

Preface

Analytical chemistry plays an important role in many branches of chemistry, biochemistry, pharmacy, life science and food production, as well as in monitoring of our environment, our health, etc. Many decisions are based on the results of quantitative chemical analysis, and it is important to be aware of the quality of the results whenever analytical chemistry methods are used. The development of analytical chemistry is thus increasingly characterized by the introduction of analytical quality assurance principles. The harmonization of European and international markets is triggering this process, and analytical laboratories in the chemical and pharmaceutical industries, as well as analytical routine laboratories in other disciplines such as environmental and food analysis, have generally accepted and introduced the appropriate standards, norms, and principles in the analytical process.

Nowadays, the analyst is not only expected to understand modern instrumental methods, they are also expected to understand and follow the regulatory requirements: for example, good laboratory practice (GLP) used in pharmaceutical analysis and elsewhere. This is a wide field, starting with the planning and selection of methods and sampling protocols. Next, the analyst has to validate the method and to test whether the approach is fit-for-purpose. This means they must use appropriate, calibrated equipment for the analytical measurements and must complete documentation at the end of the process, according to the stated requirements. Moreover, using principles of internal quality assurance, the analyst must be able to prove that the analytical methods are fit-for-purpose at any time. In addition, the work of the laboratory should be checked by interlaboratory comparison.

Despite its increasing importance, analytical quality assurance is hardly covered in university education. The beginner working in a chemical analytical laboratory will therefore face many issues for which they have not been trained. This book tries to help overcome this deficiency. Approaches are introduced and explained in detail on the basis of challenges as they appear to an analytical chemist in analytical practice. Most of the examples result from research in cooperation with industry and non-university laboratories. They have also been successfully applied in practical student courses in analytical quality assurance at our university.

Objective decisions require statistical tests. Therefore, all the challenges are solved by appropriate statistical tests which must be applied according to the regulatory requirements or which are recommended to establish the analyst's decision. Considerable weight is placed on solutions obtained according to these regulatory requirements.

Clearly, nowadays there are software packages for most of the problems, but we present each solution in detail in order to recalculate the results from first principles, because we believe that the analyst should know what the software program calculates. There are software packages, for example, for the calculation of the limit of detection. However, is it calculated on the basis of the German norm (DIN) or the IUPAC recommendations? Here, the analyst will obtain different results and therefore, in case of doubt, should be able to check the calculations. Besides the solutions given immediately following the challenges, MS Excel[®] spreadsheet functions can be found on the internet for solving the challenges, and these can also be applied to the reader's own problems.

As mentioned above, analytical quality assurance is a wide field which includes, besides the experimental requirements, the creation of documents according to regulatory requirements such as standard operation procedures (SOPs). Therefore, we had to make a selection of topics, and omitted this important documentation, which the analyst will learn, for example, in special workshops. We have only briefly introduced the extensive field of method development and tool qualification. However, the reader will find good books written by specialists in these fields.

Method validation is one of our main objectives. As all decisions must be taken with the help of statistical tests, the reader will find a comprehensive overview of method validation, taking into account all regulatory requirements. Thus the analyst will find, for example, all six methods for checking the trueness of analytical methods, and all the tests for linearity. The reader will find suitable methods for their own analytical approaches, as each test is supported by practical challenges.

We also point out that some frequently used procedures in statistics might not be the correct approach in analytical chemistry. For example, linearity is almost always checked by the correlation coefficient r . However, we argue that this is false, and discuss it in detail.

For further information on each chapter, there are many good books written by specialists. We apologize to colleagues whose work we could not cite because of space limitations. We wanted to introduce the reader to the wide field of analytical quality assurance in the style of a textbook rather than present a monograph with an exhaustive bibliography.

A comment on the symbols: we endeavored to apply unified symbols but we sometimes used the symbols suggested in documents such as DIN in order to retain compliance with the regulations. Last but not least, we have presented about 80 complex challenges. As there may be mistakes remaining, the authors will be grateful for any readers' comments.

Thus, we hope that beginners will find these inspiring challenges a positive and helpful introduction to the experimental work of analytical quality assurance.

Advanced analysts will also find suggestions and statistical tests necessary to ensure objectivity in their decisions.

Finally, we would like to express our thanks to the staff at Springer for all their help and courtesy, especially with regard to correction of the English.

Jena, January 2011

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Challenges in Analytical Quality Assurance

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2011, XIX, 356 p., Hardcover

ISBN: 978-3-642-16594-8