# Prompt Gamma Spectroscopy Retrieval Algorithm for Element and Density Measurements

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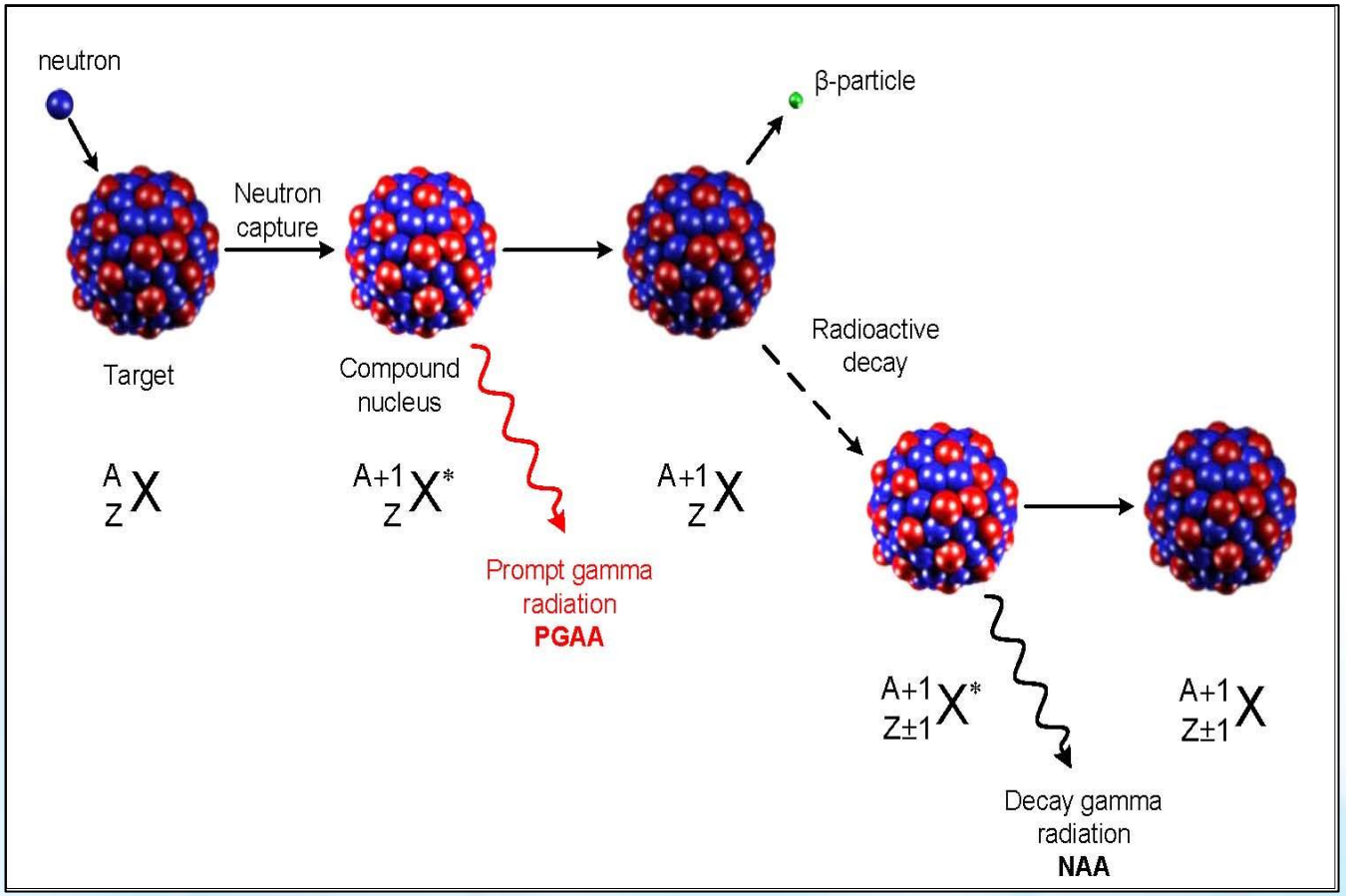
**2023 7 6@YIWS**

# Contents

# Background

## prompt gamma-ray neutron activation analysis (PGNAA)

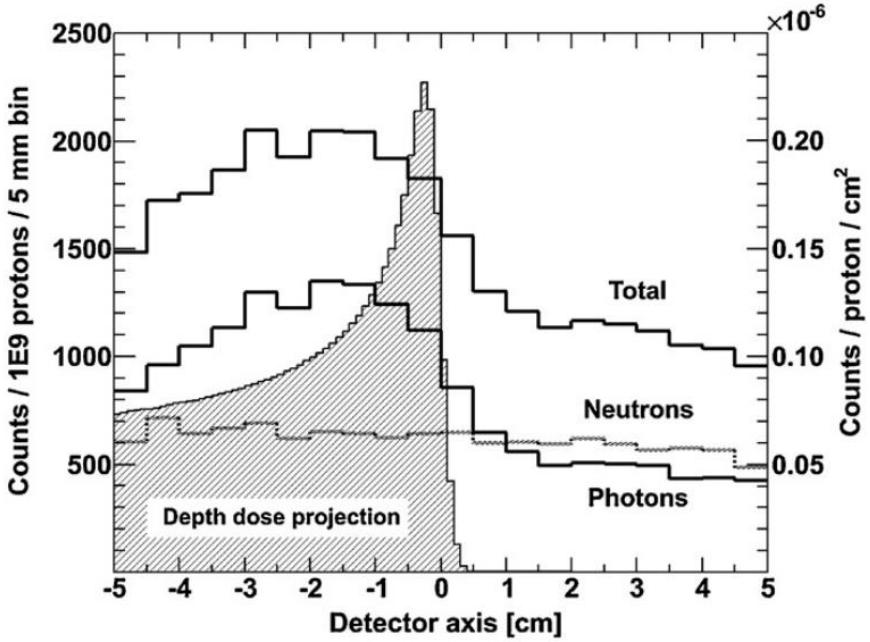



**Prompt Gamma + Decay Gamma**

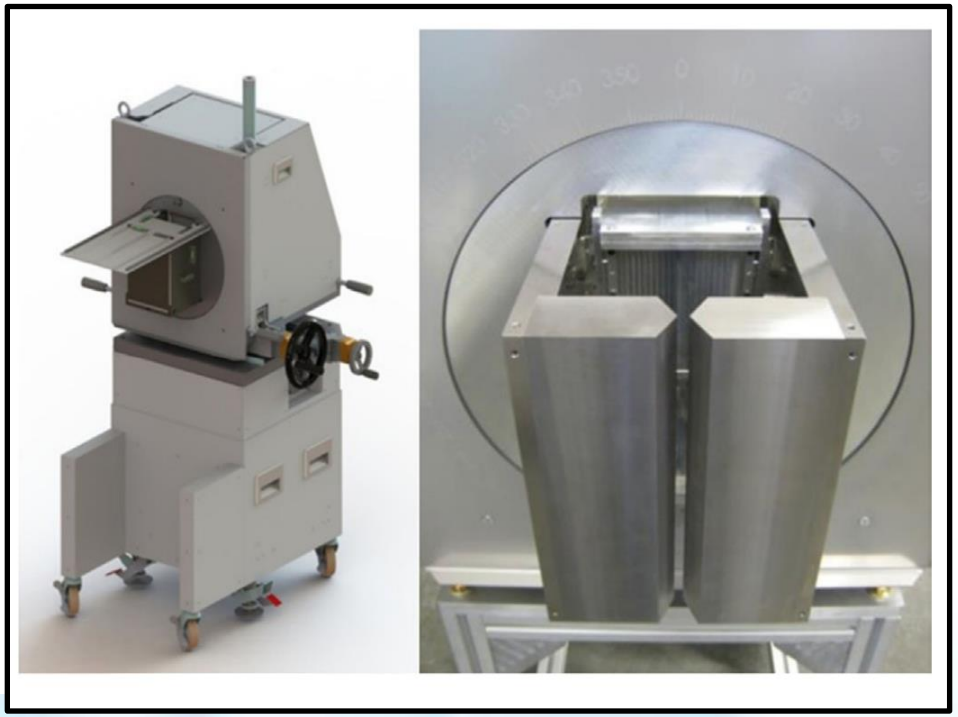
A.A. Naqvi. Appl. Radiat. Isot. 70, 882–887 (2012).

