

SUPPLEMENTAL INFORMATION:

**Circulating oxidized LDL increased in patients with acute myocardial infarction is accompanied by heavily modified HDL.**

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**Supplemental Table S1. List of variable modifications**

<b>Biological Modification Set</b>		
Modification	Residue	Specificity
1 Acetyl		Protein N-term
2 Acetyl		N-term
3 Acetyl	Lysine	
4 Acetyl	Serine	
5 AMP	Histidine	
6 AMP	Lysine	
7 AMP	Threonine	
8 AMP	Tyrosine	
9 Arg->Orn	Arginine	
10 Biotin		Protein N-Term
11 Biotin	Lysine	
12 Bromo	Histidine	
13 Bromo	Phenylalanine	
14 Bromo	Tyrosine	
15 Bromo	Tryptophan	
16 Carboxy	Aspartic Acid	
17 Carboxy	Glutamic Acid	
18 Chloro	Tyrosine	
19 Cysteinylyl	Cysteine	
20 Cys->Oxoalanine	Cysteine	
21 Deamidated	Arginine	
22 dHex	Asparagine	
23 dHex	Serine	
24 dHex	Threonine	
25 Dibromo	Tyrosine	
26 Dichloro	Tyrosine	
27 Diiodo	Histidine	
28 Diiodo	Tyrosine	
29 Dimethyl	Arginine	
30 Dimethyl	Lysine	
31 Dioxidation	Arginine	
32 Dioxidation	Lysine	
33 Dioxidation	Proline	
34 Dioxidation	Tyrosine	
35 Diphthamide	Histidine	
36 FAD	Cysteine	
37 FAD	Histidine	
38 Farnesyl	Cysteine	
39 Iodo	Histidine	
40 Iodo	Tyrosine	
41 FormaldehydeAdduct	Tryptophan	
42 Formyl		Protein N-Term
43 FormylMet		Protein N-Term

**Supplemental Table S1. List of variable modifications**

<b>Biological Modification Set (continued)</b>		
Modification	Residue	Specificity
44 Geranylgeranyl	Cysteine	
45 Glucuronyl		Protein N-Term
46 Glucuronyl	Serine	
47 Glutathione	Cysteine	
48 GlyGly	Lysine	
49 Hex		Protein N-Term
50 Hex	Asparagine	
51 Hex	Lysine	
52 Hex	Serine	
53 Hex	Threonine	
54 Hex	Tryptophan	
55 Hex(1)HexNAc(1)	Asparagine	
56 Hex(1)HexNAc(1)	Serine	
57 Hex(1)HexNAc(1)	Threonine	
58 Hex(1)HexNAc(1)NeuAc(1)	Asparagine	
59 Hex(1)HexNAc(1)NeuAc(1)	Serine	
60 Hex(1)HexNAc(1)NeuAc(1)	Threonine	
61 Hex(1)HexNAc(1)NeuAc(2)	Asparagine	
62 Hex(1)HexNAc(1)NeuAc(2)	Serine	
63 Hex(1)HexNAc(1)NeuAc(2)	Threonine	
64 HexNAc	Asparagine	
65 HexNAc	Serine	
66 HexNAc	Threonine	
67 Hydroxyfarnesyl	Cysteine	
68 LeuArgGlyGly	Lysine	
69 Lipoyl	Lysine	
70 Lys->Hydroxyallysine	Lysine	
71 Methyl		Protein N-Term
72 Methyl	Arginine	
73 Methyl	Asparagine	
74 Methyl	Aspartic Acid	
75 Methyl	Cysteine	
76 Methyl	Glutamic Acid	
77 Methyl	Glutamine	
78 Methyl	Histidine	
79 Methyl	Isoleucine	
80 Methyl	Leucine	
81 Methyl	Lysine	
82 Methyl	Serine	
83 Methyl	Threonine	
84 Methyl		Protein C-Term
85 Methylthio	Asparagine	
86 Methylthio	Aspartic Acid	

**Supplemental Table S1. List of variable modifications**

**Biological Modification Set** (*continued*)

Modification	Residue	Specificity
87 Myristoyl	Glycine	Protein N-Term
88 Myristoyl	Lysine	
89 NeuAc	Serine	
90 NeuAc	Threonine	
91 NeuAc	Asparagine	
92 NeuGc	Serine	
93 NeuGc	Threonine	
94 NeuGc	Asparagine	
95 Nicotinyl	Lysine	
96 Nitro	Tryptophan	
97 Nitro	Tyrosine	
98 Oxidation	Arginine	
99 Oxidation	Asparagine	
100 Oxidation	Aspartic Acid	
101 Oxidation	Lysine	
102 Oxidation	Phenylalanine	
103 Oxidation	Tyrosine	
104 Palmitoyl	Cysteine	
105 Palmitoyl	Lysine	
106 Palmitoyl	Serine	
107 Palmitoyl	Threonine	
108 Phospho	Arginine	
109 Phospho	Aspartic Acid	
110 Phospho	Histidine	
111 Phospho	Lysine	
112 Phospho	Serine	
113 Phospho	Threonine	
114 Phospho	Tyrosine	
115 Phosphopantetheine	Serine	
116 Ser->Oxoalanine	Serine	
117 Succinyl		Protein N-Term
118 Sulfo	Serine	
119 Sulfo	Threonine	
120 Sulfo	Tyrosine	
121 Trimethyl	Arginine	
122 Trimethyl	Lysine	
123 Trioxidation	Tyrosine	
124 Tripalmitate	Cysteine	Protein N-Term
125 Ammonia-loss	Serine	N-term
126 Ammonia-loss	Threonine	N-term

