De Stefano Concetta

Curriculum Vitae

Born in Messina, Italy, November 01, 1958.
Laurea magna cum laude, in Chemistry (1982), University of Messina.

Academic positions
Researcher Analytical Chemistry, University of Messina (1990-1998).
Associate Professor of Analytical Chemistry, University of Messina (1998-2001).
Full Professor of Analytical Chemistry, University of Messina (since 2001 -).

Teaching activity
Since 1995 she taught courses in the subject areas CHIM/01 and CHIM/12, including Analytical Chemistry and Laboratory, Characterization Technology and Quality Control, Environmental Chemistry, Characterization and Remediation of Contaminated Sites, Quality Control and data validation, Environmental Monitoring.

Research interests
- solution equilibria thermodynamics, with particular attention to the problems regarding the speciation of natural fluids;
- equilibrium data analysis by means of computer programs;
- acid-base properties of different ligand classes (polyamines, polycarboxylates, amino acids, complexones);
- hydrolysis of metal and organometal cations;
- supramolecular chemistry (interactions of polyamine with protonated organic and inorganic anions);
- sequestration of toxic metals by selective ligands;
- weak complexation (weak ion pair formation) of alkali metals and alkaline earth metals with inorganic and organic ligands;
- speciation of natural ligands such as phytic acid and glutathione;
- speciation studies in natural and biological fluids (quantitative description of the chemical species in a system, using suitable statistical and mathematical tools)

Publications/Bibliometric parameters (SCOPUS),

274 papers (**H-index = 37; Total No. of Citations = 5596**), published in international specialized journals and three chapters of books.
Her research activity was often developed together with researchers from other Italian and foreign Universities.

Funding
- PRIN, "Thermodynamics of complexes in natural and synthetic fluids: models of and structure of species in solution". Component of the University of Messina research unit (1998).
- PRIN 2015: "Multiple equilibria in natural and biological fluids: from speciation to selective sequestering" – responsible of the University of Messina research unit (2015 - prot. 2015MP34H3).
- "Research &Mobility" 2017: P.I. of the project ARCADIA - smARt materials for landfill leaChAte remediation

- COST Action CA18202 – NECTAR - Network for Equilibria and Chemical Thermodynamics Advanced Research. Demetrio Milea: Action Chair and grant Holder Scientific representative. 02/10/2019-01/10/2023.
- PRIN 2022 PNRR "GADOlinium (Gd), an emergent contaminant, is a new threat to the living beings: a comparative study to assess its biological TOXicity in animal models (GADOTOX)" CUP J53D23014240001 - ID: P2022JLE99, component of Messina University research unit.
- PRIN 2022 "Wastezilla: Recycled waste biomass for efficient recovery of critical elements CUP J53D2300754006, component of Messina University research unit.

Positions in National and International Bodies

- member of Advisor Board of Journal of Chemical and Engeneering Data (2004 -2009);
- deputy director of the Department of Inorganic Chemistry, Analytical Chemistry and Physical Chemistry -University of Messina(2007-2012);
- 2008-2010 member of the organizing committee of the "Research Nights" - Faculty of science MM.FF.NN. of the Messina University;
- chairman of the II level "Eurofos" Master in Forensic Sciences – University of Messina (2001);
- deputy director of the Department of Chemical Science-University of Messina (2013 -2015);
- member elected of the Analytical Chemistry Division of the Italian Chemical Society since 2013;
- she was member of the Organizing Secretariat of the Analytical Chemistry Division of the Italian Chemical Society, from 2019 to January 2022
- deputy Chairman of the Analytical Chemistry Division of the Italian Chemical Society (SCI) 2022-2024.
- dean of the school "Faculty of Science and Technology" of Messina University, from 2013 to 2016.
- member of the ASN 2016 Scientific Committee;
- chairman of the University committee for the "24 CFU" Course;
- chairman of the Orientation and Tutoring committee of the Department CHIBIOFARAM since genuary 2024;
- responsible of the tutoring projects (MIUR funds), since 2016;
- component, since 2017, of the scientific board of the University of Messina for the remediation of the "Falcata area";
- 2019 - Member of the organizing committee of "*One night for research @unime*".
- Member of the University committee for Sustainability and assignment to be part of the RUS RESOURCES AND WASTE Working Group, since June 2021.
- Member of the Scientific Committee for the support to the Extraordinary Commissioner of the Government for the rehabilitation of the slums of the city of Messina - Decree No. 3/2021
- Since 1/10/2022 she is the coordinator of the PhD course in Chemical Sciences
- Since January 2024 she is deputy director of the department of Chemical, Biological, Pharmaceutical and Environmental Sciences of Messina University.
- since 2024 she is the coordinator of the bachelor degree course "Marine Biology and Blue Biotechnologies"