# 1 Background

## Range and PGs



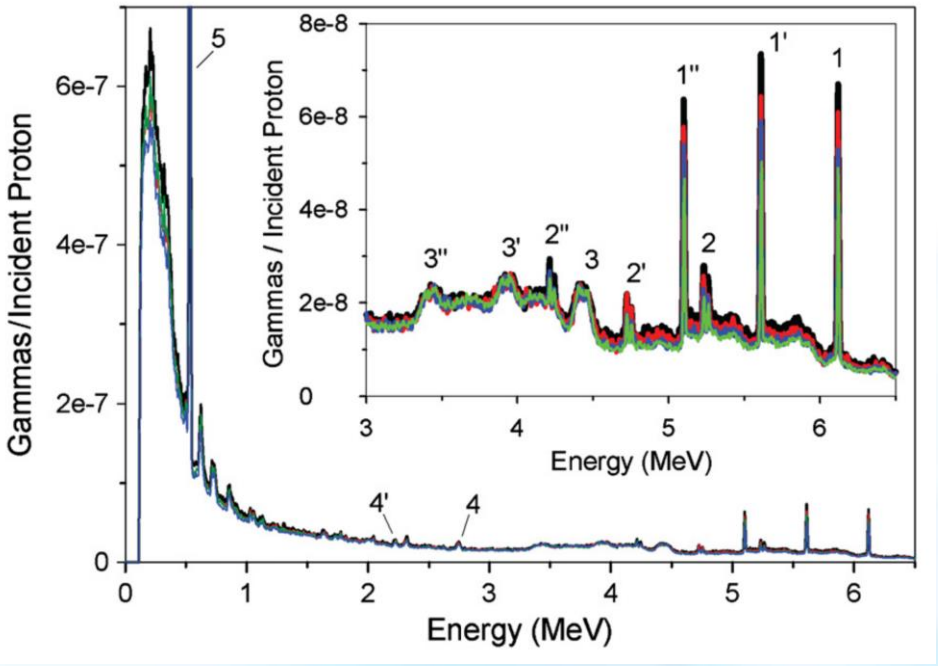

J Smeets 2012

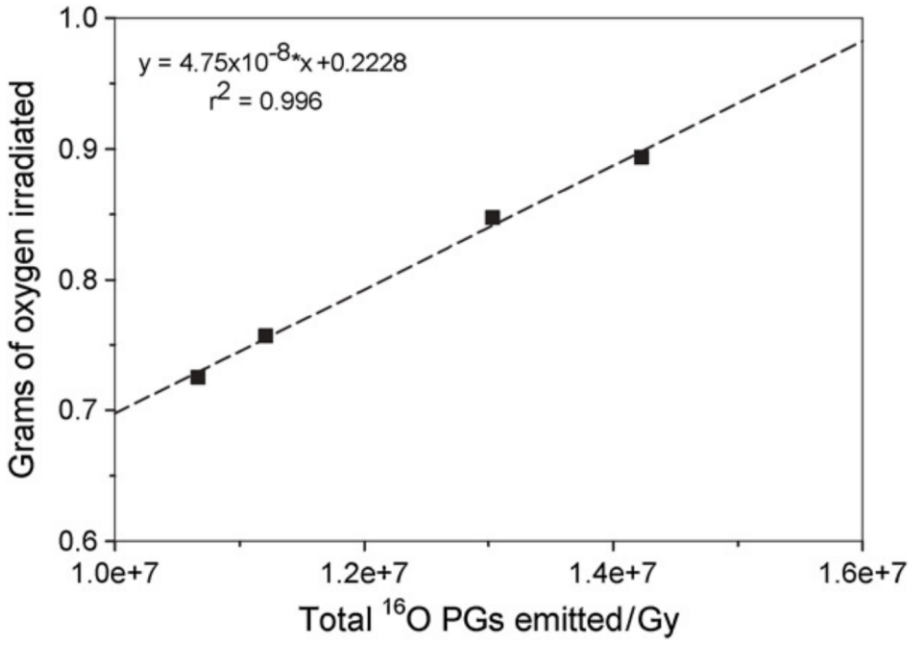


J Smeets 2016

# 1 Background

## PGs and elements



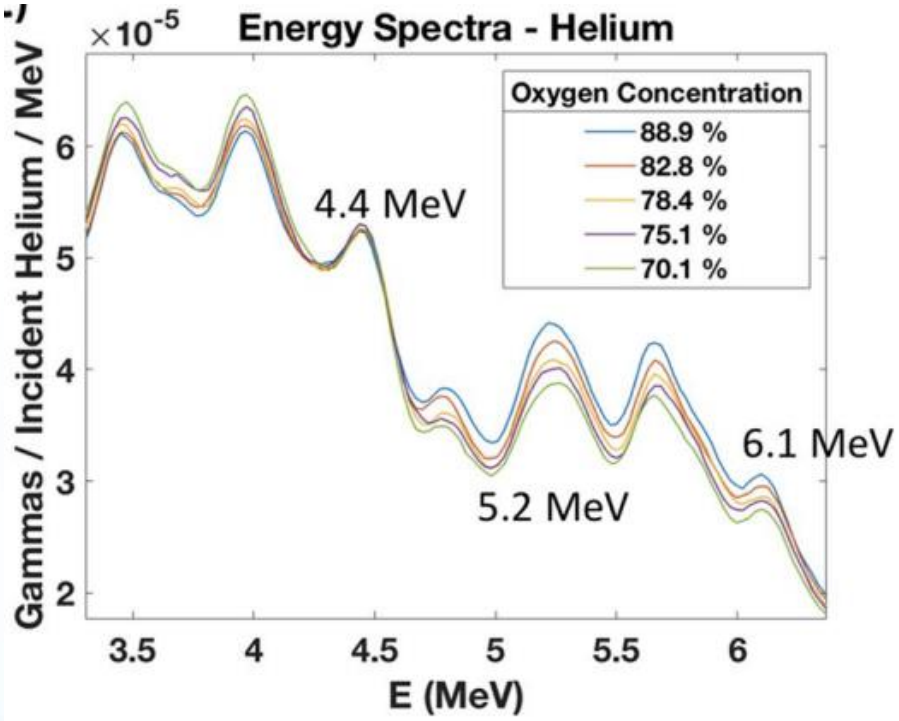



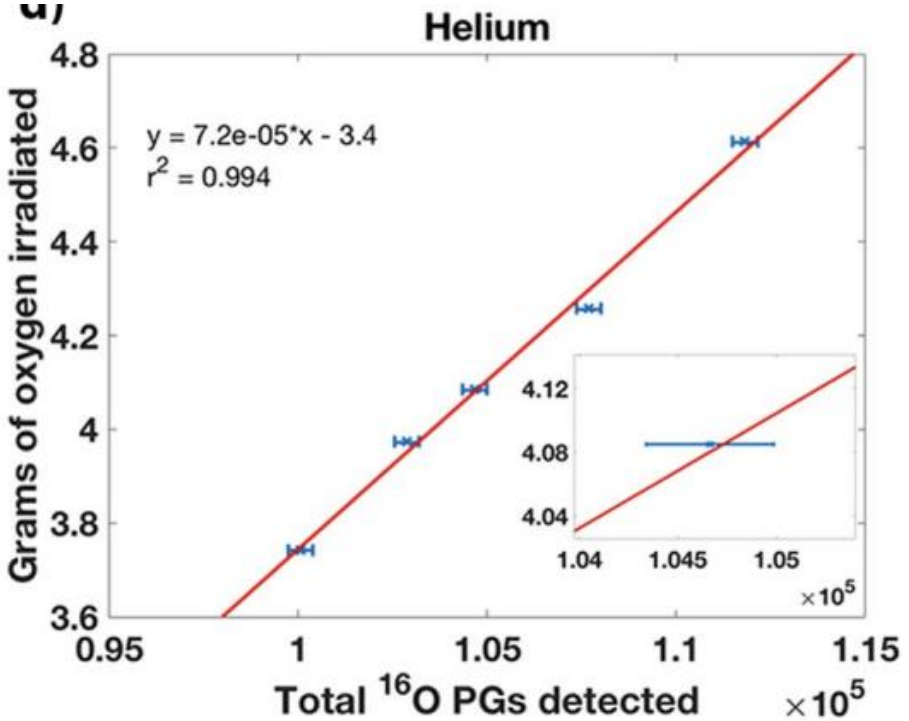

Jerimy C Polf 2013

# 1 Background

## PGs and elements

Paulo Magalhaes Martins 2020



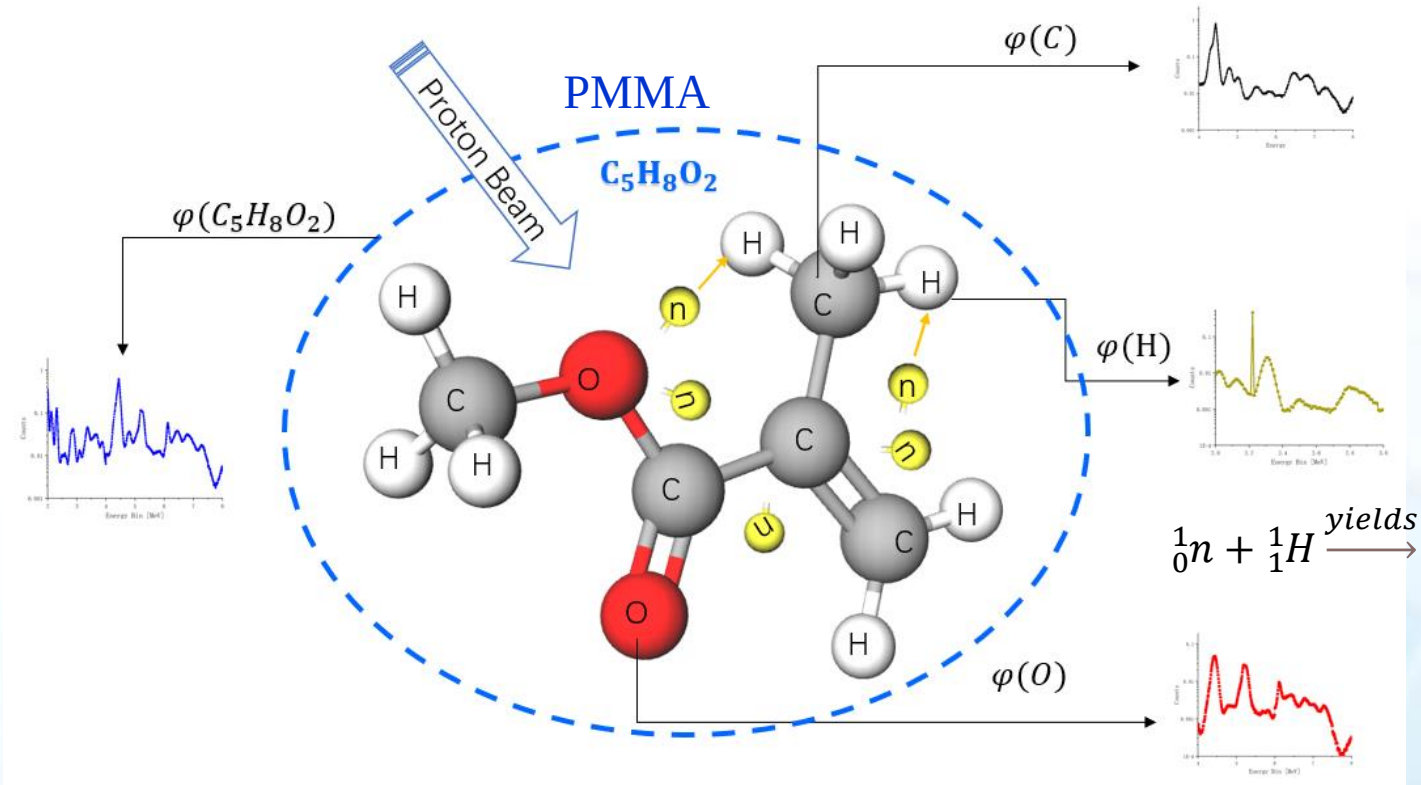

**A linear relationship** was demonstrated between the **amounts of irradiated oxygen** in tissue-equivalent samples and the **total emission** of prompt gamma radiation during irradiation by particles.

# Contents

# Prompt gamma spectroscopy retrieval algorithm

## Basics & Mathematical form

Spectroscopy directly generated by $C(p,\gamma)C^*$




$$ {}_0^1n + {}_1^1H \xrightarrow{yields} \left({}_1^2H\right) \xrightarrow{yields} {}_1^2H + \gamma_{2.23} \quad (1) $$

Spectroscopy directly generated $by\ O(p,\gamma)O^*$

# 2 Prompt gamma spectroscopy retrieval algorithm

## Basics & Mathematical form

Formalize a mathematical model from a **phase-only perspective** which could be solved by the numerical method:

Basic assumptions:

1) the sample material has a relationship with its element molar gamma lines in prompt gamma spectroscopy
2) The dominant factor is the number of element atoms in the molecule
3) for carbon and oxygen, this relationship is linear, and
4) for hydrogen, this relationship is nonlinear and is based on a neutron absorption reaction

$$\varphi(C_5H_8O_2) = N_c\varphi(C) + N_O\varphi(O) + f(N_c, N_O)\varphi(H) \quad (2)$$

The dominant factor is the number of element atoms in the molecule

# Prompt gamma spectroscopy retrieval algorithm

## Basics, Mathematical form

**linear components** **Non-linear components neutron absorption**

$$\varphi\left(C_{N_C}H_{N_H}O_{N_O}\right) = N_C\varphi(C) + N_O\varphi(O) + f_c(N_c, N_O, N_H)\varphi(HC) + f_o\,(N_c, N_O, N_H)\varphi(HO) \quad (3)$$

$$f_c(N_c, N_O, N_H) = N_H \frac{N_c}{N_O+N_c}\frac{N_H}{N_O+N_c} \quad (4)$$

$$f_o(N_c, N_O, N_H) = N_H \frac{N_O}{N_O+N_c}\frac{N_H}{N_O+N_c} \quad (5)$$

- $N_H$ : The dominant parameter is the number of hydrogen atoms $N_H$ in the molecule;
