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### 1) N-Heterocyclic Silylenes as Ligands in Transition Metal Carbonyl Chemistry: Nature of Their Bonding and Supposed Innocence

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* Chemistry - A European Journal
* https://doi.org/10.1002/chem.202001062
* Corresponding author: Radius, U.
* Published 1 Sep 2020 (early online 31 Mar 2020)
* Processed: 2020-9

A study on the reactivity of the N-heterocyclic silylene Dipp2NHSi (1,3-bis(diisopropylphenyl)-1,3-diaza-2-silacyclopent-4-en-2-yliden) with the transition metal complexes [Ni(CO)4], [M(CO)6] (M=Cr, Mo, W), [Mn(CO)5(Br)] and [(η5-C5H5)Fe(CO)2(I)] is reported. We demonstrate that N-heterocyclic silylenes, the higher homologues of the now ubiquitous NHC ligands, show a remarkably different behavior in coordination chemistry compared to NHC ligands. Calculations on the electronic features of these ligands revealed significant differences in the frontier orbital region which lead to some peculiarities of the coordination chemistry of silylenes, as demonstrated by the synthesis of the dinuclear, NHSi-bridged complex [{Ni(CO)2(μ-Dipp2NHSi)}2] (2), complexes [M(CO)5(Dipp2NHSi)] (M=Cr 3, Mo 4, W 5), [Mn(CO)3(Dipp2NHSi)2(Br)] (9) and [(η5-C5H5)Fe(CO)2(Dipp2NHSi-I)] (10). DFT calculations on several model systems [Ni(L)], [Ni(CO)3(L)], and [W(CO)5(L)] (L=NHC, NHSi) reveal that carbenes are typically the much better donor ligands with a larger intrinsic strength of the metal–ligand bond. The decrease going from the carbene to the silylene ligand is mainly caused by favorable electrostatic contributions for the NHC ligand to the total bond strength, whereas the orbital interactions were often found to be higher for the silylene complexes. Furthermore, we have demonstrated that the contribution of σ- and π-interaction depends significantly on the system under investigation. The σ-interaction is often much weaker for the NHSi ligand compared to NHC but, interestingly, the π-interaction prevails for many NHSi complexes. For the carbonyl complexes, the NHSi ligand is the better σ-donor ligand, and contributions of π-symmetry play only a minor role for the NHC and NHSi co-ligands.

### 2) Understanding the 1,3-Dipolar Cycloadditions of Allenes

* Yu, S., Vermeeren, P., van Dommelen, K., Bickelhaupt, F. M., Hamlin, T. A.
* Theoretical Chemistry, AIMMS, Chemistry and Pharmaceutical Sciences, VU University
* Chemistry - A European Journal
* https://doi.org/10.1002/chem.202000857
* Corresponding author: Bickelhaupt, F. M.
* Published 4 Sep 2020 (early online 27 Mar 2020)
* Processed: 2020-9

We have quantum chemically studied the reactivity, site-, and regioselectivity of the 1,3-dipolar cycloaddition between methyl azide and various allenes, including the archetypal allene propadiene, heteroallenes, and cyclic allenes, by using density functional theory (DFT). The 1,3-dipolar cycloaddition reactivity of linear (hetero)allenes decreases as the number of heteroatoms in the allene increases, and formation of the 1,5-adduct is, in all cases, favored over the 1,4-adduct. Both effects find their origin in the strength of the primary orbital interactions. The cycloaddition reactivity of cyclic allenes was also investigated, and the increased predistortion of allenes, that results upon cyclization, leads to systematically lower activation barriers not due to the expected variations in the strain energy, but instead from the differences in the interaction energy. The geometric predistortion of cyclic allenes enhances the reactivity compared to linear allenes through a unique mechanism that involves a smaller HOMO–LUMO gap, which manifests as more stabilizing orbital interactions.

