

directDIA .json settings file

This document contains instructions for adjusting settings for directDIA pipeline using a .json file.

JSON settings file import-export

A .json file can be generated using Spectronaut GUI: **Settings** perspective → **directDIA™** → **Export schema...** → Save as type: **Json Settings File (*.json)** → **Save**.

JSON settings file for BGS Factory Settings (default) contains fields as below:

```
1 {
2   "DIA_Analysis": {
3     "Identification": {
4       "Precursor_PEP_Cutoff": 0.2,
5       "Precursor_Qvalue_Cutoff": 0.01,
6       "Protein_Qvalue_Cutoff_Experiment": 0.01,
7       "Protein_Qvalue_Cutoff_Run": 0.05,
8       "Protein_PEP_Cutoff": 0.75,
9       "Exclude_Single_Hit_Proteins": false
10    },
11    "Quantification": {
12      "Proteotypicity_Filter": "none",
13      "Data_Filtering": "qvalue",
14      "Cross_Run_Normalization": true,
15      "Imputation_Strategy": "none"
16    },
17    "PTM_Workflow": {
18      "PTM_Localization": false,
19      "Probability_Cutoff": 0.0
20    },
21    "Pipeline_Mode": {
22      "Generate_SNE_File": true
23    },
24    "XIC_Extraction": {
25      "MS1_Mass_Tolerance_Strategy": "dynamic",
26      "MS2_Mass_Tolerance_Strategy": "dynamic"
27    }
28  },
29  "Pulsar_Search": {
30    "Peptides": {
31      "Enzymes_Cleavage_Rules": [
32        "Trypsin/P"
33      ],
34      "Digest_Type": "Specific",
35      "Max_Peptide_Length": 52,
36      "Min_Peptide_Length": 7,
37      "Missed_Cleavages": 2,
38      "Toggle_NTerminal_M": true
39    },
40    "Modifications": {
41      "Max_Variable_Modifications": 5,
42      "Fixed_Modifications": [
43        "Carbamidomethyl (C)"
44      ],
```

```

45     "Variable_Modifications": [
46         "Acetyl (Protein N-term)",
47         "Oxidation (M)"
48     ]
49 },
50 "Identification": {
51     "DirectDIA_Workflow": "directdia_deep"
52 }
53 }
54 }

```

JSON file can be imported into Spectronaut in the command-line mode using the `-j` option. These settings will override the default settings or settings specified in the `.prop` file (imported using the `-s` option).

Possible field values

Name	Possible values
Precursor_PEP_Cutoff	Double between 0 and 1
Precursor_Qvalue_Cutoff	Double between 0 and 1
Protein_Qvalue_Cutoff_Experiment	Double between 0 and 1
Protein_Qvalue_Cutoff_Run	Double between 0 and 1
Protein_PEP_Cutoff	Double between 0 and 1
Exclude_Single_Hit_Proteins	true, false
Proteotypicity_Filter	"none", "only_proteotypic", "only_protein_group_specific", "only_gene_specific"
Data_Filtering	"qvalue", "qvalue_complete", "qvalue_percentile"
Cross_Run_Normalization	true, false
Imputation_Strategy	"none", "background", "global", "runwise"
PTM_Localization	true, false
Probability_Cutoff	Double between 0 and 1
Generate_SNE_File	true, false
MS1_Mass_Tolerance_Strategy	"dynamic", "relative", "static"
MS2_Mass_Tolerance_Strategy	"dynamic", "relative", "static"
Enzymes_Cleavage_Rules	"GluC", "LysC", "LysC/P", "Trypsin", "Trypsin/P"
Digest_Type	"Specific", "Semi-specific (free N-terminus)", "Semi-specific (free C-terminus)", "Semi-specific", "Unspecific"
Max_Peptide_Length	Non-negative integer

Min_Peptide_Length	Non-negative integer
Missed_Cleavages	Non-negative integer
Toggle_NTerminal_M	true, false
Max_Variable_Modifications	Integer between 0 and 15
Fixed_Modifications	A list of modification names
Variable_Modifications	A list of modification names
DirectDIA_Workflow	"directdia_deep", "directdia_fast", "directdia"

Settings applicability

Pipeline	Example command	Applicable settings
directDIA	direct -r <raw_file> -fasta <fasta_file>	"Pulsar_Search" settings are affecting search archive generation, "DIA_Analysis" affects later stages of a pipeline
Search archive merging	lg -se Pulsar -sa search_arch1.psar -k output_lirary	No applicable setting
DIA Analysis	diaanalysis -r <raw_file> -a <library>	"DIA_Analysis"
SNE-combine	combine -f <SNE_file> -fasta <fasta_file>	"DIA_Analysis" → "Identification" "DIA_Analysis" → "Quantification"

Possible modifications

Values of "Fixed_Modifications" and "Variable_modifications" may contain modification names from the table below.

