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### 1) Iodine Gauche Effect Induced by an Intramolecular Hydrogen Bond

* Martins, F. A., De Azevedo Santos, L., Rodrigues Silva, D., Fonseca Guerra, C., Bickelhaupt, F. M., Freitas, M. P.
* Theoretical Chemistry, AIMMS, Chemistry and Pharmaceutical Sciences, Universidade Federal de Lavras
* Journal of Organic Chemistry
* https://doi.org/10.1021/acs.joc.2c01258
* Corresponding author: Freitas, M. P.
* Published 2 Sep 2022 (early online 19 Aug 2022)
* Processed: 2022-9

The gauche conformer in 1-X,2-Y-disubstituted ethanes, that is, the staggered orientation in which X and Y are in closer contact, is only favored for relatively small substituents that do not give rise to large X···Y steric repulsion. For more diffuse substituents, weakly attractive orbital interactions between antiperiplanar bonds (i.e., hyperconjugation) cannot overrule the repulsive forces between X and Y. Our quantum chemical analyses of the rotational isomerism of XCH2CH2Y (X = F, OH; Y = I) at ZORA-BP86-D3(BJ)/QZ4P reveal that indeed the anti conformer is generally favored due to a less destabilizing I···F and I···O-H steric repulsion. The only case when the gauche conformer is preferred is when the hydroxyl hydrogen is oriented toward the iodine atom in the 2-iodoethanol. This is because of the significantly stabilizing covalent component of the I···H-O intramolecular hydrogen bond. Therefore, we show that strong intramolecular interactions can overcome the steric repulsion between bulky substituents in 1,2-disubstituted ethanes and cause the gauche effect. Our quantum chemical computations have guided nuclear magnetic resonance experiments that confirm the increase in the gauche population as X goes from F to OH.

### 2) Optical control of the β2-adrenergic receptor with opto-prop-2: A cis-active azobenzene analog of propranolol

* Bosma, R., Dijon, N. C., Zheng, Y., Schihada, H., Hauwert, N. J., Shi, S., Arimont, M., Riemens, R., Custers, H., van de Stolpe, A., Vischer, H. F., Wijtmans, M., Holliday, N. D., Kuster, D. W. D., Leurs, R.
* Innovations in Human Health & Life Sciences, AIMMS, Medicinal chemistry, University of Nottingham, Vrije Universiteit Amsterdam, Karolinska Institutet, University of Marburg, Amsterdam UMC
* iScience
* https://doi.org/10.1016/j.isci.2022.104882
* Corresponding author: Leurs, R.
* Published 16 Sep 2022 (early online 5 Aug 2022)
* Processed: 2022-9

In this study, we synthesized and evaluated new photoswitchable ligands for the beta-adrenergic receptors β1-AR and β2-AR, applying an azologization strategy to the first-generation beta-blocker propranolol. The resulting compounds (Opto-prop-1, -2, -3) have good photochemical properties with high levels of light-induced trans-cis isomerization (>94%) and good thermal stability (t1/2 > 10 days) of the resulting cis-isomer in an aqueous buffer. Upon illumination with 360-nm light to PSScis, large differences in binding affinities were observed for photoswitchable compounds at β1-AR as well as β2-AR. Notably, Opto-prop-2 (VUF17062) showed one of the largest optical shifts in binding affinities at the β2-AR (587-fold, cis-active), as recorded so far for photoswitches of G protein-coupled receptors. We finally show the broad utility of Opto-prop-2 as a light-dependent competitive antagonist of the β2-AR as shown with a conformational β2-AR sensor, by the recruitment of downstream effector proteins and functional modulation of isolated adult rat cardiomyocytes.