### 3) Diastereoselective Synthesis of β-Lactams by Ligand-Controlled Stereodivergent Intramolecular Tsuji-Trost Allylation

* Faltracco, M., Sukowski, V., Van Druenen, M., Hamlin, T. A., Bickelhaupt, F. M., Ruijter, E.
* Organic Chemistry, AIMMS, Theoretical Chemistry, Chemistry and Pharmaceutical Sciences, VU University
* Journal of Organic Chemistry
* https://doi.org/10.1021/acs.joc.0c00575
* Corresponding author: Ruijter, E.
* Published 7 Aug 2020 (early online 25 Jun 2020)
* Processed: 2020-8

The diastereoselective synthesis of highly substituted β-lactams by intramolecular Tsuji-Trost allylation is reported. Judicious selection of the ligand on palladium allows selective access to either the trans isomer (in generally good to excellent yield with very high diastereomeric excess) or cis isomer (with yields and diastereoselectivity ranging from modest to excellent depending on the substrate). The reaction proceeds under exceedingly mild conditions (rt, no additives) with a broad range of substrates, which are readily accessible by the Ugi reaction.

### 4) Structure and Function of the Mycobacterial Type VII Secretion Systems

* Bunduc, C. M., Bitter, W., Houben, E. N. G.Pages:315-335
* Molecular Microbiology, AIMMS
* Annual Review of Microbiology
* https://doi.org/10.1146/annurev-micro-012420-081657
* Corresponding author: None
* Published 13 Jul 2020 (early online None)
* Processed: 2020-7

Bacteria have evolved intricate secretion machineries for the successful delivery of large molecules across their cell envelopes. Such specialized secretion systems allow a variety of bacteria to thrive in specific host environments. In mycobacteria, type VII secretion systems (T7SSs) are dedicated protein transport machineries that fulfill diverse and crucial roles, ranging from metabolite uptake to immune evasion and subversion to conjugation. Since the discovery of mycobacterial T7SSs about 15 y ago, genetic, structural, and functional studies have provided insight into the roles and functioning of these secretion machineries. Here, we focus on recent advances in the elucidation of the structure and mechanism of mycobacterial T7SSs in protein secretion. As many of these systems are essential for mycobacterial growth or virulence, they provide opportunities for the development of novel therapies to combat a number of relevant mycobacterial diseases. Expected final online publication date for the Annual Review of Microbiology, Volume 74 is September 8, 2020. Please see http://www.annualreviews.org/page/journal/pubdates for revised estimates.

### 5) Vibrational circular dichroism spectroscopy for probing the expression of chirality in mechanically planar chiral rotaxanes

* Koenis, M. A., Chibueze, C. S., Jinks, M. A., Nicu, V. P., Visscher, L., Goldup, S. M., Buma, W. J.
* Theoretical Chemistry, AIMMS, University of Amsterdam, University of Southampton, Lucian Blaga University of Sibiu, Radboud University Nijmegen
* Chemical Science
* https://doi.org/10.1039/d0sc02485f
* Corresponding author: Buma, W. J.
* Published 28 Aug 2020 (early online 23 Jul 2020)
* Processed: 2020-8

Mechanically interlocked molecules can exhibit molecular chirality that arises due to the mechanical bond rather than covalent stereogenic units. Developing applications of such systems is made challenging by the absence of techniques for assigning the absolute configuration of products and methods to probe how the mechanical stereogenic unit influences the spatial arrangements of the functional groups in solution. Here we demonstrate for the first time that Vibrational Circular Dichroism (VCD) can be used to not only discriminate between mechanical stereoisomers but also provide detailed information on their (co)conformations. The latter is particularly important as these molecules are now under investigation in catalysis and sensing, both of which rely on the solution phase shape of the interlocked structure. Detailed analysis of the VCD spectra shows that, although many of the signals arise from coupled oscillators isolated in the covalent sub-components, intercomponent coupling between the macrocycle and axle gives rise to several VCD bands.

