Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Effects of Polydopamine-Passivation on the Optical Properties of Carbon Dots and its Potential Use *In Vivo*

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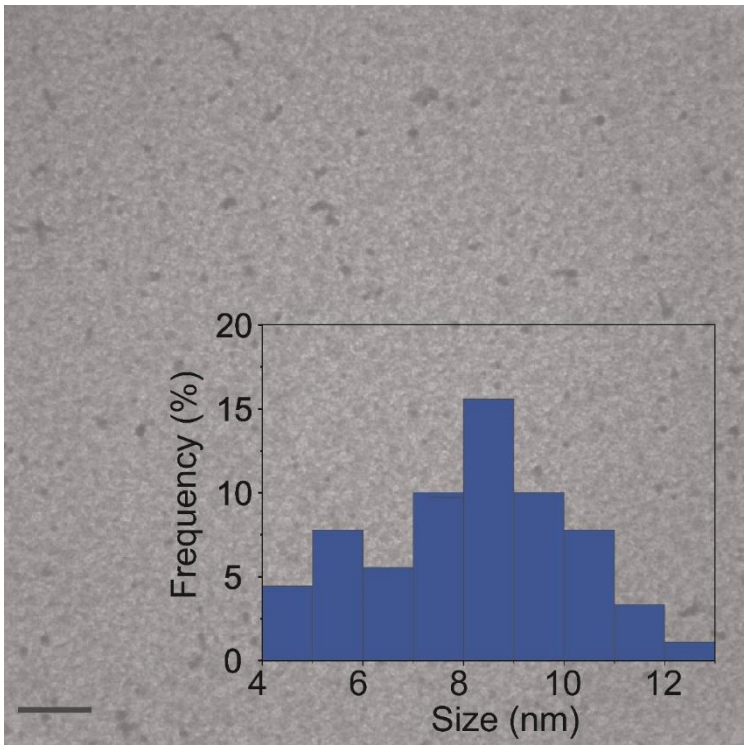

Figure S1. TEM image of uCDot dispersion in water prepared at a concentration of 2 mg/mL. Scale bar = 200 nm

