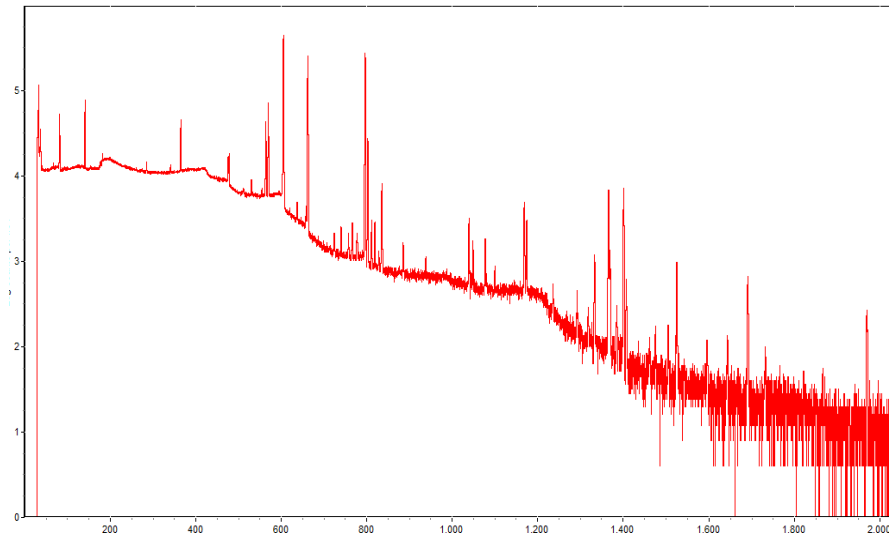**Gamma-ray spectrometry basics #2:**
Gamma spectrum analysis and activity calculations

Alexander Mauring
NKS GammaSkill Training Day, 26.09.2023

What this lecture is basically about…

How do we go from this…

… to this?

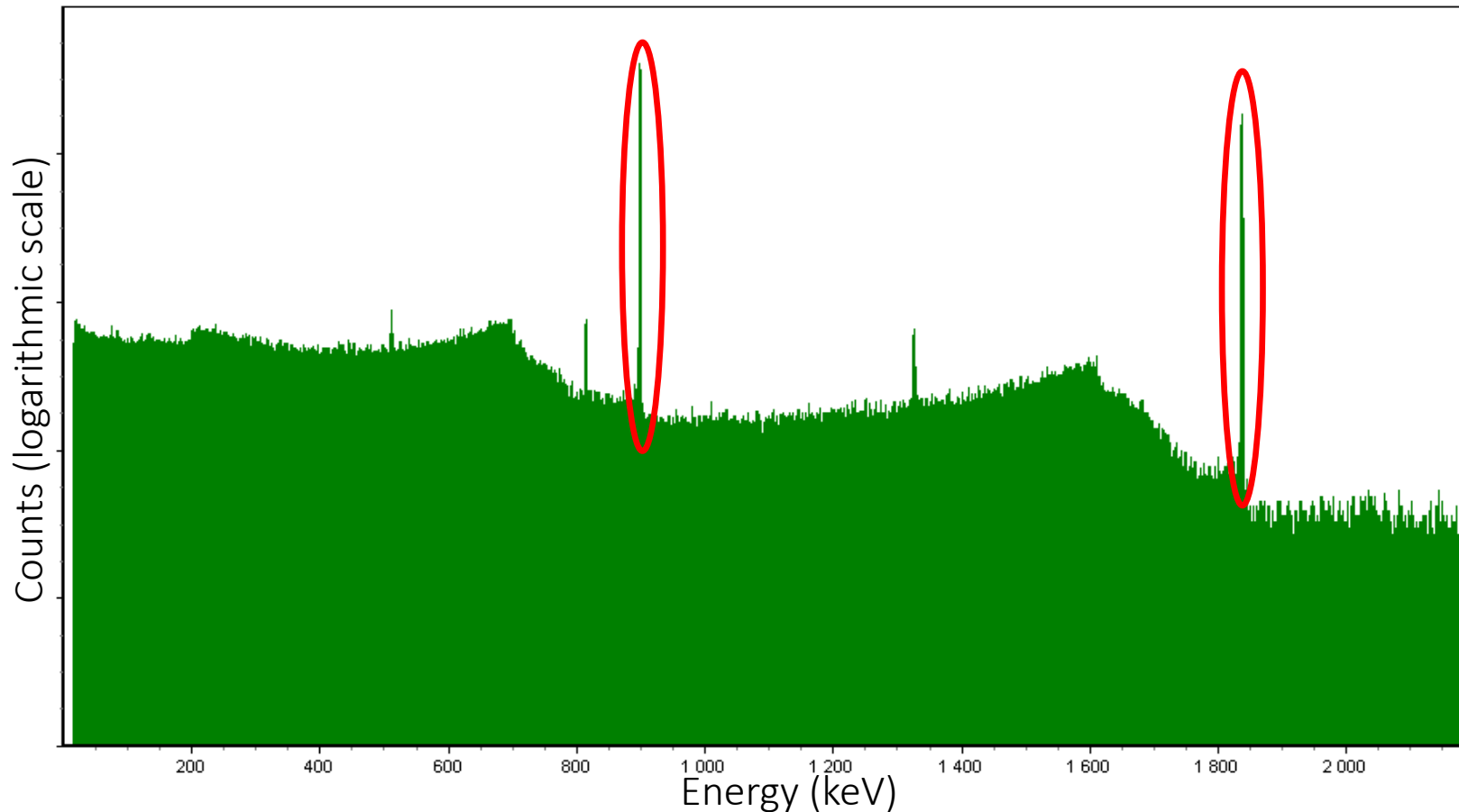| Nuclide	Activity [Bq/kg]
K-40	512 ± 29
Co-60	63 ± 6
Cs-134	104 ± 7
Cs-137	338 ± 11
Pb-210	273 ± 19
Am-241	< 12

Agenda

The gamma spectrum

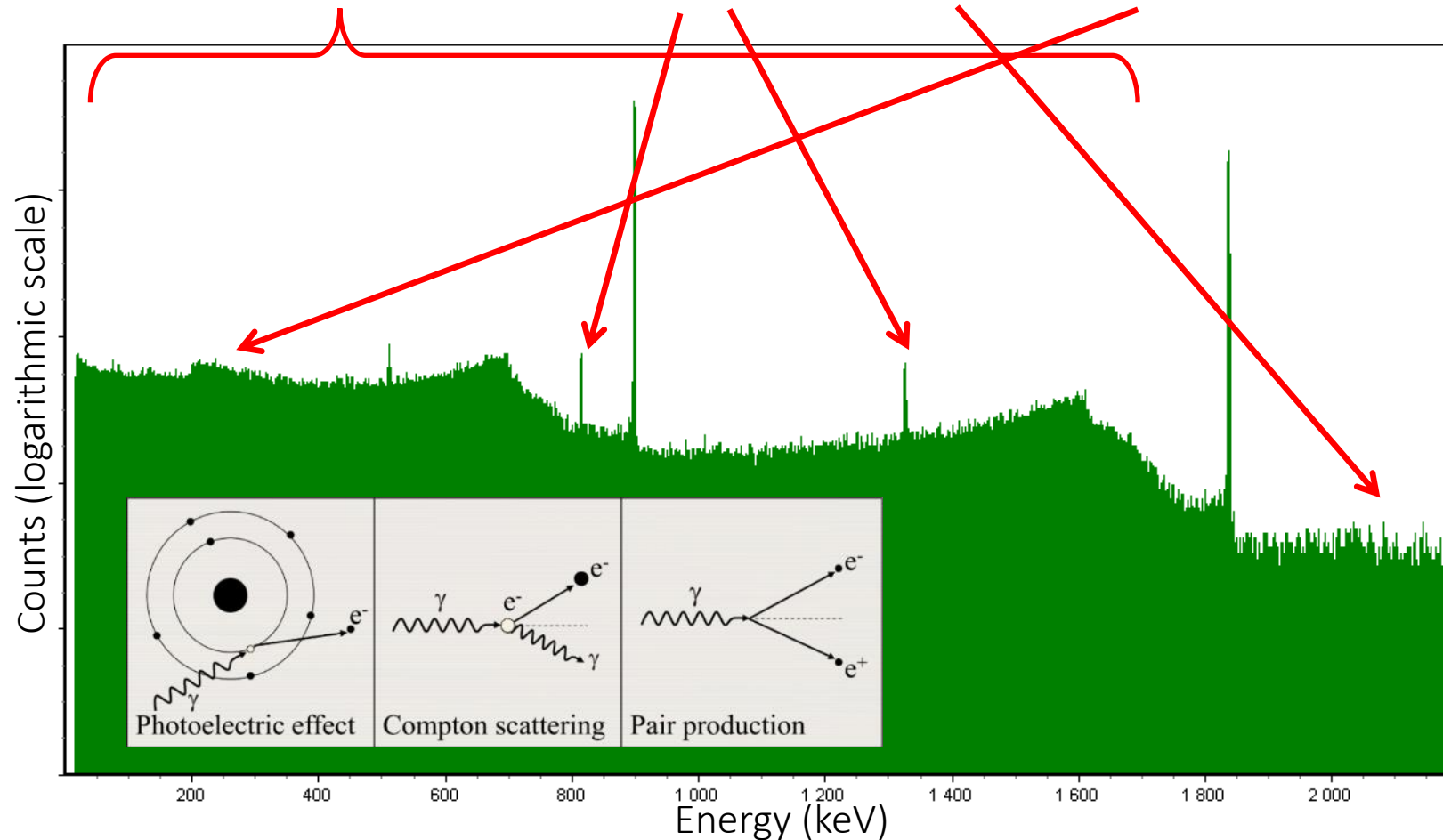- The location (energy) of full energy peaks tells us which nuclide(s) are in the spectrum
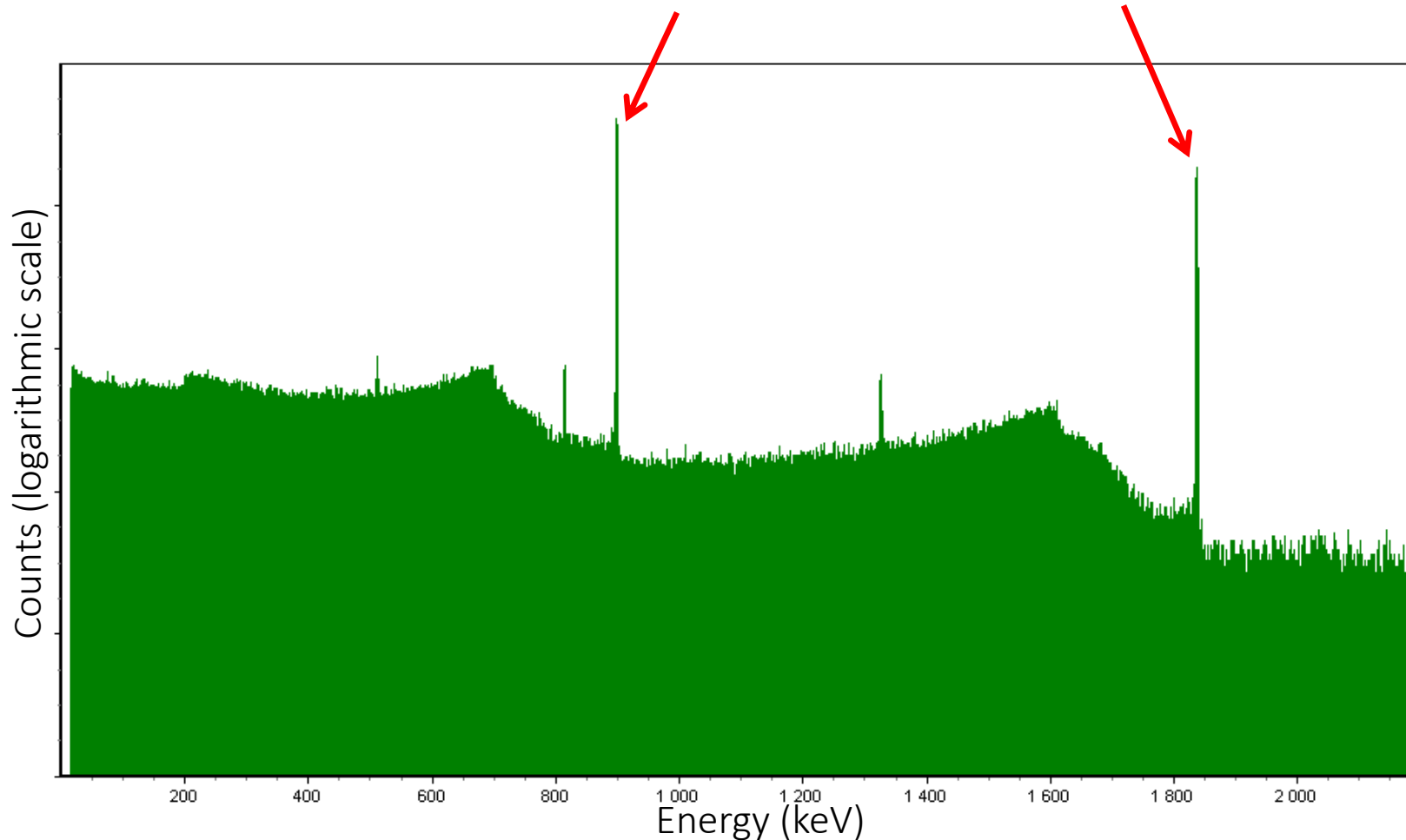
The gamma spectrum