### 6) Environmental Effects with Frozen-Density Embedding in Real-Time Time-Dependent Density Functional Theory Using Localized Basis Functions

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* Theoretical Chemistry, AIMMS, University of Perugia, Technical University of Braunschweig, Universite de Lille 2, Gabriele d’Annunzio University
* Journal of chemical theory and computation
* https://doi.org/10.1021/acs.jctc.0c00603
* Corresponding author: None
* Published 8 Sep 2020 (early online 27 Jul 2020)
* Processed: 2020-9

Frozen-density embedding (FDE) represents a versatile embedding scheme to describe the environmental effect on electron dynamics in molecular systems. The extension of the general theory of FDE to the real-time time-dependent Kohn-Sham method has previously been presented and implemented in plane waves and periodic boundary conditions [Pavanello, M.; J. Chem. Phys. 2015, 142, 154116]. In the current paper, we extend our recent formulation of the real-time time-dependent Kohn-Sham method based on localized basis set functions and developed within the Psi4NumPy framework to the FDE scheme. The latter has been implemented in its "uncoupled" flavor (in which the time evolution is only carried out for the active subsystem, while the environment subsystems remain at their ground state), using and adapting the FDE implementation already available in the PyEmbed module of the scripting framework PyADF. The implementation was facilitated by the fact that both Psi4NumPy and PyADF, being native Python API, provided an ideal framework of development using the Python advantages in terms of code readability and reusability. We employed this new implementation to investigate the stability of the time-propagation procedure, which is based on an efficient predictor/corrector second-order midpoint Magnus propagator employing an exact diagonalization, in combination with the FDE scheme. We demonstrate that the inclusion of the FDE potential does not introduce any numerical instability in time propagation of the density matrix of the active subsystem, and in the limit of the weak external field, the numerical results for low-lying transition energies are consistent with those obtained using the reference FDE calculations based on the linear-response TDDFT. The method is found to give stable numerical results also in the presence of a strong external field inducing nonlinear effects. Preliminary results are reported for high harmonic generation (HHG) of a water molecule embedded in a small water cluster. The effect of the embedding potential is evident in the HHG spectrum reducing the number of the well-resolved high harmonics at high energy with respect to the free water. This is consistent with a shift toward lower ionization energy passing from an isolated water molecule to a small water cluster. The computational burden for the propagation step increases approximately linearly with the size of the surrounding frozen environment. Furthermore, we have also shown that the updating frequency of the embedding potential may be significantly reduced, much less than one per time step, without jeopardizing the accuracy of the transition energies.

### 7) Light-Matter Hybrid-Orbital-Based First-Principles Methods: The Influence of Polariton Statistics

* Buchholz, F., Theophilou, I., Giesbertz, K. J., Ruggenthaler, M., Rubio, A.
* Theoretical Chemistry, AIMMS, Max Planck Institute for the Structure and Dynamics of Matter, Simons Foundation
* Journal of chemical theory and computation
* https://doi.org/10.1021/acs.jctc.0c00469
* Corresponding author: None
* Published 8 Sep 2020 (early online 21 Jul 2020)
* Processed: 2020-9

A detailed understanding of strong matter-photon interactions requires first-principle methods that can solve the fundamental Pauli-Fierz Hamiltonian of nonrelativistic quantum electrodynamics efficiently. A possible way to extend well-established electronic-structure methods to this situation is to embed the Pauli-Fierz Hamiltonian in a higher-dimensional light-matter hybrid auxiliary configuration space. In this work we show the importance of the resulting hybrid Fermi-Bose statistics of the polaritons, which are the new fundamental particles of the "photon-dressed" Pauli-Fierz Hamiltonian for systems in cavities. We show that violations of these statistics can lead to unphysical results. We present an efficient way to ensure the correct statistics by enforcing representability conditions on the dressed one-body reduced density matrix. We further present a general prescription how to extend a given first-principles approach to polaritons and as an example introduce polaritonic Hartree-Fock theory. While being a single-reference method in polariton space, polaritonic Hartree-Fock is a multireference method in the electronic space, i.e., it describes electronic correlations. We also discuss possible applications to polaritonic QEDFT. We apply this theory to a lattice model and find that, the more delocalized the bound-state wave function of the particles is, the stronger it reacts to photons. The main reason is that within a small energy range, many states with different electronic configurations are available as opposed to a strongly bound (and hence energetically separated) ground-state wave function. This indicates that under certain conditions coupling to the quantum vacuum of a cavity can indeed modify ground state properties.

