Dopamine sensing by fluorescent carbon nanoparticles synthetized by artichoke extract

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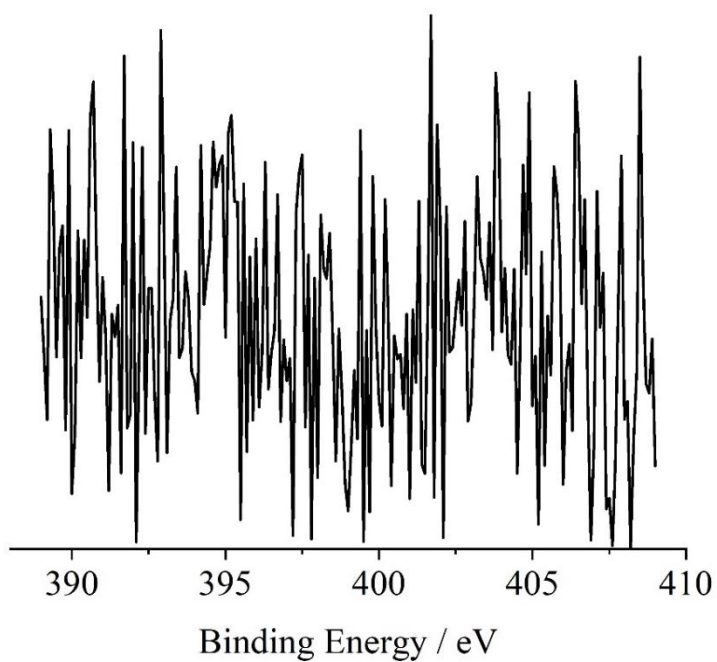[5] R&D Department, Bionap S.r.l., 95032 Belpasso, CT, Italy

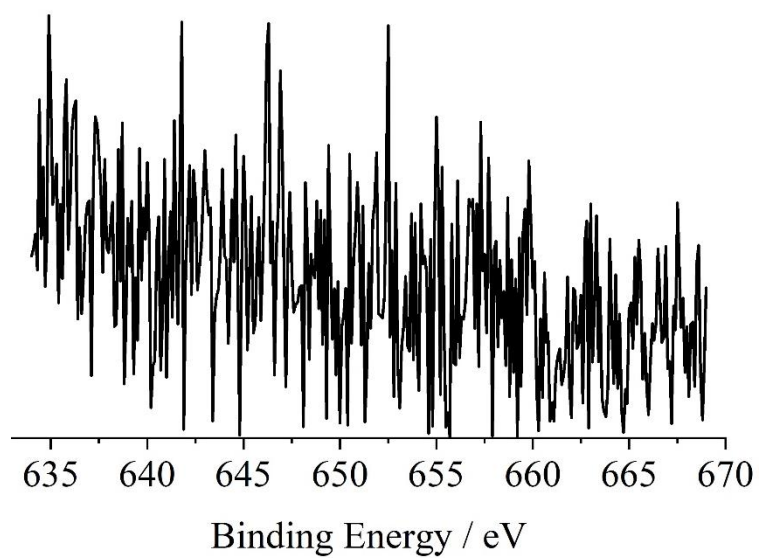**Figure S1**. Al Kα excited XPS of the CNPs in the N 1s binding energy region.

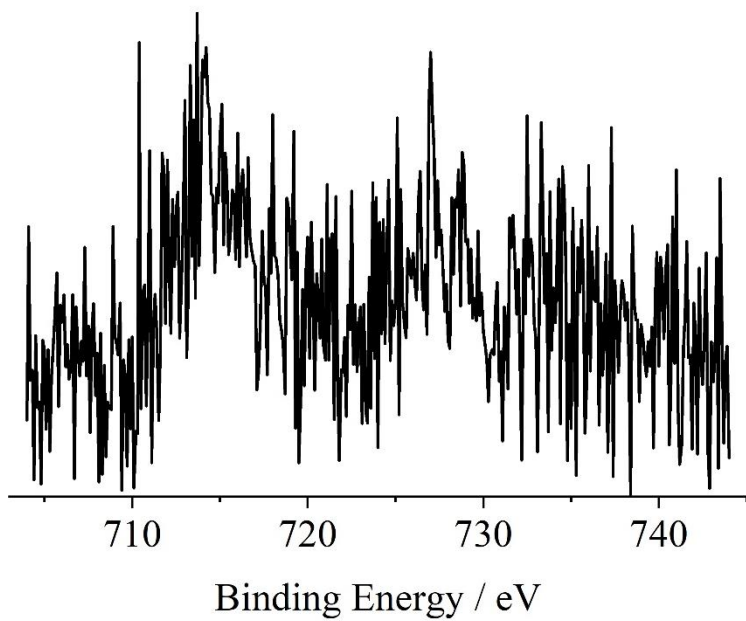**Figure S2**. Al Kα excited XPS of the CNPs in the Mn 2p binding energy region.

