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### 1) Easy Access to Phosphine-Borane Building Blocks

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* Chemistry - A European Journal
* https://doi.org/10.1002/chem.202002367
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* Published 4 Dec 2020 (early online 30 Jun 2020)
* Processed: 2020-12

In this paper, we highlight the synthesis of a variety of primary phosphine-boranes (RPH2⋅BH3) from the corresponding dichlorophosphines, simply by using Li[BH4] as reductant and provider of the BH3 protecting group. The method offers facile access not only to alkyl- and arylphosphine-boranes, but also to aminophosphine-boranes (R2NPH2⋅BH3) that are convenient building blocks but without the protecting BH3 moiety thermally labile and notoriously difficult to handle. The borane-protected primary phosphines can be doubly deprotonated using n-butyllithium to provide soluble phosphanediides Li2[RP⋅BH3] of which the phenyl-derivative Li2[PhP⋅BH3] was structurally characterized in the solid state.

### 2) A Unified Framework for Understanding Nucleophilicity and Protophilicity in the SN2/E2 Competition

* Vermeeren, P., Hansen, T., Jansen, P., Swart, M., Hamlin, T. A., Bickelhaupt, F. M.
* Theoretical Chemistry, AIMMS, Chemistry and Pharmaceutical Sciences, Vrije Universiteit Amsterdam, Swiss Federal Institute of Technology Zurich, ICREA, University of Girona
* Chemistry - A European Journal
* https://doi.org/10.1002/chem.202003831
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* Published 1 Dec 2020 (early online 31 Aug 2020)
* Processed: 2020-12

The concepts of nucleophilicity and protophilicity are fundamental and ubiquitous in chemistry. A case in point is bimolecular nucleophilic substitution (SN2) and base-induced elimination (E2). A Lewis base acting as a strong nucleophile is needed for SN2 reactions, whereas a Lewis base acting as a strong protophile (i.e., base) is required for E2 reactions. A complicating factor is, however, the fact that a good nucleophile is often a strong protophile. Nevertheless, a sound, physical model that explains, in a transparent manner, when an electron-rich Lewis base acts as a protophile or a nucleophile, which is not just phenomenological, is currently lacking in the literature. To address this fundamental question, the potential energy surfaces of the SN2 and E2 reactions of X−+C2H5Y model systems with X, Y = F, Cl, Br, I, and At, are explored by using relativistic density functional theory at ZORA-OLYP/TZ2P. These explorations have yielded a consistent overview of reactivity trends over a wide range in reactivity and pathways. Activation strain analyses of these reactions reveal the factors that determine the shape of the potential energy surfaces and hence govern the propensity of the Lewis base to act as a nucleophile or protophile. The concepts of “characteristic distortivity” and “transition state acidity” of a reaction are introduced, which have the potential to enable chemists to better understand and design reactions for synthesis.

### 3) NMR in target driven drug discovery: why not?

* Keiffer, S., Carneiro, M. G., Hollander, J., Kobayashi, M., Pogoryelev, D., Ab, E., Theisgen, S., Müller, G., Siegal, G.
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* Journal of Biomolecular NMR
* https://doi.org/10.1007/s10858-020-00343-9
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* Published Nov 2020 (early online 8 Sep 2020)
* Processed: 2020-11

No matter the source of compounds, drug discovery campaigns focused directly on the target are entirely dependent on a consistent stream of reliable data that reports on how a putative ligand interacts with the protein of interest. The data will derive from many sources including enzyme assays and many types of biophysical binding assays such as TR-FRET, SPR, thermophoresis and many others. Each method has its strengths and weaknesses, but none is as information rich and broadly applicable as NMR. Here we provide a number of examples of the utility of NMR for enabling and providing ongoing support for the early pre-clinical phase of small molecule drug discovery efforts. The examples have been selected for their usefulness in a commercial setting, with full understanding of the need for speed, cost-effectiveness and ease of implementation.