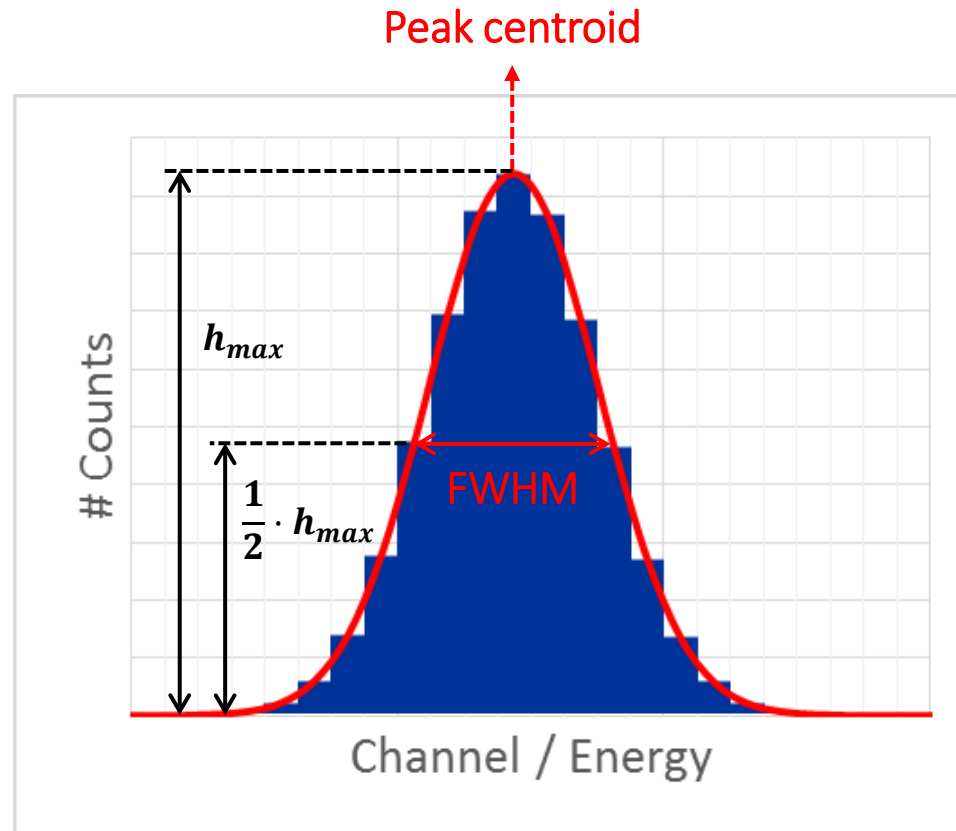- The size (area) of the peaks tells us something about the nuclide activity

The gamma spectrum

- We can also see many other effects in the spectrum

Shape of full energy peaks in the spectrum

- The peak shape is typically "Gaussian"

Peak centroid

h_{max}

$\frac{1}{2} \cdot h_{max}$

FWHM

Channel / Energy

FWHM = "Full Width at Half Maximum"

The "low tail" effect:

Counts

Channel / Energy
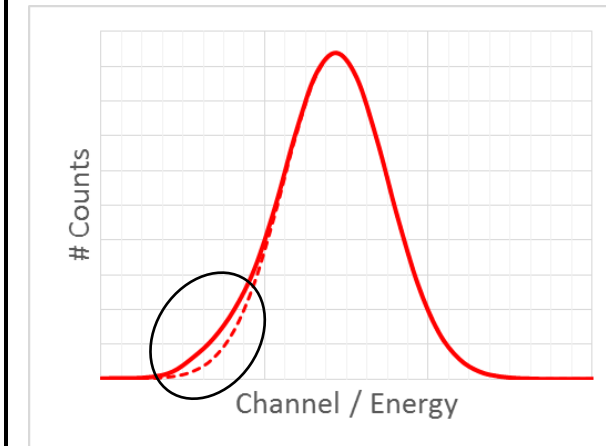
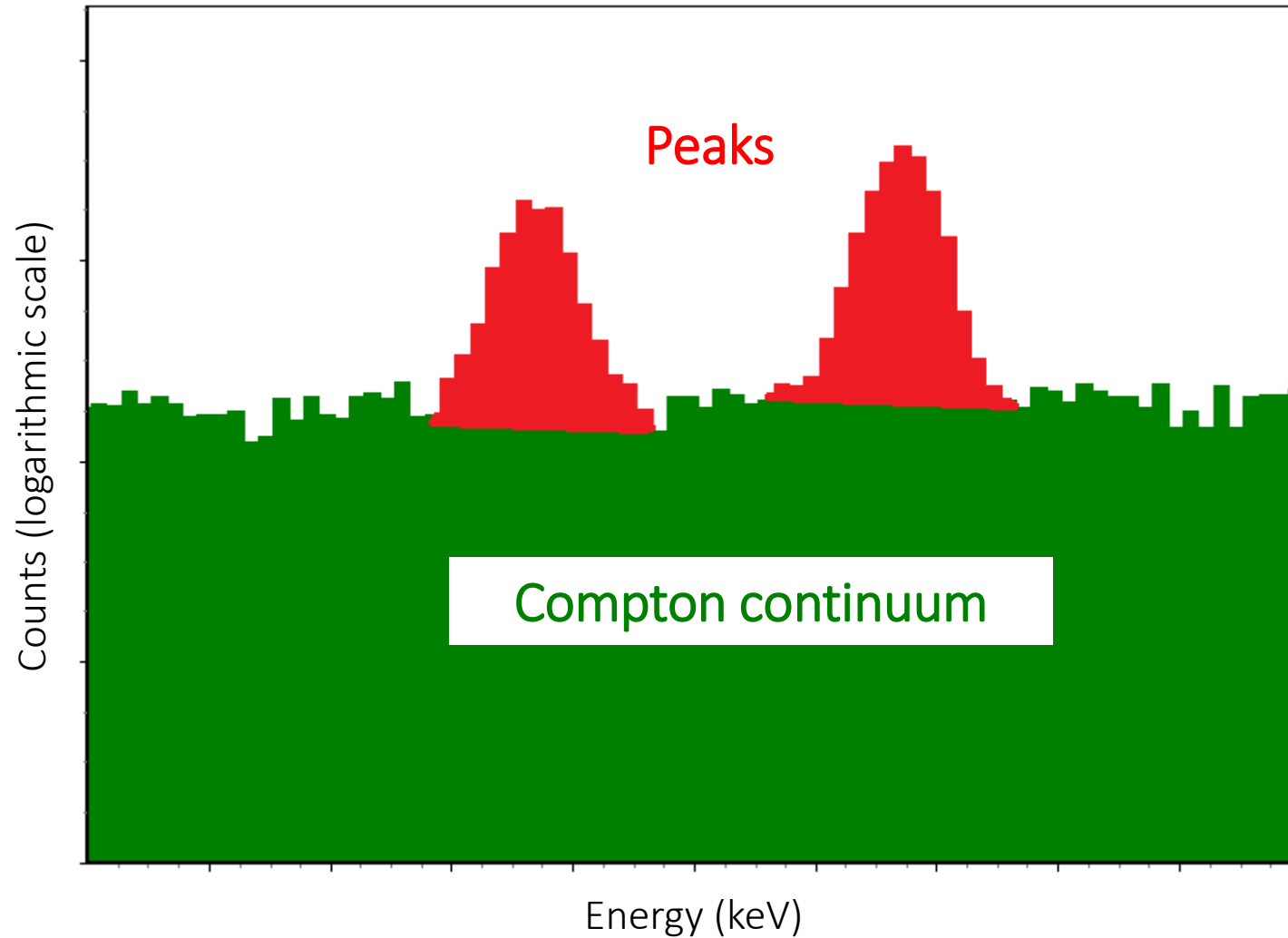**Occurs due to incomplete charge collection in the detector.**

