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### 1) A centrifugation-based clearing method allows high-throughput acidification and growth-rate measurements in milk

* Douwenga, S., Janssen, P., Teusink, B., Bachmann, H.
* AIMMS, Systems Bioinformatics, Systems Bioinformatics, TI Food and Nutrition, NIZO food research
* Journal of Dairy Science
* https://doi.org/10.3168/jds.2020-20108
* Corresponding author: Bachmann, H.
* Published Aug 2021 (early online 30 Apr 2021)
* Processed: 2021-8

The turbidity of milk prohibits the use of optical density measurements for strain characterizations. This often limits research to laboratory media. Here, we cleared milk through centrifugation to remove insoluble milk solids. This resulted in a clear liquid phase, termed milk serum, in which optical density measurements can be used to track microbial growth until a pH of 5.2 is reached. At pH 5.2 coagulation of the soluble protein occurs, making the medium opaque again. We found that behavior in milk serum was predictive of that in milk for 39 Lactococcus lactis (R2 = 0.81) and to a lesser extent for 42 Lactiplantibacillus plantarum (formerly Lactobacillus plantarum; R2 = 0.49) strains. Hence, milk serum can be used as an optically clear alternative to milk for comparison of microbial growth and metabolic characteristics. Characterization of the growth rate, specific acidification rate for optical density at a wavelength of 600 nm, and the amount of acid produced per unit of biomass for all these strains in milk serum, showed that almost all strains could grow in milk, with higher specific acidification and growth rates of Lc. lactis strains compared with Lb. plantarum strains. Nondairy Lc. lactis isolates had a lower growth and specific acidification rate than dairy isolates. The amount of acid produced per unit biomass was relatively high and similar for Lc. lactis dairy and nondairy isolates, as opposed to Lb. plantarum isolates. Lactococcus lactis ssp. lactis showed slightly lower growth and acidification rates when compared with ssp. cremoris. For Lc. lactis strains a doubling of the specific acidification rate occurred with a doubling of the maximum growth rate. This relation was not found for Lb. plantarum strains, where the acidification rate remained relatively constant across 39 strains with growth rates ranging from 0.2 h−1 to 0.3 h−1. We conclude that milk serum is a valuable alternative to milk for high-throughput strain characterization during milk fermentation.

### 2) A push–pull mechanism helps design highly competent G-quadruplex-DNA catalysts

* Chen, J., Wang, J., van der Lubbe, S. C., Cheng, M., Qiu, D., Monchaud, D., Mergny, J. L., Fonseca Guerra, C., Ju, H., Zhou, J.
* Theoretical Chemistry, AIMMS, Nanjing University, Université de Bourgogne-Franche Comté
* CCS Chemistry
* https://doi.org/10.31635/ccschem.020.202000473
* Corresponding author: Fonseca Guerra, C.
* Published Aug 2021 (early online 1 Aug 2021)
* Processed: 2021-8

Massive efforts are currently being invested to improve the performance, versatility, and scope of applications of nucleic acid catalysts. G-quadruplex (G4)/hemin DNAzymes are of particular interest owing to their structural programmability and chemical robustness. However, optimized catalytic efficiency is still bottleneck and the activation mechanism is unclear. Herein, we have designed a series of parallel G4s with different proximal cytosine (dC) derivatives to fine-tune the hemin-binding pocket for G4-DNAzymes. Combining theoretical and experimental methods, we have assessed the dependence of catalytic enhancement on the electronic properties of proximal dCs and demonstrated how proximal dCs activate catalytic proficiency. These results provide interesting clues in recapitulating the push–pull mechanism as the basis of peroxidase activity and help to devise a new strategy to design highly competent DNA catalysts whose performances are of the same order as protease.