### 8) Scientific Perspectivism in Secondary-School Chemistry Education: Integrating Concepts and Skills in Chemical Thinking

* Landa, I., Westbroek, H., Janssen, F., van Muijlwijk-Koezen, J. E., Meeter, M.
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* Science & Education
* https://doi.org/https://doi.org/10.1007/s11191-020-00145-3
* Corresponding author: Westbroek, H.
* Published 7 Aug 2020 (early online None)
* Processed: 2020-8

The importance of learning chemical ways of thinking is widely recognized. Various frameworks have been developed to address the essence of chemistry and chemical thinking. However, very few studies have focused on how chemical ways of thinking can be defined. To elaborate chemical ways of thinking, this paper draws on scientific perspectivism (Giere 2010; Wimsatt 2007; Thagard 2012). Scientific perspectivism states that, within each general domain, several broadly accepted theoretical models exist side by side. These general theoretical models, or theoretical perspectives, determine which research questions are generated, which types of models are developed, and which criteria are important for evaluating models. A theoretical perspective can be captured in a core reasoning that embodies the fundamental relationship between model and the “real world.” Starting with their most basic form, perspectives can be used in learning how to reason about all types of ill-structured problems, directing and organizing knowledge development, and integrating knowledge and skills. The study is part of a research project on how perspectivism can be applied to the design of secondary-school chemistry education. This particular study concerns the identification, elaboration, and validation of four chemical perspectives for secondary-school chemistry education. We use these perspectives to indicate the consequences of taking a perspectivism approach to a curriculum framework. We conclude with discussing the consequences for secondary chemistry curriculum.

### 9) MS-Based Allotype-Specific Analysis of Polyclonal Ig

* Sénard, T., Gargano, A. F., Falck, D., de Taeye, S. W., Rispens, T., Vidarsson, G., Wuhrer, M., Somsen, G. W., Domínguez-Vega, E.
* BioAnalytical Chemistry, AIMMS, Leiden University, Sanquin Blood Supply Foundation
* Frontiers in Immunology
* https://doi.org/10.3389/fimmu.2020.02049
* Corresponding author: Domínguez-Vega, E.
* Published 21 Aug 2020 (early online None)
* Processed: 2020-8

G-Fc N-GlycosylationCurrent approaches to study glycosylation of polyclonal human immunoglobulins G (IgG) usually imply protein digestion or glycan release. While these approaches allow in-depth characterization, they also result in a loss of valuable information regarding certain subclasses, allotypes and co-occuring post-translational modifications (PTMs). Unfortunately, the high variability of polyclonal IgGs makes their intact mass spectrometry (MS) analysis extremely challenging. We propose here a middle-up strategy for the analysis of the intact fragment crystallizable (Fc) region of human plasma IgGs, with the aim of acquiring integrated information of the N-glycosylation and other PTMs of subclasses and allotypes. Human plasma IgG was isolated using Fc-specific beads followed by an on-bead CH2 domain digestion with the enzyme IdeS. The obtained mixture of Fc subunits was analyzed by capillary electrophoresis (CE) and hydrophilic interaction liquid chromatography (HILIC) hyphenated with MS. CE-MS provided separation of different IgG-subclasses and allotypes, while HILIC-MS allowed resolution of the different glycoforms and their oxidized variants. The orthogonality of these techniques was key to reliably assign Fc allotypes. Five individual donors were analyzed using this approach. Heterozygosis was observed in all the analyzed donors resulting in a total of 12 allotypes identified. The assignments were further confirmed using recombinant monoclonal IgG allotypes as standards. While the glycosylation patterns were similar within allotypes of the same subclass, clear differences were observed between IgG subclasses and donors, highlighting the relevance of the proposed approach. In a single analysis, glycosylation levels specific for each allotype, relative abundances of subclasses and information on co-occurring modifications are obtained. This middle-up method represents an important step toward a comprehensive analysis of immunoglobulin G-Fc variants.

