

## Curriculum Vitae Károly Héberger

**Name:** Károly (Charles) Héberger

**Date of birth:** 16 Aug. 1953

**Universities:** Sept. 1972 - June 1977

Technical University of Budapest

Faculty of Chemical Engineering

Section of Organic and Synthetic Chemistry

Pharmaceutical Branch

Diploma Work was made in the Polytechnic University of Tallinn (Estonia) 1977

topic: Characterization of Systematic Errors During Measuring and Evaluation of Vapor-Liquid Equilibrium Data by Mathematical Statistical Methods

### Working Places:

- Central Research Institute for Chemistry of the Hungarian Academy of Sciences, Budapest, Hungary. Supervisor: Prof. Dr. D. Gál, from the 1st of Sept. 1977. (Ph.D. student, research associate, senior research associate and finally scientific advisor) Since the reorganization of the Institute, its name has been changed into Chemical Research Center, Hungarian Academy of Sciences, Research Centre for Natural Sciences, Hungarian Academy of Sciences and now: Research Centre for Natural Sciences, Hungarian Academy of Sciences, Centre of Excellence.
- Max-Planck-Institut für Strömungsforschung, Göttingen, Germany. Supervisor: Prof. Dr. H. Gg. Wagner, between Jan. 1987 - Aug. 1989. (Post. doc.)
- Physikalisch-Chemisches Institut der Universität Zürich, Zürich, Switzerland. Supervisor: Prof. Dr. H. Fischer, between Apr. 1990 - Aug. 1992. (~Assistant professor) and between Sept. 1997 - Jan. 1998 (Private docent).
- European Commission, Joint Research Centre, Institute for Health and Consumer Protection, Physical and Chemical Exposure Unit, BEVABS, Ispra (VA), Italy, between July 01, 2004 – June 30, 2005 (visiting scientist).
- European Commission, Joint Research Centre, Institute for Health and Consumer Protection, Physical and Chemical Exposure Unit, BEVABS, Ispra (VA), Italy, between Sept. 16, 2005 – Sept. 15, 2006 (contract agent).

**Degrees:**

- *Ph.D.*, May 1981, "suma cum laude"  
Topic: Thermal Decomposition of  $\alpha$ -Phenyl-ethyl Hydroperoxide
- *Candidate of Chemical Science*, June 1990  
Topic: Reactions of Methylene Radical with Benzenes and Alkylbenzenes
- *Doctor of the Hungarian Academy of Sciences* (Feb. 2000)  
Topic: Empirical Correlation Equations in the Physical Organic Chemistry (Chemometric Approach)
- *Titular Professor* (Budapest University of Technology and Economics, June 28 / 2011).

**Knowledge of languages:** German (high degree), English, Russian (medium degree)

**Paper-reviews for:**

Acta Alimentaria (10), Acta Silvatica et Lignaria Hungarica (1), Acta Chimica Slovenica (1), Advances in Meteorology (1), Analytica Chimica Acta (54), Analyst (>1), Analytical Chemistry (8), Analytical & Bioanalytical Chemistry (30), Analytical Letters (8), Analytical Methods (13), Annals of Medicine (1), Applied sciences (2), Arabian Journal of Chemistry (1), Arabian Journal of Scientific Engineering (1), Beverages (2), Biomedical Chromatography (2), Bioorganic Chemistry (1), Bioorganic & Medicinal Chemistry (3), Biotechnology Progress (2), BMC Chemistry (1) Bulletin of the Chemical Society of Ethiopia (3), Chemical Industry and Chemical Engineering Quarterly (3), Chemical Papers (2), Chemical Reviews (1), Chemistry Central Journal (10), Chemistry Central Journal - Heritage Science (5), Chemometrics and Intelligent Laboratory Systems (61), Chemosphere (4), Chromatographia (39), Chromatography Research International (2), Computational Biology and Chemistry (1), Computer Methods and Programs in Biomedicine (1), Computational Concepts in Magnetic Resonance Part A (1), Croatica Chemica Acta (12), Current Computer Aided Drug Design (7), Ecotoxicology and Environmental Safety (5), Environmental Engineering and Management Journal (2), Food Analytical methods (5), Food and Chemical Toxicology (1), Food Chemistry (59), Food Control (3), Food Research International (1), Food Science and Technology International (2), Fresenius Environmental Bulletin (2), Fuel (2), Geophysics Research Letters (2), Heritage Science (7), IEEE Access (1), Information Fusion (1), International Conference on Biological Information and Biomedical Engineering, BIBE 2018 (1), Industrial Crops and Products (1), Interdisciplinary Sciences: Computational Life Sciences (1), International Journal of Analytical Chemistry (1), International Journal of Chemical Kinetics (2), International Journal of Environmental Analytical Chemistry (1), International Journal of Environmental Analytical Chemistry (2), International Journal of Industrial Chemistry (1), International Journal of

