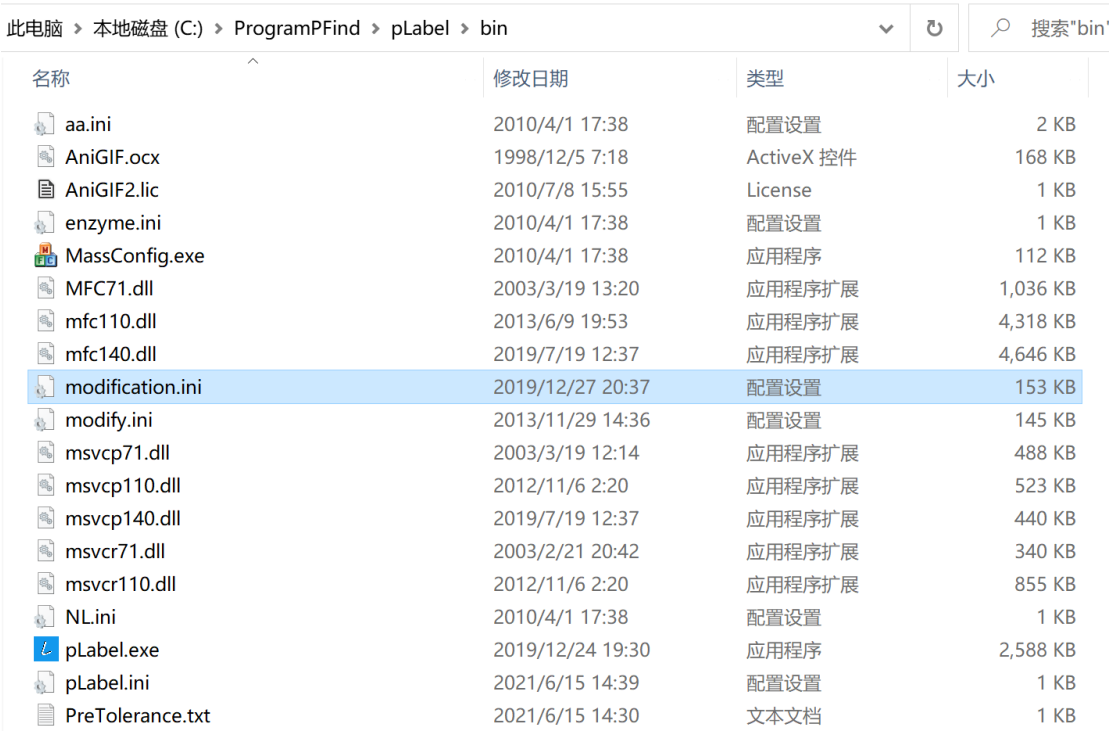
1. Open the pLabel installation directory. Go to the ./bin/ directory. Find the modification.ini file.



名称	修改日期	类型	大小
aa.ini	2010/4/1 17:38	配置设置	2 KB
AniGIF.ocx	1998/12/5 7:18	ActiveX 控件	168 KB
AniGIF2.lic	2010/7/8 15:55	License	1 KB
enzyme.ini	2010/4/1 17:38	配置设置	1 KB
MassConfig.exe	2010/4/1 17:38	应用程序	112 KB
MFC71.dll	2003/3/19 13:20	应用程序扩展	1,036 KB
mfc110.dll	2013/6/9 19:53	应用程序扩展	4,318 KB
mfc140.dll	2019/7/19 12:37	应用程序扩展	4,646 KB
modification.ini	2019/12/27 20:37	配置设置	153 KB
modify.ini	2013/11/29 14:36	配置设置	145 KB
msvcp71.dll	2003/3/19 12:14	应用程序扩展	488 KB
msvcp110.dll	2012/11/6 2:20	应用程序扩展	523 KB
msvcp140.dll	2019/7/19 12:37	应用程序扩展	440 KB
msvcr71.dll	2003/2/21 20:42	应用程序扩展	340 KB
msvcr110.dll	2012/11/6 2:20	应用程序扩展	855 KB
NL.ini	2010/4/1 17:38	配置设置	1 KB
pLabel.exe	2019/12/24 19:30	应用程序	2,588 KB
pLabel.ini	2021/6/15 14:39	配置设置	1 KB
PreTolerance.txt	2021/6/15 14:30	文本文档	1 KB

