

^{47}Sc production for medical applications: cross-section optimization based on genetic algorithms

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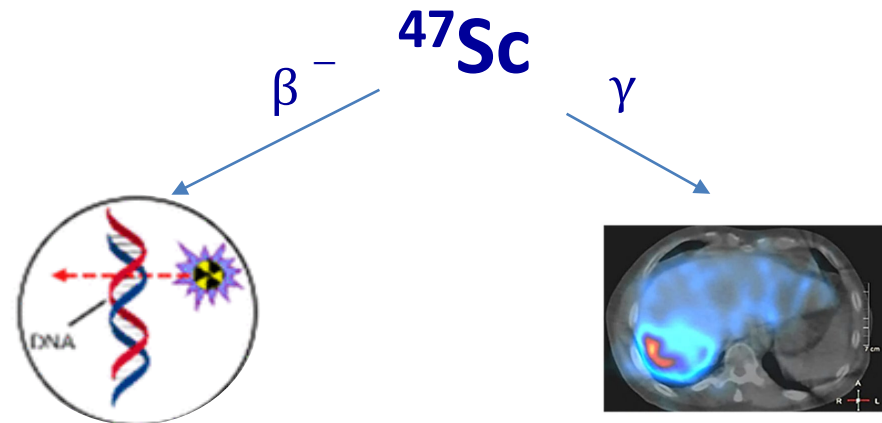
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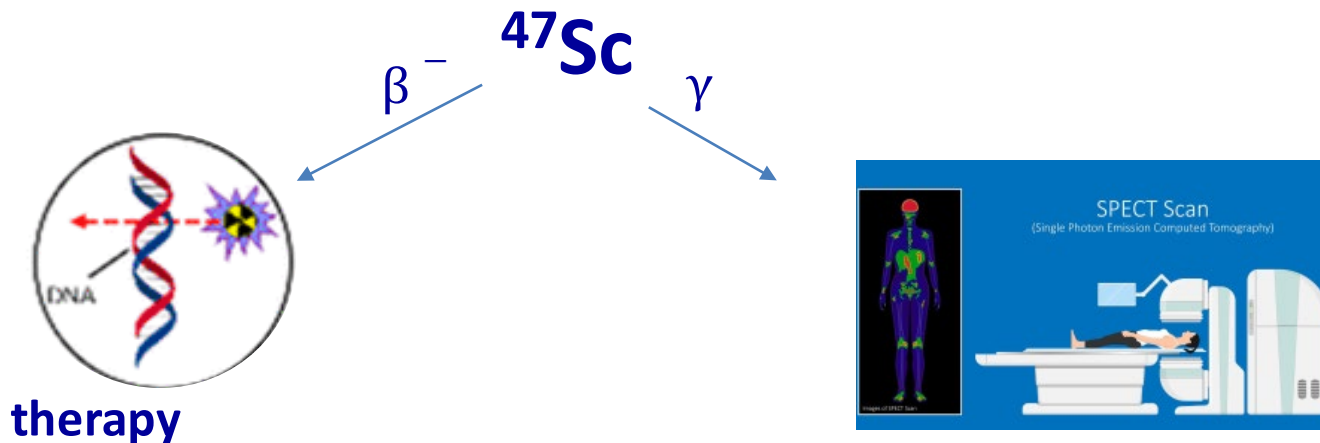
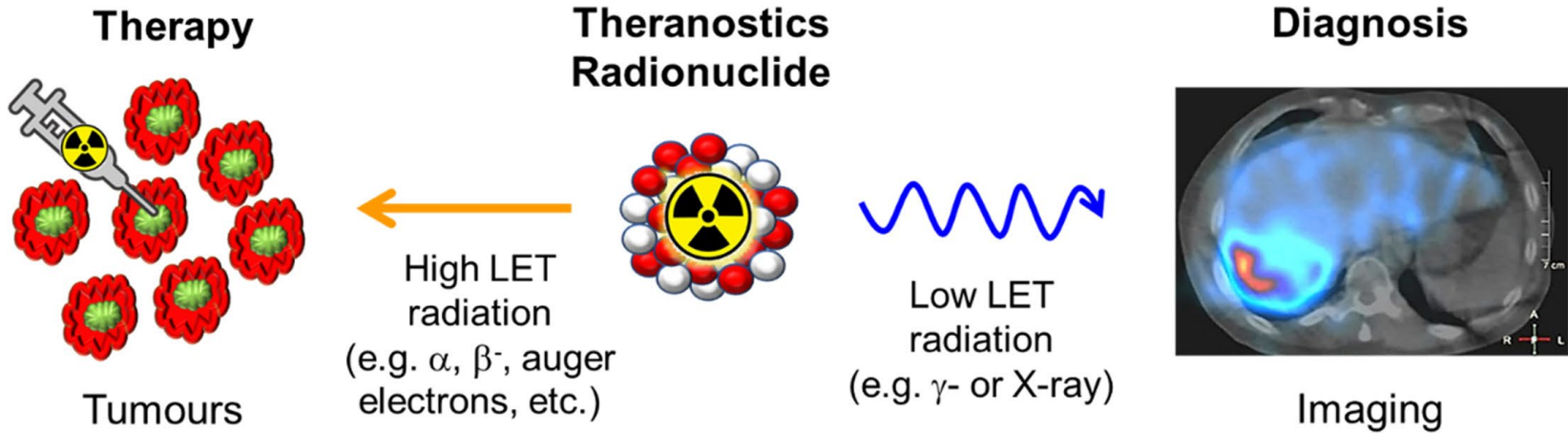
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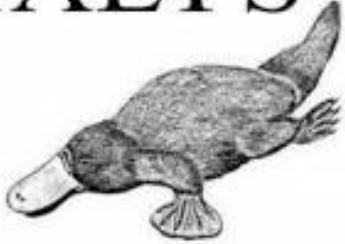
		<ul style="list-style-type: none"> <li style="margin-right: 10px;">● PET <li style="margin-right: 10px;">● Beta Therapy <li style="margin-right: 10px;">● SPECT <li style="margin-right: 10px;">● Alpha Therapy <li style="margin-right: 10px;">● Auger e⁻ Therapy 																	
H	He																	He	
Li	Be																	Ne	
Na	Mg																	Ar	
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr		
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe		
Cs	Ba	57-71	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn		
Fr	Ra	89-103	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Nh	Fl	Mc	Lv	Ts	Og		
*Lanthanoids		La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu			
**Actinoids		Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr			

