

Effect of *Vicia sativa* L. allelochemicals on *Lens culinaris* L. growth and molecular docking against tryptophane synthase β subunit of *Pyrococcus furiosus*

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Vicia sativa is a common weed that grows luxuriously with the lentil (*Lens culinaris* L.) crop. According to literature studies, the plant can produce a negative allelopathic effect on lentil crops. Because both of these plants have the same morphology, and removal through manually picking of the weed is very difficult. The present investigation was framed to identify the allelopathic effect of *V. sativa* by growing lentil plants under the different dilutions of its whole plant extract. We analyzed growth on the 5th and 20th day after seed germination. We estimated the total carbohydrate, nitrogen, and proline contents to assess the potential impact of weed on photosynthesis and respiration. All concentrations of the extract strongly inhibited the growth of the test plant, resulting in a reduction of 3.0 and 2.7 cm in shoot and root length, respectively. The carbohydrate, and nitrogen accumulations decreased in a similar way as compared to its control. The steady increase in free proline contents indicates that whole plant extracts have a negative allelopathic effect. LC/MS analysis of extract revealed presence of various allelochemicals, including luteolin, naringenin, ferulic acid, 3,4-dihydrocinnamic acid, vanillic acid, 3,4-dihydroxyacetophenone, succinic acid, and benzaldehyde, among others. These allelochemicals were docked by the tryptophan synthase beta-subunit from *Pyrococcus furiosus* that stimulate tryptophane biosynthesis and auxin production and disturb the phytohormone balance in test plants. Luteolin and naringenin when docked with the target protein (PDB ID 5dw3), show high binding affinity (-9.2 kcal/mol) as compared to their natural ligands.

Keywords: Lentil, Extracts, Allelopathy, Weeds, Carbohydrates, Nitrogen