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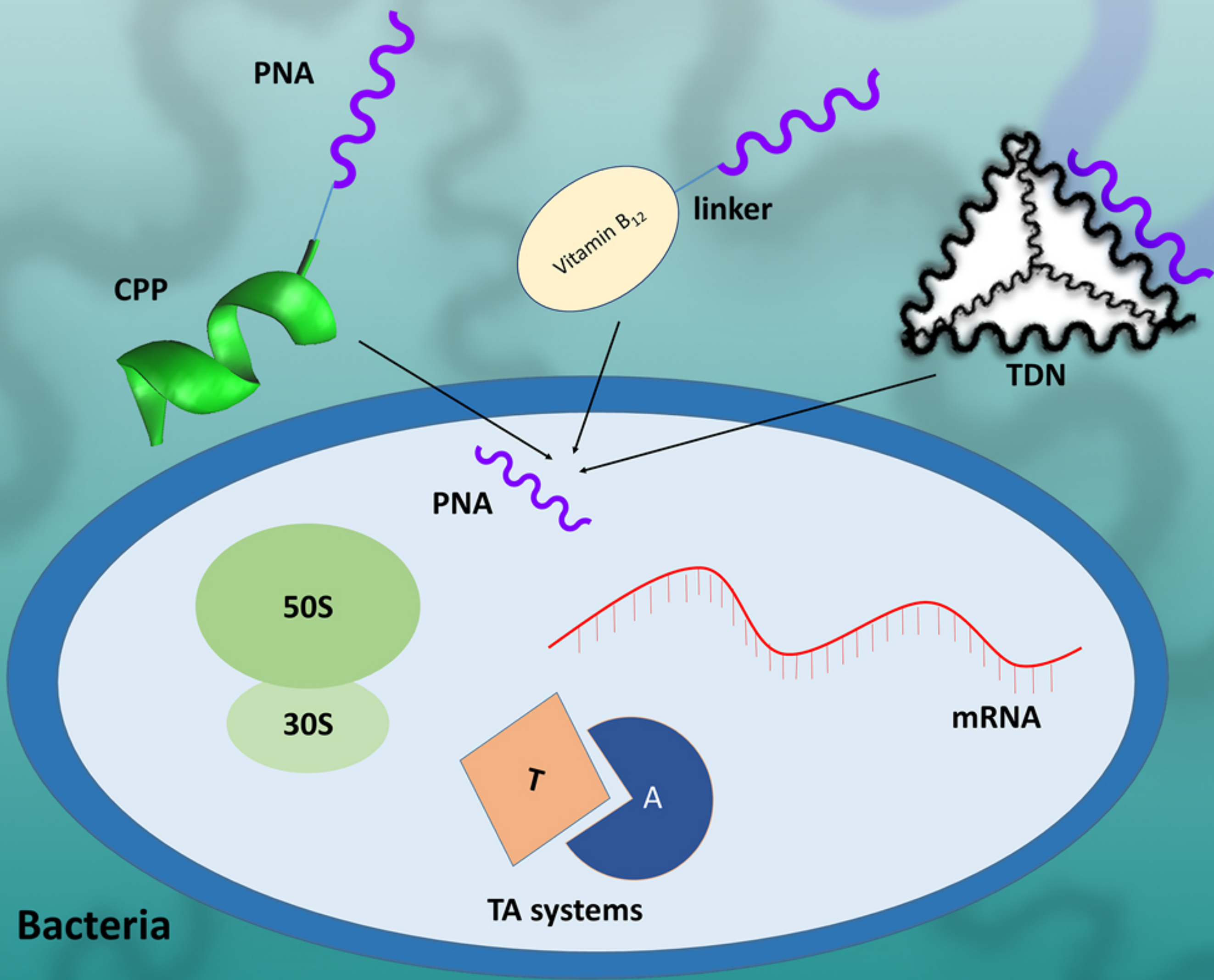

Antibacterial Peptide Nucleic Acids—Facts and Perspectives

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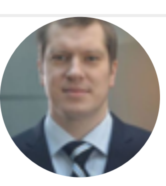
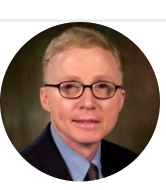
Senior Director, Technology Strategy, Amyris, Inc., 5885 Hollis St, Suite 100, Emeryville, CA 94608, USA
Interests: organic synthesis; medicinal chemistry; biotechnology



Prof. Dr. Michal Szostak *
Website (https://sasn.rutgers.edu/about-us/faculty-staff/michal-szostak)
Section Editor-in-Chief
Department of Chemistry, Rutgers University, 73 Warren St, Newark, NJ 07102, USA
Interests: amide bonds; N-heterocyclic carbenes; C-N activation; C-H activation; C-O activation; lanthanides; cross-coupling; catalysis; reductions; reductive couplings; radical chemistry; synthetic methodology; natural products
* Organometallic Chemistry
Special Issues and Collections in MDPI journals



Prof. Dr. Rudy J. Richardson *
Website (https://sph.umich.edu/faculty-profiles/richardson-rudy.html)
Section Editor-in-Chief
University of Michigan, Ann Arbor, Department of Environmental Health Sciences, Ann Arbor, United States
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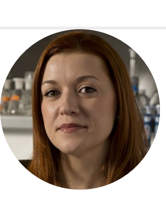
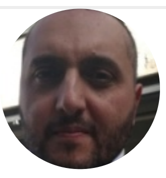
* Molecular Structure
Special Issues and Collections in MDPI journals



Prof. Dr. Mara Guadalupe Freire Martins
Website (http://www.ciceco.ua.pt/MaraFreire)

Section Editor-in-Chief
Department of Chemistry, University of Aviero, Potugal
Interests: green chemistry; separation processes; biopharmaceuticals; ionic liquids; deep eutectic solvents
Special Issues and Collections in MDPI journals



Prof. Dr. Giuseppe Cirillo
Website (https://www.unical.it/portale/strutture/dipartimenti_240/dfssn/areastudenti/avvisi_docenti/cirillo/)
Section Editor-in-Chief
Department of Pharmacy, Health and Nutritional Sciences, University of Calabria, Rende (CS), Italy
Interests: nanoparticles; carbon nanomaterials; hybrid materials; hydrogels; polymer therapeutics; self-assembling materials; stimuli-responsive drug delivery systems; cancer; infectious diseases
Special Issues and Collections in MDPI journals

Prof. Dr. Anan Yaghmur *
Website (https://research.ku.dk/search/?pure=en%2Fpersons%2Fanan-yaghmur(a910866e-d3b9-4a69-b238-005ea9906b8f)%2Fcv.html)
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Section Editor-in-Chief
Kobenhavns Universitet, Department of Pharmacy, Copenhagen, Denmark
Interests: biophysical characterization of nano-self-assemblies, cubosomes, hexosomes; nanodispersions of inverse non-lamellar liquid crystalline phases; drug and functional food soft self-assembled nanocarriers; lyotropic liquid crystalline phases; microemulsions
* Physical Chemistry
Special Issues and Collections in MDPI journals

Prof. Dr. Vadim A. Soloshonok *
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Section Editor-in-Chief
Previous research and teaching experience in Ukraine, Poland, Italy, Japan and USA. Ikerbasque Research Professor at the Department of Organic Chemistry I, University of the Basque Country, UPV/EHU in San Sebastian.
Interests: Organic Chemistry
* Organic Chemistry
Special Issues and Collections in MDPI journals

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Australian Centre of Research on Separation Science, School of Physical Science, University of Tasmania, Hobart, Tasmania, Australia
Interests: capillary electrophoresis; liquid chromatography; mass spectrometry; sample concentration; green sample preparation
* Analytical Chemistry
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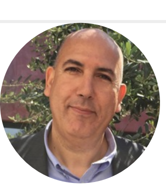

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Green Extraction Team, Avignon University, INRAE, Avignon Cedex 84029, France
Interests: green extraction; alternative solvents; innovative technologies; original procedures; microwave; ultrasound; intensification.
* Green Chemistry
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GlcNAcylation
* Chemical Biology
Special Issues and Collections in MDPI journals

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Interests: drug discovery, glycobiology, chemoenzymatic transformations, chemical virology, infectious diseases, cancer
* Bioorganic Chemistry
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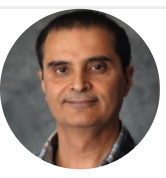

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Interests: nanostructures; soft nanoparticles; macromolecules; dendrimers; miktoarm polymers; telodendrimers, naked nanocarriers; metal nanoparticles; gold nanoshells; iron oxide nanoparticles; nanomedicine; drug delivery; diagnostics
* Nanochemistry
Special Issues and Collections in MDPI journals

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Section Editor-in-Chief
Department of Chemistry and Biochemistry, University of Windsor, Windsor, Ontario N9B 3P4, Canada
Interests: computational chemistry; quantum mechanics/molecular mechanics; molecular dynamics; docking; catalysis; enzymology; thermochemistry; reaction mechanisms; sulfur biochemistry
* Theoretical Chemistry
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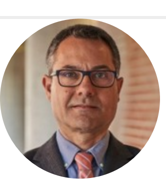

Prof. Dr. Diego Muñoz-Torrero *
Website (http://www.ub.edu/farmaco/ca/farmaceutica/recerca/multitarget_antialzheimer_and_chemotherapeutic_compounds/3/)
Section Editor-in-Chief
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Interests: multitarget anti-Alzheimer agents; hybrid compounds; cholinesterase inhibitors; amyloid anti-aggregating compounds; BACE-1 inhibitors; antiprotozoan compounds
* Medicinal Chemistry
Special Issues and Collections in MDPI journals

Prof. Dr. Roman Dembinski *
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Interests: organic, organometallic, and medicinal chemistry; organic synthesis; nucleosides; heterocycles; alkynes; fluorine and fluorous; cycloisomerizations; cyclizations
* Organic Chemistry
Special Issues and Collections in MDPI journals

Prof. Dr. Thomas J. Schmidt *
Website (http://www.uni-muenster.de/Chemie.pb/en/forschung/schmidt/index.html)

Interests: heterocyclic synthesis; strained rings; azirine; aziridine; azoles; N-ylides; carbenes; diazo compounds

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Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 82234 Weßling, Germany

Interests: classical strongly coupled systems; plasmas and complex plasmas; soft condensed matter; phase transitions; thermodynamics and transport properties of fluids

Special Issues and Collections in MDPI journals:

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RIKEN Center for Biosystems Dynamics Research (BDR) 1-7-22 Suehiro-cho, Tsurumi-ku, Yokohama 230-0045, JAPAN

Interests: structural biology; NMR; protein; structure; dynamics; protein in living cells; protein synthesis; cell-free protein synthesis; stable-isotope labeling; enzymes

Dr. Isao Kii

Website (https://www.riken.jp/en/research/labs/rch/integr/common_fac/)

Common Facilities Unit, Integrated Research Group, Compass to Healthy Life Research Complex Program, RIKEN Cluster for Science and Technology Hub, Kobe, Japan

Interests: kinase, protein folding; folding intermediate; activation mechanism; autophosphorylation; chaperone; structural analysis; protein quality control; ubiquitin proteasome pathway; Small molecule inhibitor; neurogenesis; intellectual disability; down syndrome; autism spectrum disorders; click reaction; protein modification; immuno-PET imaging

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Prof. Dr. Anake Kijjoa

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Departamento de Química, Instituto de Ciências Biomédicas de Abel Salazar and CIIMAR, Universidade do Porto, Rua Jorge de Viterbo Ferreira, nº228, 4050-313 Porto, Portugal

Interests: antibacterial compounds from higher plants； marine invertebrates；soil and marine-derived fungi； cosmetic ingredients from marine resources； natural biopesticides

Special Issues and Collections in MDPI journals:

Special Issue in ***Molecules*: Selected Papers from the 6th International Conference on Natural Products for Health and Beauty (NATPRO 6) (/journal/molecules/special_issues/NATPRO_6)**

Special Issue in ***Marine Drugs*: Marine Products for Health and Beauty (/journal/marinedrugs/special_issues/health_beauty)**

