

Supplementary Materials: Matrix Effect of Diverse Biological Samples Extracted with Different Extraction Ratios on the Detection of β -N-methylamino-L-alanine by Two Common LC-MS/MS Analysis Methods

Peng Zhao, Jiangbing Qiu, Aifeng Li, Guowang Yan, Min Li and Ying Ji

Table S1. The MRM transitions used for detection of BMAA and its isomers.

Methods	Precursor ion (<i>m/z</i>)	Product ion (<i>m/z</i>)	DP (V)	CE (eV)
HILIC	119	102	30	13
	119	101	30	11
	119	88	30	17
	119	56	30	24
	119	44	30	24
AQC	459	119	30	25
	459	188	30	25
	459	214	30	40
	459	258	30	30
	459	289	30	25
	459	171	30	40

Table S2. The MRM transitions used for detection of amino acids.

Methods	Precursor ion (<i>m/z</i>)	Product ion (<i>m/z</i>)	DP (V)	CE (eV)
Glycine	76	30	20	10
	117	76	20	10
Alanine	90	44	40	15
	90	45	20	45
Serine	106	60	40	15
	106	42	40	30
Proline	116	70	40	20
	157	70	20	40
Valine	118	72	40	20
	118	55	40	30
Threonine	120	74	40	15
	120	56	40	25
Cysteine	122	59	40	35
	163	122	20	10
Isoleucine	132	69	40	30
	132	86	40	15
Leucine	132	86	40	15
	132	44	40	35
Asparagine	133	87	30	12
	133	74	30	16
Aspartic acid	134	74	30	15

	134	88	30	18
Glutamine	147	84	40	20
	147	130	40	15
Lysine	147	67	40	14
	147	84	40	30
Glutamic amid	148	84	30	16
	148	56	30	28
Methionine	150	61	40	35
	150	56	40	20
Histidine	156	110	40	20
	156	82	40	45
Phenylalanine	166	120	40	15
	166	103	40	40
Arginine	175	70	20	35
	175	60	20	15
Tyrosine	182	91	40	25
	182	136	40	30
Tryptophan	205	146	40	20
	205	118	40	35

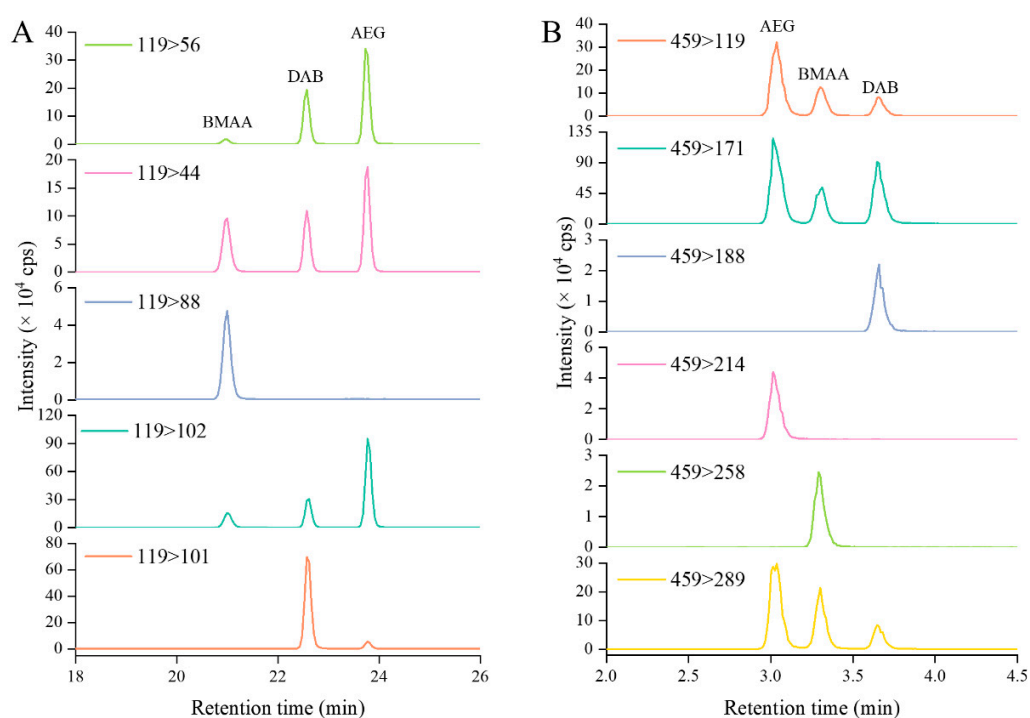


Figure S1. The LC-MS/MS chromatograms of BMAA, DAB and AEG standard detected by the HILIC direct analysis (A) and AQC derivatization method (B).