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

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* 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 protein-protein interaction (PPI) interface. The ubiquitous availability of sequence data, allows us to predict epitopes from sequence in order to focus time-consuming wet-lab experiments towards the most promising epitope regions. Here, we extend our previously developed sequence-based predictors for homodimer and heterodimer PPI interfaces to predict epitope residues that have the potential to bind an antibody.RESULTS: We collected and curated a high quality epitope dataset from the SAbDab database. Our generic PPI heterodimer predictor obtained an AUC-ROC of 0.666 when evaluated on the epitope test set. We then trained a random forest model specifically on the epitope dataset, reaching AUC 0.694. Further training on the combined heterodimer and epitope datasets, improves our final predictor to AUC 0.703 on the epitope test set. This is better than the best state-of-the-art sequence-based epitope predictor BepiPred-2.0. On one solved antibody-antigen structure of the COVID19 virus spike RNA binding domain, our predictor reaches AUC 0.778. We added the SeRenDIP-CE Conformational Epitope predictors to our webserver, which is simple to use and only requires a single antigen sequence as input, which will help make the method immediately applicable in a wide range of biomedical and biomolecular research.AVAILABILITY: Webserver, source code and datasets at www.ibi.vu.nl/programs/serendipwww/.

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

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* 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 ingredients (e.g., vitamins) degrade. It is often challenging to establish a strong link between photodegradation products and their parent molecules due to the complexity of the sample. To allow effective study of light-induced degradation (LID), a low-volume exposure cell was created in which solutes are efficiently illuminated (especially at low concentrations) while simultaneously analysed by absorbance spectroscopy. The new LID cell encompasses a gas-permeable liquid-core waveguide (LCW) connected to a spectrograph allowing collection of spectral data in real-time. The aim of the current study was to evaluate the overall performance of the LID cell by assessing its transmission characteristics, the absolute photon flux achieved in the LCW, and its capacity to study solute degradation in presence of oxygen. The potential of the LID set-up for light-exposure studies was successfully demonstrated by monitoring the degradation of the dyes eosin Y and crystal violet.

### 3) Lysosome-targeted photodynamic treatment induces primary keratinocyte differentiation

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* Journal of Photochemistry and Photobiology B: Biology
* https://doi.org/10.1016/j.jphotobiol.2021.112183
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* 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, it unavoidably affects some of the healthy cells surrounding the tumor as well. However, data on the effects of PDT to normal cells are scarce, and the characterization of the pathways activated after the photodamage of normal cells may help to improve clinical photodynamic therapy. In our study, primary human epidermal keratinocytes were used to evaluate photodynamic treatment effects of photosensitizers with different subcellular localization. We compared the response of keratinocytes to lysosomal photodamage induced by phthalocyanines, aluminum phthalocyanine disulfonate (AlPcS2a) or aluminum phthalocyanine tetrasulfonate (AlPcS4), and cellular membrane photodamage by m-tetra(3-hydroxyphenyl)-chlorin (mTHPC). Our data showed that mTHPC-PDT promoted autophagic flux, whereas lysosomal photodamage induced by aluminum phthalocyanines evoked differentiation and apoptosis. Photodamage by AlPcS2a, which is targeted to lysosomal membranes, induced keratinocyte differentiation and apoptosis more efficiently than AlPcS4, which is targeted to lysosomal lumen. Computational analysis of the interplay between these molecular pathways revealed that keratin 10 is the coordinating molecular hub of primary keratinocyte differentiation, apoptosis and autophagy.

