

Supporting Information

Chemically induced crosslinked enhanced emission of carbon polymer dots discerning healthy and cancer cells through pH dependent tunable photoluminescence

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Materials

Citric acid anhydrous, Urea, 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (EDC.HCl), Coumarin-153, Quinine sulphate, Dimethyl Sulfoxide-d₆ were purchased from Sigma-Aldrich. All the organic solvents were obtained from Sisco Research Laboratories (SRL, India). Chemicals are used as received. Millipore water was used for synthesis and dilutions during spectroscopic analysis.

Instrumentation

The morphological characterization was done by Atomic Force Microscopy (AFM, Model: Keysight 5500 Scanning Probe Microscope and Agilent Technologies 5500), Transmission Electron Microscopy (TEM, Model: JEM-F200), and Field Emission Scanning Electron Microscopy (FESEM, Model: Gemini SEM 500 microscope, ZEISS). The topography images were captured in the non-contact mode after the spin coating on a silicon wafer. TEM analysis was done after the drop-casting of a diluted sample on a carbon-coated copper TEM grid. FESEM images were also acquired after the spin coating of the sample on a silicon wafer followed by gold coating. The hydrodynamic diameter of the samples was analyzed by Anton Paar (Litesizer 500) instrument. Reverse Phase High-Performance Liquid Chromatography (RP-

HPLC) was done on a Shimadzu Prominence analytical HPLC system. The mobile phase contained (95:5) % of 10mM Tris.HCl buffer (pH 7.4) as eluent A and acetonitrile as eluent B. The flow rate was 0.2 ml/min with 25±1 °C column temperature and 10 µl injection volumes. Powder XRD (p-XRD, Model: Empyrean, Malvern Panalytical) analysis of the CPD was done with Cu-Kα (λ=1.54°A) X-ray source. Fourier transform- infrared spectroscopy (FT-IR, Model: Parkin Elmer Spectrum-400) experiment was done on KBr mode within the range of 400-4000 cm⁻¹. UV-Visible absorption spectra data were recorded on a UV-2550 spectrophotometer (Shimadzu, Japan). Steady-state fluorescence spectra were done on a Fluoromax-400 spectrofluorometer (Horiba, Japan). Time-resolved fluorescence decay was measured by a time-resolved fluorescence spectrophotometer from Edinburgh Instruments (LifeSpec-II, UK) working on the time-correlated single-photon counting (TCSPC) technique. Raman spectra (STR 750 RAMAN spectrograph, Seki Technotron Corporation Japan) were recorded with a 633 nm laser. NMR experiment was done on a BRUKER NMR AVANCE-400 MHz. Digital images were taken on a Canon D60 digital camera exposed to a UV transilluminator. For the determination of the quantum yield of CPD in water, a solution of quinine sulfate (QY= 0.55) in 0.5 M H₂SO₄ was used as standard. Quantum yield was calculated by using the following equation,

$$\Phi_x = \Phi_s \times (I_x f_s \eta_x^2 / I_s f_x \eta_s^2)$$

Where subscript x and s denote test and standard sample respectively; Φ is fluorescence quantum yield; I is the integrated fluorescence intensity; f is absorption factor ($f = 1 - 10^{-A}$, where A = absorbance); and η is the refractive index of the solvent. For QY calculation of green-CPD, we used coumarin-153 as a standard.

Confocal Microscopy:

Incubated cells were washed thrice in 1×PBS (pH 7.4) by centrifuging at 300×g for 5 min. The washed cells were fixed with 4% paraformaldehyde for 4 min. The cells were again washed 3× in 1×PBS. 10 µl of the cell pellet was placed on a clean microscopic slide and stained with DAPI to stain the nucleus and mounted in ProLong Gold Antifade mounting solution (Invitrogen). The slides were then examined using LSM 880 confocal microscope (Zeiss). Stained cells were viewed at 405, 458, and 543 excitations and 460, 519, and 621 nm emissions.

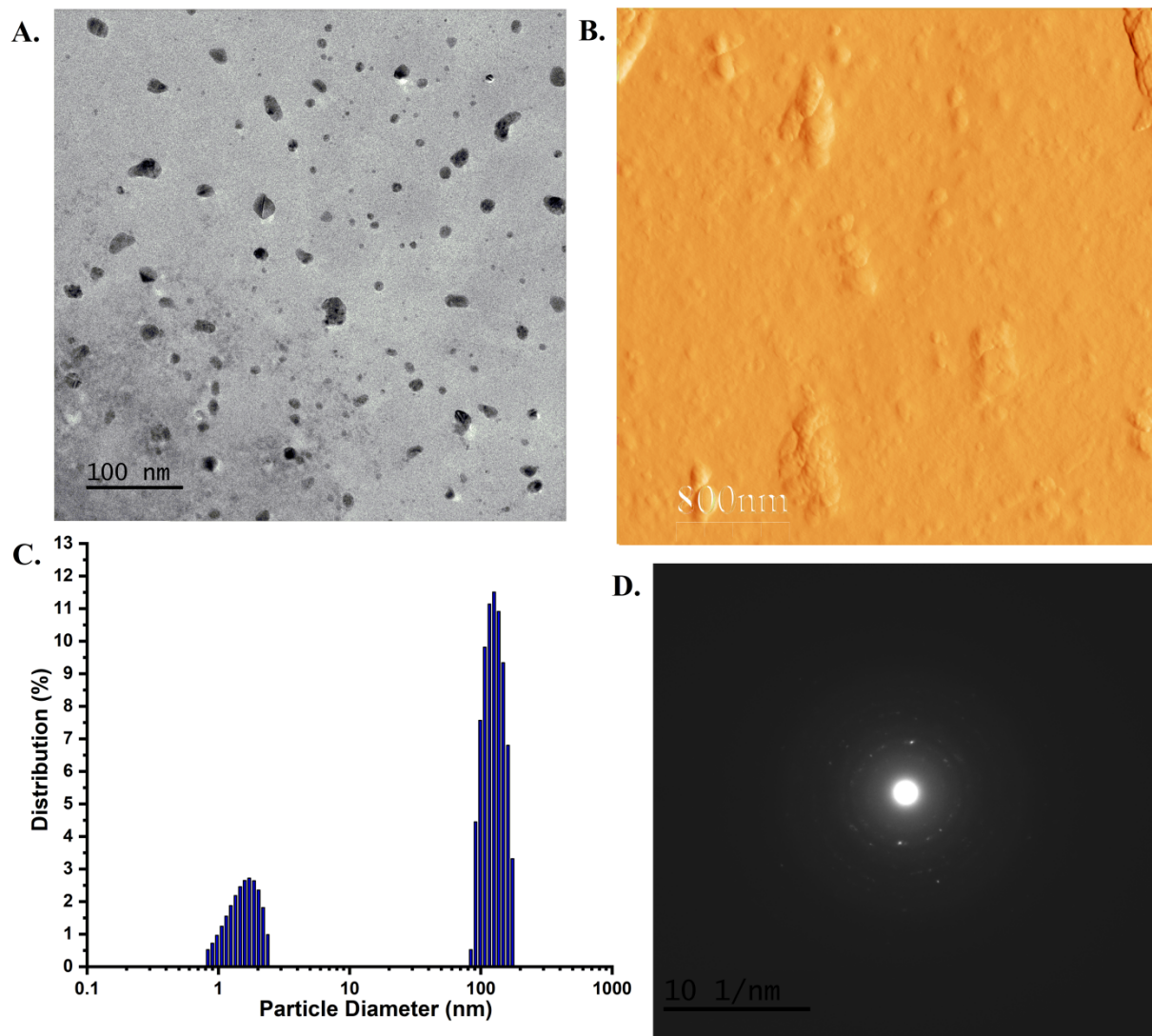


Figure S1: A. TEM image of CPD in 100nm scale showing heterogeneous size distributions. B. 2D AFM of CPD (800nm scale). C. DLS spectra of CPD. D. SEAD pattern of CPD.

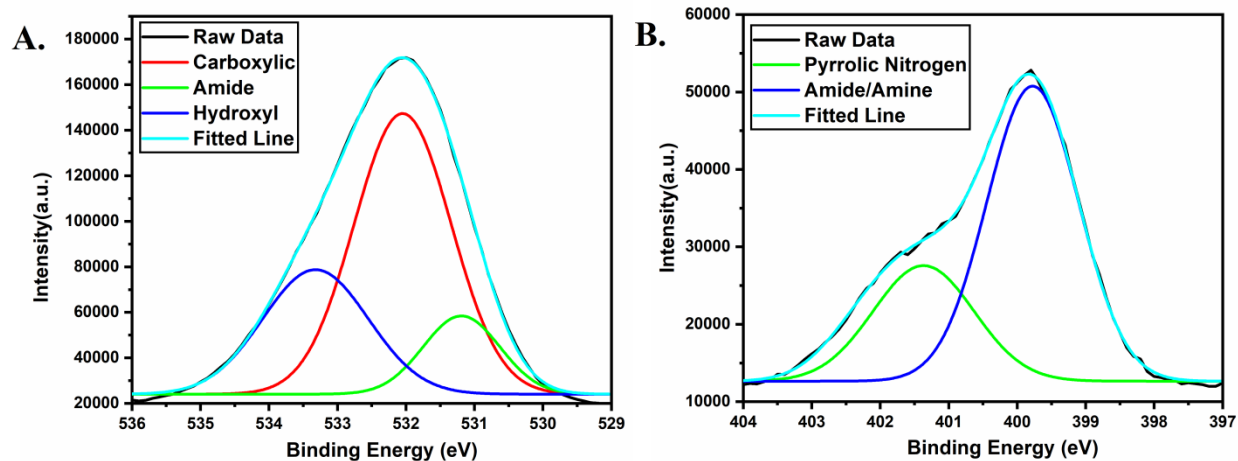


Figure S2: A. High-resolution deconvoluted XPS spectra of O1s. B. High-resolution deconvoluted XPS spectra of N1s

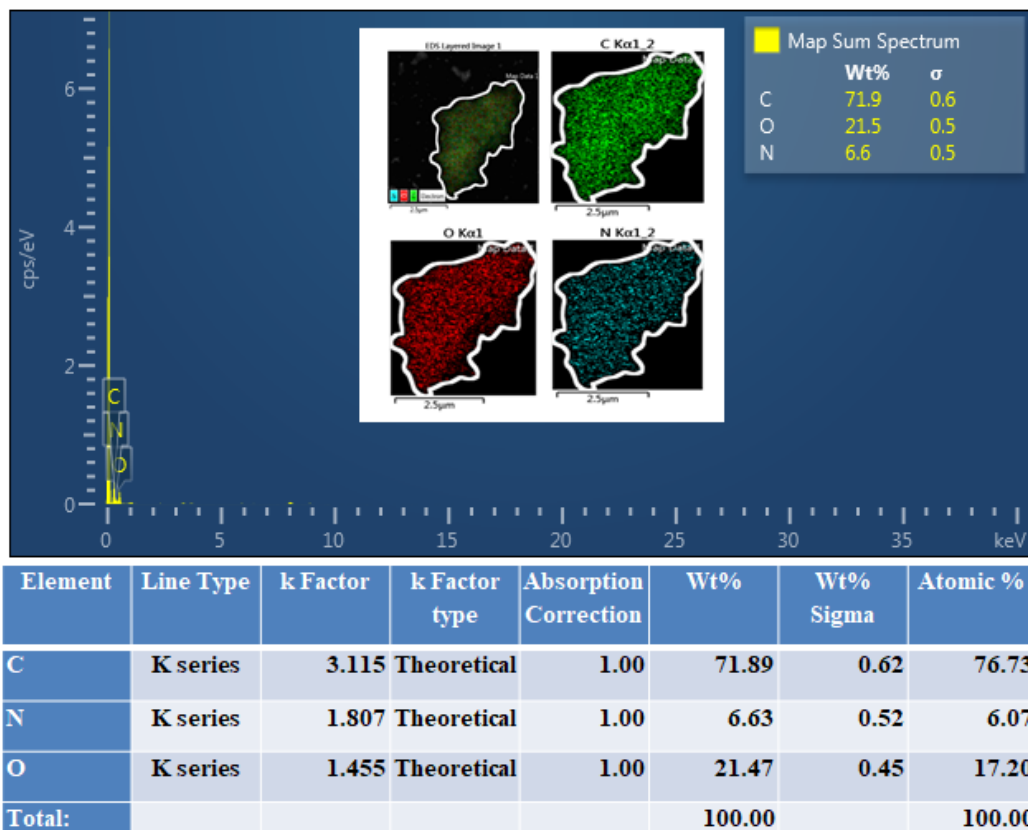
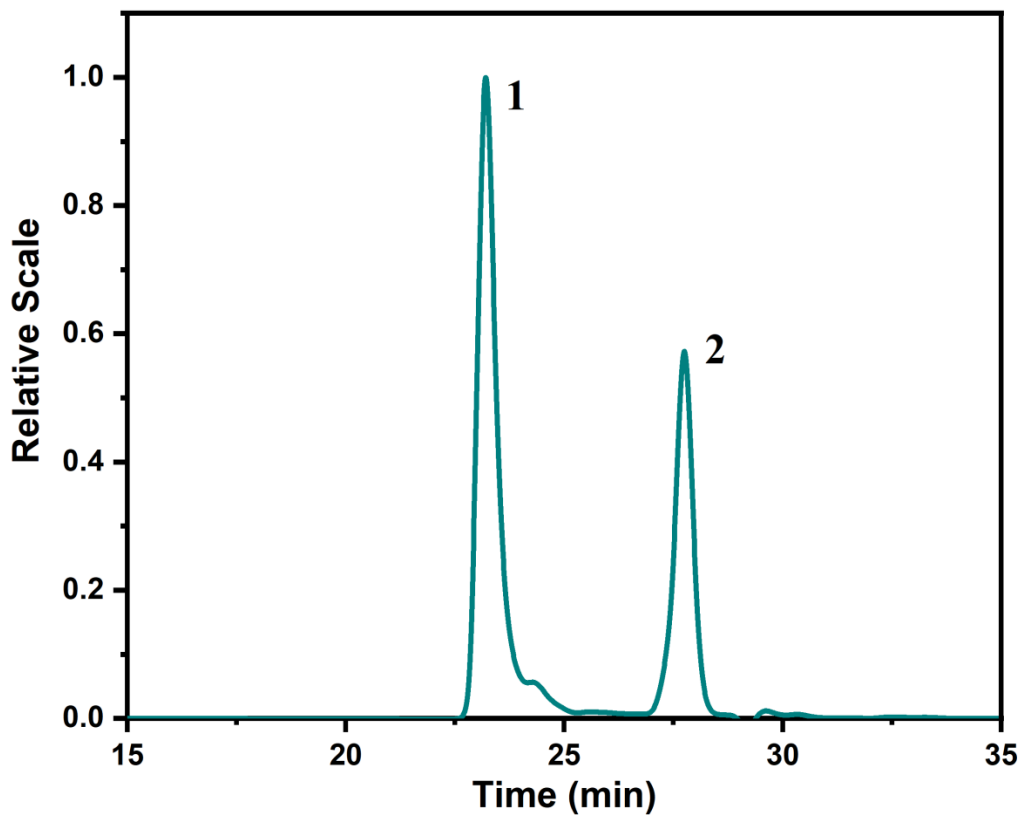


Figure S3: The energy dispersive spectrometry (EDS) analysis of the CPD



Peak-1: $M_n - 5.18 \times 10^3$	Peak-2: $M_n - 4.28 \times 10^2$
$M_w - 5.28 \times 10^3$	$M_w - 4.35 \times 10^2$
PDI - 1.019	PDI - 1.016

