# AIMMS publication report for: 2021-06-28

1. Noncovalent Interactions from Models for the Møller-Plesset (2021-5)
2. Generation and characterization of iPSC-derived renal proxim (2021-6)
3. Stimulated Raman scattering simulation for imaging optimizat (2021-6)
4. *Evaluation of chemicals of environmental concern in crumb ru (2021-5)*
5. *A bifunctional iminophosphorane squaramide catalyzed enantio (2021-5)*
6. *Anticoagulant Activity of Naja nigricollis Venom Is Mediated (2021-5)*
7. *Understanding FBA solutions under multiple nutrient limitati (2021-5)*
8. *SeRenDIP-CE: Sequence-based Interface Prediction for Conform (2021-5)*
9. *Endocrine, metabolic and apical effects of in utero and lact (2021-5)*
10. *Erratum: "Large coupling-strength expansion of the Møller-Pl (2021-5)*
11. *Characterization of a liquid-core waveguide cell for studyin (2021-5)*
12. *Lysosome-targeted photodynamic treatment induces primary ker (2021-5)*
13. *IL-1R1-Dependent Signals Improve Control of Cytosolic Virule (2021-5)*
14. *Salivary biomarkers of stress and inflammation in first grad (2021-5)*
15. *Different resource allocation in a bacillus subtilis populat (2021-6)*
16. *Evaluation of a human iPSC-derived BBB model for repeated do (2021-6)*
17. *Growth, dormancy and lysis: the complex relation of starter (2021-6)*
18. *Synergistic DNA‐ and Protein‐Based Recognition Promote an RN (2021-6)*
19. *Corrigendum to “Bioactivation of trichloroethylene to three (2021-6)*
20. *Se (2021-5)*
21. *High-resolution infrared spectroscopy of naphthalene and ace (2021-1)*
22. *Synthesis of Carbazoles by a Diverted Bischler-Napieralski C (2021-4)*

### 1) Noncovalent Interactions from Models for the Møller-Plesset Adiabatic Connection

* Daas, T. J., Fabiano, E., Della Sala, F., Gori-Giorgi, P., Vuckovic, S.
* AIMMS, Theoretical Chemistry, Institute for Microelectronics and Microsystems (CNR-IMM), Center for Biomolecular Nanotechnologies
* The journal of physical chemistry letters
* https://doi.org/10.1021/acs.jpclett.1c01157
* Corresponding author: None
* Published 27 May 2021 (early online 18 May 2021)
* Processed: 2021-5

Given the omnipresence of noncovalent interactions (NCIs), their accurate simulations are of crucial importance across various scientific disciplines. Here we construct accurate models for the description of NCIs by an interpolation along the Møller-Plesset adiabatic connection (MP AC). Our interpolation approximates the correlation energy, by recovering MP2 at small coupling strengths and the correct large-coupling strength expansion of the MP AC, recently shown to be a functional of the Hartree-Fock density. Our models are size consistent for fragments with nondegenerate ground states, have the same cost as double hybrids, and require no dispersion corrections to capture NCIs accurately. These interpolations greatly reduce large MP2 errors for typical π-stacking complexes (e.g., benzene-pyridine dimers) and for the L7 data set. They are also competitive with state-of-the-art dispersion enhanced functionals and can even significantly outperform them for a variety of data sets, such as CT7 and L7.

### 2) Generation and characterization of iPSC-derived renal proximal tubule-like cells with extended stability

* Chandrasekaran, V., Carta, G., da Costa Pereira, D., Gupta, R., Murphy, C., Feifel, E., Kern, G., Lechner, J., Cavallo, A. L., Gupta, S., Caiment, F., Kleinjans, J. C., Gstraunthaler, G., Jennings, P., Wilmes, A.
* Molecular and Computational Toxicology, AIMMS, Maastricht University, Innsbruck Medical University, AstraZeneca Sweden
* Scientific Reports
* https://doi.org/10.1038/s41598-021-89550-4
* Corresponding author: Jennings, P.
* Published Dec 2021 (early online 2 Jun 2021)
* Processed: 2021-6

The renal proximal tubule is responsible for re-absorption of the majority of the glomerular filtrate and its proper function is necessary for whole-body homeostasis. Aging, certain diseases and chemical-induced toxicity are factors that contribute to proximal tubule injury and chronic kidney disease progression. To better understand these processes, it would be advantageous to generate renal tissues from human induced pluripotent stem cells (iPSC). Here, we report the differentiation and characterization of iPSC lines into proximal tubular-like cells (PTL). The protocol is a step wise exposure of small molecules and growth factors, including the GSK3 inhibitor (CHIR99021), the retinoic acid receptor activator (TTNPB), FGF9 and EGF, to drive iPSC to PTL via cell stages representing characteristics of early stages of renal development. Genome-wide RNA sequencing showed that PTL clustered within a kidney phenotype. PTL expressed proximal tubular-specific markers, including megalin (LRP2), showed a polarized phenotype, and were responsive to parathyroid hormone. PTL could take up albumin and exhibited ABCB1 transport activity. The phenotype was stable for up to 7days and was maintained after passaging. This protocol will form the basis of an optimized strategy for molecular investigations using iPSC derived PTL.