### 3) Analytical investigation of cannabis biomarkers in raw urban wastewater to refine consumption estimates

* Campos-Mañas, M. C., Wichelen, N. V., Covaci, A., Nuijs, A. L. N. V., Ort, C., Béen, F., Castiglioni, S., Hernández, F., Bijlsma, L.
* E&H: Environmental Chemistry and Toxicology, AIMMS
* Water Research
* https://doi.org/10.1016/j.watres.2022.119020
* Corresponding author: None
* Published Sep 2022 (early online None)
* Processed: 2022-9

### 4) Quantum cascade laser imaging (LDIR) and machine learning for the identification of environmentally exposed microplastics and polymers

* Tian, X., Beén, F., Bäuerlein, P. S.
* E&H: Environmental Chemistry and Toxicology, AIMMS
* Environmental Research
* https://doi.org/10.1016/j.envres.2022.113569
* Corresponding author: None
* Published Sep 2022 (early online None)
* Processed: 2022-9

### 5) Approximate Circular Pattern Matching

* Charalampopoulos, P., Kociumaka, T., Radoszewski, J., Pissis, S. P., Rytter, W., Waleń, T., Zuba, W.
* Bioinformatics, AIMMS, Bio Informatics (IBIVU), Birkbeck University of London, Reichman University, Max Planck Institute for Informatics, University of Warsaw, Samsung R&D Institute Poland, Centrum voor Wiskunde en Informatica
* None
* https://doi.org/10.4230/LIPIcs.ESA.2022.35
* Corresponding author: None
* Published 1 Sep 2022 (early online None)
* Processed: 2022-9

We investigate the complexity of approximate circular pattern matching (CPM, in short) under the Hamming and edit distance. Under each of these two basic metrics, we are given a length-n text T, a length-m pattern P, and a positive integer threshold k, and we are to report all starting positions (called occurrences) of fragments of T that are at distance at most k from some cyclic rotation of P. In the decision version of the problem, we are to check if there is any such occurrence. All previous results for approximate CPM were either average-case upper bounds or heuristics, with the exception of the work of Charalampopoulos et al. [CKP+, JCSS'21], who considered only the Hamming distance. For the reporting version of the approximate CPM problem, under the Hamming distance we improve upon the main algorithm of [CKP+, JCSS'21] from O(n+(n/m) k4) to O(n+(n/m) k3 log log k) time; for the edit distance, we give an O(nk2)-time algorithm. Notably, for the decision versions and wide parameter-ranges, we give algorithms whose complexities are almost identical to the state-of-the-art for standard (i.e., non-circular) approximate pattern matching: For the decision version of the approximate CPM problem under the Hamming distance, we obtain an O(n + (n/m) k2 log k/ log log k)-time algorithm, which works in O(n) time whenever k = O( p mlog log m/logm). In comparison, the fastest algorithm for the standard counterpart of the problem, by Chan et al. [CGKKP, STOC'20], runs in O(n) time only for k = O(√ m). We achieve this result via a reduction to a geometric problem by building on ideas from [CKP+, JCSS'21] and Charalampopoulos et al. [CKW, FOCS'20]. For the decision version of the approximate CPM problem under the edit distance, the O(nk log3 k) runtime of our algorithm near matches the O(nk) runtime of the Landau-Vishkin algorithm [LV, J. Algorithms'89] for approximate pattern matching under edit distance; the latter algorithm remains the fastest known for k = Ω(m2/5). As a stepping stone, we propose an O(nk log3 k)-time algorithm for solving the Longest Prefix k-Approximate Match problem, proposed by Landau et al. [LMS, SICOMP'98], for all k ∈ {1, , k}. Our algorithm is based on Tiskin's theory of seaweeds [Tiskin, Math. Comput. Sci.'08], with recent advancements (see Charalampopoulos et al. [CKW, FOCS'22]), and on exploiting the seaweeds' relation to Monge matrices. In contrast, we obtain a conditional lower bound that suggests a polynomial separation between approximate CPM under the Hamming distance over the binary alphabet and its non-circular counterpart. We also show that a strongly subquadratic-time algorithm for the decision version of approximate CPM under edit distance would refute the Strong Exponential Time Hypothesis.