### 3) Bistability in fatty-acid oxidation resulting from substrate inhibition

* Abegaz, F., Martines, A. C. M., Vieira Lara, M. A., Morales, M. R., Reijngoud, D. J., Wit, E. C., Bakker, B. M.
* Molecular Cell Physiology, AIMMS, University of Groningen, Università della Svizzera italiana
* PLoS Computational Biology
* https://doi.org/10.1371/journal.pcbi.1009259
* Corresponding author: Bakker, B. M.
* Published Aug 2021 (early online None)
* Processed: 2021-8

In this study we demonstrated through analytic considerations and numerical studies that the mitochondrial fatty-acid β-oxidation can exhibit bistable-hysteresis behavior. In an experimentally validated computational model we identified a specific region in the parameter space in which two distinct stable and one unstable steady state could be attained with different fluxes. The two stable states were referred to as low-flux (disease) and high-flux (healthy) state. By a modular kinetic approach we traced the origin and causes of the bistability back to the distributive kinetics and the conservation of CoA, in particular in the last rounds of the β-oxidation. We then extended the model to investigate various interventions that may confer health benefits by activating the pathway, including (i) activation of the last enzyme MCKAT via its endogenous regulator p46-SHC protein, (ii) addition of a thioesterase (an acyl-CoA hydrolysing enzyme) as a safety valve, and (iii) concomitant activation of a number of upstream and downstream enzymes by short-chain fatty-acids (SCFA), metabolites that are produced from nutritional fibers in the gut. A high concentration of SCFAs, thioesterase activity, and inhibition of the p46Shc protein led to a disappearance of the bistability, leaving only the high-flux state. A better understanding of the switch behavior of the mitochondrial fatty-acid oxidation process between a low- and a high-flux state may lead to dietary and pharmacological intervention in the treatment or prevention of obesity and or non-alcoholic fatty-liver disease.

### 4) Effects of DNA preservation solution and DNA extraction methods on microbial community profiling of soil

* Iturbe-Espinoza, P., Brandt, B. W., Braster, M., Bonte, M., Brown, D. M., van Spanning, R. J.
* Systems Bioinformatics, AIMMS, Bioinformatics, Molecular Cell Physiology, Royal Dutch Shell PLC, Ricardo
* Folia Microbiologica
* https://doi.org/10.1007/s12223-021-00866-0
* Corresponding author: Iturbe-Espinoza, P.
* Published Aug 2021 (early online None)
* Processed: 2021-8

Microbial community profiling using high-throughput sequencing relies in part on the preservation of the DNA and the effectiveness of the DNA extraction method. This study aimed at understanding to what extent these parameters affect the profiling. We obtained samples treated with and without a preservation solution. Also, we compared DNA extraction kits from Qiagen and Zymo-Research. The types of samples were defined strains, both as single species and mixtures, as well as undefined indigenous microbial communities from soil. We show that the use of a preservation solution resulted in substantial changes in the 16S rRNA gene profiles either due to an overrepresentation of Gram-positive bacteria or to an underrepresentation of Gram-negative bacteria. In addition, 16S rRNA gene profiles were substantially different depending on the type of kit that was used for extraction. The kit from Zymo extracted DNA from different types of bacteria in roughly equal amounts. In contrast, the kit from Qiagen preferentially extracted DNA from Gram-negative bacteria while DNA from Gram-positive bacteria was extracted less effectively. These differences in kit performance strongly influenced the interpretation of our microbial ecology studies.

### 5) Using functional annotations to study pairwise interactions in urinary tract infection communities

* Lara, E. G., van der Windt, I., Molenaar, D., de Vos, M. G., Melkonian, C.
* Systems Bioinformatics, AIMMS, Vrije Universiteit Amsterdam, University of Groningen
* Genes
* https://doi.org/10.3390/genes12081221
* Corresponding author: de Vos, M. G.
* Published Aug 2021 (early online 6 Aug 2021)
* Processed: 2021-8