Figure S4: Size exclusion chromatography (SEC) data of the CPD

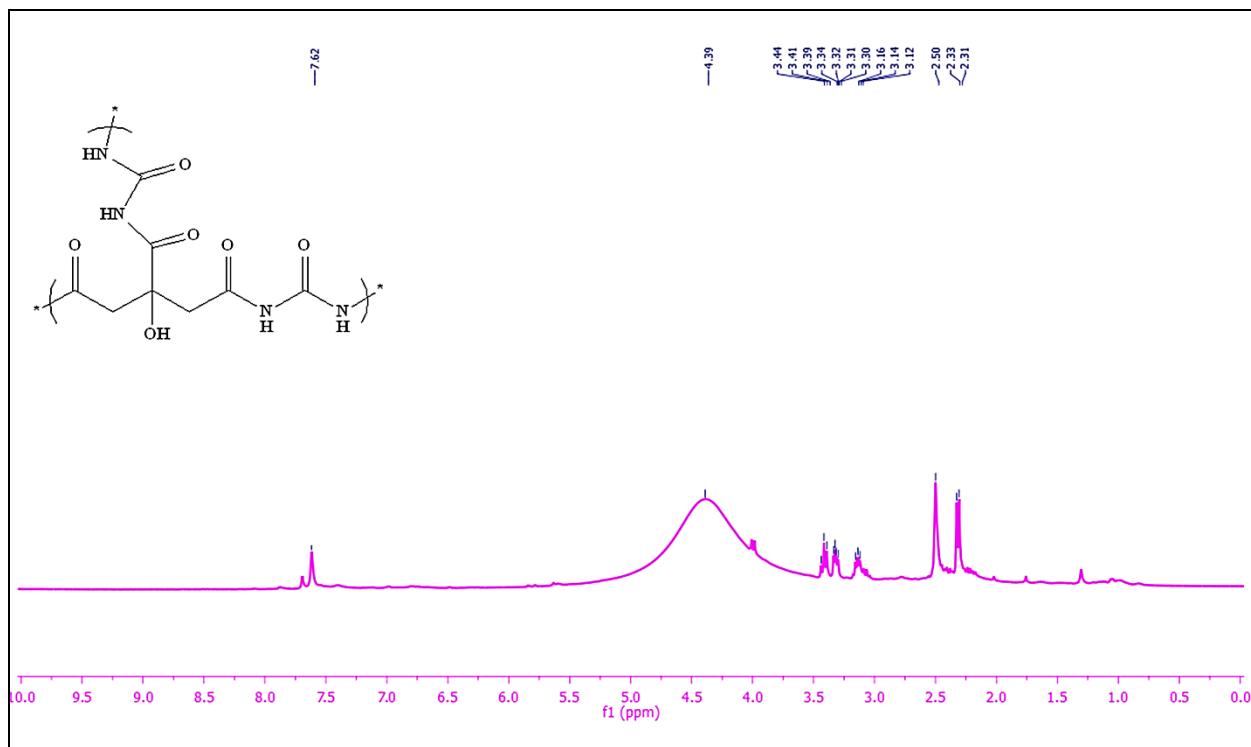


Figure S5: Proton NMR of CPD

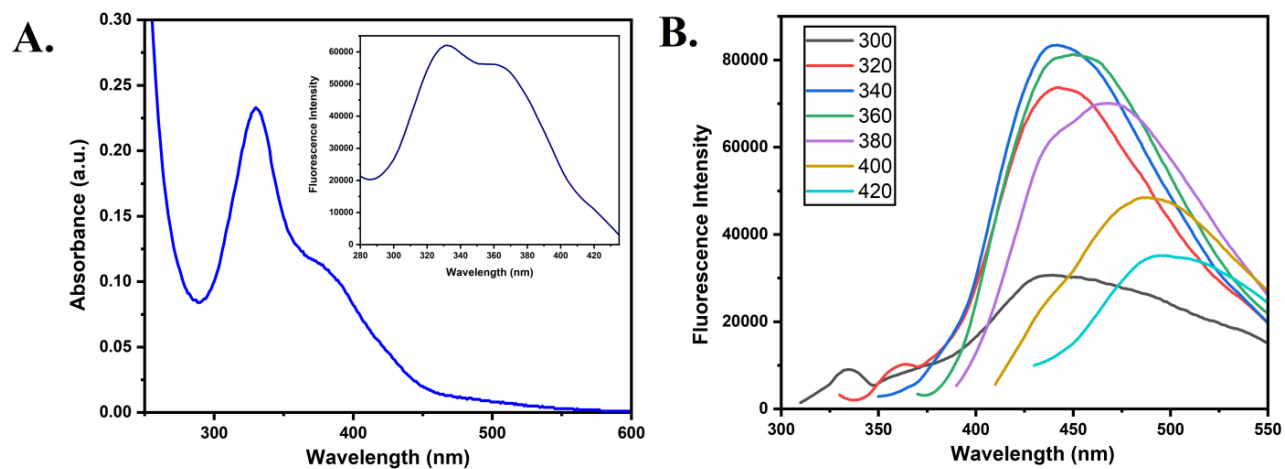


Figure S6: **A.** UV-Vis absorption spectra (excitation spectra inset) of CPD and **B.** Fluorescence spectra of CPD

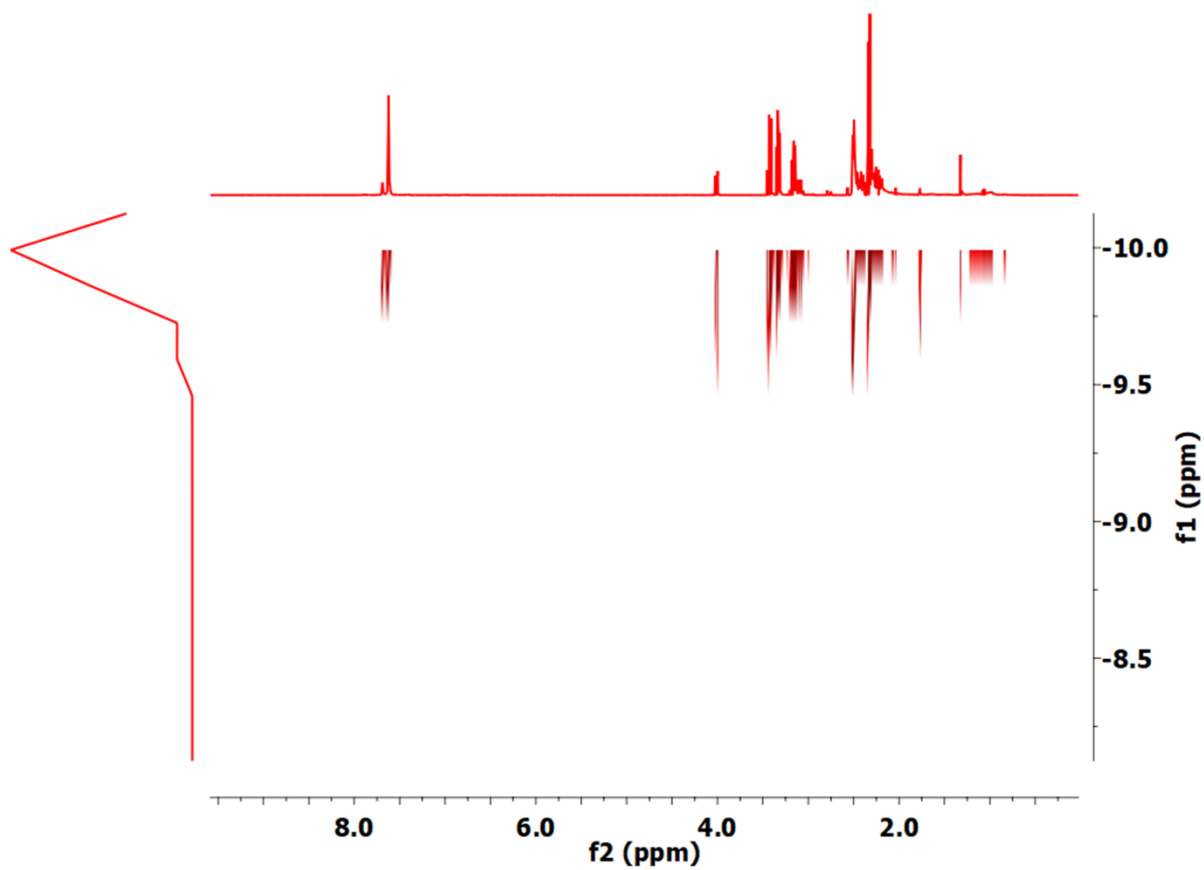


Figure S7: ^1H DOSY NMR spectrum of CPD

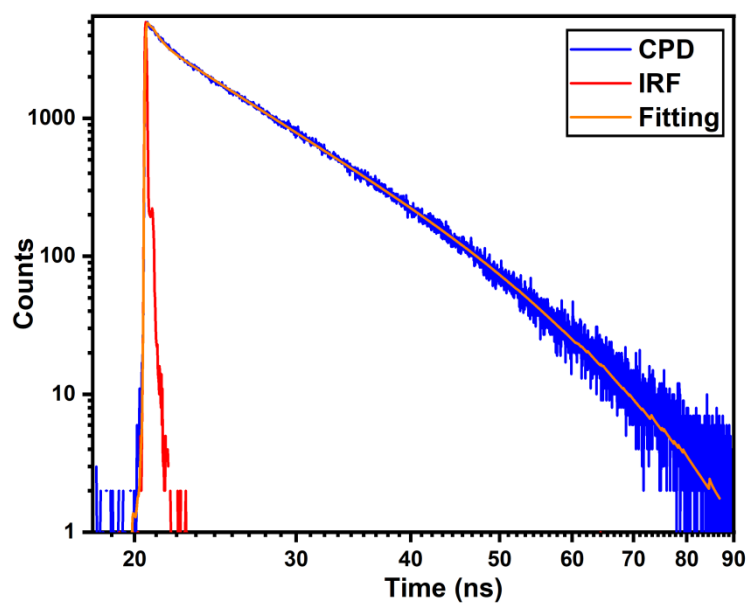


Figure S8: The time-resolved PL of CPD

Sample Name	Lifetime (ns)			T _{average} (ns)	a(%)	χ^2
	T ₁	T ₂	T ₃			
CPD	0.59	4.14	9.14	7.001	10, 26.05, 63.95	1.053
Green-CPD	2.01	5.50	-	5.29	5.96, 94.04	1.127
orange-CPD	0.21	2.76	4.77	3.58	2.07, 54.38, 43.55	1.040
Blue-CPD	0.44	3.19	8.28	6.286	7.51, 27.6, 64.89	1.192

Table S1: Lifetime data of CPD, green-CPD, yellow-CPD, and blue-CPD

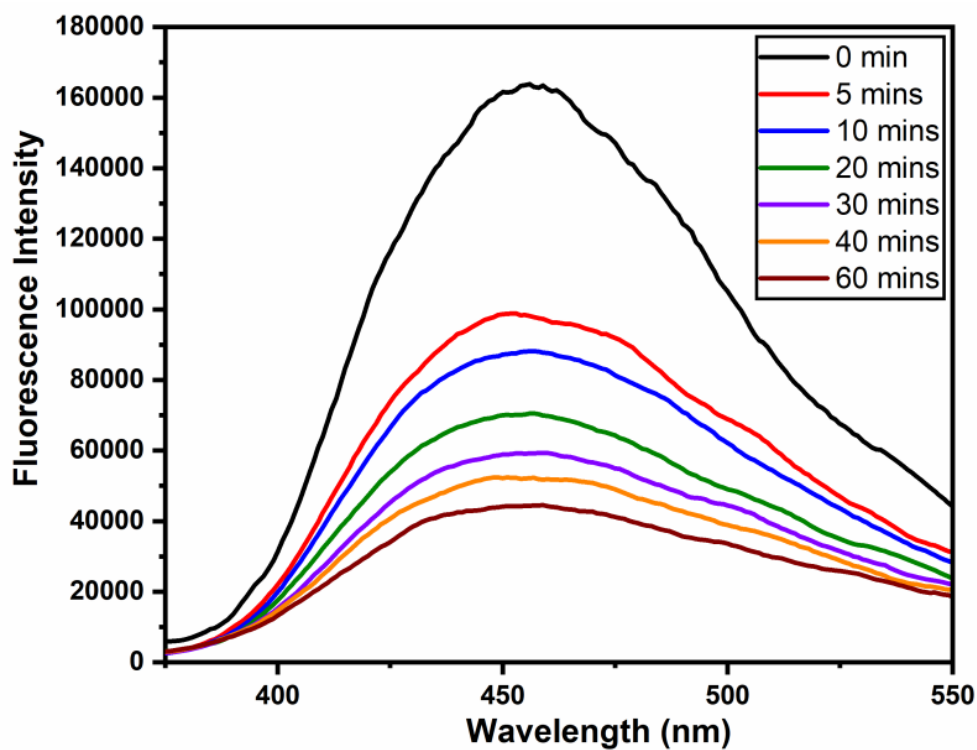


Figure S9: UV light dependent PL of CPD

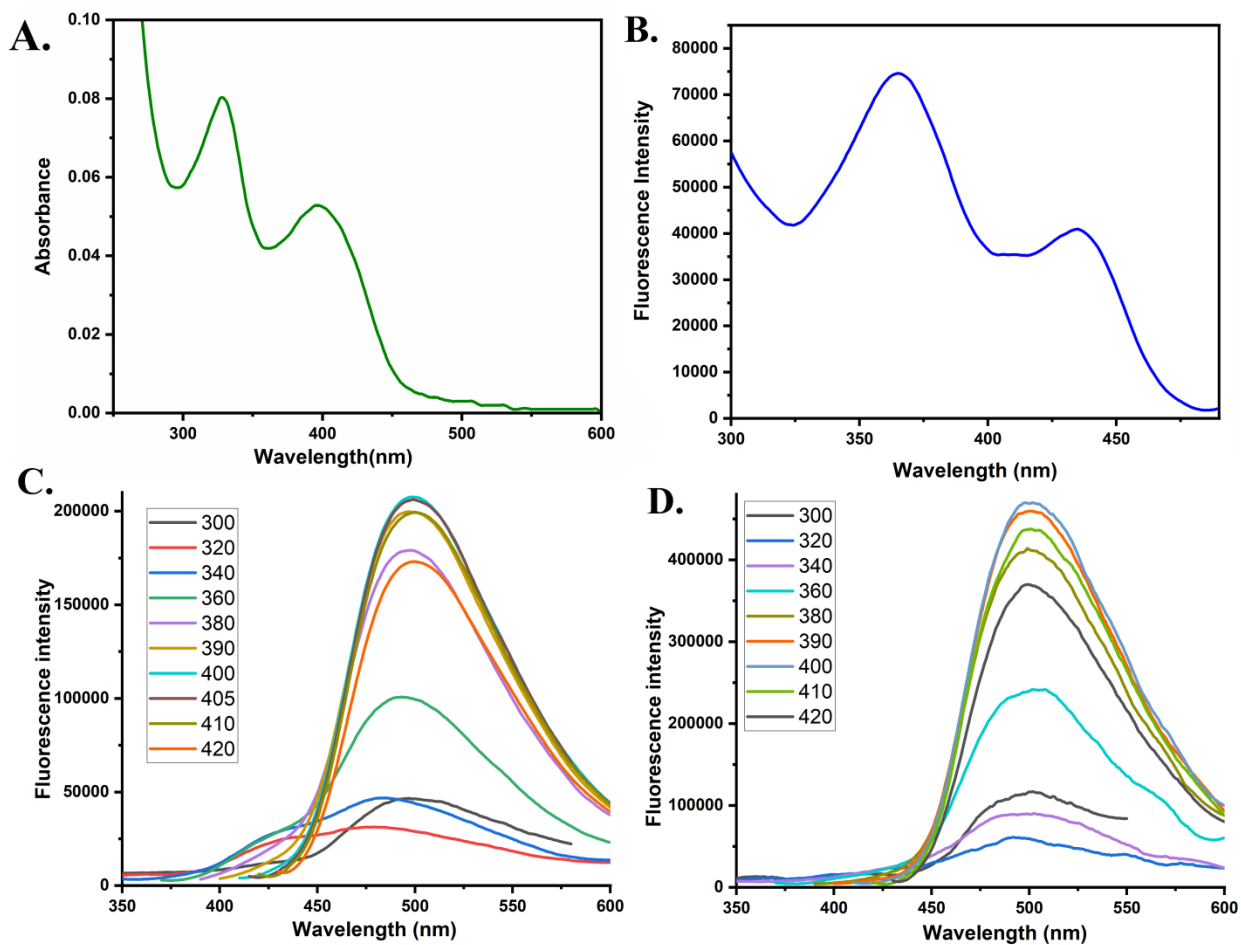


Figure S10: **A.** The UV-Vis absorption spectra of green-CPD. **B.** Excitation spectra of green-CPD at 500nm emission. **C.** Fluorescence spectra of green-CPD before dialysis. **D.** Fluorescence spectra of green-CPD after dialysis.

