

Controlling the Electroactive Performance of Polypyrrole through 3- and 3, 4- Methyl Substituted Copolymers.

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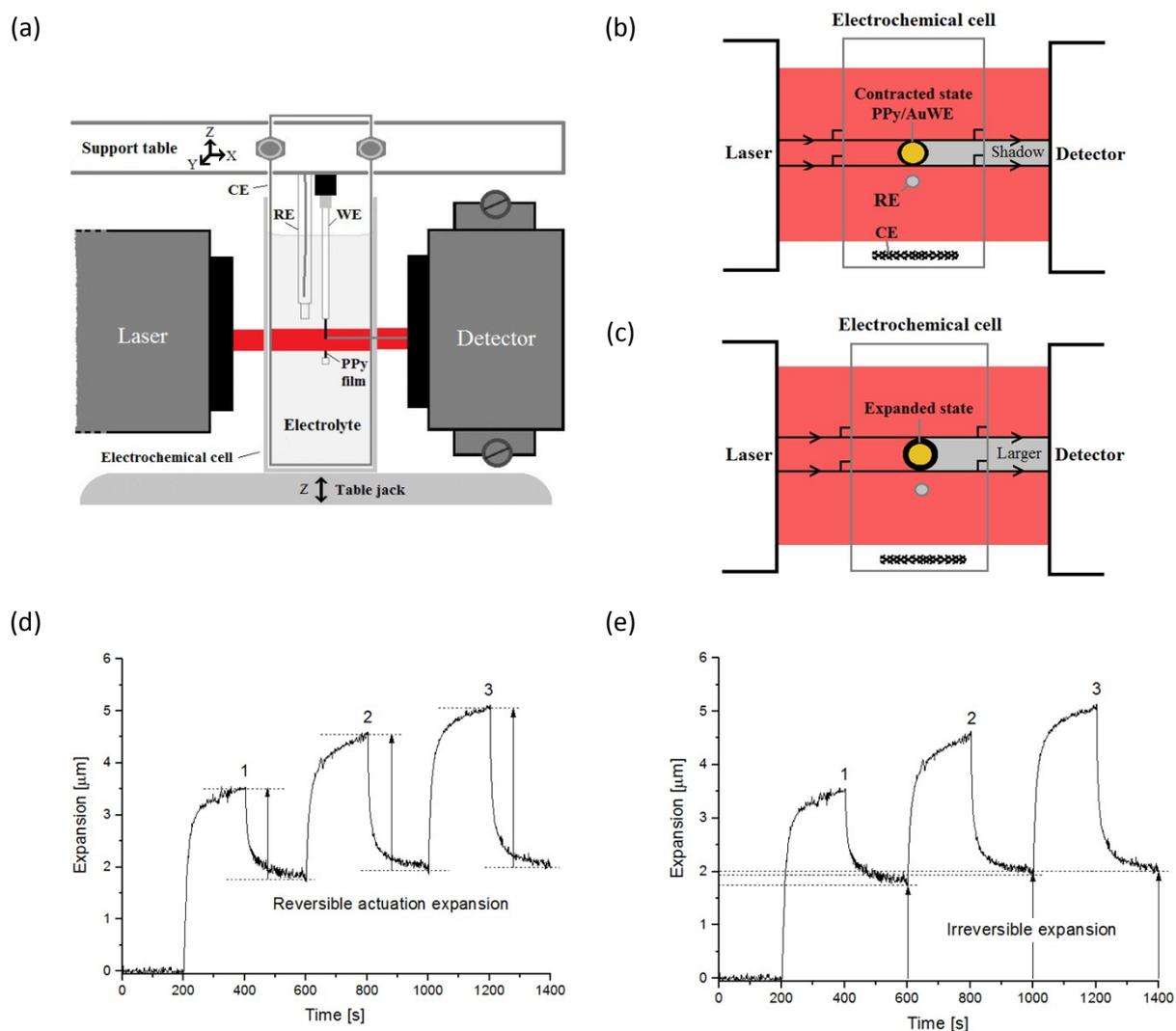


Figure S1. (a) Schematic of Laser Scanning Micrometry (LSM) setup for characterisation of electroactive performance showing a side view of the electrochemical cell and LSM micrometer. Schematics (plan view) showing the principle of LSM measurement: (b) contracted PPy film (c) expanded PPy film. (d) A typical actuation sequence for the first three cycles of PPy showing: (d) the reversible component of the expansion and (e) the irreversible component of the expansion.

