**Table S1.** Amino acids transformation using Tukey’s Ladder of Power:

, where y – new value, x – original value.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Amino acid** | **Number of iterations** | **λ** | **W statistic** | ***p*-value** |
| Asp | 2078 | 0.385 | 0.9857 | 0.2798 |
| Glu | 2042 | 0.205 | 0.9822 | 0.1411 |
| Asn | 2048 | 0.235 | 0.9867 | 0.3380 |
| Ser | 2038 | 0.185 | 0.9811 | 0.1139 |
| Gln | 2055 | 0.270 | 0.9795 | 0.08244 |
| His | 2063 | 0.310 | 0.9863 | 0.3146 |
| Gly | 2065 | 0.320 | 0.9686 | 0.009655 |
| Thr | 2079 | 0.390 | 0.9756 | 0.03763 |
| Cit | 2083 | 0.410 | 0.8806 | 5.183e-08 |
| Arg | 2090 | 0.445 | 0.9517 | 0.0004818 |
| Ala | 1989 | -0.060 | 0.9839 | 0.1981 |
| Tau | 2111 | 0.550 | 0.9699 | 0.01231 |
| GABA | 2081 | 0.400 | 0.9497 | 0.0003495 |
| BABA | 2103 | 0.510 | 0.8189 | 2.054e-10 |
| Tyr | 2074 | 0.365 | 0.8103 | 1.053e-10 |
| AABA | 2103 | 0.510 | 0.8793 | 4.537e-08 |
| Cys | 2020 | 0.095 | 0.9920 | 0.7597 |
| Val | 2075 | 0.370 | 0.9718 | 0.01793 |
| Met | 2167 | 0.830 | 0.9497 | 0.0003468 |
| Nva | 2075 | 0.370 | 0.7778 | 9.977e-12 |
| Trp | 2092 | 0.455 | 0.9845 | 0.2221 |