List of publications 2017-2025

1. Bretti C., Cigala R.M., Crea F., De Stefano C., Gattuso G., Irto A., Lando G., Milea D., Sammartano S. *Thermodynamic Properties of O-Donor Polyelectrolytes: Determination of the Acid-Base and Complexing Parameters in Different Ionic Media at Different Temperatures.* Journal of Chemical and Engineering Data, 2017. **62**(9): p. 2676-2688.
2. Bretti C., Cigala R.M., De Stefano C., Lando G., Sammartano S., *Understanding the bioavailability and sequestration of different metal cations in the presence of a biodegradable chelant MGDA in biological fluids and natural waters.* Chemosphere, 2017. **183**: p. 107-118.
3. Bretti C., Cigala R.M., De Stefano C., Lando G., Sammartano S. *Thermodynamic solution properties of a biodegradable chelant (MGDA) and its interaction with the major constituents of natural fluids.* Fluid Phase Equilibria, 2017. **434**: p. 63-73.
4. Bretti C., De Stefano C., Lando G., Majlesi K., Sammartano S. *Thermodynamics (Solubility and Protonation Constants) of Risedronic Acid in Different Media and Temperatures (283.15–318.15 K).* Journal of Solution Chemistry, 2017. **46**(9-10): p. 1903-1927.
5. Cardiano P., Cigala R.M., Cordaro M., De Stefano C., Milea D., Sammartano S., *On the complexation of metal cations with "pure" diethylenetriamine-N,N,N′,N″,N″-pentakis(methylenephosphonic) acid.* New Journal of Chemistry, 2017. **41**(10): p. 4065-4075.
6. Cardiano P., Cigala R.M., Crea F., De Stefano C., Giuffrè O., Sammartano S., Vianelli G. *Potentiometric, UV and 1H NMR study on the interaction of penicillin derivatives with Zn(II) in aqueous solution.* Biophysical Chemistry, 2017. **223**: p. 1-10.
7. Cigala R.M., Crea F., De Stefano C., Sammartano S., Vianelli G. *Thermodynamic Parameters for the Interaction of Amoxicillin and Ampicillin with Magnesium in NaCl Aqueous Solution, at Different Ionic Strengths and Temperatures.* Journal of Chemical and Engineering Data, 2017. **62**(3): p. 1018-1027.
8. Crea F., De Stefano C., Irto A., Milea D., Pettignano A., Sammartano S. *Modeling the acid-base properties of molybdate(VI) in different ionic media, ionic strengths and temperatures, by EDH, SIT and Pitzer equations.* Journal of Molecular Liquids, 2017. **229**: p. 15-26.
9. Bretti C., Cardiano P., Cigala R.M., De Stefano C., Irto A., Lando G., Sammartano S. *Exploring various ligand classes for the efficient sequestration of stannous cations in the environment.* Science of the Total Environment, 2018. **643**: p. 704-714.
10. Bretti C., De Stefano C., Lando G., Sammartano S. *Solubility, acid-base properties and thermodynamics of interaction between three NTA-phosphonate derivatives and the main cationic components (H^+, Na^+, Mg^{2+} and Ca^{2+}) of natural fluids.* Journal of Chemical Thermodynamics, 2018. **123**: p. 117-127.
11. Cardiano P., De Stefano C., Foti C., Giacobello F., Giuffrè O., Sammartano S. *Sequestration of HEDPA, NTA and phosphonic NTA derivatives towards Al3+ in aqueous solution.* Journal of Molecular Liquids, 2018. **261**: p. 96-106.
12. Cigala R.M., Crea F., De Stefano C., Irto A., Sammartano S. *Use of Gantrez Copolymers as Potential Chelating Agent for the Selective Sequestration of Metal Ions. Studies of the Interactions in Aqueous Solution at Different Ionic Strengths and Temperatures.* Journal of Chemical and Engineering Data, 2018. **63**(11): p. 4193-4204.
13. Crea F., De Stefano C., Milea D., Sammartano S. *Phytate-molybdate(VI) interactions in NaCl (aq) at different ionic strengths: Unusual behaviour of the protonated species.* New Journal of Chemistry, 2018. **42**(10): p. 7671-7679.
14. Irto A., Cardiano P., Chand K., Cigala R.M., Crea F., De Stefano C., Gano L., Gattuso G., Sammartano S., Santos M.A. *New bis-(3-hydroxy-4-pyridinone)-NTA-derivative: Synthesis, binding ability towards Ca^{2+}, Cu^{2+}, Zn^{2+}, Al^{3+}, Fe^{3+} and biological assays.* Journal of Molecular Liquids, 2018. **272**: p. 609-624.
15. Irto A., Cardiano P., Chand K., Cigala R.M., Crea F., De Stefano C., Gano L., Sammartano S., Santos M.A. *Bifunctional 3-hydroxy-4-pyridinones as effective aluminium chelators: synthesis, solution equilibrium studies and in vivo evaluation.* Journal of Inorganic Biochemistry, 2018. **186**: p. 116-129.