### 10) The constitutive activity of the viral-encoded G protein-coupled receptor US28 supports a complex signalling network contributing to cancer development

* Daly, C. A., Smit, M. J., Plouffe, B.
* Medicinal chemistry, AIMMS, Queen's University Belfast
* Biochemical Society transactions
* https://doi.org/10.1042/BST20190988
* Corresponding author: None
* Published 28 Aug 2020 (early online None)
* Processed: 2020-8

US28 is a viral G protein-coupled receptor (GPCR) encoded by the human cytomegalovirus (HCMV). This receptor, expressed both during lytic replication and viral latency, is required for latency. US28 is binding to a wide variety of chemokines but also exhibits a particularly high constitutive activity robustly modulating a wide network of cellular pathways altering the host cell environment to benefit HCMV infection. Several studies suggest that US28-mediated signalling may contribute to cancer progression. In this review, we discuss the unique structural characteristics that US28 acquired through evolution that confer a robust constitutive activity to this viral receptor. We also describe the wide downstream signalling network activated by this constitutive activation of US28 and discuss how these signalling pathways may promote and support important cellular aspects of cancer.

### 11) Neutralizing effects of small molecule inhibitors and metal chelators on coagulopathic Viperinae snake venom toxins

* Xie, C., Albulescu, L. O., Bittenbinder, M. A., Somsen, G. W., Vonk, F. J., Casewell, N. R., Kool, J.
* AIMMS, BioAnalytical Chemistry, Liverpool School of Tropical Medicine, VU University, Centre for Analytical Sciences Amsterdam (CASA), Naturalis Biodiversity Center
* Biomedicines
* https://doi.org/10.3390/BIOMEDICINES8090297
* Corresponding author: Kool, J.
* Published Sep 2020 (early online 20 Aug 2020)
* Processed: 2020-9

Animal-derived antivenoms are the only specific therapies currently available for the treatment of snake envenoming, but these products have a number of limitations associated with their efficacy, safety and affordability for use in tropical snakebite victims. Small molecule drugs and drug candidates are regarded as promising alternatives for filling the critical therapeutic gap between snake envenoming and effective treatment. In this study, by using an advanced analytical technique that combines chromatography, mass spectrometry and bioassaying, we investigated the effect of several small molecule inhibitors that target phospholipase A2 (varespladib) and snake venom metalloproteinase (marimastat, dimercaprol and DMPS) toxin families on inhibiting the activities of coagulopathic toxins found in Viperinae snake venoms. The venoms of Echis carinatus, Echis ocellatus, Daboia russelii and Bitis arietans, which are known for their potent haemotoxicities, were fractionated in high resolution onto 384-well plates using liquid chromatography followed by coagulopathic bioassaying of the obtained fractions. Bioassay activities were correlated to parallel recorded mass spectrometric and proteomics data to assign the venom toxins responsible for coagulopathic activity and assess which of these toxins could be neutralized by the inhibitors under investigation. Our results showed that the phospholipase A2-inhibitor varespladib neutralized the vast majority of anticoagulation activities found across all of the tested snake venoms. Of the snake venom metalloproteinase inhibitors, marimastat demonstrated impressive neutralization of the procoagulation activities detected in all of the tested venoms, whereas dimercaprol and DMPS could only partially neutralize these activities at the doses tested. Our results provide additional support for the concept that combinations of small molecules, particularly the combination of varespladib with marimastat, serve as a drug-repurposing opportunity to develop new broad-spectrum inhibitor-based therapies for snakebite envenoming.

### *12) Toddler behavior, the home environment, and flame retardant exposure*

* Sugeng, E. J., de Cock, M., Leonards, P. E., van de Bor, M.
* Environmental Health and Toxicology, AIMMS, Environmental Bioanalytical Chemistry, Environment and Health
* Chemosphere
* https://doi.org/10.1016/j.chemosphere.2020.126588
* Corresponding author: Sugeng, E. J.
* Published Aug 2020 (early online 23 Mar 2020)
* Processed: 2020-8

Toddlers are at increased risk of dust ingestion and subsequently flame retardant (FR) exposure because they often play close to the floor and mouth hands and objects. Exposure to some FRs have been a ...

