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### 1) No associations between microbiota signaling substances and cognitive, language and motor development among three-year-old rural Ugandan children

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* Acta Paediatrica
* https://doi.org/10.1111/apa.15330
* Corresponding author: None
* Published 29 Apr 2020 (early online None)
* Processed: 2020-4

### 2) MAP: An MP2 Accuracy Predictor for Weak Interactions from Adiabatic Connection Theory

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* Journal of chemical theory and computation
* https://doi.org/10.1021/acs.jctc.0c00049
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* Published 14 Jul 2020 (early online 7 May 2020)
* Processed: 2020-7

Second-order Møller-Plesset perturbation theory (MP2) approximates the exact Hartree-Fock (HF) adiabatic connection (AC) curve by a straight line. Thus, by using the deviation of the exact curve from the linear behavior, we construct an indicator for the accuracy of MP2. We then use an interpolation along the HF AC to transform the exact form of our indicator into a highly practical MP2 accuracy predictor (MAP) that comes at a negligible additional computational cost. We show that this indicator is already applicable to systems that dissociate into fragments with a nondegenerate ground state, and we illustrate its usefulness by applying it to the S22 and S66 datasets.

### 3) 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

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* The journal of physical chemistry letters
* https://doi.org/10.1021/acs.jpclett.0c01616
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* 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 correlation (EDC) effects. We reveal that there exists a connection between the ionic character of a wave function and EDC. Following this finding we introduce a quantitative measure of ionicity based solely on local functions without referring to valence bond models. The ability to recognize both the SDC and EDC regions underlies the presented method, named CASΠDFT, combining complete active space (CAS) wave function and density functional theory (DFT) via the on-top pair density (Π) function. We extend this approach to excited states by devising an improved representation of the EDC effect in the correlation functional. The generalized CASΠDFT uses different DFT functionals for ground and excited states. Numerical demonstration for singlet π → π\* excitations shows that CASΠDFT offers satisfactory accuracy at a fraction of the cost of the ab initio approaches.

### 4) Cloning and functional complementation of ten Schistosoma mansoni phosphodiesterases expressed in the mammalian host stages

* Munday, J. C., Kunz, S., Kalejaiye, T. D., Siderius, M., Schroeder, S., Paape, D., Alghamdi, A. H., Abbasi, Z., Huang, S. X., Donachie, A. M., William, S., Sabra, A. N., Sterk, G. J., Botros, S. S., Brown, D. G., Hoffman, C. S., Leurs, R., de Koning, H. P.
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* PLoS Neglected Tropical Diseases
* https://doi.org/10.1371/journal.pntd.0008447
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* Published 30 Jul 2020 (early online None)
* Processed: 2020-7

Only a single drug against schistosomiasis is currently available and new drug development is urgently required but very few drug targets have been validated and characterised. However, regulatory systems including cyclic nucleotide metabolism are emerging as primary candidates for drug discovery. Here, we report the cloning of ten cyclic nucleotide phosphodiesterase (PDE) genes of S. mansoni, out of a total of 11 identified in its genome. We classify these PDEs by homology to human PDEs. Male worms displayed higher expression levels for all PDEs, in mature and juvenile worms, and schistosomula. Several functional complementation approaches were used to characterise these genes. We constructed a Trypanosoma brucei cell line in which expression of a cAMP-degrading PDE complements the deletion of TbrPDEB1/B2. Inhibitor screens of these cells expressing only either SmPDE4A, TbrPDEB1 or TbrPDEB2, identified highly potent inhibitors of the S. mansoni enzyme that elevated the cellular cAMP concentration. We further expressed most of the cloned SmPDEs in two pde1Δ/pde2Δ strains of Saccharomyces cerevisiae and some also in a specialised strain of Schizosacharomyces pombe. Five PDEs, SmPDE1, SmPDE4A, SmPDE8, SmPDE9A and SmPDE11 successfully complemented the S. cerevisiae strains, and SmPDE7var also complemented to a lesser degree, in liquid culture. SmPDE4A, SmPDE8 and SmPDE11 were further assessed in S. pombe for hydrolysis of cAMP and cGMP; SmPDE11 displayed considerable preferrence for cGMP over cAMP. These results and tools enable the pursuit of a rigorous drug discovery program based on inhibitors of S. mansoni PDEs.

