The Medical Isotope Browser

An app for prediction of radioisotope production yields

Arjan Koning and Marco Verpelli

Nuclear Data Section, IAEA

INTERNATIONAL SYMPOSIUM ON TRENDS IN RADIOPHARMACEUTICALS

#ISTR2019

28 October – 1 November 2019

Contents

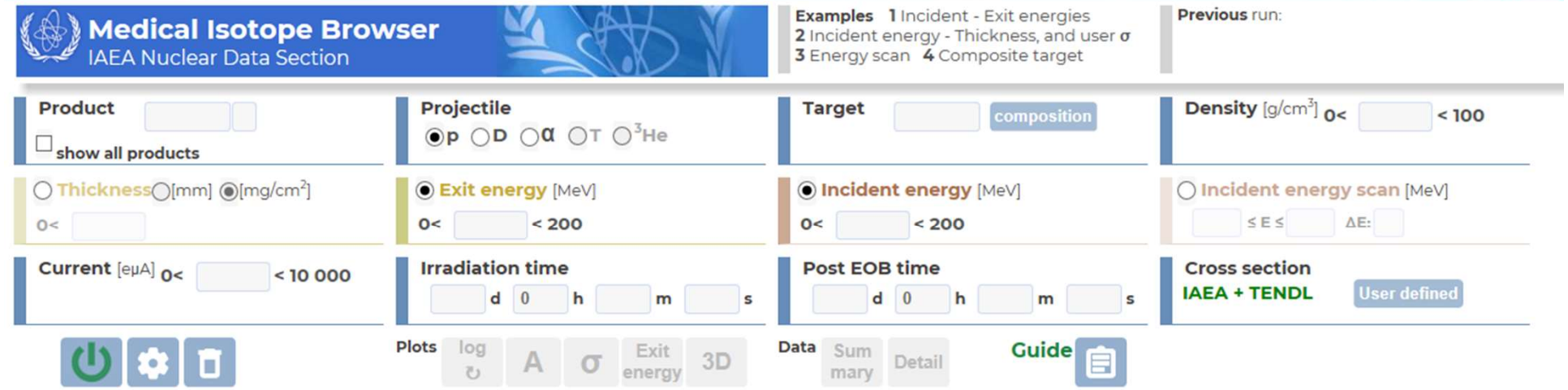
- The medical isotope browser
- Physics and nuclear data input
- Current status of visual software
- Future extensions

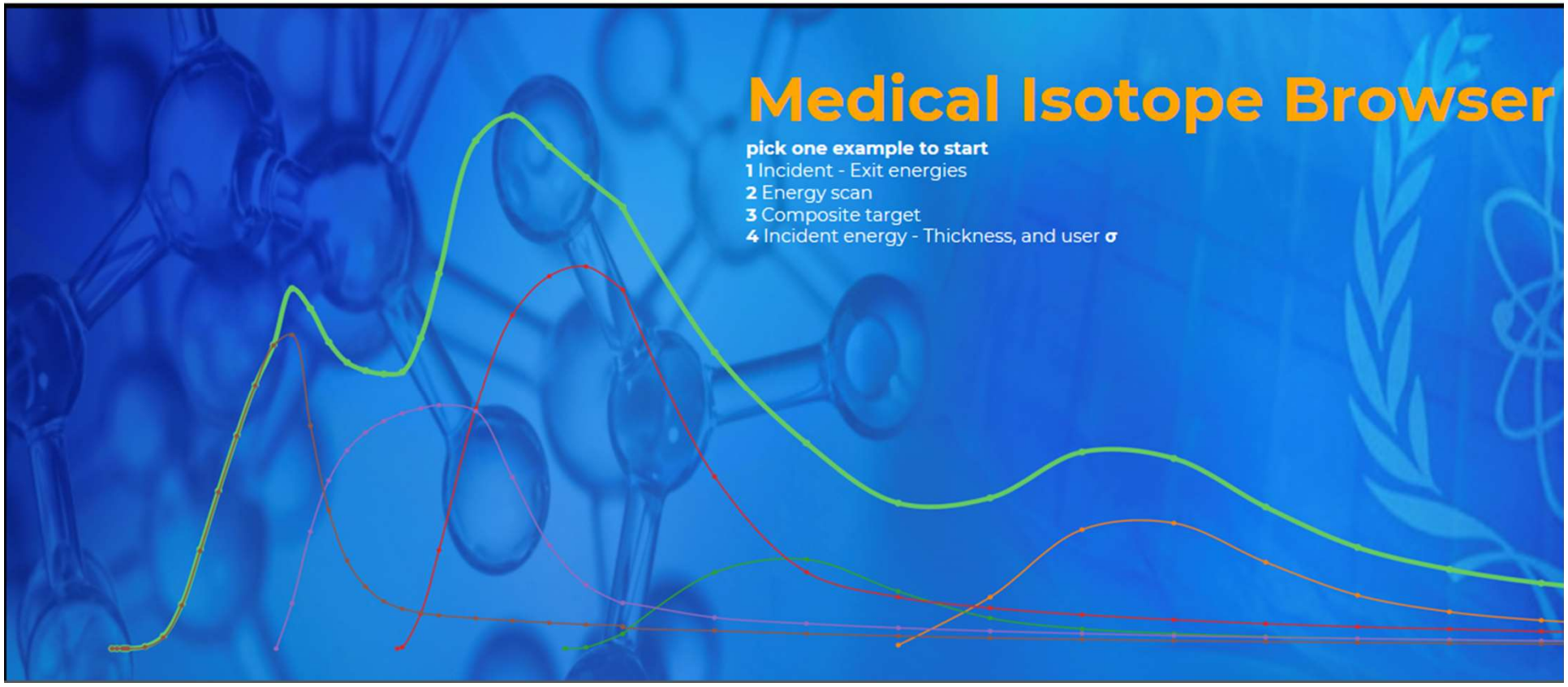
The medical isotope browser

A web application for medical isotope production on the basis of user input:

- User provides characteristics of the incident particle source:
  - Energy range
  - Specification of the target material
  - Power of the accelerator
  - Irradiation time and cooling time
- Software returns, virtually instantaneously:
  - Yield of desired isotope
  - Contaminations (unwanted side-products)
  - …in a visually attractive and descriptive way

www-nds.iaea.org/mib





Medical Isotope Browser
IAEA Nuclear Data Section

Examples 1 Incident - Exit energies
2 Incident energy - Thickness, and user σ
3 Energy scan 4 Composite target

Previous run: • 1

Product TC99 M
☐ show all products

Projectile ◉p ○D ○α ○T ○^{3}He

Target MO100 composition

Density [g/cm^3] 0< 10.3 < 100

○ Thickness ○[mm] ◉[mg/cm^2]
0<

◉ **Exit energy** [MeV]
0< 15.0 < 200

◉ **Incident energy** [MeV]
0< 22 < 200

○ Incident energy scan [MeV]
≤ E ≤ ΔE:

