**Nicholas J. Peraino, PhD**

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Chemical Engineer, Organic Chemist, and Analytical Chemist trained in biomedical and environmental applications of chemistry. Mass Spectrometry Laboratory Manager responsible for procurement and maintenance of instruments, expanding facilities research protocols, and consulting research groups on how to design their experiments within instrument limitations and abilities.

**Education**

*Oakland University; Rochester, MI*

**Ph.D. Biomedical Sciences: Health and Environmental Chemistry, 2017**

* Dissertation: Asymmetric Synthesis using Sulfoxonium Ylides

*Western Michigan University; Kalamazoo, MI*

**B.S. Chemical Engineering: Life Sciences, 2009**

* Minors in Chemistry and Mathematics
* Senior Design: Methanol distillation recovery loop optimization for biodiesel reactor.

**Work History**

*Lumigen Instrument Center, Wayne State University, Detroit,MI*

**Mass Spectrometry Laboratory Manager, 2017 to present**

* Maintained, Calibrated, and Trained students on instruments in the LIC at Wayne State.
* Managed instrument use for billing.
* Conducted research in the development of analytical methods in molecular biology and environmental sciences.
* Designed MALDI sprayer project for summer research student. (Arduino/C++)
* Write programs for spectral analysis (Python/Rust)

*Department of Chemistry, Oakland University, Rochester, MI*

**Assistant Instrumentation Engineer and Organic Chemistry TA, 2012 to 2017**

* Maintained gases and coolants, Calibrated, and Trained students on NMR, GCMS, LCMS, IR, chiral HPLC/GC.

**Organic Synthesis Research Assistant, 2011 to 2017**

* Researched novel synthesis protocols for cyclic moieties common in APIs
* Determined Intrinsic Reaction Coordinates using Gaussain to predict selectivity
* Conducted Molecular Dynamics simulations using PROGDYN

*Department of Paper Engineering, Chemical Engineering, and Imaging, WMU, Kalamazoo, MI*

**Senior Design Project, 2009**

* Modeled and optimized methanol recovery and purification loop for biodiesel processing plant.

*Department of Chemistry, Western Michigan University, Kalamazoo, MI*

**Organic Synthesis Research Assistant, 2008**

* Conducted organic synthesis of rhizopines for metabolic testing.

*Serv-U-Success, Southeast Michigan Territory,* **2006-2011**

**Sales Representative**

* Managed crew and scheduled ordering for high volume Meijer merchandise.

**Summary of Skills**

* Programming (Python mostly, C++, Rust, and Visual Basic (Excel), R-Studio)
  + Scikit-learn, Numpy, Numba, SciPy, PyTorch, RDKit, Pyteomics, QT, OpenGL, Cython for RUST/C++
* Chemical synthesis, reaction kinetics profiling, and unknown characterization. (DFT in Gaussian)
* Quantitation, statistical analysis, and metabo/proeto/lipidomics and bioniformatics (GNPS, XCMS, MaxQuant)
* Quantum mechanical approaches to solving reaction thermodynamics for product distribution optimization.
* Process control and design. (LabView, Pumping, reactor, temperature control, and separation processes.)
* Microelectronic design (Digital logic, microcontrollers (Arduino), FPGA with (Alchitry))
* Cell culture and transfection for biochemical probes (CHO-K1, serotonin receptor agonists)
* Passed NCEES FE Chemical Engineering exam.

**Instrumentation**

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| **LC/MSMS** – Shimadzu 840, Thermo Quantiva, Altis | **GCMS** – Agilent 6890/5973, 7890/5975 |
| **LCMS** – Waters ZQ, Shimadzu 2010 | **GC/MSMS**– Thermo TSQ Duo/Trace 1310 |
| **LC-TOF** – Waters LCT XE, Agilent QTOF | **Head Space** **GC**- Perkin Elmer ECD/FID |
| **FTIR** – Varian, Bruker | **MALDI-TOF**– Bruker Ultraflextreme |
| **IonTrap MSn** – Thermo Orbitrap | **Chiral HPLC and GC** – Perkin Elmer Flexar |
| **EDX** – Shimadzu | **NMR** – Bruker Avance (200, 400, 700, TDNMR), JEOL 400 MHz |
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| **LC-UV/PDA-** Waters 2795, 2695, 996 PDA, Varian 920 with dual channel UV/VIS, Shimadzu LC-8A preparative HPLC/PDA | |
| **Plate Reader-** Spectra Max M2e UV/VIS, Fluorescence, Luminescence. | |
| Attended Seminar on Perkin Elmer’s DMA, TGA-IR, and DSC. | |

**Continued Training**

“Advanced Metabolomics and Systems Biology” Gary Sizudak, Scripps Institute, June 2, 2019