### 5) 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

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

* Keating, S. M., Waltemath, D., König, M., Zhang, F., Dräger, A., Chaouiya, C., Bergmann, F. T., Finney, A., Gillespie, C. S., Helikar, T., Hoops, S., Malik-Sheriff, R. S., Moodie, S. L., Moraru, I. I., Myers, C. J., Naldi, A., Olivier, B. G., Sahle, S., Schaff, J. C., Smith, L. P., Swat, M. J., Thieffry, D., Watanabe, L., Wilkinson, D. J., Blinov, M. L., Begley, K., Faeder, J. R., Gómez, H. F., Hamm, T. M., Inagaki, Y., Liebermeister, W., Lister, A. L., Lucio, D., Mjolsness, E., Proctor, C. J., Raman, K., Rodriguez, N., Shaffer, C. A., Shapiro, B. E., Stelling, J., Swainston, N., Tanimura, N., Wagner, J., Meier-Schellersheim, M., Sauro, H. M., Palsson, B., Bolouri, H., Kitano, H., Funahashi, A., Hermjakob, H., Doyle, J. C., Hucka, M., Adams, R. R., Allen, N. A., Angermann, B. R., Antoniotti, M., Bader, G. D., Červený, J., Courtot, M., Cox, C. D., Dalle Pezze, P., Demir, E., Denney, W. S., Dharuri, H., Dorier, J., Drasdo, D., Ebrahim, A., Eichner, J., Elf, J., Endler, L., Evelo, C. T., Flamm, C., Fleming, R. M., Fröhlich, M., Glont, M., Gonçalves, E., Golebiewski, M., Grabski, H., Gutteridge, A., Hachmeister, D., Harris, L. A., Heavner, B. D., Henkel, R., Hlavacek, W. S., Hu, B., Hyduke, D. R., de Jong, H., Juty, N., Karp, P. D., Karr, J. R., Kell, D. B., Keller, R., Kiselev, I., Klamt, S., Klipp, E., Knüpfer, C., Kolpakov, F., Krause, F., Kutmon, M., Laibe, C., Lawless, C., Li, L., Loew, L. M., Machne, R., Matsuoka, Y., Mendes, P., Mi, H., Mittag, F., Monteiro, P. T., Natarajan, K. N., Nielsen, P. M., Nguyen, T., Palmisano, A., Pettit, J. B., Pfau, T., Phair, R. D., Radivoyevitch, T., Rohwer, J. M., Ruebenacker, O. A., Saez-Rodriguez, J., Scharm, M., Schmidt, H., Schreiber, F., Schubert, M., Schulte, R., Sealfon, S. C., Smallbone, K., Soliman, S., Stefan, M. I., Sullivan, D. P., Takahashi, K., Teusink, B., Tolnay, D., Vazirabad, I., von Kamp, A., Wittig, U., Wrzodek, C., Wrzodek, F., Xenarios, I., Zhukova, A., Zucker, J.
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* Molecular Systems Biology
* https://doi.org/10.15252/msb.20199110
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* Published 1 Aug 2020 (early online None)
* Processed: 2020-8

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 model descriptions. We review the latest edition of the Systems Biology Markup Language (SBML), a format designed for this purpose. A community of modelers and software authors developed SBML Level 3 over the past decade. Its modular form consists of a core suited to representing reaction-based models and packages that extend the core with features suited to other model types including constraint-based models, reaction-diffusion models, logical network models, and rule-based models. The format leverages two decades of SBML and a rich software ecosystem that transformed how systems biologists build and interact with models. More recently, the rise of multiscale models of whole cells and organs, and new data sources such as single-cell measurements and live imaging, has precipitated new ways of integrating data with models. We provide our perspectives on the challenges presented by these developments and how SBML Level 3 provides the foundation needed to support this evolution.

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

* de Araújo, J. S., França da Silva, C., Batista, D. D. G. J., Nefertiti, A., Fiuza, L. F. D. A., Fonseca-Berzal, C. R., Bernardino da Silva, P., Batista, M. M., Sijm, M., Kalejaiye, T. D., de Koning, H. P., Maes, L., Sterk, G. J., Leurs, R., Soeiro, M. D. N. C.
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* Antimicrobial agents and chemotherapy
* https://doi.org/10.1128/AAC.00414-20
* Corresponding author: None
* Published 20 Aug 2020 (early online None)
* Processed: 2020-8

Pyrazolones are heterocyclic compounds with interesting biological properties. Some derivatives inhibit phosphodiesterases (PDEs) and thereby increase the cellular concentration of cyclic AMP (cAMP), which plays a vital role in the control of metabolism in eukaryotic cells, including the protozoan Trypanosoma cruzi, the etiological agent of Chagas disease (CD), a major neglected tropical disease. In vitro phenotypic screening identified a 4-bromophenyl-dihydropyrazole dimer as an anti-T. cruzi hit and 17 novel pyrazolone analogues with variations on the phenyl ring were investigated in a panel of phenotypic laboratory models. Potent activity against the intracellular forms (Tulahuen and Y strains) was obtained with 50% effective concentration (EC50) values within the 0.17 to 3.3 μM range. Although most were not active against bloodstream trypomastigotes, an altered morphology and loss of infectivity were observed. Pretreatment of the mammalian host cells with pyrazolones did not interfere with infection and proliferation, showing that the drug activity was not the result of changes to host cell metabolism. The pyrazolone NPD-227 increased the intracellular cAMP levels and was able to sterilize T. cruzi-infected cell cultures. Thus, due to its high potency and selectivity in vitro, and its additive interaction with benznidazole (Bz), NPD-227 was next assessed in the acute mouse model. Oral dosing for 5 days of NPD-227 at 10 mg/kg + Bz at 10 mg/kg not only reduced parasitemia (>87%) but also protected against mortality (>83% survival), hence demonstrating superiority to the monotherapy schemes. These data support these pyrazolone molecules as potential novel therapeutic alternatives for Chagas disease.

### *8) 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 ...

### *9) 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 ...

### *10) 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.
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* 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 ...

### *11) 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.
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* 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 ...

### *12) 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.
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* 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 ...

### *13) 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 ...