A successful establishment of the symbiosis between nitrogen fixing bacteria and the plant requires a complex exchange of molecular signals between both partners. It is well-known that during the first steps of the interaction, nodulation (Nod) factors are secreted by *Rhizobium* sp. These Nod factors are lipo-oligosaccharide signals, essential for initiating early plant responses during nodulation. However, recent reports have shown that other bacteria-derived bio molecules also act as important signals in the recognition events. Most molecules acting as important signals in symbiotic process also seem to be activators of the plant’s defence mechanism to biotic and abiotic stresses. Despite important advances in the molecular and biochemical events behind this biological process, the economical and environmental potential of these molecules is not yet well-explored. Our consortium of scientific institutions aims to investigate the structural-bioactivity relationship for these molecules and how they could be used to improve commercial bio-fertilizers. In this work, a summary of the results obtained in the set up of the isolation methods, structural analysis and biological validation of bio-molecules derived from *B. japonicum* fermentation broth will be presented.