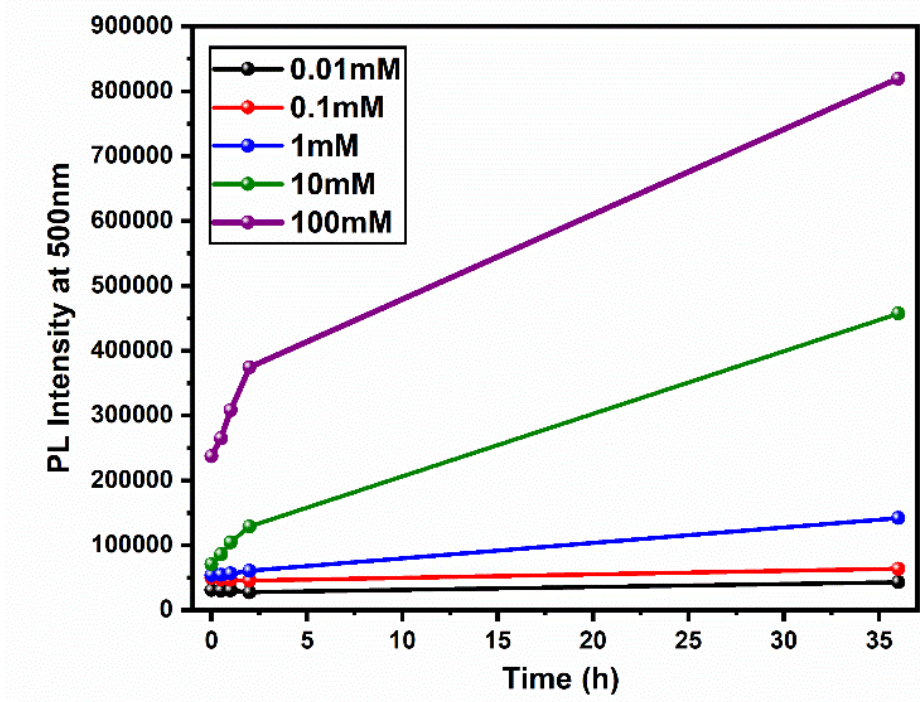


Figure S11: Study the effect of varying EDC concentrations on CPD with respect to time

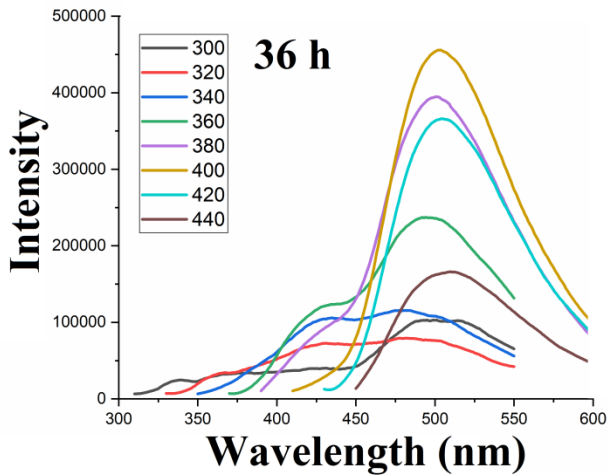
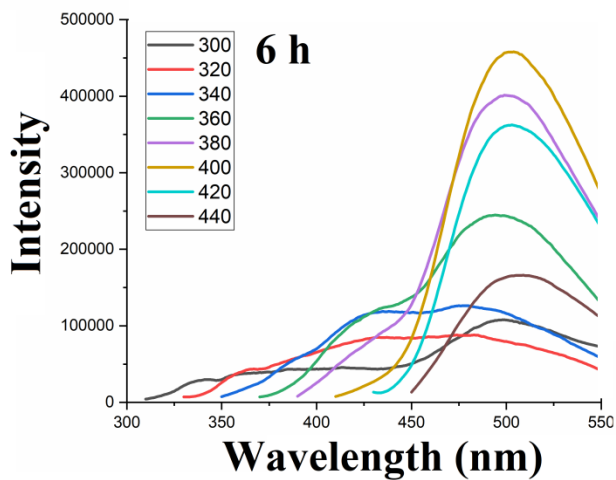
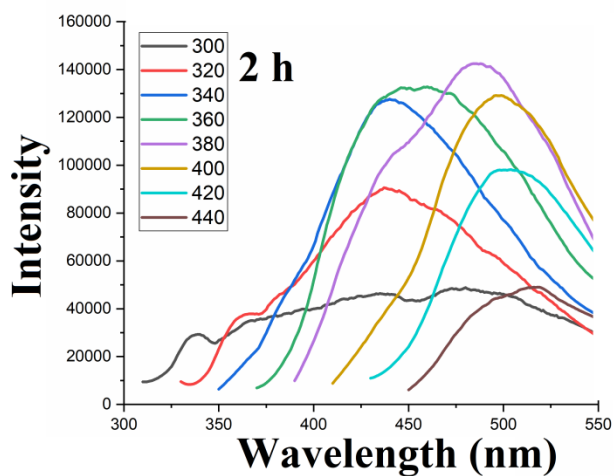
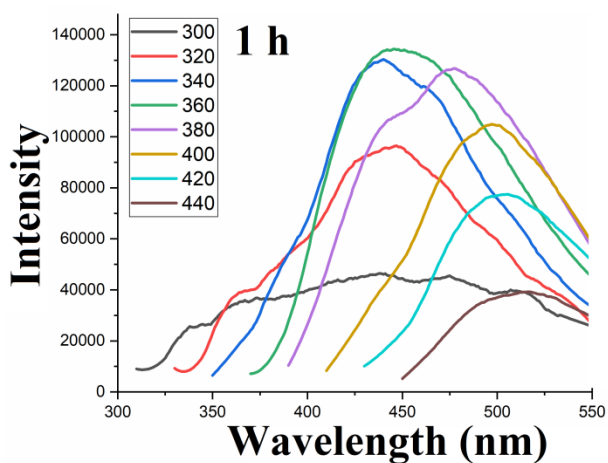
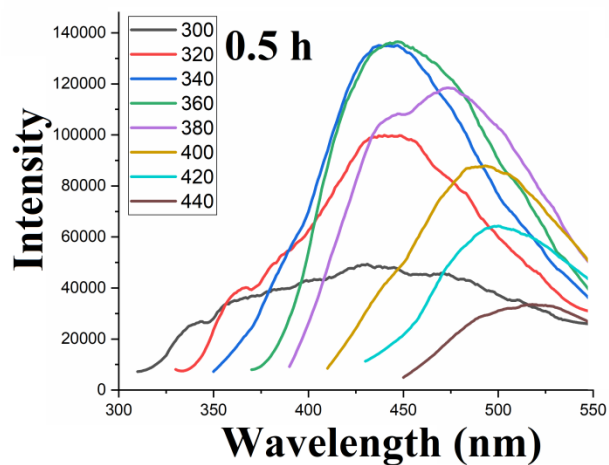
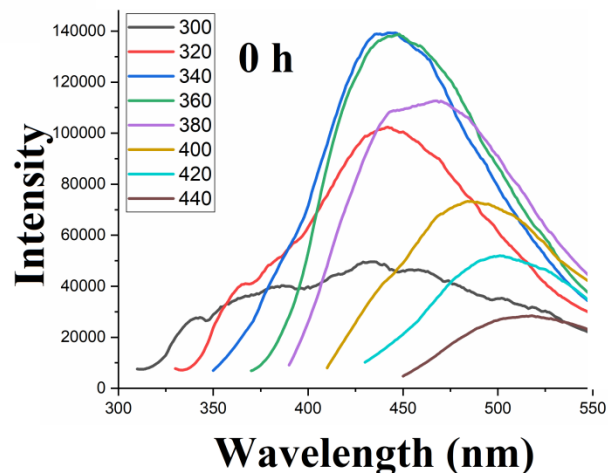


Figure S12: Study the effect of EDC on CPD with respect to time

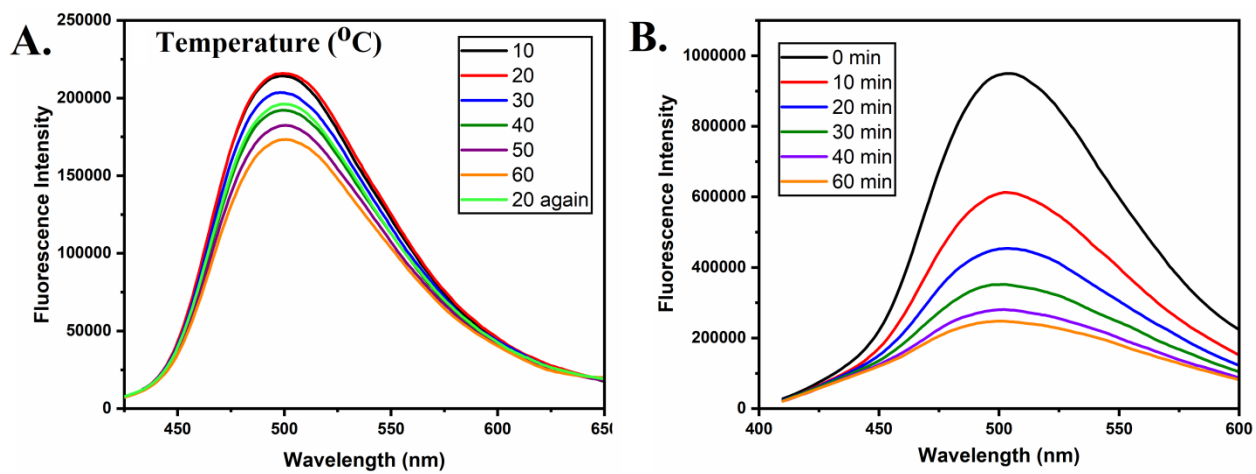


Figure S13: A. Temperature dependent and **B.** UV dependent PL of green-CPD

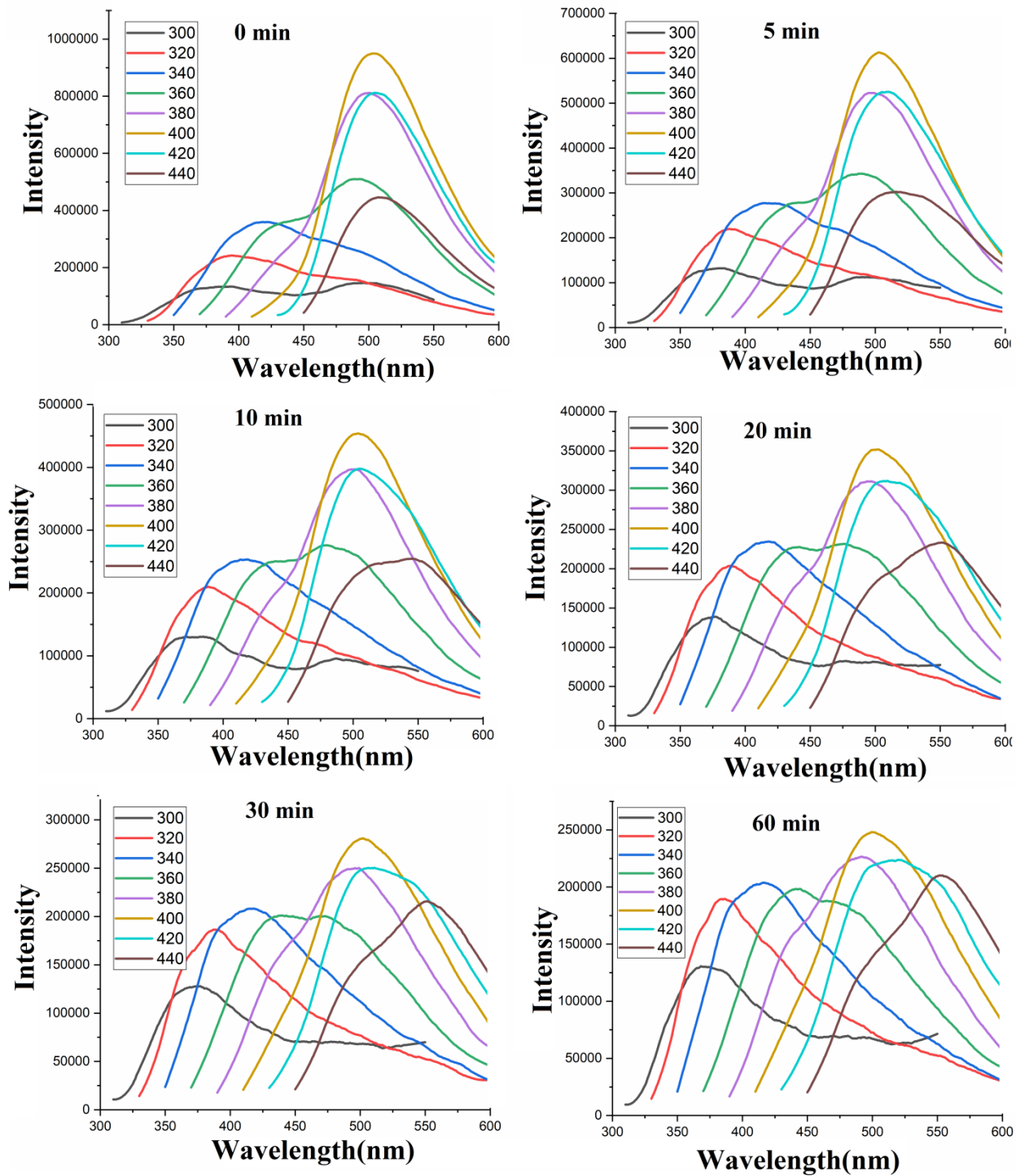


Figure S14: Study the excitation dependent emission properties of green-CPD upon UV irradiation, with respect to time.

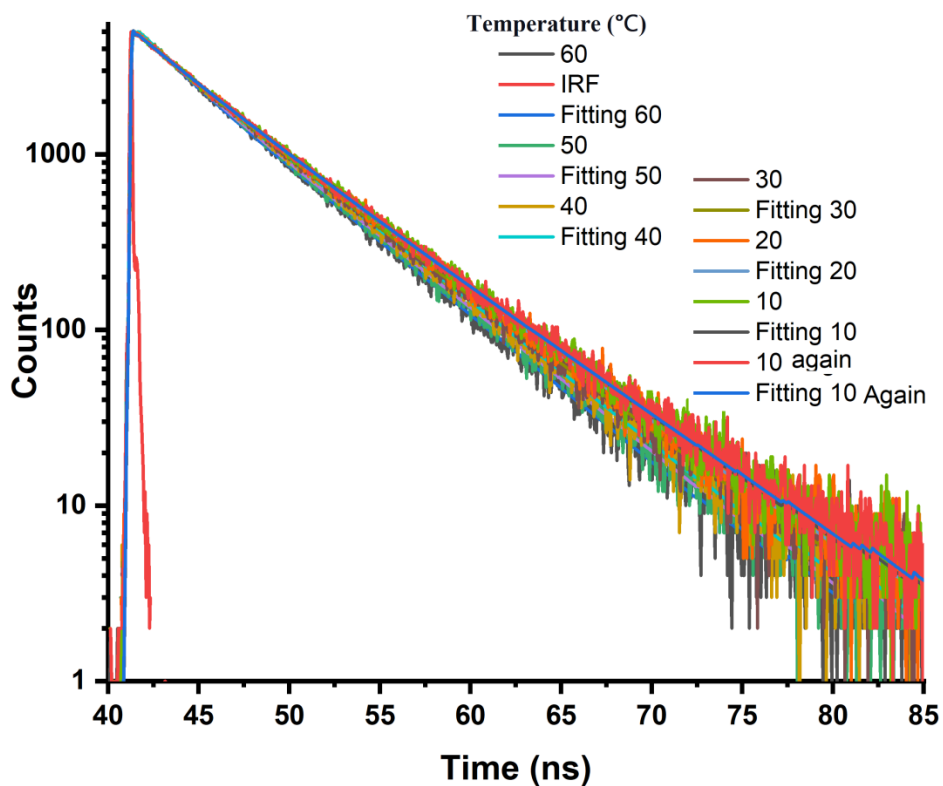


Figure S15: The time resolved PL lifetime of green-CPD at different temperatures

Sample Name	Lifetime (ns)			χ^2
	T ₁	T ₂	T ₃	
10°C	0.08	3.42	5.97	1.051
20°C	2.24	5.73	-	1.136
30°C	0.12	3.77	5.84	0.968
40°C	1.54	5.35	-	1.15
50°C	2.17	5.30	-	1.18
60°C	2.09	5.16	-	1.09
10°C again	0.12	3.83	6.16	0.98

