Table 2. Continued

Compound	Fraction	EE (%)	RSD of EE (%)	R^2	LOD (nM)
L-lysine	HILIC positive	56.2	39.1	0.888	1.5
L-methionine S-oxide	HILIC positive	72.6	18.6	0.973	0.16
L-ornithine	HILIC positive	47.2	30.7	0.907	6.8
L-phenylalanine	RP	128	21.0	0.914	0.20
L-proline	HILIC positive	104	16.4	0.984	0.51
L-serine	HILIC positive	75.3	38.4	0.919	4.0
L-threonine	HILIC positive	62.2	17.5	0.942	0.21
L-tyrosine	HILIC positive	28.6	26.7	0.938	0.88
Melamine	HILIC positive	60.2	18.2	0.975	0.36
Muramic acid	HILIC positive	14.6	25.5	0.968	0.046
N6-acetyl-L-lysine	HILIC positive	37.8	26.4	0.984	0.015
N6-Methyladenine	HILIC positive	15.8	29.2	0.917	0.020
Nicotinic acid	RP	102	12.2	0.894	1.1
O-Methylmalonyl-L-carnitine	HILIC positive	47.4	20.7	0.989	0.0064
Ophthalmic acid	HILIC positive	23.0	27.8	0.959	0.020
Proline betaine	HILIC positive	58.2	17.3	0.985	0.022
Sarcosine	HILIC positive	41.0	14.4	0.968	0.32
Trigonelline	HILIC positive	53.3	15.7	0.987	0.057
TMAO	HILIC positive	54.7	33.0	0.946	0.13
Urocanic acid	HILIC negative	65.6	17.6	0.939	0.73
Xanthine	RP	69.2	22.7	0.965	0.055

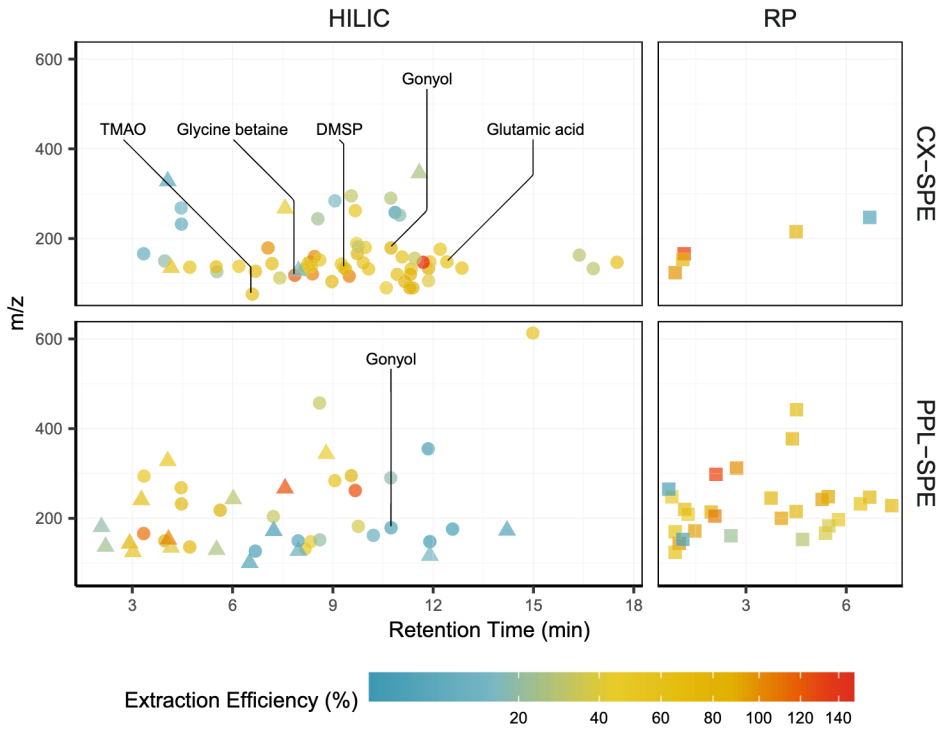

Fig. 2. Extraction efficiency of targeted compounds extracted by CX-SPE and PPL-SPE shown by the compounds' m/z and RT for both types of chromatography. Different analytical fractions are denoted by shape (HILIC positive, circle; HILIC negative, triangle; RP, square). Several compounds representative of various functional classes of metabolites extracted by CX-SPE (TMAO, amine oxides; homarine and glycine betaine, betaines; DMSP and gonyol, sulfoniums; glutamic acid, amino acids) are annotated. Note that the color bar has a square root transformation.

