



**National Institute for Advanced Analytical Science and Technology -
INCTAA**

**Annual Activity Report
(March 2009 – March 2010)**

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I. Introductory Remarks

This report describes the achievements of the National Institute for Advanced Analytical Science and Technologies (INCTAA) during its first year of activity between March 2009 and March 2010.

The major results attained in this period and their relevance for analytical science and technology are highlighted. In the following, future activities and perspectives of the INCTAA are described.

II. Presentation of the INCTAA

II. 1. The INCTAA

The National Institute of Advanced Analytical Science and Technology (INCTAA) is hosted at the Chemistry Institute of the State University of Campinas (UNICAMP) and acts by fostering synergistic actions, within a modern inter- and multi-disciplinary approach, leading to scientific advancements and technological innovations of analytical instrumentation and methods to face the challenges that arise nowadays in several fields of interest to the social and economic development of Brazil. Among these fields, it is worth citing: the environment, new materials and nanotechnology (concerning its use and environmental impact, still unknown), biochemical processes, quality control of industrial products and processes (such as those of the pharmaceutical, petrochemical and fossil/renewable fuel sectors), commercialization of food and agricultural products, and forensic investigation. By meeting the demands from these various areas, the Institute shall provide solutions to analytical problems of priority to the country, which will be of value to maintain the current trend of social and economic growth, by means of both a significant scientific and technology advancement and the formation of qualified human resources.

II.2. Research Lines

In order to fulfil the objectives and goals established for the INCTAA the institute will initially pursue four research lines, which are associated with presently existing *demands* (i.e, urgent requirements) that shall require the synergistic and complementary efforts of its researchers working in teams. These lines of research not only involve fundamental scientific aspects, but are also aimed at achieving

technological breakthroughs of relevance to the economic and social development of Brazil.

The research lines presently being developed by the INCTAA are the following:

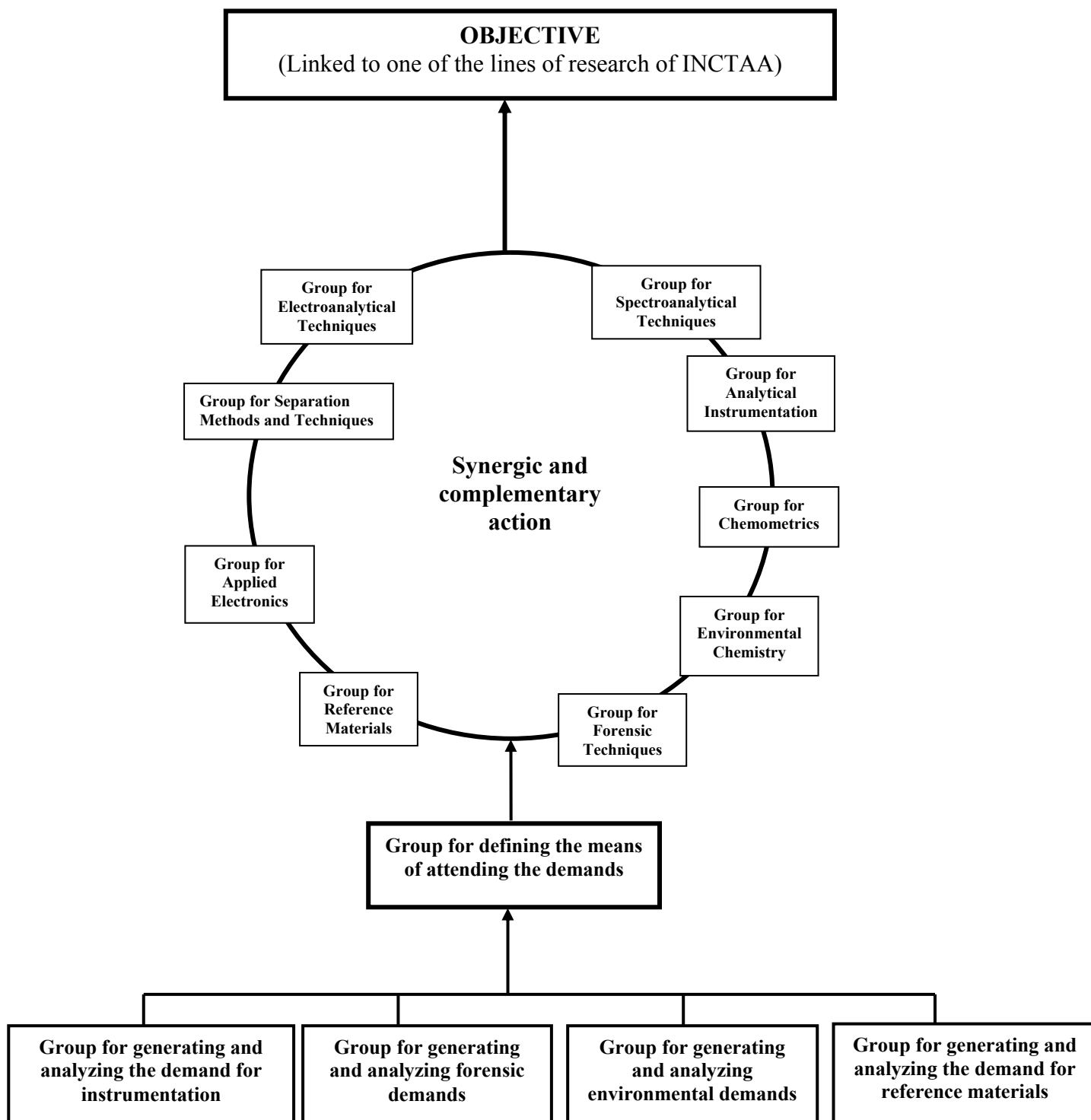
- 1. Development of analytical process instrumentation and robust workbench instrumentation for monitoring of agricultural and industrial feedstocks and products.*
- 2. Development of analytical instrumentation and methods for forensic use.*
- 3. Development of remote sensing instruments and methods for applications in environmental monitoring and in the understanding of environmental processes.*
- 4. Production of reference materials and creation of a national inter-laboratorial network.*

II.3. *Modus Operadi*

Perhaps the most remarkable and innovative feature of the INCTAA is in the way it operates to elect and achieve its objectives. The figure below is a schematic representation of the INCTAA operational mode. Because of the extensive the INCTA research group, constituted by more than 50 researchers in university level teaching/research institutions, industries and research centers, summing 20 entities widely distributed around Brazil, it is necessary to act synergistically to attend the real *demands* for analytical science and technology. It is thus of fundamental importance that the *demands* be carefully selected according to the initial premises of the INCTAA.