^{47}Sc holds potential for dual-purpose radiopharmaceuticals—**therapy** and **diagnostics** (theranostics)



For the evaluation of the cross sections we used TALYS code

TALYS



Hartree-Fock level densities from numerical tables

Geometry-dependent hybrid model
for the pre-equilibrium process

Level densities are adjusted to experimental data via a scaling function:

$$\rho(E) = \exp\left(c\sqrt{E-p}\right) \rho_{\text{HFM}}(E-p)$$

We optimized 6 pairs of **c** & **p** parameters with genetic algorithm to fit a large set of measured cross sections relevant for ^{47}Sc production from ^{49}Ti target

The genetic algorithm is a random-based evolutionary algorithm inspired by Darwin's theory of natural selection



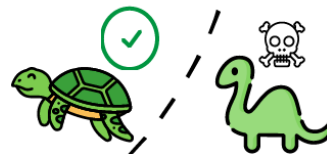
gene



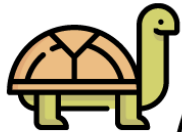
new generation



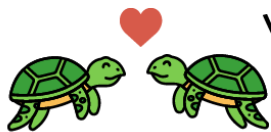
evaluation of each individual



selection

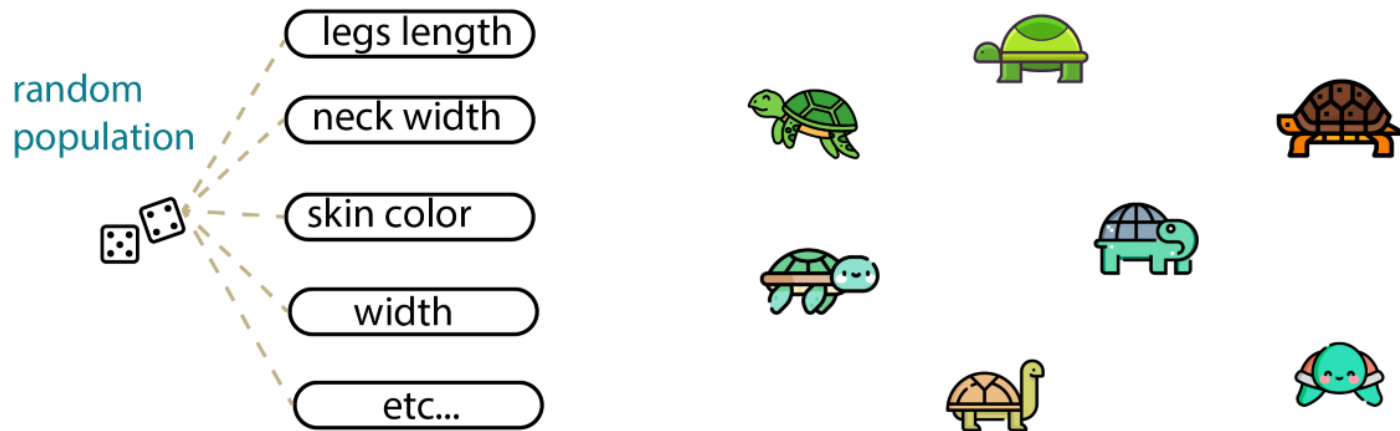


mutation



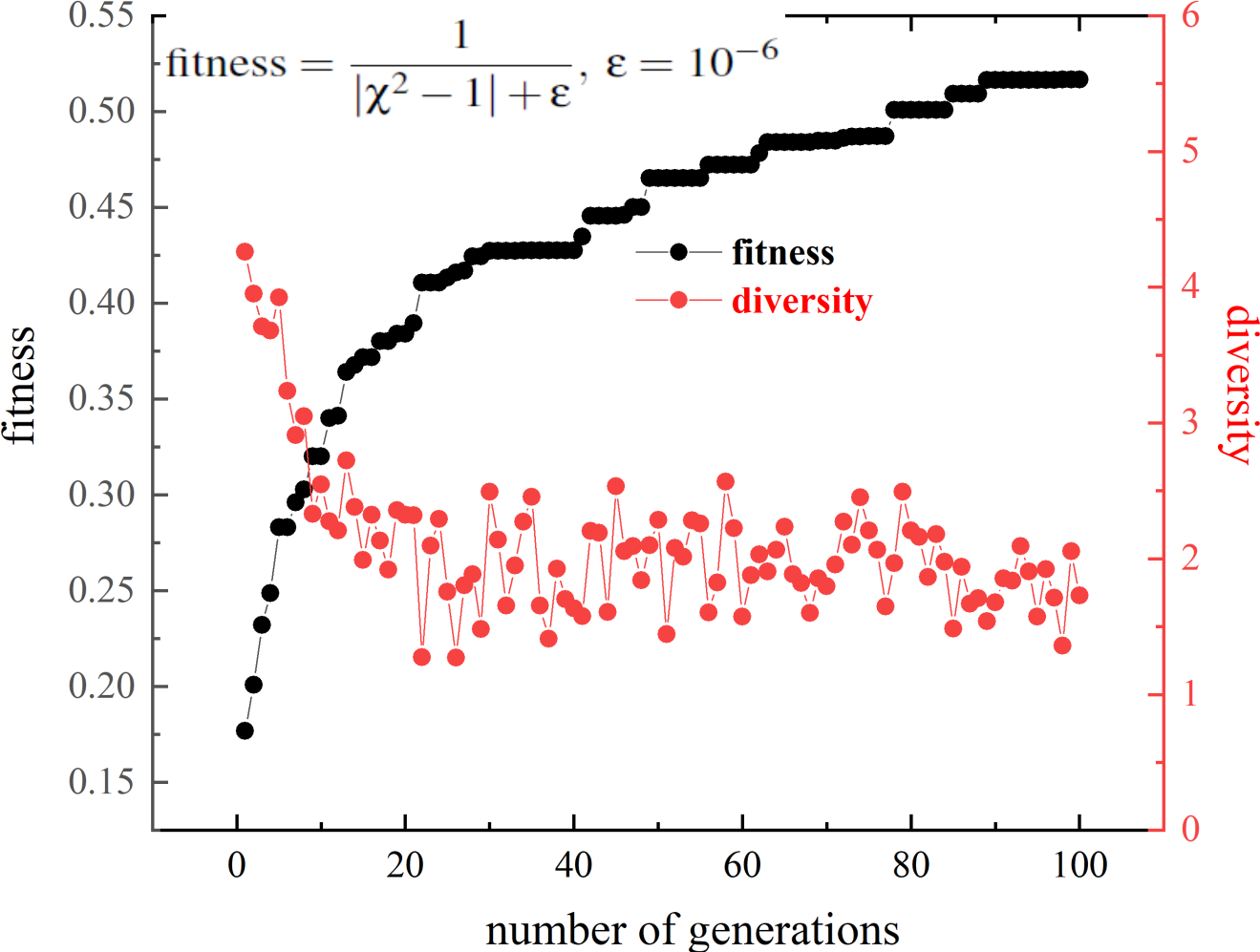
reproduction

In the initialization phase, it is important to consider how this initial population might vary



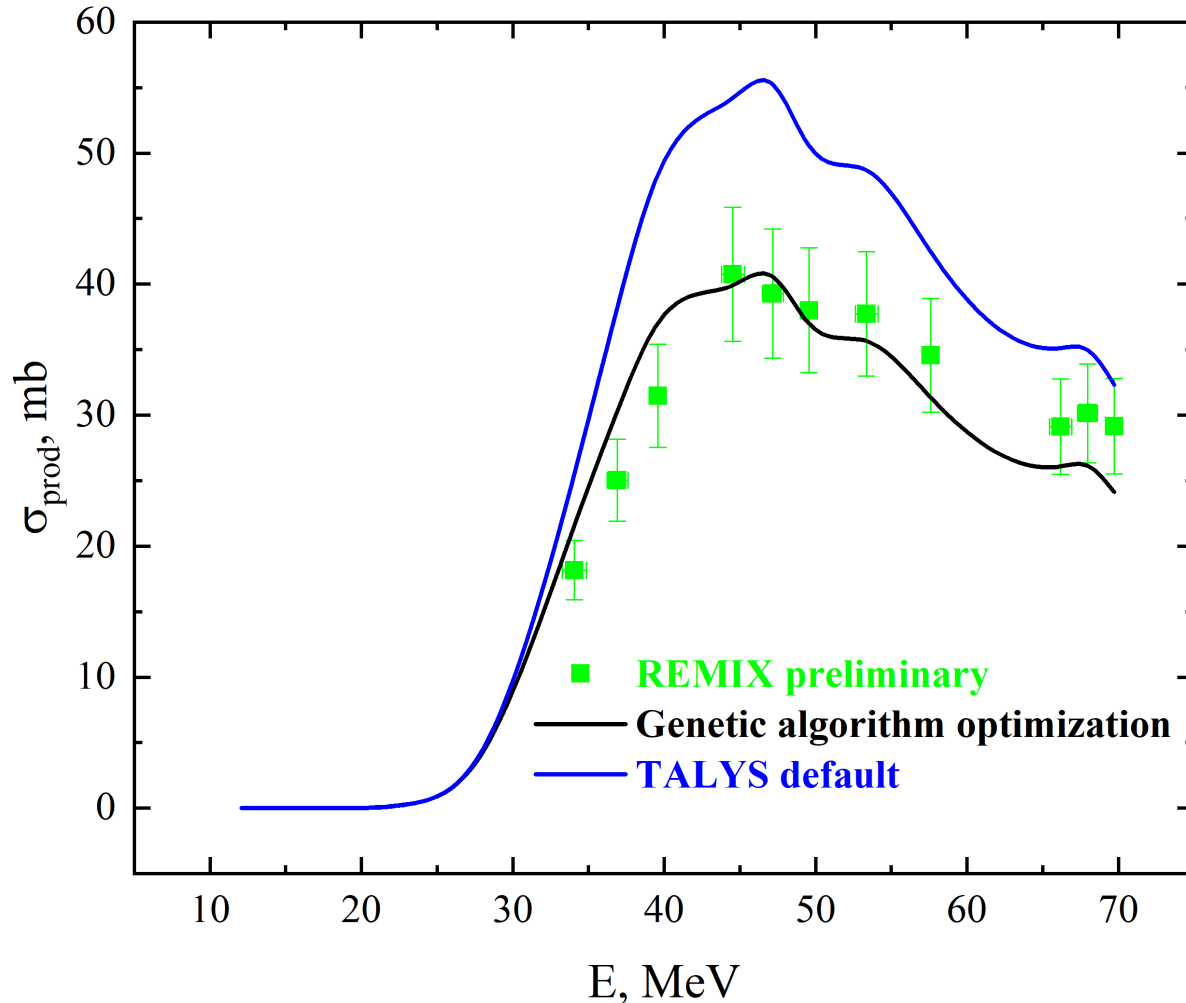
Maintaining population diversity is essential for preventing premature convergence to suboptimal solutions

