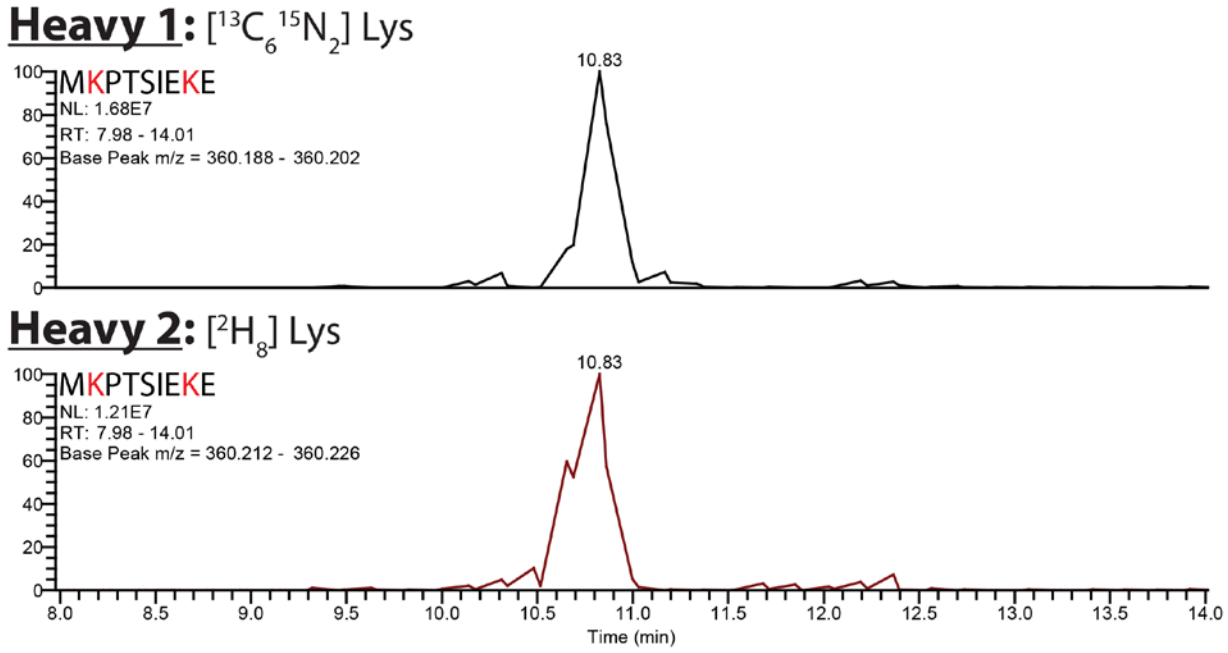
Neutron Encoded Labeling for Peptide Identification