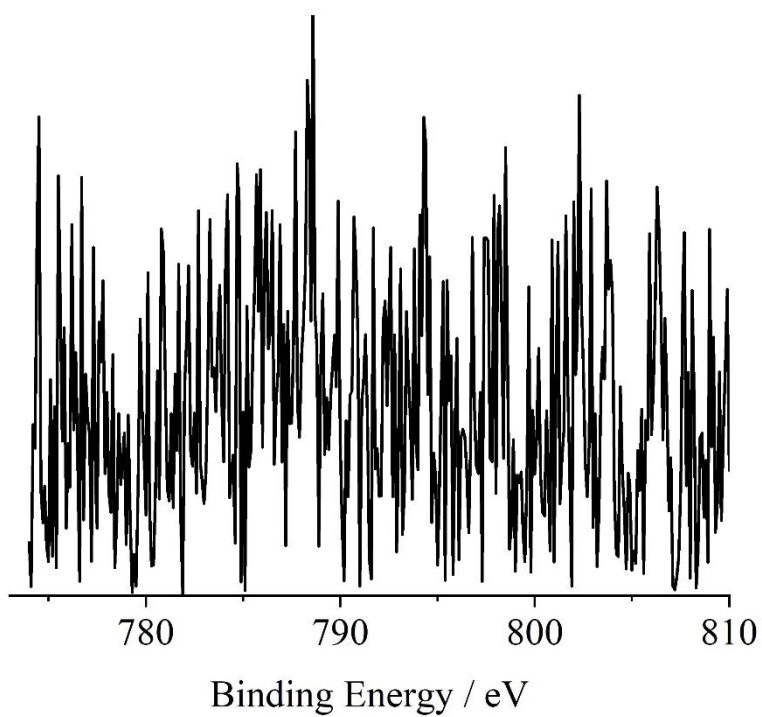**Figure S3**. Al Kα excited XPS of the CNPs in the Fe 2p binding energy region.

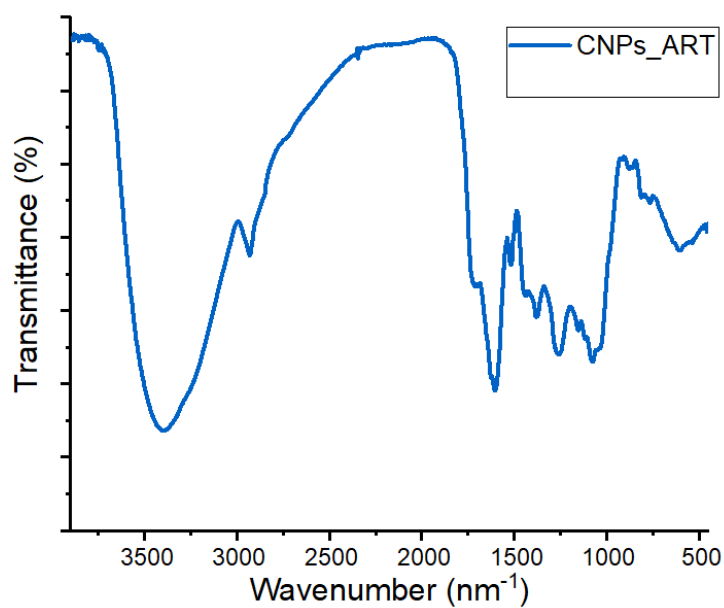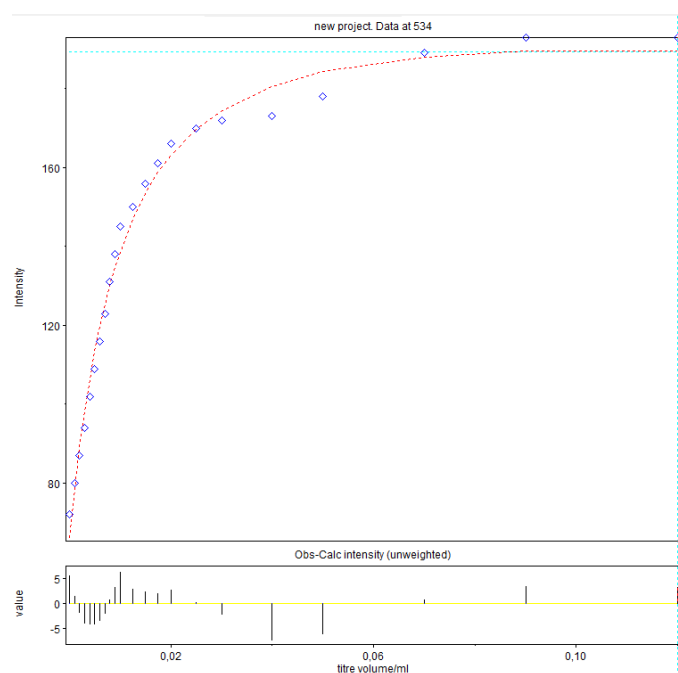**Figure S4**. Al Kα excited XPS of the CNPs in the Co 2p binding energy region.