Increasing the diversity of the initial population often results in a faster convergence of the fitness function



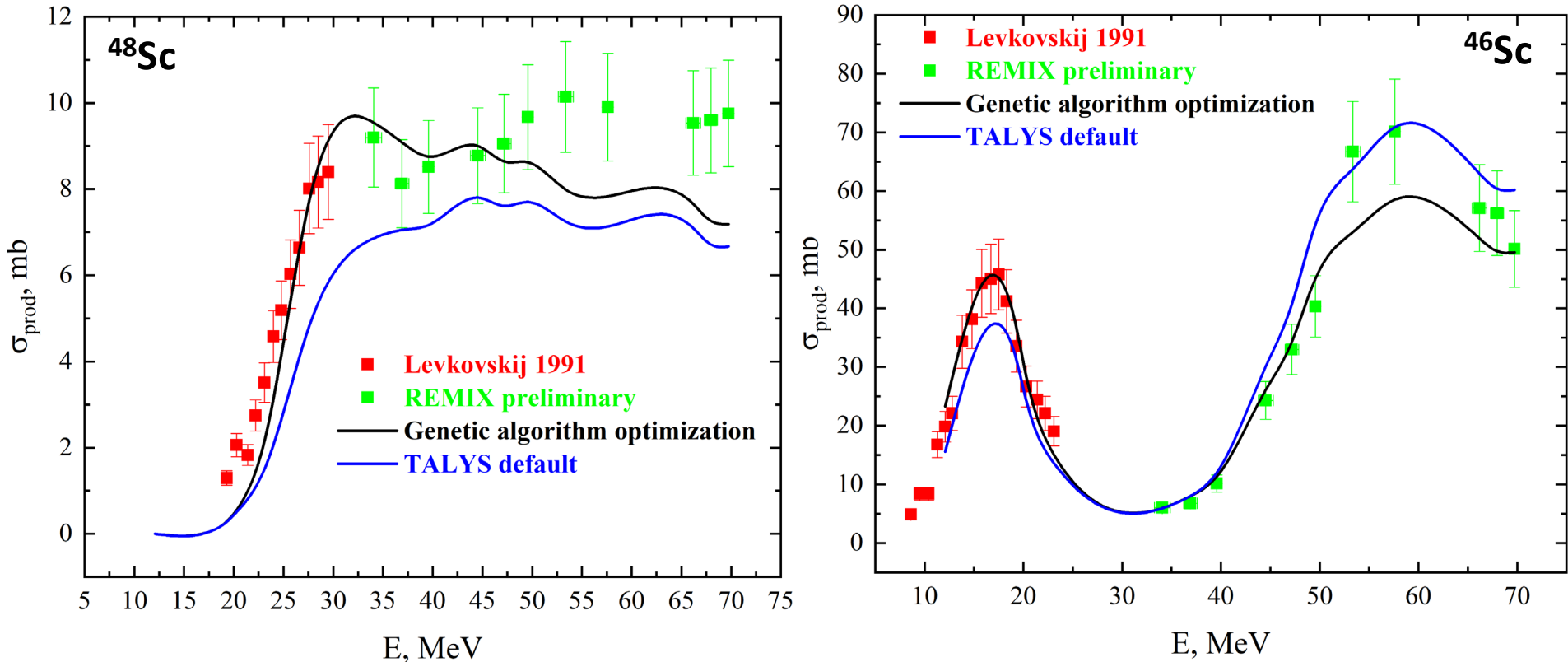
Convergence of fitness function in p-⁴⁹Ti cross section optimization vs. initial population diversity