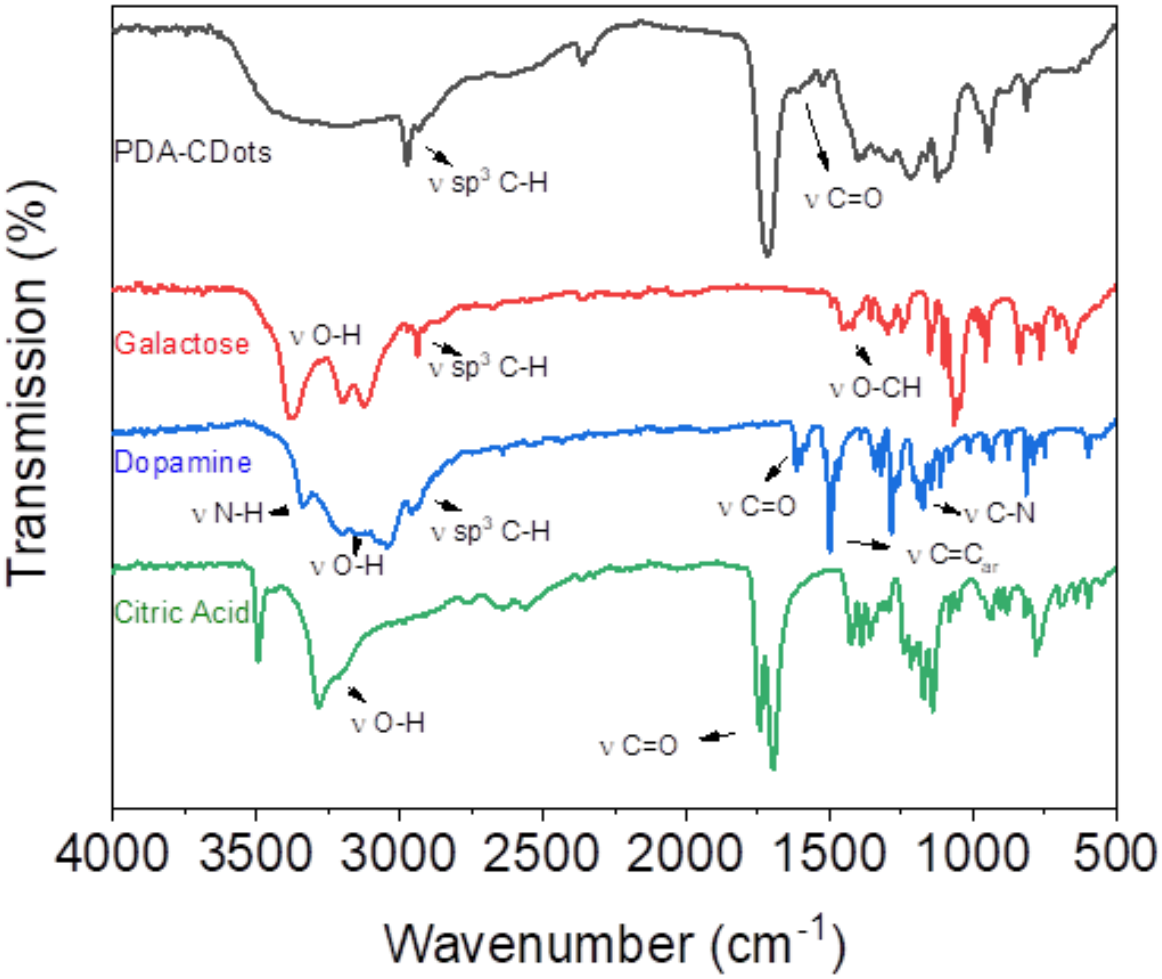

Figure S2. Overlaid FT-IR spectra of PDA-Dots and the corresponding starting materials. It is noted that the stretching vibrations at ~1600 cm^{-1} stem from the C=O of dopamine (and polydopamine). In addition, the C-H stretching vibrations are contributed by galactose and dopamine. The FTIR profile for galactose illustrates the stretching vibration associated to the OH groups at ~ 3400 cm^{-1}, 3200 cm^{-1} and 3130 cm^{-1}, the stretching vibration associated to O-CH bonds are present at ~1420 cm^{-1} and 1390 cm^{-1}. The FTIR profile for dopamine illustrates a stretching vibration at ~ 3300 cm^{-1} associated to the OH groups, at ~ 3400 cm^{-1} and ~ 3200 cm^{-1} associated to the N-H bonds of the primary amine in the dopamine structure, furthermore the stretching vibration associated to the C-N bond is present at ~ 1280 cm^{-1} and at ~ 1500 cm^{-1} the stretching vibrations associated to $(C=C)_{ar}$. The FTIR profile for citric acid illustrates the stretching vibration for free O-H at ~3500 cm^{-1} and the C=O stretching vibration at ~1650 cm^{-1}.

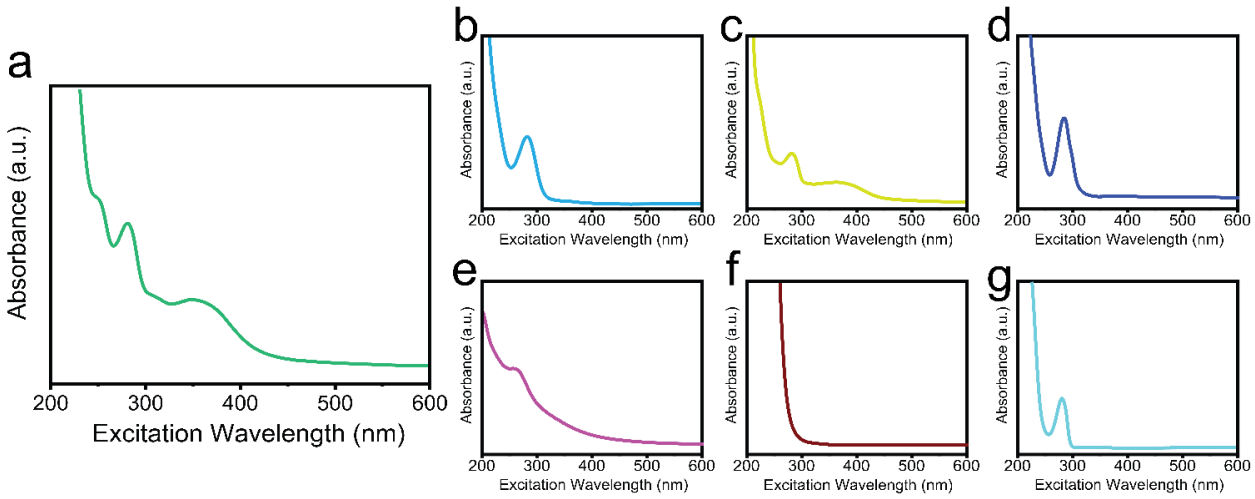

Figure S3. UV-Vis absorbance spectra of PDA-CDots and various control samples: (a) PDA-CDots; (b) uCDots; (c) PDA + Galactose; (d) PDA + CA; (e) Galactose alone; (f) CA alone; (g) PDA alone.

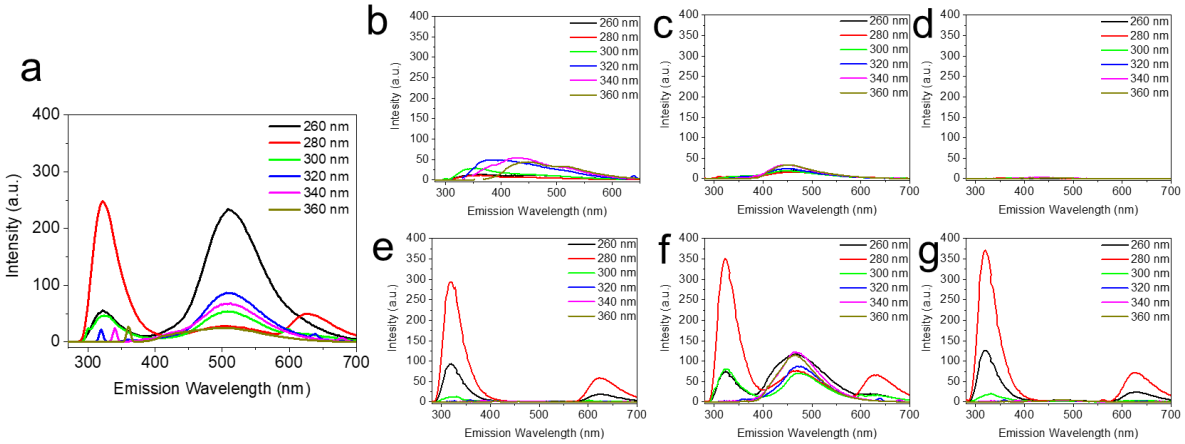

Figure S4. Fluorescence spectra of PDA-CDots and various control samples (50 µg/mL concentration): (a) PDA-CDots; (b) uCDots; (c) Galactose; (d) Citric acid (CA); (e) PDA; (f) PDA and galactose; (g) PDA and citric acid. A strong emission is noted centered at 322 nm stemming from PDA.

