

# Annals of West University of Timisoara

## Series of Chemistry

AN INTERNATIONAL JOURNAL

Published by:

West University of Timisoara

Faculty of Chemistry – Biology - Geography

and

Romanian Academy

Institute of Chemistry Timisoara



---

### CONTENTS & SHORT SUMMARY

---

Quantitative Analysis of Gallic Acid from *Apium Graveolens*, *Equisetum Arvense* L. and *Petroselinum Crispum* Using High Performance Liquid Chromatography      Condrat D., Crişan F., Harja F.      1-5

Nr.	Vegetal extract	Retention time $t_r$ , [min]	Content in gallic acid [mg/mL]
1	<i>Apium graveolens</i> – celery	4.543	0.0052
2	<i>Equisetum arvense</i> L. – horsetail	4.490	0.0037
3	<i>Petroselinum crispum</i> – parsley	4.522	0.0179

*This paperwork is aiming to bring forth information regarding the chemical composition of Apium graveolens, Equisetum arvense L. and Petroselinum Crispum and their content in gallic acid.*

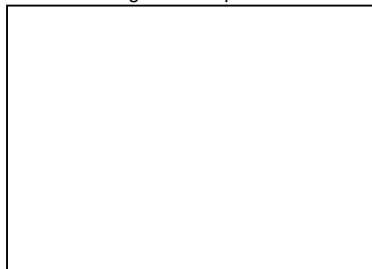
Research on the Systems Used to Evaluate the Personnel Operating in Toxic / Explosive / Flammable Atmospheres      Ilie C., Găman A. G., Pupăzan D.      7-12

*The evaluation systems represent an essential component part of artificial intelligence that cover the expert knowledge for a specific domain; subsequently, this knowledge shall be dynamically capitalized by a reasoning mechanism. Thus, an artificial reasoning is implemented whose idea is to simulate natural reasoning triggered by the human brain.*

Preliminary MLR Study of Phosphoramidate Derivatives Based on Dragon Descriptor

Petric M., Crişan L., Micle A., Crişan M., Maranescu B., Ilia G.

13-18

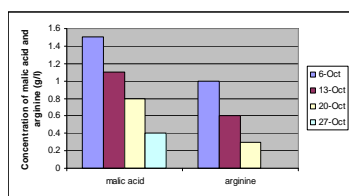


*Phosphoramidates are important biologically active compounds, often used as intermediates in organic synthesis. Our goal is to identify theoretical descriptors that can be correlated with the capacity factor ( $k$ ). For this reason a large amount of 2D descriptors using the DRAGON software were calculated. The statistical qualities of MLR have been evaluated by several parameters such as: the squares of correlation coefficient ( $R^2$ ), standard error of estimate (see), Fischer test ( $F$ ).*

Estimation of Arginine Degradation During Malolactic Fermentation of Wine

Popescu-Mitroi I., Stoica F.

19-26

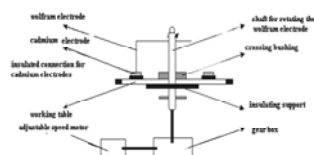


*This paper follows the arginine metabolism dynamic during the malolactic fermentation in a comparative study with the degradation of the malic acid, as well as the forming risks of some compounds with a high toxicological potential, as a result of the degradations in wine.*

Minimum Ignition Energy for a Fuel-Air Mixture by Electrical Spark Initiation

Prodan M., Szöllösi-Moţă A., Nălboc I., Jurca A, Lupu L.

27-34

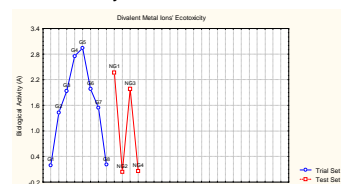


*The most important aspects of explosion initiations by electrical sparks are reviewed in connection with the minimum ignition energy characteristic parameter of the ignition source. Original data are presented and discussed for a fuel-air mixture initiated by electrical spark. Experiments in this work are preliminary tests in order to improve the experimental equipments to achieve the best possible correlation with the literature data and further research on the determination and assessment of explosion initiation characteristic parameters in fuel-air mixture.*

QSAR Study on Divalent Metal Ions' Ecotoxicity

Saitos Z., Lazea M., Chiriac A.

35-40



The present analysis enlighten on the fact the parabolic dependence on activity respecting the acidity and electronegativity seems to be the most preferred (selected) model for higher prediction based on a collection of QSAR trial equation. Our results (models of metal ions' (eco) toxicity using ion characteristics) agree with the target theory respecting the increase and decrease of the electrical and electronic effects of a toxicant as reflected into its organism activity.

Aspects Concerning the Estimation of Uncertainty of Measurement Issues for Determination of Sulphate in Waste Waters Through Spectrophotometric Method

Toth L., Ghetie G., Kovacs M., Morar M.

41-46

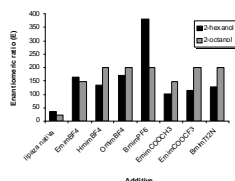


This paper aims to present a model of estimation of the uncertainty for the determination of sulphate in wastewater made in a test laboratory accredited by RENAR. One of the fundamental requirements placed before testing laboratories ISO 17025 standard is the estimation and reporting of budget uncertainty and traceability to international standards. Measurement uncertainty is a parameter associated with the outcome of a measurement, which characterizes the scattering of which could reasonably be attributed to the measure. It is important to take into account not only one measurement, but the overall result of the measurement. Test results must represent the best approximation to the true value.

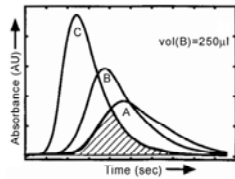
Solid-Phase Immobilized Biocatalysts for Optical Resolution of Secondary Alcohols

Ursoiu A, Paul C., Marcu C., Kurtán T., Zamfir A., Péter F.

47-52



We carried out sol-gel entrapment of *Candida antarctica* B lipase in matrices derived from ternary silane precursor systems and then adsorbed on Celite. Several ionic liquids have been employed as structure-directing additives and stabilizers against lipase inactivation during the sol-gel immobilization process. The obtained biocatalysts were investigated in the kinetic resolution of model secondary alcohols. The addition of an ionic liquid during the immobilization process resulted in preparations with higher activities and better enantioselectivity, compared to the native lipase.



*Such studies are necessary in order to highlight and take corresponding measures regarding the protection of land and buildings from the surface thus reducing the subsidence damages caused by the movement of land surface and rock coverings over the environment and population in mining areas.*