The mechanism starts by searching among the internal and external contributors of the INCTAA for real multi- and inter-disciplinary *demands*. After evaluation, these *demands* are presented to the researchers of the institute who will attend the *demand* by using the network facilities in terms of hardware and intellectual expertise.

The mechanism intends to permanently link the efforts of the INCTAA to attend real *demands* in an effective manner, according to the requirements of the field of interest which initially indicated their relevance. Experience has shown that, as far as the field of analytical science and technology is concerned, the *modus operandi* of the INCTAA can contribute both to find urgently needed solutions to analytical problems and to generate original academic contributions to the field, both to the benefit of Brazil.



III. Some Words from the Coordinator

The first year of the existence of the INCTAA has been marked by the challenge of launching the institute, ensuring that the original premises that guided its proposal were fully embodied in its members. This is not a simple task as the *modus operandi* of the INCTAA is somewhat innovative for the Brazilian community involved in analytical science and technology.

In order to start to move the INCTAA on its tracks, the first workshop of the institute took place between 30th July and 1st August 2009 at the host institution (the Chemistry Institute - UNICAMP). 64 attendees were registered in the event, including the whole research team of the INCTAA (16 researchers from São Paulo State and 34 from rest of the country), invited guests that represented important sectors of government (National Petroleum Agency - ANP) and industry (Petrobras SA) and some students from IQ-UNICAMP.

By the end of the first day of work the group produced an expressive number of 30 possible *demands*, aligned within the four research lines of the INCTAA; all would require networking to be attended to and, therefore, fulfilled the initial INCTAA premises. Due the budget restrictions, the group then selected 20 *demands* to be attended in the next three years.

The selected *demands* are now the research goals of the INCTAA. They are listed below, where the number in parentheses indicates the number of researchers of the INCTAA committed to attending this *demand*:

Research line I. Development of analytical process instrumentation and robust workbench instrumentation for monitoring of agricultural and industrial feedstock and products.

I.1. Development of instrumentation for determination of moisture in gases. (7)

I.2. Development of instrumentation for determination metals in biofuel by electrochemical techniques. (5)

I.3. Development of instrumentation for comparison between different types of bioethanol (organic and inorganic compounds) (5)

I.4. Development of instrumentation for determination for identification of variety and geographical origin of biofuels.

I.5. Development of a on-line analyzer for determination of Pt/Co color and Saybolt color in thinner streams. Typical range for the Pt/Co color: <5 to 50. (4)

I.6. Development of a on-line analyzer for determination of total iron, soluble aluminum, chlorine, fluorine and turbidity in demineralized drinking water clarified. Typical content (mg L^{-1}): iron (<0.6 – 3), aluminium (<1 – 2), chlorine (<2 – 5), turbidity (NTU) (< 2 -40). (7)

I.7. Development of analytical methods for determination of grouped composition (PIONA), class composition (ex. isoparaffins) or individual components (ex. butadiene, isoprene, etc.) in naphtha. (6)

I.8. Development of a portable instrument for determination of benzene and ethanol in gasoline. (9)

I.9. Development of a portable instrument for determination of water in diesel and biodiesel. (9)

I.10. Development of analytical methods and studies of distribution of chemical species (ex. Si, As, Hg and Pb), to determine the total content or perform the speciation across a petrochemical process in diverse matrices (organics, lime, aqueous effluents, gases etc.). Distinct techniques may be employed: ICP-MS, FAAS, ETAAS and Voltammetry. (11)

Research line II. Development of analytical instrumentation and methods for forensic use.

II.1. Development and field testing of low cost, easy to use and disposal units for (5)

- a) Field equipment for drug identification
- b) Aqueous biphasic systems for drugs
- c) Environmental parameters in field such as BTEX, metals, leachates and pesticides)

II.2. Development of instrumentation and methods for authentication for (6)

- a) Authentication of documents
- a) Images – e.g. analysis of printing material and signatures

II.3. Environmental analysis, including sampling (transport), analytical methods (extraction) and interpretations including determination of origin of contamination (9)

- a) Leachates (metals, organic load), pesticides.
- b) Trace analysis (organics and inorganic)
- c) Pesticides and impurities (smuggled samples with distinct impurities)

II.4. Validation of imported fuels (RR) (4):

- a) FTIR calibration – model transference to 35 laboratories of the Brazilian Federal Police

Research line III. Development of remote sensing instruments and methods for applications in environmental monitoring and understanding of environmental processes.

III.1. Emerging Contaminants (8)

Sources, methods, new technologies for mitigation, ecotoxicology.

III.2. Sensors, analytical methods and instruments for environmental monitoring (in situ and real time / remote). Indications of pollution sources and time-space evaluation of contaminations. (10)

III.3. New materials of environmental interest. (9)

Catalysts, adsorbents, sensors, environmental impacts

Research line IV. Production of reference materials and creation of a national inter-laboratorial network.

IV.1. Reference materials for forensic use.

IV.2. Reference materials of food matrices.

IV.3. Reference materials of organics in fuels and petroleum products.

A preliminary evaluation of the contents of the selected *demands* shows agreement between their contents and the major interest of Brazil regarding its social and economic impact. This synchronicity comes from the way INCTAA plans to act, which makes demand selection, with the help of its members from several federal institutions (e.g., Brazilian Federal Police, EMBRAPA and INMETRO) and representative industries that will be the final users of the analytical techniques (p.e. BRASKEM, PETROBRAS).

During the workshop the directors and coordinators of the selected *demands* and for administrative functions of the INCTAA organizational structure were chosen. The INCTAA is now fully functional in terms of organization and promotion of its actions at the different levels from research to secondary education, passing through divulgation of the INCTAA. The structure of the INCTAA can be found at <http://www.inctaa.iqm.unicamp.br/estrutura.php>.

In a second stage, after the *demands* have been selected, the members of the INCTAA applied for financial support of the institute in order to develop the actions necessary to attend the selected *demands*. The Managing Committee evaluated the applications and decided to initially apply R\$ 1.041.000,00 from the INCTAA budget to support the development of the four research lines and their respective workpackages.

The first workshop can be considered the main action of this first year, because it was extremely relevant to organizing the institute, other significant actions and results have been produced by the INCTAA in the period. Some of them are highlighted in this report. Even though the institute is now read to go forward with its activities, its Managing Committee is concerned to report only the activities and results which can be really associated with the INCTAA and not with many previous actions which have been developed before the INCTAA come into existence. That is because the INCTAA presents a breakthrough in the way analytical scientists will work in Brazil, bypassing individual actions (although these will be always a part of the activities of the researchers of the institute) and enhancing network actions.

