Searching for Nanostructured or pOre fOrming Peptides for therapY COST Action

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Introduction

Peptide science increasingly relies on the integration of design, synthesis, characterization, biological evaluation, and computational prediction within unified research workflows [1,2]. Functional peptides, including self-assembling, antimicrobial, and pore-forming systems, are of particular interest because of their potential in biomedical and materials-related applications [2,3]. The field is highly interdisciplinary, reflecting the structural diversity of peptides and the wide range of available experimental methods, computational tools and application contexts. At the same time, this diversity can hamper progress by making it more difficult to integrate approaches, compare results, and establish common workflows.

COST Action CA23111, *Searching for Nanostructured or pOre fOrming Peptides for therapY* (SNOOPY), running from 2024 to 2028, was established to address these challenges through a coordinated international network bringing together researchers from institutions across Europe and beyond. The Action is chaired by Daniela Kalafatovic, University of Rijeka, Faculty of Engineering, and co-chaired by Paula Gomes, Faculty of Sciences, University of Porto, and currently comprises more than 600 participants from 48 countries. The network brings together researchers, innovators, stakeholders, and industry representatives, with the aim of connecting fundamental peptide research with real-world applications.

COST Actions are designed as European networking frameworks supporting collaboration among researchers and innovators. Their main role is to create international networks, facilitate knowledge exchange and training, connect academic, industrial, and societal stakeholders, and promote collaborative approaches to common scientific challenges. Within this framework, SNOOPY aims to strengthen interactions across peptide-related disciplines while creating opportunities for mobility, knowledge transfer, career development, and wider scientific and societal impact.

Structure of the SNOOPY network and goals

SNOOPY is organized into interconnected Working Groups (WGs), each addressing a complementary aspect of the peptide research pipeline (Figure 1): computational approaches (WG1), synthesis and characterization (WG2), biological applications (WG3), and WG4, fully dedicated to dissemination.

WG1 focuses on computational approaches for understanding, predicting and designing bioactive peptides and peptide nanostructures. Its activities encompass *in silico* prediction and design, molecular dynamics (MD) simulations, data mining and database development, machine learning (ML) and deep learning (DL), and the integration and sharing of computational data. Emphasis is placed on linking peptide sequence, structure, dynamics and function, while developing computational resources, workflows and recommended practices that support reproducibility and accelerate peptide discovery.

A central challenge is the enormous size of peptide sequence and structural search spaces, making computational approaches increasingly important for prioritizing candidates before experimental validation [4, 5, 6, 7]. An emerging WG1 contribution, entitled *Solving the Computational Peptide Design Puzzle: Challenges and Opportunities* under consideration in *ACS Omega*, considers peptide discovery as an interconnected process involving artificial intelligence (AI), MD simulations, experiments, and automation. Each approach provides complementary information: AI identifies patterns in data, MD provides

microscopic insight, experiments provide macroscopic validation, and automation creates opportunities for autonomous experimental workflows [8]. A key objective is to improve integration across these components and, ultimately, enable closed-loop peptide design.



Figure 1. Overview of the CA23111 COST Action generated using OpenAI ChatGPT's image-generation tool, based on the input form the MoU and information available on the Action website (https://cost-snoopy.eu/).

WG2 focuses on the production and characterization of bioactive peptides and peptide-based nanostructures. Its activities encompass synthetic strategies, with interest in development of greener approaches, purification and quality control, optimization of production efficiency and sustainability, and the application of advanced analytical and automated characterization methods. In addition, WG2 focuses on design, formation and characterization of self-assembled peptide nanostructures, including nanofibrils, nanoparticles, and nanotubes, as well as on understanding how the self-assembly process can be controlled through sequence design and experimental conditions.

A major WG2 initiative, *From Community Experience to Best Practices,* aims to convert community experience into guidelines for peptide synthesis and characterization. The initiative is based on a survey involving more than 100 participants and includes respondents from academia and industry. The survey captures current approaches, challenges, and priorities across key areas including synthetic strategies, purification, quality control, characterization methods, and common limitations. By analyzing the responses, WG2 aims to assess the current state of the field, identify key challenges and sources of variability, and use these insights to guide the development of practical, community-driven recommendations and best practices. This is especially important in peptide science, where variations in synthesis, purification, sample preparation, and characterization can strongly influence reproducibility.

