

LIST OF LECTURES

- 1./ K. Héberger, I. Nencsev, P. Hajdu, D. Sopov, D. Gál, Putyi obrazovaniya szvabodnikh radikalov iz gidroperekisi etilbenzola pri ivo avtookiszljeniya, Activation of Molecules by Metal Complexes IV. International Seminar, **Sofia**, Bulgaria, May 21, 1980 [in Russian]. (lecture)
- 2./ Héberger K., Experiments to Elaborate a Chemical Ignition Method for *in situ* Combustion, Petrochemical Industry and Related Fields, Forum, **Csopak**, Hungary, Jun. 11-12, 1980 [in Hungarian]. (lecture)
- 3./ Héberger K., Hajdu P., Thermal Decomposition of α -Phenyl-ethyl Hydroperoxide. Effect of Concentration of Ethylbenzene, Hydroperoxide and Alcohol on the Rate of Initiation, Lectures in Chemistry, V. Scientific Symposium /MKE/ **Szeged**, Hungary, Apr 1-3, 1981 [in Hungarian]. (lecture)
- 4./ Héberger K., Analytical Methods to Follow Liquid Phase Oxidation of Ethylbenzene, Publication Forum for Young Organic Analysts, **Budapest**, Hungary, Dec. 15, 1981 [in Hungarian]. (lecture)
- 5./ Héberger K., Danóczy R., Gál D., A Chemical Ignition Process for Oil Recovery by *in situ* Combustion, Thermal Methods for Oil Recovery, Seminar, **Nagykanizsa**, Hungary, May 27-28, 1982 [in Hungarian]. (lecture)
- 6./ K. Héberger, P. Hajdu, Determination of the Initiation Rates in the Liquid Phase Oxidation of Ethylbenzene III. Rate Constants of Elementary Steps Resulting in Secondary Initiation, Second Int. Spec. Meeting of the Combustion Institute on Oxidation, **Budapest**, Hungary, Aug. 18-22, 1982. (lecture)
- 7./ K. Héberger, E. Hubert-Noszek, D. Gál, Interactions of Hydroperoxide with Alcohol and Inhibitor Molecules, International Symposium on the Mechanism of Additives, **Bourgas**, Bulgaria, Sept. 12-17, 1983. (lecture)
- 8./ É. Danóczy, K. Héberger, P. Kalocsai, M. Tóth, D. Gál, Modelling of *in situ* Combustion Processes and Their Chemical Ignition, International Symposium on the Mechanism of Additives, **Bourgas**, Bulgaria, Sept. 12-17, 1983. (lecture)
- 9./ D. Gál, K. Héberger, G. Vasvári, T. Vidóczy, Transient species in Hydrocarbon Oxidation. Generation of Radicals and Their Combination Processes, 16th International Symposium of Free Radicals, **Ottignies**, Belgium, 1983. (lecture)
- 10./ Héberger K., Hubertné-Noszek E., Alcohol Induced Decomposition of Hydroperoxides as well as Interaction between Inhibitors and Hydroperoxide, Lectures in Chemistry, VI. Scientific Symposium /MKE/ , **Szeged**, Hungary, Nov. 9-10, 1983 [in Hungarian]. (lecture)
- 11./ K. Héberger, J. Lukács, T. Vidóczy, On the Limitations of Evaluation Methods of Inhibition Measurements in Oxidation Systems, Oxydation of Hydrocarbons by Molecular Oxygen, Microsymposium, **Merseburg**, Germany, March 26-28, 1985. (lecture)
- 12./ Héberger K., Kemény S., Vidóczy T., Problems of Parameter Estimation. On the Uncertainties of Arrhenius Type Fits, Association of Hungarian Chemists, **Budapest**, Hungary, Sept. 16. 1985. [in Hungarian] (lecture)
- 13./ K. Héberger, S. Kemény, T. Vidóczy, On the Errors of Arrhenius Parameters and Estimated Rate Constant Values,
 - a.) 9th International Symposium on Gas Kinetics, **Bordeaux**, France, July 20-25, 1986.
 - b.) XXth International Symposium on Combustion, **München**, Germany, Aug. 3-8, 1986.