Special Issue in ***Molecules*: Selected Papers from the Joint Symposia of MESMAP-5 & ISPBS-5 (/journal/molecules/special_issues/MESMAP-5_ISPBS-5)**

Special Issue in ***Molecules*: Selected Papers from the 6th International Mediterranean Symposium on Medicinal and Aromatic Plants (MESMAP-6) (/journal/molecules/special_issues/MESMAP-6)**

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Website (http://web.skku.edu/~polyphysics/01/)

School of Chemical Engineering, Sungkyunkwan University, Suwon, Gyeonggi 16419, Korea

Interests: polymer electrolyte; membrane; battery; fuel cell; electrolysis, ion transfer

Special Issues and Collections in MDPI journals:

Special Issue in ***Membranes*: Polymer Electrolyte Membranes (/journal/membranes/special_issues/polymer_electrolyte_membranes)**

Prof. Dr. Cheal Kim

Website (https://blog.naver.com/only4u870)

Development of chemical sensors; reactivity study of the transition metal complexes; DNA cleavage by their metal complexes; MOF

Interests: Development of chemical sensors, reactivity study of the transition metal complexes, DNA cleavage by their metal complexes, and MOF

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Interests: electrochemical energy storage and conversion system; energy nanomaterials, nanocarbons and carbon fibers; functional nanofibers; supercapacitors; electrocatalysts, metal nanoparticles; biosensors; fuel cells; layer-by-layer self-assembled thin films and capsules; nanostructured molecular nanocomposites; hydrogels; and hybrid POSS materials

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Department Chemistry and Physics, McNeese State University, Lake Charles, LA, USA
Interests: Nanocatalysis; Hydrogen Storage; Cluster-assembled materials; Quantum Dots; Aluminum Hydrides; Nanocatalysis with special emphasis on gold and gold-metal alloy nanoparticles; Green Chemistry; Structure and reactivity of clusters and cluster-assembled-materials

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UNC Eshelman School of Pharmacy, Division of Chemical Biology and Medicinal Chemistry, Center for Integrative Chemical Biology and Drug Discovery, University of North Carolina at Chapel Hill, Chapel Hill 27599, NC, USA
Interests: computational biophysics; computer-aided drug design; molecular simulations; chromatin structure and dynamics; histone code; virtual screening; machine learning

Assoc. Prof. Dr. Evgueni Kirillov
[**Website (https://iscr.univ-rennes1.fr/evgueni-kirillov)**](https://iscr.univ-rennes1.fr/evgueni-kirillov)
Catalysis & Organometallics - UMR 6226, Center of Catalysis and Green Chemistry, Institut des Sciences Chimiques de Rennes, University of Rennes 1, Rennes, France
Interests: Organometallic and coordination chemistry; "oscillating" and polynuclear polymerization catalysis; mechanistic studies and stereochemistry of polymerization; prediction of chemical reactivity using QM methods; activation of CO2 via coupling with unsaturated substrates; C-H and C-O bond activation reactions with rare-earths

Prof. Masato Kitamura
[**Website (http://www.ps.nagoya-u.ac.jp/teaching_staff/kitamura/)**](http://www.ps.nagoya-u.ac.jp/teaching_staff/kitamura/)
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Interests: molecular catalyst; reaction mechanism, environmentally friendly organic synthesis; total synthesis

Prof. Dr. Arjan W. Kleij
[**Website (http://www.iciq.org/research/research_group/prof-arjan-w-kleij/)**](http://www.iciq.org/research/research_group/prof-arjan-w-kleij/)
Institute of Chemical Research of Catalonia (ICIQ), The Barcelona Institute of Science and Technology, Tarragona, Spain
Interests: biopolymers; CO_2 conversion; renewable compounds; sustainable catalysis

Prof. Dr. Axel Klein
[**Website (http://www.klein.uni-koeln.de/)**](http://www.klein.uni-koeln.de/)
Department für Chemie, Institut für Anorganische Chemie, Universität zu Köln, Greinstraße 6, 50939 Köln, Germany
Interests: transition metal complexes (including organometallic); platinum, palladium, nickel; synthesis; electrochemistry; photophysics; spectroscopy; modelling of catalytic processes
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Prof. Dr. Frank Ko
[Website (http://mtrl.ubc.ca/faculty/frank-ko/)]
Department of Materials Engineering, University of British Columbia, Vancouver, BC V6T 1Z4, Canada
Interests: nanofibre technology; biomaterials/surgical implants; textile structural composites
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Dr. Mihkel Koel
[Website (https://www.ttu.ee/en/personnel-search/&kood=T000901)]
Department of Chemistry and Biotechnology, Tallinn University of Technology, Akadeemia tee 15, 12618 Tallinn, Estonia
Interests: analytical chemistry; chemometrics; alternative solvents

Prof. Dr. René Michael Koenigs
[Website (http://www.koenigslab.rwth-aachen.de)]
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Interests: organic synthesis; reactive intermediates; catalysis; method development; medicinal chemistry; carbene transfer reactions

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Interests: materials chemistry; inorganic chemistry; solid-state chemistry; X-ray diffraction; superconductors; material characterization; DFT calculations; crystal structure; synthesis; perovskites; oxides; fluorides; crystallography
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Prof. Dr. Chojiro Kojima
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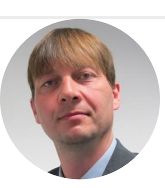
Graduate School of Engineering, Yokohama National University, Tokiwadai 79-5, Hodogaya-ku, Yokohama 240 8501, Japan
Interests: structural biology; NMR, protein; nucleic acids; structure; dynamics; interaction; drug screening
Special Issues and Collections in MDPI journals:
Special Issue in ***Molecules*: Recent Advances in Biomolecular NMR Spectroscopy (/journal/molecules/special_issues/NMR)**



Prof. Dr. Ladislav Kokoska
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Interests: biologically active natural products; phytochemistry; food and agricultural chemistry; ethnobotany and ethnopharmacology
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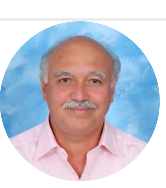

Prof. Dr. George Kokotos
[Website (http://users.uoa.gr/~gkokotos/)]
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Interests: design, synthesis and study of enzyme inhibitors; synthesis of bioactive lipids; phospholipase A2; lipases; fatty acids; lipidomics; therapeutic molecules
Special Issues and Collections in MDPI journals:
Special Issue in ***Biomolecules*: Bioactive Lipids in Inflammation, Diabetes and Cancer (/journal/biomolecules/special_issues/Bioactive_Lipids_Inflammation)**

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Prof. Dr. Marek M. Kowalczuk
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2. School of Biology, Chemistry and Forensic Science, Faculty of Science and Engineering, University of Wolverhampton, Wolverhampton, UK
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Special Issues and Collections in MDPI journals:
Special Issue in ***Materials*: Biodegradable and Bio-Based Polymers (/journal/materials/special_issues/Biodegradable_Bio-Based_Polymers)**
Special Issue in ***Molecules*: Advances in Biodegradable Polymers (/journal/molecules/special_issues/Biodegradable_Polymers)**
Special Issue in ***Polymers*: Intrinsically Biocompatible Polymer Systems (/journal/polymers/special_issues/biocompatible_polymers)**
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Special Issues and Collections in MDPI journals:
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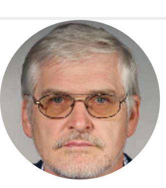
Institute of Chemistry, Saint Petersburg State University, Russian Federation
Interests: new heterocyclic compounds; scaffold-oriented synthesis; multi-component reactions



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Interests: electrical; thermal and magnetic properties of new materials; magnetic systems with unusual ground stats properties; low-dimensional and frustrated quantum antiferromagnets; multiferroics; new superconductors
Special Issues and Collections in MDPI journals:
Special Issue in ***Molecules*: Inorganic Materials Chemistry (/journal/molecules/special_issues/molecules_InorganicMaterialsChemistry)**

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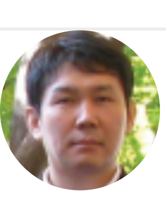
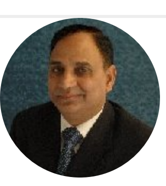
Stony Brook University, Stony Brook, United States
Interests: Nanobiotechnology; Plasma-material interface; Transition dynamics in molecules



Prof. Dr. Takaaki Kubota
Website (https://www.shoyaku.ac.jp/en/laboratory/natural_products_chemistry/)
Showa Pharmaceutical University, 3-3165 Higashi-Tamagawagakuen, Machida, Tokyo 194-8543, Japan
Interests: natural products; isolation; structure elucidation; bioactivity; biosynthesis

Prof. Dr. Kamil Kuca
Website (http://eng.fnhk.cz/cbv/our-team/kuca-kamil)
University of Hradec Kralove, Hradec Kralove, Czech Republic
Interests: Antidotes for pesticide and nerve agent poisonings; Alzheimer’s disease treatment; Detergents as disinfectants, nanoparticles; decontamination means; Toxins; Drug design and development; Nanotechnology; IT, parallel computing, ANN; Project management; Scientific management; Technology Transfer; Health economics and Pharmacoeconomics
Special Issues and Collections in MDPI journals:
Special Issue in ***International Journal of Molecular Sciences*****: Biochemistry, Molecular Biology and Toxicology of Natural and Synthetic Toxins (/journal/ijms/special_issues/natural-synthetic_toxins)**
Special Issue in ***International Journal of Molecular Sciences*****: Development of Novel Drugs for Alzheimer's Disease and Myasthenia Gravis (/journal/ijms/special_issues/AD_MG)**
Special Issue in ***Economies*****: Innovation and Socioeconomic Development (/journal/economies/special_issues/Innovation_socioeconomic_development)**
Special Issue in ***Biomolecules*****: Advances in Cholinesterases (/journal/biomolecules/special_issues/Advances_in_Cholinesterases)**
Special Issue in ***Molecules*****: Development of Novel Drugs for Alzheimer´s Disease (/journal/molecules/special_issues/Drugs_AD)**
Special Issue in ***Sustainability*****: Problems of Selected Industries on the Way to Suitable Development (/journal/sustainability/special_issues/selected_industries_way_to_suitable_development)**
Special Issue in ***International Journal of Molecular Sciences*****: Natural and Synthetic Toxins: Molecular Aspects and Development Treatment Strategy (/journal/ijms/special_issues/natural_synthetic_toxins)**
Special Issue in ***Toxins*****: Mycotoxins and Their Metabolites Biochemistry, Molecular Biology and Toxicology (/journal/toxins/special_issues/Mycotoxins_metabolites)**

Prof. Dr. Thomas D. Kühne
Website (https://chemie.uni-paderborn.de/arbeitskreise/theoretische-chemie/kuehne/prof-dr-thomas-d-kuehne/)
Dynamics of Condensed Matter, Chair of Theoretical Chemistry, University of Paderborn, D-33098 Paderborn, Germany
Interests: theoretical chemistry; computational physics; Car-Parrinello ab-initio molecular dynamics; dynamics of condensed matter; hydrogen bonding in aqueous systems; sustainable systems; on-water catalysis



Prof. Dr. Krishan Kumar
Website (https://www.researchgate.net/profile/Krishan_Kumar25)
Associate Professor of Radiology, The Wright Center of Innovation in Biomedical Imaging, The Ohio State University, Columbus, United States
Interests: drug discovery and development; targeted peptides and proteins for diagnosis and treatment of cancer; bioconjugation chemistry; imaging pharmaceuticals; PET probes; radiochemistry and radiolabeling of biomolecules
Special Issues and Collections in MDPI journals:
Special Issue in ***Diagnostics*****: NMR in Medicine (/journal/diagnostics/special_issues/nmr_in_medicine)**
Special Issue in ***Diagnostics*****: Radiopharmaceuticals for Cancer Diagnosis (/journal/diagnostics/special_issues/radiopharmaceuticals)**
Special Issue in ***Molecules*****: Radiolabeled Compounds for Diagnosis and Treatment of Cancer (/journal/molecules/special_issues/Radiolabeled_Compounds)**