- $\frac{N_c}{N_O+N_c}$ : Represents the factor of the neutron, i.e., the neutron absorption reaction (Equation 1) , where the neutron is emitted from the $C(p,n)C^*$ reaction.
- $\frac{N_H}{N_O+N_c}$ : is a hydrogen enhancement factor because when there are more hydrogens in a molecule with the same number of carbon or oxygen, the neutron absorption probability will increase.

# Prompt gamma spectroscopy retrieval algorithm

## Basics, Mathematical form

linear components

Non-linear components neutron absorption

$$\varphi\left(C_{N_C}H_{N_H}O_{N_O}\right) = N_c\varphi(C) + N_O\varphi(O) + f_c(N_c, N_O, N_H)\varphi(HC) + f_o\,(N_c, N_O, N_H)\varphi(HO) \quad (3)$$

For hydrogen, there is **only one peak at 2.23 MeV** in its PGS, and it does not contribute to the other characteristic gamma lines in the carbon and oxygen spectra

Transform unknown material $x$

$C_{N_C}H_{N_H}O_{N_O} \rightarrow x$, $\varphi(HC) \rightarrow \varphi_{HC}^{2.23}$, $\varphi(HO) \rightarrow \varphi_{HO}^{2.23}$, $\varphi_{HC}^{2.23}$ and $\varphi_{HO}^{2.23}$ are 2.23 MeV gamma counts originating from carbon and oxygen per molecule or per mol.

Mathematically separated linear and non-linear part

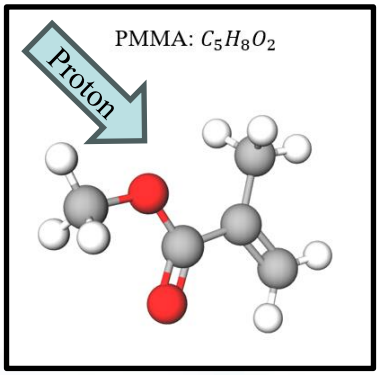
$$\boldsymbol{\varphi(x) - \varphi_x^{2.23} = N_c\varphi(C) + N_O\varphi(O)}$$

$$\boldsymbol{\varphi_x^{2.23} = f_c\varphi_{HC}^{2.23} + f_o\,\varphi_{HO}^{2.23}} \quad (6)$$

# Prompt gamma spectroscopy retrieval algorithm

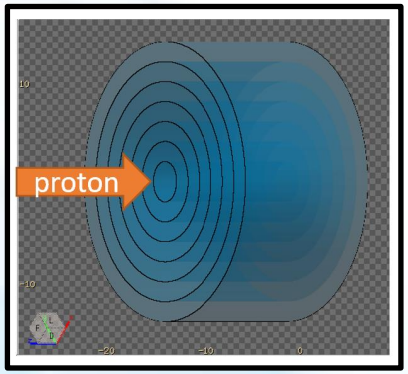
## Basics, Mathematical form

Shoot a single molecule target with a single proton




$$\varphi(x) - \varphi_x^{2.23} = N_c\varphi(C) + N_O\varphi(O)$$
$$\varphi_x^{2.23} = f_c\varphi_{HC}^{2.23} + f_o\,\varphi_{HO}^{2.23} \quad (6)$$

Shoot target phantom has $M$ mol molecules with proton beam




$$\psi_x^{FullEnergy} - \psi_x^{2.23} = M_c\varphi(C) + M_O\varphi(O) \quad (7a)$$
$$\psi_x^{2.23} = F_C\varphi_{HC}^{2.23} + F_O\,\varphi_{HO}^{2.23} \quad (7b)$$

$$\psi_x^{FullEnergy} = M * \varphi(x)$$

$$F_C = M * f_c = M_H \frac{M_c}{M_O+M_c}\frac{M_H}{M_O+M_c} \quad (8)$$

$$F_O = M * f_o = M_H \frac{M_O}{M_O+M_c}\frac{M_H}{M_O+M_c} \quad (9)$$

There are only two unknown variables $M_c$ and $M_O$ in Equation (7a). Thus, for a binary linear equation, we need at least two peak points to solve the equation.

