Green Synthesis, antioxidant, and plant growth regulatory Activities of Novel afurfuryl-2-alkylaminophosphonates

A series of novel a-furfuryl-2-alkylaminophosphonates have been efficiently synthesized from the one-pot threecomponent classical Kabachnik-Fields reaction in a green chemical approach by addition of an in situ generated dialkylphosphite to Schiff's base of aldehydes and amines by using environmental and eco-friendly silica gel supported iodine as a catalyst by microwave irradiation. The advantage of this protocol is simplicity in experimental procedures and products were resulted in high isolated yields. The synthesized a-furfuryl-2alkylaminophosphonates were screened to in vitro antioxidant and plant growth regulatory activities and some are found to be potent with antioxidant and plant growth regulatory activities. These in vitro studies have been further supported by ADMET (absorption, distribution, metabolism, excretion, and toxicity), quantitative structure-activity relationship, molecular docking, and bioactivity studies and identified that they were potentially bound to the GLN340 amino acid residue in chain C of 1DNU protein and TYR597 amino acid residue in chain A of 4M7E protein, causing potential exhibition of antioxidant and plant growth regulatory activities. Eventually, title compounds are identified as good blood – brain barrier (BBB)-penetrable compounds and are considered as proficient central nervous system active and neuroprotective antioxidant agents as the neuroprotective property is determined with BBB penetration thresholds.