### 3) Stimulated Raman scattering simulation for imaging optimization

* Zada, L., Fokker, B., Leslie, H. A., Vethaak, A. D., De Boer, J. F., Ariese, F.
* Biophotonics and Medical Imaging, LaserLaB - Biophotonics and Microscopy, E&H: Environmental Chemistry and Toxicology, AIMMS, Environment and Health, Amsterdam Neuroscience - Brain Imaging, Deltares
* Journal of the European Optical Society. Rapid Publications
* https://doi.org/10.1186/s41476-021-00155-w
* Corresponding author: None
* Published 16 Jun 2021 (early online None)
* Processed: 2021-6

Two simulation programs of a stimulated Raman scattering microscopy (SRS) imaging system with lock-in amplifier (LIA) detection were developed. SRS is an imaging technique based on the vibrational Raman cross-section as the contrast mechanism and enables fast, label-free imaging. Most SRS implementations are based on LIA detection of a modulated signal. However, building and operating such SRS set-ups still poses a challenge when selecting the LIA parameter settings for optimized acquisition speed or image quality. Moreover, the type of sample, e.g. a sparse sample vs. a densely packed sample, the required resolution as well as the Raman cross-section and the laser powers affect the parameter choice.A simulation program was used to find these optimal parameters. The focal spot diameters of the individual lasers (pump and Stokes) were used to estimate the effective SRS signal focal spot and the (optical) spatial resolution. By calibrating the signal and noise propagation through an SRS system for a known molecule, we estimated the signal and noise input to the LIA. We used a low pass filter model to simulate the LIA behavior in order to find the optimal parameters (i.e. filter order and time constant).Optimization was done for either image quality (expressed as contrast to noise ratio) or acquisition time. The targeted object size was first determined as a measure for the required resolution. The simulation output consisted of the LIA parameters, pixel dwell time and contrast to noise ratio.In a second simulation we evaluated SRS imaging based on the same principles as the optimal setting simulation, i.e. the signals were propagated through an imaging system and LIA detection. The simulated images were compared to experimental SRS images of polystyrene beads.Finally, the same software was used to simulate multiplexed SRS imaging. In this study we modeled a six-channel frequency-encoded multiplexed SRS system demodulated with six LIA channels. We evaluated the inter-channel crosstalk as a function of chosen LIA parameters, which in multiplex SRS imaging also needs to be considered.These programs to optimize the contrast to noise ratio, acquisition speed, resolution and crosstalk will be useful for operating stimulated Raman scattering imaging setup, as well as for designing novel setups.

### *4) Evaluation of chemicals of environmental concern in crumb rubber and water leachates from several types of synthetic turf football pitches*

* Celeiro, M., Armada, D., Ratola, N., Dagnac, T., de Boer, J., Llompart, M.
* Environment and Health, AIMMS, University of Santiago de Compostela, University of Porto, Agronomic Research Centre (AGACAL-CIAM) – Unit of Organic Contaminants
* Chemosphere
* https://doi.org/10.1016/j.chemosphere.2020.128610
* Corresponding author: Llompart, M.
* Published May 2021 (early online 19 Oct 2020)
* Processed: 2021-5

Nowadays concern exists about the safety for both football players and the environment of recycled tire rubber used as infill in synthetic turf football pitches. In this study 40 target compounds, inc ...

### *5) A bifunctional iminophosphorane squaramide catalyzed enantioselective synthesis of hydroquinazolines: Via intramolecular aza-Michael reaction to α,β-unsaturated esters*

* Su, G., Thomson, C. J., Yamazaki, K., Rozsar, D., Christensen, K. E., Hamlin, T. A., Dixon, D. J.
* Chemistry and Pharmaceutical Sciences, Theoretical Chemistry, AIMMS, University of Oxford
* Chemical Science
* https://doi.org/10.1039/d1sc00856k
* Corresponding author: Dixon, D. J.
* Published 7 May 2021 (early online 18 Mar 2021)
* Processed: 2021-5

An efficient synthesis of enantioenriched hydroquinazoline cores via a novel bifunctional iminophosphorane squaramide catalyzed intramolecular aza-Michael reaction of urea-linked α,β-unsaturated ester ...