Linear vs. logarithmic y-axis for the spectrum

Shape of peak
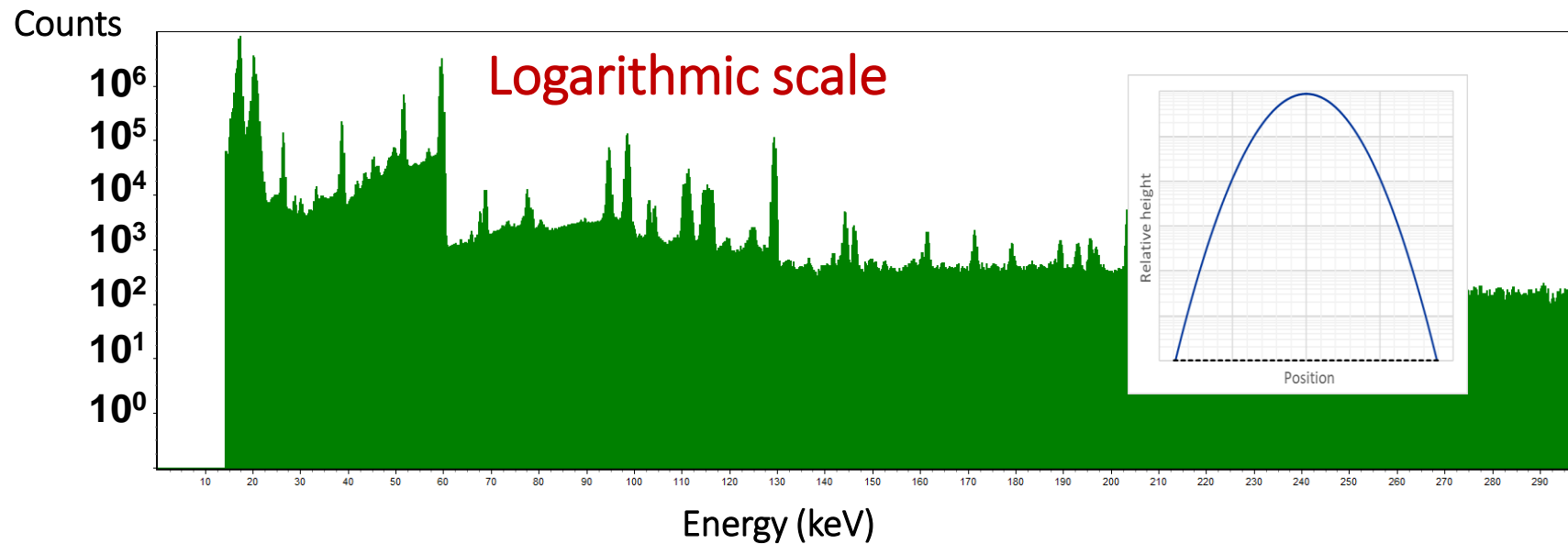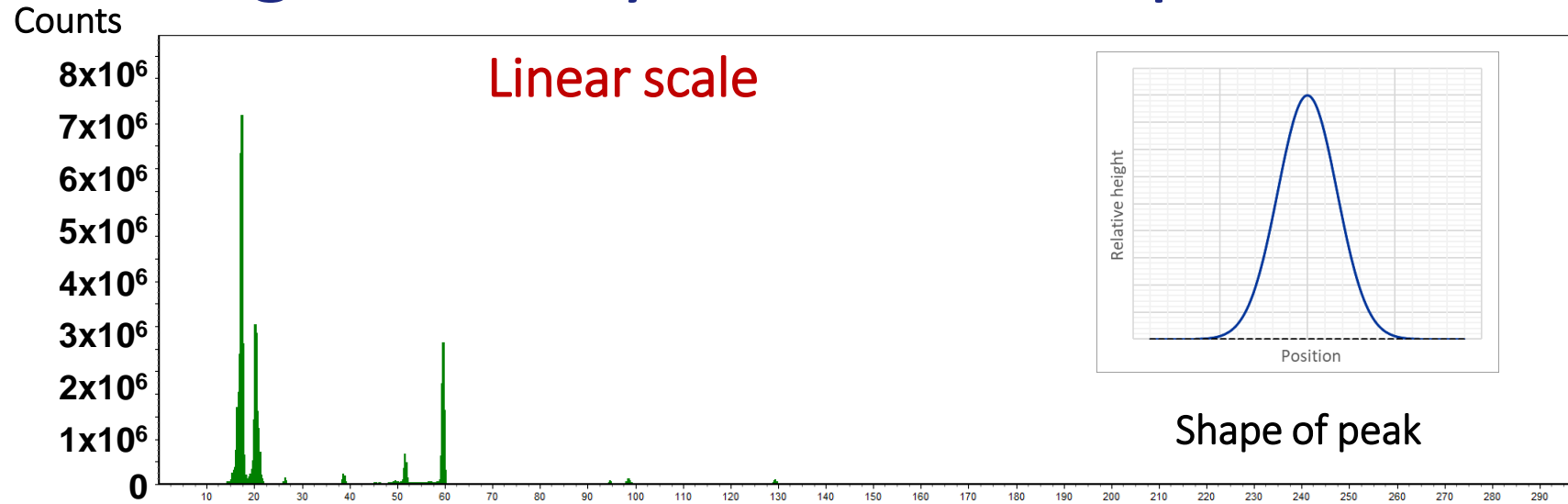
A closer look at full energy peaks in the spectrum

Peaks

Compton continuum

Counts (logarithmic scale)

Energy (keV)

Agenda

Energy calibration

- The MCA sorts each event into an appropriate channel in the spectrum
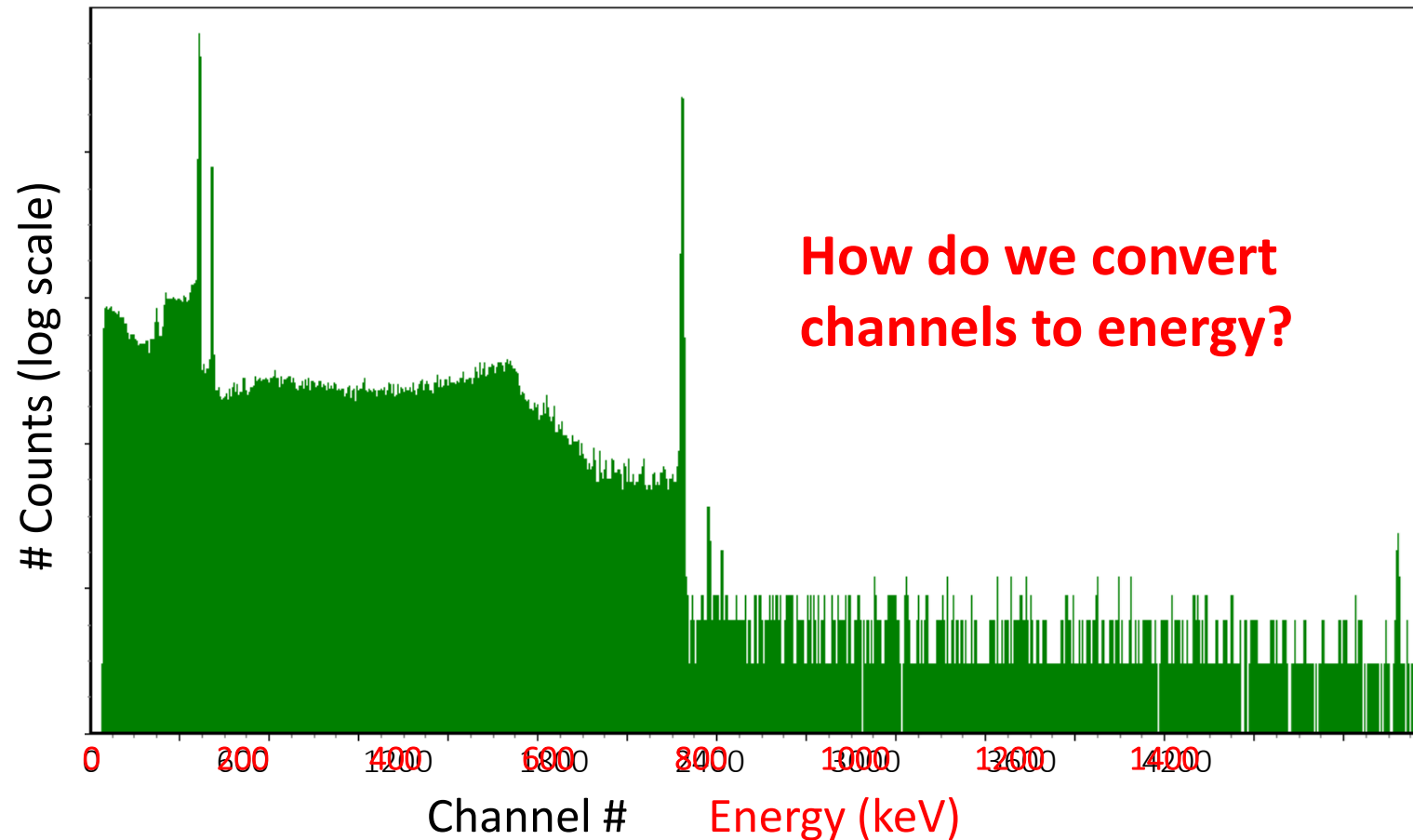
How do we convert channels to energy?

Energy calibration

- Energy calibration relates the channel number to the photon energy. It is done by measuring known gamma sources at several energies

Formula:

$$E = a \cdot (Ch) + b$$
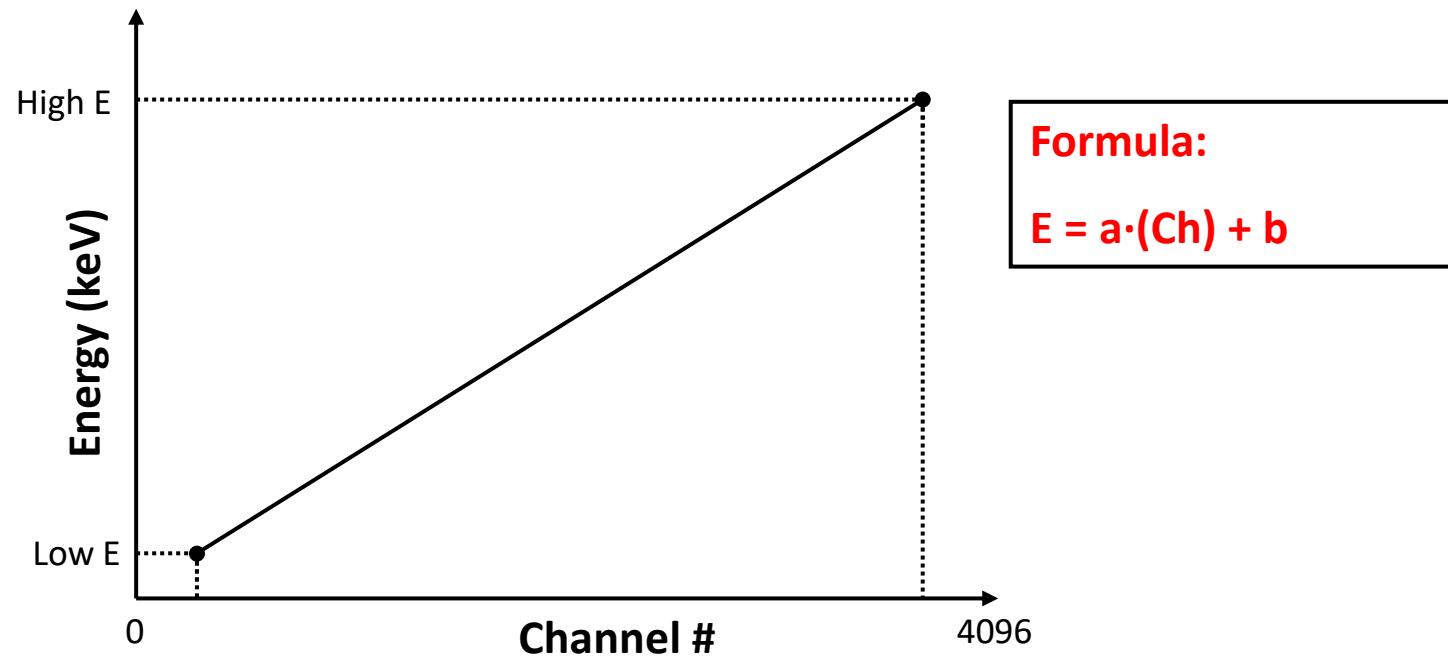
Energy calibration

- Energy calibration relates the channel number to the photon energy. It is done by measuring known gamma sources at several energies

- The curve can then be used to predict the energy of a peak in any channel

Formula:

$E = a \cdot (Ch) + b$

Energy calibration

- The "straight line hypothesis" also holds true when using many peaks:
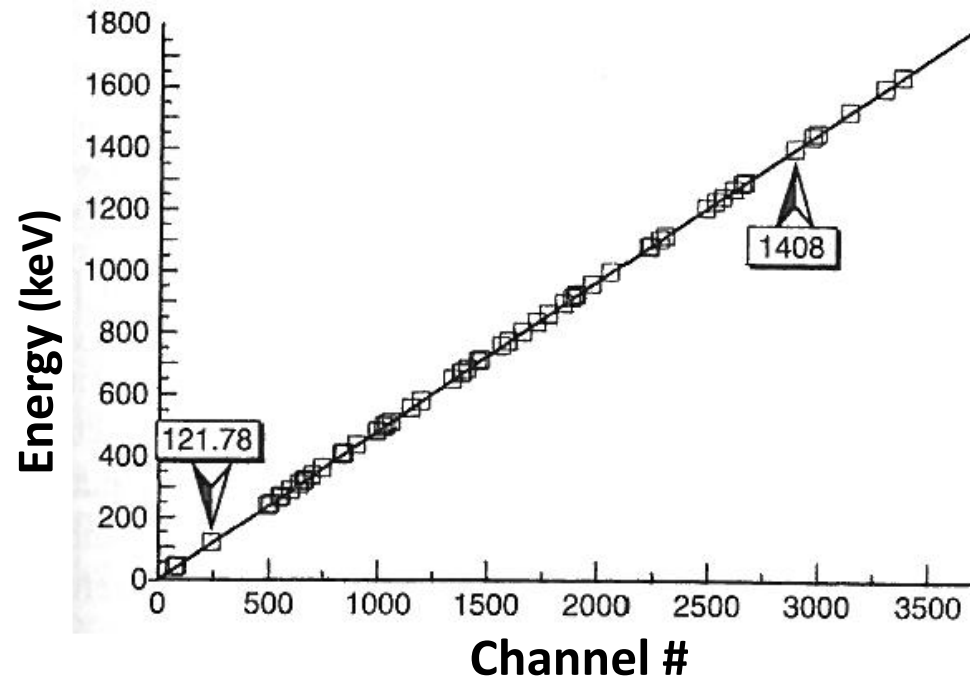
Source: Gilmore, 2008. "Practical gamma-ray spectrometry"

