**Supplementary Materials**

# Chitosan-Derived Carbon Dots for Fluorescence Detection of $Hg^{2+}$: Selectivity, Real-Water Assessment, and Computational Insights

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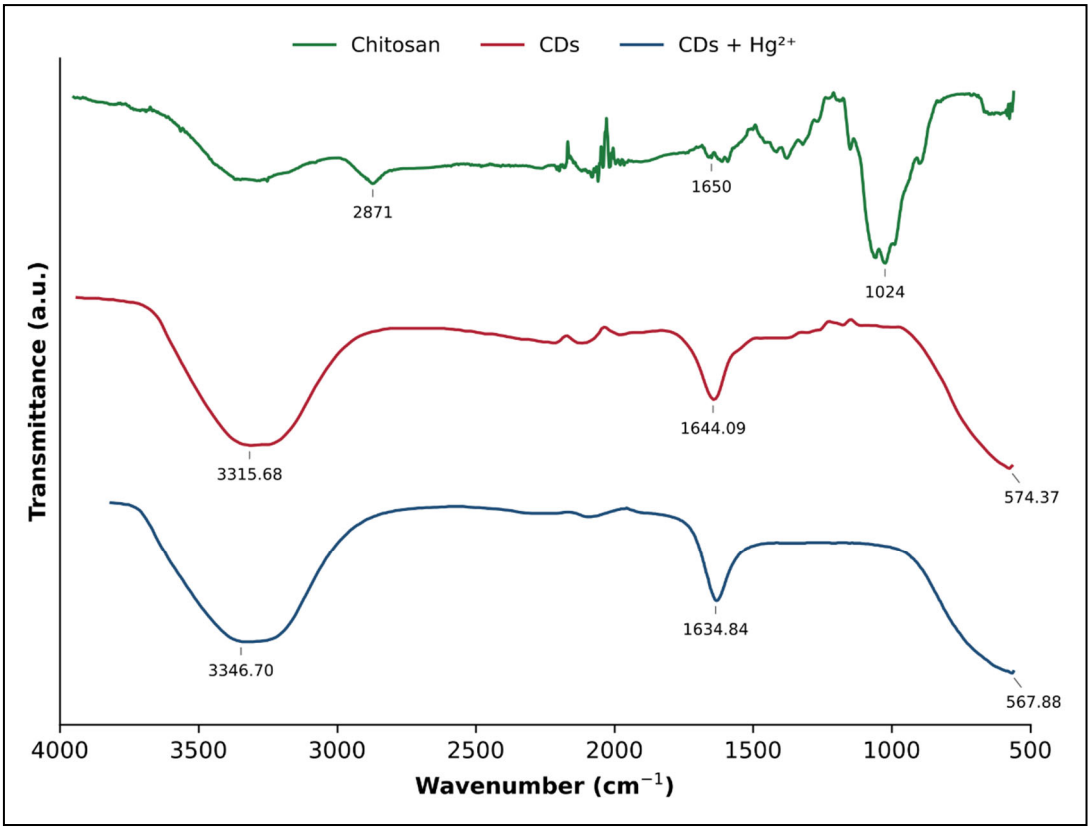


**Figure S1.** FTIR spectra of pristine chitosan, the CDs, and the CDs after $Hg^{2+}$ exposure. Both CD samples were prepared by the same drying procedure. After $Hg^{2+}$ exposure, the O–H/N–H stretching band shifted from 3315.68 to 3346.70 $cm^{-1}$ and the band at 1644.09 $cm^{-1}$ shifted to 1634.84 $cm^{-1}$.

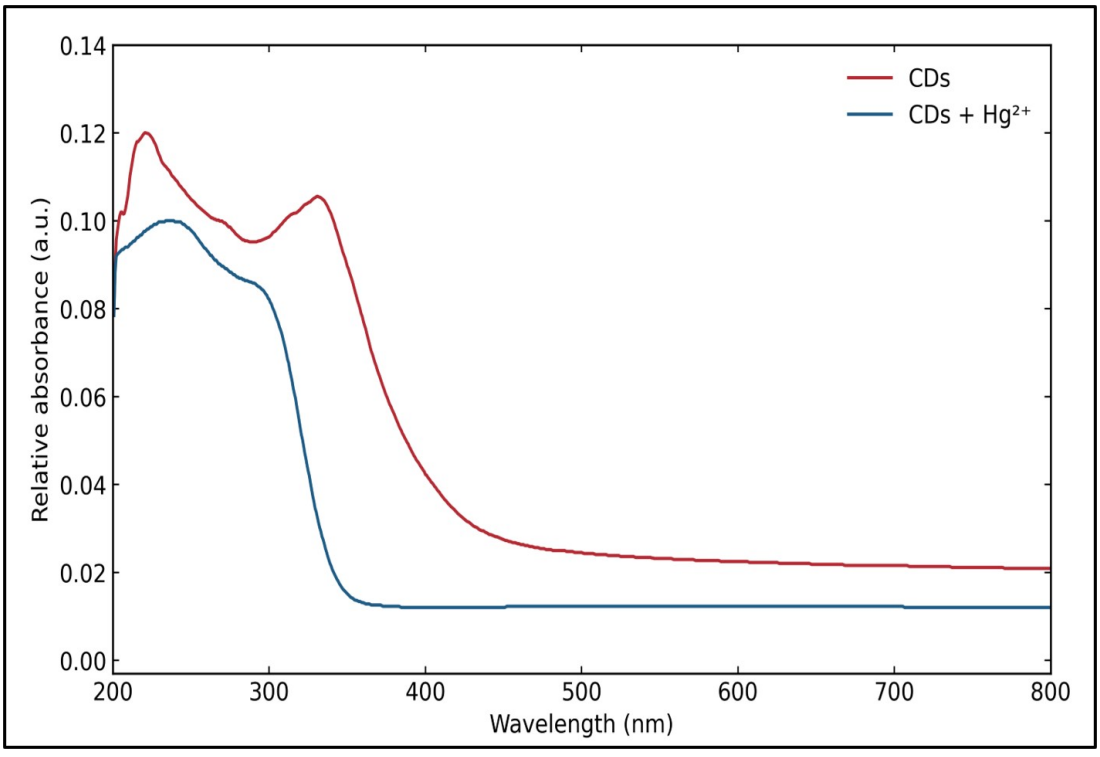

**Figure S2.** UV–Vis absorption spectra of the CDs before and after $Hg^{2+}$ addition. The band near 330 nm becomes less pronounced after $Hg^{2+}$ addition.

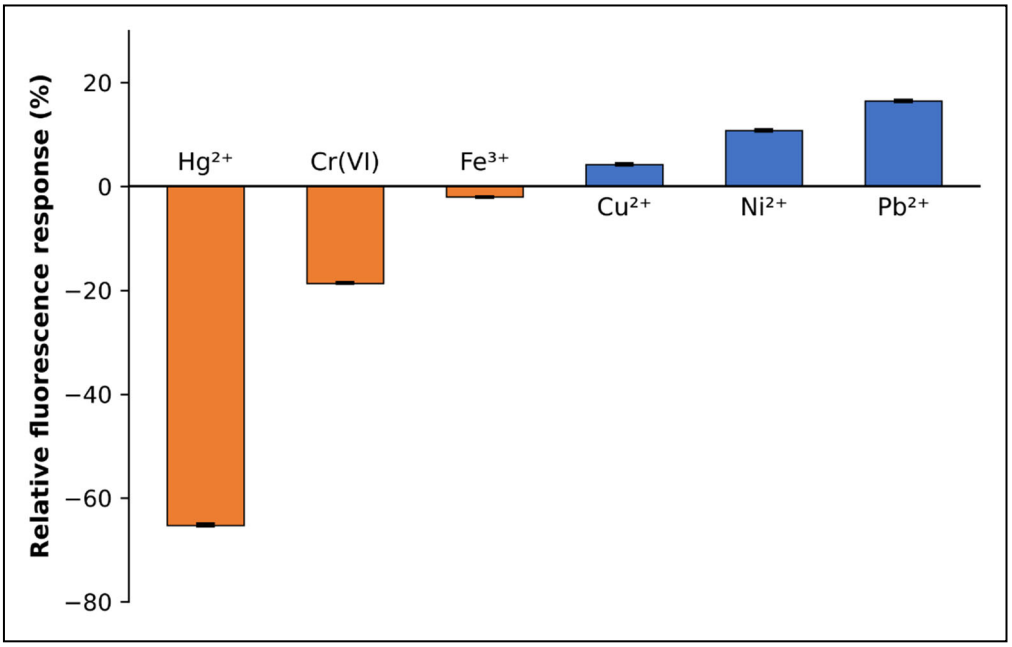


**Figure S3.** Relative fluorescence response, $100(F - F_0)/F_0$, of the CDs to $Hg^{2+}$, Cr(VI), $Fe^{3+}$, $Cu^{2+}$, $Ni^{2+}$, and $Pb^{2+}$ (each at 100 μM; λex = 340 nm, λem = 436 nm). Negative values indicate quenching and positive values indicate enhancement. Error bars represent the standard deviation (n = 3).

