

# Validation of the Geant4 radioactive decay and emission of Auger electrons

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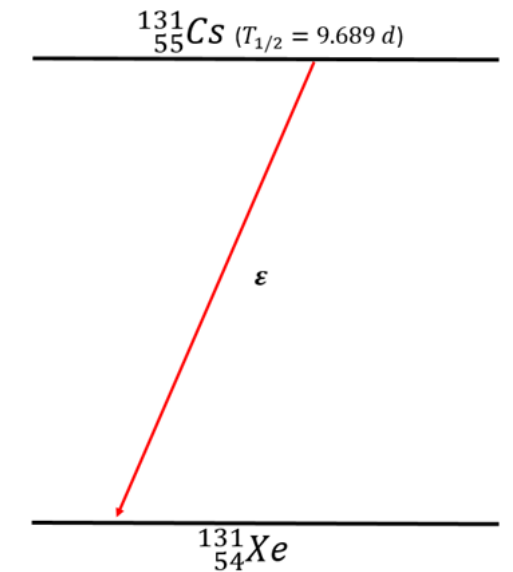
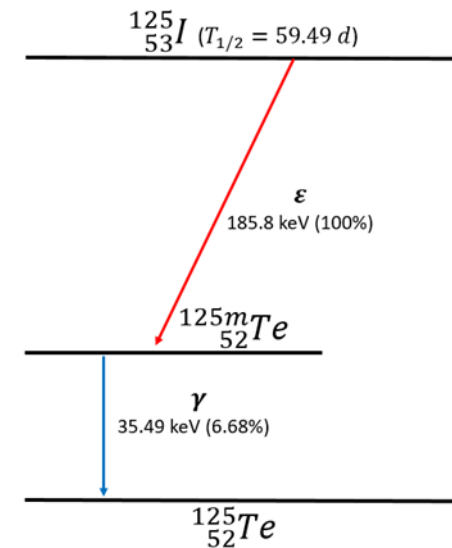
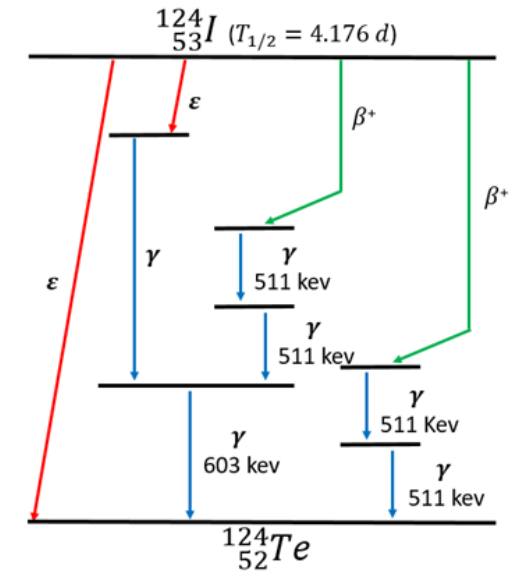
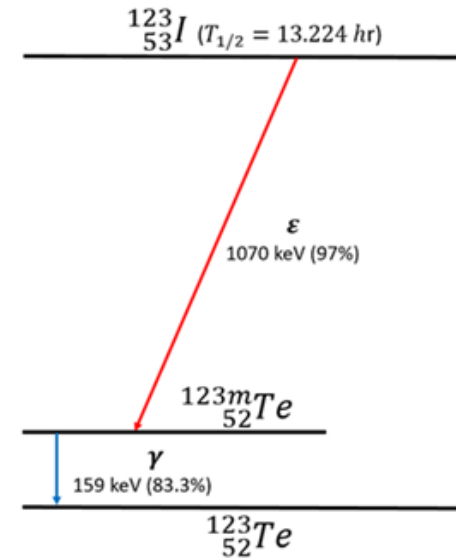
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# Benchmarking: radioisotopes

- I-123, I-124, I-125
  - widely used in nuclear medicine
- Cs-131
  - attractive radioisotope for brachytherapy of malignant tumours
- Comparison of Auger  $e^-$ , X and gamma rays, IC  $e^-$  yields w.r.t.
  - Other theoretical approaches
  - Experimental measurements in the case of I-125 and Cs-131
- rdecay01 example, Geant4 10.4

The uncertainty in the Auger yields calculated by means of EADL is  $\sim 15\%$  for K and L shells. In the case of Coster-Kronig The uncertainty could be as high as factor two.



# Benchmarking: reference data

- Pomplun [13] and Stepanek [12]
- BrlccEmis model by ANU[14]

[12] J. Stepanek, *Med. Phys.*, vol. 27, no. 7, pp. 1544–1554, 2000.

[13] E. Pomplun, *Acta Oncol. (Madr)*., vol. 39, no. 6, pp. 673–679, 2000.

[14] B. Q. Lee, H. Nikjoo, J. Ekman, P. Jonsson, A. E. Stuchbery, and T. Kibedi, *Int J Radiat Biol*, vol. 92, no. 11, pp. 641–653, 2016.

