# Tamás Milán Nagy

Date of birth: 26/03/1993 | **Nationality:** Hungarian | **Gender:** Male |

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Egyetem tér 1., Debrecen, Hungary

About me: predoctoral fellow in the MTA-DE Molecular Interaction and Recognition Group, Chemistry Institute, University of Debrecen.

## WORK EXPERIENCE

29/08/2017 – 31/07/2022 – Debrecen, Hungary

**PHD IN CHEMISTRY –** UNIVERSITY OF DEBRECEN, MTA-DE MOLECULAR INTERACTION AND RECOGNITION GROUP

Structure, dynamics and interactions of peptides and proteins with NMR spectroscopy and molecular dynamics (MD).
PI: Prof. Katalin E. Kövér.

11/11/2021 – 11/02/2022 – Boulder, CO, United States

**VISITING SCHOLAR (CAMPUS MUNDI GRANT) –** UNIVERSITY OF COLORADO BOULDER, HEINZ LAB

Development of a zirconia INTERFACE force field to study the interactions between biomolecules and a nanovaccine platform.
PI: Prof. Hendrik Heinz.

## EDUCATION AND TRAINING

30/08/2012 – 29/06/2017 – Debrecen, Hungary

**BSC AND MSC IN CHEMISTRY –** University of Debrecen

Majoring in radiochemistry.
Final grade: with honour.

31/08/2017 – 31/07/2022 – Debrecen, Hungary

**PHD IN CHEMISTRY –** University of Debrecen

Richter Talentum Doctoral Grant.

## LANGUAGE SKILLS

Mother tongue(s): **HUNGARIAN**

Other language(s):

**ENGLISH (PROFICIENCY LEVEL)** | **GERMAN (INTERMEDIATE LEVEL)**

## DIGITAL SKILLS

linux | python | high-performance computing | shell scripting

## PUBLICATIONS

### List of Publications (Google Scholar)

https://bit.ly/3gGr1aK

**Distinguished publications:**

The First Dimeric Derivatives of the Glycopeptide Antibiotic Teicoplanin
Bereczki, Ilona, Zsolt Szűcs, Gyula Batta, Tamás M. Nagy, Eszter Ostorházi, Katalin E. Kövér, Anikó Borbás,Pál Herczegh
*Pharmaceuticals*. 15(1), 77, (2022).

NORD: NO Relaxation Delay NMR spectroscopy
Tamás Milán Nagy, Katalin E. Kövér, Ole W. Soerensen
Angew. Chem.Int. Ed. 60(24), 13699-13702 (2021).

Double and adiabatic BANGO for concatenating two NMR experiments relying on the same pool of magnetization
Tamás Milán Nagy, Katalin E. Kövér, Ole W. Soerensen
J. Magn. Res. 316, 106767 (2020)

BANGO SEA XLOC/HMBC–H2OBC: complete heteronuclear correlation within minutes from one NMR pulse sequence
Tamás Milán Nagy, Tamás Gyöngyösi, Katalin E. Kövér, Ole W. Soerensen
Chem. Comm 55 (81), 12208-12211 (2019).

Distinguishing between two- and three-bond correlations for all 13C multiplicities in heteronuclear NMR spectroscopy
Tamás Gyöngyösi, Tamás Milán Nagy, Katalin E. Kövér, Ole W. Soerensen
Chem. Comm. 54:(70), 9781-9784. (2018).

Photochemical and Structural Studies on Cyclic Peptide Models
Tamás Milán Nagy, Krisztina Knapp, Eszter Illyés, István Timári, Gitta Schlosser, Gabriella Csík, Attila Borics, Zsuzsa Majer, Katalin E. Kövér
Molecules 23:(9) Paper 2196. 20 p. (2018).

## CONFERENCES AND SEMINARS

2016 – 2020 – Balatonszemes, Hungary.
**Hungarian NMR working committee**

Talks on a yearly basis. Main topics: *Structural analysis of small cyclic peptides using NMR and computational techniques. The fuzziness of MEF2D β-domain and its role in biological activity: NMR and in-silico studies.*

2016 – Niederöblarn, Austria
**NMR Summer School**

Attendant. Organized by the University of Graz.

2017 – Budapest, Hungary.
**Magnetic Moments in Central Europe**

First poster presentation: *Double perfect-echo INEPT based HSQMBC experiment: more efficient detection of heteronuclear multiple bond correlations and measurement of coupling constants.*

2018 – edX e-learning
**Introduction to Computer Science and Programming Using Python**

Completed and received a passing grade in the online course provided by MITx, Massachusetts Institute of Technology.
https://courses.edx.org/certificates/84e536a8e7c84b5d87311b9a6955c20a

2018 – Orlando FL, USA
**59th Experimental Nuclear Magnetic Resonance Conference (ENC, 2018)**

Poster presentation: *Boosting the NMR assignment of small to medium-sized molecules with different edited variants of HSQC-CLIP-COSY experiment.*

2018 – Nantes, France
**European Magnetic Resonance Meeting (EUROMAR, 2018)**

Poster presentation: *Dynamical studies of the Mef2D β-domain by NMR and computational methods.*

2018 – Budapest, Hungary
**9th Chemistry towards Biology Conference (CTB9)**

Talk: *Determining fuzziness of the Mef2D β-domain by NMR-experiments and MD-calculations.*

2019 – Helsinki, Finland
**Spring School in Computational Chemistry**

Attendant. Organized by CSC-IT Center for Science, PRACE.

