Thick Target Yield Analysis of Proton-Induced Reactions on Selenium for Theranostic Bromine Radioisotopes Based on Machine Learning Results

Parichehr Khalilzadeh[1], S. Farhad Masoudi[1], Hassan Yousefnia[2], Fatemeh S. Rasouli[1]

[1]Department of Physics, K.N. Toosi University of Technology, Tehran, Iran
[2] Radiation Application Research School, NSTRI, Tehran, Iran

CCP 2025 – XXXVI IUPAP Conference on Computational Physics
Virtual Conference, November 3–7, 2025

Abstract

This work investigates the thick target yield (TTY) of proton-induced reactions on selenium for the production of theranostic bromine radioisotopes $^{76}\mathrm{Br}$ and $^{77}\mathrm{Br}$. Cross-section data were obtained from two sources: experimental data reconstructed using machine learning models and theoretical predictions from the TALYS-2.0 code. Two main reactions, $^{76}\mathrm{Se}(p,n)^{76}\mathrm{Br}$ and $^{77}\mathrm{Se}(p,n)^{77}\mathrm{Br}$, along with their impurity-producing competing channels, were analyzed to determine the optimal energy ranges for high-yield and high-purity production. Stopping power data from SRIM were used to account for proton energy loss through a 1 mm selenium target. The results define the effective energy windows suitable for cyclotron production of bromine radioisotopes.

Introduction

Bromine radioisotopes $^{76}\mathrm{Br}$ and $^{77}\mathrm{Br}$ are of significant interest in nuclear medicine due to their complementary imaging and therapeutic properties; $^{76}\mathrm{Br}$ (half-life ≈ 16 h) is a positron emitter suitable for PET imaging, while $^{77}\mathrm{Br}$ (half-life ≈ 57 h) is a beta-minus emitter useful for targeted radiotherapy. They can be produced via proton-induced reactions on selenium isotopes $^{76}\mathrm{Se}$ and $^{77}\mathrm{Se}$, where evaluating the TTY and isotopic purity is essential for optimizing production efficiency. Impurity formation through competing channels, such as $^{76}\mathrm{Se}(p,2n)^{75}\mathrm{Br}$ and $^{77}\mathrm{Se}(p,2n)^{76}\mathrm{Br}$, can reduce the final product quality. While the TALYS nuclear reaction code provides theoretical cross-section predictions, its accuracy may decrease in resonance regions. ML models have recently emerged as complementary tools for reconstructing and predicting reaction data. This study compares TTY results derived from TALYS and ML-based cross-sections to identify optimal proton energy ranges for the efficient production of bromine theranostic isotopes [1, 2].

Materials and Methods

The yield was determined using the following relation:

$$Y = \frac{N_A H}{M z q_e} \int_{E_{\text{em}}}^{E_{\text{inc}}} \left(\frac{dE}{dx}\right)^{-1} \sigma(E)\, dE,$$

where N_A is Avogadro's number, H is the isotopic enrichment fraction, M is the molar mass of the target isotope, z is the projectile charge, q_e is the elementary charge, $\frac{dE}{dx}$ is the stopping power, and $\sigma(E)$ represents the reaction cross-section as a function of proton energy. The integration limits E_{inc} and E_{em} correspond to the incident and emergent proton energies, respectively. The reaction cross-section data were obtained from two sources: theoretical calculations using the TALYS-2.0 nuclear reaction code [3] and machine learning predictions based on the Random Forest model developed in our previous work [4]. Stopping power data were obtained from the SRIM software [5]. The integration limits were determined based on the calculated energy loss and projectile motion through a 1 mm selenium target using the SRIM stopping power data. The integral was evaluated numerically to obtain the thick target yield.

Results and Discussion

The calculated thick target yields for both reactions are shown in Figure 1. The left panel corresponds to the $^{77}\mathrm{Se}(p,n)^{77}\mathrm{Br}$ reaction and its impurity channel $^{77}\mathrm{Se}(p,2n)^{76}\mathrm{Br}$, while the right panel presents the $^{76}\mathrm{Se}(p,n)^{76}\mathrm{Br}$ and $^{76}\mathrm{Se}(p,2n)^{75}\mathrm{Br}$ reactions.

