O.27 - *p*-Hydroxyphenylpyruvate dioxygenase, a herbicide target site for natural β-triketones

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Weed control relies primarily on the use of synthetic herbicides. However, concerns over their potential impact on the environment and health necessitate the development of alternative and safer weed management tools. Natural herbicides present themselves as a potential bridge between traditional and organic agriculture (Duke et al. 2000). *p*-Hydroxyphenylpyruvate dioxygenase (HPPD) is a key enzyme in the biosynthesis of prenyl quinones. Inhibition of HPPD reduces plastoquinone levels and has deleterious effects on carotenoid synthesis and the photosynthetic apparatus. This enzyme is the target site of β-triketone herbicides (e.g., sulcotrione and mesotrione) (Lee et al., 1997). The inhibitory activity of natural β-triketones (e.g., flavesone, grandiflorone and leptospermone) and several analogues against HPPD was tested. Modeling of the binding of the triketones to HPPD and conformational molecular field analysis (CoMFA) determined that bulky substituents on the ring structure hindered binding to HPPD. The length of the aliphatic tail also modulated the activity of the compounds. Preliminary greenhouse data indicates that while these natural β-triketones may not have optimal structural features of their synthetic counterparts for *in vivo* herbicidal activity, the activity of the β-triketone enriched essential oil can be improved with the use of surfactants to a level sufficiently high to be potentially developed as natural tools for weed management.