# Prompt gamma spectroscopy retrieval algorithm

## Basics, Mathematical form

$$\psi_x^{FullEnergy} - \psi_x^{2.23} = M_c\varphi(C) + M_O\varphi(O) \quad (7a)$$

Solve $M_c$ and $M_O$

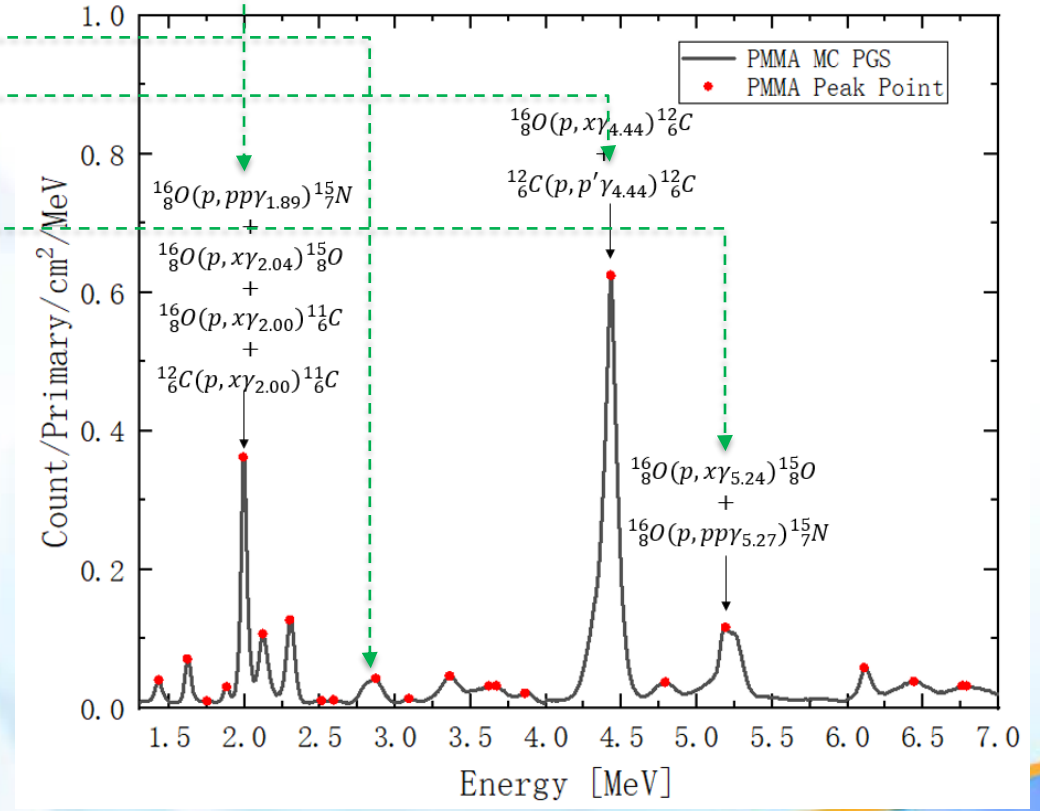
To obtain a numerical solution, we discretize Equation 7(a)

$$\begin{bmatrix} \varphi_c^1 & \varphi_o^1 \\ \varphi_c^2 & \varphi_o^2 \\ \varphi_c^3 & \varphi_o^3 \\ \vdots & \vdots \\ \varphi_c^i & \varphi_o^i \\ \vdots & \vdots \end{bmatrix} \begin{bmatrix} M_C \\ M_O \end{bmatrix} = \begin{bmatrix} \psi_x^1 \\ \psi_x^2 \\ \psi_x^3 \\ \vdots \\ \varphi_x^i \\ \vdots \end{bmatrix} \quad (10)$$

Can be determined by the least square method

$$A = \begin{bmatrix} \varphi_c^1 & \varphi_o^1 \\ \varphi_c^2 & \varphi_o^2 \\ \varphi_c^3 & \varphi_o^3 \\ \vdots & \vdots \\ \varphi_c^i & \varphi_o^i \\ \vdots & \vdots \end{bmatrix} \quad B = \begin{bmatrix} \psi_x^1 \\ \psi_x^2 \\ \psi_x^3 \\ \vdots \\ \varphi_x^i \\ \vdots \end{bmatrix} \quad m = \begin{bmatrix} M_C \\ M_O \end{bmatrix}$$

$$Object: \min(Am - B) \quad (11)$$



# Prompt gamma spectroscopy retrieval algorithm

## Basics, Mathematical form

$$\psi_x^{2.23} = F_C\varphi_{HC}^{2.23} + F_O\,\varphi_{HO}^{2.23} \quad \textbf{(7b)}$$

Solve $M_H$

Bring coefficients $F_C$ and $F_O$ into Equation (7b):

$$\psi_x^{2.23} = M_H * \left(\frac{M_O}{M_O+M_C}\varphi_{HO}^{2.23} + \frac{M_C}{M_O+M_C}\varphi_{HC}^{2.23}\right)\frac{M_H}{M_O+M_C} \quad (12)$$

Now, only $M_H$ is an unknown variable, and the analytical solution of $M_H$ is

$$M_H = (M_O + M_C)\sqrt{\frac{\psi_x^{2.23}}{M_O\varphi_{HO}^{2.23}+M_C\varphi_{HC}^{2.23}}} \quad \textbf{(13).}$$

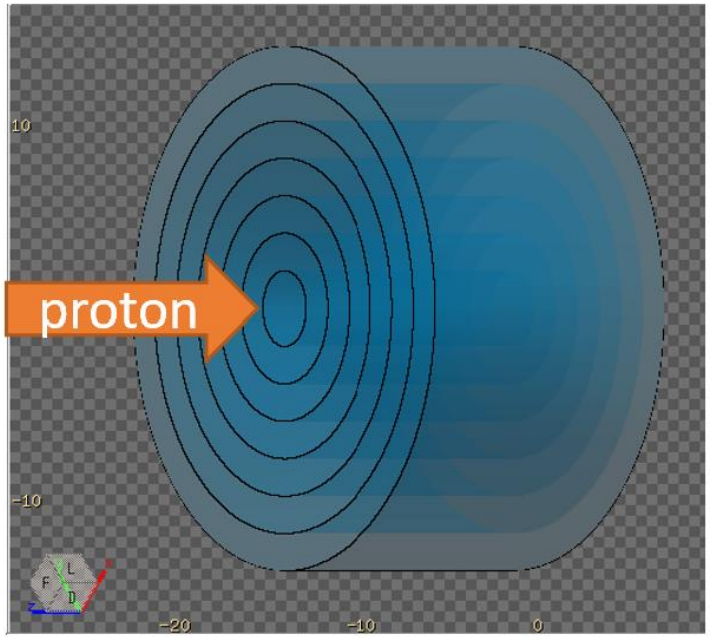
$$\rho = \frac{Mass}{V} = \frac{12 * M_C + 16 * M_O + M_H}{S * R} \quad (15)$$

- Where $\psi_x^{2.23}$ is the peak point count at 2.23 MeV for target material $x$, which is determined by **neutron distribution (energy, time, and lateral distribution) inside the phantom**.
- $\varphi_{HC}^{2.23}$ and $\varphi_{HO}^{2.23}$ are the PG counts per mol hydrogen with **neutrons originating from carbon and oxygen**.