The behaviour of microbial communities depends on environmental factors and on the interactions of the community members. This is also the case for urinary tract infection (UTI) microbial communities. Here, we devise a computational approach that uses indices of complementarity and competition based on metabolic gene annotation to rapidly predict putative interactions between pair of organisms with the aim to explain pairwise growth effects. We apply our method to 66 genomes selected from online databases, which belong to 6 genera representing members of UTI communities. This resulted in a selection of metabolic pathways with high correlation for each pairwise combination between a complementarity index and the experimentally derived growth data. Our results indicated that Enteroccus spp. were most complemented in its metabolism by the other members of the UTI community. This suggests that the growth of Enteroccus spp. can potentially be enhanced by complementary metabolites produced by other community members. We tested a few putative predicted interactions by experimental supplementation of the relevant predicted metabolites. As predicted by our method, folic acid supplementation led to the increase in the population density of UTI Enterococcus isolates. Overall, we believe our method is a rapid initial in silico screening for the prediction of metabolic interactions in microbial communities.

### 6) Imaging and modelling of poly(3-hydroxybutyrate) synthesis in Paracoccus denitrificans

* Bordel, S., van Spanning, R. J., Santos-Beneit, F.
* Systems Bioinformatics, AIMMS, University of Valladolid, Institute of Sustainable Processes, Vrije Universiteit Amsterdam
* AMB Express
* https://doi.org/10.1186/s13568-021-01273-x
* Corresponding author: Santos-Beneit, F.
* Published Dec 2021 (early online 9 Aug 2021)
* Processed: 2021-8

Poly(3-hydroxybutyrate) (PHB) granule formation in Paracoccus denitrificans Pd1222 was investigated by laser scanning confocal microscopy (LSCM) and gas chromatography analysis. Cells that had been starved for 2days were free of PHB granules but resynthesized them within 30min of growth in fresh medium with succinate. In most cases, the granules were distributed randomly, although in some cases they appeared in a more organized pattern. The rates of growth and PHB accumulation were analyzed within the frame of a Genome-Scale Metabolic Model (GSMM) containing 781 metabolic genes, 1403 reactions and 1503 metabolites. The model was used to obtain quantitative predictions of biomass yields and PHB synthesis during aerobic growth on succinate as sole carbon and energy sources. The results revealed an initial fast stage of PHB accumulation, during which all of the acetyl-CoA originating from succinate was diverted to PHB production. The next stage was characterized by a tenfold lower PHB production rate and the simultaneous onset of exponential growth, during which acetyl-CoA was predominantly drained into the TCA cycle. Previous research has shown that PHB accumulation correlates with cytosolic acetyl-CoA concentration. It has also been shown that PHB accumulation is not transcriptionally regulated. Our results are consistent with the mentioned findings and suggest that, in absence of cell growth, most of the cellular acetyl-CoA is channeled to PHB synthesis, while during exponential growth, it is drained to the TCA cycle, causing a reduction of the cytosolic acetyl-CoA pool and a concomitant decrease of the synthesis of acetoacetyl-CoA (the precursor of PHB synthesis).

### *7) 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

...

### *8) Different resource allocation in a Bacillus subtilis population displaying bimodal motility*

* Hamoen, L. W., Wang, B., Staal, J., Gao, Y., Kort, R., Syvertsson, S.
* Bioinformatics, Molecular Cell Physiology, AIMMS, UvA, Amsterdam
* bioRxiv
* https://doi.org/10.1101/2021.01.21.427716
* Corresponding author: None
* Published 22 Jan 2021 (early online None)
* Processed: 2021-1

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 ...

### *9) From recipe to research: introducing undergraduate students to the nature of science using a hybrid practical course centred on drug discovery for neglected diseases: introducing undergraduate students to the nature of science using a hybrid practical course centred on drug discovery for neglected diseases*

* Wijtmans, M., Edink, E., van Linden, O. P., Zheng, Y., Blaazer, A. R., Siderius, M., van Muijlwijk-Koezen, J. E.
* Medicinal chemistry, AIMMS, Innovations in Human Health & Life Sciences
* Drug Discovery Today
* https://doi.org/10.1016/j.drudis.2021.02.012
* Corresponding author: van Muijlwijk-Koezen, J. E.
* Published Jun 2021 (early online 18 Feb 2021)
* Processed: 2021-6

Highlights•A hybrid undergraduate laboratory course combines laboratory skills and exposure to research.•Students experience the nature of science first-hand by synthesising hit derivatives.•A neglect ...