Peak width (FWHM) calibration

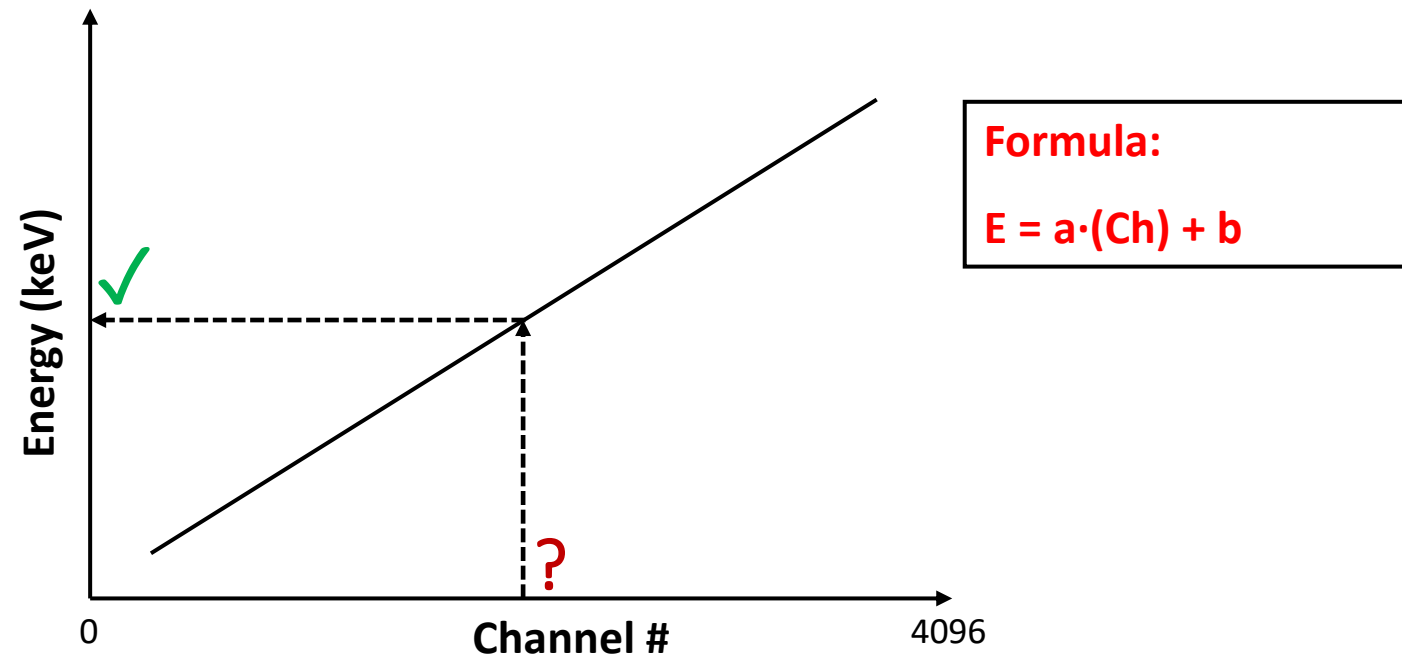- Plot of observed FWHM values as a function of energy from measurement of one or several known sources, fitted with a mathematical function:
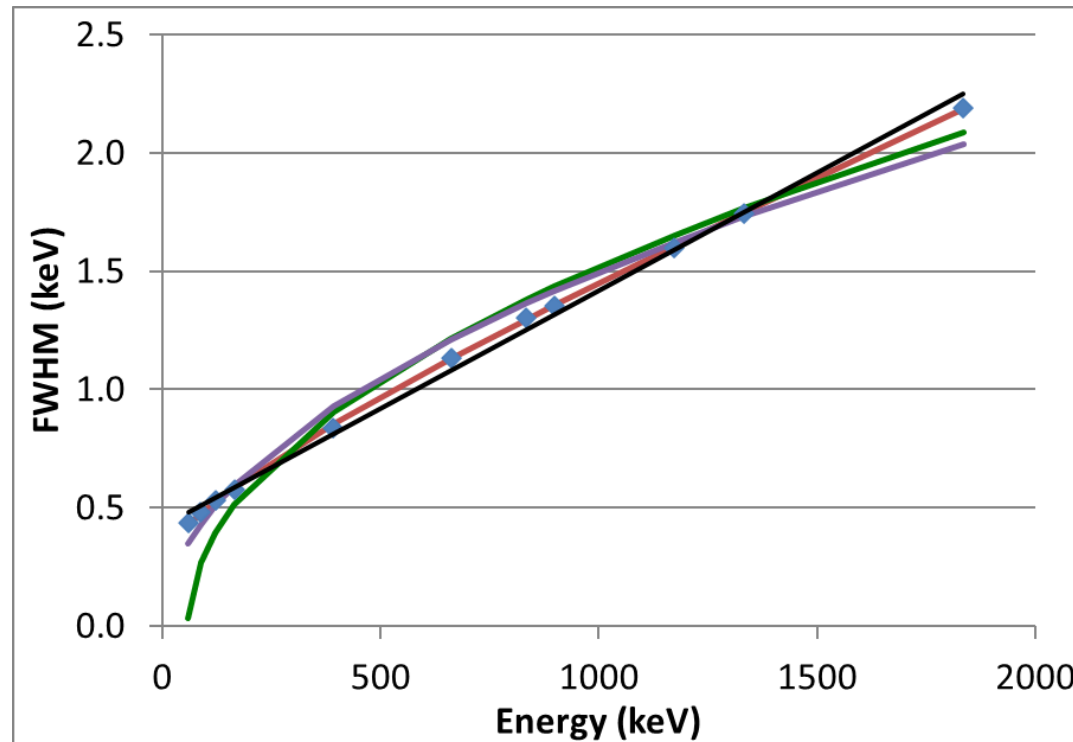
Gilmore

$$FWHM = \sqrt{a \cdot E^2 + b \cdot E + c}$$

Debertin & Helmer

$$FWHM = \sqrt{a \cdot E + b}$$

Genie2000

$$FWHM = \sqrt{a \cdot E} + b$$

Agenda

The spectrum analysis process

Computer with gamma spectrum acquisition and analysis software
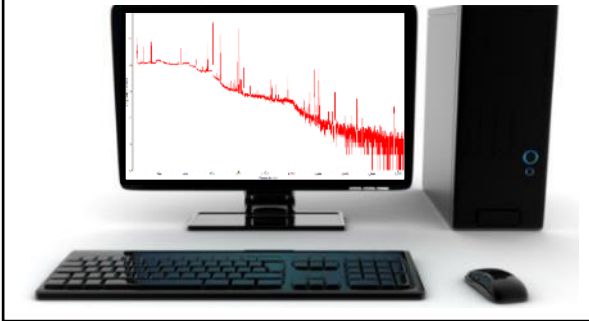
First part: Determining peak areas

Peak search

↓

Peak area determination

↓

Background subtraction

↓

Efficiency correction / calibration

↓

Nuclide identification & activity calculation

↓

Reporting the results

Second part: Converting areas to activities

Searching for peaks: Visual method

- *Where are the peaks in the spectrum?*
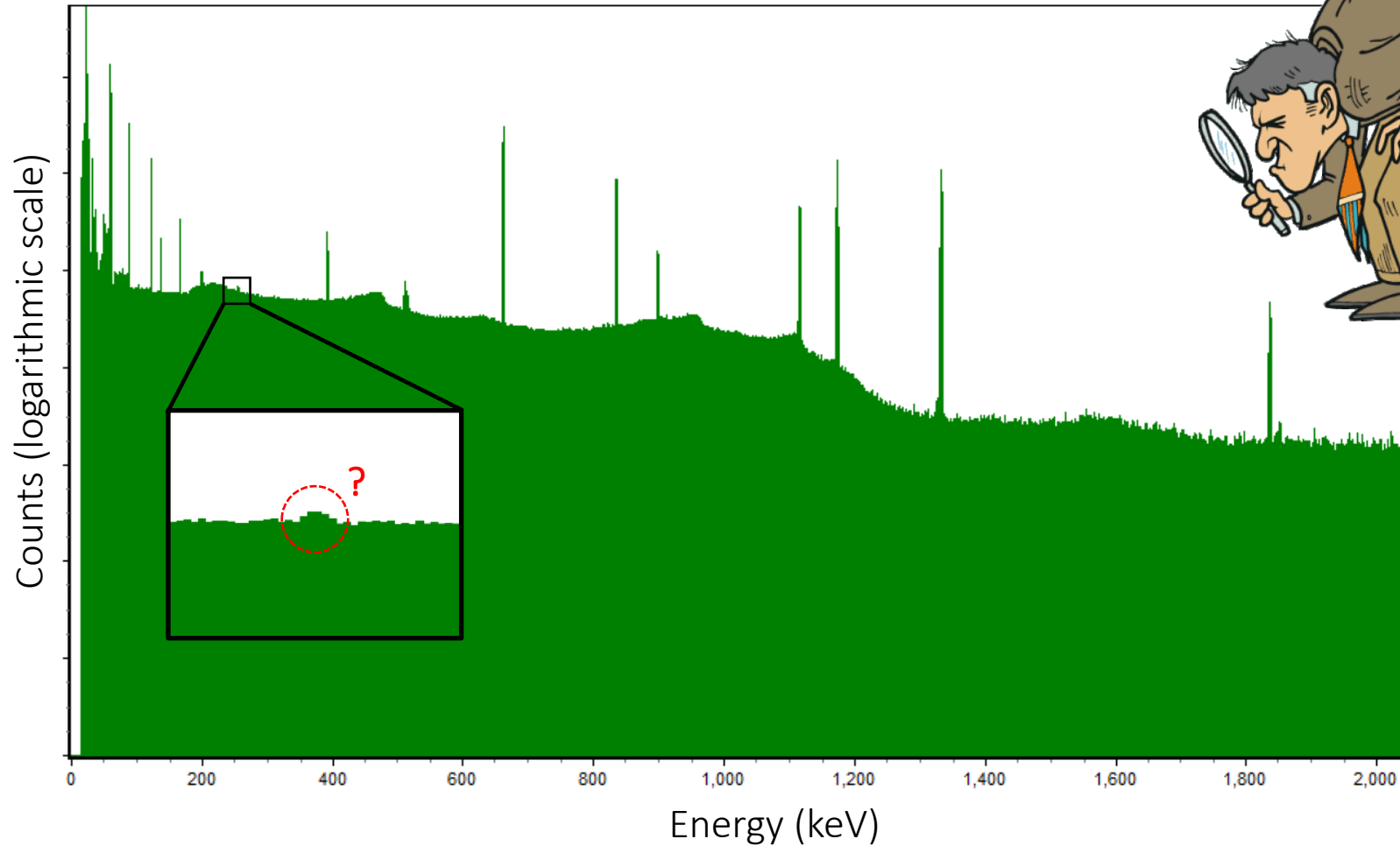
Searching for peaks: "Second difference method"