| Phe | 2078 | 0.385 | 0.9725 | 0.02038 |
| Ile | 2070 | 0.345 | 0.9882 | 0.4378 |
| Orn | 2078 | 0.385 | 0.9294 | 1.682e-05 |
| Leu | 2062 | 0.305 | 0.9868 | 0.3403 |
| Lys | 2059 | 0.290 | 0.9722 | 0.01927 |
| Pro | 2061 | 0.300 | 0.9819 | 0.134 |

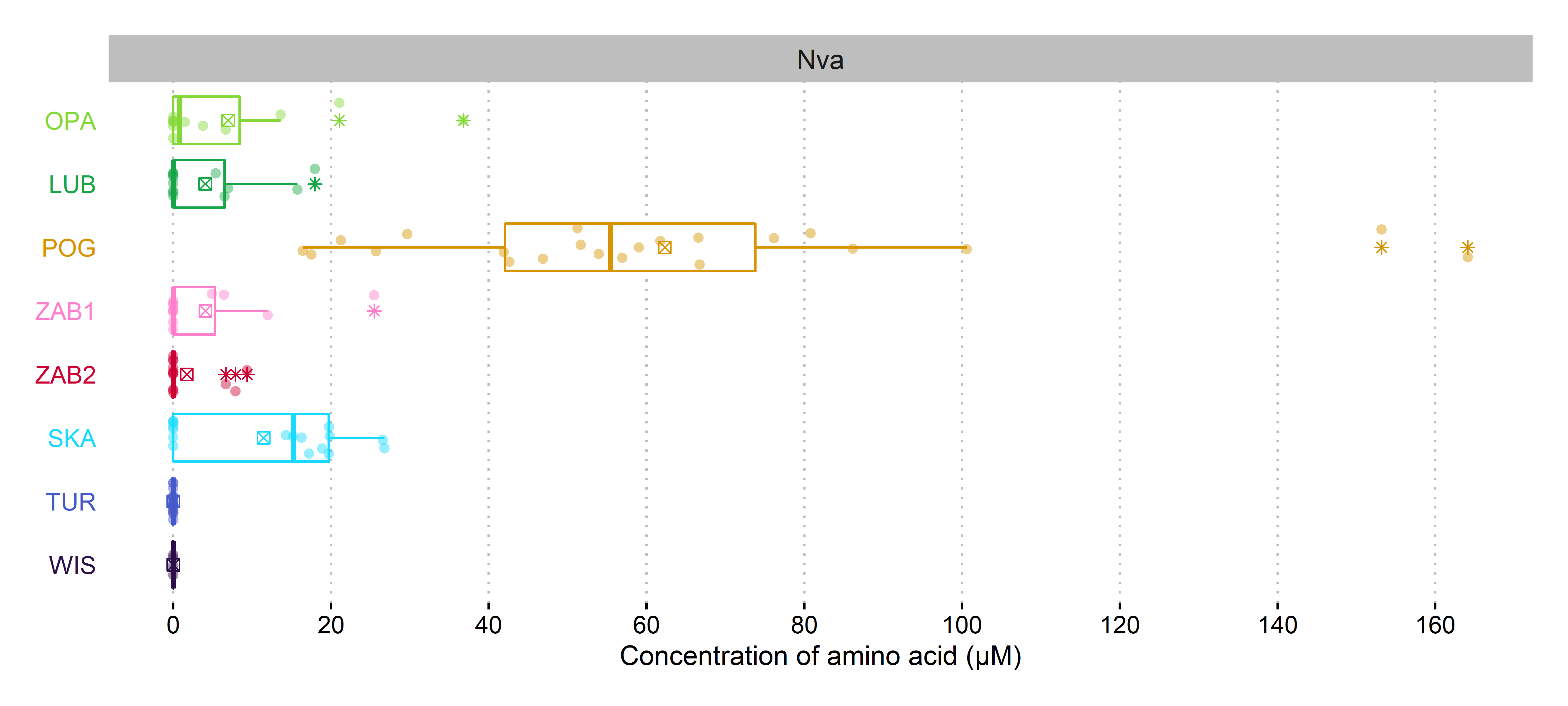
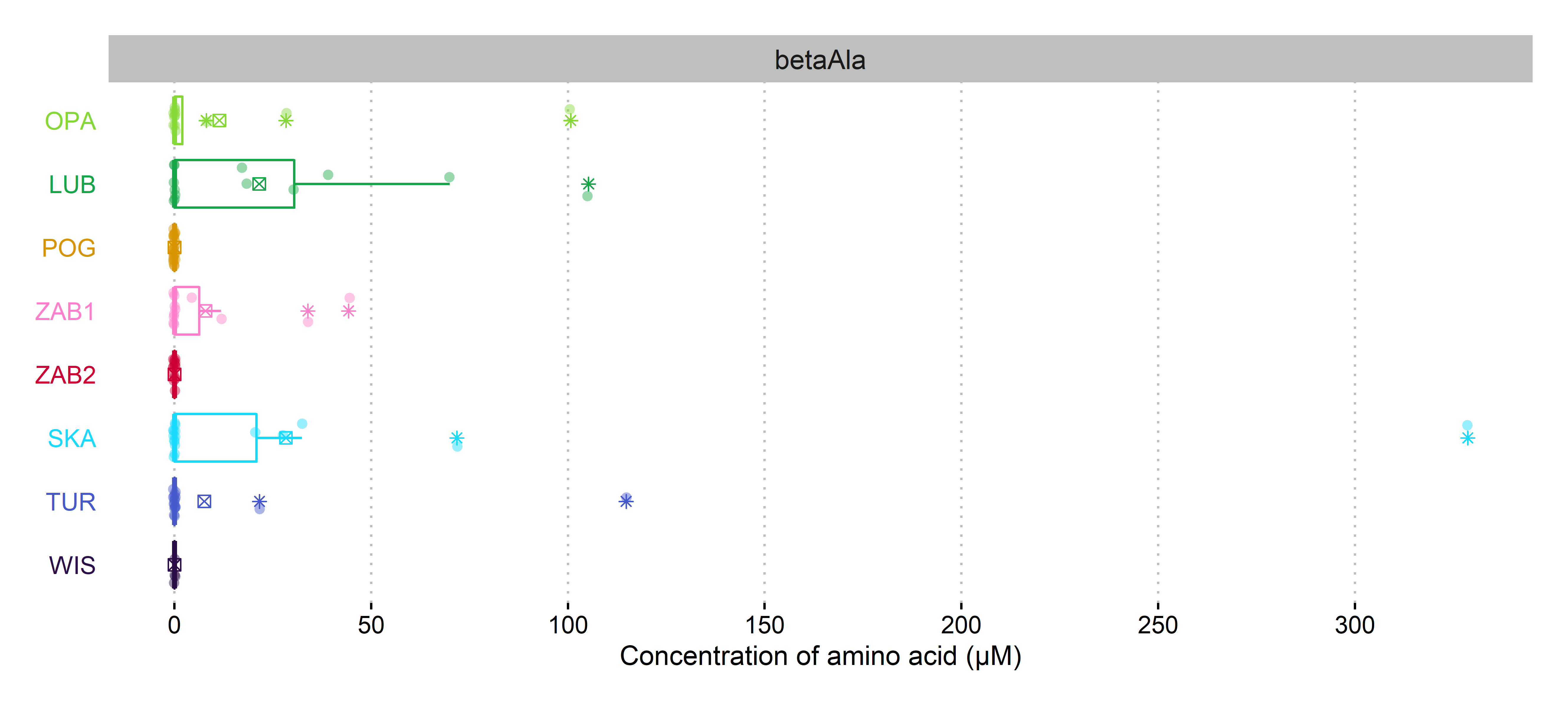
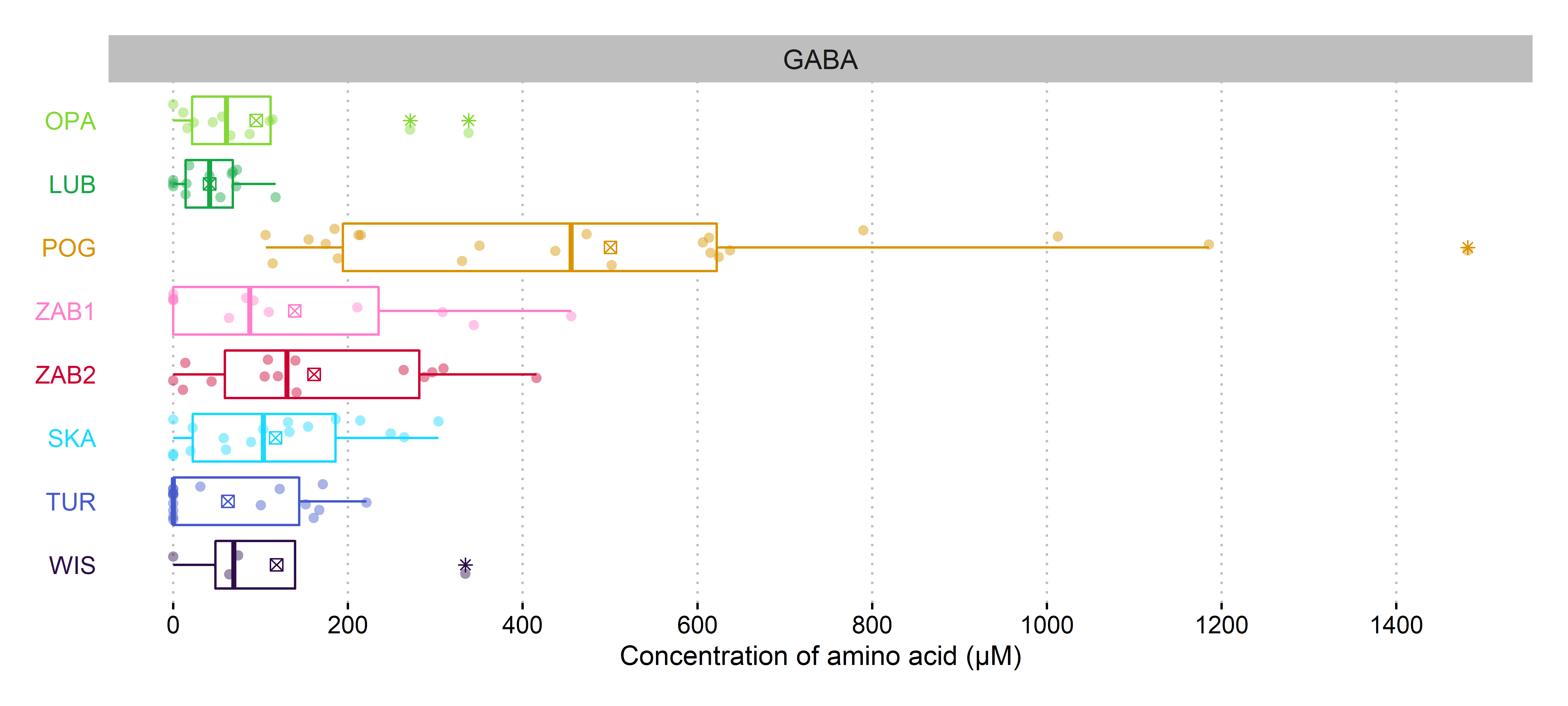
