Supporting Information

Synthesis and Characterisation of Isothiocyanate Functionalised Silicon Nanoparticles and their uptake in cultured colonic cells

Yimin Chao[a†], Ashley I. Marsh[a], Mehrnaz Behray[a], Feng Guan[ab], Anders Engdahl[c], Yueyang Chao[d], Qi Wang[e], and Yongping Bao[e]

[a] *School of Chemistry, University of East Anglia, Norwich NR4 7TJ, United Kingdom.*
[b] *MAX IV laboratory, Lund University, P. O. Box 118, 22100 Lund, Sweden.*
[c] *School of Pharmacy, Heilongjiang University of Chinese Medicine, Haerbin 150040, China.*
[d] *Birmingham Heartlands Hospital, Bordesley Green E, Birmingham B9 5SS, United Kingdom.*
[e] *Norwich Medical School, University of East Anglia, Norwich NR4 7TJ, United Kingdom.*

corresponding author: Y.chao@uea.ac.uk

1. EDX analysis

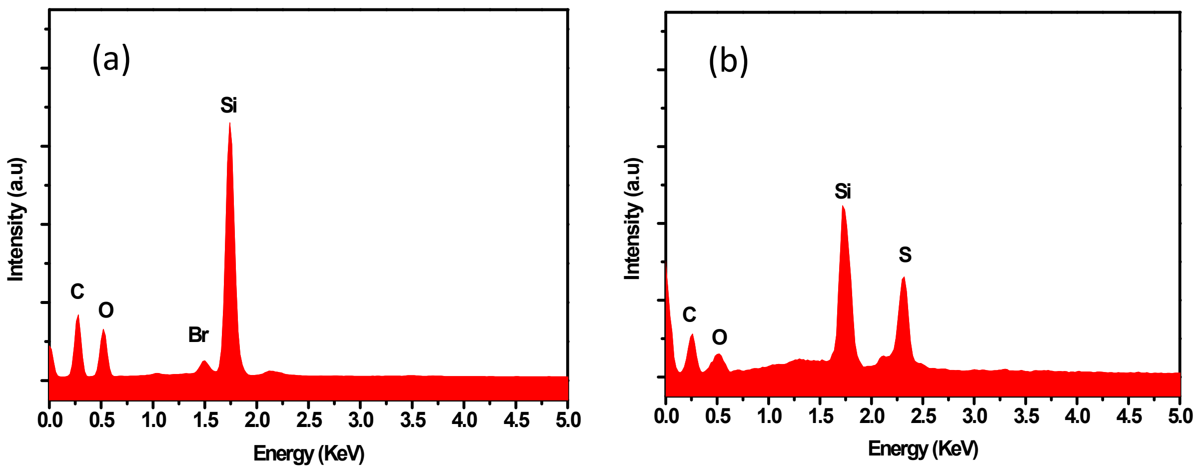

Figure S1. EDX spectrum of bromine-functionalised SiNPs (a) and ICT SiNP (b)

2. Quantum Yield measurement

The quantum yield of ITC SiNPs was calculated using the following equation:

$$Q = Q_{Ref}\left(\frac{Grad_{SiNPs}}{Grad_{Ref}}\right)\left(\frac{\eta_{Toluene}^{2}}{\eta_{Ref}^{2}}\right)$$

Equation 1

Where Q_{Ref} is the quantum yield of the standard reference Quinine Sulphate (QS) and was considered to be 54.6% when dissolved in 0.5M H_2SO_4. ηToluene is the refractive index of the solvent = 1.497 and ηRef is the refractive index of the reference = 1.346.

A quantum yield of 13% was calculated which is in agreement with the previously reported quantum yields for SiNPs which typically lie between 2% and 25%. These calculated quantum yields are bright enough for biological applications, however they may vary with different excitation wavelengths.

