Chemical characterization and quality control of toxic glycoalkaloids in *Solanum scabrum* berries using LC-MS techniques

Bo Yuan [a, b], David R. Byrnes [a], Fekadu F. Dinssa [c], James E. Simon [a, *], Qingli Wu [a, b]

[a] New Use Agriculture and Natural Plant Products Program, Department of Plant Biology, Rutgers University, 59 Dudley Road, New Brunswick, NJ 08901, USA

[b] Department of Food Science, Rutgers University, 65 Dudley Road, New Brunswick, NJ 08901, USA

[c] WorldVeg Center, Eastern and Southern Africa, P.O. Box 10 Duluti, Arusha, Tanzania

Abstract Body (249 words)

Solanum scabrum is a popular leafy vegetable in sub-Saharan Africa. While the leaves are consumed, the prolific berries are generally discarded without consumption due to conceptual toxicity [1] and remain an abundant yet underutilized resources. Such neglect in Africa is in stark contrast to recognition and consumption in some south American and European cultural practices. In order to facilitate re-evaluation of the berry edibility and consumption safety and to encourage new applications of the untapped berry resource in Africa, this study aimed to systematically investigate the toxins in berries of different maturity and genotypes using LC-MS techniques. In the phase-one study [2], three different and complementary HPLC-ion trap MS or MS/MS methods with or without acid-assisted hydrolysis were developed for berry phytochemical identification. Apart from twenty-four polyphenols and saponins identified, thirty toxic glycoalkaloids were profiled including glycosides of solasodine and uncommon analogues with hydroxylation and methylation modification. The structures were identified based on scaffold-fragmentation pattern [3]. Berries from different maturity and genotypes presented dramatically varied profile of the toxic glycoalkaloids, which could account for the associated berry consumption controversy and meanwhile sounded the alarm demanding rigorous quality control of berry safety. Thus, in phase-two study, aiming for sensitive and rapid analysis of the toxic glycoalkaloids, a UHPLC-triple quadrupole MS/MS method was developed, featuring in-source glycosidic bond cleavage and subsequent aglycone-based fragmentation pathway-specified multiple reaction monitoring (MRM). The characteristic in-source fragmentation behavior was fully optimized using fractional factorial design, projection analysis, and Box-Behnken design, allowing for a superior femtogram-level sensitivity.

Figures

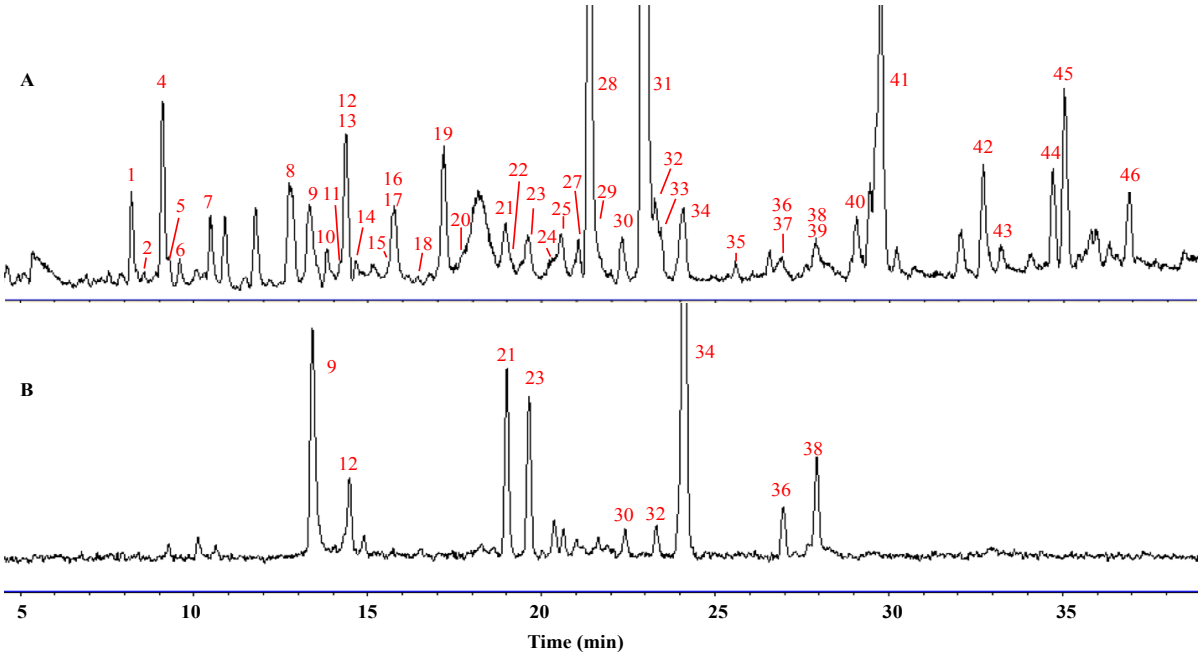


Figure 1. Representative chromatograms of glycoalkaloids, flavonoids and saponins in *Solanum scabrum* SS 04.2 berries. (A) total ion chromatogram (TIC) and (B) UV-vis chromatogram at 370 nm.

