

Correcting transmission losses in short-wave infrared spatially offset Raman spectroscopy measurements to enable reduced fluorescence through-barrier detection

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Supplementary Information

Name/Brand	Ref	Material	Physical Description			
			<i>Opacity</i>	<i>Colour</i>	<i>Texture</i>	<i>Thickness (mm)</i>
Small chemical drum (VWR)	1	HDPE	Opaque	Blue	Dimpled on outside, smooth inside	2.06
Hessian sack, brown vegetable sack	2	Hessian	Opaque	Brown	Large, loose weave	N/A
Plastic woven sack	3	Unknown	Opaque	Yellow	Close weave	N/A
300 ml drinks bottle (Sprite™ original)	4	PET	Transparent	Green	Smooth, large patterned dimples	0.30
500 ml Plastic box (Tesco)	5	PP	Transparent	White	Smooth	1.30
Brown plastic padded envelope/jiffy™ (Banner)	6	Paper/plastic	Opaque	Brown/ clear	Paper outside, plastic bubble wrap interior	1.54
Herbal Essences™ Shampoo: Vibrant Colour	7	PET	Transparent	Pink	Smooth	0.63
Herbal Essences™ Shampoo: Straightening	8	PET	Transparent	Pink	Smooth	0.58-0.89
Herbal Essences™ Shampoo: Tousled	9	PET	Transparent	Pink	Smooth	0.41-0.69
Herbal Essences™ Shampoo: Volumizing	10	PET	Transparent	Pink	Smooth	0.60-0.88
Herbal Essences™ Shampoo: Moisture & Shine	11	PET	Transparent	Blue	Smooth	0.80
Herbal Essences™ Shampoo: Shine Reflecting	12	PET	Transparent	Blue	Smooth	0.83
Herbal Essences™ Shampoo: Clarifying	13	PET	Transparent	Blue	Smooth	0.64
Herbal Essences™ Shampoo: Smooth	14	PET	Transparent	Orange	Smooth	0.63-1.06
Herbal Essences™ Shampoo: Split End	15	PET	Transparent	Red	Smooth	0.65
Herbal Essences™ Conditioner: Vibrant	16	HDPE	Opaque	Bright Pink	Smooth	0.62-0.72
Herbal Essences™ Conditioner: Straightening	17	HDPE	Opaque	Fuschia Pink	Smooth	0.68
Herbal Essences™ Conditioner: Tousle	18	HDPE	Opaque	Purple	Smooth	0.62
Herbal Essences™ Conditioner: Moisture & Shine	19	HDPE	Opaque	Light Blue	Smooth	0.67-0.87
Herbal Essences™ Conditioner: Balancing	20	HDPE	Opaque	Green	Smooth	0.68

Herbal Essences™ Conditioner: Shine	21	HDPE	Opaque	Pale Green	Smooth	0.86
Herbal Essences™ Conditioner: Lightweight	22	HDPE	Opaque	Light Orange	Smooth	0.70
Herbal Essences™ Conditioner: Soft	23	HDPE	Opaque	Dark Orange	Smooth	0.55-0.75
Herbal Essences™ Conditioner: Split End	24	HDPE	Opaque	Red	Smooth	0.70
Herbal Essences™: Normal	25	HDPE	Opaque	Pearly Light Yellow	Dimpled on outside, smooth inside	0.96
12 samples of HDPE (domestic containers e.g. bleach bottle)	26 – 37	HDPE	Opaque	Various	Various	Various
Sparkling Water, 200ml (Perrier™)	38	Glass	Transparent	Green	Smooth	1.90
50 ml chemical bottle (Sigma)	39	Glass	Transparent	Brown	Smooth	Up to 1.79
Square 100 ml chemical bottle (VWR)	40	Glass	Transparent	Clear	Smooth	1.00
20 L Jerry can (VWR)	41	HDPE	Semi-transparent	White	Smooth inside, textured exterior	2.85
10 L Jerry can (VWR)	42	HDPE	Semi-transparent	White	Smooth inside, textured exterior	1.00
Nivea™ Soft, Moisturising Cream, 200 ml tub	43	PP	Transparent	White	Smooth	1.20
Nivea™ Crème, Moisturising Cream, 200 ml tub	44	PP	Transparent	Dark Blue	Smooth	1.25
Radox™ Handwash	45	PP	Semi-transparent	White	Smooth	0.65
250 ml square chemical tub (VWR)	46	PVC	Transparent	Brown	Smooth	0.71-1.06

Table S1 – Details of containers studied.