- Method was first proposed by Mariscotti in 1967, now used for finding peaks in all major spectrum analysis software

Theoretical basis of method
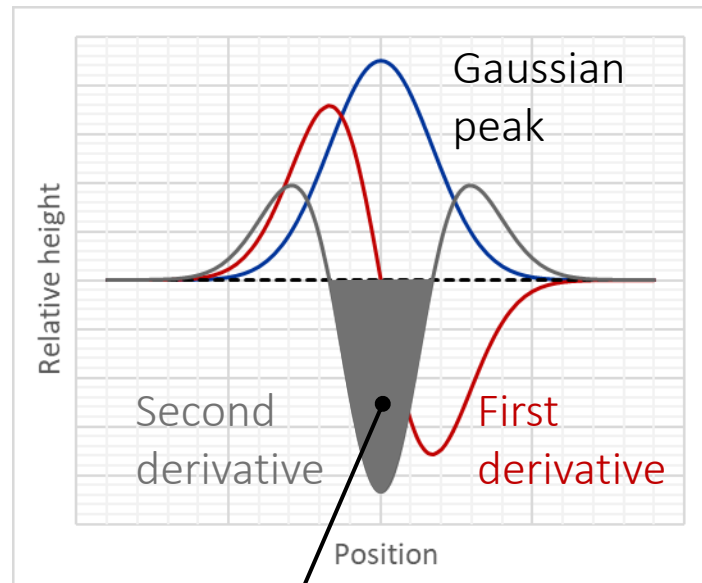
Larger area = higher significance

The method in practice
(Derivatives → differences)
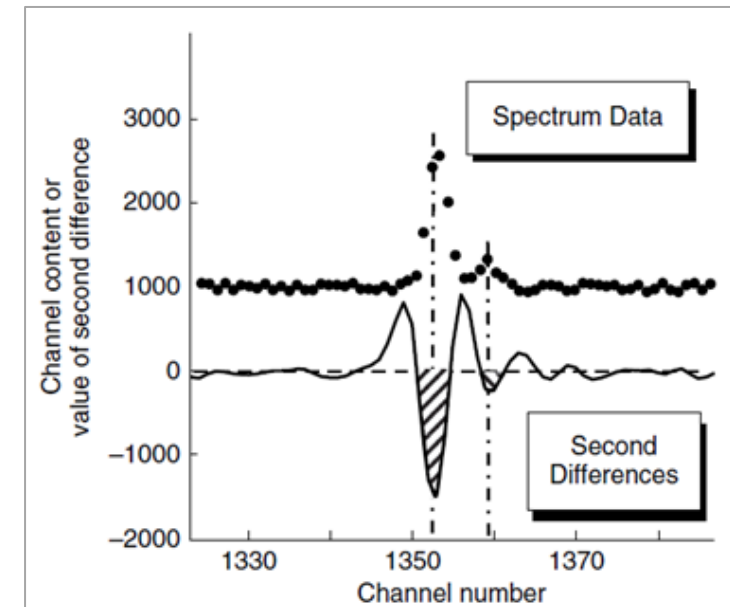
Figure source: Gilmore, 2008. "Practical gamma-ray spectrometry"

Peak area determination by two different methods

- Method one: "Simple" ROI based method
- Method two: Fitting a Gaussian function
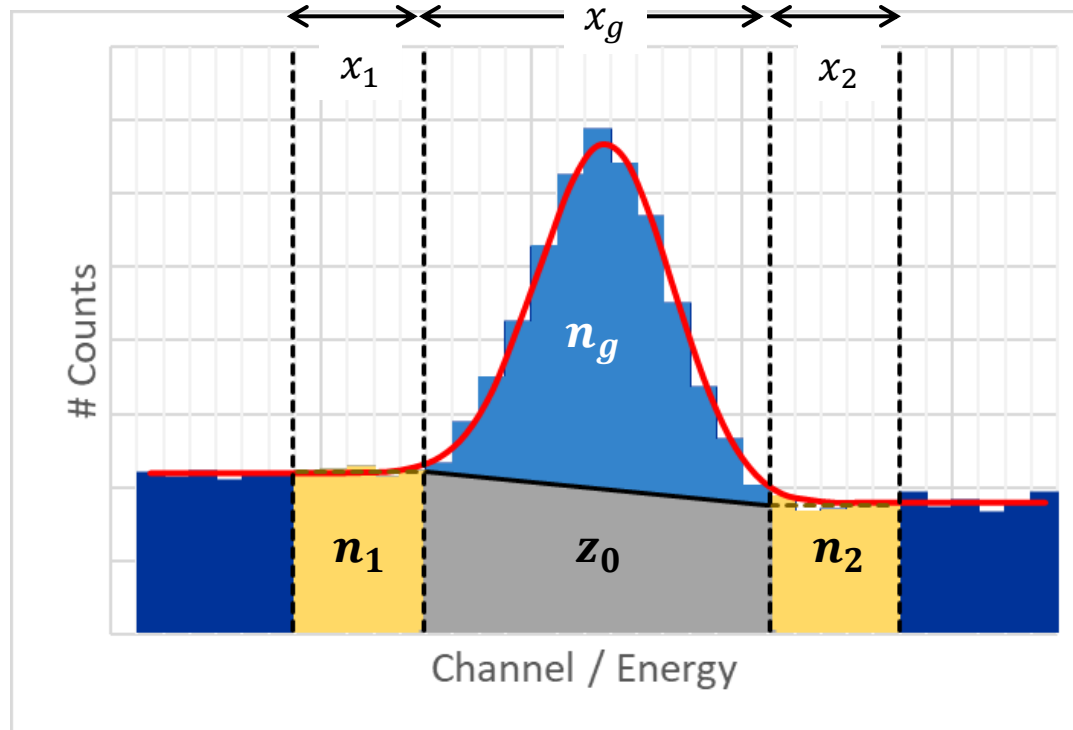
Some mathematics:

$$x_0 = x_1 + x_2$$

$$n_0 = n_1 + n_2$$

$$z_0 = \frac{x_g}{x_0} \cdot n_0$$

$$\boxed{n_E = n_g - z_0}$$

$$u(n_E) = \sqrt{u^2(n_g) + u^2(z_0)}$$

$$= \sqrt{n_g + \left(\frac{x_g}{x_0}\right)^2 \cdot n_0}$$

Because count numbers are **Poisson distributed** ⟵

Peak area determination by Gaussian fitting

- If several peaks are located close together, Gaussian fitting is often the only way to determine their respective areas. But be careful to not "over-fit" something!

Peak area:

$$n_E = h \cdot \sigma \cdot \sqrt{2\pi}$$

where

$$\sigma = \frac{FWHM}{2\sqrt{2\ln 2}}$$
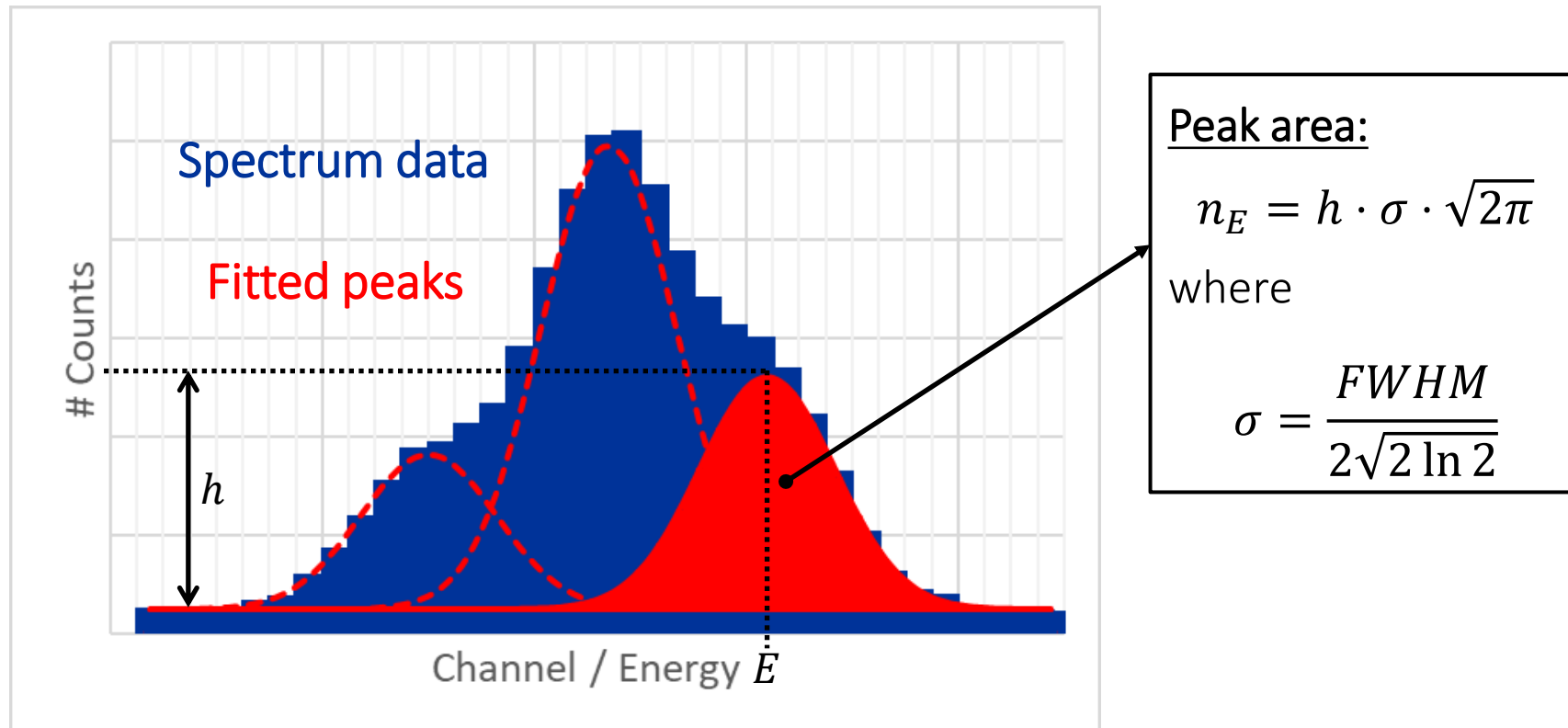
Detector background and need for correction
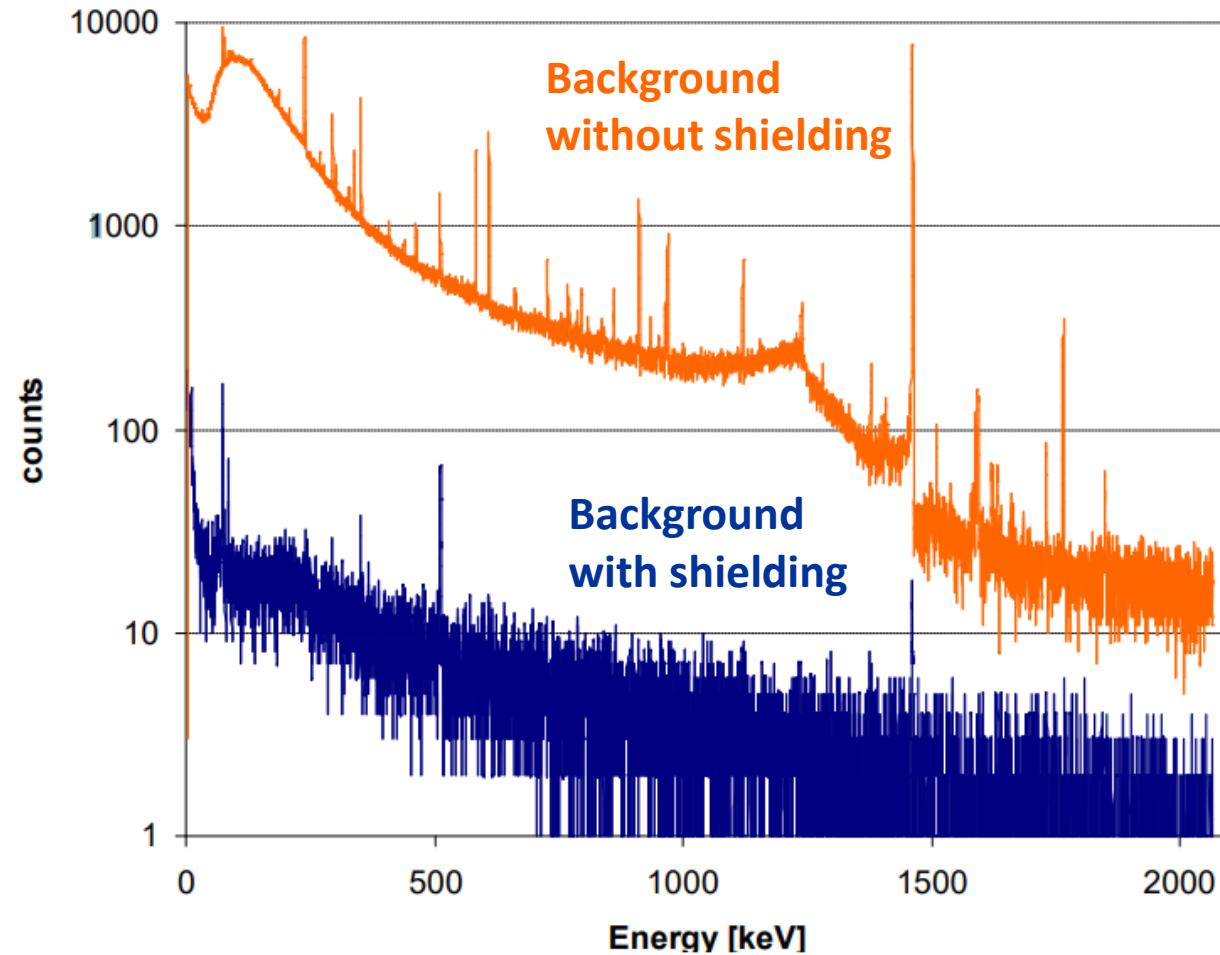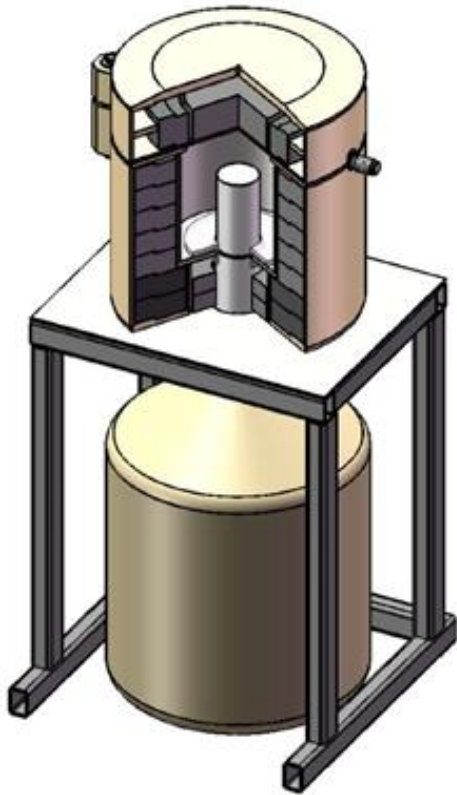
Peaked background subtraction

