SUPPORTING INFORMATION

Supramolecular-Enhanced Charge Transfer within Entangled Polyamide Chains as Origin of the Universal Blue Fluorescence of Polymer Carbon Dots

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1.- Influence of the reaction time on the formation of CDs1

In the following study **CDs1** are obtained from citric acid and ethylenediamine under microwave irradiation at 140°C, respectively for 1, 2 and 3 minutes. The resulting materials are labeled **CDsA**, **CDsB**, **CDsC**. The characterization of the three samples allowed to investigate the influence of the reaction time on the CDs features, i.e. their size, structure and optical properties. Finally **CDsC** was chosen for the experiments described in the article, renamed **CDs1**.

Synthesis of CDsA,CDsB,CDsC. 2.0 g of citric acid monohydrate (9.5 mmol, 1 eq.) were dissolved in 15 ml of ultrapure water. Upon addition of 0.64 ml of EDA (1 eq.) the solution was heated up to 140°C through microwave irradiation (stirring, open batch), causing the evaporation of the water. The temperature was kept constant for 1 minute, after that the irradiation was stopped and the mixture cooled down. This yields in a yellow, transparent solid product **CDsA**, insoluble in most common organic solvents but highly soluble in water. In the case of **CDsB**, after the first minute of heating, the mixture was redissolved in 10 ml of water and put one additional minute at 140°C under microwave irradiation, for a total of 2 minutes. **CDsC** was prepared as **CDsB**, but one additional step of redissolution and heating at 140°C for 1 minute was effectuated, for a total of 3 minutes. The redissolution step is an important adjustment that allows the reagents to reorganize randomly in the liquid phase before increasing the time of the reaction, that instead takes place in the solid phase. The solid products were diluted with ultrapure water, filtrated on 0.45 µm PTFE membrane and dialyzed against ultrapure water (MWCO = 0.5-1.0 KDa, 3 days, twice a day). The dry products were obtained by freeze-drying.

Atomic force microscopy (AFM)

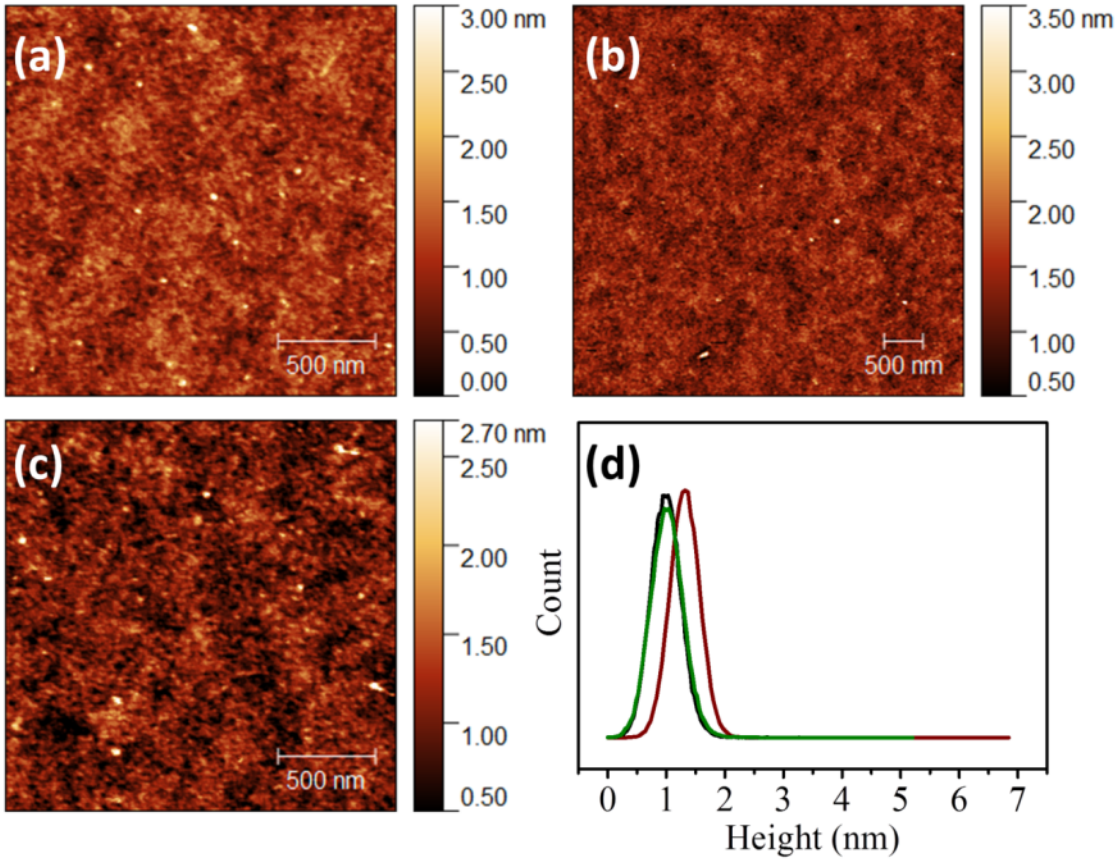

Figure S1. AFM images of **CDs1** samples obtained at different reaction times: **CDsA** (a), **CDsB** (b), **CDsC** (c) and their respective height distribution (d) in green, brown and black.

Dynamic light scattering (DLS)

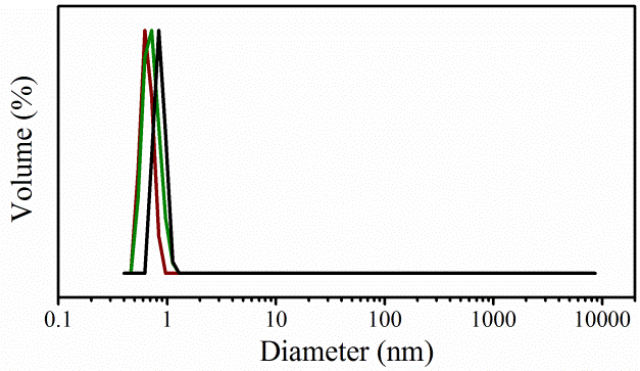

Figure S2. DLS size distribution of **CDs1** samples obtained at different reaction times: **CDsA** (green), **CDsB** (brown) and **CDsC** (black). All the samples show a diameter of about 1 nm.

Diffusion ordered spectroscopy (DOSY)

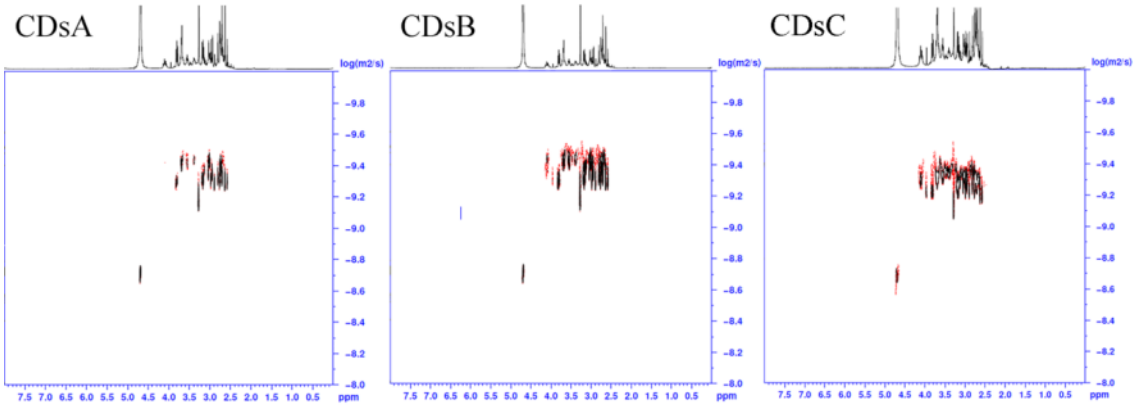

Figure S3. DOSY spectra of **CDs1** samples obtained at different reaction times: **CDsA**, **CDsB**, **CDsC**.

The diffusion coefficients (D) found from the DOSY experiments were related to the hydrodynamic radius (rH) through the Stokes-Einstein equation (Equation 1), assuming the particles spherical.

$$rH = \frac{kT}{6\pi\eta D} \qquad \text{Equation 1.}$$

k = Boltzmann constant = $1.3806*10^{-23}$ $m^2kg\ s^{-2}K^{-1}$
T = temperature (K) = 298K
η = dynamic viscosity. For water at 298 K = $0.89*10^{-3}$ $kg\ m^{-1}s^{-1}$
D = diffusion coefficient (m^2s^{-1})

Table S1. Measured diffusion coefficient (D) and the calculated hydrodynamic radius (rH) and diameter of **CDs1** samples obtained at different reaction times: **CDsA**, **CDsB**, **CDsC**.

	D (m^2/s)	rH (nm)	Diameter (nm)
CDsA	$10^{-9.4}$	0.6	1.2
CDsB	$10^{-9.4}$	0.6	1.2
CDsC	$10^{-9.4}$	0.6	1.2

All the samples show a diameter between 1.2-1.6 nm.

Size exclusion chromatography (SEC/RI)

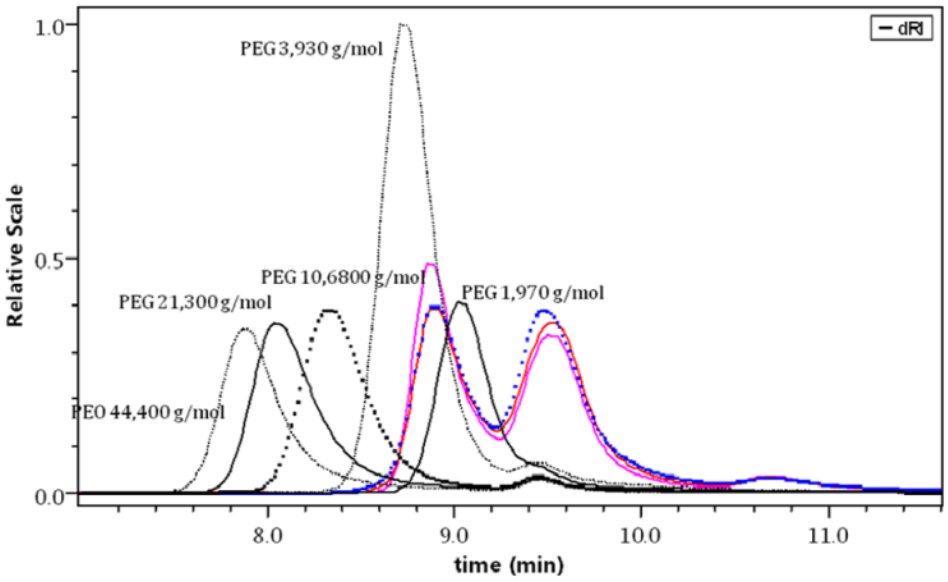

Figure S4. SEC/RI chromatograms of **CDs1** samples obtained at different reaction times: **CDsA** (pink), **CDsB** (red), **CDsC** (blue). The profiles are identical. The first eluition peak at 8.9 min, in the same position for all the samples, appear between the peaks of PEG 3930 g/mol and PEG 1970 g/mol. A second peak of much smaller molecular mass (out of calibration) at 9.6 min could be due to the salt employed in the mobile phase (0.1 M sodium acetate) or to the CDs' counter ions.

