

## Supplementary Figures

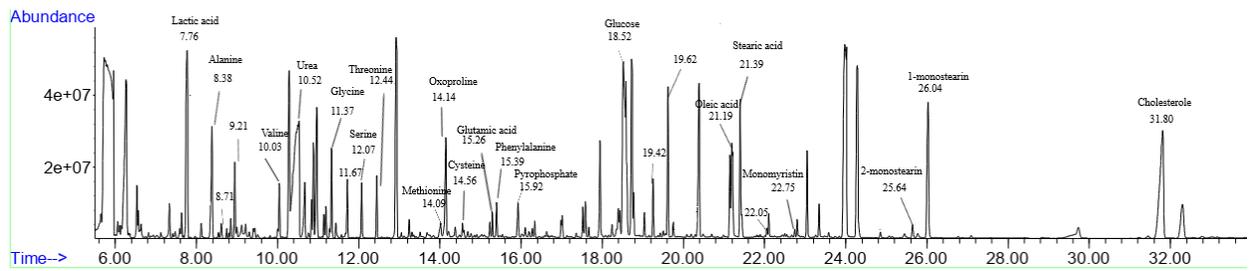
**Supplementary Figure S1.** The GC-Q-MS total ion current (TIC) chromatograms of plasma from a healthy subject.

**Supplementary Figure S2.** The principal component analysis (PCA) scores plot obtained from GC-Q-MS data of all samples.

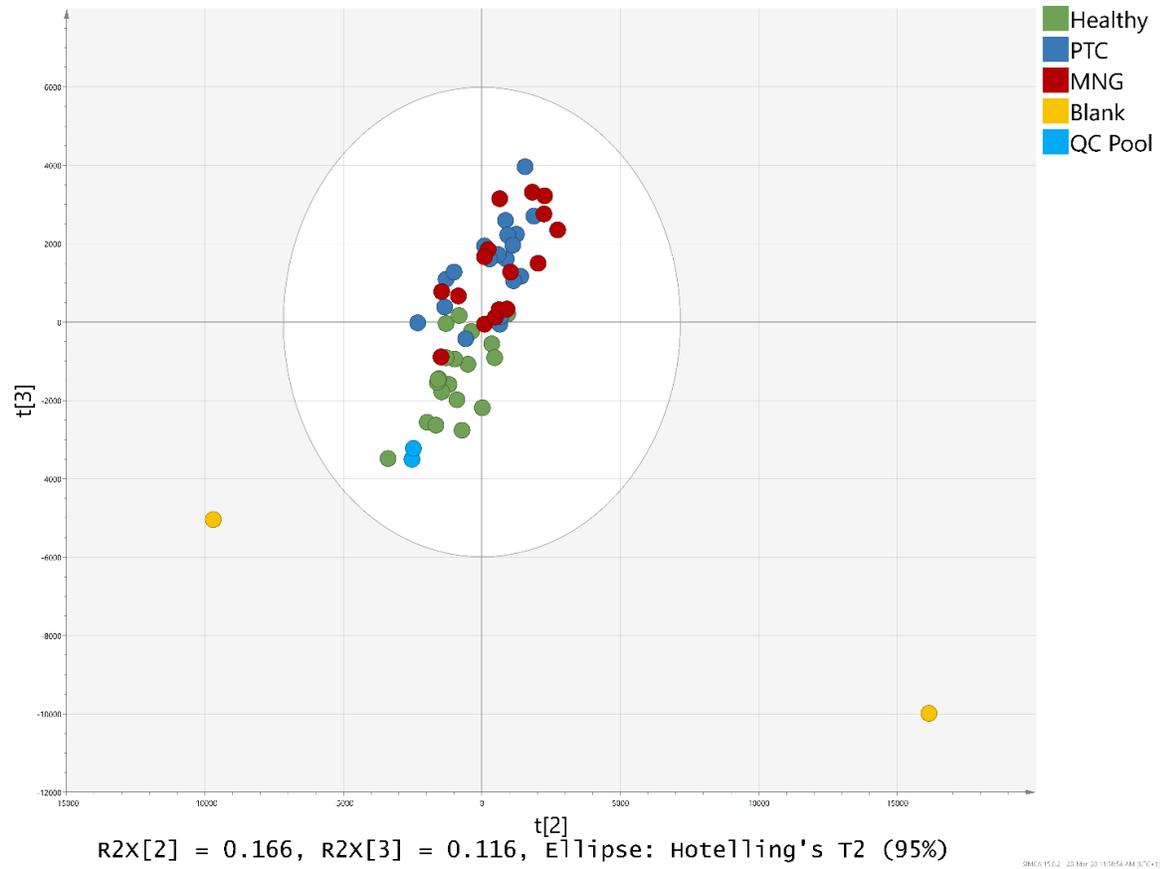
**Supplementary Figure S3.** Validation plot of a 100 permutation test for OPLS-DA model built for plasma samples among three groups.

**Supplementary Figure S4.** Validation plot of 100 permutation tests for OPLS-DA models built for plasma samples between two groups separately.

