Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information

Realisation and Advanced Engineering of True Optical Rugate Filters Based on Nanoporous Anodic Alumina by Sinusoidal Pulse Anodisation

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S1. Summary of Results

Table S1 compiles a comprehensive summary of the experiments carried out in our study, where the effect of the main anodisation parameters on the position of the characteristic reflection peaks of NAA-RFs was systematically analysed. To this end, a NAA-RF produced with T_p = 650 s, A_J = 0.420 mA cm^{-2}, J_{Offset} = 0.28 mA cm^{-2}, N_P = 150 pulses, T_{An} = -1°C and t_{pw} = 0 min was chosen as the reference structure. From this, the anodisation period (T_p), the anodisation amplitude (A_J), the anodisation offset (J_{Offset}), the number of pulses (N_P), the anodisation temperature (T_{An}) and the pore widening time (t_{pw}) were systematically modified from 450 to 1400 s (ΔT_P = 50 s), from 0.105 to 0.735 mA cm^{-2} (ΔA_J = 0.105 mA cm^{-2}), from 0.14 to 0.98 mA cm^{-2} (ΔJ_{Offset} = 0.14 mA cm^{-2}), from 100 to 300 pulses (ΔN_P = 50 pulses), from -1 to 6°C (ΔT_{An} = 1°C) and from 0 to 10 min (Δt_{pw} = 2 min), respectively.

S2. Refractive Index of Aqueous Solutions of Glucose

Figure S1 shows a fitting line between the concentration of glucose and the refractive index of the solution. This relationship was used to establish a direct correlation between the level of change in λ_{Peak} and the refractive index of the medium filling the nanopores of NAA-RFs.

S3. Estimation of $\Delta\lambda_{Peak}$ in Real-Time by RIfS

NAA-RFs were functionalised with HSA via APTES silanization using GTA as a coupling agent. The reversible binding affinity between HSA and indomethacin molecules was assessed by measuring changes in the position of the characteristic reflection peak (1st order) of NAA-RFs in real-time by RIfS. **Figure S2** shows representative RIfS spectra from which $\Delta\lambda_{Peak}$ associated with each stage of the sensing process was estimated.

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Table S1. Comprehensive summary of the effect of the different anodisation parameters on the position of the characteristic reflection peaks of NAA-RFs analysed in this study.

Analysed Parameter	**Range and Step Size**	**Peaks**	**Fitting Parameters**	**Range of λ_{Peak}**
Anodisation Period – T_P	From 450 to 1400 s	1st Order	*Slope* = 0.67 ± 0.01 nm s^{-1}	401 – 1036 nm
	ΔT_P = 50 s		*Intercept* = 130.21 ± 13.95 nm	(Red Shift)
			R^2 = 0.9912	
		2nd Order	*Slope = 0.29 ± 0.01 nm* s^{-1}	260 – 513 nm
			Intercept = 98.93 ± 7.25 nm	(Red Shift)
			R^2 *= 0.9899*	
		3rd Order	*Slope = 0.16 ± 0.02 nm* s^{-1}	278 – 347 nm
			Intercept = 109.11 ± 26.41 nm	(Red Shift)
			R^2 *= 0.8537*	
Anodisation Amplitude - A_J	From 0.105 to 0.735 mA cm^{-2}	1st Order	*Slope* = 970.74 ± 28.13 nm (mA cm^{-2})$^{-1}$	283 – 886 nm
	ΔA_J = 0.105 mA cm^{-2}		*Intercept* = 166.22 ± 13.21 nm	(Red Shift)
			R^2 = 0.9950	
		2nd Order	*Slope* = 464.60 ± 47.99 nm (mA cm^{-2})$^{-1}$	289 – 443 nm
			Intercept = 98.03 ± 28.28 nm	(Red Shift)
			R^2 = 0.9687	
Anodisation Offset - J_{Offset}	From 0.14 to 0.98 mA cm^{-2}	1st Order	*Slope* = 865.48 ± 23.83 nm (mA cm^{-2})$^{-1}$	431 – 1163 nm
	ΔJ_{Offset} = 0.14 mA cm^{-2}		*Intercept* = 303.44 ± 14.92 nm	(Red Shift)
			R^2 = 0.9955	
		2nd Order	*Slope* = 435.32 ± 24.27 nm (mA cm^{-2})$^{-1}$	290 – 587 nm
			Intercept = 152.29 ± 16.35 nm	(Red Shift)
			R^2 = 0.9847	
Number of Pulses - N_P	From 100 to 300 pulses	1st Order	*Slope* = -0.97 ± 0.11 nm $pulse^{-1}$	623 – 525 nm
	ΔN_P = 50 pulses		*Intercept* = 715.37 ± 17.27 nm	(Blue Shift)
			R^2 = 0.9740	
			NB: Fitting from 100 to 200 pulses	
		2nd Order	*Slope* = -0.54 ± 0.03 nm $pulse^{-1}$	318 – 263 nm
			Intercept = 369.50 ± 4.63 nm	(Blue Shift)
			R^2 = 0.9939	
			NB: Fitting from 100 to 200 pulses	
Anodisation Temperature - T_{An}	From -1 to 6°C	1st Order	*Slope* = -20.37 ± 1.57 nm $^oC^{-1}$	562 – 421 nm
	ΔT_{An} = 1°C		*Intercept* = 537.31 ± 5.34 nm	(Blue Shift)
			R^2 = 0.9597	
		2nd Order	*Slope* = -5.26 ± 0.87 nm $^oC^{-1}$	286 – 270 nm
			Intercept = 280.57 ± 1.06 nm	(Blue Shift)
			R^2 = 0.9229	
Pore Widening Time - t_{pw}	From 0 to 10 min	1st Order	*Slope* = -15.15 ± 1.10 nm min^{-1}	563 – 401 nm
	Δt_{pw} = 2 min		*Intercept* = 560.40 ± 6.67 nm	(Blue Shift)
			R^2 = 0.9741	
		2nd Order	*Slope* = -10.06 ± NA nm min^{-1}	286 – 266 nm
			Intercept = 287.32 ± NA nm	(Blue Shift)
			R^2 = NA	
			NB: Only two points	