In both cases, ML-based results predict slightly higher yields near the peak energy region compared with TALYS, indicating better agreement with the experimental trend at moderate proton energies.

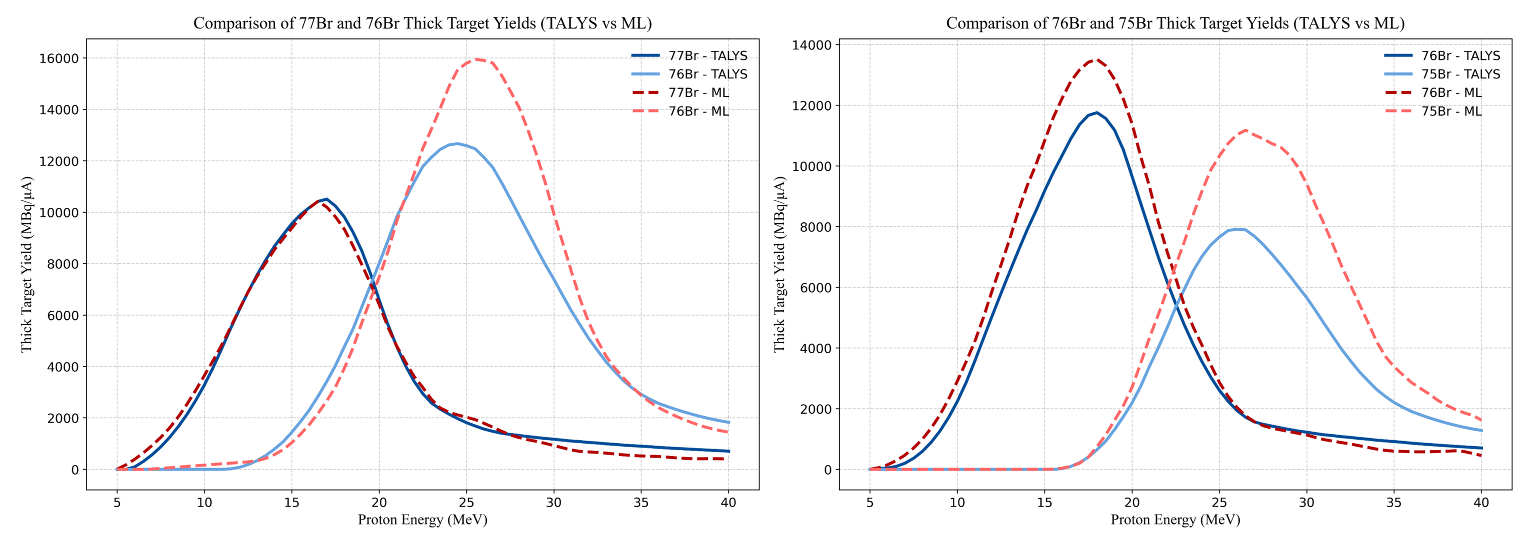

Figure 1: Thick target yield comparison for $^{77}\mathrm{Br}$ (left) and $^{76}\mathrm{Br}$ (right) reactions based on TALYS and ML data.

The isotopic purity analysis for both reactions is presented in Figure 2. The left panel corresponds to the $^{77}\mathrm{Se}(p,n)^{77}\mathrm{Br}$ reaction and its impurity $^{76}\mathrm{Br}$, while the right panel shows the $^{76}\mathrm{Se}(p,n)^{76}\mathrm{Br}$ reaction and its impurity $^{75}\mathrm{Br}$. For both reactions, the purity remains above 98% within the low-energy region, indicating that optimal production conditions lie below approximately 16 MeV for $^{76}\mathrm{Br}$ and 8 MeV for $^{77}\mathrm{Br}$.

