Electronic Supplementary Material (ESI) for Analytical Methods

Supporting Information

Discrimination and identification of different amines by pattern recognition of kinetic spectral data

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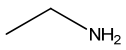
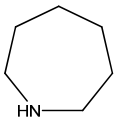
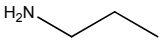
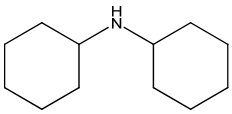
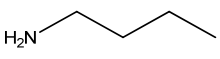
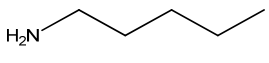
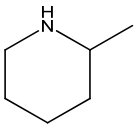
Table S1. Aliphatic amine samples evaluated

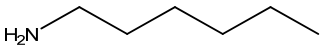
 Ethylamine	 Hexamethylenimine
 n-Propylamine	 Dicyclohexylamine
 n-Butylamine	



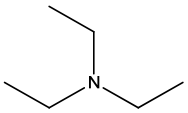
n-Pentylamine

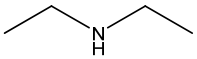


2-Methyl-pipyridine



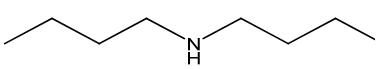
n-Hexylamine



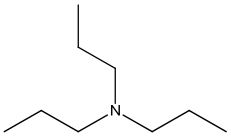


Diethylamine

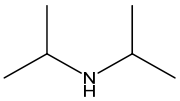
Triethylamine



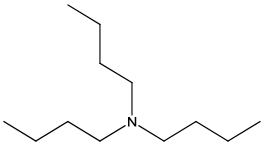
Dibutylamine



Tripropylamine

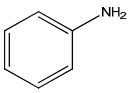


Diisopropylamine

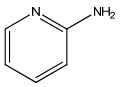


Tributylamine

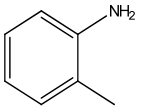
Table S2. Aromatic amine samples evaluated



