

De Stefano Concetta

Curriculum Vitae

Laurea magna cum laude, 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 (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 Analytical data validation.

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

Over 250 papers (H-index = 34; Total No. of Citations = 4607) 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: responsible of the project ARCADIA - smARt materials for landfill leachate remediation

Positions in National and International Bodies

- member of Advisor Board of Journal of Chemical and Engineering 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 Board of the Italian Chemical Society since 2013;
- dean of the school “Faculty of Science and Technology” of Messina University
- member of the ASN 2016 Committee;
- chairman of the University Commission for the “24 CFU” Course;
- chairman of the Orientation and Tutoring Commission of the Department CHIBIOFARAM since 2018;
- referent of the tutoring projects (MIUR funds), since 2016;
- component, since 2017, of the scientific commission of the University of Messina for the remediation of the “Falcata area”;
- 2019 - Member of the organizing committee of “One night for research @unime”.

List of publication (2014-2020)

1. Bergamasco, A., et al., *Composition, Distribution, and Sources of Polycyclic Aromatic Hydrocarbons in Sediments of the Gulf of Milazzo (Mediterranean Sea, Italy)*. Polycyclic Aromatic Compounds, 2014. **34**(4): p. 397-424.
2. Bretti, C., et al., *Thermodynamics for proton binding of pyridine in different ionic media at different temperatures*. Journal of Chemical and Engineering Data, 2014. **59**(1): p. 143-156.
3. Bretti, C., et al., *The effect of the tetraalkylammonium salts on the protonation thermodynamics of the phytate anion*. Fluid Phase Equilibria, 2014. **383**: p. 126-133.
4. Bretti, C., et al., *Solubility, activity coefficients, and protonation sequence of risedronic acid*. Journal of Chemical and Engineering Data, 2014. **59**(11): p. 3728-3740.
5. Cigala, R.M., et al., *Acid-base properties and alkali and alkaline earth metal complex formation in aqueous solution of diethylenetriamine- N, N, N', N'', N'''-pentakis(methylenephosphonic acid) obtained by an efficient synthetic procedure*. Industrial and Engineering Chemistry Research, 2014. **53**(23): p. 9544-9553.
6. Crea, F., et al., *Chelating agents for the sequestration of mercury(II) and monomethyl mercury(II)*. Current Medicinal Chemistry, 2014. **21**(33): p. 3819-3836.
7. Cucinotta, D., et al., *Formation, stability and empirical relationships for the binding of Sn²⁺ by O-, N- and S-donor ligands*. Journal of Molecular Liquids, 2014. **200**(PB): p. 329-339.
8. De Stefano, C., et al., *Acid-base and UV behavior of 3-(3,4-dihydroxyphenyl)-propenoic acid (caffeic acid) and complexing ability towards different divalent metal cations in aqueous solution*. Journal of Molecular Liquids, 2014. **195**: p. 9-16.
9. De Stefano, C., et al., *Evaluation of the sequestering ability of different complexones towards Ag⁺ ion*. Journal of Molecular Liquids, 2014. **199**: p. 432-439.
10. De Stefano, C., et al., *Sequestering ability of aminopolycarboxylic (APCs) and aminopolyphosphonic (APPs) ligands toward palladium(II) in aqueous solution*. Journal of Chemical and Engineering Data, 2014. **59**(6): p. 1970-1983.
11. Bretti, C., et al., *Thermodynamics of Zn²⁺ 2-mercaptopyridine-N-oxide and 2-hydroxypyridine-N-oxide interactions: Stability, solubility, activity coefficients and medium effects*. Journal of Molecular Liquids, 2015. **211**: p. 876-884.
12. Bretti, C., et al., *Solubility and modeling acid-base properties of adrenaline in NaCl aqueous solutions at different ionic strengths and temperatures*. European Journal of Pharmaceutical Sciences, 2015. **78**: p. 37-46.
13. Bretti, C., et al., *On the interaction of phytate with proton and monocharged inorganic cations in different ionic media, and modeling of acid-base properties at low ionic strength*. Journal of Chemical Thermodynamics, 2015. **90**: p. 51-58.
14. Cigala, R.M., et al., *Zinc(II) complexes with hydroxocarboxylates and mixed metal species with tin(II) in different salts aqueous solutions at different ionic strengths: Formation, stability, and weak interactions with supporting electrolytes*. Monatshefte für Chemie, 2015. **146**(4): p. 527-540.
15. Cigala, R.M., et al., *Modelling the Hydrolysis of Mixed Mono-, Di- and Trimethyltin(IV) Complexes in Aqueous Solutions*. Journal of Solution Chemistry, 2015. **44**(8): p. 1611-1625.
16. Cigala, R.M., et al., *Thermodynamic data for the modeling of lanthanoid(III) sequestration by reduced glutathione in aqueous solution*. Journal of Chemical and Engineering Data, 2015. **60**(1): p. 192-201.
17. Crea, F., et al., *SALMO and S₃M: A saliva model and a single saliva salt model for equilibrium studies*. Bioinorganic Chemistry and Applications, 2015. **2015**.
18. Bretti, C., et al., *Polycarboxylic acids in sea water: acid-base properties, solubilities, activity coefficients, and complex formation constants at different salinities*. Monatshefte für Chemie, 2016. **147**(9): p. 1481-1505.

