Connection between the Molecular Structure and the Gas Chromatograph - Mass Spectrometer Response

Extended Abstract of the PhD dissertation

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1. Introduction

Gas chromatography-mass spectrometry (GC-MS) is one of the most frequently used analytical techniques because of its high sensitivity, selectivity and flexibility. This combination can provide the required and sufficient analytical information, even about complicated samples. The qualitative information can be obtained by interpretation of mass spectra. The quantitative results can be originated from the measurement of area under the gas chromatographic peak of the respective compound in total ion current chromatogram (TIC). However, in both cases, but first of all in quantitation, the use of suitable standard substances is important. Most of them are available in trade, but in many cases there are no standard materials with suitable quality in the market because of their difficult or impossible synthesis. They are those components of organic synthetic materials which are present in the product of some technology in l area % quantity or less but they have to be taken into consideration in the mapping of contamination profile at the product-qualification.

But if the response factors for respective molecules are known, their quantity can be calculated without standards. The question is how an MS response factor can be calculated based on chemical structure under respective measurement conditions; i.e. GC-MS system, column, injector and ion source temperature. The response factor depending on these conditions can apparently be determined in a particular compound group. If the apparent response factor differences are calculated between the members of this group, a few members can be enough to measure on another GC-MS system (under the same conditions) to obtain other apparent response factors by means of differences.

2. Literature review

There are close connection between the molar sensitivity (S) and the electron impact ionization cross section (Q). As in previous study[1], at the low pressures of EI experiments the total ion current is directly related to the ionization cross section, by the equation

$$\sum I_i^+ = Q_i I_e [n_i] d$$

in which $\sum I_i^+$ is the total positive ion current (pA), Q_i is the ionization cross section (10^{-16} cm^2), $[n_i]$ is the concentration of sample molecules of species i (cm^{-3}), I_e is the electron current (pA), and d is the ionization path length (cm).

Naphthalene was used as internal standard. The fundamental equations of quantitative analysis are

$$A_i = S_i n_i$$
$$A_j = S_j n_j$$

where S_i and S_j are the individual sensitivities of sample molecules and naphthalene (pA*cm^3*mmol^{-1} or μV*cm^3*mmol^{-1}), A_i is the area under the peak of the compound in TIC chromatogram (pAs), A_j is the area of naphthalene peak in TIC chromatogram (pAs), n_i and n_j are the concentration (mmolmL^{-1} or mmol) of the compound and naphthalene (mmolmL^{-1} or mmol), respectively.

For the calculation of relative molar response (*RMR*, relative sensitivity) in the present experiments the following formula was used

$$RMR_i = \frac{A_i}{A_j} \frac{n_j}{n_i}$$

where RMR_i is the relative molar response of the investigated compound (*i*) related to naphthalene (*j*). The sum of total ion current of the component *i* provides the area under the peak $\sum I_i^+ = A_i$.

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[1] A Harrison, E Jones, S Gupta, G Nagy; *Can J Chem*, (1966); 44: 1967-1973.

The ionization path length and the electron current are constant in case of a respective instrument. Thus, they are no need for the calculation of relative sensitivity and cross section. The ratio of component concentrations in the solution and the ion source is considered also constant. Based on the above mentioned equations, the ratio of the ionization cross sections for two different molecules and the ratio of their molar responses are equal.

$$RMR_i = \frac{A_i}{A_j}\frac{n_j}{n_i} = \frac{S_i}{S_j} = \frac{Q_i}{Q_j}$$

In the literature numerous studies were published about cross sections, as contrasted with few publications about *RMRs*. The reason of this difference is that the cross section data are utilized for many other scientific fields[2]. The known of cross sections can help to model the plasma state, the density and temperature of plasma[3]. The cross section also takes a prominent part in the working of the hollow-cathode lamp.

The cross sections found in the literature concern organic compounds only in a minor part thus they cannot be utilized for determination of *RMR*s in the daily routine analysis. My study refers to the *RMR*s of those compounds that have not been investigated yet and the applicability of published cross section data were also investigated in case of GC-MS system.

