Supporting Information

Molecularly Imprinted Polymer-Coated Hybrid Optical Waveguide for Sub-aM Fluorescent Sensing

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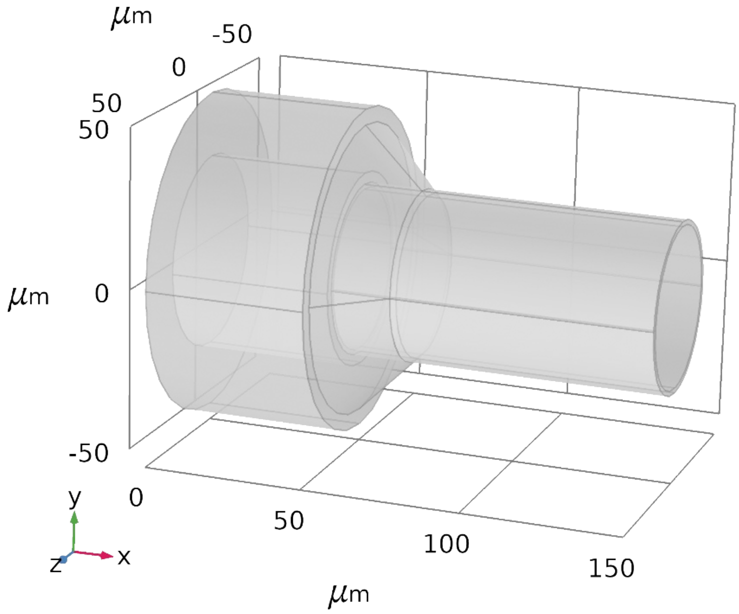

Figure S1. 3-D simulation model of MIP coated optical fibre waveguide structure.

Table S1. Simulation parameters used for the optical fibre-waveguide structure simulation

$n_{waveguide}$	1.44	$r_{waveguide}$	25 µm	$r_{tapertop}$	25 µm	t_{MIP}	1.5 µm
$n_{fibrecladding}$	1.45	$r_{fibrecore}$	30 µm	$l_{waveguide}$	100 µm	Wavelength	550 nm
$n_{fibrecore}$	1.455	$r_{fibrecladding}$	50 µm	l_{taper}	20 µm	Method	Beam envelopes
n_{MIP}	1.57	$r_{taper\ bottom}$	45 µm	l_{fibre}	50 µm		

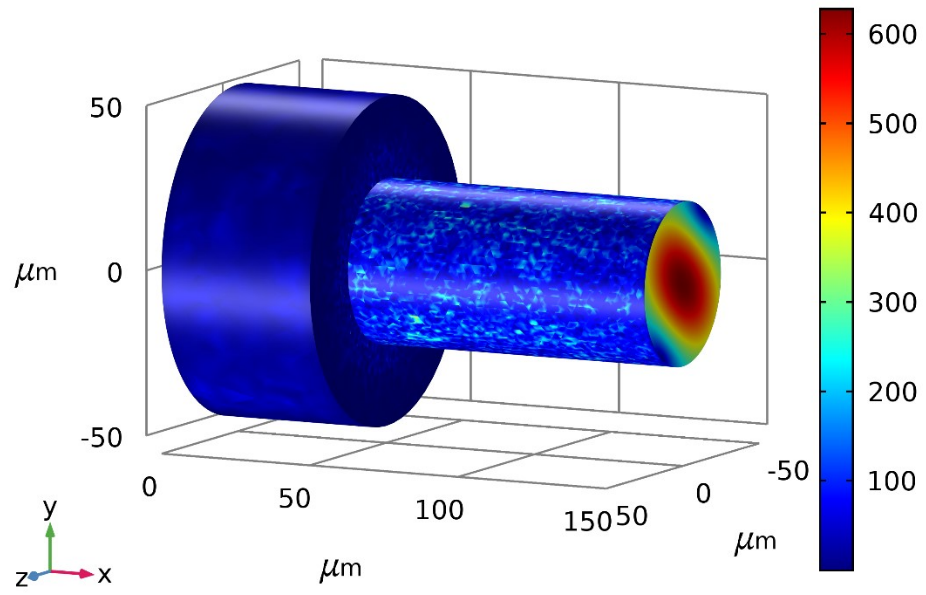

Figure S2. A typical simulation result of optical fibre-waveguide structure without high-n MIP coating layer. The propagation light is confined in the waveguide core, which is distinguished with that of MIP coated model.

