

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, “*summa cum laude*”
Topic: Thermal Decomposition of α -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).
- *Professor Emeritus* (Aug. 16. 2023)

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

Paper-reviews for:

Acta Alimentaria (22), AI (1), Acta Silvatica et Lignaria Hungarica (1), Acta Chimica Slovenica (1), Advances in Meteorology (1), Algorithms (2), American Journal of Biochemistry and Biotechnology (2), Analytical & Bioanalytical Chemistry (38), Analytica Chimica Acta (60), Analyst (1), Analytical Chemistry (13), Analytical Letters (13), Analytical Methods (16), Annals of Medicine (1), Applied Sciences (11), Arabian Journal of Chemistry (1), Arabian Journal of Scientific Engineering (1), Arabian Journal for Science and Engineering (1), Artificial Intelligence Chemistry (3), Beverages (5), Bioengineering (1), Biomedical Chromatography (2), Biomedical and Environmental Sciences (1), Bioorganic Chemistry (1), Bioorganic & Medicinal Chemistry (3), Bioorganic & Medicinal Chemistry Letters (3), Biotechnology Progress (2), BMC Chemistry (13), Bulletin of the Chemical Society of Ethiopia (3), Chemical Industry and Chemical Engineering Quarterly (3), Chemical Engineering Science (1), Chemical Papers (3), Chemical Research in Toxicology (2), Chemical Reviews (1), Chemistry Central Journal (10), Chemistry Central Journal - Heritage Science (5), Chemometrics and Intelligent Laboratory Systems (72), Chemosphere (4), Chiang Mai University Journal of Natural Sciences (1), Chromatographia (41), Chromatography Research International (2), Coatings (1), Communications in Statistics - Simulation and Computation (1), Comprehensive Reviews in Food Science and Food Safety (1), Computational Biology and Chemistry (1), Computer Methods and Programs in Biomedicine (2), Computational and Structural Biotechnology Journal (3), Computational and Theoretical Chemistry (2), Computational Concepts in Magnetic Resonance Part A (1), Croatica Chemica Acta (12), Current Computer Aided Drug Design (10), Current Research in Food Science (1), Ecotoxicology and Environmental Safety (10), Electronics (2), Entomological Research (1), Entropy (1), Environmental Engineering and

Management Journal (3), Evidence-Based Complementary and Alternative Medicine (1), Expert systems (2), Food Analytical methods (5), Food and Chemical Toxicology (4), Food Chemistry (74), Food Chemistry: X (1), Food Chemistry Advances (1), Food Control (8), Food Research International (1), Foods (2), Food Science and Technology International (2), Fresenius Environmental Bulletin (2), Fuel (2), Geophysics Research Letters (2), Heritage Science (8), IEEE Access (7), IEEE Transactions on Systems Man and Cybernetics: Systems (4), Information Fusion (5), Interdisciplinary Sciences: Computational Life Sciences (3), Industrial Crops and Products (1), International Conference on Biological Information and Biomedical Engineering, Information Sciences (1), BIBE 2018 (1), International Journal of Analytical Chemistry (2), International Journal of Chemical Kinetics (2), International Journal of Environmental Analytical Chemistry (4), International Journal of Gastronomy and food Science (1), International Journal of Industrial Chemistry (1), International Journal of Information Technology and Decision Making (1) International Journal of Molecular Sciences (5), International Journal of Quantitative Structure-Property Relationships (3), International Journal of Quantum Chemistry (5), Internet Electronic Journal of Molecular Design and Internet Electronic Journal of Theoretical Chemistry (1), Heliyon (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] (7), Journal of AOAC International (1), Journal of Applied Statistics (4), Journal of Chemical Information and [Computer Sciences] Modeling (22), Journal of Chemical and Engineering Data (2), Journal of Chemical Sciences (1), Journal of Cheminformatics (8), Journal of Chemometrics (55), Journal of Chromatographic Science (84), Journal of Chromatography A (>194), Journal of Chromatography B (22), 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 Experimental & Theoretical Artificial Intelligence (1), Journal of Food Biochemistry (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 (5), Journal of Liquid Chromatography and Related Technologies (1), Journal of Molecular Structure (26), Journal of Nanomaterials (1), Journal of Pharmaceutical Analysis (1), Journal of Pharmaceutical and Biomedical Analysis (29), Journal of Pharmaceutical Innovation (1), Journal of Pharmacy and Pharmacology (1), Journal of Physical Organic Chemistry (6), Journal of Planar Chromatography – Modern TLC (2), Journal of Radioanalytical and Nuclear chemistry (1), Journal of Separation Science (19), Journal of the Iranian Chemical Society (5), Journal of the Serbian Chemical Society (2), 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 (7), Materials Science and Engineering B (2), Measurement (32), Medicinal Chemistry (1), Metabolites (2), Metabolomics (1), Microchemical Journal (2), Mini Reviews in Medicinal Chemistry (1), ACH Models in Chemistry (4), Molecular Biosystems (1), Molecular Diversity (14), Molecular Informatics (6), Molecular Pharmaceutics (2), Molecules (7), Multimodal Technologies and Interactions (1), Nitric Oxide (1), Nitrogen (2), Nuclear Science and Techniques (1), Nutrition and Dietary Supplements (1), Organic Chemistry (1), Pattern Recognition Letters (1), Periodica Polytechnica (2), Pharmaceutics (3), Political Analysis (2), Polymer Bulletin (8), Polymer Testing (1), Processes (2), Qeios Open review (2), 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 (11), Scientific Reports (1), Scientometrics (2), Sensors (14), Sensors & Actuators B: Chemical (14), Separations (3), Separation Science and Technology (1), SN Applied Sciences (1), Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy (4), Spectroscopy Letters (6), Statistics and Operation Research Transactions (1), Structural Chemistry (1), Symmetry (2), Talanta (33), 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; Czech Science Foundation, GACR (2)