18O	2-dimethylsuccinyl	2-monomethylsuccinyl	2-nitrobenzyl
2-succinyl	2HPG	3-deoxyglucosone	3-phosphoglyceryl
3sulfo (Any N-term)	4-ONE	4-ONE+Delta:H(-2)O(-1)	4AcAllylGal
a-type-ion (Any C-term)	AccQTag	AccQTag (Any N-term)	Acetyl
Acetyl (K)	Acetyl (N-term)	Acetyl (Protein N-term)	Acetyl:13C(2)
Acetyl:13C(2) (Protein N-term)	Acetyl:2H(3)	Acetyl:2H(3) (Any N-term)	Acetyl:2H(3) (Protein N-term)
Acetyldeoxyhypusine	Acetylhypusine	ADP-Ribosyl	AEBS
AEBS (Protein N-term)	AEC-MAEC	AEC-MAEC:2H(4)	AHA-Alkyne
AHA-Alkyne-KDDDD	AHA-SS	AHA-SS_CAM	Ahx2+Hsl (Any C-term)
Ala->Arg	Ala->Asn	Ala->Asp	Ala->CamCys
Ala->Cys	Ala->Gln	Ala->Glu	Ala->Gly

Ala->His	Ala->Lys	Ala->Met	Ala->Phe
Ala->Pro	Ala->Ser	Ala->Thr	Ala->Trp
Ala->Tyr	Ala->Val	Ala->Xle	Amidated (C-term)
Amidated (Protein C-term)	Amidine	Amidine (Any N-term)	Amidino
Amino	Ammonia-loss	Ammonia-loss (Any N-term)	Ammonia-loss (Protein N-term)
Ammonium	Ammonium (Any C-term)	AMTzHexNAc2	Archaeol
Arg (Any N-term)	Arg->Ala	Arg->Asn	Arg->Asp
Arg->CamCys	Arg->Cys	Arg->Gln	Arg->Glu
Arg->GluSA	Arg->Gly	Arg->His	Arg->Lys
Arg->Met	Arg->Npo	Arg->Orn	Arg->Phe
Arg->Pro	Arg->Ser	Arg->Thr	Arg->Trp
Arg->Tyr	Arg->Val	Arg->Xle	Arg-add (Any N-term)
Arg-loss (Any C-term)	Arg10	Arg2PG	Arg6
Argbiotinhydrazide	AROD	Asn->Ala	Asn->Arg
Asn->Asp	Asn->CamCys	Asn->Cys	Asn->Gln
Asn->Glu	Asn->Gly	Asn->His	Asn->Lys
Asn->Met	Asn->Phe	Asn->Pro	Asn->Ser
Asn->Thr	Asn->Trp	Asn->Tyr	Asn->Val
Asn->Xle	Asp->Ala	Asp->Arg	Asp->Asn
Asp->CamCys	Asp->Cys	Asp->Gln	Asp->Glu
Asp->Gly	Asp->His	Asp->Lys	Asp->Met
Asp->Phe	Asp->Pro	Asp->Ser	Asp->Thr
Asp->Trp	Asp->Tyr	Asp->Val	Asp->Xle
Atto495Maleimide	azole	Bacillosamine	BADGE
BDMAPP	BDMAPP (Protein N-term)	Benzoyl	Benzoyl (Any N-term)
Benzyl	benzylguanidine	Benzyloxycarbonyl (Protein N-term)	BHAc
BHT	BHTOH	Biotin	Biotin (Any N-term)
Biotin-HPDP	Biotin-PEG-PRA	Biotin-PEO-Amine	Biotin-PEO-Amine (Protein C-term)
Biotin-phenacyl	Biotin:Cayman-10013	Biotin:Cayman-10141	Biotin:Invitrogen-M1602

Biotin:Sigma-B1267	Biotin:Thermo-21325	Biotin:Thermo-21345	Biotin:Thermo-21360
Biotin:Thermo-21901+2H2O	Biotin:Thermo-21901+H2O	Biotin:Thermo-21911	Biotin:Thermo-33033
Biotin:Thermo-33033-H	Biotin:Thermo-88310	Biotin:Thermo-88317	biotinAcrolein298
biotinAcrolein298 (Protein N-term)	BisANS	bisANS-sulfonates	BITC
BITC (Any N-term)	BMOE	BMP-piperidinol	Boc (Protein N-term)
Bodipy	Bromo	Bromobimane	BuUrBU
BuUrBu Amidated	BuUrBu Hydrolyzed	BuUrBu Tris	C8-QAT
C8-QAT (Any N-term)	CAF (Any N-term)	CamCys->Ala	CamCys->Arg
CamCys->Asn	CamCys->Asp	CamCys->Gln	CamCys->Glu
CamCys->Gly	CamCys->His	CamCys->Lys	CamCys->Met
CamCys->Phe	CamCys->Pro	CamCys->Ser	CamCys->Thr
CamCys->Trp	CamCys->Tyr	CamCys->Val	CamCys->Xle
CAMthiopropionyl	CAMthiopropionyl (Protein N-term)	Can-FP-biotin	Carbamidomethyl
Carbamidomethyl (Any N-term)	Carbamidomethyl (C)	CarbamidomethylDTT	Carbamyl
Carbamyl (N-term)	Carbamyl (Protein N-term)	Carbamylation (KR)	Carbofuran
Carboxy	Carboxy (Protein N-term)	Carboxy->Thiocarboxy (Protein C-term)	Carboxyethyl
Carboxymethyl	Carboxymethyl (Any N-term)	Carboxymethyl:13C(2)	CarboxymethylDMAP (Any N-term)
CarboxymethylDTT	Cation:Ag	Cation:Ag (Any C-term)	Cation:Ca[II]
Cation:Ca[II] (Any C-term)	Cation:Cu[I]	Cation:Cu[I] (Any C-term)	Cation:Fe[II]
Cation:Fe[II] (Any C-term)	Cation:K	Cation:K (Any C-term)	Cation:Li
Cation:Li (Any C-term)	Cation:Mg[II]	Cation:Mg[II] (Any C-term)	Cation:Na (Any C-term)
Cation:Na (DE)	Cation:Ni[II]	Cation:Ni[II] (Any C-term)	Cation:Zn[II]
Cation:Zn[II] (Any C-term)	cGMP	cGMP+RMP-loss	CHDH
Chlorination	Chlorpyrifos	Cholesterol (Protein C-term)	CLIP_TRAQ_2