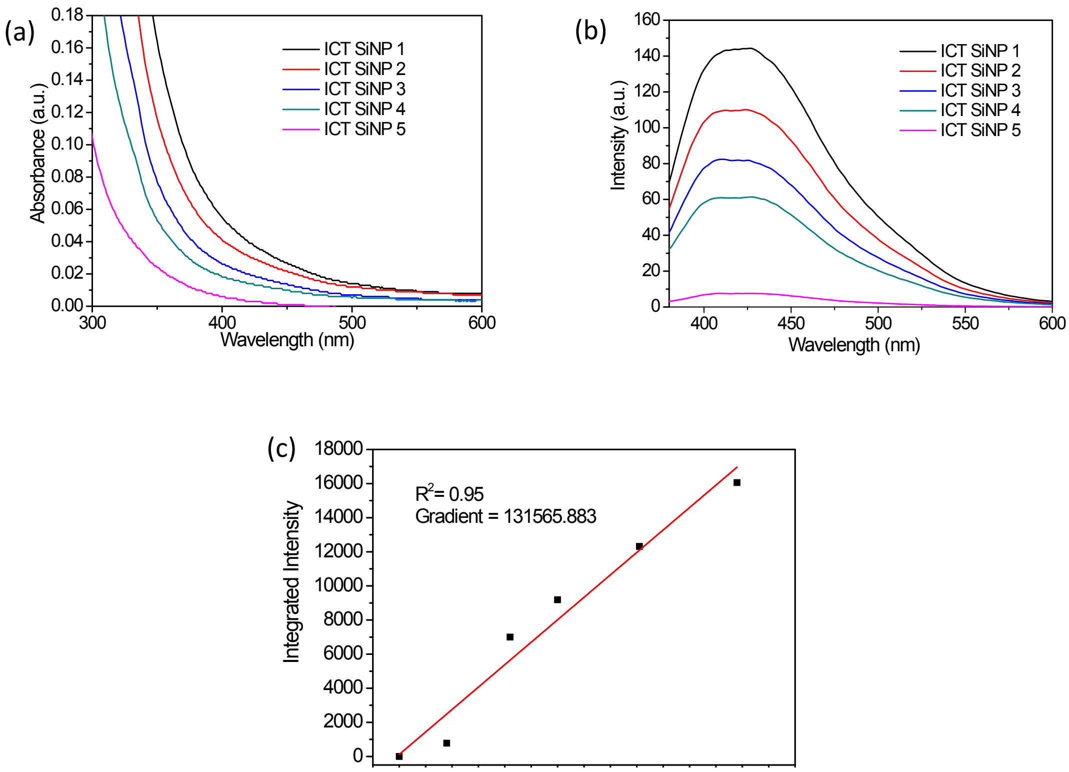

Figure S2. Absorption (a) and emission spectra (b) for various concentrations of ICT SiNP in toluene. Plotted integrated intensity of emission against absorbance for ITC-functionalized SiNPs in toluene (c).

