此电	◎ > 本地磁盘 (C:) > ProgramPFind > pLabel > bin v ひ 2 提案"bin							
순	~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~	修改日期	类型		大小			
8	] aa.ini	2010/4/1 17:38	配置设置		2 K	B		
W	AniGIF.ocx	1998/12/5 7:18	ActiveX 控件		168 K	B		
	AniGIF2.lic	2010/7/8 15:55	License		1 K	В		
8	] enzyme.ini	2010/4/1 17:38	配置设置		1 K	(B		
d	🖁 MassConfig.exe	2010/4/1 17:38	应用程序		112 K	(B		
	MFC71.dll	2003/3/19 13:20	应用程序扩展		1,036 K	(B		
	🗟 mfc110.dll	2013/6/9 19:53	应用程序扩展		4,318 K	(B		
w.	🗟 mfc140.dll	2019/7/19 12:37	应用程序扩展		4,646 K	(B		
1	] modification.ini	2019/12/27 20:37	配置设置		153 K	B		
	] modify.ini	2013/11/29 14:36	配置设置		145 K	В		
	svcp71.dll	2003/3/19 12:14	应用程序扩展		488 K	(B		
4	svcp110.dll	2012/11/6 2:20	应用程序扩展		523 K	(B		
ter all all all all all all all all all al	svcp140.dll	2019/7/19 12:37	应用程序扩展		440 K	B		
w.	svcr71.dll	2003/2/21 20:42	应用程序扩展		340 K	В		
W	svcr110.dll	2012/11/6 2:20	应用程序扩展		855 K	B		
1	NL.ini	2010/4/1 17:38	配置设置		1 K	В		
	🖉 pLabel.exe	2019/12/24 19:30	应用程序		2,588 K	B		
	] pLabel.ini	2021/6/15 14:39	配置设置		1 K	B		
	PreTolerance.txt	2021/6/15 14:30	文本文档		1 K	B		

1. Open the pLabel installation directory. Go to the ./bin/ directory. Find the modification.ini file.

## 2. The example of adding a custom modification

First, change the total number of modifications in the first line.

## For example:

"@NUMBER\_MODIFICATION=1609" to "@NUMBER\_MODIFICATION=1610"

Then, add self-defined modification by imitating previous modification to the end of the file.

For example: name1610=galactosylation[K] 1 galactosylation[K]=K NORMAL 178.047738 178.140000 0 O(1)Hex(1)

🧾 modification.ini - 记事本	
文件(F) 编辑(E) 格式(O) 查看(V) 帮助(H)	
pyrophospho[T]=T NORMAL 159.932662 159.932662 1 176.935402 176.935402 name1607=sulfo+amino[Y] 1	H(2)O(6)P(2 ^
sulfo+amino[Y]=Y NORMAL 94.967714 94.967714 0 H(1)N(1)O(3)S(1) name1608=thioacylPA[K] 1	
thioacylPA[K]=K NORMAL 159.035399 159.035399 0 H(9)C(6)N(1)O(2)S(1) name1609=trifluoro[L] 1	
trifluoro[L]=L NORMAL 53.971735 53.971735 0 H(-3)F(3)	
name1610=galactosylation[K] 1 galactosylation[K]=K NORMAL 178.047738 178.140000 0 0(1)Hex(1)	-
<	E. ▲

- R pLabel 2.4 MS/MS Labeling System F\EcoliN15\02N1403N15\MG1655\_3N15\_2N14\_01\_090731\_rep1\_01.RAW\_out\2015\_07\_31\_10\_23\_34\2015\_07\_31\_10\_23\_34\_pLabel\inputFlLE1.plai P 63 ? , Li OL. 00007 800 000 0077900 CIELP MG1655\_3N15\_2N14\_01\_090731\_rep1\_01.1462.1462.2 Seq: GSALINDKR Mod: 6,Deamidated[N] 5 5e+002 < 8-2+ > All 8 + 8 Modification 2 Relative Intensity (%) Modifica 8 N-term 1 2 3 4 5 6 7 8 9 8 4 Deamidated[N] 8 20 2 Can htd/Ns-... eth/su/ordet/n ipercondet/i iPercondet/i iPercondet/i iPercondet/i iPercondet/i iPercondet/i iPercondet/i iPercondet/i miTRAQB/ Main Info Ion Type Select Ion Mass Ion M/Z Deviation Statistics Normal/Cross-Link SEQ GSALINDKR Display Match Type 🛛 Highest 💌 CID/ETD Show Info Normal Precursor Info MH+ -974 523546 Peak Width CID Show Peak Mass () XLink Update Charge 2 O ETD Show Neutral Loss XL-Reagent 2 🔹 Mass Deviation[Da] -0.002971 Possible link Show AA Sequence Immonium Ions Reset SCRL Matched Intensity = 31.56% 🛃 pLabel 2.4 - MS/MS Labe liN15\02N1403N15\MG1655\_3N15\_2N14\_01\_090731\_rep1\_01.RAW\_out\2015\_07\_31\_10\_23\_34\2015\_07\_31\_10\_23\_34\_pLa ng System F:\E P ? 1 , di ti ti ti ti FALG 800 000 ۵L OPTIOD 00007 000 MG1655\_3N15\_2N14\_01\_090731\_rep1\_01.1462.1462.2 Seq: GSALINDKR Mod: 6, Deamidated[N] 5.5e+002 < 1<sup>2</sup> >All 8 + 8 Modification 20 Intensity (%) ۵۵ Modification # 0 1 8 N-te G Relative 8 9 Deamidated[N] 8 R C-term 10 8 10 Cancel OK 600 m/z Main Info Ion Type Select Ion Mass Ion M/Z Deviation Statistics SFD GSALINDKR Display Normal/Cross-Link SEQ GSALINDKR TOL 0.5 Da 🔹 Match Type Highest 💌 CID/ETD Show Info O Normal Precursor Info MH+ Threshold(%) 1.0 Peak Width 974 523546 Update CID Show Peak Mass XLink Mass Measurement Monoisotopic 