16. Majlesi K., Bretti C., Cigala R.M., De Stefano C., Majlesi K., Sammartano S. *Thermodynamic Study on the Protonation and Na^+, Ca^{2+}, Mg^{2+}-Complexation of a Biodegradable Chelant (HEIDA) at Different Ionic Strengths and Temperatures.* Journal of Solution Chemistry, 2018. **47**(3): p. 528-543.
17. Majlesi K., Bretti C., De Stefano C., Majlesi K., Sammartano S., Zeighaminezhad S. *Complexation of Molybdenum(VI) with GLDA at Different Ionic Strengths.* Journal of Solution Chemistry, 2018. 47(12): p. 1965-1979.
18. Bretti C., Cigala R.M., De Stefano C., Lando G., Sammartano S. *Thermodynamic study on polyaspartic acid biopolymer in solution and prediction of its chemical speciation and bioavailability in natural fluids.* Journal of Molecular Liquids, **2019**. **274**: p. 68-76.
19. Cardiano P., Cigala R.M., Crea F., De Stefano C., Milea D., Sammartano S. *Characterization of the thermodynamic properties of some benzenepolycarboxylic acids: Acid-base properties, weak complexes, total and neutral species solubility, solubility products in $NaCl_a$, $(CH_3)_4NCl_{aq}$ and Synthetic Sea Water (SSW).* Fluid Phase Equilibria, 2019. **480**: p. 41-52.
20. De Stefano C., Lando G., Malegori C., Oliveri P., Sammartano S. *Prediction of water solubility and Setschenow coefficients by tree-based regression strategies.* Journal of Molecular Liquids, 2019. **282**: p. 401-406.
21. Irto A., Cardiano P., Chand K., Cigala R.M., Crea F., De Stefano C., Gano L., Gattuso G., Sammartano S., Santos M.A. *A new bis-(3-hydroxy-4-pyridinone)-DTPA-derivative: Synthesis, complexation of di-/tri-valent metal cations and in vivo M^{3+} sequestering ability.* Journal of Molecular Liquids, 2019. **281**: p. 280-294.
22. Irto A., Cardiano P., Cataldo S., Chand K., Cigala R.M., Crea F., De Stefano C., Gattuso G., Muratore N., Pettignano A., Sammartano S., Santos M.A. *Speciation studies of bifunctional 3-hydroxy-4-pyridinone ligands in the presence of Zn^{2+} at different ionic strengths and temperatures*, Molecules, **2019**, 24(22), pp. 4084
23. Majlesi K., Bretti C., De Stefano C., Lando G., Majlesi K., Sammartano S., *Thermodynamic Study on the Interaction of Nicotinic Acid with H^+, Na^+, Ca^{2+} and Mg^{2+} at Different Temperatures and Ionic Strengths*, Journal of Solution Chemistry, **2019**, 48, pp 1671-1684
24. Crea F., De Stefano C., Irto A., Lando G., Materazzi S., Milea D., Pettignano A., Sammartano S., *Understanding the solution behavior of epinephrine in the presence of toxic cations: A thermodynamic investigation in different experimental conditions*, Molecules, **2020**, 25, 3, pp. 511.
25. Irto A., Cardiano P., Chand K., Cigala R.M., Crea F., De Stefano C., Gattuso G., Sammartano S., Santos M.A.,*Complexation of environmentally and biologically relevant metals with bifunctional 3-hydroxy-4-pyridinones*, Journal of Molecular Liquids, 2020, ,319.
26. Majlesi K., Bretti C., De Stefano C., Sammartano S., *Thermodynamic Study on the Protonation and Complexation of the Neuroleptic Drug, Gabapentin with Na^+, Ca^{2+} and Mg^{2+} at Various Temperatures and Ionic Strengths*, Journal of Solution Chemistry 2020, 49, 1225-1236.
27. Arena K., Brancato G., Cacciola F., Crea F., Cataldo S., De Stefano C., Gama S., Lando G., Milea D., Mondello L., Pettignano A., Plass W., Sammartano S., *8-hydroxyquinoline-2-carboxylic acid as possible molybdophore: A multi-technique approach to define its chemical speciation, coordination and sequestering ability in aqueous solution*, Biomolecules, 2020, 10, 930, 1-21.
28. Cernaro V., Loddo S., Macaione V., Ferlazzo V.T., Cigala R.M., Crea F., De Stefano C., Genovese A.R.R., Gembillo G., Bolignano D., Santoro D., Vita R., Buemi M., Benvenga S., *RAS inhibition modulates kynurenine levels in a CKD population with and without type 2 diabetes mellitus*, International Urology and Nephrology ,2020, 52, 1125-1133".
29. Cigala R.M., Crea F., De Stefano C., Irto A., Milea D., Sammartano S., *Thermodynamic Behavior of Polyalcohols and Speciation Studies in the Presence of Divalent Metal Cations*, Journal of Chemical and Engineering Data, 2020, 65, 2805-2812.