CLIP_TRAQ_2 (Any N-term)	CLIP_TRAQ_3	CLIP_TRAQ_3 (Any N-term)	CLIP_TRAQ_4
CLIP_TRAQ_4 (Any N-term)	CoenzymeA	Cresylphosphate	CresylSaligeninPhosphate
Crotonaldehyde	Crotonyl	CuSMo	Cy3-maleimide
Cy3b-maleimide	Cyano	CyDye-Cy3	CyDye-Cy5
Cys->Ala	Cys->Arg	Cys->Asn	Cys->Asp
Cys->Dha	Cys->ethylaminoAla	Cys->Gln	Cys->Glu
Cys->Gly	Cys->His	Cys->Lys	Cys->Met
Cys->methylaminoAla	Cys->Oxalanine	Cys->Phe	Cys->Pro
Cys->PyruvicAcid (Protein N-term)	Cys->Ser	Cys->Thr	Cys->Trp
Cys->Tyr	Cys->Val	Cys->Xle	Cys-Cys
CysteinyI	CysteinyI - carbamidomethyl	cysTMT	cysTMT6plex
Cytopiloyne	Cytopiloyne (Any N-term)	Cytopiloyne+water	Cytopiloyne+water (Any N-term)
DAET	Dansyl	Dansyl (Any N-term)	Dap-DSP
Deamidated	Deamidated (Protein N-term)	Deamidated:18O(1)	Deamidation (N)
Deamidation (NQ)	Deamidation 18O (N)	Decanoyl	DEDGFLYMVYASQETFG
Dehydrated	Dehydrated (Any N-term)	Dehydrated (Protein C-term)	Dehydrated (ST)
Delta:H(2)C(2)	Delta:H(2)C(2) (N-term)	Delta:H(2)C(2) (Protein N-term)	Delta:H(2)C(3)
Delta:H(2)C(3)O(1)	Delta:H(2)C(5)	Delta:H(4)C(2)	Delta:H(4)C(2) (Any N-term)
Delta:H(4)C(2)O(-1)S(1)	Delta:H(4)C(3)	Delta:H(4)C(3) (Protein N-term)	Delta:H(4)C(3)O(1)
Delta:H(4)C(6)	Delta:H(5)C(2)	Delta:H(6)C(3)O(1)	Delta:H(6)C(3)O(1) (Protein N-term)
Delta:H(6)C(6)O(1)	Delta:H(8)C(6)O(1)	Delta:H(8)C(6)O(1) (Protein N-term)	Delta:H(8)C(6)O(2)
Delta:Hg(1)	Delta:S(-1)Se(1)	Delta:Se(1)	Deoxy
Deoxyhypusine	Desthiobiotin - carbamidomethyl	DeStreak	Dethiomethyl (M)
DFDNB	dHex	dHex(1)Hex(1)	dHex(1)Hex(2)

dHex(1)Hex(3)	dHex(1)Hex(3)HexNAc(4)	dHex(1)Hex(4)	dHex(1)Hex(4)HexNAc(4)
dHex(1)Hex(5)	dHex(1)Hex(5)HexNAc(4)	dHex(1)Hex(6)	DHP
Diacylglycerol	DiART6plex	DiART6plex (Any N-term)	DiART6plex (Protein N-term)
DiART6plex115	DiART6plex115 (Any N-term)	DiART6plex115 (Protein N-term)	DiART6plex116/119
DiART6plex116/119 (Any N-term)	DiART6plex116/119 (Protein N-term)	DiART6plex117	DiART6plex117 (Any N-term)
DiART6plex117 (Protein N-term)	DiART6plex118	DiART6plex118 (Any N-term)	DiART6plex118 (Protein N-term)
Dibromo	Dicarbamidomethyl	Dicarbamidomethyl (Any N-term)	dichlorination
Didehydro	Didehydro (Any C-term)	Didehydroretinylidene	Diethyl
Diethyl (Any N-term)	Diethylphosphate	Diethylphosphate (Any N-term)	Difuran
Dihydroxyimidazolidine	Diiodo	Diironsubcluster	Diisopropylphosphate
Diisopropylphosphate (Any N-term)	DiLeu4plex	DiLeu4plex (Any N-term)	DiLeu4plex115
DiLeu4plex115 (Any N-term)	DiLeu4plex117	DiLeu4plex117 (Any N-term)	DiLeu4plex118
DiLeu4plex118 (Any N-term)	DimethLys0	DimethLys2	DimethLys4
DimethLys6	DimethLys8	DimethNter0	DimethNter2
DimethNter4	DimethNter6	DimethNter8	Dimethyl
Dimethyl (K)	Dimethyl (KR)	Dimethyl (Protein N-term)	Dimethyl:2H(4)
Dimethyl:2H(4) (Protein N-term)	Dimethyl:2H(4)13C(2)	Dimethyl:2H(4)13C(2) (Any N-term)	Dimethyl:2H(6)
Dimethyl:2H(6)13C(2)	Dimethyl:2H(6)13C(2) (Protein N-term)	DimethylamineGMBS	DimethylArsino
DimethylpyrroleAdduct	Dioxidation	Dioxidation (MW)	Diphthamide
Dipropionyl (Any N-term)	Dipyridyl	Dipyrrolylmethanemethyl	DMPO
DNCB_hapten	dNIC (Any N-term)	DNPS	DSBU
DSBU Amidated	DSBU Hydrolyzed	DSBU Tris	DSS
DSS Amidated	DSS Tris	DSSO	DSSO Hydrolyzed
DTBP	DTBP (Protein N-term)	DTT_C	DTT_C:2H(6)

