If statistical properties of experimental data are poorly known, the standard statistical procedures often lead to doubtful results. The report is concentrated at a few procedures which allow to decrease the level of uncertainty connected with extracting meaningful information from data with overcome some drawbacks of standard statistical procedures. The main attention is paid to regression analysis applied to treatment data of quantitative physico-chemical analysis (QPCA) and QSAR. The first task considered is the robust estimation of fitting parameters. The Huber’s approach to representation of density function \( p \) of experimental random errors \( \epsilon \) is used:

\[
p(\epsilon) = (1 - \delta) \cdot \varphi(\epsilon) + \delta \cdot h(\epsilon),
\]

where \( \varphi(\epsilon) \) is the Gaussian density function with zero mean, \( h(\epsilon) \) is density of “outliers” (density function with long tails) and \( \delta \) is intensity of outliers. The variation of hypotheses on \( \delta \) allows to search for the Huber’s maximum likelihood estimations (\( M \)-estimations) of fitting parameters with acceptable level of robustness. The QPCA and QSAR data were used to compare comprehensively the properties of robust \( L_1 (\delta=1) \), \( M \)-estimations (\( \delta>0 \)) with the least-square (LS) ones (\( \delta=0 \)).

Also the properties robust and unrobust estimations were compared in respect to their ability to provide the prognostic power of models. In particular, the prognostic features of QSAR models were studied by leave-one-out (LOO) and leave-many-out cross-validation methods. In the case of noisy and/or heterogeneous data the LS procedures were shown to give unsatisfactory results and should be replaced by the robust ones. The especially noticeable distinctions between results of applying the LS and \( L_1 \) methods were detected with the use of the LOO CV criterion.