2. The example of adding a custom modification

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

For example:

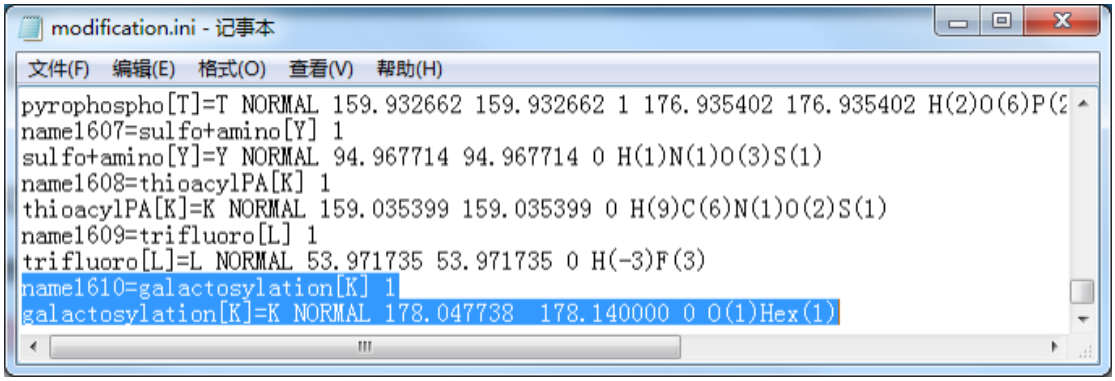
"@NUMBER_MODIFICATION=1609" to "@NUMBER_MODIFICATION=1610"

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

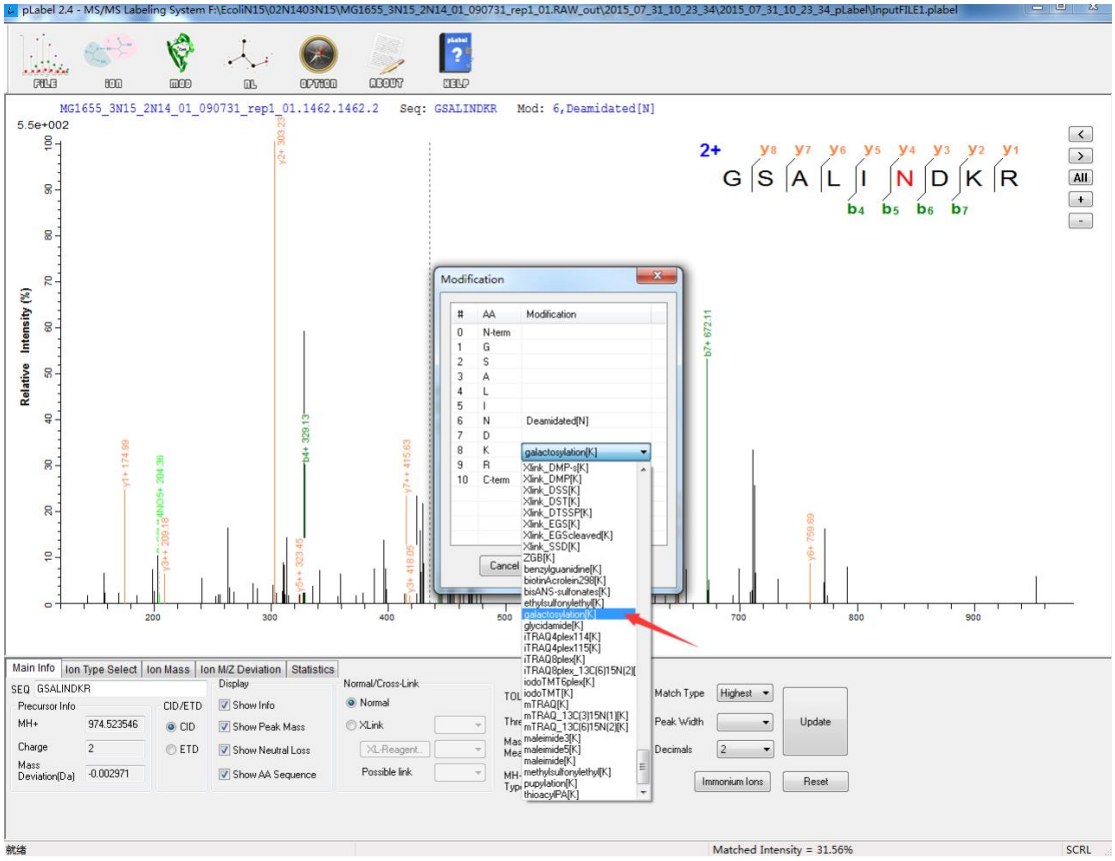
For example:

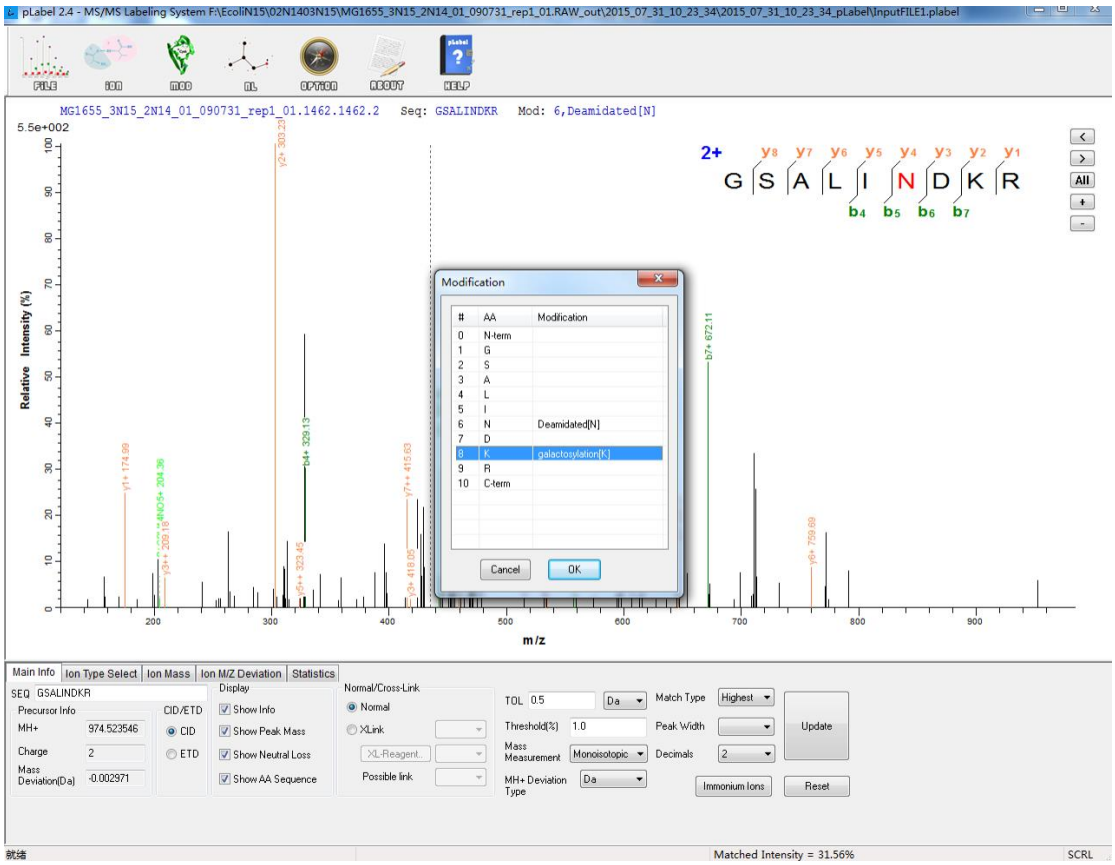
name1610=galactosylation[K] 1