Reference	Container
2	
3	

4	
5	
6	
7 – 15	
16 – 25	
26 – 37	
42	

Table S2 – Photographs of some of the containers studied.

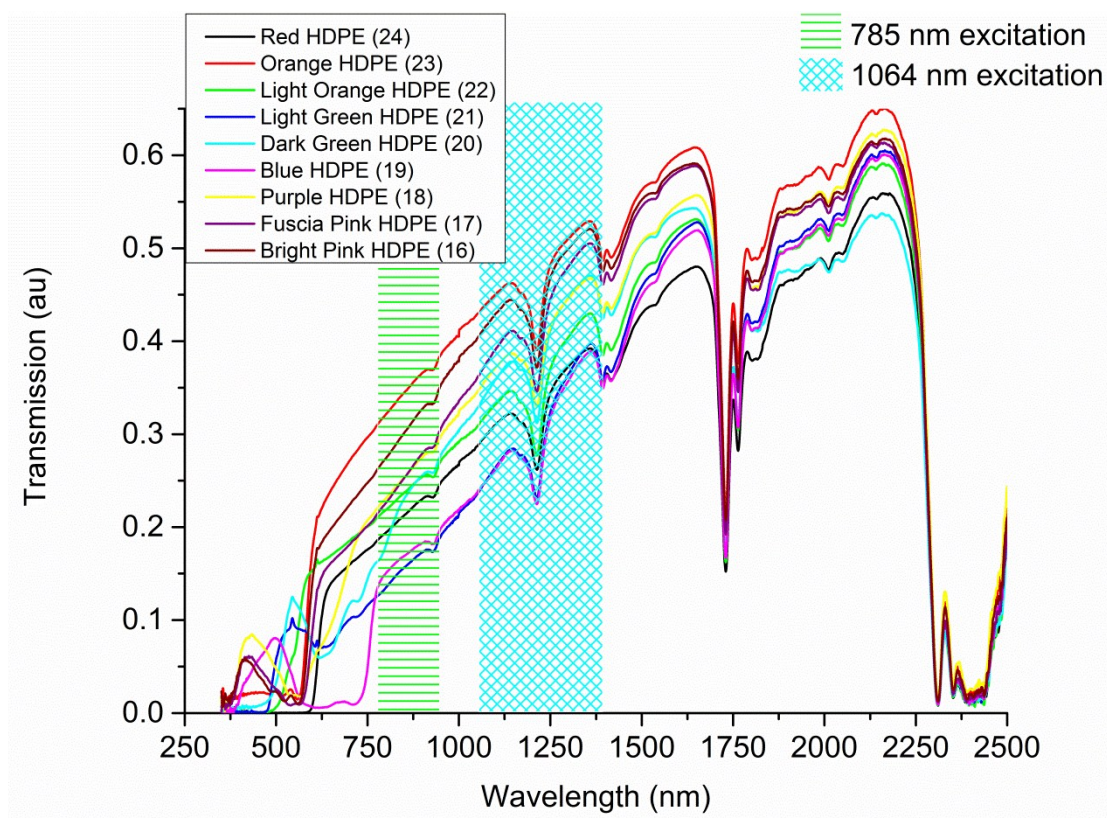


Figure S1 - Transmission spectra of coloured HDPE containers (Herbal Essence range of hair conditioners, reference 16 – 25, Table S2). These containers have similar thickness, but are different colours.