WG3 focuses on the biological evaluation and application of bioactive peptides and peptide-based nanostructures, with emphasis on their therapeutic potential and translation toward clinical applications. Its activities encompass peptide bioactivity and mechanisms of action, interactions with biological membranes and other biomolecular targets, antimicrobial and antiviral activity, drug delivery and cellular transport, as well as amyloid-related systems and emerging therapeutic and diagnostic applications. A central aim of WG3 is to connect molecular and materials-level properties with biologically relevant function and performance. In this way, WG3 complements the computational design activities of WG1 and the production and characterization efforts of WG2 by evaluating how peptide properties translate into activity in increasingly complex biological systems. A major WG3 contribution will be the *Roadmap on the Biological Applications of Peptides and Peptide Nanostructures*, which will assess the current landscape of biomedical applications, identify key scientific and translational challenges, and define priorities and opportunities for future development.

WG4 supports the activities of WG1, WG2 and WG3 through dissemination, scientific communication, career development, inclusiveness, and engagement with industry and wider society. It promotes knowledge exchange across the network through initiatives that strengthen skills, visibility, collaboration, and career development, particularly for young researchers.

From innovation to standardization and best practices

Methodological innovation is particularly challenging in peptide research because of the broad diversity of scientific questions, experimental and computational techniques, disciplinary expertise, and application areas that must be integrated across the field. SNOOPY promotes integration of computational and experimental approaches with the long-term goal to establish closed-loop peptide discovery systems in which design, synthesis, testing, and model refinement become progressively interconnected. Such approaches could substantially accelerate the discovery of peptides with desired structural, functional, or therapeutic properties.

In parallel with methodological innovation, SNOOPY recognizes that progress in peptide science requires reproducible and transferable experimental procedures. The WG2 community survey therefore represents an important effort to collect practical experience from peptide researchers and transform it into shared recommendations. By developing such resources collectively, SNOOPY seeks to improve reliability and comparability between laboratories. This network-driven approach also enables expertise from different countries, institutions, and research environments to contribute to the development of common standards.

Scientific dissemination is supported through meetings, publications, joint activities, and dedicated journal collections. Two SNOOPY-associated special issues highlight this effort: a WG2 collection in *Materials Advances (RSC)* on supramolecular peptide and protein systems, and a WG1 special issue in *Journal of Peptide Science* (Wiley) on computational approaches for the assessment of peptides and peptide nanostructures. Together, these collections provide focused platforms for sharing advances across design, synthesis, characterization, computation, and applications.

Networking, Mobility, and Capacity Building

A defining feature of SNOOPY is its emphasis on researcher mobility and international network building. The Action supports Short-Term Scientific Missions, conference participation, meetings, workshops, and training schools. These mobility mechanisms allow researchers to visit partner laboratories, acquire new experimental or computational skills, access complementary infrastructure, initiate collaborations, and present results at international conferences. To date, SNOOPY has approved 70 grant applications. The number of approved grants increased from 20 in 2025 to 50 in 2026, reflecting growing participation and connections within the network. SNOOPY also promotes industry engagement to strengthen knowledge

transfer, connect academic research with practical challenges, and support the translation of peptide technologies toward real-world applications.

SNOOPY has also developed a dedicated “Find the Partner” platform (https://cost-snoopy.eu/find-the-partner/), enabling researchers to identify collaborators by research topic, technique, country, WG, or individual expertise. The tool reflects the Action’s broader objective of making scientific capabilities visible across the network and facilitating the formation of new collaborations.

WG meetings and training activities form another major component of the network. Activities highlighted include a WG1 meeting in Cres, Croatia (2025), a WG2 meeting in Nottingham, UK (2026), an upcoming WG3 meeting in Granada (2027), and training activities in Porto (2026) and Lyon (2027). These events are designed not only to present scientific results, but also to encourage methodological exchange and strengthen interactions between researchers at different career stages.

Conclusions

COST Action CA23111 SNOOPY provides an interdisciplinary framework for advancing research on peptides through coordinated European collaboration with connections across continents. SNOOPY combines complementary areas: computational design, synthesis and characterization and biological applications. Beyond its scientific goals, SNOOPY is designed as a community-building platform. Through researcher mobility, training schools, WG meetings, conference grants, partner-search tools, surveys, journal collections, and industry participation, the network aims to create a sustainable collaborative ecosystem for peptide science. At the same time, the development of shared experimental guidelines and standards should improve reproducibility and facilitate translation between laboratories. SNOOPY represents not only a coordinated scientific effort in peptide research, but also an infrastructure for knowledge exchange, inclusiveness, training, and long-term European and global collaboration.

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