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### 1) Fluorescent tagging of endogenous Heme oxygenase-1 in human induced pluripotent stem cells for high content imaging of oxidative stress in various differentiated lineages

* Snijders, K. E., Fehér, A., Táncos, Z., Bock, I., Téglási, A., van den Berk, L., Niemeijer, M., Bouwman, P., Le Dévédec, S. E., Moné, M. J., Van Rossom, R., Kumar, M., Wilmes, A., Jennings, P., Verfaillie, C. M., Kobolák, J., ter Braak, B., Dinnyés, A., van de Water, B.Pages:3285-3302
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* Archives of Toxicology
* https://doi.org/10.1007/s00204-021-03127-810.1007/s00204-021-03127-8
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* Published 4 Sep 2021 (early online 4 Sep 2021)
* Processed: 2021-9

Tagging of endogenous stress response genes can provide valuable in vitro models for chemical safety assessment. Here, we present the generation and application of a fluorescent human induced pluripotent stem cell (hiPSC) reporter line for Heme oxygenase-1 (HMOX1), which is considered a sensitive and reliable biomarker for the oxidative stress response. CRISPR/Cas9 technology was used to insert an enhanced green fluorescent protein (eGFP) at the C-terminal end of the endogenous HMOX1 gene. Individual clones were selected and extensively characterized to confirm precise editing and retained stem cell properties. Bardoxolone-methyl (CDDO-Me) induced oxidative stress caused similarly increased expression of both the wild-type and eGFP-tagged HMOX1 at the mRNA and protein level. Fluorescently tagged hiPSC-derived proximal tubule-like, hepatocyte-like, cardiomyocyte-like and neuron-like progenies were treated with CDDO-Me (5.62-1000 nM) or diethyl maleate (5.62-1000 µM) for 24 h and 72 h. Multi-lineage oxidative stress responses were assessed through transcriptomics analysis, and HMOX1-eGFP reporter expression was carefully monitored using live-cell confocal imaging. We found that eGFP intensity increased in a dose-dependent manner with dynamics varying amongst lineages and stressors. Point of departure modelling further captured the specific lineage sensitivities towards oxidative stress. We anticipate that the newly developed HMOX1 hiPSC reporter will become a valuable tool in understanding and quantifying critical target organ cell-specific oxidative stress responses induced by (newly developed) chemical entities.

### 2) A method for intuitively extracting macromolecular dynamics from structural disorder

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* https://doi.org/10.1038/s41467-021-25814-x
* Corresponding author: Pearce, N. M.
* Published Dec 2021 (early online 17 Sep 2021)
* Processed: 2021-9

Macromolecular dynamics manifest as disorder in structure determination, which is subsequently accounted for by displacement parameters (also called temperature factors, or B-factors) or alternate conformations. Though B-factors contain detailed information about structural dynamics, they are the total of multiple sources of disorder, making them difficult to interpret and thus little-used in structural analysis. We report here an analytical approach for decomposing molecular disorder into a parsimonious hierarchical series of contributions, providing an intuitive basis for quantitative structural-dynamics analysis. We demonstrate the decomposition of disorder on example SARS-CoV-2 and STEAP4 structures, from both crystallographic and cryo-electron microscopy data, and reveal how understanding of the macromolecular disorder leads to deeper understanding of molecular motions and flexibility, and suggests hypotheses for molecular mechanisms.

### 3) The analytical quest for sub-micron plastics in biological matrices

* Abdolahpur Monikh, F., Vijver, M. G., Mitrano, D. M., Leslie, H. A., Guo, Z., Zhang, P., Lynch, I., Valsami-Jones, E., Peijnenburg, W. J.
* E&H: Environmental Chemistry and Toxicology, AIMMS, University of Eastern Finland, Leiden University, Swiss Federal Institute of Technology Zurich, University of Birmingham, National Institute of Public Health and the Environment
* Nano Today
* https://doi.org/10.1016/j.nantod.2021.101296
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* Published Dec 2021 (early online 23 Sep 2021)
* Processed: 2021-9

The current debate on hazards associated with sub-micron sized plastics is hampered by a lack of quantitative data on the uptake and biological fate of plastics in organisms. Analytical methods should be developed to identify, characterize, and quantify sub-micron particulate plastic in biota to understand their biological fate in terms of biodistribution, localization, bioaccumulation and clearance. Here we give a perspective on a promising workflow of sample preparation methods and techniques that could enable analysis of sub-micron plastics in biological matrices and discuss their application for biological fate studies of particulate plastic in organisms. We also expect these methods to be largely transferrable to studies considering sub-micron plastics in food, consumer products, human and some environmental compartments.