Current [eμA] 0< 100 < 10 000

Irradiation time 1d
1 d 0 h 0 m 0 s

Post EOB time 1d
1 d 0 h 0 m 0 s

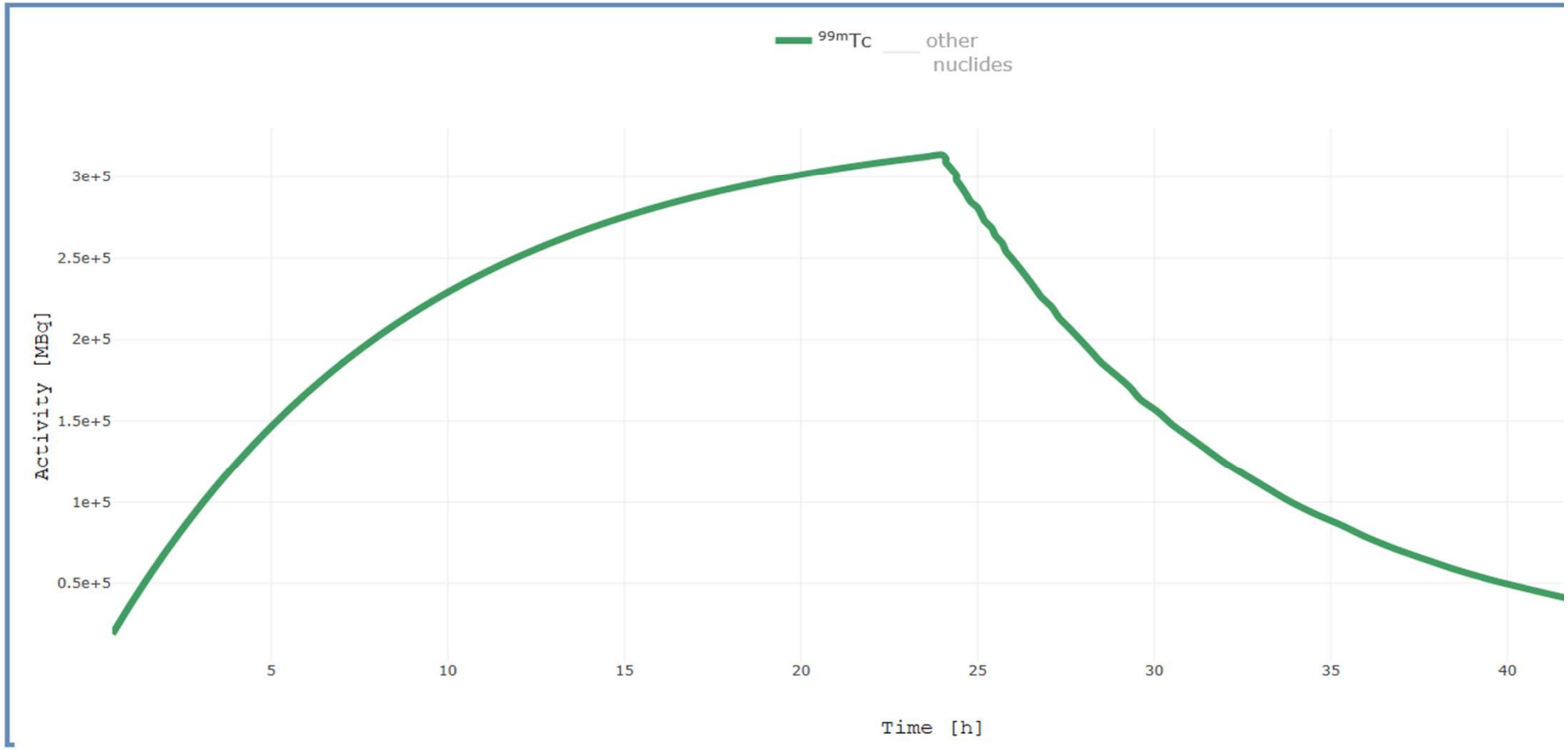
Cross section
IAEA + TENDL User defined

Plots log ↻ A σ Exit energy 3D

Data Sum mary Detail

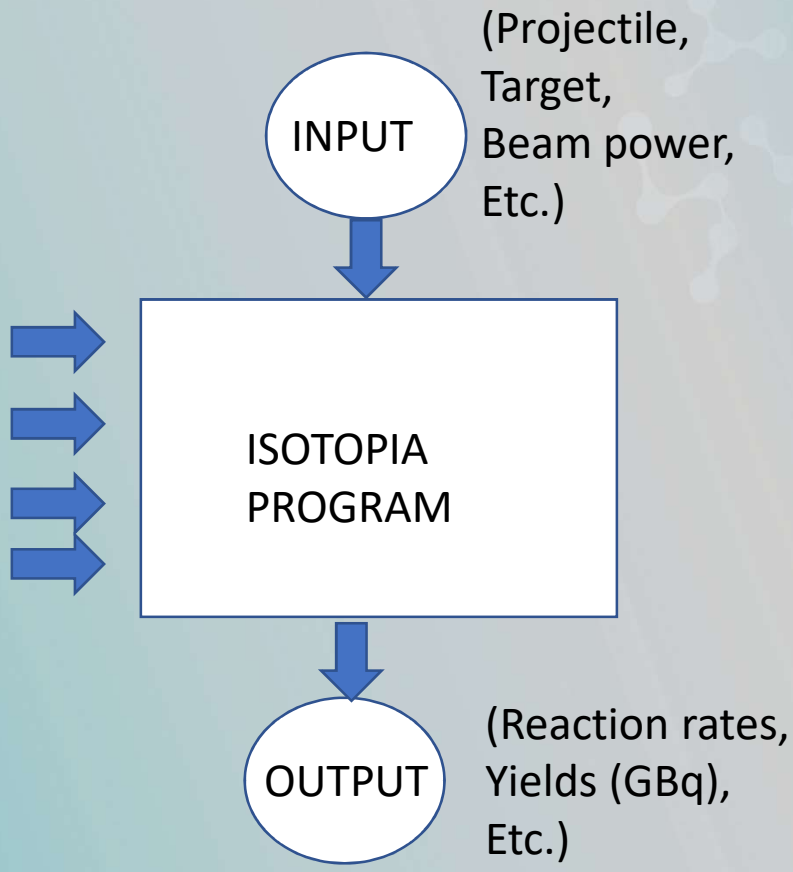
Guide

• Effective target thickness : 0.045 cm • # incident particles: 6.24151E+14 [s^-1] • Produced heat in target : 0.700 kW • Activities less than 1.0E-6 MBq are not displayed



ISOTOPIA: Predicts radioisotope yield

- Radioactive Decay Data
- Production and depletion equations
- Stopping power
- Cross section data



Calculation time: < 0.2 sec.

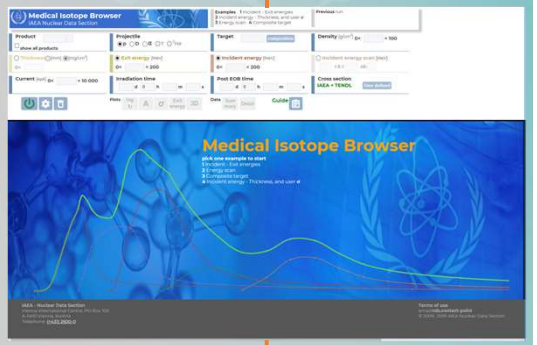
Medical Isotope Browser: GUI around ISOTOPIA

- Radioactive Decay Data
- Production and depletion equations
- Stopping power
- Cross section data

INPUT

(Projectile,
Target,
Beam power,
Etc.)

ISOTOPIA PROGRAM



OUTPUT

(Reaction rates,
Yields (GBq),
Etc.)

Calculation time: < 0.2 sec.

