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HOW TO CREATE AN INSTRUMENTAL DATA BASE FOR VERIFICATION? Working Paper

1. Introduction

The necessity of creating a computerized data base containing information about chemical warfare (CW) agents and related compounds was expressed by the Technical Group on Instrumentation during their meetings in Geneva in 1989 and 1990 (1,2). In addition to more general information about the compiled compounds, this data base should contain the spectrometric and chromatographic data which may serve as references in order to identify unequivocally a compound of CW interest.

Basically, there are two ways to create such an instrumental data base :

- Existing data from various laboratories with experience in the field of identification of CW agents could be taken on, provided that the data meet certain quality requirements.
- The data could be recorded anew, using generally accepted operational procedures. In this case the compounds of interest have to be collected. The task of recording the data could be carried out by one or more accredited laboratories.

The Netherlands is in favour of the first option. The reasons for this choice will be presented in this working paper. Furthermore, some remarks will be made about which data should be collected as well as about the way the data should be distributed to laboratories operating under the CW Convention. Finally, as a possible contribution to an instrumental data base for verification, a survey of data digitally available in The Netherlands will be given.

2. The creation of an instrumental data base from existing data

The basic idea of creating an instrumental data base from new recorded spectrometric and chromatographic data according to standard operational procedures using high quality analytical equipment is attractive. It might appeal to a general human quality to make a fresh start every now and then. However, the following arguments may be raised against this approach:

- The workload will be enormous. This will especially be caused by collecting and preparing the compounds. It may take weeks to prepare a few compounds in a sufficiently pure form.
- The laboratory or laboratories providing the data bear(s) a great responsibility on the usability of these, whereas in the case of compiling existing data from various laboratories a comparison can be made. Possible differences can be discussed by experts, thus leading to more reliable or better applicable data.