	Calculations	Experimental
I-123	BrlccEmis [14], Pomplun [13]	-
I-124	BrlccEmis [14]	-
I-125	BrlccEmis [14], Stepanek [12], Pomplun [13] (K lines)	ANU [4]
Cs-131	-	JINR [8]

	Stepanek [12]	Pomplun [13]	BrlccEmis
Nuclear decay/structure data	ENSDF	ICRP38	ENSDF
Electron capture probabilities	N. B. Gove and M. J. Martin. Log-f tables for beta decay  M. J. Martin and P. H. Blichert-toft. Radioactive atoms: Auger-Electron, $\alpha$ , $\beta$ , $\gamma$ and X-Ray Data.	N. B. Gove and M. J. Martin. Log-f tables for beta decay	E. Schonfeld. Tables for the calculation of electron capture probabilities.
Atomic shells	K-N	K-N	K-O
Atomic transition rates	S. T. Perkins et al (EADL)	Krause et al. Chen et al. McGuire et al.	S. T. Perkins et al (EADL)
Atomic transition energies	Dirac-Fock calculations	Dirac-Fock calculations	Dirac-Fock calculations

[12] J. Stepanek, *Med. Phys.*, vol. 27, no. 7, pp. 1544–1554, 2000.

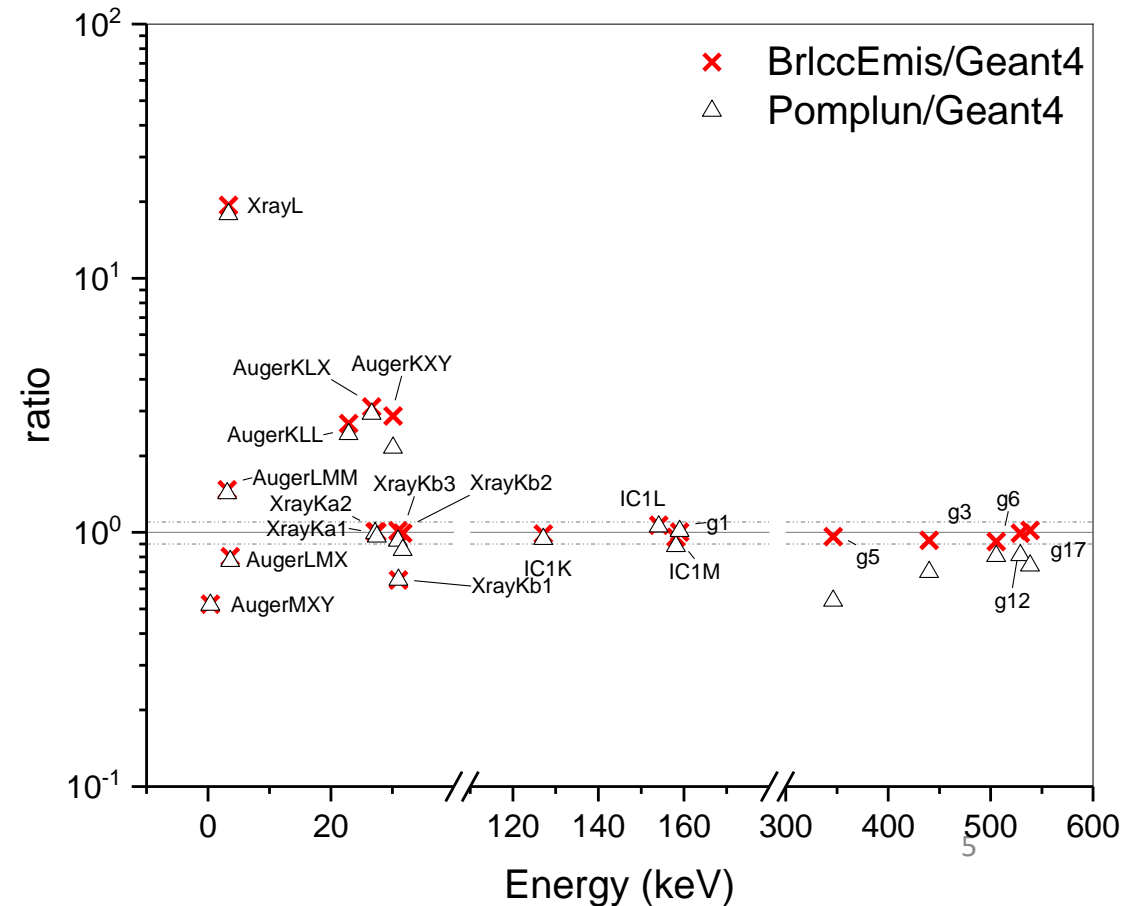
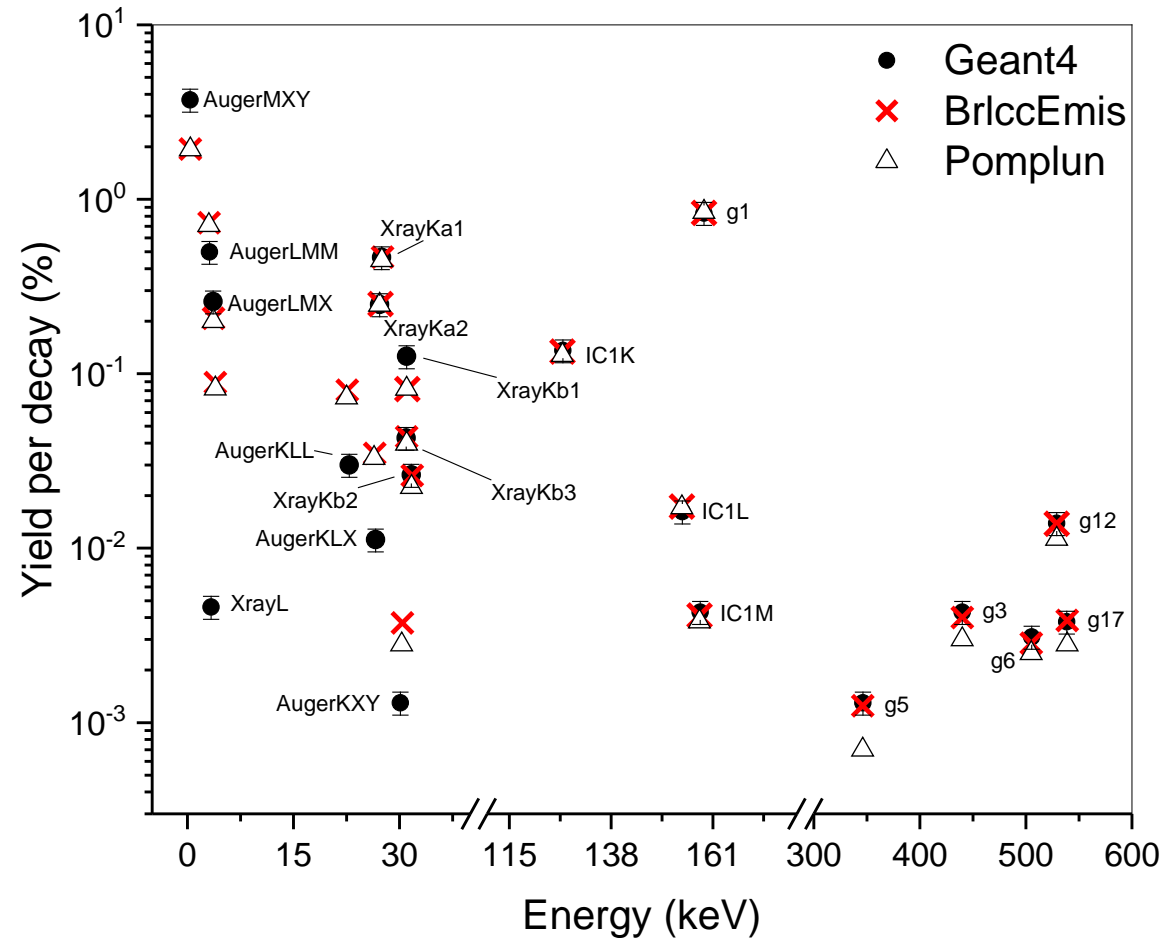
[13] E. Pomplun, *Acta Oncol. (Madr.)*, vol. 39, no. 6, pp. 673–679, 2000.

