



Initializing a digital chromatography data archive for tropospheric air samples on Taunus Observatory Frankfurt by GC-TOF-MS

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The inception of a digital air archive for halogenated hydrocarbons will be presented. This archive is based on weekly samples taken at the Taunus Observatory on “Kleiner Feldberg” near Frankfurt/ Main, i.e. a very central position in Germany. The station is characterized by a mixture of clean air, moderately polluted air and occasional influence from the nearby city of Frankfurt. Regular meteorological and air quality data are available from the German Weather service (DWD) and the regional air quality monitoring (Hessische Landesanstalt für Umwelt und Geologie, HLUG). Two air samples are collected in parallel in 2 l stainless steel flasks using a metal bellows pump. The air samples are analysed in the laboratory by gas chromatography coupled with Time of Flight Mass Spectrometry (GC TOF MS) and Quadrupole Mass Spectrometry (GC QUAD MS) for halogenated trace gases. Analysis is carried out no later than a month after sampling. Our current target species which will be measured by both mass spectrometers contain a wide range of halogenated trace gases, with calibration scales linked to both global monitoring networks, i.e. NOAA and AGAGE. A Time of Flight Mass Spectrometer has the advantage to measure a full mass range with a high sensitivity. Other measuring networks use Quadrupole mass spectrometers which need to be tuned to selected masses in order to achieve sufficient sensitivity. The full mass scan information available in the TOF data in combination with the high sensitivity of the instrument opens the possibility for retrospective analysis of the data in the future, as information on all substances which can be trapped and desorbed using our sampling technique are recorded, even though they may not be retrieved at the time of measurements. This will open the opportunity to have a look on historical developments even of yet undiscovered halogenated trace gases or those, which have not been subject to one’s research focus until a certain time point but have become interesting later. The full resolution mass spectrometric data will be stored together with all meteorological and other information necessary for later reprocessing. This will constitute a digital air archive, which can also be made available to other research groups for reanalysis.