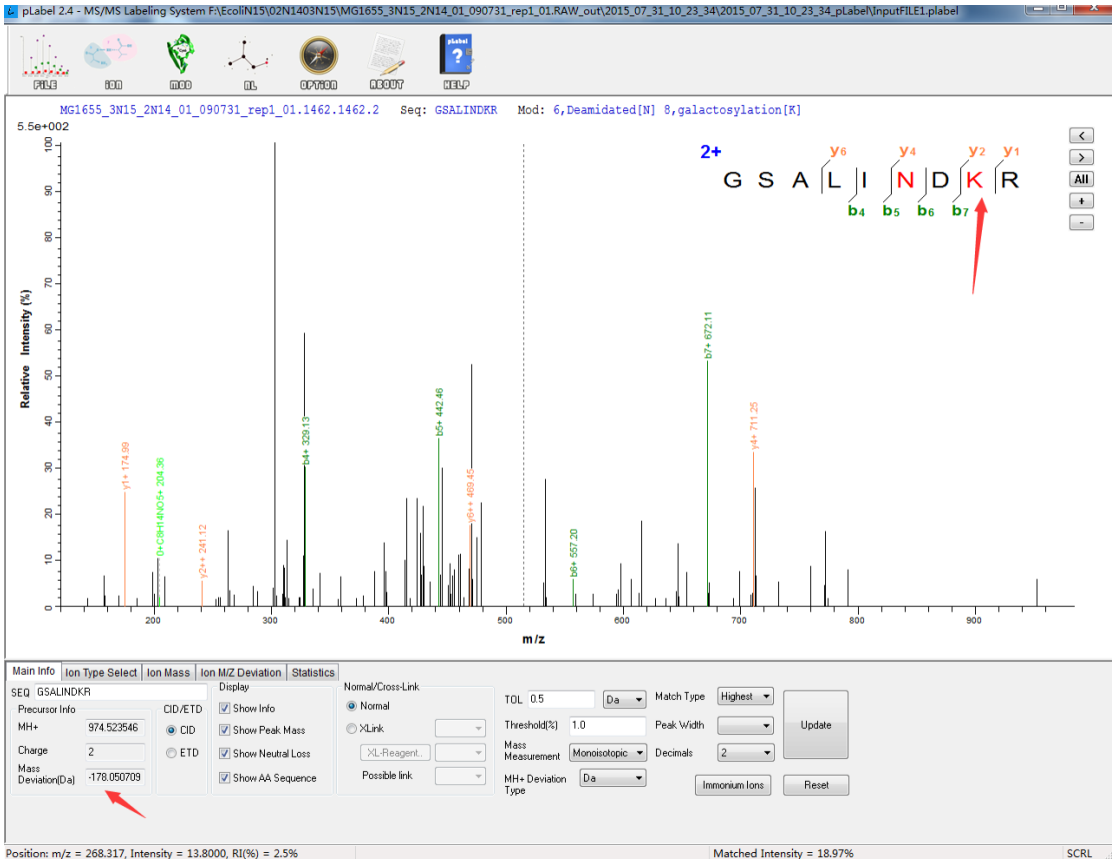
galactosylation[K]=K NORMAL 178.047738 178.140000 0 O(1)Hex(1)



