

Electronic Supplementary Information

Surface-enhanced Raman spectroscopy (SERS) characterisation of abasic sites in DNA duplexes

*Luca Guerrini,^{*a} and Ramon A. Alvarez-Puebla.^{*a,b}*

^a Department of Physical and Inorganic Chemistry and EMaS, Universitat Rovira I Virgili,
Carrer de Marcel·lí Domingo s/n, 43007 Tarragona, Spain.

^b ICREA, Passeig Lluís Companys 23, 08010 Barcelona, Spain.

Corresponding Author

*Email: luca.guerrini@urv.cat

*Email: ramon.alvarez@urv.cat

Experimental methods

Materials. All materials were of the highest purity available and obtained from Sigma-Aldrich and Fisher Scientific. DNA oligonucleotides were purchased from Eurofins Genomics and Life Technologies. Stock solutions (400 μM) of each strand were prepared in Milli-Q water. Subsequent hybridization was conducted by heating to 90° C for 10 minutes an equimolar solution (20 μM) of complementary strands in PBS 1 M (pH 7.4). The solution was then slowly cooled down to room temperature.

Synthesis of silver colloids and SERS measurements. Positively-charged spermine coated-silver nanoparticles (AgSp) were synthesized as previously illustrated.¹⁻³ Nanoparticles of ca. 22 nm and a localized surface plasmon resonance centered at ca. 391 cm^{-1} are obtained, displaying a positive ζ -potential of ca. + 40 mV. For SERS measurements, 8 μL of a 4 μM solution of the duplex in PBS 0.1 M were added to 140 μL of AgSp colloids. Samples were left to equilibrate for 2 hours and quickly sonicated before performing the SERS measurements. SERS measurements of the homopolymeric strand ssG were performed by adding an aliquot of a ssG solution submitted to thermal treatment (60°C, 10 min).

Instrumentation. SERS spectra were acquired using a Renishaw InVia Reflex confocal microscope equipped with a high-resolution grating consisting of 1800 grooves/cm for visible wavelengths, additional band-pass filter optics, and a CCD camera. A 514 nm laser was focused onto the sample by a lens for macrosampling (30 mm focal length, 0.17 NA). SERS spectra were acquired with 5 \times 10 s exposure time and 6 accumulations. UV-vis spectra were obtained using a Thermo Scientific Evolution 201 UV-visible spectrophotometer.

ssA = AAA AAA AAA AAA AAA AAA AAA

ssC = CCC CCC CCC CCC CCC CCC CCC

ssT = TTT TTT TTT TTT TTT TTT TTT

ssG = GGG GGG GGG GGG GGG GGG GGG

**dsCG = CCG CGC CGC GCG CGC GGC GCGG
GGC GCG GCG CGC GCG CCG CGCC**

**dsAT = AAT ATA ATA TAT ATA TTA TATT
TTA TAT TAT ATA TAT AAT ATAA**

Figure S1. Sequences of the reference DNA samples.

References

1. J. Morla-Folch, P. Gisbert-Quilis, M. Masetti, E. Garcia-Rico, R. A. Alvarez-Puebla and L. Guerrini, *Angew. Chem.-Int. Edit.*, 2017, **56**, 2381.
2. J. Morla-Folch, R. A. Alvarez-Puebla and L. Guerrini, *J. Phys. Chem. Lett.*, 2016, **7**, 3037.
3. D. van Lierop, Z. Krpetic, L. Guerrini, I. A. Larmour, J. A. Dougan, K. Faulds and D. Graham, *Chem. Commun.*, 2012, **48**, 8192.