Alterations of metabolic and lipid profiles in polymyxin-resistant *Pseudomonas aeruginosa*

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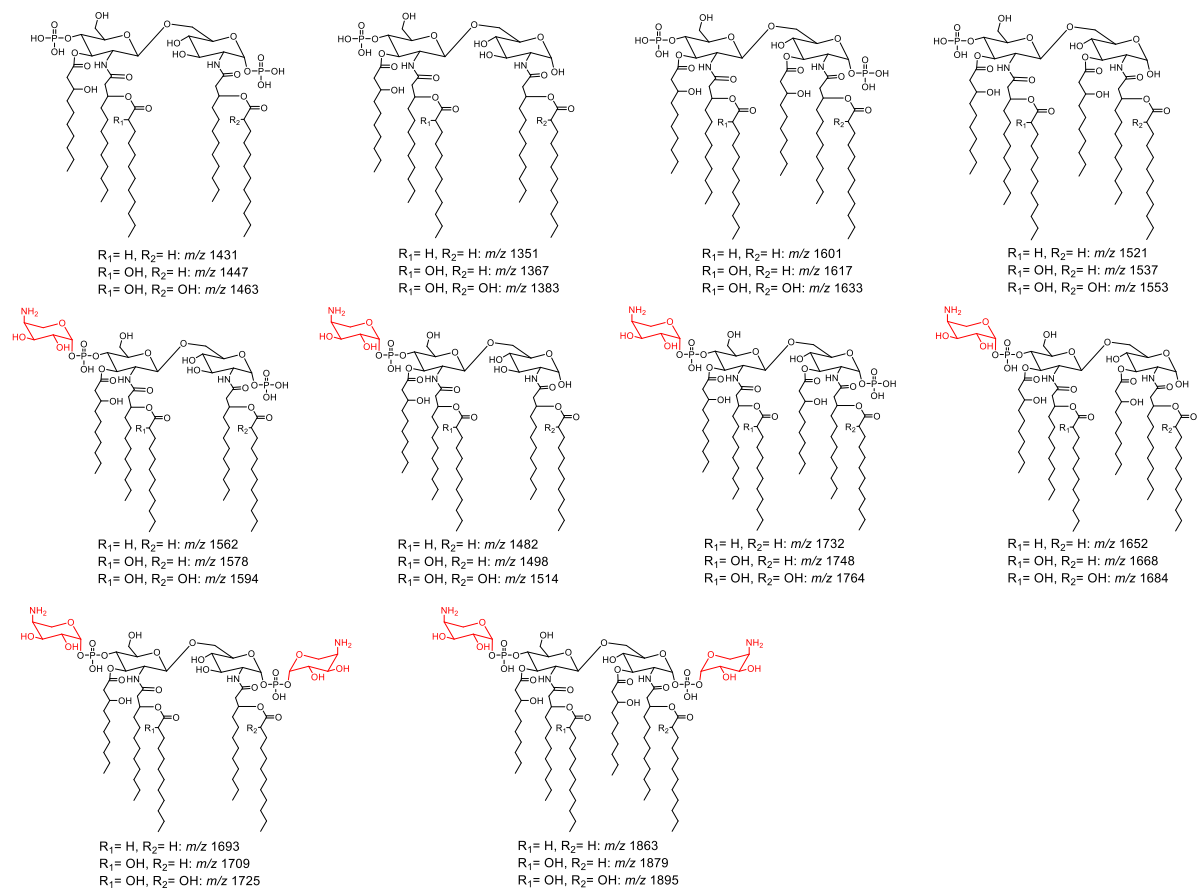
Figure S1