# Contents

# Neutron & Gamma Distributions

## Where and When




150 MeV proton to water phantom with 7 layers ranging from a radii of 2 cm to 14 cm

**Neutron distribution inside the phantom:**

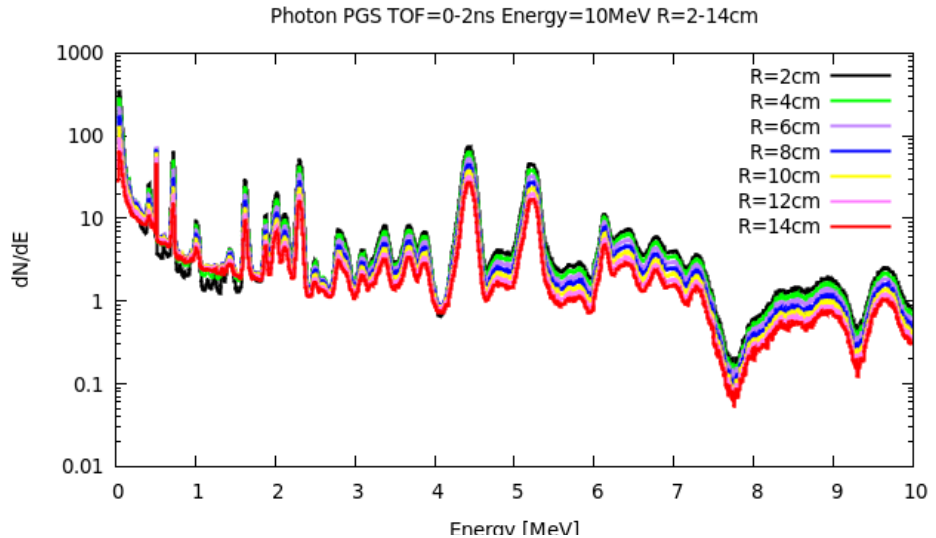
- energy
- time
- lateral distribution

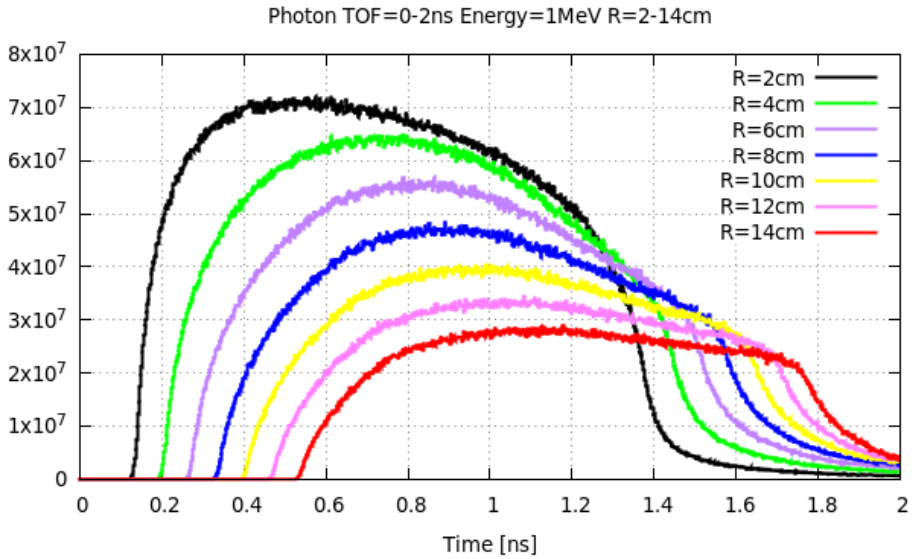
2.23 MeV Gamma from the phantom**:**

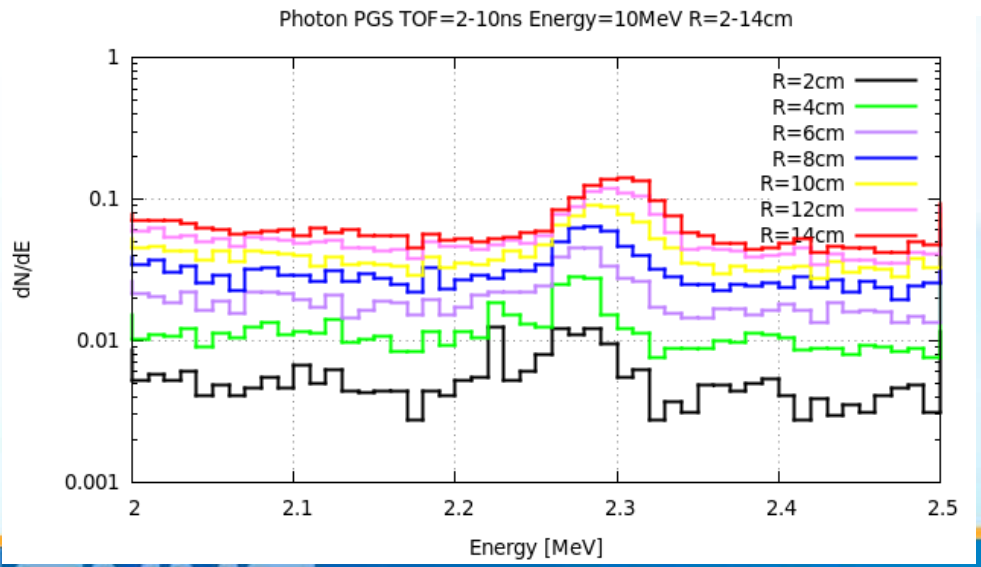
- **Where**
- **When**

# 3 Neutron & Gamma Distributions

## Where and When



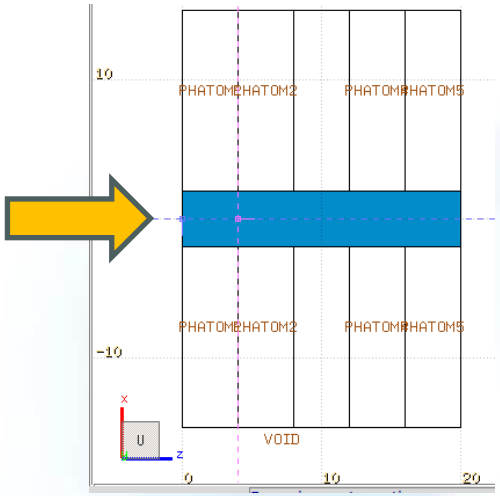



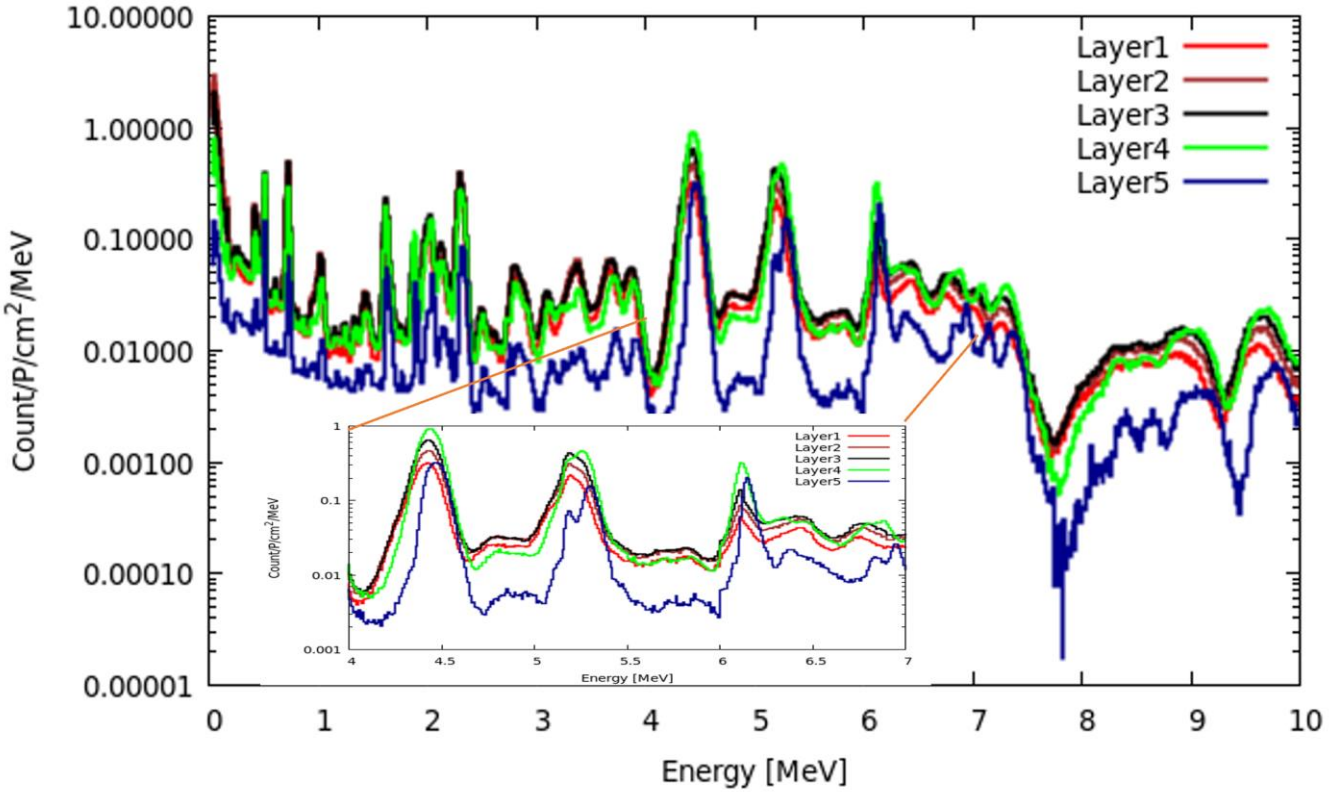

- PGS at different layers have the same shape.
- most photons are generated in the center layer R=2 cm from 0.1 ns to 1.4 ns. The outside layers will start generating photons slightly later, within 0.6 ns, as neutron and other secondary particles require a short time to travel in the lateral direction in the water phantom;