Essential 1: High-quality cross section data

1. E. Betak, A.D. Caldeira, R. Capote, B.V. Carlson, H.D. Choi, F.B. Guimaraes, A.V. Ignatyuk, S.K. Kim, B. Kiraly, S.F. Kovalev, E. Menapace, A.L. Nichols, M. Nortier, P. Pompeia, S.M. Qaim, B. Scholten, Yu. N. Shubin, J-Ch. Sublet, F. Tarkany et al, **Nuclear data for the production of therapeutic radionuclides**. In: S.M. Qaim, F. Tarkanyi, R. Capote (Technical editors) , IAEA Technical Reports Series no. 473, IAEA, scientific and technical report STI/DOC/010/473, IAEA Vienna, Austria (2011)

2. F. T. Tarkanyi, A. V. Ignatyuk, A. Hermanne, R. Capote, B. V. Carlson, J. W. Engle, M. A. Kellett, T. Kibedi, G. N. Kim, F. G. Kondev, M. Hussain, O. Lebeda, A. Luca, Y. Nagai, H. Naik, A. L. Nichols, F. M. Nortier, S. V. Suryanarayana, S. Takacs, and M. Verpelli**: Recommended nuclear data for medical radioisotope . production: diagnostic positron emitters**, J. Rad.Nucl.Chem. 319 (2019) 487-531.

3. A. Hermanne, A. V. Ignatyuk, R. Capote, B. V. Carlson, J. W. Engle, M. A. Kellett, T. Kibedi, G. N. Kim, F. G. Kondev, M. Hussain, O. Lebeda, A. Luca, Y. Nagai, H. Naik, A. L. Nichols, F. M. Nortier, S. V. Suryanarayana, S. Takacs, F. T. Tarkanyi, and M. Verpelli: **Reference cross sections for charged-particle monitor reactions**, Nucl. Data Sheets 148 (2018) 338-382.

4. F. T. Tarkanyi, A. V. Ignatyuk, A. Hermanne, R. Capote,B. V. Carlson, J. W. Engle, M. A. Kellett, T. Kibedi, G. N. Kim, F. G. Kondev, M. Hussain, O. Lebeda, A. Luca, Y. Nagai, H. Naik, A. L. Nichols, F. M. Nortier, S. V. Suryanarayana, S. Takacs, and M. Verpelli: **Recommended nuclear data for medical radioisotope production: diagnostic gamma emitters**, J. Rad. Nucl. Chem. 319 (2019) 533-666;

5. J. W. Engle, A. V. Ignatyuk, R. Capote, B. V. Carlson, A. Hermanne, M. A. Kellett, T. Kibedi, G. N. Kim, F. G. Kondev, M. Hussain, O. Lebeda, A. Luca, Y. Nagai, H. Naik, A. L. Nichols, F. M. Nortier, S. V. Suryanarayana,S. Takacs, F. T. Tarkanyi, and M. Verpelli: **Recommended Nuclear Data for the Production of Selected Therapeutic Radionuclides**, Nucl. Data Sheets 155 (2019) 56-74.

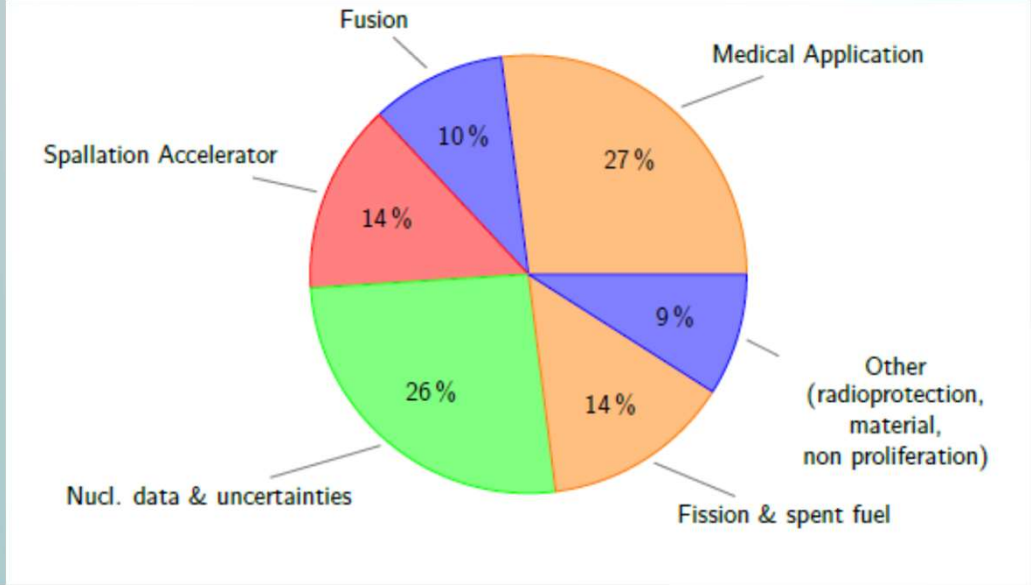
20 years of IAEA CRP's and other meetings led to ~150 high-quality nuclear reaction channels

Essential 2: Complete and good/reasonable quality cross section data

TENDL: TALYS Evaluated Nuclear Data Library

- Produced by TALYS nuclear model code + other sources
- Complete in projectile (n, g, p, d, t, h, a), target (2813 nuclides) and energy range (0-200 MeV)
- 1000-1500 citations, current version TENDL-2017
- Globally good predictive power