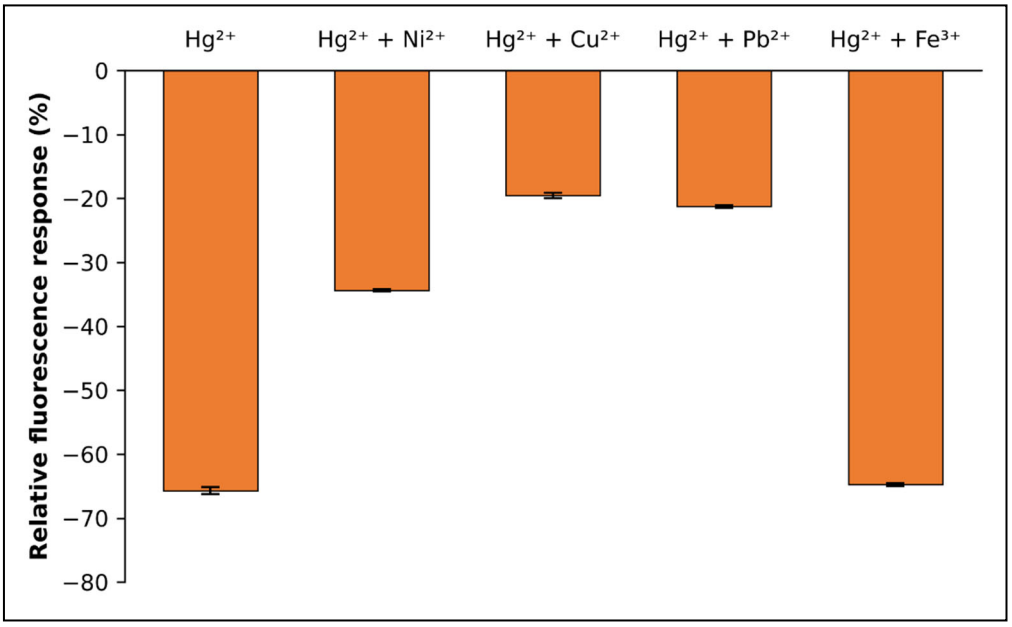


**Figure S4.** Relative fluorescence response (%) of the CDs to $Hg^{2+}$ (100 μM) alone and in the presence of $Ni^{2+}$, $Cu^{2+}$, $Pb^{2+}$, or $Fe^{3+}$ (each at 1 mM). Error bars represent the standard deviation of triplicate measurements.

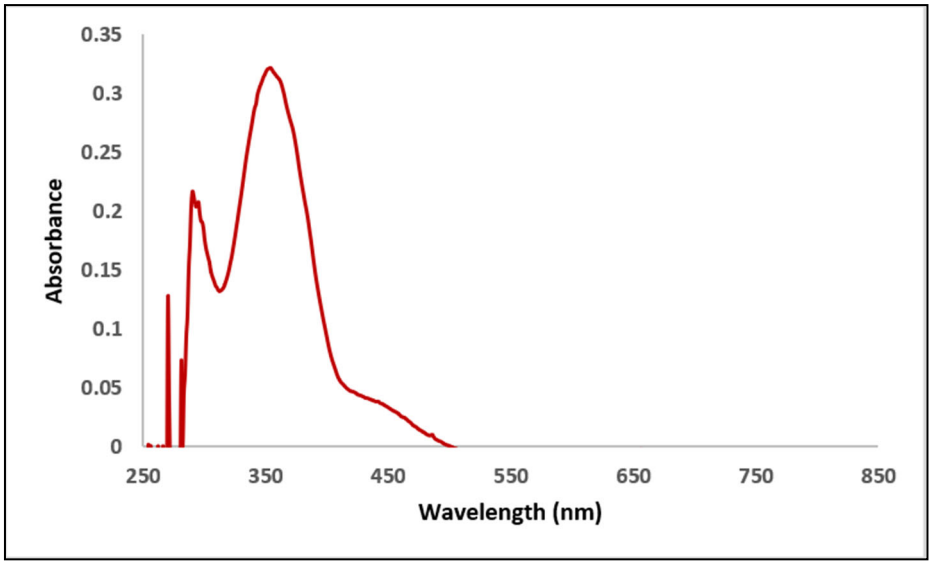


**Figure S5.** UV–Vis absorption spectrum of $K_2Cr_2O_7$ (100 μM). The strong absorption near the 340 nm excitation wavelength (A ≈ 0.29 at 340 nm and 0.04 at 436 nm) produces an inner filter effect in the fluorescence measurements.

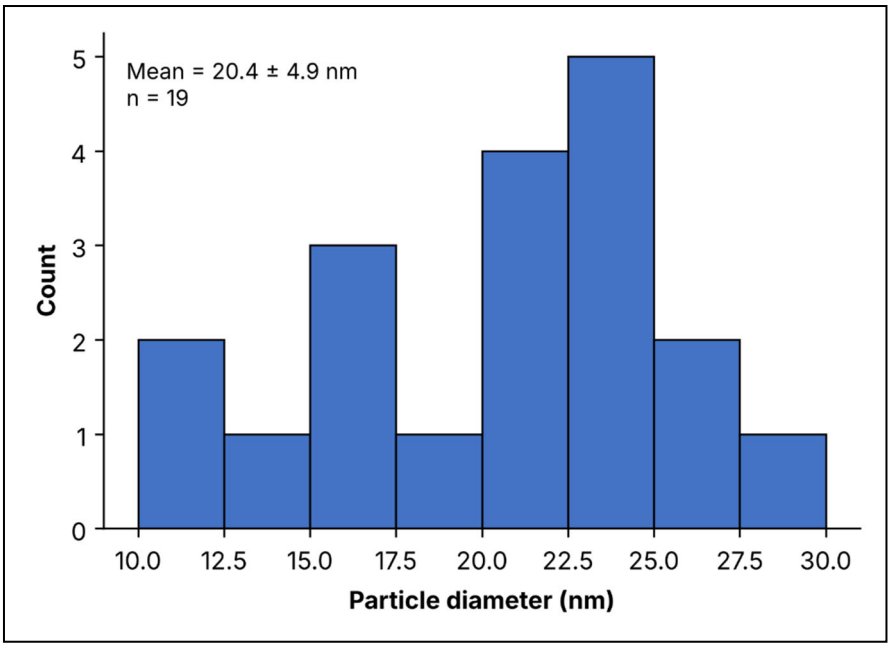


**Figure S6.** Size histogram of the CD particles with clearly resolved boundaries at aggregate edges (n = 19, from two non-overlapping TEM images). Diameters were obtained by fitting a circle to each particle edge (mean 20.4 ± 4.9 nm; range 10.8–28.3 nm). Because of the small sample and the selection of edge particles, the histogram is a limited estimate and may not represent the size distribution of the whole sample.