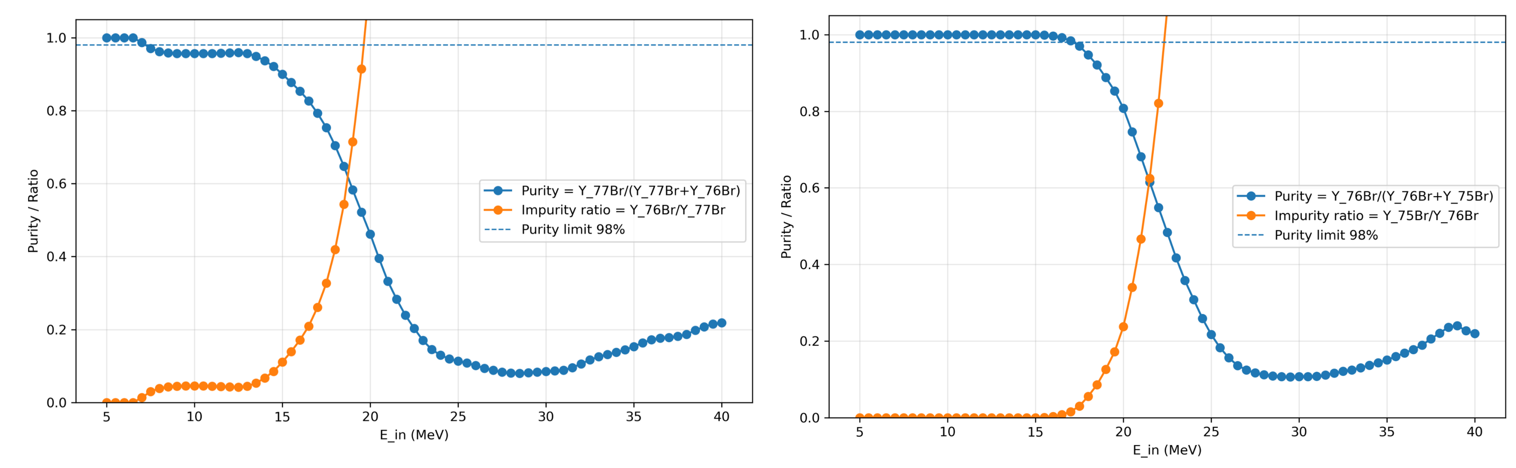

Figure 2: Isotopic purity and impurity ratio for $^{77}\mathrm{Br}$ (left) and $^{76}\mathrm{Br}$ (right) production as functions of incident proton energy.

Conclusions

In this study, the thick target yields of proton-induced reactions on selenium for the production of $^{76}\mathrm{Br}$ and $^{77}\mathrm{Br}$ were calculated using both TALYS theoretical data and ML predictions. The ML-based results generally showed higher agreement with experimental trends and slightly greater yield values in the peak regions compared to TALYS. Isotopic purity analysis indicated that optimal proton energy ranges for high-purity production are below 16 MeV for $^{76}\mathrm{Br}$ and below 8 MeV for $^{77}\mathrm{Br}$. These results demonstrate the potential of ML-assisted nuclear data reconstruction to enhance predictive accuracy.

References

[1] Şevki Şentürk, Tuncay Bayram, and Anes Hayder. Production cross-section and reaction yield of 76 br for nat se (p, xn) 76 br reaction channels. *Iranian Journal of Science*, 49(1):259–267, 2025.

[2] Serkan Akkoyun, Cafer Mert Yeşilkanat, and Tuncay Bayram. Machine learning predictions for cross-sections of 43, 44sc radioisotope production by alpha-induced reactions on ca target. *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms*, 549:165293, 2024.

[3] Arjan J Koning and Dimitri Rochman. Modern nuclear data evaluation with the talys code system. *Nuclear data sheets*, 113(12):2841–2934, 2012.

[4] Parichehr Khalilzadeh, S Farhad Masoudi, Hassan Yousefnia, and Fatemeh S Rasouli. Machine learning-based prediction of proton-induced reaction cross-sections for medically relevant bromine radioisotopes. *Results in Physics*, page 108357, 2025.

[5] James F Ziegler, Matthias D Ziegler, and Jochen P Biersack. Srim–the stopping and range of ions in matter (2010). *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms*, 268(11-12):1818–1823, 2010.

For correspondence: par.khalilzadehvaneghi@email.kntu.ac.ir