

## 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







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Task Group – Software Development
September 2020

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Development of software for microspeciation analysis from NMR data fitting

Project start 02/10/2019





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On-line Meeting of WG4
Task Group – Software Development
17/02/2021



- ✓ SpectrApp v.0 presentation
- ✓ Agreement to:
  - prepare survey on current software
  - test the available software on a dataset
  - develop software for potentiometric data analysis





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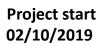
September 2020

✓ Survey results

NECTAR Spring Web-Meeting 25-26/03/2021

Valencia:

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WG2 - WG4 meeting, Valencia 9-10/06/2022

✓ Presentation of 1<sup>st</sup> version of PyES







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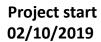
✓ Survey results

NECTAR Spring Web-Meeting

25-26/03/2021

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

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



On-line Meeting of WG4
Task Group – Software Development
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#### https://www.uv.es/supramol/pages/software.html





GEMS, a tool for microspeciation analysis from NMR data fitting  $^{\mbox{\tiny $\alpha$}}$ 

Salvador Blasco <sup>(h. )</sup>, Mario Inclán <sup>(h. )</sup>, Begoña Verdejo <sup>(h</sup>, Enrique García-España <sup>(h. )</sup> <sup>(h. )</sup> bustuse of Molecular Sciences, University of Videntia, c/Candrigico José Belirin Martine 2, 40880, Fearms, Videntia, Spain



GEMS publication 15 December 2022





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Champagaria and Intelligent Inhoration Systems 231 (2022) 164672



GEMS, a tool for microspeciation analysis from NMR data fitting  $^{\pm}$  Salvador Blasco  $^{\rm a,*}$ , Mario Inclán  $^{\rm a,b}$ , Begoña Verdejo  $^{\rm a}$ , Enrique García-España  $^{\rm a}$ 



GEMS publication 15 December 2022

SpectrApp available on-line 1 January 2023





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#### https://github.com/Kastakin/PyES



 $\mbox{\sc PyES}-\mbox{\sc An open-source}$  software for the computation of solution and precipitation equilibria



Lorenzo Castellino<sup>®</sup>, Eugenio Alladio <sup>®</sup>, Stefano Bertinetti <sup>®</sup>, Gabriele Lando <sup>®</sup>, Concetta De Stefano <sup>®</sup>, Salvador Blasco <sup>®</sup>, Enrique García-España <sup>®</sup>, Sofia Gama <sup>®</sup>, Silvia Berto <sup>®</sup> <sup>®</sup>, Demetrio Milea <sup>®</sup>

\* Dipartemento di Cherico, Diovendo di Torino, via P. Gueria T, 19225, Terina, Italy
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PyES publication 17 May 2023





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

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\* Dipartimento di Chinica, Università di Torino, via P. Giaria 7, 10125, Torino, Italy.
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\* Pagramono di Science Charleck, Bologhek, Franscontale ed Archiental, CHIDIOTRAM, Università deffi Studi di Massim, Viale Ferdanado Siagno d'Alcoures 21, 20166. Massim, Viale Ferdanado Siagno d'Alcoures 21, 20166. Massim, Viale servicio de Marcine, Vialencia, «Cardericio Just Belevis Merdire», 2 4,000 p. Parenta, Vialencia, Spain de Marcine, Spain de Mercules Science, Invatato Superior Terinoti, Universidade de Labor, Barnal Nacional D des 1729/7, 2015-066. Bibahdia LES, Parend Carlesia extractionipa Nacional D des 1729/7, 2015-066.

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A tutorial on potentiometric data processing.

Analysis of the current tools for optimization of protonation constants

S. Berto, S. Blasco, L. Castellino, A. Cvetkovski, C. De Stefano, S. Gama, E. García-España, P. Hermann, G. Lando, M. Marafante, M. Meyer, W. Plass, L. Quinodoz, D. Milea





### 4th European NECTAR Conference and Final Action Meeting Milazzo, February 26th-27th 2024

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Chemometrics and Intelligent Laboratory Systems

GEMS, a tool for microspeciation analysis from NMR data fitting\* Salvador Blasco a, Mario Inclán a, Begoña Verdejo a, Enrique García-España



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NECTAR WG1 meeting, Zagreb 28-29/09/2023

- Agreement to:
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  - apply FAIR principles to equilibrium data





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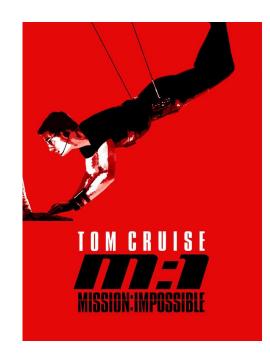
4<sup>th</sup> European NECTAR Conference and Final Action Meeting, Milazzo, 26-27/02/2024





4th European NECTAR Conference and Final Action Meeting Milazzo, February  $26^{th}$ - $27^{th}$  2024

### 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





## We still have many more missions to solve



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

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



Department Chemistry





Dr. Eugenio Alladio



Dr. Stefano Bertinetti



Dr. Lorenzo Castellino



Dr. Matteo Marafante

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