Table S2: Life time data of green-CPD at different temperatures

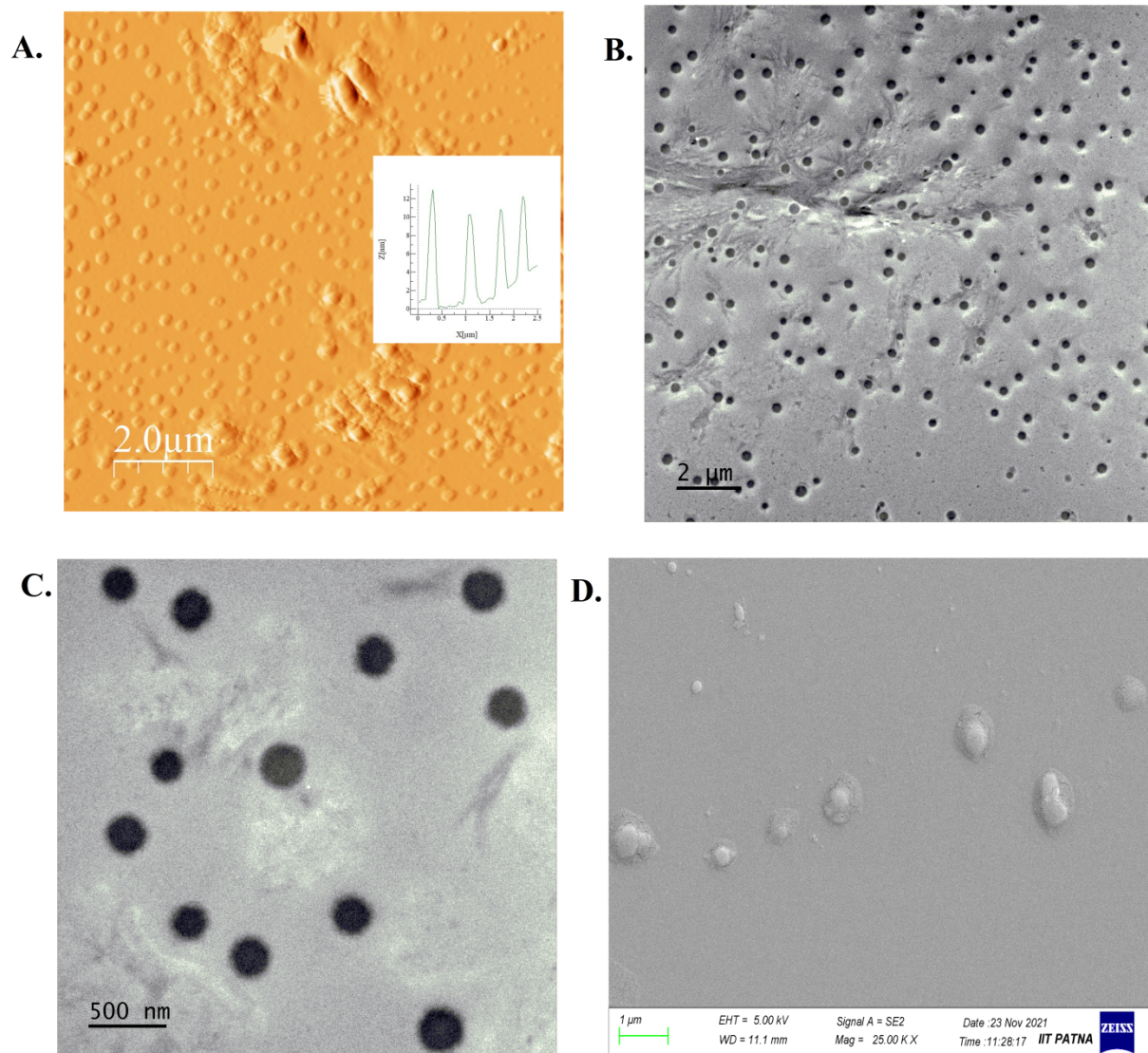


Figure S16: **A.** AFM and height profile (inset) of green-CPD **B.** TEM images of green-CPD in at $2\mu\text{m}$ scale. **C.** TEM images of green-CPD in at 500nm scale. **D.** FESEM image of green-CPD

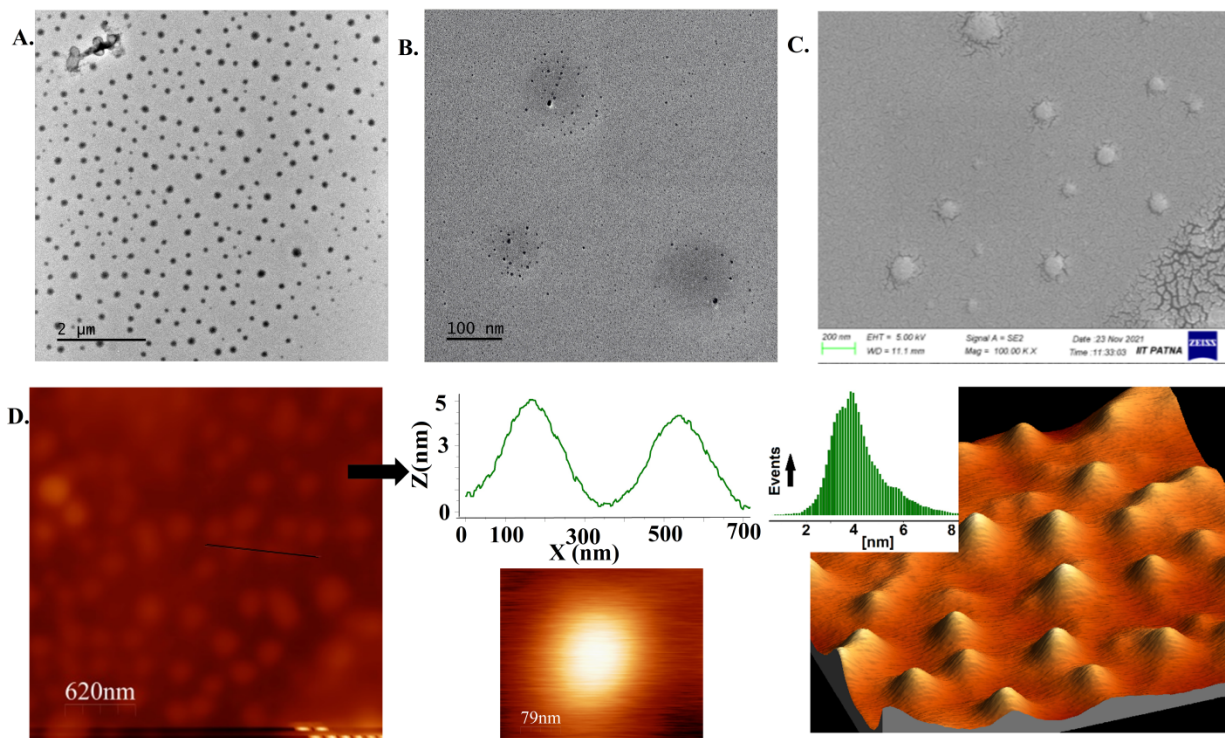


Figure S17: **A.** TEM images of orange-CPD in at 2 μ m scale. **B.** TEM images of orange-CPD in at 100nm scale. **C.** FESEM image of orange-CPD. **D.** AFM images and height profile (inset) of orange-CPD

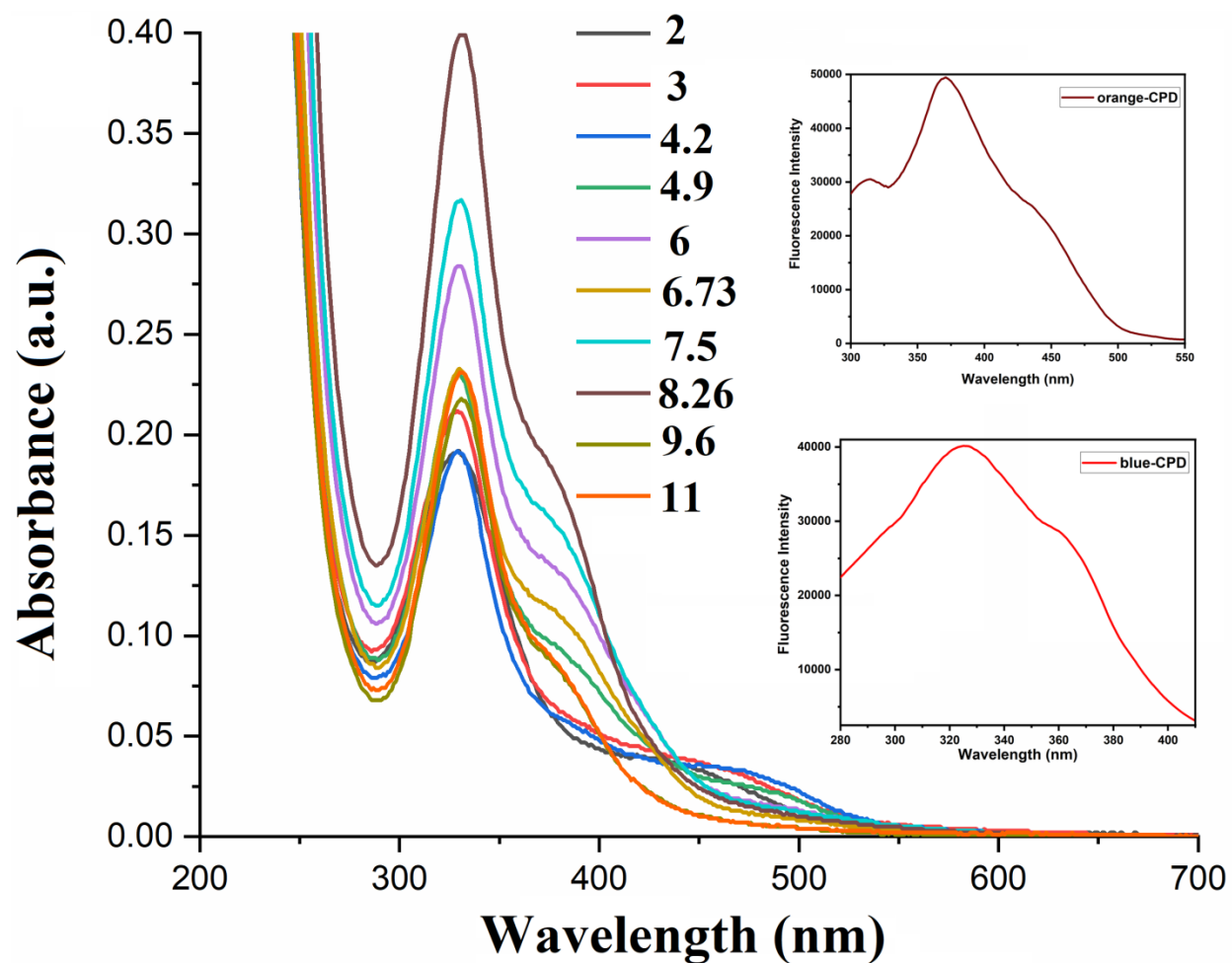


Figure S18: The absorption peak of green-CPD at different pH conditions (Inset-Excitation spectra of orange-CPD at 560nm emission and Excitation spectra of blue-CPD at 445nm emission.)

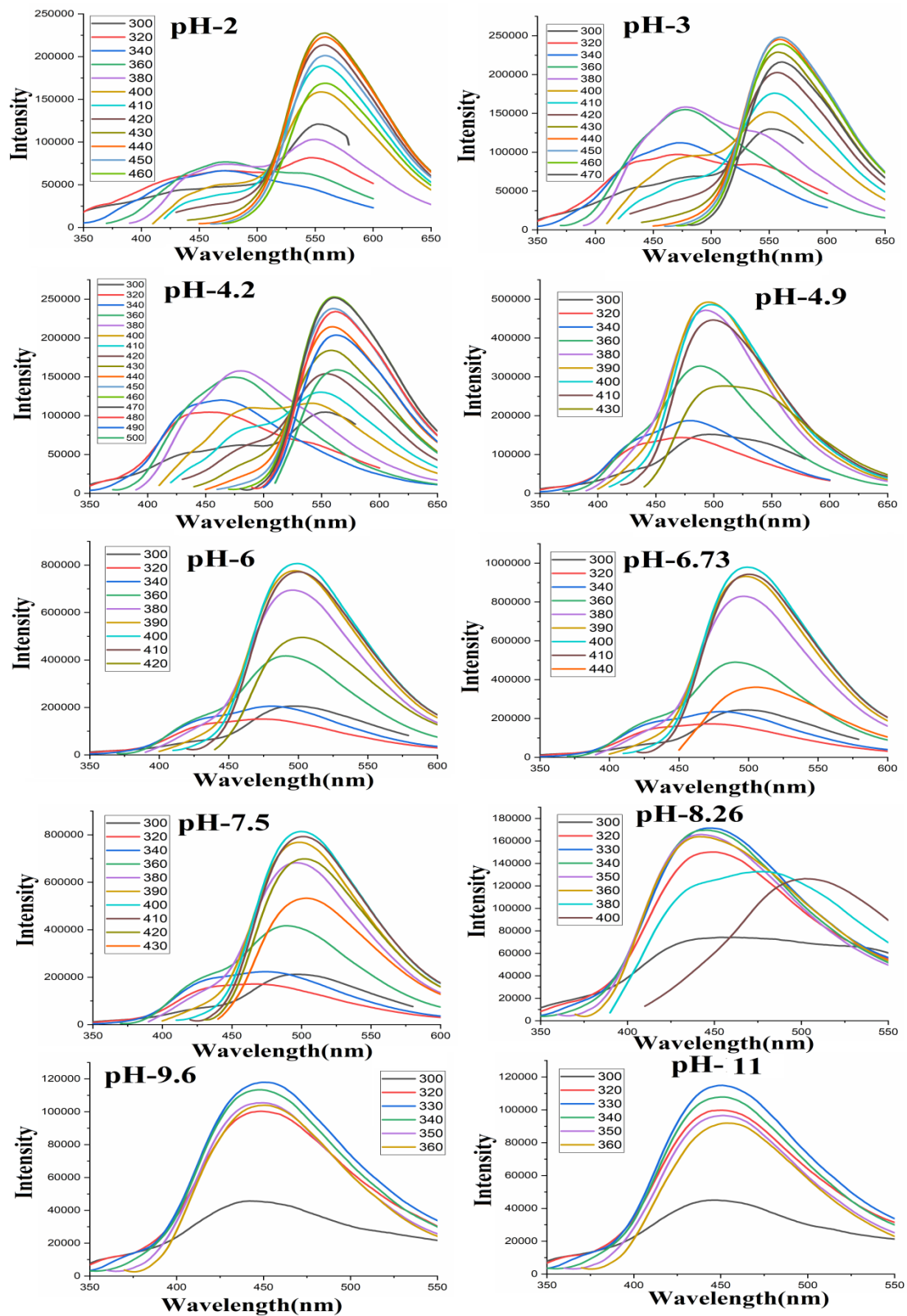


Figure S19: pH dependent fluorescence emission of green-CPD

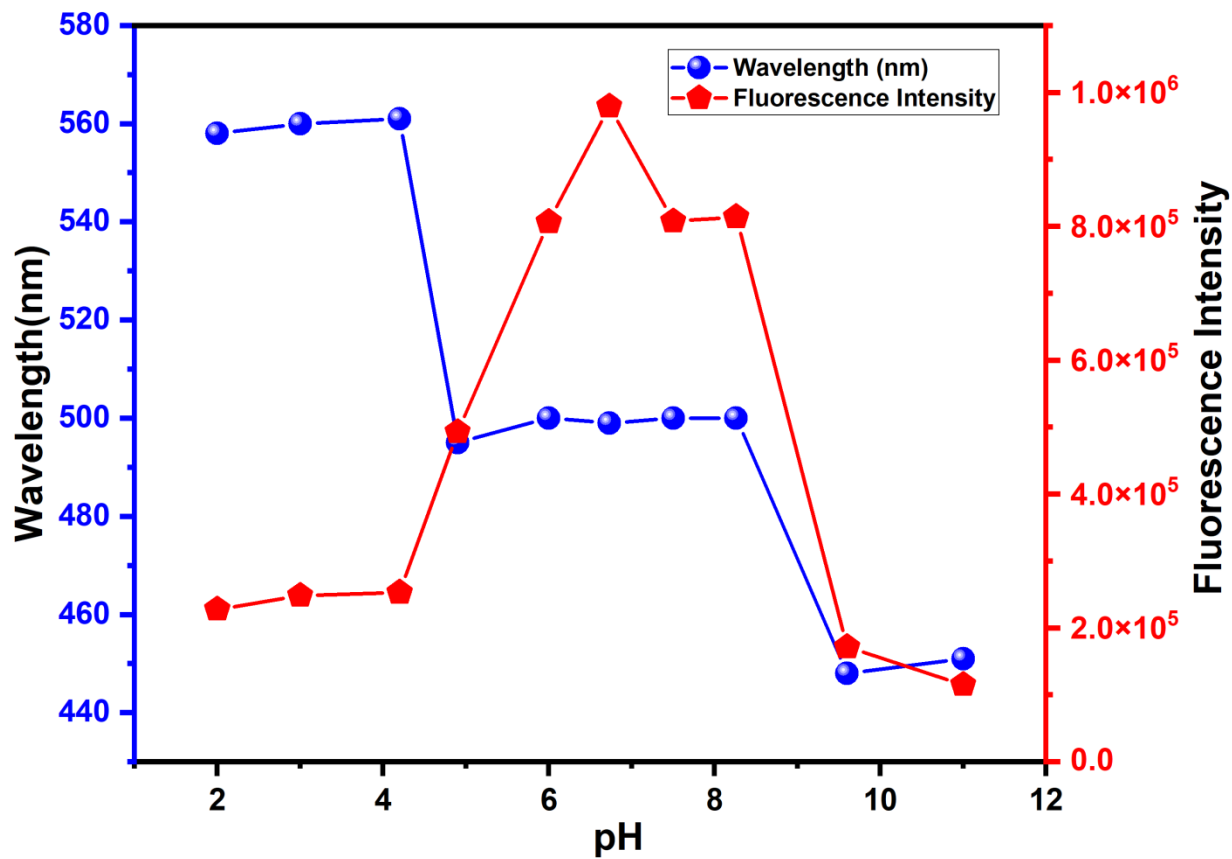


Figure S20: pH dependent emission maximum wavelength shift (pH vs lambda max) and intensity shift (pH vs Fl. Intensity) of green-CPD.