Use of TENDL in 2019

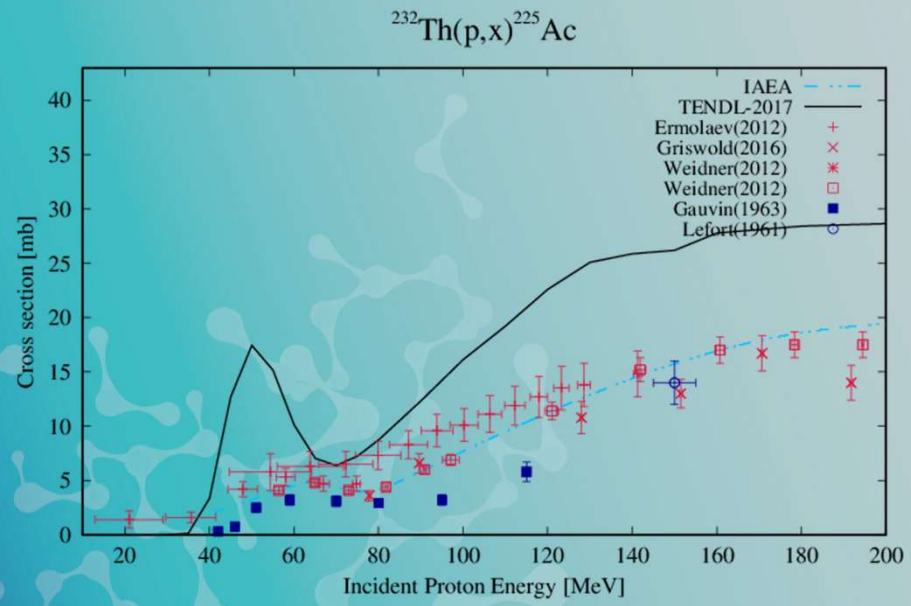


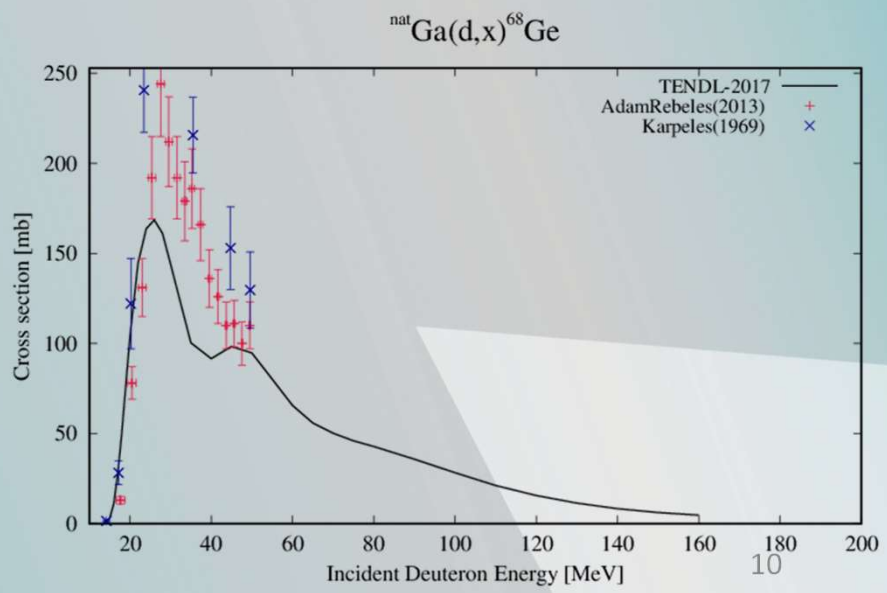
Medical isotope data library: combine the best with the most complete

IAEA high-quality evaluations (150 reaction channels)

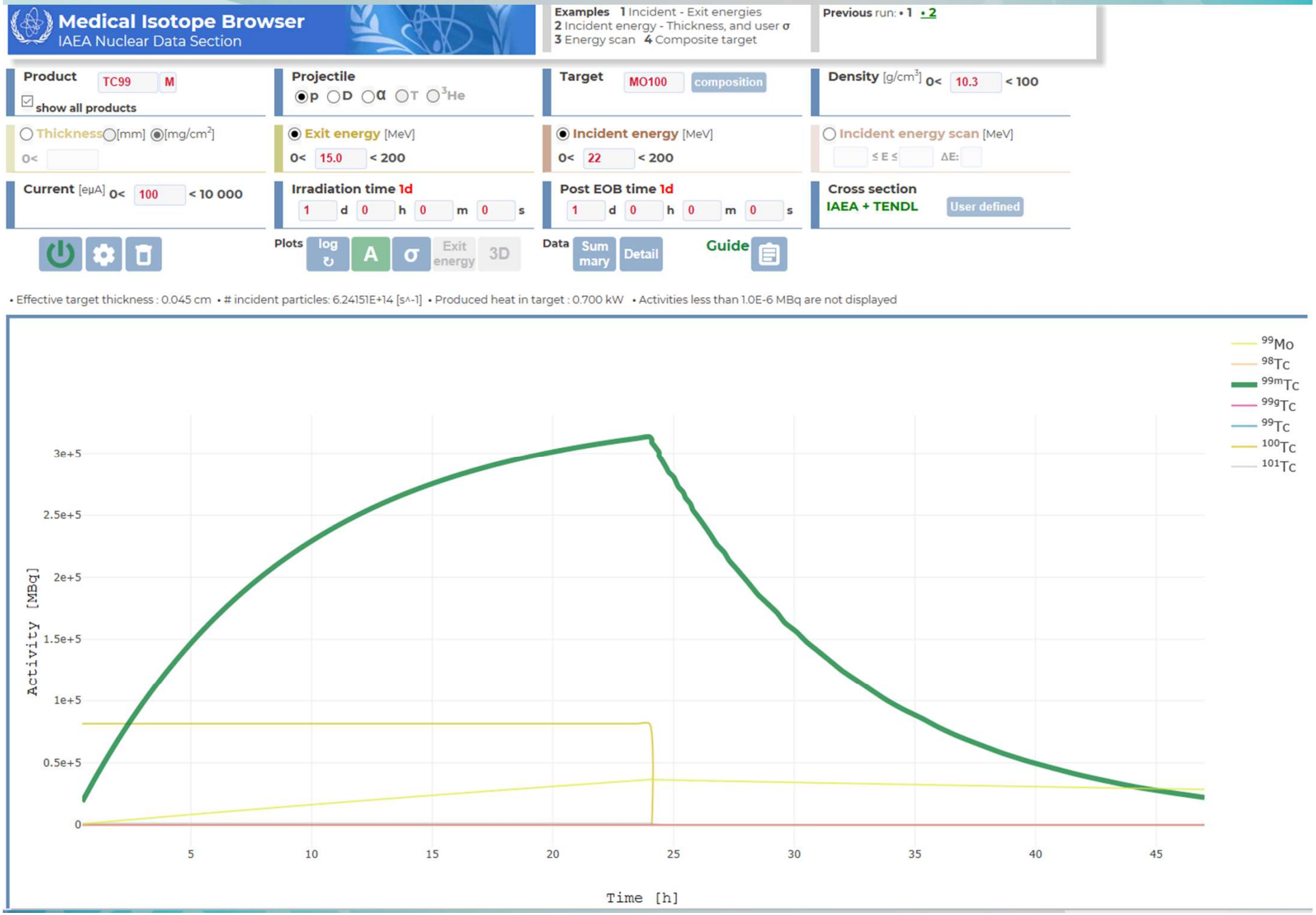
TENDL-2017

IAEA-2019 Medical Isotope Data Library





p + Mo-100: production of all isotopes



p + Mo-100 → Tc-99m: plot of cross sections

Medical Isotope Browser
IAEA Nuclear Data Section

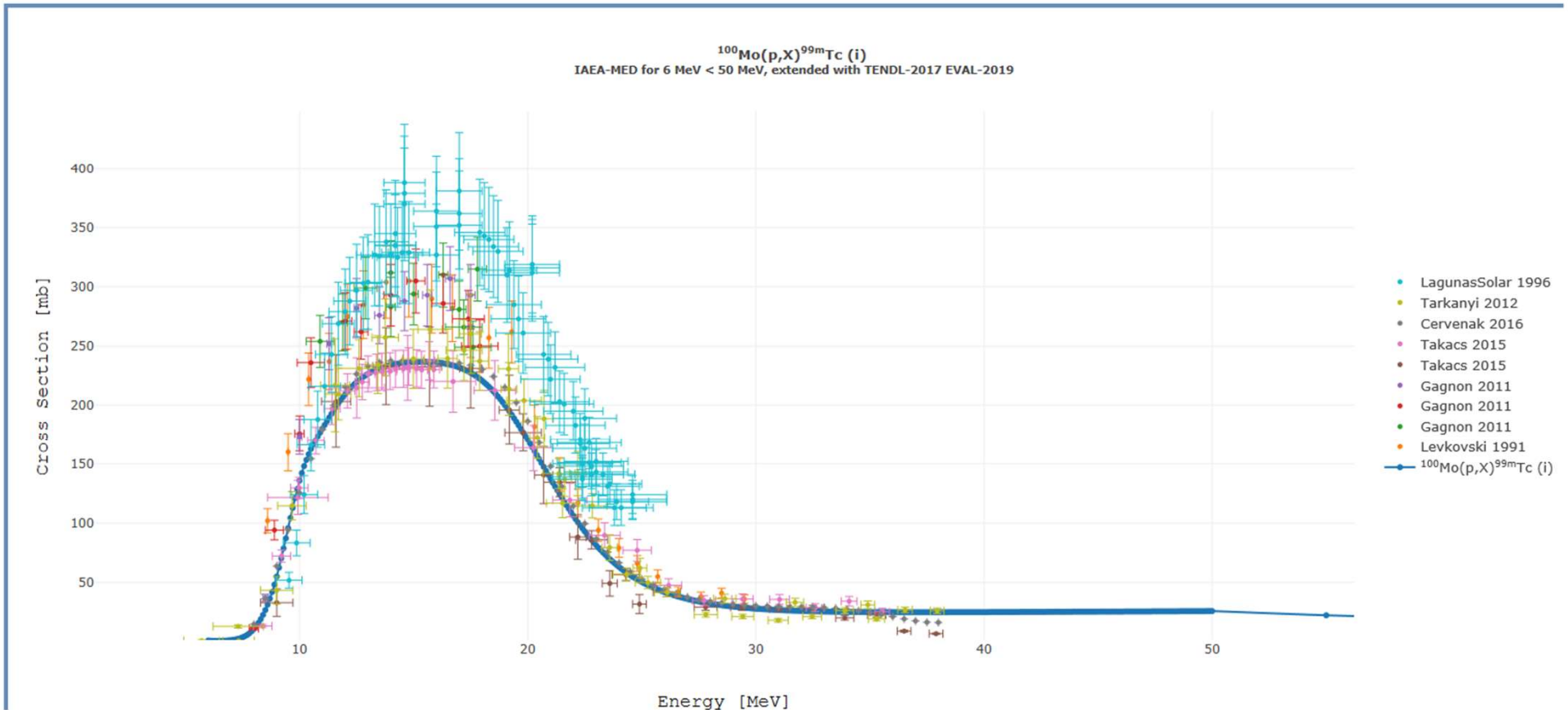
Examples 1 Incident - Exit energies
2 Incident energy - Thickness, and user σ
3 Energy scan 4 Composite target

