A Ubiquitous but Overlooked Side Reaction in Dimethyl Labeling of Peptides

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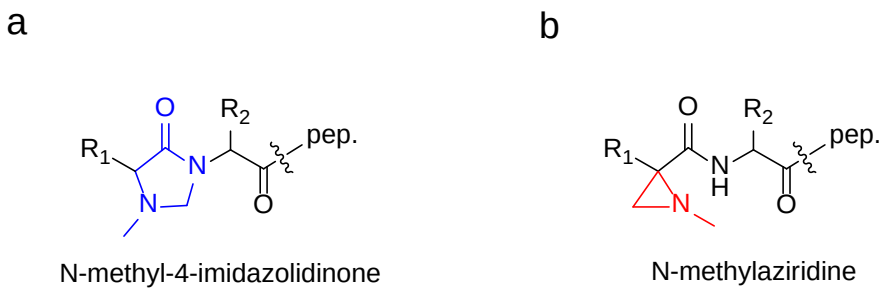

Figure S1. The two possible structures for the +26 Da modification at peptide N-termini occurring in peptide dimethylation with formaldehyde and $NaBH_3CN$.

Figure S2. a, ^{1}H spectrum

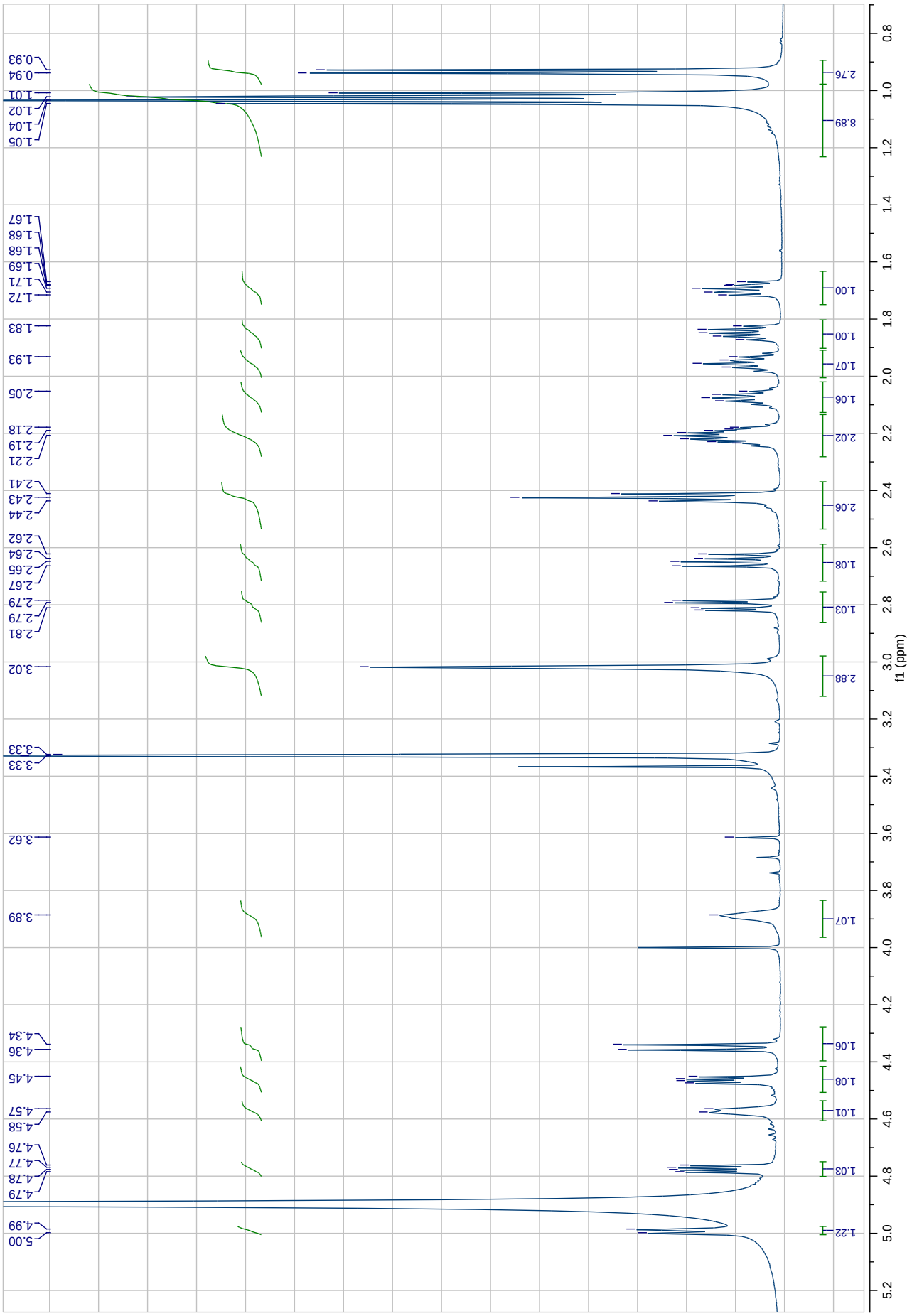

Figure S2. b, ^{13}C spectrum

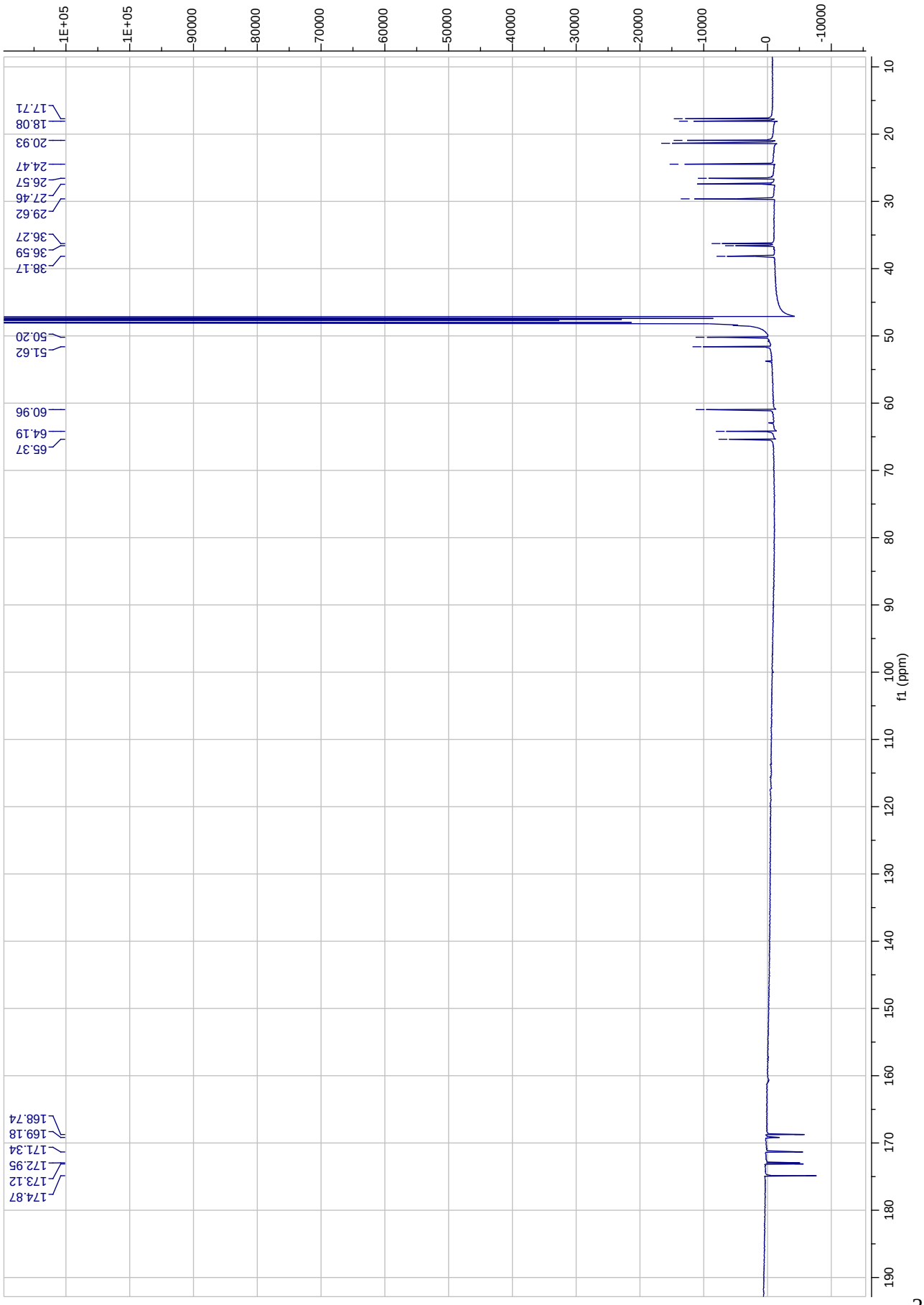

Figure S2. c, ^{1}H-^{13}C HSQC spectrum

