

Public Abstract

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Title:Identification and Characterization of Atrazine-Degrading Phytochemicals in Eastern Gamagrass

Naturally occurring phytochemicals of the 1,4-benzoxazin-3-one (Bx) class exhibit broad chemical reactivity that includes detoxification of chloro-triazine herbicides. Atrazine (6-chloro-N-ethyl-N'-(1-methylethyl)-1,3,5-triazine-2,4-diamine) contamination of surface and ground water remains an environmental concern that warrants continued research to identify mitigation and decontamination strategies. In this research, the Bx compound DIBOA-Glc (2-B-D-glucopyranosyloxy-4-hydroxy-1,4-benzoxazin-3-one) was identified as the atrazine-degrading compound present in eastern gamagrass roots (EG, *Tripsacum dactyloides* (L.) L.); identifying Bx compounds in the *Tripsacum* species for the first time. In order to further characterize the reaction between atrazine and DIBOA-Glc, methodology was developed in which bulk quantities of highly pure DIBOA-Glc were produced using HPLC separation of crude methanol extracts of EG roots. The resulting pure DIBOA-Glc was then used to characterize the atrazine-DIBOA-Glc reaction in terms of reaction kinetics, identification of intermediates and products, and pH effects. Findings from these studies demonstrated that DIBOA-Glc was consumed in the reaction and was not acting catalytically. A conjugate of DIBOA-Glc and atrazine was identified as a stable reaction intermediate. Additionally, the formation of hydroxyatrazine (2-hydroxy-4-ethylamino-6-isopropylamino-s-triazine) and Cl⁻ as reaction products confirmed that the reaction mechanism was a nucleophilic attack of the hydroxamic acid moiety at the C-2 position. Use of naturally occurring phytochemicals, such as DIBOA-Glc, in concert with existing mitigation practices may allow producers to continue the use of atrazine as a valuable crop protection tool while simultaneously protecting the soil and water resources in environments where atrazine is used.