Table 2. *Analysis fraction*, EE, RSD_{EE}, R^2 values, and LODs for compounds meeting quality control thresholds using CX-SPE. Isoleucine and leucine are not fully separated with our chromatography and are treated together as (iso)leucine.

Compound	Fraction	EE (%)	RSD of EE (%)	R^2	LOD (nM)
(3-Carboxypropyl)trimethylammonium	HILIC positive	46.8	27.6	0.964	0.012
(Iso)leucine	HILIC positive	59.7	17.6	0.949	0.23
3′,5′-Cyclic adenosine monophosphate	HILIC negative	5.92	39.7	0.886	0.0071
4-Aminobutyric acid	HILIC positive	89.2	16.9	0.934	0.67
5-Hydroxyectoine	HILIC positive	47.2	16.0	0.994	0.0074
5-Methylcytosine	HILIC positive	21.0	15.1	0.962	0.042
5-Oxoproline	HILIC negative	18.1	38.5	0.912	17
Abscisic acid	RP	4.77	38.1	0.925	0.62
Adenine	HILIC positive	49.1	18.4	0.954	0.23
Adenosine	HILIC positive	10.6	20.9	0.953	0.12
Adenosine monophosphate	HILIC negative	23.0	39.3	0.961	0.027
Allopurinol	HILIC negative	46.0	38.6	0.859	1.2
Arsenobetaine	HILIC positive	88.9	14.1	0.992	0.0013
β-Alanine	HILIC positive	82.1	15.4	0.977	1.3
β-Alaninebetaine	HILIC positive	66.2	15.1	0.991	0.014
β-Glutamic acid	HILIC positive	52.9	12.7	0.843	1.0
Betonicine	HILIC positive	89.2	14.1	0.996	0.0059
Butyrylcarnitine	HILIC positive	5.56	39.2	0.930	0.0090
Citrulline	HILIC positive	40.2	27.7	0.857	1.5
Creatine	HILIC positive	50.4	19.5	0.980	0.047
Cytidine	HILIC positive	19.9	21.3	0.970	0.038
Cytosine	HILIC positive	30.8	15.2	0.969	0.050
Desthiobiotin	RP	66.1	38.3	0.784	0.0042
Dimethylglycine	HILIC positive	65.1	14.9	0.993	0.70
DMS-Ac	HILIC positive	94.8	12.6	0.996	0.00013
DMSP	HILIC positive	55.5	15.5	0.973	0.00010
Ectoine	HILIC positive	47.6	12.5	0.990	0.025
Glucosamine	HILIC positive	49.4	15.9	0.988	0.21
Glutamylphenylalanine	HILIC positive	26.0	23.4	0.923	0.012
Glycerophosphocholine	HILIC positive	2.24	47.8	0.931	0.25
Glycine betaine	HILIC positive	100	20.6	0.969	0.38
Gonyol	HILIC positive	71.0	26.2	0.974	0.17
Guanine	HILIC positive	47.1	26.0	0.955	0.35
Guanosine	HILIC positive	13.2	30.0	0.952	0.17
Homarine	HILIC positive	50.0	15.2	0.995	0.15
Hordenine	HILIC positive	7.29	41.9	0.732	0.060
Hydroxyisoleucine	HILIC positive	63.2	39.1	0.916	0.25
Hydroxyproline	HILIC positive	54.5	16.1	0.965	0.041
Hypoxanthine	HILIC positive	59.6	18.7	0.978	0.39
Inosine	HILIC negative	36.7	28.2	0.950	0.023
L-alanine	HILIC positive	106	30.3	0.974	1.8
L-asparagine	HILIC positive	82.7	14.4	0.916	0.49
L-aspartic acid	HILIC positive	67.2	18.5	0.963	3.4
L-glutamic acid	HILIC positive	53.7	22.4	0.850	2.0
L-glutamine	HILIC positive	131	16.8	0.988	0.024
L-histidine	HILIC positive	33.0	36.8	0.969	0.66
L-Homoserine	HILIC positive	68.8	18.1	0.986	0.18
L-Hydroxylysine	HILIC positive	38.2	23.4	0.732	0.0026

(Continues)