- c.) International Summer School on Chemical Physics, **Leipzig**, Germany, Aug. 21-28, 1986. (posters)
- 14./ K. Héberger, On the Errors of Estimated Arrhenius Parameters, Kinetik-Seminar, Phys.-Chem. Institut der Universität Göttingen, **Göttingen**, Germany, Apr. 15, 1987 [in English]. (lecture)
- 15./ K. Héberger, Several Radical-Molecule Reactions of Phenolic Antioxidants, International Summer School on Lasers in Polymer Research, **Leipzig**, Germany, July 5-11, 1987. (poster)
- 16./ K. Héberger, A. Lopata, J. Müller, Linear Free Energy Relationships for Peroxy Radicals - Phenol Reactions, WATOC Conference **Budapest**, Hungary, Aug. 12-15, 1987. (poster)
- 17./ K. Héberger, Utilization of Gas Chromatography in Chemical Kinetics. Product Identification by Correlation Equations, Arbeitstagung, Schloss **Ringberg**, Germany, Sept. 6-9, 1987. (lecture)
- 18./ K. Héberger, On the Errors of Arrhenius Parameters and Estimated Rate Constant Values, Seminarvortrag, Phys.- Chem. Instiut der Universität Zürich, **Zürich**, Switzerland, Nov. 24, 1987. (invited lecture)
- 19./ Héberger K., Irinyi Gy., Keszler A., Gál D., Studies of Photooxidation Reactions by Intermittent Illuminations, X. Spectroscopic School on Luminescence, **Pécs-Komló**, Hungary, Oct. 8-10, 1987. (poster)
- 20./ T. Böhland, K. Héberger, M. Koch, F. Temps, Kinetik und Produkte der Reaktion von CH_2 (X^3B_1)-Radikalen mit Benzol, Bunsentagung, **Passau**, Germany, May 12-14, 1988 [in German]. (lecture)
- 21./ K. Héberger, Empirical Correlation Between Retention Data and Physical or Topological Properties of Solute Molecules, CAC88, 4th International Conference on Chemometrics in Analytical Chemistry, **Amsterdam**, The Netherlands, May 18-20, 1988. (lecture)
- 22./ K. Héberger, On the Errors of Arrhenius Parameters and Estimated Rate Constant Values, Seminarvortrag, Physikalisch - Chemisches Institut der Universität Heidelberg, **Heidelberg**, Germany, May 27, 1988. (lecture)
- 23./ K. Héberger, F.Temps, Primary Products of the Reactions of CH_2 Radicals with Aromatic Hydrocarbons, 22nd International Symposium on Combustion, **Seattle**, USA, Aug.14-19, 1988. (poster)
- 24./ K. Héberger, Comparisons Between Linear and Nonlinear Models for Fitting Retention Data of Alkylbenzenes, COMPANA 88, 4. Tagung Computereinsatz in der Analytik, **Jena**, Germany, Sept. 5-8, 1988. (poster)
- 25./ K. Héberger, H. Jander, Product Analysis of the Reaction, CH_2 + Alkylbenzenes by GC and GC-MS Technique, 17th International Symposium on Chromatography, **Wien**, Austria, Sept. 25-30, 1988. (poster)
- 26./ K. Héberger, New Developments in Fitting of Arrhenius Parameters, Seminarvortrag, Fraunhofer Institut für Toxikologie und Aerosolforschung, **Hannover**, Germany, Okt. 18, 1988. (invited lecture)
- 27./ K. Héberger, Discrimination Between Linear and Nonlinear Models Describing Retention Data of Alkylbenzenes in Capillary Gas Chromatography, 10th International Symposium on Capillary Chromatography, **Riva del Garda**, Italy, May 22-25, 1989. (poster)
- 28./ K. Héberger, Identification of C_5H_8 Isomers with Test Reactions CH_2 (a^1A_1) + Butyne-1, Butyne-2 and Butadiene-1,3, 3rd International Symposium on Kinetics in

- Analytical Chemistry, **Dubrovnik-Cavtat**, Yugoslavia, Sept. 25-28, 1989.
(poster)
- 29./ a.) Héberger K., Reaction of Methylene Radical with Selected Hydrocarbons, Kinetics and Catalysis Scientific Community, Central Research Institute for Chemistry HAS **Budapest**, Hungary, Nov 1, 1989. [in Hungarian] (lecture)
- b.) Héberger K., Reaction of Methylene Radical with Benzene and Alkylbenzenes, Lecture for Receiving "Cand. Sci." Degree, Great Room of Hungarian Academy of Sciences, **Budapest**, Hungary, June 4, 1990. [in Hungarian] (lecture)
- 30./ K. Héberger, Methylen-Biradikale und ihre Reaktion mit Alkyl-aromaten., Seminarvortrag, Phys.- Chem. Institut der Universität Zürich, **Zürich**, Switzerland, May 8, 1990 [in German]. (lecture)
- 31./ K. Héberger, F. Temps, S. Völker, M. Wolf, H.Gg. Wagner, A Direct Study of the Reaction of CH_2 (X^3B_1)-Radicals with Toluene in the Temperature Range $296 \text{ K} < T < 623 \text{ K}$, 23rd Symposium (International) on Combustion, University of Orleans, **Orleans**, France, July 22-27, 1990. (lecture)
- 32./ K. Héberger, Empirische Korrelationsgleichungen in der Physikalisch - Organischen Chemie, Institutvortrag, Phys. - Chem. Institut der Universität Zürich, **Zürich**, Switzerland, Febr 14. 1991, [in German] (lecture)
- 33./ H. Fischer, K. Héberger, H. Rubin, M. Walbiner, Additionskonstanten einiger Radikale an Alkene und Alkine, Symposium "Organische Radikale und Radikationen. Präparative und mechanistische Aspekte", Universität Oldenburg, **Oldenburg**, Germany, Febr. 28 - March 2, 1991 [in German]. (lecture)
- 34./ K. Héberger, Addition Substituierter Benzyl Radikale on Alkene, Seminarvortrag, Phys.- Chem. Institut der Universität Zürich, **Zürich**, Switzerland, May 24, 1991. [in German] (lecture)