State of PPy(DBS)

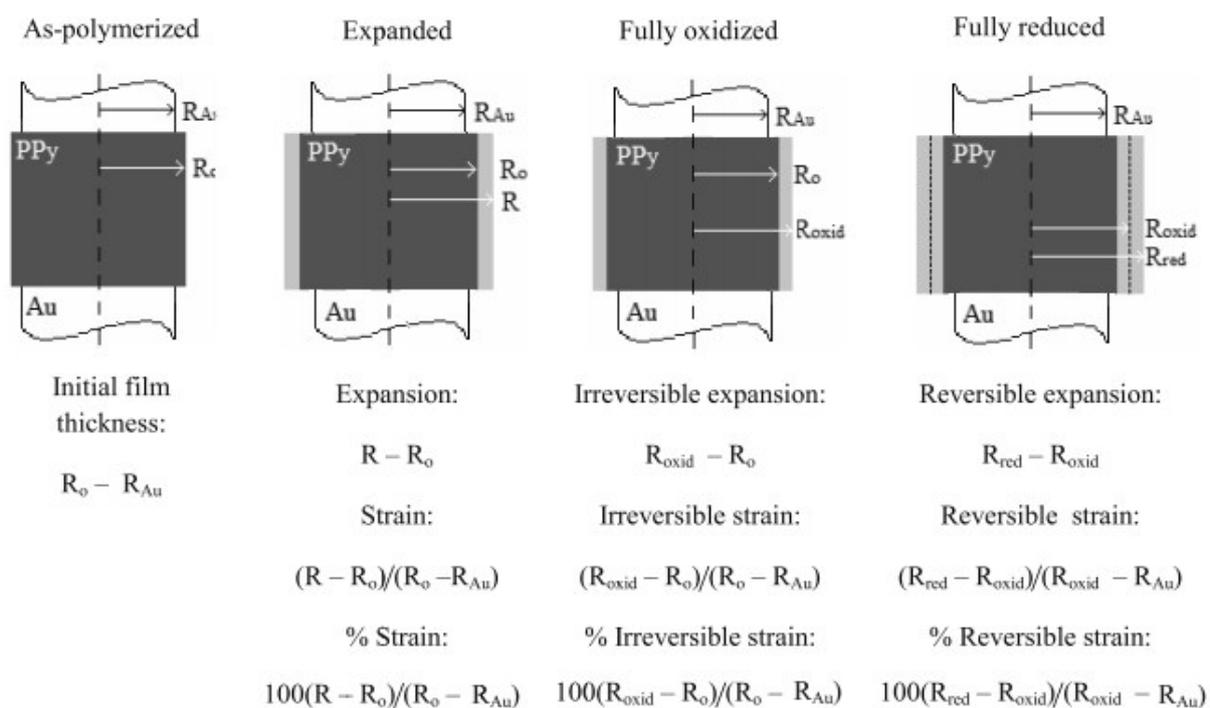
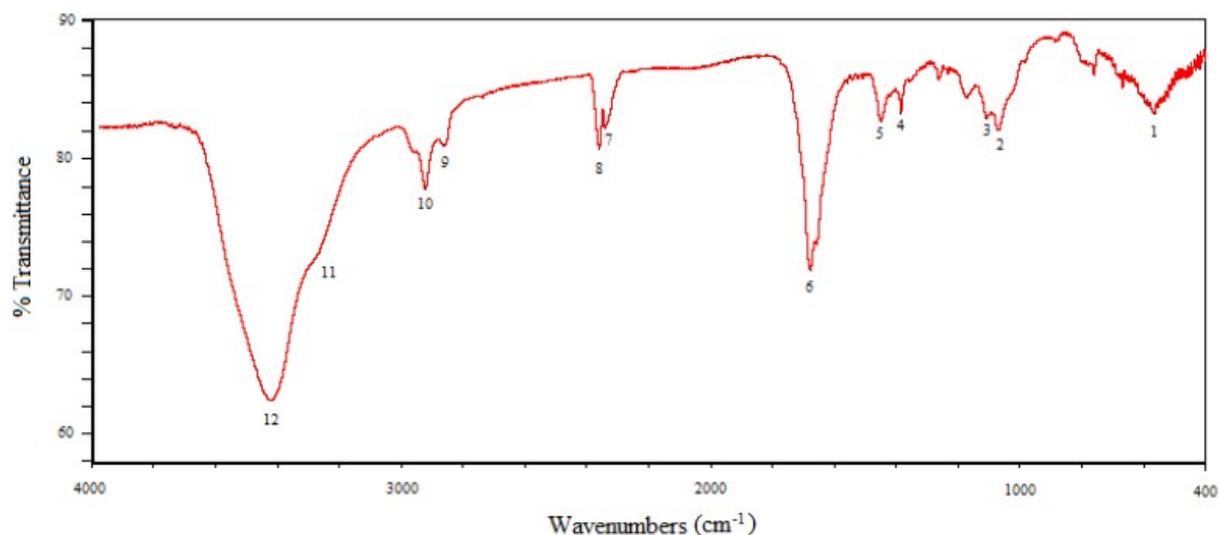