19. Bretti, C., et al., *Understanding the bioavailability and sequestration of different metal cations in the presence of a biodegradable chelant S,S-EDDS in biological fluids and natural waters*. *Chemosphere*, 2016. **150**: p. 341-356.
20. Bretti, C., et al., *Acid-base and thermodynamic properties of d-gluconic acid and its interaction with Sn²⁺ and Zn²⁺*. *Journal of Chemical and Engineering Data*, 2016. **61**(6): p. 2040-2051.
21. Bretti, C., et al., *Thermodynamic Study on the Protonation and Complexation of GLDA with Ca²⁺ and Mg²⁺ at Different Ionic Strengths and Ionic Media at 298.15 K*. *Journal of Chemical and Engineering Data*, 2016. **61**(5): p. 1895-1903.
22. Crea, F., et al., *Alkali Metal Ion Complexes with Phosphates, Nucleotides, Amino Acids, and Related Ligands of Biological Relevance. Their Properties in Solution*, in *Metal Ions in Life Sciences*. 2016. p. 133-166.
23. De Stefano, C., et al., *Complexation of Hg²⁺, CH₃Hg⁺, Sn²⁺ and (CH₃)₂Sn²⁺ with phosphonic NTA derivatives*. *New Journal of Chemistry*, 2016. **40**(2): p. 1443-1453.
24. Bretti, C., et al., *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.
25. Bretti, C., et al., *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.
26. Bretti, C., et al., *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.
27. Bretti, C., et al., *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.
28. Cardiano, P., et al., *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.
29. Cardiano, P., et al., *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.
30. Cigala, R.M., et al., *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.
31. Crea, F., et al., *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.
32. Bretti, C., et al., *Exploring various ligand classes for the efficient sequestration of stannous cations in the environment*. *Science of the Total Environment*, 2018. **643**: p. 704-714.
33. Bretti, C., et al., *Solubility, acid-base properties and thermodynamics of interaction between three NTA-phosphonate derivatives and the main cationic components (H⁺, Na⁺, Mg²⁺ and Ca²⁺) of natural fluids*. *Journal of Chemical Thermodynamics*, 2018. **123**: p. 117-127.
34. Cardiano, P., et al., *Sequestration of HEDPA, NTA and phosphonic NTA derivatives towards Al³⁺ in aqueous solution*. *Journal of Molecular Liquids*, 2018. **261**: p. 96-106.
35. Cigala, R.M., et al., *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.
36. Crea, F., et al., *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.
37. Irto, A., et al., *New bis-(3-hydroxy-4-pyridinone)-NTA-derivative: Synthesis, binding ability towards Ca²⁺, Cu²⁺, Zn²⁺, Al³⁺, Fe³⁺ and biological assays*. *Journal of Molecular Liquids*, 2018. **272**: p. 609-624.
38. Irto, A., et al., *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.
39. Majlesi, K., et al., *Thermodynamic Study on the Protonation and Na⁺, Ca²⁺, Mg²⁺-Complexation of a Biodegradable Chelant (HEIDA) at Different Ionic Strengths and Temperatures*. *Journal of Solution Chemistry*, 2018. **47**(3): p. 528-543.
40. Majlesi, K., et al., *Complexation of Molybdenum(VI) with GLDA at Different Ionic Strengths*. *Journal of Solution Chemistry*, **2018**. **47**(12): p. 1965-1979.
41. Bretti, C., et al., *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.
42. Cardiano, P., et al., *Characterization of the thermodynamic properties of some benzenepolycarboxylic acids: Acid-base properties, weak complexes, total and neutral species solubility, solubility products in NaCl_{aw} (CH₃)₄NCl_{aq} and Synthetic Sea Water (SSW)*. *Fluid Phase Equilibria*, 2019. **480**: p. 41-52.
43. De Stefano, C., et al., *Prediction of water solubility and Setschenow coefficients by tree-based regression strategies*. *Journal of Molecular Liquids*, 2019. **282**: p. 401-406.
44. Irto, A., et al., *A new bis-(3-hydroxy-4-pyridinone)-DTPA-derivative: Synthesis, complexation of di-/tri-valent metal cations and in vivo M³⁺ sequestering ability*. *Journal of Molecular Liquids*, 2019. **281**: p. 280-294.
45. 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 Zn²⁺ at different ionic strengths and temperatures*, *Molecules*, **2019**, 24(22), pp. 4084
46. Majlesi K., Bretti C., De Stefano C., Lando G., Majlesi K., Sammartano S., *Thermodynamic Study on the Interaction of Nicotinic Acid with H⁺, Na⁺, Ca²⁺ and Mg²⁺ at Different Temperatures and Ionic Strengths*, *Journal of Solution Chemistry*, **2019**, 48, pp 1671-1684
47. 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.
48. 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.

49. Majlesi K., Bretti C., De Stefano C., Sammartano S., *Thermodynamic Study on the Protonation and Complexation of the Neuroleptic Drug, Gabapentin with Na⁺, Ca²⁺ and Mg²⁺ at Various Temperatures and Ionic Strengths*, Journal of Solution Chemistry 2020, 49, 1225-1236.
50. 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.
51. 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".
52. 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.
53. Lando G., Gomez-Laserna O., Proverbio E., Khaskhoussi A., Iannazzo D., Plutino M.R., De Stefano C., Bretti C., Cardiano P. *Towards a rational design of materials for the removal of environmentally relevant cations: polymer inclusion membranes (PIMs) and surface-modified PIMs for Sn²⁺ sequestration in aqueous solution*, Environmental Science and Pollution Research, 2021,- DOI: 10.1007/s11356-021-14328-0

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