- 35./ K. Héberger, H. Fischer, Rate constants for the Addition of Substituted Benzyl Radicals to Olefins by Kinetic ESR, International Symposium on Recent Advances in ESR Spectroscopies, Applications to Chemistry, Physics and Biology, University of Padua, **Padova**, Italy Sept. 8-12, 1991. (poster)
- 36./ K. Héberger, Empirical Correlation Equations in Physical Organic Chemistry, Seminare de l'ITODYS, University of Paris VIII. **Paris**, France, Apr. 22, 1992. (invited lecture)
- 37./ K. Héberger, Enthalpie kontrollierte Addition von 2-Cyano-2-Propyl Radikalen an Alkene, Phys.- Chem. Institut der Universität Zürich, **Zürich**, Switzerland, June 19, 1992. Seminarvortrag [in German]. (lecture)
- 38./ K. Héberger, F. Temps, S. Völker, H. Gg. Wagner, R. Koch, Kinetics and Product Distribution of Reactions of Some Aromatic Hydrocarbons with CH_2 (X^3B_1) in the Gas Phase, 12th International Symposium on Gas Kinetics, University of Reading, **Reading**, England, July 19-24, 1992. (lecture)
- 39./ K. Héberger, H. Fischer, Absolute Rate Constants for Radical Addition Reactions, Enthalpy Control for 2-Cyano-2-Propyl Radical, 6th International Symposium on Organic Free Radicals, **Nordwijkerhout**, The Netherlands, Aug. 23-28, 1992. (poster)
- 40./ K. Héberger, Linear Free Energy Relationships in Radical Reactions. Hydrogen Abstraction from Substituted Toluenes by *tert*-Butyl, *tert*-Butoxyl and *tert*-Butyl Peroxy Radicals, 6th International Symposium on Organic Free Radicals, **Nordwijkerhout**, The Netherlands, Aug. 23-28, 1992. (poster)

- 41./ K. Héberger, Prediction of Gas Chromatographic Retention Indices for Alkylbenzenes on OV-101 Using Nonlinear Functions 19th International Symposium on Chromatography, **Aix-en-Provence**, France, Sept. 13-18, 1992. (poster)
- 42./ Héberger K. and Lukovits I., Decomposition of a Graph Invariant into a Sum of Substitution and Bonding Increments. Interpretation of Gas-Chromatographic Retention Indices for Alkylbenzenes, Workshop on Theoretical Organic Chemistry of Hungarian Academy of Sciences, ELTE TTK, Chemistry Building, **Budapest**, Hungary, Nov. 6-7, 1992 [in Hungarian]. (lecture)
- 43./ Héberger K., Addition Reactions of Carbon Centered Radicals on Alkenes. Determination of Absolute Rate Constants by Kinetic ESR Spectroscopy, JATE Department of Physical Chemistry, Seminar, **Szeged**, Hungary, May 5, 1993 [in Hungarian]. (lecture)
- 44./ K. Héberger, H. Fischer, Addition Rate Constants of 2-Hydroxy-2-Propyl Radical to Alkenes, GORDON Research Conference, Free Radical Reactions, **Plymouth**, USA, New Hampshire, July 25-30, 1993. (poster)
- 45./ K. Héberger, A. Lopata, Principal Component Analysis of Rate Constants for Radical Addition Reactions, GORDON Research Conference, Free Radical Reactions, **Plymouth**, USA, New Hampshire, July. 25-30, 1993. (poster)
- 46./ I. Nemes, K. Héberger, Á. Keszler, T. Vidóczy, D. Gál, L. Cotarca, P. Delogu, Various Types of Free Radicals and Their Role in the Oxidative Decarboxylation of Cyclohexane Monocarboxylic Acid, 22nd Symposium on Free Radicals, **Doorwerth**, The Netherlands, Sept. 6-10. 1993. (poster)
- 47./ Héberger K., Combinatoric Method to Discriminate Statistically Equivalent Quantities (Factors), Hungarian Chemometric Workshop, Kemometria'93, MKE, **Balatonfüred**, Hungary, Oct. 18-20, 1993 [in Hungarian]. (lecture)
- 48./ Héberger K., Addition of Carbon Centered Radicals on Alkenes, Workshop on Reaction Kinetics and Photochemistry of HAS, **Kecskemét**, Hungary, Apr. 22, 1994 [in Hungarian]. (lecture)
- 49./ K. Héberger and A Lopata, Separation of Polar and Enthalpic Effects on Radical Addition Reactions Using Principal Component Analysis, 10th European Symposium on Structure - Activity Relationships, QSAR and Molecular Modelling, **Barcelona**, Sept. 4-9, 1994. (poster)
- 50./ K. Héberger, Discrimination of Statistically Equivalent Variables in QSAR, 10th European Symposium on Structure - Activity Relationships, QSAR and Molecular Modelling, **Barcelona**, Spain, Sept. 4-9, 1994. (poster)
- 51./ K. Héberger, Comparison of Hammett Type Scales in Describing Rate Constants of Radical Reactions, 10th European Symposium on Structure - Activity Relationships, QSAR and Molecular Modelling, **Barcelona**, Spain, Sept. 4-9, 1994. (poster)
- 52./ K. Héberger, "Pair-Correlation Method for Choosing the Decisive Factor" 6th International Workshop on Quantitative Structure-Activity Relationships (QSAR) in Environmental Sciences, **Belgirate**, Italy, Sept. 13-17, 1994. (poster)
- 53./ Héberger K. and Lopata A., Separation of Polar and Enthalpic Effect in Radical Addition Reactions by Principal Component Analysis, Hungarian Chemometric Workshop, Kemometria'93, MKE, **Zamárdi**, Hungary, Oct. 5-7, 1994 [in Hungarian]. (lecture)
- 54./ Héberger K. and Németh A., Principal Component Analysis in Kinetic Systems, Hungarian Chemometric Workshop, Kemometria'93, MKE, **Zamárdi**, Hungary, Oct. 5-7, 1994 [in Hungarian]. (lecture)

- 55./ Héberger K., Determination and Evaluation of Rate Constants for Radical Addition Reactions, Institute Workshop, **Budapest**, Hungary, March. 22-23. 1995, [in Hungarian]. (lecture)