### 4) Population dynamics of microbial cross-feeding are determined by co-localization probabilities and cooperation-independent cheater growth

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* Systems Bioinformatics, AIMMS, Systems Bioinformatics, Vrije Universiteit Amsterdam
* ISME Journal
* https://doi.org/10.1038/s41396-021-00986-y
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* Published Oct 2021 (early online None)
* Processed: 2021-10

As natural selection acts on individual organisms the evolution of costly cooperation between microorganisms is an intriguing phenomenon. Introduction of spatial structure to privatize exchanged molecules can explain the evolution of cooperation. However, in many natural systems cells can also grow to low cell concentrations in the absence of these exchanged molecules, thus showing “cooperation-independent background growth”. We here serially propagated a synthetic cross-feeding consortium of lactococci in the droplets of a water-in-oil emulsion, essentially mimicking group selection with varying founder population sizes. The results show that when the growth of cheaters completely depends on cooperators, cooperators outcompete cheaters. However, cheaters outcompete cooperators when they can independently grow to only ten percent of the consortium carrying capacity. This result is the consequence of a probabilistic effect, as low founder population sizes in droplets decrease the frequency of cooperator co-localization. Cooperator-enrichment can be recovered by increasing the founder population size in droplets to intermediate values. Together with mathematical modelling our results suggest that co-localization probabilities in a spatially structured environment leave a small window of opportunity for the evolution of cooperation between organisms that do not benefit from their cooperative trait when in isolation or form multispecies aggregates.

### 5) Systematic assessment of variability in the proteome of iPSC derivatives

* Beekhuis-Hoekstra, S. D., Watanabe, K., Werme, J., de Leeuw, C. A., Paliukhovich, I., Li, K. W., Koopmans, F., Smit, A. B., Posthuma, D., Heine, V. M.
* Complex Trait Genetics, Amsterdam Neuroscience - Complex Trait Genetics, Molecular and Cellular Neurobiology, AIMMS, Amsterdam Neuroscience - Cellular & Molecular Mechanisms, Amsterdam Neuroscience - Neurodegeneration, Center for Neurogenomics and Cognitive Research
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* Published Oct 2021 (early online None)
* Processed: 2021-10

The use of induced pluripotent stem cells (iPSC) to model human complex diseases is gaining popularity as it allows investigation of human cells that are otherwise sparsely available. However, due to its laborious and cost intensive nature, iPSC research is often plagued by limited sample size and putative large variability between clones, decreasing statistical power for detecting experimental effects. Here, we investigate the source and magnitude of variability in the proteome of parallel differentiated astrocytes using mass spectrometry. We compare three possible sources of variability: inter-donor variability, inter- and intra-clonal variability, at different stages of maturation. We show that the interclonal variability is significantly smaller than the inter-donor variability, and that including more donors has a much larger influence on statistical power than adding more clones per donor. Our results provide insight into the sources of variability at protein level between iPSC samples derived in parallel and will aid in optimizing iPSC studies.

### *6) 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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### *7) Lack of Cooperativity in the Triangular X3Halogen-Bonded Synthon?*

* Dominikowska, J., Rybarczyk-Pirek, A. J., Fonseca Guerra, C.
* Theoretical Chemistry, AIMMS, University of Łódź
* Crystal Growth and Design
* https://doi.org/10.1021/acs.cgd.0c01410
* Corresponding author: Dominikowska, J.
* Published 6 Jan 2021 (early online 16 Dec 2020)
* Processed: 2021-1

We have investigated 44 crystal structures, found in the Cambridge Structural Database, containing the X3 synthon (where X = Cl, Br, I) in order to verify whether three type II halogen-halogen contact ...