Table S2. Average molecular weight in number ($\overline{M_n}$), in weight ($\overline{M_w}$) and polydispersity (Đ) of **CDs1** samples obtained at different reaction times: **CDsA**, **CDsB** and **CDsC**.

	$\overline{M_n}$ (g/mol)	$\overline{M_w}$ (g/mol)	Đ
CDsA	2300	2500	1.07
CDsB	2300	2500	1.08
CDsC	2300	2600	1.09

Absorbance and fluorescence

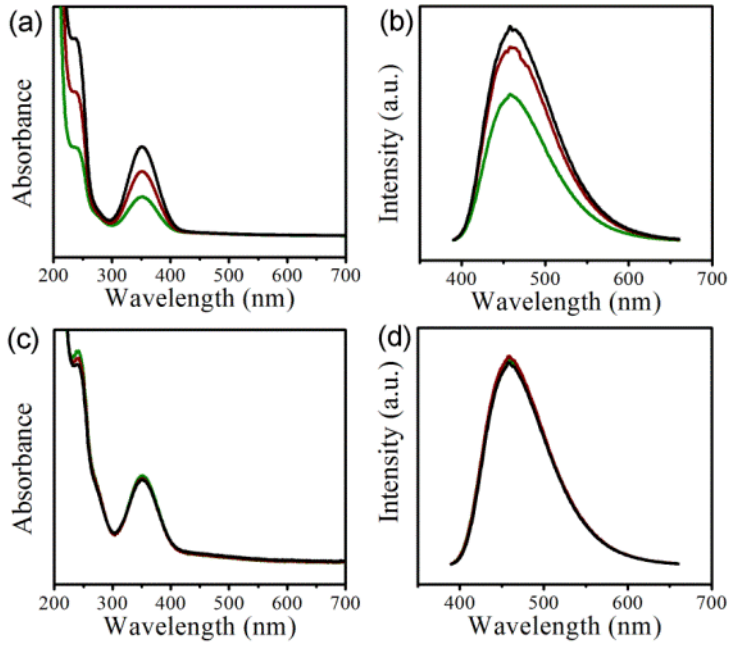

Figure S5. (a) UV/vis and (b) emission spectra of **CDs1** samples obtained at different reaction times: **CDsA** (green), **CDsB** (brown), **CDsC** (black) at the same mass concentration of 0.05 mg/mL. (c) UV/Vis and (d) emission spectra of **CDsA** (green), **CDsB** (brown), **CDsC** (black) at the same optical concentration.

While for solution with the same mass concentration absorption and emission increase from **CDsA** to **CDsC**, when the solution are prepared with the same absorption (optical concentration) the emission intensity is the same for all the samples. This means that increasing the reaction time the same fluorophore is forming in larger amounts, without changing its nature.

Fluorescence decay

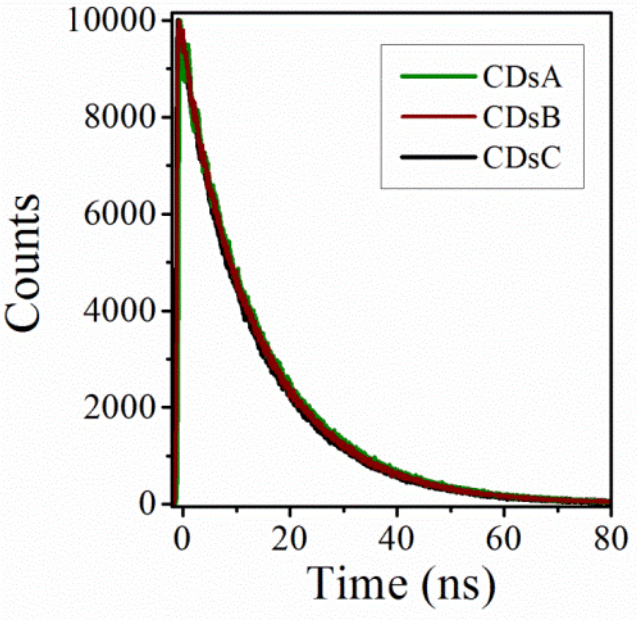

Figure S6. Fluorescence decay of **CDs1** samples obtained at different reaction times: **CDsA** (green), **CDsB** (brown) and **CDsC** (black).

Elemental analysis

Table S3. Elemental Analysis of **CDs1** samples obtained at different reaction times: **CDsA**, **CDsB**, and **CDsC.**

	C (mol%)	H (mol%)	N (mol%)	O (mol%)
CDsA	26,3	47,0	6,9	20,0
CDsB	27,9	45,8	7,2	19,2
CDsC	30,0	44,3	8,0	17,7
$C_8H_{12}N_2O_5$	29,6	44,4	7,4	18,5

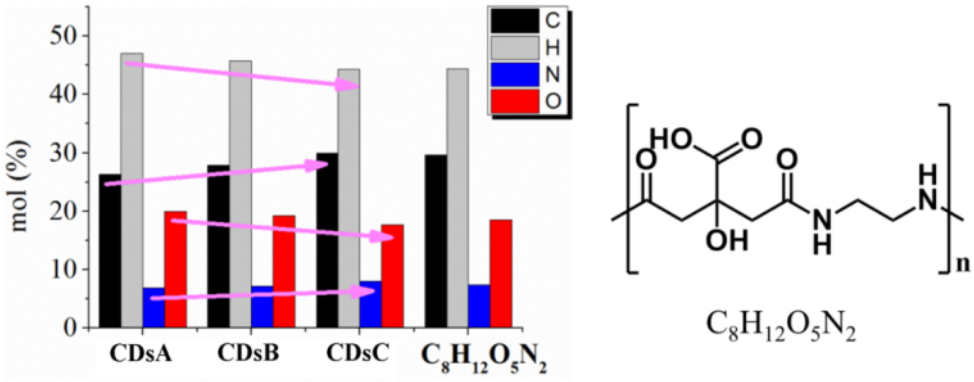

Figure S7. Mole percentages of C, H, N, O of **CDs1** samples obtained at different reaction times, i.e. **CDsA**, **CDsB** and **CDsC**, and the calculated values of the polymeric repetitive unit $C_8H_{12}O_5N_2$. From **CDsA** to **CDsC** it can be observed the relative increase of C and N and decrease of H and O. These changes are due to the loss of water happening during the condensation of the reagents that forms the CDs. In fact the amount of unreacted material (CA and EDA retained on the CDs as counter ions) diminuishes from **CDsA** to **CDsC** forming new particles.

Nuclear Magnetic resonance (NMR)

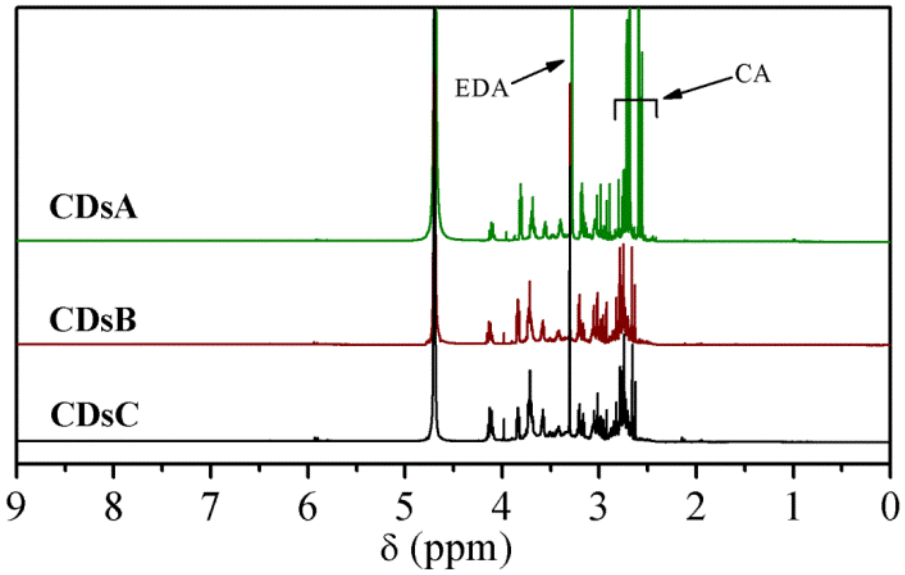

Figure S8. ^{1}H NMR of **CDs1** samples obtained at different reaction times: **CDsA**, **CDsB** and **CDsC**. The nanoparticles have the same profile in the three cases, but the presence of unreacted EDA and CA decreases considerably from **CDsA** to **CDsC**. These reagents could be present in the samples in the form of CDs counter ions, in the way that dialysis cannot remove them completely. Increasing the reaction time, the consumption of the reagent towards the formation of the CDs removes the most part.

Infrared spectroscopy (IR)

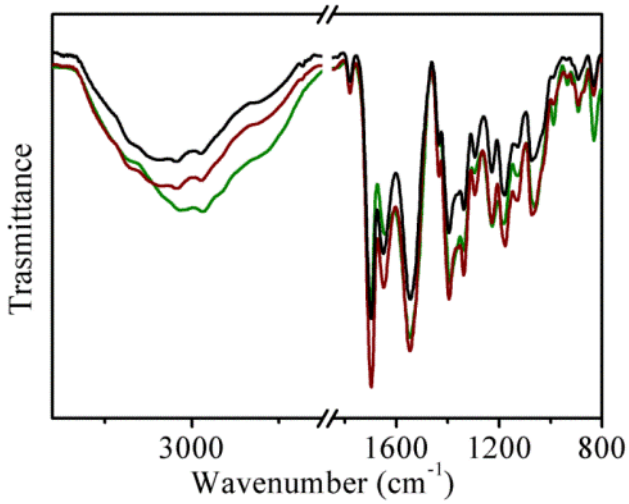

Figure S9. IR spectra of **CDs1** samples obtained at different reaction times: **CDsA** (green), **CDsB** (brown), **CDsC** (black). The profile is the same for all the samples.

