

Table 1. The mix of pesticides used as the analytical standard.

Name	Molecular formula	m/z [M+H]	Retention time, min
Pymetrozine	C10H11N5O	218.1036	4.7
Formetanate	C11H15N3O2	222.1237	4.88
Fenuron	C9H12N2O	165.1022	4.89
Carbendazim	C9H9N3O2	192.0768	6.4
2-Hydroxyatrazine	C8H15N5O	198.1349	6.99
Atrazine-Desisopropyl	C5H8ClN5	174.0541	7.21
Metamitron	C10H10N4O	203.0927	7.71
Acetamiprid	C10H11ClN4	223.0745	7.86
Chloridazone	C10H8ClN3O	222.0429	7.88
Crimidine	C7H10ClN3	172.0636	7.89
Pirimicarb	C11H18N4O2	239.1503	8.13
Atrazine-Desethyl	C6H10ClN5	188.0697	8.16
Atraton	C9H17N5O	212.1506	8.29
Metoxuron	C10H13ClN2O2	229.0738	8.54
2-4-Dimethylphenylformamide	C9H11NO	150.0913	8.75
Metolcarb	C9H11NO2	166.0863	8.75
Nicosulfuron	C15H18N6O6S	411.1081	8.96
Carbofuran	C12H15NO3	222.1125	9.08
Carboxin	C12H13NO2S	236.074	9.26
Fenpropidin	C19H31N	274.2529	9.32
Fosthiazate	C9H18NO3PS2	284.0538	9.45
Cyprazin	C9H14ClN5	228.101	9.69
DEET (diethyltoluamide)	C12H17NO	192.1383	9.71
Diuron	C9H10Cl2N2O	233.0243	9.76
Cycluron	C11H22N2O	199.1805	9.82
Phenmedipham	C16H16N2O4	301.1183	9.87
Azoxystrobin	C22H17N3O5	404.1241	10.01
Isoxaben	C18H24N2O4	333.1809	10.23
Methoxyfenozide	C22H28N2O3	369.2173	10.27
Chromafenozide	C24H30N2O3	395.2329	10.42
Metolachlor	C15H22ClNO2	284.1412	10.65
Fenothiocarb	C13H19NO2S	254.1209	10.78
Pencycuron	C19H21ClN2O	329.1415	11.05

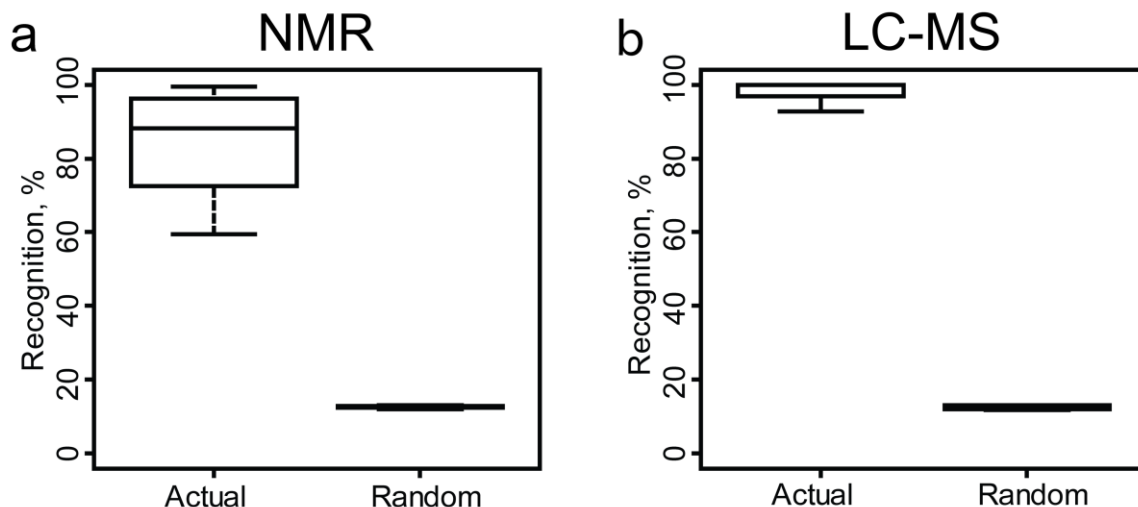


Figure 1. Person recognition based on ^1H NMR and LC-MS data of urine samples from 8 individuals. (a) Boxplot of the recognition accuracy based on ^1H NMR spectra for actual (left) and permuted (right) person labels. (b) Boxplot of the recognition accuracy based on LC-MS data for actual (left) and permuted (right) person labels.

