



Transformation of agricultural waste into nutraceutical and pharmaceutical products with the aid of In-silico methods

Tumwesigye R^{1,2,3}, Akello R. O^{2,3}, Gumula I^{2,3}, Akampurira D², Patrick O^{2,3}, Asiimire B^{2,3}, Kikonyogo I^{2,3}

¹Makerere University, ²Kyambogo University, ³Reflora Labs (U) Ltd

Abstract:

This project transforms Ugandan agricultural waste, such as pineapple and soursop residues, into valuable nutraceuticals and pharmaceuticals. By combining green chemistry, LC-MS/MS & GC-MS/MS analysis with in-silico molecular docking and toxicity profiling, we identify bioactive compounds with high therapeutic potential. This sustainable, circular model provides a scalable, cost-effective framework for drug discovery, offering an affordable approach to health innovation that aligns with global sustainability goals.

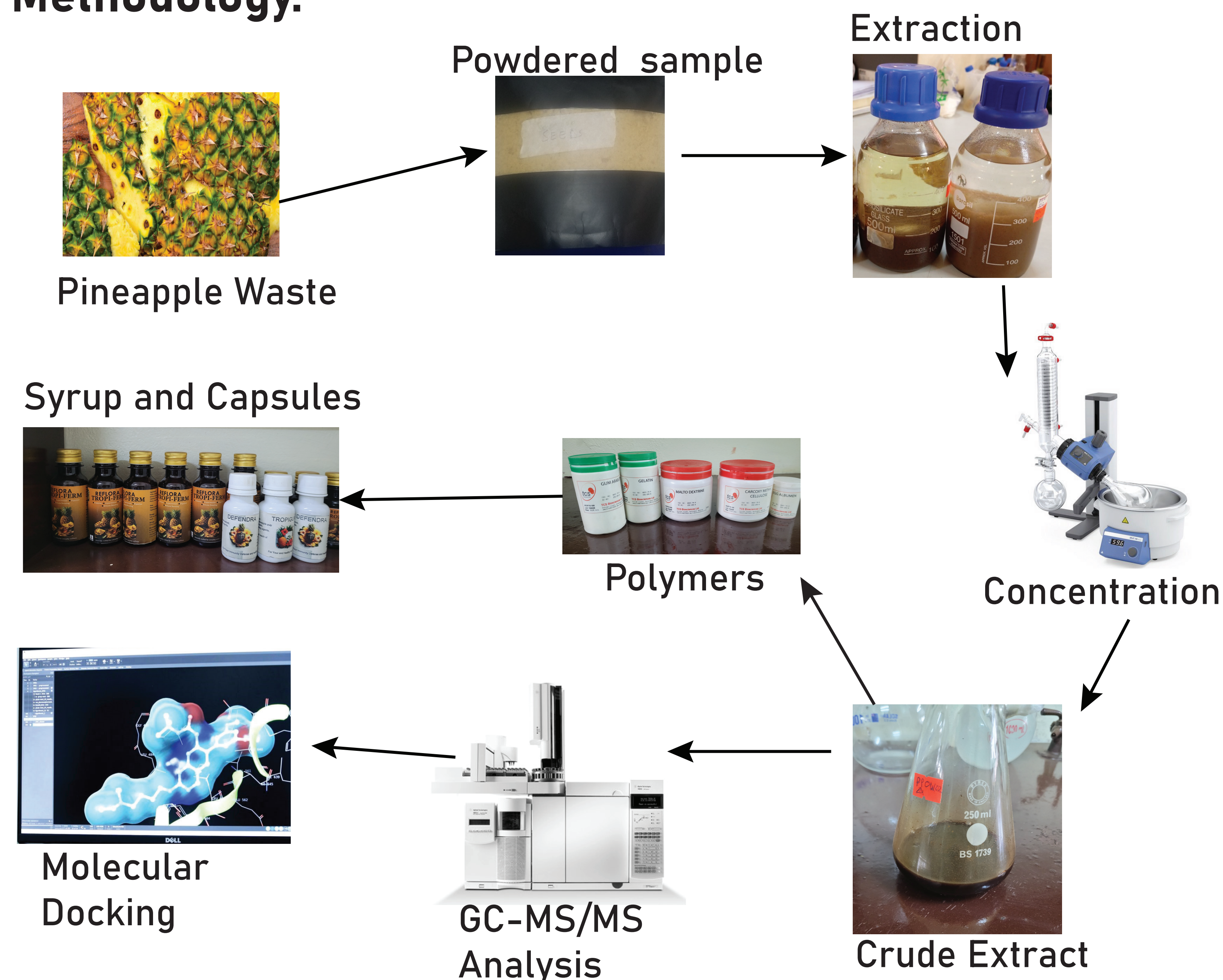
Introduction:

Agricultural waste, particularly from pineapple and soursop processing, represents a significant environmental burden in Uganda, where improper disposal, often via open burning contributes to greenhouse gas emissions and pollution. Simultaneously, Uganda faces a mounting health crisis, with non-communicable diseases (NCDs) such as cardiovascular disease, cancer, and diabetes now accounting for approximately 36% of national deaths. As the demand for affordable, locally sourced therapeutic agents rises, there is a critical need to transition from traditional waste disposal to a circular bioeconomy model. This project leverages green chemistry and in-silico computational tools to valorize these residues, transforming agricultural biomass into high-value nutraceutical and pharmaceutical products through an efficient, data-driven discovery pipeline.

Specific Objective:

1. Quantify and identify the chemical profile of bioactive metabolites in pineapple and soursop residues using LC-MS/MS and GC-MS/MS.
2. Conduct molecular docking studies for the identified lead compounds to determine their binding affinities against priority targets
3. Perform comprehensive in-silico ADME and safety profiling via ProTox-II to validate the therapeutic suitability of lead candidates

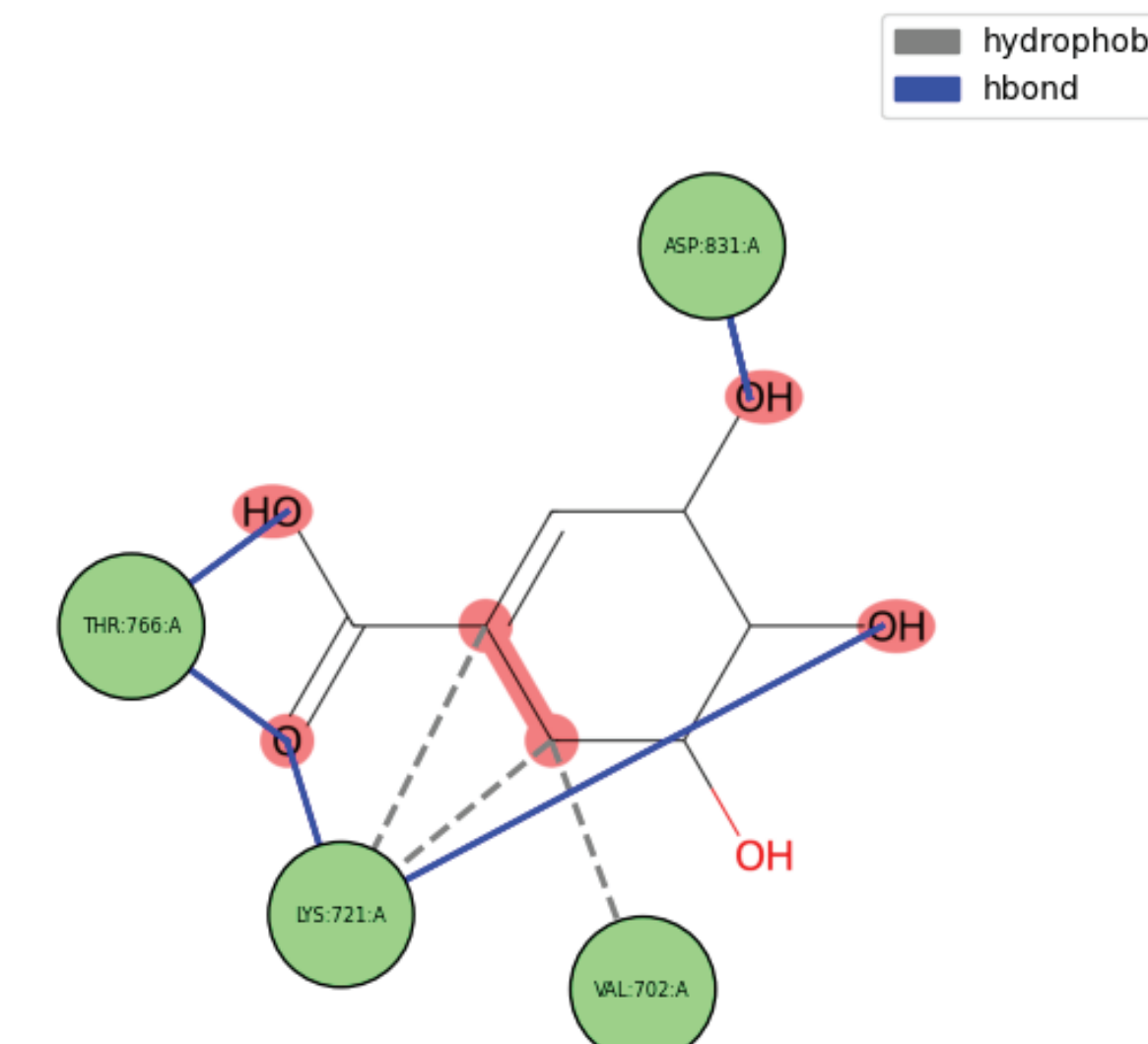
Methodology:



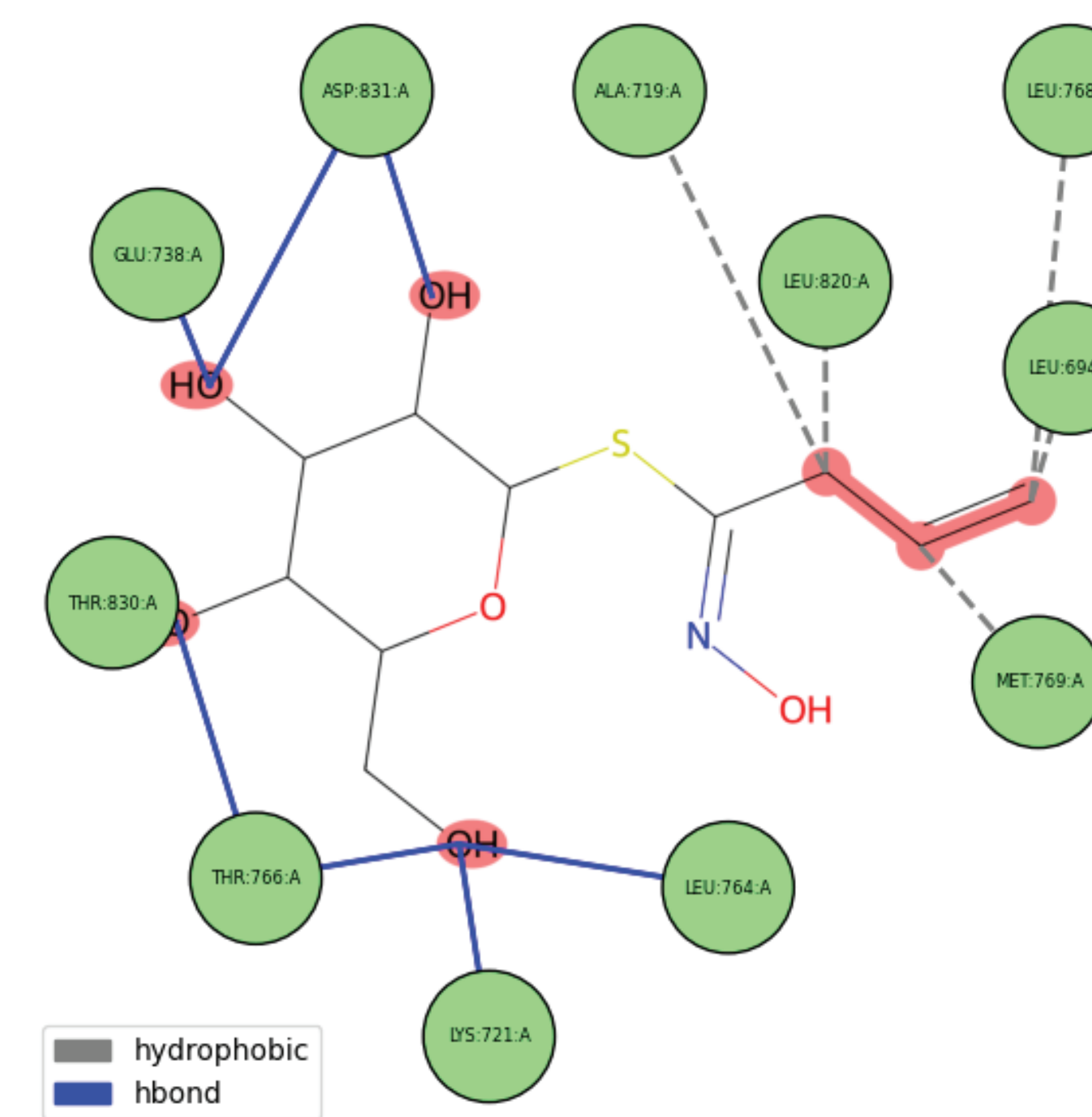
Results:

Name	m/z	Found RT	Area
2,3-Dimethylpentanoic acid	74.00	3.000	15,179
3,4-Dimethoxycinnamic acid	208.00	3.011	48,083
2,2'-Bioxirane	55.00	3.011	220,291
2,2'-Bioxirane	55.00	3.132	32,105
Butanoic acid, 2-methyl-3-oxo-, ethyl ester	74.00	3.256	42,018
Shikimic acid	98.00	4.182	35,185
Furfural	96.00	3.672	160,886
Methylenecyclopropanecarboxylic acid	98.00	4.185	10,620
2H-Pyran-2-one, tetrahydro-4-hydroxy-6-pentyl-	86.00	4.358	51,704
4-Cyclopentene-1,3-dione	96.00	4.478	193,929
2(5H)-Furanone	55.00	5.151	179,634
3-Deoxy-d-mannonic lactone	281.00	5.788	86,037
6-Oxa-bicyclo[3.1.0]hexan-3-one	98.00	5.470	257,070

GC-MS/MS analysis of the fermented ethanol:water extract



Shikimic Acid docked to EGFR



desulphonigrin docked to EGFR

ProTox-3.0 - Prediction of TOXicity of Shikimic Acid

Target	Prediction	Probability
Hepatotoxicity	Inactive	0.70
Neurotoxicity	Inactive	0.88
Nephrotoxicity	Active	0.64
Respiratory toxicity	Inactive	0.54
Cardiotoxicity	Inactive	0.61
Carcinogenicity	Inactive	0.66
Mutagenicity	Inactive	0.94
Androgen Receptor (AR)	Inactive	0.95
Aromatase	Inactive	0.99
Estrogen Receptor Alpha (ER)	Inactive	0.90

References:

1. Abdullahi, M., Ndagi, U., & Ibrahim, Z. G. (n.d.). The prostate cancer-fighting powers of soursop fruit: in silico evaluation to give insight into binding affinity of selected bioactive compounds on selected prostate cancer targets. sciforum. <https://sciforum.net/manuscripts/15618/manuscript.pdf>
2. Dattani, S., Samborska, V., Ritchie, H., & Roser, M. (2024). Cancer. Our World in Data. Retrieved May 30, 2025, from <https://ourworldindata.org/cancer>

Acknowledge:

