

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    "Workflow": {
22      "Method_Evaluation": false
23    },
24    "Pipeline_Mode": {
25      "Generate_SNE_File": true
26    },
27    "XIC_Extraction": {
28      "MS1_Mass_Tolerance_Strategy": "dynamic",
29      "MS2_Mass_Tolerance_Strategy": "dynamic"
30    }
31  },
32  "Pulsar_Search": {
33    "Peptides": {
34      "Enzymes_Cleavage_Rules": [
35        "Trypsin/P"
36      ],
37      "Digest_Type": "Specific",
38      "Max_Peptide_Length": 52,
39      "Min_Peptide_Length": 7,
40      "Missed_Cleavages": 2,
41      "Toggle_NTerminal_M": true
42    },
43    "Modifications": {
44      "Max_Variable_Modifications": 5,
```

```

45     "Fixed_Modifications": [
46         "Carbamidomethyl (C)"
47     ],
48     "Variable_Modifications": [
49         "Acetyl (Protein N-term)",
50         "Oxidation (M)"
51     ]
52 "DIA_Analysis": {
53     "Identification": {
54         "Precursor_PEP_Cutoff": 0.2,
55         "Precursor_Qvalue_Cutoff": 0.01,
56         "Precursor_Qvalue_Cutoff_Experiment": 0.01,
57         "Protein_Qvalue_Cutoff_Experiment": 0.01,
58         "Protein_Qvalue_Cutoff_Run": 0.05,
59         "Protein_PEP_Cutoff": 0.75,
60         "Single_Hit_Protein_Rule": "StratifiedFDR",
61         "Run_Level_Protein_Scoring": "all_observation"
62     },
63     "Quantification": {
64         "Proteotypicity_Filter": "none",
65         "Data_Filtering": "qvalue",
66         "Cross_Run_Normalization": true,
67         "Imputation_Strategy": "none",
68         "Perform_IM_Peak_Picking": true,
69         "Perform_background_noise_removal": true
70     },
71     "PTM_Workflow": {
72         "PTM_Localization": false,
73         "Probability_Cutoff": 0.0
74     },
75     "Workflow": {
76         "Method_Evaluation": false
77     },
78     "Pipeline_Mode": {
79         "Generate_SNE_File": true
80     },
81     "XIC_Extraction": {
82         "MS1_Mass_Tolerance_Strategy": "dynamic",
83         "MS2_Mass_Tolerance_Strategy": "dynamic"
84     }
85 },
86 "Pulsar_Search": {
87     "Peptides": {
88         "Enzymes_Cleavage_Rules": [
89             "Trypsin/P"
90         ],
91         "Digest_Type": "Specific",
92         "Max_Peptide_Length": 52,
93         "Min_Peptide_Length": 7,
94         "Missed_Cleavages": 2,
95         "Toggle_NTerminal_M": true
96     },
97     "Modifications": {
98         "Max_Variable_Modifications": 5,
99         "Fixed_Modifications": [
100             "Carbamidomethyl (C)"
101         ],
102         "Variable_Modifications": [

```

```

103     "Acetyl (Protein N-term)",
104     "Oxidation (M)"
105 ],
106 "Search_Mode": "Closed Search"
107 },
108 "Identification": {
109     "PSM_FDR": 0.01,
110     "Peptide_FDR": 0.01,
111     "Protein_Group_FDR": 0.01,
112     "DirectDIA_Workflow": "directdia_deep",
113     "RT_Sampling_Reduction": 1
114 },
115 "Tolerances": {
116     "Thermo_IonTrap": {
117         "Calibration_Search": "dynamic",
118         "Calibration_Search_MS1_Correction_Factor": 1.0,
119         "Calibration_Search_MS2_Correction_Factor": 1.0,
120         "Main_Search": "dynamic",
121         "Main_Search_MS1_Correction_Factor": 1.0,
122         "Main_Search_MS2_Correction_Factor": 1.0
123     },
124     "Thermo_OrbiTrap": {
125         "Calibration_Search": "dynamic",
126         "Calibration_Search_MS1_Correction_Factor": 1.0,
127         "Calibration_Search_MS2_Correction_Factor": 1.0,
128         "Main_Search": "dynamic",
129         "Main_Search_MS1_Correction_Factor": 1.0,
130         "Main_Search_MS2_Correction_Factor": 1.0
131     },
132     "TOF": {
133         "Calibration_Search": "dynamic",
134         "Calibration_Search_MS1_Correction_Factor": 1.0,
135         "Calibration_Search_MS2_Correction_Factor": 1.0,
136         "Main_Search": "dynamic",
137         "Main_Search_MS1_Correction_Factor": 1.0,
138         "Main_Search_MS2_Correction_Factor": 1.0
139     }
140 },
141 "MS2": {
142     "Ion_Types": [
143         "b",
144         "y"
145     ]
146 }
147 }
148 }
149
150

```

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", "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_NTerminalM | 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 |
| PSM_FDR | Double between 0 and 1 |
| Peptide_FDR | Double between 0 and 1 |
| Protein_Group_FDR | Double between 0 and 1 |
| Calibration_Search | "relative", "static", "dynamic" |
| Main_Search | "relative", "static", "dynamic" |
| Calibration_Search_MS1_Correction_Factor | Double between 0.1 and 100 |
| Calibration_Search_MS2_Correction_Factor | Double between 0.1 and 100 |
| Main_Search_MS1_Correction_Factor | Double between 0.1 and 100 |
| Main_Search_MS2_Correction_Factor | Double between 0.1 and 100 |
| Calibration_Search_MS1_Tolerance | Non-negative double |
| Calibration_Search_MS2_Tolerance | Non-negative double |
| Main_Search_MS1_Tolerance | Non-negative double |
| Main_Search_MS2_Tolerance | Non-negative double |
| 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> | r_Search" |
| Search archive merging | lg -se Pulsar -sa search_arch1.psar -k output_lirary | "Pulsar_Search" settings are affecting library generation from search archive |
| 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 |
| α-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 | DEDGFLYMVYASQETF G |
| 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 | GPAnchor (Protein C-term) | Guanidinyl |
| Guanidinyl (Any N-term) | HCysteinylyl | 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 |

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|-----------------------------------|-------------------------------------|-----------------------------|------------------------------|
| 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-anhyropyrrrole |
| LG-anhyropyrrrole (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 |

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|---|---------------------------|---------------------------|--|
| 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:alpha: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 |
| Myristoyl (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) |

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|---------------------------------------|------------------------------------|-------------------------------------|--------------------------------------|
| 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 |

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|----------------------------|------------------------------------|-----------------------------------|-------------------------------|
| 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 |

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|---------------------------|------------------------------------|---------------------------|-------------------------------------|
| 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 |

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| 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 |

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|------------------------------|----------------------------|-----------------------------------|----------------|
| 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) | |