R₁= H, R₂= H: *m/z* 1431
R₁= OH, R₂= H: *m/z* 1447
R₁= OH, R₂= OH: *m/z* 1463

R₁= H, R₂= H: *m/z* 1351
R₁= OH, R₂= H: *m/z* 1367
R₁= OH, R₂= OH: *m/z* 1383

R₁= H, R₂= H: *m/z* 1601
R₁= OH, R₂= H: *m/z* 1617
R₁= OH, R₂= OH: *m/z* 1633

R₁= H, R₂= H: *m/z* 1521
R₁= OH, R₂= H: *m/z* 1537
R₁= OH, R₂= OH: *m/z* 1553

R₁= H, R₂= H: *m/z* 1562
R₁= OH, R₂= H: *m/z* 1578
R₁= OH, R₂= OH: *m/z* 1594

R₁= H, R₂= H: *m/z* 1482
R₁= OH, R₂= H: *m/z* 1498
R₁= OH, R₂= OH: *m/z* 1514

R₁= H, R₂= H: *m/z* 1732
R₁= OH, R₂= H: *m/z* 1748
R₁= OH, R₂= OH: *m/z* 1764

R₁= H, R₂= H: *m/z* 1652
R₁= OH, R₂= H: *m/z* 1668
R₁= OH, R₂= OH: *m/z* 1684

R₁= H, R₂= H: *m/z* 1693
R₁= OH, R₂= H: *m/z* 1709
R₁= OH, R₂= OH: *m/z* 1725

R₁= H, R₂= H: *m/z* 1863
R₁= OH, R₂= H: *m/z* 1879
R₁= OH, R₂= OH: *m/z* 1895

Figure S1. Structures of wild-type lipid A presented in PAK and L-Ara4N modified lipid A in PAK*pmrB6* and PAK*pmrB12*. L-Ara4N moiety is highlighted in red.
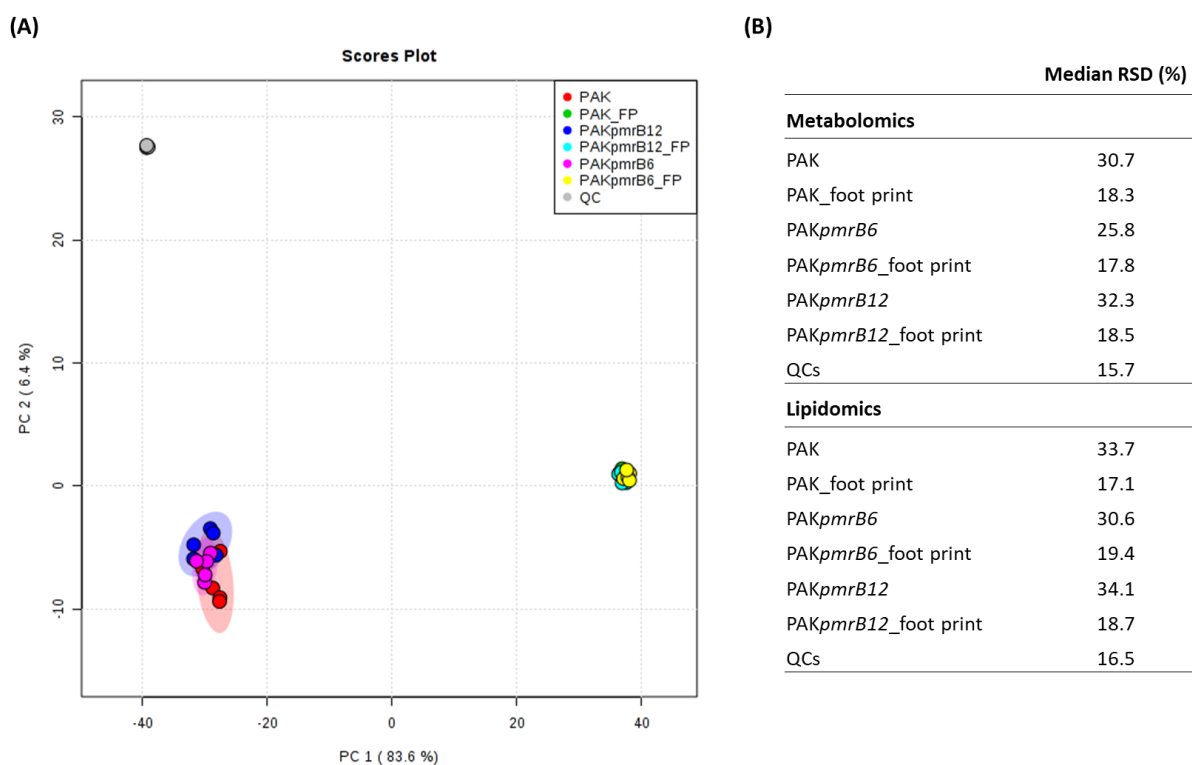
Figure S2