- **10ns is TOF window** to select 2.23 MeV gamma.

# 3 Neutron & Gamma Distributions

## Where and When

150 MeV proton to water



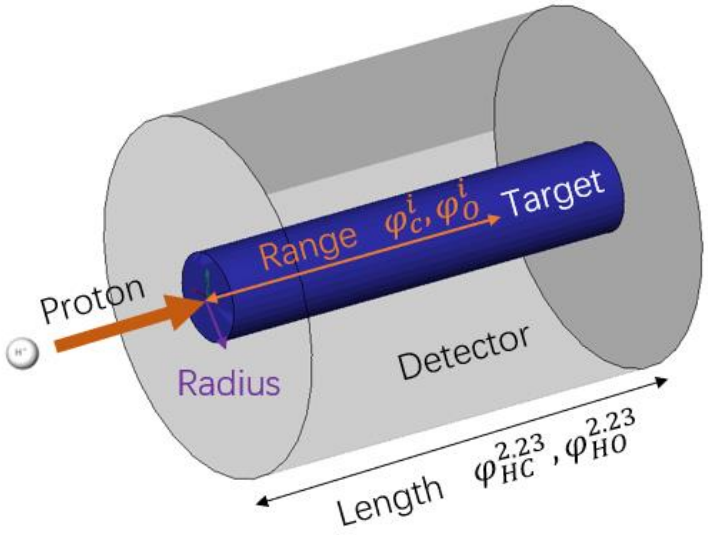




- Layer 1-4 >10 MeV proton has similar PGs
- Layer 5 at distal fall off region PGs decreases obviously.

# Contents

# FLUKA Simulations and Results

## Elements and Density



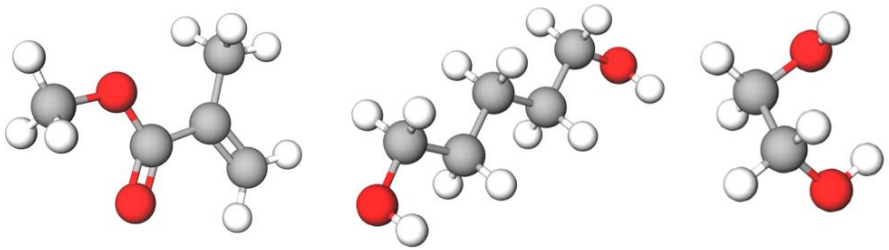

Molar PGS

- hydrocarbons: $C,\ HC,\ H_2C,\ H_3C, \ldots,\ H_{20}C$
- hyd*roxygens*: $O,\ HO,\ H_2O,\ H_3O, \ldots,\ H_{20}O$

Sample Materials x

- PMMA ($C_5H_8O_2$), 1.18 $g/cm^3$
- pentanediol ($C_5H_{12}O_2$) 0.9939 $g/cm^3$
- ethanediol ($C_2H_6O_2$). 1.1088 $g/cm^3$

PMMA: $C_5H_8O_2$ | Pentanediol: $C_5H_{12}O_2$ | Ethanediol: $C_2H_6O_2$

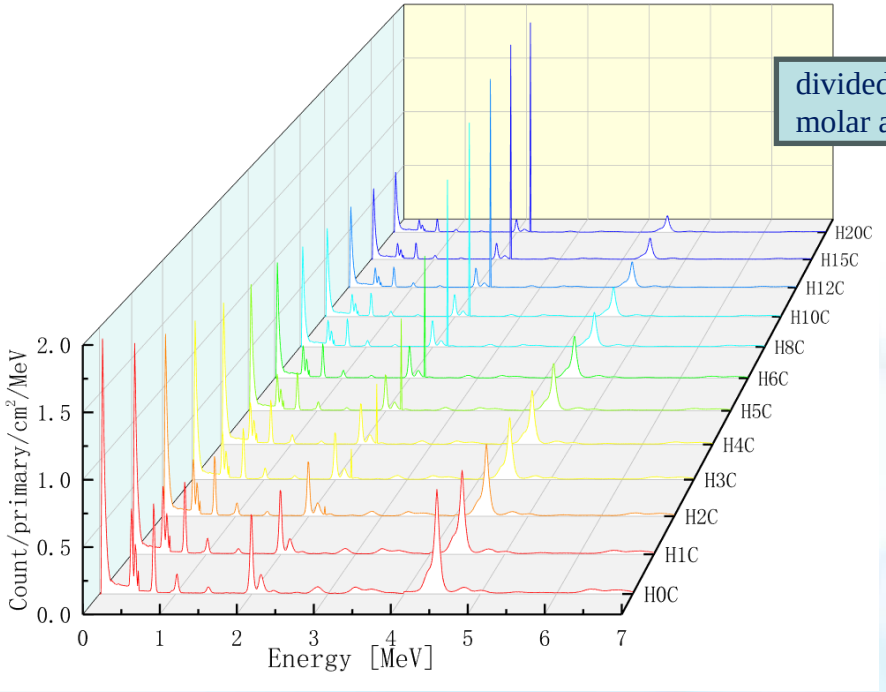


- molar PGS for carbon and oxygen range mass
- molar PGS for hydrogen target mass