- 56./ Héberger K., Investigations on Chemometrics in the Department of Oxidation Processes (HAS) Workshop on Reaction Kinetics and Photochemistry of HAS, **Veszprém**, Hungary, Apr. 14-15. 1995, [in Hungarian]. (lecture)
- 57./ K. Héberger, Evaluation of Stationary Phase Polarity by Principal Component Analysis in Gas-Liquid Chromatography, Chemometrics '95 (Czech Chemical Society) **Pardubice**, Bohemia, July 3-7, 1995. (poster)
- 58./ Héberger K., Combinatoric Generation of Reaction Mechanism and its Reduction by Various Methods Chemometrics '95 (Czech Chemical Society) **Pardubice**, Bohemia, July 3-7, 1995. (software presentation)
- 59./ K. Héberger, A. Lopata, Assessment of Nucleophilicity and Electrophilicity of Radicals, Is Cyanomethyl Really Electrophilic? GORDON Research Conference, Free Radical Reactions, **Plymouth**, USA, New Hampshire, July 16-21, 1995. (poster)
- 60./ K. Héberger, I. Nemes A. Keszler, T. Vidóczy and D. Gál, "Oxidative Decarboxylation of Cyclohexane Acid, Kinetics, Mechanism and Modelling" GORDON Research Conference, Free Radical Reactions, **Plymouth**, USA, New Hampshire, July 16-21, 1995. (poster)
- 61./ K. Héberger, Characterization of Gas-Chromatographic Stationary Phases and Polarity Indicators by Principal Component Analysis, Hungarian Chemometric Workshop, Kemometria'95 MKE, **Veszprém**, Hungary, Oct. 18-21, 1995 [in Hungarian]. (lecture)
- 62./ K. Héberger and R. Rajkó, Generalization of the Pair-Correlation Methods for More Variables in QSAR, Hungarian Chemometric Workshop, Kemometria'95 MKE, **Veszprém**, Hungary, Oct. 18-21, 1995 [in Hungarian]. (lecture)
- 63./ K. Héberger, Empirical Correlations between Retention Indices and Physical as well as Topological Properties of Alkylbenzene Molecules, Institute of Chemistry, Estonian Academy of Sciences, **Tallinn**, Estonia, Nov. 9, 1995. (invited lecture)
- 64./ K. Héberger, Evaluation of Polarity Indicators and Stationary Phases by Principal Component Analysis in Gas-Liquid Chromatography, V Ogólnopolska Konferencja Chromatograficzna, **Katowice-Szczyrk**, June 12-14, 1996. (plenary lecture)
- 65./ K. Héberger, Generalization of the Pair Correlation Method for Variable Selection in QSAR, 7th International Workshop on QSARs in Environmental Sciences. QSAR 96 "Past, Present and Future", **Elsinore**, Denmark, June 24-28, 1996. (lecture)
- 66./ K. Héberger, Frequent Errors and Artifacts in Modelling, Conference of Chemists, Hungarian Chemical Society, **Eger**, Hungary, July 2-4, 1996 [in Hungarian]. (lecture)
- 67./ K. Héberger, A. Lopata, Classification of Radicals According to Their Nucleophilicity and Electrophilicity, 11th European Symposium on QSAR, Computer Assisted Lead Finding and Optimization, **Lausanne**, Switzerland, Sept. 1-6, 1996. (poster)
- 68./ K. Héberger, Errors and Artifacts in Modeling, Institute for Drug Research, LTD., **Budapest**, Hungary, Sept. 19, 1996 [in Hungarian]. (invited lecture)
- 69./ K. Héberger and T. Kowalska, Thermodynamic Properties of Alkylbenzenes from Retention - Boiling Point Correlations in Gas Chromatography, XXI Symposjum Naukowe Chromatograficzne Metody Badania Zwiaskow Organicznych, **Katowice**, Poland, Jun. 12-13, 1997. (poster)

- 70./ K. Héberger and T. Kowalska, Thermodynamic Properties of Alkylbenzenes from Kováts Retention Index - Boiling Point Correlations in Gas Chromatography, XXI Symposjum Naukowe Chromatograficzne Metody Badania Zwiaskow Organicznych, **Katowice**, Poland, Jun. 12-13, 1997. (poster)
- 71./ K. Héberger, A. Lopata, Assessment of Nucleophilicity and Electrophilicity of Radicals and of Polar and Enthalpy Effects on Radical Addition Reactions, GORDON Research Conference, Free Radical Reactions, **Plymouth**, USA, New Hampshire, July. 13-18. 1997, (poster)
- 72./ K. Héberger and T. Kowalska, Non-Linear Fitting of Relative Retention Time - Boiling Point Relations in Gas Chromatography, CC'97 Conferentia Chemometrica, **Budapest**, Hungary, Aug. 20-23, 1997. (poster)
- 73./ K. Héberger and T. Kowalska, Residual Analysis for Kováts Retention Index - Boiling Point Correlations in Gas Chromatography", CC'97 Conferentia Chemometrica, **Budapest**, Hungary, Aug. 20-23, 1997. (poster)
- 74./ Á. Keszler, K Héberger, and M Gude, Quantitative Analysis of Aliphatic Aldehydes using Headspace SPME Sampling and Ion-Trap GC/MS Detection, Balaton Symposium'97 on High Performance Separation Methods, **Siófok**, Hungary, Sept. 3-5, 1997. (poster)
- 75./ K Héberger, and T. Kowalska, Determination of Heats of vaporization and the Gibbs Free Energies of Alkylbenzenes on GC Stationary Phases of Different Polarity, Balaton Symposium'97 on High Performance Separation Methods, **Siófok**, Hungary, Sept. 3-5, 1997. (poster)
- 76./ K. Héberger, A Predictive Analysis of Radical Addition Reaction Rates, Phys.-Chem. Institut der Universität Zürich, **Zürich**, Switzerland, Jan 23, 1998, Seminarvortrag, [in English] (lecture)