Nevertheless, several results of this first year reflect actions initiated before the INCTAA was fully installed. These actions and results are in agreement with the institute premises, have been included in the INCTAA, and will be mentioned here as examples of the type of action and expected results that the INCTAA wishes to encourage in the near future.

Other actions were initiated after the INCTAA was launched and cover many other aspects of the global actions dedicated to institute divulgation and to overall divulgation of analytical science and technology.

In summary, the coordinator considers the INCTAA has, during its first year of life, fully accomplished its original premises and established the grounds to ensure the success of its further activities.

IV. Highlights

IV.1. Scientific and Technological Activities

As pointed out before, the first year of activity of the INCTAA was dedicated mostly to organizing and to facilitating the INCTAA for network operation. However, there are some impacting results obtained during this first year, some coming from actions initiated before the INCTAA was formally launched, but which have been

included to serve as good examples of the type of product the institute intend to generate. Several of these actions, now concluded, have inspired the elaboration of the INCTAA proposal.

IV.1.1. Development of a process analyzer based on near infrared spectroscopy (NIR) for monitoring hydrocarbons and fuels derived from petroleum.



The development of a process analyzer based on near infrared spectroscopy for monitoring hydrocarbons and fuel derived from petroleum may be taken as an example of the results the INCTAA intends to produce related to its research line in instrumentation and analytical methods. The construction of the process analyzer began as a primary activity of a collaborative research project between IQ-UNICAMP/PETROBRAS and has recently been supported by the INCTAA. The development of this analyzer means the knowhow associated with the construction and integration of this type of instrument in the process is now dominated by Brazil. This instrument can be considered the first one

entirely constructed in Brazil employing state-of-the-art technology available to the area. The development of the analyzer generated many innovative advances which will be subject of patents in the near future. The multidisciplinary action of the INCTAA was fully embodied and identified in this analyzer. The figure shows the process NIR spectrophotometer and its cabinet, designed to permit the installation of the instrument in a risk area of a petroleum refinery.

IV.1.2. Emerging Contaminants.



The research line on emerging contaminants shows some significant results consolidated in the period and relevant to the comprehension of the potential risk of the presence of such species in water designated for human consumption. The presence of emerging contaminants in fresh water sources and in drinking water provided to the

Brazilian population is basically unknown. There are few groups in Brazil acting in this area at a time when a whole picture of the quality of these waters is becoming extremely

relevant in order to predict possible damages to the aquatic communities of the fresh water sources as well as its probable risk to human health. In view of the low number of groups working on the subject in Brazil, the INCTAA is consolidating three new laboratories, distributed around the country (in Pernambuco and in Paraíba, in Paraná and in the north of Rio de Janeiro state) that have started a preliminary evaluation of the quality of the water in those regions.

Furthermore, the innovative and pioneering work developed by the INCTAA supports the definition of public policy regarding standards for some of these emerging contaminants. The proposal of the INCTAA is to promote an integrated study involving several groups within its network, using the same analytical procedures to access the present stage of the sources of drinking water in several locations in Brazil. As far as this subject is concerned, the INCTAA supported ABES (Brazilian Association of Sanitary Engineering) in generating a document “Grounds for a National Policy for Water for Human Consumption”, produced by the Technical Chamber for Public Health (Year I, No. 1, March 2010).

IV.1.3. Analytical Methods for Forensic Analysis.



The line of analytical methods for forensic analysis highlight the recent results attained in the use of Laser Induced Breakdown Spectroscopy (LIBS) for detection of gunshot residues on the hands of suspects of criminal acts. The impact of analytical science and technology in the forensic area has been demonstrated with increased frequency and its relevance on the final decisions of the criminal investigations and public trials is noticeable. Close collaboration with the Brazilian Federal Police, a partner of the INCTAA network,

will make certain that sure the analytical methods developed by the INCTAA could really fulfill the requirements of the security agencies.

IV.1.4. Reference Materials.

The research line on reference materials (RM) has been involved in the development of two strategies for sample treatment that will allow for launching network activities related to the production of RMs. The center for sample treatment assembled in EMBRAPA, São Carlos, shown in the picture is a relevant result of the INCTAA activities in the field of reference materials.



V. Facilities

During its first year the INCTAA has increased its facilities to sustain its network efforts toward the goals established during the I Workshop. The Managing Committee has authorized the acquisition of several instruments and allocated them to a number of institutions. The guide lines for the distribution followed mainly the criteria of attending the network operational requirements. Nevertheless, a few instruments were allocated to encourage a few emerging research groups.



It is worth emphasizing that the set up of the Center for Sample Treatment located at EMBRAPA, São Carlos as being an effective action that will enable further actions to attend the *demands* related to the production of reference materials. The equipment acquired include: a cryogenic ball mill, an automatic quarterer, a sieve for assay with an automatic mill, and an ultra-centrifuge mill. The center is fully operational and is serving INCTAA

members in any matter requiring sample treatment. A number of the instrument located at the center is shown in the picture.

Other imported instruments included in the INCTAA facilities were:

An Atomic Absorption Spectrophotometer located at the Federal University of Viçosa – MG.

Two Spectrofluorimeters, one located at the Chemistry Institute of UNICAMP and the other at CENA-USP-Piracicaba.

Two microwave digestion ovens, one located at the Chemistry Institute of UNICAMP and the other at EMBRAPA, São Carlos, in the Center for Sample Treatment of the INCTAA.

VI. Divuligation of Science and Technology

The divulgation of the INCTAA and of the actions performed by the institute is viewed as a key activity regarding the premises of the INCTAA. During this last year the institute has promoted and attended several events where its members had the opportunity to divulge the concept of the INCTAA. Also the research activities of the institute have been divulged according to its initial proposal, including the following actions:

VI.1. Organization of the 1st Workshop in Emerging Contaminants in Water for Human Consumption. 7th October 2009. Campinas - SP

VI.2. Organization of the 1st Workshop in Proficiency Assay for Animal Nutrition Laboratories (EPLNA). EMBRAPA Pecuária Sudeste, São Carlos - SP. 12th and 13th April 2010. This workshop included a course on sample preparation which employed the equipment acquired by the INCTAA, installed in the Center for Sample Treatment.

VI.3. Organization of the IV Workshop in Near Infrared Spectroscopy (NIR). 17th and 18th October of 2009. Salvador - BA

VI.4. Organization of the Workshop “Materials for Chemical Sensors and Environmental Processes”. 6th August 2009. Campinas – SP. CAPES-DGU (Spain) also supported this activity.