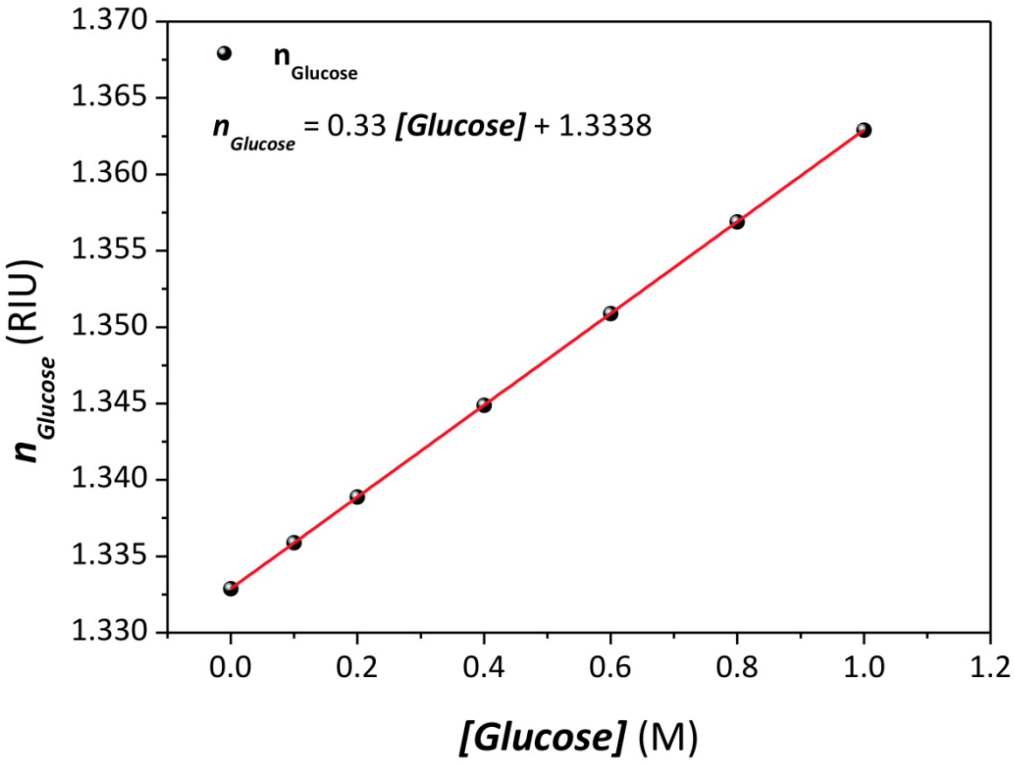

Figure S1. Estimation of the refractive index of aqueous solutions of glucose ($n_{Glucose}$) as a function of their concentration (*[Glucose]*).