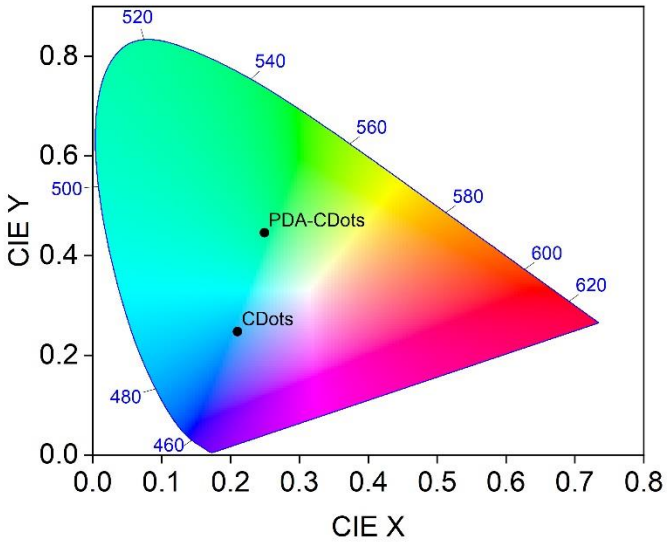

Figure S5. CIE diagram illustrating the blue fluorescence observed for the uCDots and the green fluorescence upon passivation with PDA (λ_{ex} = 340 nm).

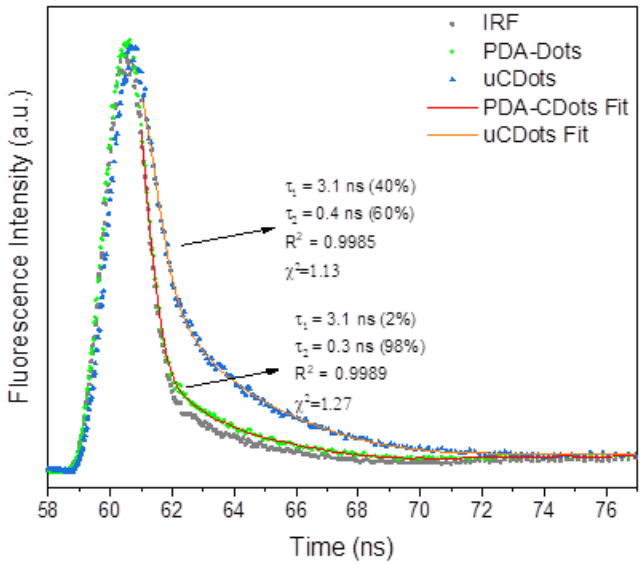

Figure S6. Fluorescence lifetime decays for PDA-CDots and uCDots at λ_{ex} = 368 nm. Both systems possess a short and long lifetime component.

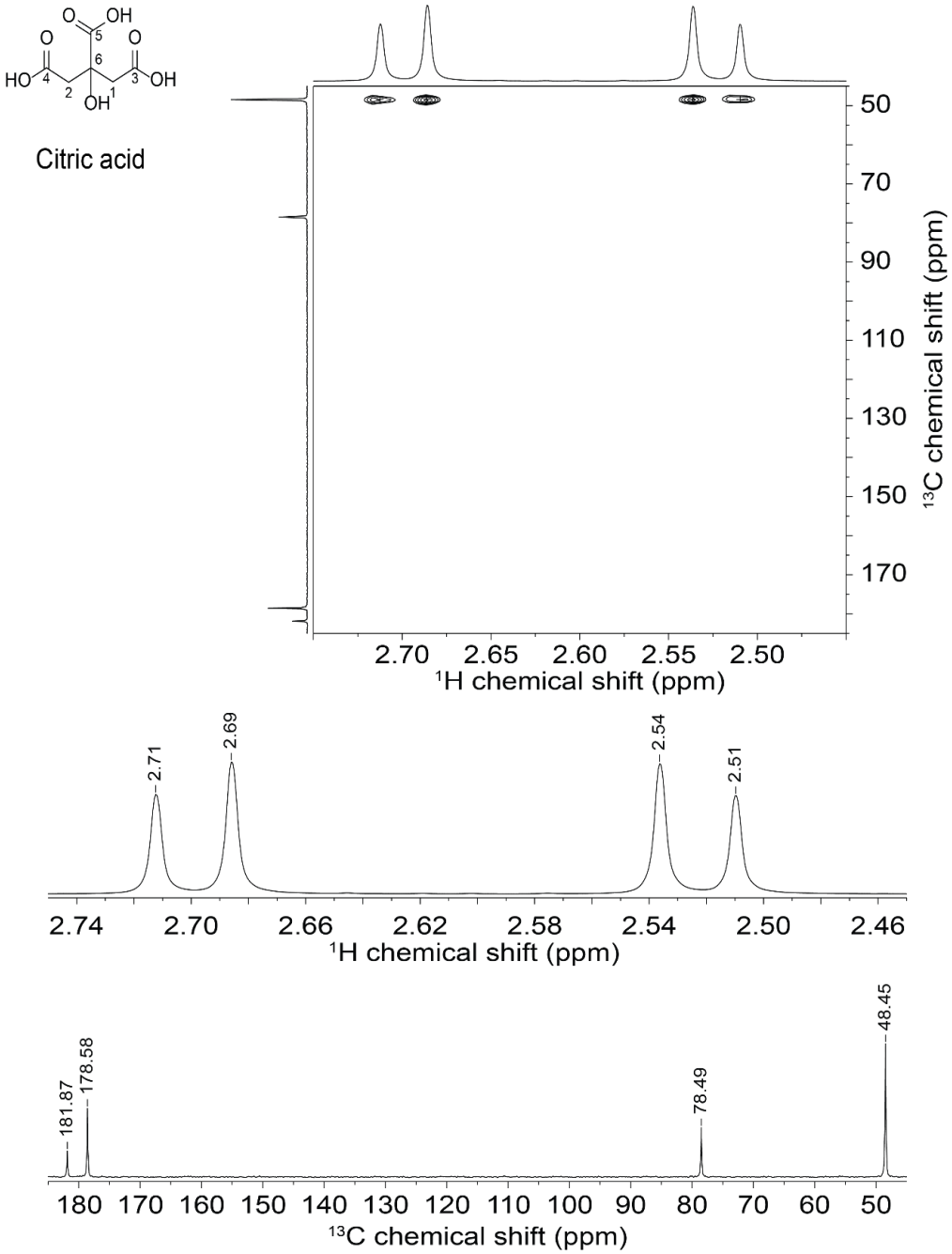

Figure S7. Assignment of the 2D heteronuclear single quantum coherence (HSQC) NMR spectrum of citric acid in D_2O.