The cross sections of hydrocarbons

Harrison *et al.*[1] investigated some members of homologous series of n-alkanes, n-alkenes and n-alkynes. Direct sample introduction was applied; the related compound was Kr and its cross section was obtained from the literature. A linear correlation was found between the cross sections and the carbon atom numbers in the respective homologous series. The highest cross sections are given by n-alkanes, followed by n-alkanes and n-alkynes in decreasing order according to the decreasing number of hydrogen atom.

Cross sections of n-Alkylbenzenes were discussed in two earlier studies. In both cases the related compounds arose from the literature and a direct sample introduction was applied. The date of issue of the studies can show the development of the instruments, the data from 1957[4] (Ar related compound) are smaller consecutively than that from 1966[1] (Kr related compound). But in both cases the correlations are linear between the cross sections and the

[2] W Hwang, YK Kim, ME Rudd; *J Chem Phys*, (1996); 104: 2956-2966.
[3] TD Märk, GH Dunn; Electron Impact Ionization, Springer-Verlag Wien-New York, (1985)
[4] R Alberti, MM Genoni, C Pascual, J Vogt; *Int J Mass Spec Ion Phys,* (1974); 14: 89-98.

carbon atom numbers and the cross sections of n-alkanes are higher than that of n-alkylbenzenes.

The cross sections of halogenated compounds

Alberti *et al.*[4] measured relative cross sections of some monohalogenated n-alkanes related to Ar. After that by means of literary cross section of Ar the absolute cross sections can be calculated from the relative data. From the literary cross sections of Ar it was chosen $2,81*10^{-16}$ cm^2. In this study there are some other cross section data for Ar that are between $2,54-3,76*10^{-16}$ cm^2. The applied instrument was mass spectrometry without a separation system and so direct sample introduction was chosen. Similarly to the hydrocarbons, a linear correlation was found between the cross sections and the carbon atom numbers in the respective homologous series; n-iodoalkanes, n-bromoalkanes, n-chloroalkanes and n-alkanes in decreasing order. The lines are parallel to each other. The molecule size increases with a CH_2 group in a respective homologous series thus the rise of a line is equivalent of the partial cross section of CH_2 group. Based on this observation an additivity rule is valid for the cross section of CH_2 group. This is very important fact from the point of view of analytical methods because the cross section is proportional to the molar response. This value is valid not only for one homologous series but also rise of the line of every group of compounds has the similar partial cross section for CH_2 group ($2,4*10^{-16}$ cm^2).

Polyhalogenated hydrocarbons having small carbon atom number were also investigated. In this case the compounds contain halogen atom having various qualities and quantities, no homologous series were measured. There is no additivity rule for halogen atoms in these compounds at all. The partial cross section of any halogen atom does not give a permanent data by means of calculation from these compounds.

Polychlorinated biphenyls were investigated by Sauter *et al.* [5]. Their cross sections were calculated and furthermore, *RMR*s were measured. As compared to the earlier study, not only MS instrument was utilized but a GC separation system was connected to it. In this case the errors of the measurement arise from both GC (the place of the sample evaporation) and MS instrument thus the number of these errors can be higher than that without GC. Two related compounds (phenantrene-*d10* and chrysene-*d12*) were utilized. The number of the chlorine atom of the respective PCBs was various; and their positions on the ring are unmethodical. The calculated cross sections are in a linear correlation with the chlorine atom

[5] AD Sauter, JJ Downs, JD Buchner, NT Ringo, DL Shaw, JG Dulak; *Anal Chem*, (1986); 58: 1665-1670.

number, independent of their positions. Interestingly, the measured *RMR*s decrease while the number of the chlorine atom increases (see in details Results section).

