

**Table S3. Calibration and linearity parameters.** Limits of detection (LLOD) and quantification (LLOQ), upper limit of quantification (ULOQ), and linear regression coefficient ( $R^2$ ) for each target compound's calibration curve. All analytes demonstrated good linear response ( $R^2 \geq 0.990$ ) across the quantified range.

Compound (Abbrev)	LLOD (nmol/L)	LLOQ (nmol/L)	ULOQ (nmol/L)	$R^2$
5DS	0.02	0.04	606.061	0.9942
ABA	0.05	0.09	757.576	0.9925
ACC	0.6	1.21	9900.99	0.99
BAP	0.22	0.43	111.111	0.9921
BAP9G	0.03	0.06	129.199	0.9981
BAPR	0.02	0.03	559.91	0.9906
BL	0.13	0.25	4166.67	0.9986
DHZR	0.02	0.03	566.572	0.9923
DZ	0.03	0.06	904.977	0.9936
GA1	1.12	2.24	143.596	0.9977
GA20	0.18	0.37	188.196	0.999
GA3	0.07	0.14	72.2335	0.9975
GA4	0.15	0.29	602.047	0.992
GA7	0.15	0.3	605.694	0.9904
GA9	0.19	0.39	3162.56	0.9993
H2JA	0.03	0.06	29.4811	0.992
IA	0.13	0.26	1069.52	0.9994
IAA	0.56	1.12	1142.86	0.9903
IAA-Ala	12.7	25.41	813.008	0.9944
IAA-Asp	0.34	0.67	689.655	0.994
IAA-Glu	51.38	102.76	3288.39	0.9961
IAA-Gly	0.03	0.05	53.8793	0.9922
IAA-Leu	0.04	0.08	693.963	0.9932
IAA-Phe	0.02	0.04	620.732	0.9968
IAA-Trp	0.03	0.07	553.863	0.9916
IAA-Val	0.04	0.09	729.927	0.9923
IAM	2.24	4.49	574.713	0.9924
IAN	0.31	0.63	641.026	0.9953
IBA	0.6	1.2	4926.11	0.9942
ICA	38.82	77.64	1242.24	0.9936
ICAlD	0.08	0.17	1379.31	0.9913
ILA	1.91	3.81	243.902	0.9926
IP	0.03	0.06	985.222	0.9983
IPA	0.03	0.06	1058.2	0.9905
IPR	0.02	0.04	597.015	0.9926
JA	0.47	0.93	952.381	0.9939
JA-ILE	0.6	1.21	618.62	0.9978
K	0.06	0.11	930.233	0.9957
KR	0.02	0.04	144.092	0.9902
OxIAA	16.36	32.72	1047.12	0.9958
SA	70.82	141.63	290065	0.9906

SAG	20.83	41.67	666.667	0.9916
TRA	19.53	39.06	1250	0.995
TRP	0.6	1.2	9803.92	0.9904
cZ	0.03	0.06	913.242	0.9956
cZR	0.02	0.03	284.899	0.9946
mT	0.03	0.05	829.187	0.9903
mTR	0.03	0.07	67.0241	0.9962
oT	0.03	0.05	207.469	0.9997
oTR	0.02	0.03	134.048	0.9906
pT	0.03	0.05	207.469	0.991
pTR	0.02	0.03	516.662	0.9903
tZ	0.03	0.06	913.238	0.9927
tZR	0.02	0.03	284.9	0.9924