### *8) Hide and mine in strings: Hardness and algorithms*

* Bernardini, G., Conte, A., Gourdel, G., Grossi, R., Loukides, G., Pisanti, N., Pissis, S. P., Punzi, G., Stougie, L., Sweering, M.
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* None
* https://doi.org/10.1109/ICDM50108.2020.00103
* Corresponding author: None
* Published 9 Feb 2021 (early online None)
* Processed: 2021-2

We initiate a study on the fundamental relation between data sanitization (i.e., the process of hiding confidential information in a given dataset) and frequent pattern mining, in the context of seque ...

### *9) Business model innovation for sustainability: The role of stakeholder interaction and managerial cognitive change*

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* None
* https://doi.org/10.4324/9780429299506-4
* Corresponding author: Oskam, I.
* Published Apr 2021 (early online None)
* Processed: 2021-4

Business model innovations emerge over time and are influenced by managerial interaction with stakeholders. Especially with regard to business model innovation for sustainability, manager–stakeholder ...

### *10) Imaging of Genetically Encoded FRET-Based Biosensors to Detect GPCR Activity*

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* Systems Bioinformatics, AIMMS, University of Amsterdam
* None
* https://doi.org/10.1007/978-1-0716-1221-7\_11
* Corresponding author: Goedhart, J.
* Published 2021 (early online None)
* Processed: 2021-6

A wealth of assays for screening GPCR activity have been developed. Biosensors that employ Förster Resonance Energy transfer (FRET) are specific and enable dynamic measurements. Moreover, FRET biosens ...

### *11) NanoLuc-Based Methods to Measure β-Arrestin2 Recruitment to G Protein-Coupled Receptors*

* Ma, X., Leurs, R., Vischer, H. F.
* Medicinal chemistry, AIMMS
* None
* https://doi.org/10.1007/978-1-0716-1221-7\_16
* Corresponding author: Vischer, H. F.
* Published 2021 (early online None)
* Processed: 2021-6

Cytosolic β-arrestins are key regulators of G protein-coupled receptors (GPCRs) by sterically uncoupling G protein activation, facilitating receptor internalization, and/or acting as G protein-indepen ...

### *12) Constructing strings avoiding forbidden substrings*

* Bernardini, G., Marchetti-Spaccamela, A., Pissis, S. P., Stougie, L., Sweering, M.
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* None
* https://doi.org/10.4230/LIPIcs.CPM.2021.9
* Corresponding author: Bernardini, G.
* Published 1 Jul 2021 (early online None)
* Processed: 2021-7

We consider the problem of constructing strings over an alphabet Σ that start with a given prefix u, end with a given suffix v, and avoid occurrences of a given set of forbidden substrings. In the dec ...

### *13) String sanitization under edit distance: Improved and generalized*

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* None
* https://doi.org/10.4230/LIPIcs.CPM.2021.19
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* Published 1 Jul 2021 (early online None)
* Processed: 2021-7

Let W be a string of length n over an alphabet S, k be a positive integer, and S be a set of length-k substrings of W. The ETFS problem (Edit distance, Total order, Frequency, Sanitization) asks us to ...

### *14) Inter-laboratory mass spectrometry dataset based on passive sampling of drinking water for non-target analysis*

* Schulze, B., van Herwerden, D., Allan, I., Bijlsma, L., Etxebarria, N., Hansen, M., Merel, S., Vrana, B., Aalizadeh, R., Bajema, B., Dubocq, F., Coppola, G., Fildier, A., Fialová, P., Frøkjær, E., Grabic, R., Gago-Ferrero, P., Gravert, T., Hollender, J., Huynh, N., Jacobs, G., Jonkers, T., Kaserzon, S., Lamoree, M., Le Roux, J., Mairinger, T., Margoum, C., Mascolo, G., Mebold, E., Menger, F., Miège, C., Meijer, J., Moilleron, R., Murgolo, S., Peruzzo, M., Pijnappels, M., Reid, M., Roscioli, C., Soulier, C., Valsecchi, S., Thomaidis, N., Vulliet, E., Young, R., Samanipour, S.
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* https://doi.org/10.1038/s41597-021-01002-w
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* Published Dec 2021 (early online 24 Aug 2021)
* Processed: 2021-8

Non-target analysis (NTA) employing high-resolution mass spectrometry is a commonly applied approach for the detection of novel chemicals of emerging concern in complex environmental samples. NTA typi ...