X-ray photoelectron spectroscopy (XPS)

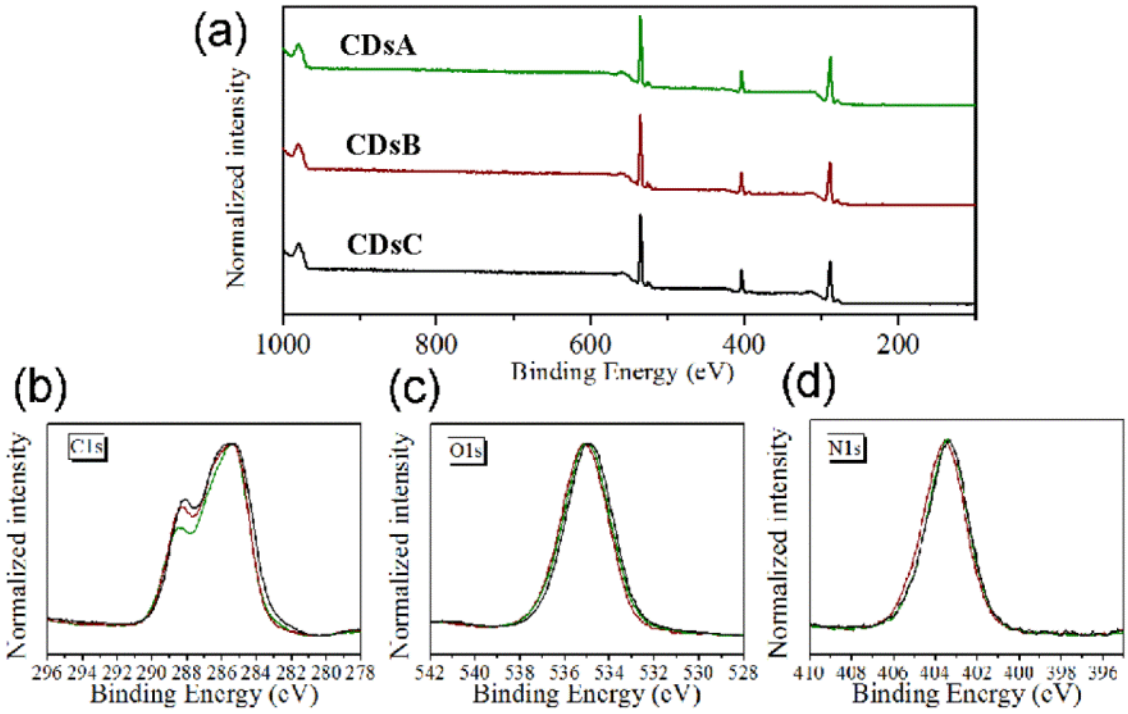

Figure S10. XPS spectra of **CDs1** samples obtained at different reaction times: **CDsA** (green), **CDsB** (brown), **CDsC** (black). The profile is the same for all the samples.

2.- Characterization of CDs1, CDs2 and CDs3

Atomic force microscopy (AFM)

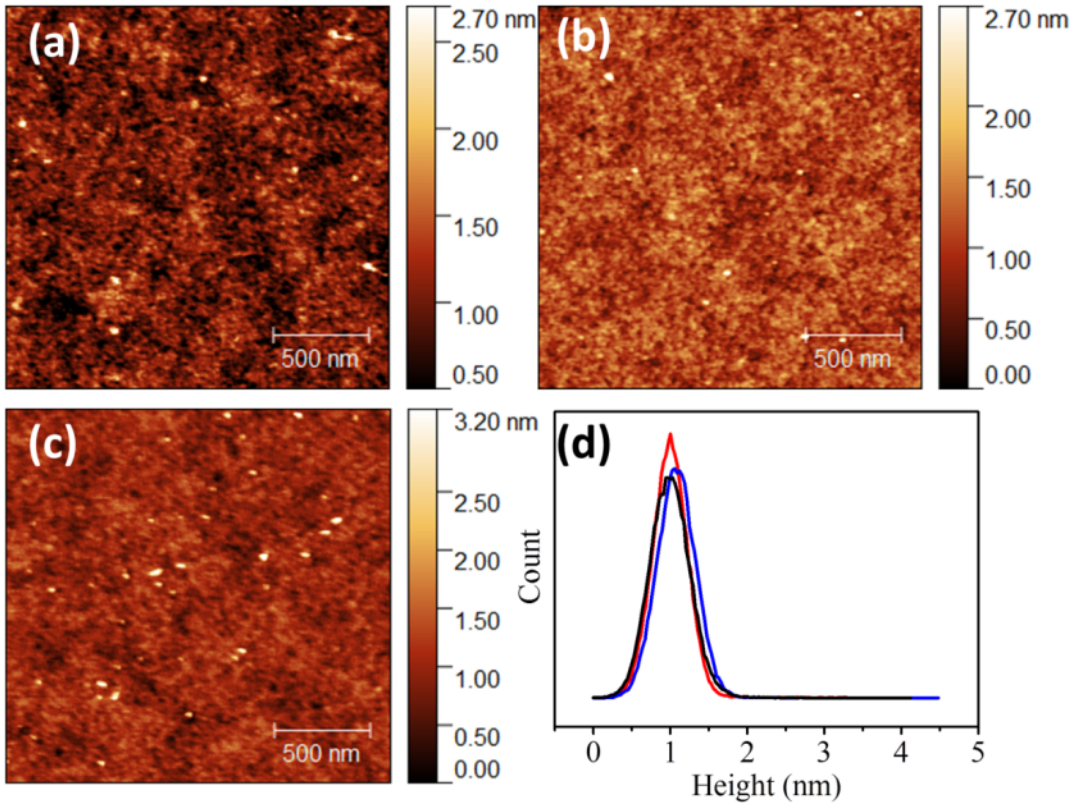

Figure S11. AFM images of **CDs1** (a), **CDs2** (b), **CDs3** (c) and their respective height distribution (d) in black, blue and red, respectively.

Dynamic light scattering (DLS)

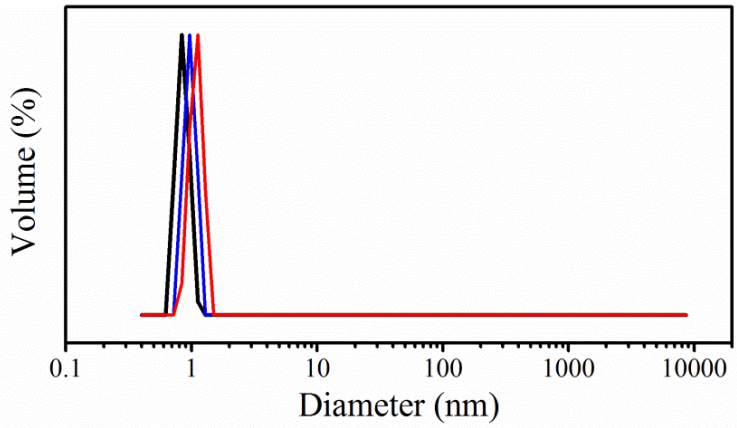

Figure S12. DLS size distribution of **CDs1** (black), **CDs2** (blue), **CDs3** (red). All the samples show a diameter of about 1 nm.

Diffusion ordered spectroscopy (DOSY)

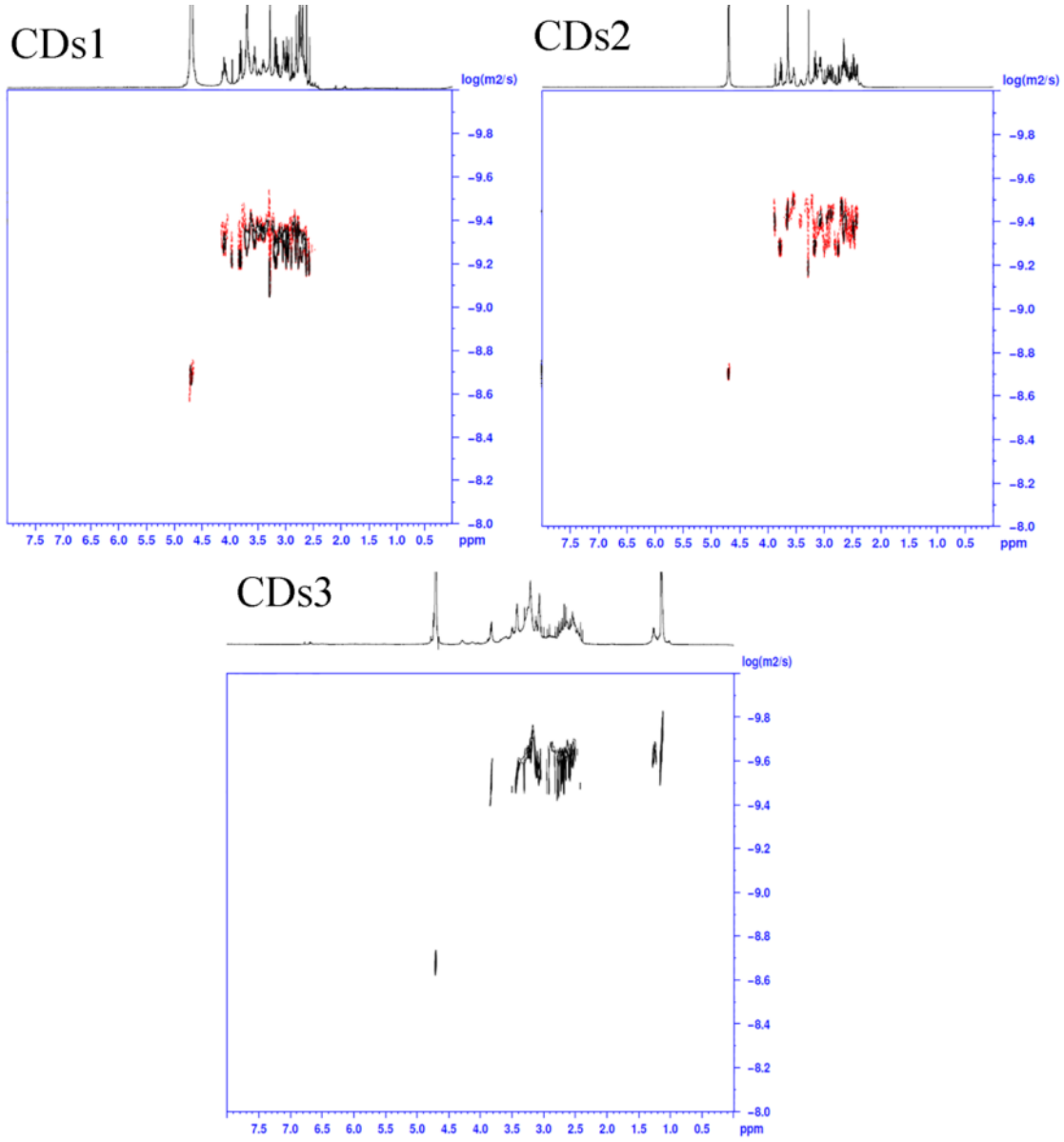

Figure S13. DOSY spectra of **CDs1**, **CDs2**, and **CDs3**.