- Subtracting a background contribution to the FEP area, peak by peak:

Input to the activity equation $\longleftarrow$ $\underline{n_{\mathrm{N},E}} = n_E - n_{0,E} \cdot \dfrac{t_g}{t_0}$

$n_{\mathrm{N},E}$	net peak area (background corrected)
n_E	peak area (not background corrected)
$n_{0,E}$	area of peak in background spectrum
t_g	"live time" of sample spectrum measurement
t_0	"live time" of background spectrum measurement

In case of no background peak ($n_{0,E} = 0$): $n_{N,E} = n_E$

Measurement live time, t_g
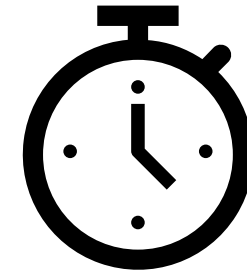
- Measured by the internal clock of the MCA

- Corrected for "dead time" (when system still busy with previous signal and cannot process a new one)

- Reported directly in the acquisition software:

		Elapsed	Preset
Acq. Start: 10/14/2018 8:47:03 AM			
Dead Time: 2.61%	Live (secs.):	86400.000	0
Comp. Preset Region:	Real (secs.):	88715.380	0
0 - 0 (channels)	Total (cnts.):	0.00	0

Going from peak area to activity: Key principle

- The area of a full energy peak tells us about the activity concentration of a nuclide of interest:

$$\boxed{\text{Activity concentration (for example [Bq/kg])}} \leftarrow \enspace \textcircled{a} \propto \frac{\textcircled{$n_{\text{N},E}$} \rightarrow \boxed{\text{Net full energy peak area}}}{\textcircled{t_g} \rightarrow \boxed{\text{Measurement live time [s]}}}$$
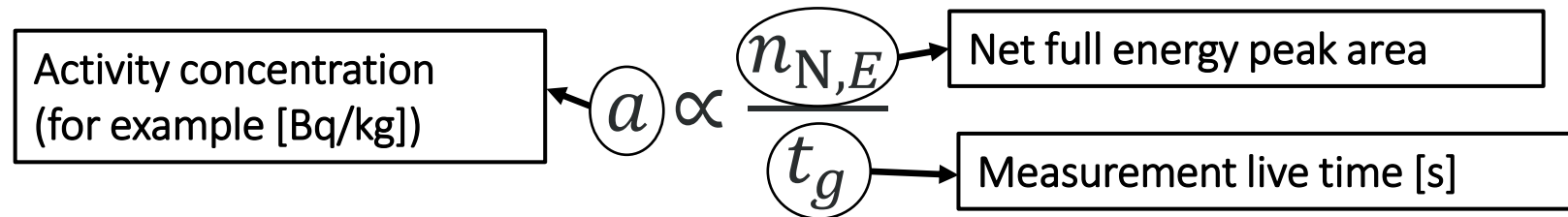
- However, to calculate a, we must consider several other factors as well...

Agenda

The full activity equation

- Typical activity equation in gamma-ray spectrometry:

$$a = \frac{n_{\mathrm{N},E}/t_g}{P_E \cdot \varepsilon_E \cdot q \cdot f_E}$$

- $n_{\mathrm{N},E}$ net peak area of the peak of interest
- t_g measurement live time of the spectrum
- P_E emission probability of gamma line of interest
- ε_E full energy peak efficiency at energy E
- q sample quantity (for example kg, l, m³, …)
- f_E all other necessary correction factors
  (more details later)

Gamma emission probability

$$a = \frac{n_{\mathrm{N},E}/t_g}{P_E \cdot \varepsilon_E \cdot q \cdot f_E}$$

A decay may not always result in the emission of a specific gamma-ray photon.

- Also known as "Intensity", "Abundance", "Yield", etc.
- Nuclear data quantity stored in the nuclide library. <u>Example:</u>

Energy (keV)	Intensity (%)	Type	Origin*	Levels		Possible coincidence with (keV) / Possible sum of (levels)
				Start*	End*	
661.657 (3)	84.99 (20)	γ	Ba-137	2	0	

- What does this tell us?

  The emission probability of the 661.657 keV gamma line of Cs-137 is **0.8499 ± 0.0020**
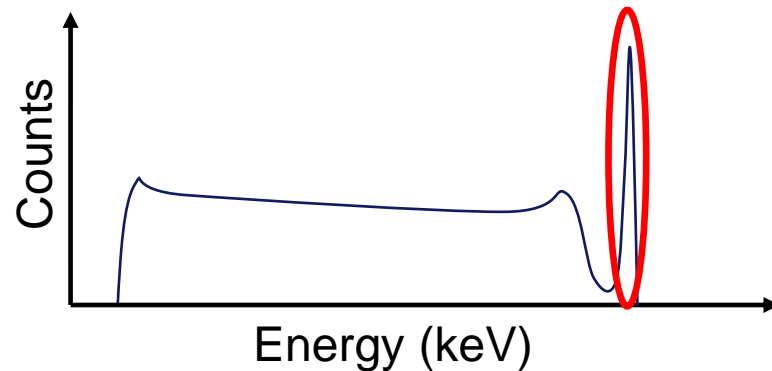 - OR -
  There's around 85 % chance that the decay of Cs-137 will result in the emission of a 661.657 keV gamma-ray photon.

Full energy peak (FEP) efficiency

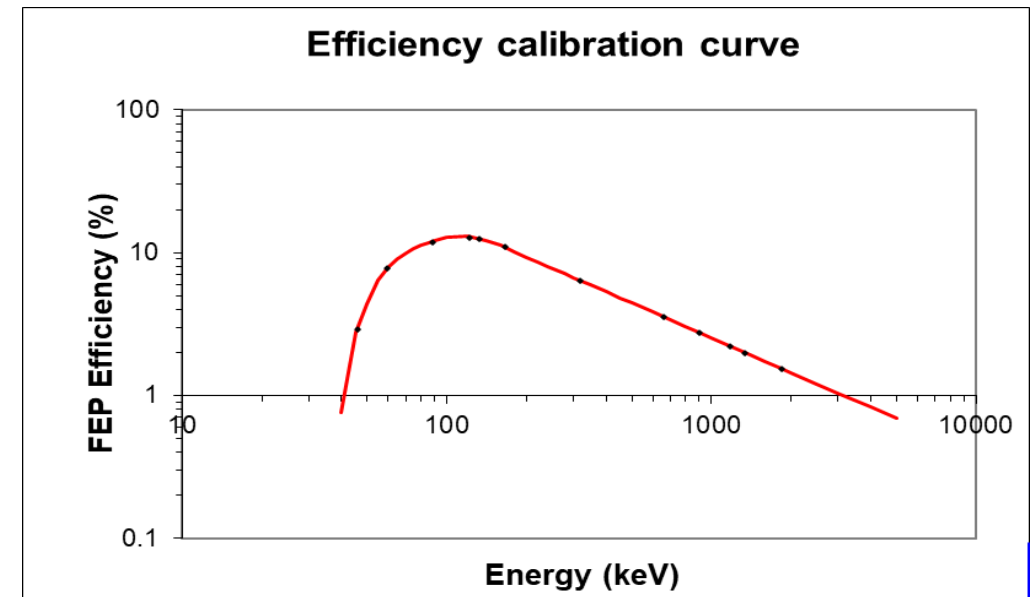$$a = \frac{n_{\mathrm{N},E}/t_g}{P_E \cdot \varepsilon_E \cdot q \cdot f_E}$$

Only a certain fraction of gamma-ray photons emitted by the sample will give a count in the corresponding full energy peak in the gamma spectrum.

$$\varepsilon_E = \frac{\text{\# events regisered as counts in the full energy peak*}}{\text{\# gamma} - \text{ray photons emitted by the source*}}$$

* At the energy of interest (E)

Sample quantity

$$a = \frac{n_{\mathrm{N},E}/t_g}{P_E \cdot \varepsilon_E \cdot \boldsymbol{q} \cdot f_E}$$

Needed to calculate the activity concentration of radionuclides in a sample material.

