

Supporting Information (48 pages)

Triplet Exciton Delocalization in Organic-Quantum Dots Hybrid Photo-Systems: A Pathway to Improved Phototherapy and Theragnostics

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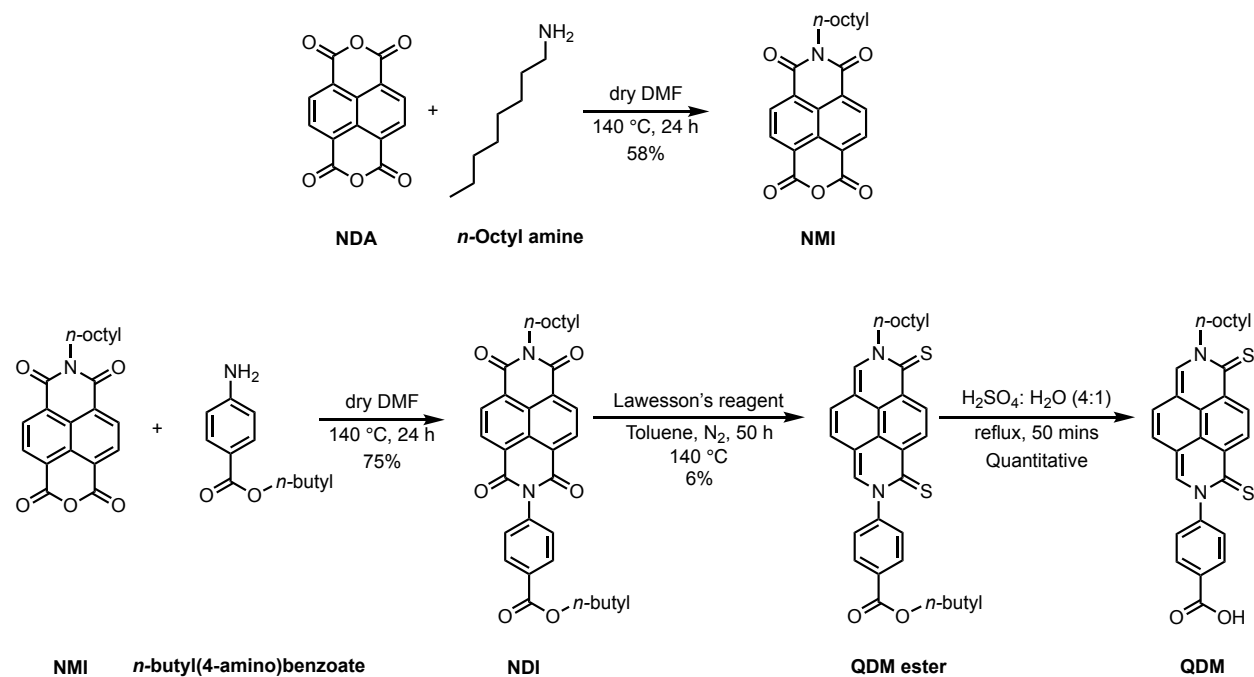
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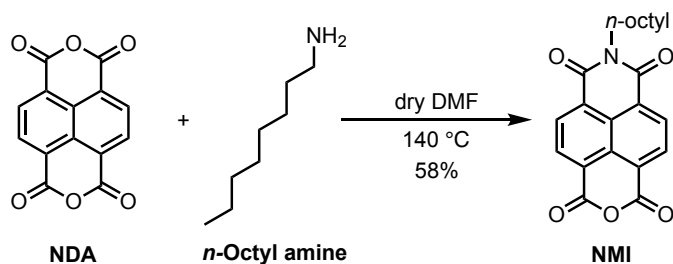
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SYNTHESIS SCHEME



Scheme S1. Synthetic route for **QDM**.

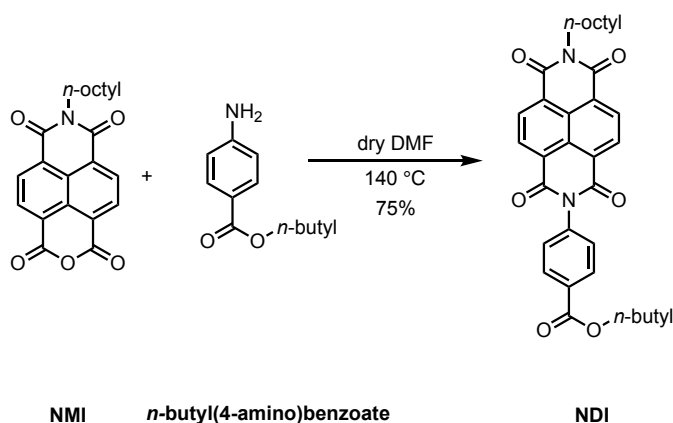
SYNTHETIC PROCEDURES & CHARACTERIZATION



Scheme S2. Synthetic route for **NMI**.

Naphthalene-4,5,8,9-tetracarboxylic dianhydride (**NDA**) (5.0 g, 18.6 mmol, 1 equiv.) was dissolved in *anhyd.* dimethylformamide (DMF) in a round-bottom flask with an attached

condenser under an inert atmosphere. The reaction mixture was heated up to 140 °C. *n*-octylamine (2.8 mL, 16.8 mmol, 0.9 equiv.) was added dropwise at 140 °C. The mixture was stirred at 140 °C for 24 h. After the reaction, the solution was cooled down to room temperature and kept in the fridge for 2 h for complete precipitation. The resultant mixture was filtered. The filtrate was collected and concentrated in a vacuum to obtain a brown crude solid mixture which was then extracted with ethyl acetate (3 X 25 mL). The organic layer was dried over *anhyd.* Na₂SO₄ and was concentrated. The expected compound (naphthalene mono imide, **NMI**) was obtained as a pale yellowish crystalline solid. It is used for the second step without further purification. Yield: 2.87 g, 58%.

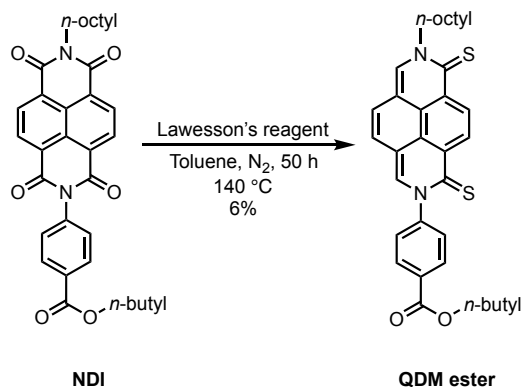


Scheme S3. Synthetic route for **NDI**.

NMI (2.85 g, 10.7 mmol, 1 equiv.) and butyl 4-aminobenzoate (2.2 g, 16.1 mmol, 1.5 equiv.) were added to *anhyd.* DMF in a round-bottom flask with an attached condenser under an inert atmosphere. The mixture was stirred at 140 °C for 24 h. After the reaction, the solution was cooled down to room temperature. DMF was evaporated and ethyl acetate (EtOAc) was poured into the crude product to precipitate the product. The light green precipitate (naphthalene diimide, **NDI**) was collected by suction filtration. Yield: 3.1 g, 75%.

¹H NMR (500 MHz, Chloroform-*d*) δ = 8.79 (s, 4H), 8.24 (d, *J* = 6.8 Hz, 2H), 7.42 (d, *J* = 8.5 Hz, 2H), 4.37 (t, *J* = 6.6 Hz, 2H), 4.19 (d, *J* = 7.9 Hz, 2H), 1.00 (t, *J* = 7.4 Hz, 3H), 0.89–0.85 (m, 3H) ppm.

^{13}C NMR (125 MHz, Chloroform-*d*) δ = 165.9, 162.9, 162.8, 138.7, 131.6, 131.4, 131.1, 131.0, 130.9, 128.9, 127.2, 127.2, 126.9, 126.6, 65.3, 41.2, 31.9, 30.9, 29.4, 29.3, 28.2, 27.2, 22.8, 19.4, 14.2, 13.9 ppm.

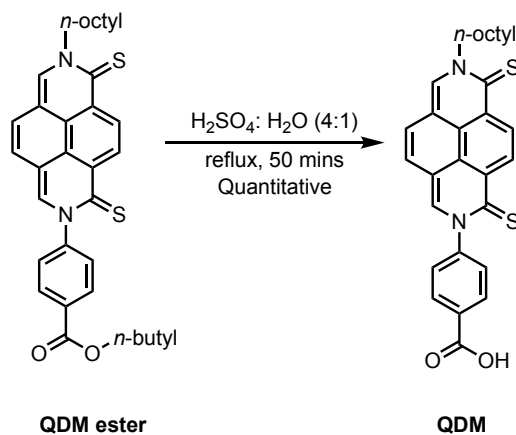


Scheme S4. Synthetic route for **QDM** ester.

NDI (3.0 g, 5.4 mmol, 1.0 equiv.) and Lawesson's reagent (11.0 g, 27.1 mmol, 5 equiv.) were added to anhydrous toluene in a two-neck round bottom flask with an attached condenser under an inert atmosphere. The mixture was stirred at 140 °C for 50 h. The resulting solution was cooled down to room temperature and concentrated under reduced pressure to give a dark red-brown sticky solid. The solid was then precipitated into methanol and filtered to remove excess Lawesson's reagent and Lawesson's reagent byproducts. The precipitated product was purified by column chromatography with toluene to get a dark wine-red colored solid to afford (naphthoquinodimethyl-*bis*-thioamide, **QDM ester**). Yield: 180 mg, 6%.

^1H NMR (500 MHz, Chloroform-*d*) δ = 9.03 (dd, J = 41.0, 9.1 Hz, 2H), 8.27 (d, J = 7.7 Hz, 2H), 7.80 (d, J = 38.1 Hz, 2H), 7.56 (d, J = 7.9 Hz, 2H), 7.04 (d, J = 21.8 Hz, 2H), 4.78 (s, 2H), 4.38 (t, J = 6.7 Hz, 2H), 1.99 (s, 2H), 1.86 – 1.73 (m, 2H), 1.55 – 1.44 (m, 4H), 1.39 (s, 3H), 1.30 (d, J = 9.9 Hz, 6H), 1.00 (t, J = 7.4 Hz, 3H), 0.88 (t, J = 6.9 Hz, 3H) ppm.

^{13}C NMR (125 MHz, Chloroform-*d*) δ = 181.6, 179.4, 165.9, 149.7, 134.5, 132.8, 132.1, 131.7, 131.2, 127.6, 125.6, 124.0, 123.3, 119.3, 65.7, 59.1, 32.2, 31.1, 29.6, 28.6, 27.2, 23.0, 19.7 (2C), 14.5, 14.2, 7.4 ppm.



Scheme S5. Synthetic route for **QDM**.

QDM ester (180 mg, 0.32 mmol) was dissolved in a solution of $\text{H}_2\text{SO}_4\text{:H}_2\text{O}$ (4:1) and refluxed for 50 min. The reaction was quenched with water to precipitate the desired dark red colored solid (naphthoquinodimethyl-*bis*-thioamide, **QDM**). The solid was further purified by multiple solvent washes with dichloromethane and methanol. Yield: Quantitative.

^1H NMR (500 MHz, Chloroform-*d*) δ = 9.09 (d, J = 9.2 Hz, 1H), 8.99 (d, J = 9.4 Hz, 1H), 8.45 (s, 2H), 8.31 – 8.18 (m, 4H), 7.69 (d, J = 8.3 Hz, 2H), 4.87 (t, J = 7.9 Hz, 2H), 1.48 (d, J = 6.9 Hz, 4H), 1.42 (s, 4H), 1.35 (s, 4H), 0.87 (d, J = 6.9 Hz, 3H) ppm.

^{13}C NMR (125 MHz, Chloroform-*d*) δ = 184.15, 169.93, 165.46, 156.39, 148.97, 138.74, 134.80, 131.74, 131.37, 130.36, 127.12, 126.75, 125.93, 123.32, 118.78, 73.03, 65.33, 30.75, 30.32, 19.26 (2C), 18.29, 13.75 ppm.

NMR SPECTRA

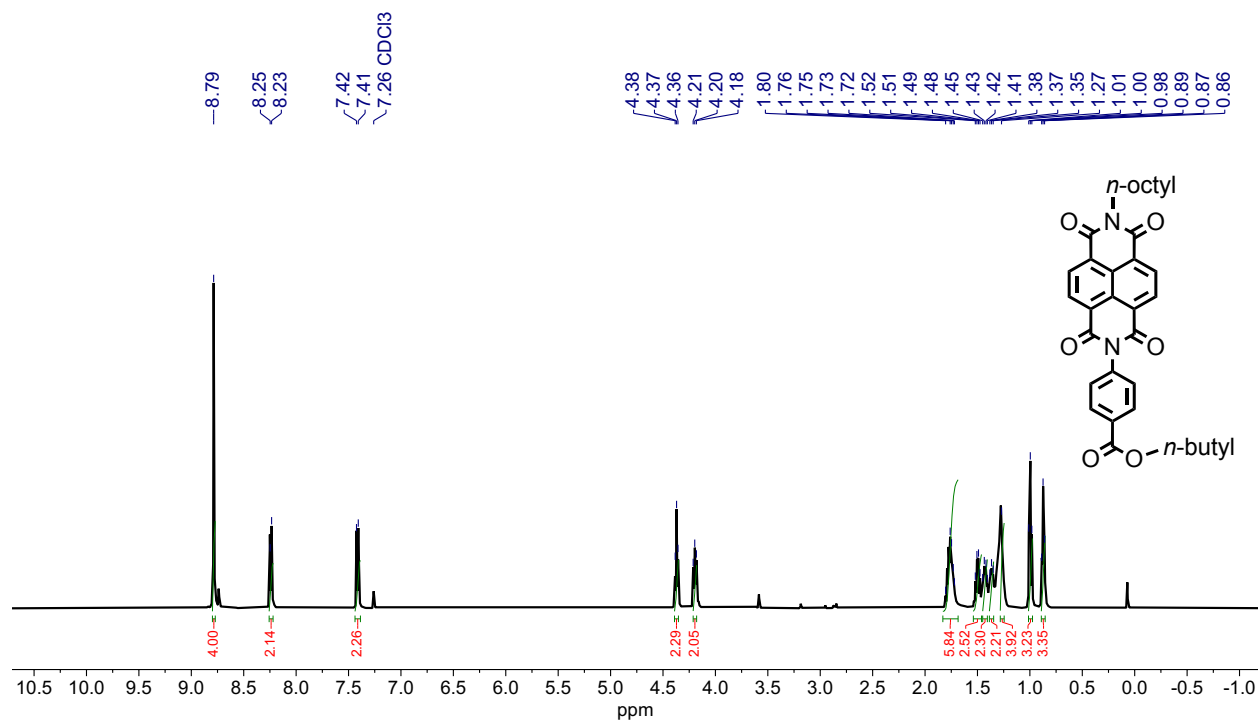


Figure S1. ¹H NMR spectrum (500 MHz) of NDI in CDCl₃. *Residual solvent peak of CHCl₃.