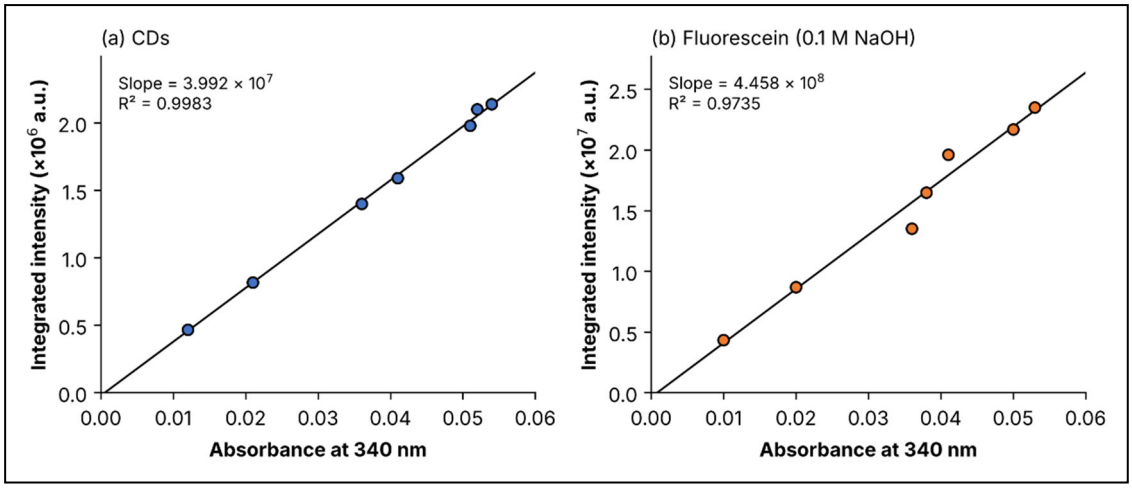


**Figure S7.** Integrated fluorescence intensity versus absorbance at 340 nm for the CDs and the fluorescein reference (0.1 M NaOH, Φref = 0.925). Slopes: $3.992 \times 10^7$ ($R^2 = 0.9983$) for the CDs and $4.458 \times 10^8$ ($R^2 = 0.9735$) for fluorescein, giving a quantum yield of 8.28%.

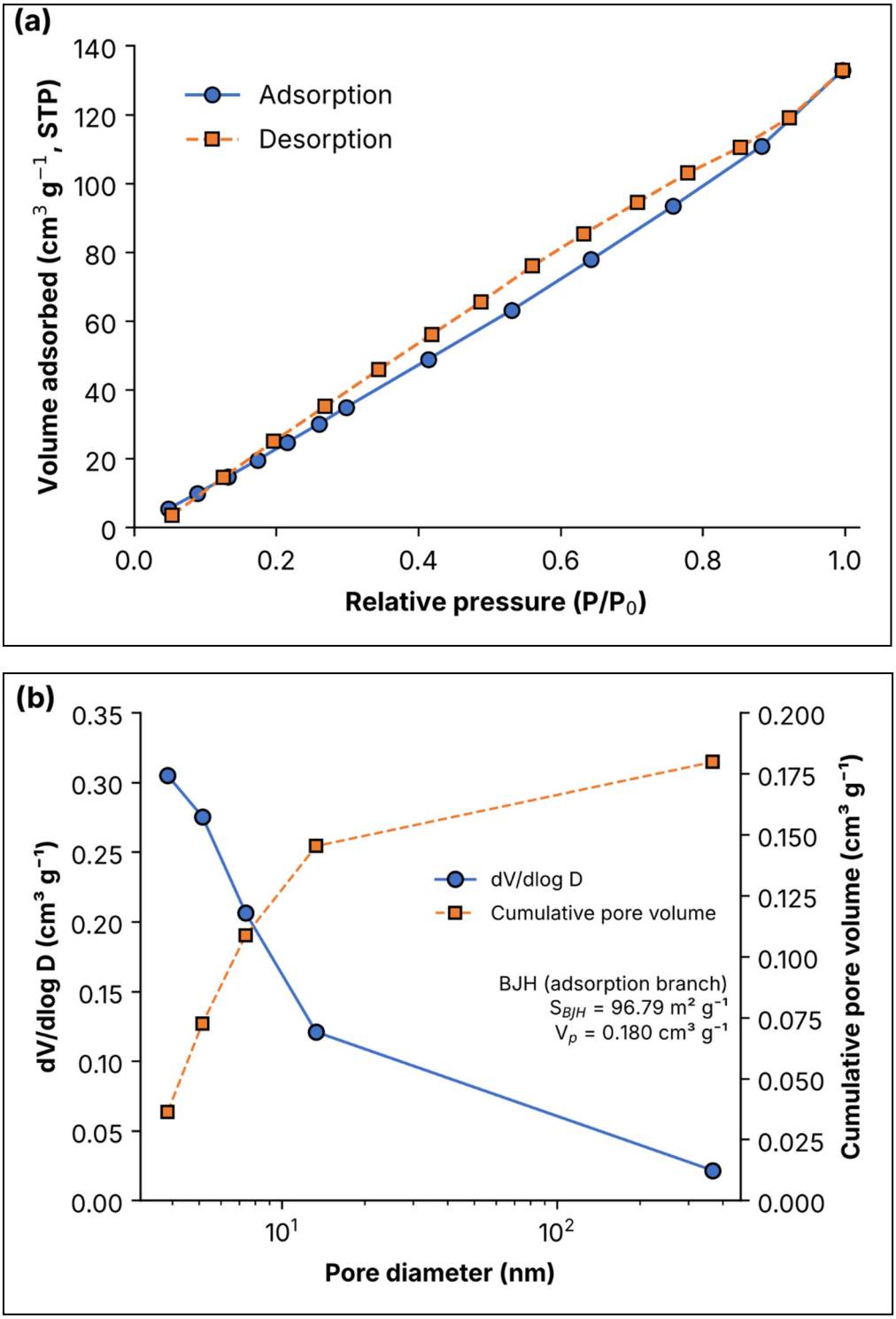


**Figure S8.** (a) $N_2$ adsorption–desorption isotherm of the freeze-dried CDs at 77.35 K (type III-like; BET C constant = 2.2; apparent BET surface area 223.18 $m^2\ g^{-1}$). (b) BJH pore-size distribution from the adsorption branch (pore volume 0.180 $cm^3\ g^{-1}$; BJH surface area 96.79 $m^2\ g^{-1}$).

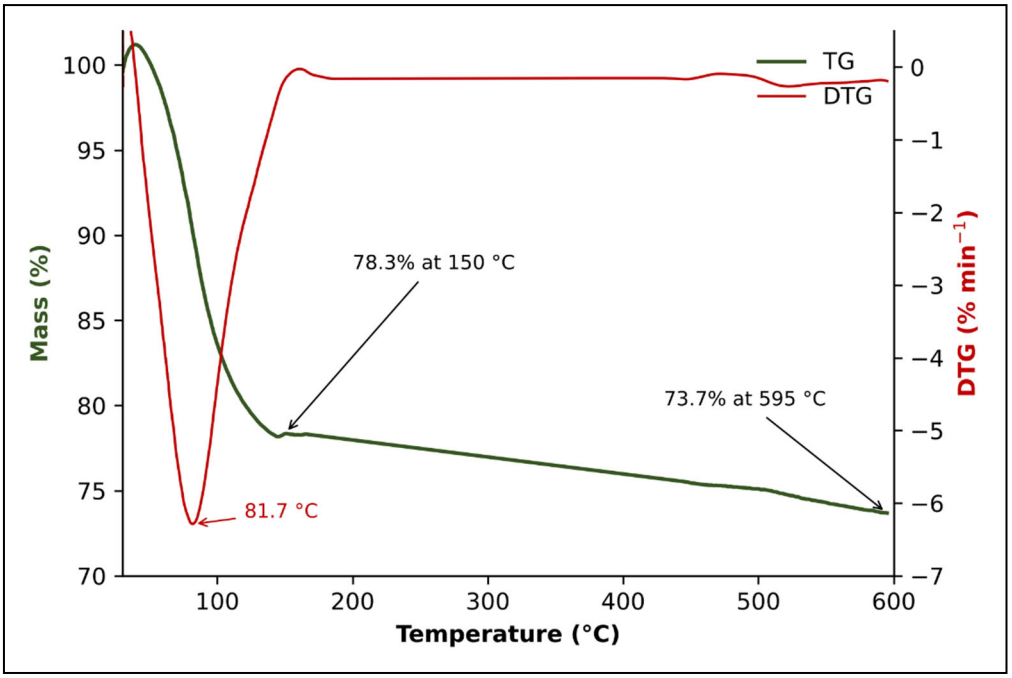


**Figure S9.** TGA curve of the freeze-dried CDs (10.1 mg; 30–595 °C; heating rate 20 °C min$^{-1}$; nitrogen atmosphere; Linseis thermal analyzer).

