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### 1) Past, present, and future developments in enantioselective analysis using capillary electromigration techniques

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* https://doi.org/10.1002/elps.202000151
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* Published Jan 2021 (early online 11 Sep 2020)
* Processed: 2021-1

Enantioseparation of chiral products has become increasingly important in a large diversity of academic and industrial applications. The separation of chiral compounds is inherently challenging and thus requires a suitable analytical technique that can achieve high resolution and sensitivity. In this context, CE has shown remarkable results so far. Chiral CE offers an orthogonal enantioselectivity and is typically considered less costly than chromatographic techniques, since only minute amounts of chiral selectors are needed. Several CE approaches have been developed for chiral analysis, including chiral EKC and chiral CEC. Enantioseparations by EKC benefit from the wide variety of possible pseudostationary phases that can be employed. Chiral CEC, on the other hand, combines chromatographic separation principles with the bulk fluid movement of CE, benefitting from reduced band broadening as compared to pressure-driven systems. Although UV detection is conventionally used for these approaches, MS can also be considered. CE-MS represents a promising alternative due to the increased sensitivity and selectivity, enabling the chiral analysis of complex samples. The potential contamination of the MS ion source in EKC-MS can be overcome using partial-filling and counter-migration techniques. However, chiral analysis using monolithic and open-tubular CEC-MS awaits additional method validation and a dedicated commercial interface. Further efforts in chiral CE are expected toward the improvement of existing techniques, the development of novel pseudostationary phases, and establishing the use of chiral ionic liquids, molecular imprinted polymers, and metal-organic frameworks. These developments will certainly foster the adoption of CE(-MS) as a well-established technique in routine chiral analysis.

### 2) The CXCL12/CXCR4/ACKR3 Axis in the Tumor Microenvironment: Signaling, Crosstalk, and Therapeutic Targeting

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* Annual Review of Pharmacology and Toxicology
* https://doi.org/10.1146/annurev-pharmtox-010919-023340
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* Published 6 Jan 2021 (early online 21 Sep 2020)
* Processed: 2021-1

Elevated expression of the chemokine receptors CXCR4 and ACKR3 and of their cognate ligand CXCL12 is detected in a wide range of tumors and the tumor microenvironment (TME). Yet, the molecular mechanisms by which the CXCL12/CXCR4/ACKR3 axis contributes to the pathogenesis are complex and not fully understood. To dissect the role of this axis in cancer, we discuss its ability to impinge on canonical and less conventional signaling networks in different cancer cell types; its bidirectional crosstalk, notably with receptor tyrosine kinase (RTK) and other factors present in the TME; and the infiltration of immune cells that supporttumor progression. We discuss current and emerging avenues that target the CXCL12/CXCR4/ACKR3 axis. Coordinately targeting both RTKs and CXCR4/ACKR3 and/or CXCL12 is an attractive approach to consider in multitargeted cancer therapies. In addition, inhibiting infiltrating immune cells or reactivating the immune system along with modulating the CXCL12/CXCR4/ACKR3 axis in the TME has therapeutic promise.

### 3) Neurotoxicity and underlying cellular changes of 21 mitochondrial respiratory chain inhibitors

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* Archives of Toxicology
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* Published Feb 2021 (early online 29 Jan 2021)
* Processed: 2021-2

Inhibition of complex I of the mitochondrial respiratory chain (cI) by rotenone and methyl-phenylpyridinium (MPP +) leads to the degeneration of dopaminergic neurons in man and rodents. To formally describe this mechanism of toxicity, an adverse outcome pathway (AOP:3) has been developed that implies that any inhibitor of cI, or possibly of other parts of the respiratory chain, would have the potential to trigger parkinsonian motor deficits. We used here 21 pesticides, all of which are described in the literature as mitochondrial inhibitors, to study the general applicability of AOP:3 or of in vitro assays that are assessing its activation. Five cI, three complex II (cII), and five complex III (cIII) inhibitors were characterized in detail in human dopaminergic neuronal cell cultures. The NeuriTox assay, examining neurite damage in LUHMES cells, was used as in vitro proxy of the adverse outcome (AO), i.e., of dopaminergic neurodegeneration. This test provided data on whether test compounds were unspecific cytotoxicants or specifically neurotoxic, and it yielded potency data with respect to neurite degeneration. The pesticide panel was also examined in assays for the sequential key events (KE) leading to the AO, i.e., mitochondrial respiratory chain inhibition, mitochondrial dysfunction, and disturbed proteostasis. Data from KE assays were compared to the NeuriTox data (AO). The cII-inhibitory pesticides tested here did not appear to trigger the AOP:3 at all. Some of the cI/cIII inhibitors showed a consistent AOP activation response in all assays, while others did not. In general, there was a clear hierarchy of assay sensitivity: changes of gene expression (biomarker of neuronal stress) correlated well with NeuriTox data; mitochondrial failure (measured both by a mitochondrial membrane potential-sensitive dye and a respirometric assay) was about 10-260 times more sensitive than neurite damage (AO); cI/cIII activity was sometimes affected at > 1000 times lower concentrations than the neurites. These data suggest that the use of AOP:3 for hazard assessment has a number of caveats: (i) specific parkinsonian neurodegeneration cannot be easily predicted from assays of mitochondrial dysfunction; (ii) deriving a point-of-departure for risk assessment from early KE assays may overestimate toxicant potency.