Prof. Dr. Naresh Kumar
Website (http://www.chemistry.unsw.edu.au/research/research-groups/kumar-group)
School of Chemistry, University of New South Wales, UNSW Sydney, Australia
Interests: Biologically active molecules; Heterocyclic chemistry; Medicinal chemistry; Design and synthesis of quorum-sensing inhibitors; antimicrobial peptides and mimics; Biomimetic synthesis; Development of new synthetic methodologies; antimicrobial biomaterials
Special Issues and Collections in MDPI journals:
Special Issue in ***Antibiotics*****: Antibiotic Synthesis (/journal/antibiotics/special_issues/antibiotic_synthesis)**
Special Issue in ***Molecules*****: Design and Synthesis of Quorum-Sensing Inhibitors (/journal/molecules/special_issues/DS_QSI)**
Special Issue in ***Molecules*****: Recent Advances in Antimicrobial Biomaterials (/journal/molecules/special_issues/Antimicrobial_Biomaterials)**
Special Issue in ***Molecules*****: Modulation of Quorum Sensing in Bacteria (/journal/molecules/special_issues/QS_Bacteria)**

Prof. Dr. Jolanta Kumirska

[Website (https://ug.edu.pl/pracownik/1656/jolanta_kumirska)](https://ug.edu.pl/pracownik/1656/jolanta_kumirska)

University of Gdansk, Faculty of Chemistry, Department of Environmental Analysis, Wita Stwosza 63, 80-308 Gdansk, Poland

Interests: analytical chemistry; methods development; environmental protection; pharmaceutical analysis

Special Issues and Collections in MDPI journals:

Special Issue in ***Molecules*: Pharmaceutical Residues in the Environment (/journal/molecules/special_issues/pharmaceutical_residues_environment)**

Dr. Dmitry Kurouski

[Website (https://kurouskilab.com/research/)](https://kurouskilab.com/research/)

Department of Biochemistry and Biophysics, Texas A&M University, College Station, Texas 77843, United States

Interests: nanoscale vibrational spectroscopy; tip-enhanced Raman spectroscopy (TERS); atomic force microscope infrared spectroscopy (AFM-IR); Raman-based plant disease diagnostics; electrochemistry; plasmonics

Special Issues and Collections in MDPI journals:

Special Issue in ***Molecules*: Raman Spectroscopy: An Important Technique in Medicine, Agriculture, and Biochemistry (/journal/molecules/special_issues/raman_spectrosc)**

Prof. Dr. Tibor Kurtán

[Website (http://szerves.science.unideb.hu/english/index.php/prof-dr-tibor-kurtan/)](http://szerves.science.unideb.hu/english/index.php/prof-dr-tibor-kurtan/)

Department of Organic Chemistry, University of Debrecen, Debrecen, Hungary

Interests: stereochemistry; chiroptical spectroscopy; natural products; DFT calculation; O- and O,N-heterocycles; domino cyclization reaction; antiproliferative activity; neuroprotective activity; axial chirality; stereochemistry-activity relationship

Priv.-Doz. Dr. Souvik Kusari

[Website (http://www.ccb.tu-dortmund.de/fb03/en/Fields_of_research/AU/M-Uebersicht/M-Leitung/Kusari_Souvik)](http://www.ccb.tu-dortmund.de/fb03/en/Fields_of_research/AU/M-Uebersicht/M-Leitung/Kusari_Souvik)

[SciProfiles (https://sciprofiles.com/profile/962599)](https://sciprofiles.com/profile/962599)

Department of Chemistry and Chemical Biology, TU Dortmund University, Otto-Hahn-Str. 6, 44221 Dortmund, Germany

Interests: plant-microbe interaction; chemical ecology; endophytes; phytopathogens; microbial drug discovery; antimicrobials; metabolomics; imaging mass spectrometry; natural product chemistry

Prof. Dr. Leonid Kustov

[Website (https://www.researchgate.net/profile/Leonid_Kustov)](https://www.researchgate.net/profile/Leonid_Kustov)

1. National University of Science and Technology, Moscow 119049, Russia
2. Department of Chemistry, M. V. Lomonosov Moscow State University, Moscow 119992, Russia
3. N. D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, Moscow 119991, Russia

Interests: catalysis; nanomaterials; renewables; green chemistry

Special Issues and Collections in MDPI journals:

Special Issue in ***Crystals*: New Horizons in Zeolites and Zeolite-Like Materials (/journal/crystals/special_issues/zeolite_materials)**

Special Issue in ***Molecules*: Activation of Small Molecules: Challenges and Solutions (/journal/molecules/special_issues/Activation_small_molecules)**

Dr. Andrzej Kutner

[Website (http://analizalekow.wum.edu.pl/content/pracownicy)](http://analizalekow.wum.edu.pl/content/pracownicy)

Department of Bioanalysis and Drug Analysis, The Medical University of Warsaw, Faculty of Pharmacy, 1 Stefana Banacha, 02-097 Warsaw, Poland

Interests: medicinal chemistry; drug discovery; structure-activity relationships; design and synthesis of biologically active compounds; anticancer agents; crystal structure of biomolecules and ligand-receptor interactions, vitamin D analogs, pharmaceutical syntheses

Prof. Dr. Masayasu Kuwahara

[Website (http://kenkyu-web.cin.nihon-u.ac.jp/Profiles/149/0014837/prof_e.html)](http://kenkyu-web.cin.nihon-u.ac.jp/Profiles/149/0014837/prof_e.html)

Graduate School of Integrated Basic Sciences, Nihon University, 3-25-40 Sakurajosui, Setagaya-ku, Tokyo 156-8550, Japan

Interests: bioanalytical chemistry; nucleic acid aptamers; xenonucleic acids; polymerases

Special Issues and Collections in MDPI journals:

Special Issue in ***Molecules*: Nucleic Acid Aptamers (/journal/molecules/special_issues/nucleic_acid_aptamers)**

Dr. Maxim L. Kuznetsov
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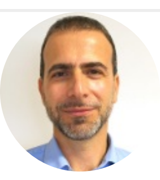
Centro de Química Estrutural, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1049-001, Lisbon, Portugal
Interests: computational chemistry; coordination chemistry; molecular catalysis; oxidation of hydrocarbons; activation of small molecules; reaction mechanism; chemical bond nature; cycloaddition; nitriles; non-covalent interactions
Special Issues and Collections in MDPI journals:
Special Issue in ***Molecules*: Computational Chemistry (/journal/molecules/special_issues/computational_chemistry_2013)**
Special Issue in ***Molecules*: Metal Mediated Activation of Small Molecules (/journal/molecules/special_issues/Metal_Mediated_Activation_Molecules)**
Special Issue in ***Molecules*: Theoretical Investigations of Reaction Mechanisms (/journal/molecules/special_issues/theor_mech)**
Special Issue in ***Molecules*: Metal-Induced Molecule Activation and Coupling Reactions (/journal/molecules/special_issues/Metal_Activation_Coupling)**

Prof. Dr. Akinori Kuzuya
Website (http://wps.itc.kansai-u.ac.jp/mol-mach2/group-members/kuzuya/)
Organization for Research and Development of Innovative Science and Technology (ORDIST), Kansai University, Suita, Osaka 564-8680, Japan
Interests: nucleic acid chemistry; DNA nanotechnology; supramolecular chemistry; molecular machines; molecular robotics; molecular technology
Special Issues and Collections in MDPI journals:
Special Issue in ***Molecules*: Feature Review Papers in Chemical Biology (/journal/molecules/special_issues/review_chemical_biology)**



Assoc. Prof. Dr. Massimo La Deda
Website1 (https://www.unical.it/portale/strutture/dipartimenti_240/ctc/didattica/homedid/docenti/associati/ladedam/) **Website2 (https://www.scopus.com/authid/detail.uri?authorId=6603129582)**
Department of Chemistry and Chemical Technologies, University of Calabria, I – 87036 Rende (CS) Italy
Interests: photochemistry; plasmonics; nanoparticles; photodynamic therapy; fluorescence; coordination compounds; electrochromic devices

Dr. Carmelo La Rosa
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Dipartimento di Scienze Chimiche, Universita' di Catania, Viale A. Doria 6, Italy
Interests: Protein Folding-Misfolding and Aggregation; Lyotropic Liquid crystals – model membrane. Methods: experimental and computer simulations.
Special Issues and Collections in MDPI journals:
Special Issue in ***Molecules*: Cutting-Edge Physical Chemistry Research in Europe (/journal/molecules/special_issues/Cutting-Edge_PC)**

Dr. Jalel Labidi
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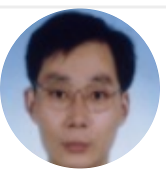
Department of Chemical and Environmental Engineering, Faculty of Engineering Gipuzkoa, University of the Basque Country, Plaza Europa 1, 20018 Donostia-San Sebastián, Gipuzkoa, Spain
Interests: biomaterials; nanomaterials; polysaccharide; lignin; biorefinery; green chemistry
Special Issues and Collections in MDPI journals:
Special Issue in ***Materials*: Advances in Functionalization of Lignocellulosic Materials (/journal/materials/special_issues/lignocellulosic_materials)**
Special Issue in ***Molecules*: Biorefineries (/journal/molecules/special_issues/biorefineries)**
Special Issue in ***Forests*: Methods and New Technologies for Wood Modification (/journal/forests/special_issues/wood_modification)**

Dr. Sami Lakhdar
Website (https://www.lcmt.ensicaen.fr/cv-sami-lakhdar/)
Ecole Nationale Superieure d'Ingenieurs de Caen, Caen, France
Interests: Organic physical chemistry; Phosphorus chemistry; Photoredox catalysis; organocatalysis

Prof. Dr. Mahesh K. Lakshman
Website (http://rcmiccny.org/wordpress1/researchers/biomolecular-structure-and-function/dr-mahesh-lakshman/)
Department of Chemistry, The City College and The City University of New York, New York, NY 10031, USA
Interests: Nucleoside modification via metal-catalyzed and uncatalyzed processes, synthesis of novel nucleoside structures, chemical carcinogenesis, site-specific DNA modification, synthesis of polycyclic aromatic hydrocarbons and their metabolites, aryne chemistry, and generally applicable synthetic methodology
Special Issues and Collections in MDPI journals:
Special Issue in ***Molecules*: Nucleoside Modifications (/journal/molecules/special_issues/Nucleoside_Modifications)**

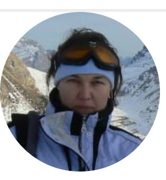
Prof. Dr. Jacques Lalevee
Website (http://www.iufrance.fr/les-membres-de-liuf/membre/776-jacques-lalevee.html)
Universite de Haute-Alsace (UHA), Centre National de la Recherche Scientifique (CNRS), UMR 7361, IS2M, 15 Rue Jean Starcky, F-68057 Mulhouse, France
Interests: photopolymerization; photochemistry; polymers & lights; photoinitiators; 3D printing (stereolithography)
Special Issues and Collections in MDPI journals:
Special Issue in ***Catalysts*: Recent Advances in Photoredox Catalysts (/journal/catalysts/special_issues/Photoredox_Catalysts)**



Prof. Dr. Yucheng Lan
Website1 (https://scholar.google.com/citations?user=xtJ-O98AAAAJ&hl=en) Website2 (https://www.morgan.edu/school_of_computer_mathematical_and_natural_sciences/departments_and_programs/physics/faculty_and_staff/yucher
Department of Physics and Engineering Physics, Morgan State University, Baltimore, 21251 Maryland, US
Interests: nanomaterials; nanodevices; thermoelectrics; photovoltaics; photocatalytics; electron microscopies; crystallography
Special Issues and Collections in MDPI journals:
Special Issue in ***Molecules*: Nanostructured Carbon-base Compounds in Renewable Energy Conversion, Energy Storage, and Environment Applications (/journal/molecules/special_issues/carbon_nanostructure)**