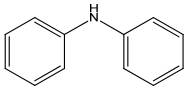
Aniline



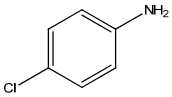
Pyridine-2-amine



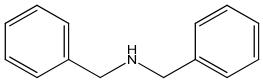
o-Toluidine



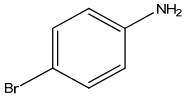
Diphenylamine



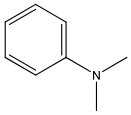
4-Chlroaniline



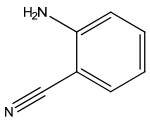
Dibenzylamine



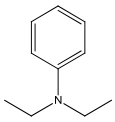
4-Bromoaniline



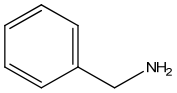
N,N-Dimethylaniline



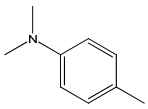
2-minobenzonitrile



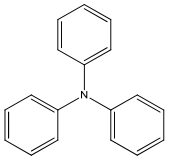
N,N-Diethylaniline



Benzylamine



N,N-Dimethyl-p-toluidine



Triphenylamine

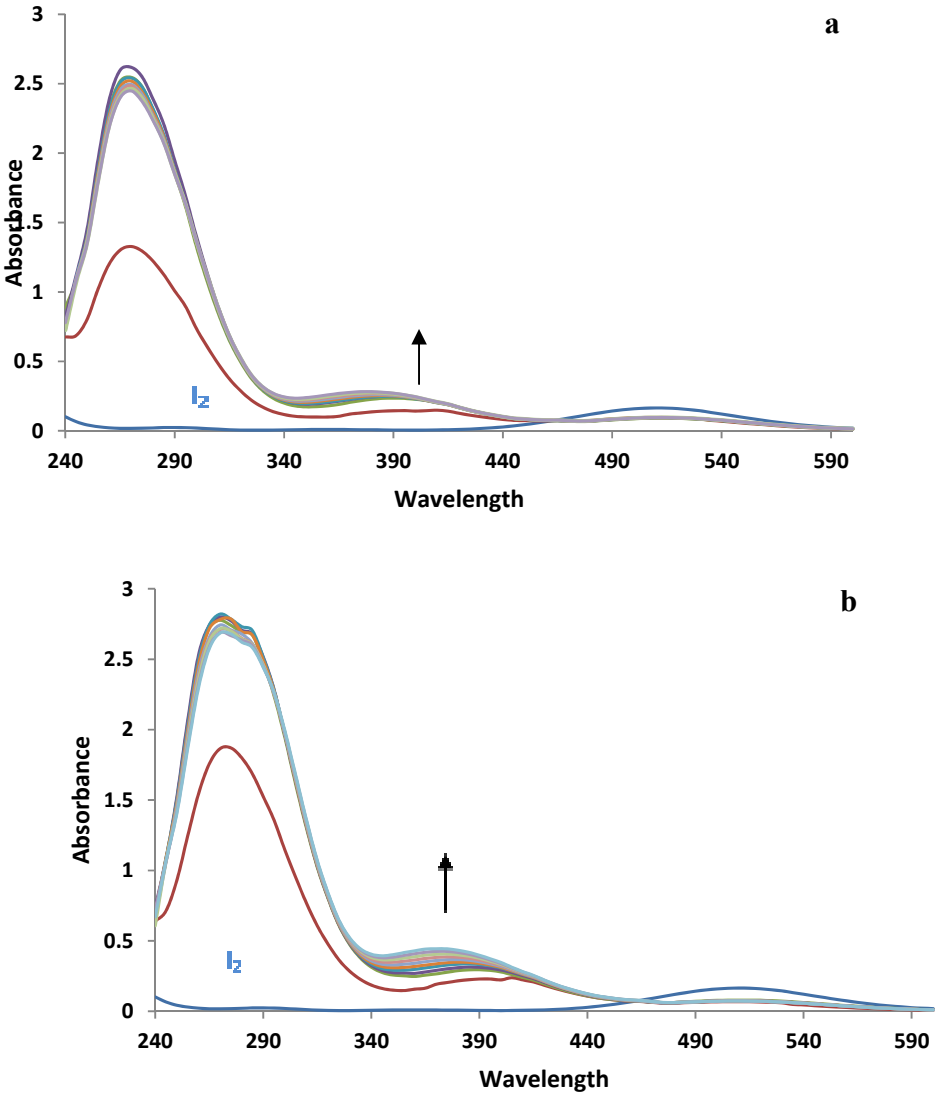


Figure S1. The electronic absorption spectra of iodine (2.0×10^{-4} M) and (a) Dibutylamine (2.0×10^{-4} M), (b) Hexamethyleneimine (2.0×10^{-4} M) in chloroform solution in during 10 min.

