WG4 DEVELOPMENT OF TOOLS, SERVICES AND FACILITIES FOR THE NECTAR COMMUNITY

TASK: PROVIDING UPDATED GUIDELINES, SOFTWARE AND SERVICES TO ENHANCE THE EFFECTIVENESS OF OUR RESEARCH INTO EQUILIBRIUM THERMODYNAMICS AND THE APPLICATION OF THE OUTCOMES

ONCE UPON A TIME;

Turin:
Master thesis on the development of a new version of ES4 software

Valencia:
Development of software for microspeciation analysis from NMR data fitting

Project start
02/10/2019

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September 2020

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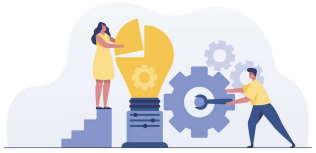

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- ✓ Agreement to:
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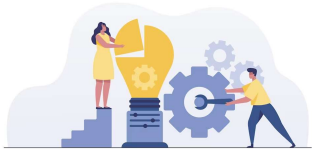

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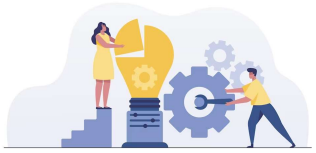

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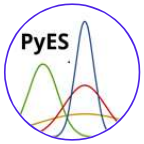

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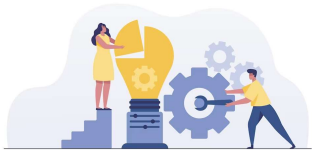

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- ✓ Presentation of 1st version of PyES

- ✓ Presentation of preliminary results of a comparative study on the current tools for optimization of stability constants from potentiometric data

3rd European NECTAR Conference
Ljubljana, 24-26/10/2022

https://www.uv.es/supramol/pages/software.html

Chemometrics and Intelligent Laboratory Systems 231 (2022) 104672

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GEMS, a tool for microspeciation analysis from NMR data fitting☆

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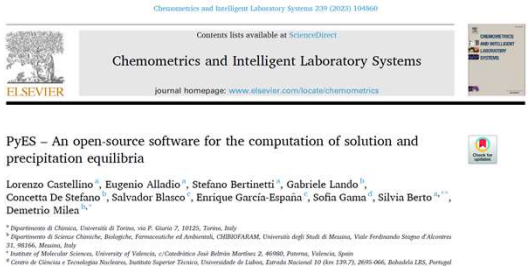
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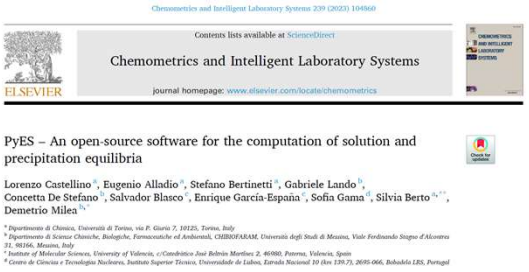
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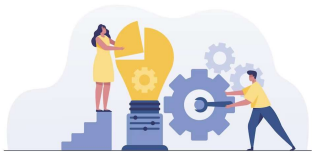

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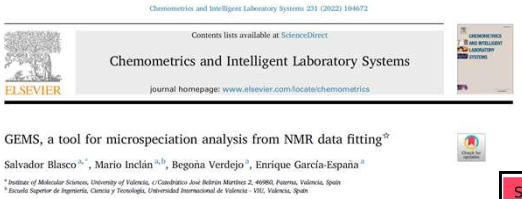
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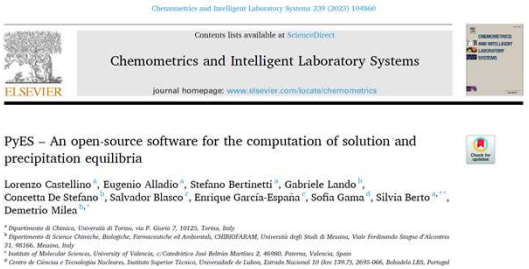
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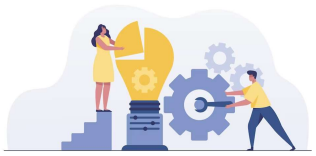

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4th European NECTAR Conference and Final Action Meeting,
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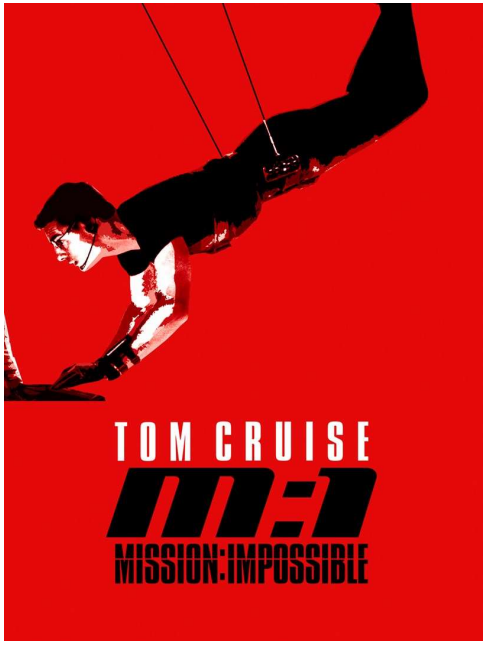
We feel like Ethan Hunt at the end of his first mission



We still have many more missions to solve

1. **SpectrAPP development**
   - Insertion of MCR-ALS
2. **Database searching software**
3. **PyES development and integration with related software:**
   - Follow up and application of the (solved) **issues and guidelines** coming from the different **interlab experiments** carried out within NECTAR
   - Implementing the **experimental design** function by suitably tuning the concentration of the reactants and the observable to be measured
   - Multiple species and stoichiometry, no binding models
   - Integration of PyES with related software for the analysis of potentiometric, UV-vis/fluo and calorimetric data also as a function of ionic strength and temperature

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4 **Survey**

What data do you consider necessary to completely define the experimental conditions?

How to compile metadata files

Potentiometry and UV-vis experiments

Deadline: May 2024

5 Analysis of the current tools for optimization of **formation constants** from potentiometric data on a more complex system.

Acknowledgments


Prof. Demetrio Milea


Dr. Sofia Gama

Prof. Winfried Plass


Prof. Aleksandar Cvetkovski

and all the colleagues who actively collaborated to achieve these outcomes;

by measurements, tests, discussions, revisions and much food for thought!

Acknowledgments

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2023 - 2027 DEPARTMENT OF EXCELLENCE
Ministero dell'Università e della Ricerca


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Dr. Lorenzo Castellino


Dr. Matteo Marafante