Figure S5. FT-IR spectrum of CNPs_ART


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Converged in 1 iteration with sigma = 6,2468

                        standard
Log beta    value       deviation
AB          5.7639      0.0238
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Figure S6 HypSpec output of the Fulorescence titration data of CNPs_ART (0.05mg/mL in MilliQ water) upon progressive addition of DA (0-12μM).
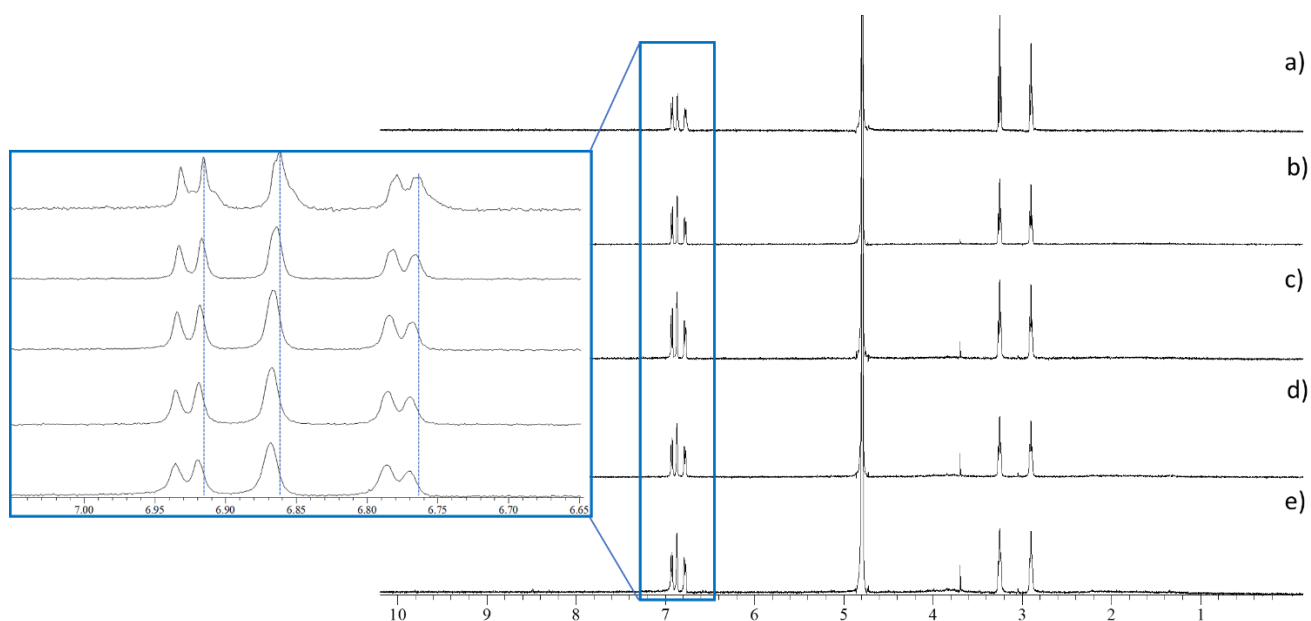
Figure S7. ^{1}H NMR titration of dopamine: a) DA 1mM in D_2O; b) DA 1mM in D_2O + CNPs_ART 0.0625mg/mL; c) DA 1mM in D_2O + CNPs_ART 0.125mg/mL; d) DA 1mM in D_2O + CNPs_ART 0.187mg/mL; e) DA 1mM in D_2O + CNPs_ART 0.250mg/mL.
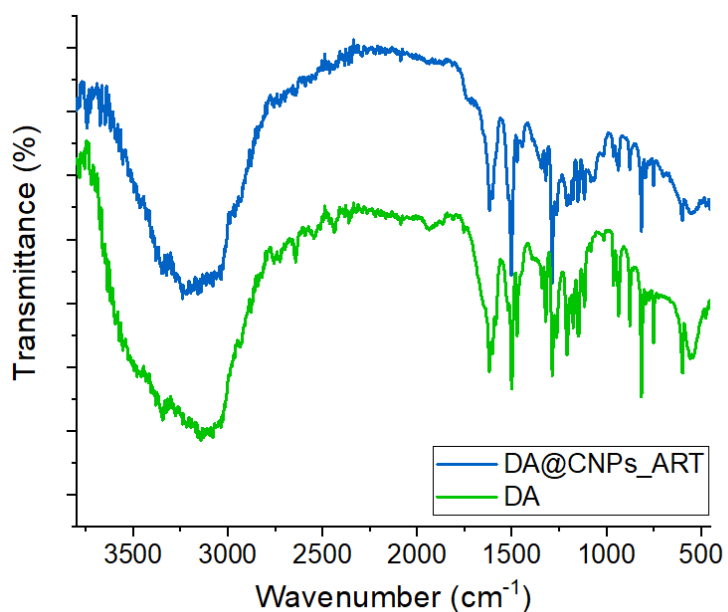