Figure S2. Actuation metrics used to characterise actuation performance.



Peak positions (cm ⁻¹)	Peak intensity and description	Peak assignment
1384.32	Medium	1395-1365: -CH ₃ γ
1448.29	Medium	1470-1430: -CH ₃ δ
2863.05 and 2922.04	Medium, possible multiplet	3100: pyrrollic CH stretch
3250 (shoulder)	Strong	3400-2800: pyrrollic NH (H-bonded) stretch
3420.61	Strong, broad	3500-3400: pyrrollic NH (free) stretch

Figure S3. FTIR spectrum of the product (3,4-dimethyl-1H-pyrrole) prepared as a KBr disc and potential peak assignments. Peak assignments were made using p. 301-303 of *The Handbook of Infrared and Raman Characteristic Frequencies of Organic Molecules*. Lin-Vien, D., Colthup, N. B., Fateley, W. G., Grasselli, J. G. (1991). Academic Press, San Diego, USA.

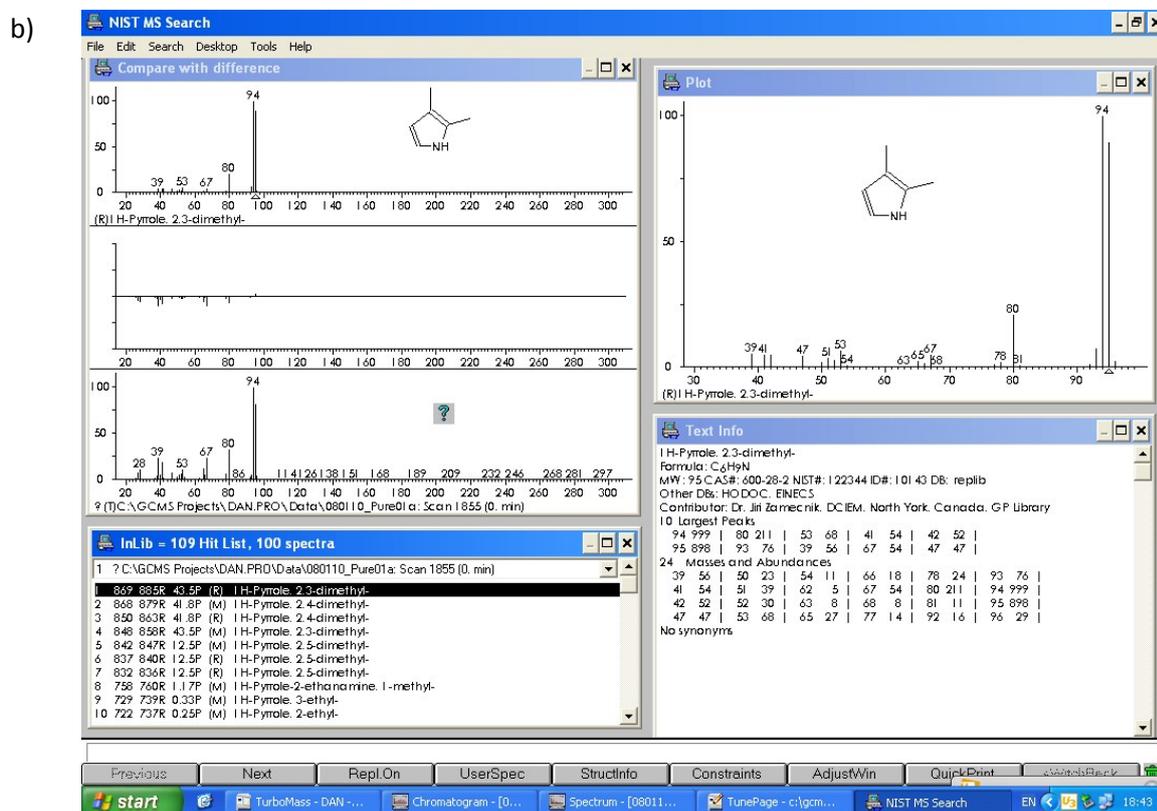
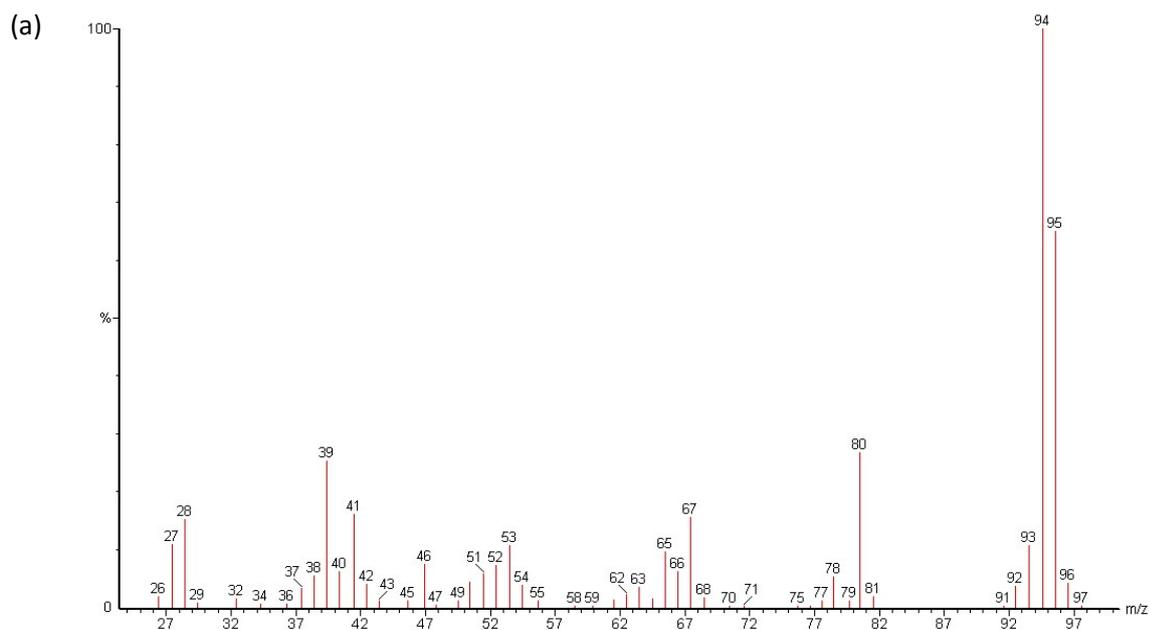


Figure S4. (a) Mass spectrum of the product (3,4-dimethyl-1H-pyrrole) displaying a peak corresponding with the molecular ion at $m/z = 95$. (b) NIST MS database search showing the closest matches for the product as the 2,3- and 2,4- isomers of dimethyl-1H-pyrrole. (Note: the 3,4- isomer was not in the NIST database and therefore an exact match was not possible).