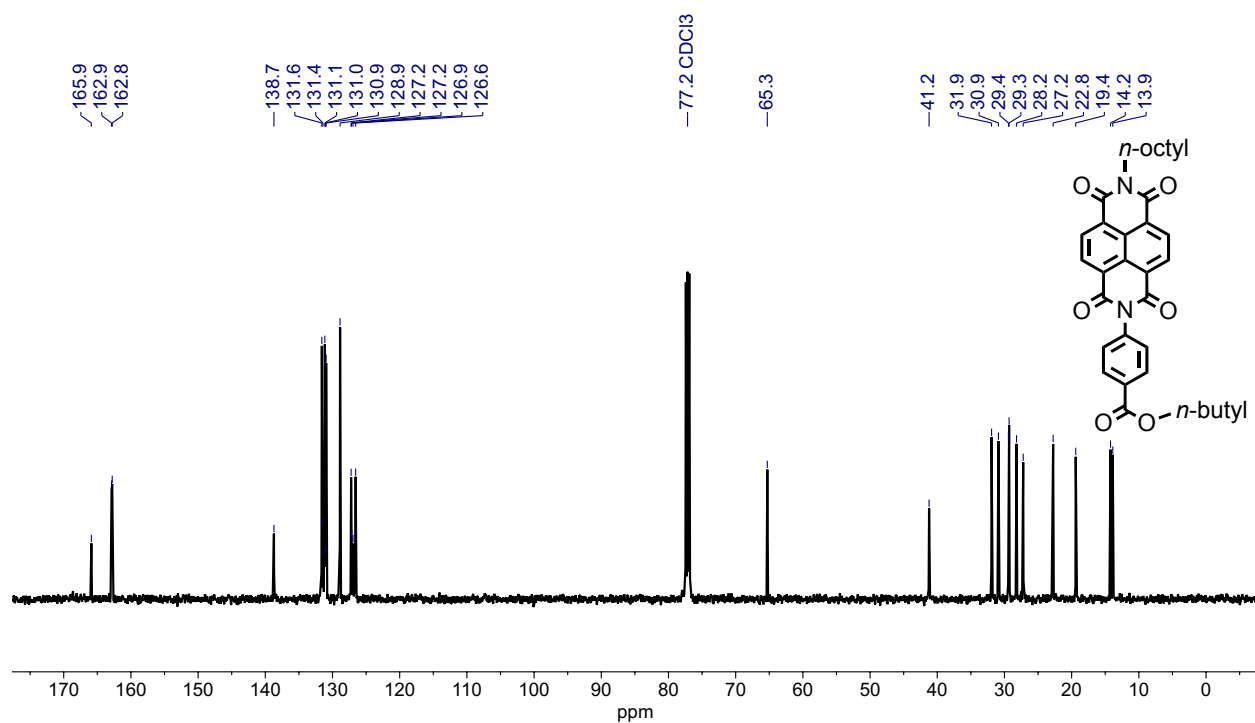


Figure S2. ¹³C NMR spectrum (125 MHz) of NDI in CDCl₃. *Residual solvent peak of CHCl₃.

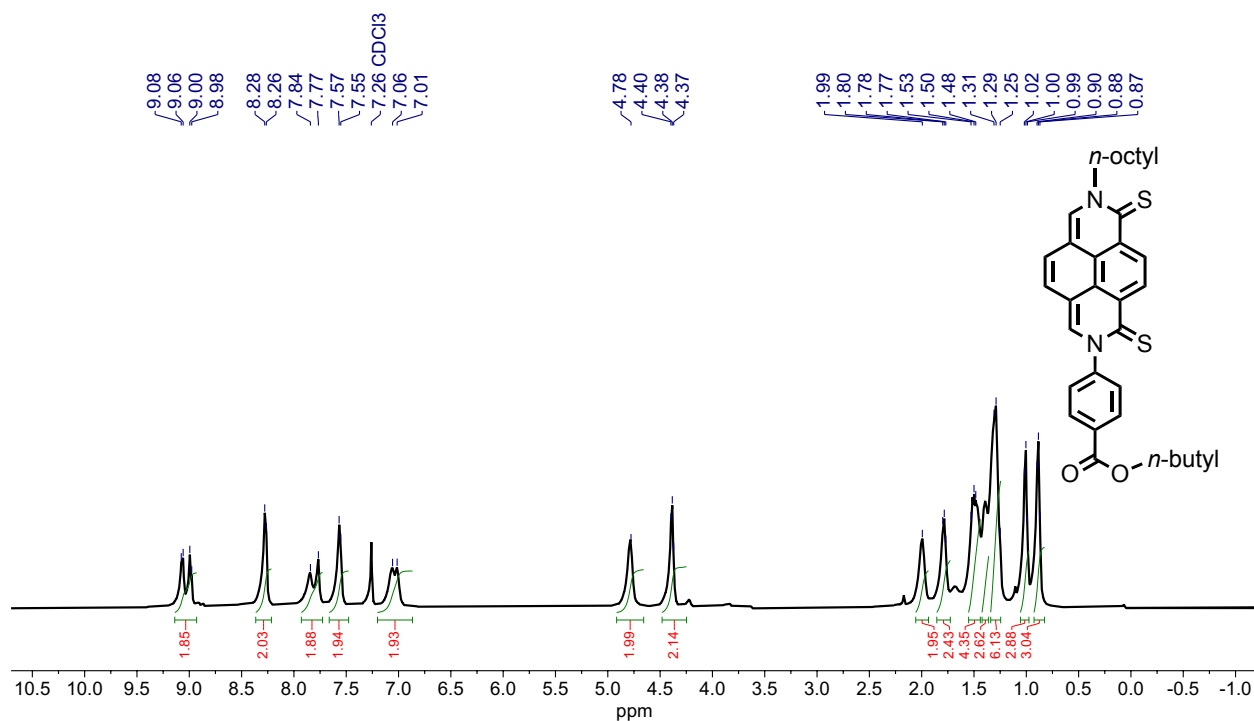


Figure S3. ¹H NMR spectrum (500 MHz) of **QDM ester** in CDCl₃. *Residual solvent peak of CHCl₃.

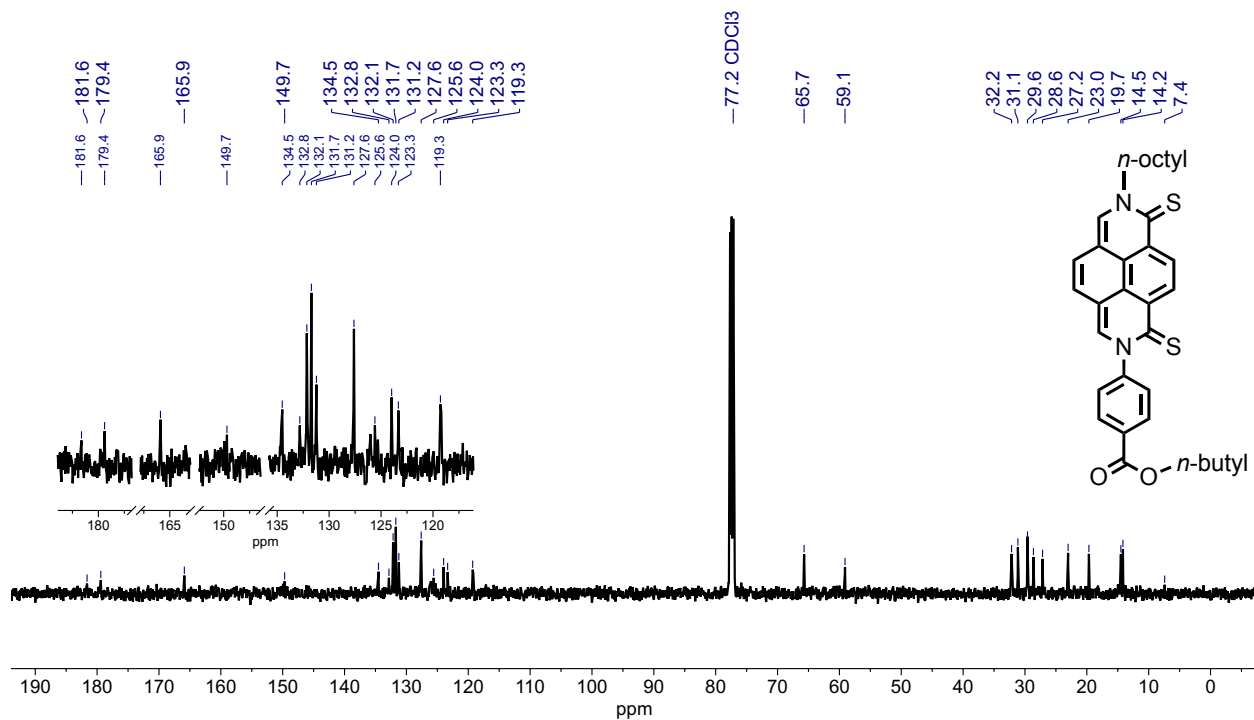


Figure S4. ¹³C NMR spectrum (125 MHz) of **QDM ester** in CDCl₃. *Residual solvent peak of CHCl₃.

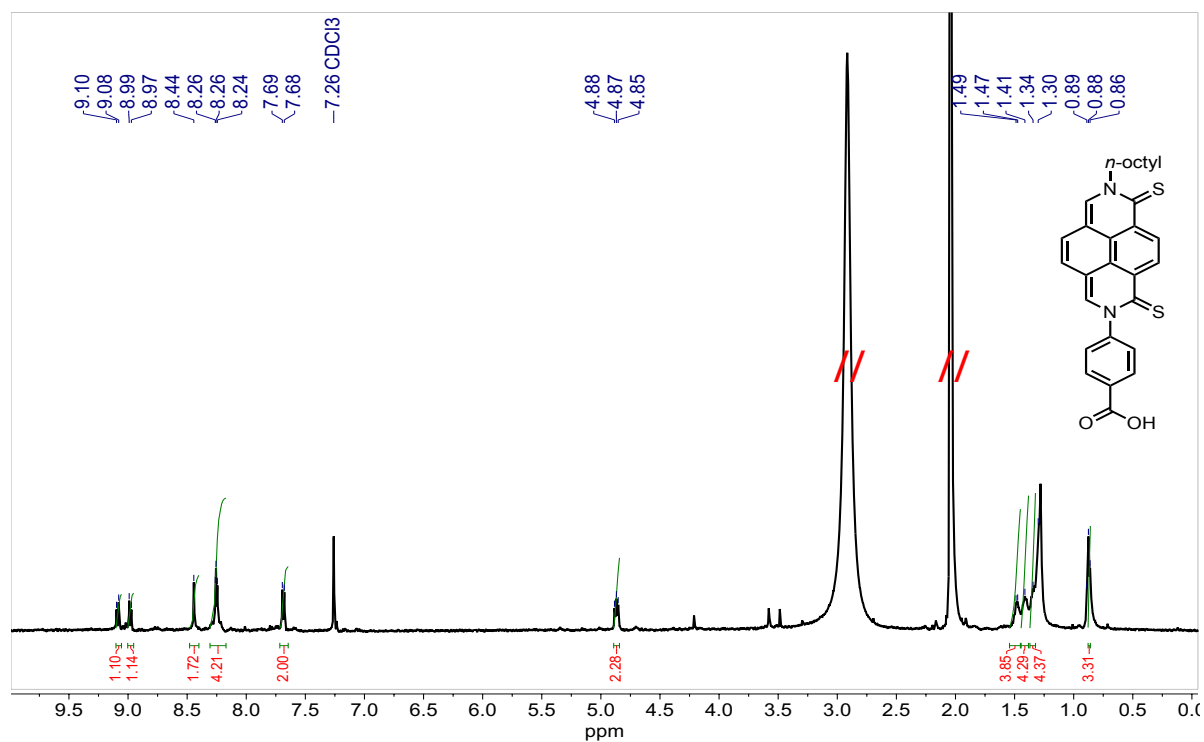


Figure S5. ¹H NMR spectrum (500 MHz) of **QDM MA** in CDCl₃. *Residual solvent peak of CHCl₃.

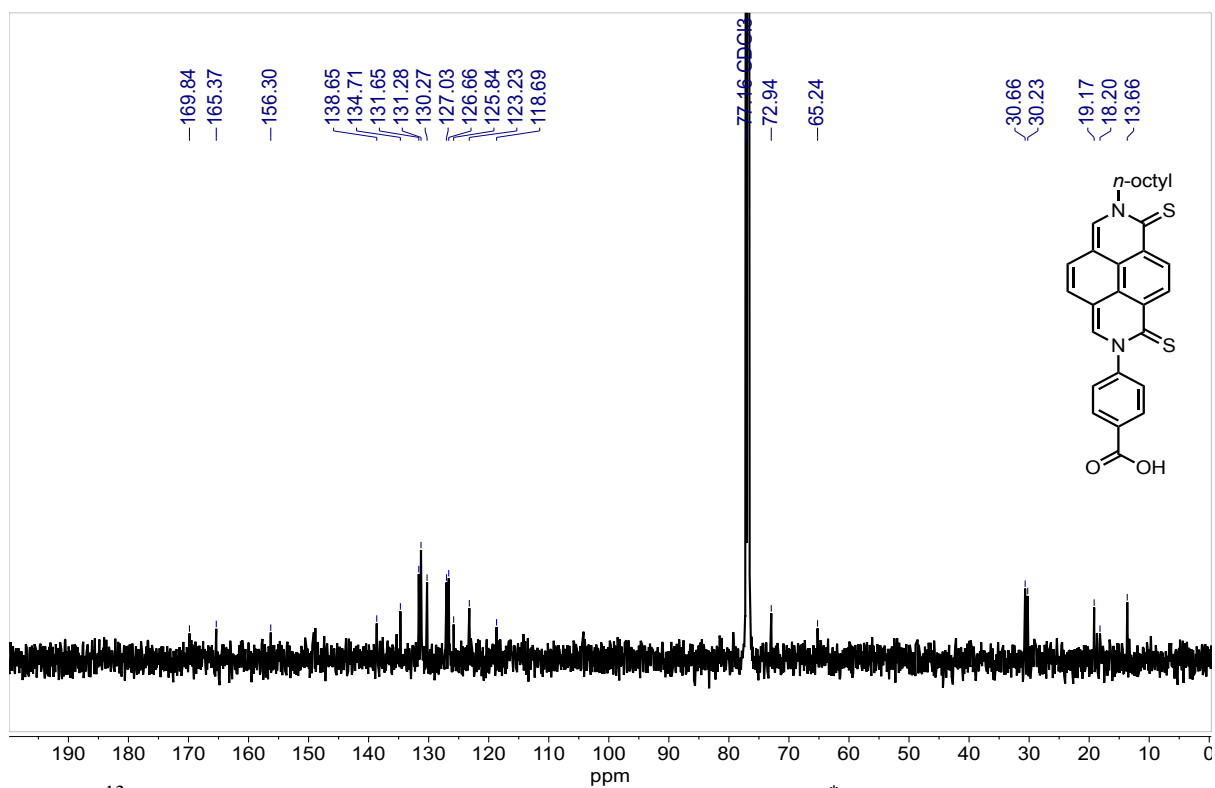


Figure S6. ¹³C NMR spectrum (500 MHz) of **QDM MA** in CDCl₃. *Residual solvent peak of CHCl₃.

