NATIONAL NUCLEAR LABORATORY

CARP

Development of a new tool for modelling medical radionuclide production

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Acknowledgements

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"Strengthening the European Chain of sUpply for the generation medical RadionuclidEs"

- **Sustainability of medical isotope production**
- **Focus on irradiation target and production route developments**

Presentation Contents

1. What is CARP?
2. How does CARP work? (ish)
3. Example inputs and outputs
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What is CARP

Computational Assessment of Radionuclide Production

- **New tool for modelling the nuclide composition of irradiated target materials**
- **Inputs:**
  - Target information (geometry, composition, mass etc.)
  - Irradiation conditions
- **Outputs**
  - Stepwise evolution of the target nuclide inventory
  - Inc. parameters of interest e.g per nuclide contributions to alpha, beta and gamma emissions
  - Nuclide agnostic

What is CARP?

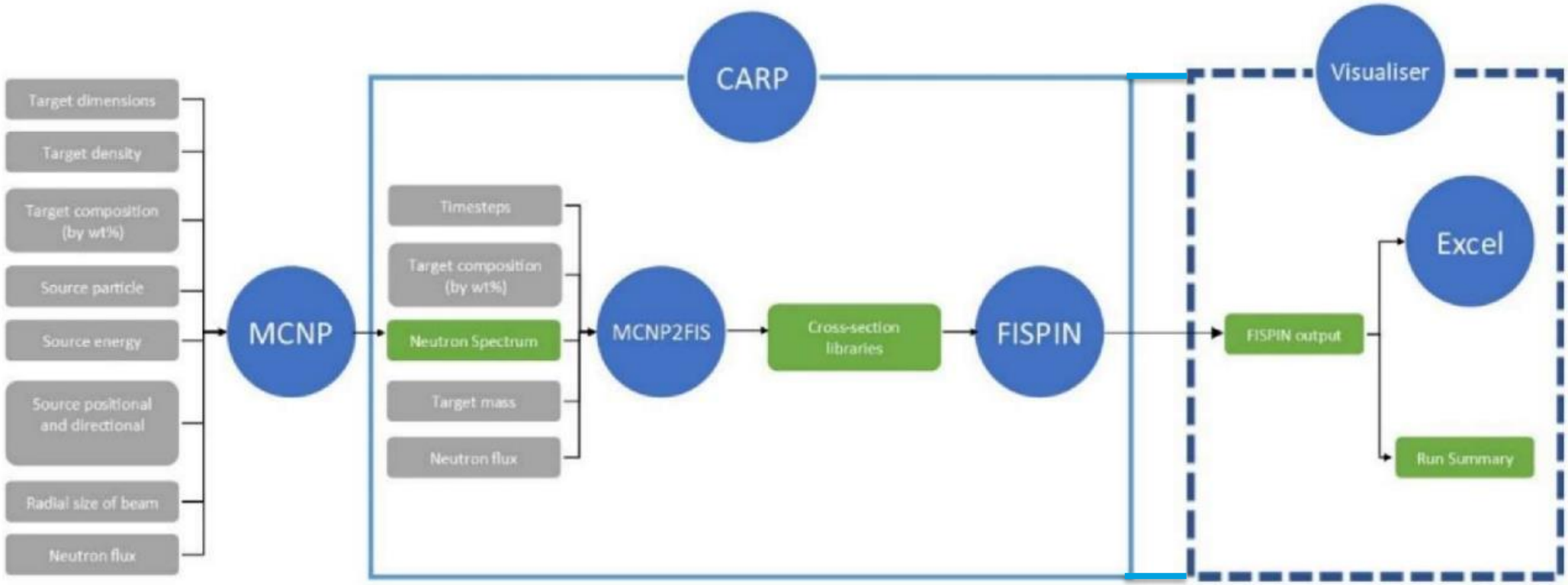
Aims:

To produce a flexible, batch operable, and easy to use tool for the quick assessment and optimisation of radionuclide production routes by incident particle beams.

To produce simple, human readable and flexible outputs to advise on the pitfalls and benefits of production routes.