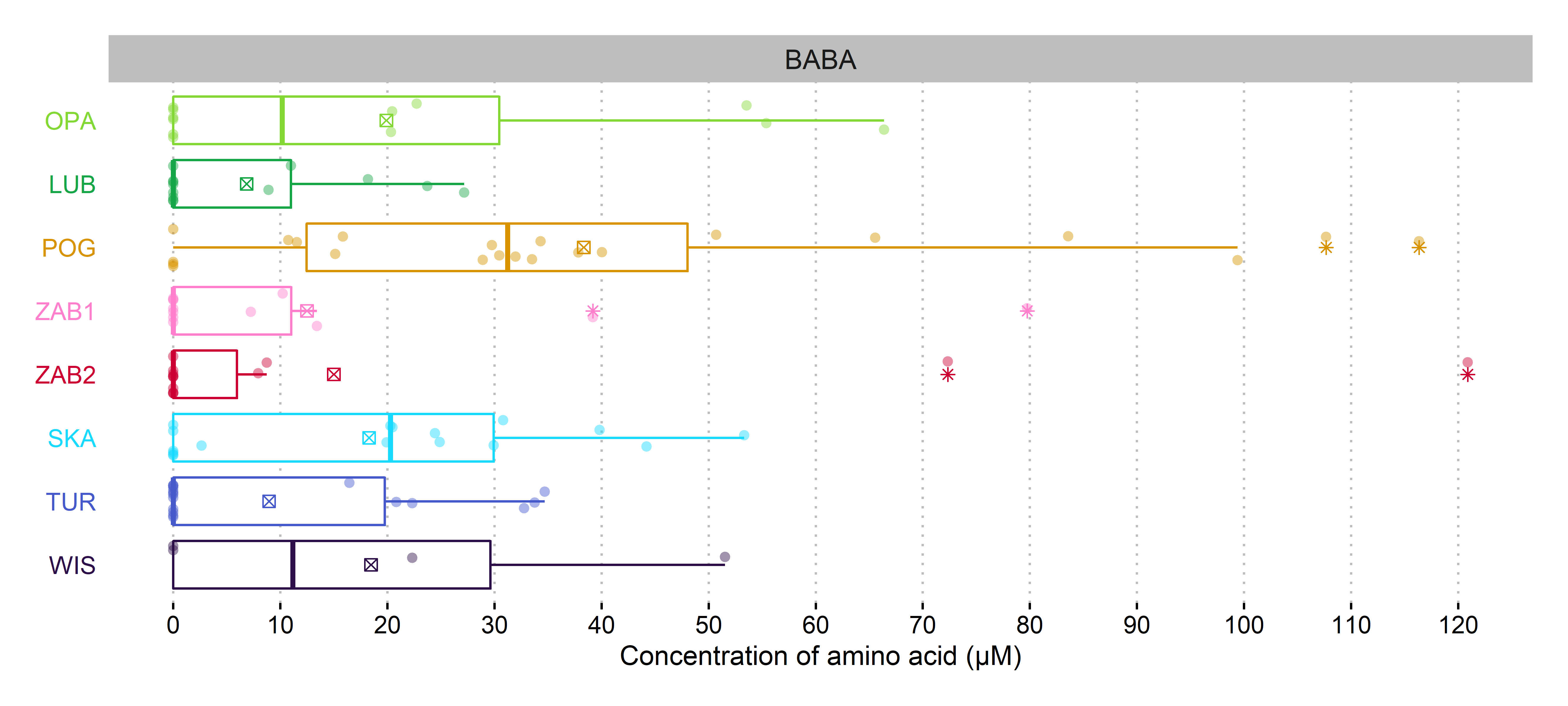
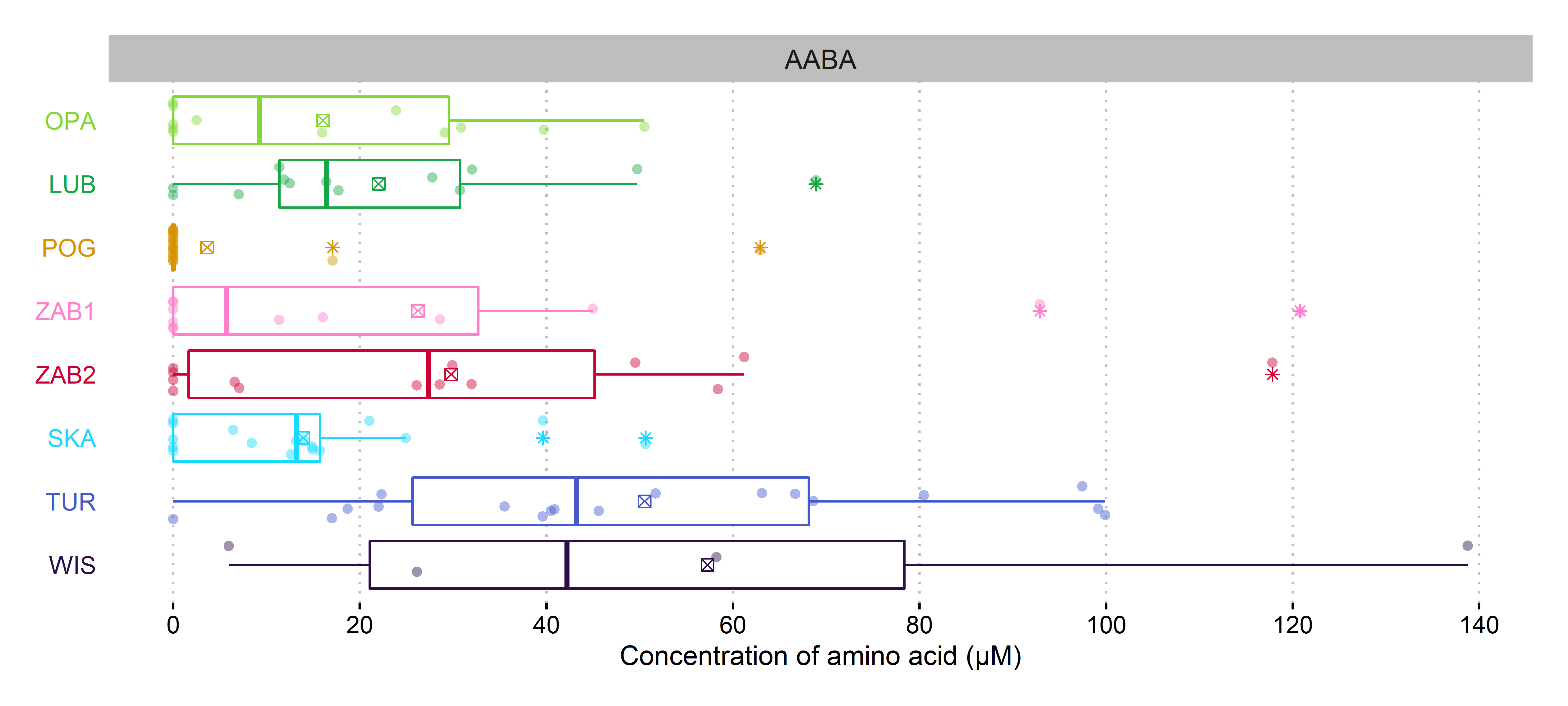
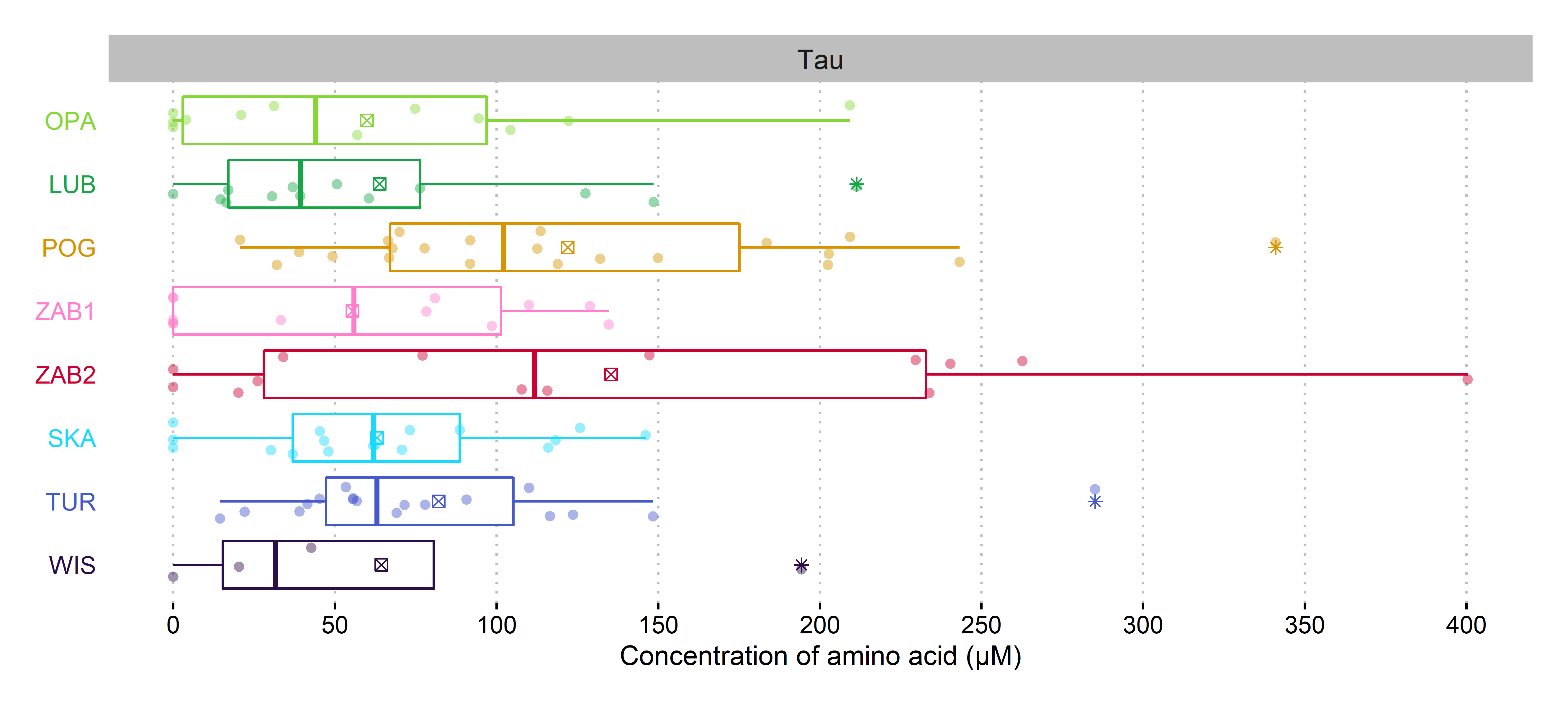
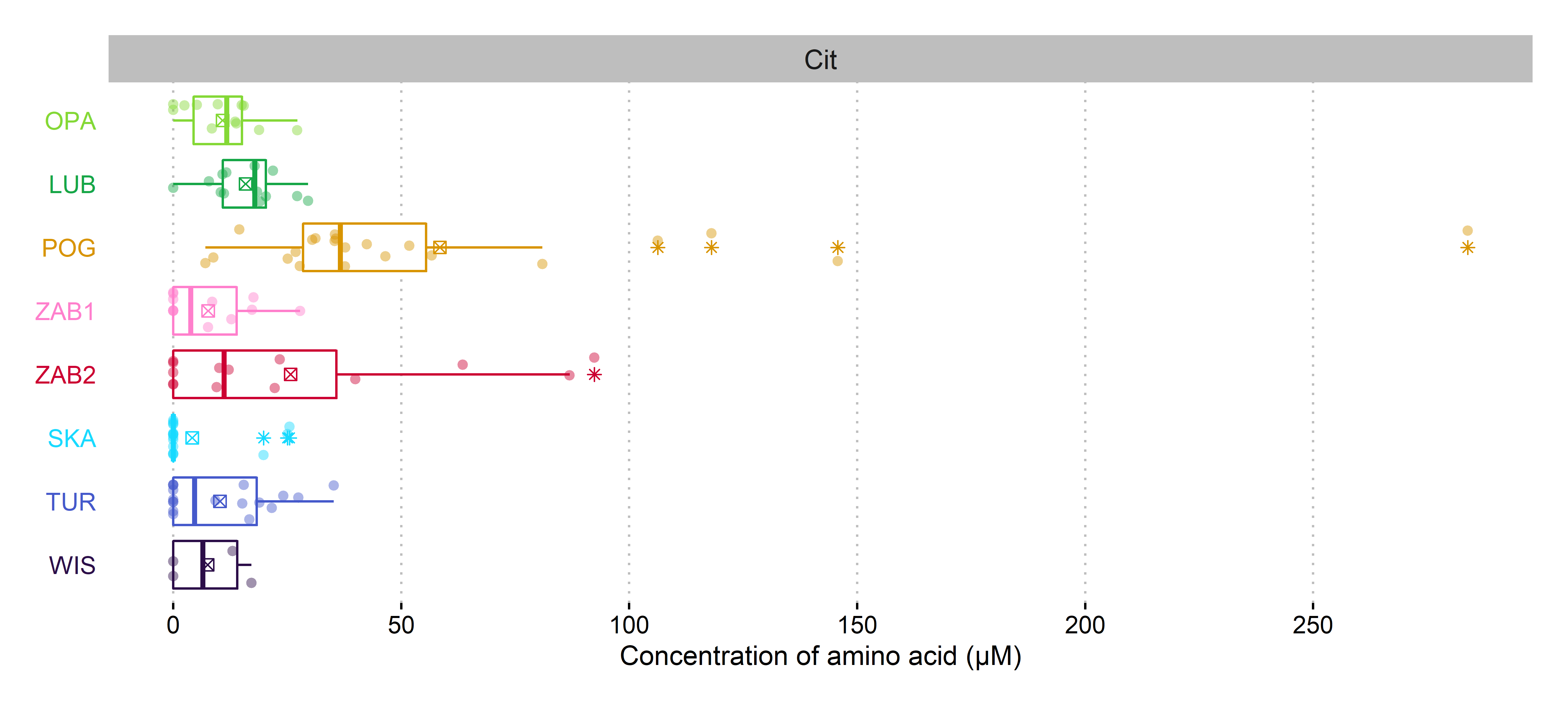
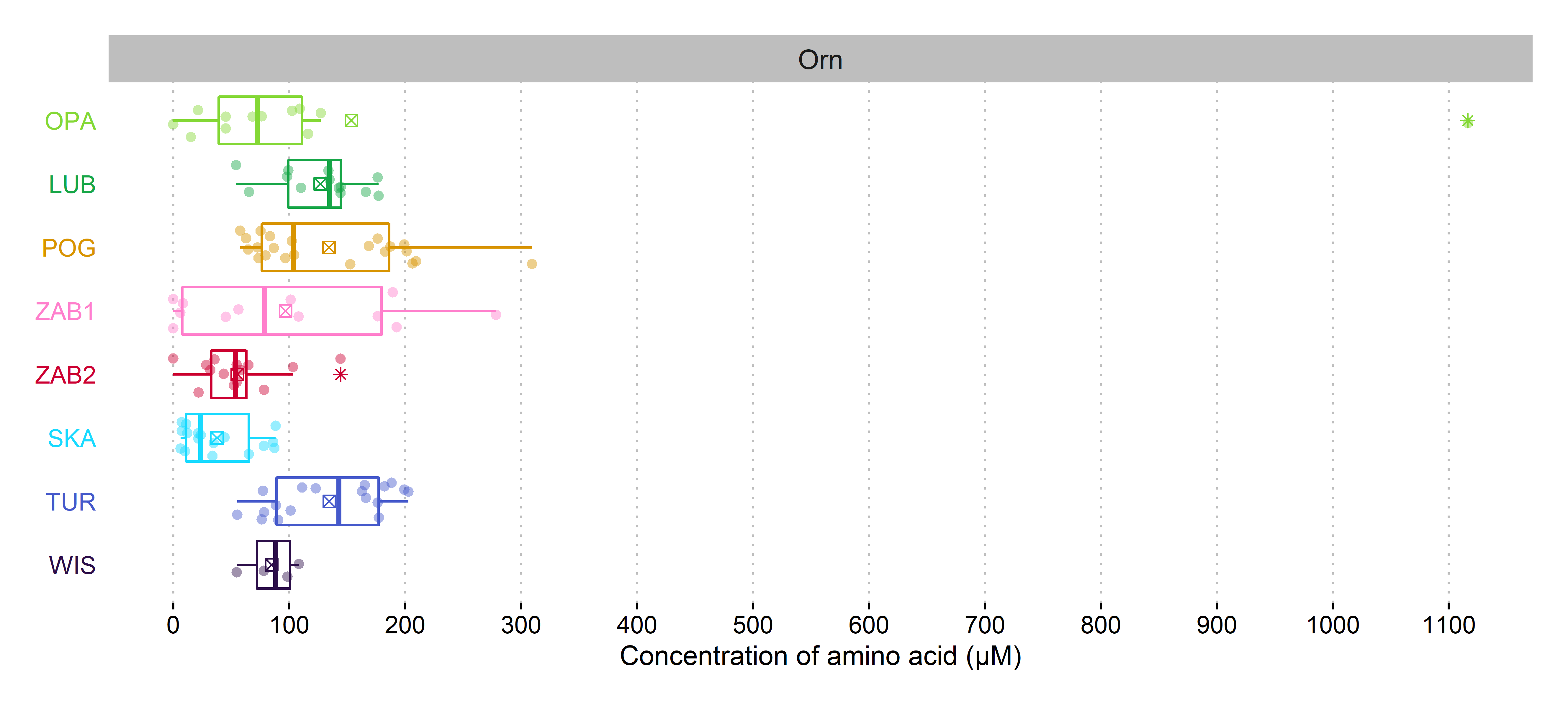
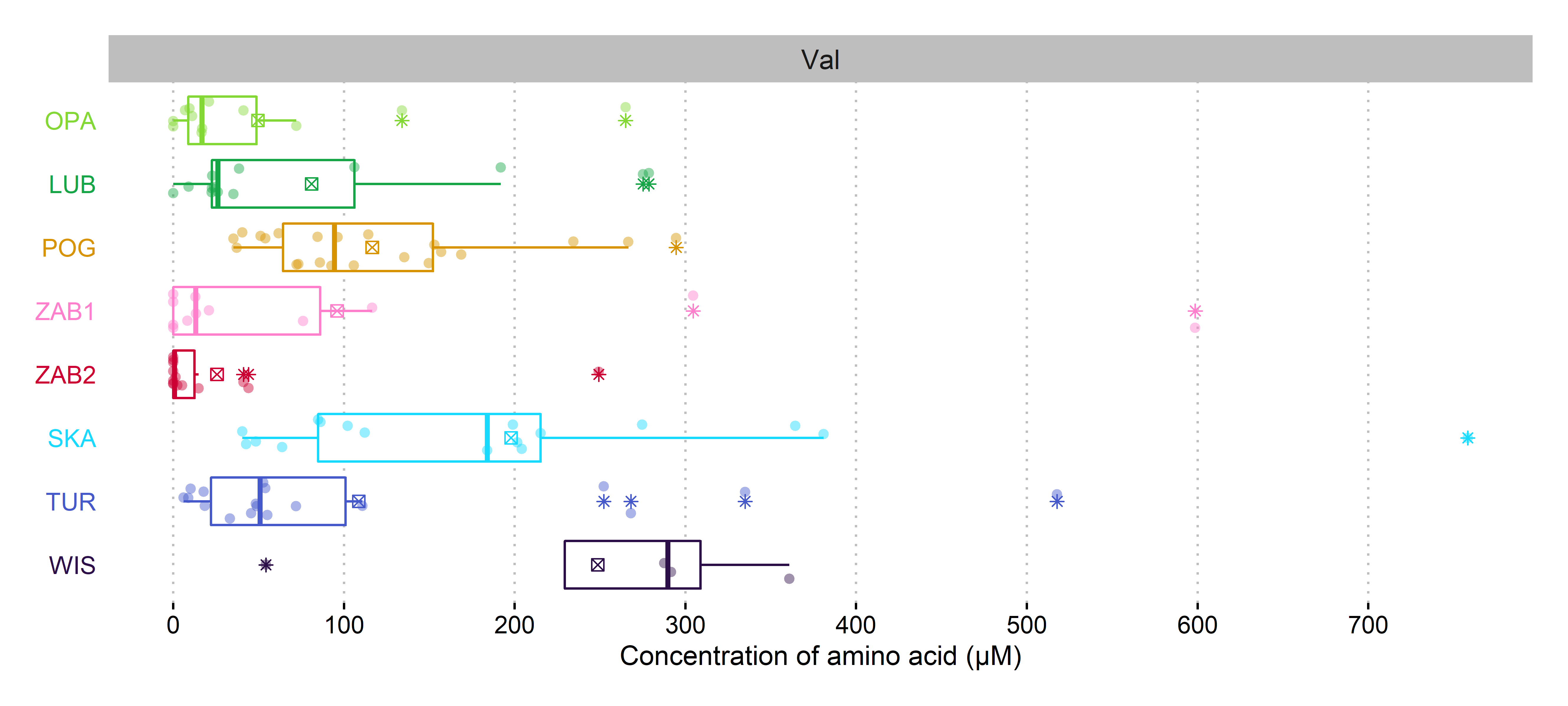
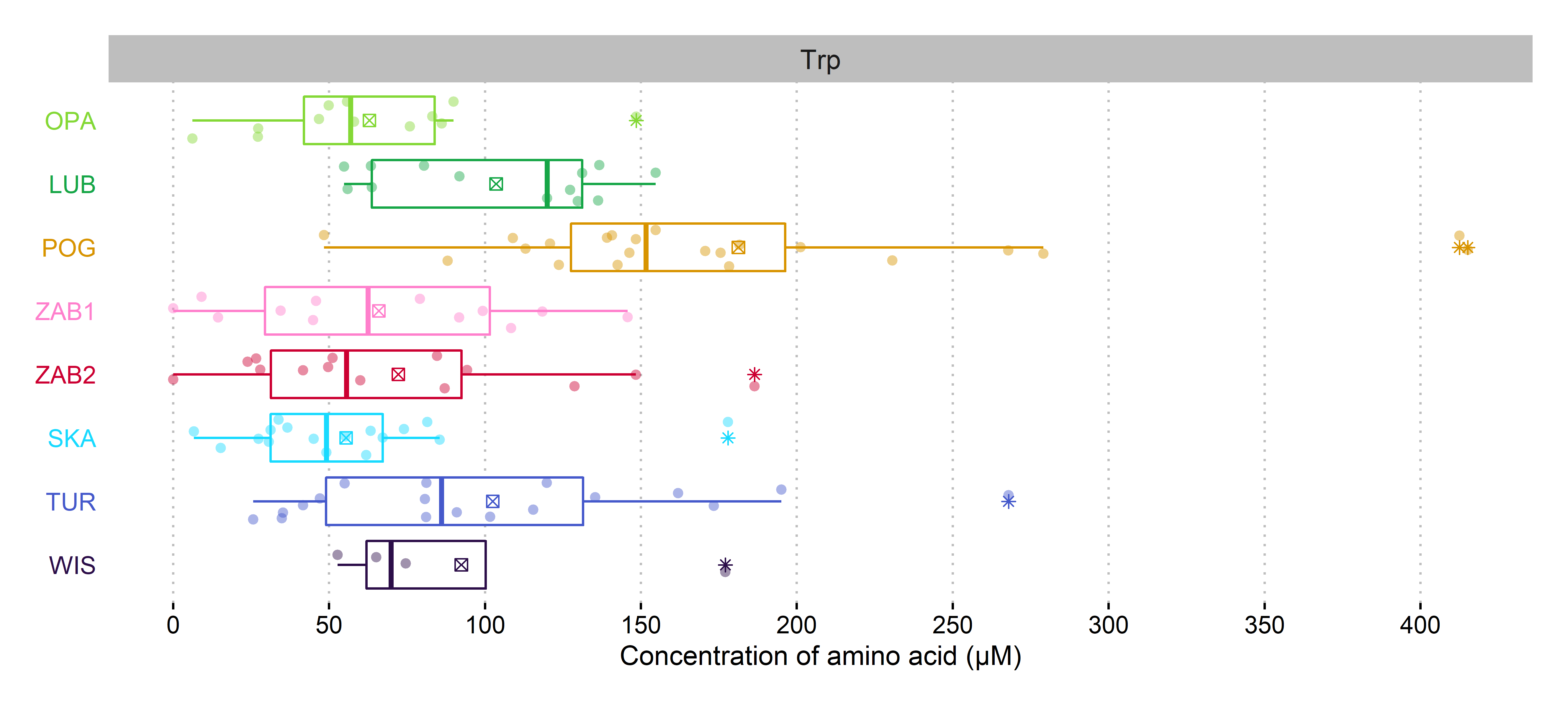
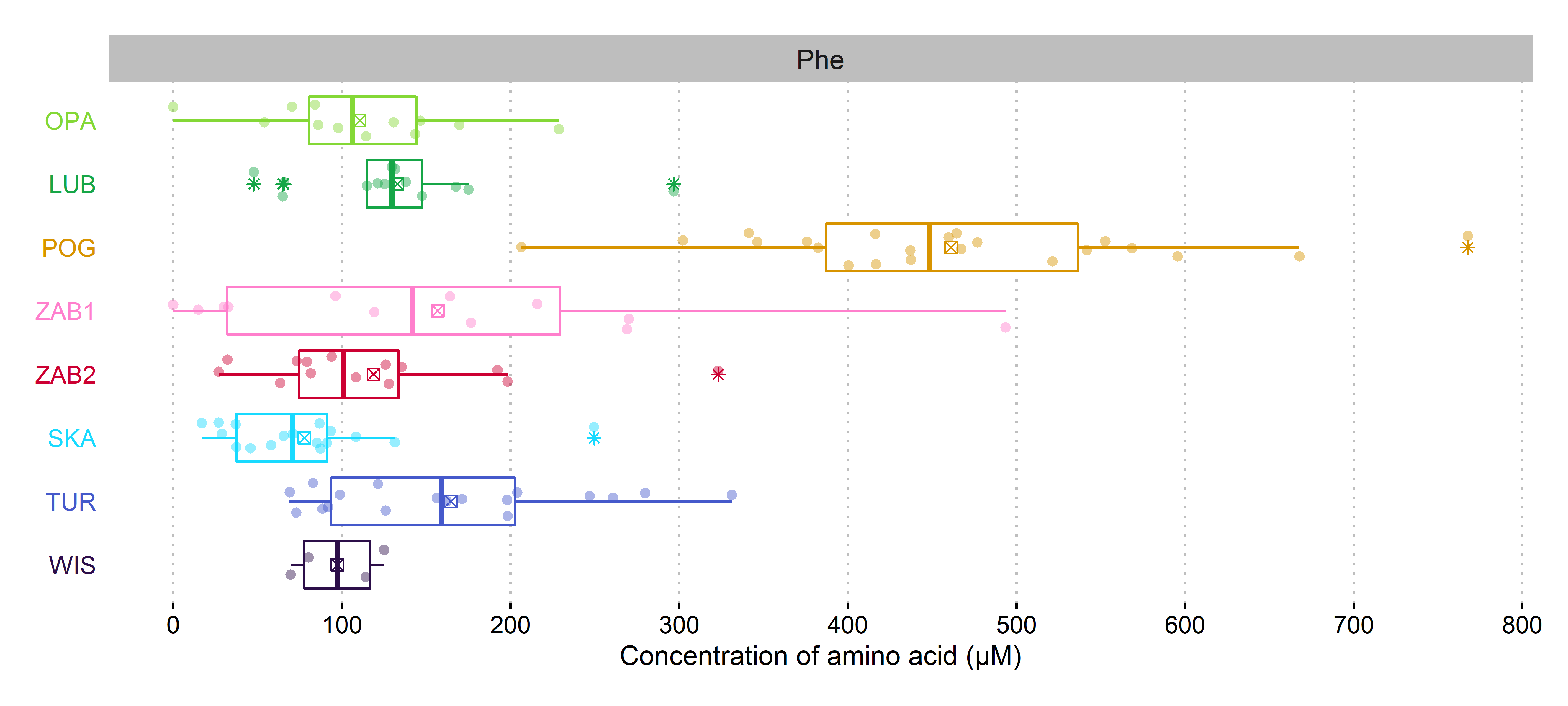
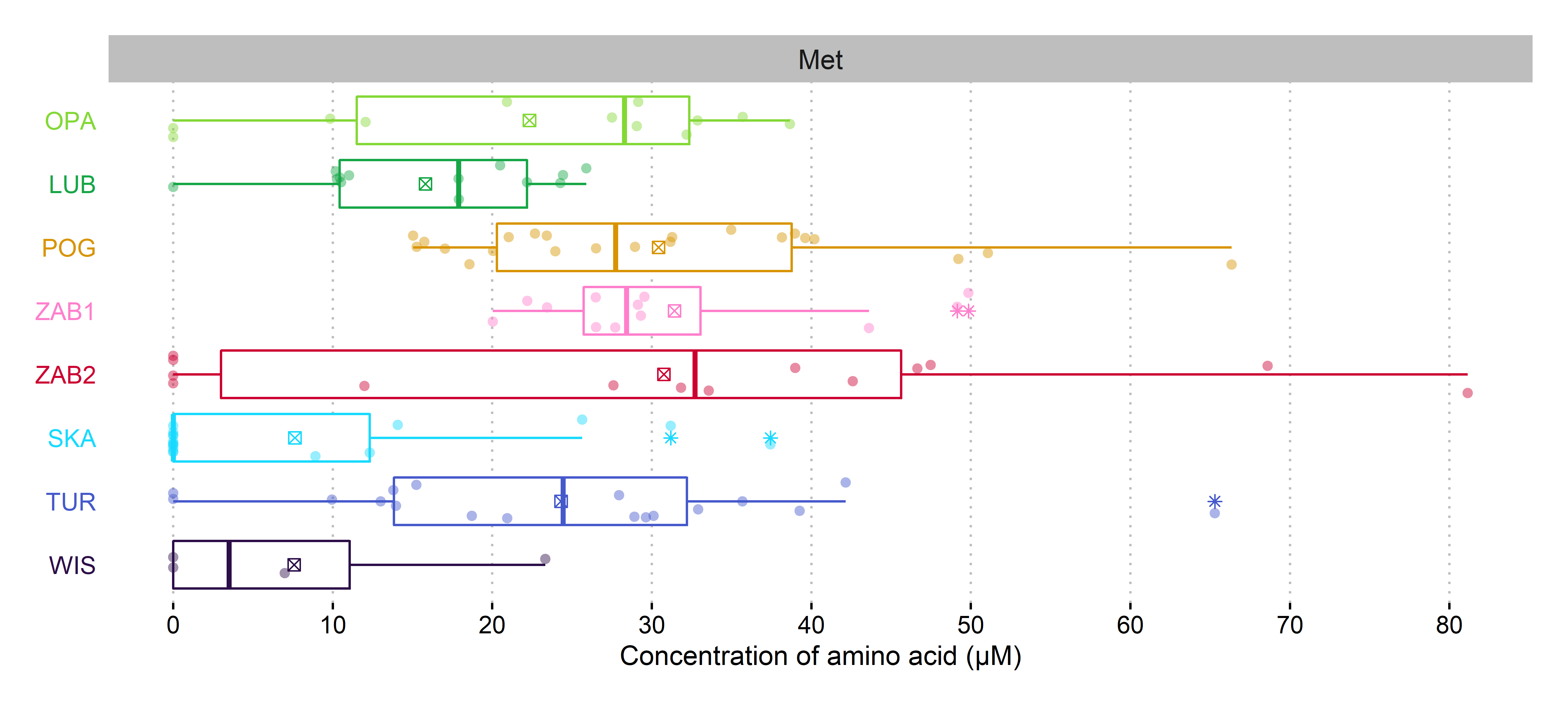
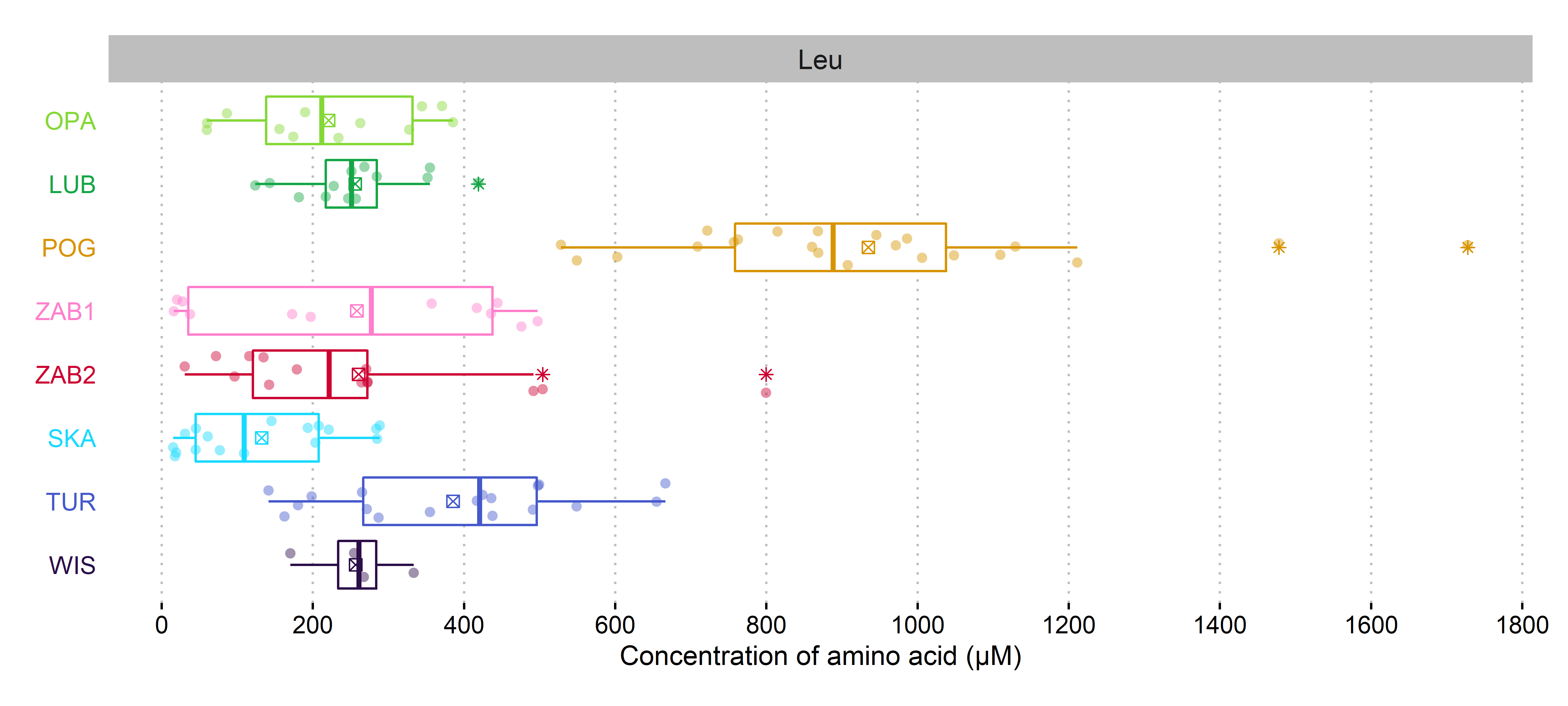