[14] B. Q. Lee, H. Nikjoo, J. Ekman, P. Jonsson, A. E. Stuchbery, and T. Kibedi, *Int J Radiat Biol*, vol. 92, no. 11, pp. 641–653, 2016.

# I-123

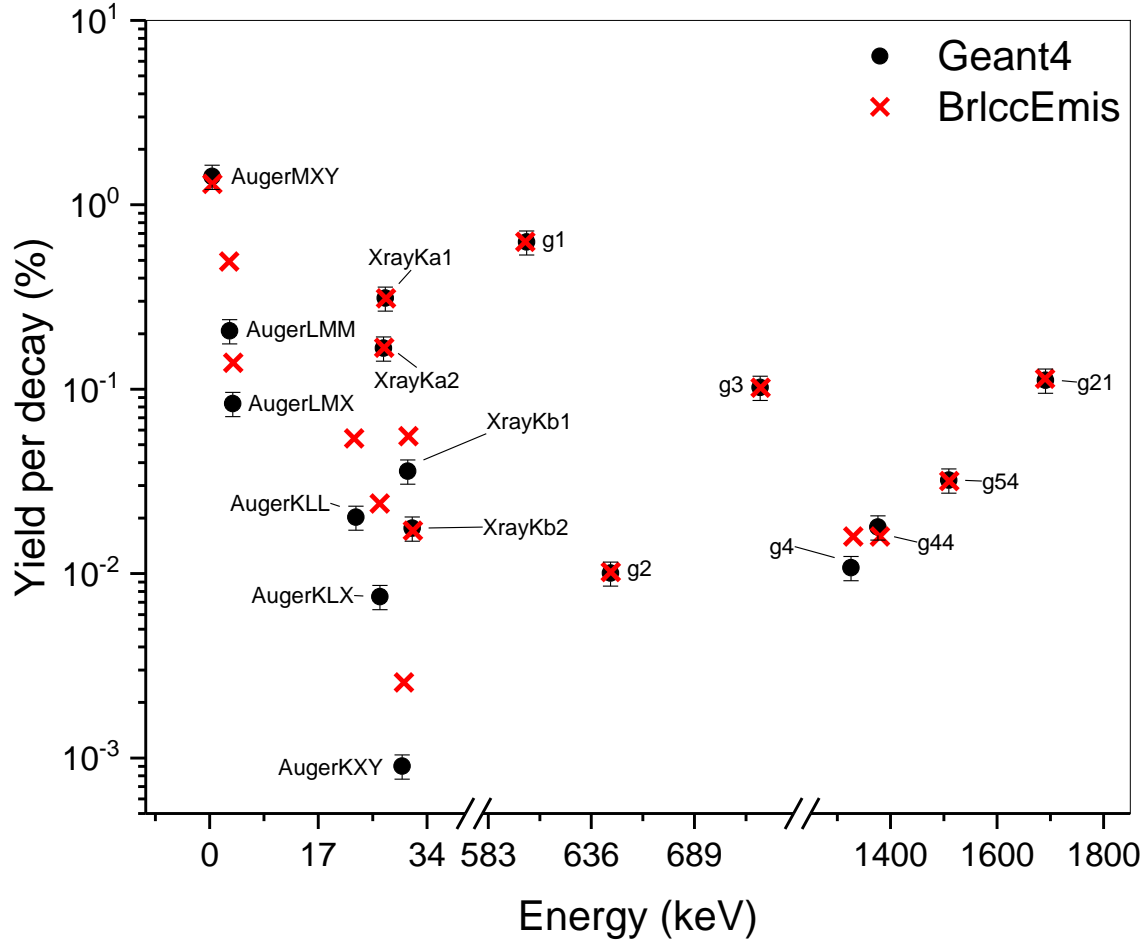
## G4.10.04

Line	Geant4		BrlccEmis		Pomplun			
	Energy $\pm 0.125$ (keV)	Yield %	Energy (keV)	Yield %	Energy (keV) BrlccEmis- Geant4	Energy (keV)	Yield %	Energy (keV) Pomplun - Geant4
Auger MXY	0.375	3.4	0.411	1.94	0.036	0.394	1.93	0.019
Auger LMM	3.125	0.46	3.05	0.734	-0.075	3.03	0.711	-0.095
Auger LMX	3.63	0.24	3.68	0.208	0.055	3.66	0.2	0.035
Auger KLL	22.88	0.03	22.6	0.0804	-0.275	22.5	0.0731	-0.375
Auger KLX	26.6	0.01	26.5	0.0349	-0.125	26.4	0.0328	-0.225
Auger KXY	30.1	0.001	30.4	0.00373	0.275	30.3	0.0028	0.175



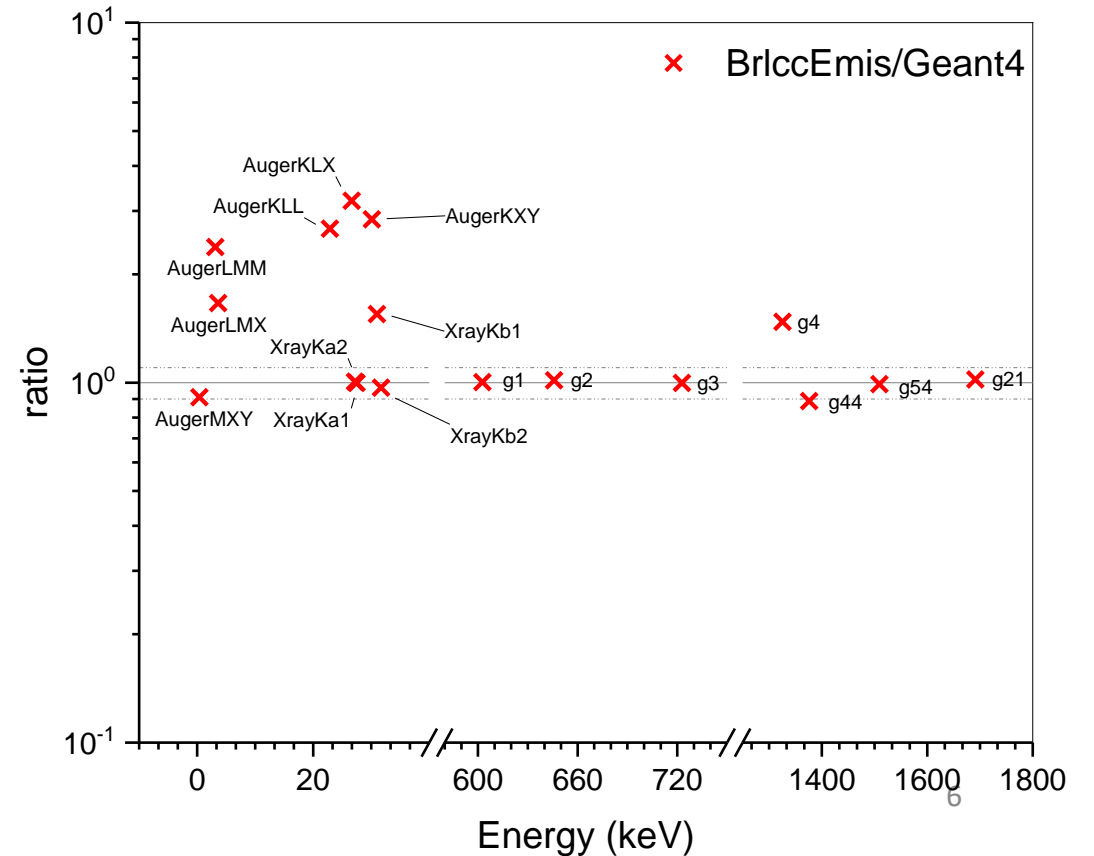
G4.10.04

The uncertainty in the Auger yields calculated by means of EADL is ~15% for K and L shells. In the case of Coster-Kronig The uncertainty could be as high as factor two.