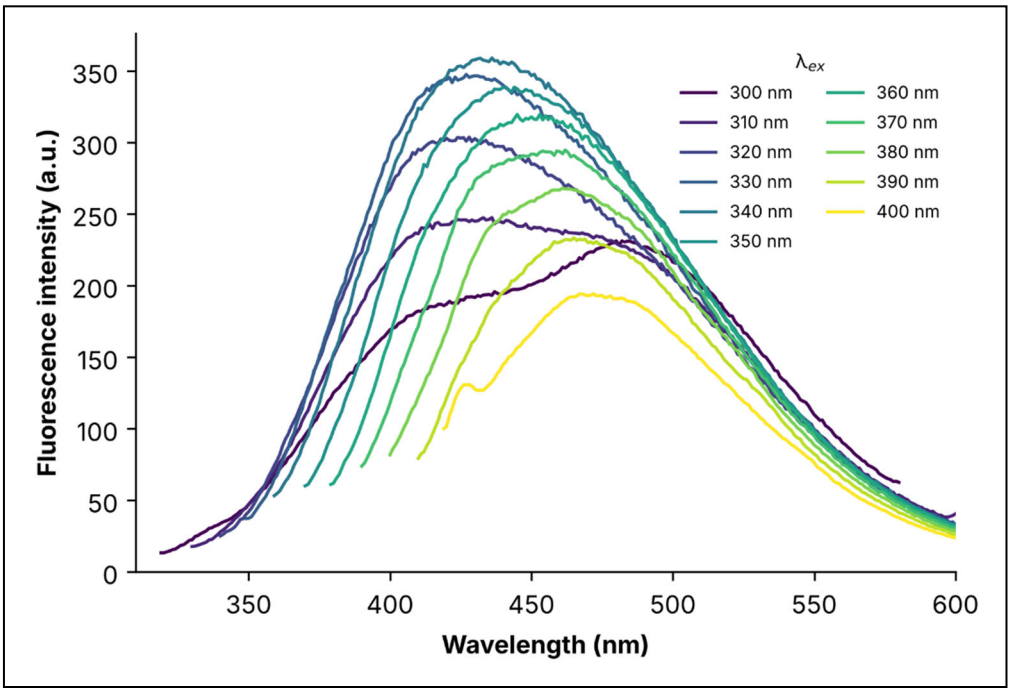


**Figure S10.** Emission spectra of the CDs at excitation wavelengths of 300–400 nm (10 nm steps). The strongest emission was obtained with excitation at 340 nm (emission maximum at 436 nm).

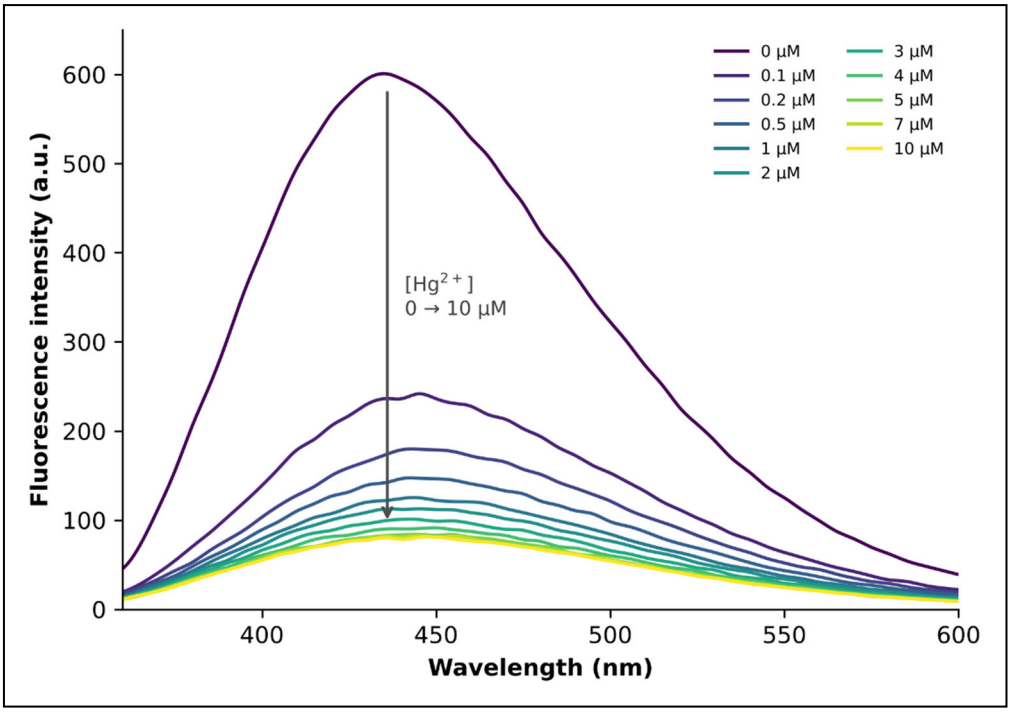


**Figure S11.** Emission spectra of the CDs (λex = 340 nm) in the presence of 0–10 µM $Hg^{2+}$ (concentrations in the analyte solution before 1:1 mixing).

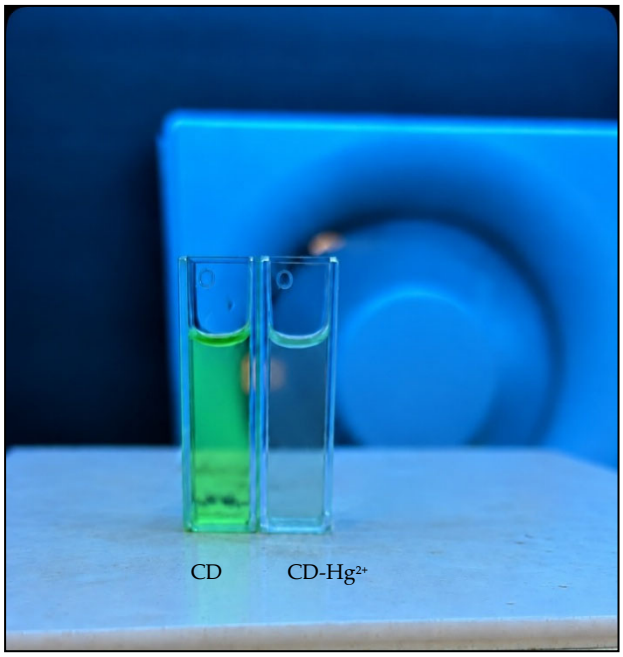


**Figure S12.** Photograph of the CD dispersion (left) and the CD dispersion with 100 µM $Hg^{2+}$ (right) under a UV lamp (16 W), showing quenching of the fluorescence visible to the naked eye. To the naked eye, the CD emission appears blue-green; the greener hue in the photograph results from the automatic white balance and colour processing of the smartphone camera (iPhone 15). The emission maximum measured by spectrofluorometry is 436 nm (Figure S10).