To produce a collaborative tool for research purposes to support the medical radionuclide production community, and accelerator system and research reactor beam communities.

How does CARP work?

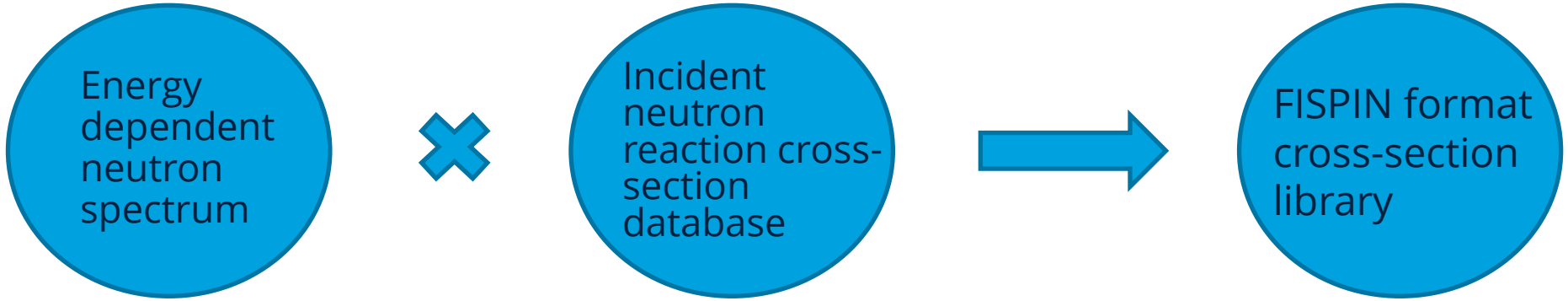


How does CARP work? - FISPIN

- **So what is FISPIN?**
  - **UK nuclear fuel inventory code – used for validation of UK reactors, reprocessing facilities etc.**
  - **In development since the 70's, FISPIN 10 (90's/00's) was used for various reactor validation cases throughout Europe**
  - **New version FISPIN 11 – acts as a calculation kernel – not constrained to reactors – can model incident particle scenarios**

0 dimensional...

How does CARP work? – MCNP -> CARP



- **Uses recommended NJOY equations to emulate continuous neutron flux – as in ORIGEN**
- **Translates beam and target information into a FISPIN usable format**
- **TENDL-2017, 2021, ENDFB-VIII**
- **Energy bin agnostic**

How does CARP work? - Summary

- MCNP generates a beam specific particle spectrum across the target
- This particle spectrum is cross-referenced against a cross-section database to produce a FISPIN cross-section library containing the beam data
- The FISPIN kernel calculates the stepwise inventories of the target using this data, producing inventories at the user specified timesteps
- A number of behind the scenes calculations e.g. activity, mass
  - Visualised into a user friendly excel file

Example inputs/outputs - Input

```
////////////////////////
//Output file name
////////////////////////

NAME

Example_case

////////////////////////
//Target and irradiation data
////////////////////////

TARGET

Zn64    47.509620
Zn66    28.125974
Zn67    4.195971
Zn68    19.526883
Zn70    0.641552
O compound with Zn 1

TOTAL MASS

2.22e-3 g

PARTICLE

neutron

FLUX

0 seconds 6.73E+13
0.5 hours 6.75E+13
0.5 hours 0

TIME

0.5 h
20 d
```

Target information

Beam information

Calculation times

```
////////////////////////
//Energy boundaries (eV)
////////////////////////

TRF

0.625
8000

BW

0.1
820300

////////////////////////
//Directories and files
////////////////////////

MCNP

C:\dummy_directory\dummy_data\dummy_mcnp_file.txt

NUCLIDES

C:\dummy_directory\dummy_data\nuclides_file.txt

REACTIONS

C:\dummy_directory\dummy_data\reactions_file.txt

XSEC

C:\dummy_directory\dummy_data\TENDL17_processed\
```