Figure S8. FT-IR spectra of DA (green line) and DA@CNPs_ART (blue line).
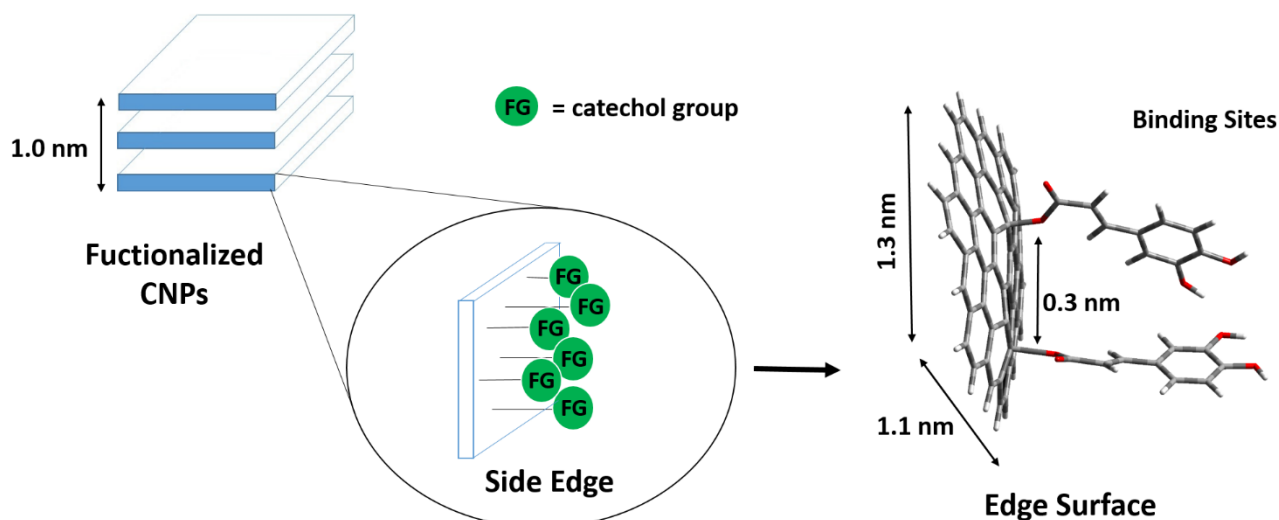
Figure S9: Schematic representation of the investigated system (functionalized CNPs with catechol units), taking in account the distances found in the XPS and TEM analyses.
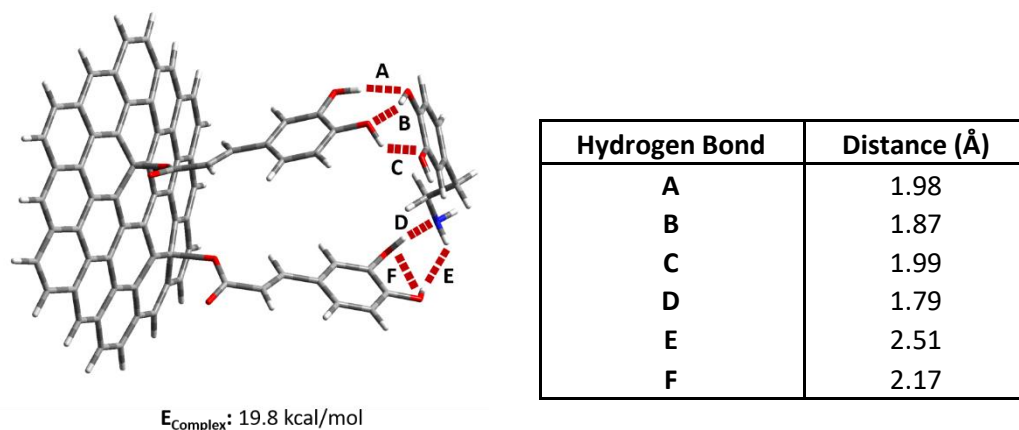

