151	WFLEAAKDPSAVAKHF
P52792	172	NWTKGFKASGAEGNNI
G3UW86	286	DRLEELKMQNIKQVIE
P50247	388	GVHFLPKKLDEAVAEA

77	P62702	71	CMQRFIKIDGKVRTDI
78	Q9JLF6	565	AAAHGSKPNVYATRDS
79	P58252	330	DSEDKDKEGKPLLKAV
80	P63038	387	TTSEYEKEKLNERLAK
81	P30115	195	SNLPTVKKFLQPGSQR
82	Q9D8N0	275	ALAAEPKAKDPFAHLP
83	Q922D8	228	VKGEWIKPGAVVIDCG
84	D3YWR7	99	IGYMAKGAHVHQLCQS
85	B1AU25	469	NMTGAAPYWHQSMFW
86	P09411	17	KLDVKGKRVMRVDFN
87	D6RHN2	69	LPMPYLKDELHHSWGN
88	P58252	688	GFQWATKEGALCEENM
89	P19096	802	FLTNLGKVHLTGINVN
90	D3Z1U3	110	THTLVEKINYTGRFLP
91	P97352	39	LNINEFKELATQQLPH
92	P24549	128	DLGGCIKALKYCAGWA
93	Q9CZX8	41	DTVKLAKHKELAPYDE
94	Q5SXR6	1167	LQMARKKARESIVETE
95	P24549	363	LIESGKKEGAKLECGG
96	P07901	632	MGYMAAKKHLEINPDH
97	P19096	1545	WVSSPLKHTQPSSSGA
98	J3QNG0	316	KQGLGLKFAELVYTFG
99	D3Z6F5	191	GTDEKKKLYCIYVAIG
100	F8WIT2	601	PLFFADKLYKSMKGAG
101	E9PZJ8	57	VKFLNEKLEKNKMQNI
102	A2AQN4	67	FWGNIAKEFYWKTACP
103	P63017	423	NTTIPTKQTQTFTTY
104	J3QNG0	400	INSLRLKEYHRLQSKV
105	Q8JZR0	536	LPNGTLKIVDRKKNIF
106	Q8VCW8	339	SPSFNGKKALEAISRE
107	Q8CHT0	129	RAQVFLKAADMLSGPR
108	Q64459	116	PVGIMSKAISISKDDE
109	Q5SXR6	100	IFNIEMKSKMKAHTMT
110	Q8JZR0	517	TQEVLDKDGWLHTGDI
111	D3Z3F7	363	DYERIHKKMLKPAFIF
112	Q3U2G2	800	PKKEPKHAEQNGPVD
113	Q3U367	340	KQTQKIKLGDPLEDT
114	P97872	347	DSVKVVKNKVS LYKVV
115	O35490	327	LPPASEKHGWSWGLD
116	Q9D0F9	24	GTSGLRKRKRVFQSN
117	Q8BH59	370	VGELMYKNSFDCFKV
118	D3Z3F7	262	FNTVTDKKAIALGFAF
119	G3X982	99	EGIGSTKTRIHVPQER
120	A6ZI44	67	ALTPEQKKELSDIAHR
121	O88451	72	AEQLRNKTSDRLETVI
122	Q9CZX8	122	DQDGRKLTTPQGQRDL
123	P24549	255	QVGKLIKEAAGKSNLK
124	E9Q509	278	PEGRGIKIISKIENHE
125	P28271	852	RMTVQIKLDTGKTFQA
126	A2A974	366	TWNDLDMKMPYTTMCIK
127	P05201	318	SDPELFKEWKGNVKTM
128	Q3U2G2	329	SVLEQSKLKKEDIYAV
129	Q9DCD0	375	RSVFLGKIKDAFERNP
130	Q9EP89	283	ARCRSAKPGKKKNDFE
131	Q9D6Y7	212	HQQYLKSNPDGYCGLG
132	O09173	304	FTVLTAKSLRPGVAIA
133	G3X982	860	GFMNNGKIKAAADIQLY
134	P19096	1386	LHLVGLKRSFYGTALF
135	Q62446	70	NHLFESKRFGKTETIS
136	P58252	366	SPVTAQKYRCELLYEG
137	Q8C196	942	NIHPWVKQIDTLAAEY
138	F8WIT2	99	LAYCDAKEIKDAISGV
139	Q8VC30	372	AGGVTSKQMALVLDRI
140	P24270	430	QCAVDVKRFNSANEDN
141	Q8VCR2	271	ISLILEKGPGFSSKHP
142	O35215	110	EAWQIGKKGTVMTFLX
143	Q9DD20	33	CWQPICKTYFPYFMAM
144	P19157	55	LYGQLPKFEDGDLTLY
145	B1AU25	350	SNWTEKVKREGVKVM
146	Q3V117	948	AAKMFSAFDSGIIPM
147	P10854	6	XMPEPTKSAPAPKKGS
148	A2AQN4	669	NAPGLPKTRSGKIMRR