30. Cigala R.M., Crea F., De Stefano C., Irto A., Sammartano S. Nature as Resource. Thermodynamic characterization of natural and synthetic polymers and their sequestering ability towards some bivalent metal cations. Journal of Chemical Thermodynamics ,2020, 150, 106205.
31. Berto, S., Marangella, M., De Stefano, C., Milea, D., Daniele, P.G. Critical reappraisal of methods for measuring urine saturation with calcium salts. 2021, Molecules 26(11),3149,
32. Gigliuto, A., Cigala R.M., Irto A, Felice, M. R., Pettignano A., Milea D., Materazzi S., De Stefano C., Crea F. The solution behavior of dopamine in the presence of mono and divalent cations: A thermodynamic investigation in different experimental conditions. 2021, Biomolecules 11(9),1312.
33. Lando, G., Gomez-Laserna, O., Proverbio, E., Khaskhoussi, A., Iannazzo, D., Plutino, M.R., De Stefano, C., Bretti, C. , Cardiano, P. 2021. Towards a rational design of materials for the removal of environmentally relevant cations: polymer inclusion membranes (PIMs) and surface-modified PIMs for Sn^{2+} sequestration in aqueous solution. 2021, Environmental Science and Pollution Research, 28(37), pp. 51072-51087.
34. Crea, F., De Stefano, C., Gigliuto, A., Irto, A., Behavior of Antibacterial Ofloxacin; Hydronation Constants and Solubility in Aqueous Solutions of Sodium Chloride at Different Temperatures. 2021. Journal of Solution Chemistry. 50(9-10), pp. 1236-1257.
35. Bretti, C., De Stefano, C., Cardiano, P., Cataldo, S., Pettignano, A., Arena, G., Sgarlata,C., Ida Grasso, G., Lando, C., Sammartano, S., Risedronate complexes with Mg^{2+}, Zn^{2+}, Pb^{2+}, and Cu^{2+}: Species thermodynamics and sequestering ability in $NaCl_{(aq)}$ at different ionic strengths and at T = 298.15 K., 2021, Journal of Molecular Liquids. 343,117699.
36. Bretti, C., Di Pietro, R., Cardiano, P., Gomez-Laserna, O., Irto A., Lando, G., De Stefano, C. Thermodynamic solution properties of a biodegradable chelant (L-glutamic-n,n-diacetic acid, l-glda) and its sequestering ability toward Cd^{2+}. 2021. Molecules. 26(23),7087.
37. Irto, A., Cardiano, P., Chand, K., Cigala, R.M., Crea, F., De Stefano, C., Santos, M.A. Bifunctional 3-hydroxy-4-pyridinones as potential selective iron(Iii) chelators: Solution studies and comparison with other metals of biological and environmental relevance. 2021. Molecules. 26(23),7280.