ADDITIONAL SPECTRA

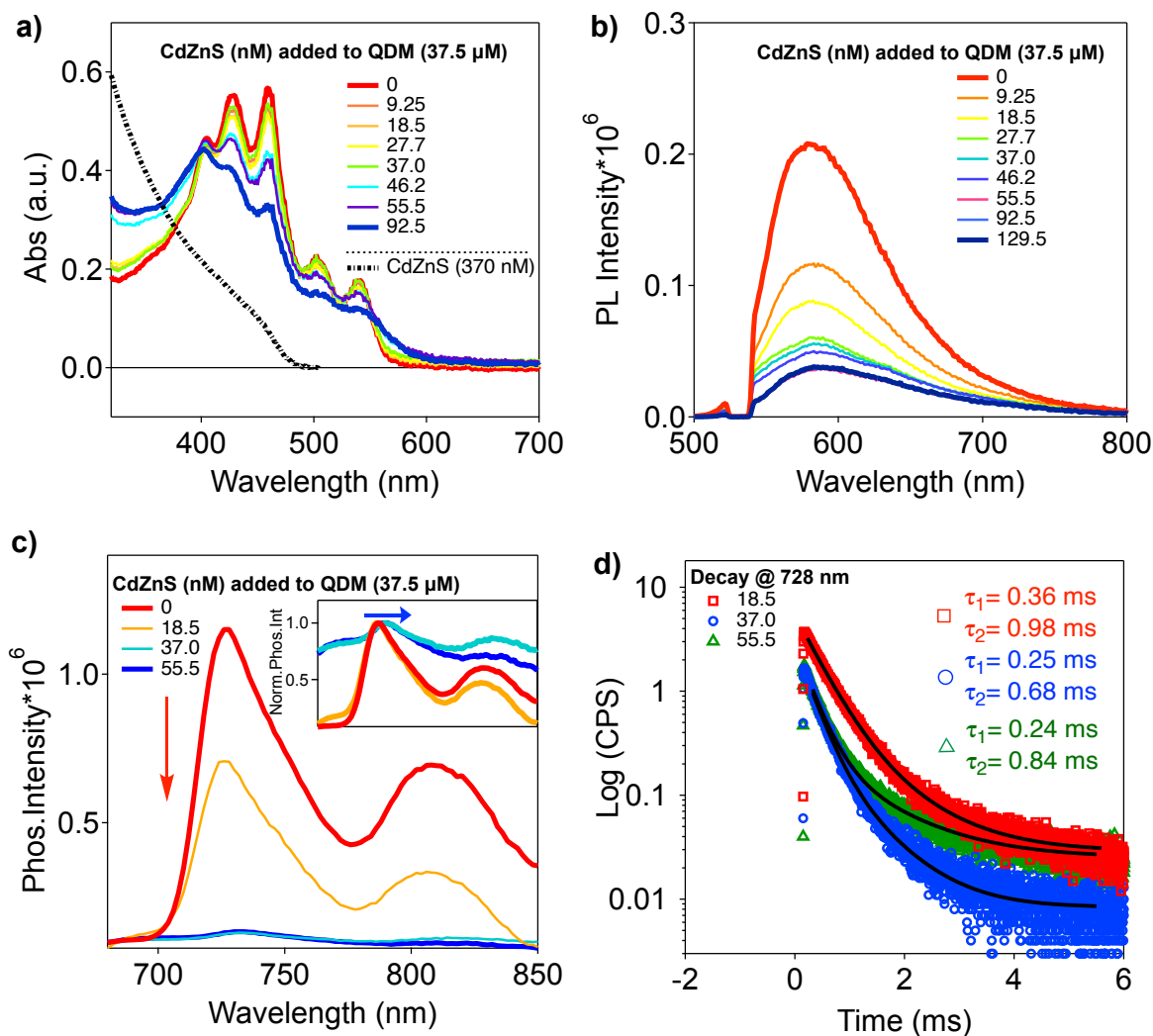


Figure S7. (a) UV-vis abs spectra of **CdZnS** added to **QDM** (37.5 μM) in toluene (b) FL emission spectra of **CdZnS** added to **QDM** (37.5 μM) in toluene with OD = 0.15 at $\lambda_{\text{Exc}} = 532$ nm. A 532 nm notch filter with 17 nm bandwidth was used for recording FL emission. (c) Phos. emission spectra of **CdZnS** added to **QDM** (37.5 μM) recorded in MCH at 77 K at $\lambda_{\text{Exc}} = 532$ nm (μs Flashlamp frequency = 40 Hz and Detector delay = 140 μs , inset: Normalised phosphorescence emission spectra). (d) Bi-exponential phos. decay kinetic at 728 nm of **CdZnS-QDM** hybrid.

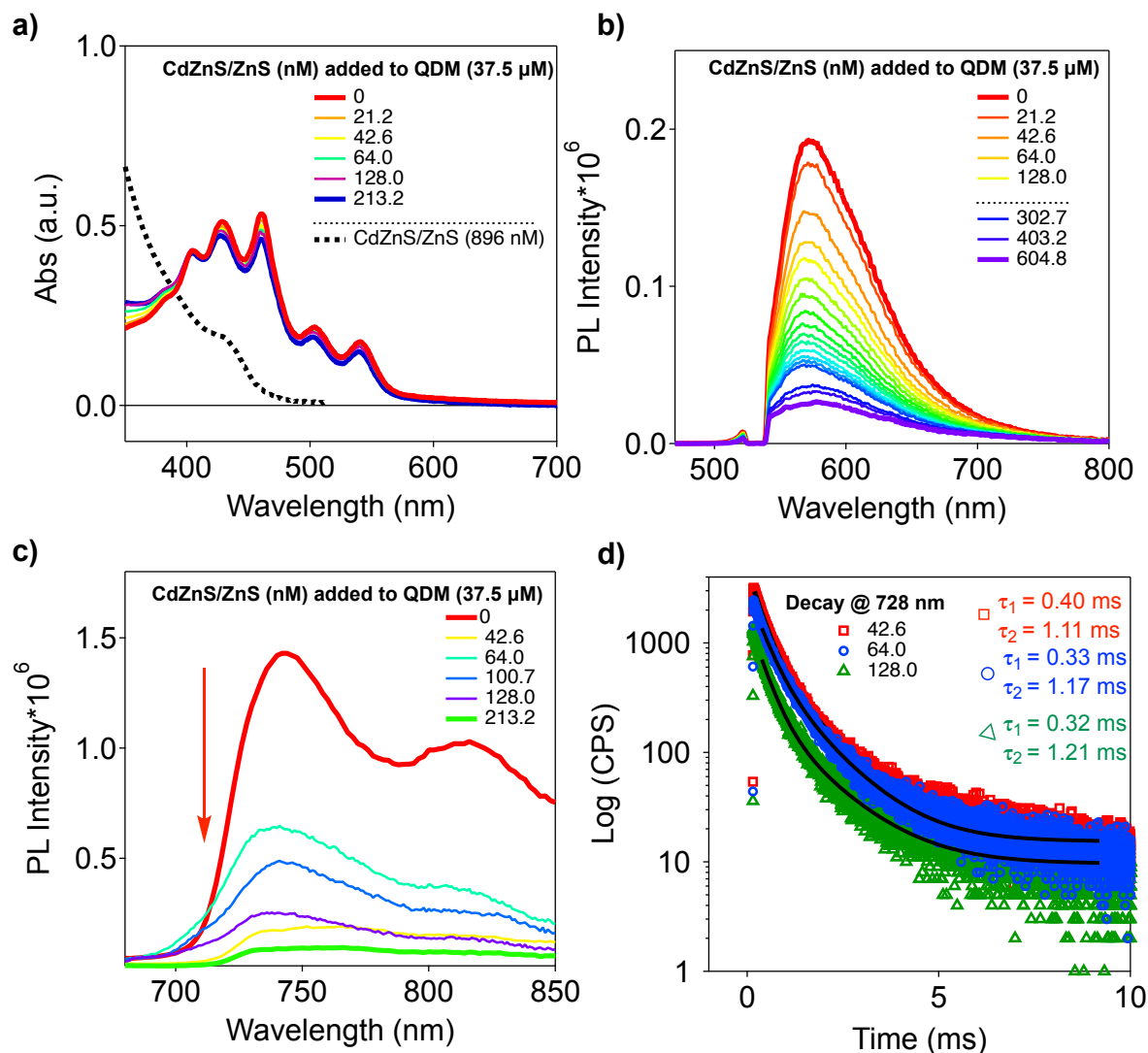


Figure S8. (a) UV-vis abs spectra of **CdZnS/ZnS** added to **QDM** (37.5 μM) in toluene (b) FL emission spectra of **CdZnS/ZnS** added to **QDM** (37.5 μM) in toluene with OD = 0.15 at $\lambda_{\text{Exc}} = 532$ nm. A 532 nm notch filter with 17 nm bandwidth was used for recording FL emission. (c) Phos. emission spectra of **CdZnS/ZnS** added to **QDM** (37.5 μM) recorded in MCH at 77 K at $\lambda_{\text{Exc}} = 532$ nm (μs Flashlamp frequency = 40 Hz and Detector delay = 140 μs). (d) Bi-exponential phos. decay kinetic at 728 nm of **CdZnS/ZnS-QDM** hybrid.

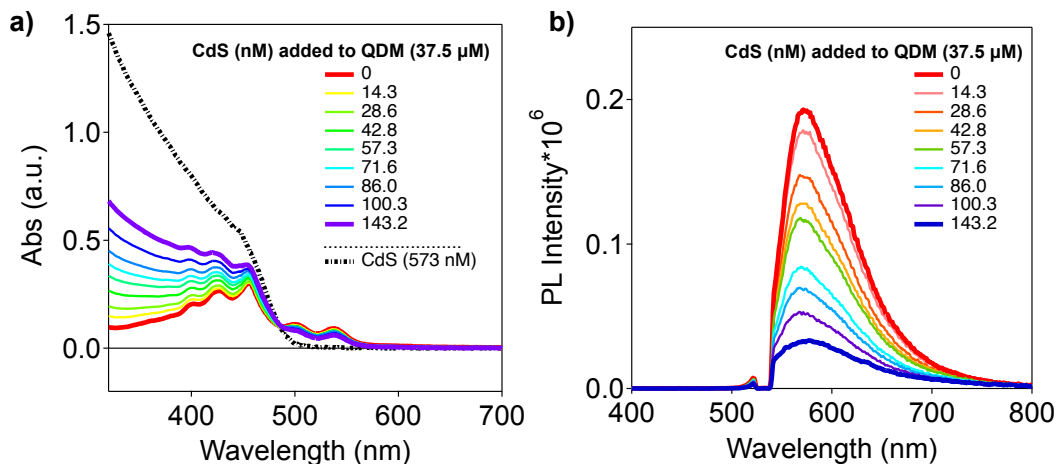


Figure S9. (a) UV-vis abs spectra of **CdS** added to **QDM** (37.5 μM) in DCM (b) FL emission spectra of **CdS** added to **QDM** (37.5 μM) in DCM with OD = 0.15 at $\lambda_{\text{Exc}} = 532$ nm. A 532 nm notch filter with 17 nm bandwidth was used for recording FL emission.

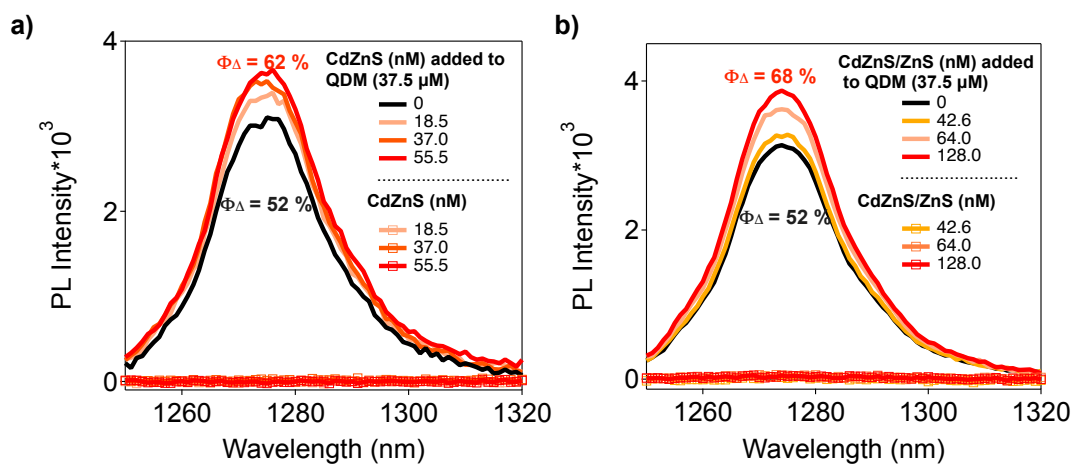


Figure S10. Singlet oxygen emission spectra of (a) **CdZnS** added to **QDM** (37.5 μM) and free **CdZnS** (b) **CdZnS/ZnS** added to **QDM** (37.5 μM) and free **CdZnS/ZnS** recorded in air-saturated toluene. ($\lambda_{\text{exc}} = 532$ nm).