Table S4. Measured diffusion coefficient (D), calculated hydrodynamic radius (rH) and diameter of **CDs1**, **CDs2**, and **CDs3**. All samples show a diameter between 1.2-1.6 nm.

	D (m^2/s)	rH (nm)	Diameter (nm)
CDs1	$10^{-9.4}$	0.6	1.2
CDs2	$10^{-9.4}$	0.6	1.2
CDs3	$10^{-9.5}$	0.8	1.6

Fluorescence decay

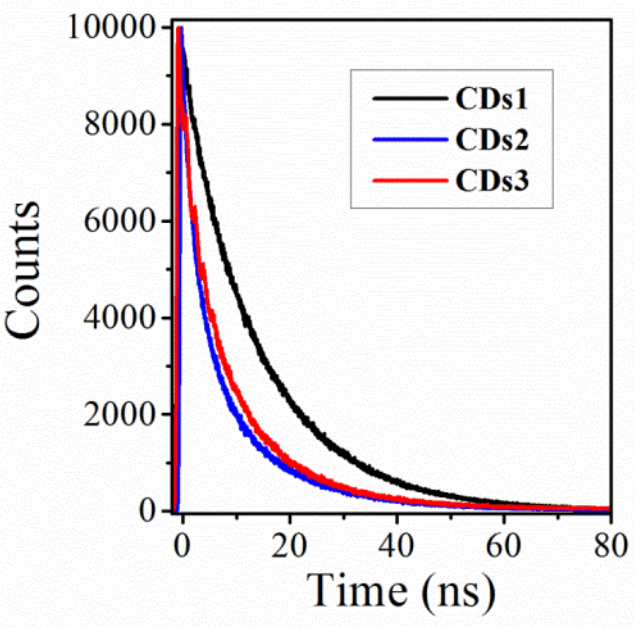

Figure S14. Fluorescence decay of **CDs1** (black), **CDs2** (blue) and **CDs3** (red).

Excitation dependance and quantum yield

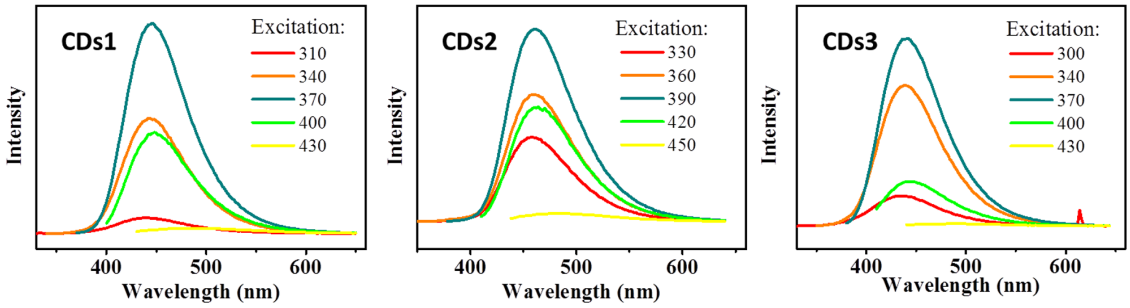

Figure S15. Emission spectra of **CDs1** (left), **CDs2** (center), **CDs3** (right) at various excitation wavelengths.

The quantum yield measurements were performed with quinine sulphate in 0.10 M H_2SO_4 (literature quantum yield 0.54 at 350 nm) as the standard. The quantum yields were calculated from Equation 2, where Φ is the quantum yield, *Grad* is the slope from the plot of integrated intensity vs absorbance and η the refractive index of the solvent. The indices *x* and *st* denote the sample and the standard, respectively.

$$\Phi_x = \Phi_{st}\left(\frac{Grad_x}{Grad_{st}}\right)\left(\frac{\eta_x^2}{\eta_{st}^2}\right) \quad \text{Equation 2.}$$

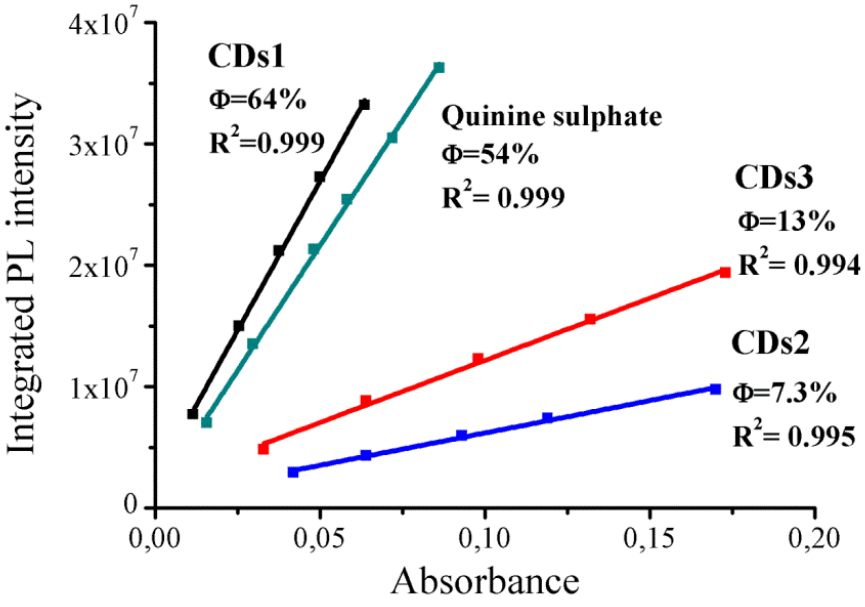

Figure S16. Different concentrations of **CDs1** (black), **CDs2** (blue), **CDs3** (red) and quinine sulfate (cyan), plotted by integrated PL intensity vs. absorbance and fitted for calculating the quantum yield, expressed in %.

pH dependance of the fluorescence emission

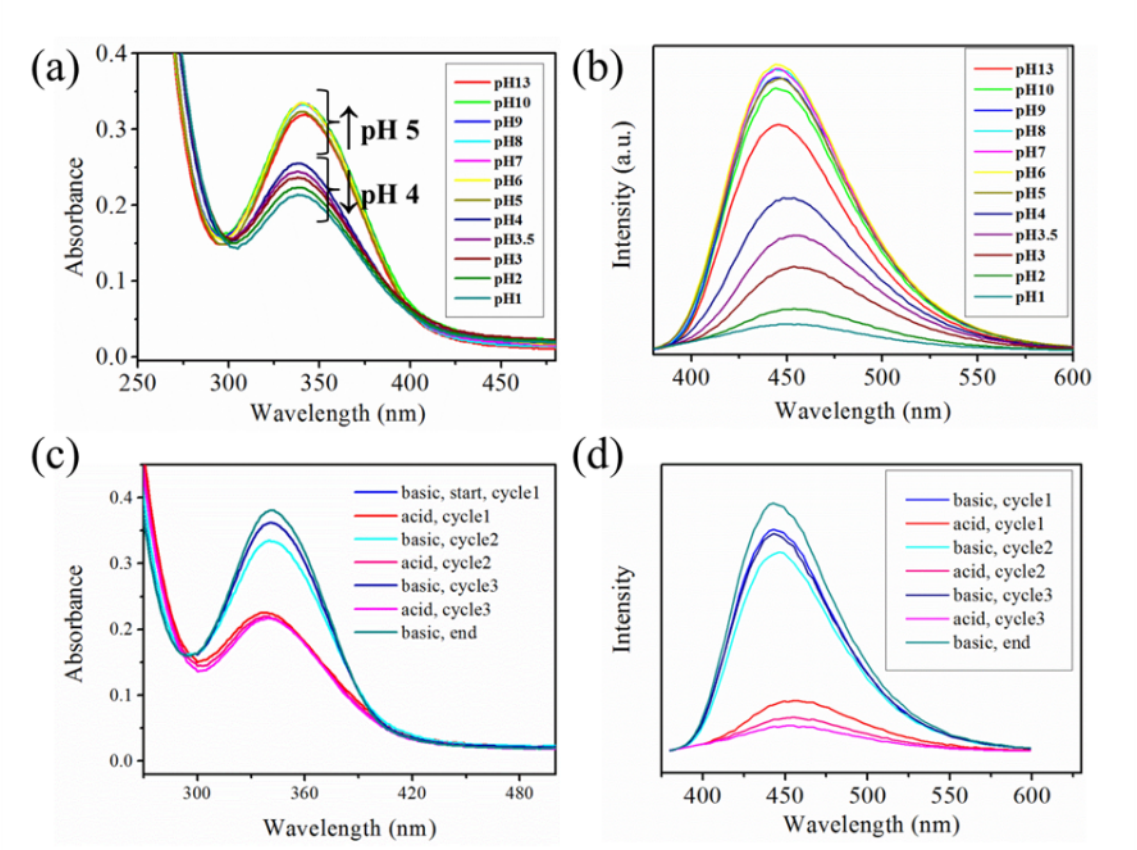

Figure S17. (a) UV/Vis and (b) fluorescence emission of a 0.5 mg/mL solution of **CDs1** at various pH. (c) UV/Vis and (d) fluorescence emission of a 0.5 mg/mL solution of **CDs1** changes during base (pH>12)/acid (pH<2) cycles.

Elemental analysis

Table S5: Elemental analysis of **CDs1**, **CDs2** and **CDs3** and the calculated percentage for the repetitive unit of the corresponding polymeric condensation products.