“Advanced Imaging Mass Spectrometry” Vanderbilt University, April 24, 2018

“Metabolomics and Orbitrap Training” Thermo Fisher Scientific, May 1, 2018

“Sample Prep and LC Column Solutions for Forensic Toxicology Applications” Waters, November 29, 2017

“Accelerating Innovation Chromatography Symposium” ThermoFisher Scientific, September 14, 2017

“Advanced GCMSMS with TSQ Duo/Trace 1310 and Chromeleon” ThermoFisher Scientific, June 12, 2017

**Projects Worked**

* Derivitization of myoinositol for nitrogen fixing bacteria attractant.
* Methanol distillation recovery loop optimization for biodiesel manufacturing plant.
* Isotopic labeling and mechanistic studies of reaction of ylides with aldehydes and ketenes.
* Development of asymmetric one pot synthesis of γ-lactones from α,β-unsaturated sulfoxonium salts.
* Quantum molecular dynamics and IRC mapping of alkaloid catalyzed ketene heterodimerization.
* Computational modeling of NMR monitored reaction kinetics for phosphine catalyzed cycloaddition of ketenes and aldehydes. Gaussian
* Determination of Benzyl Alcohol content in off label drug application by GCMS.
* Testing of phthalates in food products by GCMSMS.
* Functionalized microcystins/nodularin by LCMS
* Pesticides from active air sampling filters for AchE Inhibition study by LCMSMS
* CyP450 assay for drug metabolism interactions LCMSMS
* Bacteria speciation and biomarker discovery by Orbitrap and MALDI-TOF
* Glucose metabolism assay on LCMSMS
* Cannabinoid metabolite analysis by LCMSMS
* Short chain fatty, amino, and bile acid analysis (methyl esterifaction and MTBSTFA).
* Camelid trypsin wool digest analysis for archaeological artifact fingerprinting.
* VOC ground sampling using passive air monitors. GCMS
* Mechanistic validation of diammonium catalyzed esterification of carbohydrates. Orbitrap
* Validation of monocolonal antibody conjugation site by deglycosylation and trypsin digestion for targeting of triple negative breast cancer. MALDI-TOF/Orbitrap
* MALDI Imaging of microplastic damage to zebra mussels.
* Data Dependent Acquisition for MSn analysis of bacterial extracts for bioactive compounds.
* Analysis of plumbing systems for uptake of methylcyclohexylmethanol into rubber components by GCMS.
* Analysis of drinking and source water samples for cyanotoxins.
* Analysis of mouse urine for Glycans.
* Thermal Desorption of 100 uL samples of mouse blood for trace levels of toluene.
* Purge and trap of water samples for 60 VOC compounds.
* Developed quantitative method by relative response factor for unisolable homo and heteronitrene coupling products by GCMS.
* SPME of mouse serum for VOCs
* Targeted metabolomic profiling for dehydration status and cancer incidence.
* Book binder protein characterization by trypsin digestion and MALDI
* Detection of enzyme mutation in patients by whole red blood cell lysate trypsin digestion and targeted analysis.
* Purge and Trap analysis of TTHMS in water before and after exposure to animals in aquarium.
* Characterization of acid/microwave mediated decomposition of cyanotoxins for class quantification.
* MALDI imaging mass spectrometry of tissue damage and metabolomics from cyanotoxin exposure.
* Recovery of microcystin stored in tissue and plasma by maceration, extraction, and trypsin digestion.
* 5-HT receptor fluorescence assay for compound screening in HEPG2, MCF-7, and orthologous transfection of CHO-K1 cells.
* Comparative quantitation of sphingosine-1-phosphate in serum in obese and healthy patients using ELISA and LCMSMS
* LCMSMS trace analysis of pesticides in water using online sample concentration.
* Identification and semi quantitative assessment of VOCs enriched in trees.
* Identification of oxidation byproducts of toxins in KMnO4 water treatment.
* Cys34 adduct identification in mouse, bovine, and human serum albumin as marker for exposure to and secondary endogenous release of microcystins.
* Identification of signaling molecules in freshwater broadcast spawners with cyanobacteria.
* Developing modified PAMPA assay for compound discovery.
* Participating in combined research efforts with Virginia Tech and University of Michigan to assess aerosol exposure of microcystins.
* Writing software suite in python to analyze HRMS data against a database to account for ion speciation, potential fragmentation patterns, and statistical analysis.(PyQT, OpenGL)
* Neural network training for predictive parent compound from fragmentation data. (PyTorch, SciKit-Learn, RDKit, Pyteomics)
* Quantification of shortchain fatty acids in reactor feed and product streams.
* Synthesis of swellable silicagel derivatives for hazardous material recovery and value added waste streams.
* Analysis of VOCs in cell culture media.
* 18O2, 16O2, 16O18O ratio analysis in catalytic oxidation of heavy water.