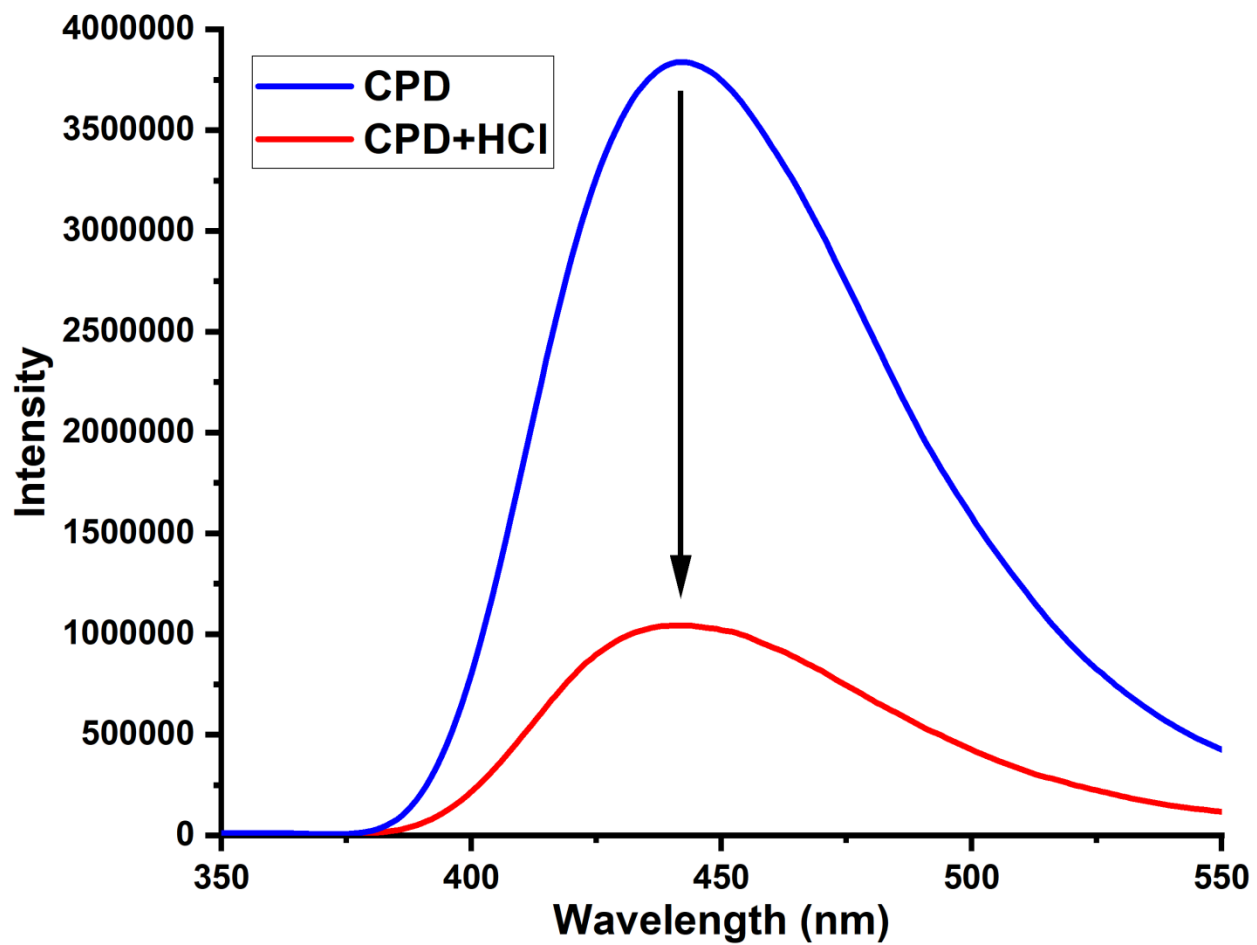


Figure S21: Acid sensitive fluorescence quenching of CPD.

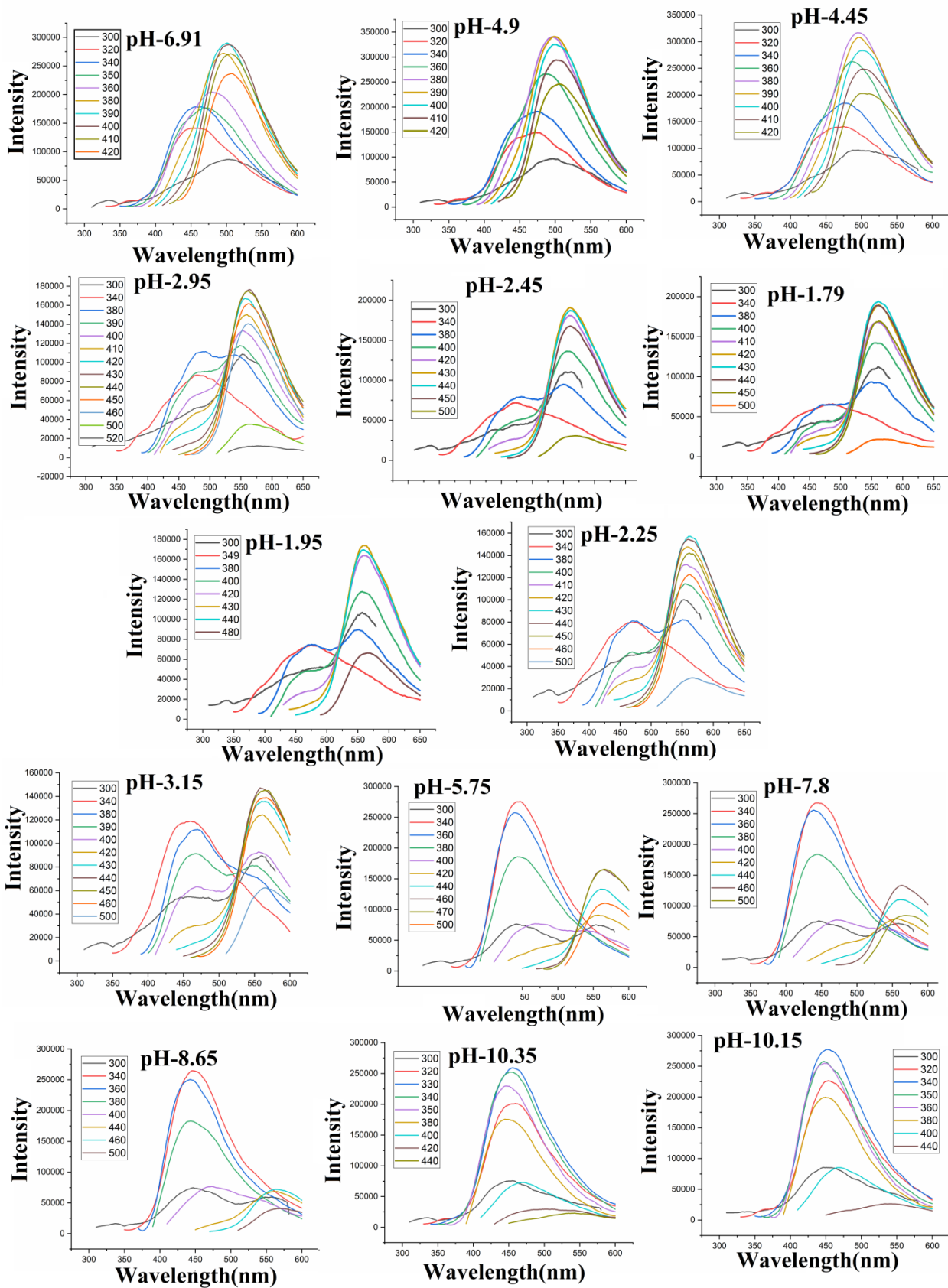


Figure S22: Study the reversibility of optical properties by titrating the green-CPD with HCl and NaOH

