

Additional File S5 – statistical procedure

Statistical analysis has been conducted with MATLAB version R2015b. Next, details and test specific MATLAB functions (set in `'typewriter'`) are outlined.

Use case 1

The tissue dataset has been downloaded from <https://www.ncbi.nlm.nih.gov/geo/query/acc.cgi?acc=GSE7905> as indicated in the main text. One-way ANOVA (`'anova1'`) had been applied to check for differences of variances of kynurenine and serotonin concentrations among different tissues. Subsequent multiple comparison test with applied Bonferroni multiple test correction (`'multcompare'`) was applied to check for pairwise statistical significance of differences in free concentrations of kynurenine or serotonin among different tissues. Results are detailed out in Additional File: Table S6.

Use case 2

RNASeq data were downloaded from <http://cancergenome.nih.gov>. The corresponding patient identifiers are listed in Additional File S7. For each patient a separate model was generated and respective steady state metabolite concentrations calculated. The initial tryptophan concentration was set to 5 μM , which corresponds to the median concentration of free tryptophan measured in blood [1].

As Komolgorov-Smirnov test (`'kstest'`) and Levene test (`'vartestn'` with `'TestType'` set to `'LeveneAbsolute'` option) revealed that assumptions for one-way ANOVA are violated, non-parametric Kruskal-Wallis test has been applied to check for differences of variances of kynurenine and serotonin concentrations between different cancer types. Finally, a multiple comparison test with Bonferroni multiple test correction (`'multcompare'`) was applied to check for pairwise statistical significance of differences in free concentrations of kynurenine or serotonin between different cancer types.

References

- [1] Chen, Y., Guillemin, G.J.: Kynurenine pathway metabolites in humans: disease and healthy States. *Int J Tryptophan Res* **2**, 1–19 (2009)