**Instrument Repair**

* Salvaged ECD, FID, and ALS from a corroded old Perkin Elmer GC for installation into a new GC-Headspace system.
* Replaced pump seals and motherboard in PerkinElmer Flexar HPLC.
* Replaced pneumatic flow controller in Waters ZQ.
* Replaced injection module and pump seals in Waters 2695.
* Replaced injection port seals, pump seals, and degassing pump in Shimadzu Sil-30ACMP, LC-20AD, and DGU.
* Performed PMs on Shimadzu 8040, Shimadzu 2010, LTQ XL, Waters ZQ, TSQ Quantiva, TSQ Duo, Agilent 6890/5973N, and Ultraflextreme.
* Cleaned and rebuilt Edwards roughing pump seals, gaskets, etc.
* Assessed damage to MALDI from power bump, replaced high voltage power supply, and retuned methods for various mass ranges for new voltage supply.
* Salvaged a broken down Agilent6890N/5973N from a faculty member. Returned to working order and updated the software for everyone in the department to use. Determined a method for updating IP address to firmware via bootP service because the front screen was not operable on the MS.
* Restored connectivity to a Waters GCT via restoring proper FTP protocol and VXWorks files and repaired pneumatic valve controller.
* Removed and retuned probe in Bruker and Varian NRMS when student dropped sample tube into machine.
* Setup and restored Velocity XPT/Solatek 72 purge and trap system.
* Setup and restored CDS 8000 concentrator.
* Reconfigured Varian Excalibur for NIR/FarIR/MidIR as necessary.
* Installed Waters 2795 HPLC that was not being used and interfaced with LTQ Orbitrap. Worked around Firmware incompatibility to allow automatic HPLC injections for metabolomics.
* Repaired Waters 2695/960 HPLC-PDA to operating condition.
* Installed Varian 920 LC for semipreparative work.
* Replaced Turbo molecular pump in Orbitrap and LTQ.
* Salvaged HP6890 for use with GCT and set up GC-APCI-Orbitrap system for HRMS lipid analysis.
* Modified Shimadzu AC30 and pumping program to allow for large volume injection outside of specs to allow for sub ppt level detection of pesticides by online solid phase extraction within the autosampler.
* Repaired LCT Premier XE by transferring motherboard from GCT EPC.
* Moved, installed, and qualified, Thermo LTQ-XL fitted with Acquity UPLC.
* Installed and qualified Shimadzu 2010EV.
* Repaired chiller loop on Thermo LTQ Orbitrap XL.
* Configured Equan LC system for LTQ Orbitrap XL and wrote Sampler Scripts for preparative and 2D LC.

**Publications**

“Identification of Novel Microcystins Using High-Resolution MS and MSn with Python Code.” In Environmental Science & Technology, **2022**, Baliu-Rodriguez, D., Peraino, N. J., Premathilaka, S. H., Birbeck, J. A., Baliu-Rodriguez, T., Westrick, J. A., & Isailovic, D.

“Toward Revealing Microcystin Distribution in Mouse Liver Tissue Using MALDI-MS Imaging.” Toxins, **2021**, Kucheriavaia, D., Veličković, D., Peraino, N., Lad, A., Kennedy, D. J., Haller, S. T., Westrick, J. A., & Isailovic, D.

“Negative Regulation of Human Hepatic Constitutive Androstane Receptor by Cholesterol Synthesis Inhibition: Role of Sterol Regulatory Element Binding Proteins.” Drug Metabolism and Disposition. American Society for Pharmacology & Experimental Therapeutics, **2021**, Cuko, L., Duniec-Dmuchowski, Z., Rondini, E. A., Pant, A., Fallon, J. K., Wilson, E. M., Peraino, N. J., Westrick, J. A., Smith, P. C., & Kocarek, T. A.

“Pesticide exposure and adverse health effects associated with farmwork in Northern Thailand.” Journal of Occupational Health, **2021**, Forté, C. A., Colacino, J., Polemi, K., Guytingco, A., Peraino, N. J., Jindaphong, S., Kaviya, T., Westrick, J., Neitzel, R., & Nambunmee, K.

“Diastereoselective Synthesis of γ‐Lactones through Reaction of Sulfoxonium Ylides, Aldehydes, and Ketenes: Substrate Scope and Mechanistic Studies.” European Journal of Organic Chemistry, **2020**, Peraino, N. J., Mondal, M., Ho, H., Beuque, A., Viola, E., Gary, M., Wheeler, K. A., & Kerrigan, N. J

“Obesity and impaired barrier function after shock,” Journal of Trauma and Acute Care Surgery, **2020**, L. N. Diebel, N. Peraino, J. Westrick, K. Shinki, and D. M. Liberati.