Genetic algorithm optimization yields a superior cross-section fit compared to the default TALYS model



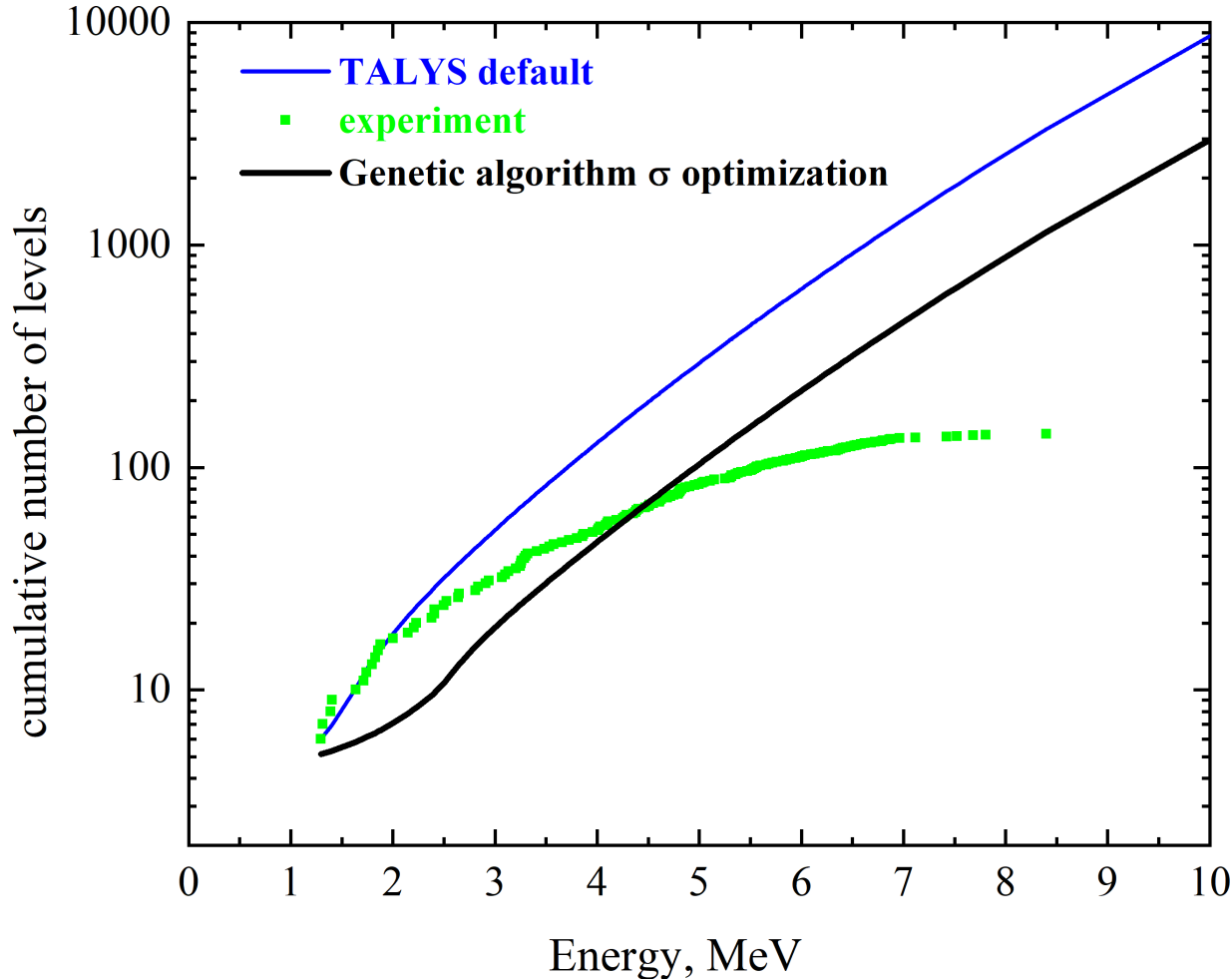
Fit of the $^{49}\text{Ti}(p,n2p)^{47}\text{Sc}$ cross section using GA optimization for level-density parameters compared to default LD model 4 values