### 6) Nuclear magnetic resonance as a tool to determine chlorine percentage of chlorinated paraffin mixtures

* Valderhaug, S., Liu, H., Gorovoy, A., Johansen, J. E., van Mourik, L., de Boer, J., Gautun, O. R.
* E&H: Environmental Bioanalytical Chemistry, AIMMS, E&H: Environmental Health and Toxicology, Amsterdam Sustainability Institute, Norwegian University of Science and Technology, CHIRON AS
* Chemosphere
* https://doi.org/10.1016/j.chemosphere.2022.136312
* Corresponding author: Gautun, O. R.
* Published Dec 2022 (early online 9 Sep 2022)
* Processed: 2022-9

A new simple method for chlorine percentage calculations (method C), from proton nuclear magnetic resonance (1H NMR) spectroscopy, has been established and applied to an industrial chlorinated paraffin (CP) mixture and 13 single-chain CPs of known carbon chain lengths. Two modified methods (method A and B), originating from the work of Sprengel et al., have been utilized on the same single-chain mixtures. All samples were analysed by 1H NMR and two-dimensional heteronuclear quantum coherence (HSQC) for this purpose. All three methods worked well for medium chlorinated (45–55% Cl) single-chain mixtures of known carbon chain lengths. Method A yielded the best result for mixtures of lower chlorine content (<45% Cl), method C gave better estimations for higher chlorine contents (>55% Cl). Compared to Mohr's titration, method A showed a deviation of 0.7–7.8% (3.6% average), method B 4.1–11.3% (7.0% average) and method C 0.6–11.6% (5.2% average), for all 13 single-chain mixtures. The new method C is the only method that could be applied for determining the chlorine percentage of industrial mixtures of multiple, unknown chain lengths.

### *7) Methyl Substitution Destabilizes Alkyl Radicals*

* Blokker, E., van Zeist, W. J., Sun, X., Poater, J., van der Schuur, J. M., Hamlin, T. A., Bickelhaupt, F. M.
* Theoretical Chemistry, Chemistry and Pharmaceutical Sciences, AIMMS, Nouryon
* Angewandte Chemie - International Edition
* https://doi.org/10.1002/anie.202207477
* Corresponding author: Bickelhaupt, F. M.
* Published 5 Sep 2022 (early online 12 Jul 2022)
* Processed: 2022-9

We have quantum chemically investigated how methyl substituents affect the stability of alkyl radicals MemH3−mC⋅ and the corresponding MemH3−mC−X bonds (X = H, CH3, OH; m = 0 – 3) using density functi ...

### *8) Full humanization of the glycolytic pathway in Saccharomyces cerevisiae*

* Boonekamp, F. J., Knibbe, E., Vieira-Lara, M. A., Wijsman, M., Luttik, M. A., van Eunen, K., Ridder, M. D., Bron, R., Almonacid Suarez, A. M., van Rijn, P., Wolters, J. C., Pabst, M., Daran, J. M., Bakker, B. M., Daran-Lapujade, P.
* Molecular Cell Physiology, AIMMS, Delft University of Technology, University of Groningen
* Cell Reports
* https://doi.org/10.1016/j.celrep.2022.111010
* Corresponding author: None
* Published 28 Jun 2022 (early online None)
* Processed: 2022-6

Although transplantation of single genes in yeast plays a key role in elucidating gene functionality in metazoans, technical challenges hamper humanization of full pathways and processes. Empowered by ...

### *9) Front Cover: How Ionization Catalyzes Diels‐Alder Reactions (Chem. Eur. J. 40/2022)General information*

* Vermeeren, P., Hamlin, T. A., Bickelhaupt, F. M.
* Theoretical Chemistry, AIMMS, Chemistry and Pharmaceutical Sciences
* Chemistry – A European Journal
* https://doi.org/10.1002/chem.202201619
* Corresponding author: None
* Published 15 Jul 2022 (early online None)
* Processed: 2022-7

Front Cover: How Ionization Catalyzes Diels‐Alder Reactions (Chem. Eur. J. 40/2022) ...