- We distinguish between the total activity of a source, A, with units [Bq]:

- ... and the activity concentration, a, of a sample material with units [Bq/quantity]:

[Bq/kg]　　　　　　　　[Bq/l]　　　　　　[Bq/m^3]

Correction factors

$$a = \frac{n_{\mathrm{N},E}/t_g}{P_E \cdot \varepsilon_E \cdot q \cdot \textcolor{red}{f_E}}$$

Correcting the calculated activity for various effects.

- f_E actually consists of three different factors which are multiplied together:

$$f_E = f_d \cdot f_{\mathrm{att},E} \cdot f_{\mathrm{tcs},E}$$

Where:

f_d is the correction factor for **radioactive decay**

$f_{\mathrm{att},E}$ is the correction for **sample self-attenuation (geometry)**

$f_{\mathrm{tcs},E}$ is the correction for **true coincidence summing**

Radioactive decay correction, f_d

- Radioactive decay is a random process.

- We **cannot** predict exactly <u>when</u> a radioactive nucleus will decay, but we **can** say something about the general behavior of many radioactive nuclei over time.

 # Atoms

N_o

$\dfrac{N_o}{2}$

$N = N_o \cdot e^{-\lambda \cdot t}$

$t_{1/2}$

Radioactive half-life

Time
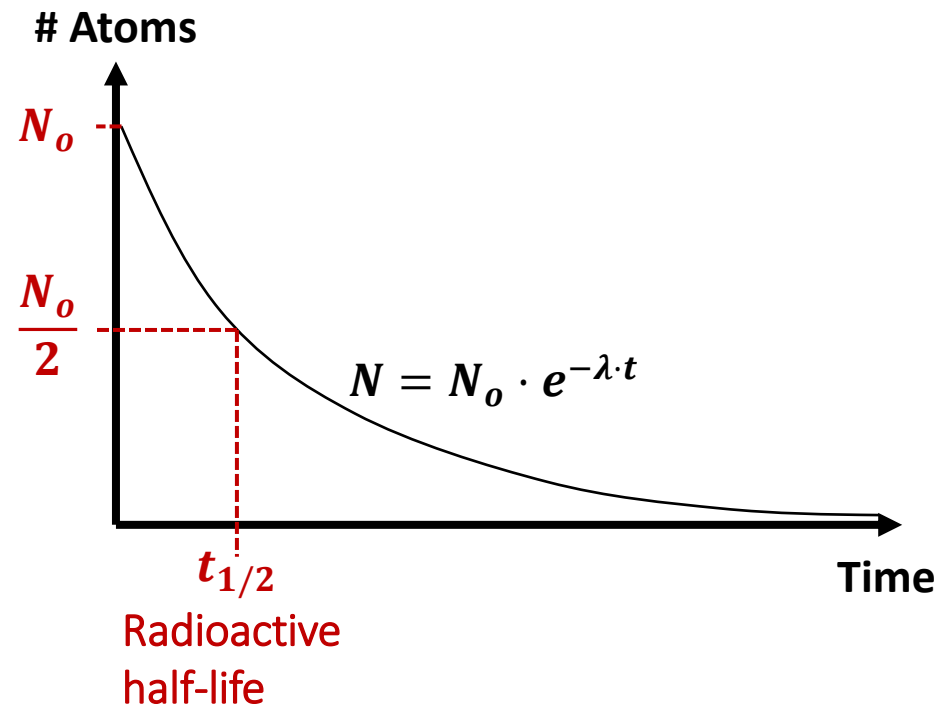
Relation between activity and number of atoms:
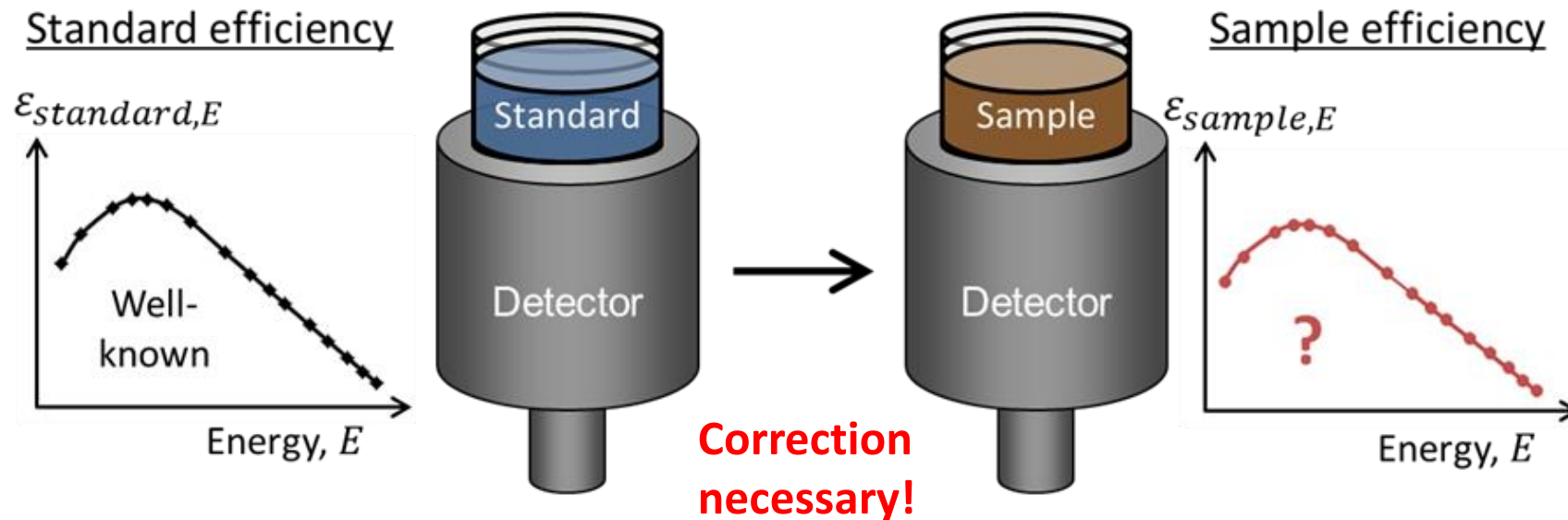
$$A = \lambda \cdot N$$

Decay constant:
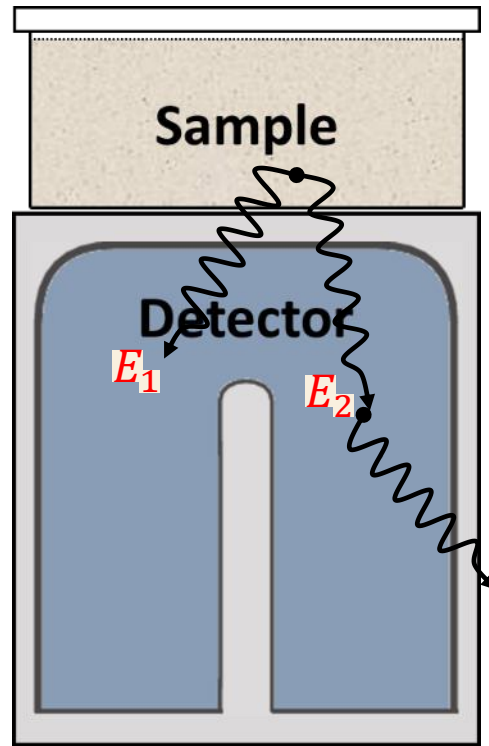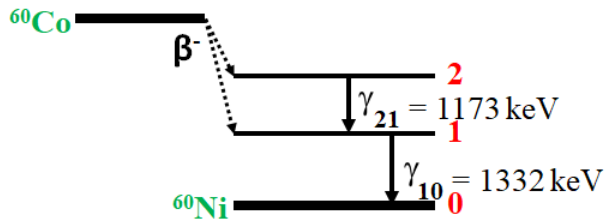
$$\lambda = \frac{\ln(2)}{t_{1/2}}$$

Self-attenuation (geometry) correction, $f_{\text{att},E}$

- Corrects for differences in FEP efficiency between the **calibration standard** and the **sample of interest**, caused by differences in self-attenuation and geometries.

True coincidence summing correction, $f_{\text{tcs},E}$

- Two or more photons from the same radionuclide are emitted in **cascade** (one directly after the other) and interact in the detector "simultaneously"

- The time between the two gamma emissions is much shorter than the resolving time of the detector, and they are therefore registered as one event.

- The individual counts at E_1 and E_2 are lost and instead a count is gained at $(E_1 + E_2)$

  Correction necessary!

Putting it all together…

$$a = \frac{n_{N,E}/t_g}{P_E \cdot \varepsilon_E \cdot q \cdot f_d \cdot f_{att,E} \cdot f_{tcs,E}}$$
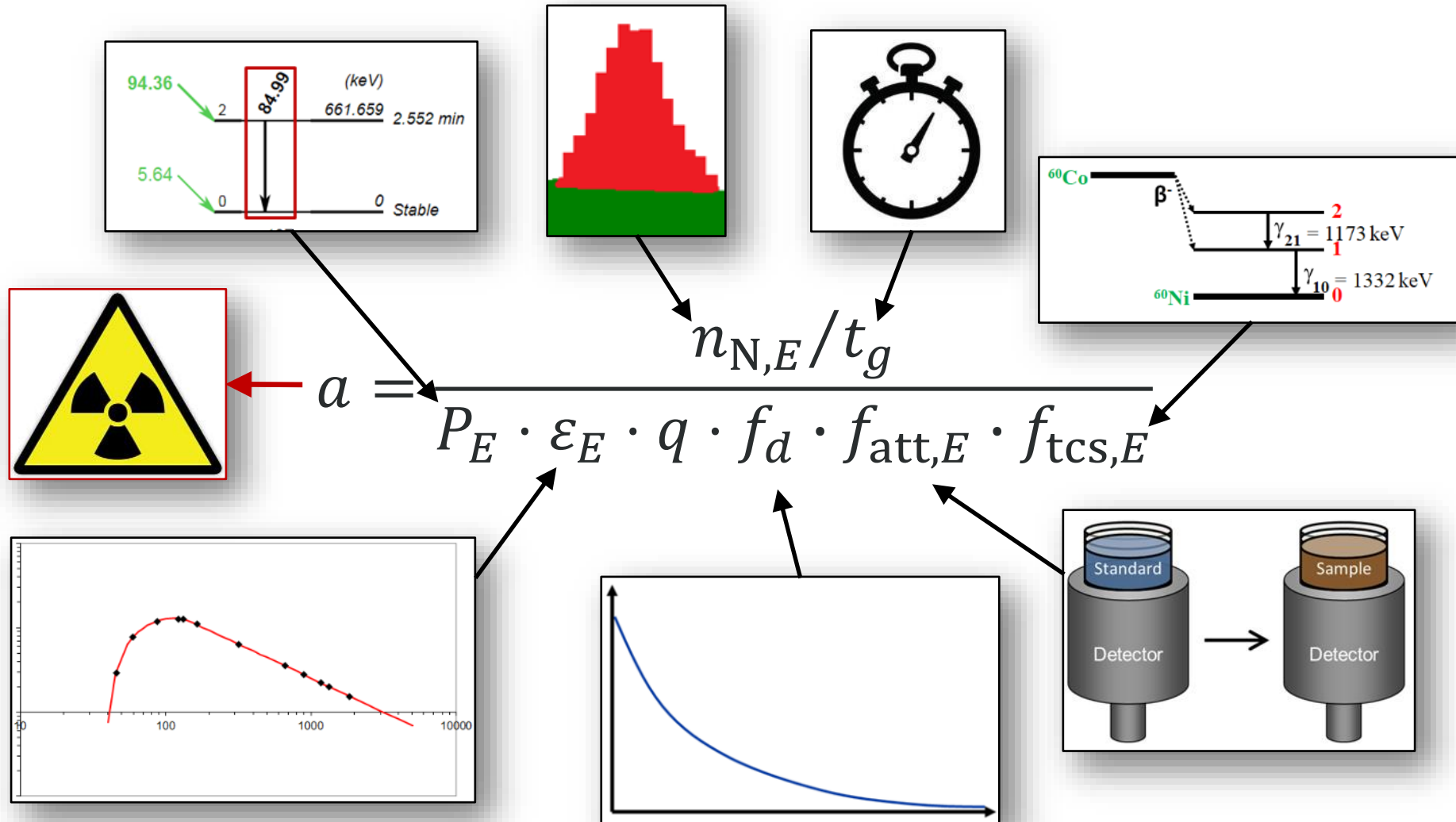
Calculating measurement uncertainties

