Macrocycles, as important and powerful ligands, are applied in many areas such as ion and molecular sensing, metal ion protection in biomedical imaging, treatment of heavy metal waste streams, drug delivery and increase of drug efficacy, etc. Considerable effort has been directed towards the design and synthesis of sulfur and selenium containing macrocyclic ligands. The objective of this research is to synthesize novel macrocycles containing mixed atoms such as N, O, S, Se and Si atoms and study their coordination chemistry with metal ions. The incorporation of the Si atom is to increase the coordination ability of the ligand due to the beta-silicon effect.

Several macrocycles containing mixed Si/S/N, Si/S/O, Si/Se/N or Si/Se/O are designed. The designed macrocycles contain mixed-donor functionalities with both hard and soft donor atoms. Therefore they can potentially bind two metals of differing character and oxidation state within the same cavity. These macrocycles can be used for complexation with heavy metals due to (1) higher stability constant of the complexes over their open chain analogs due to macrocyclic effect and (2) selectivity of the metal ion binding can be achieved by varying macrocyclic ring sizes and donor atom set combinations. Also, sulfur and selenocrown ethers should bind strongly to precious metals like Cu, Ag, Au, Pd and Pt since these metals prefer soft donor atoms. The synthesis of these macrocycles will be described. The obtained macrocycles will further react with various metal ions since all of them are tetra-dentate ligands with mixed soft and hard donors.