GCxIMS Library Search

Compound Identification Software for Gas Chromatograph-Ion Mobility Spectrometer

The new software ***GCxIMS Library Search*** makes identification and characterization of volatile organic compounds (VOC's) easy and fast. Using both, a Gas-Chromatographic and Ion Mobility based separation leads in 2-dimensional data of the sample; in combination with a high sensitive detection via Ion-Mobility-Spectrometry at the same time (Fig. 1). Identification of compounds is supported by matching both (GC & IMS) compound-specific separation properties. The gas-chromatographic retention times can be normalized to retention indices (RI) [1], that can be matched to literature- and database- values (Fig.2).

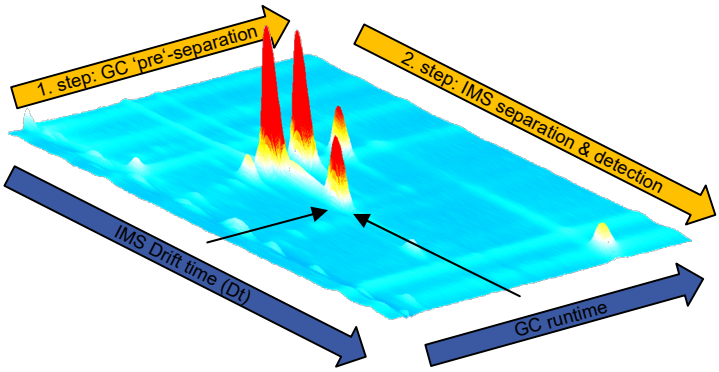

Fig.1: 3-dimensional representation of a GC-IMS measurement. The separating effect of both techniques, GC & IMS, can be clearly seen. A signal is defined by one or more vector pairs (Dt, RI), which is unique for a defined substance.

Implemented NIST2014 RI DATABASE (non-restricted)

The NIST GC Method and Retention Index Database provides retention index data and gas chromatographic conditions for **~83.000** compounds on polar and non-polar stationary phase used with packed and open tubular columns.

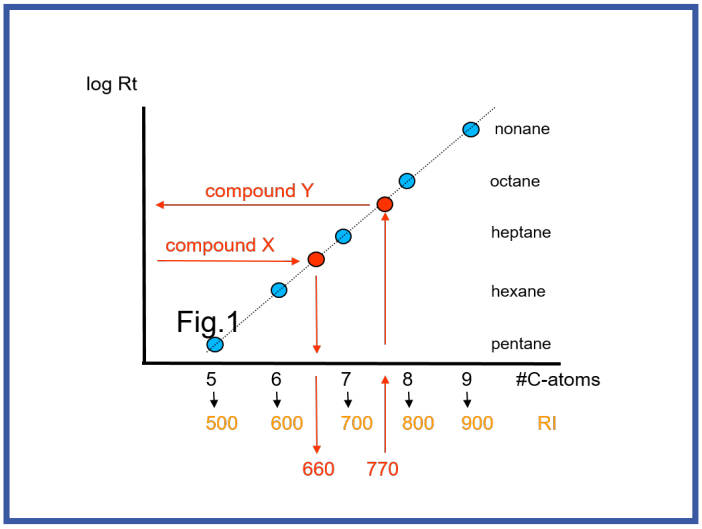

Fig.2: Substance retention times (Rt) strongly depend on system parameters, such as temperature or the chemical properties of the used GC column, e.g. Therefore the retention time is converted into a system-independent constant, the Kovats retention index, based on a series of adjacently eluting alkanes and there arbitrarily assigned RI values. [1]

The software comes with a full non-restricted version of the NIST2014 Retention Index Database including NIST search software. The database includes ~400.000 annotated Kovats/Lee retention indices and ~83.000 compounds. The ion mobility drift time (Dt) is also a specific parameter for a compound at constant measurement conditions. The measurement condition- based shift can be overcome by normalization of Dt values when related to the reactant ion peak (RIP), which is directly accessible in IMS spectra in positive polarization (Fig.3).