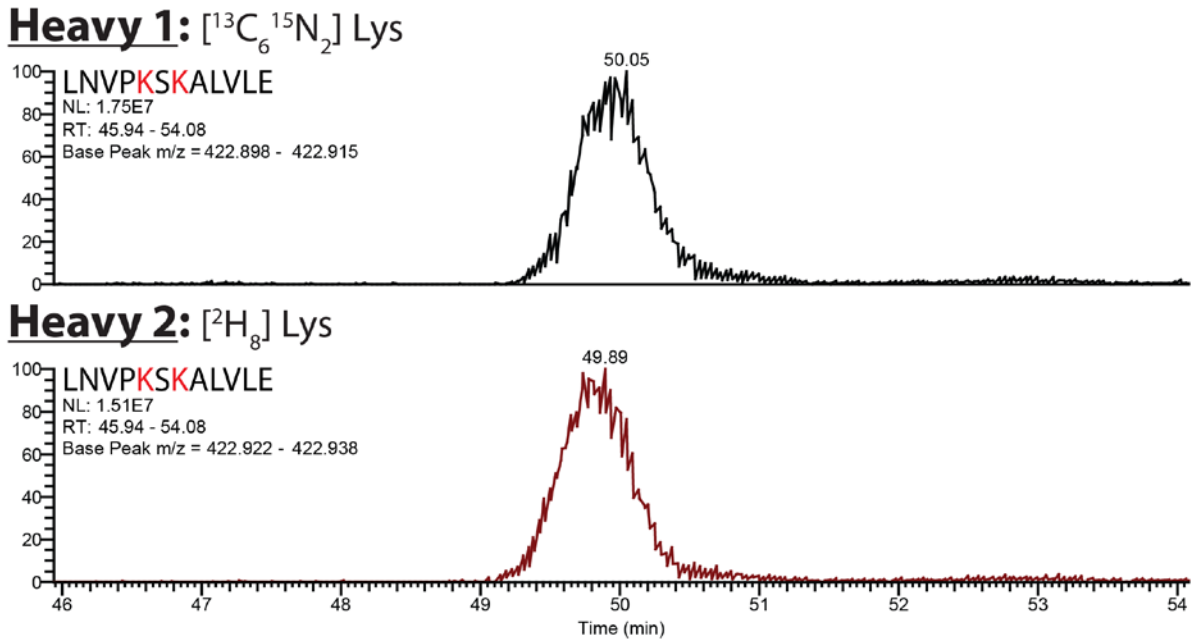
Supplementary Material

Mass Shift mDa	# of Leucines					
# of Lysines	0	1	2	3	4	5
0	0.0	26.8	53.5	80.3	107.1	133.9
1	36.0	62.8	89.6	116.3	143.1	169.9
2	72.0	98.8	125.6	152.4	179.1	205.9
3	108.0	134.8	161.6	188.4	215.1	241.9
4	144.1	170.8	197.6	224.4	251.2	277.9
5	180.0	206.8	233.6	260.4	287.2	313.9

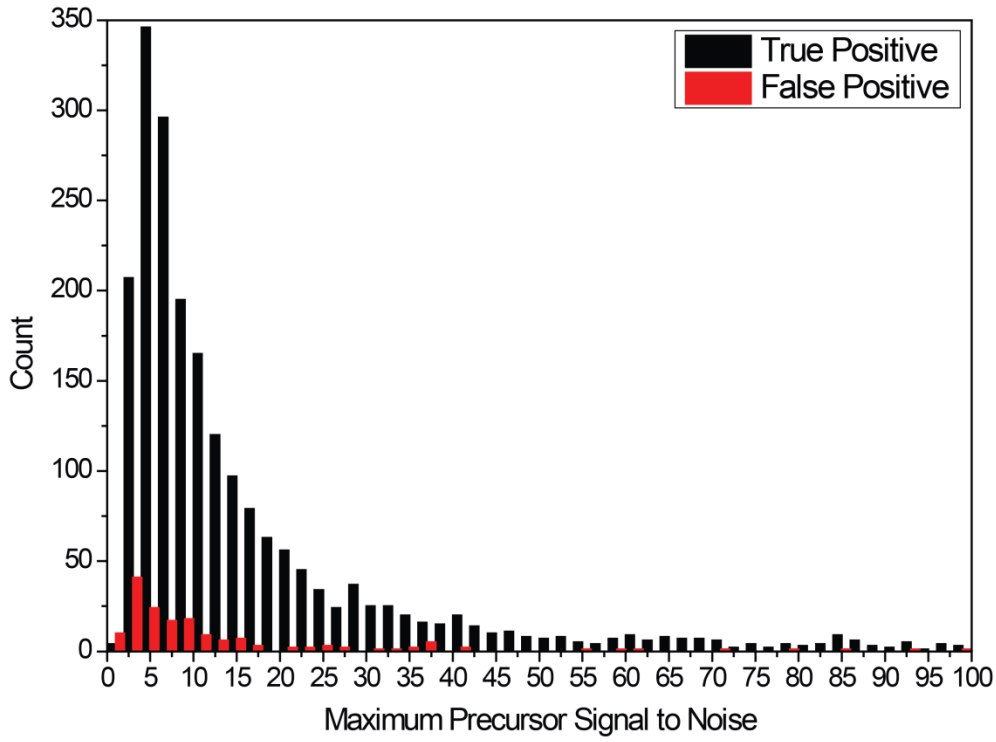
Supplementary Figure 1. Mass Shifts of NeuCode Lysine and Leucine Combinations.