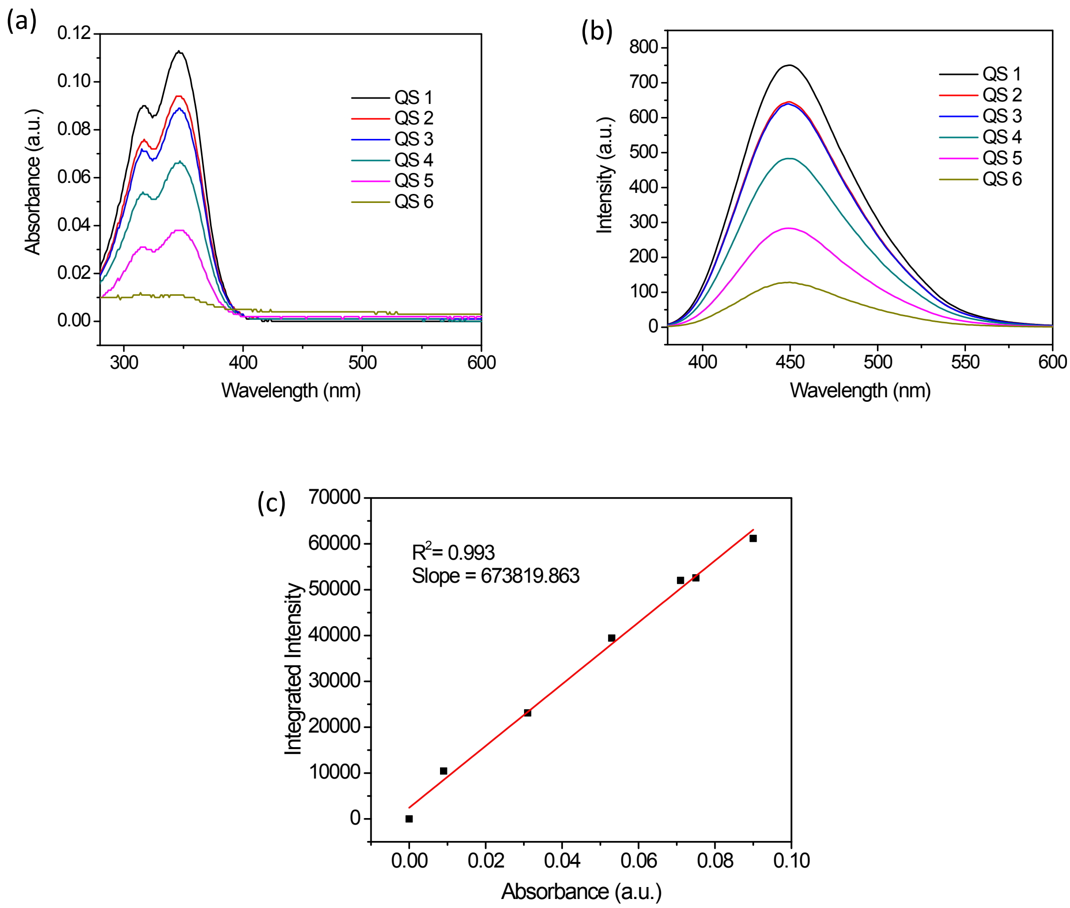

Figure S3. Absorption (a) and emission spectra (b) for various concentrations of standard Quinine Sulphate in 0.1 M H_2SO_4. Plotted integrated intensity of emission against absorbance for Quinine Sulphate in 0.1 M H_2SO_4(c).

3. DLS measurements

The hydrodynamic diameter of ITC SiNPs and polydispersity index were determined by dynamic light scattering (DLS) measurement with Zetasizer Nano ZS (Malvern Instruments Ltd, UK) at room temperature, equilibrating samples for 120 seconds prior to the measurement. 1 mg/mL of ITC SiNP solution was measured in toluene and DMSO as well as RPMI and complete RPMI (supplemented with 10% FBS) media. Size measurements were performed in triplicates.
Polydispersity index (PdI), which is an indicator of the particle size distribution, was equal or less than 0.1 in toluene, DMSO and RPMI demonstrating the high monodispersibility of the prepared nanoparticle suspensions. The normal centrifugation before the measurement promoted the limited aggregation leading to the formation of ITC SiNPs with lower PdI.

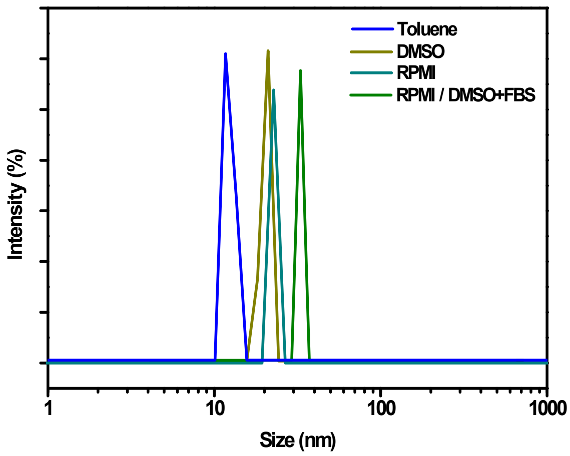

Figure S4. Hydrodynamic diameter of ITC SiNPs in different dispersing solvents.