38. Gigliuto, A., Cigala, R.M., Irto, A., Felice, M. R., Pettignano, A., , De Stefano, C., Crea, F., The effect of metal cations on the aqueous behavior of dopamine. Thermodynamic investigation of the binary and ternary interactions with Cd^{2+}, Cu^{2+} and UO_2^{2+} in NaCl at different ionic strengths and temperatures. 2021. Molecules. 26(24),7679.
39. Arciszewska, Ż., Gama, S., Kalinowska, M., Świderski, G., Świsłocka, R., Gołębiewska, E., Naumowicz, M., Worobiczuk, M., Cudowski, A., Pietryczuk, A., De Stefano, C., Caffeic Acid/Eu(III) Complexes: Solution Equilibrium Studies, Structure Characterization and Biological Activity. 2022. International Journal of Molecular Sciences 23(2),888.
40. Cernaro V., Calabrese, V. , Loddo S., Corsaro, R., Macaione V., Ferlazzo V.T., Cigala R.M., Crea F., De Stefano C., Gembillo, G., Romeo,A., Longhitano, E. Indole-3-acetic acid correlates with monocyte-to-high-density lipoprotein (HDL) ratio (MHR) in chronic kidney disease patients. 2022. International Urology and Nephrology, 54, 2355-2364.
41. Cigala R.M., De Stefano C., Irto A., Lanzafame P., Papanikolaou G., Crea F. Environmental behaviour of a pesticide metabolite, the AMPA. Sequestration of Ca^{2+}, Mg^{2+}, Cu^{2+}, Zn^{2+} and Al^{3+}. ***Chemosphere*** Volume 306 (2022) Article number 135535
42. Irto A., Cigala R.M., Alessandrello C., De Stefano C., Gattuso G., Crea F. Binary and ternary complexes of epinephrine with alginate and biologically and environmentally relevant metal cations. Frontiers in Chemistry Volume 11 (2023) article number 1189308.
43. Lando G., Bretti C., Milea D., De Stefano C., Gómez-Laserna, O., Cardiano P. Thermodynamic insights into Trans-Aconitate interactions with H^+, Cd^{2+}, Mn^{2+}, and Pb^{2+}: Equilibrium constants, enthalpy changes and sequestering ability. (2023) Journal of Molecular Liquids. 387, 122702.
44. Irto, A., Raccuia, S.G. M.; Lando G., De Stefano C., Arena K., Salerno T.M.G., Pettignano a., Cacciola C., Mondello L., Cardiano P. Valorization of citrus waste for circular economy: A case study on bergamot