Molecular Sciences (2), International Journal of Quantitative Structure-Property Relationships (3), International Journal of Quantum Chemistry (1), Internet Electronic Journal of Molecular Design and Internet Electronic Journal of Theoretical Chemistry (1), Journal of Agricultural and Food Chemistry (21), Journal of Alloys and Compounds (1), Journal of Analytical Methods in Chemistry (former Journal of Automated Methods and Management in Chemistry) (4), Journal of Applied Statistics (2), Journal of Chemical Information and (Computer Sciences) Modeling (13), Journal of Chemical and Engineering Data (2), Journal of Chemical Sciences (1), Journal of Cheminformatics (4), Journal of Chemometrics (50), Journal of Chromatographic Science (73), Journal of Chromatography A (172), Journal of Chromatography B (21), Journal of Colloid and Interface Science (2), Journal of Computational Chemistry (2), Journal of Computer-Aided Molecular Design (1), Journal of Ecology and the Natural Environment (1), Journal of Food Science (7), Journal of Functional Foods (1), Journal of Hazardous Materials (1), Journal of Inclusion Phenomena (1), Journal of the Iranian Chemical Society (4), Journal of Molecular Structure (23), Journal of Nanomaterials (1), Journal of Pharmaceutical and Biomedical Analysis (22), Journal of Pharmacy and Pharmacology (1), Journal of Physical Organic Chemistry (5), Journal of Planar Chromatography – Modern TLC (2), Journal of Radioanalytical and Nuclear chemistry (1), Journal of Separation Science (18), Journal of the Iranian Chemical Society (5), Kuwait Journal of Science and Engineering (1), Letters in Drug Design & Discovery(online) (3), LWT - Food Science and Technology (2), Magyar Kémiai Folyóirat (1), MATCH - Communications in Mathematical and in Computer Chemistry (5), Materials Science and Engineering B (2), Measurement (26), Medicinal Chemistry (1), Microchemical Journal (1), Mini Reviews in Medicinal Chemistry (1), ACH Models in Chemistry (4), Molecular Biosystems (1), Molecular Diversity (9), Molecular Informatics (4), Molecules (6), Nitric Oxide (1), Nutrition and Dietary Supplements (1), Pattern Recognition Letters (1), Polymer Bulletin (7), Polymer Testing (1), QSAR and Combinatorial Sciences (7), Química Nova (1), Reaction Kinetics and Catalysis Letters (1), Reaction Kinetics, Mechanism and Catalysis (7), RSC Advances (23), SAR and QSAR in Environmental Sciences (7), Scientific Reports (1), Scientometrics (2), Sensors (7), Sensors & Actuators B: Chemical (13), Separations (3), Separation Science and Technology (1), SN Applied Sciences (1), Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy (3), Spectroscopy Letters (2), Statistics and Operation Research Transactions (1), Structural Chemistry (1), Symmetry (1), Talanta (26), Termochimica Acta (3), Trends in Analytical Chemistry (7), Water Science and Technology (4).