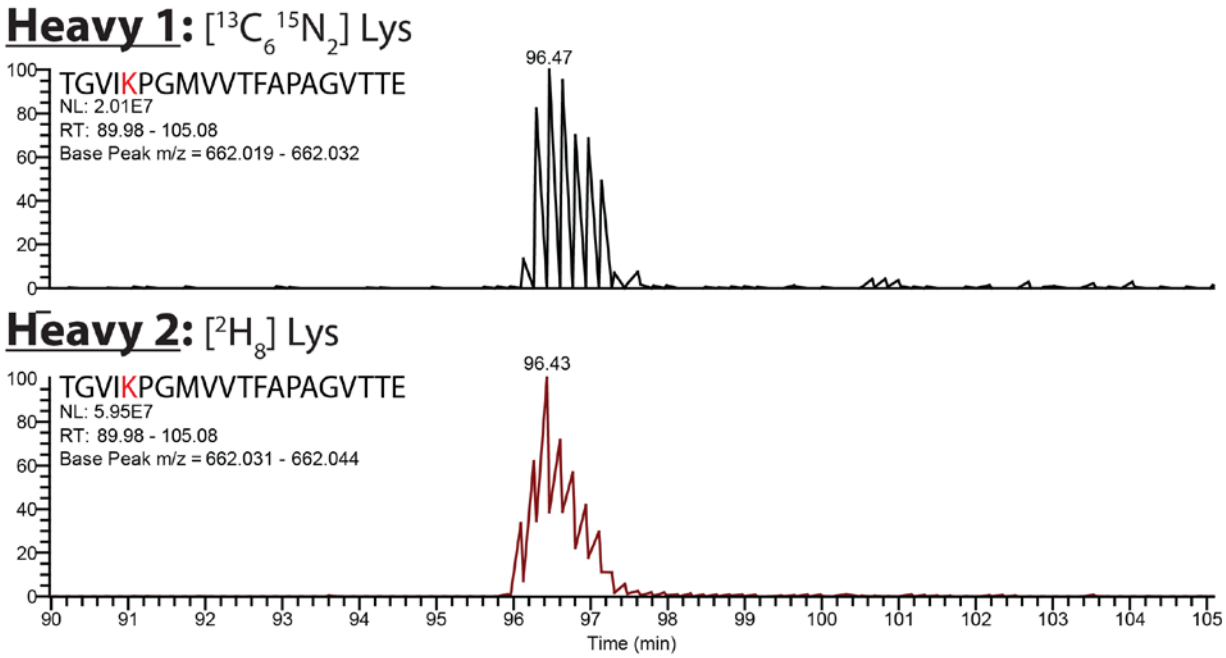
Supplementary Figure 2. XIC of the peptide MKPTSIEKE labeled with lysine isotopologues.



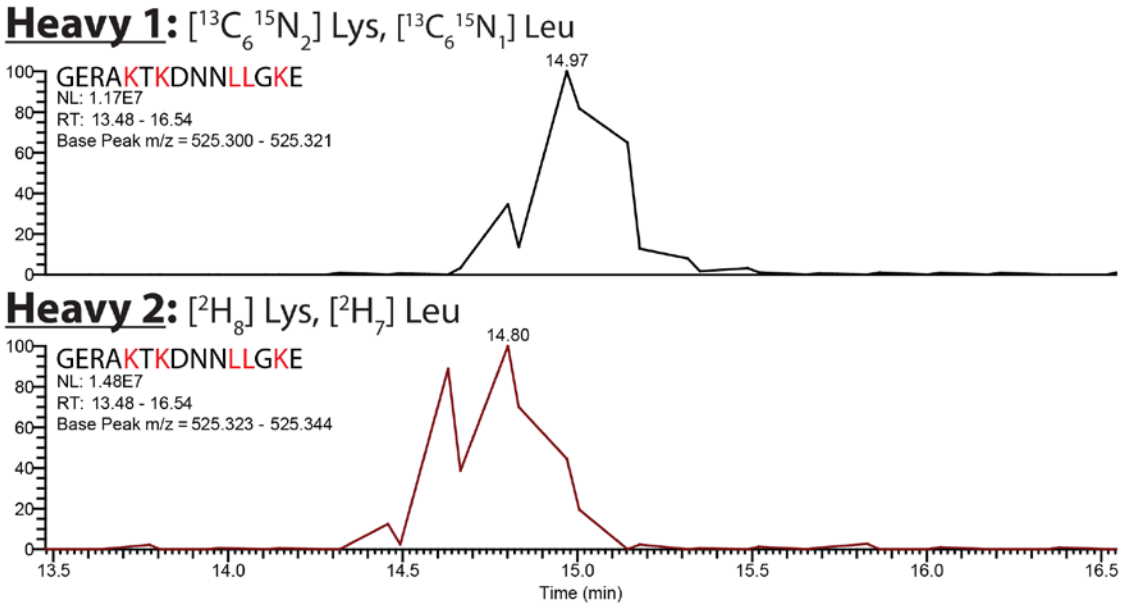
Supplementary Figure 3. XIC of the peptide LNVPKSKALVLE labeled with lysine isotopologues.



Supplementary Figure 4. Number of true and false positive results as a function of maximum precursor signal to noise. For all scored precursors AAC determined the likely number of lysine residues and filtered possible peptide matches based on that information in addition to accurate mass. True positives represent cases where the peptide identified by database search is still under consideration, whereas false positives represent cases where the correct peptide was eliminated as a choice.



Supplementary Figure 5. . XIC of the peptide TGVIKPGMVVTFAPAGVTTE labeled with lysine isotopologues. Note, that these species are not separated in the 30K MS^1 resulting in zero signal for the "Heavy 1" peptide isotopologue in the 30K MS^1 spectra.



Supplementary Figure 6. XIC of the peptide GERAKTKDNNLLGKE labeled with lysine and leucine isotopologues.