VI.5. Course: “Production and certification of Reference Materials”. 12th and 14th May 2009. INMETRO. Xerém – RJ.

VI.6. Training in the use of Multivariate Calibration Software and Calibration Transference Procedures. UFPE, Recife – PE. Offered to BRASKEM staff involved in the INCTAA.

VII. Perspectives

The INCTAA is presently finalizing the organization of network actions necessary to attend the *demands* for analytical solutions selected during its first workshop. The acquisition of consumables and several other equipments necessary to facilitate the necessary actions is in an advanced stage.

The financial management of the institute, a complex task considering the number of institutions, researchers and their geographical distribution, and the mechanism to apply and obtain financial support are being assimilated by the financial director, the managing committee, the coordinator, and by the institute's members, accelerating the practical procedures related to the operation of the INCTAA.

The interaction among the members of the institute should be intensified in the next months as the actions required for the several workpackages begin to be executed. The web page of the institute will be up-graded to become a more effective way to promote interaction among the groups. A Bulletin of the INCTAA will be launched to improve the communication both inside and outside the institute.

With its operational mechanism well tuned, allowing for faster and prompter actions, several interesting results regarding the development of analytical science and technology are expected to come from the multidisciplinary work in development. The next annual report should show results directly obtained under the scope of the INCTAA. They should demonstrate that the premises of the original proposal of the institute were correct and that the benefits of actions driven by demand will be confirmed. In summary, we are confident that the *modus operandi* of the INCTAA, involving a new way of thinking about how to develop analytical science and technology in Brazil, will be demonstrated.

After the first year, a significant number of new members, ranging from undergraduate students, to academic researchers and to people from industry, have been included in the institute. This is evidence of the effective divulgation of the institute and of the common goals that it represents: a new proposal capable of reaching new standards.

As the institute has a fixed budget, new actions aimed to raise funds for support of the new members and new workpackages will be implemented. These actions include writing up complementary proposals to FAPESP and CNPq, based on new *demands* that will be identified as the INCTAA expands.

The benchmarks indicated for the next year include the effective beginning of the activities directed toward education at several levels by offering short courses and lectures and by involving the institute in both academic and public events.

In addition, the managing committee and the institute coordinator will promote interaction with other INCTs, as some of them present several points which allow foreseeing a number of opportunities regarding the development of common actions.

Finally, the managing committee and the institute coordinator will continue to emphasize the need for a true network of multidisciplinary collaboration, according to its original proposal, and for a balanced development of the four research lines presently incorporated in the INCTAA.

VIII. List of the Academic and Technical Production of the Year

VIII.1. Papers published in international journals as result of activities developed by the INCTAA:

VIII.1.1. Sodré F. F.; Locatelli M. A. F.; Jardim W. F. (2010) Emerging contaminants in the drinking water supplied to the city of Campinas, Brazil: from sewage to tap; *Water Air Soil Pollut.*; 206; 57-67.

VIII.1.2. Sodré, Fernando F. ; Pescara, Igor C. ; Montagner, Cassiana C. ; Jardim, Wilson F. (2010). Assessing selected estrogens and xenoestrogens in Brazilian surface waters by liquid chromatography-tandem mass spectrometry. *Microchemical Journal*, *in press*.

VIII.1.3. Silva, M. J. ; Coetez, J. ; Pasquini, C. ; Honorato, R. S. ; Paim, A. P. S. ; Pimentel, M. F. Gunshot residues - screening analysis by laser-induced breakdown spectroscopy. *Journal of the Brazilian Chemical Society*, v. 20, p. 1887-1894, 2009.

VIII.1.4. Barbieri, F.B., and Pasquini, C. A Low Cost Short Wave Near Infrared Spectrophotometer: Application for Determination of Quality Parameters of Diesel Fuel”, submetido para publicação na *Analytica Chimica Acta*, *Accept for publication* (2010).

VIII.1.5. M. F. Mesko, J. S. F. Pereira, D. P. Moraes, J. S. Barin, P. A. Mello, J. N. G. Paniz, J. A. Nóbrega, M. G. A. Korn e É. M. M. Flores, Focused Microwave-Induced Combustion: A New Technique for Sample Digestion. *Anal. Chem.*, 82:2155-2160, 2010.

VIII.1.6. J. A. Nóbrega, C. Bizzi, R. Picoloto, J. S. Barin, É. M. M. Flores, Microwave-assisted digestion in closed vessels: effect of pressurization with oxygen on digestion process with diluted nitric acid. *Anal. Meth.*, *in press*.

VIII.2. Papers published in national journals as result of activities developed by the INCTAA:

VIII.2.1. Sodré F. F.; Locatelli M. A. F.; Jardim W. F. (2010) Sistema limpo em linha para extração em fase sólida de contaminantes emergentes em águas naturais; *Quim. Nova*; 33; 216-219.

VIII.3. Papers published in international journals as result of activities developed before the INCTAA has been launched:

VIII.3.1. Souza, G.B.; Nogueira, A.R.A.; Del-Santo, V.R. ; Picchi, C.M.C.; Guimarães, E.S.; Barioni, W. Proficiency testing of animal nutrition laboratories. *Accreditation and Quality Assurance*, v. 14, p. 455-460, 2009.

VIII.3.2. Rodrigues, G. D. ; De Lemos, L. R. ; da Silva, L. H. M. ; da Silva, M.C.H. ; Minim, L. A. ; Coimbra, J. S. R. . A green and sensitive method to determine phenols in water and wastewater samples using an aqueous two phase system. *Talanta (Oxford)*, v. 80, p. 1139-1144, 2010.