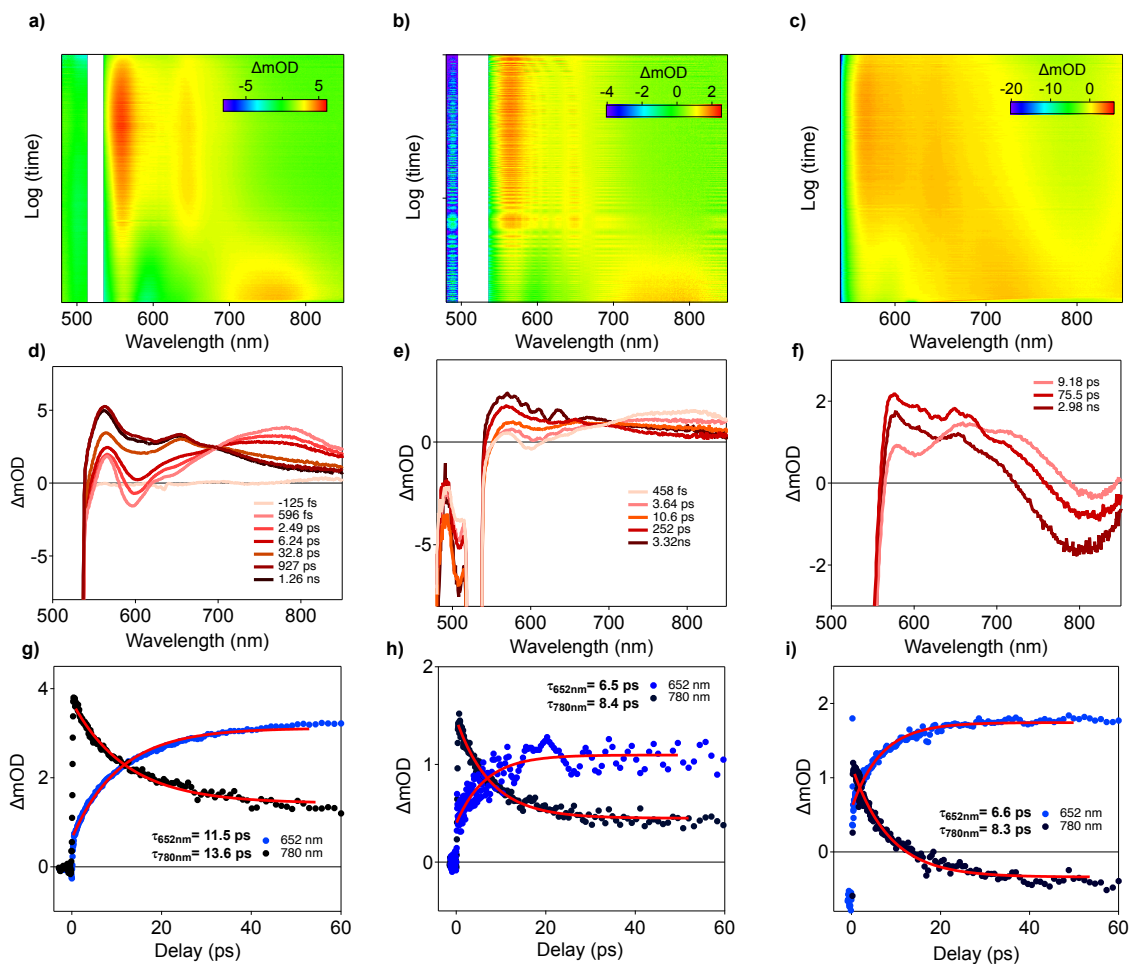


Figure S11. Femtosecond time-resolved transient absorption (fsTA) 2D intensity map of (a) **QDM** (37.5 μM) (b) **QDM + QD** (8.75 nM), and (c) **QDM + QD** (35.0 nM) respectively, and (d-i) their corresponding transient absorption features and kinetics recorded in oxygen-free toluene with samples of OD = 0.45 at $\lambda_{\text{Exc}} = 532\text{ nm}$, 0.1 $\mu\text{J/pulse}$, and 2.5 kHz repetition rate.

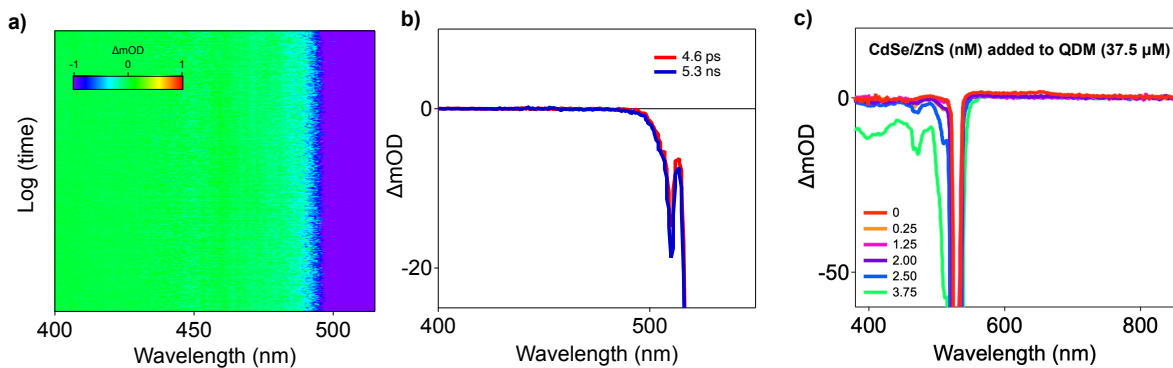


Figure S12. (a) Femtosecond time-resolved transient absorption 2D intensity map of **CdSe/ZnS QD** recorded in toluene pumped at 532 nm. (b) Corresponding transient absorption features recorded in oxygen-free toluene with samples of O.D. = 0.4 at $\lambda_{Exc} = 532$ nm, 0.1 $\mu J/pulse$, and 2.5 kHz repetition rate. (c) nsTA spectra of **CdSe/ZnS** added to **QDM** (37.5 μM) selected at 4 μs .

ELECTROCHEMICAL DATA

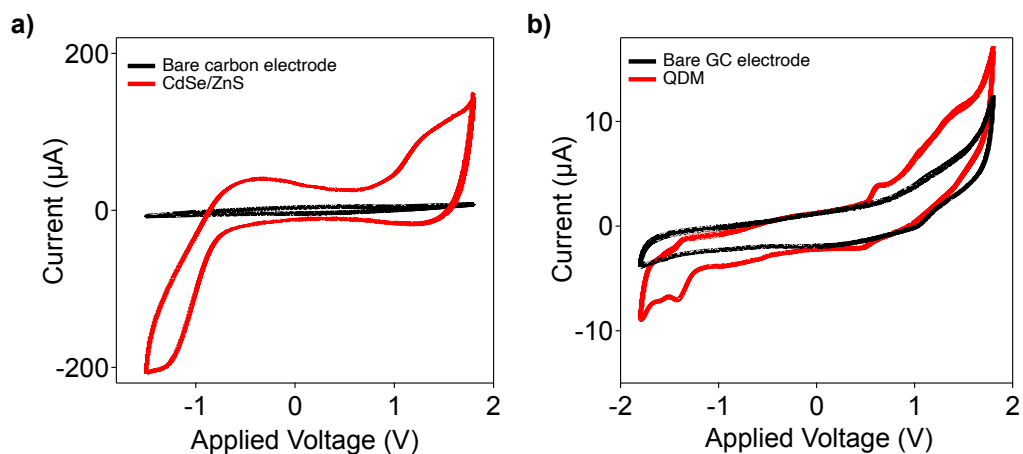


Figure S13. Cyclic voltammograms of (a) **CdSe/ZnS** measured at carbon fiber paper electrode vs Ag/AgCl/3M KCl; (b) **QDM** measured at glassy carbon (GC) electrode vs Ag/AgCl/3M KCl. CV parameters were as follows: potential window applied -1.8 V to +1.8 V, scan rate 100 mV/s, counter electrode Pt wire. All experiments were carried out in air-free ACN at room temperature (22-25 °C). Supporting electrolyte 0.1 M TBAPF₆ was used for the measurements of **QDM**.

DETERMINATION OF QDM:QD RATIO IN THE HYBRID SAMPLE

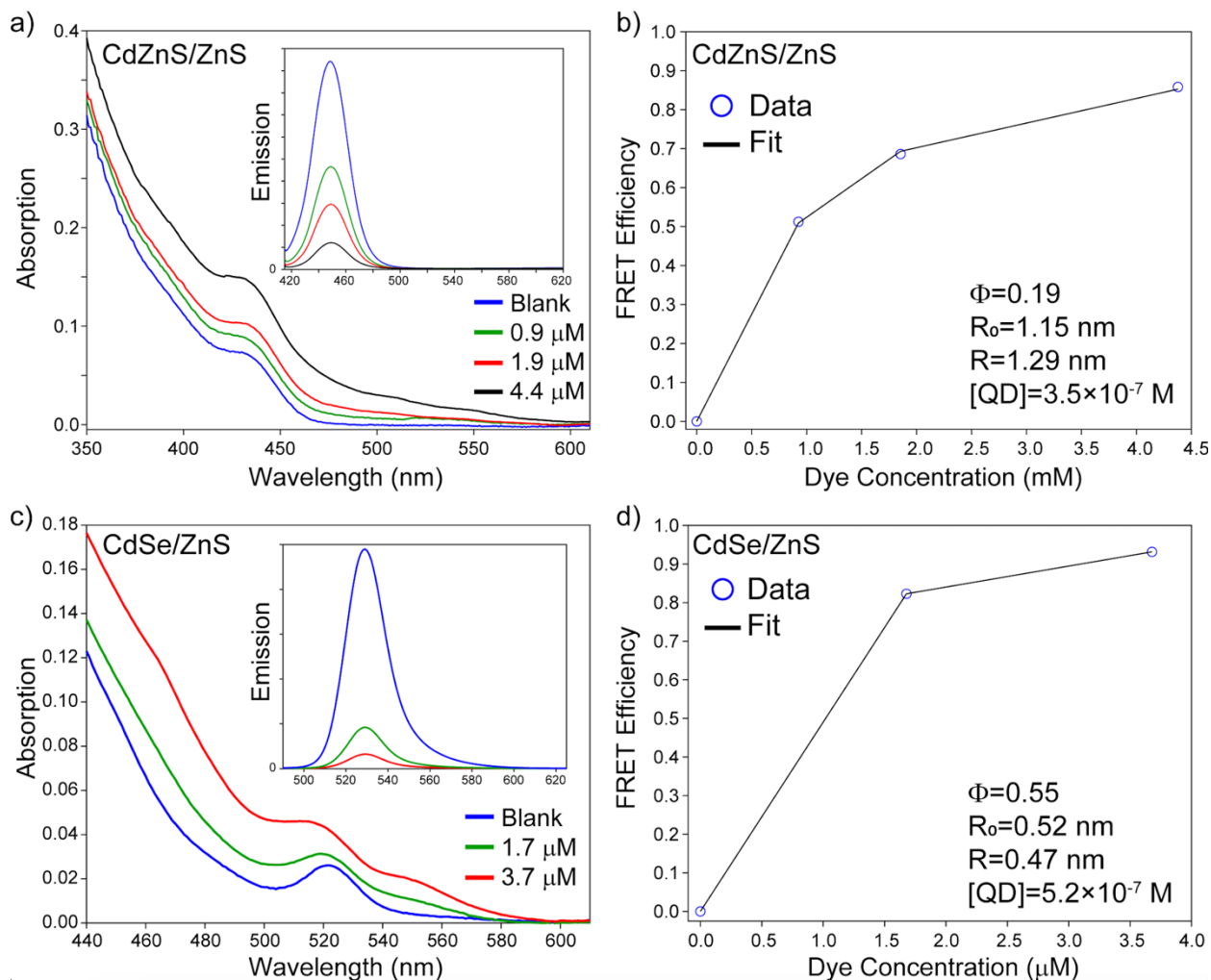


Figure S14. Determination of QDM/QD ratio for CdZnS/ZnS and CdSe/ZnS dots. Using the method¹, a series of QDs were water solubilized using 40% octylamine-modified poly(acrylic acid) with additional QDM dye. Co-localization within micelles was achieved by dissolving a mixture of QD and QDM chromophores with the amphiphilic polymer in chloroform before vacuum removal and dissolution into basic water. The non-specific interaction is robust, as extensive dialysis did not fully desorb the dye. (a,c) Absorption spectra of a constant concentration of QDs as a function of increasing QDM dye loading. Insets: Emission of the blank and QDM/QD conjugates reveals quenching. (b,d) Fitting the quenching (FRET) efficiency with Poisson statistical correction yields the QDM-QD distance and the QD concentrations, which enables the determination of the QDM/QD ratio for the materials prepared in this study.

CELL VIABILITY RAW DATA

Table S1. Cell viability data for DC2.4 using 250 nM of **QD**, **QDM**, and the **QDM-QD** hybrid after 24 h incubation (a) without photo-irradiation (b) with photo-irradiation using 100 mW green LED for 30 minutes.

Without Irradiation

		<i>Blank</i>			<i>QD</i>			<i>QDM</i>			<i>Hybrid</i>		
		T	D	%	T	D	%	T	D	%	T	D	%
<i>CdZnS/ZnS</i>	Trial 1	296	5	98.3	599	23	96.2	244	31	87.3	256	26	89.8
	Trial 2	327	15	95.4	351	12	96.6	185	26	85.9	125	15	88.0
	Trial 3	351	3	99.1	366	6	98.4	146	13	91.1	161	13	91.9
<i>CdSe/ZnS</i>	Trial 1	41	0	100	49	1	97.9	31	1	96.7	33	1	96.9
	Trial 2	31	0	100	36	1	97.2	33	1	96.9	66	2	96.9
	Trial 3	34	2	94.1	91	2	97.8	77	2	97.4	58	4	93.1

With Irradiation

		<i>Blank</i>			<i>QD</i>			<i>QDM</i>			<i>Hybrid</i>		
		T	D	%	T	D	%	T	D	%	T	D	%
<i>CdZnS/ZnS</i>	Trial 1	28	5	82.1	25	5	80	42	11	73.8	17	14	17.6
	Trial 2	87	10	88.5	29	6	79.3	29	11	62.1	16	15	6.3
	Trial 3	204	15	92.6	248	28	88.7	70	13	81.4	9	9	0
<i>CdSe/ZnS</i>	Trial 1	164	10	93.9	105	10	90.4	113	10	91.1	23	21	8.7
	Trial 2	65	4	93.8	151	8	94.7	73	7	90.4	13	13	0
	Trial 3	160	10	93.7	70	3	95.7	61	7	88.5	17	17	0

T: Total cells, *D*: Dead cells, *%*: Live cells/Total cells

CELL VIABILITY AND IMAGING EXPERIMENT WITH JURKAT CELLS

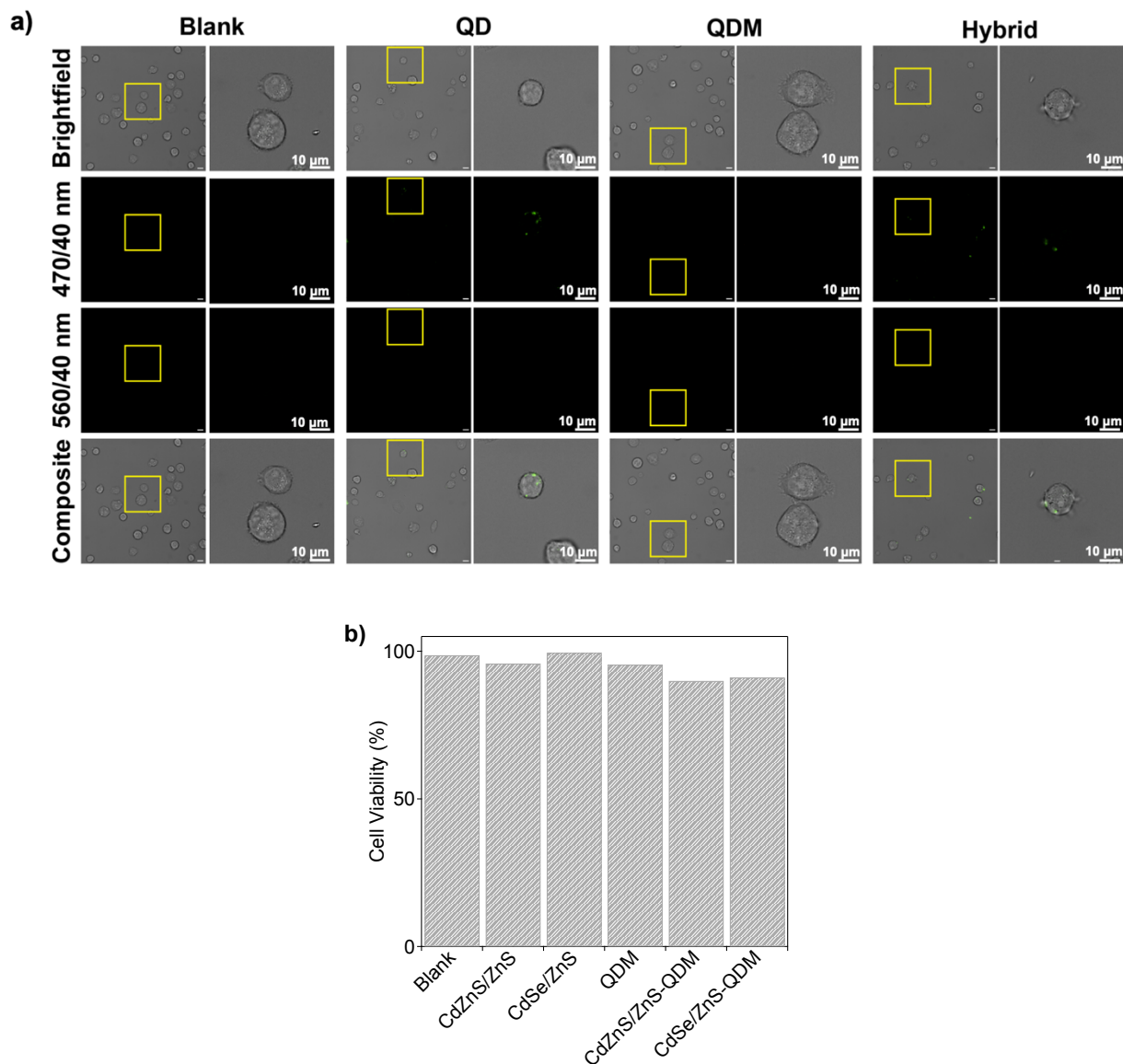
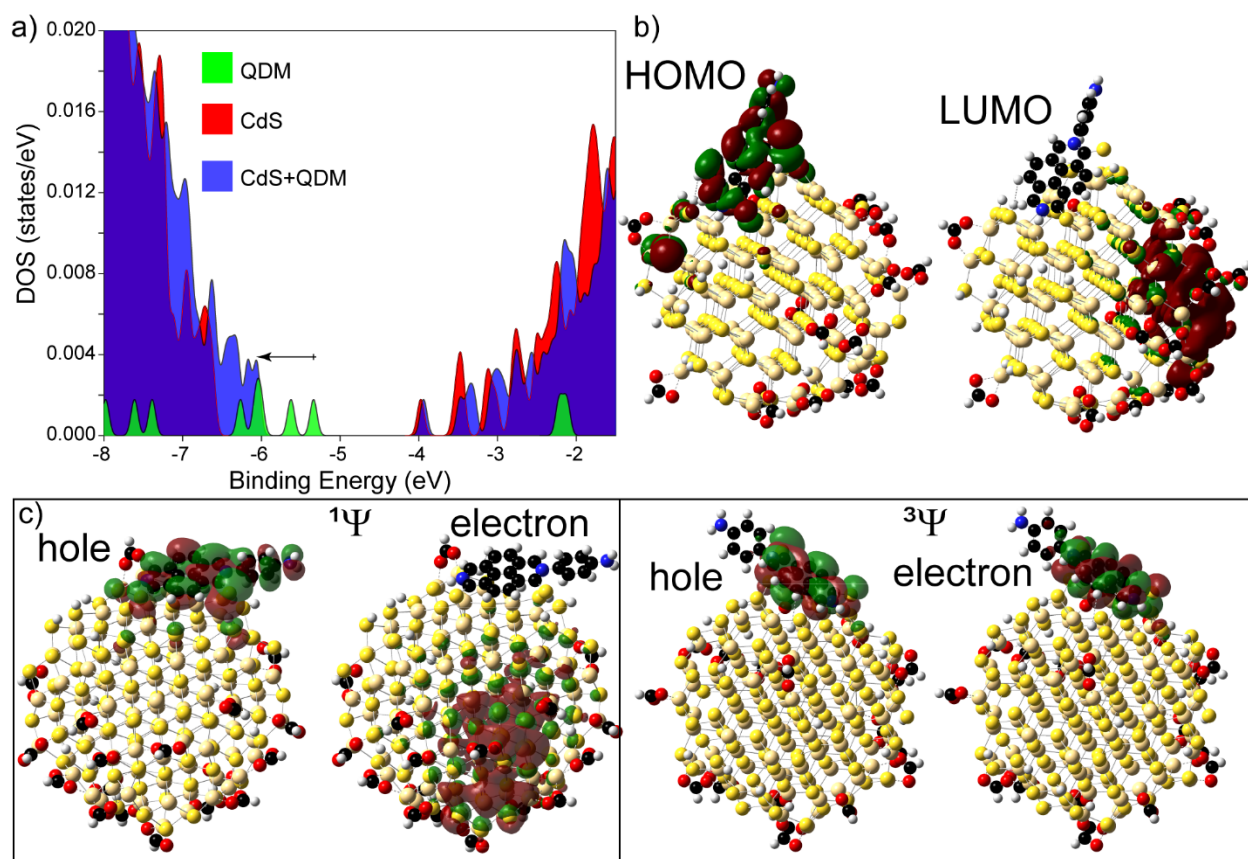
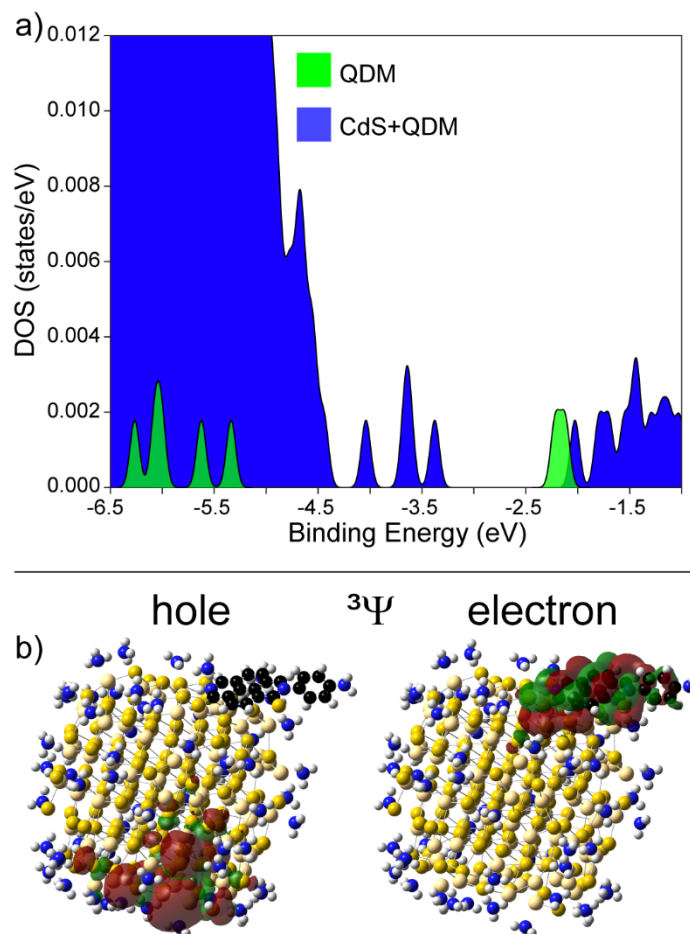


Figure S15. (a) Brightfield, fluorescence images excited at 470/40 nm and 560/40 nm, and composite images of Jurkat cells loaded with 100 nM **CdSe/ZnS**, **QDM**, and **QDM-CdSe/ZnS** hybrid and equal volume of blank media. Magnified views of the yellow box in each condition are shown to the right. Scale Bars: 10 μm . (b) Cell viability (%) of Jurkat cells for 100 nM of **CdZnS/ZnS**, **CdSe/ZnS**, **QDM**, **QDM-CdZnS/ZnS** hybrid, and **QDM-CdSe/ZnS** hybrid after 24 h incubation without photo-irradiation. An equal volume of blank media was added to blank wells.

ADDITIONAL COMPUTATIONAL DATA



Scheme S6. (a) Density of states for a **CdS** cluster (red), **CdS-QDM** hybrid, and **QDM** dye alone. (b) DFT orbital visualization reveals a **QDM**-centered HOMO and **QD**-centered LUMO. (c) TDDFT with NTO analysis reveals a split exciton state for the 1st optically allowed transition, while the lowest excited state is triplet and is centered on the **QDM** component.



Scheme S7. (a) Density of states for an amine-ligated **CdS-QDM** hybrid (blue) and **QDM** dye alone (green). (b) TDDFT with NTO analysis reveals a **QD**-centered hole state and a **QDM**-centered electron in the lowest excited triplet state. The 1st optically allowed singlet state's electron and hole densities were essentially identical to these results.

CARTESIAN COORDINATES

CdSe/formic acid ligand + QDM complex:

Cd	1.28413600	-2.43578000	-0.00817500
Se	-1.01863800	2.22510700	0.07603300
Cd	0.06577300	1.04682200	2.33032200
Cd	-1.78068200	0.19255400	-1.61929900
Se	2.21819700	-0.54021000	1.75074100
Se	0.31134200	-1.40053200	-2.36767300
Cd	0.91927500	3.69681100	-1.11306600
Se	-1.87294100	-0.42240100	3.50838700
Se	-3.71402700	-1.27278500	-0.42756800
Cd	4.10283200	1.00098500	0.54654000
Cd	2.22584400	0.13455500	-3.52733800
Se	-0.64095500	-3.92203300	1.17017100
Cd	-4.22512000	-0.30918900	2.09741000
Se	1.35817100	2.74469900	-3.65305500
Se	3.21608000	3.59535200	0.36567100
Cd	-3.01255500	-3.95396500	-0.23012100
Cd	-1.10097000	-3.07603400	3.75499000
Se	4.51195100	0.13147300	-2.02308800
Cd	-3.20139100	3.77577300	0.77805100
Se	0.87919200	2.99838000	4.11244400
Se	-2.87778500	1.28937200	-3.92336200
Cd	3.12891600	-1.76502700	4.09887800
Cd	-0.61470600	-3.48285200	-3.98258200
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Se	-5.11480800	2.28237400	1.93348300
Cd	-0.89775100	2.71374000	-5.17756000
Cd	2.87943000	4.48450100	2.92456900
Se	1.16669500	-3.18167500	5.24282600
Se	-2.51494000	-4.90825600	-2.73751000
Cd	5.31687200	-2.47887500	-1.84715300
Se	0.14369000	6.32801800	-1.35085300
Cd	-6.01821500	-1.14990200	-1.84344600
Cd	-2.32704300	0.50541000	6.02280600
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Cd	1.72843600	1.64188500	6.37114600
Se	-1.71717200	-2.45451800	-6.28749200
Se	3.92489800	0.11718800	5.92921800

Se	5.33913400	-3.27526100	3.46918500
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Cd	4.30031400	-5.10097300	1.73834900
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Se	-5.76403300	-2.28261300	-4.32937600
Se	-0.19682500	0.28675100	7.72068200
Cd	0.13644100	-0.80431600	-7.23678500
Cd	5.59406100	1.69209600	4.59325100
Cd	7.04313600	-1.69053800	2.11976500
Cd	3.43148500	-3.34529700	-5.71132100
Se	0.64105100	-7.63954800	-1.15369900
Se	2.45351900	-6.72528500	2.89238300
Cd	-7.49560800	2.45203900	0.53299300
Cd	-5.68235100	3.25647500	4.46056300
Se	-1.85154200	5.32781400	-5.24120400
Se	1.95962200	7.06617500	2.74592400
Se	-0.43939700	1.83677100	-7.72695300
Se	5.17275600	4.39020100	4.41839300
Cd	-4.79724400	-5.01884000	-4.29647100
Cd	0.74473300	-2.44772700	7.89340300
Cd	2.02760600	-5.78921800	5.58481700
Cd	-1.74345800	-7.58184300	-2.74084800
Se	5.82781200	-3.35156200	-4.40046200
Se	7.65184300	-2.52613000	-0.41212600
Se	4.15020700	6.20852800	-3.15742700
Cd	-7.05055100	-3.86919900	1.74564400
Cd	-5.19430800	-3.05936100	5.54476900
Se	5.45756100	2.69683600	-5.56311300
Se	7.26550500	3.63437500	-1.42296100
Cd	-3.97149200	-6.52520400	3.31797200
Cd	2.08108800	7.94145300	-2.54497100
Se	-7.94793600	-2.64586300	-0.60847600
Se	-4.32210800	-0.94511200	7.16905600
Cd	4.55736600	0.76541500	-7.43765500
Cd	8.39007200	2.56888900	0.95551100
Se	-1.73248500	-8.00049600	2.53731600

Cd	-8.30950100	-0.27681600	3.90466200
Se	2.27564000	5.51735800	-7.01281500
Se	5.81176300	7.25610500	0.88647000
Cd	-5.65756700	-7.48692900	-0.84422500
Cd	-2.07992200	-5.75828400	7.30589100
Se	8.58792500	0.13232400	-3.86790000
Cd	-6.48377200	6.59664100	-0.65574000
Cd	-4.66273100	7.40412400	3.12211900
Se	-6.10690800	3.93578400	-5.42661100
Se	-0.55914400	6.41936800	6.48267000
Se	-4.83025500	0.28715200	-7.76145000
Se	2.54197700	3.64297200	8.17295000
Cd	-2.50596300	-4.60917700	-8.09489000
Cd	5.01385100	-1.20052400	8.29477300
Cd	0.54774200	-7.05817700	-6.54810400
Cd	6.30211400	-4.45100300	5.95456300
Se	6.49193000	-6.72884400	1.02221600
Se	4.65592700	-7.57365200	-3.01109200
Se	-9.43685800	1.04143500	1.77975300
Se	-7.76663400	1.85567400	5.55794600
Cd	0.25166100	6.83217700	-5.84685200
Cd	3.59134800	8.80608600	1.39225200
Cd	2.55376000	4.28182700	-9.46841400
Cd	8.04304700	6.82331700	2.43467600
Se	-6.74452800	-6.51972200	-3.15000000
Se	-1.20567200	-3.88990000	9.08971700
Se	-3.63516400	-9.12044000	-1.57995600
Se	0.14429500	-7.27996000	6.83066200
Cd	7.69207600	-1.67336000	-5.64507600
Cd	9.56206000	-0.84407900	-1.55757400
Se	-6.35259400	5.88350800	4.53211900
Se	-8.42529500	4.99536100	0.26493500
Cd	-4.16132200	5.28775900	-6.70930000
Cd	1.47225700	7.79469100	5.31154800
Cd	-2.88120800	1.83055400	-8.86145600
Cd	4.39773000	5.16170900	6.88260500
Se	-4.53131900	-5.79001100	-6.84486100
Se	2.94808600	-2.42840300	9.42202200
Se	-1.11835300	-8.58148100	-5.15041900
Se	4.39234200	-6.08878700	6.81861500
Cd	8.30660500	-5.15500100	-0.27288800
Cd	6.56671400	-5.94481000	-4.08230300
Se	-3.01644900	8.91802100	-2.85918300
Se	-1.09247300	9.76413600	1.09748600
Cd	-9.43152800	1.38443400	-3.57239100
Cd	-3.77264600	3.96057100	8.56372900