149	P19096	1780	GMAIFLKNVTFHGILL
150	G3UW86	167	ATLRETKESTRREEFVN
151	Q9D8E6	106	RMFAPTKTWRRWHRV
152	Q3UPL0	518	GPDVALKDSQVAQSD

153	E0CXN5	217	EMIAFAKLFCSGTVSS
154	E9PVP0	286	LAPKAMKKMYKACIKY
155	Q9DBP5	150	NRESLEKRIQTYLEST
156	P16858	257	AKYDDIKKVVKQASEG
157	P62754	188	PRVLQHKRRRIALKKQ
158	Q5SXR6	86	IALKGIKDSGKTLQIF
159	Q8VDG5	115	GPAQSGKLSLEAEENA
160	P62301	93	DLYHLIKKAVAVRKHL
161	P40142	603	KPAELLKMFIDKDAI
162	P19096	235	VAVLLTKKSLARRVYA
163	P40142	499	KVVLKSKDDQVTVIGA
164	Q3V117	355	NVAATFKGIVRAIRDY
165	Q922D8	175	VVGRSKIVGAPMHD
166	F6SAC3	122	VNRVLDKMKSFQCQLT
167	Q3V117	178	HAPEDKKEVLASFISG
168	P07901	357	DLFENRKKKNNIKLYV
169	P56480	350	ERITTTKKSITSVQA
170	Q3V117	1017	EKITTSKKNLILNVD
171	P06801	330	KENARKKIWLVDKGL
172	E9PZF0	250	EIHLWFKPEELIDYKS
173	P05201	207	PTPEQWKQIAAVMQRR
174	D3Z492	349	LESCCKAEELGRGIA
175	A2ANX6	199	RDHKVKKALGNLGRD
176	E0CXN5	259	AFARTGKSIEQLEKEM
177	Q91V76	244	LHFYEMKAPLVCLPVF
178	Q8BWT1	212	IEVKTKKGKQTMQVDE
179	P19096	1516	FQLEQDKPKEQTAHAF
180	E9PZJ8	48	DFGLTWKKIVKFLNEK
181	Q9D0F9	457	DRSFVKGQFSANDKVY
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183	A2ANX6	312	KTQTEKKKLRDVFCKG
184	Q93092	7	MSGSPVKRQRMESALD
185	Q8BMS1	166	IATKDRKTVLGVPEVL
186	P48962	171	FKSDGLKGLYQGFSVS
187	J3QNG0	50	FEEARKKALKLGAKKV
188	G3UWE1	148	PLRNIFKNCTYYWGFA
189	G3X9Y6	179	LEKILNKPGLKYKPVK
190	D3Z563	48	SKESAMKTYVEKVDL
191	E9PZJ8	861	GRPQFDKFGEGIIIT
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322	P97494	475	NMKVAQKRDAVLQGMF
323	E9PZJ8	1630	LHERDRKTVEELFVNC
324	Q5SXR6	250	NQPFPKKAVDVFFPPE
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331	Q8CGC7	581	NITKIHKNDGKITSL
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372	Q8C196	42	IRLLSVKAKTAHIVLE
373	Q3V117	562	MADAMKKHPEVDVLIN
374	H7BXC3	137	VTGATCKELASQPDVD
375	Q91ZJ5	184	YNHCRVKIYTFNQSRV
376	P05201	236	ASGDLEKDAWAIRYFV
377	Q8BP40	383	PRGCPDKLCLDKFLN
378	Q6P2B2	8	DHSNREKDDRQRTTKT
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380	F8VPN3	137	RNGKTSKKITISDSEQ

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KMINQDKLEKERNDK
QVLRIRIKNFERLNSDF
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VKSSHAKCRTSIECLP
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KSTPRPKFSVCVLGDQ
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VNSPHLKPAWVLDRAL
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AREEMAKRYVDSQRHT
IQKAVKNFTDVHPDY
LDKLDVKGKRVVMRVD
HLRDVLKVQEQLKYE