	C (mol%)	H (mol%)	N (mol%)	O (mol%)
CDs1	30,0	44,3	8,0	17,7
CDs3	26,5	48,0	7,0	18,5
$C_8H_{12}N_2O_5$	29,6	44,4	7,4	18,5
CDs2	30,8	45,4	8.4	15.4
$C_8H_{12}N_2O_4$	30,8	46,2	7.7	15.4

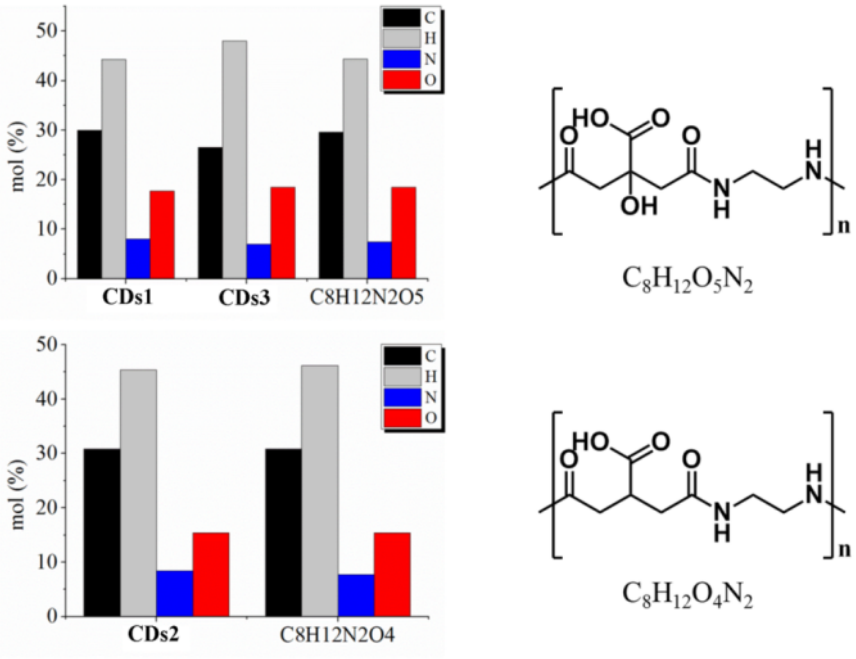

Figure S18. Mole percentages of C,H,N,O of **CDs1**, **CDs2** and **CDs3**, and the calculated percentages for the repetitive unit of the corresponding polymeric condensation product.

X-ray photoelectron spectroscopy (XPS)

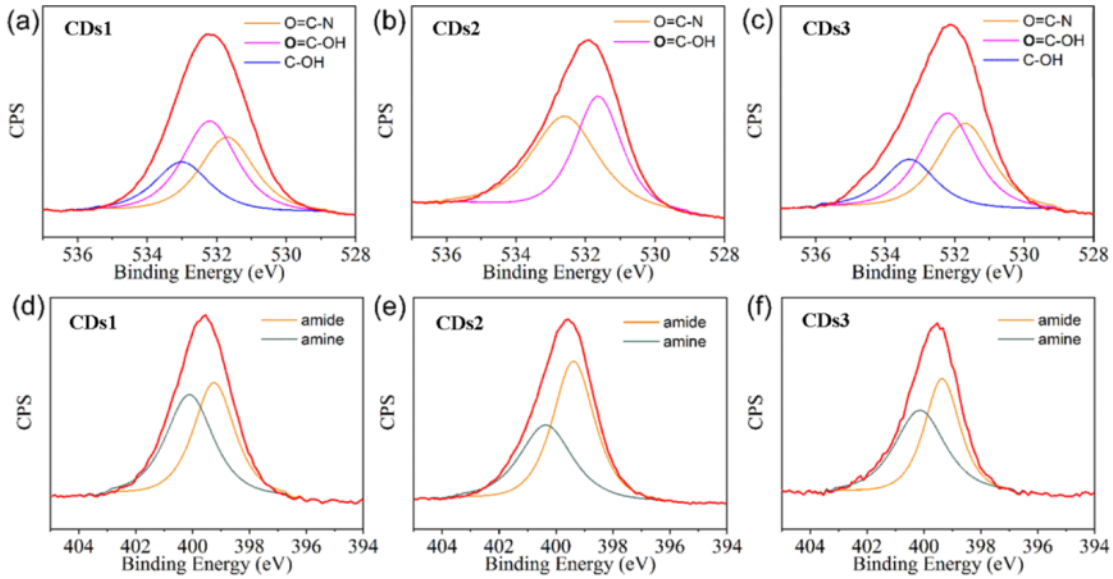

Figure S19. XPS O1*s* spectra of (a) **CDs1**, (b) **CDs2**, (c) **CDs3**. The peak was deconvoluted into three components: amide (orange), carboxylic acid (magenta), alcohol (blue), absent for **CDs2**. XPS N1*s* spectra of (d) **CDs1**, (e) **CDs2**, (f) **CDs3**. The peak was deconvoluted into two components: amide (orange) and amine (green).

Fitting was performed using GL(70) profiles (70% Gaussian and 30% Lorentzian) after substraction of a Shirley background. Full-width-half-maximum (FWHM) of contributions was constrained to a maximum of 2 eV.

Meaningful fittings rely on pre-existing structural information obtained from NMR studies: Absence of C=C; presence of amines and amides.

C1s results (see main manuscript): satisfying deconvolution for all CDs is obtained with 5 components. Control fits using a sixth component corresponding to a C=C contribution, do not lead to further improvements, thus validating the absence of C=C and the developed structural model.

N1s results: satifsying deconvolution for all CDs is obtained with 2 contributions belonging to amines and amides, thus validating the developed structural model.

Nuclear magnetic resonance (NMR)

CDs1

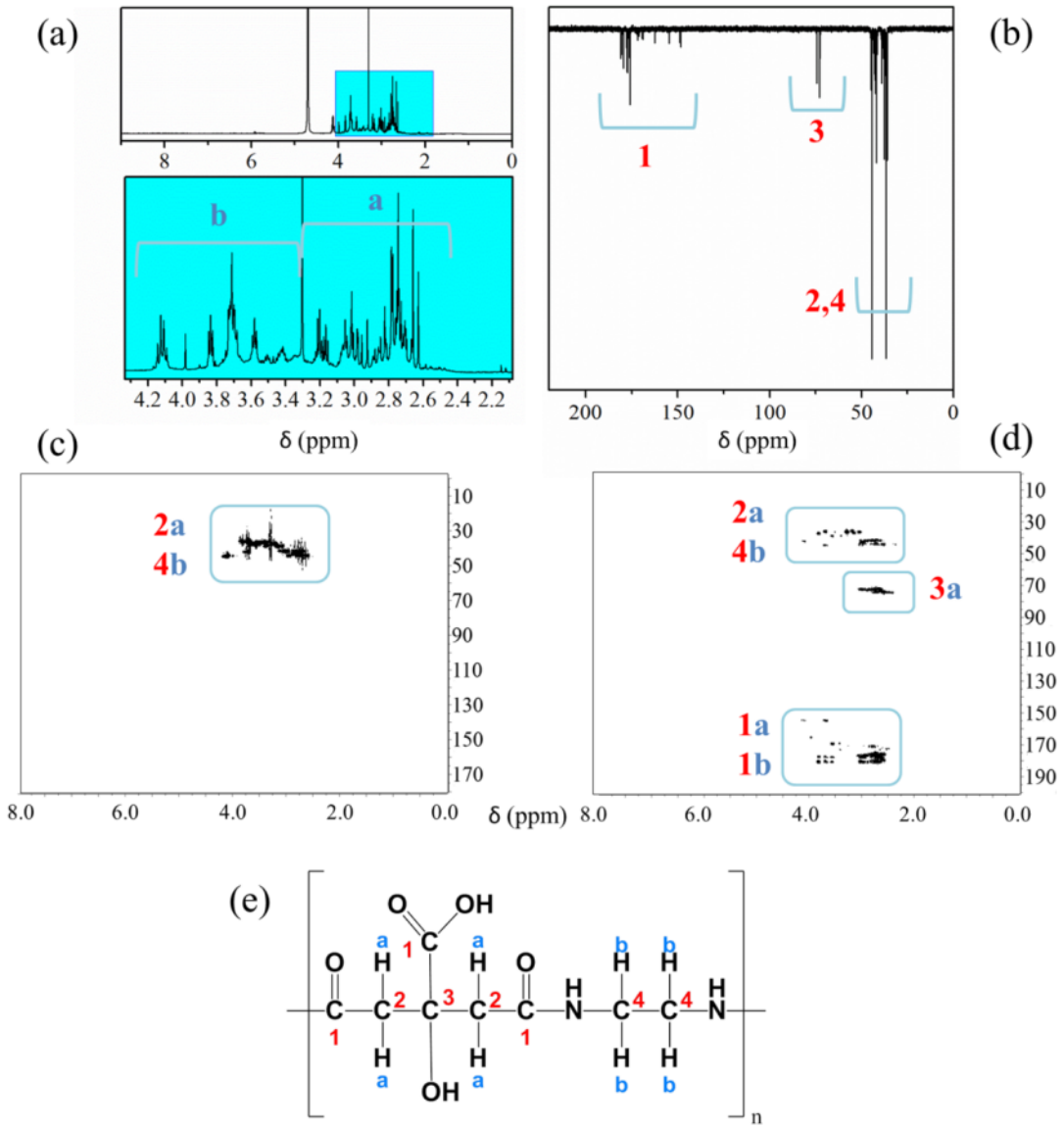

Figure S20. (a) ^{1}H NMR. (b) APT ^{13}C NMR, (c) ^{1}H-^{13}C HSQC and (d) ^{1}H-^{13}C HMBC spectra of **CDs1**. (e) one of the possible chain isomers of the **CDs1** repetitive unit, with C and H assignation. ^{1}H NMR. Hb: 4.2-3.4 ppm (m), EDA 3.3 ppm (s), Ha: 3.2-2.5 ppm (s or d). APT ^{13}C NMR shows in-phase signals, belonging to secondary or quaternary carbons. C1: 182-148 ppm, C2 and C4: 46-35 ppm, C3: 75-71 ppm. ^{1}H-^{13}C HSQC shows the ^{1}J coupling of Ha and Hb with C2 and C4 respectively. ^{1}H-^{13}C HMBC shows the ^{2}J of Ha with C3, the ^{2}J and ^{3}J coupling of Ha with C1 and C2, the ^{3}J coupling of Hb with C1 and C4.