- 77./ K. Héberger, Assessment of Nucleophilicity and Electrophilicity of Radicals, and of Polar and Enthalpy Effects on Radical Addition Reactions, Institut für Physikalische Chemie der Universität Basel, **Basel**, Switzerland, Febr. 12, 1998 Institutsvortrag, [in English]. (invited lecture)
- 78./ Á. Keszler, K Héberger, and L. Kótai, On the Mass Spectral Detection in Gas Chromatography Workshop on Mass Spectrometry, MKE Mass Spectroscopist Society, **Budapest**, Hungary, March 26, 1998 [in Hungarian]. (lecture)
- 79./ R. Rajkó and K. Héberger, Application of Test Statistics on the Pair-Correlation Method, Days of Chemical Industry in Veszprém, **Veszprém**, Hungary, Apr. 16-17, 1998 [in Hungarian]. (lecture)
- 80./ Héberger K., Prediction of Activation Energies of Radical Addition Reactions, Workshop on Reaction Kinetics and Photochemistry of HAS, **Balatonalmádi**, Hungary, Apr. 16-17, 1998 [in Hungarian]. (lecture)
- 81./ A. Borosy and K. Héberger, Comparison of Chemometric Methods for Prediction of Activation Energy of Radical Addition Reactions, 2nd Int. Chemometrics Research Meeting, ICRM'98 **Veldhoven**, the Netherlands May 24-28, 1998 (poster)
- 82./ K. Héberger and T. Kowalska, Empirical Retention - Boiling Point Correlations and Explanation of Their Constants in Gas Chromatography, XXII Symposjum Naukowe Chromatograficzne Metody Badania Zwiaskow Organicznych, **Katowice-Szczyrk**, Poland, Jun. 8-10, 1998. (poster)
- 83./ K. Héberger and T. Kowalska, Thermodynamic Significance of the Kováts Retention Index - Boiling Point Correlations in Gas Chromatography. Application of Trouton - Hildebrand - Everett's Rule for Alkylbenzenes, XXII Symposjum

- Naukowe Chromatograficzne Metody Badania Związków Organicznych, **Katowice-Szczyrk**, Poland, Jun. 8-10, 1998. (poster)
- 84./ K. Héberger and T. Kowalska, Empirical Retention - Boiling Point Correlations and Interpretation of Their Constants in Gas-Liquid Chromatography, Advances in Chromatography and Electrophoresis, ACE'98, an International Symposium, **Szeged**, Hungary, June 18-20, 1998. (poster)
- 85./ K. Héberger and T. Kowalska, Kováts Retention Index - Boiling Point Correlations in Gas Chromatography. Application of Trouton - Hildebrand - Everett's Rule, Advances in Chromatography and Electrophoresis, ACE'98, an International Symposium, **Szeged**, Hungary, June 18-20, 1998. (poster)
- 86./ K. Héberger and M. Görgényi, Principal Component Analysis of Kováts Indices for Carbonyl Compounds in Capillary Gas Chromatography, Advances in Chromatography and Electrophoresis, ACE'98, an International Symposium, **Szeged**, Hungary, June 18-20, 1998. (poster)
- 87./ K. Héberger and H. Fischer, Predictive Analysis of Radical Addition Reaction Barriers, EUACHEM Conference on „Organic Free Radicals” **Grottaferrata - Rome**, Italy, July 4-9, 1998. (poster)
- 88./ A. Lopata, I. Novak, Z. Szántó, and K. Héberger, Assessment of Nucleophilicity and Electrophilicity of Radicals and of Polar and Enthalpy Effects on Radical Addition Reactions Using Comparative Molecular Field Analysis, 12th European Symposium on Quantitative structure - Activity Relationships, „Molecular Modeling and Prediction of Bioactivity” **Copenhagen**, Denmark, Aug. 23-28, 1998. (poster)
- 89./ Á. Keszler and K. Héberger, Influence of the Extraction Parameters and of the Medium on the Efficiency of SPME Sampling in the Quantitative Analysis of Aliphatic Aldehydes, 22th International Symposium on Chromatography, ISC'98, **Rome**, Italy Sept. 13-18, 1998. (poster)
- 90./ K. Héberger and T. Kowalska, On the Thermodynamic Significance of Boiling Point Correlations for Alkylbenzenes in Gas Chromatography. Extension of the Trouton's Rule, 22th International Symposium on Chromatography, ISC'98, **Rome**, Italy Sept. 13-18, 1998. (poster)
- 91./ K. Héberger and M. Görgényi, Principal Component Analysis of Kováts Indices for Carbonyl Compounds in Capillary Gas Chromatography, 22th International Symposium on Chromatography, ISC'98, **Rome**, Italy Sept. 13-18, 1998. (poster)
- 92./ Héberger K. and Keszler Á., Principal Component Analysis of Measured Quantities during Degradation of Hydroperoxides in Oxidized Vegetable Oils, Hungarian Chemometric Workshop, Kemometria'98, **Miskolc**, Hungary, Oct. 7-9, 1998 [in Hungarian]. (lecture)
- 93./ Borosy A. and Héberger K., Comparison of Chemometric Methods for Prediction of Activation Parameters of Radical Addition Reactions, Hungarian Chemometric Workshop, Kemometria'98, **Miskolc**, Hungary, Oct. 7-9, 1998 [in Hungarian]. (lecture)
- 94./ Rajkó R. and Héberger K., MS Excel VBA Code for Pair Correlation Method with New Test Statistics, Hungarian Chemometric Workshop, Kemometria'98, **Miskolc**, Hungary, Oct. 7-9, 1998 [in Hungarian]. (lecture)
- 95./ Héberger K. Physical Significance of Gas Chromatographic Retention and Boiling Point Correlations, Institute Workshop, **Budapest**, Hungary, March. 30-31. 1999, [in Hungarian]. (lecture)