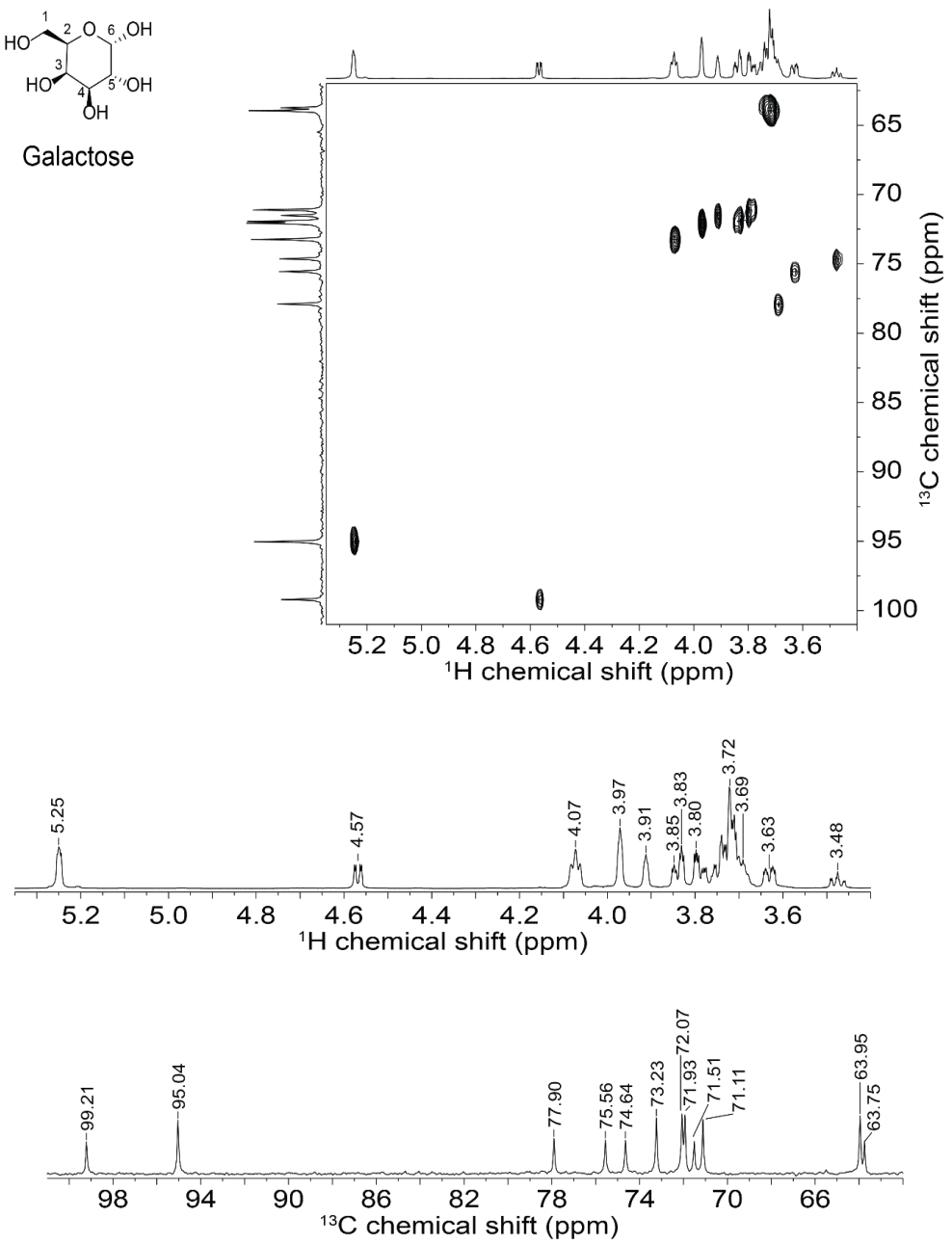

Figure S8. Assignment of the the 2D heteronuclear single quantum coherence (HSQC) NMR spectrum of galactose in D_2O.