CDs2

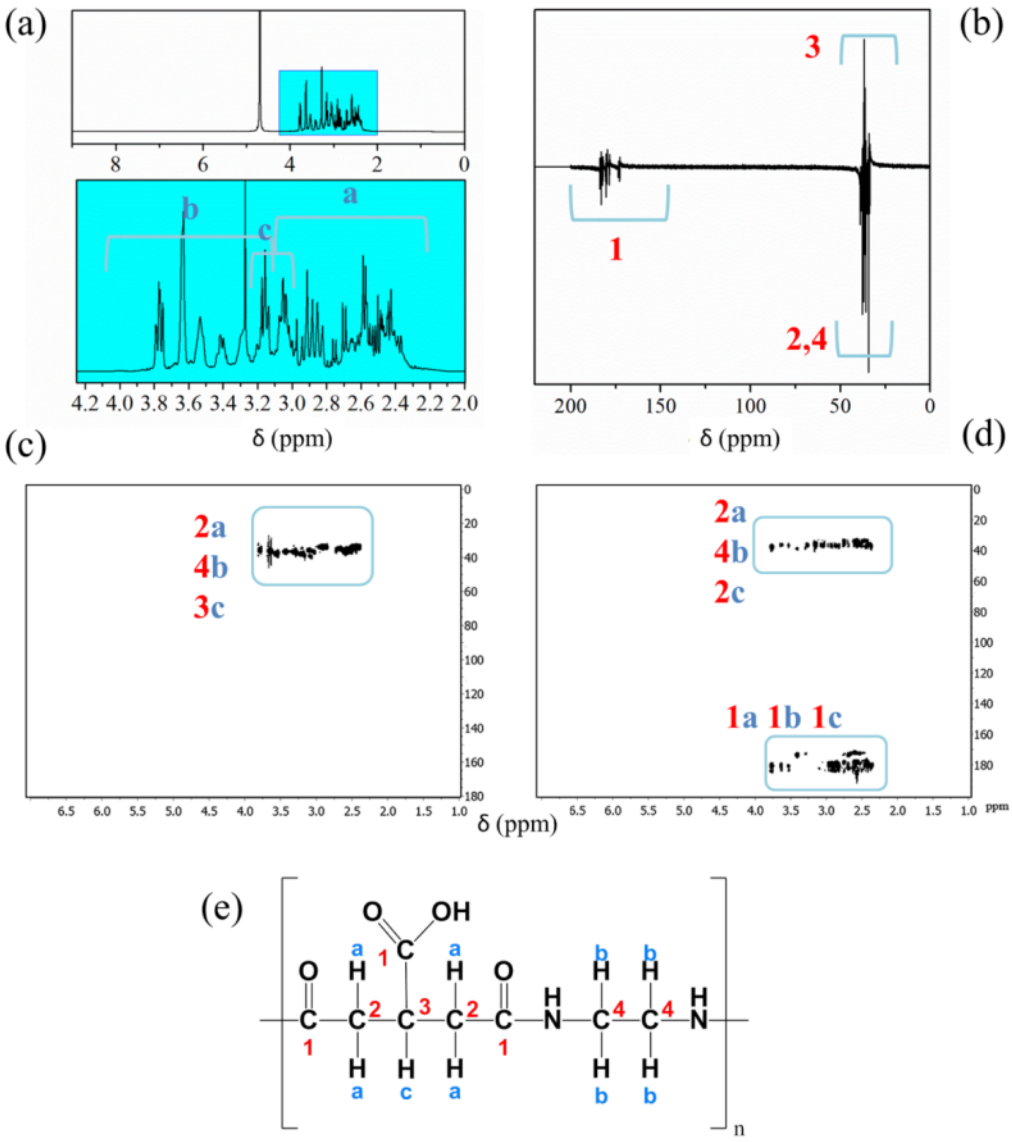

Figure S21. (a) ^{1}H NMR. (b) APT ^{13}C NMR, (c) ^{1}H-^{13}C HSQC and (d) ^{1}H-^{13}C HMBC spectra of **CDs2**. (e) one of the possible chain isomers of the **CDs2** repetitive unit, with C and H assignation. ^{1}H NMR. Hb: 3.8-3.3 ppm (t), EDA 3.25 ppm (s), Hc: 3.2-3.0 ppm (m), Ha: 3.2-2.3 ppm (s or d). APT ^{13}C NMR shows in-phase signals, belonging to secondary or quaternary carbons. APT also shows an antiphased signal, assigned to C3, at about 36 ppm. C1: 184-171 ppm, C2 and C4: 40-32 ppm, C3: 38-34 ppm. ^{1}H-^{13}C HSQC shows the ^{1}J coupling of Ha, Hb and Hc with C2, C4 and C3 respectively. ^{1}H-^{13}C HMBC shows the ^{2}J of Ha with C3, the ^{2}J coupling of Hc with C1 and C2, the ^{2}J and ^{3}J coupling of Ha with C1 and C2, the ^{3}J coupling of Hc with C1 and the ^{3}J coupling of Hb with C1 and C4.

CDs3

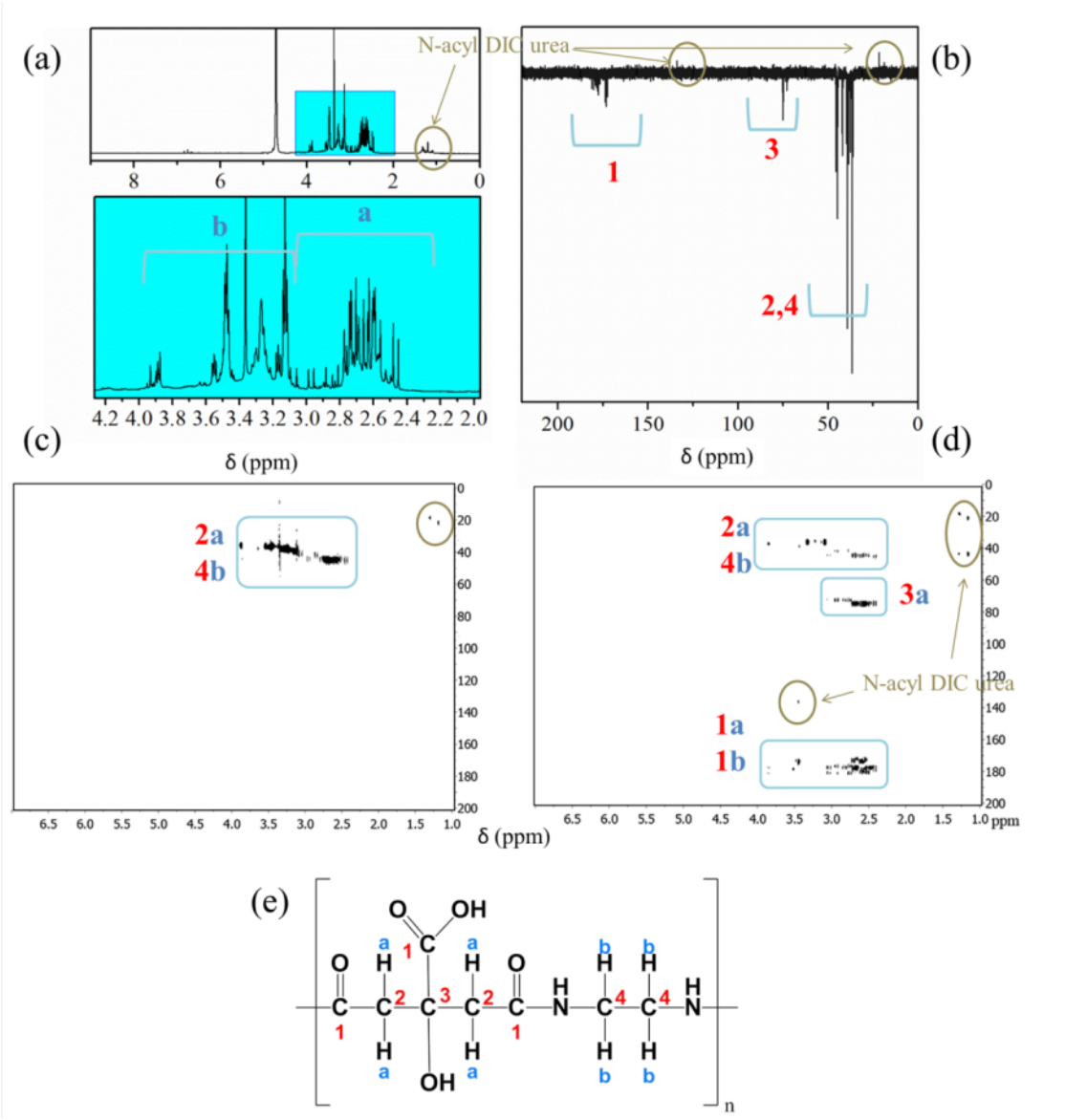

Figure S22. (a) ^{1}H NMR. (b) APT ^{13}C NMR, (c) ^{1}H-^{13}C HSQC and (d) ^{1}H-^{13}C HMBC spectra of **CDs3**. (e) one of the possible chain isomers of the **CDs3** repetitive unit, with C and H assignation. ^{1}H NMR. Hb: 4.0-3.2 ppm (m), EDA 3.35 ppm (s), Ha: 3.2-2.4 ppm (s or d). APT ^{13}C NMR shows in-phase signals, belonging to secondary or quaternary carbons. C1: 182-171 ppm, C2 and C4: 47-35 ppm, C3: 76-71 ppm. ^{1}H-^{13}C HSQC shows the ^{1}J coupling of Ha and Hb with C2 and C4 respectively. ^{1}H-^{13}C HMBC shows the ^{2}J of Ha with C3, the ^{2}J and ^{3}J coupling of Ha with C1 and C2, the ^{3}J coupling of Hb with C1 and C4. N-acyl DIC urea side-product has formed in little amount during the reaction, incorporated into the CDs5 structure (1H NMR: 1.20, 1.32, 6.72 ppm, in APT: 137, 21

ppm). Some of the proton signals of **CDs3** are right-shifted with respect to **CDs1**, probably because of the different charged form due to the final addition of NaOH.