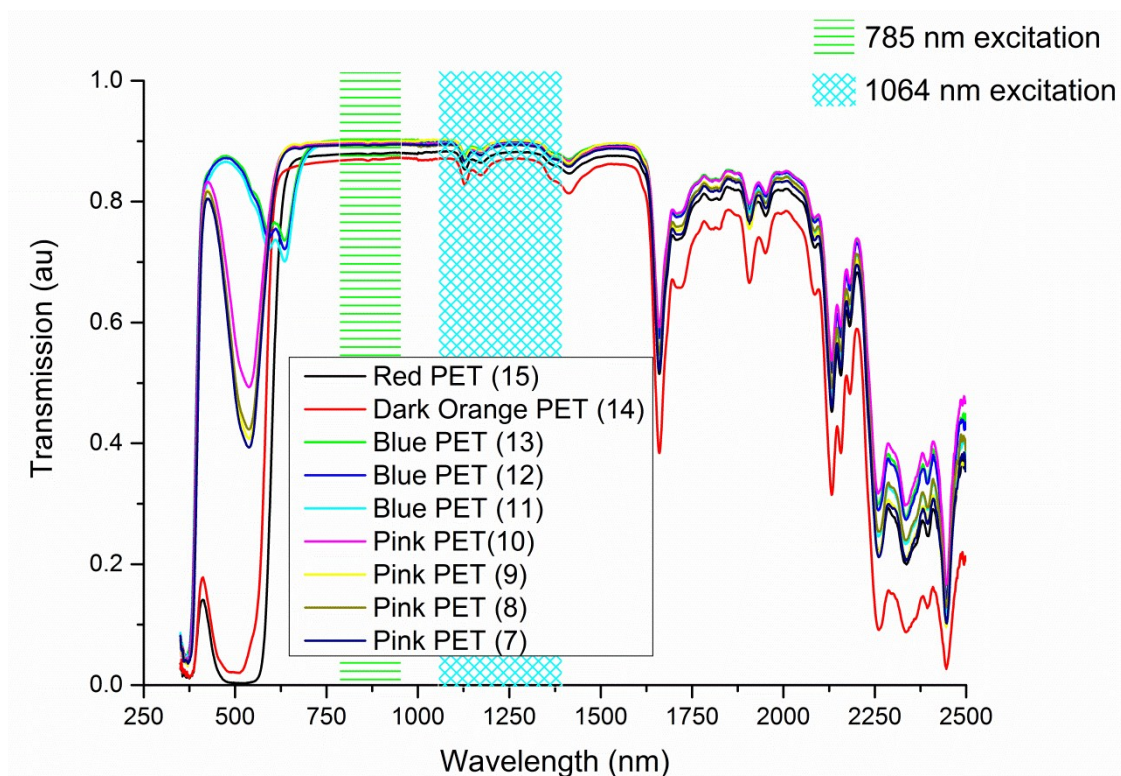


Figure S2 - Transmission spectra of coloured PET containers (Herbal Essence range of hair shampoo, reference 7 – 15, Table S2). These containers have similar thickness, but are different colours.