### *6) Anticoagulant Activity of Naja nigricollis Venom Is Mediated by Phospholipase A2 Toxins and Inhibited by Varespladib*

* Kazandjian, T. D., Arrahman, A., Still, K. B., Somsen, G. W., Vonk, F. J., Casewell, N. R., Wilkinson, M. C., Kool, J.
* BioAnalytical Chemistry, AIMMS, Chemistry and Pharmaceutical Sciences, Liverpool School of Tropical Medicine
* Toxins
* https://doi.org/10.3390/toxins13050302
* Corresponding author: None
* Published May 2021 (early online 23 Apr 2021)
* Processed: 2021-5

Bites from elapid snakes typically result in neurotoxic symptoms in snakebite victims. Neurotoxins are, therefore, often the focus of research relating to understanding the pathogenesis of elapid bite ...

### *7) Understanding FBA solutions under multiple nutrient limitations*

* van Pelt-KleinJan, E., de Groot, D. H., Teusink, B.
* Systems Bioinformatics, AIMMS, Systems Bioinformatics
* Metabolites
* https://doi.org/10.3390/metabo11050257
* Corresponding author: Teusink, B.
* Published May 2021 (early online 21 Apr 2021)
* Processed: 2021-5

Genome-scale stoichiometric modeling methods, in particular Flux Balance Analysis (FBA) and variations thereof, are widely used to investigate cell metabolism and to optimize biotechno-logical process ...

### *8) SeRenDIP-CE: Sequence-based Interface Prediction for Conformational Epitopes*

* Hou, Q., Stringer, B., Waury, K., Capel, H., Haydarlou, R., Xue, F., Abeln, S., Heringa, J., Feenstra, K. A.
* Computer Science, Bioinformatics, AIMMS, Integrative Bioinformatics, Bio Informatics (IBIVU), IBIVU - Center for Integrative Bioinformatics, Shandong University
* Bioinformatics (Oxford, England)
* https://doi.org/10.1101/2020.11.19.390500
* Corresponding author: None
* Published 11 May 2021 (early online 11 May 2021)
* Processed: 2021-5

MOTIVATION: Antibodies play an important role in clinical research and biotechnology, with their specificity determined by the interaction with the antigen's epitope region, as a special type of prote ...

### *9) Endocrine, metabolic and apical effects of in utero and lactational exposure to non-dioxin-like 2,2´,3,4,4´,5,5´-heptachlorobiphenyl (PCB 180): A postnatal follow-up study in rats*

* Alarcón, S., Esteban, J., Roos, R., Heikkinen, P., Sánchez-Pérez, I., Adamsson, A., Toppari, J., Koskela, A., Finnilä, M. A., Tuukkanen, J., Herlin, M., Hamscher, G., Leslie, H. A., Korkalainen, M., Halldin, K., Schrenk, D., Håkansson, H., Viluksela, M.
* E&H: Environmental Chemistry and Toxicology, AIMMS, Miguel Hernández University, Karolinska Institutet, Finnish Institute for Health and Welfare, University of Turku, University of Oulu, Justus Liebig University Giessen, University of Kaiserslautern, University of Eastern Finland
* Reproductive Toxicology
* https://doi.org/10.1016/j.reprotox.2021.04.004
* Corresponding author: Esteban, J.
* Published Jun 2021 (early online 13 May 2021)
* Processed: 2021-5

PCB 180 is a persistent and abundant non-dioxin-like PCB (NDL-PCB). We determined the developmental toxicity profile of ultrapure PCB 180 in developing offspring following in utero and lactational exp ...

### *10) Erratum: "Large coupling-strength expansion of the Møller-Plesset adiabatic connection: From paradigmatic cases to variational expressions for the leading terms" [J. Chem. Phys., 153, 214112 (2020)]*

* Daas, T. J., Grossi, J., Vuckovic, S., Musslimani, Z. H., Kooi, D. P., Seidl, M., Giesbertz, K. J., Gori-Giorgi, P.
* Theoretical Chemistry, AIMMS, Vrije Universiteit Amsterdam
* Journal of Chemical Physics
* https://doi.org/10.1063/5.0053838
* Corresponding author: Gori-Giorgi, P.
* Published 14 May 2021 (early online 10 May 2021)
* Processed: 2021-5

We correct an error in Eq. (19) of the article, namely, a missing factor 1/2. The correct equation reads (Farmula Presenred) This is only a misprint in the article and does not affect any of the resul ...

