

## ***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, 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.

### **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 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

### **List of publication (2017-2012)**

1. 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, pp. 107-118.
2. 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), pp. 1-25.
3. 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), pp.4065-40754.
4. 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, 63-735.
5. Cardiano, P.; Cigala, R. M.; Crea, F.; De Stefano, C.; Giuffrè, O.; Sammartano, S.; Vianelli, G., Potentiometric, UV and <sup>1</sup>H NMR study on the interaction of penicillin derivatives with Zn(II) in aqueous solution. *Biophysical Chemistry* 2017,223, 1-10.
6. 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.
7. 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.
8. De Stefano, C.; Foti, C.; Giuffrè, O.; Milea, D., Complexation of Hg<sup>2+</sup>, CH<sub>3</sub>Hg<sup>+</sup>, Sn<sup>2+</sup> and (CH<sub>3</sub>)<sub>2</sub>Sn<sup>2+</sup> with phosphonic NTA derivatives. *New Journal of Chemistry* 2016, 40, 1443-1453.
9. 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.
10. 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, pp133-166.
11. Bretti, C.; Majlesi, K.; De Stefano, C.; Sammartano, S., Thermodynamic Study on the Protonation and Complexation of GLDA with Ca<sup>2+</sup> and Mg<sup>2+</sup> at Different Ionic Strengths and Ionic Media at 298.15 K. *Journal of Chemical and Engineering Data* 2016,61, 1895-1903.
12. 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.
13. 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 Sn<sup>2+</sup> and Zn<sup>2+</sup>. *Journal of Chemical and Engineering Data* 2016,61, 2040-2051.
14. 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 fur Chemie* 2016, 1-25.
15. 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.

16. 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.
17. 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.
18. 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.
19. 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.
20. 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, 37-46.21.
21. 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.
22. 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.
23. 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.
24. 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.
25. 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.
26. 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.
27. 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.
28. 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.
29. 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.
30. 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, 126-133.31.

31. 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.
32. 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.
33. Cigala, R. M.; De Stefano, C.; Giacalone, A.; Gianguzza, A.; Sammartano, S., Enhancement of hydrolysis through the formation of mixed heterometal species:  $Al^{3+}/CH_3Sn^{3+}$  mixtures. *Journal of Chemical and Engineering Data* 2013,58, 821-826.
34. 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 fur Chemie* 2013,144, 761-772.
35. 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.
36. Bretti, C.; De Stefano, C.; Lando, G.; Sammartano, S., Thermodynamics for proton binding of phytate in  $KNO_3(aq)$  at different temperatures and ionic strengths. *Thermochimica Acta* 2013,566, 193-202.
37. 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.
38. Bretti, C.; De Stefano, C.; Foti, C.; Sammartano, S., Acid-base properties, solubility, activity coefficients and  $Na^+$  ion pair formation of complexons in  $NaCl(aq)$  at different ionic strengths. *Journal of Solution Chemistry* 2013,42, 1452-1471.
39. 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.
40. Bretti, C.; Cigala, R. M.; De Stefano, C.; Lando, G.; Sammartano, S., Potentiometric determination of some solution thermodynamic parameters of three hydroxypyron derivatives. *International Journal of Electrochemical Science* 2013,8, 10621-10649.
41. 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.
42. 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  $NaCl(aq)$  at different ionic strengths and temperatures. *European Journal of Pharmaceutical Sciences* 2012,47, 661-677.
43. 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.
44. 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.
45. 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.
46. 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.
47. Cataldo, S.; De Stefano, C.; Gianguzza, A.; Pettignano, A., Sequestration of  $(\text{CH}_3)\text{Hg}^+$  by amino-polycarboxylic chelating agents. *Journal of Molecular Liquids* 2012,172, 46-52.
  48. Bretti, C.; De Stefano, C.; Foti, C.; Sammartano, S.; Vianelli, G., Protonation thermodynamics of some aminophenol derivatives in NaCl (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.
  49. 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 temperature on the solubility and acid-base properties. *Fluid Phase Equilibria* 2012,314, 185-197.
  50. 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.
  51. Bretti, C.; Cigala, R. M.; De Stefano, C.; Lando, G.; Sammartano, S., Interaction of phytate with  $\text{Ag}^+$ ,  $\text{CH}_3\text{Hg}^+$ ,  $\text{Mn}^{2+}$ ,  $\text{Fe}^{2+}$ ,  $\text{Co}^{2+}$ , and  $\text{VO}^{2+}$ : Stability constants and sequestering ability. *Journal of Chemical and Engineering Data* 2012,57,2838-2847.
  52. Berto, S.; Crea, F.; Daniele, P. G.; De Stefano, C.; Prenesti, E.; Sammartano, S., Potentiometric and spectrophotometric characterization of the  $\text{UO}_2^{2+}$ -citrate complexes in aqueous solution, at different concentrations, ionic strengths and supporting electrolytes. *Radiochimica Acta* 2012,100, 13-28