### *13) Development of a high-throughput bioassay for screening of antibiotics in aquatic environmental samples*

* Jonkers, T. J., Steenhuis, M., Schalkwijk, L., Luirink, J., Bald, D., Houtman, C. J., Kool, J., Lamoree, M. H., Hamers, T.
* AIMMS, Environmental Chemistry and Toxicology, Molecular Microbiology, LaserLaB - Molecular Biophysics, Structural Biology, BioAnalytical Chemistry, Environmental Health and Toxicology, VU University, The Water Laboratory
* Science of the Total Environment
* https://doi.org/10.1016/j.scitotenv.2020.139028
* Corresponding author: Jonkers, T. J.
* Published 10 Aug 2020 (early online 28 Apr 2020)
* Processed: 2020-8

The goal of the present study was to select a Gram-positive (Gram+) and Gram-negative (Gram−) strain to measure antimicrobial activity in environmental samples, allowing high-throughput environmental ...

### *14) Human exposure to synthetic endocrine disrupting chemicals (S-EDCs) is generally negligible as compared to natural compounds with higher or comparable endocrine activity. How to evaluate the risk of the S-EDCs?*

* Autrup, H., Barile, F. A., Berry, S. C., Blaauboer, B. J., Boobis, A., Bolt, H., Borgert, C. J., Dekant, W., Dietrich, D., Domingo, J. L., Gori, G. B., Greim, H., Hengstler, J., Kacew, S., Marquardt, H., Pelkonen, O., Savolainen, K., Heslop-Harrison, P., Vermeulen, N. P.
* Chemistry and Pharmaceutical Sciences, AIMMS, Aarhus University, St. John's University, Queen Mary University of London, Utrecht University, Imperial College London, Dortmund University, Applied Pharmacology and Toxicology, Inc. Gainesville, University of Würzburg, University of Konstanz, Pere Virgili Health Research Institute, The Health Policy Center, University of Ottawa, Toxicology, University of Oulu, Finnish Institute of Occupational Health, University of Leicester
* Environmental Toxicology and Pharmacology
* https://doi.org/10.1016/j.etap.2020.103396
* Corresponding author: Dekant, W.
* Published Aug 2020 (early online 29 Apr 2020)
* Processed: 2020-8

Theoretically, both synthetic endocrine disrupting chemicals (S-EDCs) and natural (exogenous and endogenous) endocrine disrupting chemicals (N-EDCs) can interact with endocrine receptors and disturb h ...

### *15) Human exposure to synthetic endocrine disrupting chemicals (S-EDCs) is generally negligible as compared to natural compounds with higher or comparable endocrine activity. How to evaluate the risk of the S-EDCs?*

* Autrup, H., Barile, F. A., Berry, S. C., Blaauboer, B. J., Boobis, A., Bolt, H., Borgert, C. J., Dekant, W., Dietrich, D., Domingo, J. L., Gori, G. B., Greim, H., Hengstler, J., Kacew, S., Marquardt, H., Pelkonen, O., Savolainen, K., Heslop-Harrison, P., Vermeulen, N. P.
* Chemistry and Pharmaceutical Sciences, AIMMS, Aarhus University, St. John's University, Queen Mary University of London, Utrecht University, Imperial College London, Dortmund University, Applied Pharmacology and Toxicology, Inc., University of Würzburg, University of Konstanz, Pere Virgili Health Research Institute, The Health Policy Center, Technical University of Munich, University of Ottawa, Toxicology, University of Oulu, Finnish Institute of Occupational Health, University of Leicester
* Chemico-Biological Interactions
* https://doi.org/10.1016/j.cbi.2020.109099
* Corresponding author: Greim, H.
* Published 1 Aug 2020 (early online 1 May 2020)
* Processed: 2020-8

Theoretically, both synthetic endocrine disrupting chemicals (S-EDCs) and natural (exogenous and endogenous) endocrine disrupting chemicals (N-EDCs) can interact with endocrine receptors and disturb h ...