Previous run: • 1 • 2 • 3 • 4 • 5 • 6 • 7 • 8 • 9 • 10 • 11 • 12 • 13 • 14 • 15 • 16 • 17 • 18 • 19 • 20 • 21 • 22 • 23

Product TC99 M; show all products	Projectile ◉p ○D ○α ○T ○^{3}He	Target MO100 composition	Density [g/cm^3] 0< 10.3 < 100
○ Thickness ○[mm] ◉[mg/cm^2] 0<	◉ Exit energy [MeV] 0< 15.0 < 200	◉ Incident energy [MeV] 0< 35.0 < 200	○ Incident energy scan [MeV] ≤ E ≤ ΔE:
Current [eμA] 0< 100 < 10 000	Irradiation time 1d: 1 d 0 h 0 m 0 s	Post EOB time 1d: 1 d 0 h 0 m 0 s	Cross section IAEA + TENDL User defined

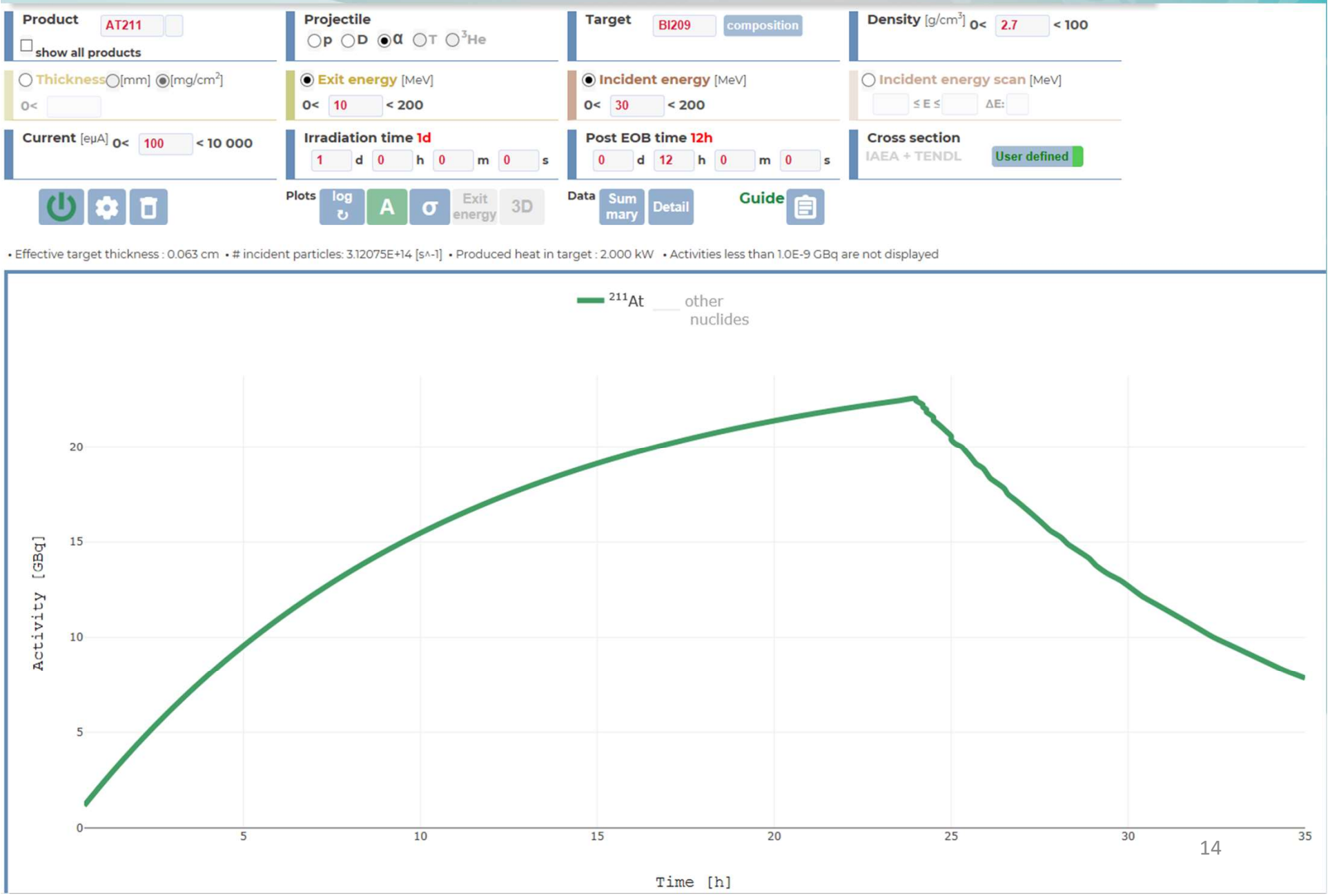
Plots: log ↻ A σ Exit energy 3D Data: Sum mary Detail Guide

