

De Stefano Concetta

Curriculum Vitae

Born in [REDACTED]

Laurea magna cum laude, Chemistry (1982), University of Messina.

Academic positions

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

Research interests:

- thermodynamics of solution equilibria, 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 240 papers (H-index = 32; Total No. of Citations = 4209; Citations/paper = 17.5) 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" (1998).
- Research agreement with the multinational company Procter&Gamble (since 2008)
- PRIN, "Multiple equilibria in natural and biological fluids: from speciation to selective sequestering" (2015)

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)
- 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 Board of Directors of the Division of Analytical Chemistry-Italian Chemical Society form 2013.
- dean of the school "Faculty of Science and Technology" of Messina University (December 2013-February 2017).

List of publication (2017-2012)

1. 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, 63-73.
2. 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, 1-10.
3. 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, 1018-1027.
4. 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, 15-26.
5. De Stefano, C.; Foti, C.; Giuffrè, O.; Milea, D., Complexation of Hg²⁺, CH₃Hg⁺, Sn²⁺ and (CH₃)₂Sn²⁺ with phosphonic NTA derivatives. *New Journal of Chemistry* **2016**, 40, 1443-1453.
6. Crea, F.; De Stefano, C.; Foti, C.; Lando, G.; Milea, D.; Sammartano, S., Alkali Metal Ion Complexes with Phosphates, Nucleotides, Amino Acids, and Related Ligands of Biological Relevance. Their Properties in Solution. *Metal ions in life sciences* **2016**, 16, 133-166.
7. Crea, F.; De Stefano, C.; Foti, C.; Lando, G.; Milea, D.; Sammartano, S., 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; Vol. 16, pp 133-166.
8. Bretti, C.; Majlesi, K.; De Stefano, C.; Sammartano, S., 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, 1895-1903.
9. 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 S,S-EDDS in biological fluids and natural waters. *Chemosphere* **2016**, 150, 341-356.
10. Bretti, C.; Cigala, R. M.; De Stefano, C.; Lando, G.; Sammartano, S., Acid-base and thermodynamic properties of d-gluconic acid and its interaction with Sn²⁺ and Zn²⁺. *Journal of Chemical and Engineering Data* **2016**, 61, 2040-2051.
11. Bretti, C.; Cigala, R. M.; Crea, F.; De Stefano, C.; Foti, C.; Pettignano, A.; Sammartano, S., Polycarboxylic acids in sea water: acid-base properties, solubilities, activity coefficients, and complex formation constants at different salinities. *Monatshefte für Chemie* **2016**, 1-25.
12. Crea, F.; De Stefano, C.; Milea, D.; Pettignano, A.; Sammartano, S., SALMO and S₃M: A saliva model and a single saliva salt model for equilibrium studies. *Bioinorganic Chemistry and Applications* **2015**, 2015.
13. Cigala, R. M.; De Stefano, C.; Irto, A.; Milea, D.; Sammartano, S., Thermodynamic data for the modeling of lanthanoid(III) sequestration by reduced glutathione in aqueous solution. *Journal of Chemical and Engineering Data* **2015**, 60, 192-201.
14. Cigala, R. M.; Crea, F.; De Stefano, C.; Sammartano, S., Modelling the Hydrolysis of Mixed Mono-, Di- and Trimethyltin(IV) Complexes in Aqueous Solutions. *Journal of Solution Chemistry* **2015**, 44, 1611-1625.