2019 – Berlin, Germany
**European Magnetic Resonance Meeting (EUROMAR, ISMAR, 2019)**

Poster presentation: *The fuzzy β-domain of MEF2D: NMR and computational studies.*

2019 – Prague, Czech Republic
**Instruct-ERIC workshop on computational approaches in integration of structural biology techniques**

Attendant.

2020 – Online meeting
**European Magnetic Resonance Meeting (EUROMAR online, 2020)**

Presentation: *The fuzzy β-domain of MEF2D: altering function via dynamics.*

## PROJECTS

2013 – 2016
**Photochemical and structural studies on cyclic peptide models**

https://www.researchgate.net/project/Photochemical-and-Structural-Studies-on-Cyclic-Peptide-Models

2015 – CURRENT
**Dynamical studies on the intrinsically disordered β-domain of MEF2D**

- dynamical characterization of various disordered peptide constructs

- NMR $^{15}$N-relaxation measurements: T1,T2,hetNOE, reduced spectral density function calculation
- predicting dynamics and disorder based on chemical shifts
- diffusion NMR (DOSY)

- *in silico* investigations: molecular dynamics (MD)
- order parameters, radius of gyration, secondary structure content
- contact map, cluster analysis
- distance analysis (interactions)

2016 – CURRENT
**Participation in the development of novel NMR supersequences**

- seperate echo-antiecho (SEA-XLOC) for distingushing between two and three bond heteronuclear couplings
- NOAH-type experiments introducing the BANGO selective excitation module
- No Relaxation Delay (NORD) spectroscopy

2013 – CURRENT
**Minor projects**

- saturation difference spectroscopy (STD) measurements on the interaction between TRPM8 receptor and an antibiotic (in vivo NMR)
- studying the oligomerization processes of disordered peptide models with NMR and computation
- STD experiments on μ-opioid receptors (in vivo NMR)
- qualitative (qNMR) measurements of mycotoxines
- zirconia INTERFACE moelcular mechanics force field parametrization
- MD simulations of the interactions between biomolecules and a nanovaccine platform

## HONOURS AND AWARDS

09/2016
**Scholarship of The Republic of Hungary – The Republic of Hungary**

09/2017
**Richter Talentum Doctoral Grant – Gedeon Richter Plc.**

2017- present

10/2017
**Theses Award – Hungarian Chemical Society**

03/2019
**Campus Mundi short study – Tempus Public Foundation**

Spring School in Computational Chemistry (Helsinki, Finland)

09/2019
**ÚNKP-2019 New National Excellence Program – Hungarian Ministry of Human Capacities**

NMR and computational studies on peptides and peptide-protein interactions.

09/2020
**ÚNKP-2020 New National Excellence Program – Hungarian Ministry of Human Capacities**

What is the role of aggregation in the biological activity of intrinsically disordered proteins?
NMR methodology and computational chemistry studies.

2021
**Campus Mundi Internship – Tempus Public Foundation**

Internship in the Heinz Laboratory, Boulder, CO, USA.

## TEACHING EXPERIENCE

2015 – 2021
**University of Debrecen**

- NMR Operator Training
- Quantitative Analytical Chemistry Practice
- General Chemistry Practice

## RELATED SKILLS

2015 – CURRENT
**Molecular Dynamics (MD) simulations**

Molecular simulations of proteins with AMBER and GROMACS engines:

- building solution state systems
- energy optimization
- equilibration
- production runs with classical and scaled MD protocols
- trajectory analysis
- data visualization
- high-performance computing
- parametrizing new compounds in INTERFACE FF

2015 – CURRENT
**NMR-spectroscopy**

NMR-spectroscopy of proteins:

- sample preparation
- 1D and 2D homo- and heteronuclear experiments
- e.g. COSY, TOCSY, HSQC, NOESY, T1,T2 relaxation, hetNOE, STD, DOSY
- spectral data evaluation
- homo- and heteronuclear resonance assignment
- protein 3D structure calculation based on NMR data
- data visualization.

## HOBBIES AND INTERESTS

### Sports

Athletics, hiking, tennis, basketball.

### Music

Member of a music group (piano) and choirs in Debrecen, Hungary.

## PROJECTS ON GITHUB

2017 – 2021
**Collection of my simple but useful shell and python scripts created during my graduate student years.**

https://github.com/ocel0t/abyss0fPhD