• Effective target thickness : 0.161 cm • # incident particles: 6.24151E+14 [s^-1] • Produced heat in target : 2.000 kW • Activities less than 1.0E-9 GBq are not displayed



p + Ca-44 → Sc-44 : finding the optimal incident energy

α + Bi-209 → At-211



p + Ga-69 → Ge-68: 3D plot – Activity, time, energy

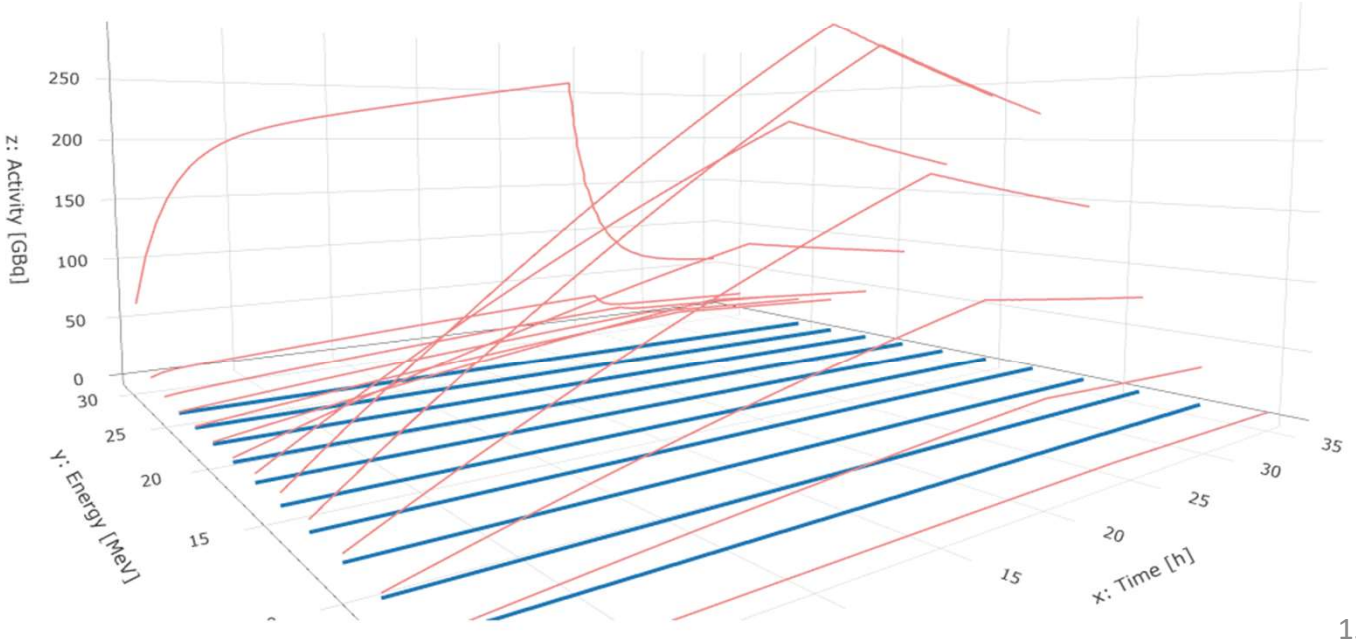
Medical Isotope Browser
IAEA Nuclear Data Section

Examples 1 Incident - Exit energies
2 Incident energy - Thickness, and user σ
3 Energy scan 4 Composite target

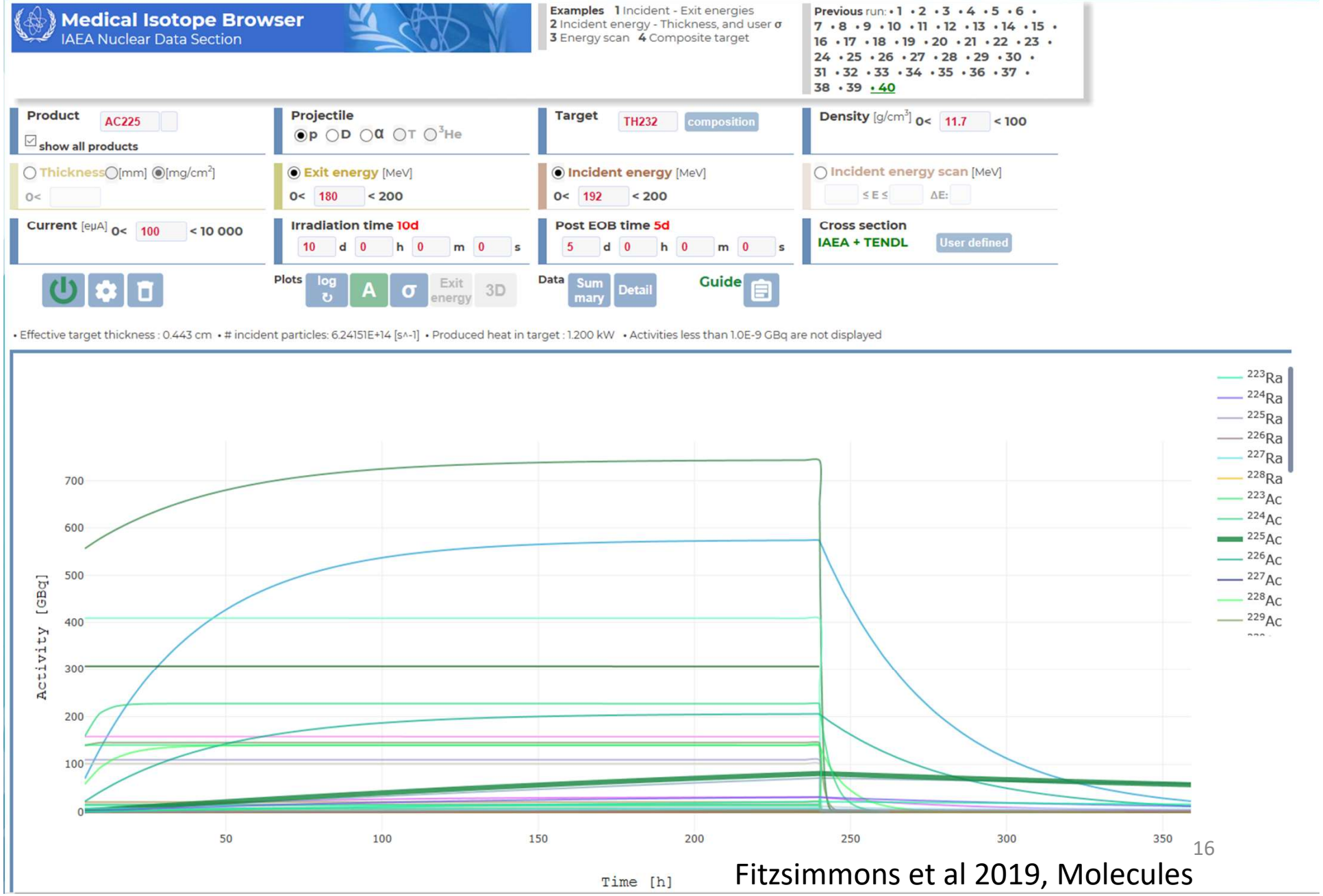
Previous run: • 1 • 2 • 3 • 4 • 5 • 6 • 7 • 8 • 9 • 10 • 11

Product GE68 ☐ show all products	Projectile ◉p ○D ○α ○T ○^{3}He	Target GA69 composition	Density [g/cm^3] 0< 2.7 < 100
◉ Thickness ○[mm] ◉[mg/cm^2] 0< 300	○ Exit energy [MeV] 0< < 200	○ Incident energy [MeV] 0< < 200	◉ Incident energy scan [MeV] 5 ≤ E ≤ 30 ΔE: 2
Current [eμA] 0< 100 < 10 000	Irradiation time 1d 1 d 0 h 0 m 0 s	Post EOB time 12h 0 d 12 h 0 m 0 s	Cross section IAEA + TENDL User defined

Plots log A σ Exit energy 3D Data Sum mary Detail Guide



p + Th-232 → Ac-225 at 192 MeV



Fitzsimmons et al 2019, Molecules

Click on radioisotope: direct link to IAEA's Livechart webpage with all decay information