# FLUKA Simulations and Results

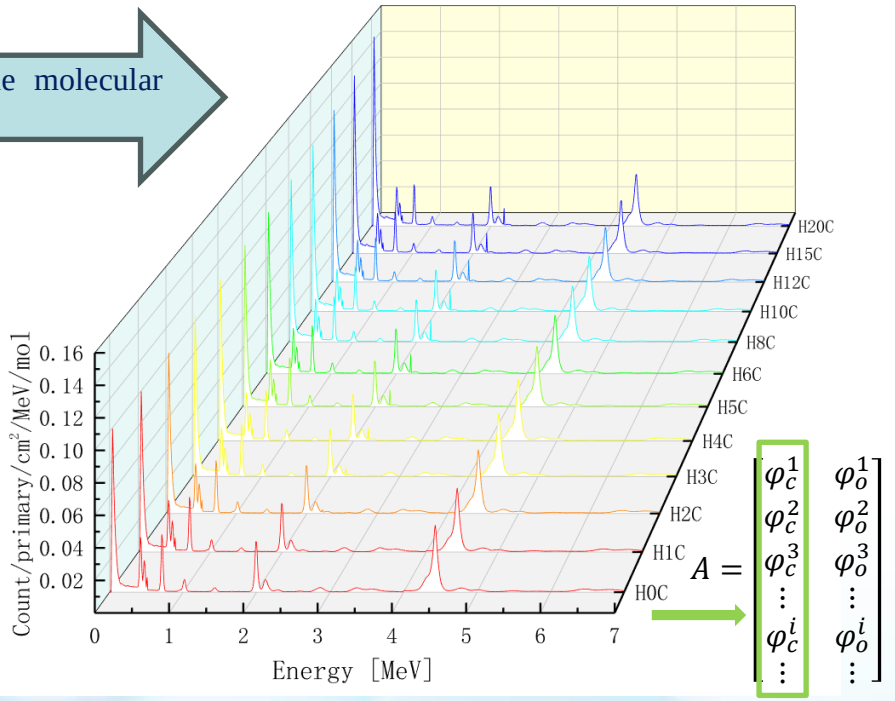
## Elements and Density

PGS spectra
from combinations of carbon and hydrogen




divided by the molecular molar amount

Molar PGS spectra
from combinations of carbon and hydrogen



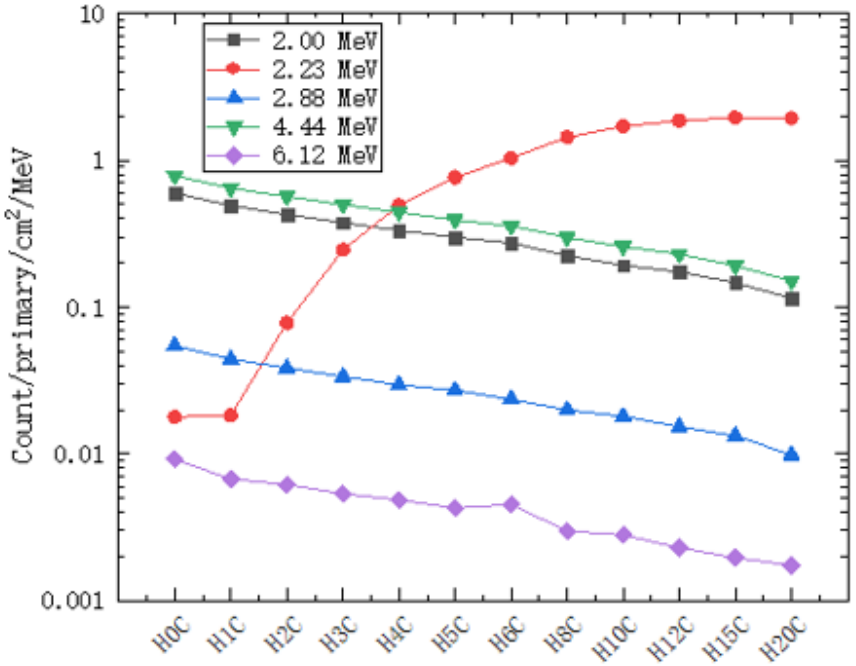

- Characteristic gamma lines from carbon **decrease** with an increasing number of hydrogen atoms,
- while 2.23 MeV gamma lines **increase** as the number of hydrogen atoms increases.

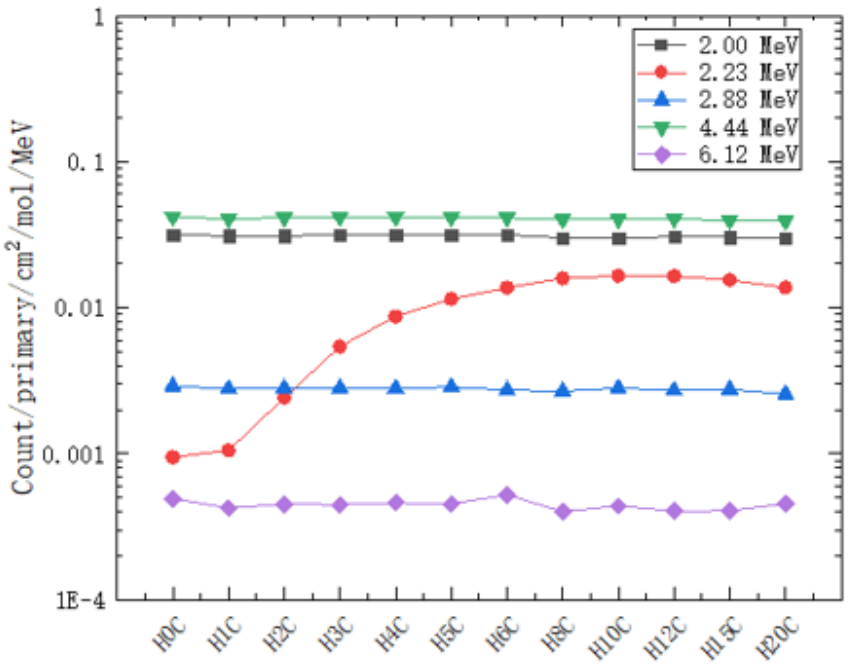
- Characteristic gamma lines from carbon come to the same level in molar PGS
- except at energy of approximately 2.23 MeV

# FLUKA Simulations and Results

## Elements and Density

Extract peak gamma lines (2.00 MeV, 2.23 MeV, 2.88 MeV, 4.44 MeV and 6.12 MeV)



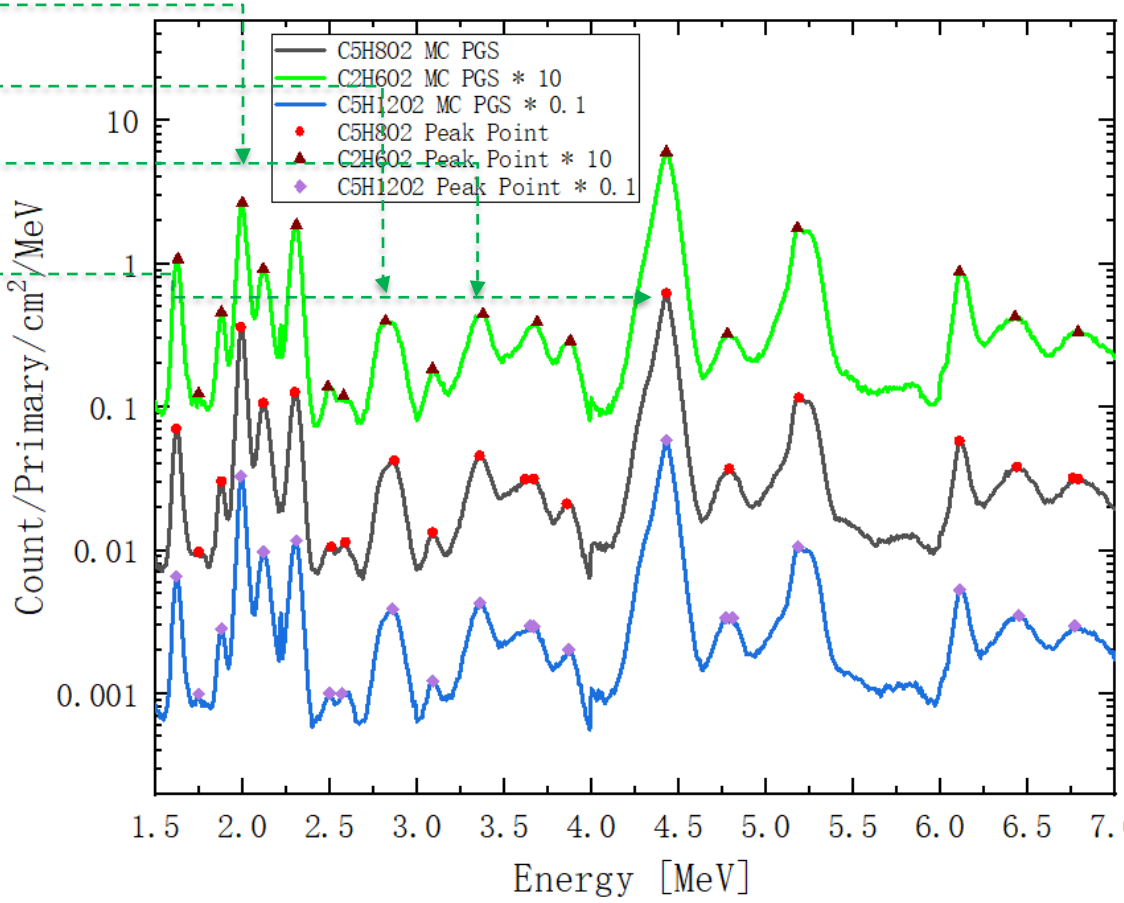

- ✓ 2.00 MeV, 2.88 MeV, 4.44 MeV and 6.12 MeV counts **have a linear relationship** with carbon concentration, which has been confirmed by experiments
- ✓ 2.23 MeV is **non-linear**

# 4 Results

## Elements and Density

Full energy PGS spectra of PMMA ($C_5H_8O_2$ in dark), ethanediol ($C_2H_6O_2$ in green) and pentanediol ($C_5H_{12}O_2$ in blue)

$$B = \begin{bmatrix} \psi_x^1 \\ \psi_x^2 \\ \psi_x^3 \\ \vdots \\ \varphi_x^i \\ \vdots \end{bmatrix}$$




- **Low:** low-energy peaks from 1.5~4 MeV.
- **High:** high-energy peaks from 4~7 MeV.
- **Medium-High:** peaks of medium energy 2 MeV to high energy 7 MeV.

