One-Pot Shotgun Quantitative Mass Spectrometry Characterization of Histones

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Supplemental Table 1. Summary of H2A/H2B variants detected through analysis of the HPLC purified proteins and one-pot analyses of unfractionated bulk histones acid extracted from HeLa cells.

Histone Variants	Accession Number	H2A HPLC purified	H2B HPLC purified	One-pot Shotgun (CAD-MS/MS)	One-pot Shotgun Decision-tree (CAD/ETD)
Histone H2A					
H2AM_HUMAN Histone H2A.m (H2A/m)	121986	+	+	+	+
histone H2a	15617199	+	+	+	+
histone H2A	25092737	+		+	+
H2A histone family, member C	4504239	+		+	+
H2A histone family, member O	4504251	+	+	+	+
H2A histone family, member Y isoform 2	93141020	+	+	+	+
Core histone macroH2A2.2	8923920	+	+		
H2A histone family, member Z	4504255	+	+	+	+
H2A histone family, member V isoform 4	41406069	+	+		
H2A histone family, member V isoform 5	41406071	+			
H2AFX	48146275	+		+	+
histone H2A/r	49659927	+		+	+
Histone H2a	12654707			+	+
H2A histone family, member J isoform 1	8922758			+	+
histone H2A	28195394			+	+
Histone H2B					
H2B histone family, member B	20336752		+	+	+
H2B histone family, member C	4504259	+	+	+	+
H2B histone family, member R	20336754		+	+	+
H2B histone family, member E	4504263		+	+	+
HIST1H2BA protein	42542679		+	+	+

Supplemental Table 2. Summary of abundant post-translational modifications detected on histone H3

through analysis of HPLC purified histone H3.2 protein and one-pot analyses of bulk histones coupled

to nanoLC-MS/MS.

Histone H3 peptides	H3 HPLC purified	One-pot Shotgun (CID-MS/MS)	One-pot Shotgun Decision-tree (CID/ETD)
TKQTAR			
Unmod	+	+	+
K4me1	+	+	+
K4me2	+	+	+
K4me3	+	-	-
K4ac	+	+	+
KSTGGKAPR			
Unmod	+	+	+
K9me1	+	+	+
K9me2	+	+	+
K9me3	+	+	+
K9ac	+	+	+
K14ac	+	+	+
K9me1 K14ac	+	+	+
K9me2 K14ac	+	+	+
K9me3 K14ac	+	+	+
K9acK14ac	+	+	+
KQLATKAAR			
Unmod	+	+	+
K18me1	+	+	+
K23me1	+	+	+
K18ac	+	+	+
K23ac	+	+	+
K18acK23ac	+	+	+
KSAPATGGVKKPHR			
Unmod	+	+	+
K27me1	+	+	+
K27me2	+	+	+
K27me3	+	+	+
K27ac	+	+	+
K36me1	+	+	+
K36me2	+	+	+
K36me3	+	+	+
K27me1K36me1	+	+	+
K27me1K36me2	+	+	+
K27me1K36me3	+	+	-
K27me2K36me1	+	+	+
K27me2K36me2	+	+	-
K27me2K36me3	+	-	+
K27me3K36me1	+	+	+
K27me3K36me2	+	+	-
K27me3K36me3	-	-	
YQKSTELLIR			
Unmod	+	+	+
K56me1	+	+	+
K56ac	+	+	+
KLPFQR			
Unmod		+	+
K65me1	+	+	+
	+		
EIAQDFKTDLR			
Unmod	+	+	+
K79me1	+	+	+
K79me2	+	+	+
K79ac	+	+	+