Gamma ray energies and IC e- energies are the same  
Differences in X-ray and Auger e-

Line	Geant4		BrlccEmis		Energy (keV) BrlccEmis- Geant4
	Energy ±0.125 (keV)	Yield %	Energy (keV)	Yield %	
Auger MXY	0.375	1.4	0.413	1.3	0.038
Auger LMM	3.13	0.21	3.05	0.493	-0.075
Auger LMX	3.63	0.084	3.68	0.139	0.055
Auger KLL	22.88	0.02	22.6	0.0541	-0.275
Auger KLX	26.6	0.006	26.6	0.024	-0.025
Auger KXY	30.1	9E-04	30.4	0.00257	0.275



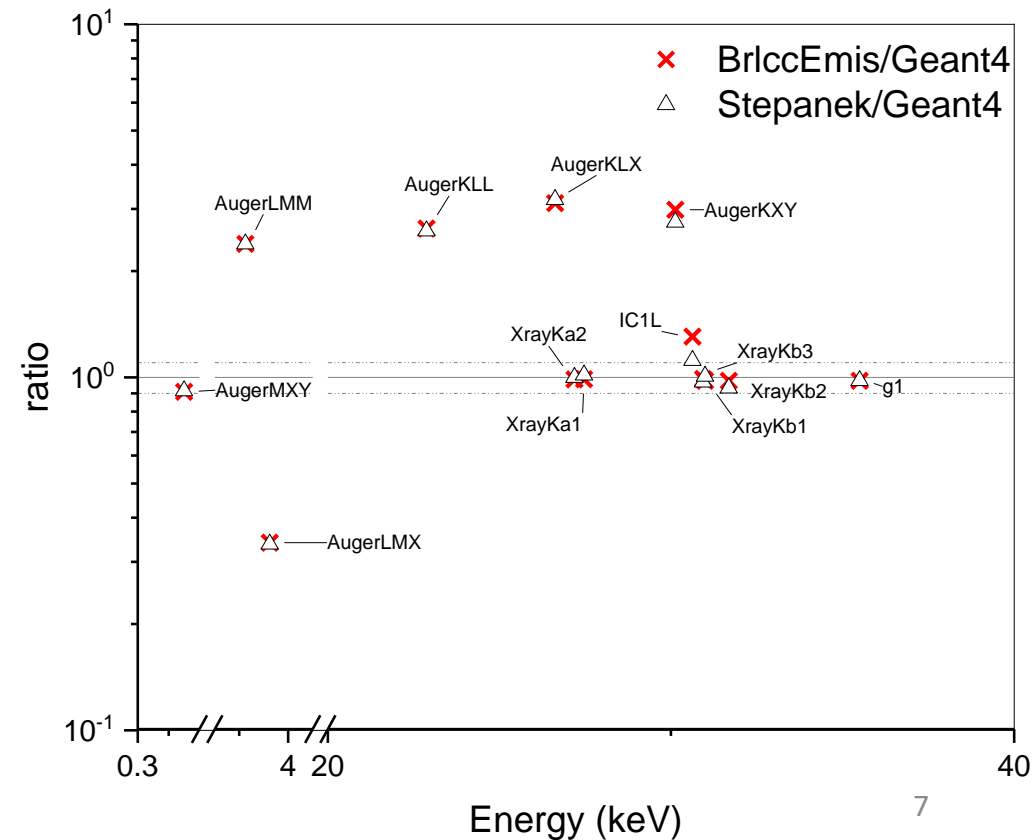
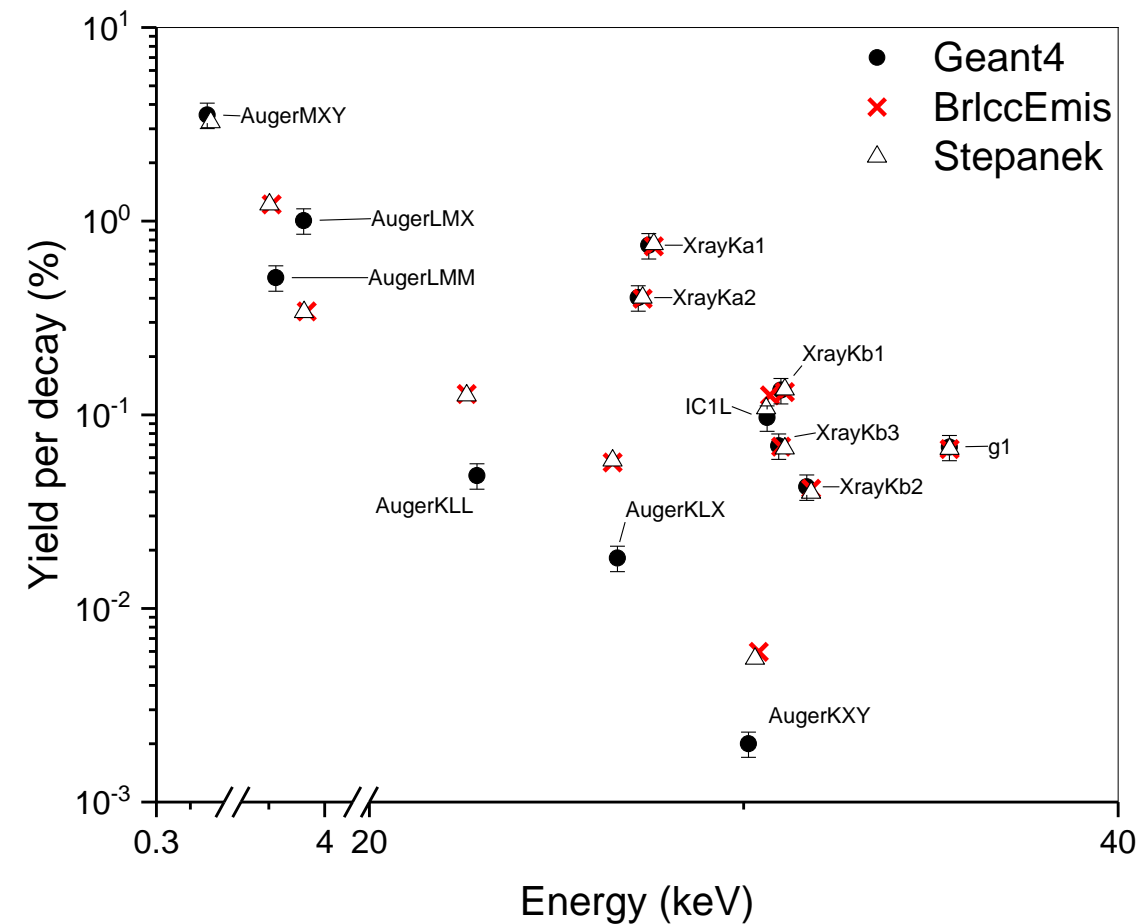
I-125