### 4) 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
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* mSphere
* https://doi.org/10.1128/mSphere.00153-21
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* 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 the cytosol upon phagocytosis by macrophages. Translocation from the phagolysosome to the cytosol is an ESX-1-dependent process, as previously shown in vitro Here, we show that in vivo, mycobacteria also translocate to the cytosol but mainly when host immunity is compromised. We observed only low numbers of cytosolic bacilli in mice, armadillos, zebrafish, and patient material infected with M. tuberculosis, M. marinum, or M. leprae In contrast, when innate or adaptive immunity was compromised, as in severe combined immunodeficiency (SCID) or interleukin-1 receptor 1 (IL-1R1)-deficient mice, significant numbers of cytosolic M. tuberculosis bacilli were detected in the lungs of infected mice. Taken together, in vivo, translocation to the cytosol of M. tuberculosis is controlled by adaptive immune responses as well as IL-1R1-mediated signals.IMPORTANCE For decades, Mycobacterium tuberculosis has been one of the deadliest pathogens known. Despite infecting approximately one-third of the human population, no effective treatment or vaccine is available. A crucial pathogenicity factor is subcellular localization, as M. tuberculosis can translocate from phagolysosome to the cytosol in macrophages. The situation in vivo is more complicated. In this study, we establish that high-level cytosolic escape of mycobacteria can indeed occur in vivo but mainly when host resistance is compromised. The IL-1 pathway is crucial for the control of the number of cytosolic mycobacteria. The establishment that immune signals result in the clearance of cells containing cytosolic mycobacteria connects two important fields, cell biology and immunology, which is vital for the understanding of the pathology of M. tuberculosis.

### 5) 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.
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* 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 economically-disadvantaged schools in an urban setting in Côte d′Ivoire. For one semester, children in one school were randomized to receive a probiotic (N = 79) or placebo (N = 85) fermented dairy food each day they attended school; one child (due to medical reasons) and all children in the other school (N = 98) continued their diets as usual. Children provided two saliva samples at 11:30 on consecutive days at the end of the study. Analyses revealed that the probiotic group had lower cortisol than the placebo or diet-as-usual groups (p =.015); CRP levels were comparable across groups (p =.549). Exploratory analyses suggested that dose and regularity of consumption may impact the biomarkers as well. This study provides the first evidence that a probiotic milk product may lower cortisol in a sample of young, economically-disadvantaged children.

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

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* Journal of Bacteriology
* https://doi.org/10.1128/JB.00037-21
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* 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 differentiation is generally controlled by positive feedback regulation of transcriptional activators. Due to the continuous increase in cell volume, it is difficult for these activators to reach an activation threshold concentration when cells are growing exponentially. This is one reason why bimodal differentiation is primarily observed from the onset of the stationary phase, when exponential growth ceases. An exception is the bimodal induction of motility in Bacillus subtilis, which occurs early during exponential growth. Several mechanisms have been put forward to explain this, including double-negative feedback regulation and the stability of the mRNA molecules involved. In this study, we used fluorescence-assisted cell sorting (FACS) to compare the transcriptomes of motile and nonmotile cells and noted that expression of ribosomal genes is lower in motile cells. This was confirmed using an unstable green fluorescent protein (GFP) reporter fused to the strong ribosomal rpsD promoter. We propose that the reduction in ribosomal gene expression in motile cells is the result of a diversion of cellular resources to the synthesis of the chemotaxis and motility systems. In agreement with this, single-cell microscopic analysis showed that motile cells are slightly shorter than nonmotile cells, an indication of slower growth. We speculate that this growth rate reduction can contribute to the bimodal induction of motility during exponential growth.

### 7) 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 investigate whether a compound is likely to compromise BBBs functionality, thereby probably resulting in neurotoxicity. Recently, several protocols to obtain human brain-like endothelial cells (BLECs) from induced pluripotent stem cells (iPSCs) have been reported. Within the framework of the European MSCA-ITN in3 project, we explored the possibility to use an iPSC-derived BBB model to assess the effects of repeated dose treatment with chemicals, using Cyclosporine A (CsA) as a model compound. The BLECs were found to exhibit important BBB characteristics up to 15 days after the end of the differentiation and could be used to assess the effects of repeated dose treatment. Although BLECs were still undergoing transcriptional changes over time, a targeted transcriptome analysis (TempO-Seq) indicated a time and concentration dependent activation of ATF4, XBP1, Nrf2 and p53 stress response pathways under CsA treatment. Taken together, these results demonstrate that this iPSC-derived BBB model and iPSC-derived models in general hold great potential to study the effects of repeated dose exposure with chemicals, allowing personalized and patient-specific studies in the future.

