Electronic Supplementary Material (ESI) for RSC Advances.

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

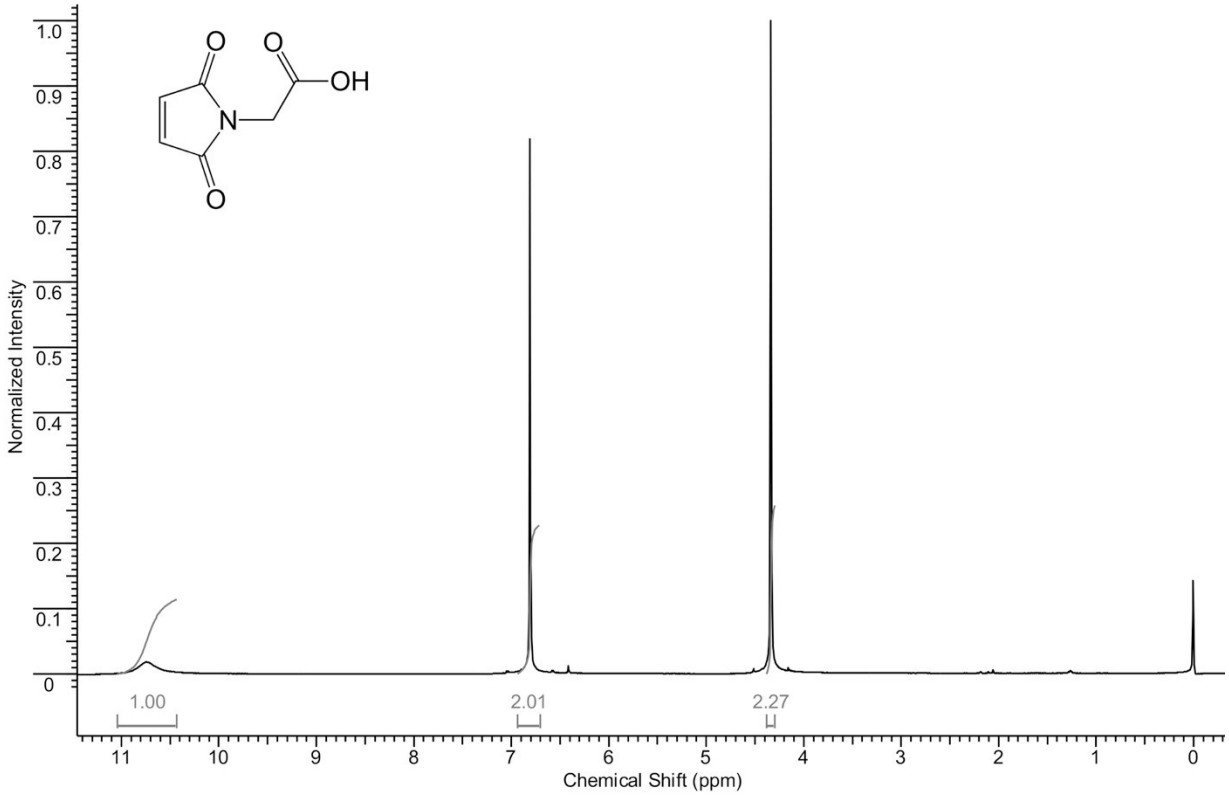

Figure S1: ^{1}H-NMR spectrum (Varian, 400MHz) of the maleimide linker used in this study.