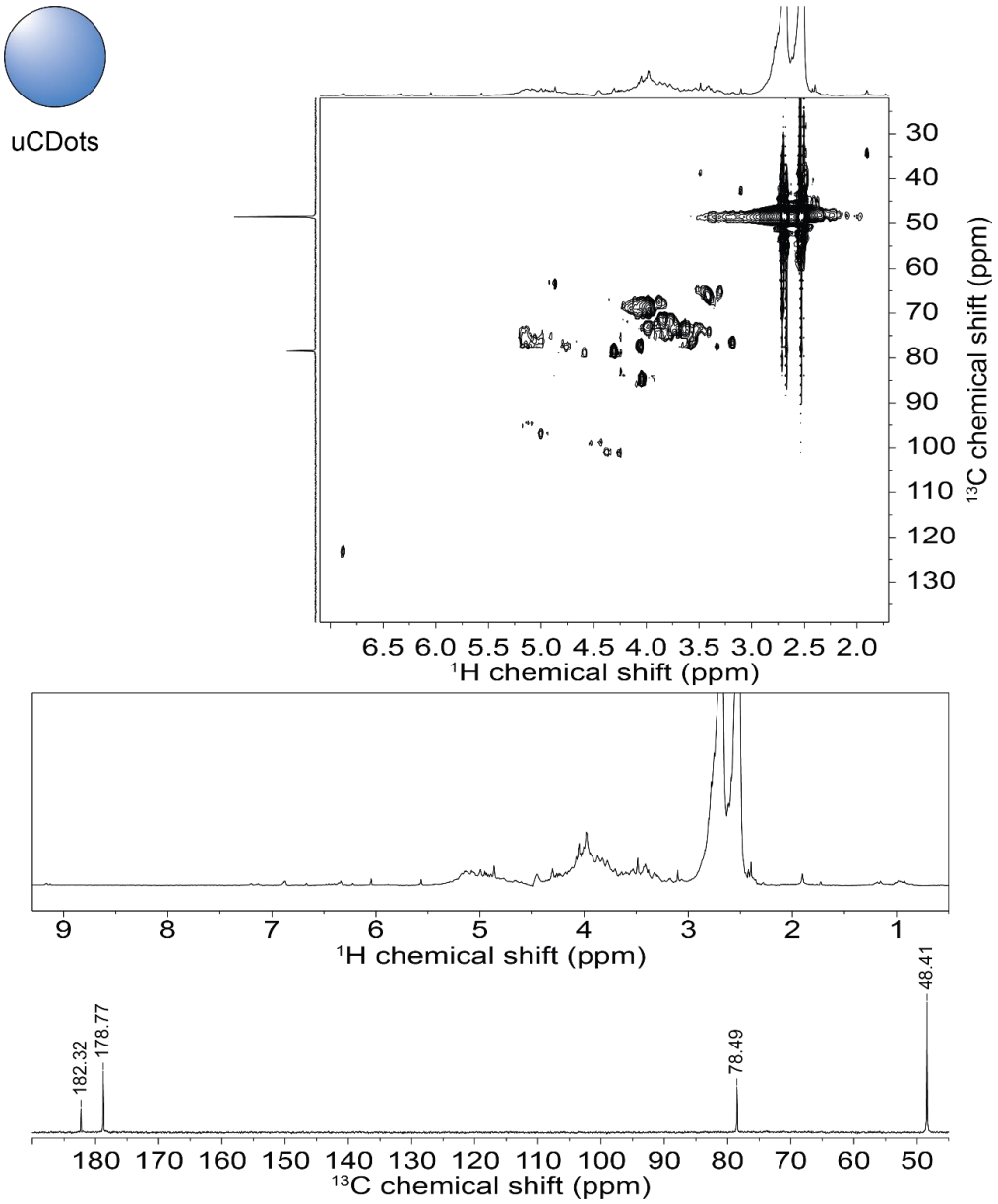

Figure S9. Assignment of the the 2D heteronuclear single quantum coherence (HSQC) NMR spectrum of unpassivated CDots in D_2O.