Review of project proposals for the International Science Foundation (Washington, DC), Hungarian Scientific Foundation (OTKA, Hungary) Ministry of Education and Science of the Republic of Serbia (New 4-year

project cycle in basic research, applied research and priority research fields, Serbia); Fundacja na rzecz Nauki Polskiej (FNP) Poland, Research Grants Council Hong Kong, China;

### **Editor**

Journal of Chemometrics (Wiley) since 2018 November

**Editorial Board member:** Accounts of Analytical Chemistry Research (The American Publishing House), Acta Chromatographica (till 2007); Beverages (since 2016); Chemical Processes and Materials (since 2016); Current Analysis on Chemistry (since July 2018), International Journal of Quantitative Structure-Property Relationships (since 2015); Journal of Analytical Methods in Chemistry (earlier Journal of Automated Methods and Management in Chemistry, since 2011); Journal of Chemometrics (since 2011); Journal of Drug Design and Medicinal Chemistry (since 2018), Journal of Metabolomics (since 2014); Molecules (Multidisciplinary Digital Publishing Institute, Basel, Switzerland, since July, 2019) SAR and QSAR in Environmental Research (Taylor and Francis, since Dec. 2019).

**Guest editor:** Chemometrics and Intell. Lab. Syst. Vol. 67 issue 1 and Vol. 72 issue 2 (ACE CC 2003), Journal of Chemometrics Vol. 22 issue 3-4 (Conferentia Chemometrica 2007), Journal of Chemometrics Vol. 23 issue 4 (4<sup>th</sup> International Symposium on Computer Applications and Chemometrics in Analytical Chemistry), Journal of Chemometrics Vol. 24 issue 3-4 (Conferentia Chemometrica 2009), Journal of Chemometrics Vol. 25 issue 5 (5<sup>th</sup> International Symposium on Computer Applications and Chemometrics in Analytical Chemistry), Journal of Chemometrics Vol. 26, issue 3-4 (Conferentia Chemometrica 2011), Analytica Chimica Acta (CAC 2012 special issue, partly), Journal of Chemometrics Vol. 28 issue 4 (Conferentia Chemometrica 2013), Journal of Chemometrics Vol. 30 issue 4, (Conferentia Chemometrica 2015) Journal of Chemometrics Vol. 32, issue 4 (Conferentia Chemometrica 2017). Journal of Chemometrics Vol. 34, (Conferentia Chemometrica 2019).

**Prizes:** “Prize for Excellent Work” Hungarian Chemical Society, May 09, 2003.

“High Standard Prize” Hungarian Chemical Society, three times: May 14, 2004, May 18, 2011 and May 23, 2013

“Excellent poster award” 2/67; Scientific days of the MTA TTK, 2012.

### **Other experiences:**

- *Teaching:* 5 semesters (terms) at Physikalisch-Chemisches Institut der Universität Zürich, Zürich, Switzerland (Physical Chemistry Laboratory

Training Course); Multivariate Data Analysis Methods (Chemometrics) 1 and 2, since 2001.

- *Organization of Conferences:*

2nd International Specialist Meeting of the Combustion Institute on Oxidation (secretary of program subcommittee, editor of abstract book) 1982, Budapest

Kemometria'94, '95, and '98 (member of the scientific committee), Zamárdi, Veszprém and Lillafüred, (Association of Hungarian Chemists) Hungary,

CC'97 Conferentia Chemometrica, 1997 Budapest (member of the scientific committee, editor of abstract book), Kemometria'99 (Szeged), Kemometria'01 (Pécs), Kemometria'02 (Tata), ACE&CC 2003 (Budapest, chair) CC 2005 (Hajdúszoboszló, chair), CC 2007 (Budapest, chair) CC 2009 (Siófok, Chair), CC 2011 (Sümege, chair), CAC 2012 ((Budapest, chair), CC 2013 (Sopron, chair), CC 2015 (Budapest, chair), CC2017 (Gyöngyös-Farkasmály, chair), CC2019 Karcag, chair, etc.