### 4) Lifestyle, metabolism and environmental adaptation in Lactococcus lactis

* Kleerebezem, M., Bachmann, H., van Pelt-KleinJan, E., Douwenga, S., Smid, E. J., Teusink, B., van Mastrigt, O.
* Systems Bioinformatics, AIMMS, Systems Bioinformatics, Wageningen University & Research, Vrije Universiteit Amsterdam, TI Food and Nutrition
* FEMS Microbiology Reviews
* https://doi.org/10.1093/femsre/fuaa033
* Corresponding author: None
* Published 24 Nov 2020 (early online 29 Sep 2020)
* Processed: 2020-11

Lactococcus lactis serves as a paradigm organism for the lactic acid bacteria (LAB). Extensive research into the molecular biology, metabolism and physiology of several model strains of this species has been fundamental for our understanding of the LAB. Genomic studies have provided new insights into the species L. lactis, including the resolution of the genetic basis of its subspecies division, as well as the control mechanisms involved in the fine-tuning of growth rate and energy metabolism. In addition, it has enabled novel approaches to study lactococcal lifestyle adaptations to the dairy application environment, including its adjustment to near-zero growth rates that are particularly relevant in the context of cheese ripening. This review highlights various insights in these areas and exemplifies the strength of combining experimental evolution with functional genomics and bacterial physiology research to expand our fundamental understanding of the L. lactis lifestyle under different environmental conditions.

### 5) Searching for principles of microbial physiology

* Bruggeman, F. J., Planqué, R., Molenaar, D., Teusink, B.
* Systems Bioinformatics, AIMMS, Mathematics, Systems Bioinformatics
* FEMS Microbiology Reviews
* https://doi.org/10.1093/femsre/fuaa034
* Corresponding author: None
* Published 24 Nov 2020 (early online 21 Sep 2020)
* Processed: 2020-11

Why do evolutionarily distinct microorganisms display similar physiological behaviours? Why are transitions from high-ATP yield to low(er)-ATP yield metabolisms so widespread across species? Why is fast growth generally accompanied with low stress tolerance? Do these regularities occur because most microbial species are subject to the same selective pressures and physicochemical constraints? If so, a broadly-applicable theory might be developed that predicts common microbiological behaviours. Microbial systems biologists have been working out the contours of this theory for the last two decades, guided by experimental data. At its foundations lie basic principles from evolutionary biology, enzyme biochemistry, metabolism, cell composition and steady-state growth. The theory makes predictions about fitness costs and benefits of protein expression, physicochemical constraints on cell growth and characteristics of optimal metabolisms that maximise growth rate. Comparisons of the theory with experimental data indicates that microorganisms often aim for maximisation of growth rate, also in the presence of stresses; they often express optimal metabolisms and metabolic proteins at optimal concentrations. This review explains the current status of the theory for microbiologists; its roots, predictions, experimental evidence and future directions.

### 6) Nature and Strength of Lewis Acid/Base Interaction in Boron and Nitrogen Trihalides

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* Theoretical Chemistry, AIMMS, Universidade Federal de Lavras
* Chemistry - An Asian Journal
* https://doi.org/10.1002/asia.202001127
* Corresponding author: Hamlin, T. A.
* Published 1 Dec 2020 (early online 5 Oct 2020)
* Processed: 2020-12

We have quantum chemically investigated the bonding between archetypical Lewis acids and bases. Our state-of-the-art computations on the X3B−NY3 Lewis pairs have revealed the origin behind the systematic increase in B−N bond strength as X and Y are varied from F to Cl, Br, I, H. For H3B−NY3, the bonding trend is driven by the commonly accepted mechanism of donor−acceptor [HOMO(base)−LUMO(acid)] interaction. Interestingly, for X3B−NH3, the bonding mechanism is determined by the energy required to deform the BX3 to the pyramidal geometry it adopts in the adduct. Thus, Lewis acids that can more easily pyramidalize form stronger bonds with Lewis bases. The decrease in the strain energy of pyramidalization on going from BF3 to BI3 is directly caused by the weakening of the B−X bond strength, which stems primarily from the bonding in the plane of the molecule (σ-like) and not in the π system, at variance with the currently accepted mechanism.