### *10) Lewis Acid-Catalyzed Diels-Alder Reactions: Reactivity Trends across the Periodic Table*

* Vermeeren, P., Dalla Tiezza, M., van Dongen, M., Fernández, I., Bickelhaupt, F. M., Hamlin, T. A.
* Theoretical Chemistry, AIMMS, Chemistry and Pharmaceutical Sciences, Vrije Universiteit Amsterdam, Complutense University
* Chemistry - A European Journal
* https://doi.org/10.1002/chem.202100522
* Corresponding author: Bickelhaupt, F. M.
* Published 21 Jul 2021 (early online 29 Mar 2021)
* Processed: 2021-7

The catalytic effect of various weakly interacting Lewis acids (LAs) across the periodic table, based on hydrogen (Group 1), pnictogen (Group 15), chalcogen (Group 16), and halogen (Group 17) bonds, o ...

### *11) Palladium-Catalyzed Cascade to Benzoxepins by Using Vinyl-Substituted Donor–Acceptor Cyclopropanes*

* Faltracco, M., van de Vrande, K. N., Dijkstra, M., Saya, J. M., Hamlin, T. A., Ruijter, E.
* Organic Chemistry, AIMMS, Theoretical Chemistry, Vrije Universiteit Amsterdam
* Angewandte Chemie - International Edition
* https://doi.org/10.1002/anie.202102862
* Corresponding author: Ruijter, E.
* Published 21 Jun 2021 (early online 6 Apr 2021)
* Processed: 2021-6

A palladium-catalyzed intermolecular cascade (4+3) cyclocondensation of salicylaldehydes and vinylcyclopropanes is reported. A key feature of the reaction is the use of a phosphonate group as an accep ...

### *12) Exploring the Effect of Cyclization of Histamine H1Receptor Antagonists on Ligand Binding Kinetics*

* Wang, Z., Bosma, R., Kuhne, S., Van Den Bor, J., Garabitian, W., Vischer, H. F., Wijtmans, M., Leurs, R., De Esch, I. J.
* Medicinal chemistry, AIMMS, Chemistry and Pharmaceutical Sciences, Vrije Universiteit Amsterdam
* ACS Omega
* https://doi.org/10.1021/acsomega.0c06358
* Corresponding author: De Esch, I. J.
* Published 18 May 2021 (early online 7 May 2021)
* Processed: 2021-5

There is an increasing interest in guiding hit optimization by considering the target binding kinetics of ligands. However, compared to conventional structure-activity relationships, structure-kinetic ...

### *13) Understanding the Relation between Structural and Spectral Properties of Light-Harvesting Complex IILight-harvesting complex II (LHCII) is a pigment-protein complex present in higher plants and green algae. LHCII represents the main site of light absorption, and its role is to transfer the excitation energy toward the photosynthetic reaction centers, where primary energy conversion reactions take place. The optical properties of LHCII are known to depend on protein conformation. However, the relation between the structural and spectroscopic properties of the pigments is not fully understood yet. In this respect, previous classical molecular dynamics simulations of LHCII in a model membrane [Sci. Rep. 2015, 5, 1-10] have shown that the configuration and excitonic coupling of a chlorophyll (Chl) dimer functioning as the main terminal emitter of the complex are particularly sensitive to conformational changes. Here, we use quantum chemistry calculations to investigate in greater detail the effect of pigment-pigment interactions on the excited-state landscape. While most previous studies have used a local picture in which electrons are localized on single pigments, here we achieve a more accurate description of the Chl dimer by adopting a supramolecular picture where time-dependent density functional theory is applied to the whole system at once. Our results show that specific dimer configurations characterized by shorter inter-pigment distances can result in a sizable intensity decrease (up to 36%) of the Chl absorption bands in the visible spectral region. Such a decrease can be predicted only when accounting for Chl-Chl charge-transfer excitations, which is possible using the above-mentioned supramolecular approach. The charge-transfer character of the excitations is quantified by two types of analyses: one focusing on the composition of the excitations and the other directly on the observable total absorption intensities. General information*