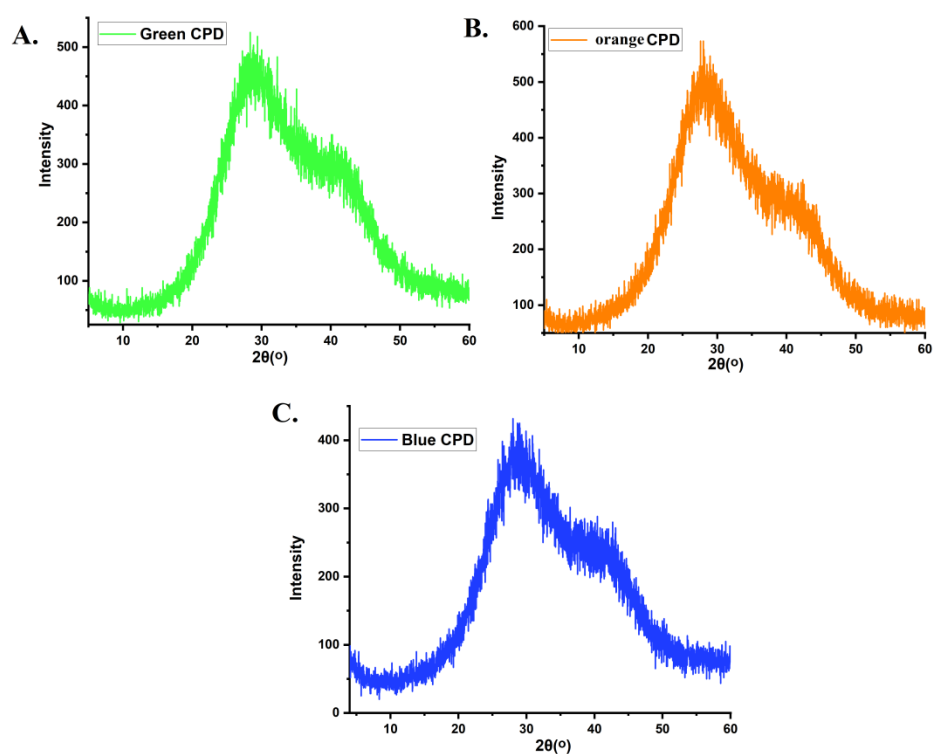


Figure S23: powder XRD data of A. green-CPD B. orange-CPD and C. blue-CPD

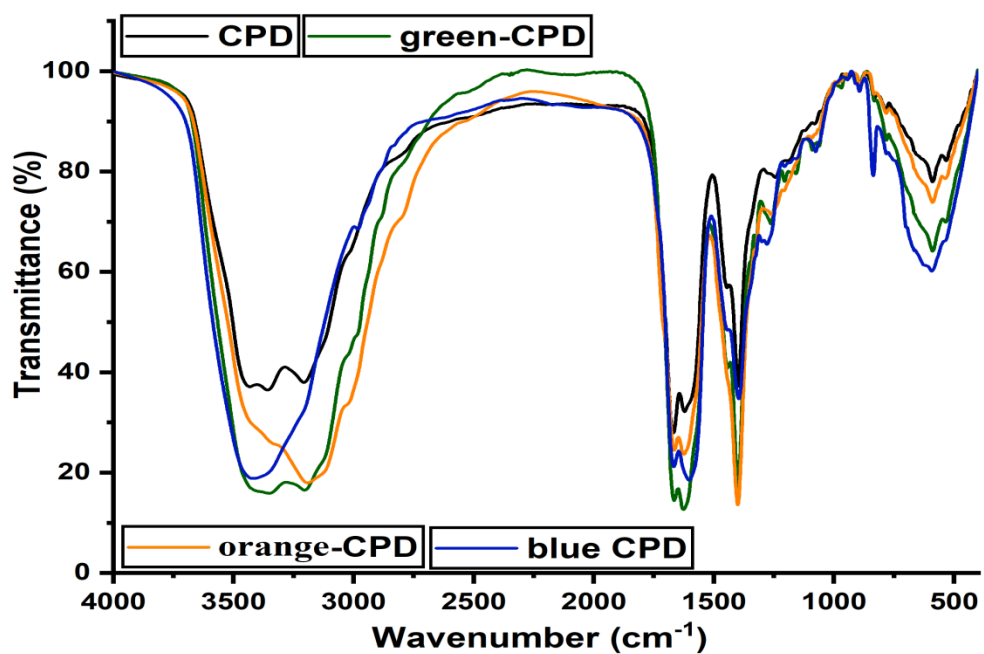


Figure S24: FTIR spectra of CPD, green-CPD, orange-CPD and blue-CPD

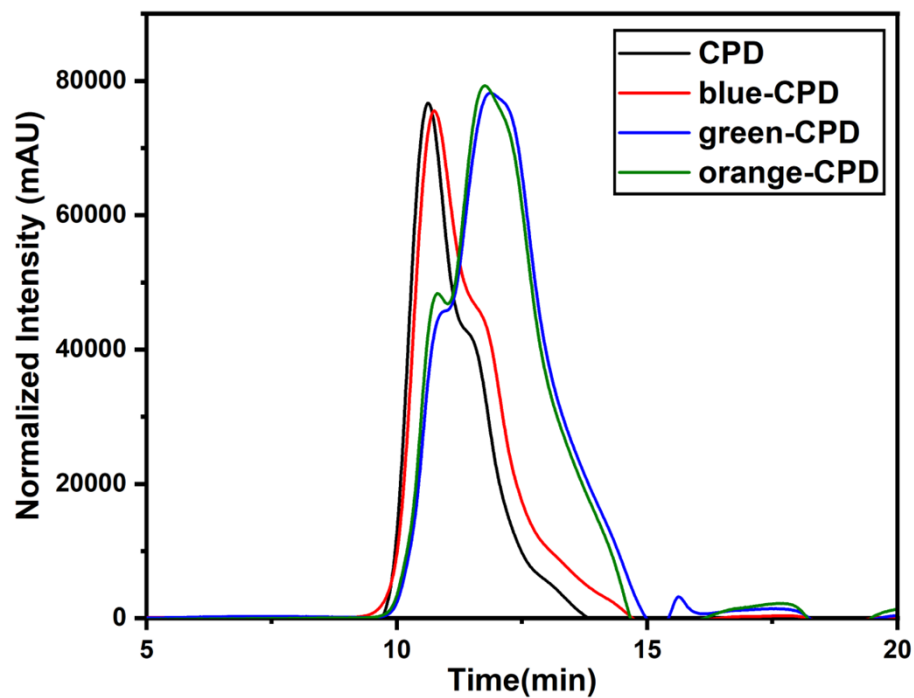


Figure S25: Reverse phase-HPLS of CPD, green-CPD, orange-CPD and blue-CPD

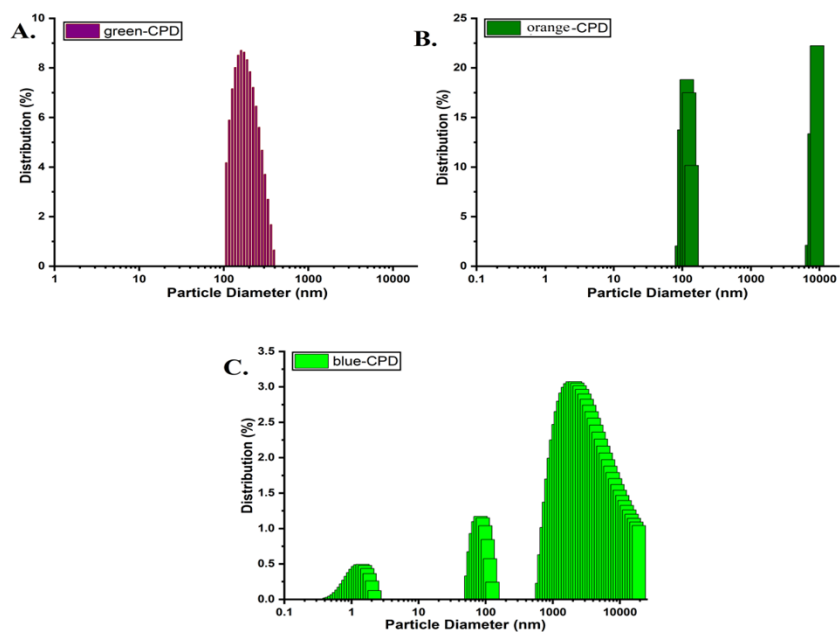


Figure S26: DLS spectra of A. green-CPD B. orange-CPD and C. blue-CPD

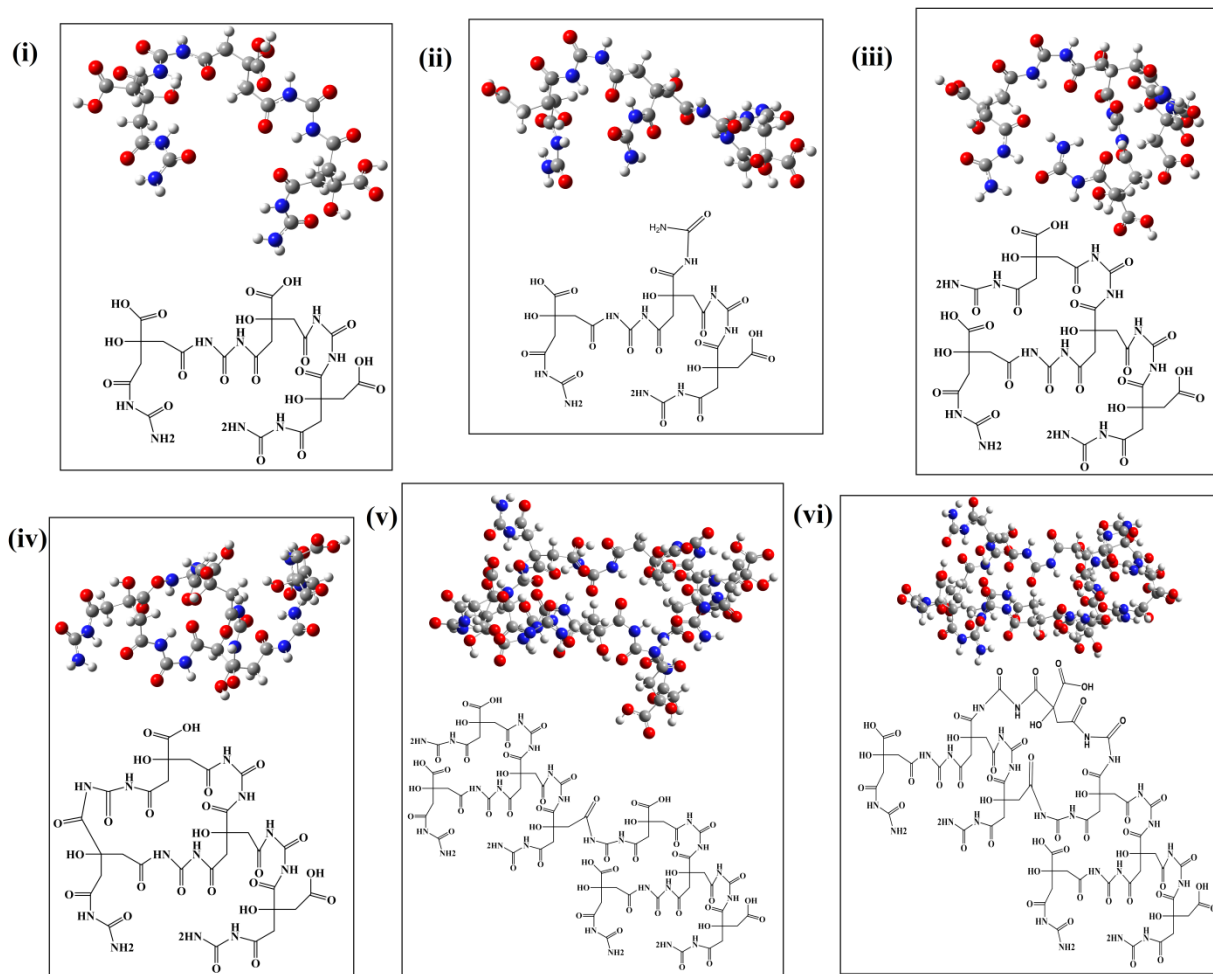


Figure S27: The optimized geometries of the polymeric units (i to vi)

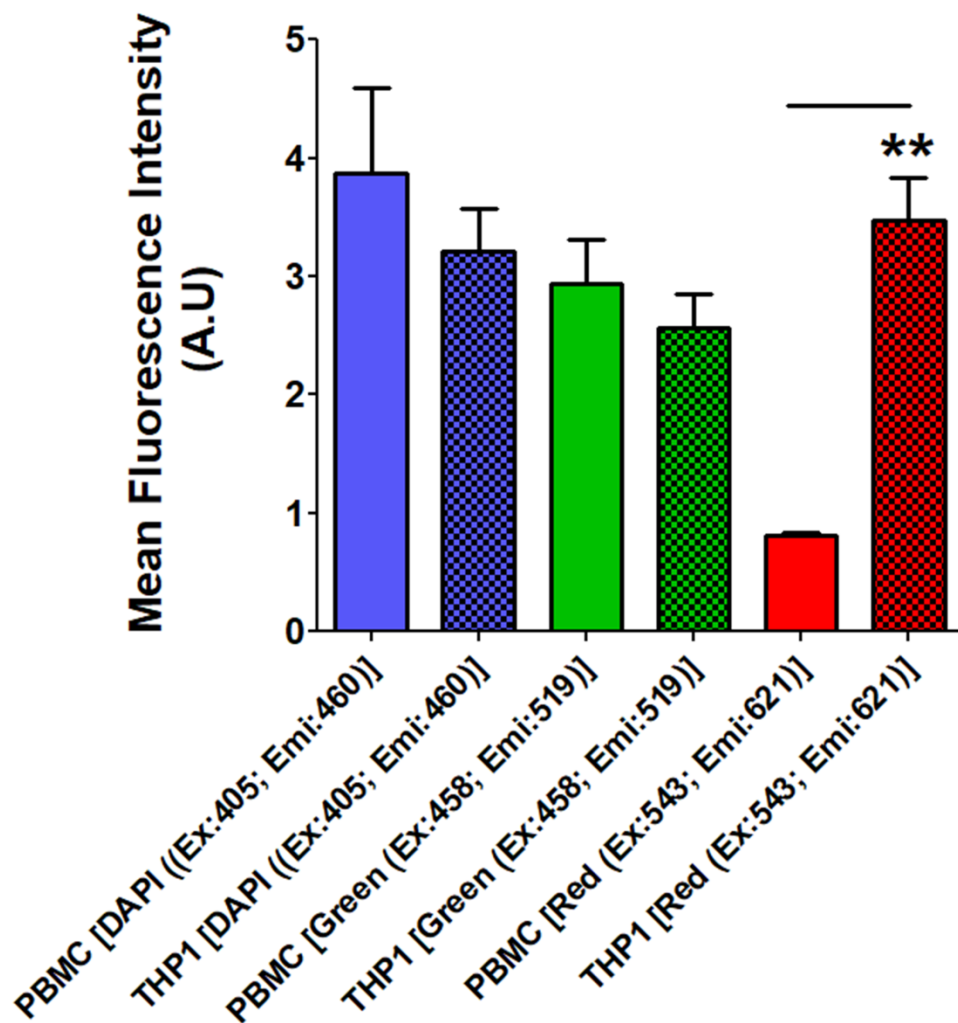


Figure S28: The comparative intensity bar graph for the fluorescence cell imaging done with One way ANOVA with Tukey's Post-Hoc test (significance: ** $p < 0.01$).

Cartesian coordinates:

Structure-(i)

Symbol	X	Y	Z
N	-3.13727600	-4.92502100	-3.17726700
H	-2.15755500	-4.93037000	-2.92973800
H	-3.57954300	-5.82766400	-3.28333900
C	-3.58837200	-3.80593300	-3.81023600

O	-2.93001200	-2.77583000	-3.89453600
N	-4.89619200	-3.95770600	-4.31842000
H	-5.33864500	-4.86438400	-4.20590300
C	-5.74179200	-3.06099300	-4.95249000
O	-6.84936700	-3.45862500	-5.30211500
C	-5.29544500	-1.63257400	-5.20067500
H	-4.23025200	-1.52538000	-5.01029600
H	-5.49749100	-1.41340900	-6.25265300
C	-6.07194600	-0.64188500	-4.30587900
O	-5.91717200	-1.07776400	-2.96321700
H	-6.02300900	-0.28430500	-2.40505400
C	-7.60135500	-0.56887900	-4.61198600
H	-8.04030500	0.11242900	-3.87661400
H	-8.00818300	-1.56736000	-4.44901100
C	-5.47808300	0.77698700	-4.39055900
O	-4.91270800	1.07175000	-5.56351100
H	-4.60394300	1.99888300	-5.52691600
O	-5.53493900	1.54001100	-3.44555100
C	-7.95950400	-0.01309400	-5.98377800
O	-7.86095300	1.17691500	-6.23147300
N	-8.40353700	-0.97026500	-6.89371400
H	-8.48052700	-1.94574400	-6.59185200
C	-8.81911400	-0.70742800	-8.19366100
N	-9.34525200	-1.81726500	-8.87893400
H	-9.64223400	-1.59959800	-9.82990500
O	-8.75543800	0.36874800	-8.75856900
C	-9.63457100	-3.08930500	-8.42541900
C	-10.22350000	-4.04207900	-9.46251300
H	-9.39460600	-4.39868100	-10.08687100
O	-9.36910200	-3.47750100	-7.29262900
C	-11.31481500	-3.50980700	-10.40264900
O	-10.71590800	-2.47501300	-11.20087200
H	-11.41620300	-2.02084600	-11.70218600
C	-11.81460600	-4.61391200	-11.36066700
H	-12.49762900	-4.16229000	-12.09107900
H	-10.95751700	-4.99503700	-11.92444300
C	-12.56840900	-5.74201800	-10.68121100
N	-12.64523200	-6.90516100	-11.41866900
H	-12.17982600	-6.93091200	-12.31958500
O	-13.08813500	-5.60990900	-9.57528300
C	-13.30981200	-8.12063600	-11.13995200
N	-13.96685300	-8.14299600	-9.91851600
H	-13.90875500	-7.29578100	-9.34625800
O	-13.26664600	-9.02567400	-11.94755200
C	-14.68981000	-9.20805200	-9.41450500
O	-14.85080800	-10.28369100	-9.96135600

C	-15.28189000	-8.94187900	-8.00219700
O	-15.20982000	-7.54883900	-7.67105200
H	-15.96017200	-7.07740100	-8.07366800
C	-14.35480200	-9.66849800	-6.99889600
H	-14.24803500	-10.71127500	-7.29324400
H	-13.36595600	-9.19596500	-7.06484800
C	-16.76465900	-9.39052000	-7.97312800
H	-17.14381700	-9.22951100	-6.95770600
H	-17.33724700	-8.74727400	-8.64752000
C	-17.08868100	-10.81982200	-8.37122300
O	-16.49452500	-11.72569100	-7.56773200
H	-16.76980800	-12.61167600	-7.87368800
O	-17.85889000	-11.12559300	-9.25614400
C	-14.75697300	-9.67018200	-5.52350900
N	-15.21544400	-8.47296100	-5.03060300
H	-15.28440700	-7.70206700	-5.69129200
O	-14.61232600	-10.68083900	-4.83863500
C	-15.60770800	-8.13596800	-3.70890800
O	-15.97915800	-6.98916900	-3.47668200
N	-15.53901900	-9.13590700	-2.80728000
H	-15.78128400	-8.93047000	-1.84945100
H	-15.19059400	-10.04727500	-3.08505000
H	-10.60930400	-4.89409600	-8.90193900
C	-12.46588900	-2.86991100	-9.59899300
O	-12.46501700	-2.67628800	-8.40461300
O	-13.44151300	-2.45806400	-10.43024300
H	-14.11695900	-1.98813500	-9.90297100

Structure-(ii)

Symbol	X	Y	Z
N	-2.88652800	-4.97976500	-3.64399500
H	-1.88736800	-4.99505400	-3.49472300
H	-3.35093200	-5.87574100	-3.69668100
C	-3.39438500	-3.85108400	-4.21183000
O	-2.74234500	-2.82316900	-4.35348500
N	-4.74886000	-3.99186500	-4.58328600
H	-5.17714100	-4.90230300	-4.44788900
C	-5.65284600	-3.08309500	-5.11013900
O	-6.78883300	-3.47572100	-5.36063600
C	-5.23521900	-1.64689200	-5.36278300
H	-4.15743300	-1.53883100	-5.26592200
H	-5.53111100	-1.40357600	-6.38680100
C	-5.93058900	-0.68200100	-4.37738300
O	-5.64777300	-1.14510600	-3.06547900
H	-5.68861200	-0.36160800	-2.48505500

C	-7.48326500	-0.61184900	-4.53511800
H	-7.85281000	0.04832800	-3.74462400
H	-7.86723300	-1.61725700	-4.35929800
C	-5.35469600	0.74205800	-4.48932500
O	-4.93605200	1.07360400	-5.71301600
H	-4.63083700	2.00233200	-5.68890100
O	-5.30206400	1.47821100	-3.52302000
C	-7.97389700	-0.02653800	-5.85261100
O	-7.94193300	1.17427000	-6.06348000
N	-8.45160500	-0.97118100	-6.75856200
H	-8.48982400	-1.95488900	-6.47646100
C	-8.95262000	-0.68665100	-8.02399600
N	-9.51074700	-1.78605200	-8.69782400
H	-9.87149800	-1.55000400	-9.62132400
O	-8.93106600	0.40138800	-8.56983000
C	-9.78076400	-3.06427100	-8.24791000
C	-10.42816600	-4.00273500	-9.26304800
H	-9.63299000	-4.34392900	-9.93781300
O	-9.44129400	-3.47373000	-7.14278300
C	-11.57427800	-3.47319800	-10.14420900
O	-11.01291800	-2.41557700	-10.93971900
H	-11.71123300	-1.94245200	-11.42390800
C	-12.06068600	-4.58885500	-11.09841900
H	-12.72814100	-4.17764500	-11.86752900
H	-11.19151800	-4.96462800	-11.64853500
C	-12.78389900	-5.73667500	-10.41114500
N	-12.97787900	-6.84328000	-11.20955100
H	-12.62088900	-6.81716200	-12.15877300
O	-13.17270200	-5.66679200	-9.24786900
C	-13.63880100	-8.06263200	-10.93583000
N	-14.15002900	-8.15806200	-9.65024800
H	-14.00566100	-7.35474000	-9.03234300
O	-13.71341600	-8.90924400	-11.80205200
C	-14.83613300	-9.24455000	-9.13949700
O	-15.09009300	-10.27275700	-9.73943800
C	-15.24504000	-9.07698100	-7.64943100
O	-15.10115100	-7.71406400	-7.22852000
H	-15.89027300	-7.20619000	-7.48657900
C	-14.21829400	-9.88967900	-6.82455200
H	-14.16770600	-10.90720400	-7.20849000
H	-13.23559900	-9.42317200	-6.97331400
C	-16.72280000	-9.50792800	-7.47089900
H	-16.97384800	-9.41199300	-6.40857700
H	-17.35978000	-8.81395300	-8.02700700
C	-17.12061000	-10.90314800	-7.92020600
O	-16.45355400	-11.86807900	-7.25441800

H	-16.78156100	-12.72816300	-7.58148800
O	-17.99618300	-11.13955700	-8.72469300
C	-14.44268400	-10.00212700	-5.31613800
N	-14.80717300	-8.83964400	-4.68165900
H	-14.93187700	-8.01766700	-5.26834600
O	-14.24611700	-11.06627500	-4.73288900
C	-15.03079800	-8.60115000	-3.30064600
O	-15.33548900	-7.46863300	-2.93788800
N	-14.89118500	-9.67223000	-2.49370700
H	-15.00278300	-9.53651900	-1.49998500
H	-14.59777500	-10.56346800	-2.87949700
H	-10.77616500	-4.86527900	-8.69473700
C	-12.69456500	-2.87469200	-9.24383900
O	-12.48645300	-2.63731400	-8.05853000
N	-13.85923200	-2.54239700	-9.88740200
H	-13.99707900	-2.81220400	-10.85326900
C	-15.02896800	-1.90574000	-9.36863700
O	-15.98114200	-1.74399200	-10.12212100
N	-14.96409300	-1.52900800	-8.07910900
H	-14.14634100	-1.74490800	-7.52020200
H	-15.78199700	-1.10254400	-7.66902300

Structure-(iii)

Symbol	X	Y	Z
N	-9.13741300	-1.39670800	0.02272000
H	-9.00188100	-1.04159900	0.95797000
H	-10.00804000	-1.86789500	-0.18965400
C	-8.03733600	-1.51957000	-0.76843600
O	-6.93343000	-1.07457400	-0.47484100
N	-8.33802300	-2.21941300	-1.95700200
H	-9.27750700	-2.63722200	-1.99834900
C	-7.59371200	-2.43555800	-3.08655600
O	-8.05325700	-3.16621400	-3.97426200
C	-6.24796400	-1.76707900	-3.27632300
H	-5.83230500	-1.45901700	-2.31947800
H	-5.59086400	-2.49983300	-3.74761300
C	-6.34457900	-0.53019100	-4.19227300
O	-7.11345500	0.44345300	-3.47979500
H	-7.10293500	1.26166700	-4.00756400
C	-7.03095900	-0.78748000	-5.55228300
H	-7.00836400	0.15190300	-6.12040000
H	-8.07924300	-1.03595900	-5.37456600
C	-4.96514300	0.11871700	-4.44179300