### 7) The Nature of Nonclassical Carbonyl Ligands Explained by Kohn–Sham Molecular Orbital Theory

* van der Lubbe, S. C., Vermeeren, P., Fonseca Guerra, C., Bickelhaupt, F. M.
* Theoretical Chemistry, AIMMS, Chemistry and Pharmaceutical Sciences
* Chemistry - A European Journal
* https://doi.org/10.1002/chem.202003768
* Corresponding author: Bickelhaupt, F. M.
* Published 1 Dec 2020 (early online 12 Oct 2020)
* Processed: 2020-12

When carbonyl ligands coordinate to transition metals, their bond distance either increases (classical) or decreases (nonclassical) with respect to the bond length in the isolated CO molecule. C−O expansion can easily be understood by π-back-donation, which results in a population of the CO's π\*-antibonding orbital and hence a weakening of its bond. Nonclassical carbonyl ligands are less straightforward to explain, and their nature is still subject of an ongoing debate. In this work, we studied five isoelectronic octahedral complexes, namely Fe(CO)62+, Mn(CO)6+, Cr(CO)6, V(CO)6− and Ti(CO)62−, at the ZORA-BLYP/TZ2P level of theory to explain this nonclassical behavior in the framework of Kohn–Sham molecular orbital theory. We show that there are two competing forces that affect the C−O bond length, namely electrostatic interactions (favoring C−O contraction) and π-back-donation (favoring C−O expansion). It is a balance between those two terms that determines whether the carbonyl is classical or nonclassical. By further decomposing the electrostatic interaction ΔVelstat into four fundamental terms, we are able to rationalize why ΔVelstat gives rise to the nonclassical behavior, leading to new insights into the driving forces behind C−O contraction.

### 8) Implications of the unitary invariance and symmetry restrictions on the development of proper approximate one-body reduced-density-matrix functionals

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* Theoretical Chemistry, AIMMS
* Physical Review A
* https://doi.org/10.1103/PhysRevA.102.052814
* Corresponding author: Giesbertz, K. J.
* Published 16 Nov 2020 (early online None)
* Processed: 2020-11

In many of the approximate functionals in one-body reduced-density-matrix (1RDM) functional theory, the approximate two-body reduced density matrix (2RDM) in the natural orbital representation only depends on the natural occupation numbers. In Phys. Rev. A 92, 012520 (2015)PLRAAN1050-294710.1103/PhysRevA.92.012520, Wang and Knowles initialized a discussion of to what extent this simplification is valid by introducing two different H4 geometries with identical natural occupation numbers but different 2RDMs. Gritsenko has argued that this feature is due symmetry [Phys. Rev. A 97, 026501 (2018)2469-992610.1103/PhysRevA.97.026501]. This work aims to contribute to the discussion on the following points: (1) one should rather speak of symmetry-restricted variants of the universal functional than saying that the universal functional is symmetry dependent; (2) the unitary invariance of degenerate NOs can lead to large deviations in the 2RDM elements, especially the phase of the NOs; (3) symmetry-restricted functionals are constructed for the H4 geometries considered by Wang and Knowles, whose structure could serve as guide in the construction of approximate 1RDM functionals.

### 9) Advanced fluorescence microscopy reveals disruption of dynamic CXCR4 dimerization by subpocket-specific inverse agonists

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* Proceedings of the National Academy of Sciences of the United States of America
* https://doi.org/10.1073/pnas.2013319117
* Corresponding author: None
* Published 17 Nov 2020 (early online 4 Nov 2020)
* Processed: 2020-11

Although class A G protein-coupled receptors (GPCRs) can function as monomers, many of them form dimers and oligomers, but the mechanisms and functional relevance of such oligomerization is ill understood. Here, we investigate this problem for the CXC chemokine receptor 4 (CXCR4), a GPCR that regulates immune and hematopoietic cell trafficking, and a major drug target in cancer therapy. We combine single-molecule microscopy and fluorescence fluctuation spectroscopy to investigate CXCR4 membrane organization in living cells at densities ranging from a few molecules to hundreds of molecules per square micrometer of the plasma membrane. We observe that CXCR4 forms dynamic, transient homodimers, and that the monomer-dimer equilibrium is governed by receptor density. CXCR4 inverse agonists that bind to the receptor minor pocket inhibit CXCR4 constitutive activity and abolish receptor dimerization. A mutation in the minor binding pocket reduced the dimer-disrupting ability of these ligands. In addition, mutating critical residues in the sixth transmembrane helix of CXCR4 markedly diminished both basal activity and dimerization, supporting the notion that CXCR4 basal activity is required for dimer formation. Together, these results link CXCR4 dimerization to its density and to its activity. They further suggest that inverse agonists binding to the minor pocket suppress both dimerization and constitutive activity and may represent a specific strategy to target CXCR4.