### 4) Bioactivation of trichloroethylene to three regioisomeric glutathione conjugates by liver fractions and recombinant human glutathione transferases: species differences and implications for human risk assessment

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* https://doi.org/10.1016/j.toxlet.2021.01.021
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* Published 1 Feb 2021 (early online None)
* Processed: 2021-2

Enzymatic conjugation of glutathione (GSH) to trichloroethylene (TCE) followed by catabolism to the corresponding cysteine-conjugate, S-(dichlorovinyl)-L-cysteine (DCVC), and subsequent bioactivation by renal cysteine conjugate beta-lyases is considered to play an important role in the nephrotoxic effects observed in TCE-exposed rat and human. In this study, it is shown for the first time that three regioisomers of GSH-conjugates of TCE are formed by rat and human liver fractions, namely S-(1,2-trans-dichlorovinyl)-glutathione (1,2-trans-DCVG), S-(1,2-cis-dichlorovinyl)-glutathione (1,2-cis-DCVG) and S-2,2-dichlorovinyl-glutathione (2,2-DCVG). In incubations of TCE with rat liver fractions their amounts decreased in order of 1,2-cis-DCVG > 1,2-trans-DCVG > 2,2-DCVG. Human liver cytosol showed a more than 10-fold lower activity of GSH-conjugation, with amounts of regioisomers decreasing in order 2,2-DCVG > 1,2-trans-DCVG > 1,2-cis-DCVG. Incubations with recombinant human GSTs suggest that GSTA1-1 and GSTA2-2 play the most important role in human liver cytosol. GSTP1-1, which produces regioisomers in order 1,2-trans-DCVG > 2,2-cis-DCVG > 1,2-cis-DCVG, is likely to contribute to extrahepatic GSH-conjugation of TCE. Analysis of the products formed by a beta-lyase mimetic model showed that both 1,2-trans-DCVC and 1,2-cis-DCVC are converted to reactive products that form cross-links between the model nucleophile 4-(4-nitrobenzyl)-pyridine (NBP) and thiol-species. No NBP-alkylation was observed with 2,2-DCVC corresponding to its low cytotoxicity and mutagenicity. The lower activity of GSH-conjugation of TCE by human liver fractions, in combination with the lower fraction of potential nephrotoxic and mutagenic 1,2-DCVG-isomers, suggest that humans are at much lower risk for TCE-associated nephrotoxic effects than rats.

### *5) A schematic sampling protocol for contaminant monitoring in raptors*

* Espín, S., Andevski, J., Duke, G., Eulaers, I., Gómez-Ramírez, P., Hallgrimsson, G. T., Helander, B., Herzke, D., Jaspers, V. L., Krone, O., Lourenço, R., María-Mojica, P., Martínez-López, E., Mateo, R., Movalli, P., Sánchez-Virosta, P., Shore, R. F., Sonne, C., van den Brink, N. W., van Hattum, B., Vrezec, A., Wernham, C., García-Fernández, A. J.
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* Published Jan 2021 (early online 12 May 2020)
* Processed: 2021-1

Birds of prey, owls and falcons are widely used as sentinel species in raptor biomonitoring programmes. A major current challenge is to facilitate large-scale biomonitoring by coordinating contaminant ...

### *6) Receptor-based in vitro activities to assess human exposure to chemical mixtures and related health impacts*

* Vinggaard, A. M., Bonefeld-Jørgensen, E. C., Jensen, T. K., Fernandez, M. F., Rosenmai, A. K., Taxvig, C., Rodriguez-Carrillo, A., Wielsøe, M., Long, M., Olea, N., Antignac, J. P., Hamers, T., Lamoree, M.
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* Environment International
* https://doi.org/10.1016/j.envint.2020.106191
* Corresponding author: Vinggaard, A. M.
* Published Jan 2021 (early online 14 Oct 2020)
* Processed: 2021-1

Humans are exposed to a large number of chemicals from sources such as the environment, food, and consumer products. There is growing concern that human exposure to chemical mixtures, especially durin ...

