

# Call for participation to IS-NMR-ILC 001\_2016 – October 27<sup>th</sup>, 2016

## **1. AIMS OF THIS INTERLABORATORY COMPARISON**

The main aim of this comparison is the validation of a combined NMR method for fingerprinting of wine grapes and quantification of some metabolites contained in the wine grapes juice. Moreover, the comparison will be the occasion to test new performance assessment criteria (see Analytical Chemistry, **2015**, *89*, 6709-6717).

Results will be published on "NMR Interlaboratory Comparisons" series, NeP Edizioni, Rome.

# 2. ANALYTICAL MATERIAL AND TECHNICAL REQUIREMENTS OF THE PARTICIPANTS

The analytical material provided to participants consists of 7 NMR tubes.

2 NMR tubes consist of aqueous solutions of wine grapes juice (buffered at pH=4.2 and containing sodium azide as biocide and 3-(trimethylsilyl)-2,2,3,3-tetradeuteropropanoic acid sodium salt in  $D_2O$  as internal reference).

5 NMR tubes consist of aqueous solutions of spiked wine grapes (buffered at pH=4.2 and containing sodium azide as biocide and 3-(trimethylsilyl)-2,2,3,3-tetradeuteropropanoic acid sodium salt in  $D_2O$  as internal reference). The solutions are spiked with five different levels of some sugars, organic acids and aminoacids. The solutions will be used to develop the calibration line for quantification of the metabolites by standard addition approach.

Any kind of high resolution NMR spectrometer can be used for this ILC without limitations in terms of magnetic field, manufacturer, age of the instrument, etc.

### **3. NMR EXPERIMENT**

1D <sup>1</sup>H NOESY experiment using presaturation of residual water signal will be run for all the 7 NMR tube.

Acquisition and processing parameters will be detailed in "Guidelines and contract terms" available in the NMR Spectrometer Profile (see IS-NMR-ILC Scheme vers2).

Processing of the NMR spectra, from Fourier transformation of the FID to signal integration, will be carried out by the participants. Calibration line development and quantification of the metabolites, along with the whole statistical elaboration, will be carried out by Innovative Solutions.

### 4. COSTS

Participation is free of charge for all participants (sample delivery is included for EU participants. Sample delivery costs for participants outside EU will be quoted after participation request. If possible, depending on the specific national regulations, Innovative Solutions S.r.l. will fund delivery costs).

Electronic version of the report is free of charge for all participants submitting the results. Hard-copy of the report is quoted at  $\notin$  15,00 (shipping costs will be quoted in case of order).

Innovative Solutions S.r.l. funds this ILC in the framework of the project "Recupero del Germoplasma Viticolo Pugliese" (Re.Ge.Vi.P.), "Progetti Integrati per la Biodiversità" - P.S.R.

www.innovative-solutions.it



FEASR 2014-2020, Misura 10.2.1 "Progetti per la conservazione e valorizzazione delle risorse genetiche in agricoltura" - Trascinamento della Mis. 214 Az. 4 sub az. a) del PSR 2007-2013.

#### **5. REGISTRATION**

The participants must email Annex 1 to *ilc@innovative-solutions.it*:

Annexes 1 must be duly filled in, signed by legal representative and sent (as pdf file) by email to <u>ilc@innovative-solutions.it</u> indicating "Participation to IS-NMR-ILC 001\_2016" as subject. More information are reported in IS-NMR-ILC Scheme vers2.

### 6. ILC COORDINATOR

Innovative Solutions S.r.l. Spin Off company of the Technical University of Bari, zona H 150/B, 70015 Noci (BA), Italy Contact person: Dr. Stefania Pontrelli Email: amministrazione@innovative-solutions.it

### 7. ILC CUSTOMER (FUNDER)

Innovative Solutions S.r.l., zona H 150/B, 70015 Noci (BA), Italy Contact person: Prof. Vito Gallo Email: direzione@innovative-solutions.it

#### 8. SCIENTIFIC COMMITTEE

Vito Gallo, Technical University of Bari and Innovative Solutions S.r.l., Italy
Nicola Intini, ARPA Puglia and Innovative Solutions S.r.l., Italy
Piero Mastrorilli, Technical University of Bari and Innovative Solutions S.r.l., Italy
Mario Latronico, Technical University of Bari and Innovative Solutions S.r.l., Italy
Pasquale Scapicchio, SAMER, LACHIMER and LCM (Laboratories of the Chamber of Commerce of Bari, Foggia and Naples, respectively) and RETELAB (Network of the laboratories of the Italian Chambers of Commerce), Italy
Antonino Rizzuti for Innovative Solutions S.r.l., Italy
Stefano Todisco for Innovative Solutions S.r.l., Italy
Rosa Ragone for Innovative Solutions S.r.l., Italy

#### 9. RIGHTS AND OBLIGATIONS OF THE PARTS

Participant must follow instructions contained in the "Guidelines and contract terms" available in the NMR spectrometer profile. If instructions will not be complied, data will not be considered for final elaboration. Participants (only those who have complied with the instructions) will be acknowledged in the final report and in any kind of publication containing their NMR data.

In case of publication of papers on peer reviewed journals, all the participants will be included in the authorship according to the rule "one NMR spectrometer, one author". For instance, if one laboratory participates with one NMR spectrometer, only one author will be considered for that lab, independently from the number of persons actually recording spectra. The name of the author will be indicated by the contact person for that lab. On the other hand, if one laboratory participates with three NMR spectrometers, a maximum of three authors will be considered according to indications of the contact person for that lab.



Innovative Solutions is the owner of the NMR data of the present ILC. NMR data will be processed anonymously (identity of the lab generating a set of NMR data will be unknown to other labs and other parties). Innovative Solutions S.r.l. has the right to share NMR data, either entirely or partly, for possible cooperation provided that identity of the lab remains undisclosed.

ILC will be carried out if the following conditions are fulfilled:

- Minimum number of participants: 10
- Maximum number of participants: 40

If the number of registered participants is lower than 10, the ILC will be cancelled. If the number of the registered participants is higher than 40, the list of laboratories will be sorted by submission date of the registration form and the first 40 labs will participate to the ILC.

In any case, registered participants will be informed on the outcome of the registration step.

9. TIMETABLE	
2016/10/24 - 2017/01/15:	Stability tests by Innovative Solutions S.r.l.
2016/11/07 - 2016/12/11:	Call open and registration of the participants (Consider the
	registration form in Annex 1)
2016/12/12 - 2017/01/31:	Recognition of the spectrometers available for the ILC and
	publication of the "Guidelines and contract terms", sample
	preparation and homogeneity tests by Innovative Solutions S.r.l.
2017/02/01 - 2017/02/28:	Sample delivery to participants
2017/03/01 - 2017/03/31:	NMR experiment registration and data submission by participants
2017/04/01 - 2017/05/31:	Data elaboration and publication of the report.

#### **10. SUBCONTRACTS**

Samples delivery will be subcontracted to qualified supplier.