pomace as sorbent for Cd^{2+} removal and source of added value compounds. (2023) Microchemical Journal, 193, 109183.

45. Irto, A., Crea, F., Alessandrello, C., Gattuso G., Cordaro M., De Stefano, C., Cigala, R.M. Characterization of thermodynamic properties on Al^{3+}/dopamine system. (2023) Journal of Molecular Liquids 386,122537.
46. Castellino L., Alladio E., Bertinetti S., Lando G., De Stefano C., Blasco S., García-España E., Gama S., Berto S., Milea D. PyES – An open-source software for the computation of solution and precipitation equilibria. (2023) Chemometrics and Intelligent Laboratory Systems, 239 104860.
47. Baryłka, A.; Bagińska-Krakówka, A.; Zuccarello, L.; Mancuso, F.; Gattuso, G.; Lando, G.; Sgarlata, C.; De Stefano, C.; Godlewska-Żyłkiewicz, B.; Milea, D., Gama, S. Protonation equilibria of the tryptophan metabolite 8-hydroxyquinoline-2-carboxylic acid (8-HQA) and its precursors: A potentiometric and calorimetric comparative study. (2023). *Thermochimica Acta* Volume 730 -Article number 179615.
48. Irto, A., Cigala, R.M., De Stefano, C., Crea, F. Advances in iron(III) hydrolysis studies. Effect of the metal concentration, ionic medium and ionic strength. (2023). Journal of Molecular Liquids 391,123361.
49. Majlesi, K., De Stefano, C., Crea, F. Bretti, C. Speciation studies of a bisphosphonate drug. New thermodynamic insights of sodium alendronate with Ca^{2+} and Mg^{2+} in NaCl aqueous solution ($0.10 \leq I/mol\ kg^{-1} \leq 1.02$) (2024) Journal of Chemical Thermodynamics, 190, 107227
50. Irto, A., Crea, F., Milone, M., Gattuso G., Bretti, C.., De Stefano, C., Cigala, R.M. Deferiprone: new environmental perspectives. Insights into its sequestering ability vs. different metal cations. (2024). Ecotoxicology and Environmental Safety, 2721,116027.
51. Irto, A., Crea, F., Alessandrello, C., De Stefano, C. Somma, R., Zaffino G., Zaccaro, S., Papanikolau, G., Cigala, R.M. Landfill leachate from Municipal Solid Waste: Multi-technique approach for its fine characterization and determination of the thermodynamic and sequestering properties towards some toxic metals. (2024) *Science of the Total Environment*, 91720 170311.
52. Berto, S., Blasco, S., Castellino, L., Cvetkovski, A., De Stefano, C.,Gama, S., García-España, E., Hermann, P., Lando, G., Marafante, M., Meyer, M., Plass, W., Quinodoz, L., Milea, D. (2024) A tutorial on potentiometric data processing. Analysis of software for optimization of protonation constants. Analytica Chimica Acta, Volume 130315 Article number 342476.
53. Cigala, R. M;, Raccuia, S. G. M.; Bretti, C.; Cardiano, P.; Lando, G.; Laserna, O.; Gómez[b] O.G.; Gattuso, G.; Irto, A.; Crea, F.; De Stefano, C. (2024). Gallic acid as potential sequestering agent for methylmercury(II) and dimethyltin(IV) removal from aqueous solutions. ***Journal of*** *Environmental Chemical Engineering* Volume 12, Article number 114620.
54. Raccuia, S. G. M.; Zanda, E.; Bretti, C.; Formica, M.;Macedi,E.; Melchior, A.; Tolazzi, M.; Sanadar, M.;Lascari, D.; De Luca, G.; Irto, A; De Stefano, C. (2024). Multi-Analytical Approach for the Acid-Base, Thermal and Surface Properties Assessment of Waste Biomasses. ***Molecules*** Volume 29, Issue 23 Article number 5735
55. Majlesi, K.; De Stefano, C.; Crea, F.;Bretti, C.; New thermodynamic insights into pregabalin interactions with H^+, Na^+, Mg^{2+}, Ca^{2+}, Cu^{2+}, Zn^{2+}: Equilibrium constants, enthalpy changes and sequestering ability.(2025). *Journal of Chemical Thermodynamics***,** Volume Article number 107411.
56. Lando, G.;Bretti, C.; Cardiano, P.;Irto, A.; Milea, D.; De Stefano, C. A Comprehensive Equilibrium Analysis of Tartronate with Proton and Major Cations in Natural Fluids. (2025). ***Molecules* ,** Volume 30, Issue 7, Article number 1497.

Messina, may 24th 2025

Concetta De Stefano

(Prof.ssa Concetta De Stefano)