### *10) Escherichia coli robustly expresses ATP synthase at growth rate-maximizing concentrations*

* Rabbers, I., Bruggeman, F. J.
* Systems Bioinformatics, AIMMS
* FEBS Journal
* https://doi.org/10.1111/febs.16401
* Corresponding author: Bruggeman, F. J.
* Published Aug 2022 (early online 17 Feb 2022)
* Processed: 2022-8

Fitness-enhancing adaptations of protein expression and its regulation are an important aspect of bacterial evolution. A key question is whether evolution has led to optimal protein expression that ma ...

### *11) Combining Photodegradation in a Liquid-Core-Waveguide Cell with Multiple-Heart-Cut Two-Dimensional Liquid Chromatography*

* Den Uijl, M. J., Van Der Wijst, Y. J. H. L., Groeneveld, I., Schoenmakers, P. J., Pirok, B. W. J., Van Bommel, M. R.
* BioAnalytical Chemistry, AIMMS, University of Amsterdam, Center for Analytical Sciences Amsterdam (CASA)
* Analytical chemistry
* https://doi.org/10.1021/acs.analchem.2c01928
* Corresponding author: Den Uijl, M. J.
* Published 9 Aug 2022 (early online 28 Feb 2022)
* Processed: 2022-8

Photodegradation greatly affects everyday life. It poses challenges when food deteriorates or when objects of cultural heritage fade, but it can also create opportunities applied in advanced oxidation ...

### *12) Fate-directed risk assessment of chemical mixtures: a case study for cedarwood essential oil*

* Sühring, R., Mayer, P., Leonards, P., MacLeod, M.
* E&H: Environmental Bioanalytical Chemistry, Amsterdam Sustainability Institute, AIMMS, Stockholm University, Ryerson University, Technical University of Denmark
* Environmental Science: Processes and Impacts
* https://doi.org/10.1039/d2em00103a
* Corresponding author: Sühring, R.
* Published 1 Aug 2022 (early online 31 May 2022)
* Processed: 2022-8

The environmental risk assessment of UVCBs (i.e., substances of unknown or variable composition, complex reaction products, or biological materials) is challenging due to their inherent complexity. A ...

### *13) Rational Tuning of the Reactivity of Three-Membered Heterocycle Ring Openings via SN2 Reactions*

* Hansen, T., Nin-Hill, A., Codée, J. D. C., Hamlin, T. A., Rovira, C.
* Organic Chemistry, AIMMS, Chemistry and Pharmaceutical Sciences, Theoretical Chemistry, University of Barcelona, Leiden University, ICREA
* Chemistry - A European Journal
* https://doi.org/10.1002/chem.202201649
* Corresponding author: Hansen, T.
* Published 27 Jul 2022 (early online None)
* Processed: 2022-7

The development of small-molecule covalent inhibitors and probes continuously pushes the rapidly evolving field of chemical biology forward. A key element in these molecular tool compounds is the “ele ...

### *14) A Computational Toolbox to Investigate the Metabolic Potential and Resource Allocation in Fission Yeast*

* Grigaitis, P., Grundel, D. A. J., van Pelt-KleinJan, E., Isaku, M., Xie, G., Mendoza Farias, S., Teusink, B., van Heerden, J. H.
* Systems Bioinformatics, AIMMS, Systems Bioinformatics, Vrije Universiteit Amsterdam
* mSystems
* https://doi.org/10.1128/msystems.00423-22
* Corresponding author: Grigaitis, P.
* Published Aug 2022 (early online 11 Aug 2022)
* Processed: 2022-8

The fission yeast, Schizosaccharomyces pombe, is a popular eukaryal model organism for cell division and cell cycle studies. With this extensive knowledge of its cell and molecular biology, S. pombe a ...