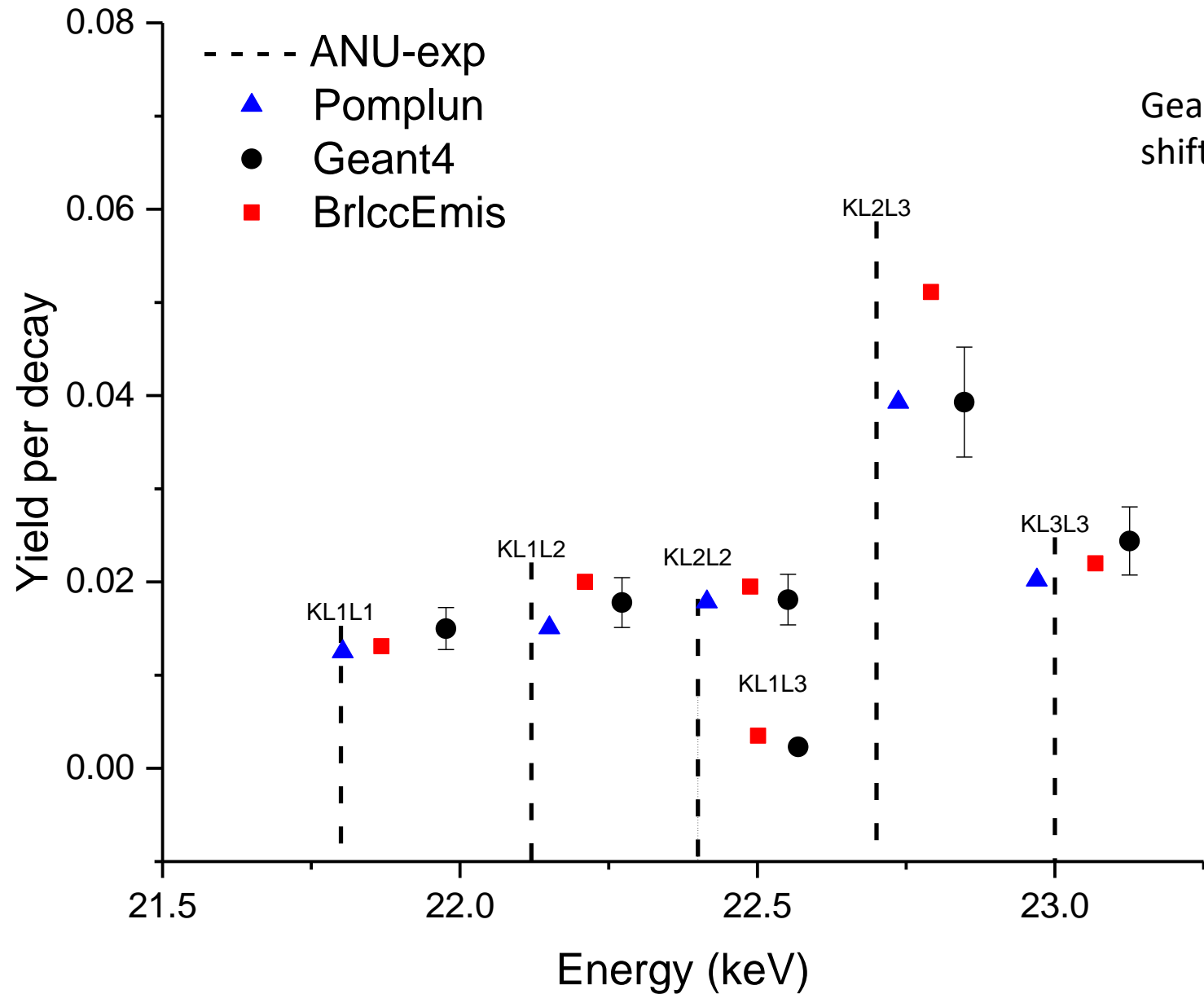
G4.10.04

Gamma ray energies and IC e- energies are the same

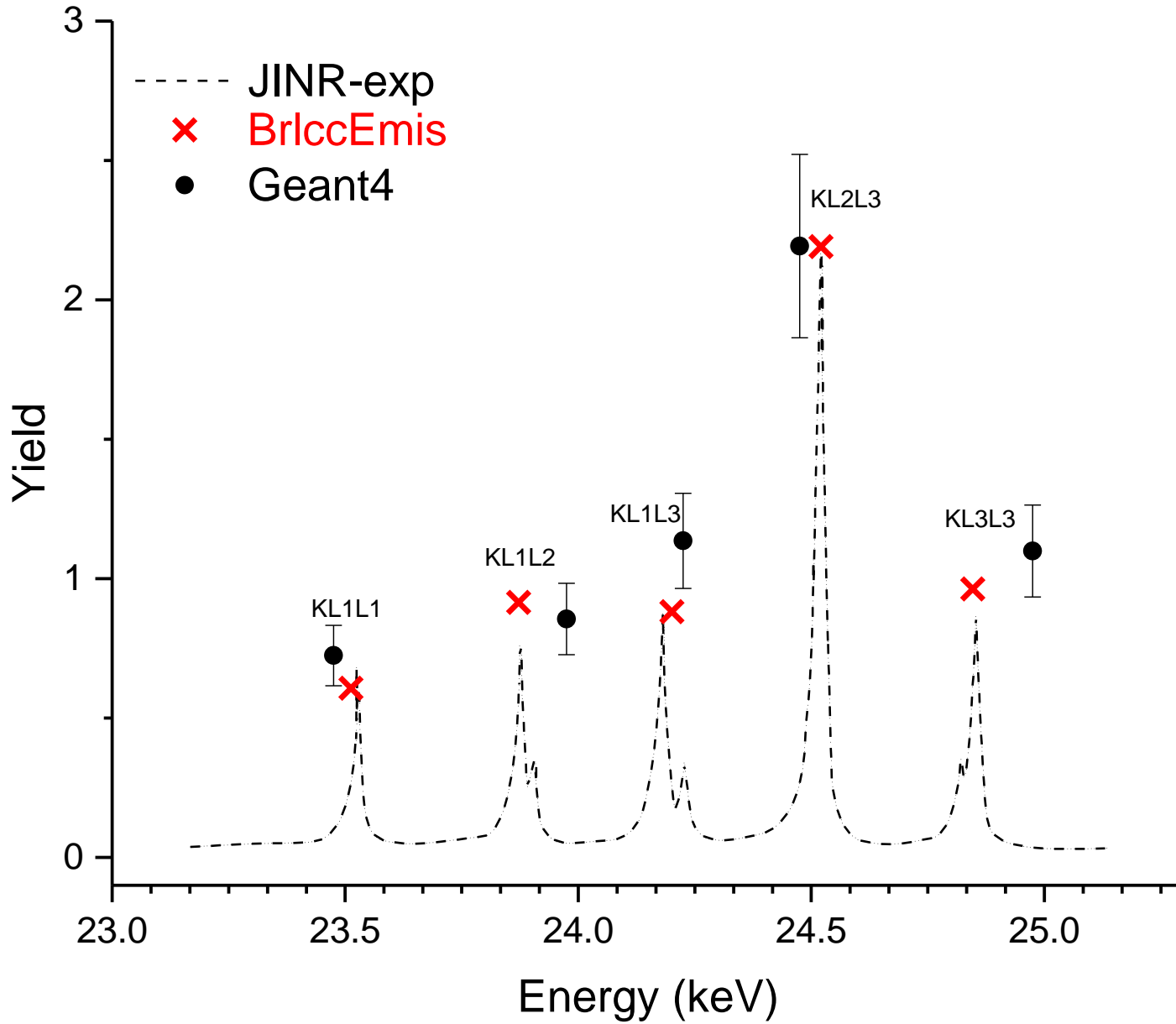
Differences in X-ray and Auger e-

Line	Geant4		BrlccEmis		Stepanek			
	Energy $\pm 0.125$ (keV)	Yield %	Energy (keV)	Yield %	Energy (keV) BrlccEmis - Geant4	Energy (keV)	Yield %	Energy (keV) Stepanek - Geant4
Auger MXY	0.38	3.5	0.408	3.22	0.033	0.38	3.24	0.005
Auger LMM	3.13	0.51	3.05	1.22	-0.075	3.01	1.22	-0.115
Auger LMX	3.63	1.0	3.68	0.342	0.055	3.63	0.339	0.005
Auger KLL	22.88	0.048	22.6	0.128	-0.275	22.6	0.126	-0.275
Auger KLX	26.6	0.018	26.5	0.0567	-0.125	26.5	0.058	-0.125
Auger KXY	30.1	2E-03	30.4	0.00597	0.275	30.3	0.0055	0.175