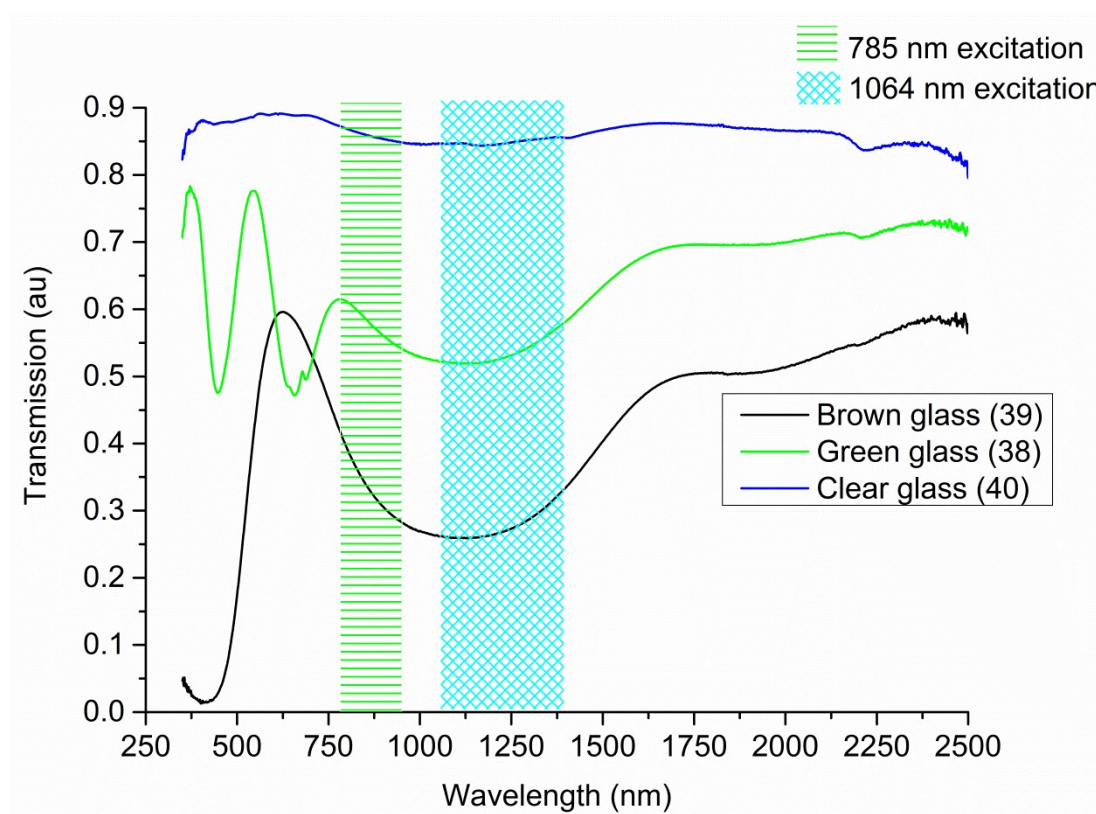


Figure S3 – Transmission spectra of coloured glass bottles (reference 38 – 40, Table S1).

