LIST OF FIGURES

CHAPTER 2

Figure 2.1 Basic schemes representing the workflow for the screening of bioactive compounds from *Indigofera caerulea*

CHAPTER 3

Figure 3.1 Pathological roles of free radicals.

Figure 3.2 *Indigofera caerulea* Roxb and its morphological properties

Figure 3.3 Flow chart of soxhlet extraction of *Indigofera caerulea leaves*

CHAPTER 4

Figure 4.1 HPLC profile of methanolic extract of *Indigofera caerulea*

Figure 4.2 Effect of MIL on hepatic antioxidant profile

Figure 4.3 Histomorphological liver sections of control and experimental rats

Figure 4.4 Effect of MIL on hepatic cytokine profile of TNF-α and IL-1β

Figure 4.5 The effect of MIL and silymarin on the expression and specific hepatic distribution of NF-κB by immunostaining.

Figure 4.6 The effect of MIL and silymarin on the expression and specific hepatic distribution of TNF-α by immunostaining

CHAPTER 5

Figure 5.1 TLC of the isolated bioactive compounds from *I. caerulea*

Figure 5.2 $^1$H NMR spectrum of the isolated bioactive compound MIL-1
Figure 5.3 $^{13}$C NMR spectrum of the isolated bioactive compound MIL-1

Figure 5.4 $^1$H- $^1$H COSY spectrum of the isolated bioactive compound MIL-1

Figure 5.5 $^{13}$C-$^1$H HSQC spectrum of the isolated bioactive compound MIL-1

Figure 5.6 $^1$H NMR spectrum of the isolated bioactive compound MIL-2

Figure 5.7 $^{13}$C NMR spectrum of the isolated bioactive compound MIL-2

Figure 5.8 $^1$H- $^1$H COSY spectrum of the isolated bioactive compound MIL-2

Figure 5.9 $^{13}$C-$^1$H HSQC spectrum of the isolated bioactive compound MIL-2

Figure 5.10 Molecular docking interaction of Tumor Necrosis Factor alpha (TNF-alpha) (PDB ID: 2AZ5) with quercetin and hydrogen bond interaction with active residues were showed

Figure 5.11 Molecular docking interaction pose of Tumor Necrosis Factor alpha (TNF-alpha) (PDB ID: 2AZ5) with silymarin and hydrogen bond interaction, bond length and active residues were labeled

Figure 5.12 Molecular docking poses of Cyclooxygenase-2 (COX-2) (PDB ID: 3LN1) with quercetin and hydrogen bond interaction and active residues were labeled

Figure 5.13 Molecular docking interaction poses of Cyclooxygenase-2 (COX-2) with Ethyl linoleate and hydrogen bond interaction and active residues were labeled

Figure 5.14 Molecular docking poses of Cyclooxygenase-2 (COX-2) with silymarin with hydrogen bond interaction and active residues were labeled
Figure 5.15  Energy peak of the TNF-α-quercetin docking complex during 20 ns MD simulation. (A) 1-10,000 picoseconds and (B) 10,000-20,000 picoseconds

Figure 5.16  MD simulation of TNF-α-quercetin complex. (A) MD simulation time Vs. RMSD of the backbone atom of TNF-α protein (B) RMSD of heavy atom (ligand) of TNF-α protein

Figure 5.17  RMSF of TNF-α-quercetin complex during 20 ns MD simulation. Blue color indicates backbone and red color indicates side chains

Figure 5.18  H-bonds formed between TNF-α-quercetin complex during 20,000 ps MD simulation

Figure 5.19  Interactions of quercetin with TNF-α active site residues showed direct H-bonds after 20.0 ns MD simulation