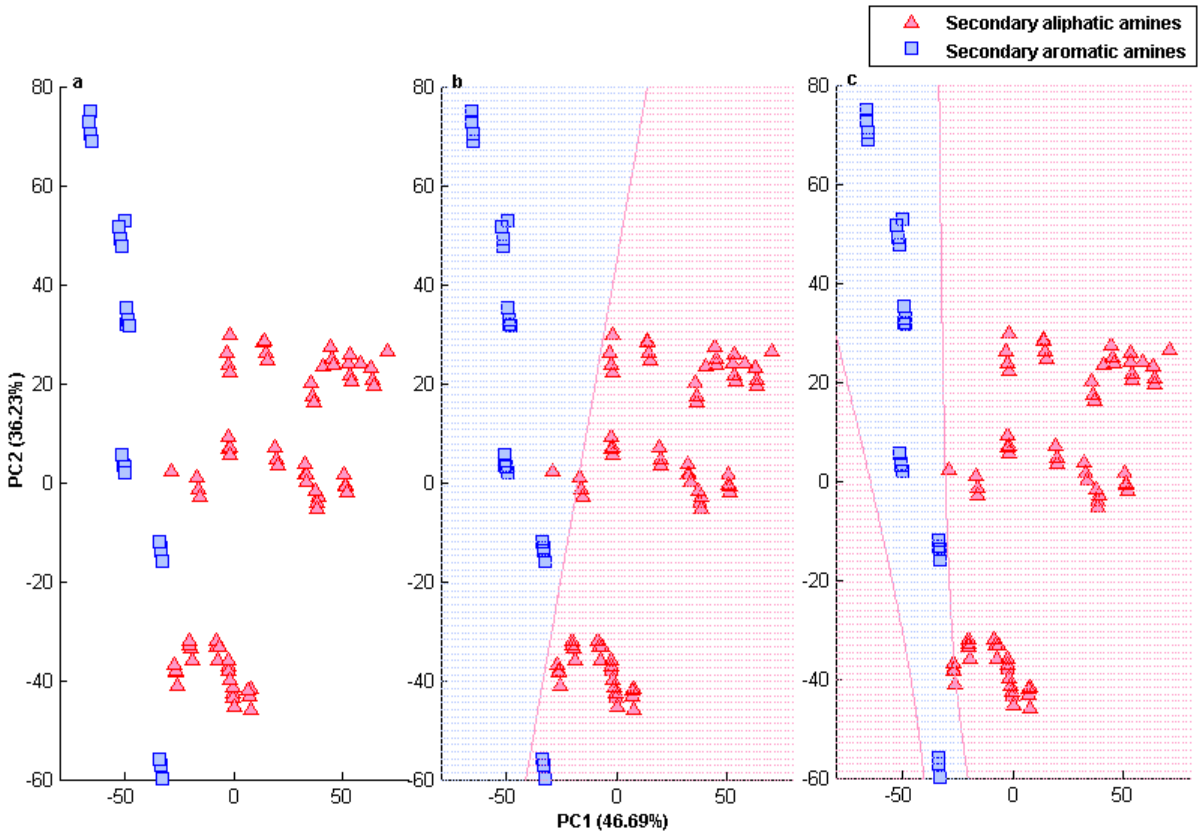


Figure S2. a) Score plot, visualisation of boundaries obtained by b) LDA and c) QDA for secondary amine complexes using default data preprocessing, and data represented by the scores of the first two PCs. Percentage on the PC axes define weight of those axes to the overall pattern. Four trials each, at three different concentrations [2.0, 4.0 and 6.0 × 10^{-4} M] for various of amines. The respective regions belonging to each class are coloured appropriately. Studies are carried out in 1:1 ratio of amine/iodine complex.

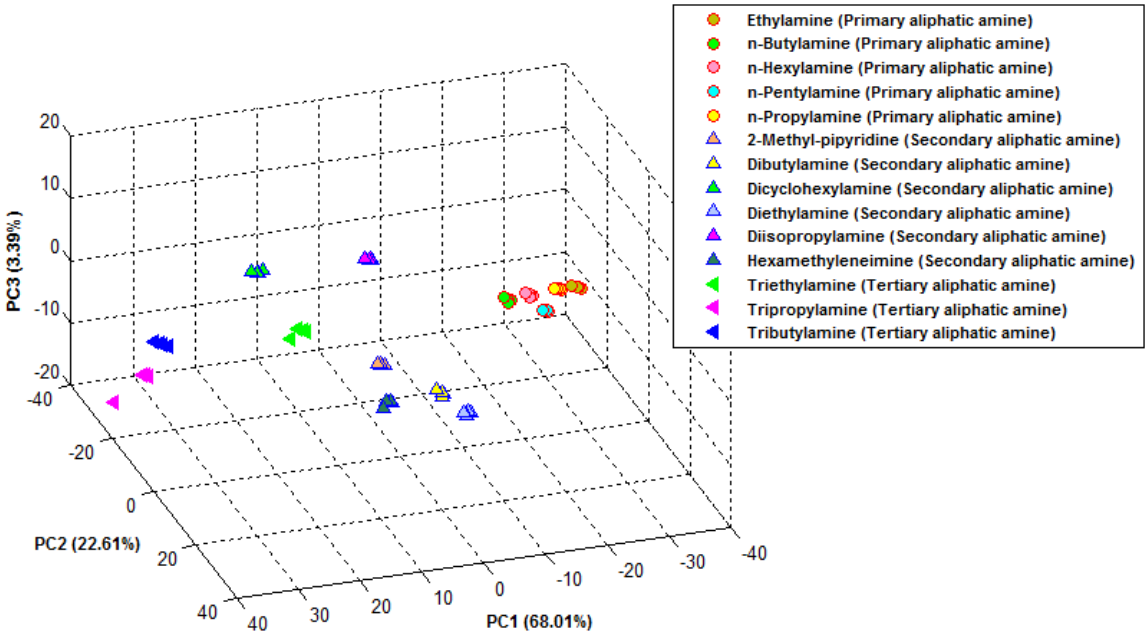


Figure S3. Three dimentional PCA plot for each aliphatic amine complex trial. Percentage on the PC axes define weight of those axes to the overall pattern. PCA score plot shows clustering for all fourtheen samples (four trials each, 2×10^{-4} M of amines and iodine). The additional dimention further separates the amines.