- 96./ K. Héberger and T. Kowalska, Thermodynamic Interpretation of Retention – Boiling Point Correlations in Gas Chromatography, A Summary, The XXIIIrd Scientific Symposium, Chromatographic Methods of Investigating the Organic Compounds, **Katowicze–Szczyrk**, Poland, June 9-11., 1999 (plenary lecture)
- 97./ K. Héberger and T. Kowalska, Temperature Dependence of the Kováts Retention Index Based on Eyring Equation, The XXIIIrd Scientific Symposium, Chromatographic Methods of Investigating the Organic Compounds, **Katowicze–Szczyrk**, Poland, June 9-11., 1999 (poster)
- 98./ K. Héberger T. Kowalska and M. Görgényi, Temperature Dependence of Relative Retention Times Based on Eyring Equation, The XXIIIrd Scientific Symposium, Chromatographic Methods of Investigating the Organic Compounds, **Katowicze–Szczyrk**, Poland, June 9-11., 1999 (poster)
- 99./ K. Héberger T. Kowalska and M. Görgényi Temperature Dependence of Kováts Retention Indices, Chromatographic Workshop, Hungarian Chemical Society, **Budapest**, Hungary, Jul. 7-8, 1999 [in Hungarian]. (poster)
- 100./ K. Héberger and A Lopata, Separation of Polar and Enthalpic Effects in Radical Addition Reactions Using Radical Sigma (σ) scales, GORDON Research Conference, Free Radical Reactions, **Plymouth**, USA, New Hampshire, July. 11-16. 1999, (poster)
- 101./ K. Héberger, Quantitative Structure Chromatographic Retention Relationships, Retention Data as a Function of Boiling Point, Column Temperature and Other Properties CHEMOMETRICS V, **Brno**, Czech Republic, Aug. 29 – Sept. 2., 1999 (plenary lecture)
- 102./ K. Héberger and M. Görgényi, Principal Component Analysis of Kováts Indices for Oxo Compounds in Gas Chromatography, CHEMOMETRICS V, **Brno**, Czech Republic, Aug. 29 – Sept. 2., 1999 (poster)
- 103./ T. Körtvélyesi, K. Nagy and K. Héberger, Prediction of Rate Constants from Parameters Calculated by Quantum Chemical Methods, Addition of Nucleophilic and Electrophilic Radicals to Substituted Alkenes, CHEMOMETRICS V, **Brno**, Czech Republic, Aug. 29 – Sept. 2., 1999 (lecture)
- 104./ R. Rajkó and K. Héberger, Algorithmic and Statistical Problems During Development of a Nonparametric Variable selection Method, CHEMOMETRICS V, **Brno**, Czech Republic, Aug. 29 – Sept. 2., 1999 (poster)
- 105./ R. Rajkó and K. Héberger, Rapid Moisture Content Determination of Foods Using Microwave Energy and Pair-Correlation Method (PCM), CHEMOMETRICS V, **Brno**, Czech Republic, Aug. 29 – Sept. 2., 1999 (poster)
- 106./ K. Héberger and M. Görgényi, Principal Component Analysis of Kováts Indices for Oxo Compounds in Capillary Gas Chromatography, Hungarian Chemometric Workshop, Kemometria'99, **Szeged**, Hungary, Oct. 17 – Oct 19., 1999 [in Hungarian] (lecture)
- 107./ R. Rajkó and K. Héberger, Theoretical Investigation of First and Second Kind Errors for Pair Correlation Method, Hungarian Chemometric Workshop, Kemometria'99, **Szeged**, Hungary, Oct. 17 – Oct 19., 1999 [in Hungarian] (lecture)
- 108./ T. Körtvélyesi, K. Nagy and K. Héberger, Prediction of Rate Coefficients of Radical Addition and Hydrogen Transfer Reactions by Quantum Chemical Parameters, Hungarian Chemometric Workshop, Kemometria'99, **Szeged**, Hungary, Oct. 17 – Oct 19., 1999 [in Hungarian] (lecture)

- 109./ K. Héberger, Data Analysis by Multivariate Methods, Archeometric Workshop, Hungarian National Museum, **Budapest**, Hungary, Febr. 7. 2000 [in Hungarian] (lecture)
- 110./ K. Héberger, Correlation Equations in Physical Organic Chemistry (A Chemometric Approach). Lecture for Receiving "Doctor of the Academy" Degree, Great Room of Hungarian Academy of Sciences, **Budapest**, Hungary, Febr. 25, 2000. [in Hungarian] (lecture)
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- 224./ O. Farkas, I. G. Zenkevich, F. Strout, J. H. Kalivas, K. Héberger, Prediction of Kováts indices for fatty acid methyl esters. Optimal or parsimonious models? , Conferentia Chemometrica 2007, **Budapest** (Hungary), September 2-5, 2007 (poster)
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- 227./ Károly Héberger, Comparison of Methods for Column Selection in Chromatography, Invited lecture at Rugjer Boskovic Institute, **Zagreb**, Croatia, November 05, 2007 (lecture)
- 228./ Károly Héberger, What kind of information can be gathered if analyzing chromatographic data? Three examples., 7th KeMoMo - QSAR minisymposium, **Szeged**, (Hungary) Dec. 06-07, 2009. [in Hungarian] (lecture)
- 229./ Károly Héberger, Objective Comparison of Methods? A Novel Way of Ranking, Molecular Informatics and Bioinformatics, International symposium, Collegium Budapest - Institute for Advanced Study, **Budapest**, Hungary March, 27-29, 2008 (lecture)

- 230./ Károly Héberger, Two QSAR applications: one successful – the other not, KeMoMo - QSAR minisymposium, **Szeged**, (Hungary) April 29-30, 2009. [in Hungarian] (lecture)
- 231./ Károly Héberger, How can multivariate data analysis be useful for chromatographers? 19th International Symposium on Pharmaceutical and Biomedical Analysis, **Gdansk**, Poland, June 8-12, 2008 (invited lecture)