### 8) 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 predominant role in the formation of flavour volatiles. Recent studies in different microbial species have shown that high growth rates come at the expense of the expression level of metabolic enzymes and/or stress proteins. In starter cultures, such a trade-off would affect flavour formation, which depends on the level of flavour-forming enzymes and the prolonged survival of cells. Moreover, starter culture performance during cheese ripening could also be influenced by its cultivation history due to the low number of divisions during cheese manufacturing and limited proteome adjustment during ripening. These findings indicate that changes in (pre)-culture conditions can modulate proteome allocation and metabolic stability in starter cultures, and thereby provide novel approaches to steer flavour formation.

### 9) 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

### 10) 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. Regioselective GSH-conjugation of trichloroethylene (TCE) and subsequent processing to corresponding mercapturic acids (N-acetylcysteine S-conjugates) and beta-lyase-dependent bioactivation of cysteine S-conjugates to reactive products. Enzymes involved: a. glutathione S-transferases; b. gamma-glutamyltransferase; c. cysteinyl-glycine dipeptidase; d. cysteine conjugate beta-lyase; e. cysteine conjugate N-acetyltransferase; f. aminoacylase. Formation of sulfoxides of mercapturic acids is not shown to avoid an overcomplicated figure. The authors would like to apologise for any inconvenience caused.

### *11) 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 ...

### *12) 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 ...

### *13) 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 ...

### *14) 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 ...

### *15) 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 ...

### *16) 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 ...

### *17) 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

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### *18) Per- and polyfluoroalkyl substances (PFASs) in Swedish household dust and exposure of pet cats: Per- and polyfluoroalkyl substances (PFASs) in Swedish household dust and exposure of pet cats Per- and polyfluoroalkyl substances (PFASs) are used in a wide range of products and have been found ubiquitously in our indoor environment, and there is evidence that exposure to PFAS can lead to adverse endocrine effects, such as thyroid hormone disruption. Pet cats have a high dust intake due to their grooming behavior and have been shown to be a suitable sentinel species for assessment of toddler's exposure. Here we used paired household dust (n=46) and cat serum (n=27) samples to establish whether dust is a relevant exposure pathway to PFASs. An analytical method for PFAS analysis was optimized using a low volume of cat serum samples, combining solid-phase extraction and online sample cleanup*

* Weiss, J., Koekkoek, J., Lamoree, M., Bignert, A., Jones, B.
* E&H: Environmental Chemistry and Toxicology, AIMMS, Swedish University of Agricultural Sciences, Swedish Museum of Natural History, Department of Environmental Science and Analytical Chemistry (ACES), Stockholm University, Svante Arrhenius väg 8, 10691 Stockholm, Sweden.
* Environmental Science and Pollution Research
* https://doi.org/10.1007/s11356-021-13343-5
* Corresponding author: Weiss, J.
* Published 20 Mar 2021 (early online None)
* Processed: 2021-3

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### *19) Chlorinated paraffins and tris (1-chloro-2-propyl) phosphate in spray polyurethane foams – A source for indoor exposure?*

* Brandsma, S. H., Brits, M., de Boer, J., Leonards, P. E.
* E&H: Environmental Bioanalytical Chemistry, AIMMS, E&H: Environmental Chemistry and Toxicology, Environment and Health
* Journal of Hazardous Materials
* https://doi.org/10.1016/j.jhazmat.2021.125758
* Corresponding author: Brandsma, S. H.
* Published 15 Aug 2021 (early online 31 Mar 2021)
* Processed: 2021-3

In this study, we investigated chemical additives present in new and used spray polyurethane foams (SPFs) and assessed the dermal transfer through direct contact. This first study shows that cured do- ...