15. Cigala, R. M.; Crea, F.; De Stefano, C.; Foti, C.; Milea, D.; Sammartano, S., 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 fur Chemie* **2015**, 146, 527-540.
16. Bretti, C.; Cigala, R. M.; De Stefano, C.; Lando, G.; Milea, D.; Sammartano, S., 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, 51-58.
17. Bretti, C.; Cigala, R. M.; Crea, F.; De Stefano, C.; Vianelli, G., 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, 37-46.
18. Bretti, C.; Cigala, R. M.; Crea, F.; De Stefano, C.; Lando, G.; Sammartano, S., Thermodynamics of Zn^{2+} 2-mercaptopyridine-N-oxide and 2-hydroxypyridine-N-oxide interactions: Stability, solubility, activity coefficients and medium effects. *Journal of Molecular Liquids* **2015**, 211, 876-884.
19. De Stefano, C.; Lando, G.; Pettignano, A.; Sammartano, S., Evaluation of the sequestering ability of different complexones towards Ag^+ ion. *Journal of Molecular Liquids* **2014**, 199, 432-439.
20. De Stefano, C.; Lando, G.; Pettignano, A.; Sammartano, S., Sequestering ability of aminopolycarboxylic (APCs) and aminopolyphosphonic (APPs) ligands toward palladium(II) in aqueous solution. *Journal of Chemical and Engineering Data* **2014**, 59, 1970-1983.
21. De Stefano, C.; Foti, C.; Giuffrè, O.; Sammartano, S., 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, 9-16.
22. Cucinotta, D.; De Stefano, C.; Giuffrè, O.; Lando, G.; Milea, D.; Sammartano, S., Formation, stability and empirical relationships for the binding of Sn^{2+} by O-, N- and S-donor ligands. *Journal of Molecular Liquids* **2014**, 200, 329-339.
23. Crea, F.; De Stefano, C.; Foti, C.; Milea, D.; Sammartano, S., Chelating agents for the sequestration of mercury(II) and monomethyl mercury(II). *Current Medicinal Chemistry* **2014**, 21, 3819-3836.
24. Cigala, R. M.; Cordaro, M.; Crea, F.; De Stefano, C.; Fracassetti, V.; Marchesi, M.; Milea, D.; Sammartano, S., 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, 9544-9553.
25. Bretti, C.; Cukrowski, I.; De Stefano, C.; Lando, G., Solubility, activity coefficients, and protonation sequence of risedronic acid. *Journal of Chemical and Engineering Data* **2014**, 59, 3728-3740.
26. Bretti, C.; Cigala, R. M.; De Stefano, C.; Lando, G.; Sammartano, S., Thermodynamics for proton binding of pyridine in different ionic media at different temperatures. *Journal of Chemical and Engineering Data* **2014**, 59, 143-156.
27. Bretti, C.; Cigala, R. M.; De Stefano, C.; Lando, G.; Sammartano, S., The effect of the tetraalkylammonium salts on the protonation thermodynamics of the phytate anion. *Fluid Phase Equilibria* **2014**, 383, 126-133.
28. Bergamasco, A.; Culotta, L.; De Stefano, C.; Orecchio, S.; Sammartano, S.; Barreca, S., Composition, Distribution, and Sources of Polycyclic Aromatic Hydrocarbons in Sediments of the Gulf of Milazzo (Mediterranean Sea, Italy). *Polycyclic Aromatic Compounds* **2014**, 34, 397-424.
29. Crea, F.; De Stefano, C.; Manfredi, G.; Sammartano, S., Thermodynamic study of the non covalent interactions of phytate with xanthine derivatives and histamine in aqueous solution. *Journal of Molecular Liquids* **2013**, 178, 37-43.

