Incorporating $^{131}$I into a PAMAM (G5.0) Dendrimer-conjugate: Design of a Theranostic Nanosensor for Medullary Thyroid Carcinoma

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Supplementary Information

Figure S1: $^1$H-NMR spectrum (Varian, 400MHz) of the maleimide linker used in this study.
Figure S2: MALDI-TOF of KYKYKYC (M+ peak).

Figure S3: MALDI-TOF of GPLPLRC (M+ peak).
How many $^{131}$I atoms are bonded to each PAMAM Starburst dendrimer?

1) How many $^{131}$I atoms are present in a 3mCi $\text{Na}^{131}$I?

The Curie is defined as $3.7 \cdot 10^{10} \text{ s}^{-1}$, or 37 GBq. 3 mCi = $1.11 \times 10^8 \text{ s}^{-1}$.

The decay constant $\lambda$ of $^{131}$I is $9.94 \times 10^{-7} \text{ s}^{-1}$.

The rate of decay is defined as:

$$- \frac{dN}{dt} = \lambda N = 9.94 \times 10^{-7} \text{ s}^{-1} \times N$$

$N = 1.1167 \times 10^{14} ^{131}$I atoms. This corresponds to $1.8544 \times 10^{-10}$ moles of $^{131}$I atoms.

The molecular weight of PAMAM G5.0 is 28,826 g mol$^{-1}$. According to our ICP analysis, each dendrimer is linked to 18 units of KYKYKYC (995.20 g mol$^{-1}$ per unit). Furthermore, G5.0-VTP is additionally linked to 9 units of GPLPLRC (754.95 g mol$^{-1}$ per unit).

Therefore, the molecular weights of the functionalized dendrimers are:

- G5.0: $(28,826 + 18 \times 995.20) \text{ g mol}^{-1} = 46,739.6 \text{ g mol}^{-1}$.
- G5.0-VTP: $(28,826 + 18 \times 995.20 + 9 \times 754.95) \text{ g mol}^{-1} = 53,534.15 \text{ g mol}^{-1}$.

10 micrograms of G5.0 = $2.139 \times 10^{-10}$ moles
10 micrograms of G5.0-VTP = $1.868 \times 10^{-10}$ moles

According to our experimental design, the maximal labeling degrees are:

- G5.0: $1.8544 \times 10^{-10}$ moles of $^{131}$I atoms / $2.139 \times 10^{-10}$ moles = 0.87
- G5.0-VTP: $1.8544 \times 10^{-10}$ moles of $^{131}$I atoms / $1.868 \times 10^{-10}$ moles = 0.99.

When considering the obtained labelling rates of $93 \pm 1\%$ and $85 \pm 2\%$, respectively, each mole of G5.0 was chemically linked to 0.81 moles of $^{131}$I, whereas each mole of G5.0-VTP was coupled to 0.84 moles of $^{131}$I.

Reference: