Supplementary Material (SM) for

Cost-Effective Simultaneous Determination of τ- and π-Methylhistidine in Dairy Bovine Plasma from Large Cohort Studies Using Hydrophilic Interaction Ultra-High Performance Liquid Chromatography Coupled to Tandem Mass Spectrometry

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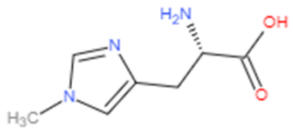
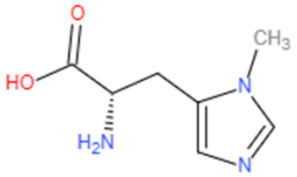
This document provides more detailed information to the main paper mentioned above.

The following information is included:



τ-methylhistidine

Name	Value
InChI	InChI=1S/C7H11N3O2/c1-10-3-5(9-4-10)2-6(8)7(11)12/h3-4,6H,2,8H2,1H3,(H,11,12)/t6-/m0/s1
InChIKey	BRMWTNUJHUMWMS-LURJTMIESA-N
molecular formula	C7H11N3O2
total exact mass	169.0851
SMILES	O=C(O)C(N)CC=1N=CN(C1)C



π-methylhistidine

Name	Value
InChI	InChI=1S/C7H11N3O2/c1-10-4-9-3-5(10)2-6(8)7(11)12/h3-4,6H,2,8H2,1H3,(H,11,12)/t6-/m0/s1
InChIKey	JDHILDINMRGULE-LURJTMIESA-N
molecular formula	C7H11N3O2
total exact mass	169.0851
SMILES	O=C(O)C(N)CC1=CN=CN1C

All information compiled from MassBank of North America (MoNA). (https://mona.fiehnlab.ucdavis.edu/)

Figure S1. Structures and identifiers for τ- and π-methylhistidine

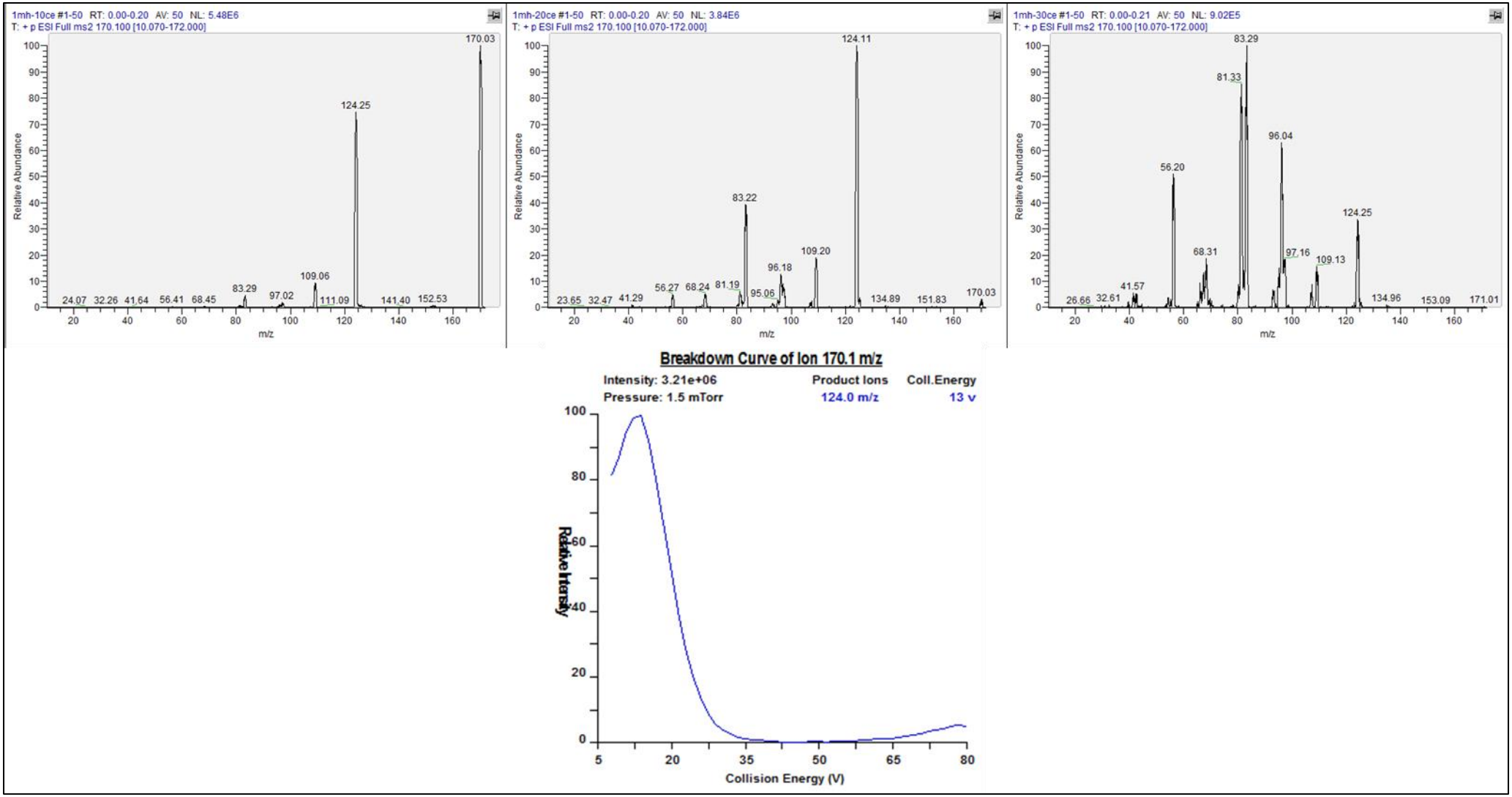


Figure S2. Fragments and abundances of τ-MH with increasing collision energy (Top from left to right: CE 10, 20 and 30 V) along with transition optimization results for ion 124m/z (Bottom). Images produced explicitly for academic review purposes from Thermo Scientific™ Qual Browser in Thermo Xcalibur version 3.063. All content remains in copyright of their respective owners.