### *15) A Functional Carbohydrate Degrading Enzyme Potentially Acquired by Horizontal Gene Transfer in the Genome of the Soil Invertebrate Folsomia candida*

* Le, N. G., van Ulsen, P., van Spanning, R., Brouwer, A., van Straalen, N. M., Roelofs, D.
* Animal Ecology, Molecular Microbiology, AIMMS, LaserLaB - Analytical Chemistry and Spectroscopy, Systems Bioinformatics
* Genes
* https://doi.org/10.3390/genes13081402
* Corresponding author: Le, N. G.
* Published Aug 2022 (early online 7 Aug 2022)
* Processed: 2022-8

Horizontal gene transfer (HGT) is defined as the acquisition by an organism of hereditary material from a phylogenetically unrelated organism. This process is mostly observed among bacteria and archae ...

### *16) Correlating biodegradation kinetics of 2,3,7,8-tetrachlorodibenzo-p-dioxin to the dynamics of microbial communities originating from soil in Vietnam contaminated with herbicides and dioxins*

* Nguyen, T. L. A., Dang, H. T. C., Dat, T. T. H., Brandt, B. W., Röling, W. F. M., Brouwer, A., van Spanning, R. J. M.
* AIMMS, Molecular Cell Physiology, Preventive Dentistry, Animal Ecology, Systems Bioinformatics, Vietnamese Academy of Science and Technology
* Frontiers in Microbiology
* https://doi.org/10.3389/fmicb.2022.923432
* Corresponding author: Nguyen, T. L. A.
* Published 11 Aug 2022 (early online None)
* Processed: 2022-8

We studied the succession of bacterial communities during the biodegradation of 2,3,7,8-tetrachlorodibenzo-p-dioxin (2,3,7,8-TCDD). The communities originated from a mesocosm with soil from Bien Hoa a ...

### *17) Competing C-4 and C-5-Acyl Stabilization of Uronic Acid Glycosyl Cations*

* Elferink, H., Remmerswaal, W. A., Houthuijs, K. J., Jansen, O., Hansen, T., Rijs, A. M., Berden, G., Martens, J., Oomens, J., Codée, J. D. C., Boltje, T. J.
* Organic Chemistry, AIMMS, Chemistry and Pharmaceutical Sciences, BioAnalytical Chemistry, Radboud University Nijmegen, Leiden University
* Chemistry - A European Journal
* https://doi.org/10.1002/chem.202201724
* Corresponding author: Boltje, T. J.
* Published 12 Aug 2022 (early online None)
* Processed: 2022-8

Uronic acids are carbohydrates carrying a terminal carboxylic acid and have a unique reactivity in stereoselective glycosylation reactions. Herein, the competing intramolecular stabilization of uronic ...

### *18) Computational Prediction of Tc-99 NMR Chemical Shifts in Technetium Complexes with Radiopharmaceutical Applications*

* De Andrade, T. F. C. B., Dos Santos, H. F., Fonseca Guerra, C., Paschoal, D. F. S.
* Theoretical Chemistry, AIMMS, Universidade Federal do Rio de Janeiro, Universidade Federal de Juiz de Fora
* Journal of Physical Chemistry A
* https://doi.org/10.1021/acs.jpca.2c01617
* Corresponding author: Paschoal, D. F. S.
* Published 18 Aug 2022 (early online 5 Aug 2022)
* Processed: 2022-8

The Tc-99m nucleus is the most used nuclide in radiopharmaceuticals designed for imaging diagnosis. The metal can exist in nine distinct oxidation states and forms distinct coordination complexes with ...

### *19) New putative phenol oxidase in ascidian blood cells*

* Daugavet, M. A., Dobrynina, M. I., Shaposhnikova, T. G., Solovyeva, A. I., Mittenberg, A. G., Shabelnikov, S. V., Babkina, I. Y., Grinchenko, A. V., Ilyaskina, D. V., Podgornaya, O. I.
* AIMMS, E&H: Environmental Bioanalytical Chemistry, RAS - Institute of Cytology, St. Petersburg State University, Russian Academy of Sciences, RAS - National Scientific Center of Marine Biology, Far Eastern Branch
* Scientific Reports
* https://doi.org/10.1038/s41598-022-18283-9
* Corresponding author: Daugavet, M. A.
* Published 22 Aug 2022 (early online None)
* Processed: 2022-8

The phenol oxidase system is ancient and ubiquitously distributed in all living organisms. In various groups it serves for the biosynthesis of pigments and neurotransmitters (dopamine), defence reacti ...