### *11) Characterization of a liquid-core waveguide cell for studying the chemistry of light-induced degradation*

* Groeneveld, I., Schoemaker, S. E., Somsen, G. W., Ariese, F., Van Bommel, M. R.
* BioAnalytical Chemistry, AIMMS, Biophotonics and Medical Imaging, LaserLaB - Biophotonics and Microscopy, Vrije Universiteit Amsterdam, University of Amsterdam
* Analyst
* https://doi.org/10.1039/d1an00272d
* Corresponding author: Groeneveld, I.
* Published 21 May 2021 (early online 7 Apr 2021)
* Processed: 2021-5

Many organic compounds undergo changes under the influence of light. This might be beneficial in, for example, water purification, but undesirable when cultural-heritage objects fade or when food ingr ...

### *12) Lysosome-targeted photodynamic treatment induces primary keratinocyte differentiation*

* Daugelaviciene, N., Grigaitis, P., Gasiule, L., Dabkeviciene, D., Neniskyte, U., Sasnauskiene, A.
* Systems Bioinformatics, AIMMS, Vilnius University, National Cancer Institute
* Journal of Photochemistry and Photobiology B: Biology
* https://doi.org/10.1016/j.jphotobiol.2021.112183
* Corresponding author: Daugelaviciene, N.
* Published May 2021 (early online None)
* Processed: 2021-5

Photodynamic therapy is an attractive technique for various skin tumors and non-cancerous skin lesions. However, while the aim of photodynamic therapy is to target and damage only the malignant cells, ...

### *13) IL-1R1-Dependent Signals Improve Control of Cytosolic Virulent Mycobacteria In Vivo*

* van der Niet, S., van Zon, M., de Punder, K., Grootemaat, A., Rutten, S., Moorlag, S. J., Houben, D., van der Sar, A. M., Bitter, W., Brosch, R., Hernandez Pando, R., Pena, M. T., Peters, P. J., Reits, E. A., Mayer-Barber, K. D., van der Wel, N. N.Pages:1-17
* Molecular Microbiology, AIMMS, University of Amsterdam, Netherlands Cancer Institute, CNRS, Instituto Nacional de Ciencias Medicas y Nutricion Salvador Zubiran, Louisiana State University, National Institutes of Health
* mSphere
* https://doi.org/10.1128/mSphere.00153-21
* Corresponding author: None
* Published 5 May 2021 (early online None)
* Processed: 2021-5

Mycobacterium tuberculosis infections claim more than a million lives each year, and better treatments or vaccines are required. A crucial pathogenicity factor is translocation from phagolysosomes to ...

### *14) Salivary biomarkers of stress and inflammation in first graders in Côte d′Ivoire: Effects of a probiotic food intervention*

* Brett, B. E., Koko, B. K., Doumbia, H. O., Koffi, F. K., Assa, S. E., Zahé, K. Y., Faye-Ketté, H., Kati-Coulibaly, S., Kort, R., Sybesma, W., Reid, G., de Weerth, C.
* Molecular Cell Physiology, AIMMS, Radboud University Nijmegen, Université de Cocody Abidjan, Centre hospitalier universitaire de Treichville, Yoba for Life foundation, Western University
* Psychoneuroendocrinology
* https://doi.org/10.1016/j.psyneuen.2021.105255
* Corresponding author: Brett, B. E.
* Published Jul 2021 (early online 12 May 2021)
* Processed: 2021-5

This semi-randomized controlled trial examined the effects of a probiotic food supplement on cortisol and C-reactive protein (CRP) in a sample of 262 four-to seven-year-old children (56% girls) in two ...

### *15) Different resource allocation in a bacillus subtilis population displaying bimodal motility*

* Syvertsson, S., Wang, B., Staal, J., Gao, Y., Kort, R., Hamoen, L. W.
* Molecular Cell Physiology, AIMMS, Bioinformatics, Bio Informatics (IBIVU), Newcastle University, University of Amsterdam, Netherlands Organisation for Applied Scientific Research
* Journal of Bacteriology
* https://doi.org/10.1128/JB.00037-21
* Corresponding author: Hamoen, L. W.
* Published Jun 2021 (early online 20 May 2021)
* Processed: 2021-6

To cope with sudden changes in their environment, bacteria can use a bet-hedging strategy by dividing the population into cells with different properties. This so-called bimodal or bistable cellular d ...