O	-3.94257800	-0.45933900	-3.80120300
H	-3.13969400	0.06382500	-3.99573200
O	-4.85642700	1.12776800	-5.11157100
C	-6.35164100	-1.84515900	-6.40402500
O	-5.16694500	-2.11418500	-6.29788600
N	-7.20931900	-2.43304100	-7.33012700
H	-8.19371300	-2.15576300	-7.33966700
C	-6.86413500	-3.39024900	-8.26811400
N	-7.94370400	-3.81758700	-9.07686500
H	-7.65106500	-4.51775500	-9.74890400
O	-5.76167100	-3.86917900	-8.44373900
C	-9.27120900	-3.44424600	-9.06982100
C	-10.14946700	-4.19964900	-10.04434700
H	-9.56174100	-4.58111200	-10.88439600
H	-10.57558300	-5.05321700	-9.51599700
O	-9.72567600	-2.59264800	-8.30551600
C	-11.24170700	-3.29699200	-10.63055800
O	-10.55830700	-2.32739800	-11.40246100
H	-11.06119600	-1.49452500	-11.28372200
C	-12.17557200	-4.07475100	-11.62906600
H	-12.87260500	-3.35176600	-12.06180800
H	-11.51944500	-4.42555200	-12.43017900
C	-12.13929100	-2.48645700	-9.63470100
O	-12.31479200	-1.30340400	-9.90018000
N	-12.91578800	-3.00531900	-8.60220500
H	-13.61771500	-2.33169600	-8.27197500
C	-12.88118800	-4.16714400	-7.85675400
N	-13.89242100	-4.25643100	-6.89469500
H	-13.74780700	-5.03386100	-6.25031600
O	-12.08774100	-5.09251800	-7.97788300
C	-14.97688900	-3.42917900	-6.64668400
C	-16.02285800	-4.00105600	-5.69535300
H	-16.94917500	-3.50834200	-6.00185600
H	-16.14899400	-5.07516000	-5.86035200
O	-15.13177600	-2.34953700	-7.20607000
C	-15.78751000	-3.71691600	-4.16739300
C	-17.17930200	-3.51679700	-3.54060700
O	-17.92801600	-4.61997900	-3.56996100
H	-18.80026900	-4.41645500	-3.17721700
O	-17.53300400	-2.44439300	-3.09349200
O	-15.05267900	-2.52823500	-3.97733900
H	-15.69067700	-1.85007900	-3.67716900
C	-15.08512700	-4.87822500	-3.39648500
H	-15.49429200	-5.83960700	-3.71542000
H	-15.29066400	-4.75121100	-2.32904300
C	-13.58489800	-4.91273600	-3.61694900

O	-13.07462800	-5.54250100	-4.55224400
N	-12.84191700	-4.19950500	-2.71749600
H	-13.33569900	-3.68390500	-1.99871900
C	-11.46052100	-3.88761500	-2.74624300
N	-10.72466100	-4.43666800	-3.71734700
H	-11.18095500	-5.00108600	-4.42556800
H	-9.76416700	-4.10552900	-3.83732700
O	-11.03630900	-3.12677400	-1.86414500
C	-12.88811700	-5.28844700	-11.06750300
N	-14.25502300	-5.15279400	-10.88558400
H	-14.71465800	-4.33309700	-11.26614700
O	-12.27883200	-6.31241100	-10.77174800
C	-15.15053100	-5.97528000	-10.16550000
N	-14.52430200	-7.00964000	-9.48321100
H	-13.52784300	-7.14295200	-9.68044300
O	-16.33335400	-5.70744800	-10.13487200
C	-15.06770900	-7.72561600	-8.43410100
O	-16.23290300	-7.69950900	-8.08247200
C	-14.02343900	-8.61618000	-7.70102000
O	-12.68992700	-8.23737300	-8.05729700
H	-12.46900600	-7.35820500	-7.69126000
C	-14.21708700	-10.05527200	-8.23416700
H	-15.25952100	-10.34763800	-8.11381100
H	-13.99042100	-10.04682900	-9.30816700
C	-14.20396500	-8.47662700	-6.16530400
H	-13.54460800	-9.20841400	-5.68571600
H	-13.86996300	-7.48680200	-5.84884700
C	-15.59826900	-8.65942200	-5.59585900
O	-16.08127600	-9.90070200	-5.79584600
H	-16.96766000	-9.94075000	-5.38669200
O	-16.19783800	-7.81823000	-4.95460900
C	-13.37830300	-11.16788200	-7.60302300
N	-12.05618000	-10.86714700	-7.38515800
H	-11.75700900	-9.92072400	-7.61083400
O	-13.87708000	-12.26738600	-7.36998100
C	-11.02031300	-11.69036500	-6.87138100
O	-9.89271000	-11.21868700	-6.75678500
N	-11.38091400	-12.94811000	-6.54694700
H	-10.67024200	-13.57104900	-6.19314100
H	-12.33689100	-13.25601300	-6.68953600

Structure-(iv)

Symbol	X	Y	Z
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C	0.03142400	0.05173600	0.02190300
O	0.03001800	0.08795800	1.43242900
H	0.96673000	0.10572600	1.72039000
C	-0.19700100	1.50869200	-0.51836800
H	0.62112300	2.12384900	-0.13426200
H	-1.12966900	1.87975600	-0.08767900
C	-0.18486900	1.64704000	-2.03731200
O	0.85720400	1.72137200	-2.67956800
N	-1.44276700	1.66448400	-2.61636400
H	-2.24831500	1.41238800	-2.03889200
C	-1.71168700	1.83672200	-3.97308300
N	-3.04437800	1.56587600	-4.33510200
H	-3.28652600	1.86534700	-5.27955700
O	-0.92088000	2.22621200	-4.80792700
C	-4.05760100	0.96651400	-3.61071600
C	-5.39232300	0.86829800	-4.33462600
H	-5.29424100	0.16706700	-5.17162400
H	-6.11065000	0.46034800	-3.63010500
O	-3.90826900	0.54858300	-2.46589800
C	-5.88292500	2.20121400	-4.93815800
O	-5.07008000	2.42961000	-6.09228100
H	-5.00046200	3.40388300	-6.18077900
C	-7.35269300	2.13381500	-5.47066200
H	-7.61929900	3.13211700	-5.83122800
H	-7.30415500	1.47437400	-6.34132800
C	-5.65311100	3.47179500	-4.04824000
O	-5.27031000	4.48580800	-4.61888200
N	-5.75729700	3.50962800	-2.66872900
H	-5.31517900	4.33110000	-2.23762600
C	-6.42175500	2.68285900	-1.77895300
N	-6.23845900	3.02141600	-0.43141200
H	-6.79121900	2.43305300	0.18115100
O	-7.14442300	1.75063200	-2.08217300
C	-5.46680900	4.03096800	0.13443400
C	-5.53570100	4.13091300	1.64854900
H	-5.63899800	5.20182900	1.84913300
H	-6.42511400	3.63341600	2.04454900
O	-4.82589600	4.82567300	-0.54245700
C	-4.26921200	3.62864500	2.42835700
C	-4.39766100	4.23804500	3.84418800
O	-5.43545400	3.76387300	4.53701200
H	-5.46239400	4.21539600	5.40410200
O	-3.62773700	5.08702300	4.24624700
O	-3.08215600	4.12518300	1.86337400
H	-2.79411200	4.85986500	2.44100700
C	-4.18723600	2.09183000	2.58786600

H	-5.06199000	1.73713200	3.13859200
H	-3.31308300	1.87406200	3.21576600
C	-3.98378500	1.27778100	1.31455600
O	-3.35779700	1.66694300	0.34216300
N	-4.54688400	0.00802000	1.39159600
H	-5.33782100	-0.10477000	2.01715600
C	-4.53996400	-0.96896300	0.36889000
N	-3.31580700	-1.46440600	-0.03084800
H	-3.20814800	-1.72836300	-1.00967900
O	-5.56446600	-1.48522600	-0.03931000
C	-8.43257100	1.55471900	-4.57120200
N	-9.33801800	2.46871000	-4.06532800
H	-9.22810300	3.44525900	-4.31295700
O	-8.51084400	0.34778400	-4.36379300
C	-10.39088200	2.28272200	-3.14557300
N	-10.56945500	0.96726700	-2.74517300
H	-9.93397000	0.27362300	-3.15250100
O	-11.04337300	3.23927900	-2.77694100
C	-11.51299700	0.51993400	-1.83969300
O	-12.33539900	1.21235700	-1.26690400
C	-11.47919100	-1.01940100	-1.62697200
O	-10.28535600	-1.59492900	-2.15479700
H	-9.55445100	-1.44993300	-1.52940300
C	-12.62291800	-1.60446400	-2.49232500
H	-13.58200200	-1.28552500	-2.07952500
H	-12.53328200	-1.19289100	-3.50183000
C	-11.57250800	-1.33556700	-0.11319900
H	-11.63699800	-2.42315500	-0.01629500
H	-10.65105700	-0.99520000	0.36815200
C	-12.71235800	-0.72726400	0.68072700
O	-13.92820600	-1.11235900	0.23549100
H	-14.59209900	-0.69003900	0.81439200
O	-12.56743000	-0.03633800	1.66792700
C	-12.60389500	-3.12787900	-2.52850000
N	-12.42631500	-3.67483700	-3.77648800
H	-12.29957100	-3.05383900	-4.56580800
O	-12.75503600	-3.80692100	-1.51297100
C	-12.38059800	-5.04290300	-4.16539600
O	-12.20792200	-5.31022300	-5.35025900
N	-12.53764300	-5.93687400	-3.17057200
H	-12.50040100	-6.91824000	-3.40292400
H	-12.66087500	-5.61974300	-2.21490400
C	-1.15666900	-0.79012300	-0.46119500
O	-1.23867600	-1.30849600	-1.55445200
O	-2.15703600	-0.81634600	0.44891700
C	1.33668400	-0.57669700	-0.52633000

H	1.42444500	-1.59179800	-0.12847500
H	1.30007900	-0.63804700	-1.61383800
C	2.53952700	0.21045100	-0.01717900
O	2.85959900	0.14185800	1.16788600
N	3.13950000	1.00944500	-0.95860900
H	2.59367500	1.15018300	-1.80946000
C	4.26193800	1.85138400	-0.75624200
O	5.06288800	1.70237500	0.15213600
N	4.37599100	2.79387100	-1.73789300
H	3.57422400	3.07506000	-2.28749400
H	5.08718800	3.49803700	-1.59486400

Structure-(v)

Symbol	X	Y	Z
N	-7.87540100	-3.80146000	-4.93871600
H	-8.85293500	-4.00527600	-4.72653300
C	-7.64309900	-2.65592300	-5.69637400
O	-6.55344400	-2.33213300	-6.16288000
N	-8.82127800	-1.95266000	-5.86837300
H	-9.65440800	-2.34996000	-5.40350700
C	-9.10198700	-0.79210800	-6.57909000
O	-10.25822400	-0.37967700	-6.53951200
C	-7.99433600	-0.13596000	-7.37577500
H	-7.09802200	-0.09283100	-6.75287000
H	-7.73538700	-0.80242200	-8.20586400
C	-8.31221600	1.27904700	-7.88804700
O	-8.56885400	2.09829700	-6.75943200
H	-8.31353900	3.00340500	-7.02114800
C	-9.54011400	1.38477900	-8.85562700
H	-9.61766800	2.43435500	-9.15447900
H	-10.42061000	1.12016800	-8.27183500
C	-7.08476300	1.88381500	-8.60426900
O	-6.29370200	0.99280400	-9.20561700
H	-5.57563100	1.47923800	-9.65765200
O	-6.88790600	3.08351900	-8.60184900
C	-9.41408800	0.57027900	-10.13317500
O	-8.69098700	0.91857800	-11.04902500
N	-10.17590100	-0.60242300	-10.14157200
H	-10.83601800	-0.77822300	-9.38108700
C	-10.13010700	-1.57916300	-11.12436000
N	-10.97811500	-2.68543700	-10.88957700
H	-10.85606900	-3.39860500	-11.59905300
O	-9.42704500	-1.57315600	-12.11501700
C	-11.90492800	-2.91678000	-9.89510800

C	-12.52327700	-4.30122500	-9.90995900
H	-12.18683200	-4.87952800	-10.77354000
H	-12.18465000	-4.81274900	-9.01076000
O	-12.18281900	-2.09038400	-9.02716100
C	-14.06026300	-4.24181600	-9.97497400
O	-14.36771500	-3.54721700	-11.16920300
H	-15.06840700	-2.90312800	-10.93476300
C	-14.70535600	-5.67286700	-10.12863200
H	-15.79279400	-5.56817800	-10.08011900
H	-14.44928900	-5.97880100	-11.14648200
C	-14.78934200	-3.45049400	-8.83332600
O	-15.52843300	-2.53753600	-9.17300900
N	-14.83972200	-3.81895400	-7.48981600
H	-15.64112700	-3.40921700	-6.99384900
C	-14.06232300	-4.63951600	-6.70745600
N	-14.62489600	-4.96425100	-5.46894600
H	-14.08216700	-5.65708000	-4.96181000
O	-12.96925400	-5.10398200	-7.01559900
C	-15.85557300	-4.59750500	-4.91913100
C	-16.20286100	-5.33778800	-3.63889600
H	-17.25023000	-5.63543300	-3.74899700
H	-15.60448700	-6.24785800	-3.54502100
O	-16.59401300	-3.78063400	-5.45018500
C	-16.10688500	-4.49698100	-2.32143900
C	-16.65895300	-5.41224600	-1.20401600
O	-15.89790600	-6.48195800	-0.96427500
H	-16.32360800	-7.01631500	-0.26452400
O	-17.70235600	-5.16326600	-0.63408300
O	-16.93903500	-3.36727100	-2.39171000
H	-17.72220900	-3.57513900	-1.84399500
C	-14.66243300	-4.08365600	-1.92299400
H	-14.04983900	-4.97747000	-1.78679800
H	-14.73143200	-3.57958900	-0.95180700
C	-13.98164100	-3.09410200	-2.86320700
O	-14.50832000	-2.04185400	-3.21139800
N	-12.71400000	-3.47132100	-3.26459500
H	-12.33494700	-4.36989100	-2.94776300
C	-11.86613200	-2.79353900	-4.15462900
N	-12.27003900	-1.61293200	-4.62975000
H	-13.17380200	-1.25028000	-4.34211200
H	-11.68129600	-1.12693800	-5.30470500
O	-10.78742000	-3.34210000	-4.45950500
C	-14.19036100	-6.76341300	-9.20683100
N	-15.08443200	-7.23432700	-8.25117900
H	-16.06313600	-6.98057600	-8.33588500
O	-13.04519900	-7.19133200	-9.29564800

C	-14.81426100	-7.92925500	-7.05494000
N	-13.45081000	-8.14265000	-6.81176000
H	-12.83747800	-8.01070600	-7.62234200
O	-15.71130500	-8.21904900	-6.29367200
C	-12.87423200	-7.92559800	-5.57654200
O	-13.49088000	-7.77325300	-4.53092400
C	-11.32358700	-7.78846900	-5.63613000
O	-10.96936500	-7.24933200	-6.91256500
H	-11.35334800	-6.35391000	-6.98938400
C	-10.69327100	-9.19824600	-5.54852500
H	-10.94962900	-9.64877300	-4.58999000
H	-11.13338400	-9.82169800	-6.33770000
C	-10.85118400	-6.80356200	-4.53749500
H	-9.75475800	-6.80110400	-4.52331200
H	-11.15639000	-5.79346700	-4.81870600
C	-11.32456600	-7.01921700	-3.11657400
O	-11.05880300	-8.24492300	-2.64415800
H	-11.37027600	-8.28514900	-1.71845900
O	-11.81826500	-6.14828500	-2.41632600
C	-9.17307600	-9.33038300	-5.70880200
N	-8.60290600	-8.55271300	-6.67363400
H	-9.19576600	-7.83222100	-7.08339600
O	-8.55590200	-10.16785200	-5.04236100
C	-7.27221300	-8.55356100	-7.17817700
O	-6.90133800	-7.58568900	-7.83926400
N	-6.55259500	-9.66856800	-6.95061100
H	-5.55521300	-9.62507800	-7.14541000
H	-6.86572000	-10.30500000	-6.22808500
N	-1.28946000	-5.46647000	2.48437100
H	-2.26569300	-5.48028600	2.74484900
H	-0.85210100	-4.55758300	2.41969000
C	-0.83350800	-6.55492600	1.80558100
O	-1.48080000	-7.58741500	1.68293900
N	0.47054700	-6.36891600	1.29351000
H	0.89238100	-5.45286900	1.41110000
C	1.30175900	-7.22249700	0.59446600
O	2.38184700	-6.77834500	0.19999300
C	0.90531300	-8.65833900	0.33180100
H	-0.14002800	-8.82297200	0.58270700
H	1.04257000	-8.83834100	-0.73578200
C	1.76736900	-9.65083000	1.14940700
O	1.54643100	-9.38424000	2.52570300
H	1.40996600	-10.25979000	2.94054700
C	3.31296400	-9.55360000	0.93015700
H	3.76547600	-10.26105000	1.62911700
H	3.60655400	-8.54354800	1.22479200