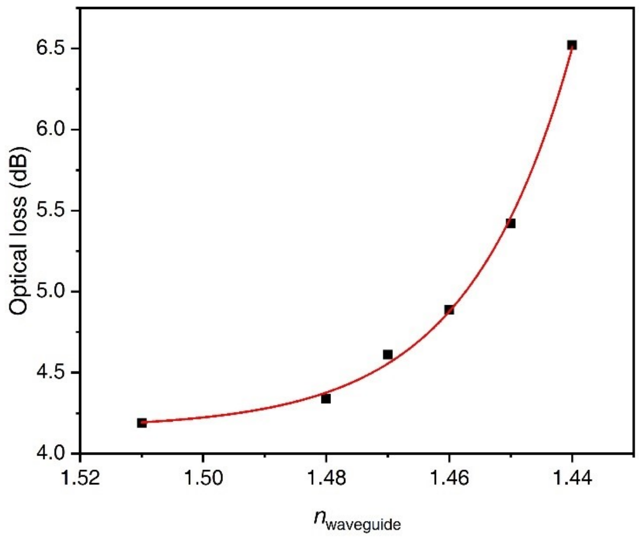

Figure S3. Optical losses of HQNPs hybrid waveguide as a function of waveguide refractive index. The hybrid waveguide lengths were fixed at 6 mm.

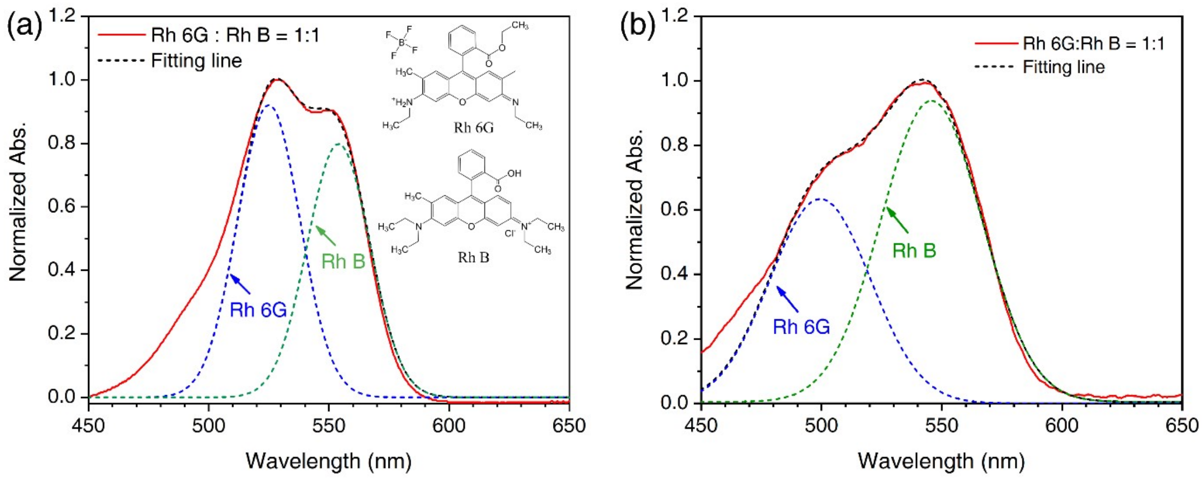

Figure S4. (a) The absorption spectrum of the Rh 6G and Rh B mixture measured by non-selective Shimadzu UV-vis 2600 spectrometer. The insets show the molecular structures of Rh 6G and Rh B, respectively. (b) The spectrum measured by MIP-OFHWF sensing system. The concentration of both Rh 6G and Rh B was 1.0×10^{-6} g/ml. The red solid line represents the experimental data, while the dashed lines represent the fitting lines. The black dashed line represents the sum of the blue and green dashed lines.