- *Leading of projects:*

“Searching quantitative - chromatographic retention relationships” Research Period: 1990-1994, Hungarian Science Foundation: OTKA No: 1782

“Application, testing and development of chemometric methods in quantitative structure - activity and in quantitative structure – retention relationships”, Research Period: 1995 –1997, prolonged till November 30, 1998, Hungarian Science Foundation: OTKA No: T016231

“Elaboration and further development of new variable selection methods for environmental sciences” Research Period: 1999–2000, Academic Research Projects: AKP No: 98-51 2,4.

“Testing and development of new chemometric methods”. Research Period: 1999 –2001, Hungarian Science Foundation: OTKA No: T029748

“Searching Quantitative Structure Activity Relationships with application of new chemometric methods” Hungarian Science Foundation: OTKA No: T037684 (2002-2005)

“Re-evaluation of fingerprints (drug design, chromatographic, foodomics, forensic): model building, method development and validation of predictive models OTKA No: K119269 (2016-2020)

“Novel fusion strategies for similarity and dissimilarity indices” KH-17, No 125608, National Science Development and Innovation Office.

- *Ph.D. Students:*

Rácz, Anita	2017 ÉDI-BCE & MTA TTK
Sági-Kiss Virág	2012 ÉDI-BCE

Farkas Orsolya	2008	OGDI
Forlay-Frick Péter	2004	OGDI
Vanyúr Rozália	2004	OGDI

### Memberships:

Head of the Chemometric and Chemoinformatic Working Group of the Hungarian Academy of Sciences

Association of Hungarian Chemists, head of the Chemometric Section (Analytical Branch) till 2018.

QSAR and Modeling Society (International),

American Association for the Advancement of Science (2000)

### 100 000 top scientists in the world (~130-150 Hungarian)

Available via: <https://doi.org/10.1371/journal.pbio.3000384>

the excel table (whole career data) is downloadable from::

<http://dx.doi.org/10.17632/btchxktzyw.1#file-ad4249ac-f76f-4653-9e42-2dfebe5d9b01>

and up-to-date data for 2017:

<http://dx.doi.org/10.17632/btchxktzyw.1#file-b9b8c85e-6914-4b1d-815e-55daefb64f5>

### Scientific interests:

- Liquid phase oxidation, radical processes, inhibition, modeling, computer simulations.
- Determination of rate constants by fast-flow technique LMR detection and by kinetic ESR spectroscopy.
- Linear free energy relationships in radical reactions
- Quantitative - structure activity (property) relationships. QSAR (QSPR).
- Quantitative - structure (gas-chromatographic) retention relationships: QSRR.
- Chemometrics: Multivariate techniques, principal component analysis, stepwise linear regression, error analyses, non-linear fits, partial least squares, variable selection, searching correlations, model building, validation, evaluation of large data sets, classification of food products, clustering, pattern recognition, ranking, method comparison, model validation, *etc.*

Scientific results were presented in >**180** papers and more than **300** lectures or posters. The papers were cited above **4300** times (without self - citations and cross - references).

	Web of Sci	Scopus	Google Scholar	Research Gate	Mendeley/ Elsevier Dashboard
No of publications	166	157	222	166	150
All citations	4752	4975	6249	4720	4976
Without self - citations	4301	4230	-	Reads: 20090	Views: 99 649
Hirsch index	36	37	40	35 2692*	37
i10-index	88	91	101	-	-

\*Research Interest, the RG score is 41.72 – higher than 97.5% of ResearchGate members

A temporarily updated list of publications, lectures and citations can be found at: <http://aki.ttk.mta.hu/scientist/heberger/>

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Web of Science Researcher ID: A-4195-2011

Scopus Author ID: 7003466436

Google scholar:

<https://scholar.google.com/citations?hl=en&user=nWaAOrsAAAAJ>

Budapest, Jan. 08 / 2019,

Károly Héberger