Dr. Daniela Lanari
Website (https://www.researchgate.net/profile/Daniela_Lanari)
Dipartimento di Scienze Farmaceutiche, Università di Perugia, Via del Liceo 1, 06123 Perugia, Italy
Interests: sustainable chemistry; heterogeneous catalysis; benign reaction media; flow chemistry
Special Issues and Collections in MDPI journals:
Special Issue in ***Molecules*: Advances in Sustainable Synthesis (/journal/molecules/special_issues/advance_sustainable_synthesis)**

Dr. Heiko Lange
Website (https://www.docenti.unina.it/#!/professor/4845494b4f4c414e47454c4e47484b4537384c33305a31313246/riferimenti)
Department of Pharmacy, University of Naples Federico II, Naples, Italy
Interests: biomaterials; natural polymers; polyphenols; lignin; tannin; micro- and nanovesicles; nanoparticles; nanofibers; targeted delivery; structure elucidation; synthetic chemistry; flow chemistry
Special Issues and Collections in MDPI journals:
Special Issue in ***Molecules*: Lignin—Chemistry and Materials: Past, Present and Future (/journal/molecules/special_issues/lignin_chem)**
Special Issue in ***Polymers*: Algae-Based Polymers: Current Trends and Emerging Opportunities (/journal/polymers/special_issues/Algae)**
Special Issue in ***Molecules*: Sustainable Approaches to Natural Product-Inspired Drug Discovery and Development (/journal/molecules/special_issues/NP_inspired)**



Prof. Dr. Anna Lankoff
Website (https://publons.com/researcher/1622770/anna-lankoff/)
1. Centre for Radiobiology and Biological Dosimetry, Institute of Nuclear Chemistry and Technology, Dorodna 16, 03-195 Warsaw, Poland
2. Department of Medical Biology, Institute of Biology, Jan Kochanowski University, Uniwersytecka 7, 25-406 Kielce, Poland
Interests: biochemistry; radiobiology; nanoparticles; toxicology; targeted cancer therapy

Special Issue in ***Molecules*: Recent Research on Neuroregeneration in Medicinal Chemistry (/journal/molecules/special_issues/Neuroregeneration_MedChemistry)**
Special Issue in ***Molecules*: Heterocyclic, Medicinal and Theoretical Chemistry: A Themed Issue in Honor of Professor Jose Elguero's Great Contribution (/journal/molecules/special_issues/jose_elguero)**

Dr. Jean-Luc Le Quéré
Website (https://www.researchgate.net/profile/J_L_Le_Quere)
Centre des Sciences du Goût et de l'Alimentation (CSGA), INRAE, Dijon, France
Interests: aroma; flavour; flavour release; in vivo flavour release; perception; direct injection mass spectrometry; PTR-MS; APCI-MS; GC-O; GC-MS; key flavour compounds; volatolomics
Special Issues and Collections in MDPI journals:
Special Issue in ***Molecules*: Selected Papers from the 16th Weurman Flavour Research Symposium (/journal/molecules/special_issues/16th_Weurman_Flavour)**

Prof. Dr. Albert Lebedev
Website (http://chem.msu.ru/eng/chairs2/organic/Buklet_eng_OrgChem.pdf)
Lomonosov Moscow State University, Moscow, Russian Federation
Interests: organic mass spectrometry; environmental chemistry; peptide sequencing; disinfection by-products

Prof. Dr. Jacques Lebreton
Website (https://www.univ-nantes.fr/site-de-l-universite-de-nantes/jacques-lebreton--594610.kjsp)
Université de Nantes, CNRS, CEISAM UMR 6230, F-44000 Nantes, France
Interests: synthetic methodologies; heterocyclic chemistry; nucleoside and nucleotide chemistry; steroid chemistry; inhibitors of protein-protein interactions; total synthesis of natural products; synthesis of non-radiolabeled compounds

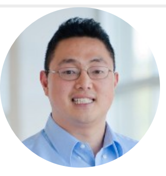
Prof. Dr. Marc Lecouvey
Website (https://cspbat.univ-paris13.fr/41-membres/132-lecouvey_marc.html)
CNRS, UMR 7244, CSPBAT, Laboratoire de Chimie, Structures et Propriétés de Biomateriaux et d'Agents Therapeutiques, Université Paris 13, Sorbonne Paris Cité, Bobigny, France
Interests: phosphorus chemistry; the synthesis of new ligands for metal complexation

Dr. Seung Seo Lee
Website (https://www.southampton.ac.uk/chemistry/about/staff/ssl1e12.page)
Lecturer in Chemical Biology, School of Chemistry, University of Southampton, UK
Interests: glycosyltransferase, glysosidase, CAZy enzymes, enzymology, biocatalysts, carbohydrate chemistry, antimicrobial resistance, two component system, enzyme inhibitors, fluorinated carbohydrate, deubiquitinase inhibitor
Special Issues and Collections in MDPI journals:
Special Issue in ***Molecules*: Chemical Biology of Antimicrobial Resistance (/journal/molecules/special_issues/chemical_biology_antimicrobial_resistance)**

Prof. Dr. Young Jin Lee
Website (https://www.ipb.iastate.edu/people/young-jin-lee)
Iowa State University, Department of Chemistry, Ames, USA
Interests: mass spectrometry imaging; matrix-assisted laser desorption ionization; plant metabolites; bio-oils; high-resolution mass spectrometry

Lecturer Vladimir Ya Lee
Website (https://trios.tsukuba.ac.jp/en/researcher/0000000622)
University of Tsukuba, Tsukuba, Japan

Interests: Experimental and theoretical studies of the low-coordinate derivatives of the main group elements: cations, free radicals, anions, carbenes, multiply-bonded species, aromatic compounds, clusters, and their transition metal complexes

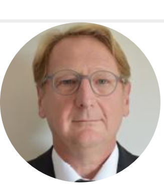


Prof. Dr. Bruce P. Lee
Website (https://www.mtu.edu/biomedical/people/faculty/lee/)
Department of Biomedical Engineering Michigan Technological University 309 M&M Building, 1400 Townsend Dr., Houghton, MI 49931, USA
Interests: biomimetic materials; antimicrobial polymers; tissue adhesives; biointerface; smart materials
Special Issues and Collections in MDPI journals:
Special Issue in ***Gels*: Tough Hydrogels for Biomedical Applications (/journal/gels/special_issues/tough_hydrogels)**
Special Issue in ***Molecules*: Antimicrobial Polymers 2020 (/journal/molecules/special_issues/antimicrobial_polym)**

Assoc. Prof. Dr. Jeongmi Lee
Website (https://skb.skku.edu/eng_pharm/intro/faculty_pharmacy.do?mode=view&perId=LZStrI4NgqgbgWgKg0gNQMoHoDmBbYMoFMCWAMgEICeSAigLxVA%20&)
School of Pharmacy, Sungkyunkwan University, Suwon, Korea
Interests: chromatography-based separation science; deep eutectic solvents; metabolomics; sample preparation methods; pharmaceutical analysis; food analysis; analytical method development, and design of experiment

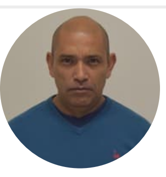
Prof. Dr. Christian Lehmann
Website (https://medicine.dal.ca/departments/department-sites/anesthesia/our-people/christian-lehmann.html)
Dalhousie University, Department of Anesthesiology, Halifax, NS, Canada
Interests: inflammation; infection; sepsis; microcirculation; intravital imaging
Special Issues and Collections in MDPI journals:
Special Issue in ***Molecules*: Cannabinoids (/journal/molecules/special_issues/molecules_cannabinoids)**
Special Issue in ***International Journal of Molecular Sciences*: Microcirculation in Inflammation (/journal/ijms/special_issues/microcirculation_inflammation)**

Dr. Zhentian Lei
Website (https://cafnr.missouri.edu/person/zhentian-lei/)
Department of Biochemistry, University of Missouri Metabolomics Center, Columbia, MO 65211, USA
Interests: bioanalytical chemistry; metabolomics and proteomics; biological mass spectrometry; GC-MS; LC-MS; LC-MS-SPE-NMR
Special Issues and Collections in MDPI journals:
Special Issue in ***Metabolites*: Mass Spectrometry-Based Metabolomics and Its Applications (/journal/metabolites/special_issues/MS_Metabolomics)**



Prof. Dr. Christophe Len
Website (https://www.lenresearch.com/)
1. Chimie ParisTech - CNRS, Institute of Chem. For Life & Health Sciences, 11 rue P&M Curie, F-75231 Paris Cedex 05, France
2. Centre de Recherche Royallieu, Université de Technologie de Compiègne – UTC, F-60200 Compiègne, France
Interests: fine chemistry from natural substances: carbohydrates, cyclodextrins, nucleosides, lipids; chemistry and processes for the sustainable development; organic chemistry in green solvents; homogeneous, heterogeneous, and micellar catalysis; continuous flow applied to organic chemistry; organic chemistry under microwave activation
Special Issues and Collections in MDPI journals:
Special Issue in ***Molecules*: Catalysis Applied to Biomass—Toward Sustainable Processes and Chemicals (/journal/molecules/special_issues/catalysis_biomass)**
Special Issue in ***Catalysts*: Catalysis of Biomass-Derived Molecules (/journal/catalysts/special_issues/catal_biomass)**
Special Issue in ***Catalysts*: Catalytic Methods in Flow Chemistry (/journal/catalysts/special_issues/catal_flow)**
Special Issue in ***Catalysts*: Catalysts for Suzuki–Miyaura Coupling Reaction (/journal/catalysts/special_issues/Suzuki%E2%80%93Miyaura_Coupling)**
Special Issue in ***Molecules*: Biorefinery and Biomass Conversion and Utilization (/journal/molecules/special_issues/biorefinery_biomass_conversion)**
Special Issue in ***Catalysts*: Selected Papers from the 2nd Edition of Global Conference on Catalysis, Chemical Engineering and Technology (CAT 2018) (/journal/catalysts/special_issues/select_cat)**

Dr. Paola Lenzi
[Website (https://www.researchgate.net/profile/Paola_Lenzi)]
Università di Pisa, Pisa, Italy
Interests: autophagy; ubiquitin proteasome pathway; transmission electron microscopy; mitochondria; cellular ultrastructure



Dr. Francisco Leon
[Website (https://pharmacy.ufl.edu/profile/leon-francisco-1/)]
Affiliation: Department of Medicinal Chemistry, College of Pharmacy, University of Florida, Gainesville, FL 32610, USA
Interests: natural products chemistry; synthesis of natural products; medicinal chemistry; alkaloids
Special Issues and Collections in MDPI journals:
Special Issue in ***Molecules*: Natural Products from Fungi (/journal/molecules/special_issues/np_fungi)**

Dr. Marilisa Leone
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Institute of Biostructures and Bioimaging (IBB), National Research Council of Italy (CNR), Via Mezzocannone 16, 80134, Naples, Italy
Interests: structural biology, NMR, drug discovery, conformational analysis of proteins & peptides, protein-protein interactions (PPIs), design and evaluation of PPI inhibitors, structure-based drug design, molecular modeling, docking, cancer
Special Issues and Collections in MDPI journals:
Special Issue in ***Molecules*: The Conformational Universe of Proteins and Peptides: Tales of Order and Disorder (/journal/molecules/special_issues/Conformational_Analysis_Proteins)**

Assoc. Prof. Dr. Marcello Leopoldo
[Website (https://persone.ict.uniba.it/rubrica/marcello.leopoldo)]
Dipartimento di Farmacia—Scienze del Farmaco, Università degli Studi di Bari, Bari, Italy
Interests: medicinal chemistry; serotonin receptors; dopamine receptors; formyl peptide receptors; positron emission tomography

Dr. Jérôme Leprince
[Website (http://anr-nemo.org/en/anr-nemo-member/leprince-j%C3%A9r%C3%B4me)]
INSERM U1239, University of Normandy, 76000 Rouen, France
Interests: Structure-activity relationship study of neuropeptides; pharmacochemistry of neuropeptides; peptide-based GPCR ligand design; bioactive peptides; neuroendocrinology; cell protection

