Aim and Objectives
Interest in discovery of natural constituents with antioxidant properties has increased globally in recent years, as they can protect the human body from free radicals and hinder the progress of many diseases including cancer and inflammation. Nowadays, the strategy of isolating the active principles from the medicinal plants and developing a pharmaceutical preparation has become trendy. Thus, the natural entities are also used as a template for the development of clinically useful therapeutic agents. *Lippia* species are being well studied and the remarkable results reported beforehand led to the conclusion that it contains more active principles. In this direction, *L. nodiflora* L. has been selected for the present study, because of multifold medicinal uses and in order to explore its phytoconstituents with valuable bioactivity. In particular, the aerial part of the plant *L. nodiflora* was selected based on its folklore use in traditional medicine and literature review. Likewise, the RAW 264.7 macrophage and MCF-7 breast cancer cell line were selected for the present study, as these cells serve as an excellent *in vitro* model for studying the inflammatory and tumor response. Moreover, MCF-7 cell line is used in several anti-cancer studies owing to its unique characteristics and being easy to culture. The present study is aimed to evaluate the antioxidant effects of extract and isolated compound of *L. nodiflora* and further, the biological activities of the isolated compound were determined experimentally by *in vitro* model in combination with molecular docking and molecular dynamics simulation. Hence, the present study was designed to achieve the following objectives:

- To assess the preliminary physicochemical and phytochemical profiles of powdered aerial parts of *L. nodiflora* L.
- To determine the *in vitro* antioxidant potential of methanol extract of *L. nodiflora* and to isolate the biologically active compound(s) through bioassay guided fractionation process using spectrophotometric DPPH assay.
Aim and Objectives

- To investigate the binding mechanism of isolated bioactive compound with model transport protein, bovine serum albumin using different kinds of spectroscopic and molecular modeling techniques.

- To evaluate the anti-inflammatory properties of isolated bioactive compound using *in vitro* enzyme assay and RAW 264.7 macrophage cells and to validate the observed activity by *in silico* analysis.

- To elucidate the bioactive potential of isolated compound in inducing apoptosis using the MCF-7 breast cancer cell line and to explore the binding interaction of isolated compound with cancer target through computational studies.