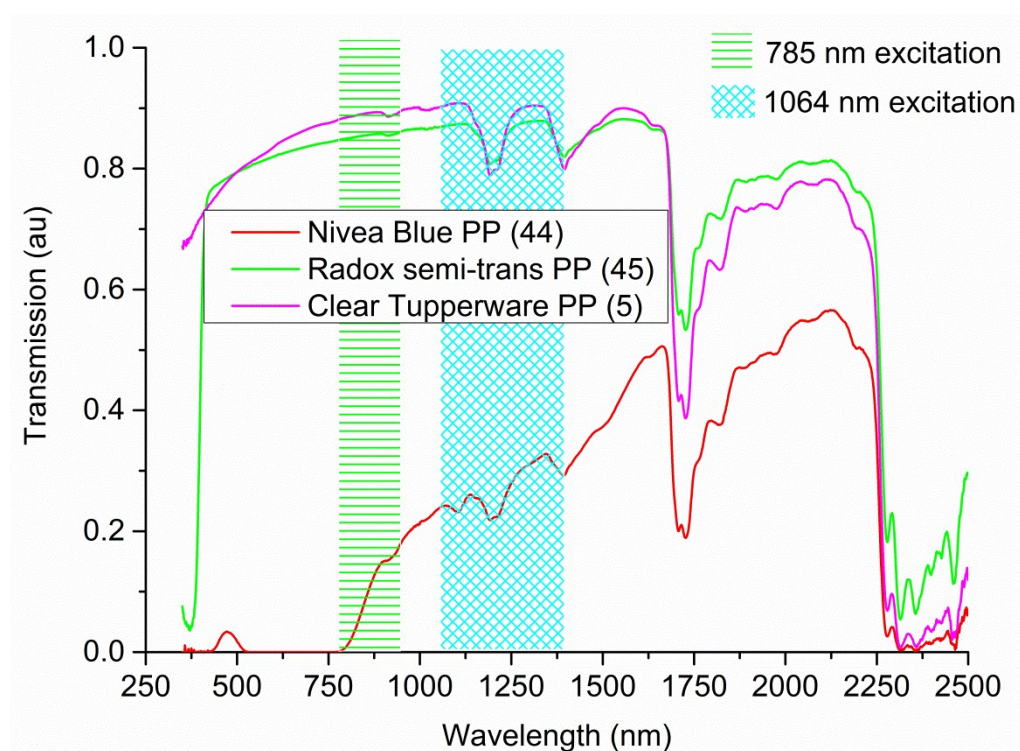


Figure S4 - Transmission spectra of coloured PP containers (reference 5, 44 and 45, Table. S1).

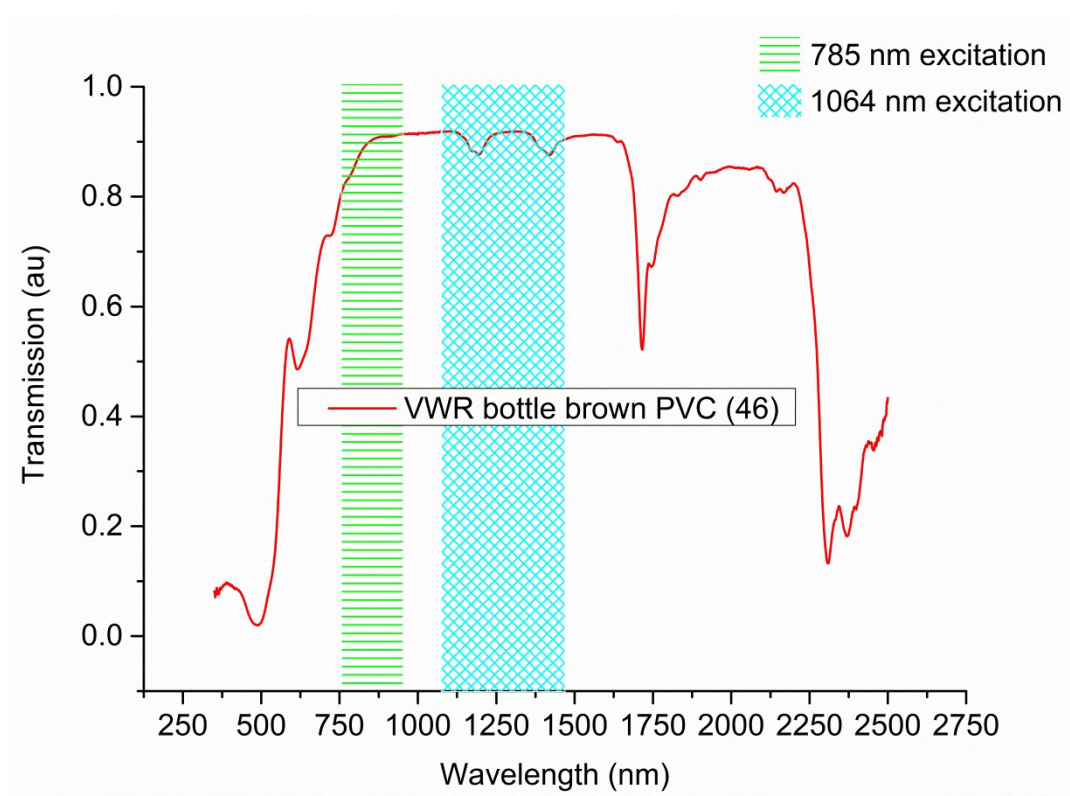


Figure S5 - Transmission spectra of coloured PVC containers (reference 46, Table S1).

