

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       "Precursor_Qvalue_Cutoff_Experiment": 0.01,
7       "Protein_Qvalue_Cutoff_Experiment": 0.01,
8       "Protein_Qvalue_Cutoff_Run": 0.05,
9       "Protein_PEP_Cutoff": 0.75,
10      "Single_Hit_Protein_Rule": "StratifiedFDR",
11      "Run_Level_Protein_Scoring": "all_observation"
12    },
13    "Quantification": {
14      "Proteotypicity_Filter": "none",
15      "Data_Filtering": "qvalue",
16      "Cross_Run_Normalization": true,
17      "Imputation_Strategy": "none",
18      "Perform_IM_Peak_Picking": true,
19      "Perform_background_noise_removal": true
20    },
21    "PTM_Workflow": {
22      "PTM_Localization": false,
23      "Probability_Cutoff": 0.0
24    },
25    "Workflow": {
26      "Method_Evaluation": false
27    },
28    "Pipeline_Mode": {
29      "Generate_SNE_File": true
30    },
31    "Tolerances": {
32      "Calibration_Tolerances": {
33        "MS1_Mass_Tolerance": {
34          "Strategy": "Dynamic",
35          "Correction_Factor": 1.0
36        },
37        "MS2_Mass_Tolerance": {
38          "Strategy": "Dynamic",
39          "Correction_Factor": 1.0
40        }
41      },
42      "Main_Search_Tolerances": {
43        "MS1_Mass_Tolerance": {
44          "Strategy": "Dynamic",
45          "Correction_Factor": 1.0
46        },
47        "MS2_Mass_Tolerance": {
```