Cd	-8.14455100	-2.06772900	-5.73761200
Cd	-0.87303100	1.30374600	10.23892100
Se	0.62507700	-1.51633600	-9.93977600
Se	8.01237800	1.84662300	6.06525800
Se	4.00609500	-4.34789500	-8.30588400
Se	9.47208800	-1.83983700	3.57758200
Cd	1.52730500	-10.27878600	-0.82860500
Cd	3.26201300	-9.38207600	2.94518200
Se	1.12803400	9.10326000	-4.87479900
Se	3.15448400	9.84658200	-1.04778900
Cd	-9.67637700	-0.65766800	-0.17189800
Cd	-6.20576200	0.91382600	7.42734100
Cd	-8.18824200	-4.46591000	-2.56524500
Cd	-2.89762200	-1.93596600	9.22938800
Se	3.76210000	1.96011800	-9.74009800
Se	9.39435800	4.55459200	2.49091800
Se	6.87254400	-0.52220400	-7.95109500
Se	10.49265600	1.17017200	-0.01494300
Cd	-2.18660900	-9.69242800	0.49806200
Cd	-0.32019300	-8.68787800	4.71811900
Se	-5.66406600	8.63646400	0.92157300
Cd	-6.84156700	1.56137700	-6.51276200
Cd	0.09020100	4.69037500	8.47287200
Se	-0.24627100	-5.88634100	-8.86761500
Se	7.28519400	-2.46905800	7.52346400
Cd	5.04058700	-8.44545900	-0.48223800
Cd	6.23980900	7.43433400	-4.32474300
Se	-7.04134500	-4.14187200	7.05052100
Se	-9.10946900	-5.25156200	2.71783200
Cd	7.32822700	4.49057300	-6.28809200
Cd	8.83214300	5.23231800	-2.91166100
Se	-5.73580400	-8.13780000	4.49053400
Cd	-3.41178400	9.24365700	-0.17719100
Se	-9.13204900	0.43858400	-6.08597700
Se	-1.64796200	3.91087400	10.22341500
Cd	1.45709300	-3.98044800	-9.19168800
Cd	8.35266600	-0.82417000	5.85175100
Se	3.85216300	-10.50012000	0.54670900
Cd	-8.39490600	5.50980500	2.86999400
Se	-3.67046500	4.46725100	-9.26188900
Se	3.72995100	7.84482800	6.84808600
Cd	-3.36022700	-8.24014500	-6.62537000
Cd	3.94202400	-4.94497900	9.24155400
Se	8.95136300	-6.16736100	-2.74374500
Se	-7.48305700	7.69392000	-3.01909000
Se	-3.78493300	9.37845400	4.86043800

Cd	-8.02183700	5.33996600	-4.04139300
Cd	-3.02346700	7.58718000	6.62265500
Cd	-5.39170400	-2.17308300	-8.88123600
Cd	3.32758200	1.79726600	10.07316700
Se	-3.65826500	-3.45740700	-10.35618300
Se	5.74436100	0.80161500	10.08464100
Se	2.72995900	-8.68389900	-7.13299500
Se	8.44048500	-6.08864900	5.23835000
Cd	3.12670200	-9.22248700	-4.59932900
Cd	6.91604600	-7.48653400	3.63073500
Cd	1.03031100	11.08118100	-0.05722900
Cd	-0.88267000	10.32162100	-3.70100100
Se	-11.36108900	-0.04597200	-2.20892700
Se	-5.73486400	2.34894900	9.68104800
Se	-10.05509500	-3.43030100	-4.26450600
Se	-2.81421700	-0.27771600	11.37703000
Cd	1.27974900	1.10938500	-10.00060600
Cd	8.07274900	4.22690700	4.75065400
Cd	6.26096200	-2.97531900	-8.53650200
Cd	10.93376200	-0.78256600	1.63662100
Se	1.16808300	-10.85114500	4.00793500
Se	-0.47633400	-11.78018300	0.30980000
Cd	-9.07313800	-4.46858200	5.33054300
Se	6.72212900	7.05172200	-6.92323800
Se	8.47670900	7.91293900	-2.97376500
Cd	-7.61422400	-7.44045400	2.78298900
Cd	-6.39960100	-6.76446700	6.75968500
Se	9.77671000	4.36727700	-5.25181500
Se	-10.25543400	-1.90731900	5.02084000
Cd	4.29062900	7.09493900	-7.87230200
Cd	7.49385800	8.66340100	-0.65743400
Se	-7.63911300	-8.91375900	0.48932200
Se	-4.15267600	-7.28083400	8.30624600
Cd	10.41754800	1.78839500	-5.01326900
Cd	-5.33984500	8.53394500	-4.21311300
Cd	-1.58940100	10.18650600	3.72385700
Se	-10.31063900	4.00881100	-3.78811700
Se	-4.76636700	6.53642400	8.35080400
Se	-7.70042300	-3.30506700	-8.15601100
Se	1.41455400	1.05351100	11.77205700
Cd	-1.88856900	-1.65557900	-10.91480600
Cd	7.05336900	2.40414600	8.52945600
Cd	4.55148300	-6.93588100	-7.66867600
Cd	9.76639200	-4.54026400	3.65291900
Se	1.89316700	-11.24779000	-3.39735500
Se	5.44077200	-9.46954000	4.62936300

C	3.44814800	7.35612600	-10.47469800
O	3.66289600	8.33454400	-9.67824100
O	3.64538200	6.13078900	-10.08446500
H	-2.26492200	4.98602900	-9.29815900
C	9.02408800	-4.05286800	-7.36113300
O	9.04708400	-3.28888700	-6.33631100
O	8.04846400	-4.18355200	-8.19321800
H	9.54671000	-4.90065600	-3.27664100
C	-0.58147800	12.80619100	-2.53046700
C	-4.90943300	8.56887700	-6.95509300
O	-0.11600500	11.82118500	-1.81680900
O	-1.14324700	12.57686800	-3.65321500
O	-5.19687600	9.58610900	-6.24681500
O	-4.75628100	7.39875700	-6.39592000
H	-10.46134400	4.35287000	-2.33718200
H	-11.20925000	-1.30901700	-3.00882700
C	12.60144100	0.52587400	-5.78041700
O	12.54033900	1.03107000	-4.59090900
O	11.61054100	0.63894000	-6.60407800
H	4.64617100	8.19071900	5.71429300
C	8.94589600	9.87641000	1.34494300
O	8.32111200	10.49162900	0.41100000
O	8.95851900	8.57822500	1.39319200
H	4.93995700	-8.52432700	5.70203400
C	2.85682800	11.81976900	2.46008000
O	3.40003200	10.66292200	2.59098800
O	1.94746800	12.15208500	1.61840200
H	-10.23511200	-4.59915300	-5.18008200
C	7.19974100	5.14633300	8.72740900
O	8.08431300	4.36529400	9.19635800
O	6.14251400	4.65339700	8.12923300
H	1.70631600	-0.39822400	11.51673500
C	0.60480900	11.03302800	5.15809600
O	0.47113100	9.74194500	4.99245600
O	-0.24337400	11.83104000	4.64992700
H	-6.93168500	-4.50933700	-7.66485800
H	1.77872000	-11.16861800	5.33578800
C	-2.37106100	0.82084800	-12.02132800
O	-2.56594500	0.70875700	-10.73016300
O	-1.99361900	-0.18646800	-12.69605600
H	-8.78106600	-8.19818000	-0.16416200
C	0.10563700	3.67942900	-11.48119600
O	0.83580600	4.49934900	-10.81965300
O	0.08966100	2.40153300	-11.35667400
H	-10.89875600	-2.21605100	3.70265700
C	12.09800900	-2.62709900	-0.69638000

C	11.20675500	-5.35598300	1.44251400
O	11.22962600	-2.30518600	-1.57904600
O	12.08328800	-2.28775300	0.54596800
O	11.70213800	-5.17856800	2.59859700
O	9.93451500	-5.13688000	1.22825100
H	-4.45782000	-6.36483100	9.45053600
C	4.98076600	-6.07901500	11.39358600
O	3.75800700	-6.33027200	11.05206700
O	5.72137500	-5.27810900	10.70305000
H	0.07218300	-11.76582600	1.70799800
C	8.06113100	7.27336600	5.64864700
O	7.94232600	7.70096500	4.44798400
O	8.11483800	6.04344900	6.01873400
H	-6.87529000	3.31252400	9.58302000
C	7.25547100	-7.14715000	-7.16315500
O	6.70327000	-7.45335600	-8.26571100
O	6.53748900	-6.68392600	-6.17198000
H	-3.97309700	0.61205300	11.03647400
C	-4.17014000	-10.11097100	-8.31022100
O	-3.26525700	-9.27855500	-8.70416200
O	-4.67678900	-10.04370100	-7.12126900
H	0.57705100	-10.83023900	-3.99567700
H	-5.74441100	6.30400800	7.22454500
H	-4.79129200	8.66788100	-8.03859500
H	-0.49021100	13.83241900	-2.16391700
H	3.19786800	12.60835400	3.14532300
H	1.44967700	11.41176200	5.74100700
H	9.47865200	10.44830000	2.11015500
H	3.09915800	7.54664900	-11.49343000
H	13.50557100	-0.00529300	-6.09414500
H	9.91478200	-4.66723300	-7.55056300
H	8.33299300	-7.27751500	-7.02968800
H	-0.57657900	4.11476700	-12.22485600
H	-2.54943800	1.78220000	-12.50758900
H	-4.51888000	-10.89238300	-8.99444400
H	11.83680700	-5.70203100	0.61798600
H	5.39287700	-6.55812100	12.28860400
H	8.11844800	8.03192700	6.44188400
H	7.30170100	6.22886500	8.82665700
H	12.93328200	-3.26206400	-1.02144100
N	-18.50852700	0.18168100	-5.09952900
H	-19.49216200	0.39080500	-5.13739000
H	-18.09136700	-0.27886400	-5.89116000
C	-17.74027100	0.56746800	-4.01583200
C	-16.35223500	0.29707000	-3.98252500
C	-18.32819000	1.23986200	-2.91796100

C -15.57912200	0.68999300	-2.88921000
H -15.88162400	-0.21409600	-4.81828000
C -17.55083700	1.63112700	-1.82783000
H -19.39245100	1.46022100	-2.92806300
C -16.18034800	1.35229400	-1.81341500
H -14.50948800	0.49747700	-2.87473500
H -18.00280300	2.16629800	-0.99811900
C -15.16953500	0.75620200	0.27914100
C -14.38257000	0.96063500	1.39414400
C -13.76555400	2.25135400	1.54288500
C -14.15766200	-0.06441400	2.38366900
C -14.81970700	3.01851700	-0.59054600
C -12.91238200	2.48892700	2.65881300
C -13.98599400	3.26392200	0.58207500
C -13.34018200	0.16276800	3.45272100
H -14.64712800	-1.02668000	2.25873800
C -12.68027300	1.43890500	3.60775600
C -12.27747000	3.75525500	2.80759800
C -13.36337000	4.53343000	0.77107400
H -13.15677500	-0.60817700	4.19454100
C -11.78165100	1.68321500	4.63591400
C -11.37725000	3.95445000	3.89768400
C -12.53955800	4.77593700	1.84738800
H -13.55757600	5.30131100	0.02932600
H -11.50193900	0.93066600	5.36323900
N -15.37198700	1.72726500	-0.66568600
S -15.11381700	4.17897400	-1.81894400
N -11.17081400	2.89917700	4.73327200
H -10.45402300	3.02280200	5.45252400
C -9.64841300	-7.14693600	7.05680300
O -10.06968600	-6.14425000	6.37304500
O -8.43371900	-7.52425800	7.20798000
H -10.41771100	-7.75124000	7.55997600
S -10.57129100	5.49204800	4.31237900
H -12.06974700	5.74414700	1.98067600
H -15.66405400	-0.18820500	0.08732300

CdS/formic acid ligand + QDM complex:

Cd	1.31401500	-2.28451100	0.73648700
S	-1.14128200	1.91055600	-0.41289200
Cd	0.19785300	1.61596100	1.87417600
Cd	-1.95163400	-0.48114600	-1.20308400
S	2.26174400	0.01413200	1.62735500
S	0.04035700	-2.14572400	-1.58894500
Cd	0.50675500	2.84720900	-2.18566000
S	-1.46100300	0.67322200	3.62936000
S	-3.60257200	-1.40606000	0.56670200
Cd	3.85992000	1.04456000	-0.15005300
Cd	1.66836900	-1.12898800	-3.34277100
S	-0.34183200	-3.24498800	2.49635000
Cd	-3.84630700	0.29207400	2.57933900
S	0.66350400	1.16979900	-4.22470700
S	2.79315900	3.31146800	-0.99936000
Cd	-2.76186500	-3.75615700	1.54331400
Cd	-0.53784700	-1.63697600	4.60125900
S	3.96999100	-0.59742500	-2.20841900
Cd	-3.20825400	3.53883400	-0.05370100
S	1.04351500	3.95967700	2.80128700
S	-3.31508500	-0.25416300	-3.50191800
Cd	3.49073900	-0.30314200	4.00535000
Cd	-0.88418100	-4.58004900	-2.25169600
S	3.39291000	-3.90535700	0.40768000
S	-4.84207500	2.56717200	1.68299300
Cd	-1.63802000	0.60115900	-5.34340300
Cd	2.77967000	4.94593100	1.06105100
S	1.77884500	-1.19020900	5.70091800
S	-2.47651100	-5.44799700	-0.43437900
Cd	5.05769800	-2.84972700	-1.35816200
S	-0.37174000	5.17789600	-3.13329700
Cd	-5.94842200	-1.75017000	-0.49552400
Cd	-1.64539100	2.31946700	5.64732800
S	6.20598800	1.55482300	0.92408500
S	1.85218800	-2.76963600	-5.40849900
Cd	0.62296400	-5.51653500	3.36657300
S	-4.50425600	3.83391400	-2.36137700
S	-2.31844100	5.90839100	0.71194000
Cd	-5.30028300	1.41978900	-3.01923200
Cd	-1.10272800	5.46356700	3.00706700
Cd	-4.16097100	-2.71388100	-4.03825700
Cd	2.18446100	3.50000100	5.15619600
S	-2.24851500	-4.40527800	-4.51558400
S	4.30050400	2.00925400	4.97270200
S	5.62294400	-1.80945800	3.58555000