**Supplemental Table S1. List of variable modifications**

<b>Generic Workup Modification Set (always invoked)</b>		
Modification	Residue	Specificity
1 Delta:H(2)C(2)		N-Term
2 Delta:H(2)C(2)	Histidine	
3 Delta:H(2)C(2)	Lysine	
4 Delta:H(4)C(2)		N-Term
5 Delta:H(4)C(2)	Histidine	
6 Delta:H(4)C(2)	Lysine	
7 Amino	Tyrosine	
8 Arg->GluSA	Arginine	
9 Carbamyl		N-term
10 Carbamyl	Arginine	
11 Carbamyl	Lysine	
13 Cation:Cu[I]	Aspartic Acid	
14 Cation:Cu[I]	Glutamic Acid	
15 Cation:Cu[I]		C-Term
16 Cation:K	Aspartic Acid	
17 Cation:K	Glutamic Acid	
18 Cation:K		C-Term
19 Cation:Na	Aspartic Acid	
20 Cation:Na	Glutamic Acid	
21 Cation:Na		C-Term
22 Cys->Dha	Cysteine	
23 Deamidated	AsnOrAsp	
24 Deamidated	Asparagine	
25 Deamidated	GlnOrGlu	
26 Deamidated	Glutamine	
27 Dehydrated	Aspartic Acid	
28 Dehydrated	Glutamic Acid	
29 Dehydrated	Serine	
30 Dehydrated	Threonine	
31 Dioxidation	Cysteine	
32 Dioxidation	Methionine	
33 Dioxidation	Tryptophan	
34 Formyl		N-Term
35 Formyl	Lysine	
36 Gln->pyro-Glu	Glutamine	N-Term
37 Glu->pyro-Glu	Glutamic Acid	N-Term
38 Lys->Allysine	Lysine	
39 Oxidation	Cysteine	
40 Oxidation	Histidine	
41 Oxidation	Methionine	
42 Oxidation	Proline	
43 Oxidation	Tryptophan	
44 Pro->pyro-Glu	Proline	

## Supplemental Table S1. List of variable modifications

### **Generic Workup Modification Set (always invoked) (continued)**

Modification	Residue	Specificity
45 Pro->Pyrrolidinone	Proline	C-Term
46 Trioxidation	Cysteine	
47 Trioxidation	Tryptophan	
48 Trp->Hydroxykynurenin	Tryptophan	
49 Trp->Kynurenin	Tryptophan	
50 Dethiomethyl	Methionine	
51 Met->Hse	Methionine	

### **Iodoacetamide Cysteine Alkylation Modification Set**

Modification	Residue	Specificity
1 Ammonia-loss	Cysteine	N-term
2 Carbamidomethyl		N-term
3 Carbamidomethyl	Aspartic Acid	
4 Carbamidomethyl	Cysteine	
5 Carbamidomethyl	Glutamic Acid	
6 Carbamidomethyl	Histidine	
7 Carbamidomethyl	Lysine	
8 Carbamyl	Methionine	
9 Iodo	Histidine	
10 Iodo	Tyrosine	

### **User defined Modification Set**

Modification	Residue	Specificity
1 acrolein addition +38	lysine	
2 acrolein addition +56	lysine	
3 acrolein addition +76	lysine	
4 acrolein addition +94	lysine	
5 acrolein addition +112	lysine	
6 reduced acrolein addition +lysine		
7 reduced acrolein addition +lysine		
8 reduced HNE +158	histidine	
9 ONE addition +154	lysine	
10 hexanoyl addition +98	lysine	
11 HPNE addition +172	lysine	
12 MDA adduct +54	lysine	
13 MDA adduct +62	lysine	

**Supplemental Table S2. List of 45 species monitored by LC-MS/MS**

m/z	Molecular species	m/z	Molecular species
S/MUFA-PC		Long chain oxPC	
732.6	32:1	722.6	34:2+14
734.6	32:0	774.6	34:2+16
760.6	34:1	790.6	34:2+32
788.6	36:1	796.6	36:4+14
790.6	36:0	798.6	36:4+16
678.4	28:0	814.6	36:4+32
		800.6	36:2+14
		802.6	36:2+16
PUFA-PC			
756.6	34:3	818.6	36:2+32
758.6	34:2	824.6	38:4+14
780.6	36:5	826.6	38:4+16
782.6	36:4	842.6	38:4+32
784.6	36:3		
786.6	36:2	Cleaved oxPC	
806.6	38:6	594.6	1-palmitoyl-2-(5-oxovaleroyl) PC
808.6	38:5	610.6	1-palmitoyl-2-glutaroyl PC
810.6	38:4	622.6	1-stearoyl-2-(5-oxovaleroyl) PC
834.6	40:6	638.6	1-stearoyl-2-glutaroyl PC
838.6	40:4	650.6	1-palmitoyl-2-(9-oxo-nonanoyl) PC
		664.6	1-palmitoyl-2-(5-oxo-octenoyl) PC
LysoPC		666.6	1-palmitoyl-2-azelaoyl PC
496.2	16:0-LPC	692.6	1-stearoyl-2-(5-oxo-octenoyl) PC
524.2	18:0-LPC	706.6	1-stearoyl-2-(6-oxo-nonenoyl) PC
494.2	16:1-LPC	652.6	1-O-hexadecyl-2-azelaoyl PC
522.2	18:1-LPC		
482.2	16:0-LPC-alkyl		
510.2	18:0-LPC-alkyl		