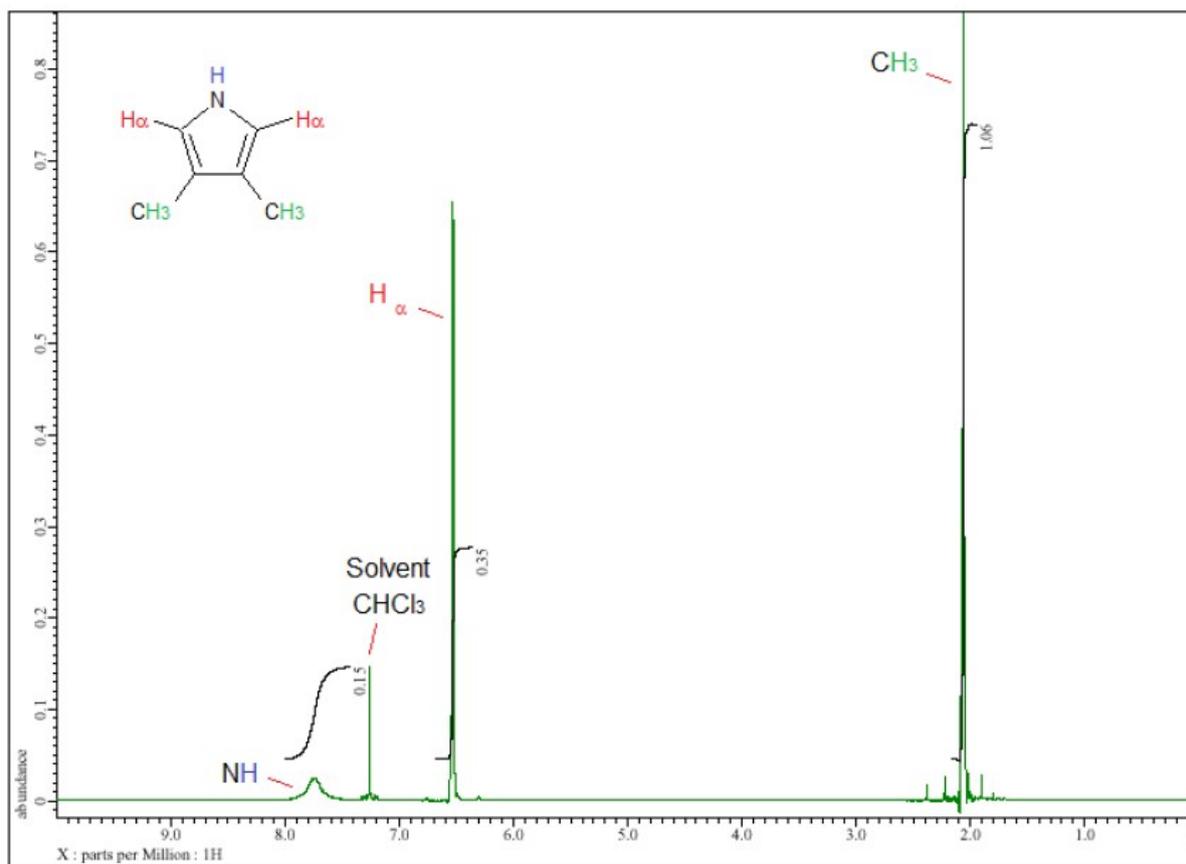


Figure S5. ¹H NMR spectrum of the product (3,4-dimethyl-1H-pyrrole).

Summary:

¹H NMR (400 MHz, CDCl₃, δ): 7.75 (s, br, 1H, NH), 6.53 (d, J = 2.52 Hz, 2H, C_α), 2.05 (s, 6H; CH₃).