S	1.19014200	-6.15579000	-2.69620900
Cd	2.34959400	-6.21666600	-0.34486300
Cd	4.52088700	-4.04257500	2.80317900
S	-5.47562900	-0.66376700	4.33396500
Cd	4.42394400	4.37096400	-2.71947200
Cd	2.35256800	2.07928900	-5.97777900
S	-4.40613900	-4.72841800	3.30522900
S	-2.16123900	-2.59392900	6.36091400
Cd	5.59385300	0.45312200	-3.94697700
Cd	-2.75713000	4.62901000	-4.06824800
Cd	-0.54445500	6.69108300	-0.98160300
S	-2.71983300	4.62263000	4.88361900
S	-7.14369000	0.45464300	-1.42609100
S	-5.88958600	-3.63504200	-2.33110100
S	0.54384100	2.74057200	7.02790300
Cd	-0.64245300	-3.24328100	-6.10652300
Cd	5.69540700	2.97944800	3.08417500
Cd	7.05783100	-0.82650300	1.65706300
Cd	2.80068800	-4.97127900	-4.32202600
S	0.87842800	-7.35461700	1.48609700
S	2.94677300	-5.15679300	4.55867300
Cd	-7.26630700	2.26791200	0.60548700
Cd	-5.10698100	4.26250000	3.71751100
S	-2.62643100	2.97285200	-6.13415300
S	1.66316700	7.21902600	0.29634300
S	-1.43996400	-1.06498600	-7.36977200
S	5.07252200	5.38160700	2.22875300
Cd	-4.81095900	-6.06761000	-1.53608000
Cd	1.62300400	0.33712600	7.90682900
Cd	2.79515300	-3.43332800	6.70215300
Cd	-1.56138400	-7.84652300	0.34287200
S	5.20799200	-4.53678300	-3.40129100
S	7.46833500	-2.36659500	-0.42500400
S	3.26336000	4.41177800	-5.15904100
Cd	-6.40228900	-3.04129300	3.72313900
Cd	-4.25881000	-1.05788000	6.65997000
S	4.40787700	0.54265000	-6.34762100
S	6.46619500	2.80681100	-3.12557100
Cd	-3.14904000	-4.91761200	5.65259200
Cd	1.34431900	6.16737200	-4.90348500
S	-7.57214500	-2.71501400	1.33093400
S	-3.39364200	1.38556900	7.34881700
Cd	3.44967700	-1.79422000	-7.33882900
Cd	7.89080000	2.71675300	-0.82889900
S	-1.02518100	-6.47979600	5.19306100
Cd	-7.57304200	0.89570600	4.60573500

S	1.14900600	2.63333200	-8.27804700
S	5.17092100	6.72726200	-1.89250800
Cd	-5.15138500	-7.19850200	2.46439600
Cd	-0.96074100	-2.88399800	8.76817800
S	7.58418500	-1.15840600	-4.32521500
Cd	-6.54796000	5.63340300	-1.90480200
Cd	-4.44219200	7.62331400	1.00352800
S	-6.66777100	1.64335200	-5.34796100
S	-0.27071300	7.84157100	4.01285700
S	-5.51412700	-2.46817100	-6.38493700
S	3.03948400	5.91802100	6.04604600
Cd	-3.05824000	-6.97095300	-5.35954000
Cd	5.70618300	1.59970900	7.36866600
Cd	0.14778400	-8.62753400	-3.53741500
Cd	6.88445800	-2.03509600	6.09279700
S	6.64200000	-5.69912900	2.40494600
S	4.48176900	-7.86496300	-0.69078100
S	-8.89109000	1.32984500	2.38292500
S	-6.95438000	3.33875000	5.34760500
Cd	-0.73343700	4.11283400	-7.39485300
Cd	3.14785400	8.28285500	-1.51006100
Cd	1.07823700	0.70864700	-10.07945100
Cd	7.63498100	7.19443300	-1.09245000
S	-6.47114600	-7.00742800	0.22891400
S	-0.11031500	-0.57650200	9.59720300
S	-3.15782600	-8.79188800	2.13874800
S	1.17027400	-4.36321000	8.49313700
Cd	6.71719800	-3.37402400	-5.26094500
Cd	9.29168900	-1.25785700	-2.31506500
S	-5.75324800	6.69080500	2.99509200
S	-8.14202100	4.57252500	-0.21782400
Cd	-5.00386500	2.43929500	-7.14519400
Cd	1.50631700	8.77048000	2.39083600
Cd	-3.88437400	-1.46250000	-8.13475600
Cd	4.64224100	6.92779800	4.25664100
S	-4.75265000	-7.61473200	-3.57871000
S	3.92258000	0.75940000	8.96367600
S	-1.26340600	-9.47972600	-1.61318400
S	5.19857800	-3.22932500	7.58663100
Cd	8.18084800	-4.66804800	0.53853200
Cd	6.12145300	-6.76876800	-2.40052200
S	-3.58350200	7.02086100	-5.06574200
S	-1.22953700	9.09905700	-2.03279000
Cd	-9.55115300	-0.15450300	-2.55408300
Cd	-2.98339500	6.27230900	6.98285700
Cd	-8.29086800	-4.02353700	-3.41550400

Cd	0.08966000	4.44697100	9.07841900
S	-0.44558200	-4.75654400	-8.38004700
S	8.14991000	3.73064800	3.96622400
S	3.15092800	-6.71608400	-6.42563300
S	9.53226800	-0.39297200	2.77124900
Cd	1.87787600	-9.62587600	2.57330100
Cd	3.89902000	-7.49858800	5.42790900
S	0.13802100	6.47317900	-7.23810100
S	2.61295700	8.29699500	-4.13916900
Cd	-9.30829100	-0.84282700	1.26175800
Cd	-5.31614200	3.04173800	7.21166100
Cd	-7.93107500	-5.03044100	0.29816100
Cd	-1.85214100	1.16519800	9.41102900
S	2.30208400	-1.44343400	-9.64091800
S	8.79410500	5.07836600	-0.27958300
S	5.63321000	-3.14350000	-7.60420300
S	9.83754600	1.14842600	-1.46268900
Cd	-1.60623700	-8.73114300	4.07041800
Cd	0.52899900	-6.38223400	7.23816100
S	-5.55455900	7.95781700	-1.31351000
Cd	-7.35414700	-0.85957200	-5.52968700
Cd	0.70817500	6.96655300	6.26417300
S	-0.87269600	-8.24849300	-5.89297400
S	7.83473000	0.30101000	6.67292800
Cd	5.23798000	-7.78260800	1.78617400
Cd	4.93712000	5.26904800	-6.96482900
S	-5.87007600	-1.58765700	8.51319800
S	-8.19361500	-3.96953100	5.29721800
Cd	6.07507900	1.93659400	-7.72310200
Cd	7.62145100	4.08986400	-5.04048700
S	-4.70299200	-5.91420600	7.41862400
Cd	-3.57465900	8.24551100	-2.75050100
S	-9.32281300	-1.89770500	-4.45287000
S	-0.77871100	6.74920600	8.22571600
Cd	0.63929600	-6.72211600	-7.09457200
Cd	8.69318900	1.28058400	4.57919700
S	4.25201100	-9.23106100	3.53414200
Cd	-7.92121200	5.87813900	1.94639000
S	-4.69678400	0.84392200	-9.19481400
S	3.83344000	9.31318200	3.43287800
Cd	-3.60373300	-9.79700200	-2.68986700
Cd	4.94077400	-1.55629400	9.57662400
S	8.51966600	-6.44070400	-1.39092400
S	-7.78292500	5.76723500	-4.25790900
S	-3.41902300	9.93893700	1.77492900
Cd	-8.49830600	3.37210700	-4.41270800

Cd	-2.64421200	8.96124800	3.96047500
Cd	-6.04009100	-5.05675500	-6.55337200
Cd	4.12594400	4.89273600	8.23762000
S	-4.43991700	-6.65700800	-7.61453500
S	6.46140800	4.01543700	8.17725800
S	2.27857000	-10.20008200	-3.76554500
S	8.91640100	-3.69714000	5.68844600
Cd	2.96117800	-9.90679300	-1.37327700
Cd	7.40580900	-5.53845800	4.92180900
Cd	0.66650200	9.95194000	-3.68222200
Cd	-1.72135700	8.00933700	-6.53536700
S	-11.08248600	-1.08872800	-0.61776000
S	-4.60106800	5.05381700	8.70793300
S	-9.90319500	-4.63983900	-1.38463300
S	-1.66240700	3.39103300	10.72756500
Cd	-0.01311100	-2.42388100	-9.39905100
Cd	7.83157200	5.50080700	2.02069800
Cd	5.20065900	-5.58207000	-7.40636400
Cd	10.71975200	0.04481900	0.56377000
S	2.03080900	-8.50770800	7.03092200
S	0.20466400	-10.54605500	4.37957500
Cd	-8.03398400	-2.38468000	7.38110500
S	5.24710100	3.96442700	-9.12044000
S	6.84239200	6.42299200	-5.80762300
Cd	-6.73244400	-5.94898900	5.93093400
Cd	-5.15678600	-4.01237600	9.15877100
S	8.42328400	2.38685600	-6.81464300
S	-9.31154200	-0.25379400	6.27056800
Cd	2.86905200	3.78259200	-9.85687200
Cd	5.36992500	7.88184900	-4.23208900
S	-6.84903700	-8.02175800	4.35056900
S	-2.78955200	-3.94753400	10.35389900
Cd	9.25964600	0.25040900	-5.72346900
Cd	-5.96363000	6.30212500	-5.85595400
Cd	-1.53764400	10.39468700	0.21280800
S	-10.47994200	1.89445200	-3.94023600
S	-4.11843200	8.45388200	5.97866000
S	-7.94292200	-5.98548100	-5.12415100
S	2.48280800	4.70831900	10.18002200
Cd	-2.88393900	-5.35023800	-9.01674100
Cd	7.61947100	4.94892800	6.19227800
Cd	3.83403100	-8.89372300	-5.16084800
Cd	10.07728300	-2.74778500	3.72269000
S	1.96958600	-11.29175000	0.51226500
S	6.11658700	-6.86013000	6.68486900
C	1.67537500	3.21625700	-12.23962800

O	1.94888300	4.40300500	-11.84300700
O	1.98106800	2.18990700	-11.50115100
H	-3.45487900	1.27633100	-9.61027400
C	8.14945100	-6.06452700	-6.32661900
O	8.18485800	-5.01972400	-5.59020600
O	7.12240700	-6.51668000	-6.96140100
H	9.06942100	-5.61630400	-2.34879100
C	-1.18605300	10.71946100	-6.41565300
C	-5.87509400	5.43315000	-8.47918800
O	-0.63027100	10.02968400	-5.45974200
O	-1.93325200	10.14056700	-7.27159900
O	-6.10479100	6.63365200	-8.12165400
O	-5.61152300	4.52064400	-7.58442100
H	-11.43454300	2.58618300	-3.18645600
H	-10.96262900	-2.44002400	-0.91287600
C	11.40718300	-1.31217000	-5.15215200
O	10.76656800	-0.85919400	-4.12533800
O	11.06755400	-0.96056700	-6.34394300
H	4.57328300	9.40630100	2.27365100
C	7.74171600	9.64651400	-3.31472900
O	6.61542700	9.64852900	-3.93985800
O	8.17843100	8.71759400	-2.55346600
H	5.74539500	-5.69152600	7.36034800
C	2.65482400	11.52587600	-1.82688400
O	3.07909200	10.47134600	-1.23129600
O	1.73941700	11.57579600	-2.72569300
H	-10.33214900	-5.90280300	-1.71961200
C	7.64675000	7.62041100	5.57478100
O	8.64289100	7.02210600	6.08746400
O	6.53753700	6.96033700	5.34647100
H	2.80563900	3.40819400	10.51619000
C	0.66961500	11.76664500	1.08730900
O	0.54693100	10.51679100	1.44996400
O	-0.20072300	12.29240800	0.32339200
H	-7.08062000	-6.84781200	-4.44275900
H	2.68277400	-8.58976400	8.23877900
C	-3.69953300	-3.46001100	-10.83822700
O	-3.74842400	-3.11103100	-9.57750500
O	-3.29104300	-4.61935500	-11.16153600
H	-8.03100700	-7.79793100	3.67979500
C	-1.51334400	-0.52246000	-11.48491500
O	-0.81015000	0.50806800	-11.18479600
O	-1.38697100	-1.69749800	-10.98560700
H	-9.97941400	-0.99793200	5.31979700
C	11.81653300	-2.59440100	-0.80920800
C	11.25380800	-4.48236700	1.93790200

O	10.83550400	-2.71344800	-1.62117700
O	11.96358800	-1.67697800	0.08162000
O	11.88437100	-3.88902200	2.86778000
O	9.98438300	-4.23887400	1.74059000
H	-2.90401500	-2.93334600	11.27759100
C	6.12261800	-2.00383100	11.89751800
O	4.88873800	-2.35034800	11.71813000
O	6.80494100	-1.43647200	10.96018700
H	0.85423400	-10.11710100	5.52613300
C	7.84544100	8.63547900	1.86891600
O	7.61697300	8.60200800	0.61375800
O	7.95628600	7.61826900	2.65187000
H	-5.69245000	5.88994000	8.74159800
C	6.57829100	-8.93232700	-4.97519800
O	5.90820700	-9.58327500	-5.83807000
O	5.96842700	-8.16122300	-4.11321100
H	-2.79166100	4.07953600	10.32180700
C	-4.59174600	-12.14477000	-3.39165200
O	-3.77965900	-11.55372700	-4.20239100
O	-4.92064800	-11.61171200	-2.25916200
H	0.67405800	-11.25306100	0.02908600
H	-5.11260100	7.89493500	5.17941100
H	-5.89987800	5.15873800	-9.53809500
H	-1.01051000	11.79669900	-6.48097000
H	3.10739400	12.48322300	-1.53789900
H	1.52110000	12.34775100	1.45224800
H	8.38200300	10.52674900	-3.45747200
H	1.18624400	3.05919400	-13.20454000
H	12.24436000	-2.00262900	-5.01434100
H	9.07743200	-6.64420000	-6.42471300
H	7.66742300	-9.02039000	-4.94068400
H	-2.30166400	-0.38115200	-12.23733100
H	-4.02951200	-2.75416700	-11.60310100
H	-5.01354000	-13.11844300	-3.66426200
H	11.76359700	-5.20954600	1.29840300
H	6.59464200	-2.19786000	12.86700500
H	7.95201100	9.62641400	2.33331500
H	7.69512500	8.68360800	5.33358400
H	12.61341600	-3.34932700	-0.86419600
N	-17.37783500	-1.36077800	-4.52966300
H	-18.26760600	-0.99138200	-4.82062300
H	-17.03269100	-2.18482000	-4.99316800
C	-16.62640300	-0.72468100	-3.55924600
C	-15.36504500	-1.23359600	-3.17299300
C	-17.10589700	0.45066200	-2.93130800
C	-14.60819100	-0.58646000	-2.19511100