DTT_ST	DTT_ST:2H(6)	DyLight-maleimide	EASI-tag_Lys
EASI-tag_Nter	EDT-iodoacetyl-PEO-biotin	EDT-maleimide-PEO-biotin	EGCG1
EGCG2	EHD-diphenylpentanone	EQAT	EQAT:2H(5)
EQIGG	ESP	ESP (Any N-term)	ESP:2H(10)
ESP:2H(10) (Any N-term)	Ethanedithiol	Ethanolamine	Ethanolamine (Any C-term)
Ethanolyl	Ethanolyl (Any N-term)	Ethoxyformyl	Ethyl
Ethyl (Any C-term)	Ethyl (Any N-term)	Ethyl (Protein N-term)	Ethyl+Deamidated
ethylamino	Ethylphosphate	Ethylphosphate (Any N-term)	ethylsulfonylethyl
ExacTagAmine	ExacTagThiol	FAD	Farnesyl
Fluorescein	Fluoro	FMN	FMNC
FMNH	Fmoc (Protein N-term)	FNEM	Formyl
Formyl (Any N-term)	Formyl (Protein N-term)	FormylMet (Protein N-term)	FP-Biotin
FTC	Furan	G-H1	Galactosyl
GeranylGeranyl	GGQ	GIST-Quat	GIST-Quat (Any N-term)
GIST-Quat:2H(3)	GIST-Quat:2H(3) (Any N-term)	GIST-Quat:2H(6)	GIST-Quat:2H(6) (Any N-term)
GIST-Quat:2H(9)	GIST-Quat:2H(9) (Any N-term)	Gln->Ala	Gln->Arg
Gln->Asn	Gln->Asp	Gln->CamCys	Gln->Cys
Gln->Glu	Gln->Gly	Gln->His	Gln->Lys
Gln->Met	Gln->Phe	Gln->Pro	Gln->pyro-Glu
Gln->Ser	Gln->Thr	Gln->Trp	Gln->Tyr
Gln->Val	Gln->Xle	Glu	Glu (Protein C-term)
Glu->Ala	Glu->Arg	Glu->Asn	Glu->Asp
Glu->CamCys	Glu->Cys	Glu->Gln	Glu->Gly
Glu->His	Glu->Lys	Glu->Met	Glu->Phe
Glu->Pro	Glu->pyro-Glu	Glu->Ser	Glu->Thr
Glu->Trp	Glu->Tyr	Glu->Val	Glu->Xle
Gluconoylation	Gluconoylation (Any N-term)	glucosone	Glucosylgalactosyl

Glucuronyl	Glucuronyl (Protein N-term)	GluGlu	GluGlu (Protein C-term)
GluGluGlu	GluGluGlu (Protein C-term)	GluGluGluGlu	GluGluGluGlu (Protein C-term)
Glutathione	Gly	Gly->Ala	Gly->Arg
Gly->Asn	Gly->Asp	Gly->CamCys	Gly->Cys
Gly->Gln	Gly->Glu	Gly->His	Gly->Lys
Gly->Met	Gly->Phe	Gly->Pro	Gly->Ser
Gly->Thr	Gly->Trp	Gly->Tyr	Gly->Val
Gly->Xle	Gly-loss+Amide (Any C-term)	Glycerophospho	GlycerylPE
glycidamide	glycidamide (Any N-term)	Glycosyl	GlyGly
GlyGly (K)	GlyGly (K)_1	GPIanchor (Protein C-term)	GuanidinyI
GuanidinyI (Any N-term)	HCysteinyI	HCysThiolactone	Heme
Hep	Hex	Hex (Any N-term)	Hex (K)
Hex 4	Hex(1)HexNAc(1)	Hex(1)HexNAc(1) (ST)	Hex(1)HexNAc(1)dHex(1)
Hex(1)HexNAc(1)NeuAc(1)	Hex(1)HexNAc(1)NeuAc(2)	Hex(1)HexNAc(2)	Hex(1)HexNAc(2)dHex(1)
Hex(1)HexNAc(2)dHex(1)Pent(1)	Hex(1)HexNAc(2)dHex(2)	Hex(1)HexNAc(2)Pent(1)	Hex(2)
Hex(2)HexNAc(2)	Hex(2)HexNAc(2)dHex(1)	Hex(2)HexNAc(2)Pent(1)	Hex(3)
Hex(3)HexNAc(1)Pent(1)	Hex(3)HexNAc(2)	Hex(3)HexNAc(2)P(1)	Hex(3)HexNAc(4)
Hex(4)HexNAc(4)	Hex(5) HexNAc(4) NeuAc(2) (N)	Hex(5) HexNAc(4) NeuAc(2) Sodium (N)	Hex(5)HexNAc(2)
Hex(5)HexNAc(4)	Hex1HexNAc1	HexN	HexNAc
HexNAc (ST)	HexNAc (ST)_1	HexNAc(1)dHex(1)	HexNAc(1)dHex(2)
HexNAc(2)	HexNAc(2)dHex(1)	HexNAc(2)dHex(2)	His->Ala
His->Arg	His->Asn	His->Asp	His->CamCys
His->Cys	His->Gln	His->Glu	His->Gly
His->Lys	His->Met	His->Phe	His->Pro
His->Ser	His->Thr	His->Trp	His->Tyr
His->Val	His->Xle	HMVK	HN2_mustard