- VIII.3.3. Rodrigues, G. D. ; De Lemos, L. R. ; da Silva, L. H. M. ; da Silva, M.C.H. ; Minim, L. A. ; Coimbra, J. S. R. . A green and sensitive method to determine phenols in water and wastewater samples using an aqueous two phase system. *Talanta* (Oxford), v. 80, p. 1139-1144, 2010.
- VIII.3.4. Rodrigues, G. D. ; Teixeira, L. S. ; Ferreira, G. M. D. ; da Silva, M.D.H. ; da Silva, L. H. M. ; de Carvalho, R. M. M. . Phase Diagrams of Aqueous Two-phase Systems with Organic Salts and F68 Triblock Copolymer at Different Temperatures. *Journal of Chemical and Engineering Data*, v. 55, p. 1158-1165, 2010.
- VIII.3.5. De Lemos, L. R. ; Santos, I. J. B. ; Rodrigues, G. D. ; Ferreira, G. M. D. ; da Silva, L. H. M. ; da Silva, M.D.H. ; de Carvalho, R. M. M. . Phase Compositions of Aqueous Two phase Systems Formed by L35 and Salts at Different Temperatures. *Journal of Chemical and Engineering Data*, v. 55, p. 1193-1199, 2010.
- VIII.3.6. da Silva, L. H. M. ; da Silva, M.C.H. ; de Sousa, R. C. S. ; Martins, J. P. ; Rodrigues, G. D. ; Coimbra, J. S. R. ; Minim, L. A. . Surface Excess Enthalpy of PEO + Salt + Water and L35 + Salt + Water Aqueous Two-Phase Systems. *Journal of Chemical and Engineering Data*, v. 54, p. 531-535, 2009.
- VIII.3.7. Rodrigues, G. D. ; da Silva, M.D.H. ; da Silva, L. H. M. ; Teixeira, L. S. ; de Andrade, V. M. . Liquid-Liquid Phase Equilibrium of Triblock Copolymer L64, Poly(ethylene oxide-b-propylene oxide-b-ethylene oxide), with Sulfate Salts from (278.15 to 298.15) K. *Journal of Chemical and Engineering Data*, v. 54, p. 1894-1898, 2009.
- VIII.3.8. Lacerda, V. G. ; Mageste, A. B. ; Santos, I. J. B. ; da Silva, L. H. M. ; da Silva, M.C.H. . Separation of Cd and Ni from Ni-Cd batteries by an environmentally safe methodology employing aqueous two-phase systems. *Journal of Power Sources* (Print), v. 193, p. 908-913, 2009.
- VIII.3.9. Mageste, A. B. ; De Lemos, L. R. ; Ferreira, G. M. D. ; da Silva, M.C.H. ; da Silva, L. H. M. ; Bonomo, R. C. F. ; Minim, L. A. . Aqueous two-phase systems: an efficient, environmentally safe and economically viable method for purification of natural dye carmine. *Journal of Chromatography* (Print), v. 1216, p. 7623-7629, 2009.
- VIII.3.10. Martins, J. P. ; da Silva, M.D.H. ; da Silva, L. H. M. ; Senra, T. D. A. ; Ferreira, G. M. D. ; Coimbra, J. S. R. ; Minim, L. A. . Liquid Liquid Phase Equilibrium of Triblock Copolymer F68, Poly(ethylene oxide) b poly(propylene oxide) b poly(ethylene oxide), with Sulfate Salts. *Journal of Chemical and Engineering Data*, v. 55, p. 1618-1622, 2009.
- VIII.3.11. Sivanildo S. Borges, Jailson de Souza Peixoto, Mário A. Feres, Boaventura F. Reis, Downscaling a multicommutated flow injection analysis system for the photometric determination of iodate in table salt, *Anal. Chim. Acta*, *in press*, Corrected Proof available online 15 March 2010.
- VIII.3.12. dos Santos, Edmilson Oliveira ; Silva, Andréa Monteiro Santana ; Fragoso, Wallace Duarte ; Pasquini, C. ; Pimentel, Maria Fernanda . Determination of degree of polymerization of insulating paper using near infrared spectroscopy and multivariate calibration. *Vibrational Spectroscopy*, v. 52, p. 154-157, 2010.
- VIII.3.13. Pontes M. J. C. ; Cortez, J. ; Galvão, R. K. H. ; Pasquini, C. ; Araújo, Mário César Ugulino de ; Coelho R. M. ; Chiba M. K. ; Abreu M. F. . Classification of Brazilian Soils by Using LIBS and Variable Selection in the Wavelet Domain. *Analytica Chimica Acta*, v. 642, p. 12-18, 2009.
- VIII.3.14. Fonseca A.; Raimundo Jr. I.M.; Rohwedder J.J.R. A microfluidic device with integrated fluorimetric detection for flow injection analysis; *Anal. Bioanal. Chem.*; 396; 715-723, 2010.
- VIII.3.15. Mirian C. Santos, Martin Wagner, Bei Wu, Jessica Schneider, Miroslav Zoriy, Solange Cadore, Jörg Oehlmann, J. Sabine Becker. "Biomonitoring of Metal Contamination in a Marine Prosobranch Snail (*Nassarius reticulatus*) by Imaging Laser Ablation Inductively Coupled Plasma Mass Spectrometry (LA-ICP-MS)". *Talanta* , 80 (2009) 428-433.

VIII.1.16. Rita M. W. Nano, Roy E. Bruns, Sérgio L .C. Ferreira, Nivaldo Baccan, Solange Cadore, "Statistical mixture design development of digestion methods for Oyster tissue using inductively coupled plasma optical emission spectrometry for the determination of metallic ions". *Talanta*, 80 (2009) 559-564.

VIII.1.17. Rafael Arromba de Sousa, Mirian C. Santos, Nivaldo Baccan, Solange Cadore, "Determination of Selenium in Liquid Dietetic Sweeteners by GF AAS", *Food Analytical Methods*, 3(1) (2010) 31-35.

VIII.1.18. Mirian C. Santos, Joaquim A. Nóbrega, Nivaldo Baccan and Solange Cadore, "Determination of Toxics Elements in Plastics from Waste Electrical and Electronic Equipment by Slurry Sampling Graphite Furnace Atomic Absorption Spectrometry", *Talanta*, *in press*.

VIII.4. Papers published in national journals as result of activities developed before the INCTAA has been launched:

VIII.4.1. Dos Santos, S. R. G., Coelho, C. J. Coelho, Estudo da Relação Linear Entre Conjuntos de Dados Químicos Empregando Análise de Correlação Canônica, Revista Eletrônica de Iniciação Científica da Sociedade Brasileira de Computação, Ano X, Volume IV, Dezembro, 2009, ISSN - 1519-8219.

VIII.5. International Congress

VIII.5.1. 14th International Symposium on Toxicity Assessment; Metz; França. (2009). Title: Using bioluminescent yeast strains to verify the levels of endocrine disruptors in Brazilian waters: preliminary results. Authors: Umbuzeiro G.; Dayrell D.; Bergamasco A. M.; Sodré F. F.; Locatelli M. A. F., Quinaglia G.; Leskinen P.; Jardim W. F.

VIII.5.2. Pittcon 2010; Orlando; EUA (2010). Title : Hormones and bisphenol A in drinking waters from the State of São Paulo, Brazil. Authors: Montagner, C. C. ; Sodre, F. F. ; Pescara, I. C. ; Jardim, W. F.