**Supplementary Figure S5.** Venn diagram analysis of discriminant metabolites in different groups, (blue) PTC vs Healthy, (yellow) MNG vs Healthy and (green) MNG vs PTC.

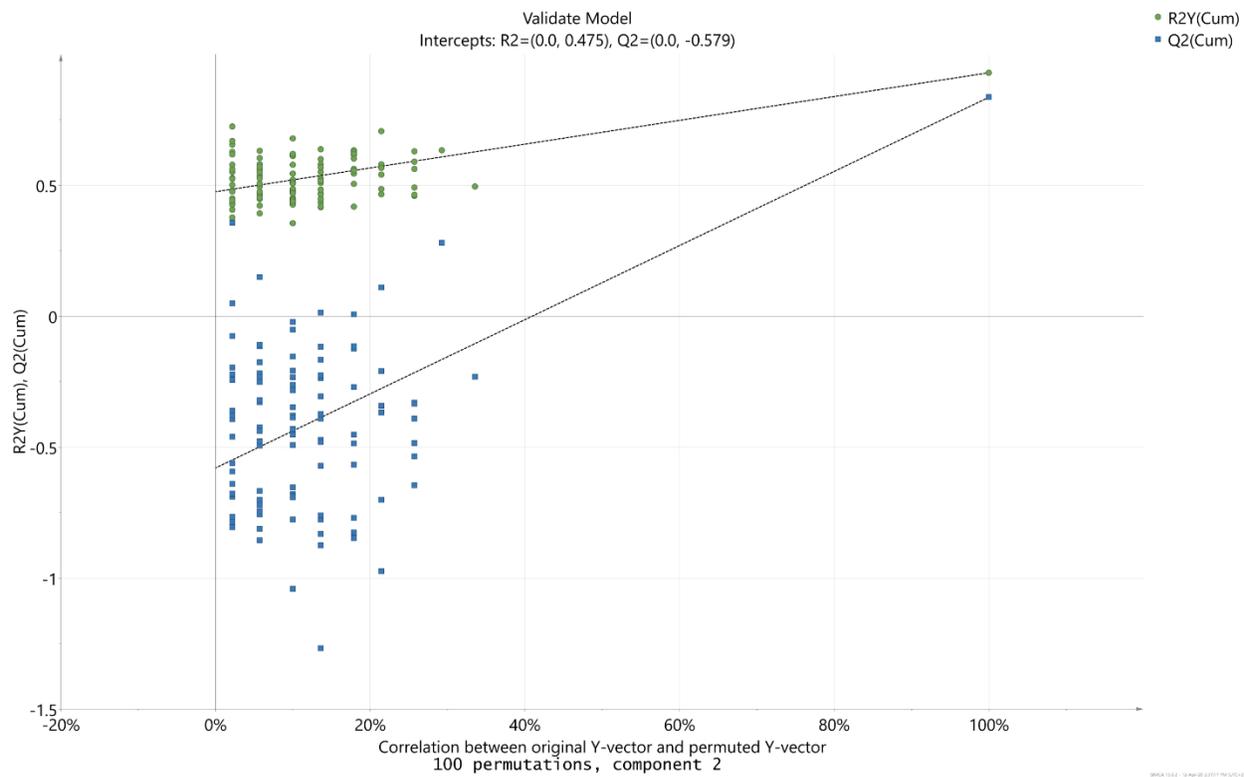


**Figure S1** The GC-Q-MS total ion current (TIC) chromatograms of plasma from a healthy subject

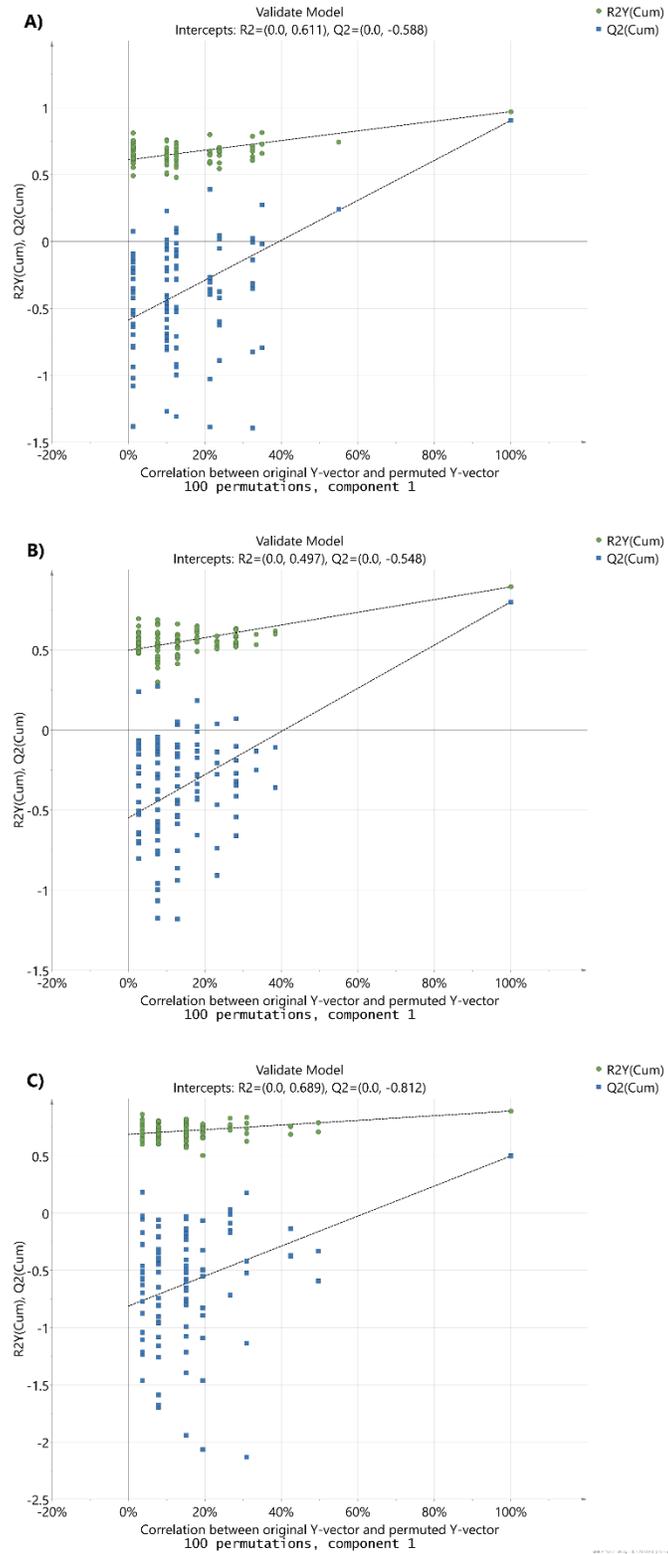


**Figure S2:** The principal component analysis (PCA) scores plot obtained from GC-Q-MS data of all samples. All quality control (QC) samples are found to cluster in the PCA plot.

PTC; papillary thyroid cancer, MNG; multi nodular goiter, QC; quality control

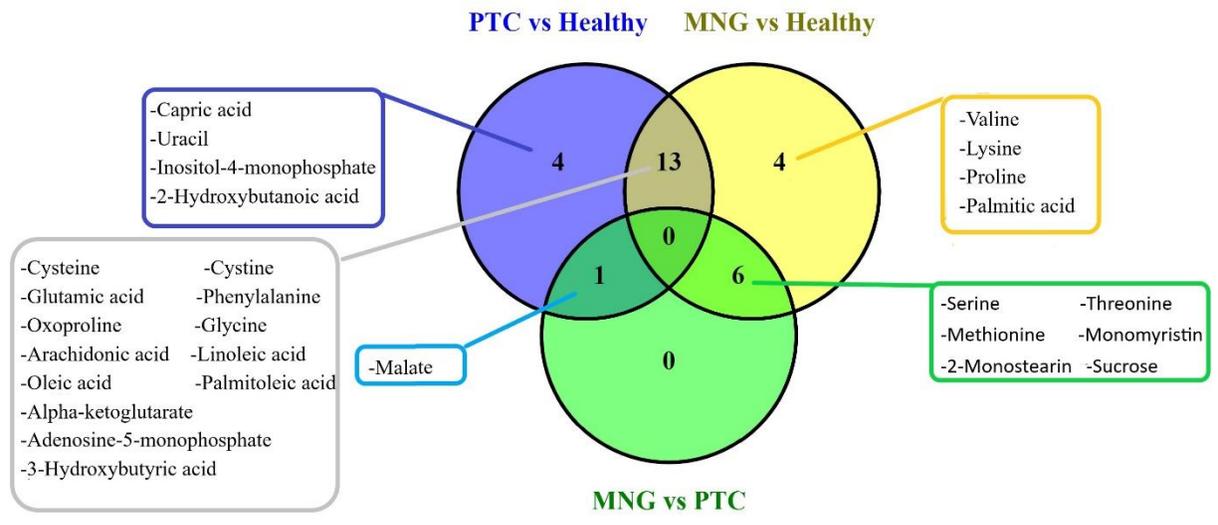


**Figure S3:** Validation plot of a 100 permutation test for OPLS-DA model built for plasma samples among three groups. Low value of R2Y and Q2-intercepts at 0.475 and -0.579 indicating a valid model.



**Figure S4.** Validation plot of 100 permutation tests for OPLS-DA models built for plasma samples **(A)** MNG vs healthy, **(B)** PTC vs healthy and **(C)** PTC vs MNG. The 3 plots assure that the 3 models were well-preserved against overfitting.

MNG; multi nodular goiter, PTC; papillary thyroid cancer



**Figure S5** Venn diagram analysis of discriminant metabolites in different groups, (blue) PTC vs Healthy, (yellow) MNG vs Healthy and (green) MNG vs PTC.

MNG; multi nodular goiter, PTC; papillary thyroid cancer