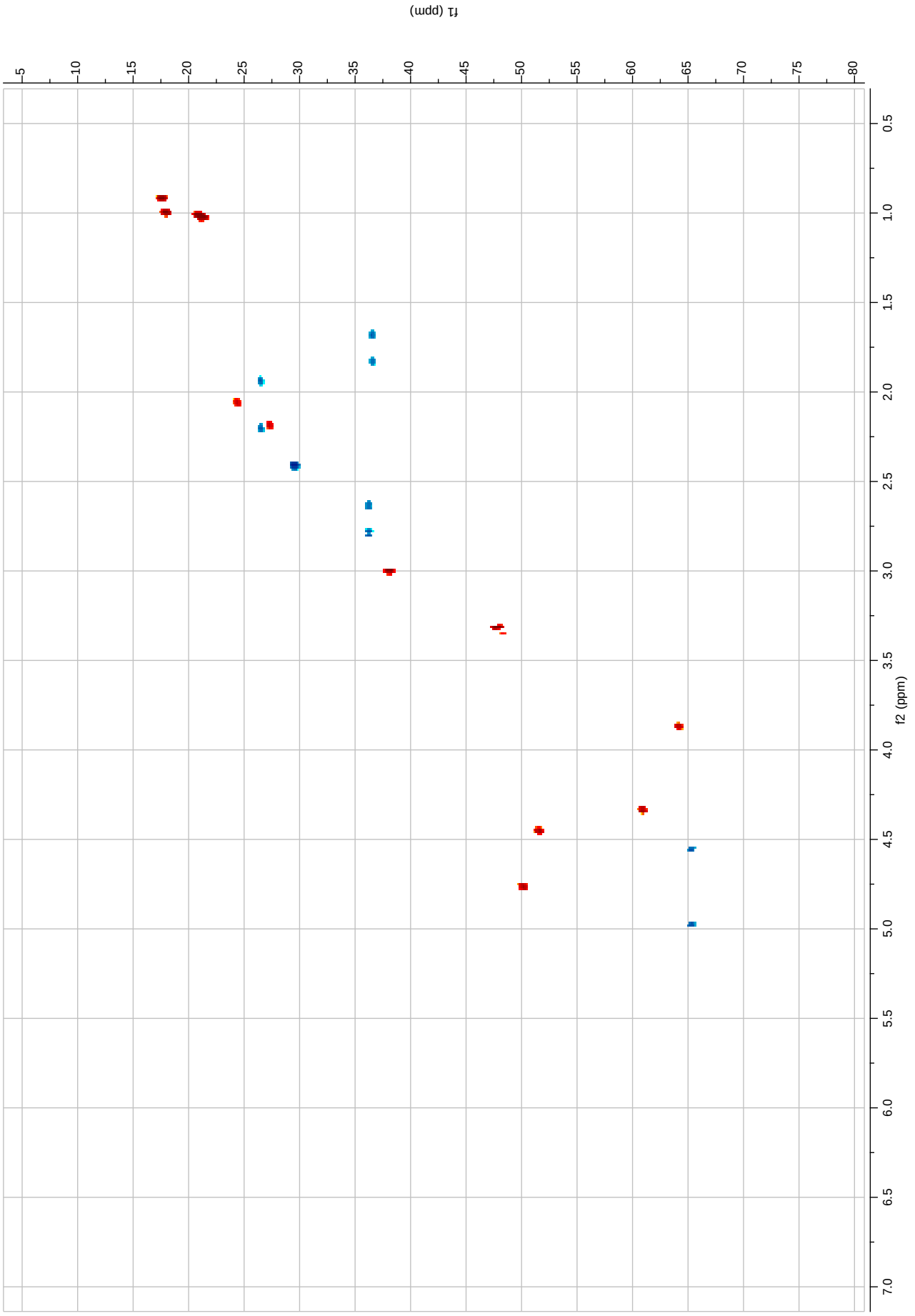

Figure S2. d, ^{1}H-^{1}H COSY spectrum

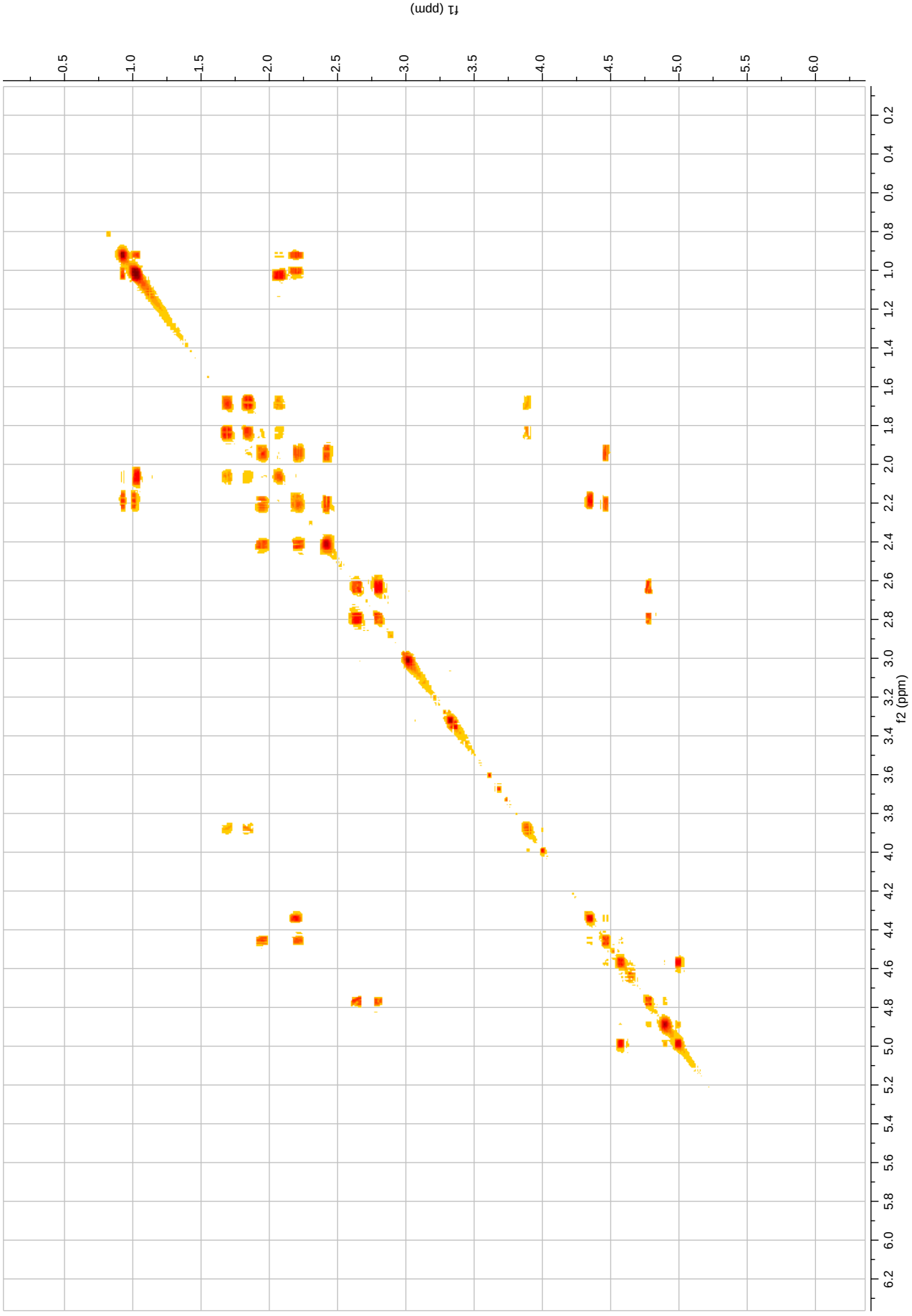

Figure S2. e, ^{1}H-^{13}C HMBC spectrum

