

Supporting Information

Surface Functionalization of Polymer Particles for Cell Targeting by Modifying Emulsifier

Chemistry

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Calculations on the mol% of PVA, and MITC used in this study and how the mass of PVA and ITC needed was calculated:

The following explains how the mole amount of PVA was calculated and how the mol% of ITC is determined.

100 mg of PVA corresponds to 5.6 μmol of PVA. To determine this, we assumed that the PVA had a molecular weight of 18,000 g/mol. Therefore, the calculation of the moles of PVA is as follows:

$$100 \text{ mg PVA} * \frac{1\text{g}}{1000\text{mg}} * \frac{1\text{mol}}{18000\text{g}} * \frac{1000000\mu\text{mol}}{\text{mol}} = 5.6 \mu\text{mol PVA} \quad (\text{S1})$$

Additionally, to understand how the mol% of ITC is determined, here is a sample calculation describing how the amount of MITC was calculated to achieve a selected mole percentage with PVA.

Assuming vinyl alcohol monomer has a molecular weight of 44g/mol,

$$\frac{18000 \left(\frac{\text{g}}{\text{mol}}\right) \text{PVA}}{44 \left(\frac{\text{g}}{\text{mol}}\right) \text{monomer}} = 409 \text{ repeating units} * 0.88 \text{ hydrolyzed} = 359 \text{ OH groups present} \quad (\text{S2})$$

If the MITC to be reacted was based on 20% of the OH groups in the PVA (MITC mol%), then:

$$359 \text{ OH} * 0.2 = 71.8 \frac{\text{molecules MITC}}{\text{molecule PVA}} \quad (\text{S3})$$

71.8 moles of MITC are needed for 1 mole of PVA

If we start with 5.6 μmol PVA then:

$$5.6 \mu\text{mol PVA} * 71.8 \frac{\text{mole MITC}}{\text{mole PVA}} = 402 \mu\text{mol MITC} * 0.00313 \left(\frac{\text{g}}{\mu\text{mol}} \right)$$

$$= 0.1258 \text{ g} = 126 \text{ mg MITC needed}$$

(S4)

Therefore, 126 mg of MITC was reacted with 100 mg of PVA when the amount of MITC in the reaction was desired to be 20% of the OH groups in the PVA.

Polymer Characterization Calculations

When characterizing FITC-PVA and MITC-PVA with NMR, we integrated the ITC phenyl peaks and the methylene proton peaks in the PVA backbone and multiplied by 0.88 (to account for the extent of hydrolysis in PVA) to get the amount of OH groups present. A ratio of ITC to OH can be calculated from these two peaks. This is shown in the NMR spectra in Figure 2 and Figure 3. This ratio gives a mol % of ITC vs OH groups present in the modified PVA. This value can be used with the mol % of ITC added to give the % of ITC reacted.

FITC and MITC conversion was calculated using the following equation.

$$\% \text{ FITC reacted} = \frac{\text{mol \% of FITC on PVA (NMR)}}{\text{mol \% of FITC added}} = \frac{4.8\%}{10\%} = 48\% \text{ of total FITC reacted} \quad (\text{S5})$$

If the ratio of MITC to OH was 5.4%, but the initial ratio of MITC to OH was 20%, then 5.4% reacted / 20% added = 27 % converted (ITC reacted column in Table 1).

$$\% \text{ MITC reacted} = \frac{\text{mol \% of MITC on PVA (NMR)}}{\text{mol \% MITC added}} = \frac{5.4\%}{20\%} = 27\% \text{ of total MITC reacted} \quad (\text{S6})$$

Described in words for FITC PVA:

FITC modified PVA was prepared by dissolving 100 mg of PVA into 10 mL of DMSO along with a mass of FITC that corresponded to 10 mol% of OH groups present in the PVA. Thus, if all the FITC would have reacted, 10% of the OH groups would have been conjugated to FITC. However, the NMR indicated that 4.8% of the OH groups were conjugated to FITC. Thus, 4.8/10*100% = 48% of the FITC reacted.