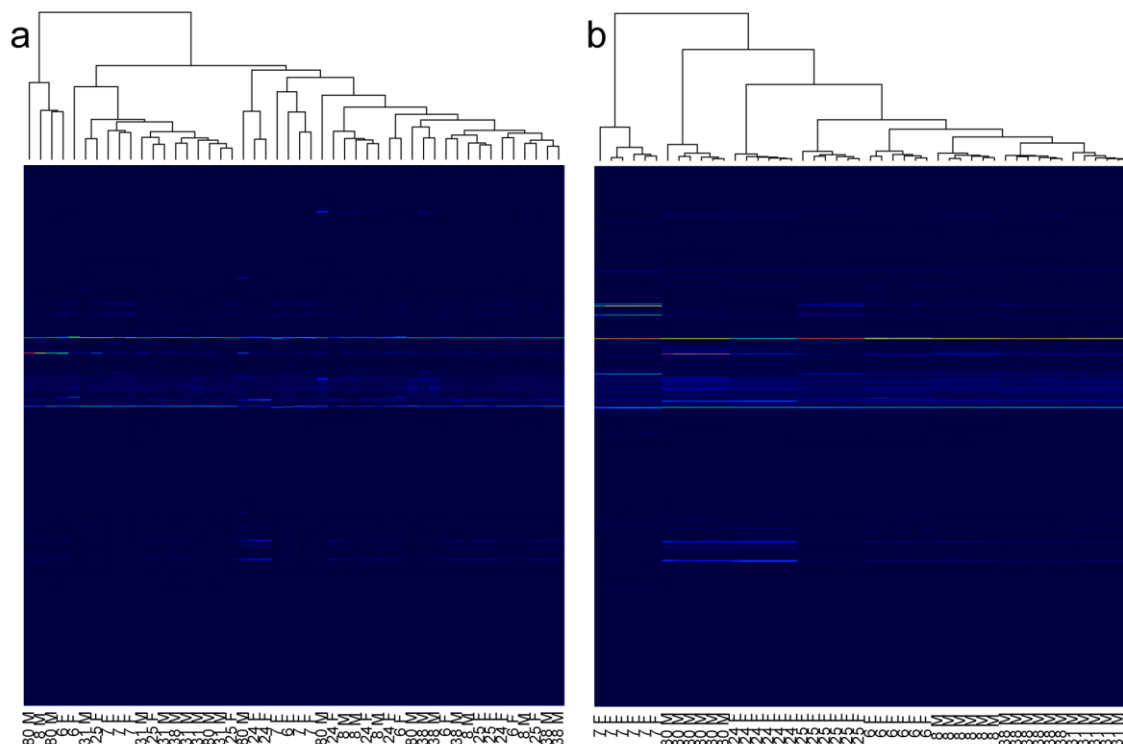


Figure 2. Heatmap and hierarchical clustering of the initial binned ^1H NMR table (a) and after back-projection (b). Samples are labeled by their ID and gender.