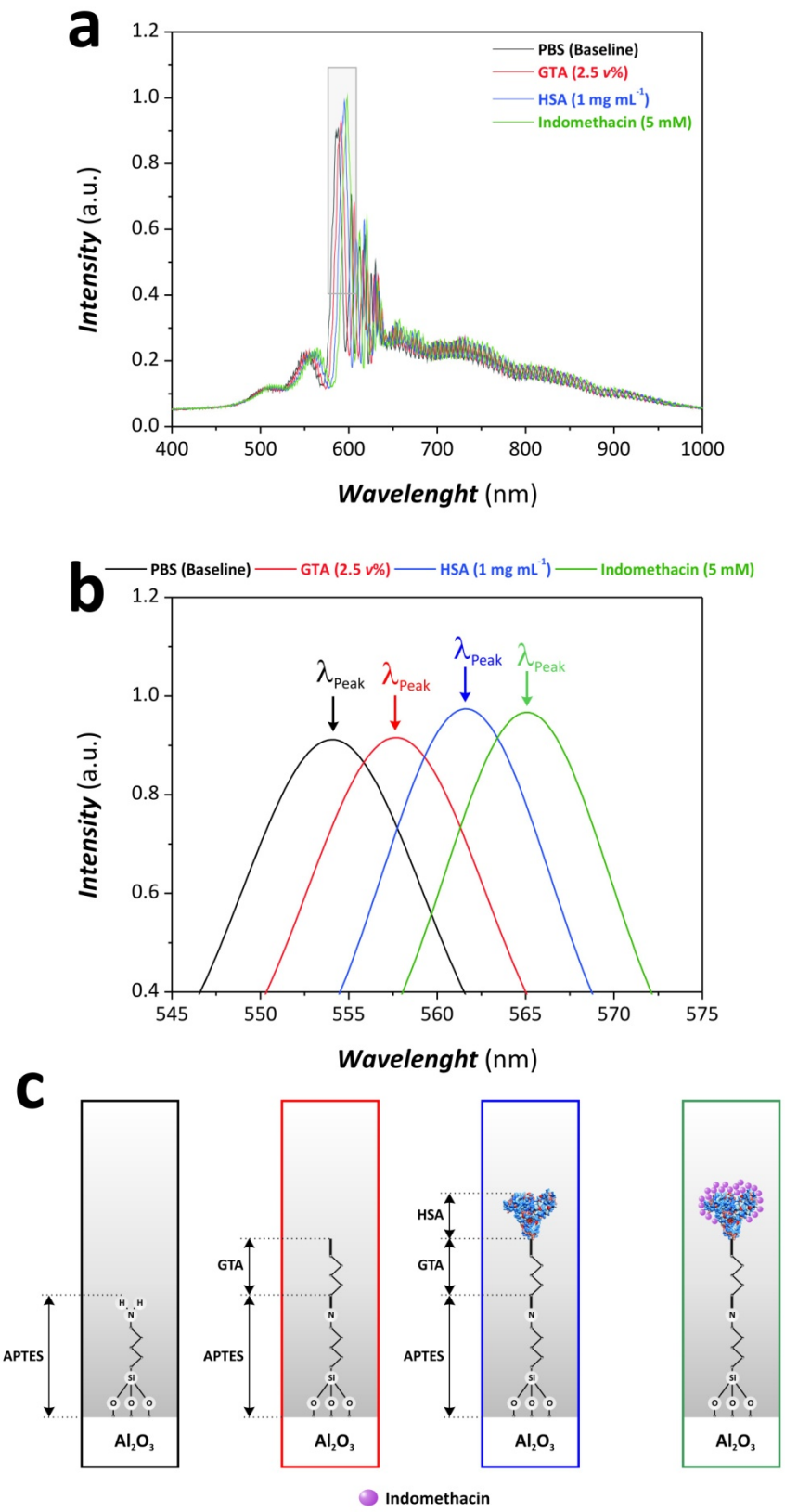

Figure S2. Example of estimation of changes in the characteristic reflection peak position (λ_{Peak}) for the assessment of the interaction between HSA molecules and indomethacin by combining APTES-functionalised NAA-RFs and RIfS. a) General RIfS spectra of a NAA-RFs at each stage of the sensing process. b) Magnified view of the 1st order reflection peak shown in (b) (grey rectangle). c) Schematic illustration showing the different stages of the sensing process.