The cross sections of oxygenated compounds

The literary cross sections refer to non-polar and volatile compounds mainly. The direct sample introduction to the MS limits the number of the compounds can be measured. Thus, only the oxygenated compounds having low carbon atom number were investigated[6]. However, the appearing of the GC allows measuring difficult compounds because an indirect sample introduction is applied in the GC. The compounds are solved and only a few amount of sample is introduced to the GC-MS. That is why component having higher boiling point than the injector temperature can be evaporated quickly.

Turecek *et al.*[6] and Hudson *et al.*[7] measured some low carbon atom number alcohols. The later one is an up-to-date study from 2003 because a new measuring method was proceeding. The fundamental equation of absolute cross section $\sum I_i^+ = Q_i I_e [n_i] d$ was applied directly to the measurement and no related compound was measured. The bombarding electron energy (I_e), the ionization pathway (d) and the number of the species in a respective volume ($[n_i]$) can be well controlled. In this way there is no need a literary cross section of the related compounds and the errors arising from this method were eliminated. The cross sections from this study are lower than the results referring to the measurements with related compounds. This systematic error can be obtained from the use of the literary cross section of related compound (benzene).

Straight chain aldehydes, ketones and ethers were also analyzed that are suitable to evaporate easily. Harrison *et al.*[1] measured relative cross sections of some above mentioned compounds related to Kr. After that by means of literary cross section of Kr the absolute cross sections can be calculated from the relative data. The applied instrument was mass spectrometry without a separation system and so direct sample introduction was chosen. A linear correlation was found between the cross sections and the carbon atom numbers in the respective homologous series; ethers, n-alkanes, ketones and aldehydes in decreasing order. Each type of homologous series contains one oxygen atom. Thus, the individual cross section of oxygen atom can be calculated from the different group. Based on the simple additivity rule the cross section for oxygen calculated from different type of compounds should be

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[6] F Tureček, L Brabec, V Hanuš, V Zima, Pytela O; *Int J Mass Spec Ion Process,* (1990); 97: 117-124.
[7] JE Hudson, ML Hamilton, C Vallance, PW Harland; *Phys Chem Chem Phys*, (2003); 5: 3162–3168.

equal. However, the individual cross section for oxygen is 0,816, 1,214 and 0,914*10^{-16} cm^2 from ethers, ketones and aldehydes, respectively.

From analytical aspects the mass spectrometer works as a detector because in general, the samples consist of more components and that should be separated after the MS. Thus the errors can increase by means of the separation system (e.g. due to the evaporation in the injector or the background contamination). In the present experiments the reference material is unvaried, which provided an opportunity for relative response factors to uniform. The internal standard method is used to compensate for the loss of analyte during the sample inlet and to eliminate random differences influencing the efficiency of ionization. Naphthalene has a very stable molecular ion with mass of *m/z* 128. Other fragments of naphthalene have a small influence on mass-spectral reactions; in practice their molecular ion abundance provides the total ion current chromatogram. Thus naphthalene is used as a stable reference material. In the literary sources the related compound and the target atom or molecule were often measured simultaneously. However, the cross section of related compound was obtained as literary data and the errors of the measuring system could not be taken into consideration.

3. Results

The compounds in the Results section can be divided in two groups. The first group contains the compounds having literary cross sections and these data were compared to the *RMR*s measured in the present study related to naphthalene. The rest of the compounds that were measured in this study had not cross section data. Some compounds needed to optimize the measurement condition that was highlighted in the respective section.

The relative molar responses of hydrocarbons

Relative molar responses of some saturated straight-chain n-alkanes were measured at the same time with the investigations of straight chain compounds. The *RMR* results for n-alkanes were mentioned in the section of respective groups. In a new publication the slope of the carbon atom number – *RMR* line is 0.215 that is similar to the present results (0.220; 0.171; 0.181 and 0.232). The reason of the different slopes is the using of the various type columns during the measurement of various types of compounds. The different columns influenced the injector temperature and this value could affect the n-alkane results.

