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<DOCHEAD>Original article

<AT>The discovery of new scaffold of plant activators: from salicylic acid to benzotriazole

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<ABS-Head><ABS-HEAD>Graphical abstract

<ABS-P>► A series of novel plant activators possessing benzotriazole scaffold was developed with the help of SHAFTS.

<ABS-HEAD>ABSTRACT
<ABS-P>Started from salicylic acid (SA) and related commercialized plant activators, based on molecular three-dimensional shape and pharmacophore similarity comparison (SHAFTS), a new lead compound benzotriazole was predicted and a series of benzotriazole derivatives were designed and synthesized. The bioassay showed that benzotriazole had high activity against a broad spectrum of diseases including fungi and oomycetes *in vivo*, but no activity *in vitro*. And the introduction of proper groups at the 1'-position and 5'-position was beneficial to the activity. So, they had the potential to be exploited as novel plant activators.
<KWD>Keywords: Plant activator Systemic acquired resistance Salicylic acid Benzotriazole Virtual screening

<H1>1. Introduction

Each year, plant diseases are responsible for billions of dollars in economic loss worldwide [1]. Therefore, agrochemicals play a critical role in the development of agriculture [2]. However, at present, traditional pesticides are less effective and will result in resistance in host plants and damages to the environment. So, the search for alternative pesticides which are effective and environmentally friendly is urgent [3]. Plant activator as an ecological pesticide has attracted more and more attention, because it has no direct bactericidal activity in vitro, but could activate the immune system[4-7] of the plant itself, such as systemic acquired resistance (SAR) [8-12], which is dependent on salicylic acid (SA), which could induce the expression of the pathogen-related proteins (*PR* proteins), and then provide defense against a broad spectrum of diseases including fungi, bacteria, viruses and insects without destroying the ecosystem [13-16]. So, it possesses better potential as a green and eco-friendly pesticide. Up to now, a variety of plant activators has been reported (Fig. 1), and some of which have come into the market, among them, benzothiadiazole (BTH) [17-19], 2,6-dichlomisonicotinic acid (INA) [20], tiadinil (TDL) [21, 22], and isotianil activate SAR at the downstream of SA, conversely, probenazole (PBZ) [23] activates SAR at the upstream of SA. As the most successful compound, BTH has been exploited in agriculture for the control of downy and powdery mildew [17]. Based on the structure of BTH, our group has also reported two series