(A)

	Median RSD (%)
Metabolomics	
PAK	30.7
PAK_foot print	18.3
PAK*pmrB6*	25.8
PAK*pmrB6*_foot print	17.8
PAK*pmrB12*	32.3
PAK*pmrB12*_foot print	18.5
QCs	15.7
Lipidomics	
PAK	33.7
PAK_foot print	17.1
PAK*pmrB6*	30.6
PAK*pmrB6*_foot print	19.4
PAK*pmrB12*	34.1
PAK*pmrB12*_foot print	18.7
QCs	16.5

Figure S2. (A) PCA score plot of all metabolites from the finger print (intracellular metabolite samples) and foot print (extracellular metabolite samples) of PAK, PAK*pmrB6* and PAK*pmrB12*. (B) Data precision of individual samples represented as the median relative standard deviation (RSD) for all metabolites based on all replicates of each group. Four quality controls (QCs) were analyzed throughout the LC-MS batch. Each dataset represents five biological replicates of finger-printing samples and three biological replicates of foot-printing samples.
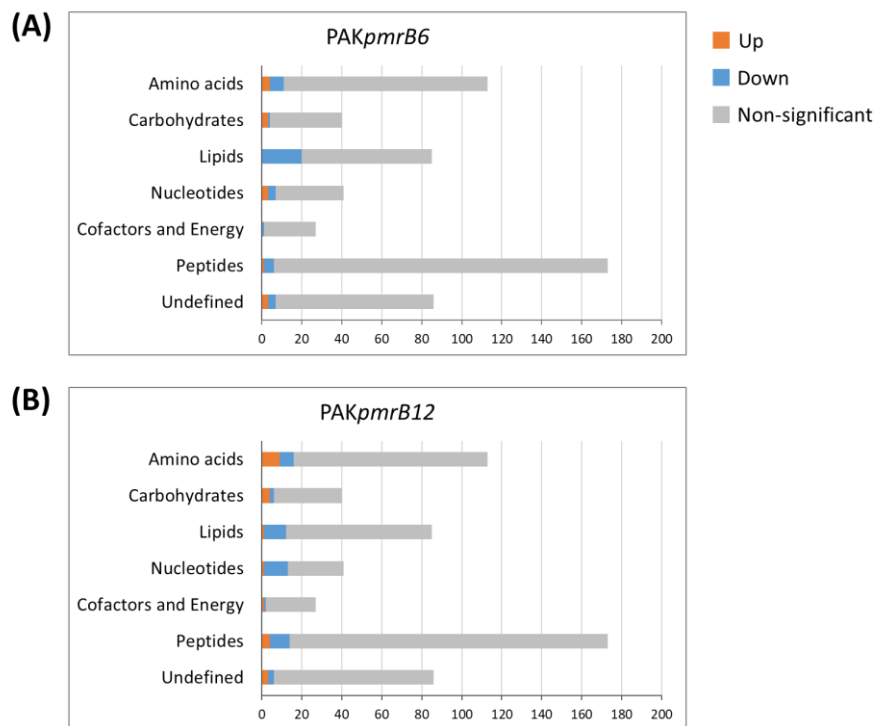
Figure S3

Figure S3. Summary number of significant metabolic changes classified according to different metabolite classes in PAK*pmrB6* (A) and PAK*pmrB12* (B) compared to the wild-type PAK strain.

Fold changes $\geq$ 1-log2-fold, $p \leq 0.05$, FDR ≤ 0.05 (one-way ANOVA for multiple comparison).