The correlation between the relative molar responses of respective compounds and the carbon atom number is linear. The slopes of the lines, i. e. the value of a CH_2 unit, are 0.220 (n-alkanes) and 0.221 (n-alkylbenzenes). The sensitivities of n-alkylbenzenes were found lower than those of n-alkanes in spite of the fact that n-alkylbenzenes provide fewer fragments with higher abundances than those of n-alkanes. Thus the cross section is the prime factor which influences the production of molecule ion and this process is the dominant, instead of the further fragmentation steps. To compare cross section and *RMRs* of n-alkylbenzenes with the current study's results, ethylbenzene was in common compound and chosen as a temporary internal standard. After this transformation the relative cross section data should be identical with the *RMR*s. The first significant digit shows good reproducibility between them.

The relative molar responses of halogenated compounds

The correlation between the relative molar responses of homologous series of monohalogenated n-alkanes and the carbon atom number is linear. In conclusion, mass spectrometric detection combined with gas chromatography was less sensitive to n-alkanes than to their derivatives containing a chlorine, bromine or iodine atom. After n-alkanes, mass spectrometric responses increase in the order of 1-chloroalkanes, 1-bromoalkanes and 1-iodoalkanes. These results are in accordance with electron ionization cross section data for n-alkyl-derivatives. The relative molar responses of the individual CH_2 groups are between 0.171 and 0.178 in the homologous series concerned. The increments of chlorine, bromine and iodine atoms to the relative molar responses are 0.081, 0.141 and 0.492, respectively.

The 1-chloro- and 1-bromoalkanes are less prone to the loss of halogen or hydrogen halide than the 1-iodoalkanes or 1-fluoroalkanes and an alternative fragmentation pathway was opened which is absent from n-alkanes. As a result of this fragmentation scheme ions containing a halogen atom appear in the mass spectra of 1-chloro- and 1-bromoalkanes by *m/z* 91, 93 and *m/z* 135, 137, respectively. A high abundant *m/z* 91, 93 associated with the molecular formula $C_4H_8Cl^+$ (similar to $C_4H_8Br^+$) appears on the mass spectra of 1-chloroalkanes containing four or more carbon atoms and, moreover, for compounds having carbon atom number of C_6-C_{12} this ion $C_4H_8Cl^+$ (**ring5**) is the basic peak[8]. The formation of *m/z* 91, 93 was described as a displacement reaction:

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[8] FW McLafferty; *Anal Chem,* (1962); 34(1): 2-15.

ring5
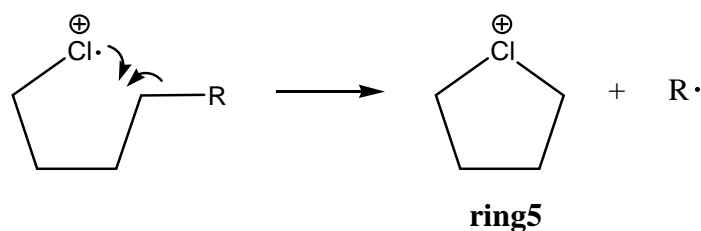
The displacement reaction of 1-chloroalkanes

The sensitivities and quantitative results can be originated from the measurement of the area under the gas chromatographic peak of the respective compound. The GC-MS chromatogram is a total ion current chromatogram (TIC). As TIC consists of absolute intensities of mass spectra, it can depend on the fragmentation pathways. Thus the fragmentation pathways can influence the sensitivity. Besides the *m/z* 91, 93, a small *m/z* 77, 79 (**ring4**, $C_3H_6Cl^+$) signal pair is present in case of each investigated molecule, furthermore with the increasing chain length peaks at *m/z* 105, 107 (**ring6**, $C_5H_{10}Cl^+$) and *m/z* 119, 121 (**ring7**, $C_6H_{12}Cl^+$) are gaining intensity. Nevertheless, even for the long-chain 1-chlorooctadecane the *m/z* 91, 93 ($C_4H_8Cl^+$) peak pair is far the most intense one. The intensities of molecule ions are negligible in case of respective 1-chloroalkanes thus these molecules rather fragment. All fragments containing chlorine atom belong to the $C_nH_{2n}Cl^+$ series.