30. Cigala, R. M.; De Stefano, C.; Giacalone, A.; Gianguzza, A.; Sammartano, S., Enhancement of hydrolysis through the formation of mixed heterometal species: $\text{Al}^{3+}/\text{CH}_3\text{Sn}^{3+}$ mixtures. *Journal of Chemical and Engineering Data* **2013**, 58, 821-826.
31. Cigala, R. M.; Crea, F.; De Stefano, C.; Milea, D.; Sammartano, S.; Scopelliti, M., Speciation of tin(II) in aqueous solution: Thermodynamic and spectroscopic study of simple and mixed hydroxocarboxylate complexes. *Monatshefte für Chemie* **2013**, 144, 761-772.
32. Cataldo, S.; De Stefano, C.; Gianguzza, A.; Pettignano, A.; Sammartano, S., Sequestration of alkyltin(IV) cations by complexation with amino-polycarboxylic chelating agents. *Journal of Molecular Liquids* **2013**, 187, 74-82.
33. Bretti, C.; De Stefano, C.; Lando, G.; Sammartano, S., Thermodynamics for proton binding of phytate in $\text{KNO}_3(\text{aq})$ at different temperatures and ionic strengths. *Thermochimica Acta* **2013**, 566, 193-202.
34. Bretti, C.; De Stefano, C.; Lando, G.; Sammartano, S., Thermodynamic properties of melamine (2,4,6-triamino-1,3,5-triazine) in aqueous solution. Effect of ionic medium, ionic strength and temperature on the solubility and acid-base properties. *Fluid Phase Equilibria* **2013**, 355, 104-113.
35. Bretti, C.; De Stefano, C.; Foti, C.; Sammartano, S., Acid-base properties, solubility, activity coefficients and Na^+ ion pair formation of complexons in $\text{NaCl}(\text{aq})$ at different ionic strengths. *Journal of Solution Chemistry* **2013**, 42, 1452-1471.
36. Bretti, C.; Crea, F.; De Stefano, C.; Foti, C.; Materazzi, S.; Vianelli, G., Thermodynamic properties of dopamine in aqueous solution. acid-base properties, distribution, and activity coefficients in NaCl aqueous solutions at different ionic strengths and temperatures. *Journal of Chemical and Engineering Data* **2013**, 58, 2835-2847.
37. Bretti, C.; Cigala, R. M.; De Stefano, C.; Lando, G.; Sammartano, S., Potentiometric determination of some solution thermodynamic parameters of three hydroxypyrrone derivatives. *International Journal of Electrochemical Science* **2013**, 8, 10621-10649.
38. Crea, F.; De Stefano, C.; Manfredi, G.; Sammartano, S., Quantitative study of the interaction between ATP and aromatic amines in aqueous solution. *Journal of Solution Chemistry* **2012**, 41, 1240-1253.
39. Crea, F.; Cucinotta, D.; De Stefano, C.; Milea, D.; Sammartano, S.; Vianelli, G., Modeling solubility, acid-base properties and activity coefficients of amoxicillin, ampicillin and (+)6-aminopenicillanic acid, in $\text{NaCl}(\text{aq})$ at different ionic strengths and temperatures. *European Journal of Pharmaceutical Sciences* **2012**, 47, 661-677.
40. Cigala, R. M.; Crea, F.; De Stefano, C.; Lando, G.; Milea, D.; Sammartano, S., The inorganic speciation of tin(II) in aqueous solution. *Geochimica et Cosmochimica Acta* **2012**, 87, 1-20.
41. Cigala, R. M.; Crea, F.; De Stefano, C.; Lando, G.; Milea, D.; Sammartano, S., Thermodynamics of binary and ternary interactions in the tin(II)/phytate system in aqueous solutions, in the presence of Cl^- or F^- . *Journal of Chemical Thermodynamics* **2012**, 51, 88-96.
42. Cigala, R. M.; Crea, F.; De Stefano, C.; Lando, G.; Milea, D.; Sammartano, S., Modeling the acid-base properties of glutathione in different ionic media, with particular reference to natural waters and biological fluids. *Amino Acids* **2012**, 43, 629-648.
43. Cigala, R. M.; Crea, F.; De Stefano, C.; Lando, G.; Manfredi, G.; Sammartano, S., Quantitative study on the interaction of Sn^{2+} and Zn^{2+} with some phosphate ligands, in aqueous solution at different ionic strengths. *Journal of Molecular Liquids* **2012**, 165, 143-153.
44. Cataldo, S.; De Stefano, C.; Gianguzza, A.; Pettignano, A., Sequestration of $(\text{CH}_3)_3\text{Hg}^+$ by amino-polycarboxylic chelating agents. *Journal of Molecular Liquids* **2012**, 172, 46-52.
45. Bretti, C.; De Stefano, C.; Foti, C.; Sammartano, S.; Vianelli, G., Protonation thermodynamics of some aminophenol derivatives in $\text{NaCl}(\text{aq})$ ($0 \leq i \leq 3 \text{ mol} \cdot \text{kg}^{-1}$) at $T = 298.15 \text{ K}$. *Journal of Chemical Thermodynamics* **2012**, 44, 154-162.
46. Bretti, C.; Crea, F.; De Stefano, C.; Sammartano, S.; Vianelli, G., Some thermodynamic properties of dl-Tyrosine and dl-Tryptophan. Effect of the ionic medium, ionic strength and

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temperature on the solubility and acid-base properties. *Fluid Phase Equilibria* **2012**, 314, 185-197.

47. Bretti, C.; Crea, F.; De Stefano, C.; Sammartano, S.; Vianelli, G., Protonation constants, activity coefficients, and chloride ion pair formation of some aromatic amino-compounds in NaCl aq ($0 \text{ mol} \cdot \text{kg}^{-1} \leq I \leq 3 \text{ mol} \cdot \text{kg}^{-1}$) at $T = 298.15 \text{ K}$. *Journal of Chemical and Engineering Data* **2012**, 57, 1851-1859.
48. Bretti, C.; Cigala, R. M.; De Stefano, C.; Lando, G.; Sammartano, S., Interaction of phytate with Ag^+ , CH_3Hg^+ , Mn^{2+} , Fe^{2+} , Co^{2+} , and VO^{2+} : Stability constants and sequestering ability. *Journal of Chemical and Engineering Data* **2012**, 57, 2838-2847.
49. Berto, S.; Crea, F.; Daniele, P. G.; De Stefano, C.; Prenesti, E.; Sammartano, S., Potentiometric and spectrophotometric characterization of the UO_2^{2+} -citrate complexes in aqueous solution, at different concentrations, ionic strengths and supporting electrolytes. *Radiochimica Acta* **2012**, 100, 13-28.

Messina, 6 Maggio 2017

C. Bretti
[Redacted Signature]