### *16) Computationally Guided Molecular Design to Minimize the LE/CT Gap in D-π-A Fluorinated Triarylboranes for Efficient TADF via D and π-Bridge Tuning*

* Narsaria, A. K., Rauch, F., Krebs, J., Endres, P., Friedrich, A., Krummenacher, I., Braunschweig, H., Finze, M., Nitsch, J., Bickelhaupt, F. M., Marder, T. B.
* Theoretical Chemistry, Chemistry and Pharmaceutical Sciences, AIMMS, University of Würzburg
* Advanced Functional Materials
* https://doi.org/10.1002/adfm.202002064
* Corresponding author: Bickelhaupt, F. M.
* Published 1 Aug 2020 (early online 2 Jun 2020)
* Processed: 2020-8

In this combined experimental and theoretical study, a computational protocol is reported to predict the excited states in D-π-A compounds containing the B(FXyl)2 (FXyl = 2,6-bis(trifluoromethyl)pheny ...

### *17) A single-step preparation of carbohydrate functionalized monoliths for separation and trapping of polar compounds*

* Wang, J., Guo, J., Chen, H., Huang, X., Somsen, G. W., Song, F., Jiang, Z.
* BioAnalytical Chemistry, AIMMS, Jinan University, Guangdong College of Pharmacy, Foshan University
* Journal of Chromatography A
* https://doi.org/10.1016/j.chroma.2020.461481
* Corresponding author: Song, F.
* Published 27 Sep 2020 (early online 16 Aug 2020)
* Processed: 2020-8

A single-step copolymerization strategy was developed for the preparation of carbohydrate (glucose and maltose) functionalized monoliths using click reaction. Firstly, novel carbohydrate-functionalize ...

### *18) Local Enhancement of Dynamic Correlation in Excited States: Fresh Perspective on Ionicity and Development of Correlation Density Functional Approximation Based on the On-Top Pair Density*

* Hapka, M., Pernal, K., Gritsenko, O. V.
* Theoretical Chemistry, AIMMS, Lodz University of Technology, University of Warsaw
* The journal of physical chemistry letters
* https://doi.org/10.1021/acs.jpclett.0c01616
* Corresponding author: None
* Published 6 Aug 2020 (early online 26 Jun 2020)
* Processed: 2020-8

We discuss the interplay between the nondynamic and dynamic electron correlation in excited states from the perspective of the suppression of dynamic correlation (SDC) and enhancement of dynamic corre ...

### *19) Correction to: Multiparametric assessment of mitochondrial respiratory inhibition in Hep*

* van der Stel, W., Carta, G., Eakins, J., Darici, S., Delp, J., Forsby, A., Bennekou, S. H., Gardner, I., Leist, M., Danen, E. H., Walker, P., van de Water, B., Jennings, P.
* Molecular and Computational Toxicology, AIMMS, Leiden University, Cyprotex Discovery Ltd, University of Konstanz, Stockholm University, Technical University of Denmark, Certara
* Archives of Toxicology
* https://doi.org/10.1007/s00204-020-02849-5
* Corresponding author: van de Water, B.
* Published Aug 2020 (early online 27 Jul 2020)
* Processed: 2020-8

G2 and RPTEC/TERT1 cells using a panel of mitochondrial targeting agrochemicals ...

### *20) SBML Level 3: an extensible format for the exchange and reuse of biological models*

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Systems biology has experienced dramatic growth in the number, size, and complexity of computational models. To reproduce simulation results and reuse models, researchers must exchange unambiguous mod ...

### *21) Efficacy of Novel Pyrazolone Phosphodiesterase Inhibitors in Experimental Mouse Models of Trypanosoma cruzi*

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Pyrazolones are heterocyclic compounds with interesting biological properties. Some derivatives inhibit phosphodiesterases (PDEs) and thereby increase the cellular concentration of cyclic AMP (cAMP), ...