- 232./ Károly Héberger, Sonja Nikolić, Comparison of Variable Selection Methods. Prediction of Toxicity of Substituted Benzenes, 23rd Math/Chem/Comp 2008: 23rd International Course on the Interfaces among Mathematics, Chemistry & Computer Sciences, **Dubrovnik**, Croatia, June 16-21, 2008 (poster)
- 233./ K. Héberger, S. Kephelopoulos, S. Kemény, H. Dymond, E. B. Wilkes, D. Kotzias, Variance analysis of nicotine and nicotine free dry particulate matter in fine-cut smoking articles, 11th International Conference on Chemometrics for Analytical Chemistry, **Montpellier**, France, Jun. 30 - Jul. 04, 2008 (poster)
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- 239./ Károly Héberger, Classification and Selection of Chromatographic Columns, Stationary Phases and Variables Characterizing Polarity, 13th Scientific Days at the Chemical Research Center, **Budapest**, Hungary, Dec. 3rd-5th, 2008 [in Hungarian]. (lecture)
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- 241./ Károly Héberger, Pattern recognition methods in medical diagnosis, KeMoMo - QSAR minisymposium, **Szeged**, (Hungary) April 29-30, 2009. [in Hungarian] (lecture)
- 242./ Carlo Bertinetto, Celia Duce, Alessio Micheli, Maria Rosaria Tiné, Roberto Solaro, Sonja Nikolić, Károly Héberger, Recursive Neural Network Modelling of Benzene Derivatives Acute Toxicity, Math/Chem/Comp 2009: 24rd International Course&Conference on the Interfaces among Mathematics, Chemistry & Computer Sciences, **Dubrovnik**, Croatia, June 08-13, 2009 (poster)

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- 244./ Károly Héberger, Igor G. Zenkevich, Comparison of physicochemical and chromatographic polarity measures for simple organic compounds, Conferentia Chemometrica 2009, **Siófok**, Hungary, September 27-30, 2009 (poster)
- 245./ Gábor P. Szijjártó, András Tompos, Károly Héberger, Combinatorial design of MgAl₂O₄ supported catalysts for steam reforming of bioethanol Conferentia Chemometrica 2009, **Siófok**, Hungary, September 27-30, 2009 (poster)
- 246./ Rosa-Maria Alonso-Salces, M-V. Holland, C. Guillou, K. Héberger, Evaluation of pattern recognition techniques for the characterization of PDO olive oils by 1H-NMR fingerprinting, Conferentia Chemometrica 2009, **Siófok**, Hungary, September 27-30, 2009 (poster)
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- 248./ Virág Sági-Kiss, Sim Fong, Andrea Pomázi, Péter Fodor, Károly Héberger, Richard G Brereton, Pattern Recognition and GCMS peak detection to predict spoilage in fruits from production of volatile organic compounds (VOC), Conferentia Chemometrica 2009, **Siófok**, Hungary, September 27-30, 2009 (poster)
- 249./ Károly Héberger, Klára Kollár-Hunek, Comparison of ranks by random numbers, Conferentia Chemometrica 2009, **Siófok**, Hungary, September 27-30, 2009 (poster)
- 250./ Károly Héberger, Klára Kollár-Hunek, Sum of ranking differences. A novel measure for comparison and grouping of methods, Analytical Days, Hungarian Chemical Society, **Budapest**, Hungary, January 28-29, 2010 (lecture)
- 251./ Károly Héberger, Klára Kollár-Hunek, Comparison of methods and models by consensus, Seventh Winter Symposium on Chemometrics, **St. Petersburg**, Russia February 15-19, 2010, (lecture)
- 252./ Károly Héberger, Klára Kollár-Hunek, How (not) to determine the number of significant latent components?, KeMoMo - QSAR minisymposium, **Szeged**, (Hungary) April 29-30, 2010. [in Hungarian] (lecture)
- 253./ Károly Héberger, Klára Kollár-Hunek, Janus-faced Cross validation. How to rank (numerical) validation methods? 5th International Symposium on Computer Applications and Chemometrics in Analytical Chemistry, **Budapest**, Hungary, Jun. 21st - 25th, 2010 (lecture)
- 254./ Sonja Nikolić, Vesna Rastija, Károly Héberger, Quantitative relationship between 3D structure and hydrophilicity and lipophilicity of polyphenols, 5th International Symposium on Computer Applications and Chemometrics in Analytical Chemistry, **Budapest**, Hungary, Jun. 21st - 25th, 2010 (poster)
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- 256./ Károly Héberger, Cross- or external validation?, Workshop on Reaction Kinetics and Photochemistry of HAS, **Gyöngyöstarján**, (Hungary), October 28-29, 2010 [in English]. (lecture)

- 257./ Károly Héberger, Data evaluation in chromatography. Validation of quantitative structure - retention relationships. Ranking of the models predicting retention data, Lecture at Poznan University of Technology, Institute of Chemical Technology and engineering, **Poznań**, Poland, November 19, 2010 (Invited lecture)
- 258./ Károly Héberger, Pattern recognition methods in medical diagnosis, 15th Scientific Days at the Chemical Research Center, **Budapest**, Hungary, Nov. 23-25, 2010 [in Hungarian]. (lecture)
- 259./ Károly Héberger, Novel Chemometric Methods, chemometric course, Faculty of Technology, University of Novi Sad, **Novi Sad**, Serbia, Dec. 04, 2010 (lectures)
- 260./ Károly Héberger, Multivariate methods for data evaluation XI. Linear discriminant analysis, Comparison of methods by consensus, Seminar at the Corvinus University, **Budapest**, Apr. 06/2011 [in Hungarian] (lecture)