A measurement result is not complete without a statement of its uncertainty!

$$a = \frac{n_{\mathrm{N},E}/t_g}{P_E \cdot \varepsilon_E \cdot q \cdot f_d \cdot f_{\mathrm{att},E} \cdot f_{\mathrm{tcs},E}}$$

For this model equation, the uncertainty can be calculated according to the Guide to Expression of Uncertainty in Measurement (GUM) uncertainty framework from simple quadratic propagation:

$$u_c(a) = \sqrt{\left(\frac{u(n_{\mathrm{N},E})}{n_{\mathrm{N},E}}\right)^2 + \left(\frac{u(P_E)}{P_E}\right)^2 + \left(\frac{u(\varepsilon_E)}{\varepsilon_E}\right)^2 + \left(\frac{u(q)}{q}\right)^2 + \left(\frac{u(f_d)}{f_d}\right)^2 + \left(\frac{u(f_{\mathrm{att},E})}{f_{\mathrm{att},E}}\right)^2 + \left(\frac{u(f_{\mathrm{tcs},E})}{f_{\mathrm{tcs},E}}\right)^2}$$

(assuming uncertainty of t_g is negligible)

Typical magnitude of uncertainty components

| Input quantity	Symbol	Typical uncertainty range (%)	Typical uncertainty value (%)
Net peak area	$n_{\mathrm{net},E}$	0.1-20	2
Counting time	t_g	0-2	-
Emission probability	P_E	0.01-5	< 0.5
FEP efficiency	ε_E	$1-5$	3
Sample quantity	m or V	0.01-5	< 0.5
Decay correction	f_d	0.01-1	< 0.2
Self-attenuation correction	$f_{\mathrm{att},E}$	0.1-10	2
TCS correction	$f_{\mathrm{cs},E}$	1-5	2
Other effects	-	0.01-1	< 0.5
Activity concentration	a	3-30	5

Agenda

Software for spectrum acquisition and/or analysis

Computer with gamma spectrum acquisition and analysis software
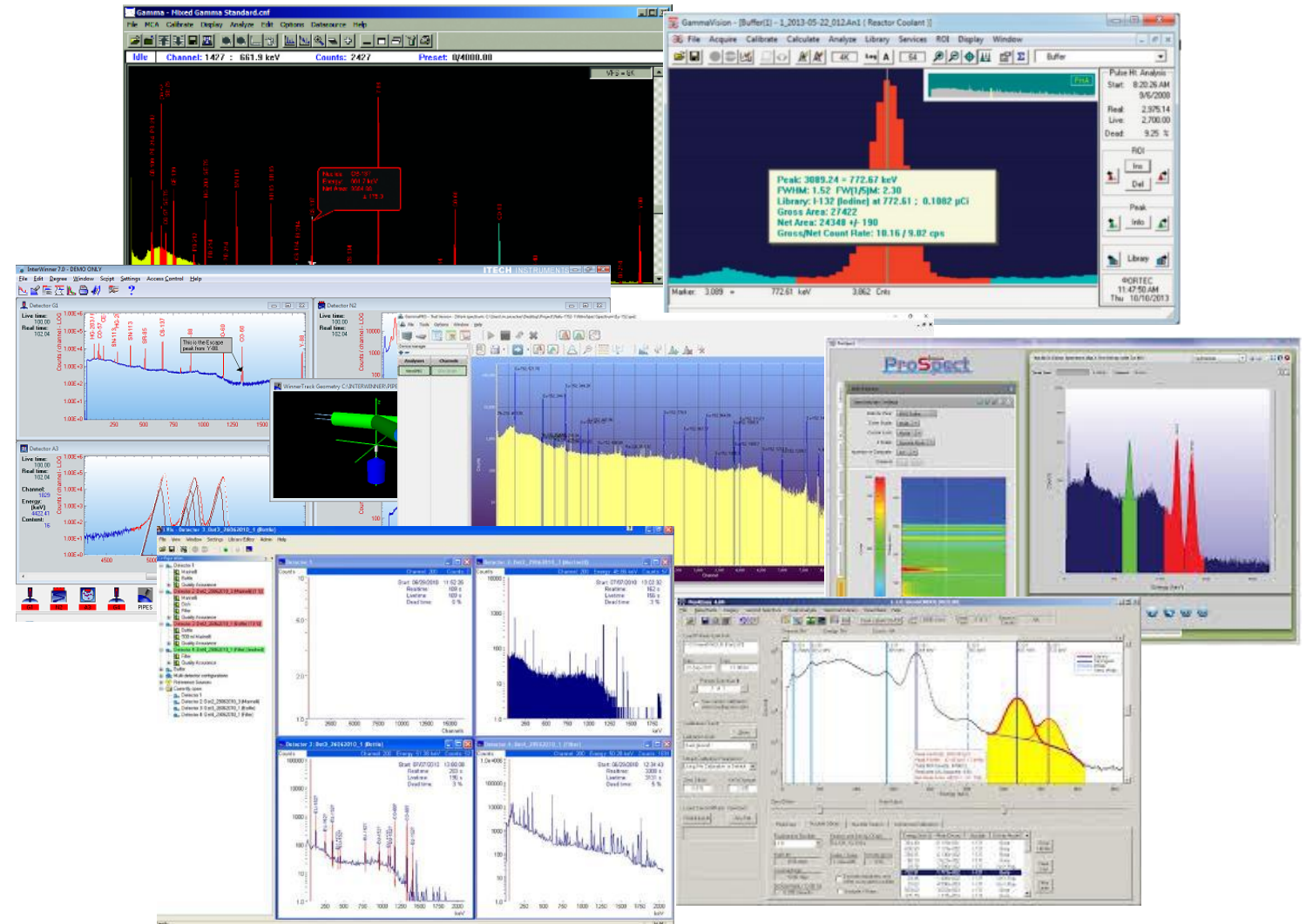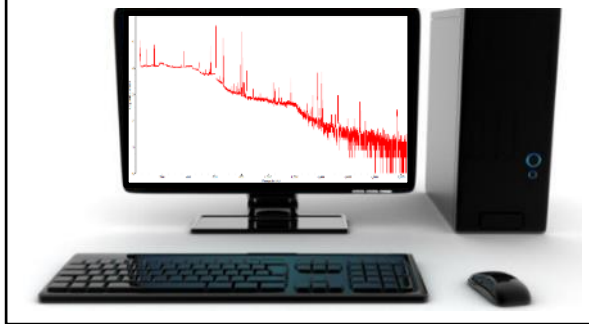
Some typical analysis software features

✓ Spectrum acquisition (MCA emulation)

✓ Storage and management of different types of files

✓ Peak search and peak area determination

✓ Energy, peak shape, efficiency calibration

✓ User configurable radionuclide libraries

✓ Radionuclide identification

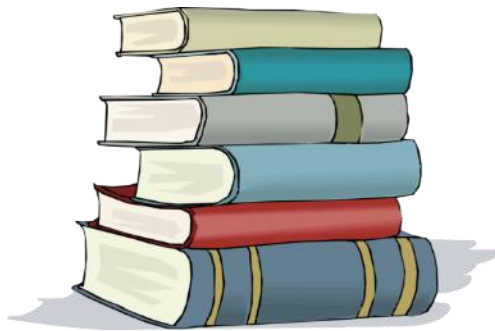✓ Calculation of activity, uncertainty and MDA

✓ Results reporting

✓ …
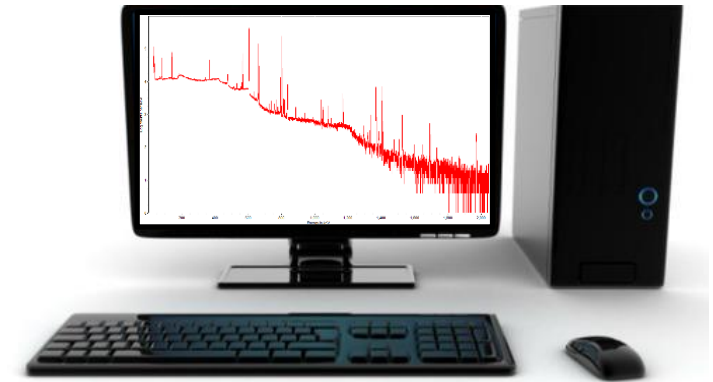
Tip: Know what your software can (and cannot) do, and how to do it!

Nuclide libraries – at the heart of the analysis

- The nuclide library contains all nuclear data parameters used by the software to carry out the analysis (nuclide identification and activity calculation)
  - Radionuclide half-lives
  - Gamma-ray energies
  - Emission probabilities
  - Related uncertainties
  - …

Screenshot of Genie2000 Nuclide Library Editor

# Nuclide libraries – recommended data sources

- Nuclide data is used as direct inputs to the activity calculation. So, it's important to use the correct data!

- <u>Some recommended data sources:</u>
  - Decay Data Evaluation Project (DDEP) / Laraweb:
    http://www.nucleide.org/DDEP.htm
    http://www.nucleide.org/Laraweb/index.php

  - IAEA Nuclear Data Services: https://www-nds.iaea.org/

- <u>Tip:</u> Check your nuclide library to be sure that it contains the radionuclides you are interested in and that they have the latest recommended data.

Reporting results

- Results should be reported **clearly** and **unambiguously**

- <u>Example</u>
  The activity concentration of Cs-137 in sample #111 is
  $$345 \pm 12 \text{ Bq/kg} \ (k = 1) \qquad \textit{on reference date 2023-09-26}$$
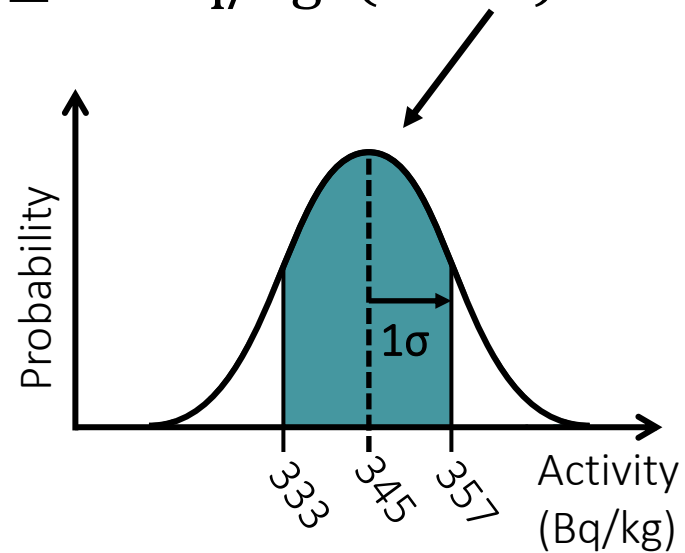
Some general tips:
- Round all values appropriately
- Include the measurement unit
- Don't forget the reference date

Final words: Trusting your software…

- The spectrum analysis process involves several steps before nuclide activities can be calculated from full energy peaks in the spectrum. Analysis software will carry out most of the steps automatically, given the correct input.

- But the software cannot think for itself. It's very important to have a qualified analyst to evaluate the results!

- Always remember:
  You are smarter than the software ☺

Thank you for the attention!

Alexander.Mauring@ife.no