VIII.5.3. Pittcon 2010; Orlando; EUA (2010). Title : Antibiotics in Brazilian surface waters. Authors: Locatelli M. A. F.; Sodré F. F.; Jardim W. F.

VIII.5.4. Flow Analysis XI, Setembro de 2009, Palma de Maiorca – Espanha. Title: Downscaling a Multicommutated Flow Injection Analysis Setup for the Photometric Determination of Iodate in Table Salt. Authors: Sivanildo S. Borges, Jailson de Souza Peixoto, Mário A. Feres, Boaventura F. Reis.

VIII.5.5. V Metrochem - International Congress on Traceability in Laboratory Measurements and Production Chains, 2009, São Paulo. Título do trabalho: Ensaio de proficiência como suporte para a produção de materiais de referência. Authors: Souza, G. B. ; Nogueira, A. R. A. ; BOSSU, C.M.; TONIOLOSILVA, P.H.; Fernandes, E.A.N. ; Barbosa Junior, F.

VIII.5.6. 12th Biological and Environmental Reference Material Symposium (BERM), 2009, Oxford, UK. Title: Development of reference materials to support the Brazilian agriculture. Authors: Fernandes, E.A.N. ; Sarriés, G.A. ; Bacchi, M.A. ; Tagliaferro, F.S. ; Barbosa Junior, F.; Nogueira, A.R.A.

VIII.5.7. 2009 International Nuclear Atlantic Conference - INAC, 2009, Rio de Janeiro. Title: Performance of IPEN-CNEN/SP Neutron Activation Analysis Laboratory for Microelement Determinations in Proficiency Testing. Authors: Armelin, M.J.A. ; Souza, G. B. ; Nogueira, A. R. A. ; Saiki, M.

VIII.5.8. X European Conference on Optical Chemical Sensors and Biosensors, República Tcheca (2010). Title: Evaluation of fluorescent reagents for simultaneous determination of heavy metals in water. Authors: Pinheiro S.C.L.; Descalzo A.B.; Raimundo Jr. I.M.; Moreno-Bondi M.C. and Orellana G.

VIII.5.9. European Winter Conference on Plasma Spectrochemistry 42. Title: Contamination in Snails by Imaging Laser Ablation Inductively Coupled Plasma Mass Spectrometry (LA-ICP-MS). Authors: Mirian C. Santos, Solange Cadore, Wu Bei, Martin Wagner, Miroslav Zoriy, J. Sabine Becker.

VIII.5.10. 3rd International IUPAC Symposium on Trace Elements in Food, Title: Determination of Mineral Nutrients in Cereal Flakes. Authors: Solange Cadore and Nilva A. R. Pedro.

VIII.5.11. Colloquium Spectroscopium Internationale XXXVI. Title: Evaluation of collision-reaction interface ICP-MS for carbon effect correction on chromium determination. Authors: R. S. Amais, C. D. Pereira, S. R. Bianchi, F. V. Silva, E. Garcia, M. C. Santos, S. Cadore, A. R. A. Nogueira, J. A. Nóbrega.

VIII.5.12. Colloquium Spectroscopium Internationale XXXVI. Title: Background spectra of acid and extractor solutions in ICP-MS with a collision-reaction Interface (CRI). Authors: C. D. Pereira, S. R. Bianchi, M. C. Santos, A. R. A. Nogueira, S. Cadore, J. A. Nóbrega.

VIII.5.13. Euroanalysis 15. Title: Evaluation of an analytical method for determination of inorganic species in enteral nutrition using ICP OES. Authors: G. T. Macarovsky, S. Cadore.,

VIII.5.14. Euroanalysis 15. Title: Determination of Inorganic Species in Bivalve Molluscs. Authors: R. M. W. Nano, R. A. Sousa, S. L. C. Ferreira, N. Baccan, S. Cadore.

VIII.5.15. Euroanalysis 15. Title: Determination of Zinc by Flame Atomic Absorption Spectrometry After On Line Preconcentration with Zincon. Authors: R. R. A. Peixoto, G. T. Macarovsky, S. Cadore.

VIII.5.16. X European Conference on Optical Chemical Sensors and Biosensors, República Tcheca (2010). Title: A portable NIR photometer for determination of aromatic hydrocarbons in water. Authors: Lima K.M.G.; Raimundo Jr. I.M.; Rohwedder J.J.R.; Pimentel M.F.

VIII.5.17. X European Conference on Optical Chemical Sensors and Biosensors, República Tcheca (2010). Title: A microfluidic device for fluorimetric determination of total calcium and magnesium in mineral Waters. Authors: Fonseca A.; Raimundo Jr. I.M.; Rohwedder J.J.R.

VIII.5.18. 14th International Conference on Near Infrared Spectroscopy – NIR 2009, Bancoc, Tailândia, 2009. Title: Classification of Brazilian Mate Tea using Linear Discriminant Analysis and Successive Projection Algorithm for Variable Selection. Authors: S.S. Simões, T.C.B. Saldanha, F.A. Hansel, C. Pasquini and K.M. dos Santos.

VIII.5.19. 14th International Conference on Near Infrared Spectroscopy – NIR 2009, Bancoc, Tailândia, 2009. Title: A New Method for Determination of the Oxidative Stability of Biodiesel using NIR Emission Spectroscopy. Authors: C. Pasquini and F. Gonzaga.

VIII.5.20. 14th International Conference on Near Infrared Spectroscopy – NIR 2009, Bancoc, Tailândia, 2009. Development of a Process NIR Analyzer for Petroleum Products. Authors: C. Pasquini, A. Bueno, J.J.R. Rohwedder and E.A. Giachero.

VIII.5.21. Pittcon 2010. Orlando, 2010. Title: Determination of Properties of Cellulose Properties by Near-Infrared Spectroscopy of Eucalyptus Wood. Authors: Celio Pasquini, Claudio J. Carneiro, Jônatas P. Araújo.

VIII.6. National Congress

VIII.6.1. V Encontro sobre Aplicações Ambientais de Processos Oxidativos Avançados (V EPOA), São Paulo, Brasil. (2009). Title: Degradação fotocatalítica de fluoroquinolonas utilizando um reator solar tipo CPC. Authors: Paschoalino, M. P.; Paschoalino, F. C. S.; Orellana, G.; Moreno-Bondi, M. C.; Jardim, W.F.

VIII.6.2. XV ENQA; Salvador; Brasil. (2009). Title: Construção de sistema limpo para extração em fase sólida de contaminantes emergentes em amostras de volume elevado. Authors: Sodré F. F.; Locatelli M. A. F.; Jardim W. F.