### 10) Universal on-top description of electron correlation in the ground and excited many-electron states with correlon quasiparticles

* Jangrouei, M. R., Pernal, K., Gritsenko, O. V.
* Theoretical Chemistry, AIMMS, Lodz University of Technology
* Physical Review A
* https://doi.org/10.1103/PhysRevA.102.052829
* Corresponding author: Gritsenko, O. V.
* Published 25 Nov 2020 (early online None)
* Processed: 2020-11

On-top conditional correlation functions of many-electron theory are rearranged into a set of correlon quasiparticles representing the local effect of electron correlation in the ground and excited states. An individual correlon is characterized with a one-particle wave function, the imaginary part of which (or covalent correlon) gives the amplitude of the on-top depletion of the (conditional electron) charge (ODC) due to (strong) electron correlation. In its turn, the real part (ionic correlon) gives the amplitude of the on-top accumulation of the (electron) charge (OAC) due to the ionic squeezing of electrons. The proposed correlon theory is applied to analyze the local correlation effects in the ground and first excited states of the hydrogen molecule as well as of the equidistant and alternate linear hydrogen chains from H4 to H12. The covalent and ionic correlons obtained at the multiconfigurational self-consistent-field level of correlated functions are demonstrated to be the robust descriptors of the covalency of the ground and the ionicity of the excited Hn states.

### 11) Fragment-derived modulators of an industrial β-glucosidase

* Makraki, E., Darby, J. F., Carneiro, M. G., Firth, J. D., Heyam, A., Ab, E., O'Brien, P., Siegal, G., Hubbard, R. E.
* Chemistry and Pharmaceutical Sciences, AIMMS, University of York, University of Sheffield, ZoBio B.V., Vernalis PLC
* The Biochemical journal
* https://doi.org/10.1042/BCJ20200507
* Corresponding author: None
* Published 27 Nov 2020 (early online None)
* Processed: 2020-11

A fragment screen of a library of 560 commercially available fragments using a kinetic assay identified a small molecule that increased the activity of the fungal glycoside hydrolase TrBgl2. An analogue by catalogue approach and detailed kinetic analysis identified improved compounds that behaved as nonessential activators with up to a 2-fold increase in maximum activation. The compounds did not activate the related bacterial glycoside hydrolase CcBglA demonstrating specificity. Interestingly, an analogue of the initial fragment inhibits both TrBgl2 and CcBglA, apparently through a mixed-model mechanism. Although it was not possible to determine crystal structures of activator binding to 55 kDa TrBgl2, solution NMR experiments demonstrated a specific binding site for the activator. A partial assignment of the NMR spectrum gave the identity of the amino acids at this site, allowing a model for TrBgl2 activation to be built. The activator binds at the entrance of the substrate-binding site, generating a productive conformation for the enzyme-substrate complex.

### 12) Supercritical fluid chromatography – Mass spectrometry in metabolomics: Past, present, and future perspectives

* van de Velde, B., Guillarme, D., Kohler, I.
* BioAnalytical Chemistry, AIMMS, Vrije Universiteit Amsterdam, Center for Analytical Sciences Amsterdam, University of Geneva
* Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences
* https://doi.org/10.1016/j.jchromb.2020.122444
* Corresponding author: Kohler, I.
* Published 15 Dec 2020 (early online 17 Nov 2020)
* Processed: 2020-12

