

Non-Targeted Analysis (NTA): Selected References
Biomonitoring California Scientific Guidance Panel Meeting
July 14, 2020

Barupal DK and Fiehn O (2019). Generating the blood exposome database using a comprehensive text mining and database fusion approach. *Environ Health Perspect* 127(9):097008. Abstract available at: <http://www.sciencedirect.com/science/article/pii/S0958166917302574> (full article available upon request).

Barupal DK, Fan S, and Fiehn O (2018). Integrating bioinformatics approaches for a comprehensive interpretation of metabolomics datasets. *Curr Opin Biotech* 54: 1-9. Available at: <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC29413745/>.

Barupal DK and Fiehn O (2017). Chemical similarity enrichment analysis (ChemRICH) as alternative to biochemical pathway mapping for metabolomic datasets. *Sci Rep* 7(1):1-11. Available at: <https://www.nature.com/articles/s41598-017-15231-w>.

Bonini P, Kind T, Tsugawa H, Barupal DK, and Fiehn O (2020). Retip: retention time prediction for compound annotation in untargeted metabolomics. *Anal Chem* 92(11):7515-7522. Abstract available at: <https://pubs.acs.org/doi/abs/10.1021/acs.analchem.9b05765> (full article available upon request).

Dennis KK, Marder E, Balshaw DM, Cui Y, Lynes MA, Patti GJ, Rappaport SM, Shaughnessy DT, Vrijheid M, and Barr DB (2017). Biomonitoring in the era of the exposome. *Environ Health Perspect* 125(4):502–510. Available at: <https://doi.org/10.1289/EHP474>.

Fan S, Kind T, Cajka T, Hazen SL, Tang WHW, Kaddurah-Daouk R, Irvin MR, Arnett DK, Barupal DK, and Fiehn O (2019). Systematic error removal using random forest for normalizing large-scale untargeted lipidomics data. *Anal Chem* 91(5):3590-3596. Abstract available at: <https://pubs.acs.org/doi/10.1021/acs.analchem.8b05592> (full article available upon request).

Grashow R, Bessonneau V, Gerona RR, Wang A, Trowbridge J, Lin T, Buren H, Rudel RA, Morello-Frosch R (2020). Integrating exposure knowledge and serum suspect screening as a new approach to biomonitoring: an application in firefighters and office workers. *Environ Sci Technol* 54(7):4344–55. Available at: <https://doi.org/10.1021/acs.est.9b04579>.

Guha N, Guyton KZ, Loomis D, Barupal DK (2016). Prioritizing chemicals for risk assessment using chemoinformatics: examples from the IARC monographs on pesticides. *Environ Health Perspect* 124(12):1823–9. Available at: <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC5132635/>.

Hedgespeth ML, Gibson N, McCord J, Strynar M, Shea D, Nichols EG (2019). Suspect screening and prioritization of chemicals of concern (COCs) in a forest-water reuse system watershed. *Sci Total Environ* 694:133378. Abstract available at: <https://www.sciencedirect.com/science/article/pii/S004896971933298X?via%3Dihub> (full article available upon request).

Hollender J, Schymanski EL, Singer HP, Ferguson PL. (2017) Nontarget screening with high resolution mass spectrometry in the environment: ready to go? *Environ Sci Technol* 51(20):11505-11512. Available at: <https://pubs.acs.org/doi/10.1021/acs.est.7b02184>.

Houtz E, Wang M, and Park JS (2018). Identification and fate of aqueous film forming foam derived per- and polyfluoroalkyl substances in a wastewater treatment plant. *Environ Sci Technol* 52(22):13212–13221. Abstract available at: <https://doi.org/10.1021/acs.est.8b04028> (full article available upon request).

McCord J and Strynar M (2019). Identifying per- and polyfluorinated chemical species with a combined targeted and non-targeted-screening high-resolution mass spectrometry workflow. *J Vis Exp* 18(146): e59142. Available at: <https://www.jove.com/video/59142/identifying-per-polyfluorinated-chemical-species-with-combined>.

McCord J and Strynar M (2019). Identification of per- and polyfluoroalkyl substances in the Cape Fear River by high resolution mass spectrometry and nontargeted screening. *Environ Sci Technol* 53(9):4717–27. Abstract available at: <https://doi.org/10.1021/acs.est.8b06017> (full article available upon request).