HN3_mustard	HNE	HNE-BAHAH	HNE-Delta:H(2)O
HNE+Delta:H(2)	Homocysteic_acid	HPG	Hydrazide
Hydroxamic_acid	Hydroxycinnamyl	Hydroxyfarnesyl	Hydroxyheme
Hydroxymethyl	HydroxymethylOP	Hydroxyproline	Hydroxytrimethyl
Hypusine	IBTP	ICAT-0	ICAT-9
ICAT-D	ICAT-D:2H(8)	ICAT-G	ICAT-G:2H(8)
ICAT-H	ICAT-H:13C(6)	ICDID	ICDID:2H(6)
ICPL	ICPL (Protein N-term)	ICPL-Lys0	ICPL-Lys10
ICPL-Lys4	ICPL-Lys6	ICPL-Nter0	ICPL-Nter10
ICPL-Nter4	ICPL-Nter6	ICPL:13C(6)	ICPL:13C(6) (Protein N-term)
ICPL:13C(6)2H(4) (Protein N-term)	ICPL:2H(4)	ICPL:2H(4) (Protein N-term)	IDeNT
IED-Biotin	IGBP	IGBP:13C(2)	Ile7
IMEHex(2)NeuAc	IMID	IMID:2H(4)	Iminobiotin
Iminobiotin (Any N-term)	Iodo	Iodoacetanilide	Iodoacetanilide (Any N-term)
Iodoacetanilide:13C(6)	Iodoacetanilide:13C(6) (Any N-term)	iodoTMT	iodoTMT6plex
iodoTMT6plex-Cys126	iodoTMT6plex-Cys127	iodoTMT6plex-Cys128	iodoTMT6plex-Cys129
iodoTMT6plex-Cys130	iodoTMT6plex-Cys131	iodoU-AMP	ISD_z+2_ion (Any N-term)
Isopropylphospho	iTRAQ_4plex_Lys	iTRAQ_4plex_Nter	iTRAQ_8plex_Lys
iTRAQ_8plex_Nter	iTRAQ4plex	iTRAQ4plex (Any N-term)	iTRAQ4plex (Protein N-term)
iTRAQ4plex-Lys114	iTRAQ4plex-Lys115	iTRAQ4plex-Lys116	iTRAQ4plex-Lys117
iTRAQ4plex-Nter114	iTRAQ4plex-Nter115	iTRAQ4plex-Nter116	iTRAQ4plex-Nter117
iTRAQ4plex114	iTRAQ4plex114 (Any N-term)	iTRAQ4plex115	iTRAQ4plex115 (Any N-term)
iTRAQ8plex	iTRAQ8plex (Any N-term)	iTRAQ8plex (Protein N-term)	iTRAQ8plex-Lys113
iTRAQ8plex-Lys114	iTRAQ8plex-Lys115	iTRAQ8plex-Lys116	iTRAQ8plex-Lys117
iTRAQ8plex-Lys118	iTRAQ8plex-Lys119	iTRAQ8plex-Lys121	iTRAQ8plex-Nter113
iTRAQ8plex-Nter114	iTRAQ8plex-Nter115	iTRAQ8plex-Nter116	iTRAQ8plex-Nter117
iTRAQ8plex-Nter118	iTRAQ8plex-Nter119	iTRAQ8plex-Nter121	iTRAQ8plex:13C(6)15N(2)

iTRAQ8plex:13C(6)15N(2) (Any N-term)	iTRAQ8plexCold	iTRAQ8plexCold (Any N-term)	iTRAQ8plexCold (Protein N-term)
K0400	K0800	K1920	K2020
K3410	K3900	K4400	K5210
K6020	K6420	Label:13C(1)2H(3)	Label:13C(1)2H(3)+Oxidation
Label:13C(3)	Label:13C(3)15N(1)	Label:13C(4)	Label:13C(4)+Oxidation
Label:13C(4)15N(1)	Label:13C(4)15N(2)+GlyGly	Label:13C(5)15N(1)	Label:13C(6)
Label:13C(6)+Acetyl	Label:13C(6)+Dimethyl	Label:13C(6)+GlyGly	Label:13C(6)15N(1)
Label:13C(6)15N(2)	Label:13C(6)15N(2)+Acetyl	Label:13C(6)15N(2)+Dimethyl	Label:13C(6)15N(2)+GlyGly
Label:13C(6)15N(4)+Dimethyl	Label:13C(6)15N(4)+Dimethyl:2H(6)13C(2)	Label:13C(6)15N(4)+Methyl	Label:13C(6)15N(4)+Methyl:2H(3)13C(1)
Label:13C(8)15N(2)	Label:13C(9)	Label:13C(9)+Phospho	Label:13C(9)15N(1)
Label:15N(1)	Label:15N(2)	Label:15N(2)2H(9)	Label:15N(3)
Label:15N(4)	Label:18O(1)	Label:18O(1) (Any C-term)	Label:2H(10)
Label:2H(3)	Label:2H(3)+Oxidation	Label:2H(4)	Label:2H(4)+Acetyl
Label:2H(4)+GlyGly	Label:2H(4)13C(1)	Label:2H(6)15N(1)	Label:2H(7)15N(4)
Label:2H(9)13C(6)15N(2)	lapachenole	Leu->MetOx	Leu7
LeuArgGlyGly	LG-anhydrolactam	LG-anhydrolactam (Any N-term)	LG-anhydropyrrole
LG-anhydropyrrole (Any N-term)	LG-Hlactam-K	LG-Hlactam-K (Protein N-term)	LG-Hlactam-R
LG-lactam-K	LG-lactam-K (Protein N-term)	LG-lactam-R	LG-pyrrole
LG-pyrrole (Any N-term)	Lipoyl	Lys (Any N-term)	Lys->Ala
Lys->Allysine	Lys->AminoadipicAcid	Lys->Arg	Lys->Asn
Lys->Asp	Lys->CamCys	Lys->Cys	Lys->Gln
Lys->Glu	Lys->Gly	Lys->His	Lys->Met
Lys->MetOx	Lys->Phe	Lys->Pro	Lys->Ser
Lys->Thr	Lys->Trp	Lys->Tyr	Lys->Val
Lys->Xle	Lys-loss (Any C-term)	Lys-loss (Protein C-term)	Lys4
Lys6	Lys8	Lysbiotinhydrazide	maleimide