Table S1. Mean hydrodynamic diameters and Polydispersity index of ITC SiNPs measured by DLS in

Solvent	Mean particle Size (nm) ± SD	Polydispersity index ± SD
Toluene	11.85 ± 0.05	0.08 ± 0.02
DMSO	21.22 ± 1.20	0.10 ± 0.02
RPMI	22.70 ± 0.50	0.10 ± 0.13
RPMI/10% FBS	33.01 ± 0.24	0.20 ± 0.08

different media.

4. XRD analysis

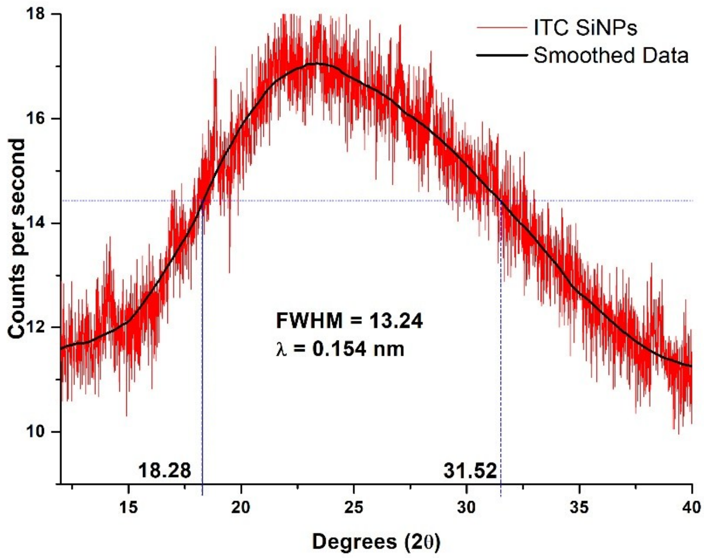

Figure S5. Zoomed in XRD Spectrum obtained from ITC-functionalized SiNPs, smoothed to obtain a value of FWHM = 13.24.

