244th American Chemical Society National Meeting
19th to 23rd August - Philadelphia, USA

FINAL REPORT to
GRAPE AND WINE RESEARCH & DEVELOPMENT CORPORATION

Project Number: GWT1202

Principal Investigator: Kerry Wilkinson

Research Organisation: The University of Adelaide

Date: 30th September 2012
Executive Summary:
Travel funding was sought to enable attendance and participation at the 244th American Chemical Society (ACS) National Meeting, held in Philadelphia, USA from August 19th to 23rd, as well as visits to several Californian Universities and wineries.

Dr Kerry Wilkinson was invited to speak at the 244th ACS National Meeting in a symposium on Fruit and Vegetable Aroma Precursors. Her presentation, titled ‘Evolution of oak lactone from glycoconjugate precursors during maturation of wine’ (Abstract provided below, comprised research findings from a University of Adelaide led oak flavour chemistry project, undertaken in collaboration with the Australian Wine Research Institute and French cooperage Seguin Moreau. The presentation was well received and generated some informative discussion, in particular concerning the potential for oak lactone glycoconjugates to be found in wine post-bottling; a theory which is now under investigation.

The symposium included another dozen presentations on topics ranging from grapes and wine, to fruit (blueberries, avocado and durian) and vegetables (asparagus and tomato). Dr John Hayes (Pennsylvania State University) gave a very interesting presentation on genetic variation in chemosensation: the copy number of the salivary amylase genes (*AMY1*) is known to vary between cultures who consume low and high starch diets; similarly there may be genetic differences in mucosal enzyme activity which affects the biotransformation of odour-active compounds (or their precursors) thereby influencing the aroma perception of individuals. The implications for wine sensory evaluation are quite interesting and this work may therefore be interesting to include within sensory science lectures (i.e. within the University of Adelaide’s oenology and wine marketing programs). Presentations by Professor Thomas Hofmann, Professor Peter Schieberle and Dr Johanna Kreissl (Technische Universität of München) described highly comprehensive approaches to the characterisation of key aroma impact compounds in fruits and vegetables. The research presented involved techniques including solvent assisted flavour evaporation (SAFE) and aroma extract dilution analysis (AEDA), together with reconstitution experiments, to facilitate identification of key aroma constituents and their sensory properties, as well as the effect of thermal processing.

The symposium presentations specific to grapes and wine included:

- Christine Mayr, The Australian Wine Research Institute, Glycoconjugates of volatile phenols: their contribution to smoke off-flavours in wine and interaction with human saliva.
- Rémi Schneider, Institut Français de la Vigne et du Vin, Varietal thiol precursors in grapes: new insights on their structure and evolution during the pre-fermentative operations of winemaking.
- David Jeffery, The University of Adelaide, Harvest, storage, and processing effects on 3-mercaptohexan-1-ol precursor concentrations in Sauvignon Blanc grape juice.
- Gal Kreitman, Pennsylvania State University, Reactivity between 1-hydroxyethyl radicals and aroma active components in wine.
In addition to the fruit and vegetable aroma precursors symposium, a range of other symposia were held throughout the 244th ACS National Meeting, across a range of chemistry themes, including aspects of food safety, the discovery of bioactive compounds, new directions in analytical chemistry and separation science, science and the law and chemical education. The National Meeting also featured a large trade exposition with several hundred chemistry related exhibitors showcasing products including analytical instrumentation, books and journals, reagents, consumables, and services. Of most interest was the analytical instrumentation, in particular the bench top nuclear magnetic resonance instrument and the portable gas chromatograph for analysis in the field.

Following the National Meeting, a series of visits were scheduled with wine researchers in California:

- Professor James Kennedy, Professor & Chair, Department of Viticulture and Enology and Director, Viticulture and Enology Research Center, California State University, Fresno;
- Mr Jim Orvis, Director, Dr John Thorngate, Research Chemist Manager, Dr Mark Kelm, Senior Research Chemist and Dr Kawaljit Tandon, Research Chemist, Research and Development Department, Constellation Brands, Madera;
- Dr Nick Dokoozlian, Vice President, Viticulture, Chemistry and Enology, and Director of Viticulture, Dr Mike Cleary, Director of Chemistry, Dr Tom Pugh, Director of Enology, David Santino, Research Winery Manager, Dr Cyd Yonker, Senior Research Scientist, Dr Martin Mendez, Senior Research Scientist, and Ms Hui Chong, Research Scientist, Research and Development Department, E. & J. Gallo Winery, Modesto;
- Professors Andrew Waterhouse, Susan Ebeler, Douglas Adams, Roger Boulton and Linda Bisson, Viticulture and Enology, University of California, Davis.

**California State University**

Professor Jim Kennedy gave a tour of the facilities at CSU Fresno, where he is responsible for the programs involving table and wine grape production and winemaking. Jim was keen to instigate collaborations, particularly with respect to student exchanges and/or co-supervision of HDR students. This could provide the opportunity for HDR students to undertake two vintages per year, thereby increasing the ability to undertake research involving vineyard trials and providing greater prospects to investigate the effects of different regional influences on grape and wine composition.