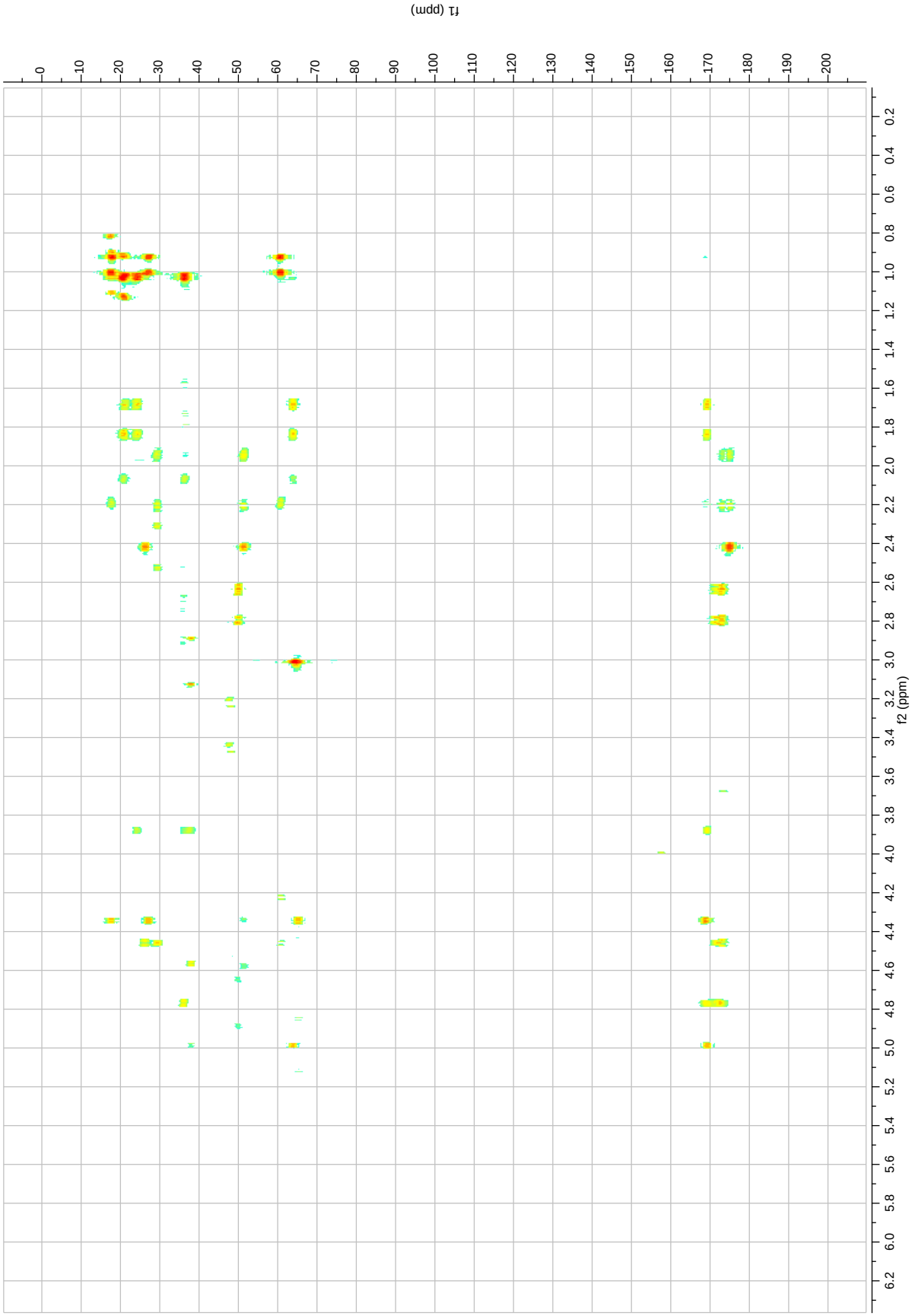

Figure S2. The ^{1}H (a), ^{13}C (b), HSQC (c), COSY (d) and HMBC (e) spectra of the side product originating from the peptide LVNE.