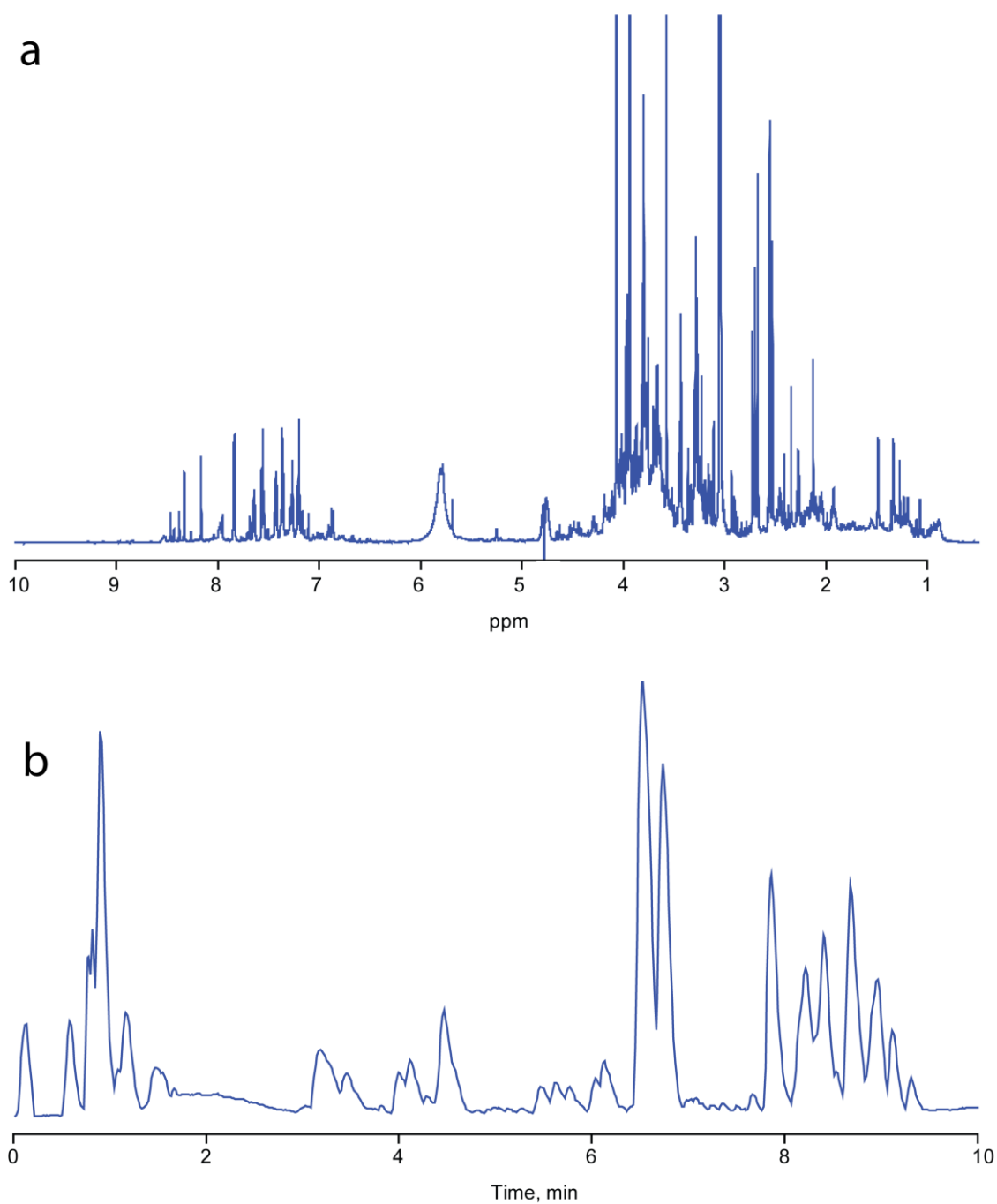


Figure 3. Sample ¹H NMR spectrum of urine (A) and LC-MS base peak chromatogram from the same urine sample (B).

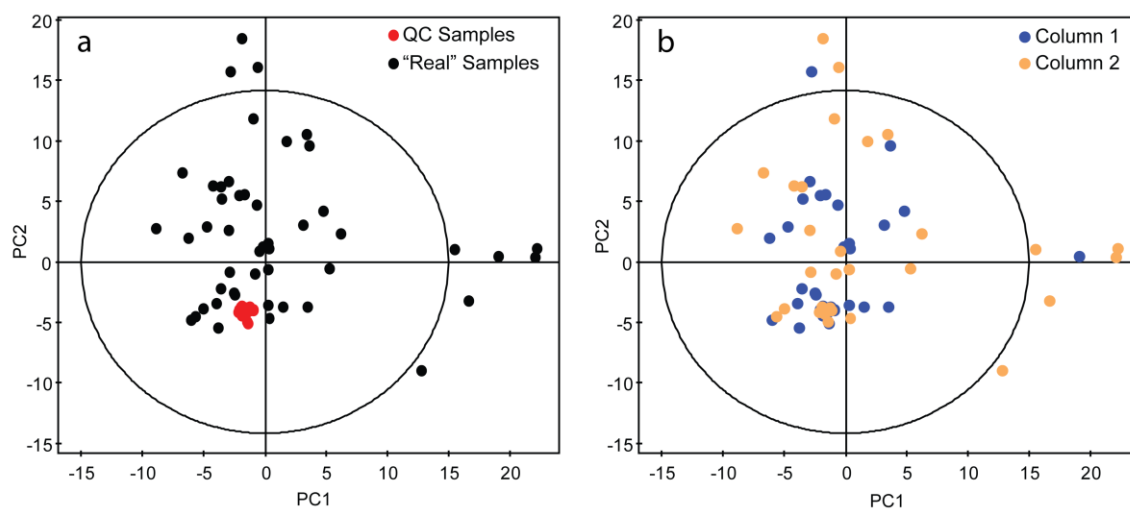


Figure 4. Scores plot of the PCA performed on the entire dataset including QC samples. (A) colored by QCs (red) and individual urine samples (black); QC samples form a tight cluster, indicating the analytical reproducibility of the method. (B) Colored by column; no separation by column is visible.

