

Calculation of cumulative Percentage Dose Recovered of $^{13}\text{C}\text{O}_2$

The enrichment of ^{13}C (atom % excess) in breath at time t was calculated from the ^{13}C abundance measurements and used, with a measure of the total CO_2 production, to calculate the cumulative percentage dose recovered (cPDR) over 240 minutes, which was expressed as a percentage of the administered ^{13}C -MTG dose as described below:

$$\text{Percent } ^{13}\text{C-dose recovered (PDR) (\%/min)} = \frac{\text{Atom \% excess} \times V\text{CO}_2 \text{ (mmol/min)} \times 100}{\text{Dose (mmol)}^1}$$

$$\text{where Atom \% excess} = \frac{\text{delta over baseline (DOB)} \times \text{RPDB} \times 100}{1000^2}$$

$\text{DOB} = \delta^{13}\text{C}_t - \delta^{13}\text{C}_0$ which is defined as the difference between the basal ^{13}C abundance of breath CO_2 before administration of ^{13}C -MTG ($\delta^{13}\text{C}_0$) and the ^{13}C -abundance of breath CO_2 at a time point after administration of ^{13}C -MTG ($\delta^{13}\text{C}_t$) relative to Vienna Pee Dee Belemnite (PDB). $\text{RPDB} = 0.0112372$ is the $^{13}\text{C}/^{12}\text{C}$ isotopic ratio of Vienna Pee Dee Belemnite.

$V\text{CO}_2$ is the total expiratory CO_2 production (mmol/h) which was assumed to be $300\text{mmol}/\text{min}^2$ multiplied by the body surface area. The body surface area was calculated by the weight-height formula of Haycock et al³.

Dose (mmol) is the amount of ^{13}C -MTG administered (mg) / molecular weight of ^{13}C -MTG $\times n \times P/100$ where n is the number of ^{13}C atoms per molecule of MTG and P is the ^{13}C isotopic purity (%) of ^{13}C -MTG.

The cPDR over the n time points up to time t was then calculated using the trapezoidal method⁴:

$$\text{cPDR over time } t = [\text{PDR}(n) + \text{PDR}(n-1)] / 2 \times \text{change in time (min)} + \text{cPDR}(n-1).$$

The results of the ^{13}C -MTG breath test were then expressed as the cumulative percentage of ^{13}C -label recovered on breath over 240 minutes (cPDR₂₄₀).

References

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3. Haycock GB, Schwartz GJ and Wisotsky DH. Geometric method for measuring body surface area: a height-weight formula validated in infants, children, and adults. *J Pediatr* 1978; 93: 62-66. 1978/07/01. DOI: 10.1016/s0022-3476(78)80601-5.
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