### *7) Asymmetrical flow field-flow fractionation to probe the dynamic association equilibria of β-D-galactosidase*

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* Journal of Chromatography A
* https://doi.org/10.1016/j.chroma.2020.461719
* Corresponding author: Ventouri, I. K.
* Published 4 Jan 2021 (early online 13 Nov 2020)
* Processed: 2021-1

Protein dynamics play a significant role in many aspects of enzyme activity. Monitoring of structural changes and aggregation of biotechnological enzymes under native conditions is important to safegu ...

### *8) Rapid Screening α-Glucosidase Inhibitors from Natural Products by At-Line Nanofractionation with Parallel Mass Spectrometry and Bioactivity Assessment*

* Liu, R., Kool, J., Jian, J., Wang, J., Zhao, X., Jiang, Z., Zhang, T.
* BioAnalytical Chemistry, AIMMS, Jinan University, SCIEX (China) Co., Ltd.
* Journal of Chromatography A
* https://doi.org/10.1016/j.chroma.2020.461740
* Corresponding author: Jiang, Z.
* Published 4 Jan 2021 (early online 23 Nov 2020)
* Processed: 2021-1

In this study, a novel at-line nanofractionation screening platform was successfully developed for the rapid screening and identification of α-glucosidase inhibitors from natural products. A time-cour ...

### *9) Reducing the influence of geometry-induced gradient deformation in liquid chromatographic retention modelling*

* Bos, T. S., Niezen, L. E., den Uijl, M. J., Molenaar, S. R., Lege, S., Schoenmakers, P. J., Somsen, G. W., Pirok, B. W.
* BioAnalytical Chemistry, AIMMS, University of Amsterdam, Centre for Analytical Sciences Amsterdam (CASA), Agilent Technologies
* Journal of Chromatography A
* https://doi.org/10.1016/j.chroma.2020.461714
* Corresponding author: Bos, T. S.
* Published 4 Jan 2021 (early online 13 Nov 2020)
* Processed: 2021-1

Rapid optimization of gradient liquid chromatographic (LC) separations often utilizes analyte retention modelling to predict retention times as function of eluent composition. However, due to the dwel ...

### *10) Influence maximization in the presence of vulnerable nodes: A ratio perspective*

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* Bioinformatics, AIMMS, Bio Informatics (IBIVU), King's College London, University of Nebraska-Lincoln
* Theoretical Computer Science
* https://doi.org/10.1016/j.tcs.2020.11.020
* Corresponding author: Loukides, G.
* Published 8 Jan 2021 (early online 20 Nov 2020)
* Processed: 2021-1

Influence maximization is a key problem seeking to identify users who will diffuse information to influence the largest number of other users in a social network. A drawback of the influence maximizat ...

### *11) Dynamic co-culture metabolic models reveal the fermentation dynamics, metabolic capacities and interplays of cheese starter cultures*

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* Biotechnology and Bioengineering
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* Published Jan 2021 (early online 14 Sep 2020)
* Processed: 2021-1

In this study, we have investigated the cheese starter culture as a microbial community through a question: can the metabolic behaviour of a co-culture be explained by the characterized individual org ...

### *12) Influence of short- And long-term exposure on the biodegradation capacity of activated sludge microbial communities in ready biodegradability tests*

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* Published Jan 2021 (early online None)
* Processed: 2021-1

Ready biodegradability tests (RBTs) are extensively used to screen the potential of chemicals to be biodegraded. The use of RBT protocols often results in large variations of test results that may lea ...

### *13) Critique of the “Comment” etitled “Pyrethroid exposure: Not so harmless after all” by Demeneix et al. (2020) published in the lancet diabetes endocrinology*

* Barile, F. A., Berry, S. C., Blaauboer, B., 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., Tsatsakis, A., Vermeulen, N. P.
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* Toxicology Letters
* https://doi.org/10.1016/j.toxlet.2020.12.020
* Corresponding author: Greim, H.
* Published 1 Apr 2021 (early online 4 Jan 2021)
* Processed: 2021-1

...