### *20) An excess of glycolytic enzymes under glucose-limited conditions may enable Saccharomyces cerevisiae to adapt to nutrient availability*

* Grigaitis, P., Teusink, B.
* Systems Bioinformatics, AIMMS, Systems Bioinformatics
* FEBS Letters
* https://doi.org/10.1002/1873-3468.14484
* Corresponding author: Grigaitis, P.
* Published 25 Aug 2022 (early online None)
* Processed: 2022-8

Microorganisms, including the budding yeast Saccharomyces cerevisiae, express glycolytic proteins to a maximal capacity that (largely) exceeds the actual flux through the enzymes, especially at low gr ...

### *21) Enantioselective Total Synthesis of (−)-Limaspermidine and (−)-Kopsinine by a Nitroaryl Transfer Cascade Strategy*

* Horst, B., Verdoorn, D. S., Hennig, S., van der Heijden, G., Ruijter, E.
* AIMMS, Organic Chemistry, Vrije Universiteit Amsterdam
* Angewandte Chemie. International Edition
* https://doi.org/10.1002/anie.202210592
* Corresponding author: Ruijter, E.
* Published 25 Aug 2022 (early online None)
* Processed: 2022-8

We report an intramolecular conjugate addition/Truce-Smiles/E1cb cascade of 2-nitrobenzenesulfonamide-functionalized cyclohexenones as a new entry to the core scaffold of monoterpene indole alkaloids. ...

### *22) Efficient simulation of resonance Raman spectra with tight-binding approximations to density functional theory*

* Ashtari-Jafari, S., Jamshidi, Z., Visscher, L.
* Theoretical Chemistry, AIMMS, Chemistry and Chemical Engineering Research Center of Iran, Vrije Universiteit Amsterdam
* Journal of Chemical Physics
* https://doi.org/10.1063/5.0107220
* Corresponding author: Visscher, L.
* Published 28 Aug 2022 (early online 22 Aug 2022)
* Processed: 2022-8

Resonance Raman spectroscopy has long been established as one of the most sensitive techniques for detection, structure characterization, and probing the excited-state dynamics of biochemical systems. ...

### *23) Density functionals based on the mathematical structure of the strong-interaction limit of DFT*

* Vuckovic, S., Gerolin, A., Daas, T. J., Bahmann, H., Friesecke, G., Gori-Giorgi, P.
* Theoretical Chemistry, AIMMS, University of Wuppertal, Technical University of Munich
* Wiley Interdisciplinary Reviews: Computational Molecular Science
* https://doi.org/10.1002/wcms.1634
* Corresponding author: Vuckovic, S.
* Published 29 Aug 2022 (early online None)
* Processed: 2022-8

While in principle exact, Kohn–Sham density functional theory—the workhorse of computational chemistry—must rely on approximations for the exchange–correlation functional. Despite staggering successes ...

### *24) Assessing the feasibility of stationary-phase-assisted modulation for two-dimensional liquid-chromatography separations*

* den Uijl, M. J., Roeland, T., Bos, T. S., Schoenmakers, P. J., van Bommel, M. R., Pirok, B. W. J.
* BioAnalytical Chemistry, AIMMS, University of Amsterdam, Center for Analytical Sciences Amsterdam (CASA)
* Journal of Chromatography A
* https://doi.org/10.1016/j.chroma.2022.463388
* Corresponding author: den Uijl, M. J.
* Published 30 Aug 2022 (early online 1 Aug 2022)
* Processed: 2022-8

Two-dimensional liquid chromatography (2DLC) offers great separation power for complex mixtures. The frequently encountered incompatibility of two orthogonal separation systems, however, makes its app ...