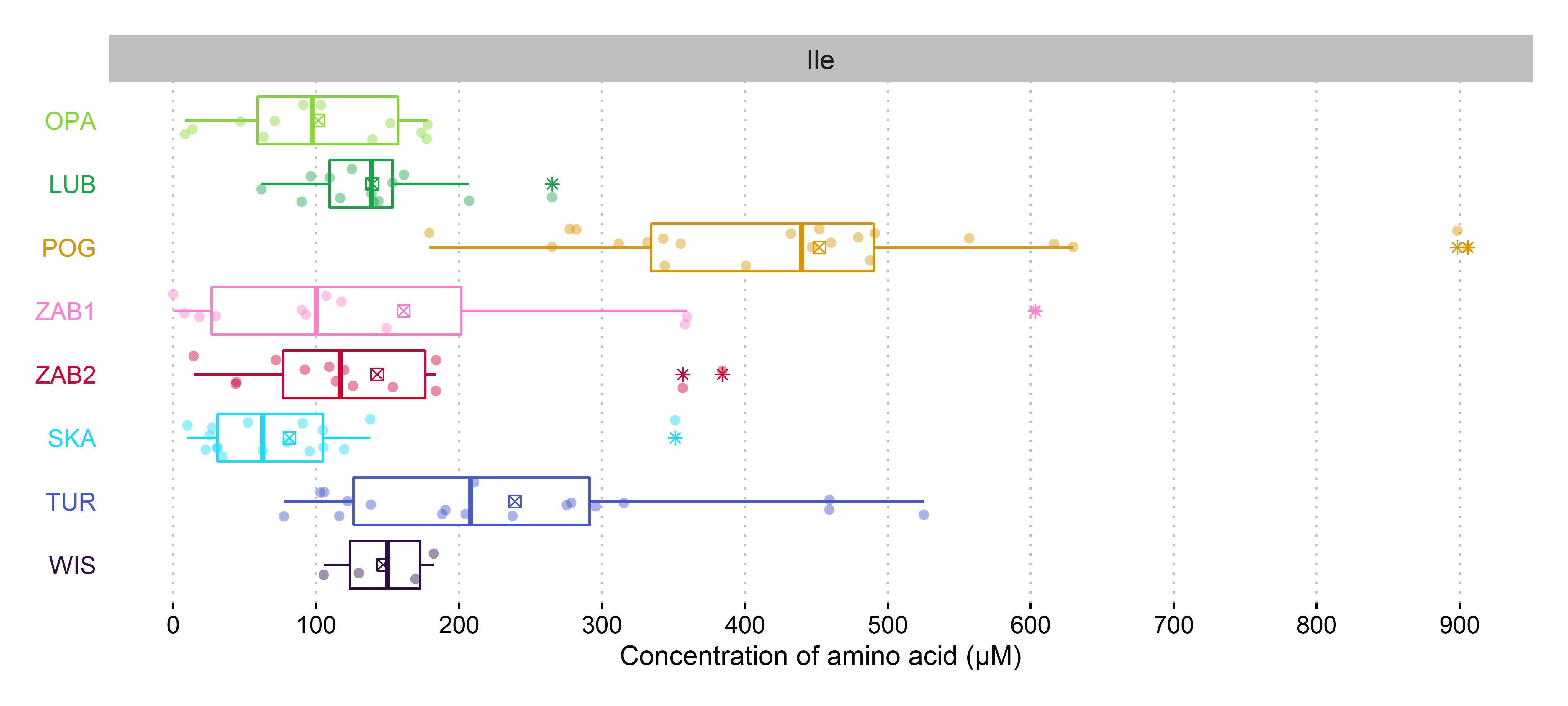
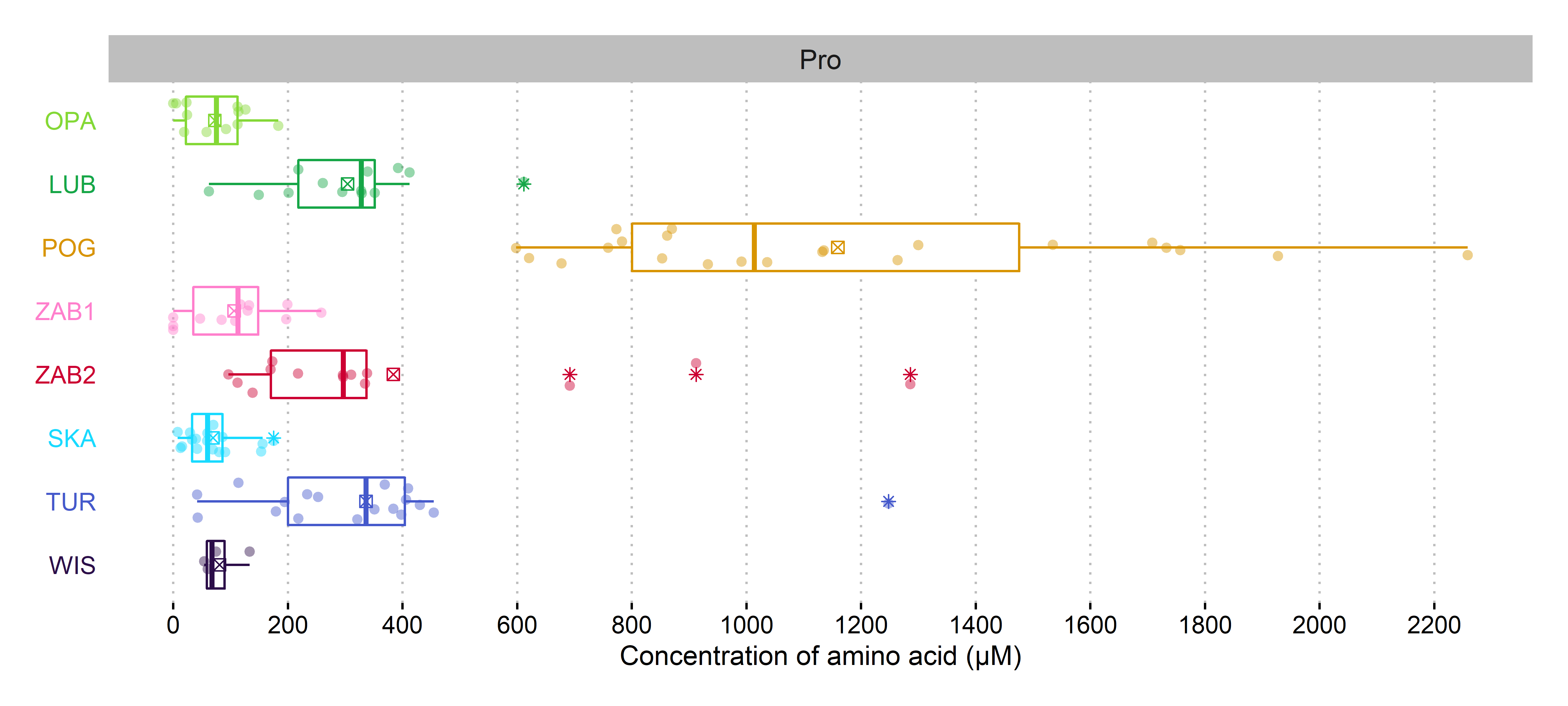
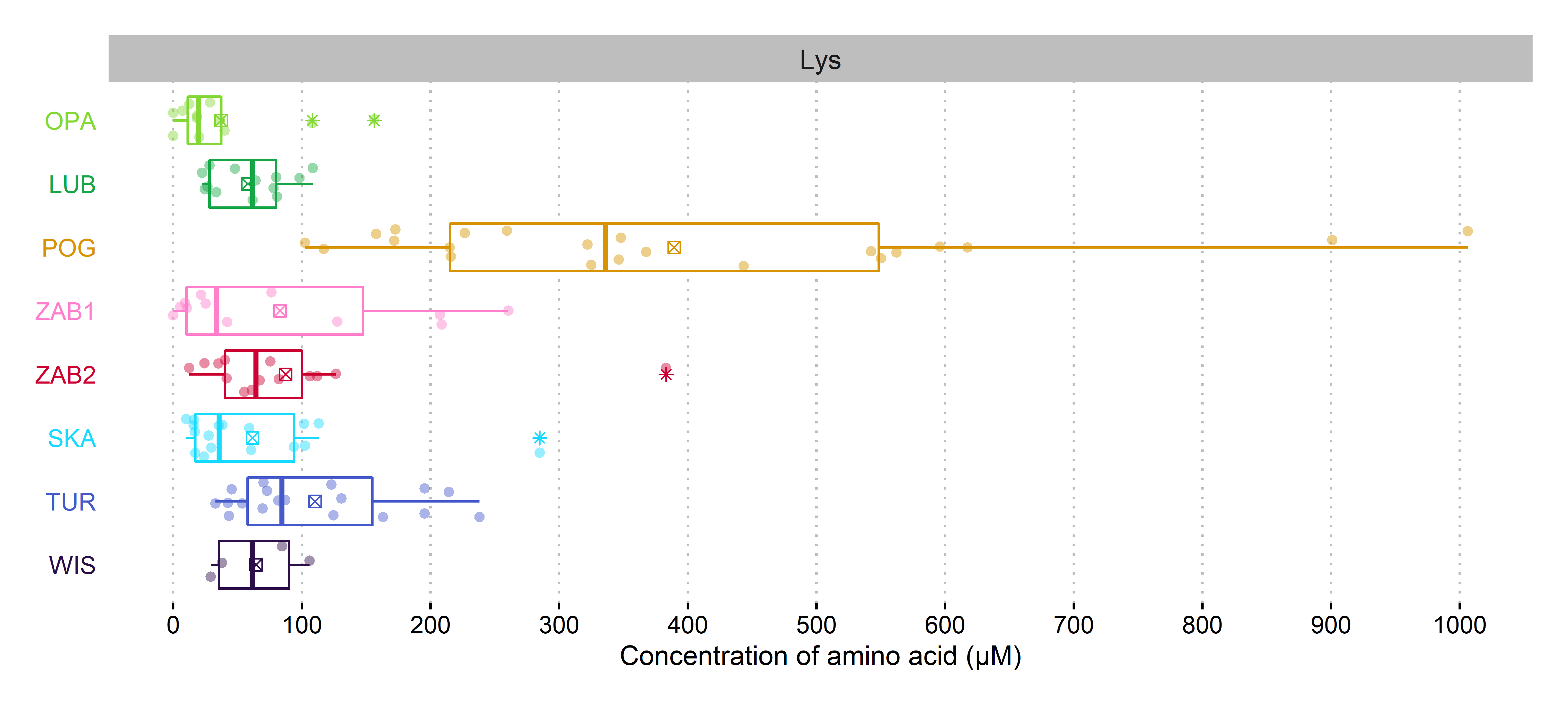
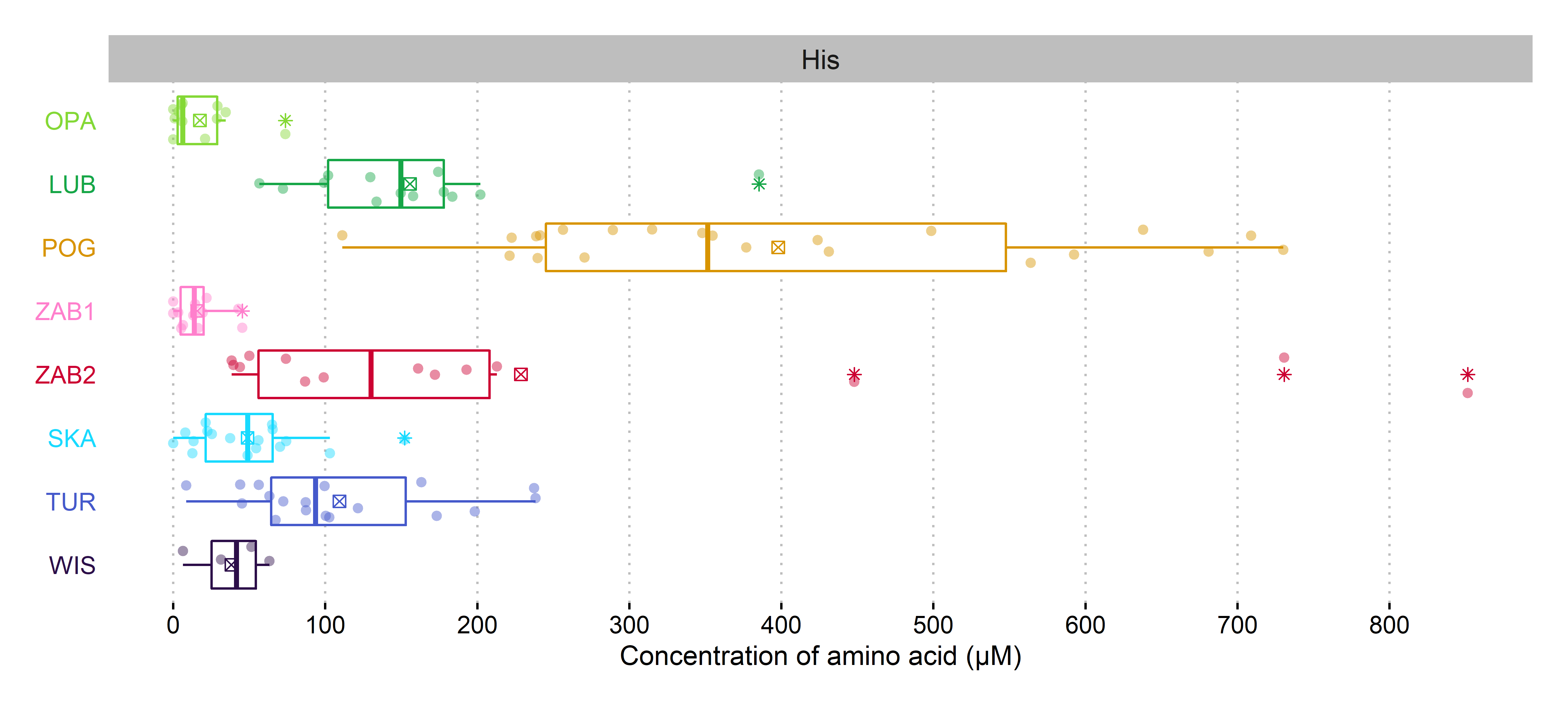
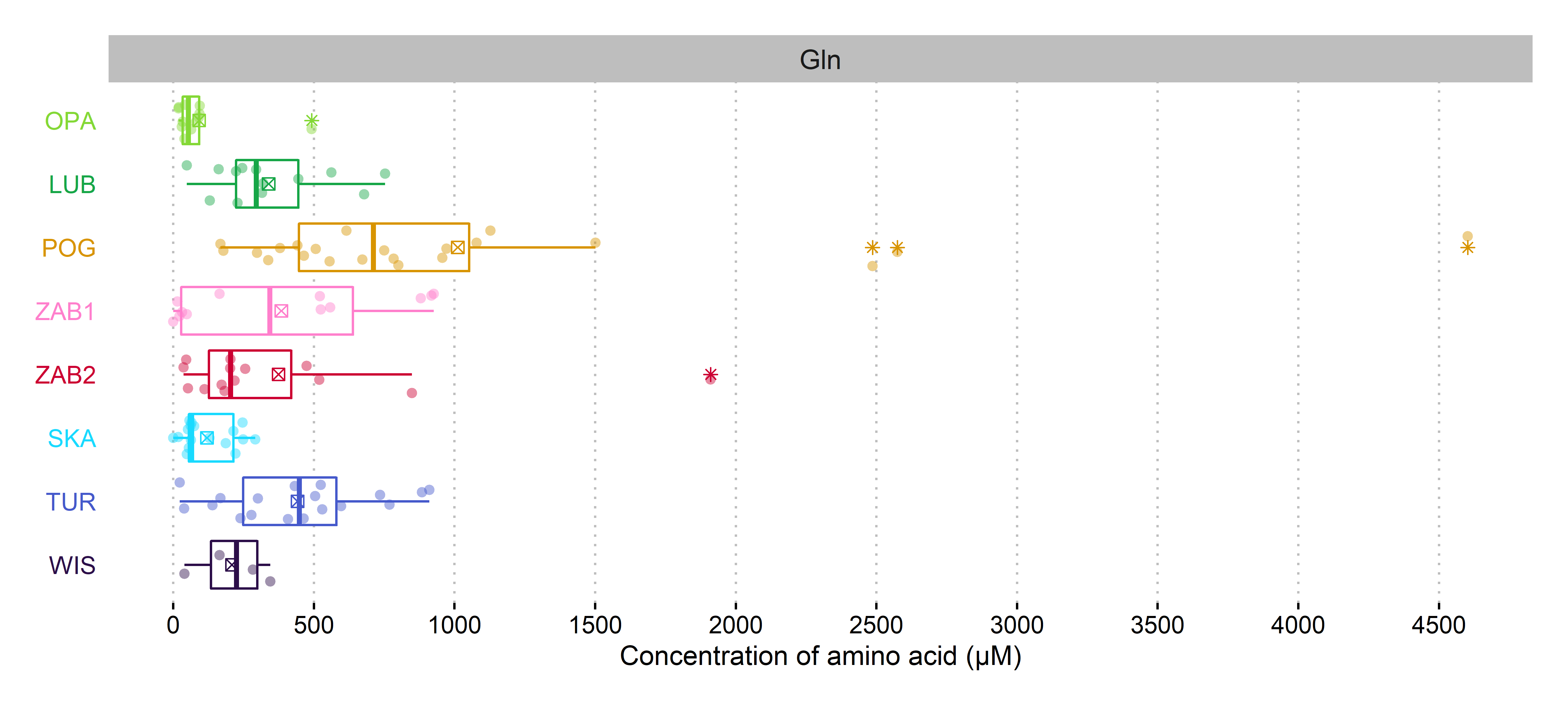
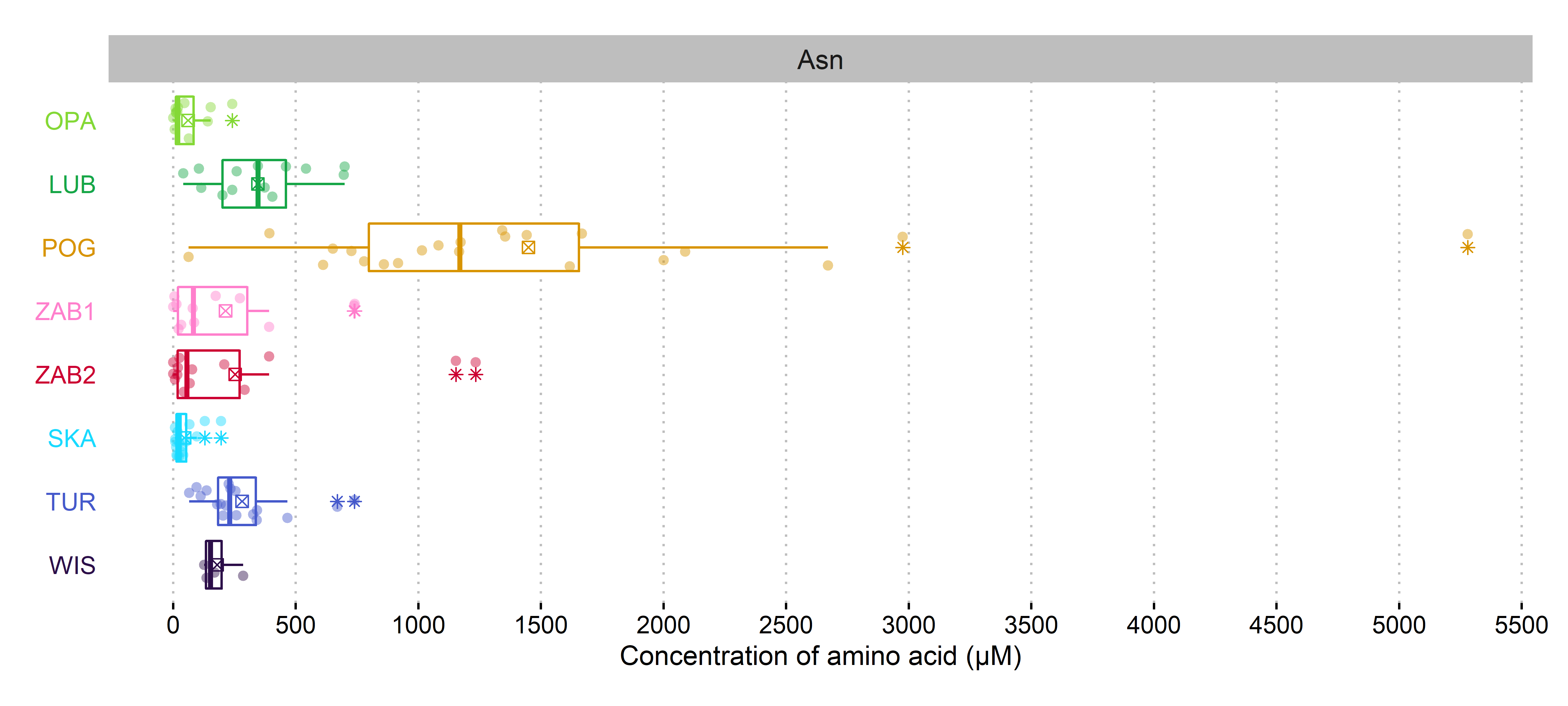
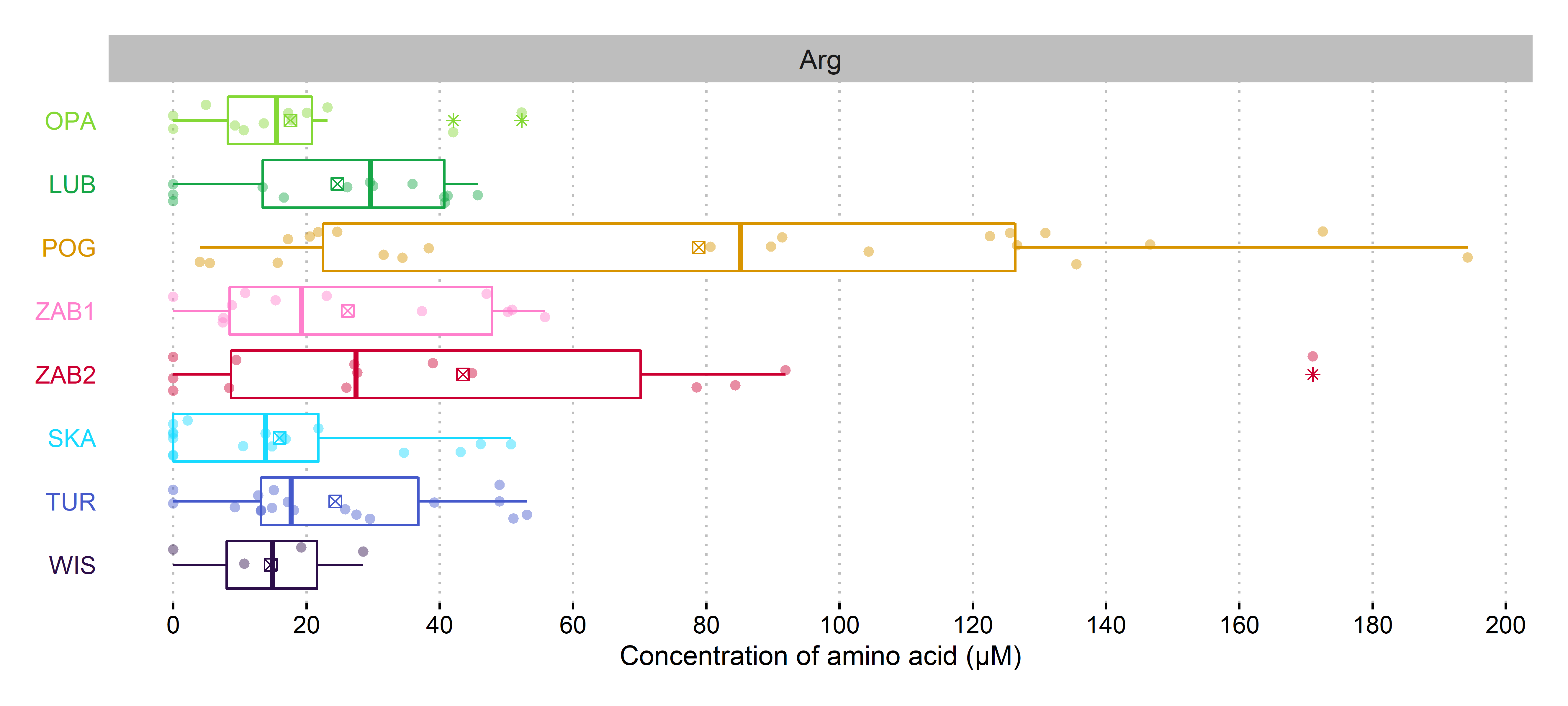
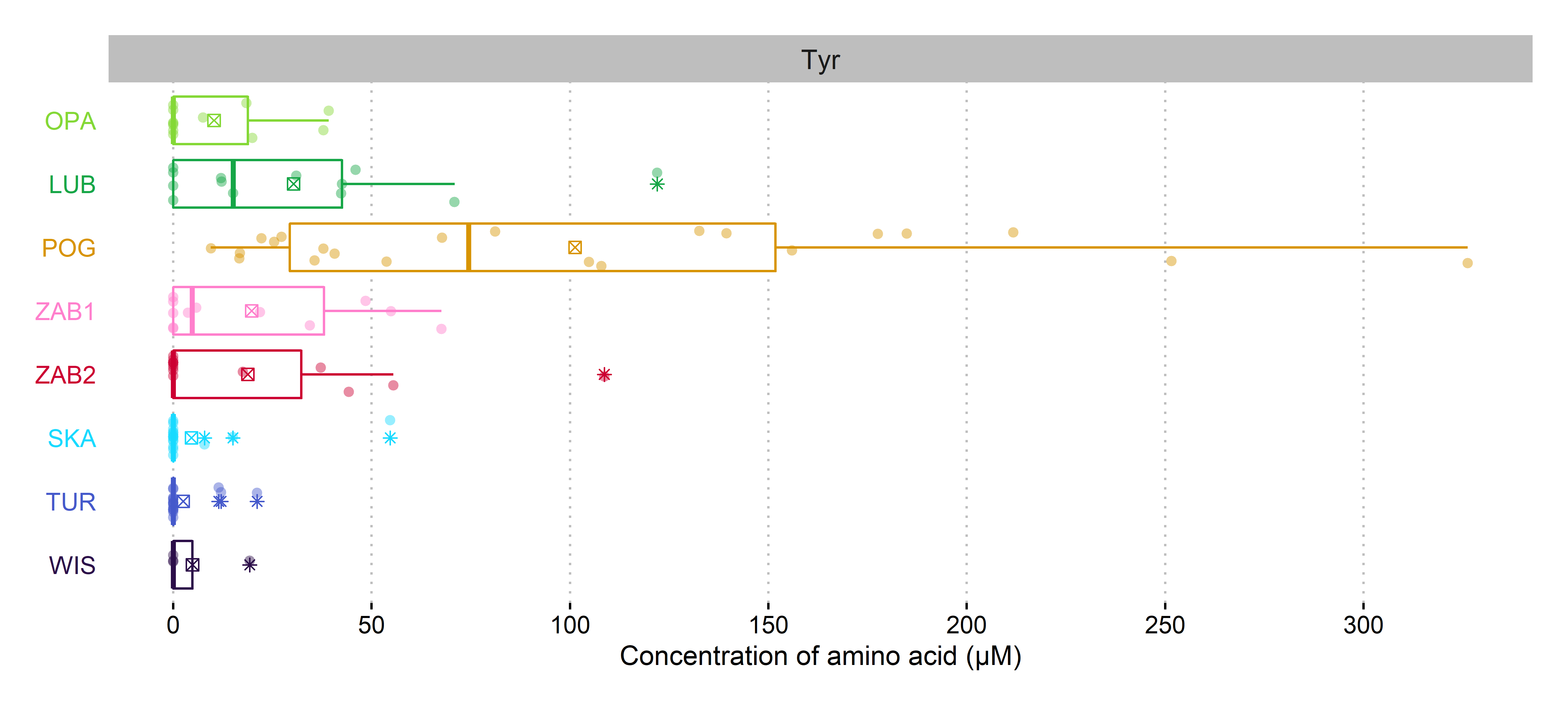
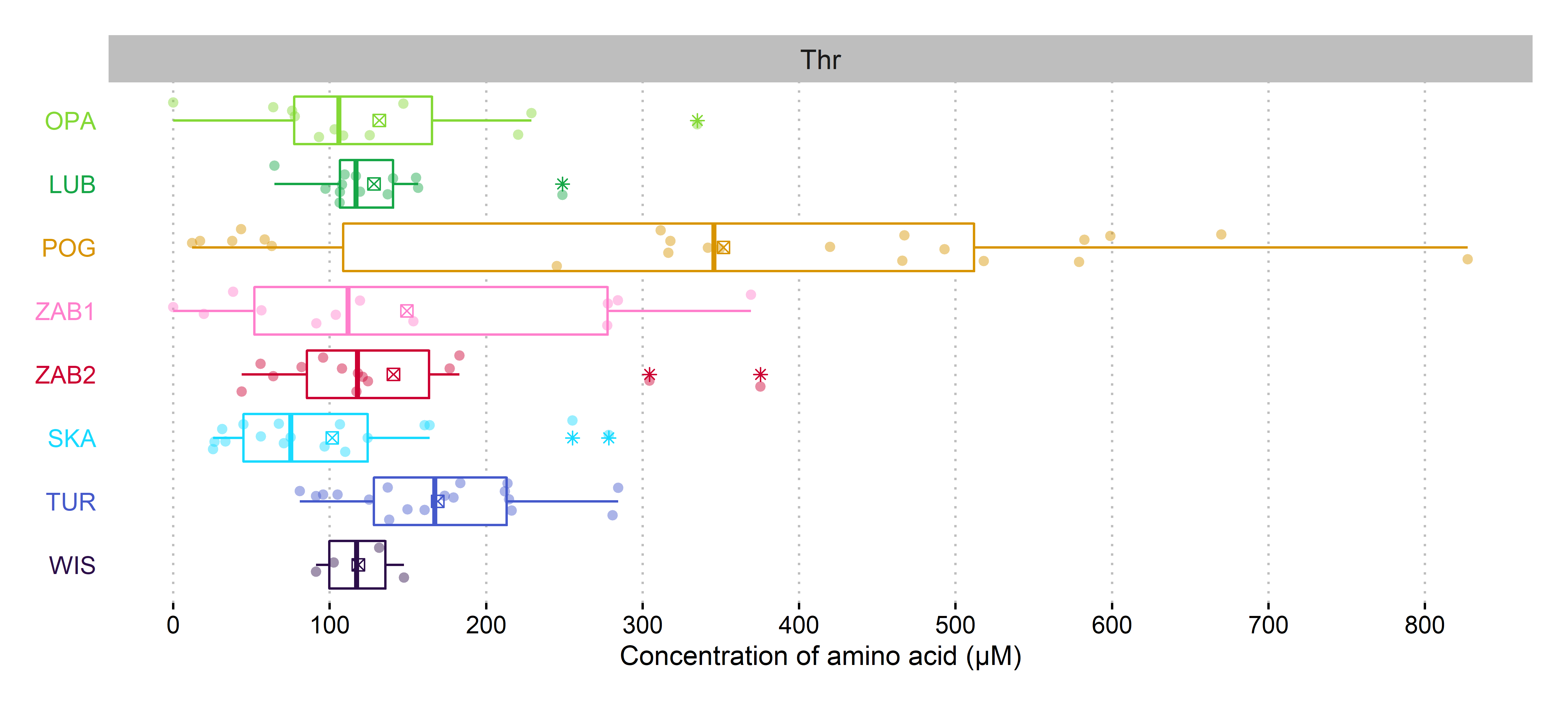
