WS16: Leveraging Large Language Models to Investigate the Novel Psychoactive Drug Ecosystem: Applications in Structural Prediction, Behavioral Analysis, and Cyber Surveillance
Date: Tuesday, October 28
Time: 1:30-5:30 PM
Audience Knowledge: Intermediate - Involves more advanced concepts requiring some technical working knowledge or prior exposure to the subject matter
Rates:

Membership	Early Bird (June 25 - Sep 10)	Late (Begins Sept 11)	Onsite (Begins Oct 9)
Member	$150	$175	$200
Student	$150	$175	$200
Non-Member	$200	$225	$250

Workshop Chairs:
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Abstract
The emergence of novel psychoactive substances (NPS), often engineered to evade regulatory controls, presents an ongoing challenge for forensic toxicologists and drug policy makers. The digital era has brought unprecedented opportunities for communication, commerce, and innovation, including new avenues for the marketing of illicit drugs. This workshop will explore the application of large language models (LLMs) as a multidisciplinary toolset for anticipating, characterizing, and monitoring trends within the illicit drug landscape. The workshop will focus on four core applications of LLMs in the context of NPS. First, it will examine the use of LLMs for structure prediction, highlighting their potential to assist in forecasting novel chemical structures and analogues of NPS by leveraging training data from pharmacological literature, patents, and open-source chemical repositories. Second, it will explore behavioral signal extraction, showcasing how LLMs can identify patterns of risky behavior and indicators of drug misuse through natural language analysis of forums, case reports, and social media discourse. Third, the session will delve into marketing and distribution monitoring, presenting methods for training LLMs to autonomously crawl and extract relevant data from social media platforms and surface web sources in order to track how NPS are marketed, branded, and sold in near real-time. Finally, the workshop will address cyber environment mapping, investigating how LLMs can be employed to analyze the broader digital landscape, including illicit online pharmacies, anonymous marketplaces, and encrypted communication channels to detect evolving supply chains and trafficking networks.

This workshop will include technical demonstrations, discussion of training architectures and data pipelines, and evaluation of the utility and limitations of LLMs in forensic contexts. Attendees will gain practical insights into how LLM-driven workflows can augment traditional toxicological methodologies and enhance early warning capabilities.

Learning Objectives

1. Understand the Application of LLMs in Structural Prediction: Participants will learn how large language models can assist in predicting and generating potential structures of novel psychoactive substances.
2. Analyze Behavioral and Market Signals Using Natural Language Processing: Attendees will explore how LLMs can be used to extract behavioral patterns, detect risky behaviors, and identify drug marketing strategies across social media and web environments.
3. Evaluate Cyber Surveillance Tools: Participants will learn about how the cyber environment is used for illicit drug distribution.

Speakers

Hande Küçük-McGinty, PhD
Assistant Professor
Department of Computer Science, Kansas State University

Michael Skinnider, PhD
Assistant Professor: Assistant Professor
Lewis-Sigler Institute for Integrative Genomics, Princeton University

Michael Young, PhD
Assistant Professor: Graduate Program Director, Psychological Sciences
Department of Psychological Sciences, Kansas State University

William Hsu, PhD
Assistant Professor: Professor
Department of Computer Science, Kansas State University

Daniel Burke
Director, Intelligence & Investigations
US Anti-Doping Agency

Workshop Agenda

Time	Topic	Speaker
1:30 – 1:40 PM	**Welcome and Opening Remarks** • Introduction to the workshop • Overview of objectives and agenda	Lynn Wagner
1:40 – 2:20 PM	**Session 1: Artificial Intelligence and the Role of Algorithms in the Creation of NPS: Mind Mapping and Ontological Structuring** • General overview of LLMs. • Explore how ontologies—structured frameworks that define relationships between concepts—can be used to standardize the categorization of NPS. • Explore how AI can generate conceptual maps that link drug structure, pharmacodynamics, user-reported effects, analogues, legal status, and common routes of administration. • Discuss how these algorithmically-generated ontologies and maps can feed into predictive models for toxicology screening, legislative scheduling, or digital market surveillance.	Hande Küçük-McGinty
2:20 – 3:00 PM	**Session 2: LLMs for Structural Predictions of NPS** • Explore how LLMs, combined with cheminformatics approaches, can be trained on molecular representations (e.g., SMILES strings) and chemical literature to generate candidate structures for unknown or emerging NPS. • Case studies and demonstrations will show how structure–activity relationships can be inferred and how such models might assist in prioritizing compounds for toxicological screening.	Michael Skinnider
3:00 – 3:30 PM	**Session 3: Behavioral Signal Extraction and Risk Detection** • Examine how LLMs can mine and analyze unstructured text data from online drug forums, case reports, and clinical literature to identify behavioral markers of drug misuse. • Participants will learn techniques for fine-tuning models on harm reduction narratives, overdose descriptions, and usage trends to detect patterns	Michael Young

	such as polysubstance use or risky administration routes.	
3:30 – 4:00 PM	**Break**	
4:00 – 4:40 PM	**Session 4: Tracking Online Drug Marketing and Distribution of NPS** • Focus on how LLMs can be deployed to crawl, monitor, and analyze drug-related content across public platforms (e.g., Reddit, Bluelight, Instagram, TikTok, YouTube) and surface web forums. • Discuss techniques for identifying euphemisms, coded language, and visual cues used in the marketing of NPS.	William Hsu
4:40 - 5:20 PM	**Session 5: Mapping the Illicit Cyber Drug Ecosystem** • Presents an integrated view of the cyber environment that supports the trade in illicit substances. • Examples from online pharmacy investigations, darknet markets, and messaging apps. • Emphasis will be placed on threat detection, signal verification, and understanding shifts in drug availability or composition.	Daniel Burke
5:20 – 5:30 PM	**Closing Remarks: Key Takeaways and Next Steps** • Recap of key insights • Open discussion on final insights and future directions • Closing remarks and participant feedback	Erin Wilfong