

## **Synthesis, Radiolabelling, and In Silico Study of the <sup>131</sup>I-(4-fluoro benzoyl)-3-methyl thiourea as a Theragnostic Radiopharmaceutical Candidate for Breast Cancer**

### **Abstract**

The chemicals produced from thiourea are actively being researched as anticancer possibilities. In complexes with radionuclides like iodine-131, the 1-(4-Fluorobenzoyl)-3-methyl thiourea is a promising ligand for theragnostic applications. This work will synthesize 1-(4-Fluorobenzoyl)-3-methylthiourea, labelled with iodine-131, and an in-silico investigation of breast cancer receptors will be conducted.

According to the results of molecular docking, this radiopharmaceutical molecule has the best activity on the HER2 receptor (PDB ID: 3PP0), with a binding affinity of -6.13 kcal/mol and a Ki value of 32.05 uM. According to the molecular dynamics data, the radiopharmaceutical molecule <sup>131</sup>I-(4-Fluorobenzoyl)-3-methylthiourea displays good stability starting from the 50ns range. The indirect radioiodination method was used to successfully manufacture and label this 1-(4-Fluorobenzoyl)-3-methylthiourea) molecule.

**Keywords:** Iodine-131, Thiourea, Radiolabelling, In Silico