To get information about the formation of the cyclic chloronium cation Van deSande and McLafferty have investigated deuterated chlorohexanes by MS, finding support for the postulated mechanism[9]. Interestingly, while this putative mechanism is generally accepted no detailed theoretical investigation was carried out to understand the cleavage of the alkyl halide radical cations resulting in the selective formation of the five membered ring. While the stability of five membered rings is generally accepted among organic compounds due to their minimised ring strain, six-membered rings are usually considered equally stable, thus the explanation of the above observations is far from being trivial.

To sum up, among the possible fragmentation products of the model compound 1-chlorohexane, the **ring5** is the most stable according to its high mass intensities. The formation of the low abundant **ring4** is inhibited thermodynamically; the formation of both **ring6** and **ring7,** that have also low intensities in the mass spectra, are inhibited kinetically.

Sauter *et al.*[5] investigated 10 polychlorinated biphenyls. One substituent chlorine atom could cause a constant increment for the absolute ionization cross section in the case of

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[9] CC Van deSande, FW McLafferty; *J Am Chem Soc,* (1975); (97):2298-2299.

biphenyls, according to the additivity rule. However, the relative molar responses of biphenyls could decrease with the increase of chlorine atom number in Sauters' study. The present relative molar responses of PCBs (EPA 525, 525.1 standard mix) increase with the increase of chlorine atom number which is according to the expectation based on their cross sections measured by Sauter *et al*. The addition of more than 3 chlorine atoms means a permanent difference in *RMR* for compounds having biphenyl skeleton. One chlorine atom contributes the value of 0.198 to *RMR* based on the respective equation (0.198x+0.555).

The *RMRs* for polychlorinated benzenes indicate diversity, and no correlation can be obtained either in the function of carbon atom number or the halogen atom number, which is because they belong to different homologous series. The isomer compounds consist of the same atoms in the same number. The relative molar responses of 1,3-dichlorobenzene (*RMR*=0.877) and 1,4-dichlorobenzene (*RMR*=1.080) related to naphthalene should be identical based on the principle of ionization cross section, but they do not fit a simple additivity postulate. The fragmentation patterns of them are almost the same. The similar fragments and abundances should indicate similar relative molar responses. According to these results, the stereoscopic structure is also an important influence factor in the formation of *RMR* or cross sections. On the other hand, the first ionization energy for 1,3-dichlorobenzene and 1,4-dichlorobenzene are 9.28 and 8.95 eV, respectively [14]. The molecular radical cation of 1,4-dichlorobenzene is very stable due to the conjugated electron system. Thus the ionization efficiency of 1,4-dichlorobenzene is higher than 1,3-dichlorobenzene. That is why the latter can produce fewer fragments than the former. The higher the ionization energy of a molecule, the lower its ionization cross section is.

The relative molar responses of oxygenated compounds

Relative molar responses of some straight chain aliphatic alkanes, ketones, aldehydes, alcohols and carboxylic acids were investigated related to naphthalene. Most of the respective compounds have not been investigated yet due to their high polarity or high boiling point. n-Alkanes are the general compounds which render possible the comparison of various homologous series. That is why besides the investigations of other homologous groups, n-alkanes were measured simultaneously.

It was found that there were linear correlations between the molecular structures, i.e. the carbon atom number and relative molar response in current homologous series. In conclusion, the n-alkanes and n-alcohols generate similar relative molar responses. The same

observation holds for n-aldehydes and n-carboxylic acids, but their relative molar responses are smaller than that of the group of n-alkanes and n-alcohols'. n-Ketones can be found between these two groups. The relative molar responses of the individual CH_2 groups are between 0.169 and 0.210 in the homologous series. The quality of the stationary phase influences the peak shape and so, the area under the peak. The wider the peak, the smaller the area under the peak is. Acidic or basic molecules are especially sensitive to the quality of the stationary phase. In order to obtain a sharp peak, a polar Stabilwax-DA column was used for acids and the other oxygenated compounds.