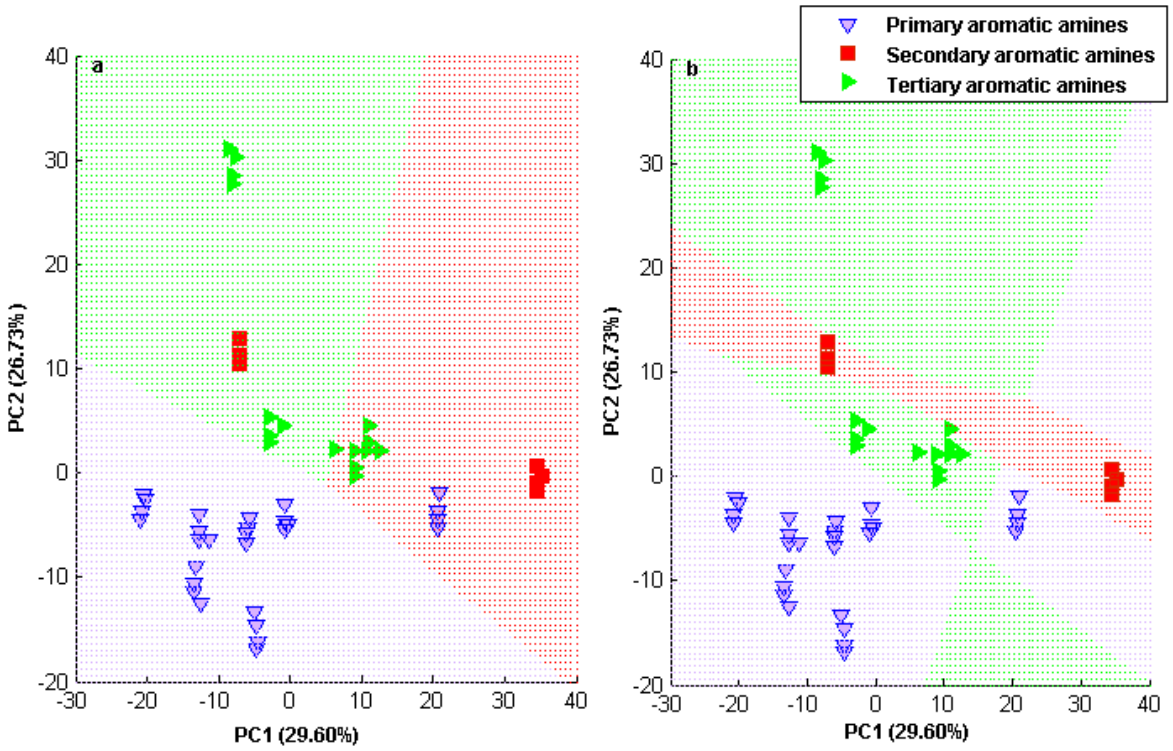


Figure S4. Visualisation of boundaries obtained by a) LDA and b) QDA for aromatic amine complexes using default data preprocessing, and data represented by the scores of PC1 and PC2. Percentage on the PC axes define weight of those axes to the overall pattern. Four trials each, at 4×10^{-4} M for various of amines. The respective regions belonging to each class are coloured appropriately. All studies carried out in 1:1 ratio of amine/iodine complex.