Maleimide-PEO2-Biotin	maleimide3	maleimide5	Malonyl
MDCC	Menadione	Menadione-HQ	MercaptoEthanol
Met->Aha	Met->Aha+tag	Met->Aha+tagMCL	Met->Ala
Met->Arg	Met->Asn	Met->Asp	Met->CamCys
Met->Carbamidomethyl-Hcy	Met->Carboxymethyl-Hcy	Met->Cys	Met->Gln
Met->Glu	Met->Gly	Met->His	Met->Hpg
Met->Hse (Any C-term)	Met->Hsl (Any C-term)	Met->Lys	Met->Phe
Met->Pro	Met->Ser	Met->Thr	Met->Trp
Met->Tyr	Met->Val	Met->Xle	Met-loss (Protein N-term)
Met-loss+Acetyl (Protein N-term)	Methyl	Methyl (Any C-term)	Methyl (Any N-term)
Methyl (E)	Methyl (KR)	Methyl (Protein C-term)	Methyl (Protein N-term)
Methyl-PEO12-Maleimide	Methyl-Propionyl (K)	Methyl:2H(2)	Methyl:2H(3)
Methyl:2H(3) (Any C-term)	Methyl:2H(3)+Acetyl:2H(3)	Methyl:2H(3)13C(1)	Methyl+Acetyl:2H(3)
Methyl+Deamidated	Methyl+Propionyl	Methylamine	Methylmalonylation
Methylphosphonate	Methylpyrroline	methylsulfonylethyl	Methylthio
Methylthio (Any N-term)	MG-H1	Microcin (Protein C-term)	MicrocinC7 (Protein C-term)
MM-diphenylpentanone	MMTS	Molybdopterin	MolybdopterinGD
MolybdopterinGD+Delta:S(-1)Se(1)	mTRAQ	mTRAQ-Lys0	mTRAQ-Lys4
mTRAQ-Lys8	mTRAQ-Nter0	mTRAQ-Nter4	mTRAQ-Nter8
mTRAQ:13C(3)15N(1)	mTRAQ:13C(6)15N(2)	MTSL	MurNAc
Myristoleyl (Protein N-term)	Myristoyl	Myristoyl (Any N-term)	Myristoyl+Delta:H(-4) (Protein N-term)
Myristoyl+Delta:H(18)C(12)N(6)O(4) (Any N-term)	N-dimethylphosphate	N-Ethylmaleimide	N-Ethylmaleimide (Any N-term)
N-Ethylmaleimide+water (Any N-term)	N-Methylmaleimide (Any N-term)	N-Methylmaleimide+water	N-Methylmaleimide+water (Any N-term)
NA-LNO2	NA-OA-NO2	Naphthyl	Naphthylacetyl
NBS	NBS:13C(6)	NDA	NDA (Any N-term)

NEIAA	NEIAA:2H(5)	NEM:2H(5)	NEM:2H(5)+H2O
NEMsulfur	NEMsulfurWater	Nethylmaleimide	Nethylmaleimide+water
NeuAc	NeuGc	NHS-fluorescein	NHS-LC-Biotin
NHS-LC-Biotin (Any N-term)	NIC (Any N-term)	NIPCAM	Nitro
Nitrosyl	Nmethylmaleimide	Nmethylmaleimide+water	NO_SMX_SEMD
NO_SMX_SIMD	NO_SMX_SMCT	O-Dimethylphosphate	O-Et-N-diMePhospho
O-Isopropylmethylphosphonate	O-Methylphosphate	O-pinacolylmethylphosphonate	Octanoyl
OxArgBiotin	OxArgBiotinRed	Oxidation	Oxidation (Any C-term)
Oxidation (M)	Oxidation (MP)	Oxidation (P)	Oxidation (W)
Oxidation+NEM	OxLysBiotin	OxLysBiotinRed	OxProBiotin
OxProBiotinRed	Palmitoleyl	Palmitoyl	Palmitoyl (Protein N-term)
PEITC	PEITC (Any N-term)	Pentylamine	PEO-Iodoacetyl-LC-Biotin
PEO-Iodoacetyl-LC-Biotin (Any N-term)	PET	Phe->Ala	Phe->Arg
Phe->Asn	Phe->Asp	Phe->CamCys	Phe->Cys
Phe->Gln	Phe->Glu	Phe->Gly	Phe->His
Phe->Lys	Phe->Met	Phe->Pro	Phe->Ser
Phe->Thr	Phe->Trp	Phe->Tyr	Phe->Val
Phe->Xle	Phenylisocyanate (Any N-term)	Phenylisocyanate:2H(5) (Any N-term)	phenylsulfonylethyl
Phospho	Phospho (ST)	Phospho (STY)	Phosphoadenosine
Phosphogluconoylation	Phosphogluconoylation (Any N-term)	Phosphoguanosine	PhosphoHex
PhosphoHexNAc	Phosphopantetheine	Phosphopropargyl	phosphoRibosyl
PhosphoribosyldephosphoCoA	PhosphoUridine	Phycocyanobilin	Phycoerythrobilin
Phytochromobilin	Piperidine	Piperidine (Any N-term)	PMC
Pro->Ala	Pro->Arg	Pro->Asn	Pro->Asp
Pro->CamCys	Pro->Cys	Pro->Gln	Pro->Glu
Pro->Gly	Pro->His	Pro->Lys	Pro->Met

Pro->Phe	Pro->pyro-Glu	Pro->Pyrrolidinone	Pro->Pyrrolidone
Pro->Ser	Pro->Thr	Pro->Trp	Pro->Tyr
Pro->Val	Pro->Xle	Pro5	Pro6
probiotinhydrazide	Propargylamine	Propargylamine (Any C-term)	Propionamide
Propionamide (Any N-term)	Propionamide:2H(3)	Propionyl	Propionyl (K)
Propionyl (Peptide N-term)	Propionyl (Protein N-term)	Propionyl:13C(3)	Propionyl:13C(3) (Any N-term)
Propionyl:2H(5)	Propionyl:2H(5) (Any N-term)	Propionyl:2H(5) (Protein N-term)	Propiophenone
Propyl (Any N-term)	Propyl:2H(6)	Propyl:2H(6) (Any N-term)	PropylNAGthiazoline
PS_Hapten	pupylation	Puromycin (Any C-term)	PyMIC (Any N-term)
PyridoxalPhosphate	PyridoxalPhosphateH2	Pyridylacetyl	Pyridylacetyl (Any N-term)
Pyridylethyl	Pyridylethyl (Any N-term)	Pyro-carbamidomethyl (Any N-term)	pyrophospho
PyruvicAcidIminyl	PyruvicAcidIminyl (Protein N-term)	QAT	QAT:2H(3)
QEQTGG	QQQTGG	QQTGG (K)	QTGG
Quinone	Retinylidene	RGG (K)	Saligenin
Sec->Dha	SecCarbamidomethyl	SecNEM	SecNEM:2H(5)
Ser->Ala	Ser->Arg	Ser->Asn	Ser->Asp
Ser->CamCys	Ser->Cys	Ser->Gln	Ser->Glu
Ser->Gly	Ser->His	Ser->LacticAcid (Protein N-term)	Ser->Lys
Ser->Met	Ser->Phe	Ser->Pro	Ser->Thr
Ser->Trp	Ser->Tyr	Ser->Val	Ser->Xle
SMA	SMA (Any N-term)	SMCC-maleimide	SPITC
SPITC (Any N-term)	SPITC:13C(6)	SPITC:13C(6) (Any N-term)	Succinyl
Succinyl (Any N-term)	Succinyl (Protein N-term)	Succinyl:13C(4)	Succinyl:13C(4) (Any N-term)
Succinyl:2H(4)	Succinyl:2H(4) (Any N-term)	SulfanilicAcid	SulfanilicAcid (Any C-term)

SulfanilicAcid:13C(6)	SulfanilicAcid:13C(6) (Any C-term)	Sulfation (Y)	Sulfide
Sulfo	Sulfo (STY)	Sulfo-NHS-LC-LC-Biotin	Sulfo-NHS-LC-LC-Biotin (Any N-term)
sulfo+amino	SulfoGMBS	SulfurDioxide	SUMO2135
SUMO3549	TAMRA-FP	Thiadiazole	Thiazolidine
Thiazolidine (Any N-term)	Thioacyl (Any N-term)	Thioacyl (DSP)	thioacylPA
Thiophos-S-S-biotin	Thiophospho	Thr->Ala	Thr->Arg
Thr->Asn	Thr->Asp	Thr->CamCys	Thr->Cys
Thr->Gln	Thr->Glu	Thr->Gly	Thr->His
Thr->Lys	Thr->Met	Thr->Phe	Thr->Pro
Thr->Ser	Thr->Trp	Thr->Tyr	Thr->Val
Thr->Xle	Thrbiotinhydrazide	Thyroxine	TMAB
TMAB (Any N-term)	TMAB:2H(9)	TMAB:2H(9) (Any N-term)	TMPP-Ac (Any N-term)
TMT	TMT (Any N-term)	TMT (Protein N-term)	TMT_Lys
TMT_Nter	TMT0plex-LysMS1	TMT10plex-Lys126C	TMT10plex-Lys127C
TMT10plex-Lys127N	TMT10plex-Lys128C	TMT10plex-Lys128N	TMT10plex-Lys129C
TMT10plex-Lys129N	TMT10plex-Lys130C	TMT10plex-Lys130N	TMT10plex-Lys131N
TMT10plex-Nter126C	TMT10plex-Nter127C	TMT10plex-Nter127N	TMT10plex-Nter128C
TMT10plex-Nter128N	TMT10plex-Nter129C	TMT10plex-Nter129N	TMT10plex-Nter130C
TMT10plex-Nter130N	TMT10plex-Nter131N	TMT11plex-Lys131C	TMT11plex-Nter131C
TMT2plex	TMT2plex (Any N-term)	TMT2plex (Protein N-term)	TMT2plex-Lys126
TMT2plex-Lys127	TMT2plex-Nter126	TMT2plex-Nter127	TMT6plex
TMT6plex (Any N-term)	TMT6plex (Protein N-term)	TMT6plex-Lys126	TMT6plex-Lys127
TMT6plex-Lys128	TMT6plex-Lys129	TMT6plex-Lys130	TMT6plex-Lys131
TMT6plex-Nter126	TMT6plex-Nter127	TMT6plex-Nter128	TMT6plex-Nter129
TMT6plex-Nter130	TMT6plex-Nter131	TMT8plex-Lys126C	TMT8plex-Lys127C
TMT8plex-Lys127N	TMT8plex-Lys128C	TMT8plex-Lys129C	TMT8plex-Lys129N
TMT8plex-Lys130C	TMT8plex-Lys131N	TMT8plex-Nter126C	TMT8plex-Nter127C
TMT8plex-Nter127N	TMT8plex-Nter128C	TMT8plex-Nter129C	TMT8plex-Nter129N