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, between 2011-2021); Journal of Chemical Reactions and Catalysis Research (JCRC since 2021); 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); Acta Alimentaria (Akadémiai Kiadó, since July 2021).

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 (4th 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 (5th 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, issue 4 (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.

☒ Officer's Cross of the Hungarian Order of Merit March 15 / 2023.

Other experiences:

- *Teaching:* 5 semesters (terms) at Physikalischem-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, CC 2023 Sopron (honorary 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 National Science Development and Innovation Office, OTKA No: K119269 (2016-2020)

“Novel fusion strategies for similarity and dissimilarity indices” National Science Development and Innovation Office KH-17, OTKA KH-125608.

“Development of soft sensor models based on in vitro experiments and creation of related metrics” National Science Development and Innovation Office, OTKA No: K134260 (2020-2024).

- *Ph.D. Students:*

Rác, 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 till 2023

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

QSAR and Modeling Society (International, 1998-2007)

American Association for the Advancement of Science (2000-2008)

100 000 top scientists in the world (~300 Hungarian)

the excel table (whole career and single year data) is downloadable from:
<https://dx.doi.org/10.17632/btchxktzyw>
for 2019, 2020, 2021, 2022.

Scientific interests:

- Liquid phase oxidation, radical processes, inhibition, modeling, computer simulations, antioxidants.
- 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,
- **Method comparison:** Pattern recognition, clustering, ranking, evaluation of large data sets, classification of food products, model validation, *etc.*
- **Ranking,** multicriteria decision making (MCDM), machine learning, sum of ranking differences, molecular similarity/diversity.

Scientific results were presented in >**200** papers and more than **300** lectures or posters. The papers were cited around or above **8000** times (without self-citations and cross - references).

	Web of Sci	Scopus	Google Scholar	Research Gate
No of publications	201	181	241	195
All citations	7983	7893	10664	8606
Without self - citations	7324	6861	-	Reads: 58795
Hirsch index	43	44	49	44 4547*
i10-index	125	124	143	-

*Research Interest score is higher than 98% of ResearchGate members. and 99% of researchers with work related to chemo-informatics.

Orcid ID: 0000-0003-0965-939X

Web of Science Researcher ID: A-4195-2011

Scopus Author ID: 7003466436

Google scholar:

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

Budapest, July 18 / 2024,

Károly Héberger