3. Save the file and reopen pLabel. You can add your modification on “K” .





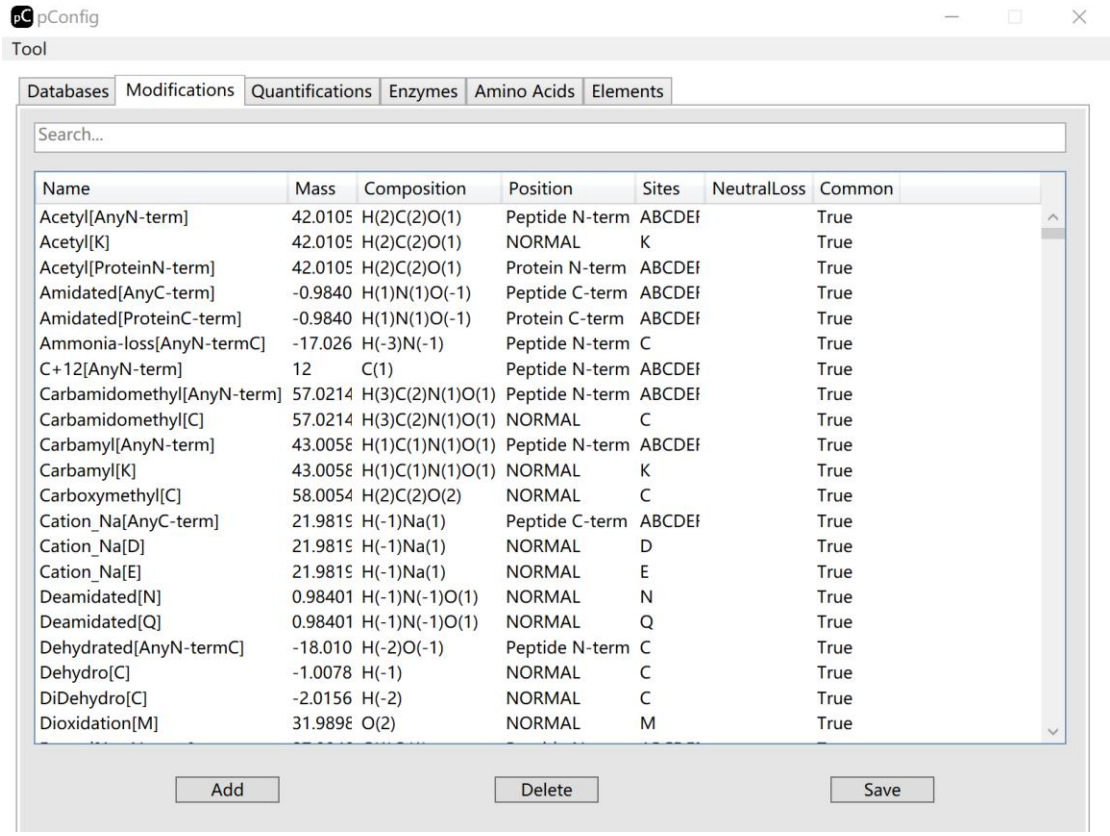


NOTE:

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.



Name	Mass	Composition	Position	Sites	NeutralLoss	Common
Acetyl[AnyN-term]	42.0105	H(2)C(2)O(1)	Peptide N-term	ABCDEF		True
Acetyl[K]	42.0105	H(2)C(2)O(1)	NORMAL	K		True
Acetyl[ProteinN-term]	42.0105	H(2)C(2)O(1)	Protein N-term	ABCDEF		True
Amidated[AnyC-term]	-0.9840	H(1)N(1)O(-1)	Peptide C-term	ABCDEF		True
Amidated[ProteinC-term]	-0.9840	H(1)N(1)O(-1)	Protein C-term	ABCDEF		True
Ammonia-loss[AnyN-termC]	-17.026	H(-3)N(-1)	Peptide N-term	C		True
C+12[AnyN-term]	12	C(1)	Peptide N-term	ABCDEF		True
Carbamidomethyl[AnyN-term]	57.0214	H(3)C(2)N(1)O(1)	Peptide N-term	ABCDEF		True
Carbamidomethyl[C]	57.0214	H(3)C(2)N(1)O(1)	NORMAL	C		True
Carbamyl[AnyN-term]	43.0058	H(1)C(1)N(1)O(1)	Peptide N-term	ABCDEF		True
Carbamyl[K]	43.0058	H(1)C(1)N(1)O(1)	NORMAL	K		True
Carboxymethyl[C]	58.0054	H(2)C(2)O(2)	NORMAL	C		True
Cation_Na[AnyC-term]	21.9819	H(-1)Na(1)	Peptide C-term	ABCDEF		True
Cation_Na[D]	21.9819	H(-1)Na(1)	NORMAL	D		True
Cation_Na[E]	21.9819	H(-1)Na(1)	NORMAL	E		True
Deamidated[N]	0.98401	H(-1)N(-1)O(1)	NORMAL	N		True
Deamidated[Q]	0.98401	H(-1)N(-1)O(1)	NORMAL	Q		True
Dehydrated[AnyN-termC]	-18.010	H(-2)O(-1)	Peptide N-term	C		True
Dehydro[C]	-1.0078	H(-1)	NORMAL	C		True
DiDehydro[C]	-2.0156	H(-2)	NORMAL	C		True
Dioxidation[M]	31.9898	O(2)	NORMAL	M		True