The relative molar responses of compounds containing nitrogen

The measurement conditions, i.e. the type of column affect the apparent relative molar responses of aliphatic primary amines. The quality of the stationary phase influences the peak shape and so, the area under the peak. The wider the peak, the smaller the area under the peak is. A midpolar column having a higher maximum operating temperature provides a more sensitive apparent relative molar response (Rtx-1701) than the basic polar column having a lower maximum temperature (Stabilwax-DB), because a high temperature allows setting a higher injector temperature and a higher amount of compound can reach the ion source. The *RMRs* decrease in function of the carbon atom number in the cases of high molecular weight amines on Stabilwax-DB. That is why the rise of amines curve is low (0.078) apparently. For another option, a modified midpolar polysiloxane stationary phase was chosen, which consists of 14% cyanopropylphenyl and 86% dimethyl substituent (Rtx-1701). For this method, the rise of amines curve was obtained 0.172.

Some other aniline and nitrobenzene derivatives were analyzed. These compounds are also difficult to measure due to their basic characteristic (aniline derivatives) and especially high boiling point (nitrobenzene derivatives). In accordance with this fact, cross sections and *RMRs* cannot be found for them in the literature. Anilines were analyzed on a Stabilwax-DB column and the *RMR* results can be seen in Table 5. Nitrobenzenes should be separated on a column having a high maximum operating temperature (Elite-5MS), thus the molecules can be evaporated in the injector. The isomer compounds consist of the same atoms in the same number. The relative molar responses of 2-chloroaniline (*RMR*=0.731), 3-chloroaniline (*RMR*=0.695) and 4-chloroaniline (*RMR*=0.666) related to naphthalene should be identical based on the principle of ionization cross sections, but they do not fit a simple additivity postulate. This observation is valid for all investigated isomer groups.

4. Theses

1. The relative molar responses related to naphthalene of homologous series of monohalogenated n-alkanes (1-iodoalkanes, 1-bromoalkanes, 1-chloroalkanes) were determined by means of indirect sample introduction on GC-MS instrument. The correlation between the relative molar responses of homologous series of monohalogenated n-alkanes and the carbon atom number is linear which refer to the literary cross section data. The GC-MS was less sensitive to n-alkanes than to their derivatives containing a chlorine, bromine or iodine atom. After n-alkanes, mass spectrometric responses increase in the order of 1-chloroalkanes, 1-bromoalkanes and 1-iodoalkanes. [1]

2. The formation of $C_nH_{2n}Cl^+$ ions from 1-chloroalkanes were investigated by means of computational chemistry. Among the possible fragmentation products of the model compound 1-chlorohexane, the $C_4H_8Cl^+$ is the most stable according to its high mass intensities. The formation of the low abundant $C_3H_6Cl^+$ is inhibited thermodynamically; the formation of both $C_5H_{10}Cl^+$ and $C_6H_{12}Cl^+$, that have also low intensities in the mass spectra, are inhibited kinetically. That is why the formation of $C_4H_8Cl^+$ ion is preferable. [2]

3. The relative molar responses related to naphthalene of some polychlorinated biphenyls were determined by means of indirect sample introduction on GC-MS instrument. The present relative molar responses of PCBs increase with the increase of chlorine atom number which is according to the expectation based on their cross sections. The addition of more than 3 chlorine atoms means a permanent difference in *RMR* for compounds having biphenyl skeleton. One chlorine atom contributes the value of 0.198 to *RMR* based on the respective equation. [3]

4. The relative molar responses of some straight chain aliphatic alkanes, ketones, aldehydes, alcohols and carboxylic acids related to naphthalene were investigated by means of indirect sample introduction on GC-MS instrument. Most of the respective compounds have not been investigated yet due to their high polarity or high boiling point. It was found that there were linear correlations between the molecular structures, i.e. the carbon atom number and relative molar response in current homologous series. In conclusion, the n-alkanes and n-alcohols generate similar

relative molar responses. The same observation holds for n-aldehydes and n-carboxylic acids, but their relative molar responses are smaller than that of the group of n-alkanes and n-alcohols'. n-Ketones can be found between these two groups. The relative molar responses of the individual CH_2 groups are between 0.169 and 0.210 in the homologous series. [4]