* Sen, S., Mascoli, V., Liguori, N., Croce, R., Visscher, L.
* Theoretical Chemistry, AIMMS, Biophysics Photosynthesis/Energy, LaserLaB - Energy
* Journal of Physical Chemistry A
* https://doi.org/10.1021/acs.jpca.1c01467
* Corresponding author: Visscher, L.
* Published 27 May 2021 (early online 12 May 2021)
* Processed: 2021-5

Understanding the Relation between Structural and Spectral Properties of Light-Harvesting Complex IILight-harvesting complex II (LHCII) is a pigment-protein complex present in higher plants and green ...

### *14) A ban on BAM: an update on inhibitors of the β-barrel assembly machinery*

* Steenhuis, M., van Ulsen, P., Martin, N. I., Luirink, J.
* AIMMS, Molecular Microbiology, LaserLaB - Analytical Chemistry and Spectroscopy, LaserLaB - Molecular Biophysics, Leiden University
* FEMS microbiology letters
* https://doi.org/10.1093/femsle/fnab059
* Corresponding author: None
* Published Jun 2021 (early online 28 May 2021)
* Processed: 2021-6

Gram-negative pathogens are a rapidly increasing threat to human health worldwide due to high rates of antibiotic resistance and the lack of development of novel antibiotics. The protective cell envel ...

### *15) Limited lactosylation of beta-lactoglobulin from cow’s milk exerts strong influence on antigenicity and degranulation of mast cells*

* Bosman, G. P., Oliveira, S., Simons, P. J., Sastre Torano, J., Somsen, G. W., Knippels, L. M., Haselberg, R., Pieters, R. J., Garssen, J., Knipping, K.
* BioAnalytical Chemistry, AIMMS, Utrecht University, Danone S.A., Polpharma Biologics
* Nutrients
* https://doi.org/10.3390/nu13062041
* Corresponding author: Knipping, K.
* Published Jun 2021 (early online None)
* Processed: 2021-6

Background: beta-lactoglobulin (BLG) is one of the major cow’s milk proteins and the most abundant allergen in whey. Heating is a common technologic treatment applied during milk transformational proc ...

### *16) Model Selection Reveals the Butyrate-Producing Gut Bacterium Coprococcus eutactus as Predictor for Language Development in 3-Year-Old Rural Ugandan Children*

* Kort, R., Schlösser, J., Vazquez, A. R., Atukunda, P., Muhoozi, G. K., Wacoo, A. P., Sybesma, W. F., Westerberg, A. C., Iversen, P. O., Schoen, E. D.
* Molecular Cell Physiology, AIMMS, Vrije Universiteit Amsterdam, KU Leuven, University of Oslo, Kyambogo acad, Yoba for Life foundation, Kristiania University College
* Frontiers in Microbiology
* https://doi.org/10.3389/fmicb.2021.681485
* Corresponding author: Kort, R.
* Published 2 Jun 2021 (early online None)
* Processed: 2021-6

Introduction: The metabolic activity of the gut microbiota plays a pivotal role in the gut-brain axis through the effects of bacterial metabolites on brain function and development. In this study we i ...

### *17) A review of bottom-up and top-down emission estimates of hydrofluorocarbons (HFCs) in different parts of the world*

* Flerlage, H., Velders, G. J., de Boer, J.
* Environment and Health, AIMMS, Vrije Universiteit Amsterdam, National Institute of Public Health and the Environment, Utrecht University
* Chemosphere
* https://doi.org/10.1016/j.chemosphere.2021.131208
* Corresponding author: Flerlage, H.
* Published Nov 2021 (early online 14 Jun 2021)
* Processed: 2021-6

Hydrofluorocarbons (HFCs) are widespread alternatives for the ozone-depleting substances chlorofluorocarbons and hydrochlorofluorocarbons. They are used mainly as refrigerants or as foam-blowing agent ...