Metabolomics, which consists of the comprehensive analysis of metabolites within a biological system, has been playing a growing role in the implementation of personalized medicine in modern healthcare. A wide range of analytical approaches are used in metabolomics, notably mass spectrometry (MS) combined to liquid chromatography (LC), gas chromatography (GC), or capillary electrophoresis (CE). However, none of these methods enable a comprehensive analysis of the metabolome, due to its extreme complexity and the large differences in physico-chemical properties between metabolite classes. In this context, supercritical fluid chromatography (SFC) represents a promising alternative approach to improve the metabolome coverage, while further increasing the analysis throughput. SFC, which uses supercritical CO2 as mobile phase, leads to numerous advantages such as improved kinetic performance and lower environmental impact. This chromatographic technique has gained a significant interest since the introduction of advanced instrumentation, together with the introduction of dedicated interfaces for hyphenating SFC to MS. Moreover, new developments in SFC column chemistry (including sub-2 µm particles), as well as the use of large amounts of organic modifiers and additives in the CO2-based mobile phase, significantly extended the application range of SFC, enabling the simultaneous analysis of a large diversity of metabolites. Over the last years, several applications have been reported in metabolomics using SFC-MS – from lipophilic compounds, such as steroids and other lipids, to highly polar compounds, such as carbohydrates, amino acids, or nucleosides. With all these advantages, SFC-MS is promised to a bright future in the field of metabolomics.

### 13) Enhancement of amino acid production and secretion by Lactococcus lactis using a droplet-based biosensing and selection system

* Hernandez-Valdes, J. A., aan de Stegge, M., Hermans, J., Teunis, J., van Tatenhove-Pel, R. J., Teusink, B., Bachmann, H., Kuipers, O. P.
* AIMMS, Systems Bioinformatics, Molecular Cell Biology, Systems Bioinformatics, University of Groningen, Faculty of Medical Sciences
* Metabolic Engineering Communications
* https://doi.org/10.1016/j.mec.2020.e00133
* Corresponding author: Kuipers, O. P.
* Published Dec 2020 (early online None)
* Processed: 2020-12

Amino acids are attractive metabolites for the pharmaceutical and food industry field. On one hand, the construction of microbial cell factories for large-scale production aims to satisfy the demand for amino acids as bulk biochemical. On the other hand, amino acids enhance flavor formation in fermented foods. Concerning the latter, flavor formation in dairy products, such as cheese is associated with the presence of lactic acid bacteria (LAB). In particular, Lactococcus lactis, one of the most important LAB, is used as a starter culture in fermented foods. The proteolytic activity of some L. lactis strains results in peptides and amino acids, which are flavor compounds or flavor precursors. However, it is still a challenge to isolate bacterial cells with enhanced amino acid production and secretion activity. In this work, we developed a growth-based sensor strain to detect the essential amino acids isoleucine, leucine, valine, histidine and methionine. Amino acids are metabolites that can be secreted by some bacteria. Therefore, our biosensor allowed us to identify wild-type L. lactis strains that naturally secrete amino acids, by using co-cultures of the biosensor strain with potential amino acid producing strains. Subsequently, we used this biosensor in combination with a droplet-based screening approach, and isolated three mutated L. lactis IPLA838 strains with 5–10 fold increased amino acid-secretion compared to the wild type. Genome re-sequencing revealed mutations in genes encoding proteins that participate in peptide uptake and peptide degradation. We argue that an unbalance in the regulation of amino acid levels as a result of these gene mutations may drive the accumulation and secretion of these amino acids. This biosensing system tackles the problem of selection for overproduction of secreted molecules, which requires the coupling of the product to the producing cell in the droplets.

### 14) Characterization of glycosyl dioxolenium ions and their role in glycosylation reactions

* Hansen, T., Elferink, H., van Hengst, J. M., Houthuijs, K. J., Remmerswaal, W. A., Kromm, A., Berden, G., van der Vorm, S., Rijs, A. M., Overkleeft, H. S., Filippov, D. V., Rutjes, F. P., van der Marel, G. A., Martens, J., Oomens, J., Codée, J. D., Boltje, T. J.
* Chemistry and Pharmaceutical Sciences, AIMMS, BioAnalytical Chemistry, Radboud University Nijmegen, Leiden University, Leiden University
* Nature Communications
* https://doi.org/10.1038/s41467-020-16362-x
* Corresponding author: Codée, J. D.
* Published 1 Dec 2020 (early online None)
* Processed: 2020-12

