Report on the outcomes of a Short-Term Scientific Mission[[1]](#footnote-1)

Action number: CA18221

Grantee name: Cynthia Munoz

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| **Details of the STSM**  Title: Predicting maternal transfer of pesticides in reptiles based on pollutant molecular structure  Start and end date: 08/07/2022 to 23/07/2022 |
| **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. |
| During the STSM preparation phase (April – June 2022), I collaborated closely online with the host, Sandrine Charles (University Lyon 1) and a colleague at Radboud University (Dr. Peter Vermeiren). We developed a database regarding the maternal transfer of organic pollutants (i.e., data on measured concentrations of pollutants in paired mother-egg tissue samples). This database was based on a systematic search of published literature and augmented by reaching out to our networks. The search resulted in 14 studies from which data were extracted and harmonized. For each of the unique organic pollutants recorded within the database, I also collected information that described the molecular structure of these compounds (specifically characteristics that might explain the differences in bioaccumulation behaviour of the pollutants). I then visualized the data to allow for a first exploration.  During the STSM visit at the University of Lyon 1, we took advantage of the developed database and preliminary data exploration, to focus our attention on the development of a predictive model. This model aimed to answer our main research questions: (1) Can we predict pollutant concentrations in eggs based on concentrations measured in females (to inform risk assessment to early life stages); (2) Can we predict concentrations in females based on measured concentrations in eggs (in the perspective of using eggs as a biomonitoring tool); and (3) Is maternal transfer species- and/or pollutant-dependent?  A main challenge in answering these questions relates to the fact that both concentrations in eggs and in females are “dependent” variables that are measured with uncertainty. Hence, a classical approach where the concentrations in one dependent variable is explained by one or more independent variables is not appropriate as such a technique only accounts for uncertainty in the dependent variable. As a solution, we developed a Gaussian orthogonal regression model in which the concentration of pollutants in both eggs and in females are associated to random variables that are linked to the observed concentrations via a Gaussian probability distribution. Additionally, to directly capture the full uncertainty in the model parameters, to further propagate it into predictions when using the model, we employed Bayesian inference to estimate all parameters. Finally, we developed and tested several model variations in the respect of the parsimony principle, that we compared based on the Widely Applicable Information Criterion (WAIC). These versions were fed with different subsets of the full DB:  (1) Data recorded in females in different studies came from different tissues (e.g., liver, blood, fat, or muscle). We extended the model equations to be able to handle data from the different types of tissue.  (2) The dataset included freshwater and marine turtles, snakes and crocodile species. We implemented a model with a species-specific intercept that explicitly capture the variability between species.  (3) The dataset included various organic pollutants, incl. PCB, OCP, PBDE, plasticizers... We made a first conceptual model of how this variety of pollutants can be accounted for in the model. Additionally, we discussed with a chemistry colleague, Prof. Florence Popowycz at INSA Lyon on further selection and refinement of molecular descriptors that are likely of highest relevance and explanatory power.  We concluded the STSM with a seminar at the host where I presented the STSM research and previous research on sea turtle ecotoxicology leading up to it. |
| **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.  The STSM resulted in practical outputs:   1. A homogenised database of paired mother-egg concentrations of organic pollutants was developed, integrating data across 14 studies. 2. R code to homogenise and integrate the data was developed. 3. An orthogonal regression model to predict concentrations of organic pollutants in both directions (e.g., in eggs from females, or in females from eggs) is developed and described, including relevant extensions. 4. The model is implemented in R computer code.   These outputs contribute to the PERIAMAR objectives: WG1.1 (identify exposure routes) and WG3.3 (minimising the use of *in vivo* reptile measurements). We are currently testing the model outcomes (model cross-validation between training and test data) in order to select the best performing model version. This version will then be implemented into the PERIAMAR project “Lifecycle energetics of reptiles under pollution stress” as an add-in module within the more general model (<https://periamar.com/projects/ttView/21>).  The outputs will be made available as follows:   1. The database (and R code used to develop it) is planned to be made publicly available and described within a Data in Brief publication. 2. The predictive model (incl. R code), incl. comparison of model extensions, will be published in open access within an international scientific journal in ecotoxicology (e.g., Ecotoxicology and Environmental Safety) 3. We are considering the options to attend the SETAC conference 2023 to present the database and the model, and will likely also have the opportunity to present at the PERIAMAR meeting in September. 4. Following discussions, a joint publication (target journal: MethodsX) on challenges in wildlife ecotoxicology between University Lyon 1 and Radboud University is underway. This will expand on ATTAC issues and best practice guidelines developed in my previous publication (Munoz et al. 2021) which relate to increasing the use and reuse of pollution biomonitoring data to support conservation and management.   Activities during the STSM allowed me to increase my knowledge of statistical modelling, particularly the formulation and implementation of regression-based models within a Bayesian framework. This greatly benefits the analysis of the data that I collected, as well as my skillset for future employment. I also enjoyed the opportunity to interact with a number of colleagues at the University of Lyon and associated institutes (e.g., INSA, VetAgro Sup, INRAE). These in person meetings will lead to closer collaboration, and are specifically useful as I am now preparing an application for a postdoctoral fellowship (e.g., Marie Curie) with the host institute. I presented my research on sea turtle ecology, maternal transfer processes, and methodologies for systematic literature synthesis during the seminar at the host, and in discussions with the team of Prof. Sandrine Charles. The outcomes of the STSM will also be presented at my home institute at a weekly seminar in a near future. |

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. [↑](#footnote-ref-1)