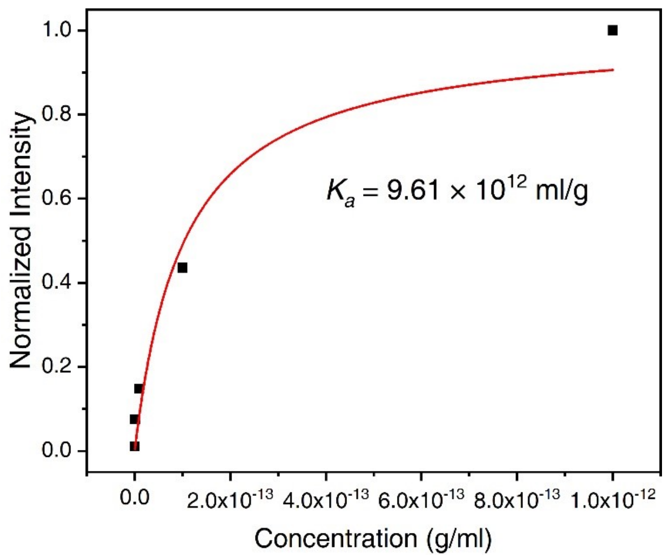

Figure S5. Correlation between normalized fluorescent intensity S and the Rh B concentration measured by NIP-OFHWF.

MIP layer coating process:

1. MIP precursor preparation

Polyethylene glycol 600 diacrylate （PEGDA, 5 g), 2-phenylphenoxyethyl acrylate (OPPEA, 10 g), ethanol (1.5 ml), and Rh B (0.005 g) were weighed into a 20 ml vial and stirred for 2 h at room temperature. Thereafter, 0.06 g of methylacrylic acid (MAA) and 0.05 g of Diphenyl(2,4,6-trimethylbenzoyl)phosphine oxide) (TPO) were added to the mixture and stirred for 1 h to achieve homogeneity. The mixture was filtered through a 0.25 μm filter to decrease the non-solvated residues.

2. MIP coating procedure

The MIP precursor e was dropped on the HQNPs hybrid waveguide section of the OFWF, after which 405 nm laser light was launched into the optical fibre, with a laser output of 20 μW, for 5 min. Under EW irradiation from the hybrid waveguide, the MIP precursor near the surface of the hybrid waveguide was cured and formed a thin MIP layer with a thickness of approximately ~1.5 μm.

3. Removal of templated molecules

The MIP-covered hybrid waveguide was immersed in ethanol for 5 min to rinse away the non-cured monomers and Rh B molecular templates. Removal of the Rh B templates was confirmed directly by microscopic observation. Under the 405 nm light irradiation, the Rh B contained waveguide emits strong yellow fluorescence, while the de-template waveguide only scatters purple laser light.

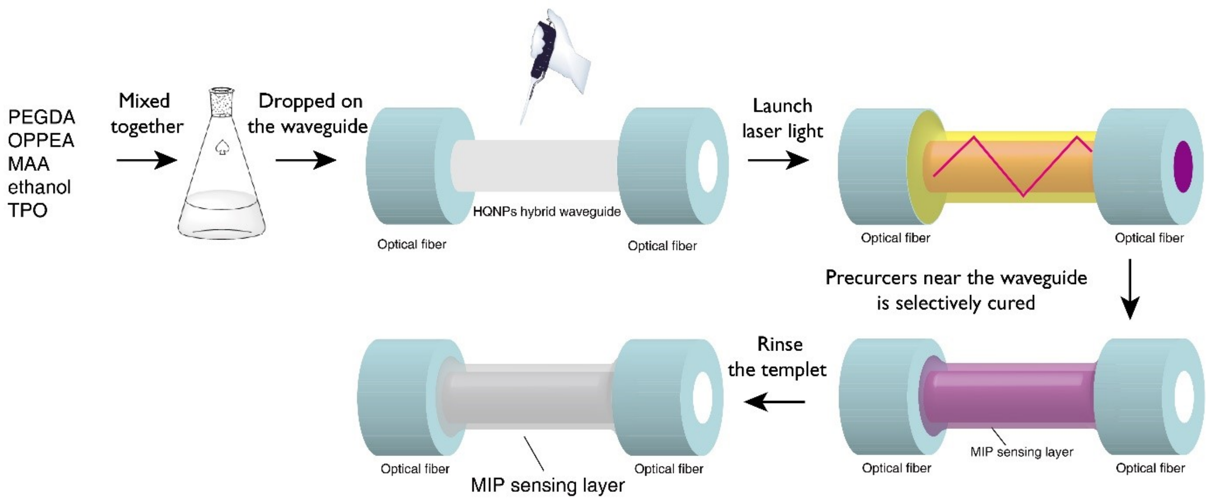

Figure S6. Process of MIP-coated waveguide fabrication