### *18) A yeast FRET biosensor enlightens c*

* Botman, D., O'Toole, T. G., Goedhart, J., Bruggeman, F. J., van Heerden, J. H., Teusink, B.
* AIMMS, Systems Bioinformatics, Systems Bioinformatics, Vrije Universiteit Amsterdam, University of Amsterdam
* Molecular Biology of the Cell
* https://doi.org/10.1091/mbc.E20-05-0319
* Corresponding author: None
* Published 15 Jun 2021 (early online None)
* Processed: 2021-6

AMP signalingThe cAMP-PKA signaling cascade in budding yeast regulates adaptation to changing environments. We developed yEPAC, a FRET-based biosensor for cAMP measurements in yeast. We used this sens ...

### *19) Author Correction: High biodiversity in a benzene-degrading nitrate-reducing culture is sustained by a few primary consumers*

* Melkonian, C., Fillinger, L., Atashgahi, S., da Rocha, U. N., Kuiper, E., Olivier, B., Braster, M., Gottstein, W., Helmus, R., Parsons, J. R., Smidt, H., van der Waals, M., Gerritse, J., Brandt, B. W., Röling, W. F., Molenaar, D., van Spanning, R. J.
* Systems Bioinformatics, Molecular Cell Physiology, AIMMS, University of Vienna, Wageningen University & Research, Vrije Universiteit Amsterdam, University of Amsterdam, Deltares
* Communications biology
* https://doi.org/10.1038/s42003-021-02311-x
* Corresponding author: None
* Published 18 Jun 2021 (early online None)
* Processed: 2021-6

...

### *20) Developmental neurotoxicity of environmentally relevant pharmaceuticals and mixtures thereof in a zebrafish embryo behavioural test*

* Atzei, A., Jense, I., Zwart, E. P., Legradi, J., Venhuis, B. J., van der Ven, L. T., Heusinkveld, H. J., Hessel, E. V.
* E&H: Environmental Health and Toxicology, AIMMS, National Institute of Public Health and the Environment
* International Journal of Environmental Research and Public Health
* https://doi.org/10.3390/ijerph18136717
* Corresponding author: Heusinkveld, H. J.
* Published 22 Jun 2021 (early online None)
* Processed: 2021-6

Humans are exposed daily to complex mixtures of chemical substances via food intake, inhalation, and dermal contact. Developmental neurotoxicity is an understudied area and entails one of the most com ...

### *21) Author Correction: A therapeutic combination of two small molecule toxin inhibitors provides broad preclinical efficacy against viper snakebite (Nature Communications, (2020), 11, 1, (6094), 10.1038/s41467-020-19981-6)The original version of this articles contained an error in Fig. 4. The graphs in panel B report the neutralization of SVSP venom by decreasing concentrations of the inhibitor nafamostat, from 150 μm to 150 nm, but the lowest concentration on the X-axis was incorrectly reported as 150 μm. This error has now been corrected on the PDF and HTML version of the article.General information*

* Albulescu, L. O., Xie, C., Ainsworth, S., Alsolaiss, J., Crittenden, E., Dawson, C. A., Softley, R., Bartlett, K. E., Harrison, R. A., Kool, J., Casewell, N. R.
* BioAnalytical Chemistry, AIMMS, Liverpool School of Tropical Medicine
* Nature Communications
* https://doi.org/10.1038/s41467-021-24308-0
* Corresponding author: Casewell, N. R.
* Published Dec 2021 (early online 24 Jun 2021)
* Processed: 2021-6

Author Correction: A therapeutic combination of two small molecule toxin inhibitors provides broad preclinical efficacy against viper snakebite (Nature Communications, (2020), 11, 1, (6094), 10.1038/s ...