MCNP file

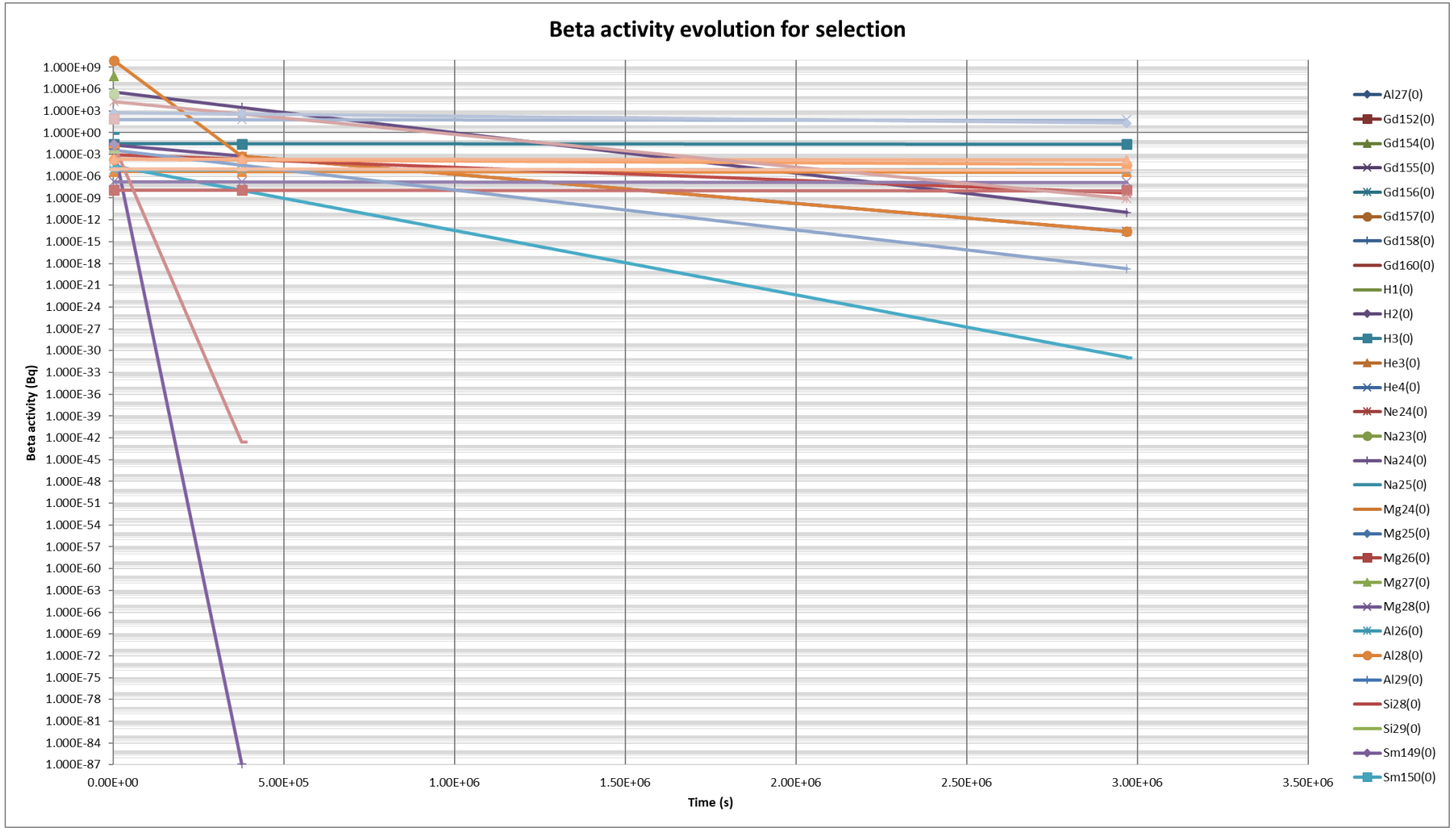
Nuclide and reaction files

Cross-section libraries

Example inputs/outputs - Output

Time (s)			7.007E+05									
Inventory			target									
Nuclide fissile are shaded	Z	ZAI	Mass kg	Moles	Atoms	Tot Activity Bq	Alpha Bq	Beta Bq	Alpha Power MeV/s	Beta Power MeV/s	Gamma+X-Ray Power MeV/s	Heat W
Eu160(0)	63	631600	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
Gd151(0)	64	641510	4.019E-17	2.663E-16	1.604E+08	1.038E+01	1.038E-07	1.038E+01	2.772E-07	4.030E-01	7.306E-01	1.816E-13
Gd153(0)	64	641530	1.851E-12	1.210E-11	7.289E+12	2.416E+05	0.000E+00	2.416E+05	0.000E+00	1.057E+04	2.577E+04	5.821E-09
Gd159(0)	64	641590	1.074E-14	6.755E-14	4.068E+10	4.220E+05	0.000E+00	4.220E+05	0.000E+00	1.302E+05	2.397E+04	2.471E-08
Gd161(0)	64	641610	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
Gd162(0)	64	641620	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
Gd163(0)	64	641630	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
Tb158(0)	65	651580	1.618E-23	1.025E-22	6.171E+01	7.504E-09	0.000E+00	7.504E-09	0.000E+00	8.384E-10	6.106E-09	1.113E-21