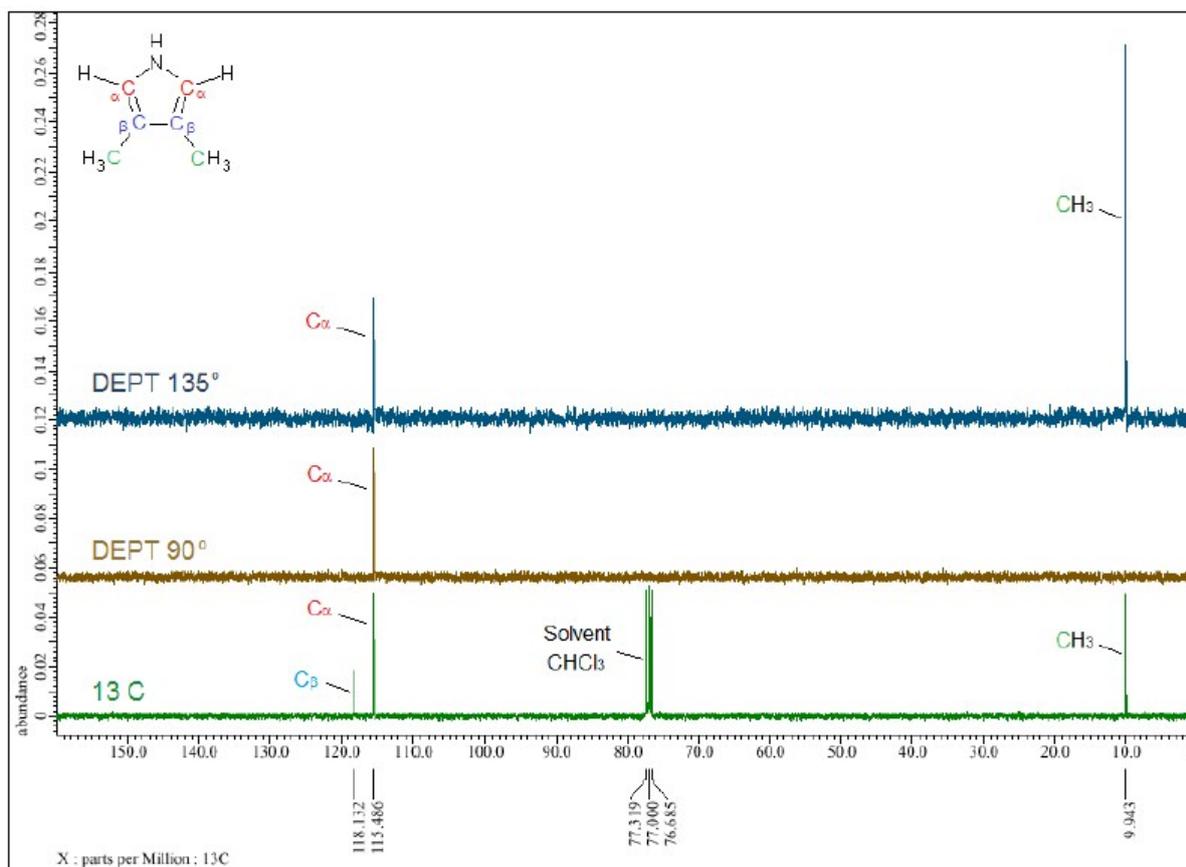


Figure S6. ¹³C NMR and Distortionless Enhancement by Polarization Transfer (DEPT 90° and 135°) ¹³C NMR spectra of the product (3,4-dimethyl-1H-pyrrole).

Summary:

¹³C NMR (400 MHz, CDCl₃, δ): 118.13 (C_β), 115.49 (C_α), 9.94 (CH₃).

ELEMENT	C	H	N	Σ	Difference
% Theory	75.74	9.53	14.71	100.00	N/A
% Found 1	75.74	9.52	14.90	100.16	0.16
% Found 2	75.73	9.51	14.83	100.07	0.07

Figure S7. Confirmation of the purity of 3,4-dimethyl-1H-pyrrole by CHN Elemental analysis.