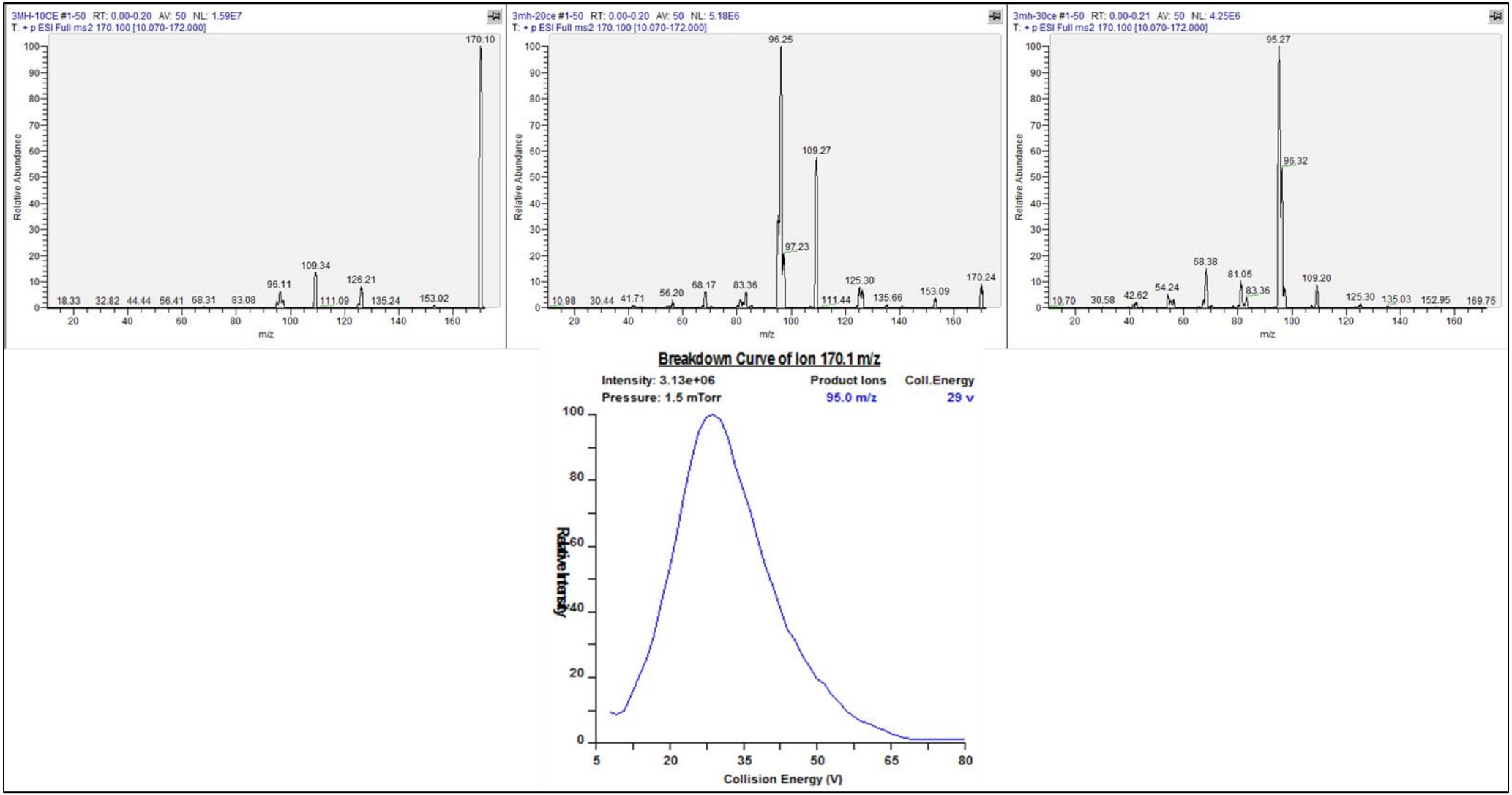


Figure S3. Fragments and abundances of π-MH with increasing collision energy (Top from left to right: CE 10, 20 and 30 V) along with transition optimization results for ion 95m/z (Bottom). Images produced explicitly for academic review purposes from Thermo Scientific™ Qual Browser in Thermo Xcalibur version 3.063. All content remains in copyright of their respective owners.

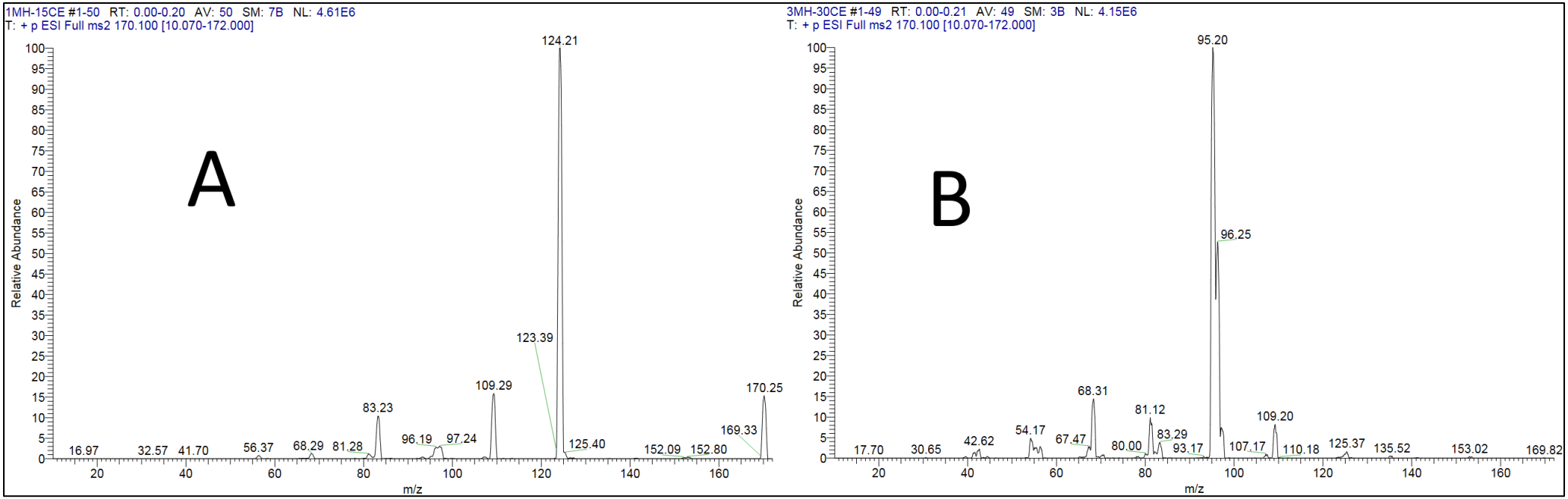


Figure S4. (A): Mass spectrum at a CE of 15 V for τ-MH. The spectrum is an average of 50 scans, from 10 to 172 m/z for the precursor 170 m/z. Ion 124 is the most intense peak in the spectrum, (B): Mass spectrum at a CE of 30 V for π-MH. The spectrum corresponds to the average of 50 scans, from 10 to 172 m/z for the precursor 170 m/z. Ion 95 is the most intense peak in the spectrum.

Table S1. Concentrations of the quality control samples for τ-MH and π-MH

Solution type	**Concentration [µg/L]**	
	τ-MH	**π-MH**
LQC	425.2	354.5
MQC	850.4	708.9
HMQC	1170.4	1028.9
HQC	1410.4	1268.9