With the genetic algorithm, we successfully fit the cross-section data for the production of 9 radionuclides



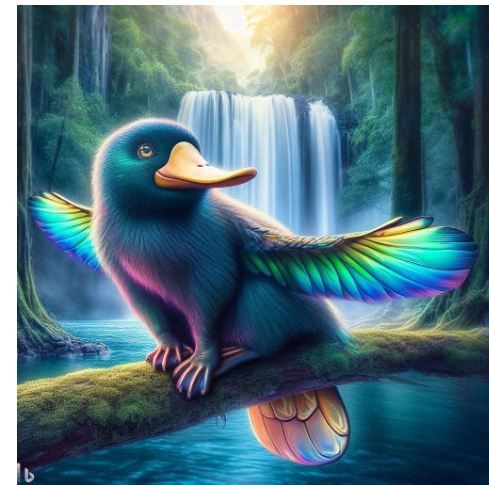
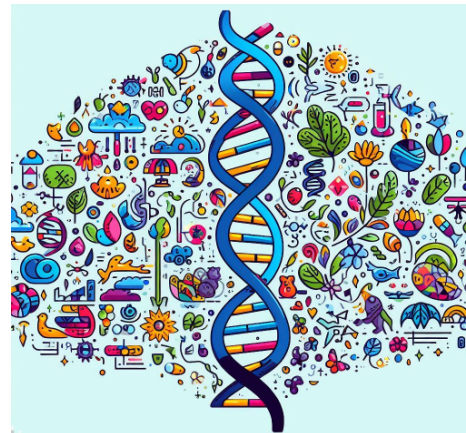
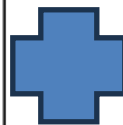
Fit of the $^{49}\text{Ti}(p,n2p)^{46,48}\text{Sc}$ cross section using GA optimization for level-density parameters compared to default LD model 4 values

TALYS default model better describes the low-energy nuclear level density of ^{47}Sc as it was tailored to fit the cumulatives



**Cumulative nuclear levels for ^{47}Sc compound nucleus:
GA-optimized vs. LD model 4 defaults**

The combination of genetic algorithm and TALYS is a powerful optimization tool for enhanced cross-section accuracy



Genetic algorithm

powerful optimization tool