[1] Kováts, E. Helv. Chim. Acta, 1958, 41 (7): 1915–32, doi:10.1002/hlca.19580410703

GCxIMS Library Search

Compound Identification Software for Gas Chromatograph-Ion Mobility Spectrometer

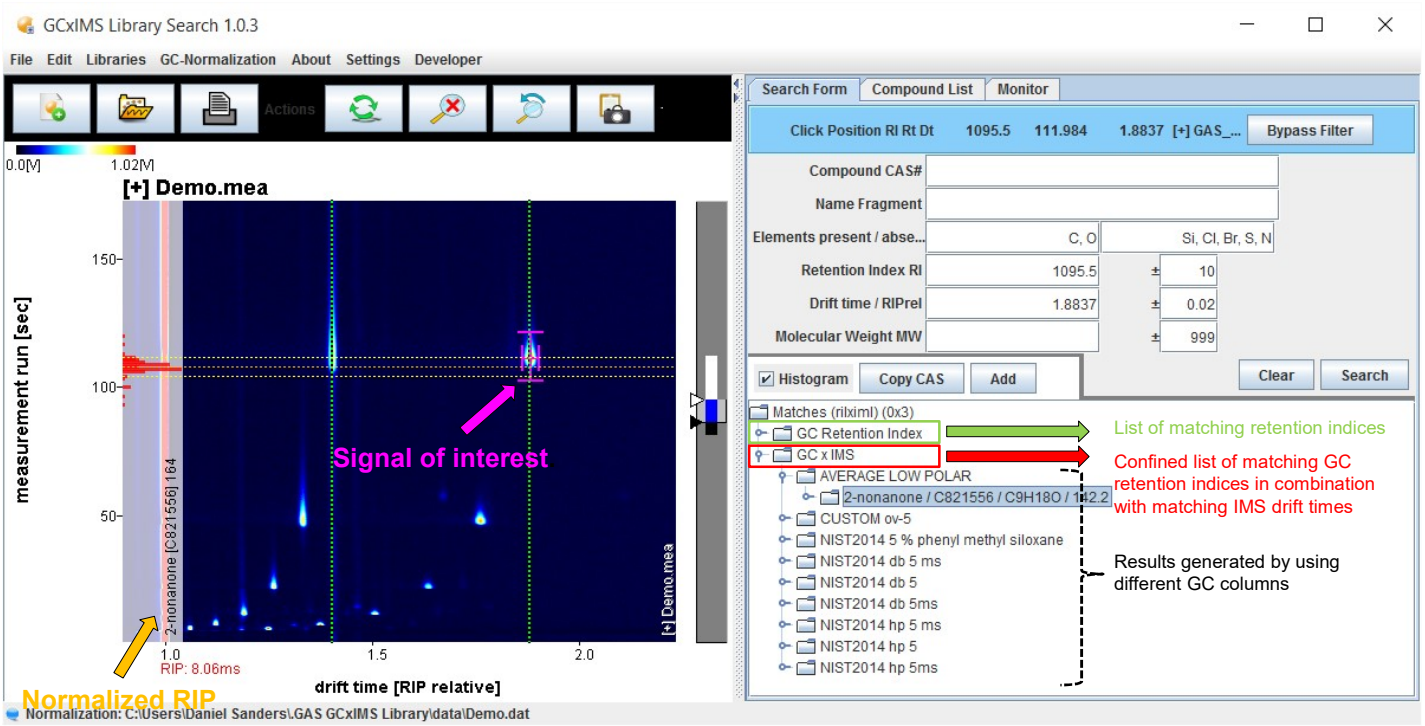

Fig.3: Screenshot of an examplary signal identification. After selecting the signal of interest the identification routine of the software starts searching for matches of retention times and IMS drift times in the NIST & GAS databases.

The search for identification of unknown compounds is initiated by clicking on the respective signal peak in the GCxIMS chromatograms. The result is the listing of i) all library compounds with matching retention indices and ii) a confined listing of compounds that match both retention index and IMS drift times (Fig. 3). The retention index match typically enfolds multiple possible compounds. Accordingly the identification of the respective compound is not possible or only feasible if compounds can be excluded by plausibility. On the other hand, when IMS drift time data are available, the matching list is confined drastically (in most cases the combination of the retention index, RI, and IMS drift time, Dt, is unique for one specific substance enabling easy and fast identification).

The ***GCxIMS Library Search*** software features all necessary tools for supporting the identification of unknown compounds in GCxIMS measurements as it comprises:

- Easy normalization of the systems gas-chromatographic properties
- RI range variable by choice of compounds
- Normalization by one single measurement possible
- Included retention index libraries (NIST 2014 Retention Index database)
- Automated normalization of IMS drift times
- *G.A.S. IMS drift time library*
- Both libraries can be customized and extended by user
- Straight *'Click-to-Search'* mode
- Search confinements e.g. by name fragments, included/excluded elements, molecular weight, CAS number

G.A.S. Gesellschaft für analytische Sensorsysteme mbH
Otto-Hahn-Straße 15, D-44227 Dortmund, Germany
Phone: +49 231 9742 6550 / Fax: +49 231 9742 6555
info@gas-dortmund.de / www.gas-dortmund.de