Report on the outcomes of a Short-Term Scientific Mission[1]

Action number: CA21126

Grantee name: Gunel Aliyeva

Details of the STSM

Title: Eco-Friendly Cross-Coupling Approaches to Mimic the Formation and Reactivity of Cosmic Nanocarbons

Start and end date: 08/12/2025 to 08/02/2026

Description of the work carried out during the STSM

Description of the activities carried out during the STSM. Any deviations from the initial working plan shall also be described in this section.

(max. 500 words)

The Short-Term Scientific Mission (STSM) was carried out at the laboratory of Prof. Vito Capriati, focusing on the development and evaluation of sustainable synthetic methodologies for the preparation of N-containing heterocyclic compounds. The activities were aligned with the initial working plan and structured around three main components: sustainable synthesis, comparative assessment, and data analysis.

During the first phase, green cross-coupling protocols were implemented using water and deep eutectic solvents (DES) as environmentally benign reaction media. A series of Suzuki–Miyaura and related cross-coupling reactions were performed to synthesize selected N-heterocyclic derivatives. Reaction parameters—including temperature, catalyst loading, base concentration, reaction time, and atmosphere—were systematically optimized to improve conversion, yield, and selectivity while ensuring reproducibility. The use of DES proved particularly advantageous due to their low toxicity, operational simplicity, and ability to stabilize catalytic species. All synthesized compounds were fully characterized using ^{1}H and ^{13}C NMR spectroscopy, mass spectrometry, and HPLC to confirm structural identity and purity.

In the second phase, conventional solvent-based methods were reproduced to enable a direct comparison with the sustainable protocols. Reactions conducted in traditional organic solvents provided a baseline for evaluating efficiency and practicality. The comparative study assessed reaction performance, operational requirements, and environmental impact using green chemistry metrics such

[1] This report is submitted by the grantee to the Action MC for approval and for claiming payment of the awarded grant. The Grant Awarding Coordinator coordinates the evaluation of this report on behalf of the Action MC and instructs the GH for payment of the Grant.

as E-factor, solvent consumption, energy usage, and process mass intensity (PMI). This analysis facilitated the identification of reaction conditions that combine high synthetic efficiency with reduced environmental footprint.
The final stage involved interpretation of the experimental data and integration of the findings within the broader scientific framework of the NanoSpace Action. The synthesized N-heterocycles serve as relevant molecular analogues for nitrogen incorporation into carbon-based systems, offering insight into chemical processes potentially occurring in extraterrestrial environments. The results highlighted the feasibility of sustainable cross-coupling strategies for generating structurally diverse heterocycles while maintaining high analytical reliability.
No major deviations from the original work plan occurred. Minor adjustments were made to reaction conditions in order to accommodate substrate-dependent reactivity and to further optimize catalytic efficiency in aqueous and DES media. These refinements enhanced the robustness of the methodologies without altering the overall objectives of the mission.
In conclusion, the STSM successfully achieved its planned activities, demonstrating that green synthetic approaches can effectively complement conventional methodologies while supporting environmentally responsible research practices and contributing valuable experimental data to the NanoSpace consortium.

Description of the STSM main achievements and planned follow-up activities

Description and assessment of whether the STSM achieved its planned goals and expected outcomes, including specific contribution to Action objective and deliverables, or publications resulting from the STSM. Agreed plans for future follow-up collaborations shall also be described in this section.

(max. 500 words)

The Short-Term Scientific Mission (STSM) successfully achieved its primary objective of developing and evaluating sustainable synthetic methodologies for the preparation of N-containing heterocyclic derivatives. The planned activities were completed in accordance with the initial proposal, resulting in significant scientific and collaborative outcomes that directly support the objectives of COST Action CA21126 “NanoSpace.”
A major achievement of the STSM was the successful implementation of green cross-coupling reactions in environmentally benign media, particularly water and deep eutectic solvents (DES). Several N-heterocyclic scaffolds were synthesized using optimized Suzuki–Miyaura and related methodologies, demonstrating that sustainable reaction conditions can provide high yields, good selectivity, and reliable reproducibility while minimizing hazardous solvent use and chemical waste. The systematic optimization of reaction parameters—including catalyst loading, temperature, reaction time, and base equivalents—enabled the identification of efficient and operationally simple protocols suitable for broader application.
A comparative evaluation between conventional solvent-based methods and sustainable approaches constituted another key outcome. The collected dataset highlighted the advantages of green methodologies in terms of reduced environmental impact, as quantified through green chemistry metrics such as E-factor, solvent consumption, and energy usage, while maintaining competitive chemical performance. These findings confirm that eco-friendly strategies can effectively complement traditional organic synthesis without compromising reaction efficiency.
All synthesized compounds were fully characterized using ^{1}H and ^{13}C NMR spectroscopy, mass spectrometry, and HPLC, generating reliable molecular reference data. These characterized heterocycles serve as valuable laboratory analogues for nitrogen incorporation into carbon-based molecular systems, contributing to a better understanding of nanocarbon functionalization processes relevant to interstellar and circumstellar environments. The experimental data therefore support the Action’s goal of integrating laboratory chemistry with astronomical observations and theoretical modelling.
The STSM also strengthened interdisciplinary collaboration within the NanoSpace network by fostering knowledge exchange between sustainable synthetic chemistry and astrochemistry. The methodologies and datasets generated during the mission represent transferable resources that can be incorporated into Action deliverables, including reaction pathway models, reference datasets, and training materials for future research activities.

Regarding dissemination, the results obtained during the STSM are expected to contribute to a peer-reviewed scientific publication focused on sustainable heterocyclic synthesis and its relevance to modelling nitrogen-containing nanocarbon species. Portions of the work may also be presented at international conferences and NanoSpace-related meetings to maximize visibility and scientific impact.
Future follow-up activities have been agreed upon with the host institution. These include extending the sustainable methodologies to a broader range of heterocyclic substrates, further mechanistic investigations of cross-coupling processes in unconventional media, and the continued exchange of expertise between the collaborating groups. Opportunities for joint publications and potential participation in future collaborative projects within the COST framework will also be explored.
Finally, the STSM met its planned goals and delivered measurable scientific progress while reinforcing the collaborative and capacity-building mission of the NanoSpace Action.