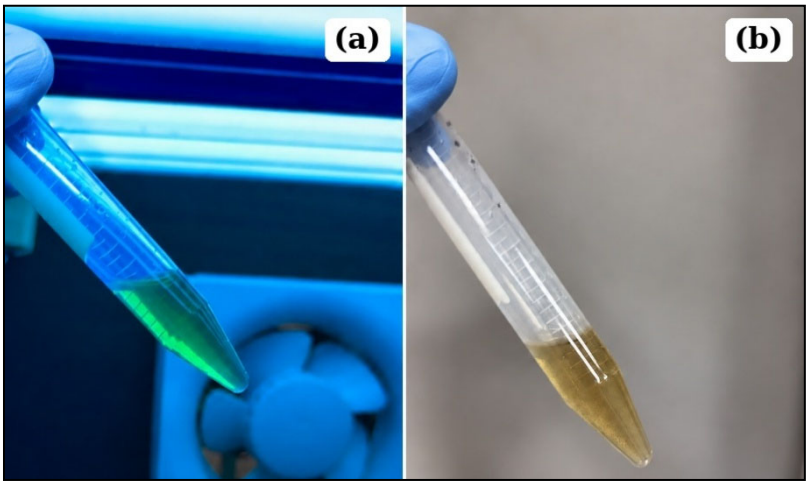


**Figure S13.** Photographs of the chitosan-derived CD dispersion (a) under a UV lamp (16 W) and (b) under ambient light. The colour under UV illumination is as recorded by the smartphone camera (see Figure S12).

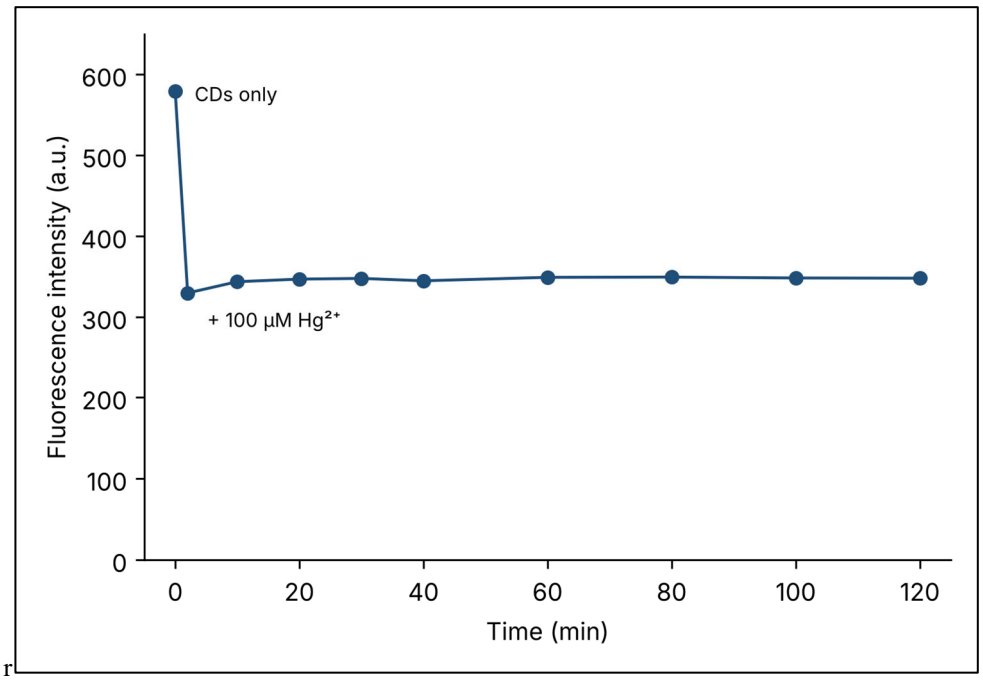


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**Figure S14.** Fluorescence intensity of the CDs (λex = 340 nm, λem = 436 nm) at different times after addition of 100 µM $Hg^{2+}$. Single measurement series (n = 1); the point at 0 min is the CD dispersion without $Hg^{2+}$.

**Table S1.** Computational details of the optimized structures at the r²SCAN-3c/CPCM(water) level.

| System | Total charge | Spin multiplicity |
|---|---|---|
| CQD ($C_{38}H_{18}N_6O_6$) | 0 | 1 |
| Hg@CQD | 0 | 1 |
| Cr@CQD | 0 | 5 and 7 |
| Isolated Hg atom | 0 | 1 |
| Isolated Cr atom | 0 | 7 |

ORCA 6.1.0 input keywords: ! r2SCAN-3c CPCM(water) Opt Freq RIJCOSX AutoAux TightSCF (complete input files in Section S2).

**Table S2.** Calibration data for $Hg^{2+}$ (mean ± SD, n = 3; λex = 340 nm, λem = 436 nm). $F_0/F$ was calculated for each replicate relative to the mean blank intensity.

| [$Hg^{2+}$] (μM) | F (a.u.) | $F_0/F$ |
|---|---|---|
| 0 | 601.81 ± 1.28 | 1.000 ± 0.002 |
| 0.1 | 235.90 ± 0.54 | 2.551 ± 0.006 |
| 0.2 | 172.75 ± 1.23 | 3.484 ± 0.025 |
| 0.5 | 141.75 ± 0.64 | 4.246 ± 0.019 |
| 1 | 128.90 ± 5.96 | 4.676 ± 0.221 |
| 2 | 112.11 ± 1.67 | 5.369 ± 0.080 |
| 3 | 101.11 ± 2.07 | 5.954 ± 0.120 |
| 4 | 92.03 ± 1.76 | 6.541 ± 0.126 |
| 5 | 83.47 ± 0.52 | 7.210 ± 0.045 |
| 7 | 83.12 ± 1.16 | 7.241 ± 0.101 |
| 10 | 81.21 ± 1.04 | 7.412 ± 0.095 |

Regression over 0.5–5 μM: $F_0/F = 0.6438[Hg^{2+}] + 4.0027$, $R^2 = 0.9976$. Residual standard deviation σ (s_y/x) = 0.0616. LOQ = 10σ/S = 0.956 μM. Linear range 0.5–5 μM; quantification range 0.956–5 μM. No LOD was derived from this regression because 3.3σ/S lies below the linear range, where the response is nonlinear; at the lowest concentration tested (0.1 μM), $F_0/F$ was approximately 2.5.

**Table S3.** Frontier molecular orbital energies of the unbound CQD model and the optimized complexes (r²SCAN-3c/CPCM(water)). For the open-shell Cr@CQD models, α and β spin channels are listed, together with the global spin-polarized gap.

| System | E(HOMO) (eV) | E(LUMO) (eV) | Gap (eV) |
|---|---|---|---|
| CQD (M = 1) | -3.914 | -2.397 | 1.517 |
| Hg@CQD (M = 1) | −3.075 | −2.864 | 0.211 |
| Cr@CQD (M = 5), α / β | −3.717 / −3.277 | −2.893 / −2.705 | 0.824 / 0.572 (global 0.384) |
| Cr@CQD (M = 7), α / β | −3.310 / −3.303 | −2.659 / −2.901 | 0.651 / 0.402 (global 0.402) |

**Section S2. ORCA input files and Cartesian coordinates (Å) of the optimized structures**
***ORCA 6.1.0; input line:***

- **CQD:**

```
! r2SCAN-3C CPCM(Water) opt freq RIJCOSX AutoAux  TightSCF
! PRINTMOS PRINTBASIS

%maxcore 2000

%pal
  nprocs 11
end

* xyzfile 0 1 GQD.xyz *
```

- **Hg@CQD 1**

```
! r2SCAN-3C CPCM(Water) opt freq RIJCOSX AutoAux  TightSCF
! PRINTMOS PRINTBASIS

%maxcore 2000

%pal
  nprocs 11
end

* xyzfile 0 1 GQD-Hg1.xyz *
```

- **Cr@CQD 5**

```
! r2SCAN-3C CPCM(Water) opt freq RIJCOSX AutoAux  TightSCF
! PRINTMOS PRINTBASIS

%maxcore 2000

%pal
  nprocs 11
end

* xyzfile 0 5 GQD-Cr5.xyz *
```