# 4 Results

## Elements and Density

| $C_5H_8O_2$ group | *Mc* [mol] | *Mo* [mol] | *Mc/Mo* | *Mc/Mo* relative error |
|---|---|---|---|---|
| All | 10.1522 | 4.2419 | 2.3933 | 4.27% |
| Low | 10.1350 | 4.2509 | 2.3842 | 4.63% |
| High | 10.2351 | 4.2068 | 2.4330 | 2.68% |
| **Medium-High** | **10.3469** | **4.1066** | **2.5196** | **0.78%** |

| $C_5H_{12}O_2$ group | *Mc* [mol] | *Mo* [mol] | *Mc/Mo* | *Mc/Mo* relative error |
|---|---|---|---|---|
| All | 9.2649 | 4.0280 | 2.3001 | 7.99% |
| Low | 9.1582 | 4.0814 | 2.2439 | 10.24% |
| **High** | **9.7719** | **3.8373** | **2.5466** | **1.86%** |
| Medium-High | 9.5617 | 3.9140 | 2.4430 | 2.28% |

| $C_2H_6O_2$ group | *Mc* [mol] | *Mo* [mol] | *Mc/Mo* | *Mc/Mo* relative error |
|---|---|---|---|---|
| All | 6.3268 | 6.6354 | 0.9535 | 4.65% |
| Low | 6.1875 | 6.6743 | 0.9271 | 7.29% |
| **High** | **6.8350** | **6.7923** | **1.0063** | **0.63%** |
| Medium-High | 6.6864 | 6.7517 | 0.9903 | 0.97% |

**Medium- and high-energy points** are preferred for the numerical solution as these characteristic gamma lines are more distinct

# 4 Results

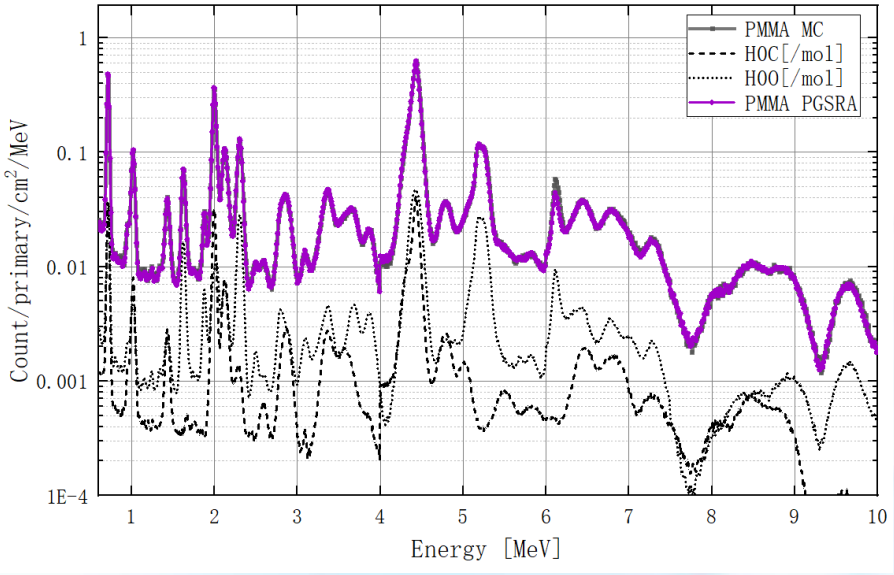
## Elements and Density

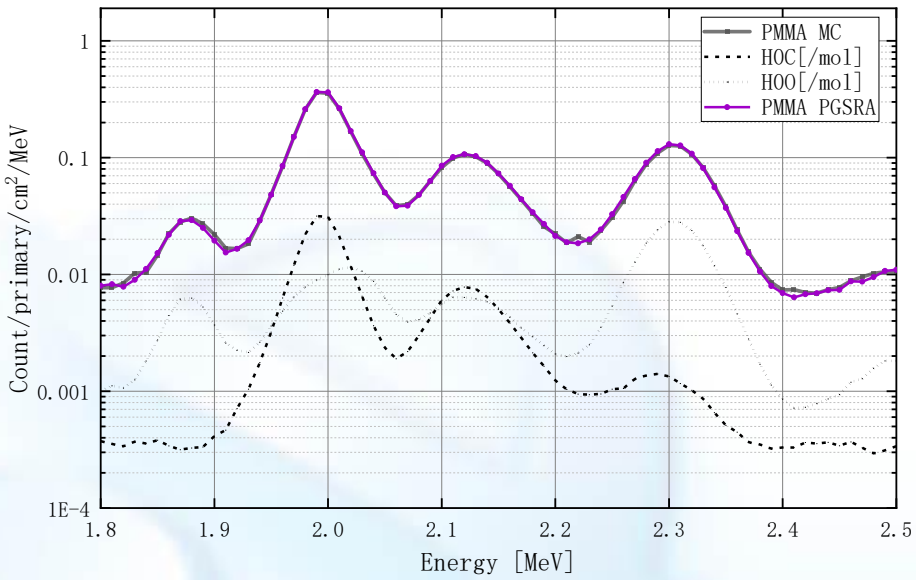
| Sample material | Variable | PGSPA result | MC setup value | Relative error |
|---|---|---|---|---|
| PMMA $\psi^{2.23}_{C_5H_8O_2}$=0.0349 | $M_O$ [mol] | 4.1066 | 4.1519 | 1.09% |
| | $M_C$ [mol] | 10.3469 | 10.3798 | 0.32% |
| | $M_H$ [mol] | 20.6003 | 21.3528 | 3.52% |
| | Sample Mass [g] | 210.4682 | 207.5964 | 1.38% |
| | **Density [g/cm$^3$]** | **1.17** | **1.18** | **1.38%** |
| Pentanediol $\psi^{2.23}_{C_5H_{12}O_2}$=0.0365 | $M_O$ [mol] | 3.8373 | 3.7901 | 1.24% |
| | $M_C$ [mol] | 9.7719 | 9.4754 | 3.13% |
| | $M_H$ [mol] | 20.4229 | 22.7409 | 10.19% |
| | Sample Mass [g] | 199.0820 | 197.0877 | 1.01% |
| | **Density [g/cm$^3$]** | **1.0040** | **0.99** | **1.01%** |
| Ethanediol $\psi^{2.23}_{C_2H_6O_2}$=0.0377 | $M_O$ [mol] | 6.7923 | 6.5758 | 3.29% |
| | $M_C$ [mol] | 6.8350 | 6.5758 | 3.94% |
| | $M_H$ [mol] | 19.8981 | 19.7273 | 0.87% |
| | Sample Mass [g] | 210.5943 | 203.8484 | 3.31% |
| | **Density [g/cm$^3$]** | **1.1455** | **1.11** | **3.31%** |

Although high atom number of hydrogen, but it has much lower weight than carbon and oxygen in materials. Thus, **density error is dominated by carbon and oxygen.**

# 4 Results

## Elements and Density




- Peak at 6.1 MeV shows a small deviation from the MC curve.
- 2.23MeV shows a small deviation from the MC curve

# Contents

# Summary and Discussion

## Experiment considerations

**For a laboratory test, there are some suggestions:**

1) Detectors must have a **good energy resolution**, such as LaBr3, HPGe, resolution could be 3.3%.

2) Detectors must have a good time resolution of approximately **5 ns** to distinguish the 2.23 MeV gamma-derived layer as a clinical target, which is approximately 30 cm in the lateral direction.

3) To obtain the molar PGS spectra, **simple substances** must be prepared, such as hydrocarbons and water.

4) The target should be a slender cylinder, and the beam range should be smaller than the target length.

# Thanks for your attention

**Contribution:**

- Jin-Long Wang: theoretical model, FLUKA simulation, and manuscript.
- Xiao-Guang Wu: physics, prompt gamma analysis, and review.
- Zuo-Feng Li: medical physics, proton therapy, and review.
- Shu-Qing Xie: data analysis.
- Zi-Hao Zhao: detector.
- Da-Qian Hei: neutron adsorption.
- Andrii Rusanov: cloud computing, FLUKA.
- ……

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