

## Readme File

These data are for the manuscript:

### Electrochemically grafted single molecule junctions exploiting a chemical protection strategy

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The following data files are included:

(1) “CV of grafting.pptx”

Cyclic voltammograms for the grafting of diazonium salts of **1** onto the gold surface at a scan rate of 50 mV/s in an acetonitrile solution containing 5 mM **1** + 5 mM NaNO<sub>2</sub> + 10 mM aq. HClO<sub>4</sub> + 0.1 M TBAB. TBAB served as the supporting electrolyte, a platinum mesh as the counter electrode, and SCE as the reference electrode.

(2) “Is data for Film-2.opj”

This can be opened with “Origin”.

This contains I(s) data and 2D conductance and distance histograms of **Film-2** (3.0 nS). The histogram consists of 336 traces. The setpoint current used was 30 nA (giving an initial calibrated tip-substrate distance,  $s_0 \approx 1$  nm) and the STM tip retraction rate was 20 nm/s.

(3) “Raman spectra for Film-1 and Film-2.pptx”

Figure A. Gap-mode Raman spectra of Film-1, Film-2 on gold substrates and a control spectrum of gold nanoparticles on a blank gold substrate. The upper curve is a normal Raman spectrum of **1**.

Figure B. SHINERS spectra of Film-1 and Film-2 on gold substrates and a control spectrum of gold nanoparticles on blank gold substrates. The upper curve is a normal Raman spectrum of **1**.