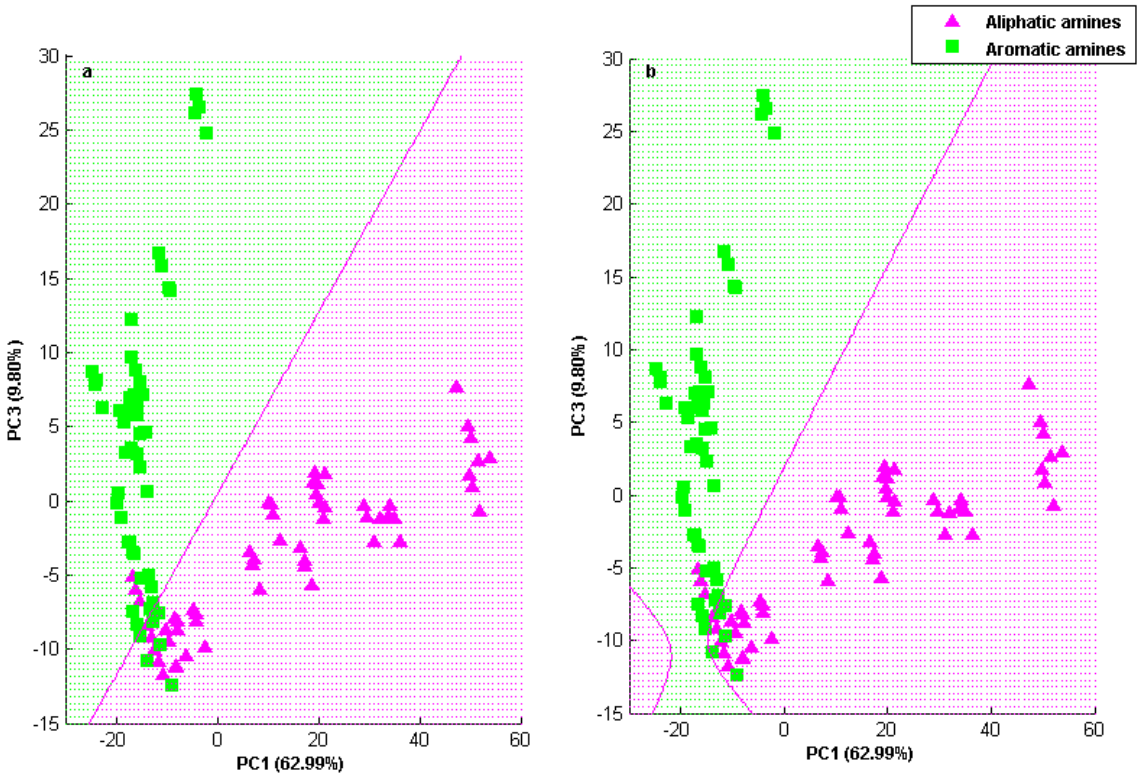


Figure S5. Visualisation of boundaries obtained by a) LDA and b) QDA for total amine complexes. Using default data preprocessing, and data represented by the scores of PC1 and PC3. Percentage on the PC axes define weight of those axes to the overall pattern. Four trials each, at 2×10^{-4} M for various of amines. The respective regions belonging to each class are coloured appropriately. All studies carried out in 1:1 ratio of amine/iodine complex.

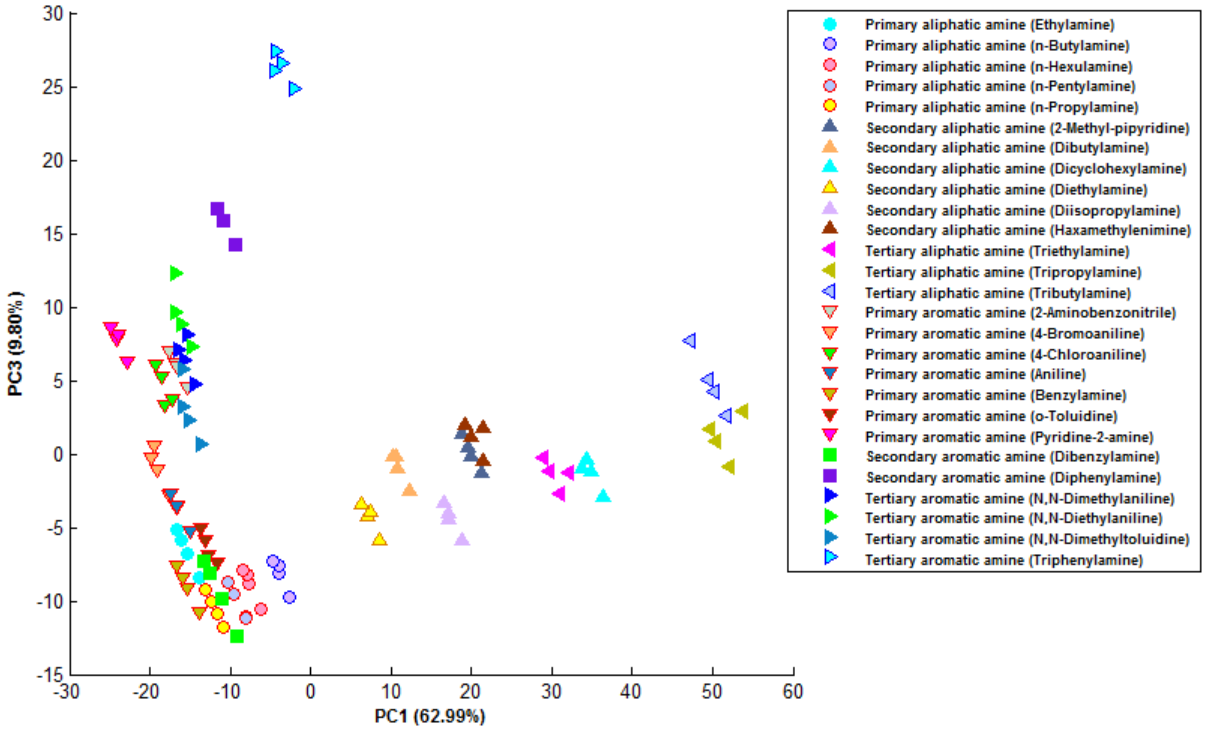


Figure S6. Two dimentional PCA plot for each total amine complex trial. Percentage on the PC axes define weight of those axes to the overall pattern. PCA score plot shows clustering for all 27 samples (four trials each, 2×10^{-4} M of amines and iodine).