Tb159(0)	65	651590	1.525E-11	9.593E-11	5.777E+13	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
Tb160(0)	65	651600	1.911E-19	1.195E-18	7.194E+05	7.983E-02	0.000E+00	7.983E-02	0.000E+00	2.054E-02	9.019E-02	1.774E-14
Tb161(0)	65	651610	8.610E-13	5.350E-12	3.222E+12	3.741E+06	0.000E+00	3.741E+06	0.000E+00	7.509E+05	1.263E+05	1.405E-07
Tb162(0)	65	651620	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
Tb163(0)	65	651630	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00

Example inputs/outputs - Output



Verification & validation work – EK data

- **Acquired V&V data from EK under the EU SECURE project:**
  - **EK run the Budapest Research Reactor (BRR)**
  - **Multiple beam lines**
  - **Irradiating samples for medical radionuclide production research**
  - **Gamma scan data and FISPACT modelled data made available**

Verification & validation work – EK data

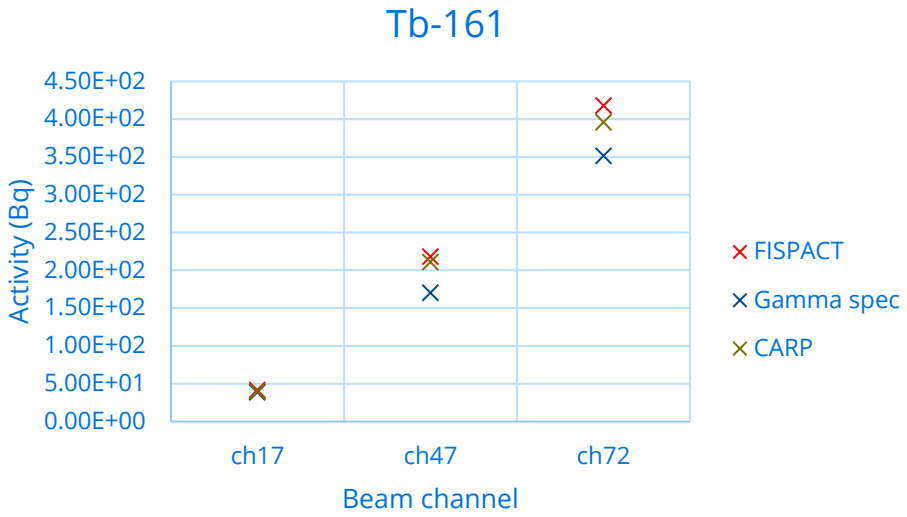
- **Three target types irradiated in three beam lines for 30-60 mins, cooled for ~4-6 days**