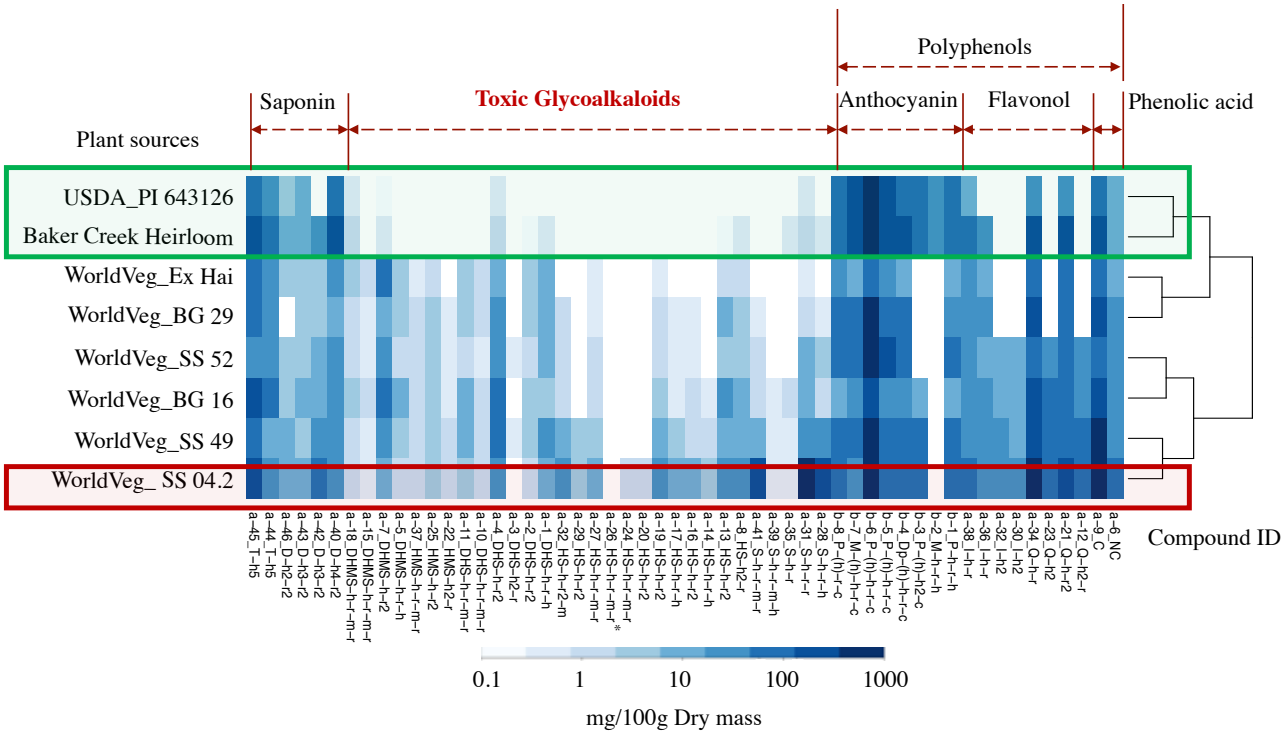


Figure 2. Heatmap of phytochemicals identified in *S. scabrum* mature berries

Reference:

1. Milner, S. E., Brunton, N. P., Jones, P. W., O'Brien, N. M., Collins, S. G., & Maguire, A. R. (2011). Bioactivities of glycoalkaloids and their aglycones from Solanum species. *Journal of Agricultural and Food Chemistry*, 59(8), 3454-3484. doi:10.1021/jf200439q

2. Yuan, B., Byrnes, D., Wu, Q., & Simon, J. E. (2018). Identification of polyphenols, glycoalkaloids and saponins in Solanum scabrum berries using HPLC-UV/Vis-MS. *Journal of Food Science* (accepted, in process)

3. Cahill, M. G., Caprioli, G., Vittori, S., & James, K. J. (2010). Elucidation of the mass fragmentation pathways of potato glycoalkaloids and aglycons using Orbitrap mass spectrometry. *Journal of Mass Spectrometry*, *45*(9), 1019-1025. doi:10.1002/jms.1785

Biography (74 words)**:**

Bo Yuan is a 5th year PhD candidate in the Department of Food Science, Rutgers University, US. During his PhD study, he's first-authored three papers, two more now under review, and two second-authored papers. There are another four first-authored papers and multiple co-authored works currently in preparation. He's proficient in different types of LC-MS techniques and is passionate in application of such high-throughput analytical platform combined with computational programming for food analysis and quality control.

Presenting author details
Full Name: **Bo Yuan**
Contact number: **(+1)732-318-9185**
Twitter account: **None**
Linked In account: **https://www.linkedin.com/in/bo-yuan-amazing/**
Session name/ number: **Session 11: Food Analysis and Quality Control**
Category: **Oral presentation**
Passport Number: **Passport not needed**