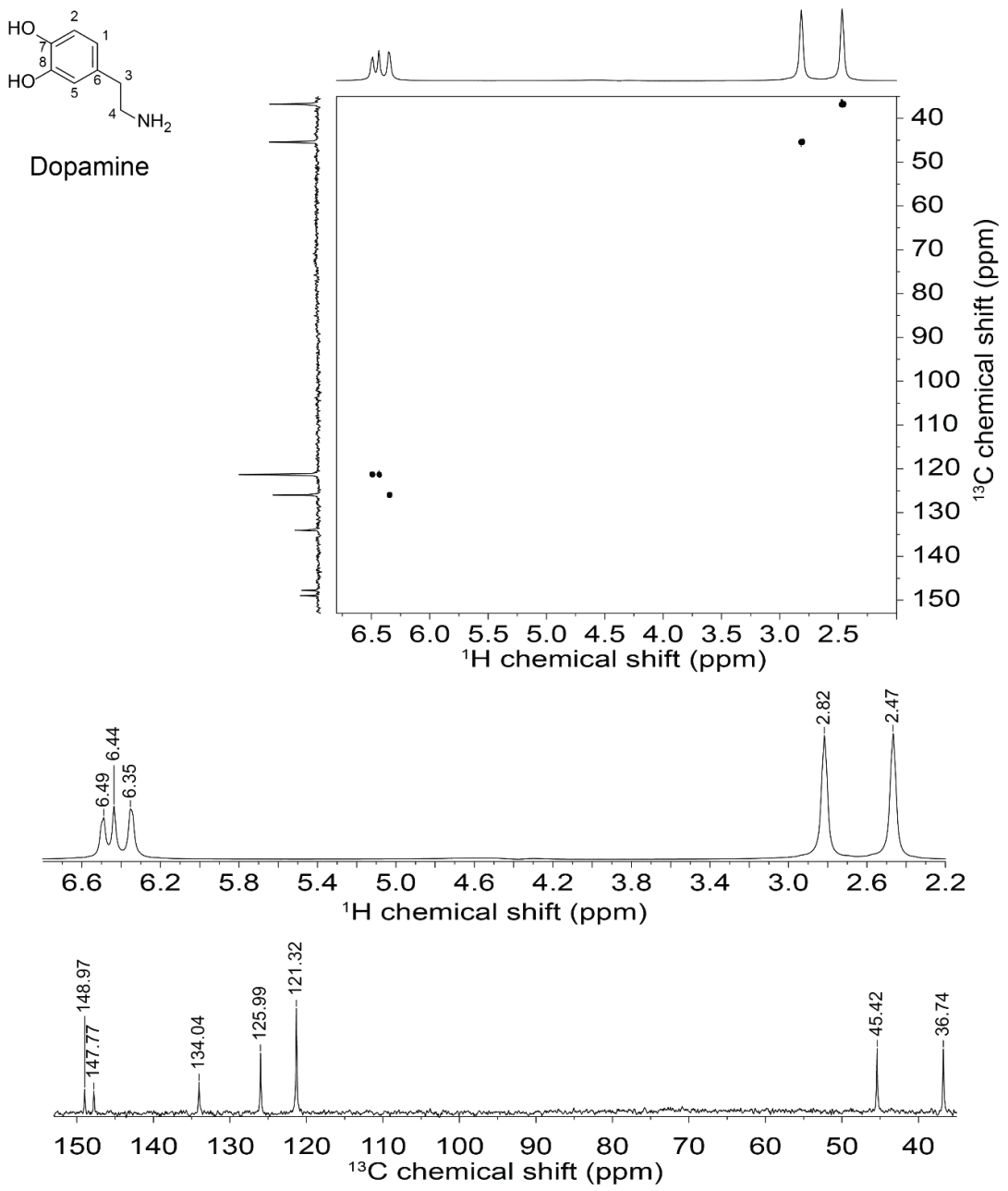

Figure S10. Assignment of the the 2D heteronuclear single quantum coherence (HSQC) NMR spectrum of dopamine in D2O.

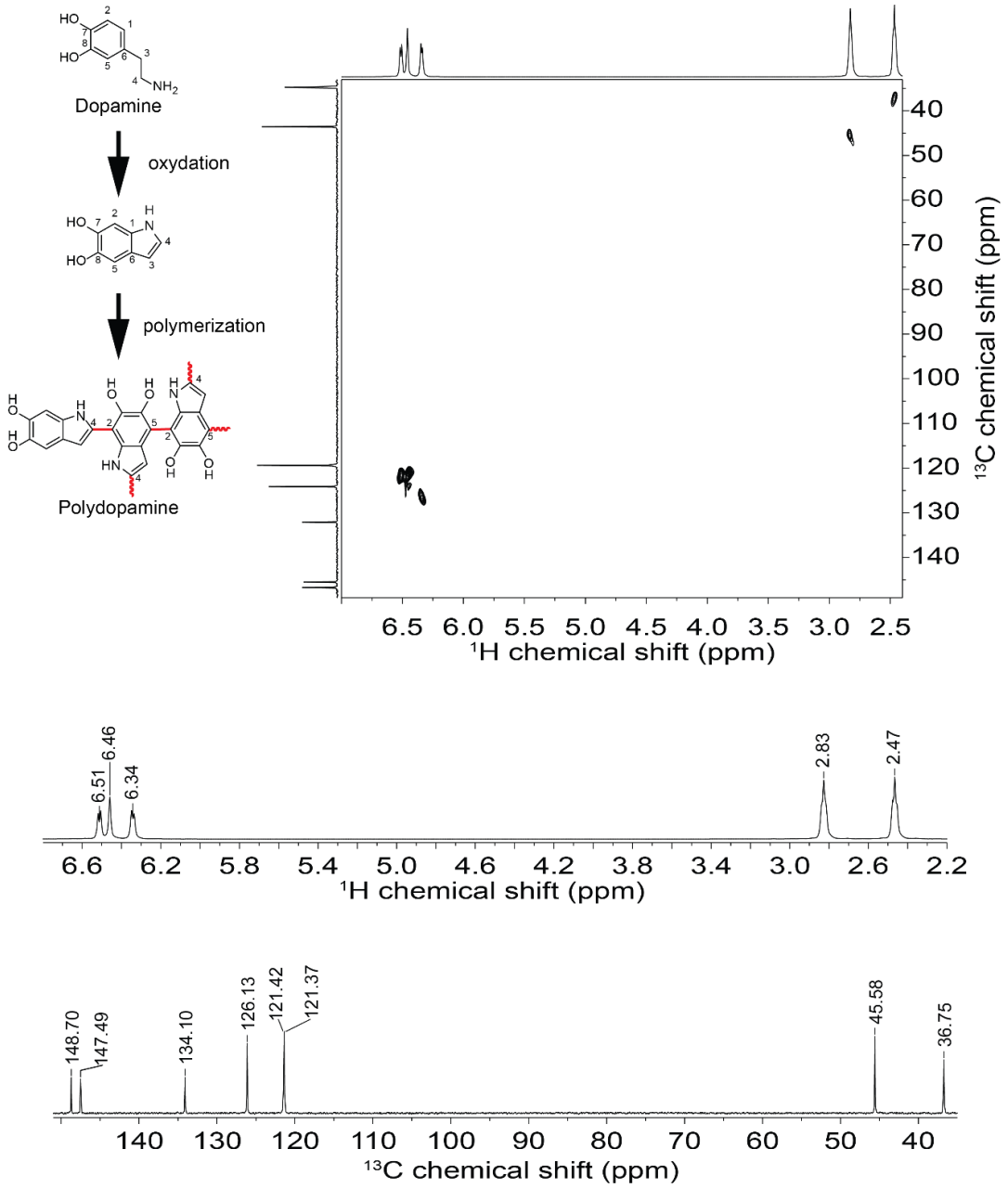

Figure S11. Assignment of the the 2D heteronuclear single quantum coherence (HSQC) NMR spectrum of soluble poly-dopamine in D_2O.