3.- Quantum chemical calculations

Geometry optimizations in the ground state were carried out within density functional theory (DFT)[1,2] using the ωB97XD functional[3] combined with the 6-31G(d) basis set.[4] Besides, time-dependent density functional theory (TDDFT)[5] has been used to compute the vertical absorption energy as well as to optimize the first excited electronic state, using the B3LYP functional[6,7,8] and the 6-31G(d) basis set. All the calculations were performed with the Gaussian 09 suite of programs.[9]

Cartesian coordinates:

Dimer one chain:

C	5.968405	0.322405	-0.827510
N	6.843575	1.473131	-0.864602
C	4.481529	0.711942	-0.785889
N	3.618649	-0.421448	-0.535721
C	3.502202	-0.932500	0.717350
O	4.085460	-0.464568	1.686040
C	2.587093	-2.146359	0.868575
C	1.463278	-2.274275	-0.165167
C	0.611373	-0.992307	-0.155927
O	0.308054	-0.531419	-1.342719
O	2.039487	-2.514505	-1.419500
C	0.503333	-3.435409	0.222520
C	-0.624499	-3.527213	-0.798361
O	-0.355143	-3.497677	-2.003011
N	-1.902274	-3.576892	-0.377255
C	-2.445680	-3.728856	0.958912
C	-2.660111	-2.435780	1.745846
N	-3.548963	-1.445260	1.156347
C	-4.192726	-1.461653	-0.035019
C	-4.724915	-0.103447	-0.504117
C	-4.067970	1.151603	0.099541
C	-2.535585	0.999144	0.001112
O	-1.984534	0.859926	-1.084223
O	0.210830	-0.514135	0.901208
O	-4.352269	-2.447546	-0.746840
C	-4.485088	2.398643	-0.705574
C	-3.894464	3.670186	-0.110471

O	-3.693879	3.778728	1.099355
O	-4.493941	1.238300	1.433113
O	-1.917736	1.011318	1.157084
N	-3.626343	4.660027	-0.988441
H	6.976903	1.945205	-1.748607
C	7.238183	2.228116	0.214208
H	6.196420	-0.279248	0.055169
H	6.169884	-0.303259	-1.703557
H	4.330943	1.444974	0.012194
H	4.180681	1.177504	-1.729487
H	3.210129	-0.942948	-1.303974
H	3.202529	-3.050844	0.805769
H	2.172331	-2.087594	1.876237
H	-0.422810	0.138570	-1.265827
H	1.086398	-4.361592	0.185770
H	0.146015	-3.287137	1.243163
H	1.304619	-2.812823	-2.001647
H	-2.602582	-3.466693	-1.103603
H	-3.392970	-4.259235	0.852366
H	-1.785108	-4.365032	1.556405
H	-3.049045	-2.718630	2.732195
H	-1.691471	-1.944230	1.904468
H	-3.621888	-0.578727	1.680793
H	-4.602055	-0.109591	-1.589213
H	-5.797134	-0.049360	-0.287063
H	-4.190615	2.274925	-1.751887
H	-5.577756	2.475727	-0.662241
H	-0.994608	0.652272	1.044148
H	-4.174143	2.104142	1.760444
C	-3.084831	5.943652	-0.586867
H	-3.773208	4.484883	-1.970248
H	-3.740044	6.757249	-0.912188
H	-3.016839	5.948341	0.501084
H	-2.086010	6.093689	-1.008277
O	7.787514	3.304939	0.051335
C	7.006373	1.625910	1.586955
H	7.673767	0.768470	1.733434
H	7.246475	2.386876	2.329751
H	5.982535	1.267509	1.736686

Dimer two chains intramolecular HB:

C	1.197417	-4.909136	-1.081842
N	2.551711	-4.643312	-0.637664
C	0.200434	-4.773460	0.074708
N	-1.170801	-4.826780	-0.369314
C	-2.149499	-5.309533	0.447848

O	-1.920451	-5.882510	1.500279
C	-3.583896	-5.094916	-0.036637
C	-3.839536	-3.776091	-0.777942
C	-3.394211	-2.588387	0.095103
O	-2.523201	-1.776850	-0.466624
O	-3.151829	-3.817861	-1.998447
C	-5.359030	-3.570517	-1.016268
C	-5.597585	-2.243859	-1.727355
O	-4.825578	-1.884521	-2.626040
N	-6.631264	-1.467559	-1.365290
C	-7.619450	-1.628063	-0.314935
C	-7.193058	-1.133842	1.072134
N	-6.658316	0.218023	1.142151
C	-6.623632	1.169386	0.181527
C	-5.678093	2.341847	0.434030
C	-4.599398	2.224456	1.527618
C	-3.832486	0.895365	1.365845
O	-3.129268	0.660889	0.387296
O	-3.880977	-2.395374	1.201684
O	-7.250784	1.129007	-0.874052
C	-3.628410	3.409348	1.375135
C	-2.504836	3.340511	2.395090
O	-2.658804	2.729957	3.460582
O	-5.250677	2.255596	2.769619
O	-4.031762	0.033569	2.336204
N	-1.377393	3.988099	2.073675
H	2.872568	-3.675248	-0.690987
C	3.350271	-5.491171	0.060428
H	1.121665	-5.903973	-1.531260
H	0.971766	-4.186976	-1.875330
H	0.341205	-5.573755	0.804949
H	0.394351	-3.831039	0.605466
H	-1.459421	-4.321027	-1.201220
H	-3.857635	-5.910373	-0.715462
H	-4.214742	-5.159650	0.851453
H	-2.564774	-0.901883	0.009727
H	-5.703020	-4.381329	-1.667893
H	-5.890809	-3.638772	-0.065906
H	-3.495321	-3.054925	-2.516943
H	-6.661353	-0.558327	-1.817319
H	-8.506114	-1.086257	-0.644370
H	-7.898085	-2.681803	-0.217933
H	-8.065213	-1.225750	1.732110
H	-6.411173	-1.795660	1.464729
H	-6.211248	0.456830	2.020814
H	-5.203486	2.530472	-0.532181
H	-6.281030	3.223685	0.674898

H	-3.230695	3.488644	0.360814
H	-4.207248	4.321084	1.563940
H	-3.737139	-0.867719	2.048195
H	-4.525072	2.296240	3.427664
C	-0.260485	4.068942	2.995101
H	-1.300645	4.427270	1.161038
H	0.442584	4.806716	2.611002
H	-0.614045	4.363581	3.986643
H	0.248904	3.103728	3.083927
O	4.360843	-5.083417	0.633337
C	2.970091	-6.956627	0.084263
H	2.902743	-7.359685	-0.931646
H	3.738715	-7.496036	0.637213
H	2.003312	-7.115953	0.572259
C	6.443244	-2.321253	0.587371
N	7.885197	-2.429165	0.633813
C	5.793982	-2.413948	1.976820
N	4.348290	-2.447835	1.866010
C	3.660939	-1.316565	1.598636
O	4.146338	-0.191870	1.665535
C	2.212590	-1.494868	1.146701
C	2.137640	-0.985967	-0.297984
C	2.435833	0.522100	-0.275536
O	3.300452	0.943924	-1.160138
O	3.078603	-1.730553	-1.024838
C	0.714789	-1.109666	-0.920710
C	0.764092	-0.699372	-2.387505
O	1.578969	-1.236360	-3.142920
N	-0.033185	0.293044	-2.850611
C	-1.237553	0.864789	-2.250416
C	-0.979057	1.982674	-1.248481
N	-0.246930	3.088375	-1.834489
C	-0.519258	4.378032	-1.498879
C	0.505539	5.399874	-1.972282
C	1.609942	5.649916	-0.915760
C	2.175085	4.268934	-0.543614
O	2.868338	3.634377	-1.339045
O	1.767380	1.250315	0.452114
O	-1.507225	4.702630	-0.848928
C	2.737067	6.504503	-1.527324
C	3.849129	6.735996	-0.512561
O	3.613976	6.768761	0.695723
O	1.012372	6.286315	0.170365
O	1.774894	3.827760	0.613465
N	5.085554	6.914971	-1.022356
H	8.413616	-1.619759	0.929946
C	8.624964	-3.582532	0.615545

H	6.034629	-3.114422	-0.043171
H	6.166550	-1.368806	0.125865
H	6.119573	-3.328543	2.480510
H	6.081269	-1.558296	2.592458
H	3.989745	-3.338814	1.534656
H	1.893924	-2.539303	1.184221
H	1.562063	-0.897684	1.789104
H	3.298170	1.937573	-1.157815
H	0.402519	-2.156479	-0.882315
H	0.004854	-0.528470	-0.332298
H	2.872928	-1.613155	-1.977466
H	0.104979	0.448006	-3.841030
H	-1.835167	1.257800	-3.076633
H	-1.833847	0.079930	-1.783332
H	-1.941683	2.361675	-0.912584
H	-0.447156	1.614233	-0.364643
H	0.655262	2.880667	-2.242179
H	0.969412	5.076832	-2.909337
H	-0.012993	6.347693	-2.130561
H	3.125968	6.027999	-2.431565
H	2.310189	7.475777	-1.802807
H	1.944147	2.841408	0.667642
H	1.751393	6.532616	0.761268
C	6.251572	7.149647	-0.192857
H	5.215651	6.807679	-2.016152
H	6.780110	8.049066	-0.521753
H	5.906858	7.286864	0.832133
H	6.934833	6.295176	-0.227344
O	9.823126	-3.564012	0.848857
C	7.890840	-4.857633	0.241365
H	6.999614	-5.035881	0.850998
H	7.560873	-4.812542	-0.802778
H	8.588331	-5.687617	0.356610

Dimer two chains intermolecular HB:

C	5.396229	4.102622	-1.964853
N	5.809927	3.056787	-1.050008
C	5.076049	2.750012	0.041086
O	4.078424	3.393216	0.365684
C	5.519250	1.513949	0.809887
C	4.813422	0.275172	0.208195
C	4.996416	-0.966079	1.112389
C	4.128345	-2.112367	0.594553
O	4.248859	-2.512703	-0.560019
O	3.453219	0.559338	0.026400
C	5.437097	-0.024561	-1.160913

O	4.538310	-0.073100	-2.152956
O	6.624932	-0.157093	-1.332120
N	3.257446	-2.636334	1.487383
C	2.185715	-3.581344	1.178133
C	2.509115	-4.745135	0.220089
N	1.978732	-4.505131	-1.111169
C	0.638119	-4.512658	-1.317469
C	0.136682	-3.826582	-2.579513
C	0.255429	-2.304556	-2.403271
C	1.733825	-1.901205	-2.495476
O	2.530219	-2.376769	-3.273310
O	-0.146456	-4.985009	-0.492767
C	-0.493771	-1.526974	-3.516467
C	-0.071773	-0.059304	-3.491723
N	-0.715739	0.711964	-2.578084
C	-0.190119	2.000525	-2.181000
C	0.477264	1.881105	-0.804029
N	1.139187	3.094728	-0.341729
C	0.463966	4.235417	-0.062220
C	1.317816	5.426703	0.318725
O	-0.256726	-1.979091	-1.120481
O	1.992714	-0.951672	-1.615256
O	0.854498	0.342119	-4.185617
O	-0.766226	4.306836	-0.090288
O	-2.603023	1.746683	-0.031841
C	-3.806898	1.752753	0.159508
O	-4.374949	1.513218	1.323397
C	-4.754534	2.048196	-0.993543
C	-4.648209	3.546391	-1.405184
N	-3.448317	4.134704	-1.381322
C	-3.292796	5.529885	-1.748881
C	-4.333797	1.153481	-2.192345
C	-4.130572	-0.281946	-1.725366
O	-3.028250	-0.830247	-1.800378
N	-5.192106	-0.882393	-1.154049
C	-4.995780	-2.075540	-0.330836
C	-4.714020	-3.340161	-1.145924
C	-4.200617	-4.488494	-0.266578
N	-2.922205	-4.185144	0.350564
C	-2.841940	-3.665299	1.596980
O	-3.815743	-3.469296	2.318038
C	-1.437004	-3.262160	2.016784
C	-1.340254	-1.719837	2.113542
O	-1.930513	-1.083344	1.004383
C	0.145995	-1.373543	2.255208
O	0.813193	-1.702916	3.213482
O	0.641619	-0.679757	1.226597