  Decimals Charge 2 C ETD Show Neutral Loss XL-Reagent. 2 • Mass Deviation(Da) -0.002971 Possible link Show AA Sequence MH+Deviation Da Immonium Ions Reset Matched Intensity = 31.56% SCRL
- 3. Save the file and reopen pLabel. You can add your modification on "K".



## NOTE:

- 1. Please remember to change the total number of modifications.
- 2. After saving the modification.ini file, you need to open the pLabel software again.

## BTW:

If you're a user of pFind or pLink, you can add custom modifications using the user interface provided by pConfig.exe. Then, copy the modification.ini file to pLabel installation ./bin/ directory. Or, use pLink's own pLabel software directly.

Databases	Modifications	Quantificatio	ons Enzymes	Amino Acids   Ele	ments			
Search								
Name		Mass	Composition	Position	Sites	NeutralLoss	Common	-
Acetyl[An	vN-term]	42.0105	H(2)C(2)O(1)	Peptide N-ter	m ABCDEF		True	
Acetyl[K]		42.010	H(2)C(2)O(1)	NORMAL	к		True	
Acetyl[Pro	oteinN-term]	42.010	H(2)C(2)O(1)	Protein N-ter	m ABCDEF		True	
Amidated	[AnyC-term]	-0.9840	H(1)N(1)O(-1)	Peptide C-ter	m ABCDEF		True	
Amidated	[ProteinC-term]	-0.9840	H(1)N(1)O(-1)	Protein C-terr	n ABCDEF		True	
Ammonia	-loss[AnyN-term	C] -17.026	H(-3)N(-1)	Peptide N-ter	m C		True	
C+12[Any	N-term]	12	C(1)	Peptide N-ter	m ABCDEF		True	
Carbamid	omethyl[AnyN-te	erm] 57.0214	H(3)C(2)N(1)O	(1) Peptide N-ter	m ABCDEF		True	
Carbamid	omethyl[C]	57.0214	H(3)C(2)N(1)O	(1) NORMAL	С		True	
Carbamyl	[AnyN-term]	43.0058	H(1)C(1)N(1)O	(1) Peptide N-ter	m ABCDEF		True	
Carbamyl	[K]	43.0058	H(1)C(1)N(1)O	(1) NORMAL	к		True	
Carboxym	ethyl[C]	58.0054	H(2)C(2)O(2)	NORMAL	С		True	
Cation_Na	[AnyC-term]	21.9819	H(-1)Na(1)	Peptide C-ter	m ABCDEF		True	
Cation_Na	[D]	21.9819	H(-1)Na(1)	NORMAL	D		True	
Cation_Na	1[E]	21.9819	H(-1)Na(1)	NORMAL	E		True	
Deamidat	ed[N]	0.9840	H(-1)N(-1)O(1)	NORMAL	N		True	
Deamidat	ed[Q]	0.9840	H(-1)N(-1)O(1)	NORMAL	Q		True	
Dehydrate	ed[AnyN-termC]	-18.010	H(-2)O(-1)	Peptide N-ter	m C		True	
Dehydro[(	<b>[</b> ]	-1.0078	H(-1)	NORMAL	С		True	
DiDehydro	o[C]	-2.0156	H(-2)	NORMAL	С		True	
Dioxidatio	n[M]	31.9898	O(2)	NORMAL	M		True	
	Add			Delete			Save	

Modification Information				
Name:	Oxidation[M]			
Composition:	O(1)	Edit		
Mass:	15.994915			
Position:	Anywhere v			
Sites:	Μ			
Neutral Loss:	63.998285;			
Is Common:	✓ Common			

Apply