VIII.6.3. 15º Encontro Nacional de Química Analítica/3º Congresso Iberoamericano de Química Analítica, Salvador, Bahia. (2009). Title: Determinação de estrogênios e bisfenol A em água superficiais por LC-MS-MS com ionização por eletrospray. Authors: Sodre, F. F. ; Montagner, C. C. ; Pescara, I. C. ; Jardim, W. F.

VIII.6.4. 3º Congresso Brasileiro de Espectrometria de Massas, Campinas, São Paulo. (2009) Title: Assessing emerging contaminants in Brazilian surface waters using ESI-LC-MS/MS in triple quadrupole. Authors: Montagner, C. C. ; Sodre, F. F. ; Pescara, I. C. ; Jardim, W. F.

VIII.6.5. V Encontro Nacional de Química Ambiental, São Pedro, São Paulo. (2010). Title: A remoção de interferentes endócrinos em uma estação de tratamento de água ETA. Authors: Pescara, I. C. ; Sodre, F. F. ; Bisinoti, M. C. ; Jardim, W. F.

VIII.6.6. 15º Encontro Nacional de Química Analítica/3º Congresso Iberoamericano de Química Analítica. Title: Uso de Análise Discriminante Linear para Distinção da Qualidade da Água de 3 Rios da Bacia do Rio Gramame/PB. Authors: Teresa C. B. Saldanha(PQ), Ilda A. S. Toscano, Danilo M. Henrique, Andréa F. Fidele, Maria M. L. M. Lúcio, Aline E. S. Anjos, Sara R. R. C. Barros, José F. Souza Filho.

VIII.6.7. 15º Encontro Nacional de Química Analítica/3º Congresso Iberoamericano de Química Analítica. Title: PCA E LDA como Ferramentas para o Estudo do Impacto da Carcinicultura sobre a Qualidade da Água do Rio da Ribeira, Santa Rita/PB. Authors: Teresa C. B. Saldanha, Aline E. S. Anjos, Ilda A. S. Toscano, Maria Mônica L. M. Lúcio, Sara R. R. C. Barros, Danielly S. Saraiva, Valmir G. Souza, Martinelly R. Teixeira, Danielle S. Nascimento.

VIII.6.8. 15º Encontro Nacional de Química Analítica/3º Congresso Iberoamericano de Química Analítica. Title: Sistema em Fluxo Multicomutado Equipado com Minibombas em Regime de Zonas Coalescentes. Authors: Sivanildo S. Borges, Boaventura F. Reis

VIII.6.9. 15º Encontro Nacional de Química Analítica/3º Congresso Iberoamericano de Química Analítica. Title: Emprego de Célula Eletrolítica para Redução de Iodato a Iodo para Determinação de Iodato em Sal de Cozinha. Authors: Jailson de Souza Peixoto, Sivanildo da Silva Borges.

VIII.6.10. 32ª Reunião Anual da Sociedade Brasileira de Química, Maio de 2009, Fortaleza – CE. Marcelo A. Teixeira, Sivanildo da S. Borges, Mário A. Feres Jr., Boaventura F. Reis, Title: Dispositivo Microcontrolado para Propulsão de Fluidos por Efeito Venturi em Sistema de Análise em Fluxo baseado em multicomutação, 32ª Reunião Anual da Sociedade Brasileira de Química, Maio de 2009, Fortaleza – CE.

VIII.6.11. 15º Encontro de Química Analítica, de 18 a 21/10/2011, Salvador, BA. Title: Análise de Enxofre em Biodiesel por ICP OES. Authors: Raquel Rainone, Pedro Vitoriano Oliveira, Danilo Luiz Flumignan, José Eduardo de Oliveira.

VIII.6.12. 1º Congresso Analítica Latin América, de 08 a 10/09/2009, São Paulo, SP. Title: Análise de Na, K, Ca, Mg e P em biodiesel por ICP OES. Authors: Raquel Rainone, Pedro Vitoriano Oliveira, Danilo Luiz Flumignan, José Eduardo de Oliveira, Mariana Ortega Garcia, Daniela Corrêa Fiaschi, Matthew Cassap.

VIII.6.13. 15º Encontro de Química Analítica, de 18 a 21/10/2011, Salvador, BA. Title: Análise Exploratória da Composição de Tijolos Antigos por Espectroscopia de Emissão em Plasma Induzido por Laser (LIBS). Authors: Borba, F. S. L. ; Cortez, J. ; Asfora, V. K. ; Pasquini, C. ; Pimentel, M. F. ; Brito, S. ; Khoury, Helen.

VIII.6.14. 32ª. Reunião Anual da Sociedade Brasileira de Química, 2009, Fortaleza. Title: Extração do corante natural carmim de cochonilha utilizando um método de baixo custo, ambientalmente seguro e reciclável. Authors: Mageste, A. B. ; Ferreira, G. M. D. ; da Silva, L. H. M. ; da Silva, M.C.H.

VIII.6.15. 32^a. Reunião Anual da Sociedade Brasileira de Química, 2009, Fortaleza. Title: Influência na região bifásica de sistemas ternários em equilíbrio termodinâmico. Authors: Patrício, P. R. ; Mageste, A. B. ; Martins, J. P. ; da Silva, M.C.H. ; da Silva, L. H. M.

VIII.6.16. 32^a. Reunião Anual da Sociedade Brasileira de Química, 2009, Fortaleza. Title: Determinação espectrofotométrica de compostos fenólicos e estudo da partição do ânion $[\text{Fe}_2(\text{CN})_{10}]^{10-}$ em SAB. Authors: De Lemos, L. R. ; Rodrigues, G. D. ; Patrício, P. R. ; Santolin, E. S. ; da Silva, L. H. M. ; da Silva, M.C.H.

VIII.6.17. 23^o Encontro Regional da SBQ-MG, 2009, Juiz de Fora. Title: Sistema aquoso bifásico: uma alternativa eficiente para a purificação do corante natural carmin. Authors: Leite, L. O. R. ; Mageste, A. B. ; Ferreira, G. M. D. ; da Silva, M.C.H. ; da Silva, L. H. M.

VIII.6.18. 15^o Encontro Nacional de Química Analítica e 3o Congresso Iberoamericano de Química Analítica, 2009, Salvador. Title: Extração seletiva de cobre em presença de concomitantes metálicos sem uso de solventes orgânicos. Authors: De Lemos, L. R. ; Santos, I. J. B. ; da Silva, L. H. M. ; da Silva, M.C.H.