NTA References for July 2020 SGP Meeting

- McEachran AD, Sobus JR, and Williams AJ (2017). Identifying known unknowns using the US EPA's CompTox Chemistry Dashboard. *Anal Bioanal Chem* 409(7):1729–35. Abstract available at: <https://link.springer.com/article/10.1007%2Fs00216-016-0139-z> (full article available upon request).
- Newton SR, Sobus JR, Ulrich EM, Singh RR, Chao A, McCord J, Laughlin-Toth S, and Strynar M (2020). Examining NTA performance and potential using fortified and reference house dust as part of EPA's Non-Targeted Analysis Collaborative Trial (ENTACT). *Anal Bioanal Chem* 412(18):4221–33. Available at: <https://doi.org/10.1007/s00216-020-02658-w>.
- Newton S, McMahan R, Sobus J, Mansouri K, Williams A, McEachran A, and Strynar M (2018). Suspect screening and non-targeted analysis of drinking water using point-of-use filters. *Environ Pollut* 234:297–306. Available at: <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC6145080/>.
- Phillips KA, Yau A, Favela KA, Isaacs KK, McEachran A, Grulke C, Richard AM, Williams AJ, Sobus JR, Thomas RS, and Wambaugh JF (2018). Suspect screening analysis of chemicals in consumer products. *Environ Sci Technol* 52(5):3125–35. Available at: <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC6168952/>.
- Rappaport SM, Barupal DK, Wishart D, Vineis P, and Scalbert A (2014). The blood exposome and its role in discovering causes of disease. *Environ Health Perspect* 122(8):769–74. Available at: <https://ehp.niehs.nih.gov/doi/full/10.1289/ehp.1308015>.
- Schymanski EL, Jeon J, Gulde R, Fenner K, Ruff M, Singer HP, and Hollender J. (2014). Identifying small molecules via high resolution mass spectrometry: communicating confidence. *Environ Sci Technol* 48(4):2097–2098. Available at: <https://doi.org/10.1021/es5002105>.
- Sobus JR, Grossman JN, Chao A, Singh R, Williams AJ, Grulke CM, Richard AM, Newton SR, McEachran AD, and Ulrich EM (2019). Using prepared mixtures of ToxCast chemicals to evaluate non-targeted analysis (NTA) method performance. *Anal Bioanal Chem* 411(4):835–51. Available at: <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC6469933/>.
- Sobus JR, Wambaugh JF, Isaacs KK, Williams AJ, McEachran AD, Richard AM, Grulke CM, Ulrich EM, Rager JE, Strynar MJ, and Newton SR (2018). Integrating tools for non-targeted analysis research and chemical safety evaluations at the US EPA. *J Expo Sci Environ Epidemiol* 28(5):411–26. Available at: <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC6661898/>.
- Ulrich EM, Sobus JR, Grulke CM, Richard AM, Newton SR, Strynar MJ, Mansouri K, and Williams AJ (2019). EPA's Non-Targeted Analysis Collaborative Trial (ENTACT): genesis, design, and initial findings. *Anal Bioanal Chem* 411(4):853–66. Abstract available at: <https://link.springer.com/article/10.1007%2Fs00216-018-1435-6> (full article available upon request).
- Walker DI, Mallon T, Hopke PK, Uppal K, Go Y-M, Rohrbeck P, Pennell KD, and Jones DP (2016). Deployment-associated exposure surveillance with high-resolution metabolomics. *J Occup Environ Med* 58(8): S12–21. Available at: <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4978191/>.
- Walker DI, Valvi D, Rothman N, Lan Q, Miller GW, and Jones DP (2019). The metabolome: A key measure for exposome research in epidemiology. *Curr Epidemiol Rep* 6:93–103. Available at: <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC6905435/>.
- Wang A, Gerona RR, Schwartz JM, Lin T, Sirota M, Morello-Frosch R, and Woodruff TJ (2018). A suspect screening method for characterizing multiple chemical exposures among a demographically diverse population of pregnant women in San Francisco. *Environ Health Perspect* 126(7). Available at: <https://ehp.niehs.nih.gov/doi/10.1289/EHP2920>.
- Washington JW, Rosal CG, McCord JP, Strynar MJ, Lindstrom AB, Bergman EL, Goodrow SM, Tadesse HK, Pilant AN, Washington BJ, Davis MJ, Stuart BG, and Jenkins TM (2020). Nontargeted mass-spectral detection of chloroperfluoropolyether carboxylates in New Jersey soils. *Science* 368:1103–1107. Abstract available at: <https://science.sciencemag.org/content/368/6495/1103> (full article available upon request).