**Constellation Brands**

The visit to Constellation primarily focussed on presentation of the talk given in Philadelphia to the small R&D department, which provided a practical introduction to the work undertaken at UA. This showcased some of UA’s research capability and led to useful discussions for how we might work with Constellation in the future. Constellation researchers currently work with Mark Downey (DPI Vic) among others in the area of grape and wine phenolic compounds, so they were mindful of encroaching on that space. Notwithstanding that sentiment, I have also worked with Mark so there is scope to explore cross-institutional collaborations over time.
E. & J. Gallo Winery

Given the existing collaborations between E. & J. Gallo and the University of Adelaide, a substantial amount of time was set aside for meetings with key E. & J. Gallo staff.

Hui Hui Chong provided a tour of the grape analysis laboratory, located at E. & J. Gallo’s Modesto facility. This included a demonstration of the high throughput sample preparation and processing system employed for basic chemistry plus grape flavour potential (i.e. the G-G assay), colour, phenolics, volatiles (methoxypyrazines, C6 compounds, norisoprenoids and terpenes) of grape samples sourced from vineyards throughout California. The quality assurance measures were particularly impressive.

Dave Santino provided a tour of the Modesto research winemaking facility. A range of prototype fermentation vessels for small-scale (50 L) red and white winemaking were inspected and the pros and cons of each were discussed. At present, the research winemaking capacity allows for approximately 50 white wine fermentations, with another 50 red wine fermentation vessels to be commissioned in the near future. A further upgrade is planned within the next 12 months to allow the research winery to undertake replicated winemaking under highly controlled conditions.

Cynthia Yonker and Martin Mendez-Costabel conducted a tour of E. & J. Gallo’s Livingstone winery, the largest winery in the world. The facilities at Livingstone include: a wine analysis laboratory, which mainly undertakes quantification of anthocyanins, tannins and flavonols by HPLC and UV/Vis spectroscopy; pilot-scale winemaking facilities (i.e. 1,000 L fermentation tanks); and commercial scale winemaking facilities (i.e. 2,000,000 L fermentation tanks). The tour certainly put the scale of E. & J. Gallo’s production into perspective.

Tom Pugh outlined the oenology research platforms and organisational structure of E. & J. Gallo’s viticulture, oenology and chemistry research areas. Tom also arranged a tour of the chemistry laboratory, highlighting the small-scale fermentation reactors and oak library. Meetings were also held with Mike Cleary and Nick Dokoozlian to discuss both existing and potential research collaborations.

University of California

The visit to Davis largely focussed on seeing the new winemaking facilities, how they were developed and funded, and how they are used for teaching. The winery in particular involved far-sighted planning in terms of sustainability (capture and use of rainwater and ground run-off, solar power, energy and water efficiency, CO2 capture) and fermentation capabilities (hardware and sensors with wifi for remote access to data and control of operations such as heating and pumping). The research fermenters are in their third generation with improvements to functionality and design features which make cleaning easy and fermentation operations effective and reproducible. Fermenters have a controller to regulate temperature
and pumping which also houses sensors to monitor temperature, colour and total soluble solids, with capability for expansion and downloading of data to a smartphone for instant feedback.

Apart from the winery tour, a short amount of time was spent with individual professors, who discussed their areas of research (polyphenols, winemaking, flavour) and gave tours of their respective laboratories. Based on these discussions, there are certainly opportunities to work collaboratively to improve our collective funding prospects and research outputs. They were also willing to host students, research fellows and staff on sabbaticals. These discussions will continue as we work towards developing joint projects in the future.
Abstract:

Evolution of oak lactone from glycoconjugate precursors during wine maturation

Kerry Wilkinson¹, Andrei Prida² and Yoji Hayasaka³

¹The University of Adelaide, Australia
²Seguin Moreau, France
³The Australian Wine Research Institute, Australia

Oak maturation plays an important role in the production of high quality wine, enhancing both physical attributes (color and stability) and sensory properties (aroma, flavor and astringency). Of the 200 oak-derived volatile compounds identified in oak-aged wine and spirits to date, the most important are considered to be the cis- and trans-isomers of oak lactone, which contribute ‘woody’, ‘citrus’, ‘vanilla’ and ‘coconut’ aromas. Oak lactone is a natural component of oak wood, but also occurs in glycoconjugate precursor forms. This study concerns the role of conjugated derivatives of 3-methyl-4-hydroxyoctanoic acid, i.e. a glucoside, gallate glucoside and rutinoside, as precursors to oak lactone. Maturation trials were conducted to investigate the evolution of oak lactone from glycoconjugate precursors. The glycoconjugate profile of oak powder and model wines were determined by liquid chromatography-tandem mass spectrometry. The effect of toasting on the glycoconjugate content of oak was also investigated.