Correlation settings	
Insertion of new peptides • do not insert new peptides • insert peptides only in range	 checked unchecked
LC peak detection • left LC window (secs) • right LC window (secs)	 30 30
„use fixed"	Wild type
Options	
Include in preselected peptides (PSPs) • bold red • light red, • bold black • parenthesized • peptide filter	 checked checked checked checked Mascot score 1 -200
Recalibration of preselected peptides • domain • peptide filter	 Frequency, 1/^0.5 (OrbiTrap) Mascot score 30 - 200
Validation of preselected peptides • peptide filter	 Mascot score 15 - 200
Classification of preselected peptides (PSPs) by Mascot score • category A • category B • category C • protein is validated by default if ABC score is greater than or equal to	 15 15 15 30
Quantitation mode	v2.2 ICAT_9C
MGF file generator	NewDTASupercharge, up to 1.18....
Raw file type	LTQ-FT/LTQ OrbiTrap (.raw)
Type(s) for quantitation	all MS spectra

SUPPLEMENTAL TABLE 1. MSQuant parameters used for quantification of LC-MS/MS data