- **Cr@CQD 7**

```
! r2SCAN-3C CPCM(Water) opt freq RIJCOSX AutoAux  TightSCF
! PRINTMOS PRINTBASIS

%maxcore 2000

%pal
  nprocs 11
end

* xyzfile 0 7 GQD-Cr7.xyz *
```

**S2.1. CQD model ($C_{38}H_{18}N_6O_6$), charge 0, multiplicity 1**

| | | | |
|---|---|---|---|
| C | 4.68474807892377 | -2.32781149673688 | -0.08080872989457 |
| C | 3.51532494253737 | -3.04416701179200 | -0.07025373650359 |
| C | 5.83709747510583 | 1.24958942241984 | -0.13034599663798 |
| C | 5.95572693683560 | -0.16212466346219 | -0.09694984078482 |
| C | 3.47075210128549 | -0.23325801037372 | -0.07550294577137 |
| C | 4.71015422062024 | -0.91056106947242 | -0.08288070005388 |
| C | 2.25706024090435 | -0.96301290598219 | -0.06401478760818 |
| C | 2.26368542649694 | -2.39015650824122 | -0.05542147401191 |

| | | | |
|---|---|---|---|
| C | -0.17453012618979 | -2.46009809296187 | -0.02550032695910 |
| C | 1.05298288728956 | -3.10254760355185 | -0.04448472000075 |
| C | -1.40453369557353 | -3.18433817124000 | 0.00949735886680 |
| C | 4.57221842564467 | 3.32470591828242 | -0.19352438427765 |
| C | 4.64277947576012 | 1.91560416516104 | -0.12915811969532 |
| C | 2.20980132235299 | 1.85238069561624 | -0.06004138464074 |
| C | 1.00592290312752 | 1.13330659457537 | -0.02182070042721 |
| C | 0.99904741933194 | -0.29702066290452 | -0.02279439832720 |
| C | -0.19105214269262 | -1.02338745946403 | -0.00338517601620 |
| C | -2.61256229516474 | -1.06220519644001 | 0.06108074502733 |
| C | -2.60174847001640 | -2.48526789561960 | 0.11812652420581 |
| C | -5.03073643504983 | -2.45112272223640 | 0.30151746450203 |
| C | -3.86635436711768 | -3.13429264289179 | 0.33265163181777 |
| C | 3.39624103455311 | 4.01651254443361 | -0.17971854236427 |
| C | 0.92883154965689 | 3.92092558183896 | -0.00013600842099 |
| C | 2.16024647852622 | 3.27781563801584 | -0.07859206679885 |
| C | -0.29234612375094 | 3.22027009821560 | 0.07003839389750 |
| C | -0.24594695148064 | 1.79762673934947 | 0.05207326285508 |
| C | -2.67807141803081 | 1.73091392937380 | 0.10734963429561 |
| C | -1.44472382228239 | 1.06268574983662 | 0.05231984344029 |
| C | -3.88956702598276 | 1.01232787763829 | 0.10729972940264 |
| C | -3.85061229823237 | -0.37085827901644 | 0.05727144029084 |
| C | -6.28264646675518 | -0.39324010409729 | -0.12008382040432 |
| C | -1.54045820601046 | 3.87669240124684 | 0.18307660974083 |
| C | -2.71151200380894 | 3.14855983981797 | 0.18704316803225 |
| C | -5.11998460660089 | 3.10313188682101 | 0.22832023501371 |
| C | -5.14068116673565 | 1.73030818549173 | 0.14723405222959 |
| C | -6.32607890837152 | 0.96310212837557 | -0.00977982106312 |
| C | -7.45341932483333 | -1.13293709003237 | -0.61062463028684 |
| O | -8.61078221105929 | -0.47722747728639 | -0.36588311487784 |
| O | -7.41905055907502 | -2.20009290422823 | -1.20590321108974 |
| N | -5.05958184880940 | -1.09813168514580 | 0.04169736162277 |
| O | 3.49258709419083 | -4.41121798313004 | -0.07110158913768 |
| H | 4.40099811976817 | -4.74256564237523 | -0.07848120835227 |
| H | 2.63352069631808 | 5.81409939731823 | -0.75520840087784 |
| O | -1.66717582525415 | 5.23950992836092 | 0.22624909398021 |
| H | -0.89898777468652 | 5.64097463600609 | 0.65431952431082 |
| C | 7.24307891352693 | -0.76843350604992 | -0.08355807285188 |
| O | 8.28415250799602 | 0.15232303653520 | -0.11096157741912 |
| O | 7.53792106787716 | -1.97970249529460 | -0.05095315553844 |
| H | -5.98296714267328 | -2.92558194762659 | 0.48684195369508 |
| H | -2.24999895115154 | -5.00906776775471 | -0.27462883684559 |
| H | 5.51850301368746 | 3.85551200579955 | -0.25729152122128 |
| H | 5.63575780045768 | -2.84774364320153 | -0.08939071443912 |
| H | 9.09480708951083 | -0.37806832127453 | -0.09820960493801 |
| H | -9.32395650220103 | -0.97652182369824 | -0.79759101748899 |
| H | 6.72775576855319 | 1.86474306376885 | -0.16174186370525 |
| H | -7.27494045563203 | 1.46870371933935 | -0.14465454837305 |
| H | 1.11558021048968 | -4.18245268024346 | -0.02696448232169 |
| H | -3.91182420144947 | -4.18740316155342 | 0.57941444253427 |
| H | -0.58526120417646 | -5.01253934916422 | -0.35515288386882 |
| H | 0.91233792777727 | 5.00398496234095 | -0.00368881897182 |
| N | -1.39932510146940 | -4.55877685772344 | 0.03080247224785 |
| N | 3.35675105484254 | 5.41342040560398 | -0.16971642101031 |
| N | -1.43706429004079 | -0.34429188430283 | 0.02734970689750 |
| N | 3.41936421072144 | 1.18859449197032 | -0.08776632582436 |
| N | -3.94806844389955 | 3.77808312651575 | 0.26870729975697 |
| H | -6.02495002435160 | 3.70019012622315 | 0.25647979030379 |
| H | 4.24828804498190 | 5.82808495981686 | -0.40974570885342 |
| H | -3.95635079914175 | 4.78624909016054 | 0.33834955588803 |