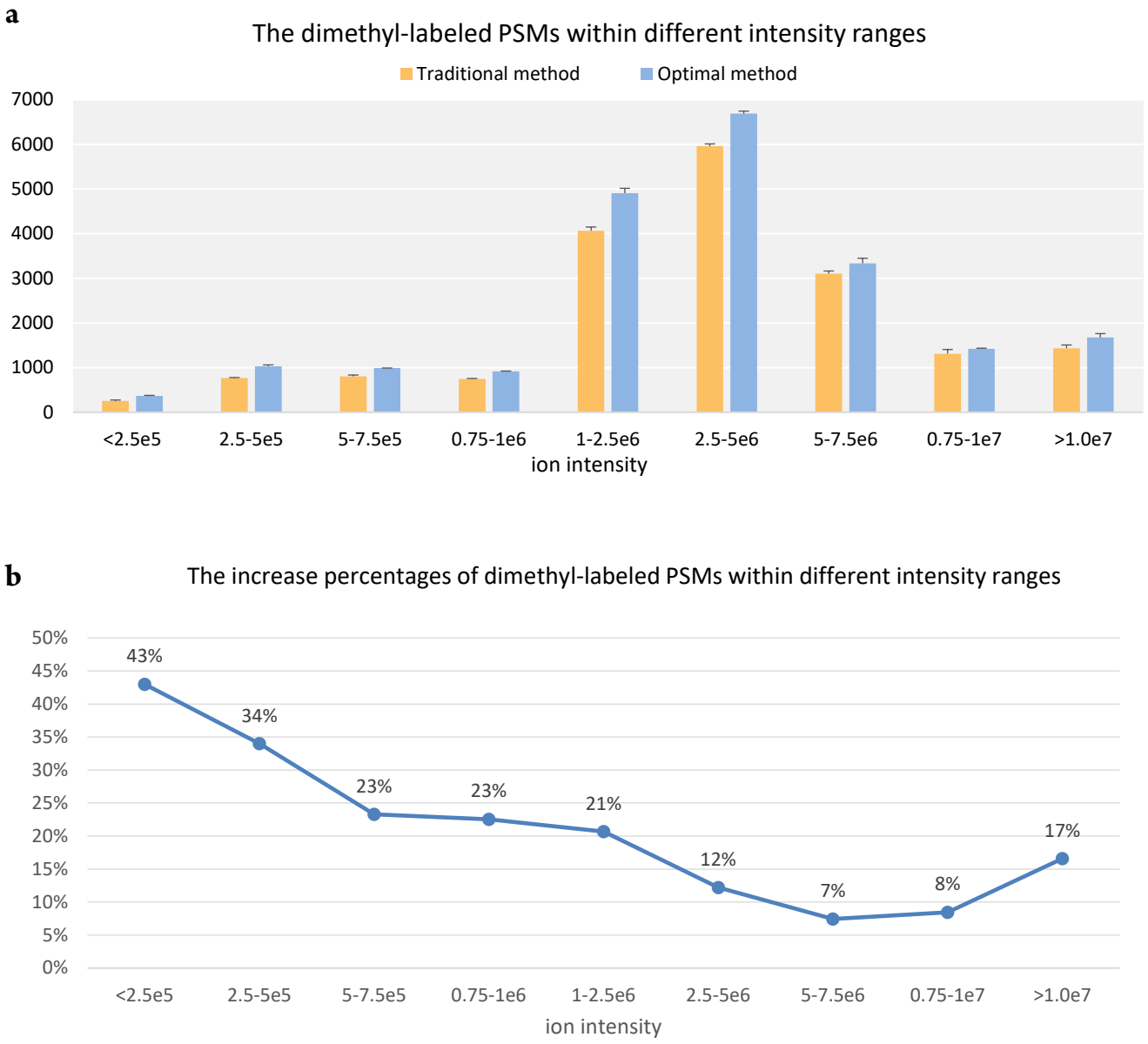

Figure S3. (a) The numbers of dimethyl-labeled PSMs within different intensity ranges from the HeLa digests labeled with traditional method or optimal method. The all numbers are the arithmetic means of 3 technical replicates. (b) The increase percentages of the dimethyl-labeled PSMs with different intensity ranges.