### *22) Author Correction: Intracellular m*

* Das, S., Vera, M., Gandin, V., Singer, R. H., Tutucci, E.
* Systems Bioinformatics, AIMMS, Yeshiva University, McGill University, Howard Hughes Medical Institute
* Nature Reviews Molecular Cell Biology
* https://doi.org/10.1038/s41580-021-00374-6
* Corresponding author: Singer, R. H.
* Published Jul 2021 (early online None)
* Processed: 2021-7

RNA transport and localized translation (Nature Reviews Molecular Cell Biology, (2021), 22, 7, (483-504), 10.1038/s41580-021-00356-8)The first sentence under the subheading ‘Regulating developmental s ...

### *23) SARS-CoV-2 Antibodies in Adult Patients with Multiple Sclerosis in the Amsterdam MS Cohort*

* Van Kempen, Z. L., Strijbis, E. M., Al, M. M., Steenhuis, M., Uitdehaag, B. M., Rispens, T., Killestein, J.
* AIMMS, Molecular Microbiology, Vrije Universiteit Amsterdam, Sanquin Blood Supply Foundation
* JAMA Neurology
* https://doi.org/10.1001/jamaneurol.2021.1364
* Corresponding author: Van Kempen, Z. L.
* Published Jul 2021 (early online None)
* Processed: 2021-7

...

### *24) Nonadditivity in public and inhouse data: implications for drug design*

* Gogishvili, D., Nittinger, E., Margreitter, C., Tyrchan, C.
* Bio Informatics (IBIVU), AIMMS, Bioinformatics, AstraZeneca Sweden
* Journal of Cheminformatics
* https://doi.org/10.1186/s13321-021-00525-z
* Corresponding author: Nittinger, E.
* Published Dec 2021 (early online 2 Jul 2021)
* Processed: 2021-7

Numerous ligand-based drug discovery projects are based on structure-activity relationship (SAR) analysis, such as Free-Wilson (FW) or matched molecular pair (MMP) analysis. Intrinsically they assume ...

### *25) PPE38-Secretion-Dependent Proteins of M. tuberculosis Alter NF-k*

* Gallant, J., Heunis, T., Beltran, C., Schildermans, K., Bruijns, S., Mertens, I., Bitter, W., Sampson, S. L.
* Molecular Microbiology, AIMMS, University of Stellenbosch, University of Oxford, Flemish Institute for Technological Research, Vrije Universiteit Amsterdam
* Frontiers in Immunology
* https://doi.org/10.3389/fimmu.2021.702359
* Corresponding author: Sampson, S. L.
* Published 2 Jul 2021 (early online None)
* Processed: 2021-7

B Signalling and Inflammatory Responses in MacrophagesIt was previously shown that secretion of PE-PGRS and PPE-MPTR proteins is abolished in clinical M. tuberculosis isolates with a deletion in the p ...

### *26) Cross platform solutions to improve the zebrafish polar metabolome coverage using LC-QTOF MS: Optimization of separation mechanisms, solvent additives, and resuspension solvents*

* Xu, M., Legradi, J., Leonards, P.
* E&H: Environmental Bioanalytical Chemistry, E&H: Environmental Health and Toxicology, AIMMS
* Talanta
* https://doi.org/10.1016/j.talanta.2021.122688
* Corresponding author: Xu, M.
* Published 1 Nov 2021 (early online 6 Jul 2021)
* Processed: 2021-7

Untargeted metabolomics has been widely used for studies with zebrafish embryos. Until now, the number of analytical approaches to determine metabolites in zebrafish is limited, and there is a lack of ...

### *27) SARS-CoV-2 neutralising antibody testing in Europe: Towards harmonisation of neutralising antibody titres for better use of convalescent plasma and comparability of trial data*

