Contribution ID: **60** Type: **not specified**

Optimized simulations of ^{50}Ti(p,α) and ^{49}Ti(d,α) reactions for hospital-cyclotron production of ^{47}Sc

Friday 16 June 2023 10:20 (20 minutes)

Radionuclide ^{47}Sc ($T_{1/2}$ = 3.35 d) represents a promising element for innovative radiopharmaceutical compounds suitable for theranostic applications, however an efficient and convenient production route has still to be identified. In this work we simulate the reactions ^{50}Ti(p,α)^{47}Sc and ^{49}Ti(d,α)^{47}Sc in view of a cyclotron production of ^{47}Sc on enriched Titanium targets. Pre-clinical and clinical applications demand a production route with high quality, minimizing the co-production of contaminants that could affect the purity of the radiolabeled compound.

The theoretical analysis has been carried out with the nuclear reaction code TALYS and the model variability of the reaction mechanisms has been investigated. Modeling the relevant cross sections, including the production of the main contaminants, namely ^{46}Sc ($T_{1/2}$ = 83.79 d) and ^{48}Sc ($T_{1/2}$ = 43.67 h), allows to select the energy interval which maximizes the production yield and the purity, for both targets. Simulations improvements are needed to reproduce the data with a high level of accuracy required for a precise estimate of yields, activities, and purities. For this purpose an optimization strategy has been adopted, based on the genetic algorithm approach.

The results indicate that both channels, ^{50}Ti(p,n)^{47}Sc and ^{49}Ti(d,α)^{47}Sc, are promising reactions for a possible production of ^{47}Sc by hospital (low-energy) cyclotrons.

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Session Classification: Medical radioisotopes

Track Classification: Medical radioisotopes