```

48         "Strategy": "Dynamic",
49         "Correction_Factor": 1.0
50     }
51 }
52 }
53 },
54 "Pulsar_Search": {
55     "Peptides": {
56         "Enzymes_Cleavage_Rules": [
57             "Trypsin/P"
58         ],
59         "Digest_Type": "Specific",
60         "Max_Peptide_Length": 52,
61         "Min_Peptide_Length": 7,
62         "Missed_Cleavages": 2,
63         "Toggle_NTerminal_M": true
64     },
65     "Modifications": {
66         "Max_Variable_Modifications": 5,
67         "Fixed_Modifications": [
68             "Carbamidomethyl (C)"
69         ],
70         "Variable_Modifications": [
71             "Acetyl (Protein N-term)",
72             "Oxidation (M)"
73         ],
74         "Search_Mode": "Closed Search"
75     },
76     "Identification": {
77         "PSM_FDR": 0.01,
78         "Peptide_FDR": 0.01,
79         "Protein_Group_FDR": 0.01,
80         "DirectDIA_Workflow": "directdia-deep",
81         "RT_Sampling_Reduction": 1,
82         "RT_Sampling_Reduction": 7
83     },
84     "MS2": {
85         "Ion_Types": [
86             "b",
87             "y"
88         ]
89     }
90 }
91 }
92
93

```

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

Precursor_Qvalue_Cutoff_Experiment	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
Single_Hit_Protein_Rule	“StratifiedFDR”, “Keep”, “Exclude”
Proteotypicity_Filter	"none", "only_proteotypic", "only_protein_group_specific", "only_gene_specific"
Data_Filtering	"qvalue", "qvalue_complete", "qvalue_percentile"
Cross_Run_Normalization	true, false
Perform_IM_Peak_Picking	true, false
Perform_background_noise_removal	true, false
Imputation_Strategy	"none", "background", "global", "runwise"
PTM_Localization	true, false
Probability_Cutoff	Double between 0 and 1
Method_Evaluation	true, false
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", "SemiSpecificFreeN", "SemiSpecificFreeC", "SemiSpecific", "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
Known_Variable_Modifications	A list of modification names. Used only when Search_mode set to "PTM Probing Search"
Search_Mode	"Closed Search", "PTM Probing Search"
DirectDIA_Workflow	"directdia_deep", "directdia_fast", "directdia"
RT_Sampling_Reduction	Non-negative integer
IM_Sampling_Reduction	Non-negative integer
PSM_FDR	Double between 0 and 1
Peptide_FDR	Double between 0 and 1
Protein_Group_FDR	Double between 0 and 1
Strategy	"Relative", "Static", "Dynamic"
Correction_Factor	Double between 0.1 and 100. Used only when Strategy is set to "Dynamic".
Tolerance_Th	Non-negative double. Used only when Strategy is set to "Static".
Tolerance_ppm	Non-negative double. Used only when Strategy is set to "Relative".
Ion_Types	"b", "y", "a", "c", "x", "z"

Settings applicability

Pipeline	Example command	Applicable settings
directDIA	direct -r <raw_file> - fasta <fasta_file>	"Pulsar_Search" settings are affecting search archive and library generation, "DIA_Analysis" affects later stages of a pipeline
Pulsar search	lg -se Pulsar -r <raw_file> -f <fasta_file>	"Pulsar_Search"
psar file merging	lg -se Pulsar -sa search_arch1.psar -k output_lirary	"Pulsar_Search" settings are affecting library generation from the psar file
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"

Breaking changes

1. Spectronaut 21.0

- "Pulsar_Search" → "Tolerances" no longer available. Use "DIA_Analysis" → "Tolerances" instead. Structure of "Tolerances" section simplified, with single schema applicable for all types of analyzers, field names and structure changed.
- "DIA_Analysis" → "XIC_Extraction" no longer available. Use "DIA_Analysis" → "Tolerances" instead.

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
CAMthiopropano yl	CAMthiopropano yl (Protein N- term)	Can-FP-biotin	Carbamidomethy l
Carbamidomethy l (Any N-term)	Carbamidomethy l (C)	Carbamidomethy IDTT	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:1 3C(2)	CarboxymethylD MAP (Any N- term)
CarboxymethylD TT	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	CresylSaligeninP hosphate
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 - carbamidomethyI	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	DEDGLYMVYA SQETFG

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	Dicarbamidomet hyl	Dicarbamidomet hyl (Any N-term)	dichlorination
Didehydro	Didehydro (Any C-term)	Didehydroretinyli dene	Diethyl
Diethyl (Any N- term)	Diethylphosphat e	Diethylphosphat e (Any N-term)	Difuran
Dihydroxyimidaz olidine	Diiodo	Diironsubcluster	Diisopropylphos phate
Diisopropylphos phate (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)13 C(2)	Dimethyl:2H(4)13 C(2) (Any N- term)	Dimethyl:2H(6)
Dimethyl:2H(6)13 C(2)	Dimethyl:2H(6)13 C(2) (Protein N- term)	DimethylamineG MBS	DimethylArsino
DimethylpyrroleA dduct	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	methylsulfonylmethyl	Methylthio
Methylthio (Any N-term)	MG-H1	Microcin (Protein C-term)	MicrocinC7 (Protein C-term)
MM-diphenylpentanone	MMTS	Molybdopterin	MolybdopterinG D
MolybdopterinG D+Delta:S(-1)Se(1)	mTRAQ	mTRAQ-Lys0	mTRAQ-Lys4
mTRAQ-Lys8	mTRAQ-Nter0	mTRAQ-Nter4	mTRAQ-Nter8

mTRAQ:13C(3)15 N(1)	mTRAQ:13C(6)15 N(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- diMePhosphate
O- Isopropylmethyl phosphonate	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)	phenylsulfonyl ethyl
Phospho	Phospho (ST)	Phospho (STY)	Phosphoadenosine
Phosphogluconylation	Phosphogluconylation (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- >Hydroxykynure nin
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	UgiJoullieProGly ProGly	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:EGScleave d	Xlink:EGScleave d (Protein N- term)	Xlink:SMCC
Xlink:SSD	ZGB	ZGB (Any N- term)	