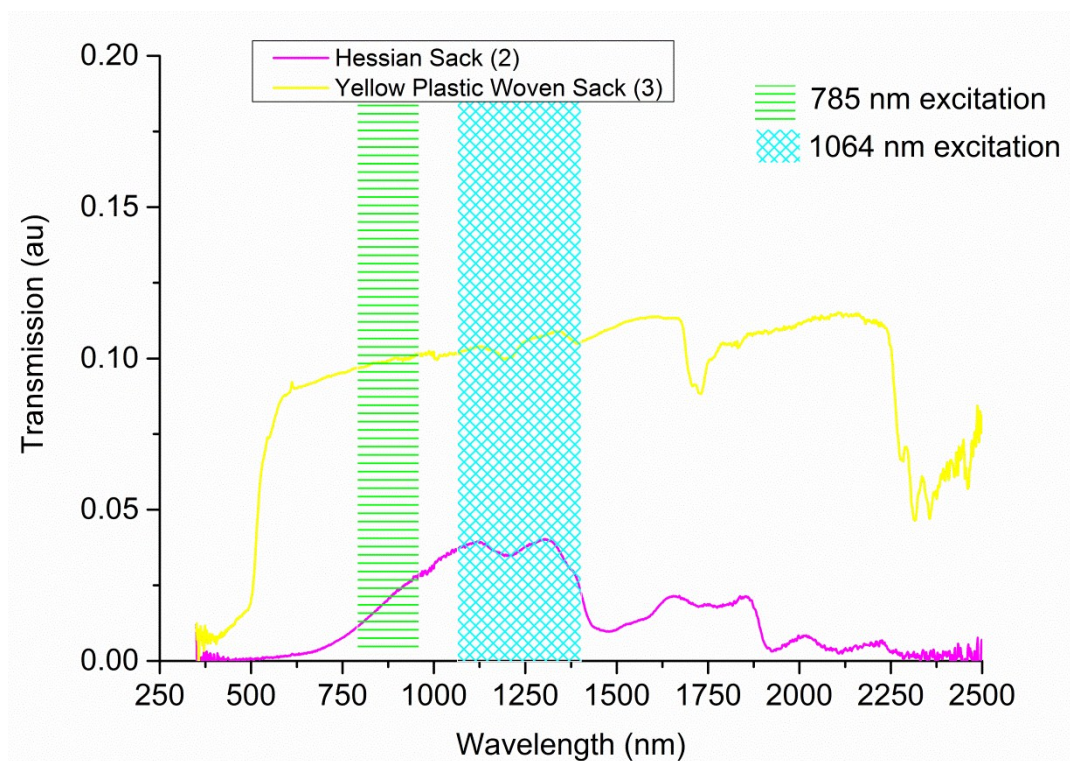


Figure S6 – Transmission spectra of fabrics (reference 2 and 3, Table S2).

Container Material (reference number from Table S1)	Transmission at 1193 nm (1015 cm ⁻¹ , urea C-N stretch)	Transmission at 1064 nm
HDPE pearlescent white (34)	0.0620	0.098
HDPE bronze	0.0746	0.098
HDPE pearlescent yellow (35)	0.0997	0.11
HDPE pink (32)	0.1034	0.11
HDPE blue (28)	0.1360	0.14
HDPE burgundy (30)	0.1810	0.2
HDPE orange (31)	0.2090	0.2
HDPE yellow (37)	0.2747	0.25
HDPE green (29)	0.3289	0.31
HDPE pearlescent blue (33)	0.3710	0.36
HDPE semi-transparent white (1 mm) (42)	0.6350	0.66
PP transparent white (43)	0.7889	0.91
PP semi-transparent white (45)	0.8081	0.87
PVC transparent brown (46)	0.8770	0.92

Table S3 - Transmission values of a range of containers at the laser excitation frequency (1064 nm, 0 cm⁻¹) and urea C-N stretch (1015 cm⁻¹).