Prof. Dr. Frederic Lesage
[Website (http://www.polymtl.ca/expertises/en/lesage-frederic)]
Biomedical Engineering, Ecloe Polytechnique de Montreal, Montreal, Quebec, Canada
Interests: biomedical engineering; molecular imaging; photoacoustics; nanomaterials design; mathematical modelling; neuronal imaging; optical coherence tomography
Special Issues and Collections in MDPI journals:
Special Issue in ***Molecules*: Metallic Nanoparticles: From Synthesis, Structure-Property Relationships to Applications (/journal/molecules/special_issues/MN)**

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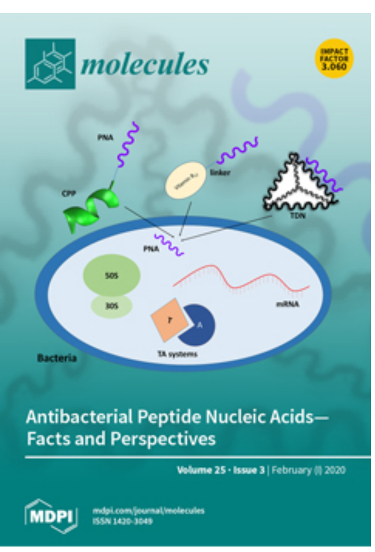

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A Density-Functional Study of the Conformational Preference of Acetylcholine in the Neutral Hydrolysis

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Abstract: Acetylcholine, which is associated with Alzheimer's disease, is widely known to have conformers. The preference of each conformer to undergo neutral hydrolysis is yet to be considered. In this study, we employed density-functional calculations to build the conformers and investigated their preference in one-step neutral hydrolysis. The results showed the preference in ten possible hydrolysis pathways involving seven acetylcholine conformers (reactant), four transition state structures, and two choline conformers (product). Three out of the seven acetylcholine conformers predicted from the results confirmed experimental findings on the conformers stability. We suggested that two out of ten possible pathways were observed in the experimental results based on agreement in reaction energy. Eventually, this study will emphasize the importance of considering acetylcholine conformers in its hydrolysis study.

Keywords: acetylcholine; conformational preference; density functional theory; neutral hydrolysis

1. Introduction

Acetylcholine (ACh^+), the organic molecule acting as neurotransmitter in the brain, is associated with the treatment of Alzheimer's disease (AD) [1]. AD is a progressive brain disease that slowly impairs coordination among neurons and leads to loss of body function [2]. A common explanation for AD is the cholinergic hypothesis, which states the cause as ACh^+ depletion [3,4]. Since the role of ACh^+ is to transmit signals among neurons [5], its depletion can disturb the signal transmission in the brain and can lead to loss of body function.

One way to treat AD is by reducing the rate of ACh^+ neutral hydrolysis [1,6], which decomposes ACh^+ into acetic acid (AA) and choline (Ch^+) [7]. The reaction is essential to return ACh^+ into its resting state after being activated during the signal transmission [8]. Because it is also important to preserve sufficient ACh^+ concentration in the brain of AD patients, reducing the rate of ACh^+ neutral hydrolysis becomes an option to compensate for ACh^+ depletion.

Generally, the rate of neutral hydrolysis depends on the conformers [9–12]. For example, the rate constant of bornyl acetate differs from iso-bornyl acetate acid hydrolysis up to 2.6×10^4/min, which has been the object of conformational study [13]. Therefore, the rate of ACh^+ neutral hydrolysis is also conformation dependent. The dependency is stronger when the reaction involves an enzyme as a catalyst [14,15]. In the ACh^+ case, at least three conformers have been investigated to understand their stability and the interconversion among the conformers and to explore the fluorination and solvent effects on each of them [16–27]. However, to the best of our knowledge, studies of ACh^+ conformers remain limited to its stability as an individual molecule. None have considered ACh^+ conformers when they interact with water in a neutral hydrolysis.

In this study, we report the preference of ACh^+ conformers in a neutral hydrolysis. We consider two important things: a one-step mechanism for the reaction model and the conformation of ACh^+ backbone dihedral angles. Despite its simplicity, the former worked well in revealing the conformational effects in the ethyl acetate neutral hydrolysis [28]. Therefore, we can focus on the conformation in one particular transition state (TS). We use the same model for ACh^+ neutral hydrolysis to obtain the standard enthalpy of reaction and standard Gibbs energy of activation.

2. Computational Methods

2.1. Reaction and Molecular Model

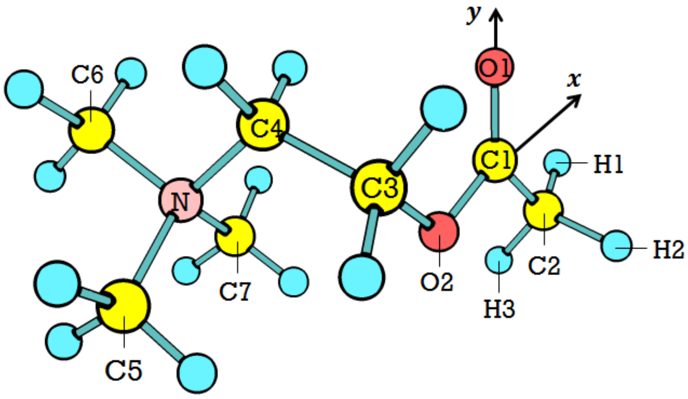
Scheme 1 represents the one-step mechanism of ACh^+ neutral hydrolysis. Our interest is the ACh^+ conformers because they potentially affect the activated complex in the TS and the final state (fs; products). In the TS, the activated complex is in the form of $[ACh^+ - H_2O]$. Consequently, they can affect the reaction energy and energy barrier. We assume that the initial state (is) and the fs of the reaction are infinitely separated molecules. Figure 1 shows the generic molecular models of ACh^+, Ch^+, and AA. Table 1 lists the geometrical parameters of interest for this study.

$$\underset{\text{acetylcholine}}{ACh^+} + \underset{\text{water}}{H_2O} \longrightarrow \underset{\text{transition state, (TS)}}{[ACh^+ - H_2O]} \longrightarrow \underset{\text{acetic acid}}{AA} + \underset{\text{choline}}{Ch^+}$$

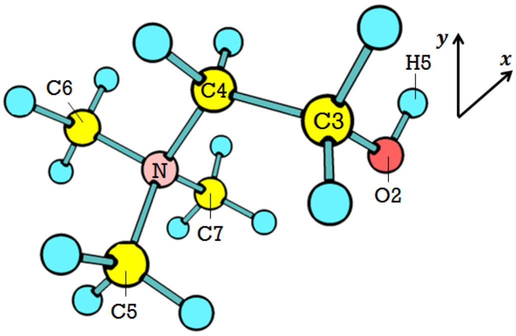
Scheme 1. A one-step mechanism for acetylcholine neutral hydrolysis.

Table 1. The geometrical parameters of interest from Figure 1 and the corresponding notations used throughout the manuscript.

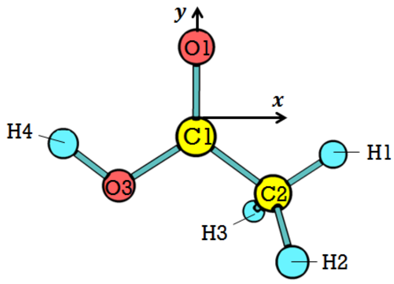
Parameter	Definition		Unit
(a) ACh^+			
*D*1	dihedral angle of C2–C1–O2–C3	(backbone)	deg.
*D*2	dihedral angle of C1–O2–C3–C4	(backbone)	deg.
*D*3	dihedral angle of O2–C3–C4–N	(backbone)	deg.
*D*4	dihedral angle of O1–C1–C2–H1	(head)	deg.
*D*5	dihedral angle of C3–C4–N–C5	(tail)	deg.
(b) Ch^+			
*D*6	dihedral angle of H5–O2–C3–C4	(backbone)	deg.
*D*7	dihedral angle of O2–C3–C4–N	(backbone)	deg.
*D*8	dihedral angle of C3–C4–N–C5	(tail)	deg.



(**a**) $C_7H_{16}NO_2^+$



(**b**) $C_5H_{14}NO^+$



(**c**) CH_3COOH

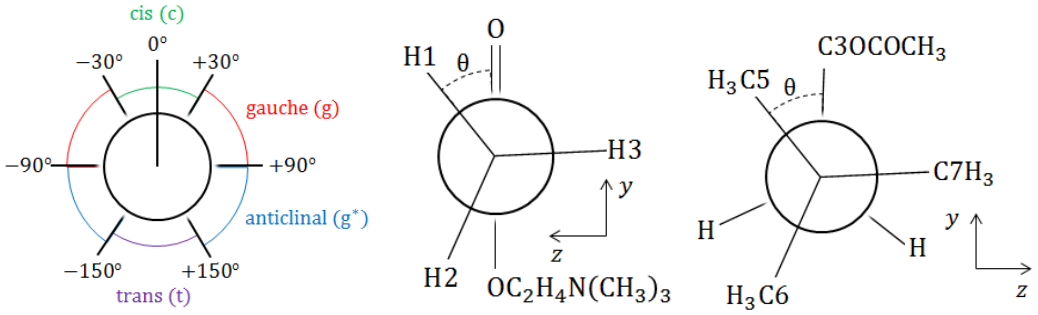
Figure 1. The molecular models of (**a**) ACh^+, (**b**) Ch^+, and (**c**) AA.

2.2. Conformer Formation

We built our initial ACh^+ conformer based on the acetylcholine bromide (ACh^+Br^-) crystal structure [29]. We removed the acetyl group (CH_3CO) from the ACh^+ initial conformer (Figure 1a) to build our Ch^+ initial conformer. We divided ACh^+ into three parts, backbone (represented by *D*1, *D*2, and *D*3), head (represented by *D*4), and tail (represented by *D*5), and Ch^+ into two parts, backbone (represented by *D*6 and *D*7) and tail (represented by *D*8), as listed in Table 1.

We varied the dihedral angles of the backbone, the head, and the tail of the initial conformer to build the potential conformers. For the ACh^+ backbone, we varied the dihedral angles (*D*1, *D*2, and *D*3) with the values of 0°, −90°, +90°, and 180° that yielded 4^3 (four values for each of the three dihedral angles) permutations. We applied the same procedure for the Ch^+ backbone (*D*6 and *D*7) that yielded 4^2 (four values for each of two dihedral angles) permutations. For the head and the tail, we varied the dihedral angles (*D*4, *D*5, and *D*8) between 0° and 180°, with increments of 20°.

Figure 2 depicts the criteria for the nomenclature of stable conformers. Figure 2a shows the criteria for each of the dihedral angles constructing the backbone. For the ACh^+ backbone, three letters representing *D*1, *D*2, and *D*3 describe the conformation type. The letters are written in a bracket following the corresponding conformer. For example, ACh^+(ctg) that indicates an ACh^+ conformer with *D*1, *D*2, and *D*3 are "c" (*cis*), "t" (*trans*), and "g" (*gauche*), respectively, and "g*" is for the *anticlinal* conformation. Figure 2b,c shows the criteria to define the head and the tail conformations, which can be eclipsed or staggered. We used the same nomenclature for Ch^+ conformers.



(**a**) For "Backbone". (**b**) For "Head". (**c**) For "Tail".

Figure 2. (**a**) The criteria to define the conformation of each dihedral angle. A line lying on 0° represents the bond of the first two atoms describing the dihedral angle. Newman projections (**b**) along C2–C1 and (**c**) along N–C4. For Figure 2b,c, $\theta \cong 0°$ means eclipsed conformation and $\theta \cong 60°$ means staggered conformation.