5. FTIR Mapping in Caco-2 and CCD-841 cells

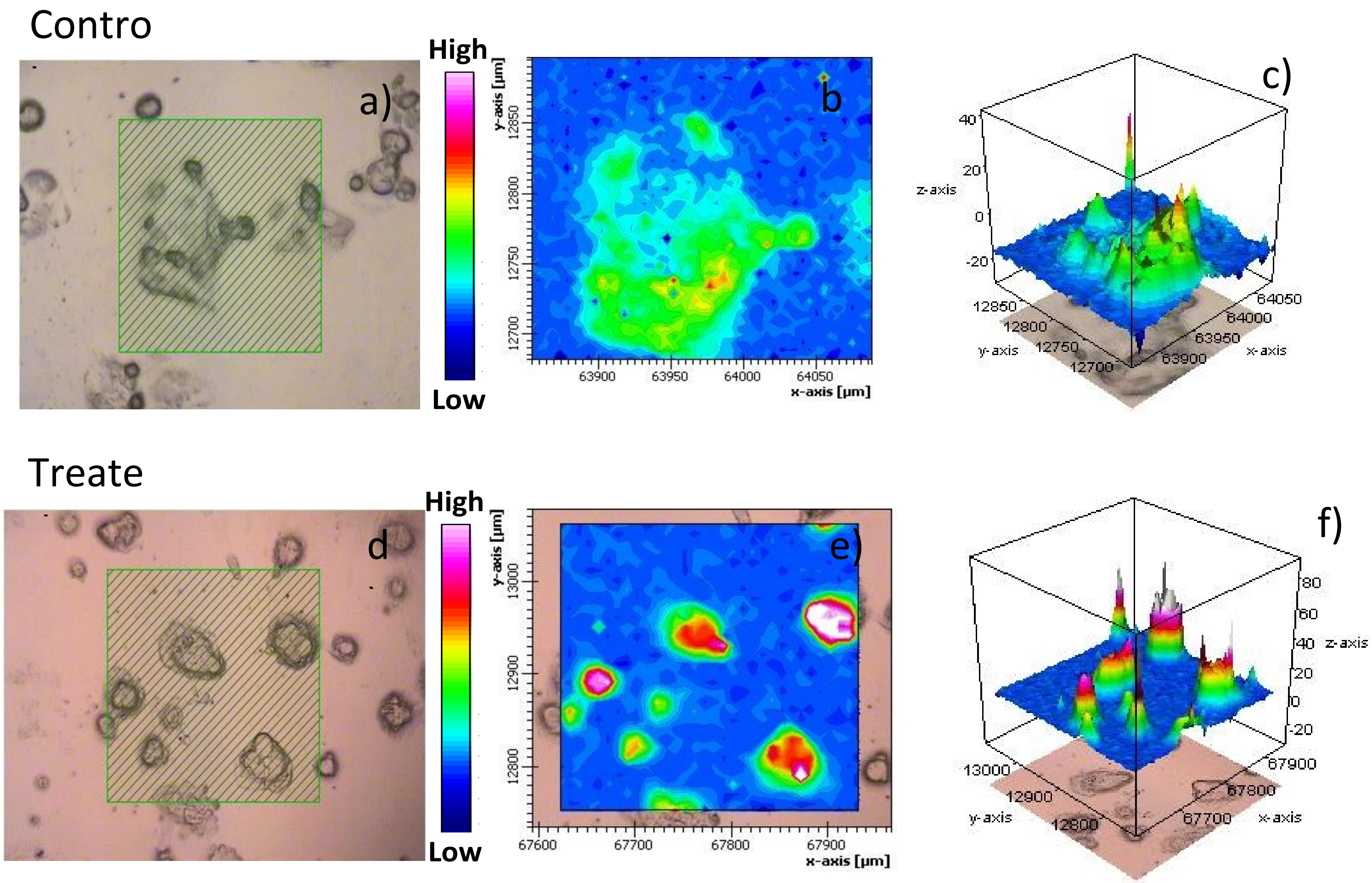

Figure S6. a) Visible image, b) FTIR 2D image and c) FTIR 3D image obtained control Caco-2 cells and d) Visible image, e) FTIR 2D image and f) FTIR 3D image of Caco-2 cells treated with ITC-functionalized SiNPs. Chemical FTIR images were obtained by application of phospholipid profile. Blue indicates low concentration and red a high concentration of phospholipid.

