

Supplementary Information: Modeling of hydrophilic interaction liquid chromatography stationary phases using chemometric approaches

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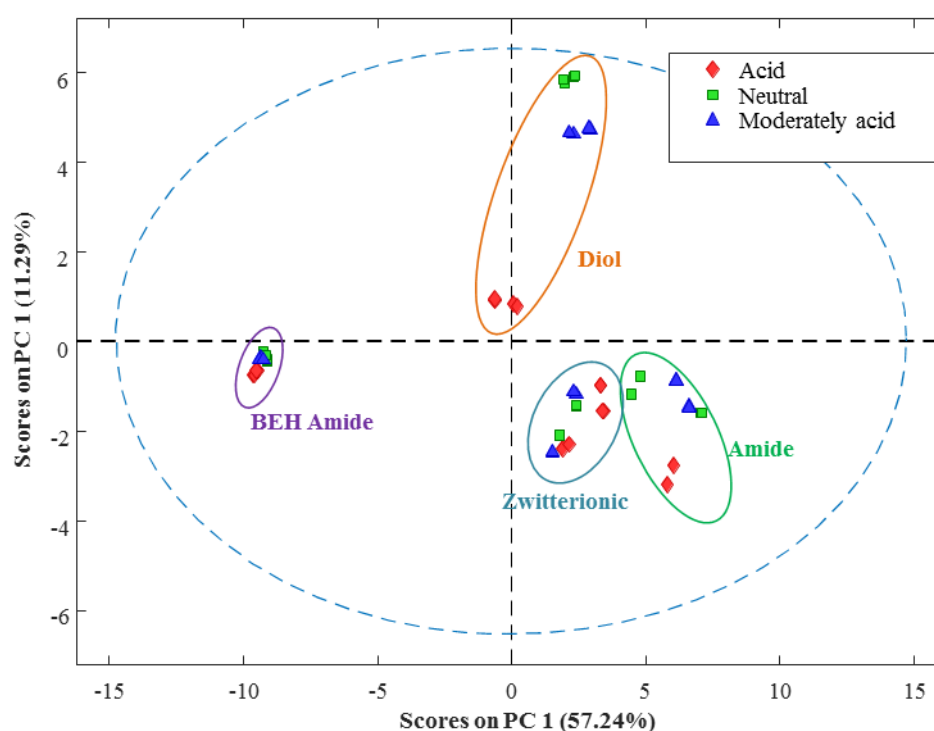


Figure S1. PCA scores plot of samples classified according to the pH of the mobile phase.

Table S1. Metabolites' logP values obtained from PCLIENT software.

Metabolites	logP
Nucleosides	
1-methyladenosine	-0.054
2''-O-methylcytidine	-0.872
2-thiocytidine	-0.427
5-methylcytidine	-0.872
cytidine	-1.176
guanosine	-0.808
inosine	-0.752

pseudouridine	-1.988
ribothymidine	-1.278
uridine	-1.582

Amino Acids

1-methyl-L-histidine	-2.704
3-methyl-L-histidine	-2.704
4-hydroxy-L-proline	-1.04
5-hydroxylysine	-3.273
β -alanine	-2.918
creatinine	-0.339
cysteine	-5.555
L(-)-proline	-0.232
L(+)-arginine	-2.934
L(+)-cystathionine	-5.202
L(+)-lysine	-2.485
L-2-aminoadipic acid	-2.568
L-2-amino-n-butyric acid	-2.465
L-alanine	-2.918
L-anserine	-0.75
L-carnosine	-1.054
L-citrulline	-3.34
L-glutamic acid	-2.946
L-histidine	-3.057
L-homocystine	-4.869
L-isoleucine	-1.677
L-leucine	-1.677
L-methionine	-2.055
L-ornithine	-2.863
L-serine	-3.726
L-threonine	-3.272
L-tryptophan	-1.267
L-valine	-2.055
taurine	-1.731
sarcosine	-0.703
L-aspartic acid	-3.356

Sugars

D(-)-ribose	-2.089
glucose	-2.483
trehalose	-3.898
mannitol	-2.497

Organic acids

citric acid	-1.169
ketoglutaric acid	-0.828
pimelic acid	0.787
succinic acid	-0.353

creatine	-0.735
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Others	
hypoxanthine	0.582
L-carnitine	-3.601
serotonin	1.006
tryptamine	1.574
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