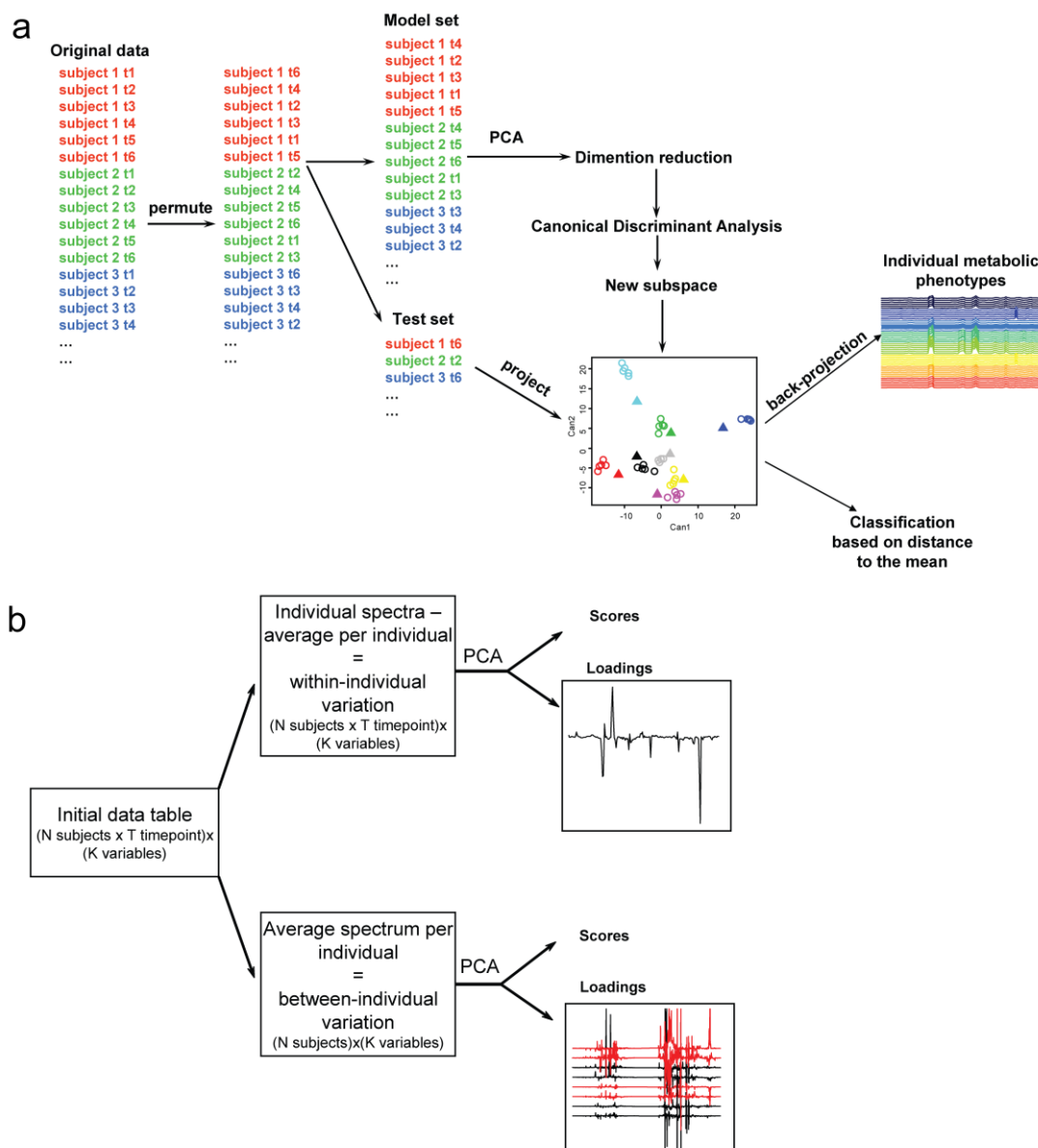


Figure 5. Schematic representation of the two statistical methods used: (a) person recognition, (b) multilevel component analysis.