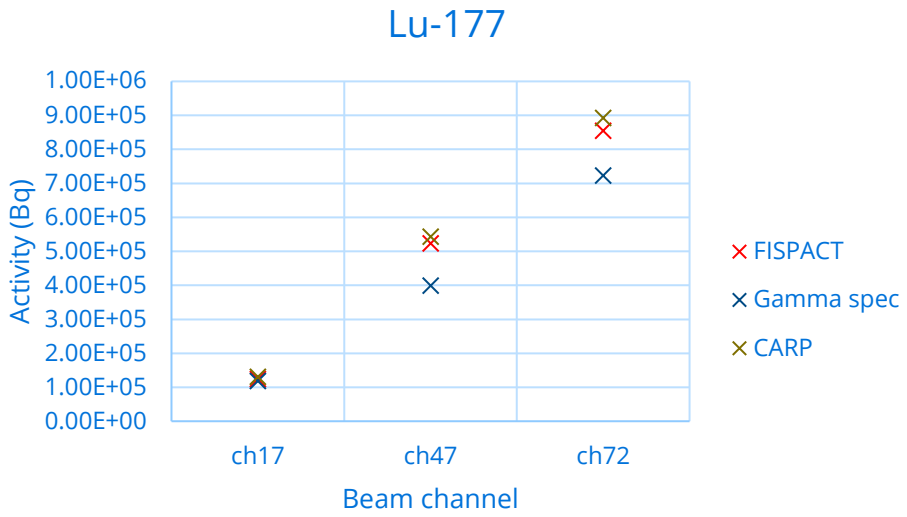
Gd diluted Al foil → Tb-161

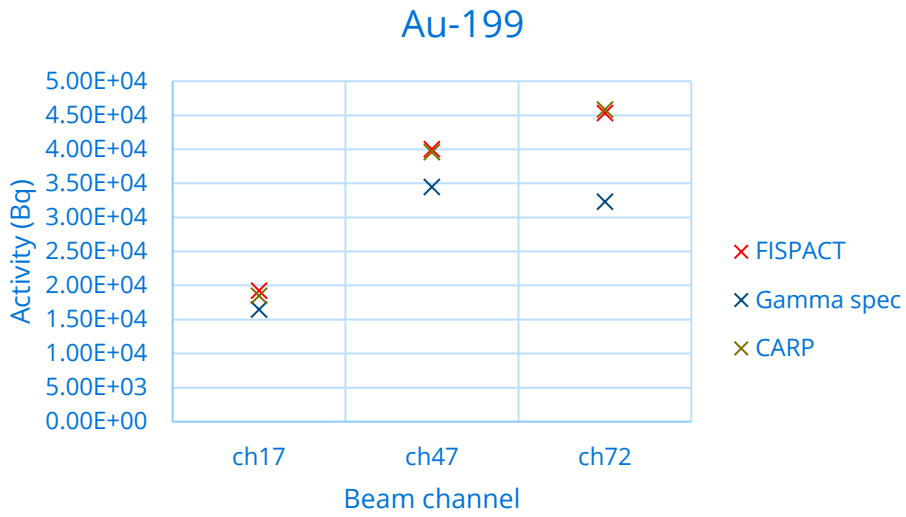
Lu diluted Al foil → Lu-177

Pt diluted Al foil → Au-199

Verification & validation work – EK data







Verification & validation work – EK data

- **Two further target types irradiated in a single beam line for 20-30 mins, cooled for 8 and 41 days**

$Gd_2O_3 \rightarrow$ Tb-161

$Lu_2O_3 \rightarrow$ Lu-177

Product nuclide	FISPACT (Bq)	Gamma spec (Bq)	CARP (Bq)
Tb-161	3.79E+06	2.87E+06	3.74E+06
Lu-177	7.26E+07	5.12E+07	6.87E+07

Verification & validation work

- **We hope to receive further reactor beam validation data from other SECURE partners**
- **Verify against FISPACT**
- **Always on the search for more!**
  - **Accelerator beam scenarios**
  - **Alternative particle types**
    (Where nuclear data is available…)

Intended uses and future work

- Future developments
  - Batch mode
  - User defined thresholds
  - Mid process separation

- Intention is to use CARP in collaborative work
  - Optimising existing experiments
  - Modelling novel and/or complex scenarios

- And to collaborate in understanding what CARP should do!

Strengthening the European Chain of sUpply for next generation medical RadionuclidEs

Thank you!

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