2.3. Energy and Structure Calculations

We employed routines of calculations based on density functional theory (DFT) [30,31] to determine the energy and the structure of molecules in the ground state and in the TS. We used B3LYP functionals and the 6-311++G(d,p) basis set integrated in Gaussian 09 software [32]. The use of B3LYP functionals follows its success in our previous similar study on chemical reactions [28,33,34] and other similar cases [35,36]. The optimization–routine calculations are to obtain the stable structures and the total electronic energy of $ACh^{+}Br^{-}$, water, and AA and, more importantly, to find the stable conformers of ACh^{+} and Ch^{+}. For the TS, we followed the same procedure used in our previous study [28], where we applied the TS optimization and the intrinsic reaction coordinate routines of calculation. Besides the energy and the structure, we also calculated the charge population using the Natural Bond Orbital (NBO) program [37].

2.4. Thermochemistry Calculations

We calculated the standard enthalpy of reaction ($\Delta_r H°$) and the standard Gibbs energy of activation ($\Delta^{\ddagger} G°$) of ACh^{+} neutral hydrolysis using the following formula:

$$\Delta_r H° = (H°_{ACh^+} + H°_{H_2O}) - (H°_{AA} + H°_{Ch^+}) \tag{1}$$

$$\Delta^{\ddagger} G° = (G°_{TS}) - (G°_{ACh^+} + G°_{H_2O}) \tag{2}$$

Both $H°$ and $G°$ in Equations (1) and (2) are temperature dependent, and we assumed the reaction occurred at room temperature (298.15 K). The values were determined from the total electronic energy of the respective systems with thermal corrections.

3. Results and Discussion

3.1. The Ground-State Structure

Table 2 presents the discrepancy in geometry between the experimental value and our calculations for $ACh^{+}Br^{-}$ in the ground state. The experimental values are from the crystal structure [29], which is comparable to our calculations in the gas phase. Overall, the values of Δ_{ba} are within the accuracy limit, according to Young [38]. It implies that B3LYP functional and the 6-311++G(d,p) basis set are appropriate for studying ACh^{+}.

Table 2. The optimized geometrical parameters of ACh^+Br^- from (a) experimental values [29] and (b) our calculations (R (in Å); A (in deg.)). The discrepancy Δ_{ba} is the value of (b) minus (a).

Parameter	(a)	(b)	Δ_{ba}
R(C1,O1)	1.192	1.202	0.010
R(C1,C2)	1.487	1.496	0.009
R(C1,O2)	1.358	1.381	0.023
R(O2,C3)	1.452	1.431	−0.021
R(C3,C4)	1.500	1.521	0.021
R(C4,N)	1.513	1.532	0.019
A(O1,C1,C2)	125.9	126.9	1.0
A(O1,C1,O2)	122.8	122.3	−0.5
A(C2,C1,O2)	111.3	110.8	−0.5
A(C1,O2,C3)	115.7	116.5	0.8
A(O2,C3,C4)	111.6	111.1	−0.5
A(C3,C4,N)	116.4	116.4	0.0

The optimization routine calculations predict the stable conformer for both ACh^+ and Ch^+. The cartesian coordinates of the stable conformers are given in the Supplementary Materials. Only seven out of 64 potential ACh^+ conformers are stable in the ground state, as shown in Figure 3. For Ch^+, there are only two possible out of 16 potential conformers. Tables 3 and 4 resume the results for ACh^+ and Ch^+, respectively. In both ACh^+ and Ch^+, the spans of the dihedral angle are more significant than those of bond lengths and bond angles, which is as expected. That is to say that the backbone determines the conformation, whereas the head (for ACh^+ only) is always eclipsed and the tail is always staggered.

Table 3. The optimized conformation type and geometrical parameters of the stable ACh^+ conformers (*R* (in Å); *A* and *D* (in deg.)).

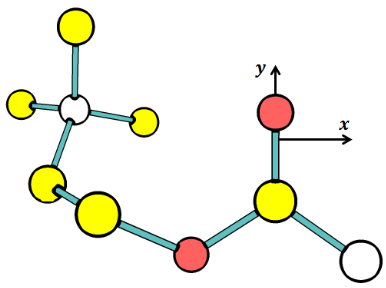
Backbone Conformation	Parameters							
	***R*1**	***R*2**	***R*3**	***A*1**	***A*2**	***D*1**	***D*2**	***D*3**
tg*g	1.497	1 369	1.532	111.5	121.8	166.6	110.4	−79.7
tgg	1.498	1.383	1.531	111.4	121.4	170.6	81.7	67.0
ttg	1.499	1.389	1.533	111.2	121.1	−178.4	166.0	65.9
tgt	1.497	1.374	1.525	111.5	121.3	174.9	80.7	−157.2
ttt	1.498	1.384	1.525	111.1	121.1	180.0	180.0	180.0
ctg	1.505	1.400	1.533	117.4	116.4	−7.4	166.7	56.7
ctt	1.507	1.397	1.523	117.3	116.8	0.0	180.0	180.0
span	0.011	0.031	0.010	6.3	5.5	180.0	99.3	124.3

*R*1 C2–C1; *R*2 C1–O2; *R*3 C4–N; *A*1 C2–C1–O2; *A*2 O1–C1–O2.

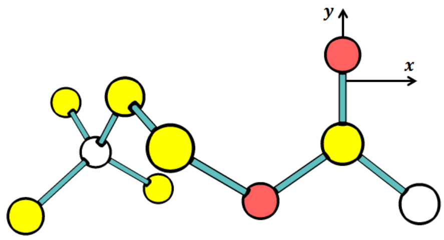
Table 4. The optimized conformation type and geometrical parameters of the stable Ch^+ conformers (*R* (in Å); *A* and *D* (in deg.)).

Backbone Conformation	Parameters						
	***R*4**	***R*5**	***R*6**	***A*3**	***A*4**	***D*6**	***D*7**
tg	1.419	1.521	1.533	110.2	109.6	167.7	58.3
tt	1.414	1.530	1.522	110.3	102.6	179.5	178.4
span	0.004	0.009	0.011	0.1	7.0	11.8	121.2

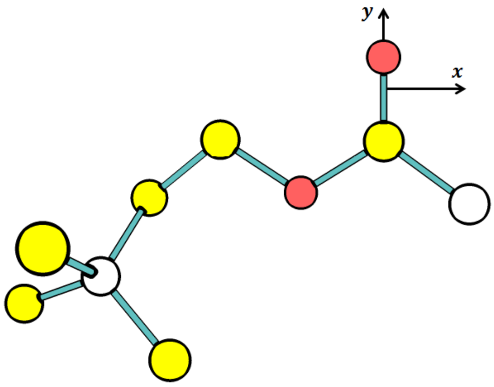
*R*4 O2–C3; *R*5 C3–C4; *R*6 C4–N; *A*3 H5–O2–C3; *A*4 C3–C4–N.



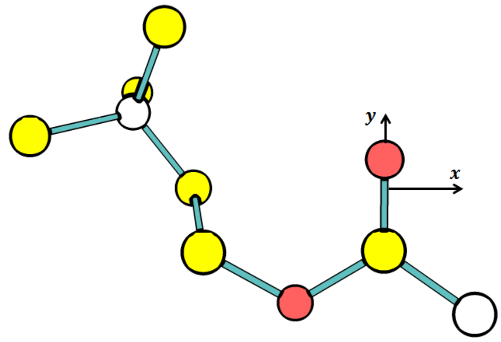
(**a**) tg*g: $d = 5.120$ Å



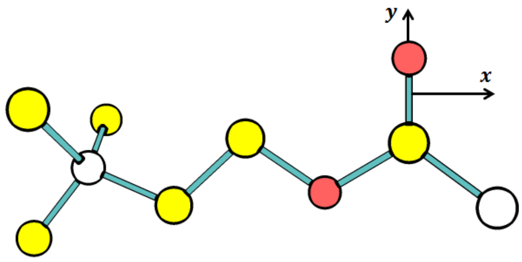
(**b**) tgg: $d = 5.188$ Å



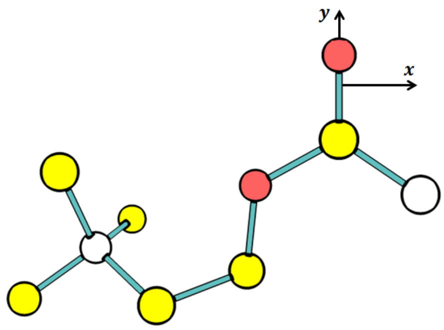
(**c**) ttg: $d = 5.303$ Å



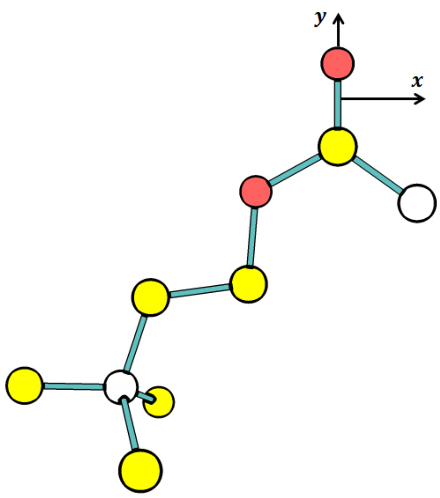
(**d**) tgt: $d = 5.688$ Å



(**e**) ttt: $d = 6.114$ Å



(**f**) ctg: $d = 5.270$ Å



(**g**) ctt: $d = 5.423$ Å

Figure 3. The optimized structure of ACh^+ conformers: For clarity, all H atoms are not displayed. The distance, d, is between C2 and N atom (white).

Figure 4 shows the energy level diagram (ELD) for the seven stable ACh^+ conformers in eV (1 eV ≈ 23.06 kcal/mol). It is clear from the energy level that there are two groups of conformers, which are low and high level. The low-level group is more stable than the high-level group. The five ACh^+ conformers (tg*g, tgg, ttg, tgt, and ttt) are in the low-level group (Figure 3a–e), and the other two conformers (ctg and ctt) are in the high-level group (Figure 3f,g). Other computational studies [20,23,39,40] also conclude the stability of the five low-level conformers. It is important to note that our results support the experiments that observed ACh^+(tg*g), (tgg), and (ttg) in their stable states [29,41,42].

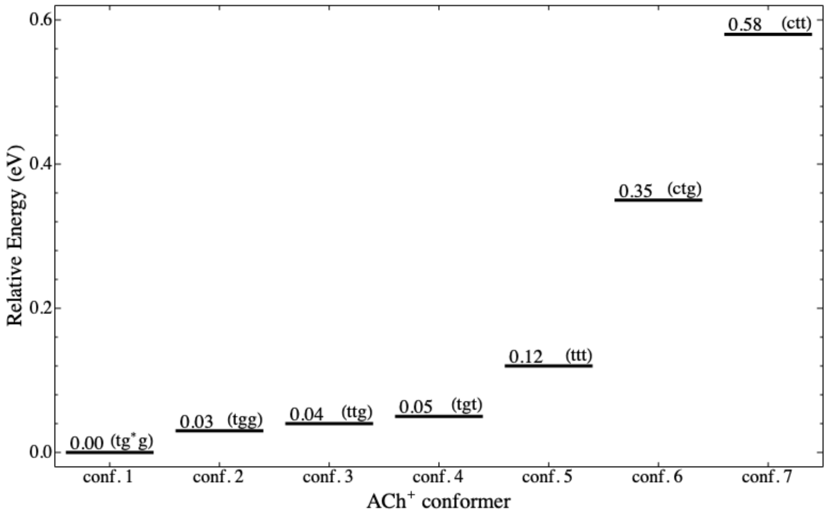


Figure 4. The energy level diagram (ELD) of the seven stable ACh^+ conformers. The energy is relative to ACh^+ (tg*g).

The ELD displays three noticeable patterns of the conformation related to ACh^+ stability as individual molecules. The first is that *gauche* conformation at *D*1 cannot achieve stability, whereas *trans* and *cis* can. The second is that *cis* at *D*2 and *D*3 cannot achieve the stability, whereas *trans* and *gauche* (and *anticlinal*) can. The second pattern is as expected because the *cis* conformation causes two bulky groups (acetyl and trimethylamine) to be ecliptic, leading to a repulsive interaction among atoms of the two groups. The third is that *gauche* conformation at *D*2 and *D*3 makes ACh^+ more stable than when they are *trans*; therefore, at the same *D*1, it is possible to arrange the order of ACh^+ stability (based on *D*2 and *D*3), from the most to the least stable, as gg, tg, gt, and tt. In addition to the third pattern, it appears that the ACh^+ stability is more dependent on *D*3 than *D*2.