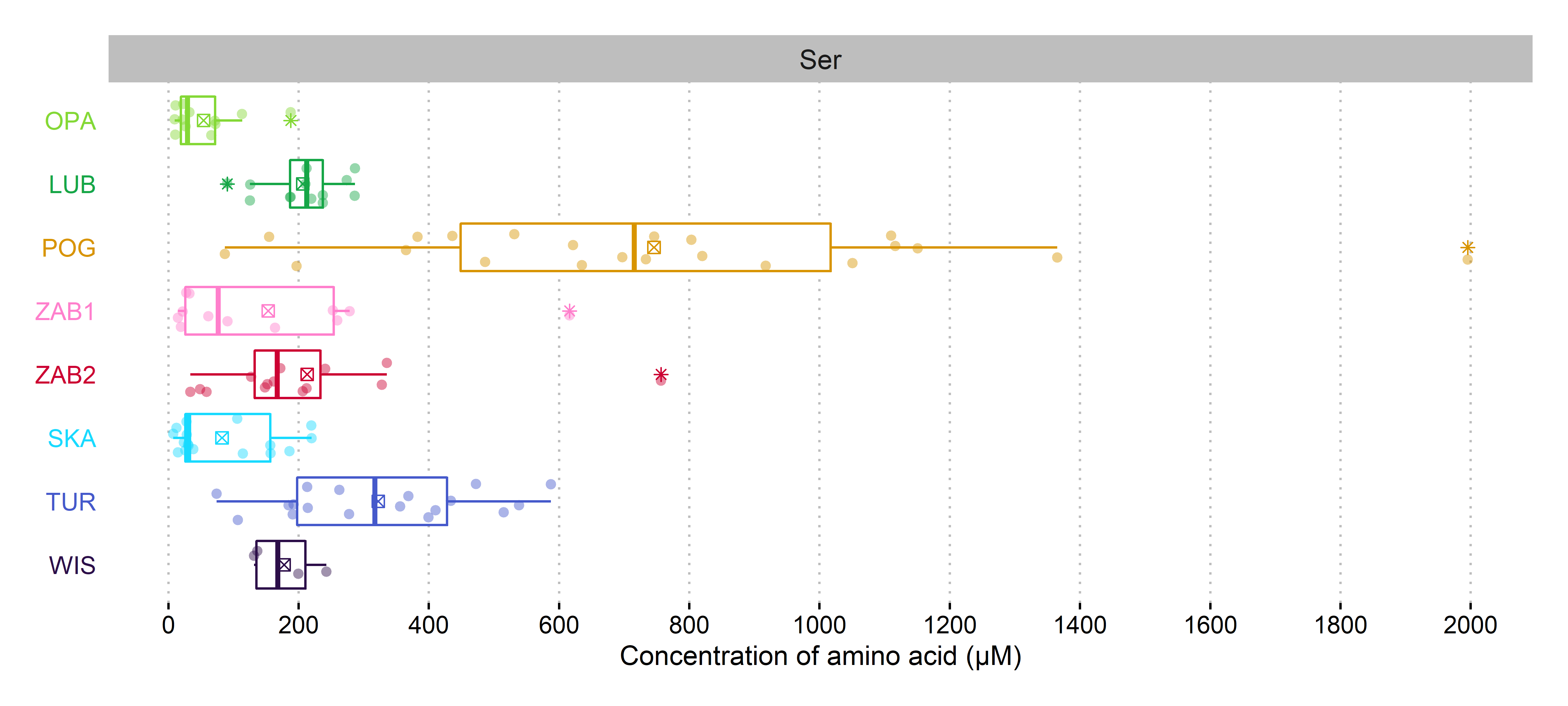
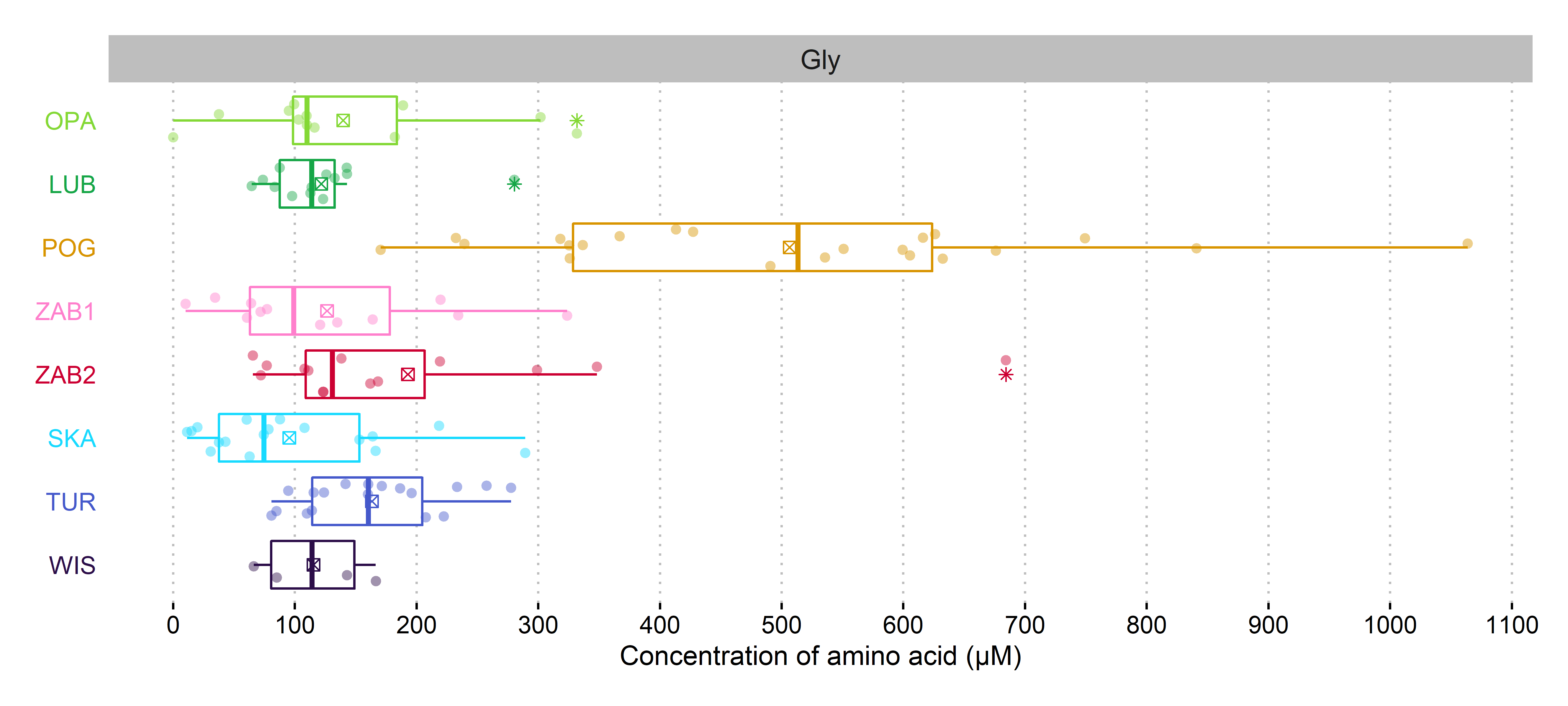
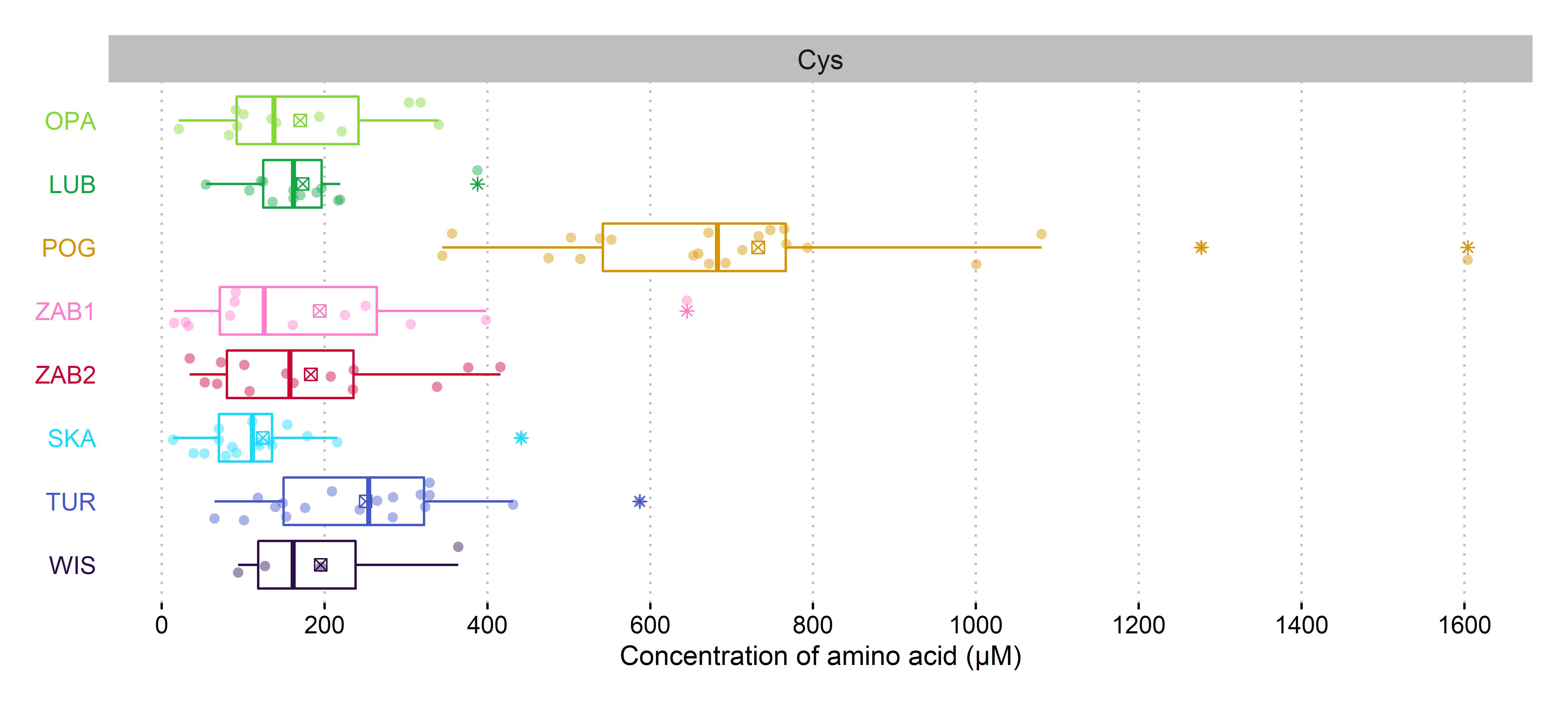
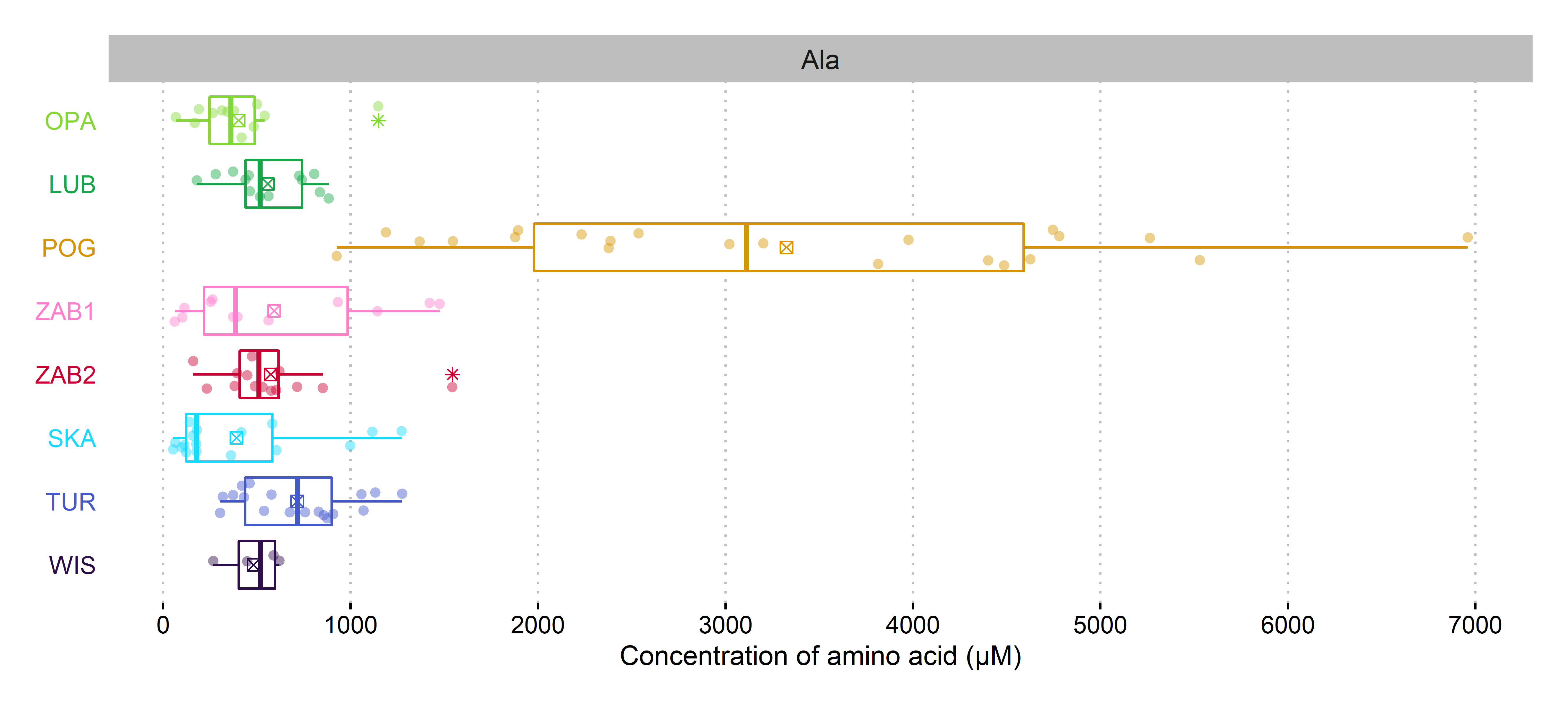
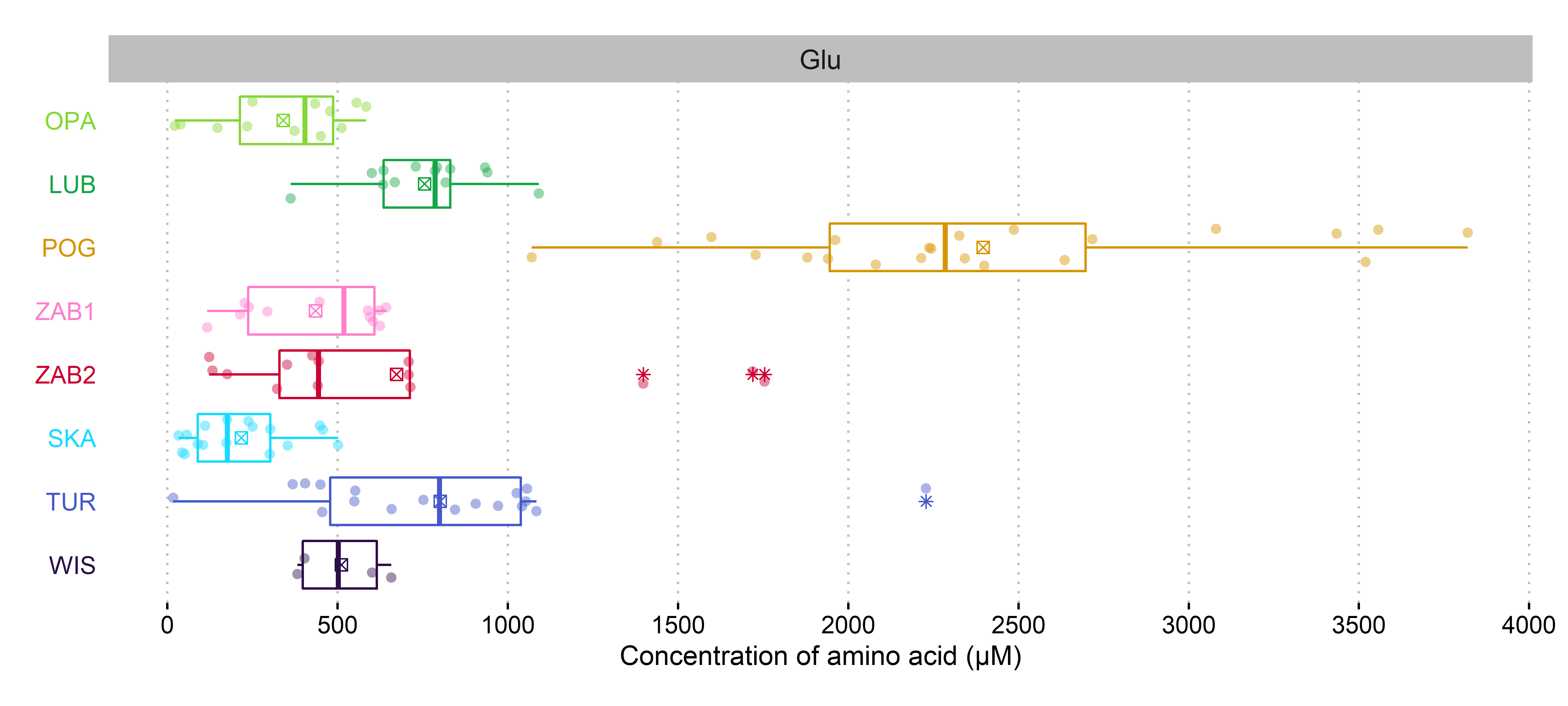
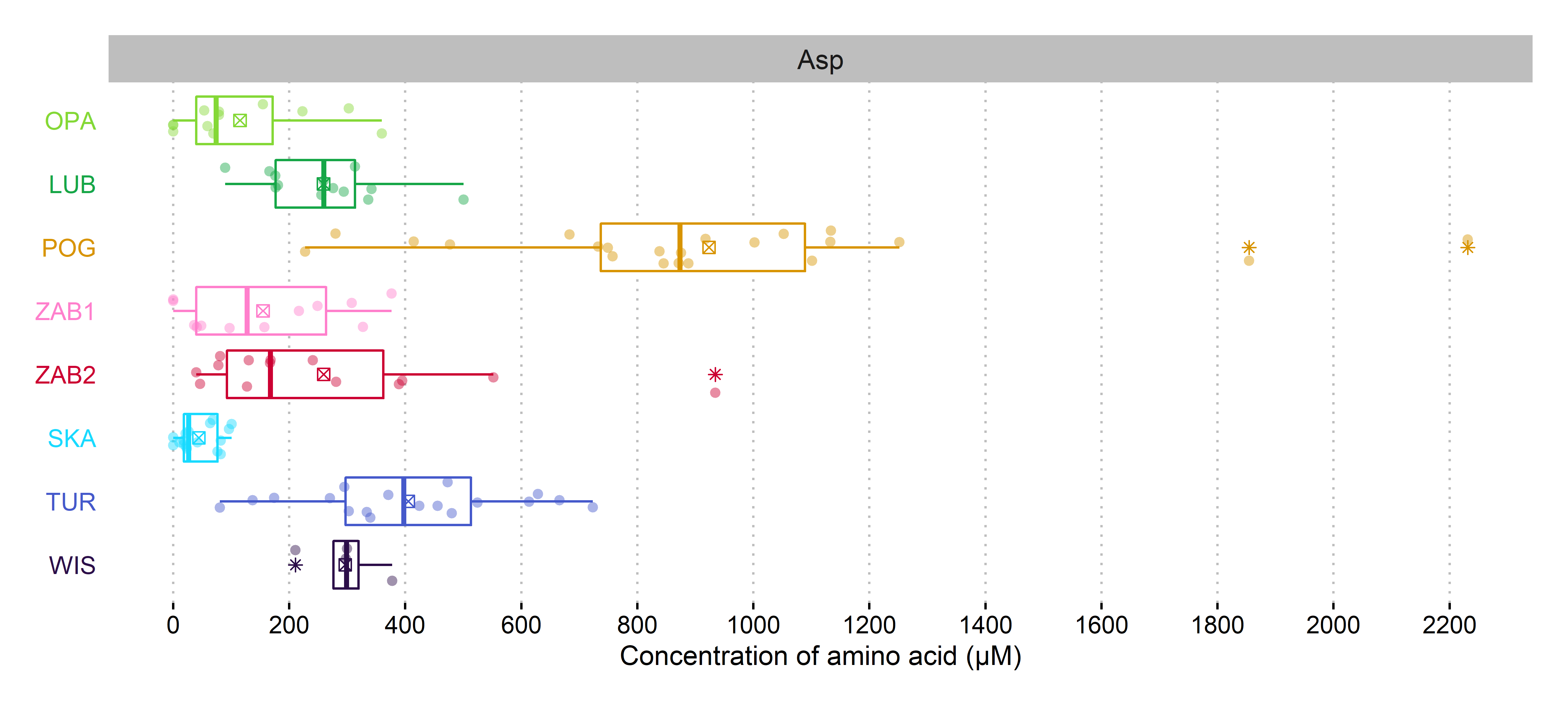
**Table S2.** Kaiser-Meyer-Olkin test results sorted in descending order by the measure of sampling adequacy (MSA) (overall MSA = 0.92).