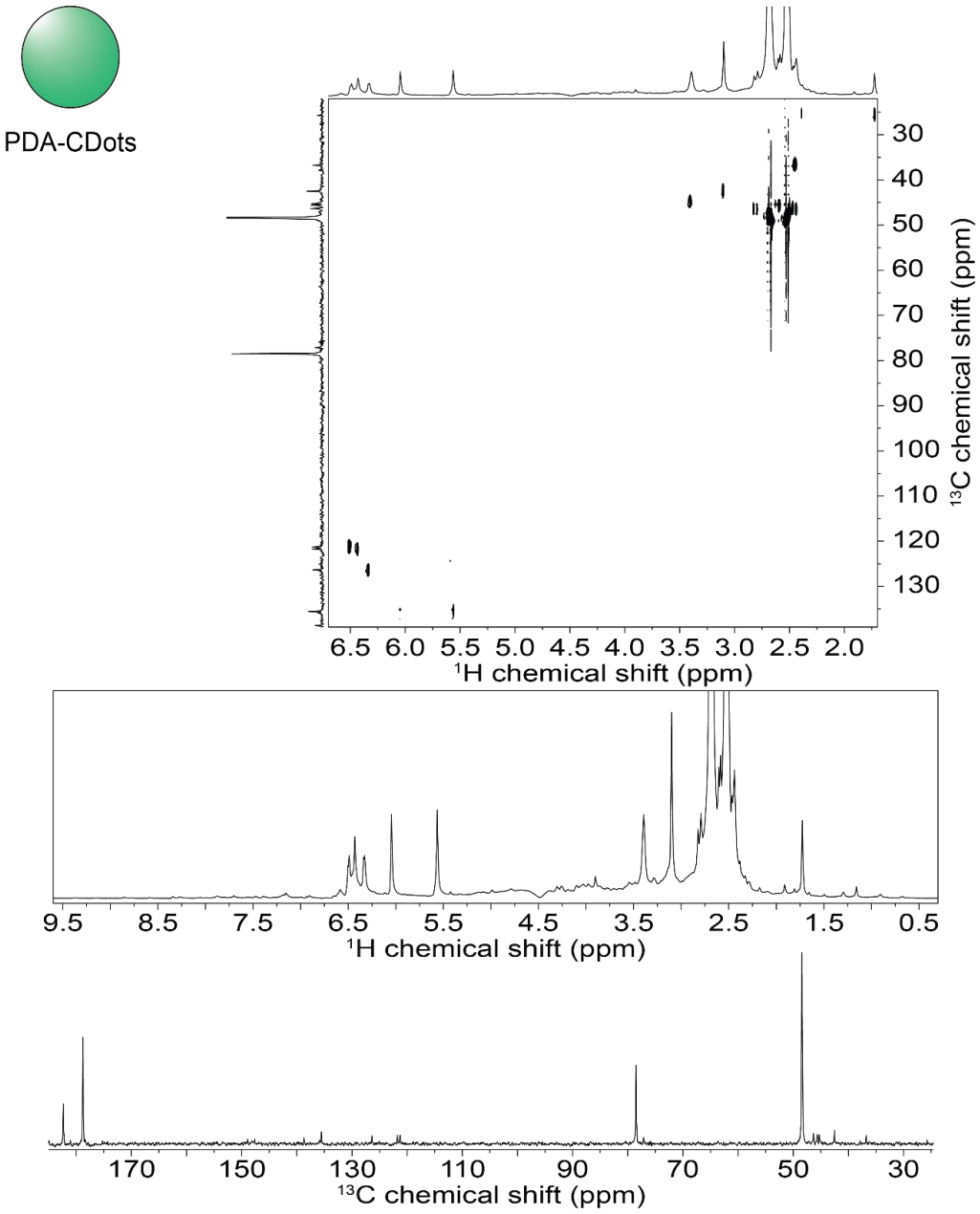

Figure S12. Assignment of the the 2D heteronuclear single quantum coherence (HSQC) NMR of PDA-CDots in D_2O.

Table S1. Table of chemical shifts of citric acid, galactose, dopamine, water soluble polydopamine, uCDots and PDA-CDots. Assignments had been done using 1D ^{1}H, ^{13}C and 2D HSQC expriments. Carbon and proton with the same index are correlated according to the HSQC spectrum.

Citric acid		**Chemical shift (ppm)**
	C1 / C2	48.45
	H1 / H2	2.51 - 2.54 - 2.69 - 2.71
	C3 / C4	178.58
	C5	181.87
	C6	78.49
Galactose		**Chemical shift (ppm)**
	C1	63.75 - 63.95
	H1	3.72
	C2 / C3 / C4 / C5	77.9 - 75.56 - 74.64 - 73.23 - 72,07 - 71.93 - 71.51 - 71.11
	H2 / H3 / H4 / H5	3.69 - 3.63 - 3.48 - 4.07 - 3,97 - 3.83 - 3.91 - 3.80
	C6a	99.21
	H6a	4.57
	C6b	95.04
	H6b	5.25
uCDots		**Chemical shift (ppm)**
Citric acid	C1 / C2	48.29
	H1 / H2	2.51 - 2.54 - 2.67 - 2.70
	C3 / C4	178.77
	C5	182.32
	C6	78.49
Galactose	C1	x
	H1	x
	C2 / C3 / C4 / C5	77.36 - 75.61 - 74.24 - 73.28 - 72.28 - 71.38 - 71.66 - 71.13
	H2 / H3 / H4 / H5	3.64 - 3.60 - 3.40 - 4.06 - 3.98 - 3.87 - 3.94 - 3.78
	C6a	99.43
	H6a	4.52
	C6b	94.92
	H6b	5.15
Galactose	Ca	100.98
	Ha	4.37 - 4.25
	Cb	96.89
	Hb	5.00
	Cc	94.34
	Hc	5.08 - 5.17
	Cd	84.58
	Hd	4.04
	Ce	78.53
	He	4.30 - 4.58
	Cf	77.24
	Hf	4.07 - 4.05 - 3.33
	Cg	75.63
	Hg	5.17 - 5.12 - 5.05 - 5.00
	Ch	73.53
	Hh	3.77 - 3.70 - 3.63
	Ci	71.78
	Hi	3.86 - 3.80
	Cj	68.53
	Hj	4.10 - 3.98 - 3.94 - 3.87
	Ck	65.49
	Hk	3.42 - 3.30
Citric acid	Ca	123.19
	Ha	6.88