**S2.2. Hg@CQD, charge 0, multiplicity 1**

| | | | |
|---|---|---|---|
| C | 4.70105545575665 | -2.32275252890122 | -0.10062090962834 |
| C | 3.53206114575683 | -3.04019696075796 | -0.09059612564010 |
| C | 5.85006358620586 | 1.25535715921837 | -0.14248630878522 |
| C | 5.97031295670118 | -0.15595760490846 | -0.11472365307174 |
| C | 3.48517448905668 | -0.22939122816447 | -0.09218740990418 |
| C | 4.72512705572720 | -0.90572722932788 | -0.10110943035618 |
| C | 2.27188339907718 | -0.96045733393927 | -0.08255627417222 |
| C | 2.28013884098002 | -2.38739020061362 | -0.07598306586333 |
| C | -0.15809414996037 | -2.45987449147378 | -0.05073902677391 |
| C | 1.06975863954963 | -3.10103262265553 | -0.06589343923950 |
| C | -1.38769827990903 | -3.18538711256280 | -0.01252574664231 |
| C | 4.58328346479435 | 3.32978227098244 | -0.19560378526681 |
| C | 4.65517276915775 | 1.92049806481422 | -0.13836759925826 |
| C | 2.22229532809701 | 1.85468200906627 | -0.07149280459089 |
| C | 1.01887213519632 | 1.13422406256276 | -0.04035116037822 |
| C | 1.01327218875217 | -0.29551222284347 | -0.04627895379805 |
| C | -0.17676891963596 | -1.02312801167924 | -0.03285582590462 |
| C | -2.59731401555888 | -1.06395025022521 | 0.02040106120248 |
| C | -2.58550764499147 | -2.48675554943678 | 0.08679712616958 |
| C | -5.01329437757190 | -2.45236443387199 | 0.28250773098384 |
| C | -3.84837963618149 | -3.13480373950025 | 0.31234343779431 |
| C | 3.40676784439287 | 4.02057336982650 | -0.17738830451365 |
| C | 0.93966233684040 | 3.92153599175705 | 0.00428752107627 |
| C | 2.17153069225744 | 3.28020569158611 | -0.08009062769307 |
| C | -0.28106066382477 | 3.21933766472594 | 0.06908682752085 |
| C | -0.23384896675032 | 1.79706461774636 | 0.03610364918997 |
| C | -2.66575723106803 | 1.72781823600548 | 0.08810555471606 |
| C | -1.43164423041492 | 1.06092915861681 | 0.02706881774931 |
| C | -3.87644826804474 | 1.00835278499470 | 0.08090381699964 |
| C | -3.83624409220049 | -0.37378009920285 | 0.01929809068352 |
| C | -6.26873997813435 | -0.39803814853539 | -0.14325028107538 |
| C | -1.52972101102867 | 3.87334728559131 | 0.18934470476084 |
| C | -2.70005246315330 | 3.14386360269609 | 0.18521354971847 |
| C | -5.10843085641139 | 3.09622060411382 | 0.22989507920897 |
| C | -5.12819582841621 | 1.72433737784730 | 0.13445617256093 |
| C | -6.31357350140454 | 0.95755409415571 | -0.02426705533680 |
| C | -7.43867841014360 | -1.13880732840564 | -0.63290861584330 |
| O | -8.59692061724797 | -0.48406703667769 | -0.38907262321132 |
| O | -7.40332133374148 | -2.20722483663878 | -1.22606837686823 |
| N | -5.04400058076493 | -1.10179656035143 | 0.01103154772313 |
| O | 3.51068950748835 | -4.40734397403636 | -0.09273076061544 |
| H | 4.41945766093954 | -4.73769403845645 | -0.09934791186882 |
| H | 2.64161975588995 | 5.82111859040011 | -0.74088476988163 |
| O | -1.65892014884303 | 5.23504557118004 | 0.24853916667748 |
| H | -0.88509509940693 | 5.63464516846759 | 0.66791039458480 |
| C | 7.25823139179288 | -0.76105473844334 | -0.10580248603432 |
| O | 8.29830522875786 | 0.16051251610462 | -0.13130084741486 |
| O | 7.55391416205356 | -1.97230468053028 | -0.07759162057299 |
| H | -5.96458954358919 | -2.92553585805944 | 0.47644971847201 |
| H | -2.23023165854535 | -5.01456427625053 | -0.28045477330707 |
| H | 5.52907523211618 | 3.86177331229784 | -0.25686719498265 |
| H | 5.65237932793377 | -2.84208651108085 | -0.10986948609552 |
| H | 9.10973769174157 | -0.36869349541118 | -0.12026684908808 |
| H | -9.30960939803130 | -0.98609569926647 | -0.81834787845213 |
| H | 6.73994240716648 | 1.87181818241782 | -0.17125059195184 |
| H | -7.26343048626670 | 1.46308190887536 | -0.15242765975739 |
| H | 1.13396553211825 | -4.18077131641316 | -0.04716553599595 |
| H | -3.89154833682480 | -4.18565039417321 | 0.56896373786040 |

| | | | |
|---|---|---|---|
| H | -0.56415926013909 | -5.01819991596411 | -0.35031287650371 |
| H | 0.92302993637587 | 5.00459362419681 | 0.00986187041084 |
| N | -1.38137098804313 | -4.55895474772304 | 0.02178828221639 |
| N | 3.36631388569157 | 5.41719275917811 | -0.15949974772899 |
| N | -1.42268238789922 | -0.34532149562131 | -0.01380510735758 |
| N | 3.43233743947934 | 1.19205075261907 | -0.10091142427775 |
| N | -3.93726003709483 | 3.77191006245108 | 0.27378008840516 |
| H | -6.01389538495193 | 3.69205508541627 | 0.26724382108514 |
| H | 4.25718167445617 | 5.83416330038851 | -0.39788369920593 |
| H | -3.94646327602593 | 4.77920604038984 | 0.35454858333335 |
| Hg | -2.37331886398063 | -0.41491727828701 | 3.42024939950456 |

**S2.3. Cr@CQD, charge 0, multiplicity 5**

| | | | |
|---|---|---|---|
| C | 4.72201573670493 | -2.32980563000490 | -0.13399245278284 |
| C | 3.54923692324039 | -3.03995316556470 | -0.12028482361772 |
| C | 5.85077139416368 | 1.24563032492447 | -0.14612760913951 |
| C | 5.96561840644085 | -0.15166550899823 | -0.13743166419557 |
| C | 3.49428542451846 | -0.23485132025984 | -0.10056324436217 |
| C | 4.73879248151304 | -0.91291521702254 | -0.12257703683700 |
| C | 2.28346932027494 | -0.96336648382988 | -0.09107664745795 |
| C | 2.29558399594125 | -2.38279878814342 | -0.09052489503572 |
| C | -0.15224892001630 | -2.45292976594224 | -0.04001119727816 |
| C | 1.08077260422299 | -3.09038754624486 | -0.06960315355198 |
| C | -1.38607307208547 | -3.19223135099737 | -0.02933509954367 |
| C | 4.58827731877592 | 3.32108972356716 | -0.16336292607939 |
| C | 4.63974656909701 | 1.90897959533049 | -0.12794215037226 |
| C | 2.22163844977803 | 1.85849091658825 | -0.05507758701141 |
| C | 1.02333016438940 | 1.13332709359376 | -0.01840222238505 |
| C | 1.02494648576492 | -0.29941512119383 | -0.03507687999388 |
| C | -0.17685180700654 | -1.01838411332746 | -0.01891428301627 |
| C | -2.60295803305723 | -1.08099906479213 | 0.33561959304607 |
| C | -2.57526460820353 | -2.52223373374776 | 0.15924863378268 |
| C | -5.00821731011983 | -2.47512598368572 | 0.31644897756089 |
| C | -3.84514394685067 | -3.17330405016262 | 0.34080382898494 |
| C | 3.41754369250932 | 4.02317473614150 | -0.14359466485157 |
| C | 0.94865544348198 | 3.93045843734190 | 0.01811489660038 |
| C | 2.17572019357405 | 3.28357726362051 | -0.05958992875573 |
| C | -0.26745792195166 | 3.22505423811025 | 0.07876572906157 |
| C | -0.21883932119702 | 1.79975503937270 | 0.06100655431010 |
| C | -2.64827126893626 | 1.71597128101243 | 0.11225378778319 |
| C | -1.42372059865748 | 1.05888167594480 | 0.07515185515909 |
| C | -3.88573996035064 | 0.98797511991976 | 0.05485406718744 |
| C | -3.84747052727056 | -0.37941396843185 | 0.10235523066164 |
| C | -6.26951347523360 | -0.41850446833552 | -0.12135516050876 |
| C | -1.52218112856266 | 3.87262538175896 | 0.16897575314372 |
| C | -2.68980195431931 | 3.13414770940231 | 0.15618095311015 |
| C | -5.11173689197404 | 3.08791271373436 | 0.09418584397516 |
| C | -5.12893973524167 | 1.71935635526652 | 0.03465101166341 |
| C | -6.31385313167693 | 0.94389420028986 | -0.08071077088154 |
| C | -7.45331281357737 | -1.17263276104567 | -0.56174995923115 |
| O | -8.60486205487732 | -0.51365806829095 | -0.30046930131195 |
| O | -7.43483188972437 | -2.25171732025348 | -1.13530275493996 |
| N | -5.04729691435702 | -1.11876115544253 | 0.05854385115576 |
| O | 3.52083723784660 | -4.40334445967693 | -0.13115300312329 |
| H | 4.42719811738437 | -4.74095148221872 | -0.14440578447559 |
| H | 2.62107132294198 | 5.85096415541482 | -0.58630821962229 |
| O | -1.65002150562863 | 5.24086929801357 | 0.17863348996502 |
| H | -0.93786055504460 | 5.64302136878719 | 0.69437804551681 |
| C | 7.28110792164033 | -0.75500456738862 | -0.14256380161367 |
| O | 8.29210646387687 | 0.17426037028906 | -0.17724496957749 |