List of updates
Mar 2018 to Jan 2019

Mass chains
β and ec decays plotting

Neutron Cross Sections
Resonance Integrals

Live Chart of Nuclides nuclear structure and decay data

Go to Nuclide: 225AC Show Chart

Ground State - Isomers | Levels | Gammas | **Decay Radiation** | Nuclear Moments | Ther. Neutrons Capture | Fission Yields | Schema Plot

Comments · **Click** on a column header to open the guide · **Uncertainty** for numeric values refers to the last digits of the value: **12.1 *23* means 12.1 ± 2.3**
Data from: ENSDF apart Q from AME2016 · **Definitions & Sources**

Evaluation: Ashok Jain, Sukhjeet Singh, Suresh Kumar, Jagdish Tuli **Publication cut-off**: 15-Jan-2007 **ENSDF insertion:** 2007-05 **Publication:** Nuclear Data Sheets 108, 883 (2007)

Parent	$T_{1/2}$	E_x [keV]	Jp order	Decay	Q_{decay} note on Q value	Daughter	Comments	Total energy by radiation type, per 100 decays of the parent [keV]										
								Alpha	Beta	CE & Auger	γ & X	Unplaced γ	Recoil	Neutrino	Absorbed	Total	Q * BR	Delta
$^{225}_{89}Ac_{136}$	9.9203 d *3*	0.0	(3/2-)	α 100 %	5935.1 *14*	$^{221}_{87}Fr_{134}$		5775.814 *1.126*	0.000 *0.000*	14.672 *1.426*	13.959 *0.496*	0.071 *0.004*	103.376 *2.271*	0.000 *0.000*	5907.821 *2.950*	5907.821 *2.950*	5935.1	27.279

see the ENSDF source

Note: Q-value used in ENSDF to determine displayed decay data is: 5935.1 *14* keV - see **note on Q value**

Alpha CSV

E_α [keV]	I_α(abs) [%]	Daughter level [keV]	J^π	HF	Comments
5021	≤ 0.001	824.2 *7*		≥ 18	
5067 *5*	0.003 *1*	780.2 *4*		11 *4*	
5092 *4*	0.006 *1*	749.16 *20*		8.7 *15*	
5131 *5*	0.0020 *8*	714.2 *6*		42 *17*	
5131 *5*	0.0020 *8*	712 *5*		44 *18*	
5202 *5*	0.0020 *5*	637.72 *11*		118 *30*	
5211 *3*	0.030 *3*	630.72 *13*	(5/2+)	8.7 *9*	
5239 *4*	0.0030 *8*	602.3 *7*	(5/2-)	128 *35*	
5270 *4*	0.014 *5*	570.83 *16*	(7/2+,5/2+)	41 *15*	
5286 *3*	0.23 *1*	552.05 *9*	(3/2)-	3.18 *15*	
5321 *3*	0.07 *1*	517.81 *12*	(5/2+)	16.3 *24*	
5436 *4*	0.07 *2*	400.62 *24*	(7/2-)	71 *21*	
5443 *3*	0.14 *1*	393.28 *15*	(7/2,5/2)+	39 *3*	
5540 *4*	0.015	294.7 *6*	(9/2)+	1225	
5545 *4*	0.03 *1*	288.14 *17*	(9/2)-	6.6E2 *23*	
5554 *4*	0.1	279.21 *11*	(7/2)+	222	
5563 *4*	0.034	272.7 *6*	(7/2-,9/2-)	698	

pop out Highlight: (keV) level Image Height: Image Width: Replot

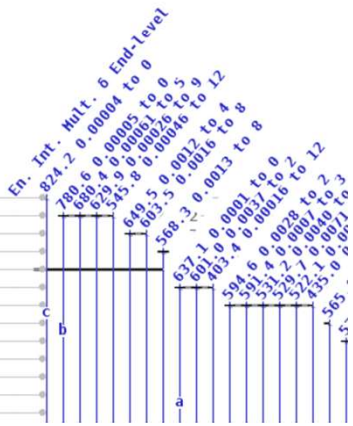
$^{225}_{89}Ac_{136}$

(3/2-) 0.0 10.0 d 1

Q⁺ 5935.1 keV 14

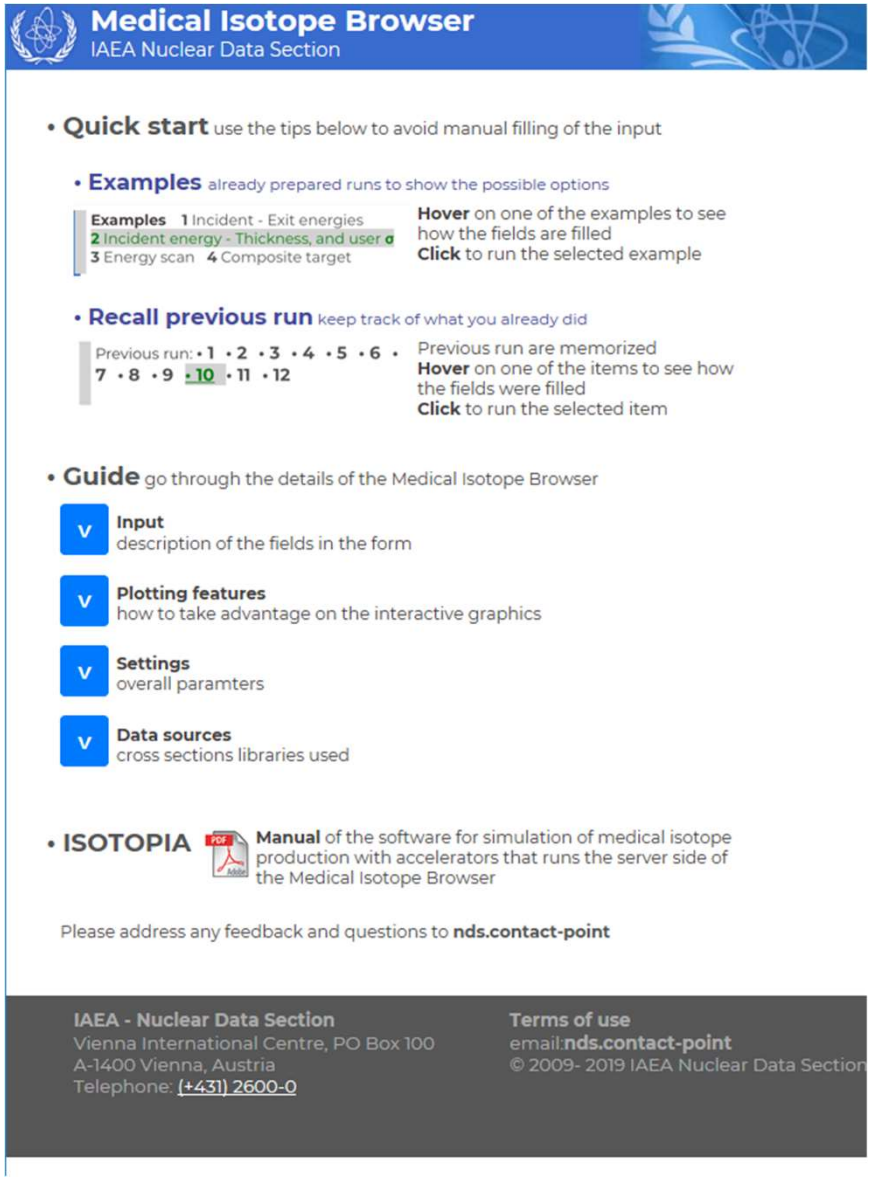
A : 100 % 0--> $^{221}_{87}Fr_{134}$

En [keV]	I%	HF	#	Jp	En [keV]
5021	≤0.001	≥18	32		824.2
5067	0.003	11	31		780.2
5092	0.006	8.7	30		749.16
5131	0.0020	42	29		714.2
5131	0.0020	44	28		712
5202	0.0020	118	27		637.72
5211	0.030	8.7	26	(5/2+)	630.72
5239	0.0030	128	25	(5/2-)	602.3
5270	0.014	41	24	(7/2+,5/2+)	570.83
5286	0.23	3.18	23	(3/2)-	552.05
5321	0.07	16.3	22	(5/2+)	517.81
5829.9			21		497.3
5829.9			20		410.3