Charge distributions align with this pattern. The overall NBO calculations determine that more electrons are distributed in the head, resulting in the tail being positively charged (see Table 5). It agrees with the typical ACh^+ structure [43]. The shorter the head–tail distance, the stronger the coulombic interaction and, consequently, the more stable the conformer. Therefore, the backbone and the tail must curl up in order to shorten the head–tail distance. Such curling behavior does not only exist in gas phase but also in solvent [18,20,23,27]. The *gauche* conformation at *D*2 and *D*3 meets the condition, particularly at *D*3, where the head–tail distance is the shortest. Figure 3 depicts the circumstance, in which the distance gradually increases from the shortest in the g*g conformation to the longest in the tt conformation for the low-level group and from the shortest tg to the longest tt for the high-level group.

Additionally, the charge distribution shown in Table 5 indicates an electrophilic site of all ACh^+ stable conformers. It is in the backbone, where C1 is located. This site is typical for the ester family. According to our study on ethyl acetate neutral hydrolysis [28], the activated complex (ACh^+–water) forms between C1 and O3, the nucleophilic site of water.

Table 5. The atomic charge populations (in unit e) of ACh^+ and water: Not available values are indicated by "n.a.".

Molecules	Head		Backbone				Tail		
	O1	**C2H$_3$**	**C1**	**O2**	**C3**	**C4**	**N**	**3(CH$_3$)**	**O3**
(a) ACh^+									
tg*g	−0.61	0.06	0.82	−0.57	−0.07	−0.18	−0.36	1.00	n.a.
tgg	−0.58	0.05	0.81	−0.59	−0.07	−0.19	−0.35	1.00	n.a.
ttg	−0.55	0.04	0.82	−0.61	−0.07	−0.17	−0.34	1.00	n.a.
tgt	−0.55	0.06	0.82	−0.61	−0.07	−0.17	−0.35	1.00	n.a.
ttt	−0.56	0.05	0.82	−0.58	−0.06	−0.17	−0.35	1.00	n.a.
ctg	−0.52	0.02	0.82	−0.62	−0.05	−0.17	−0.35	1.01	n.a.
ctt	−0.51	0.01	0.81	−0.59	−0.05	−0.17	−0.35	1.00	n.a.
(b) Water	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	−0.91

The electrophilic site of the ACh^+ conformers gives a hint to the cleaving location during the hydrolysis. The cleaving location shall be the C1–O2 bond. Therefore, we extracted the C1–O2 bonding atomic orbital from the NBO calculations as listed in Table 6. All conformers have an average bonding orbital of 0.5464 C$(sp^{2.90})$ + 0.8375 O$(sp^{2.19})$. This bonding is relatively weaker than the C1–O2 bond of ethyl acetate, which is 0.5898 C$(sp^{1.91})$ + 0.8076 O$(sp^{1.42})$ [28]. It suggests that the neutral hydrolysis of ACh^+ is easier than that of ethyl acetate.

Table 6. The Natural Bond Orbital (NBO) calculation for the C1–O2 bonding based on the linear combination of atomic orbitals $a\,\mathrm{C1}(sp^n) + b\,\mathrm{O2}(sp^m)$.

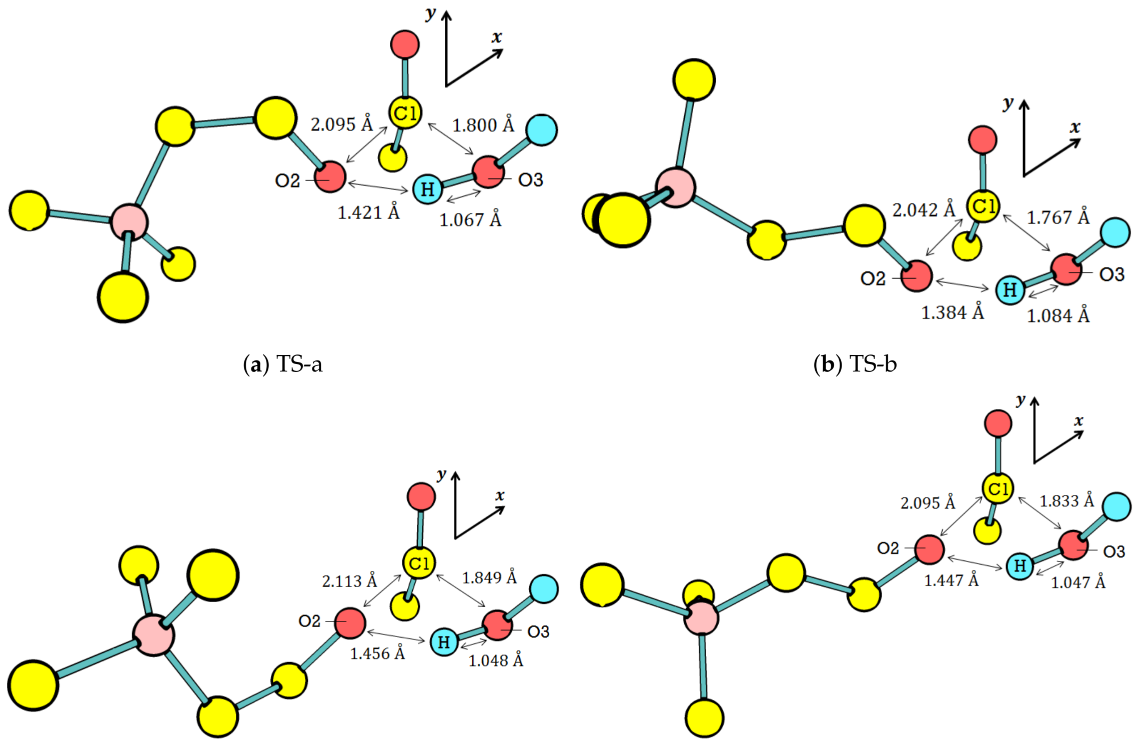
Molecules	C1		O2	
	a	sp^n	b	sp^m
(1) ACh^+				
tg*g	0.5507	2.82	0.8347	2.11
tgg	0.5481	2.87	0.8364	2.20
ttg	0.5444	2.91	0.8388	2.24
tgt	0.5503	2.84	0.8350	2.19
ttt	0.5455	2.90	0.8381	2.24
ctg	0.5419	3.01	0.8404	2.17
ctt	0.5436	2.98	0.8393	2.21
average	0.5464	2.90	0.8375	2.19
(2) Ethyl acetate				
trans	0.5901	1.91	0.8073	1.42
gauche	0.5895	1.91	0.8078	1.41
average	0.5898	1.91	0.8076	1.42

3.2. The Transition State Structure

The calculations narrow down the TS geometry from seven possible reactants to four [ACh^+–water] activated complexes. The cartesian coordinates of the four activated complexes are given in the Supplementary Materials. Table 7 lists the seven possible reactants (codes Re1–Re7). Figure 5 displays the optimized activated complex of these four [ACh^+–water]. The overall orientation of water with respect to ACh^+ is similar to our previous study on [ethyl acetate–water] activated complex [28]. This similarity suggests that ACh^+ neutral hydrolysis resembles base-induced ester hydrolysis.

Table 7. The code for reactants (initial state (is)) and products (final state (fs)) from Scheme 1.

Code	Systems	State
Re1	ACh^+(tg*g) + water	is
Re2	ACh^+(tgg) + water	is
Re3	ACh^+(ttg) + water	is
Re4	ACh^+(tgt) + water	is
Re5	ACh^+(ttt) + water	is
Re6	ACh^+(ctg) + water	is
Re7	ACh^+(ctt) + water	is
Pr1	AA + Ch^+(tg)	fs
Pr2	AA + Ch^+(tt)	fs



(**a**) TS-a (**b**) TS-b

(**c**) TS-c (**d**) TS-d

Figure 5. The four possible TS geometries.

The ACh^+–water interaction in all four possible TSs elongates C1–O2, which makes it an important parameter since it is the cleaving location, as we have discussed in Table 6. The elongation of C1–O2 is around 50% (from 1.40 Å (Table 3) to 2.10 Å (Figure 5)). It is significantly larger than that of the C1–O2 in ethyl acetate–water interaction, which is around 33% [28]. The large C1–O2 elongation is explainable according to the bonding orbital of C1–O2 described in Table 6. The bond in ACh^+ is weaker than that in ethyl acetate; therefore, the bond is easier to break in ACh^+ relative to ethyl acetate. Consequently, ACh^+ neutral hydrolysis is expected be faster than that of ethyl acetate. This expectation agrees with the experimental data showing that, at room temperature, the rate constant of the former is 10^{-9}/s [44], whereas that of the latter is 10^{-10}/s [45].

In addition to the C1–O2 elongation, there are two other similarities among the four TS geometries. First, the elongation is large enough to split the acetyl group from the rest of ACh^+. For comparison, the generalization of C–O bond lengths in saturated molecules, like ACh^+, has been widely assumed as 1.43 Å. Meanwhile, the O3 of water is still too far from C1 to form a covalent bond. The activated complex thus consists of three groups: water, acetyl, and choline. The three groups interact with each other through noncovalent interactions to form the activated complex, which lies on the TS. Second, ACh^+ prefers the curling *D*2 and *D*3 in the presence of water. The curling *D*2 and *D*3 relates the ACh^+ in the TS to the one in the ground state: (ttg), (tgt), (ctg), and (ctt). Since the curling, *D*2 and *D*3 also affect the C2–N distance and the seven ACh^+ conformers are grouped into three curling levels. The levels are extreme (d < 5.20 Å), medium (5.30 < d < 5.70 Å), and low (d > 5.70 Å). Accordingly, all TS geometries require the medium curling level of ACh^+ conformers.

Among the four TS geometries, TS-b is the most favorable one for product formation. Generally, the product formation requires the elongation of C1–O2 and O3–H in the TS with respect to the ground state, as well as shortening the distances of C1–O3 and O2–H (distances between groups in the activated complex). The shortened C1–O3 and O2–H promote the formation of AA and Ch^+, respectively. TS-b meets most of the requirements for product formation as its O3–H is the longest, whereas its C1–O3 and O2–H are the shortest among the four TS geometries.

3.3. The Reaction Coordinate

Figure 6 shows the neutral hydrolysis reaction coordinate in the ELD. The ELD involves four out of the seven potential reactants (see Table 7) capable of forming the activated complex at the TS through a one-step mechanism. The possible reactants are Re3, Re4, Re6, and Re7, which are related to the aforementioned ACh^+ curling levels. The possible products are Pr1 and Pr2, which comprise Ch^+(tg) and Ch^+(tt) from Table 4. Although the TS depends on the curling levels of *D*2 and *D*3 of the ACh^+ conformers, the products depend only on *D*3. Since *D*3 does not contain the electrophilic site, it does not change when ACh^+ is hydrolyzed into Ch^+.

Figure 7 shows the pre-hydrolysis reaction coordinate in the ELD. There are three out of seven potential reactants that require a pre-hydrolysis process (Re1, Re2, and Re5). These reactants need to undergo conformational isomerization to form either ACh^+(ttg) or (tgt) with the energy barriers at no more than 0.11 eV. It implies that the conformational isomerization can occur by thermal energy. Together with Figure 6, Figure 7 suggests that all seven potential reactants can perform hydrolysis in four pathways. The reactants with the low-level group of ACh^+ conformers go through Re3 or Re4 before going to either TS-a or TS-b. Both pathways are possible because the energy barrier to form Re3 and Re4 is no more than 0.11 eV. Meanwhile, the reactants with the high-level group of ACh^+ conformers go directly to TS-c and TS-d.

