

METROLOGICAL ASSURANCE OF QUALITY CONTROL OF PHARMACEUTICAL PRODUCTION USING POWDER XRD METHODS

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The main areas are considered here of metrological assurance of quality control for X-ray diffractometry methods when designing and manufacturing materials for biomedical purposes, including pharmaceutical products.

The first area is the control of traditional metrological characteristics of diffractometric equipment. For this purpose we have developed and certified Standard Reference Materials (SRM) on the basis of different diffraction properties of substances and materials.

Today the quality of modern diffractometric equipment has reached a high level. This made possible to lower considerably the contribution of traditional statistical uncertainties in determined characteristics. At the same time, the contribution of various methodic components has increased the contributions of the instrument uncertainties by almost an order. Therefore, the second area of metrological assurance development for this field of application is focused on elaboration of special well-described test-samples intended for development and use of measurements procedures. As more and more data on the reproducibility and stability are being collected, they also will be successively transferred to the types of certified SRMs. When choosing those types that will first be transferred we have in view their relative simplicity, multi-component nature, the presence of hydrogen chemical bonds and similarity of properties with behavior of biological substances (evolution of characteristics). We are also directly designing complex biological substances, structural characteristics of which can be reproduced with high accuracy down to mapping of distribution of electron density.

Another area is concerned with a wide application of scientific data bases for the designing of new biological substances, including pharmaceuticals. For this purpose we use the results of the experiments of higher accuracy, which are carried out on single crystals, and the results of which can then be transformed into a diffraction pattern corresponding to this polycrystalline composition. It is interesting to note the similarities of these approaches to the procedures, which have to be developed to support nanotechnologies and ensure quality control of nanomaterials. These include, above all, the necessity of development and certification of measurement procedures for nano-scale characteristics. Of importance is also a successive transition from test characteristics, associated with the functionality of specific types of nanomaterials, to certificated standard reference materials of structural characteristics of various nanomaterials.