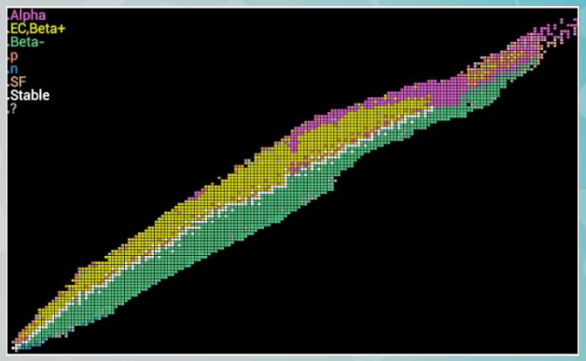
Other features

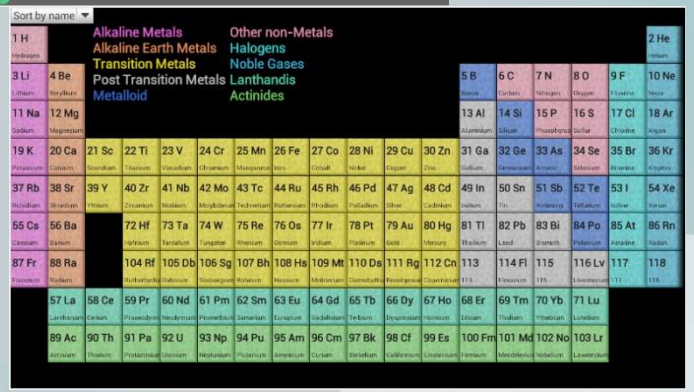
- Specify enriched targets
- Insert your own cross section files
- All important output also as text files and tables
- User guide available on the website



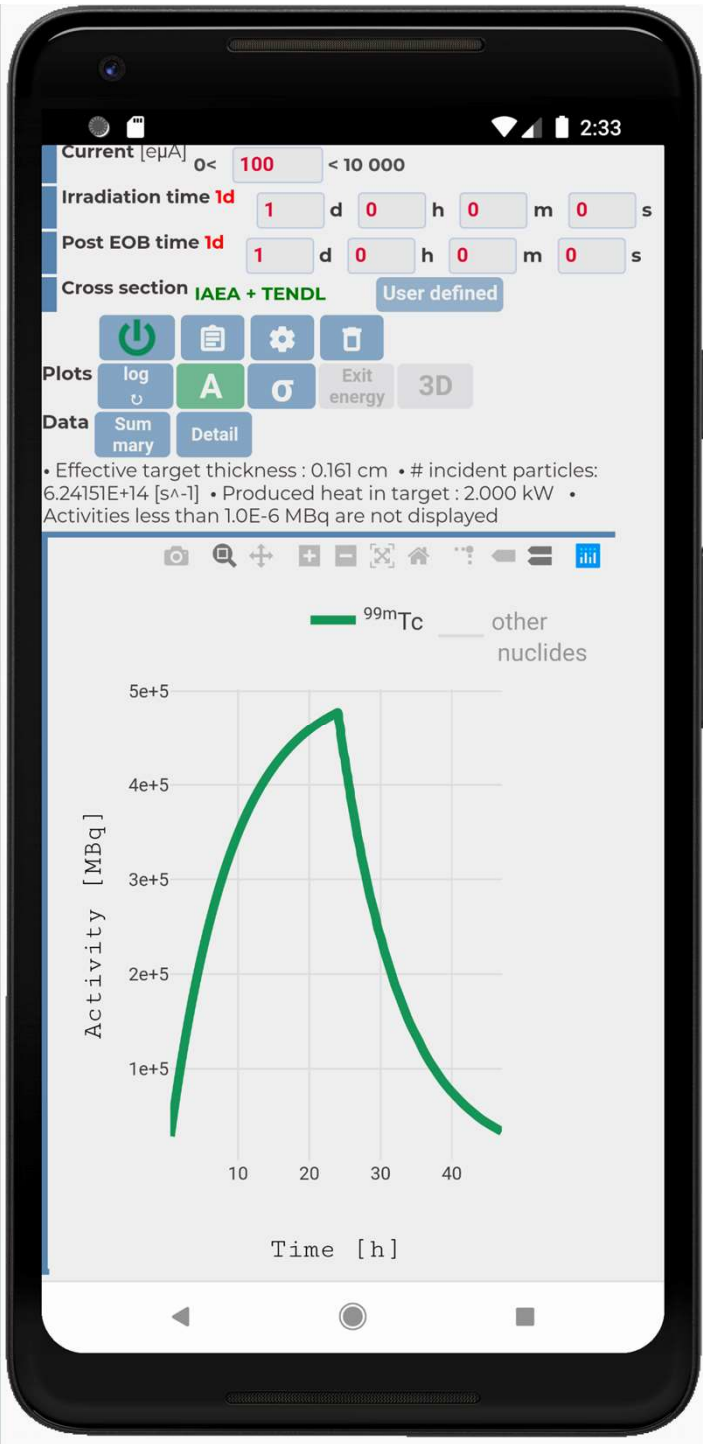
Isotope Browser – App for smart phones

- Isotope Browser; Properties of over 4,000 isotopes; Interactive App for android & Apple i devices. *http://play.google.com/store/apps*
- Independent of internet
- ~92,000 downloads in 5 y
- Now in **10 languages** (6 UN + Jap. + Slov. + Ital. + Trad. Chinese)





Yes,
it works
on your
phone



Future options (in order of priority)

- Add reactor-based production (neutrons), both for fission products and activation
- Add photonuclear route (electron accelerator)
- Improvement of the cross section data libraries
- Include uncertainties for cross sections and final yields
- (Semi-)automatically assess how hazardous the produced contaminations are
- Medical isotope “funnel”: Automatically find promising radioisotopes on the basis of their decay characteristics
- Solve the “inverse problem”: User gives a desired radioisotope and all production routes are calculated and compared

Acknowledgments to beta testers

- Participants of the Technical Meeting on Nuclear Data for Medical Applications, 10-13 December, 2018 IAEA, Vienna (R. Capote Noy et al)
- Our colleagues from Radioisotope Products & Radiation Technology Section (J. Osso et al)
- You, from now on

Summary

- The Medical Isotope Browser is accessible at
  www-nds.iaea.org/mib
- Aims to bring fundamental nuclear data directly to straightforward use in radiopharmaceutical research and industry
- Gives a direct first guess whether a production route is viable
- Your feedback will make this product better

Finally

- If you think this tool is great, tell others
- If you have complaints about this tool, tell us*

*nds.contact-point@iaea.org

THANK YOU!

INTERNATIONAL SYMPOSIUM ON TRENDS IN RADIOPHARMACEUTICALS

#ISTR2019

28 October – 1 November 2019