

**Table S2. MRM parameters for target analytes.** Optimized multiple-reaction monitoring settings for each compound, including the precursor ion  $m/z$ , product ion  $m/z$ , polarity mode, and whether the transition was used as quantifier or qualifier. (Each compound typically has two transitions listed, one quantifier and one qualifier.)

Compound (Abbrev)	Prec. Ion ( $m/z$ )	Prod. Ion ( $m/z$ )	Polarity	Transition Role
IAN-1	157	130	+	Quantifier
IAN-2	157	117	+	Qualifier
IP-1	204	136	+	Quantifier
IP-2	204	148	+	Qualifier
mTR-1	374	107	+	Quantifier
mTR-2	374	242.2	+	Qualifier
ILA-1	204	157.9	-	Quantifier
ILA-2	204	116.1	-	Qualifier
IAA-1	176	130	+	Quantifier
IAA-2	176	103.1	+	Qualifier
ICA-1	160	116	-	Quantifier
ICA-2	160	66	-	Qualifier
IA-1	188	170	+	Quantifier
IA-2	188	115.2	+	Qualifier
IAA-Ala-1	245	88	-	Quantifier
IAA-Ala-2	245	128	-	Qualifier
IAM-1	173	129.9	-	Quantifier
IAM-2	173	127.7	-	Qualifier
ABA-1	263	153	-	Quantifier
ABA-2	263	219.1	-	Qualifier
BAPR-1	358.2	226.1	+	Quantifier
BAPR-2	358.2	147.9	+	Qualifier
ACC-1	102	56	+	Quantifier
ACC-2	102	84	+	Qualifier
DZ-1	222	136	+	Quantifier
DZ-2	222	148.1	+	Qualifier
cZ-1	220	135.9	+	Quantifier
cZ-2	220	202	+	Qualifier
K-1	216	81.1	+	Quantifier
K-2	216	147.8	+	Qualifier
TRP-1	205	146.2	+	Quantifier
TRP-2	205	188.1	+	Qualifier
IAA-Asp-1	291	130.1	+	Quantifier
IAA-Asp-1	291	130.1	+	Qualifier
TRA-1	161	144.1	+	Quantifier
TRA-2	161	117.1	+	Qualifier
oT-1	242	136	+	Quantifier
oT-2	242	107.1	+	Qualifier
IAA-Phe-1	323.2	129.8	+	Quantifier
IAA-Phe-2	323.2	166.3	+	Qualifier

Compound (Abbrev)	Prec. Ion ( <i>m/z</i> )	Prod. Ion ( <i>m/z</i> )	Polarity	Transition Role
GA7-1	329.2	223.1	–	Quantifier
GA7-2	329.2	255	–	Qualifier
IAA-Trp-1	360.1	203.1	–	Quantifier
IAA-Trp-2	360.1	231	–	Qualifier
KR-1	348	216.1	+	Quantifier
KR-2	348	148.2	+	Qualifier
IAA-Val-1	275	130	+	Quantifier
IAA-Val-2	275	229.1	+	Qualifier
ICAlD-1	146	118.2	+	Quantifier
ICAlD-2	146	90.9	+	Qualifier
IPR-1	336	204.1	+	Quantifier
IPR-2	336	136.2	+	Qualifier
tZ-1	220.001	136	+	Quantifier
tZ-2	220.001	202.01	+	Qualifier
mT-1	242.2	107.1	+	Quantifier
mT-2	242.2	136	+	Qualifier
BAP-1	224	133	–	Quantifier
BAP-2	224	105.7	–	Qualifier
SA-1	136.9	92.9	–	Quantifier
SA-2	136.9	64.8	–	Qualifier
IPA-1	190.001	130.1	+	Quantifier
IPA-2	190.001	172	+	Qualifier
GA1-1	347.2	272.9	–	Quantifier
GA1-2	347.2	240.9	–	Qualifier
OxIAA-1	190	131.1	–	Quantifier
OxIAA-2	190	145.9	–	Qualifier
DHZR-1	354	222	+	Quantifier
DHZR-1	354	136.1	+	Qualifier
GA4-1	331.2	243.1	–	Quantifier
GA4-2	331.2	287.2	–	Qualifier
IBA-1	204	130	+	Quantifier
IBA-2	204	132.1	+	Qualifier
JA-1	209	58.7	–	Quantifier
JA-1	209	58.7	–	Qualifier
H2JA-1	211	59.1	–	Quantifier
H2JA-2	211	166.8	–	Qualifier
tZR-1	352	220.1	+	Quantifier
tZR-2	352	136.1	+	Qualifier
BL-1	481	315	+	Quantifier
BL-2	481	321	+	Qualifier
GA3-1	345.1	143	–	Quantifier
GA3-2	345.1	238.9	–	Qualifier
JA-ILE-1	322.3	130	–	Quantifier
JA-ILE-2	322.3	127.8	–	Qualifier
cZR-1	352.001	220.2	+	Quantifier
cZR-2	352.001	136.2	+	Qualifier

<b>Compound (Abbrev)</b>	<b>Prec. Ion (<i>m/z</i>)</b>	<b>Prod. Ion (<i>m/z</i>)</b>	<b>Polarity</b>	<b>Transition Role</b>
GA20-1	331.1	287.1	–	Quantifier
GA20-2	331.1	225	–	Qualifier
IAA-Glu-1	303.1	146	–	Quantifier
IAA-Glu-2	303.1	127.7	–	Qualifier
5DS-1	331	216	+	Quantifier
5DS-2	331	147.2	+	Qualifier
BAP9G-1	388	226	+	Quantifier
BAP9G-2	388	148.1	+	Qualifier
SAG-1	299	137	–	Quantifier
SAG-2	299	93	–	Qualifier
pT-1	240	134	–	Quantifier
pT-2	240	133	–	Qualifier
IAA-Gly-1	231	73.8	–	Quantifier
IAA-Gly-2	231	156	–	Qualifier
IAA-Leu-1	287.2	129.8	–	Quantifier
IAA-Leu-2	287.2	155.8	–	Qualifier
pTR-1	388.1	256.2	+	Quantifier
pTR-2	388.1	121	+	Qualifier
oTR-1	374.001	135.9	+	Quantifier
oTR-2	374.001	242.1	+	Qualifier
GA9-1	315.2	271.2	–	Quantifier
GA9-2	315.2	253.2	–	Qualifier