| | | | |
|---|---|---|---|
| O | 7.56498494627921 | -1.95680888693931 | -0.11778417207054 |
| H | -5.96072005362708 | -2.95596136249606 | 0.48244323083621 |
| H | -2.20643082276439 | -5.01043334478804 | -0.38065399742805 |
| H | 5.53967618229309 | 3.84210654020111 | -0.21612655677366 |
| H | 5.66914355532346 | -2.85368603262018 | -0.15454472632827 |
| H | 9.12192901600068 | -0.32798348466115 | -0.17290534507823 |
| H | -9.32761326766943 | -1.02080356245965 | -0.70668691687369 |
| H | 6.73742570764510 | 1.86536280273627 | -0.16813352398626 |
| H | -7.26815995898231 | 1.43745293415845 | -0.22257121261074 |
| H | 1.13552536385405 | -4.17116804413307 | -0.05083980105370 |
| H | -3.90475321455677 | -4.23456361469780 | 0.55079573467229 |
| H | -0.58983462948343 | -4.94142789916187 | -0.67809072945333 |
| H | 0.92250131259018 | 5.01316704465509 | 0.01831908203659 |
| N | -1.33500438820683 | -4.58617148301245 | -0.09303510389103 |
| N | 3.39795180053491 | 5.40250969938256 | -0.12194124275110 |
| N | -1.39080718574284 | -0.34690000098320 | 0.02880660705581 |
| N | 3.44439529327881 | 1.18329623174184 | -0.09520387496689 |
| N | -3.92376847215082 | 3.76629823201802 | 0.17431461805267 |
| H | -6.01203623917680 | 3.69164180708268 | 0.08554612690204 |
| H | 4.27616485974072 | 5.83712616120681 | -0.36985078929441 |
| H | -3.93062587178899 | 4.77472534133448 | 0.21614791288638 |
| Cr | -2.63598497995118 | -1.31860032068755 | 2.61440634330341 |

**S2.4. Cr@CQD, charge 0, multiplicity 7**

| | | | |
|---|---|---|---|
| C | 4.72050144667461 | -2.32738757259565 | -0.12763001193462 |
| C | 3.54694271347807 | -3.03819391285555 | -0.11137722303230 |
| C | 5.85173025459973 | 1.24632517575099 | -0.15103726124485 |
| C | 5.96984127908746 | -0.15070237944483 | -0.13916225893909 |
| C | 3.49592300116529 | -0.23272554668827 | -0.09877559793992 |
| C | 4.73882614666211 | -0.91162938137644 | -0.12083737316985 |
| C | 2.28245309573398 | -0.96330879516021 | -0.08654865409622 |
| C | 2.29507147295308 | -2.38231648784280 | -0.08315805683116 |
| C | -0.15131069131740 | -2.45312347461666 | -0.03069721651903 |
| C | 1.07841150432348 | -3.09112628662060 | -0.06150372011764 |
| C | -1.38754093835827 | -3.19268877110268 | -0.02780005181935 |
| C | 4.58781478387224 | 3.32256183963589 | -0.17498855939415 |
| C | 4.64254347644964 | 1.91002828133893 | -0.13368001330631 |
| C | 2.22482231668182 | 1.85809293764663 | -0.05651277601288 |
| C | 1.02432735200438 | 1.13076655224667 | -0.01548915117175 |
| C | 1.02676715557445 | -0.29602940526233 | -0.03081055247756 |
| C | -0.17853880771658 | -1.01779189994267 | -0.00800052139939 |
| C | -2.59885823123680 | -1.08048866717239 | 0.35770705385982 |
| C | -2.57552085552547 | -2.52432073732199 | 0.16169980708878 |
| C | -5.00875918630824 | -2.47569807687552 | 0.30875874212545 |
| C | -3.84485824209092 | -3.17520294896970 | 0.32994383073753 |
| C | 3.41759397490587 | 4.02300175602984 | -0.15501661140308 |
| C | 0.94899507857822 | 3.92886451291910 | 0.01368740376184 |
| C | 2.17575048729478 | 3.28274361586458 | -0.06524818075148 |
| C | -0.26823988131612 | 3.22248891987189 | 0.08025705584769 |
| C | -0.21988547893165 | 1.79867198979014 | 0.06447398959462 |
| C | -2.64970101704285 | 1.71565159706909 | 0.13354496434760 |
| C | -1.42312149754264 | 1.05642903053974 | 0.08963620700305 |
| C | -3.88627897423498 | 0.98581987804900 | 0.07235933316367 |
| C | -3.84894655083701 | -0.37739362916103 | 0.11403222263866 |
| C | -6.26865704104161 | -0.41771932725477 | -0.12520202157274 |
| C | -1.52159523468513 | 3.87039564589731 | 0.17516880153302 |
| C | -2.68958788920496 | 3.13147737870824 | 0.17170775635401 |
| C | -5.11016827959458 | 3.08772722998055 | 0.10608682844703 |
| C | -5.13010614786035 | 1.71991143450696 | 0.04407622583300 |
| C | -6.31363676048657 | 0.94476190901858 | -0.07977002399889 |

| | | | |
|---|---|---|---|
| C | -7.45015660226814 | -1.16947141802186 | -0.57513899704750 |
| O | -8.60294982974796 | -0.51025944174902 | -0.31846367710928 |
| O | -7.42991307447375 | -2.24658638042294 | -1.15241966328108 |
| N | -5.04715780487794 | -1.11884899260691 | 0.06017270981198 |
| O | 3.52049640348644 | -4.40238639324138 | -0.11814978175635 |
| H | 4.42748690021632 | -4.73802613166251 | -0.13238378865394 |
| H | 2.61986337348175 | 5.84509171820075 | -0.61386452950659 |
| O | -1.64972820438503 | 5.23843858206706 | 0.18191991425907 |
| H | -0.93188977476140 | 5.64212954142201 | 0.68852429918307 |
| C | 7.28069434883031 | -0.75327049955696 | -0.14651550704565 |
| O | 8.29647166311259 | 0.17462972482004 | -0.17623039090595 |
| O | 7.56542858463191 | -1.95685308293952 | -0.12630065201342 |
| H | -5.96180420058336 | -2.95857746722664 | 0.46500367077663 |
| H | -2.20509891231810 | -5.00920794777586 | -0.39699586863903 |
| H | 5.53869066701401 | 3.84433880344619 | -0.23196748918990 |
| H | 5.66781837747778 | -2.85126611799877 | -0.14731563279367 |
| H | 9.12331014987993 | -0.33212735634022 | -0.17444638892904 |
| H | -9.32349383702546 | -1.01548337465802 | -0.73086837099019 |
| H | 6.73803531995574 | 1.86689344478913 | -0.17629384640921 |
| H | -7.26731394195860 | 1.43851962280823 | -0.22507149701571 |
| H | 1.13359134916681 | -4.17178298728710 | -0.04326028773045 |
| H | -3.90660906607196 | -4.23848890238768 | 0.52887869512082 |
| H | -0.58413486031040 | -4.93476409255559 | -0.68790465277501 |
| H | 0.92271168403510 | 5.01145234155490 | 0.01132689072365 |
| N | -1.33520937602770 | -4.58258846290890 | -0.10895323449834 |
| N | 3.39353604313246 | 5.40388425109231 | -0.13664626893161 |
| N | -1.39025961340199 | -0.34628803342182 | 0.05554288559173 |
| N | 3.44411113032428 | 1.18324498013428 | -0.09707545196292 |
| N | -3.92444253519129 | 3.76619953286293 | 0.19191579937284 |
| H | -6.01080637150118 | 3.69133795903663 | 0.09553190029415 |
| H | 4.27181262989049 | 5.83789204367085 | -0.38597499802078 |
| H | -3.93093086816588 | 4.77460999627116 | 0.23200044431957 |
| Cr | -2.66094831067293 | -1.33601718271500 | 2.62936095484856 |