- 261./ Károly Héberger, How can multivariate analysis be useful for chromatographers? ICOPIC 2011: International Conference on Perspectives in Chemometrics, SRM University, **Chennai**, India, 9th - 11th April, 2011 (Invited lecture)
- 262./ Károly Héberger, Evaluation of models predicting retention indices for polycyclic aromatic hydrocarbons. Comparison of methods based on sum of ranking differences and pair-correlation, KeMoMo - QSAR minisymposium, **Szeged**, (Hungary) June 16-17, 2011. [in Hungarian] (lecture)
- 263./ Anita Rácz, János Elek, Károly Héberger, Róbert Rajkó, Adrienn Lengyel, Statistical and XRF Analyses of an silver coins of the Árpád and other dynasties, KeMoMo - QSAR minisymposium, **Szeged**, (Hungary) June 16-17, 2011. [in Hungarian] (lecture)
- 264./ Rajkó Róbert, Rácz Anita, Elek János, Héberger Károly, Lengyel Adrienn, Application of MCR-ALS to evaluate the content of coins from the Árpád and other dynasties, KeMoMo - QSAR minisymposium, **Szeged**, (Hungary) June 16-17, 2011. [in Hungarian] (lecture)
- 265./ Károly Héberger. Novel chemometric methods: Application of chemometrics in environmental and food safety domains, Tutorial II; 2nd CEFSER Workshop "Persistent organic pollutants in food and environment" **Novi Sad**, Serbia, September 08-10 2011 (lectures)
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- 270./ G. Tóth, Zs. Bodai and K. Héberger, Pre-estimation of leverage points in any data set from Q^2 AND R^2 , Conferentia Chemometrica 2011, **Sümege**, (Hungary) Sept. 18-21, 2011 (poster)
- 271./ Károly Héberger, Ranking of models (sum of ranking differences and pair-correlation metyhd), 4th CEFSER training course "Persistent organic pollutants in food and environment: risk assesment" **Novi Sad**, Serbia, September 14-15 2011 (all day, consultation included) (lectures)
- 272./ O. Ozohanics, L. Turiák, A. Puerta, M. de Frutos, J. C. Diez-Masa, K. Héberger, K. Vékey, L. Drahos Analysis of AGP glycosylation changes in cardiovascular diseases, XIIIth Chemometrics in Analytical Chemistry (CAC 2012), COO-4, **Budapest**, Hungary, June 25-29 (2012) (lecture)
- 273./ Klára Kollár-Hunek, Károly Héberger, Repeated observations and ranking (ties) for sum of ranking differences, KL-4, XIIIth Chemometrics in Analytical Chemistry (CAC 2012), **Budapest**, Hungary, June 25-29 (2012) (lecture)
- 274./ Olav H. J. Christie, Aníta Rác, János Elek, Károly Héberger, Object target rotation for principal components analysis: metal content data of Hungarian silver coins from the Árpád Dynasty, PO-4, XIIIth Chemometrics in Analytical Chemistry (CAC 2012), **Budapest**, Hungary, June 25-29 (2012) (lecture)
- 275./ Z. Niemier, A. Voelkel, M. Jędrusik, K. Héberger, Principal component analysis int he study of dental fillings stability, P-51, XIIIth Chemometrics in Analytical Chemistry (CAC 2012), **Budapest**, Hungary, June 25-29 (2012) (poster)
- 276./ K. Héberger , D. Relić, S. Sakan, B. Škrbić, D. Đorđević, Ranking and similarity for coinventional microwave and ultrasound extraction of elements, P-65, XIIIth Chemometrics in Analytical Chemistry (CAC 2012), **Budapest**, Hungary, June 25-29 (2012) (poster)
- 277./ K. Sunjog, S. Kolarević, K. Heberger, Z. Gačić, J. Knežević-Vukčević, B. Vuković-Gačić, M. Lenhardt, comparison of different methods for genotoxicity estimation based on the sum of ranking differences, P-66, XIIIth Chemometrics in Analytical Chemistry (CAC 2012), **Budapest**, Hungary, June 25-29 (2012) (poster)
- 278./ G. Tóth, Zs Bodai, K. Héberger, Pre-estimation of leverage points in any data set from Q^2 and R^2 , P-79, XIIIth Chemometrics in Analytical Chemistry (CAC 2012), **Budapest**, Hungary, June 25-29 (2012) (poster)
- 279./ Caroline West, Eric Lesellier, Károly Héberger, Sum of ranking differences to compare packed columns for supercritical fluid chromatography, P-140, XIIIth Chemometrics in Analytical Chemistry (CAC 2012), **Budapest**, Hungary, June 25-29 (2012) (poster)
- 280./ J. Kołodziejek, A. Voelkel, K. Héberger, Chemometric methods in characterization of hybride materials by means of inverse gas chromatography, P-143, XIIIth Chemometrics in Analytical Chemistry (CAC 2012), **Budapest**, Hungary, June 25-29 (2012) (poster)
- 281./ Károly Héberger, Klára Kollár-Hunek, What reasons of financial crisis in 2008? Greece and Germany in the same position?! Workshop on Reaction Kinetics and Photochemistry of HAS, **Gyöngyöstarján**, (Hungary), October 25-26, 2012 [in Hungarian]. (lecture)
- 282./ K. Héberger, Some interesting applications of chemometrics, Days of chemical engineering in Borsod, **Miskolc**, (Hungary), November 27, 2012 [in Hungarian] (lecture)

283./ Károly Héberger, Ranking of QSAR Models to Predict Minimal Inhibitory Concentrations Toward Mycobacterium tuberculosis for a Set of Fluoroquinolones, Seminar at the Institute of Materials and Environmental Chemistry, Research Centre for Natural Sciences, Hungarian Academy of Sciences, **Budapest**, Febr. 12, 2013 [in Hungarian] (lecture)