	Cb	42.48
	Hb	3.1
	Cc	38.52
	Hc	3.48
	Cd	34.33
	Hd	1.9

Dopamine		**Chemical shift (ppm)**
	C1	125.99
	H1	6.35
	C2 / C5	121.32
	H2 / H5	6.49 - 6.44
	C3	36.74
	H3	2.47
	C4	45.42
	H4	2.82
	C6	134.04
	C7 / C8	148.97 - 147.77
PDA		**Chemical shift (ppm)**
	C1	126.13
	H1	6.34
	C2 / C5	121.42 - 121.37
	H2 / H5	6.51 - 6.46
	C4	45.58
	H4	2.83
	C3	36.75
	H3	2.47
	C6	134.10
	C7 / C8	148.70 - 147.49
PDA-Cdots		**Chemical shift (ppm)**
Citric acid	C1 / C2	48.41
	H1/ H2	2.51 - 2.54 - 2.67 - 2.70
	C3 / C4	178.76
	C5	182.31
	C6	78.49
Polydopamine	C1	126.37
	H1	6.33
	C2 / C5	121.76 - 121.27
	H2 / H5	6.49 - 6.50
	C4	45.61
	H4	2.82
	C3	36.77
	H3	2.44
	C6	135.54
	H6	6.05 - 5.56
	C7 / C8	148.91 - 147.62
Polydopamine	Ca	134.04
	Ha	6.04 - 5.56
	Cb	124.63
	Hb	5.56
	Cc	42.51
	Hc	3.10
Citric acid	Ca	45.26
	Ha	3.39
	Cb	45.61
	Hb	2.60 - 2.59
	Cc	46.34
	Hc	2.47 - 2.44

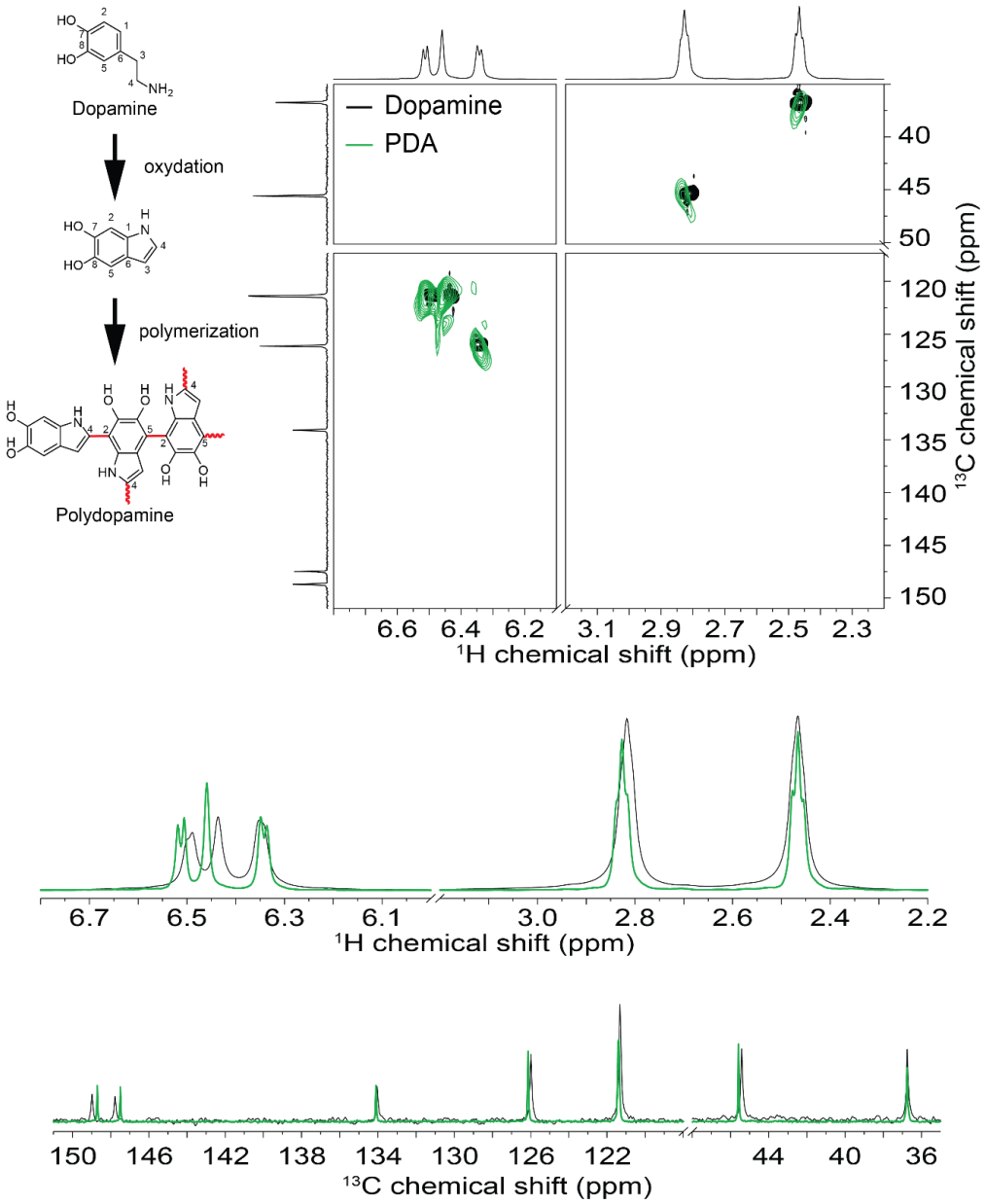

Figure S13. Assignment of the the 2D heteronuclear single quantum coherence (HSQC) NMR spectrum of PDA-CDots in D_2O.