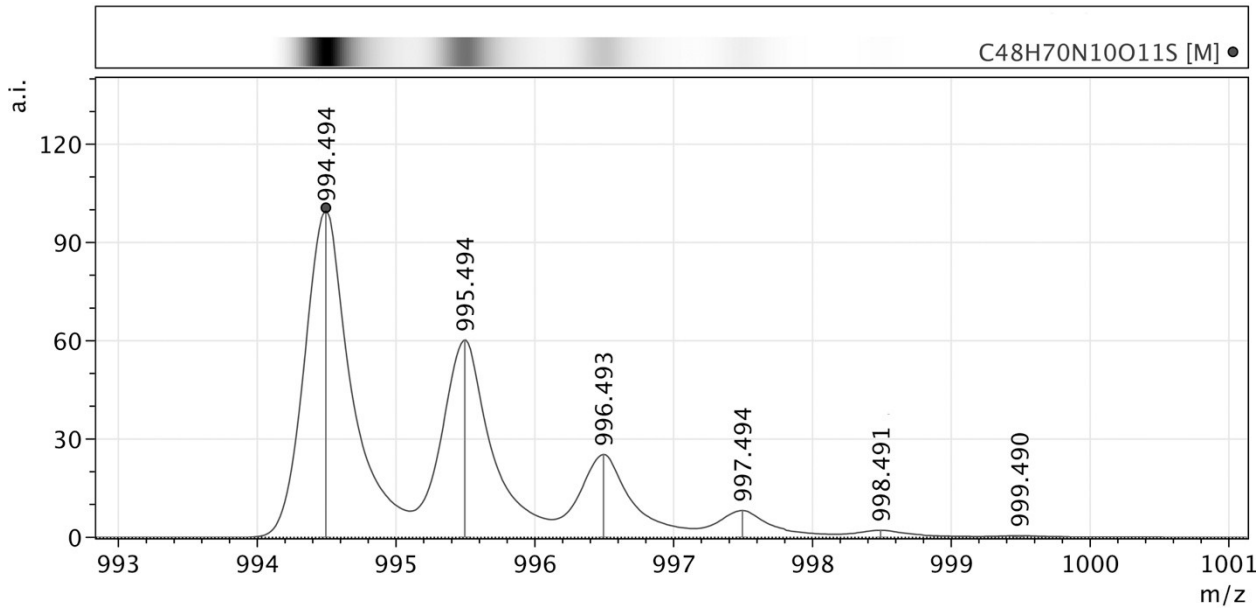

Figure S2: MALDI-TOF of KYKYKYC (M+ peak).

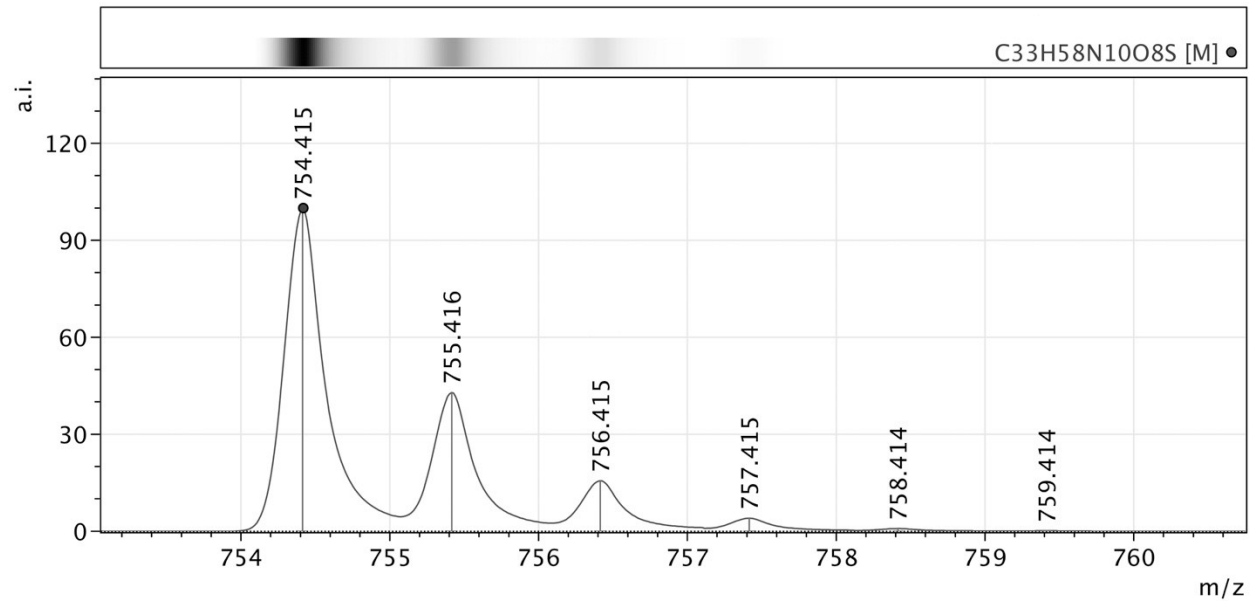

Figure S3: MALDI-TOF of GPLPLRC (M+ peak).

How many ^{131}I atoms are bonded to each PAMAM Starburst dendrimer?

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

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

The decay constant λ of ^{131}I is 9.94 x 10^{-7} s^{-1}.

The rate of decay is defined as:

$$-\frac{dN}{dt} = \lambda N = 9.94\, x\, 10^{-7} s^{-1}\, x\, \mathrm{N}$$

N = 1.1167 x 10^{14} ^{131}I atoms. This corresponds to 1.8544 x 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 x 995.20) g mol^{-1} = 46,739.6 g mol^{-1}.
G5.0-VTP: (28,826 + 18 x 995.20 + 9 x 754.95) g mol^{-1} = 53,534.15g mol^{-1}.

10 micrograms of G5.0 = 2.139 x 10^{-10} moles
10 micrograms of G5.0-VTP = 1.868 x 10^{-10} moles

According to our experimental design, the maximal labeling degrees are:
G5.0: 1.8544 x 10^{-10} moles of ^{131}I atoms / 2.139 x 10^{-10} moles = 0.87
G5.0-VTP: 1.8544 x 10^{-10} moles of ^{131}I atoms / 1.868 x 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:
CRC Handbook of Chemistry and Physics, 86th Edition, edited by David R. Lide (National Institute of Standards and Technology). CRC Press (an imprint of Taylor and Francis Group): Boca Raton, FL. 2005. 2544 pp. ISBN 0-8493-0486-5.