### *14) Serial propagation in water-in-oil emulsions selects for Saccharomyces cerevisiae strains with a reduced cell size or an increased biomass yield on glucose*

* van Tatenhove-Pel, R. J., Zwering, E., Boreel, D. F., Falk, M., van Heerden, J. H., Kes, M. B., Kranenburg, C. I., Botman, D., Teusink, B., Bachmann, H.
* AIMMS, Systems Bioinformatics, Systems Bioinformatics, Vrije Universiteit Amsterdam
* Metabolic Engineering
* https://doi.org/10.1016/j.ymben.2020.12.005
* Corresponding author: Bachmann, H.
* Published Mar 2021 (early online 5 Jan 2021)
* Processed: 2021-1

In S. cerevisiae and many other micro-organisms an increase in metabolic efficiency (i.e. ATP yield on carbon) is accompanied by a decrease in growth rate. From a fundamental point of view, studying t ...

### *15) KLIFS: an overhaul after the first 5 years of supporting kinase research*

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* Nucleic acids research
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* Corresponding author: None
* Published 8 Jan 2021 (early online None)
* Processed: 2021-1

Kinases are a prime target of drug development efforts with >60 drug approvals in the past two decades. Due to the research into this protein family, a wealth of data has been accumulated that keeps o ...

### *16) Unlocking Elementary Conversion Modes: ecmtool Unveils All Capabilities of Metabolic Networks*

* Clement, T. J., Baalhuis, E. B., Teusink, B., Bruggeman, F. J., Planqué, R., de Groot, D. H.
* Systems Bioinformatics, AIMMS, Systems Bioinformatics, Mathematics, Vrije Universiteit Amsterdam
* Patterns
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* Published 8 Jan 2021 (early online None)
* Processed: 2021-1

The metabolic capabilities of cells determine their biotechnological potential, fitness in ecosystems, pathogenic threat levels, and function in multicellular organisms. Their comprehensive experiment ...

### *17) Hazardous compounds in recreational and urban recycled surfaces made from crumb rubber. Compliance with current regulation and future perspectives*

* Celeiro, M., Armada, D., Dagnac, T., de Boer, J., Llompart, M.
* Environment and Health, AIMMS, University of Santiago de Compostela, Agronomic Research Centre (AGACAL-CIAM) – Unit of Organic Contaminants
* Science of the Total Environment
* https://doi.org/10.1016/j.scitotenv.2020.142566
* Corresponding author: Llompart, M.
* Published 10 Feb 2021 (early online 29 Sep 2020)
* Processed: 2021-2

Crumb rubber obtained from scrap tires is greatly employed for the construction of different facilities for sport, recreational and other uses. However, in recent years the concern about their safety ...

### *18) Circular pattern matching with k mismatches*

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* Bioinformatics, AIMMS, Bio Informatics (IBIVU), King's College London, University of Warsaw, Bar-Ilan University
* Journal of Computer and System Sciences
* https://doi.org/10.1016/j.jcss.2020.07.003
* Corresponding author: Pissis, S. P.
* Published Feb 2021 (early online 29 Jul 2020)
* Processed: 2021-2

We consider the circular pattern matching with k mismatches (k-CPM) problem in which one is to compute the minimal Hamming distance of every length-m substring of T and any cyclic rotation of P, if th ...

### *19) G protein-coupled receptors as promising targets in cancer*

* Perez Almeria, C. V., Setiawan, I. M., Siderius, M., Smit, M. J.
* AIMMS, Medicinal chemistry
* Current Opinion in Endocrine and Metabolic Research
* https://doi.org/10.1016/j.coemr.2020.10.005
* Corresponding author: Smit, M. J.
* Published Feb 2021 (early online 26 Oct 2020)
* Processed: 2021-2

G protein-coupled receptors (GPCRs) control diverse cellular functions, and their dysregulation is involved in a plethora of diseases including tumorigenesis. In the last decade, the association of GP ...

### *20) Metabolic cooperation and spatiotemporal niche partitioning in a kefir microbial community*

* Blasche, S., Kim, Y., Mars, R. A., Machado, D., Maansson, M., Kafkia, E., Milanese, A., Zeller, G., Teusink, B., Nielsen, J., Benes, V., Neves, R., Sauer, U., Patil, K. R.
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* NATURE MICROBIOLOGY
* https://doi.org/10.1038/s41564-020-00816-5
* Corresponding author: Patil, K. R.
* Published Feb 2021 (early online None)
* Processed: 2021-2

Microbial communities often undergo intricate compositional changes yet also maintain stable coexistence of diverse species. The mechanisms underlying long-term coexistence remain unclear as system-wi ...