TMT8plex-Nter130C	TMT8plex-Nter131N	TMTpro_Lys	TMTpro_Nter
TMTpro16plex-Lys126C	TMTpro16plex-Lys127C	TMTpro16plex-Lys127N	TMTpro16plex-Lys128C
TMTpro16plex-Lys128N	TMTpro16plex-Lys129C	TMTpro16plex-Lys129N	TMTpro16plex-Lys130C
TMTpro16plex-Lys130N	TMTpro16plex-Lys131C	TMTpro16plex-Lys131N	TMTpro16plex-Lys132C
TMTpro16plex-Lys132N	TMTpro16plex-Lys133C	TMTpro16plex-Lys133N	TMTpro16plex-Lys134N
TMTpro16plex-Nter126C	TMTpro16plex-Nter127C	TMTpro16plex-Nter127N	TMTpro16plex-Nter128C
TMTpro16plex-Nter128N	TMTpro16plex-Nter129C	TMTpro16plex-Nter129N	TMTpro16plex-Nter130C
TMTpro16plex-Nter130N	TMTpro16plex-Nter131C	TMTpro16plex-Nter131N	TMTpro16plex-Nter132C
TMTpro16plex-Nter132N	TMTpro16plex-Nter133C	TMTpro16plex-Nter133N	TMTpro16plex-Nter134N
TMTpro18plex-Lys134C	TMTpro18plex-Lys135N	TMTpro18plex-Nter134C	TMTpro18plex-Nter135N
TNBS	TNBS (Any N-term)	TransN-biotin (Protein N-term)	TransN-biotin (Protein N-term)
trifluoro	Trifluoroacetyl	Triiodo	Triiodothyronine
Trimethyl	Trimethyl (K)	Trimethyl (Protein N-term)	Trimethyl:2H(9)
Trinitrophenyl	Trinitrophenyl (Any N-term)	Trioxidation	Trioxidation (C)
Tripalmitate (Protein N-term)	Trp->Ala	Trp->Arg	Trp->Asn
Trp->Asp	Trp->CamCys	Trp->Cys	Trp->Gln
Trp->Glu	Trp->Gly	Trp->His	Trp->Hydroxykynurenin
Trp->Kynurenin	Trp->Lys	Trp->Met	Trp->Oxolactone
Trp->Phe	Trp->Pro	Trp->Ser	Trp->Thr
Trp->Tyr	Trp->Val	Trp->Xle	Tyr->Ala
Tyr->Arg	Tyr->Asn	Tyr->Asp	Tyr->CamCys
Tyr->Cys	Tyr->Dha	Tyr->Gln	Tyr->Glu
Tyr->Gly	Tyr->His	Tyr->Lys	Tyr->Met
Tyr->Phe	Tyr->Pro	Tyr->Ser	Tyr->Thr
Tyr->Trp	Tyr->Val	Tyr->Xle	Ub-amide
Ub-Br2	Ub-fluorescein	Ub-VME	UgiJoullie
UgiJoullieProGly	UgiJoullieProGlyProGly	Val->Ala	Val->Arg
Val->Asn	Val->Asp	Val->CamCys	Val->Cys
Val->Gln	Val->Glu	Val->Gly	Val->His
Val->Lys	Val->Met	Val->Phe	Val->Pro

Val->Ser	Val->Thr	Val->Trp	Val->Tyr
Val->Xle	VFQQQTGG	VIEVYQEQTGG	Withaferin
Xle->Ala	Xle->Arg	Xle->Asn	Xle->Asp
Xle->CamCys	Xle->Cys	Xle->Gln	Xle->Glu
Xle->Gly	Xle->His	Xle->Lys	Xle->Met
Xle->Phe	Xle->Pro	Xle->Ser	Xle->Thr
Xle->Trp	Xle->Tyr	Xle->Val	Xlink:B10621
Xlink:DMP	Xlink:DMP (Protein N-term)	Xlink:DMP-de (Protein N-term)	Xlink:DMP-s
Xlink:DMP-s (Protein N-term)	Xlink:DSS	Xlink:DSS (Protein N-term)	Xlink:DST
Xlink:DST (Protein N-term)	Xlink:DTSSP	Xlink:DTSSP (Protein N-term)	Xlink:EGS
Xlink:EGS (Protein N-term)	Xlink:EGScleaved	Xlink:EGScleaved (Protein N-term)	Xlink:SMCC
Xlink:SSD	ZGB	ZGB (Any N-term)	