### *16) Evaluation of a human iPSC-derived BBB model for repeated dose toxicity testing with cyclosporine A as model compound*

* Wellens, S., Dehouck, L., Chandrasekaran, V., Singh, P., Loiola, R. A., Sevin, E., Exner, T., Jennings, P., Gosselet, F., Culot, M.
* AIMMS, Molecular and Computational Toxicology, Université d'Artois, Edelweiss Connect GmbH, University of Basel
* Toxicology in Vitro
* https://doi.org/10.1016/j.tiv.2021.105112
* Corresponding author: Culot, M.
* Published Jun 2021 (early online None)
* Processed: 2021-6

The blood-brain barrier (BBB) is a highly restrictive barrier that preserves central nervous system homeostasis and ensures optimal brain functioning. Using BBB cell assays makes it possible to invest ...

### *17) Growth, dormancy and lysis: the complex relation of starter culture physiology and cheese flavour formation*

* Nugroho, A. D. W., Kleerebezem, M., Bachmann, H.
* Systems Bioinformatics, AIMMS, TI Food and Nutrition, NIZO food research, Wageningen University & Research
* Current Opinion in Food Science
* https://doi.org/10.1016/j.cofs.2020.12.005
* Corresponding author: None
* Published Jun 2021 (early online None)
* Processed: 2021-6

Fast acidification and growth are desired from lactic acid bacteria starter cultures during food fermentation to minimise the risk of spoilage and process failure. In addition, starter cultures play a ...

### *18) Synergistic DNA‐ and Protein‐Based Recognition Promote an RNA‐Templated Bio‐orthogonal Reaction*

* McLoughlin, N. M., Kuepper, A., Neubacher, S., Grossmann, T. N.
* Organic Chemistry, AIMMS, Chemistry and Pharmaceutical Sciences
* Chemistry – A European Journal
* https://doi.org/10.1002/chem.202101103
* Corresponding author: None
* Published Jun 2021 (early online None)
* Processed: 2021-6

...

### *19) Corrigendum to “Bioactivation of trichloroethylene to three regioisomeric glutathione conjugates by liver fractions and recombinant human glutathione transferases: Species differences and implications for human risk assessment” [Toxicol. Lett. 341 (2021) 94–106]*

* Capinha, L., Jennings, P., Commandeur, J. N.
* AIMMS, Molecular and Computational Toxicology
* Toxicology Letters
* https://doi.org/10.1016/j.toxlet.2021.02.011
* Corresponding author: Commandeur, J. N.
* Published 1 Jun 2021 (early online None)
* Processed: 2021-6

The authors regret that in Fig. 1 the letters indicating the enzymes involved in the reactions were not added to the arrows. A corrected Figure is shown below. [Figure presented] Fig. 1. Regioselectiv ...

### *20) Se*

* Hou, Q., Stringer, B., Waury, K., Capel, H., Haydarlou, R., Xue, F., Abeln, S., Heringa, J., Feenstra, K. A.
* Computer Science, Bioinformatics, AIMMS, Integrative Bioinformatics, Bio Informatics (IBIVU), IBIVU - Center for Integrative Bioinformatics, Shandong University
* Bioinformatics (Oxford, England)
* https://doi.org/10.1101/2020.11.19.390500v110.1093/bioinformatics/btab321
* Corresponding author: None
* Published 11 May 2021 (early online 11 May 2021)
* Processed: 2021-5

RenDIP-CE: quence-based Interface Prediction for Conformational EpitopesMOTIVATION: Antibodies play an important role in clinical research and biotechnology, with their specificity determined by the i ...

### *21) High-resolution infrared spectroscopy of naphthalene and acenaphthene dimers*

* Lemmens, A. K., Chopra, P., Garg, D., Steber, A. L., Schnell, M., Buma, W. J., Rijs, A. M.
* BioAnalytical Chemistry, AIMMS
* Molecular Physics
* https://doi.org/10.1080/00268976.2020.1811908
* Corresponding author: None
* Published 17 Jan 2021 (early online None)
* Processed: 2021-1

...

### *22) Synthesis of Carbazoles by a Diverted Bischler-Napieralski Cascade Reaction*

* Faltracco, M., Ortega-Rosales, S., Janssen, E., Cioc, R. C., Vande Velde, C. M., Ruijter, E.
* Organic Chemistry, AIMMS, Chemistry and Pharmaceutical Sciences, Vrije Universiteit Amsterdam, University of Antwerp
* Organic letters
* https://doi.org/10.1021/acs.orglett.1c00785
* Corresponding author: Ruijter, E.
* Published 16 Apr 2021 (early online 31 Mar 2021)
* Processed: 2021-4

An unforeseen twist in a seemingly trivial Bischler-Napieralski reaction led to the selective formation of an unexpected carbazole product. The reaction proved to be general, providing access to a ran ...