* Nguyen, D., Simmonds, P., Steenhuis, M., Wouters, E., Desmecht, D., Garigliany, M., Romano, M., Barbezange, C., Maes, P., Van Holm, B., Mendoza, J., Oyonarte, S., Fomsgaard, A., Lassauniere, R., Zusinaite, E., Rus, K. R., Avšic-Županc, T., Reimerink, J. H., Brouwer, F., Hoogerwerf, M., Reusken, C. B., Grodeland, G., Le Cam, S., Gallian, P., Amroun, A., Brisbarre, N., Martinaud, C., Goffart, I. L., Schrezenmeier, H., Feys, H. B., Van Der Schoot, C. E., Harvala, H.
* AIMMS, Molecular Microbiology, University of Oxford, Belgian Red Cross-Flanders, University of Liege, Immune Response Service, National Influenza Centre, KU Leuven, Vircell S.L. , Andalusian Network of Transfusion Medicine, Statens Serum Institut, University of Tartu, Institute of Microbiology and Immunology, RIVML, University of Oslo, Etablissement français du sang, Institut de recherche pour le développement, Centre de Transfusion Sanguine des Armées, Institut de recherche biomédicale des armées, Ulm University, University of Amsterdam, NHS Blood and Transplant, University College London
* Eurosurveillance
* https://doi.org/10.2807/1560-7917.ES.2021.26.27.2100568
* Corresponding author: Harvala, H.
* Published 8 Jul 2021 (early online None)
* Processed: 2021-7

We compared the performance of SARS-CoV-2 neutralising antibody testing between 12 European laboratories involved in convalescent plasma trials. Raw titres differed almost 100-fold differences between ...

### *28) Efficient workflow for the investigation of the catalytic cycle of water oxidation catalysts: Combining GFN-x*

* Menzel, J. P., Kloppenburg, M., Belić, J., de Groot, H. J., Visscher, L., Buda, F.
* AIMMS, Theoretical Chemistry, Leiden University
* Journal of Computational Chemistry
* https://doi.org/10.1002/jcc.26721
* Corresponding author: Menzel, J. P.
* Published 5 Oct 2021 (early online 18 Jul 2021)
* Processed: 2021-7

TB and density functional theoryPhotocatalytic water oxidation remains the bottleneck in many artificial photosynthesis devices. The efficiency of this challenging process is inherently linked to the ...

### *29) Targeting the latent human cytomegalovirus reservoir for T-cell-mediated killing with virus-specific nanobodies*

* De Groof, T. W., Elder, E. G., Lim, E. Y., Heukers, R., Bergkamp, N. D., Groves, I. J., Wills, M., Sinclair, J. H., Smit, M. J.
* Medicinal chemistry, AIMMS, Department of Medicine, Public Health Agency of Sweden
* Nature CommunicationsArticle number:4436
* https://doi.org/10.1038/s41467-021-24608-5
* Corresponding author: Smit, M. J.
* Published 21 Jul 2021 (early online None)
* Processed: 2021-7

Latent human cytomegalovirus (HCMV) infection is characterized by limited gene expression, making latent HCMV infections refractory to current treatments targeting viral replication. However, reactiva ...

### *30) Uncovering the effects of heterogeneity and parameter sensitivity on within-host dynamics of disease: malaria as a case study*

* Horn, S., Snoep, J. L., van Niekerk, D. D.
* Molecular Cell Physiology, AIMMS, University of Stellenbosch
* BMC Bioinformatics
* https://doi.org/10.1186/s12859-021-04289-z
* Corresponding author: van Niekerk, D. D.
* Published 24 Jul 2021 (early online None)
* Processed: 2021-7

Background: The fidelity and reliability of disease model predictions depend on accurate and precise descriptions of processes and determination of parameters. Various models exist to describe within- ...

### *31) Torpor enhances synaptic strength and restores memory performance in a mouse model of Alzheimer’s disease*

* de Veij Mestdagh, C. F., Timmerman, J. A., Koopmans, F., Paliukhovich, I., Miedema, S. S., Goris, M., van der Loo, R. J., Krenning, G., Li, K. W., Mansvelder, H. D., Smit, A. B., Henning, R. H., van Kesteren, R. E.
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* Scientific Reports
* https://doi.org/10.1038/s41598-021-94992-x
* Corresponding author: van Kesteren, R. E.
* Published 29 Jul 2021 (early online None)
* Processed: 2021-7

Hibernation induces neurodegeneration-like changes in the brain, which are completely reversed upon arousal. Hibernation-induced plasticity may therefore be of great relevance for the treatment of neu ...