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KVGELVKHLKPGDRVA
WELIKEKLILPYVELD
GVAVALKQAMTTEFKI
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VRELEKKFSGKHVFI
FIGPERKLEQGNVEEA
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KSYLLEKIKEHKEKSLD
EAFRGLKLEETYTNKD
NLQELQKWLKKEPGAY
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PWKRFEKNGIKHVHAF
TNEVGLKQADAVYFLP
SKDSVPKLVADFMACK
MASESGKLWGGRFVGA
KMYDAAKLLYNNVSNF
EEVADLKLKRSKLHEQ
AKEGFEEKISKGANPVE
CQALNRKTSSKVAQAT
IHTAFLKAMLSTGFKI
KYDLYGKDMKERALID
EELLYFKAKGGGALVE
LRQPVGKIFFAGTETA
XMVEIKKICIGAGYV
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457	Q9DCD0	184	GAGHFVKMVHNGIEYQ
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459	E9PVP0	166	HDIEYRKKWDSNVIET
460	Q8VC30	463	AAAQPLKAKTDLPTWS
461	P00186	211	GKNFPRKSEEMLNIVN
462	Q9JLF6	443	WNCWWMKRPDLPSGFD
463	P62301	78	LRILKSKGLAPDLPED
464	H7BWY3	271	ECHSNIKCCDLCMCVC
465	P19096	55	KRSGKLDLTKFDASF
466	Q8C196	1029	DFDECDKLYFEELSLE
467	Q9DBM2	673	LPTVLEKQLKYRQNP
468	G3X982	889	IEYALLKLENAYKIPN
469	E9Q800	227	EELEKMKTIIEDAKKR
470	E0CXM2	69	ILQGLDKVAEEWAQGT
471	Q8VDG5	264	NILESISFVIVTKD
472	Q3UEJ6	502	MYNR IKKDPKKFFVPR
473	P21981	414	EDGSVLKSINRSLVVG
474	Q8VCN5	211	CMCSATKYMNGHSDVV
475	P63017	102	NDAGRPKVQVEYKGET
476	Q8CGC7	974	KENKSEKQNKPKQND
477	P07724	152	AMCTSFKENPTTFMGH
478	Q3UPL0	120	VIAQKDKHTGPVRALD
479	P09411	146	VKAEPAKIDAFRASLS
480	P37040	56	EIPEFSKIQTTPAPVK
481	P21981	429	GQKISTKSVGRDDRED
482	Q8JZR0	502	KGNNVFKGYLKDPEKT
483	P21981	273	HGCQVVKYQCWVFAA
484	Q9CXW4	154	TGCI GAKHRISKEEAM
485	P55096	174	QAFTYYKMGNLDNR IA
486	P42669	272	FGHTFCKYSEEMKKIQ
487	Q8BMS1	620	GSVELLKQMVSKGFLG
488	A2AL20	77	ERVVHAKGAGAFGYFE
489	P26443	477	QESLERKFGKHGGTIP
490	Q91ZJ5	244	TFIEEGKEYIFVSNID
491	Q8C196	1222	SQGAIEKVKDATRKIA
492	D6RHN2	89	CFGDSTKSRNKLLILPG
493	D3YWR7	72	LATKHLKEGGLLTLAG
494	P06801	525	QDAYKEKMATVYPEPQ
495	Q3UPL0	470	SQTEFEKNVWSFLKVN
496	D3YZ68	129	FEAGISKNGQTREHAL
497	Q64374	253	SCCFGGKDYSEMYVTC
498	Q9CZX8	77	GVGSMTKIYGGQRNG
499	F8VPN4	1262	CGTWMDKMGESDRARN
500	A2ANX6	241	FVNYPRKIGAVGRANY
501	F6WHQ7	187	ATP IFSKMAHWSNKXX
502	P62754	195	RRRIALKKQRTKKNKE
503	Q8K4Z3	91	CATAIAKAYPPTSMSK
504	Q5XJF6	45	KNYDPQKDKRFSGTVR
505	Q8JZR0	616	CKNQCVKEAILEDLQK
506	E9PWK1	61	TSDEEIKDLHQRIDRF
507	G3UW86	573	QHNC SIKSVASTYSEF
508	P40936	19	EKEFTPKDYLTYYYSF
509	Q4LDG0	592	VPGCEGKVGMAAVKLA
510	Q91X83	266	AGVTGRKIIVDTYGGW
511			