C	1.26729800	-11.08546200	0.87247200
O	1.09393300	-11.36341500	-0.40986900
H	0.68359700	-12.27314200	-0.52292500
O	1.05484000	-11.85363500	1.79733400
C	3.90252500	-9.88888600	-0.43522800
O	4.41357300	-10.97311700	-0.66147600
N	3.81746600	-8.86955100	-1.38488400
H	3.22866100	-8.06107300	-1.16752800
C	4.36057900	-8.99309300	-2.66791900
N	3.58105700	-8.47829500	-3.71929200
H	3.94927400	-8.72255400	-4.63355000
O	5.41017600	-9.55176800	-2.91956800
C	2.24232200	-8.11405800	-3.68040800
C	1.38874900	-8.63542500	-4.82302200
H	1.72152200	-9.65387500	-5.03542000
H	0.37040100	-8.69963200	-4.45149100
O	1.77151000	-7.52644100	-2.71151100
C	1.43632700	-7.86511200	-6.16552100
O	2.79829700	-7.57181400	-6.43772300
H	2.85617200	-6.59549900	-6.51867800
C	0.95783900	-8.76030300	-7.37912300
H	0.68661200	-8.11710400	-8.22080000
H	1.86044200	-9.30702000	-7.66462000
C	0.70864600	-6.46642100	-6.14981700
O	1.40339200	-5.47544200	-6.33097600
N	-0.66370000	-6.26536700	-6.03936600
H	-0.97214500	-5.30351400	-6.21888600
C	-1.66234400	-7.14225100	-5.67466700
N	-2.97158600	-6.66729400	-5.75129100
H	-3.64105100	-7.41404400	-5.57265500
O	-1.47177500	-8.29161800	-5.30631300
C	-3.44424000	-5.37729200	-5.98253400
C	-4.95334200	-5.24624000	-5.87181900
H	-5.25334200	-4.50938000	-6.62240500
H	-5.43982200	-6.19226400	-6.13032100
O	-2.69878300	-4.44894200	-6.26402400
C	-5.49779900	-4.73746300	-4.48879400
O	-5.09390400	-3.42620200	-4.20469500
H	-5.33726800	-2.86840100	-4.97409500
C	-5.12750800	-5.60891500	-3.25815000
H	-5.59451100	-6.58922800	-3.35231600
H	-5.58760900	-5.12224200	-2.38867200
C	-3.64726100	-5.74094300	-2.93297400
O	-2.84986700	-4.81246900	-3.02829500
N	-3.28447200	-7.00346300	-2.49407900
H	-4.00958900	-7.72379000	-2.45055500

C	-1.97666400	-7.47811400	-2.25801200
N	-0.98472900	-6.57878900	-2.29520300
H	-1.20804500	-5.62187800	-2.55346000
H	-0.02831200	-6.92637900	-2.35123100
O	-1.80777400	-8.68679000	-2.02440400
C	-0.10193000	-9.81478400	-7.09981100
N	-1.31601900	-9.68073500	-7.77153500
H	-1.37490300	-9.01032800	-8.53056800
O	0.10309700	-10.74901500	-6.33524500
C	-2.57987000	-10.04221700	-7.28756700
N	-2.58481900	-10.80098600	-6.11388700
H	-1.67372200	-11.18012600	-5.84270800
O	-3.58498000	-9.65586600	-7.85834200
C	-3.45149600	-10.48910900	-5.07578600
O	-4.30399500	-9.61987500	-5.14664300
C	-3.17840000	-11.28860500	-3.76783500
O	-1.80361700	-11.04403700	-3.45045700
H	-1.72346000	-10.14791900	-3.04089100
C	-3.32564900	-12.80316100	-4.03717900
H	-4.36432000	-13.02180800	-4.29564700
H	-2.70769600	-13.08598000	-4.89761300
C	-4.09852300	-10.81809700	-2.59605000
H	-4.33166800	-11.68274800	-1.96584700
H	-3.53848800	-10.10948200	-1.98820300
C	-5.41254600	-10.14348300	-2.94564000
O	-6.28130500	-10.97172000	-3.53955200
H	-7.08542300	-10.47968000	-3.82643000
O	-5.68081900	-8.99312300	-2.63089900
C	-2.95101700	-13.75539000	-2.89693300
N	-1.78499700	-13.45312500	-2.22486400
H	-1.34483500	-12.56689000	-2.47701800
O	-3.63145100	-14.75095300	-2.66464500
C	-1.14076200	-14.18495900	-1.21352200
O	-0.08300200	-13.75993000	-0.72381600
N	-1.71698700	-15.33720200	-0.84282800
H	-1.27338500	-15.88304900	-0.11855300
H	-2.58356200	-15.63309500	-1.28066200
C	-7.05500900	-4.87924500	-4.59059400
O	-7.60369600	-5.93054400	-4.30088100

Structure-(vi)

Symbol	X	Y	Z
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N	-7.95852300	-3.32399700	-4.17636100
H	-8.96772600	-3.36556400	-4.01437000
C	-7.55099800	-2.53424600	-5.25011600
O	-6.38759500	-2.35881300	-5.60386000
N	-8.65904100	-1.98648600	-5.87177500
H	-9.57411300	-2.27896100	-5.49180000
C	-8.78615200	-1.10069200	-6.93314800
O	-9.92426500	-0.73343800	-7.21518600
C	-7.54321800	-0.68339000	-7.68936300
H	-6.77330200	-0.40513300	-6.96530000
H	-7.14906400	-1.56799900	-8.20105300
C	-7.73987100	0.47793500	-8.67799900
O	-8.15723300	1.61185900	-7.93583500
H	-7.84306900	2.38966900	-8.43503500
C	-8.79229000	0.22336300	-9.81114000
H	-8.78712900	1.10863300	-10.45391500
H	-9.76263400	0.14887500	-9.32264700
C	-6.39980200	0.85486000	-9.34675000
O	-5.54279000	-0.15804300	-9.49180400
H	-4.75090600	0.17752800	-9.95760400
O	-6.17879300	1.99559400	-9.70462400
C	-8.49018800	-0.97181400	-10.70055000
O	-7.62122800	-0.93665400	-11.55280400
N	-9.27699500	-2.09697300	-10.43371500
H	-10.05644200	-2.02103900	-9.77645700
C	-9.10955500	-3.34382100	-11.01607400
N	-10.03579200	-4.32105700	-10.58567900
H	-9.83504000	-5.22421800	-10.99912900
O	-8.24966900	-3.65562400	-11.81572900
C	-11.12075600	-4.22609000	-9.73919300
C	-11.80542300	-5.54401200	-9.43373700
H	-11.40647700	-6.35196200	-10.05156900
H	-11.59692100	-5.78080600	-8.39117400
O	-11.48464700	-3.16850500	-9.22703700
C	-13.32065500	-5.47621700	-9.69579400
O	-13.46157800	-5.14417400	-11.06463400
H	-14.14985200	-4.44694000	-11.10207100
C	-14.01795000	-6.88059000	-9.52099100
H	-15.09634900	-6.74624400	-9.64483400
H	-13.66033600	-7.46939500	-10.36968700
C	-14.12853600	-4.38015200	-8.91611600
O	-14.78624900	-3.59400400	-9.58427300
N	-14.32667000	-4.34141100	-7.53899600
H	-15.14233800	-3.77953400	-7.26677100
C	-13.68351900	-4.94502900	-6.48074700
N	-14.37783000	-4.88442900	-5.26682500

H	-13.92890700	-5.43030600	-4.53517100
O	-12.60801100	-5.52906600	-6.52864000
C	-15.62873400	-4.34315600	-4.97640600
C	-16.14666000	-4.70398400	-3.59314300
H	-17.17069000	-5.05859600	-3.74959100
H	-15.56996200	-5.52953800	-3.16867200
O	-16.25918100	-3.67323800	-5.78325400
C	-16.22749100	-3.52704300	-2.56554300
C	-16.92765200	-4.10789100	-1.31541200
O	-16.21307500	-5.04581900	-0.69056500
H	-16.72839100	-5.37216100	0.07388700
O	-18.03247800	-3.73642600	-0.97356800
O	-17.03433500	-2.48833400	-3.05835800
H	-17.88030200	-2.54862100	-2.57127100
C	-14.84705200	-2.96862400	-2.11166200
H	-14.25518100	-3.77516200	-1.67270900
H	-15.04309500	-2.23275700	-1.32414900
C	-14.05770600	-2.23467500	-3.18978800
O	-14.49180000	-1.24459700	-3.76901500
N	-12.80602700	-2.76340800	-3.44331700
H	-12.47997300	-3.58160600	-2.92269500
C	-11.89073400	-2.35568400	-4.42247500
N	-12.19813600	-1.30062000	-5.18029200
H	-13.08070900	-0.82242900	-5.02760900
H	-11.55406500	-1.02731300	-5.92024400
O	-10.84195500	-3.02248000	-4.54232400
C	-13.67905700	-7.67399400	-8.27166500
N	-14.70035200	-7.80480200	-7.33461600
H	-15.64049000	-7.53444100	-7.60380500
O	-12.56702900	-8.15945400	-8.09940800
C	-14.60197500	-8.08996200	-5.95929600
N	-13.29679900	-8.33406500	-5.51603600
H	-12.61215100	-8.55428000	-6.24482800
O	-15.58081300	-8.03904200	-5.24560500
C	-12.78302100	-7.79040100	-4.35958500
O	-13.43268100	-7.23988300	-3.48021500
C	-11.23461800	-7.87813700	-4.26778100
O	-10.66445200	-8.15125400	-5.54131700
H	-10.73183500	-7.35240700	-6.09492400
C	-10.90923100	-9.11840100	-3.38930300
H	-11.18099500	-8.91893900	-2.35094300
H	-11.50738800	-9.95851200	-3.74852600
C	-10.69256300	-6.50506700	-3.77067300
H	-9.60298000	-6.53148900	-3.86266100
H	-11.05733300	-5.72463500	-4.44218600
C	-11.01291800	-6.07204700	-2.35609700

O	-10.40587200	-6.86553200	-1.44595200
H	-10.60775100	-6.53135500	-0.54946300
O	-11.67739400	-5.11138600	-2.02246300
C	-9.46356400	-9.58055800	-3.50133400
N	-8.52086100	-8.79598200	-2.84732000
H	-8.85607200	-8.05364400	-2.23527500
O	-9.16353400	-10.58551800	-4.13451400
C	-7.12516200	-8.82939600	-2.96506500
O	-6.44272400	-7.98409300	-2.40865700
N	-6.63231600	-9.88061300	-3.72347700
H	-7.32492700	-10.59071400	-3.97829000
N	-1.65352500	-6.14877700	2.98648700
H	-2.61852700	-6.10612400	3.28220800
H	-1.08132900	-5.33785500	3.17617300
C	-1.35262400	-7.06484600	2.02623400
O	-2.13293200	-7.93609300	1.66377500
N	-0.04173100	-6.91203100	1.52080000
H	0.47701300	-6.08700300	1.80542800
C	0.66597400	-7.66822200	0.60859800
O	1.76972000	-7.25305100	0.24661300
C	0.13189800	-8.98607000	0.09775300
H	-0.93890100	-9.06927000	0.26692300
H	0.32156500	-9.01088700	-0.97568400
C	0.82835700	-10.19559700	0.76963500
O	0.48952000	-10.19541100	2.14648700
H	0.20475600	-11.11068800	2.34302800
C	2.39020400	-10.19483200	0.70386000
H	2.72074800	-11.02832700	1.32737400
H	2.73067000	-9.26522500	1.16684400
C	0.25882800	-11.48854500	0.14704200
O	0.25777900	-11.49040600	-1.17693800
H	-0.17559100	-12.31839900	-1.53600300
O	-0.14935300	-12.39295900	0.85775500
C	3.08455700	-10.39170300	-0.63800700
O	3.57821900	-11.46468100	-0.94215500
N	3.11575000	-9.27341500	-1.47381500
H	2.55455000	-8.45697900	-1.21533900
C	3.79080200	-9.28405800	-2.69500700
N	3.16866000	-8.60783800	-3.76097500
H	3.65025300	-8.78835300	-4.63510200
O	4.83148800	-9.87703400	-2.90269500
C	1.88246100	-8.09782500	-3.85345300
C	1.22060400	-8.29784900	-5.20486500
H	1.76550700	-9.05615800	-5.76951500
H	0.22854600	-8.69318100	-4.99921400
O	1.30496800	-7.61610400	-2.88394100

C	1.13689100	-7.05489700	-6.11374100
O	2.46065200	-6.56080800	-6.22218900
H	2.39715500	-5.59045400	-6.09678000
C	0.68520000	-7.44354600	-7.57654400
H	0.43848600	-6.53263500	-8.12936600
H	1.58633600	-7.86673400	-8.02871000
C	0.27963500	-5.84235700	-5.60730300
O	0.84856700	-4.76085700	-5.51773000
N	-1.09134600	-5.84384500	-5.38620000
H	-1.48683400	-4.90381800	-5.26550500
C	-1.99480000	-6.86869500	-5.18658700
N	-3.30324200	-6.46582900	-4.91056900
H	-3.90551600	-7.26508700	-4.70878600
O	-1.72954900	-8.06097100	-5.22552500
C	-3.84355200	-5.18880600	-4.83465300
C	-5.32915700	-5.15719100	-4.50345000
H	-5.80602300	-4.73862000	-5.39576900
H	-5.72755400	-6.16501400	-4.35870200
O	-3.19062200	-4.17801500	-5.06808900
C	-5.73431200	-4.27667400	-3.27064800
O	-5.16913900	-2.99046000	-3.28679000
H	-5.30167200	-2.62393100	-4.18712900
C	-5.37710100	-4.91854500	-1.90422400
H	-6.04524900	-5.75908200	-1.72711900
H	-5.57026900	-4.15792100	-1.14211700
C	-3.92326800	-5.33789400	-1.77023900
O	-3.01094000	-4.51783300	-1.67355800
N	-3.71897500	-6.70254500	-1.77400200
H	-4.52937500	-7.31184200	-1.87563000
C	-2.48844700	-7.40860100	-1.88761100
N	-1.37334500	-6.64738600	-1.89796300
H	-1.47523100	-5.63738600	-1.86691500
H	-0.50308700	-7.06951900	-2.20893500
O	-2.51691100	-8.63289800	-1.98452300
C	-0.39156200	-8.50978900	-7.69845800
N	-1.59138200	-8.12197000	-8.27184300
H	-1.64723600	-7.21881600	-8.72915900
O	-0.19455800	-9.65744800	-7.31213600
C	-2.83519800	-8.79545500	-8.25859800
N	-2.86780600	-9.89066400	-7.40542300
H	-1.99183600	-10.09850600	-6.92334500
O	-3.77163800	-8.35911200	-8.89675600
C	-4.00929300	-10.48020500	-6.89061700
O	-5.13332900	-10.36931700	-7.34207100
C	-3.71210700	-11.34327000	-5.62186100
O	-2.56320200	-10.85245800	-4.93824600

H	-2.75527900	-9.94902000	-4.60746500
C	-3.35903300	-12.77215700	-6.09569300
H	-4.17293800	-13.17228700	-6.70310800
H	-2.46825300	-12.71045900	-6.73377500
C	-4.97056300	-11.35123500	-4.73161700
H	-5.80686600	-11.80451900	-5.27072300
H	-4.78397500	-11.96963800	-3.84484100
C	-3.06627400	-13.82140400	-5.02112800
N	-2.20938200	-13.43009900	-4.01187900
H	-1.92507000	-12.45113400	-4.01137000
O	-3.53148000	-14.95379900	-5.11525600
C	-1.68208500	-14.21245500	-2.96623900
O	-0.88820100	-13.71206800	-2.15872700
N	-2.07957000	-15.49199900	-2.91389400
H	-1.69942800	-16.07916400	-2.18586200
H	-2.72163400	-15.85267600	-3.61231000
C	-7.29539800	-4.19002000	-3.30059400
O	-7.99823300	-4.85746800	-2.55737300
C	-5.35400900	-9.96614800	-4.24297300
O	-4.57764900	-9.01993200	-4.29274900