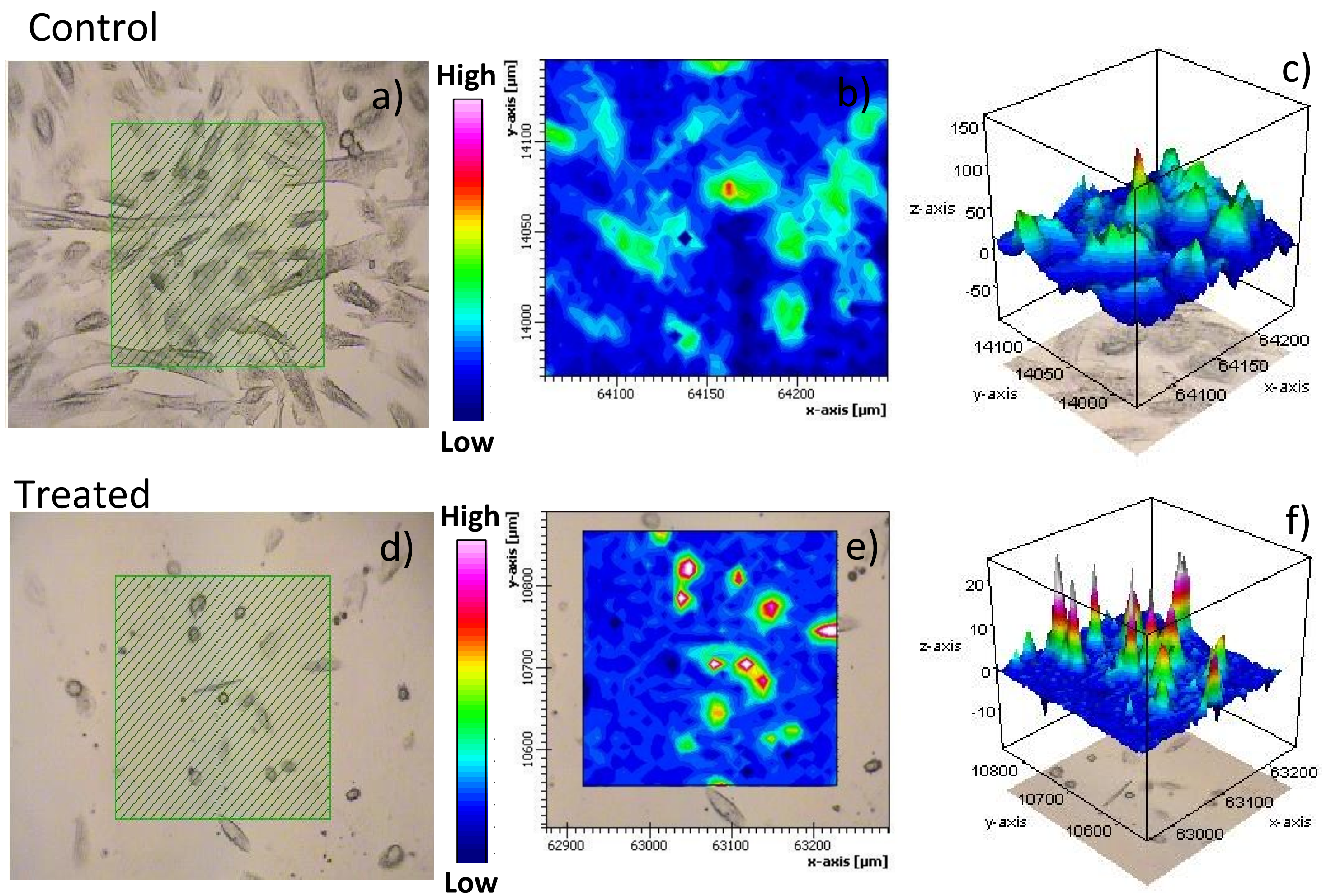

Figure S7. a) Visible image, b) FTIR 2D image and c) FTIR 3D image obtained control CCD-841 cells and d) Visible image, e) FTIR 2D image and f) FTIR 3D image of CCD-841 cells treated with ITC-functionalized SiNPs. Chemical FTIR images were obtained by application of phospholipid profile. Blue indicates low concentration and red a high concentration of phospholipid.

6. XPS spectrum of the Br(3d) region

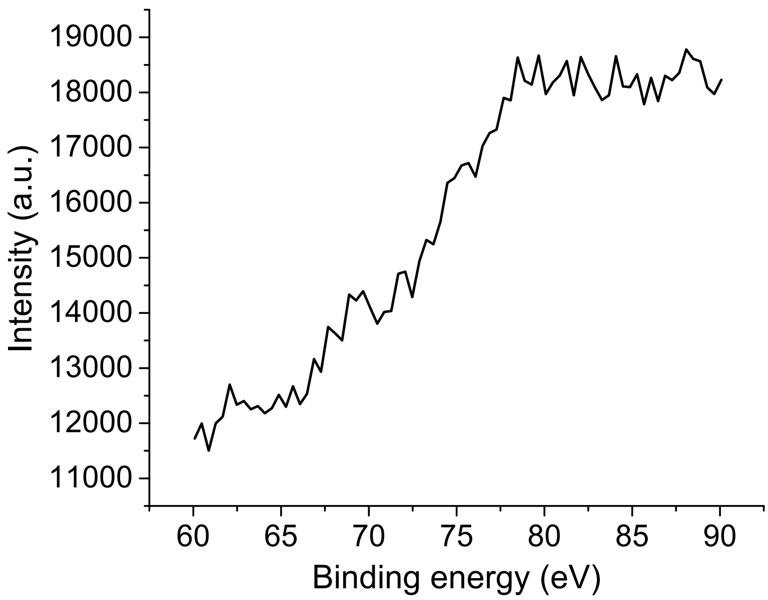

Figure S8. XPS spectrum of the Br(3d) region