VIII.6.19. 15o Encontro Nacional de Química Analítica e 3o Congresso Iberoamericano de Química Analítica, 2009, Salvador. Title: Uma metodologia verde para determinação de aminofenol em água utilizando sistemas aquosos bifásicos. Authors: Patrício, P. R. ; De Lemos, L. R. ; Rodrigues, G. D. ; da Silva, L. H. M. ; da Silva, M.C.H.

VIII.6.20. 15^o Encontro Nacional de Química Analítica e 3o Congresso Iberoamericano de Química Analítica, 2009, Salvador. Title: Extração do íon Mn(II) com 1-piridilazo-2-naftol utilizando os SAB L64/H₂O/Na₂C₄H₄O₆ ou L64/H₂O/Li₂SO₄. Authors: Santos, I. J. B. ; Mesquita, M. C. ; De Lemos, L. R. ; da Silva, L. H. M. ; da Silva, M.C.H.

VIII.6.21. Sober 47^o Congresso, 2009, Porto Alegre. Desenvolvimento Rural e Sistemas Agroalimentares: os agronegócios no contexto de integração das nações. Brasília : Sober, 2009. Title: Avaliação dos impactos econômico, social e ambiental de um programa de um ensaio de proficiência para laboratórios. Authors: Simoes, M.A.R.E. ; Vinholis, M.M.B.; Souza, G.B.; Nogueira, A.R.A.; DelSanto, V.R.

VIII.6.22. 32^a Reunião Anual da SBQ. Title: Espécies Metálicas em Cupuaçu (*Theobroma grandiflorum* Schum), Dão (*Ziziphus mauritiana* Lam) e Ingá (*Inga edulis* Mart). Authors: Vânia de Lourdes das G. Teles, Solange Cadore, Tereza Maria F. de F. Mendes.

VIII.6.23. 32^a Reunião Anual da SBQ. Title: Espécies Inorgânicas em Folhas e Polpa de “Dão” (*Ziziphus mauritiana* Lam) de Boa Vista/RR. Authors: Vânia de Lourdes das G. Teles, Victor D. Neiva, Rosana M. Doimo, Solange Cadore, Tereza Maria F. F. Mendes.

VIII.6.24. 32^a Reunião Anual da SBQ, Title: Quantificação de Lítio em Polpas de Frutas. Authors: Vânia de Lourdes das G. Teles, Mirla Janaina A. Cidade, Nivaldo Baccan, Solange Cadore, Tereza Maria F. F. Mendes.

VIII.6.25. 32^a Reunião Anual da SBQ, Title: Determinação de Espécies Metálicas em Ingá (*Inga edulis* Mart), Cupuaçu (*Theobroma grandiflorum* Schum) e Dão (*Ziziphus mauritiana* Lam) de origem amazônica por ICP OES. Authors: Greice T. Macarovscha, Vânia de Lourdes das G. Teles, Rafaella A. Peixoto, Tereza Maria F. de F. Mendes e Solange Cadore.

VIII.6.26. Analítica 2009, Title: Determinação de um método de digestão para determinação de contaminantes inorgânicos em acetato de polivinila (PVAc). Authors: Erika Matoso, Solange Cadore,

VIII.6.27. 15^o ENQA e 3^o CIAQA. Title: Mineralização de polpas de frutas e folhas para a determinação por FAAS de Cu, Mn, Ni e Zn. Authors: Vânia de Lourdes das Graças Teles, Teresa Maria Fernandes de Freitas Mendes, Mirla Janaina Augusta Cidade, Solange Cadore, Nivaldo Baccan.

VIII.6.28. 15^o ENQA e 3^o CIAQA. Title: Determinação de espécies inorgânicas em polpa de dão (*Ziziphus mauritiana* Lam) após tratamento da amostra por fotólise oxidativa UV. Authors: Vânia de

Lourdes das Graças Teles, Solange Cadore, Teresa Maria Fernandes de Freitas Mendes, Nivaldo Bacchan, Mirla Janaina Augusta Cidade, Henrique Eduardo Bezerra da Silva.

VIII.6.29. 15º ENQA e 3º CIAQA. Title: Especificação de Metais Baseada em Difusão em Filmes Finos por Gradiente de Concentração (DGT) Empregando Argilominerais. Authors: Vanessa Egéa Anjos, Marco Tadeu Grassi, Gilberto Abate, Solange Cadore, Greice Macarovscha, Lígia Marília Piai Almeida, Jarbas José Rodrigues Rohwedder.

VIII.6.30. 15º ENQAe 3º CIAQA. Title: Avaliação do Uso de ICP-MS na Determinação de Elementos Essenciais e Contaminantes em Amostras de Nutrição Enteral Industrializadas. Authors: Greice T. Macarovscha, Catarinie D. Pereira, Mirian C. Santos, Joaquim A. Nobrega e Solange Cadore.

VIII.7. Patents

VIII.7.1. Borges, S. S. ; Oliveira, F. S. ; Silva, M. B., Dispositivo de Permeação/Reação e Detecção para Acoplamento Em Sistemas De Análise Por Injeção em Fluxo para a Determinação de Analitos Voláteis Empregando Reagente Cromogênico – Depósito número PI0804881-9.

VIII.8. Software

VIII.1. Souza, G.B.; Guimarães, E.S. ; Silva, R.F.; Nogueira, A. R. A. ; Picchi, C.M.C.; Barioni Junior, W. SEPROLAB 012070000188; 11:45 h; DEDF-INPI. 2007. (This program will be employed for the proficiency assays and has become available to INCTAA in 2009)

VIII.9. International Conferences

VIII.9.1. Title: Near Infrared Spectroscopy in the Quality Control of Fossil Fuels and Biofuels. Conferencista: Celio Pasquini. SYMPOSIUM: Focus on Brazilian Analytical Chemistry: Fuel and Food. Pittcon 2009, Chicago, USA.

VIII.9.2. Title: Chemical Elements in Food: An Overview of Brazilian Contributions. Conferencista: Joaquim A. Nóbrega. SYMPOSIUM: Focus on Brazilian Analytical Chemistry: Fuel and Food. Pittcon 2009, Chicago, USA.

VIII.9.3. Title: Determination of Metals in Fuel Ethanol Using Pre-concentration by Concentration by Evaporation on Paper and Laser Induced Breakdown Spectroscopy. Conferencista: Celio Pasquini. North American Symposium on LIBS 2009 – LIBS 2009, New Orleans, USA.

Campinas, 29th March 2010.



Prof. Celio Pasquini