Hydrogen Bond	Distance (Å)
A	1.98
B	1.87
C	1.99
D	1.79
E	2.51
F	2.17

$E_{Complex}$: 19.8 kcal/mol

Figure S10: Structure of the most stable HG complex between functionalized CNPs and dopamine (DA) calcualted at B3LYP/6-31G(d,p) level of theory in gas phase. Hydrogen bonds (A-F) in the host-guest complex are marked in red. Complexation energy ($E_{complex}$) and HBs length are also reported.

Table S1: Complexation energy ($E_{complex}$) for the HG complex between dopamine and functionalized CNPs calcualted at B3LYP/6-31G(d,p) level of theory in gas phase. Complexation energy of a water dimer ($2H_2O$) is reported for a better comparison. Energy difference (ΔE) is reported, taking into account the HG complex with dopamine as a reference.

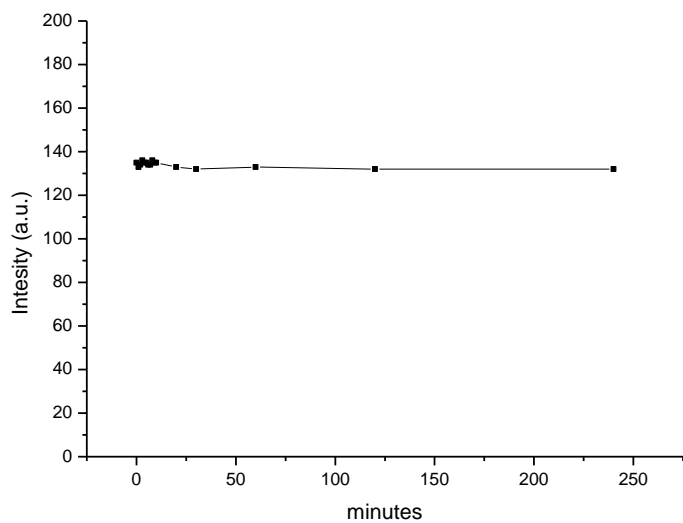| HG Complex	$E_{complex}$ (kcal/mol)	ΔE (kcal/mol)
Dopamine@CNPS	19.8	-
$2H_2O$ (dimer)	5.9	-13.9