Controlling the chemical glycosylation reaction remains the major challenge in the synthesis of oligosaccharides. Though 1,2-trans glycosidic linkages can be installed using neighboring group participation, the construction of 1,2-cis linkages is difficult and has no general solution. Long-range participation (LRP) by distal acyl groups may steer the stereoselectivity, but contradictory results have been reported on the role and strength of this stereoelectronic effect. It has been exceedingly difficult to study the bridging dioxolenium ion intermediates because of their high reactivity and fleeting nature. Here we report an integrated approach, using infrared ion spectroscopy, DFT computations, and a systematic series of glycosylation reactions to probe these ions in detail. Our study reveals how distal acyl groups can play a decisive role in shaping the stereochemical outcome of a glycosylation reaction, and opens new avenues to exploit these species in the assembly of oligosaccharides and glycoconjugates to fuel biological research.

### 15) ProVision: a web-based platform for rapid analysis of proteomics data processed by MaxQuant

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* Bioinformatics (Oxford, England)
* https://doi.org/10.1093/bioinformatics/btaa620
* Corresponding author: None
* Published 8 Dec 2020 (early online None)
* Processed: 2020-12

SUMMARY: Proteomics is a powerful tool for protein expression analysis and is becoming more readily available to researchers through core facilities or specialized collaborations. However, one major bottleneck for routine implementation and accessibility of this technology to the wider scientific community is the complexity of data analysis. To this end, we have created ProVision, a free open-source web-based analytics platform that allows users to analyze data from two common proteomics relative quantification workflows, namely label-free and tandem mass tag-based experiments. Furthermore, ProVision allows the freedom to interface with the data analysis pipeline while maintaining a user-friendly environment and providing default parameters for fast statistical and exploratory data analysis. Finally, multiple customizable quality control, differential expression plots as well as enrichments and protein-protein interaction prediction can be generated online in one platform. AVAILABILITY AND IMPLEMENTATION: Quick start and step-by-step tutorials as well as tutorial data are fully incorporated in the web application. This application is available online at https://provision.shinyapps.io/provision/ for free use. The source code is available at https://github.com/JamesGallant/ProVision under the GPL version 3.0 license.

### *16) Improving the Environmental Risk Assessment of Substances of Unknown or Variable Composition, Complex Reaction Products, or Biological Materials*

* Salvito, D., Fernandez, M., Jenner, K., Lyon, D. Y., de Knecht, J., Mayer, P., MacLeod, M., Eisenreich, K., Leonards, P., Cesnaitis, R., León-Paumen, M., Embry, M., Déglin, S. E.
* E&H: Environmental Bioanalytical Chemistry, AIMMS, Research Institute for Fragrance Materials Inc., Environment and Climate Change Canada, Givaudan, Shell Oil, National Institute of Public Health and the Environment, Technical University of Denmark, Stockholm University, United States Environmental Protection Agency, European Chemicals Agency, ExxonMobil Biomedical Sciences Inc., Health and Environmental Sciences Institute
* Environmental toxicology and chemistry
* https://doi.org/10.1002/etc.4846
* Corresponding author: Déglin, S. E.
* Published 1 Nov 2020 (early online 11 Aug 2020)
* Processed: 2020-11

Substances of unknown or variable composition, complex reaction products, or biological materials (UVCBs) pose unique risk assessment challenges to regulators and to product registrants. These substan ...

### *17) An Optimal Transport Approach for the Schrödinger Bridge Problem and Convergence of Sinkhorn Algorithm*

* Marino, S. D., Gerolin, A.
* Theoretical Chemistry, AIMMS, Scuola Normale Superiore di Pisa, University of Genoa
* Journal of Scientific Computing
* https://doi.org/10.1007/s10915-020-01325-7
* Corresponding author: Gerolin, A.
* Published 1 Nov 2020 (early online 19 Oct 2020)
* Processed: 2020-11

This paper exploit the equivalence between the Schrödinger Bridge problem (Léonard in J Funct Anal 262:1879–1920, 2012; Nelson in Phys Rev 150:1079, 1966; Schrödinger in Über die umkehrung der naturge ...