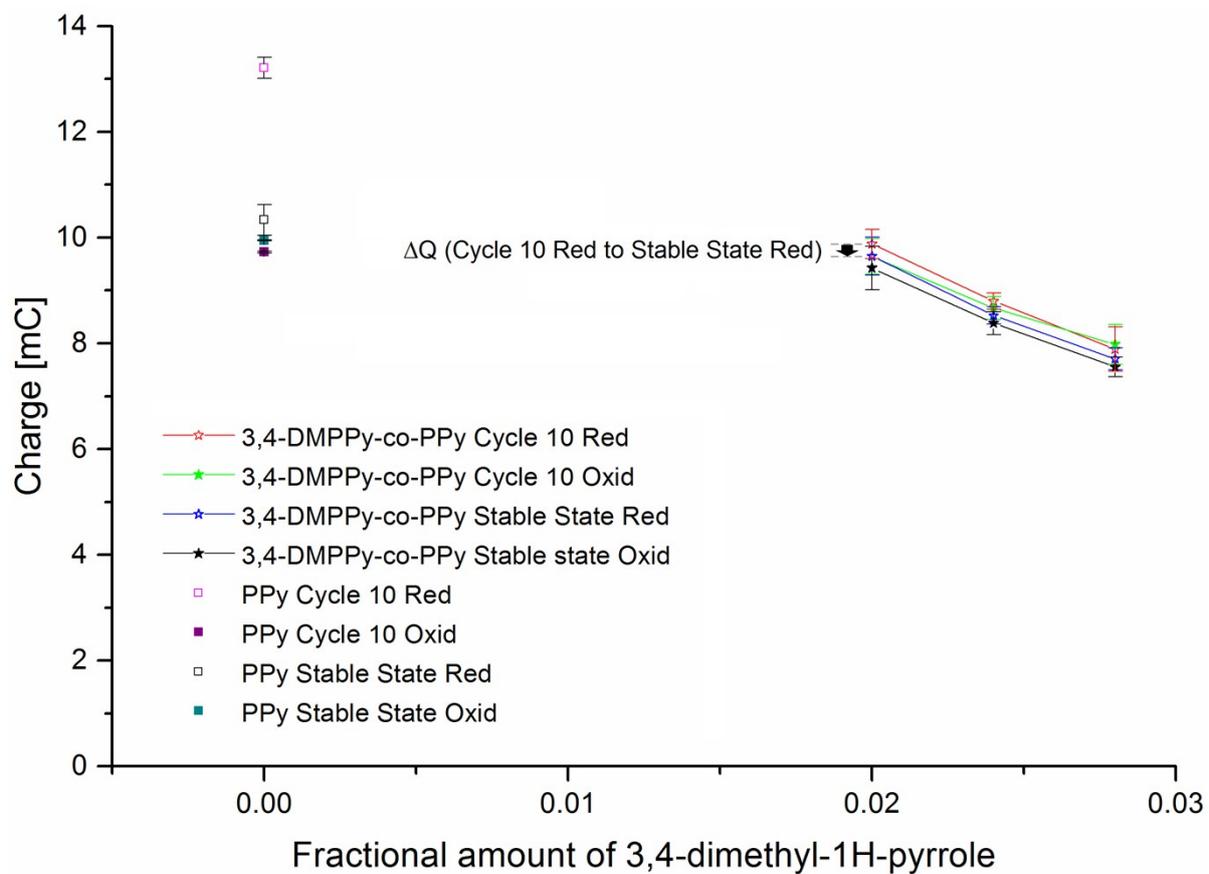


Figure S8 Charge consumed by 5 μm films of PPy(DBS) and poly(3,4-DMPy-co-Py)(DBS) whilst actuating (-1V, 200 s and 0V, 200 s) during cycle 10 and the stable state. Note: there is essentially no change in charge (ΔQ) between cycle 10 and the stable state for poly(3,4-DMPy-co-Py)(DBS).