Table 8 shows the $\Delta_r H^\circ$ for all possible reaction coordinates in Figures 6 and 7. The calculations of $\Delta_r H^\circ$ suggest that reactants with the high-level ACh^+ conformers are always exothermic and go toward either Pr1 or Pr2. Meanwhile, reactants from the low-level group are exothermic if they go toward Pr1, but they are endothermic if they go toward Pr2. Experimentally, the reaction is endothermic, with $\Delta_r H^\circ$ being $+0.28$ kcal/mol [46]. According to our results, Pr2 is mostly the product of the hydrolysis. In particular, the experiment observed mostly reactions (viii) or (ix), suggesting that the practically preferred ACh^+ conformer undergoes neutral hydrolysis, which is (tgt) or (ttt). It is worthwhile to mention that our results are in line with the study of Zhorov et al. [47], which suggest that ACh^+ with *D*2 and *D*3 being *trans* is productive for the ACh^+ hydrolysis catalyzed by acetylcholinesterase (AChE), as well as the study of Chothia and Pauling [48], which suggests that the ACh^+ conformation relevant for its interaction with AChE is the one with *D*1, *D*2, and *D*3 being *trans*.

In addition to $\Delta_r H^\circ$, Table 8 shows $\Delta^\ddagger G^\circ$. As expected, $\Delta^\ddagger G^\circ$ of reactants with the high-level ACh^+ conformers are lower than that of reactants with the low-level conformers. Consequently, reactions (v) and (x) are favorable to occur due to the low activation energy and the high exothermicity. However, the energy level of both ACh^+(ctt) and (ctg) are more than 0.30 eV higher than the most stable conformer. They can transform to ACh^+(tgt) and (ttg) via conformational isomerization according to the reaction coordinate depicted in Figure 8. The energy barrier is no more than 0.33 eV, which is still in the order of thermal energy. It implies that, despite a low $\Delta^\ddagger G^\circ$, the number of ACh^+(ctt) and (ctg) in nature is likely lower than that in the low-level group.

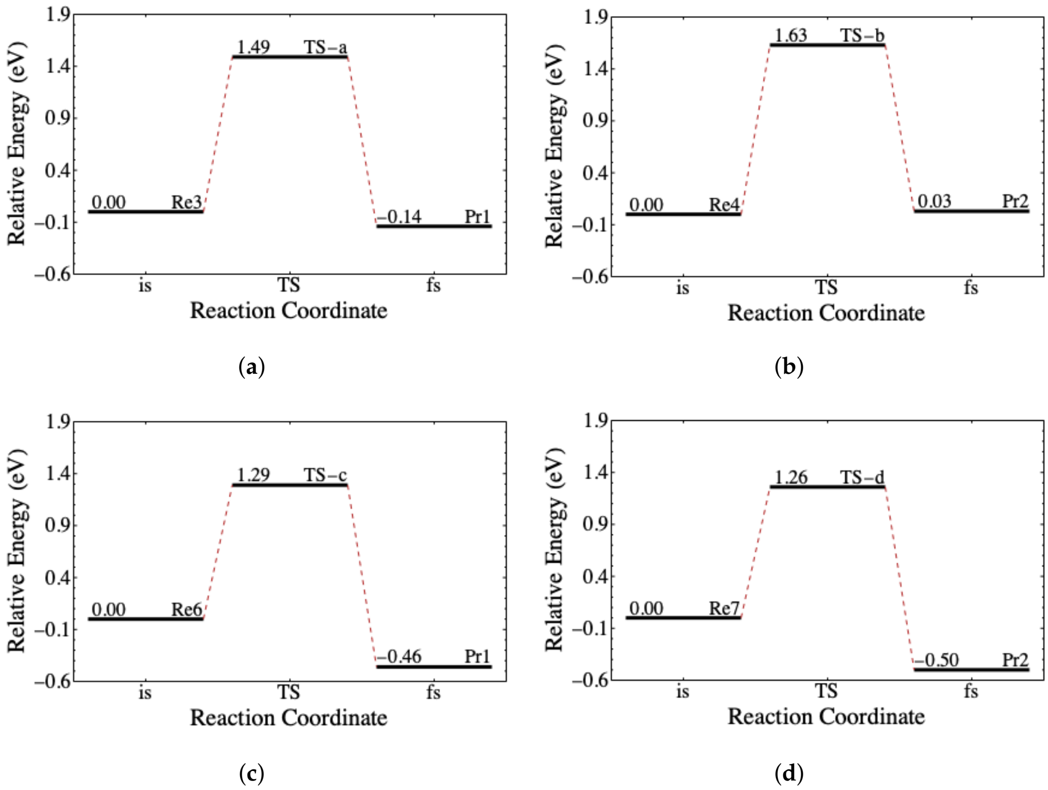


Figure 6. The ELDs for four possible TSs: (a) TS-a, (b) TS-b, (c) TS-c, and (d) TS-d, and their related initial (is) and final states (fs). The code of the reactants and the products follows Table 7. The relative energy of each TS corresponds to the energy barrier, whereas the relative energy of the fs corresponds to the reaction energy.

Table 8. The standard enthalpy of reaction ($\Delta_r H^\circ$) and the standard Gibbs energy of activation ($\Delta^\ddagger G^\circ$) at 298.15 K (in kcal/mol): For Re5, only the shortest pathway is listed.

Number	Reaction	$\Delta_r H^\circ$	$\Delta^\ddagger G^\circ$
a) Reactions that yield Pr1			
(i)	Re1 → Re2 → Re3 → Ts-a → Pr1	−1.67	45.28
(ii)	Re2 → Re3 → Ts-a → Pr1	−2.14	45.28
(iii)	Re3 → Ts-a → Pr1	−2.33	45.28
(iv)	Re5 → Re3 → Ts-a → Pr1	−4.17	45.28
(v)	Re6 → Ts-c → Pr1	−9.45	39.28
b) Reactions that yield Pr2			
(vi)	Re1 → Re4 → Ts-b → Pr2	+2.61	47.04
(vii)	Re2 → Re4 → Ts-b → Pr2	+2.14	47.04
(viii)	Re4 → Ts-b → Pr2	+1.38	47.04
(ix)	Re5 → Re4 → Ts-b → Pr2	+0.10	47.04
(x)	Re7 → Ts-d → Pr2	−10.33	38.95

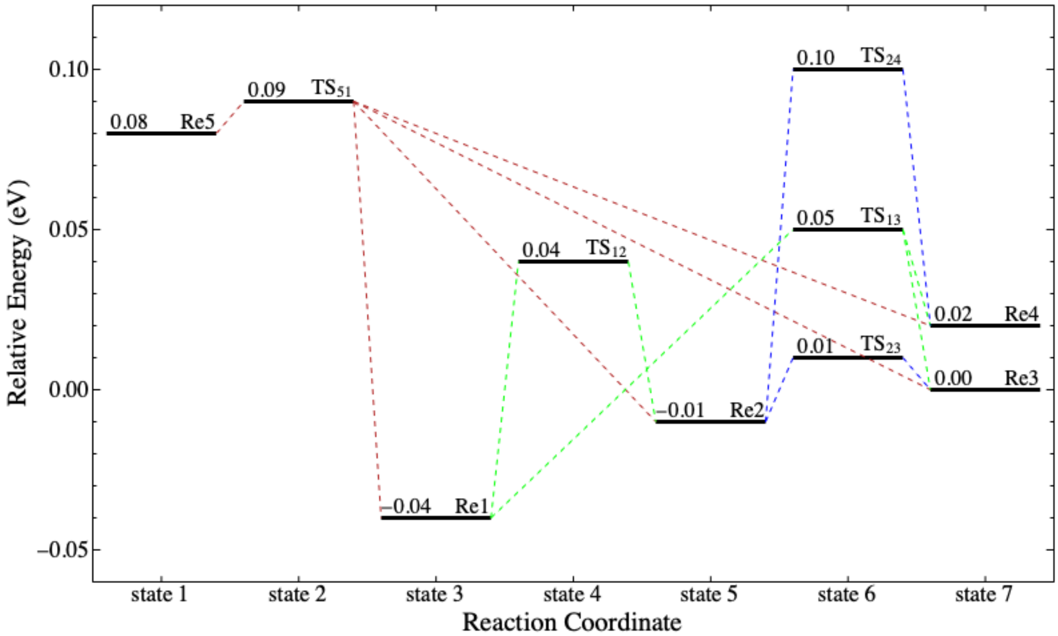


Figure 7. The reaction coordinates for all potential reactants in Table 7 before forming the activated complex (TS-a, TS-b, TS-c, and TS-d): TS_{12} means the transition state of conformational isomerization from Re1 to Re2.

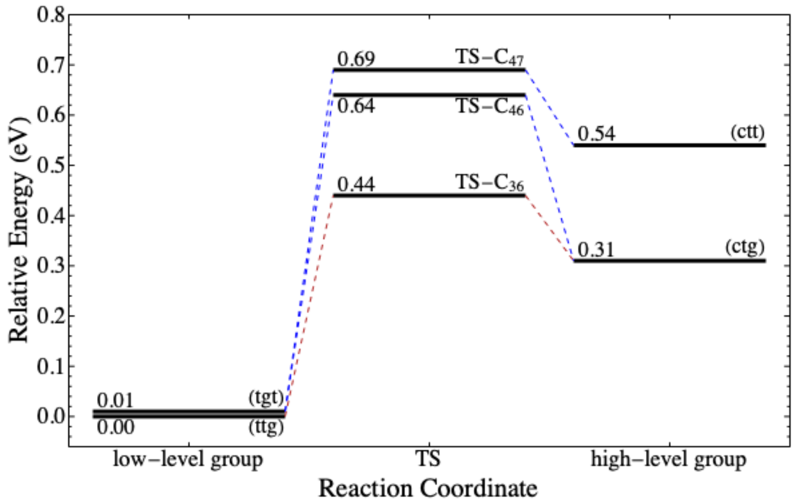


Figure 8. The reaction coordinates from low- to high-level groups of ACh^+ conformers: The TS between ACh^+(ttg) and (ctt) is almost 3 eV, and it is not displayed for the sake of clarity.

4. Conclusion

We have reported that each ACh^+ conformer exhibited different conformational preferences when existing as an individual molecule and as an activated [ACh^+–water] complex of a neutral hydrolysis. As an individual molecule, we obtained seven possible ACh^+ conformers: five low-level and two high-level conformers, each with a unique backbone conformation. Three out of the five low-level conformers were observed in the experiments. However, only four out of the seven conformers were capable of undergoing direct neutral hydrolysis via four distinct TSs, while the others had to go through some possible pre-hydrolysis pathways before forming the TS. Among the four TS structures, TS-b was the most favorable one to form the product of the neutral hydrolysis. The structure offered an insight for constructing the starting TS structure of ACh^+ neutral hydrolysis catalyzed by AChE.

In this study, we proposed ten possible reaction pathways of ACh^+ neutral hydrolysis. The most favorable reactions involved the high-level conformer with $\Delta^{\ddagger}G^{\circ}$ being 38.95 kcal/mol and $\Delta_r H^{\circ}$ being -10.33 kcal/mol. Importantly, we suggested two possible reactions involving low-level conformers ((*trans*, *gauche*, *trans*) and (*trans*, *trans*, *trans*)) with $\Delta_r H^{\circ}$ values of $+1.38$ and $+0.10$ kcal/mol, agreeing with the experimental observations. Furthermore, we argued that one had to consider ACh^+ conformers when studying its hydrolysis.

Supplementary Materials: Supplementary Materials are provided. The supplementary materials are available online.

Author Contributions: Conceptualization: F.R.; formal analysis: R.N.F., F.A., M.M., and I.P.; investigation: R.N.F., N.D.A., and V.K.; methodology: F.R. and R.N.F.; writing—original draft preparation: R.N.F.; writing—review and editing: F.R., H.K.D., and R.N.F. All authors have read and agreed to the published version of the manuscript.

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Conflicts of Interest: The authors declare no conflict of interest.

Abbreviations

The following abbreviations are used in this manuscript:

AA	Acetic Acid
ACh^+	Acetylcholine
Ch^+	Choline
ELD	Energy Level Diagram
TS	Transition State

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Sample Availability: Samples of the compounds are not available from the authors.