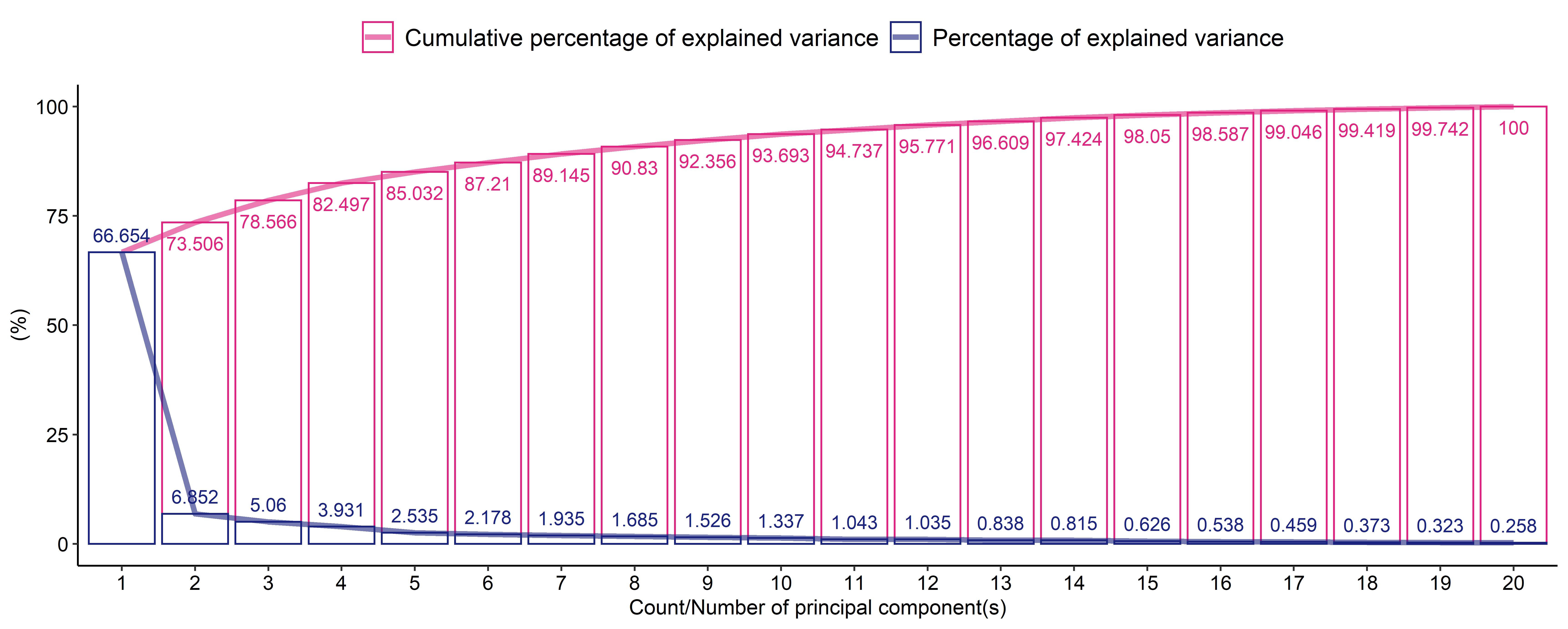
|  |  |  |
| --- | --- | --- |
| **Amino acid** | **MSA** | **Variable type** |
| Asp | 0.95 | Active |
| Glu | 0.95 | Active |
| Asn | 0.95 | Active |
| Ser | 0.95 | Active |
| Cys | 0.95 | Active |
| Trp | 0.95 | Active |
| Ile | 0.95 | Active |
| Orn | 0.95 | Active |
| Leu | 0.95 | Active |
| Lys | 0.95 | Active |
| Ala | 0.94 | Active |
| Phe | 0.94 | Active |
| Gly | 0.93 | Active |
| Cit | 0.93 | Active |
| Tyr | 0.93 | Active |
| Pro | 0.93 | Active |
| His | 0.90 | Active |
| Gln | 0.88 | Active |
| Thr | 0.88 | Active |
| GABA | 0.88 | Active |
| Nva | 0.86 | Supplementary |
| Arg | 0.85 | Active |
| Met | 0.74 | Supplementary |
| BABA | 0.69 | Supplementary |
| Val | 0.62 | Supplementary |
| AABA | 0.54 | Supplementary |
| Tau | 0.53 | Supplementary |

**Table S3.** Amino acids dataset used in PCA and UMAP analyses.

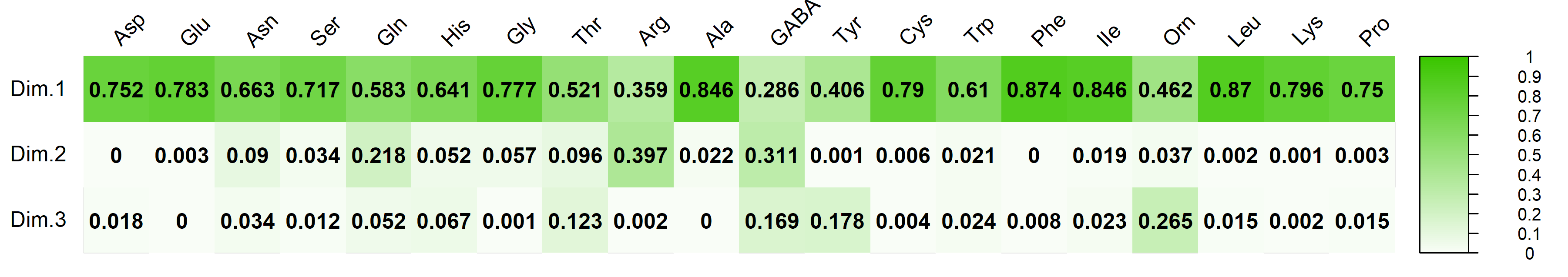
*Dataset is in Table3S.xlsx file.*

**Figure S1.** Boxplots of amino acids concentration for *Neottia ovata* populations. Colored dots are individual samples. The crossed square shows the mean. The lower and upper hinges correspond to the lower (Q1) and upper (Q3) quartiles. Thus box length shows the interquartile range (IQR). The thicker line inside boxes corresponds to the median. The lower whisker extends from the hinge to the smallest value at most Q1 - 1.5 × IQR of the hinge. The upper whisker extends from the hinge to the largest value no further than Q3 + 1.5 × IQR. Data beyond the end of the whiskers, indicated with an asterisk symbol, are outliers.

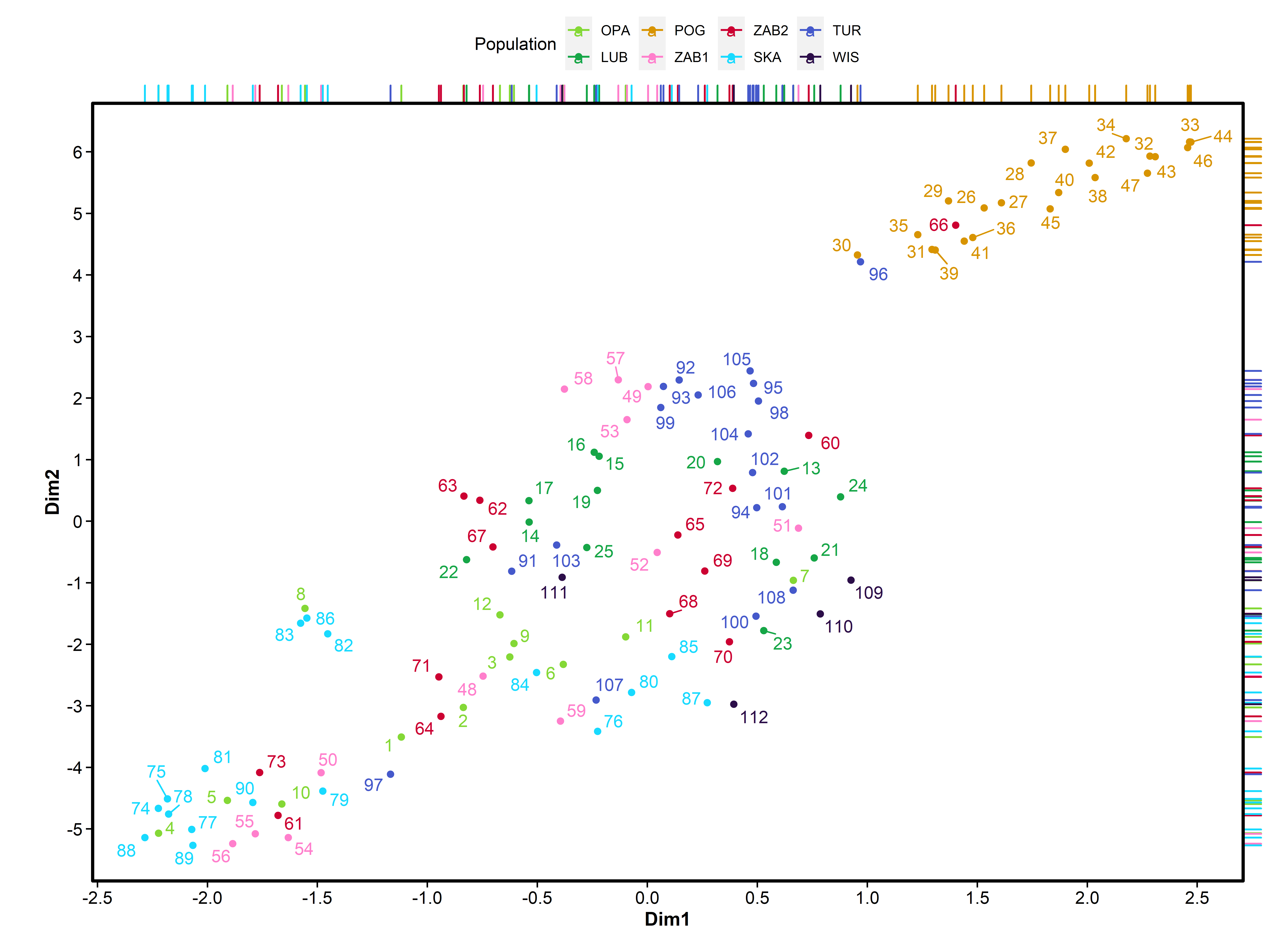




**Figure S2.** Scree plot showing the proportion of explained variance by the principal components.



**Figure S3.** Cos2 for the amino acids selected as active variables in the principal component analysis model, representing the quality of representation for variables on the factor map (Dim1-3).



**Figure S4.** Uniform manifold approximation and projection of all amino acids in *Neottia ovata* populations, except for β-Ala. Individuals (populations) are color-coded and labeled with a number corresponding to Id used in Table S3.