“Eliciting Cell Death Using Recombinant IgA Fc‐Folate Antibody Mimetics.” The FASEB Journal, **2020**, Turnbull, A., Tepe, G., Mohammed, S., Peraino, N., & Speyer, C.

“Microplastic ingestion by quagga mussels, Dreissena bugensis, and its effects on physiological processes.” *Environmental Pollution*, **2020**, Adam F. Pedersen, Kishore Gopalakrishnan, Anna G. Boegehold, Nicholas J. Peraino, Judy A. Westrick, Donna R. Kashian.

“Dhb Microcystins Discovered in USA Using an Online Concentration LC–MS/MS Platform.” *Toxins,* **2019**, Birbeck, J.A.; Peraino, N.J.; O’Neill, G.M.; Coady, J.; Westrick, J.A.

“Pesticide exposure and adverse health effects associated with farm work in Northern Thailand.” *BioRxIV*, **2019,**  A Forte, Chanese A Forte, Justin Colacino, Katelyn M. Polemi, Andrea Guytingco, Nicholas J Peraino, Siripond Jindaphong, Tharinya Kaviya, Judy Westrick, Rick Neitzel, Kowitt Nambunmee.

“Catalytic Nitrene Homocoupling by an Iron (II) Bis (alkoxide) Complex: Bulking Up the Alkoxide Enables a Wider Range of Substrates and Provides Insight into the Reaction Mechanism” *Inorganic Chemistry*, July **2017**, **2018**, Maryam Yousif, Duleeka Wannipurage, Caleb D Huizenga, Elizabeth Washnock-Schmid, Nicholas J Peraino, Andrew Ozarowski, Sebastian A Stoian, Richard L Lord, Stanislav Groysman

“Asymmetric synthesis of γ-lactones through Koga amine-controlled addition of enediolates to α,β-unsaturated sulfoxonium salts” *Journal of Organic Chemistry,* December 2, **2016**, Nicholas J. Peraino, Sven Kaster, Kraig A. Wheeler, and Nessan J. Kerrigan

"Catalytic Asymmetric Synthesis of Ketene Heterodimer β-Lactones: Scope and Limitations." *Journal of Organic Chemistry*, August 4, **2016**, Shi Chen, Ahmad A. Ibrahim, Nicholas J. Peraino, Divya Nalla, Mukulesh Mondal, Maxwell Van Raaphorst, and Nessan J. Kerrigan

“Diastereoselective Synthesis of γ-Lactones through Reaction of Enediolates with α,β-Unsaturated Sulfoxonium Salts” *Organic Letters*, March 18, **2015**, Nicholas J. Peraino, Kraig A. Wheeler, and Nessan J. Kerrigan

"Asymmetric Synthesis of γ-Lactones through Reaction of Sulfoxonium Ylides, Aldehydes and Ketenes" *Tetrahedron Letters*, June 6, **2014**, Nicholas J. Peraino, Han-Jen Ho, Mukulesh Mondal, Nessan J. Kerrigan

“Regioselective synthesis of highly substituted enol esters from ketoketene dimer β-lactones” *Archive of Organic Chemistry,* **2014**, Eric C. Salo, Kyle R. Dayak, Jacob Huxford, Pei-Hsun Wei, Nicholas J. Peraino and Nessan J. Kerrigan

“6'-Methoxy-(8S,9R)-cinchonan-9-yl N-tert-butoxycarbonyl-2-pyrrolidinecarboxylate.” *Encyclopedia of Reagents for Organic Synthesis*,April 22, **2013**, Nicholas J. Peraino and Nessan J. Kerrigan

“Diastereoselective Reaction of Sulfoxonium Ylides, Aldehydes and Ketenes: An Approach to trans-γ-Lactones.” *Journal of Organic Chemistry,* April 3, **2013**. Mukulesh Mondal, Han-Jen Ho, Nicholas J. Peraino, Melanie A. Gary, Kraig A. Wheeler, and Nessan J. Kerrigan

**Presentations and Conferences**

American Society of Mass Spectrometrists National Meeting. Atlanta GA, June 3, 2019.

“Progress in cannabis testing and regulation and Changes to new ISO 17025 requirements.” AOAC Central Meeting August 1st, 2017

“Asymmetric Synthesis of γ-lactones from Sulfoxonium Salts” *Oral Presentation at 251st ACS National Meeting Division of Organic Chemistry,* March 13, 2016

“Stereoselective Synthesis of *trans*-γ-lactones From Sulfoxonium salts” *Oral Presentation at 247th ACS National Meeting Division of Organic Chemistry,* March 18, 2014

“Optimization of Methanol Recovery Distillation Process” Senior *Design Project Day WMU*, April 14, 2009.