### *18) A protein tertiary structure mimetic modulator of the Hippo signalling pathway*

* Adihou, H., Gopalakrishnan, R., Förster, T., Guéret, S. M., Gasper, R., Geschwindner, S., Carrillo García, C., Karatas, H., Pobbati, A. V., Vazquez‐Chantada, M., Davey, P., Wassvik, C. M., Pang, J. K. S., Soh, B. S., Hong, W., Chiarparin, E., Schade, D., Plowright, A. T., Valeur, E., Lemurell, M., Grossmann, T. N., Waldmann, H.
* Organic Chemistry, AIMMS, AstraZeneca Sweden, AstraZeneca, Max Planck Institute of Molecular Physiology, Kiel University, Agency for Science, Technology and Research, National University of Singapore, Guangzhou Medical College, Dortmund University
* Nature Communications
* https://doi.org/10.1038/s41467-020-19224-8
* Corresponding author: Waldmann, H.
* Published 1 Nov 2020 (early online None)
* Processed: 2020-11

Transcription factors are key protein effectors in the regulation of gene transcription, and in many cases their activity is regulated via a complex network of protein–protein interactions (PPI). The ...

### *19) Is it worthwhile to go beyond the local-density approximation in subsystem density functional theory?*

* Grimmel, S. A., Teodoro, T. Q., Visscher, L.
* Theoretical Chemistry, AIMMS, Vrije Universiteit Amsterdam, Vrije Universiteit Amsterdam
* International Journal of Quantum Chemistry
* https://doi.org/10.1002/qua.26111
* Corresponding author: Visscher, L.
* Published 1 Nov 2020 (early online 11 Dec 2019)
* Processed: 2020-11

Frozen density embedding (FDE) theory is one of the major techniques aiming to bring modeling of extended chemical systems into the realm of high accuracy calculations. To improve its accuracy it is o ...

### *20) Efficient data structures for range shortest unique substring queries*

* Abedin, P., Ganguly, A., Pissis, S. P., Thankachan, S. V.
* Bioinformatics, AIMMS, Bio Informatics (IBIVU), University of Central Florida, University of Wisconsin-Whitewater
* Algorithms
* https://doi.org/10.3390/a13110276
* Corresponding author: Pissis, S. P.
* Published Nov 2020 (early online 30 Oct 2020)
* Processed: 2020-11

†Let T[1, n] be a string of length n and T[i, j] be the substring of T starting at position i and ending at position j. A substring T[i, j] of T is a repeat if it occurs more than once in T; otherwise ...

### *21) Bromo-cyclobutenaminones as new covalent udp-n-acetylglucosamine enolpyruvyl transferase (Mura) inhibitors*

* Hamilton, D. J., Ábrányi-Balogh, P., Keeley, A., Petri, L., Hrast, M., Imre, T., Wijtmans, M., Gobec, S., de Esch, I. J., Keserű, G. M.
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* Pharmaceuticals
* https://doi.org/10.3390/ph13110362
* Corresponding author: Keserű, G. M.
* Published Nov 2020 (early online 3 Nov 2020)
* Processed: 2020-11

Drug discovery programs against the antibacterial target UDP-N-acetylglucosamine enolpyruvyl transferase (MurA) have already resulted in covalent inhibitors having small threeand five-membered heteroc ...

### *22) Stress-based high-throughput screening assays to identify inhibitors of cell envelope biogenesis*

* Steenhuis, M., Ten Hagen-Jongman, C. M., van Ulsen, P., Luirink, J.
* Molecular Microbiology, AIMMS, LaserLaB - Analytical Chemistry and Spectroscopy, LaserLaB - Molecular Biophysics
* Antibiotics
* https://doi.org/10.3390/antibiotics9110808
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* Published Nov 2020 (early online None)
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The structural integrity of the Gram-negative cell envelope is guarded by several stress responses, such as the σE, Cpx and Rcs systems. Here, we report on assays that monitor these responses in E. co ...

### *23) Assessing the Legitimacy of Technological Innovation in the Public Sphere: Recovering Raw Materials from Waste Water*

* Blankesteijn, M., Bossink, B.
* Biophysics Photosynthesis/Energy, Science & Business Innovation, AIMMS
* Sustainability
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This paper researches legitimacy creation in a publicly-funded trajectory of innovative technological development. It develops a framework of input, throughput and output legitimacy. The framework is ...