Figure S11. Stability test: Fluorescence emission values of CNPs_ART on solid support at different time (0-240 minutes, λ_{ex} 380 nm, λ_{em} 440 nm).
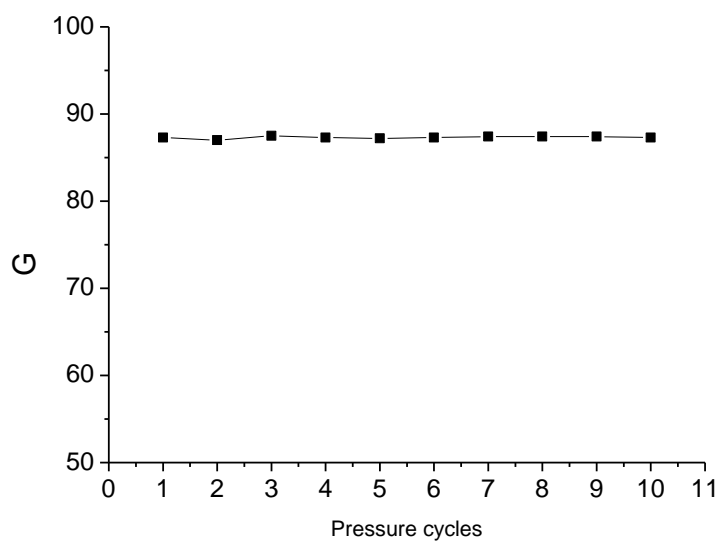

Figure S12. Mechanochromic test: G channel values of CNPs_ART on solid support obtained after progressive exposure of polycellulose filter, simulating the addition of DA.
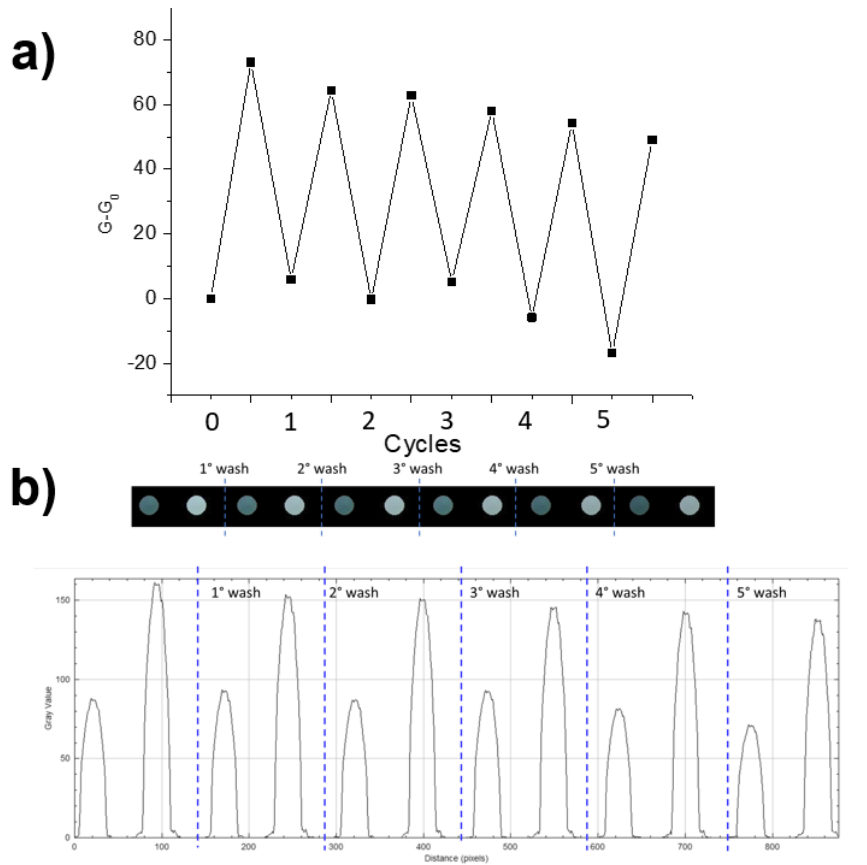
Figure S13. Recovery test: a) optical response expressed in normalised grey channel intensity values (G and G_0 are the Gray channel values after and before the exposure to the analyte, respectively) of CNPs_ART on solid support after the addition of DA 1 nM followed by washing with chloroform (simple immersion of test strip in a elution camera); b) real images and Fiji output of each cycle.