C	-2.054113	-1.189136	3.372765
C	-1.820963	0.279424	3.707436
O	-1.723389	0.668887	4.862931
N	-1.774018	1.145607	2.645979
C	-1.456071	2.554409	2.809989
C	-0.093966	2.839376	3.454971
N	0.999461	2.167767	2.775642
C	1.843656	1.264868	3.289870
O	2.687379	0.701310	2.558510
C	1.760764	0.923011	4.753756
O	-5.692072	4.091567	-1.756154
H	2.580236	-4.013176	-1.760645
H	3.581850	-4.918247	0.140488
H	2.036803	-5.651155	0.604422
H	1.347218	-3.034332	0.738020
H	1.851152	-3.973873	2.140329
H	3.134137	-2.146392	2.364311
H	4.730424	-0.682500	2.134470
H	6.043712	-1.283695	1.094207
H	4.958151	-0.445775	-2.945870
H	5.185226	1.633046	1.843431
H	6.603441	1.372570	0.792713
H	3.110362	0.852563	0.899758
H	6.581220	2.456221	-1.302621
H	6.203389	4.293442	-2.673590
H	4.494642	3.812277	-2.515618
H	5.183148	5.017908	-1.407772
H	0.705567	-4.124412	-3.464314
H	-0.912344	-4.100628	-2.711970
H	-2.059573	-4.390166	-0.149979
H	-4.910297	-4.706119	0.536924
H	-4.085004	-5.393750	-0.870663
H	-0.706437	-3.637808	1.294928
H	-1.206992	-3.697250	2.992430
H	1.569711	-0.451655	1.446083
H	-1.662350	-1.488825	0.156668
H	-3.124350	-1.380113	3.241685
H	-1.724916	-1.752856	4.245945
H	-1.678531	0.747023	1.712766
H	-1.503131	3.005777	1.814989
H	-2.216430	3.031754	3.437606
H	0.075554	3.922309	3.433757
H	-0.117322	2.518814	4.494767
H	1.139952	2.385345	1.790667
H	1.966577	1.804498	5.369803
H	0.767108	0.547009	5.015910
H	2.499769	0.150757	4.961381

H	-5.622048	-3.662042	-1.670703
H	-3.957598	-3.108972	-1.901741
H	-5.891520	-2.205701	0.281339
H	-4.163234	-1.877639	0.347861
H	-5.998648	-0.294502	-0.978143
H	0.280176	-1.260223	-0.748257
H	2.921867	-0.646095	-1.683447
H	-0.212118	-1.932413	-4.491014
H	-1.564655	-1.653188	-3.341147
H	-3.397393	1.496773	-2.634172
H	-5.129204	1.228348	-2.940008
O	-6.084766	1.808019	-0.648496
H	-3.648289	1.310715	1.956111
H	-1.484819	0.292283	-2.057439
H	0.539960	2.300436	-2.935474
H	-0.990919	2.742306	-2.151120
H	-0.278969	1.577785	-0.075452
H	1.239779	1.104248	-0.852485
H	2.156521	3.122899	-0.340564
H	2.378972	5.181484	0.405061
H	1.184113	6.206896	-0.437068
H	0.953215	5.830387	1.267495
H	-2.646796	3.663491	-0.969771
H	-2.316521	5.855939	-1.390041
H	-3.351908	5.658515	-2.834370
H	-4.079999	6.132456	-1.287657
H	-6.565996	2.575280	-1.023207

Octamer:

C	-2.468978	2.945278	-2.989126
N	-3.103272	1.630085	-2.933293
C	-3.323100	0.928556	-1.803088
C	-3.679410	-0.531388	-1.975255
C	-3.168809	-1.350336	-0.773112
C	-1.682082	-1.039714	-0.503371
O	-0.831507	-1.200237	-1.370015
O	-3.216874	1.421917	-0.672311
O	-3.940080	-1.102191	0.378479
C	-3.272410	-2.841331	-1.124006
C	-2.637069	-3.860588	-0.183031
N	-2.349608	-3.414258	1.054116
C	-1.518396	-3.989085	2.102027
C	-0.846655	-5.325699	1.791599
N	0.004996	-5.353397	0.617506
C	1.295885	-5.004394	0.460436
C	2.052477	-4.362197	1.616122

C	2.797256	-3.091436	1.115469
C	1.716585	-2.128830	0.589434
O	1.651578	-2.041976	-0.714597
O	-2.387327	-4.991361	-0.612114
O	1.862031	-5.156687	-0.626379
O	3.729472	-3.428084	0.125564
C	3.545051	-2.426408	2.276057
C	4.176434	-1.066298	1.981238
N	4.492428	-0.819866	0.682640
C	5.110171	0.430314	0.298577
C	6.595098	0.475472	0.678798
N	7.203767	1.748736	0.336415
C	7.591758	2.041091	-0.919705
O	7.446089	1.245217	-1.852693
O	4.375659	-0.260313	2.879002
C	8.196064	3.416074	-1.142362
C	9.249296	3.373023	-2.259239
C	10.378344	2.404273	-1.858830
O	11.207780	2.133713	-2.843969
O	8.685408	3.015410	-3.487282
C	9.904087	4.761623	-2.471279
C	10.784319	5.142014	-1.292205
O	10.336934	5.667281	-0.285449
O	0.956832	-1.557403	1.365882
O	-1.427003	-0.654048	0.725329
N	12.100641	4.777721	-1.413952
C	12.914818	4.618532	-0.226984
C	14.409957	4.691697	-0.547035
N	15.189895	4.301422	0.616242
C	15.615137	3.043778	0.927276
O	15.767999	2.711068	2.103067
C	15.980951	2.068902	-0.173877
C	15.152314	0.762165	-0.082680
C	13.726681	1.103305	-0.552836
O	13.526423	1.477784	-1.707481
O	10.526755	2.001211	-0.710738
C	15.675585	-0.317411	-1.056347
C	17.079275	-0.782772	-0.694518
N	17.263125	-2.086552	-0.352029
C	16.279937	-3.107587	-0.038346
C	15.745988	-2.984884	1.395037
N	14.756334	-4.002285	1.690770
C	15.113238	-5.299207	1.909249
C	13.988880	-6.237556	2.306106
O	15.162985	0.219904	1.202074
O	12.788620	0.983423	0.351055
O	18.028992	-0.011395	-0.761396

O	16.269926	-5.679537	1.805027
H	7.378865	2.419752	1.067703
H	6.692749	0.326808	1.755864
H	7.135484	-0.321237	0.159692
H	4.584721	1.248598	0.799760
H	5.005100	0.553959	-0.781806
H	4.435045	-1.586736	0.021076
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Decamer:

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H	8.933533	0.180985	-1.393872
H	4.436873	2.489305	-0.407919
H	7.940866	2.607429	-3.176768
H	7.959869	0.907415	-3.725943
H	5.543765	-0.002788	-2.124519
H	6.044703	3.827685	-3.475499
H	4.039927	4.426200	-4.522078
H	3.978688	2.834876	-5.317165
H	3.471541	2.994206	-3.622240
C	-4.659182	-5.410454	2.684867
O	-6.883149	-4.838601	1.941443
C	-5.343313	-3.035435	2.459732
H	-4.556911	-5.630885	1.616794
C	-3.360149	-4.844480	3.242423
H	-4.902806	-6.338129	3.207660
H	-6.609632	-4.606870	1.042337
O	-5.176231	-2.967826	1.126941
O	-5.038606	-2.145283	3.210679
H	-4.711629	-2.138054	0.920009
O	-3.104388	-4.842134	4.435551
N	-2.555334	-4.287081	2.294700
H	-2.808205	-4.333595	1.312374
C	-1.390442	-3.508755	2.636172
C	-0.087466	-4.277967	2.420766
H	-1.380754	-2.608473	2.006350
H	-1.476747	-3.205396	3.682489
N	1.027827	-3.371651	2.609797
H	-0.036466	-5.096144	3.145361
H	-0.084989	-4.712266	1.409708
C	2.348680	-3.706493	2.605223
H	0.889208	-2.428565	2.263193
O	3.211382	-2.844578	2.524827
C	2.690823	-5.187148	2.678562
H	2.022032	-5.733011	2.005683
C	4.155268	-5.492934	2.300779
H	2.521873	-5.562138	3.693721
C	4.231902	-6.943817	1.754322

C	4.529865	-4.570861	1.132721
O	4.965293	-5.334532	3.423465
O	5.610497	-3.838529	1.267851
O	3.862132	-4.588303	0.111402
H	5.599977	-3.203389	0.512128
H	5.762529	-5.877413	3.288276
C	5.651427	-7.265309	1.332547
H	3.959812	-7.623233	2.567478
H	3.527731	-7.080138	0.930680
O	6.546115	-7.366227	2.175624
N	5.869150	-7.390806	0.005716
C	7.199771	-7.627167	-0.523577
H	5.168408	-7.056126	-0.649567
H	7.087841	-7.817016	-1.594448
C	8.175324	-6.472356	-0.290918
H	7.614182	-8.525849	-0.057614
H	9.135724	-6.733188	-0.756084
N	7.639713	-5.246669	-0.852813
H	8.334096	-6.366888	0.785149
C	8.002101	-4.002631	-0.511263
H	6.782571	-5.318329	-1.413631
O	7.392902	-3.013623	-0.952791
C	9.161972	-3.843418	0.444007
H	8.855715	-4.160859	1.447550
H	10.020868	-4.453793	0.148893
H	9.452466	-2.792696	0.478773

[1] P. Hohenberg and W. Kohn, *Phys. Rev. B* **136**, B864 (1964)
[2] W. Kohn and L. Sham, *Phys. Rev.* **140**, A1133 (1965)
[3] J.-D. Chai and M. Head-Gordon, *Phys. Chem. Chem. Phys.*, **10**, 6615 (2008)
[4] W. J. Hehre, R. Ditchfield and J. A. Pople, *J. Chem. Phys.* **56**, 2257 (1972)
[5] E. Runge and E. K. U. Gross, *Phys. Rev. Lett.* **52**, 997 (1984)
[6] A. D. Becke, *Phys. Rev. A*, **38**, 3098 (1988)
[7] C. T. Lee, W. T. Yang and R. G. Parr, *Phys. Rev. B* **37**, 785 (1988)
[8] S. H. Vosko, L. Wilk and M. Nusair, *Can. J. Phys.* **58**, 1200 (1980)
[9] Gaussian 09, Revision A.1, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian Inc., Wallingford CT, 2009.