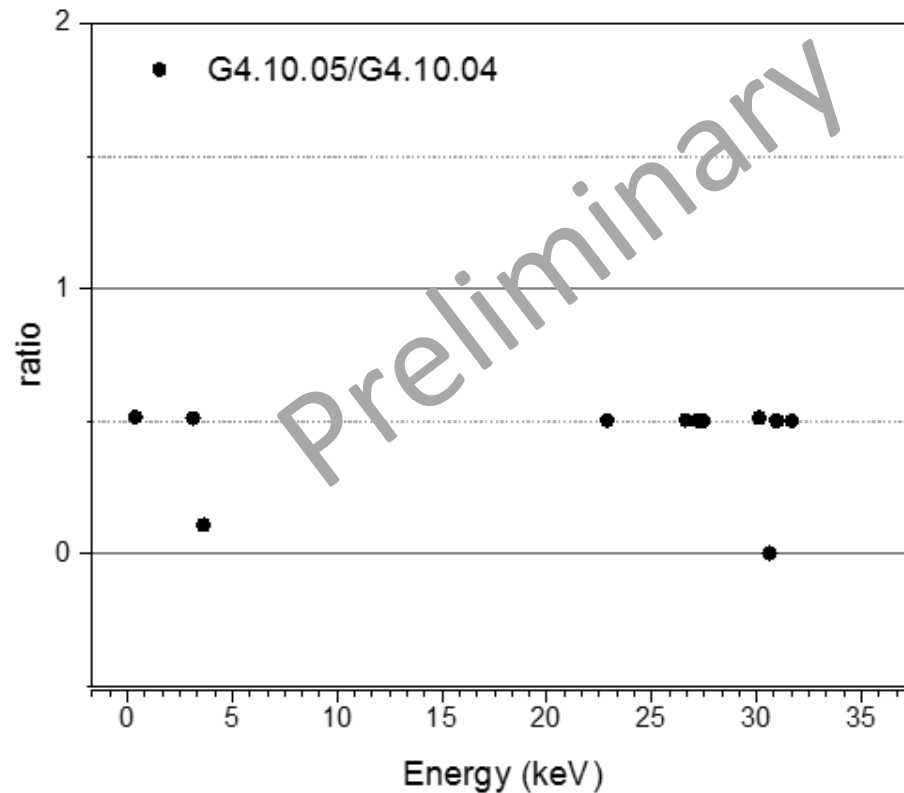
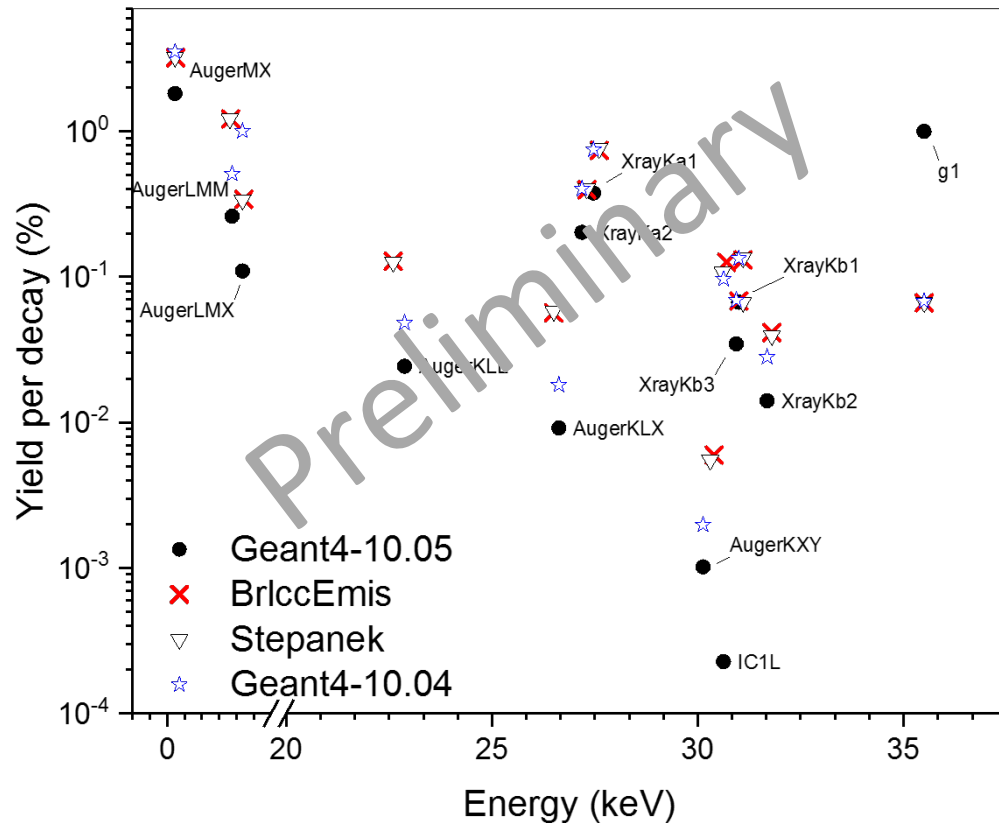


Geant4 results have a consistent energy shift of ~180 eV (BrlccEmis ~95 eV)

# Regression testing

## I-125

- Geant4 10.4 (RadioactiveDecay5.2) and 10.5 (RadioactiveDecay5.3)



# Conclusions

- Benchmarking of Geant4 for radioactive decays of I-123, I-124 and I-125
  - Against other theoretical data and exp measurements