5. The relative molar responses of aliphatic primary amines related to naphthalene were investigated by means of indirect sample introduction on GC-MS instrument. It was found that there were linear correlations between their molecular structures, i.e. the carbon atom number and relative molar response. The relative molar responses of homologous series of primary amines are smaller than that of the group of n-alkanes. In connection with this result it was found that the GC measurement conditions (injector temperature, stationary phase, efficiency of column) affect the measured relative molar responses remarkably. [4]

5. Publications

Publications on the subjects of the dissertation

[1] N **Göröcs**, D Mudri, J Mátyási, J Balla; The Determination of GC–MS Relative Molar Responses of Some n-Alkanes and their Halogenated Analogs, *J Chromatogr Sci* (2013) 51(2): 138-145. IF: 0.794. IC: 3 (Google Scholar).

[2] Z Benkő, N **Göröcs**, L Könczöl, L Nyulászi, D Szieberth, J Balla; $C_nH_{2n}Cl^+$ Ion Formation in Electron Impact MS Conditions: a Theoretical Study, *Struct Chem* (2014) 25:659-665. IF: 1.772

[3] N **Göröcs**, B Beke, J Bozsik, J Mátyási, J Balla; The Determination of GC-MS Relative Molar Responses of Benzene and their Chlorinated and Methylated Analogs, *J Anal Chem* (2014) 69 (11):1112-1121, IF: 0.616

[4] N **Göröcs**, J Mátyási, J Balla; Relative Molar Responses of some Compounds Containing Oxygen and Nitrogen in GC-MS, *Struct Chem* (2014) DOI 10.1007/s11224-014-0414-6. IF: 1.772

Presentations

Göröcs Noémi: MSD jel és a molekulaszerkezet kapcsolata – Nyílt láncú vegyületek I.; Oláh György Doktori Iskola konferenciája, 2011. febr. 3. (oral)

Göröcs N., **Bartal** M., **Balla** J.: Sterilezett kötszerek maradék etilén-oxid tartalmának a meghatározása, Magyar Elválasztástudományi Társaság Elválasztástudományi Vándorgyűlés előadásai, Sárvár, 2008. november 5-7. (poster)

Göröcs N., **Mátyási** J., **Balla** J.: Correlation between Analytical Signal and Molecular Structure in Mass Spectrometry, 8th Balaton Symposium on High Performance Separation Methods and 15th International Symposium on Separation Sciences, Siófok, Hungary, 2009. September 2-4. (poster)

Mátyási J., *Göröcs* N., **Balla** J.:Efficiency of Fast GC, 8th Balaton Symposium on High Performance Separation Methods and 15th International Symposium on Separation Sciences, Siófok, Hungary, 2009. September 2-4. (poster)

Göröcs N., **Mudri** D., **Mátyási** J., **Balla** J.: MSD jel és a molekulaszerkezet kapcsolat Nyílt láncú vegyületek I., Magyar Elválasztástudományi Társaság Elválasztástudományi Vándorgyűlés előadásai, Tapolca, 2010. november 10-12. (poster)

Göröcs N., **Beke** B., **Bozsik** J., **Mátyási** J., **Balla** J.: MSD jel és a molekulaszerkezet kapcsolata: Benzolszármazékok vizsgálata, Magyar Elválasztástudományi Társaság Elválasztástudományi Vándorgyűlés előadásai, Hajdúszoboszló, 2012. november 7-9. (poster)

Göröcs N., **Mátyási** J., **Balla** J.: The Relative Molar Sensitivity and the Electron Impact Ionization Cross Section in GC-MS, 9th Balaton Symposium on High Performance Separation Methods, Siófok, Hungary, 2013. September 4-6. (poster)