H -14.97476300	-2.12967900	-3.64803700
C -16.34582000	1.09464800	-1.95683600
H -18.07217700	0.85802200	-3.21686800
C -15.10012300	0.57376300	-1.58824000
H -13.63099500	-0.96804500	-1.91135200
H -16.71053200	2.00668000	-1.49459700
C -14.25337900	0.56776800	0.65854700
C -13.53274600	1.06195700	1.72854500
C -12.89537600	2.33698100	1.56478800
C -13.40388900	0.34855600	2.97650100
C -13.66066700	2.42687700	-0.80381100
C -12.14246300	2.88498300	2.64227100
C -12.98600200	3.02605200	0.33232700
C -12.65784700	0.86047600	3.99951500
H -13.90077700	-0.61199000	3.08234200
C -11.99434900	2.13558800	3.85449900
C -11.51292600	4.15144300	2.48975200
C -12.38547100	4.31614900	0.22194200
H -12.54086000	0.31816500	4.93296400
C -11.15666500	2.64892200	4.83490100
C -10.69117000	4.64576800	3.54519900
C -11.68756700	4.86916000	1.26919100
H -12.49143300	4.84380000	-0.71960100
H -10.91727500	2.11120100	5.74546600
N -14.32437900	1.22350100	-0.54365800
S -13.63529700	3.10633400	-2.39820200
N -10.53932900	3.84874800	4.64080300
H -9.85100100	4.16168600	5.32852500
C -8.31592000	-4.25649500	9.99382700
O -8.85749700	-3.56335700	9.05736600
O -7.07831700	-4.56426300	10.11211500
H -8.99350100	-4.63427800	10.77386000
S -9.89832600	6.24271900	3.58932300
H -11.24397800	5.85363200	1.17695300
H -14.79236200	-0.36980100	0.70778200

CdS/ammonium ligand + QDM:

N	19.74149900	-8.30088400	-5.96911800
H	20.74417700	-8.23561200	-6.02301300
H	19.30355000	-9.14729100	-6.29189600
C	18.99464500	-7.29101700	-5.38525600
C	17.59064600	-7.40455900	-5.26968300
C	19.62353600	-6.12280300	-4.89336400
C	16.84437000	-6.38397400	-4.67557400
H	17.08931300	-8.29640200	-5.63720100
C	18.87178500	-5.10853200	-4.30139500
H	20.70296300	-6.01955700	-4.96935800
C	17.48239500	-5.23685900	-4.19401800
H	15.76797400	-6.48516800	-4.56952000
H	19.36136200	-4.22461000	-3.90463900
C	16.07562400	-3.31475500	-4.50155300
C	15.29984700	-2.25418900	-4.08690100
C	15.16674300	-2.04356200	-2.66785600
C	14.63106100	-1.36934500	-5.01466100
C	16.60007200	-4.04268200	-2.22068500
C	14.38223200	-0.94806500	-2.19810600
C	15.80408400	-2.91391700	-1.75423100
C	13.87672800	-0.32819500	-4.56100500
H	14.73425800	-1.55723900	-6.07995300
C	13.73629300	-0.08479400	-3.14313800
C	14.23635000	-0.72848000	-0.80139800
C	15.64700600	-2.66956000	-0.35665000
H	13.35525300	0.33158500	-5.24753300
C	12.97442000	0.96589900	-2.65494800
C	13.43254400	0.36998600	-0.34617500
C	14.89030200	-1.61550600	0.10424500
H	16.14698900	-3.34725200	0.32766300
H	12.43152100	1.68872600	-3.29071100
N	16.69830300	-4.16351600	-3.61292800
S	17.36823200	-5.17665500	-1.17470100
N	12.86656100	1.15194900	-1.30775700
H	12.21774600	1.90601300	-1.01409700
S	13.20284100	0.74982000	1.36872700
H	14.77558400	-1.43617000	1.16784100
H	16.24151300	-3.53617700	-5.54856200
Cd	-0.57392400	1.80322500	-1.74566600
Cd	2.02620900	-0.84697400	0.06007600
S	1.22428400	-0.01520100	-2.33940200
S	0.20226400	-1.73508800	1.72666800
S	-2.58286800	1.08919900	-0.19896900
Cd	-1.55260500	0.16851800	2.06719000
Cd	0.09650800	-2.10403200	-3.46238500

S	-1.87016100	-2.73036400	-1.79908200
Cd	-0.96731600	-3.68987900	0.49977300
Cd	-3.68429000	-0.85249300	-1.51754800
S	3.30232000	1.00961100	1.35626300
S	0.55080100	3.70972400	-0.36336100
Cd	1.62996000	2.93231700	1.92897300
S	-0.36319500	2.07163500	3.36528500
Cd	3.17847900	0.86957400	-3.97002700
S	-1.61895300	2.67351900	-4.03969700
S	3.59191300	-2.90317600	-0.53091100
Cd	-4.45240400	2.89858800	0.36848100
Cd	1.09541800	-2.54165100	4.17529500
S	-3.52572600	-0.60427900	3.63811500
S	-0.99438300	-1.28080900	-5.72694000
S	1.54541700	-4.20099000	-4.07408200
Cd	-2.68555500	0.59212100	-5.21427100
Cd	2.33109900	-4.90527600	-1.67487600
S	4.31604600	2.82038000	-2.61529400
S	-4.76460400	-0.16308000	-3.83113000
S	0.56854000	-5.76408700	0.03320400
Cd	5.10462400	2.00011900	-0.25157300
Cd	2.52196000	4.52874100	-1.85512900
S	-2.98085200	-4.41864500	2.03815300
S	-5.66266600	-1.65565200	0.02708500
Cd	-1.25355100	5.48011700	0.28321300
Cd	4.38146300	0.11192500	3.65595700
Cd	-4.64832800	-2.45151800	2.27027200
S	-3.22679500	4.71329200	1.80927100
S	2.43175600	-0.56568300	5.21027500
Cd	-2.23695500	3.71930700	4.08583600
Cd	0.77831800	1.37953100	5.62709400
S	4.77387300	-1.17566000	-4.42926900
S	2.09855400	1.79837300	-6.30659300
Cd	0.36651800	3.58849000	-5.50738200
Cd	5.47058100	-1.88313800	-2.02302700
Cd	-3.03981600	-4.67434400	-3.01098700
Cd	4.52631600	-3.52565600	1.83461700
Cd	-3.27529600	4.59520100	-3.25656400
S	2.82595900	-4.42669200	3.59006800
S	-5.37622300	3.72018900	-1.97908800
S	2.80130500	4.97903400	3.04602500
S	-6.56199700	2.12003900	1.71255600
S	-0.82937800	-3.32793100	5.76442000
Cd	-2.37429900	-1.23780600	5.98578400
Cd	-5.46753000	1.17383600	3.87030300
Cd	0.87953100	-0.42612600	-7.31359300

Cd	3.47678800	-3.15894900	-5.69991100
S	1.47304300	5.45017400	-4.06990600
S	6.73428500	0.03699400	-0.80941100
Cd	-6.49040800	1.66798900	-3.11934000
Cd	1.52131900	-6.34282200	2.46968600
S	-2.13550000	6.53261000	-1.98782300
S	6.04934200	-1.81137400	3.04339900
Cd	-7.62850800	0.05490100	0.53686900
Cd	-2.03317600	-5.17988800	4.43193700
S	-4.18168100	2.73858700	5.56110300
S	-0.98503500	0.46915400	7.27300000
Cd	0.11224000	-6.41631100	-5.06108800
Cd	-2.22911000	-3.27841700	-6.93334900
S	-1.78141100	-6.97173900	-3.19066000
S	-4.17030000	-4.01324500	-5.24285900
Cd	-6.01009200	-2.21826300	-5.07786900
Cd	-0.61636200	-7.88825500	-1.04330000
S	-5.00672500	-5.74003900	-1.46493300
Cd	-6.61365100	-3.65234000	-1.27232200
Cd	-3.84889200	-6.49519100	0.83812100
S	3.63508400	6.58196600	-0.65643100
S	6.41950400	3.80830100	1.08656700
Cd	4.81286700	5.80962400	1.58040600
S	-0.16691600	7.55135100	1.50444600
S	5.53544200	2.15750600	4.79135400
Cd	3.99104800	4.19955100	5.26995800
Cd	1.00075900	6.73511700	3.76264600
S	2.04380100	3.33469500	6.73269800
S	-0.90230900	5.64639900	5.28457800
S	2.60489700	-2.19674300	-7.97410300
S	4.22417800	-6.85370600	-1.95005300
S	-3.72751000	1.54269100	-7.57188300
Cd	6.45722100	3.93867500	-3.95811800
Cd	-0.20046900	7.31120800	-3.50433500
Cd	7.73572000	-0.71384700	1.44444500
S	-8.54028100	0.78487900	-1.81787500
S	-0.50791400	-7.19300300	3.82432500
S	-6.72721800	-3.30047800	3.76536100
Cd	3.58604600	-1.20988900	7.53841300
Cd	-4.99455200	6.67439400	2.22361800
Cd	-2.38268500	1.54456500	9.15125200
S	-1.31717100	-5.71669100	-7.08227300
Cd	6.92768100	0.06309400	-5.76361600
Cd	4.49472200	3.14337800	-7.27303900
S	-0.50501600	4.77643900	-7.79065100
S	7.27094100	-3.94381200	-2.34677300

S	-4.12199600	5.55935300	-5.55904700
S	6.56788100	-5.26575100	1.67707000
S	-7.86215200	-2.89792800	-3.39906400
S	-2.55701000	-8.71239200	0.52562100
Cd	7.52347500	3.08236000	3.41851600
Cd	1.76397500	8.35414700	-0.01546500
Cd	-7.02521800	5.77795800	-1.36654200
Cd	3.73516700	-5.18468100	6.14332200
Cd	-8.37390300	4.17144000	2.33373200
Cd	0.39719600	-4.30258900	8.43863900
S	-4.65544300	-1.42448900	7.45809300
S	-7.51763100	0.27441100	5.34415500
Cd	0.36894000	5.11431900	7.59858800
S	-0.12476800	0.72250500	-9.54401200
S	5.21814900	-5.21730900	-6.02886700
Cd	5.58418000	-5.44901500	-3.58533200
Cd	-1.64246800	2.58516700	-8.71859400
S	5.13159900	5.21071500	-5.89316500
S	8.04692500	1.91665000	-4.32422200
Cd	8.78695000	1.20037100	-1.97188300
Cd	3.40604400	6.96227100	-4.96564800
Cd	-4.99716000	3.32272500	-6.29059500
Cd	5.13361900	-7.01547500	0.46496900
S	-7.36316700	2.64365700	-5.56329900
S	3.40662000	-8.23043100	1.94553900
Cd	7.62341800	-2.28172300	7.39725400
Cd	-3.90396200	8.50435900	-1.75033500
S	5.21629700	-3.08078000	6.71610600
S	-5.71450100	7.60259900	-0.09098000
S	-9.73277000	-1.11488100	1.59759000
S	-4.31457100	-5.73068100	5.80472200
Cd	-8.71931100	-1.55000300	3.94715800
Cd	-5.24505200	-3.36072900	5.91371800
S	1.90972400	-2.25065700	9.20374700
S	-6.92809100	5.87185800	3.76058800
Cd	1.25423100	-4.72601400	-8.73604800
Cd	-5.96821500	4.61938200	5.80535800
Cd	0.25298300	-0.41687700	9.56977400
S	5.76700500	1.00272300	-7.91198600
S	-3.29418500	-2.63687300	-9.22602100
S	1.95630100	-8.17744500	-5.40339900
Cd	-4.80968600	-0.74630300	-8.44410700
Cd	2.65784000	-8.70613400	-3.02075800
S	-7.06799200	-1.34615800	-7.29578500
S	1.06499800	-9.83924300	-1.31478100
Cd	-2.23601900	6.61646100	-7.07945500

Cd	8.28078300	-4.33834400	0.02957100
S	7.72204200	5.79331100	-2.57073300
Cd	5.66914300	7.13797100	-2.19941600
Cd	8.40238500	4.80715800	-0.30523900
Cd	-1.59327500	-9.47801400	3.00904600
Cd	-9.86693000	-1.09298700	-3.16876100
S	9.03478500	0.91426900	3.00069700
S	0.92231000	9.31882200	-2.34502800
S	-8.41924800	-5.07260600	0.24532800
S	-5.93084000	-7.65761200	2.17913000
Cd	-7.00092900	-5.37794200	2.36696800
S	-9.14110000	4.99400900	-0.07104900
S	1.80551000	-6.36361200	7.33728200
Cd	-2.22987200	9.11196500	1.58391200
Cd	6.62525300	1.59521600	7.11485700
S	-3.76118700	8.70089200	3.55648000
S	4.86811000	0.74553600	8.85273000
Cd	5.22398300	-1.61461300	-8.57545800
Cd	-2.41821600	7.68781500	5.48675800
Cd	3.11134300	2.60417900	8.99196500
Cd	-5.83750400	1.19396200	7.27174000
S	-0.76670500	3.61964200	9.59052800
Cd	-7.31468900	-8.55238200	-4.40511700
Cd	-4.18284400	-8.02074500	-3.00046700
Cd	-7.43371400	-7.06510100	-1.24279400
S	9.77351000	-2.13792300	0.34578900
S	-0.56196100	8.39182300	-5.92935400
Cd	-9.98767900	2.75196800	-0.90937600
Cd	-0.37328400	-7.68448000	6.51550200
S	6.07341100	7.89783300	2.51158400
S	5.18721300	6.15200300	6.54784900
S	2.16304700	8.92906200	4.57753900
Cd	-0.67075700	-3.19154600	-10.24932500
Cd	2.95388600	-6.50827600	-7.33749000
S	3.27066100	4.21540000	-9.48579700
S	8.75967800	-1.87029800	-5.97669500
S	-4.98019700	1.49177500	9.82460800
Cd	1.99125300	5.95219700	-8.15194000
Cd	8.86415300	-2.29062900	-3.55319100
Cd	-8.65875500	0.45758800	-6.40388800
Cd	1.57313600	-9.96820100	1.17828800
S	10.23723000	2.96371400	-0.67938200
S	4.78767000	8.87146700	-3.85423400
Cd	-5.81380400	7.77741800	-5.23311500
Cd	6.70186900	-4.10411200	4.54943500
S	-7.84733200	6.85987100	-3.68500100

S	5.90236000	-6.50039700	5.39127100
Cd	-10.05935700	-3.02473000	-0.04792900
Cd	-4.79543000	-8.04415900	4.59890400
S	-2.97878800	10.59591100	-0.29209000
S	8.73431600	0.08461200	7.32453800
S	-10.31426900	3.14523000	3.68732800
S	-2.10123300	-4.48409200	9.55922400
Cd	1.99140300	2.08553900	-9.24051600
Cd	6.92915300	-3.42519800	-7.33808900
Cd	-3.87989400	-6.31026000	-6.57468700
Cd	-9.08873700	2.39711600	5.79846100
Cd	-3.25756200	-2.25757200	9.65991500
S	-4.85563500	7.11797200	6.80718200
S	0.88733500	2.25122000	10.47360000
S	-5.01572400	-8.34546300	-5.44212300
S	10.30276200	-1.19286600	-1.68624900
S	1.54141800	8.17800100	-6.82809400
S	-9.14171200	-7.19235200	-3.21621800
S	-6.16397500	-9.33785900	-1.72234400
Cd	-9.78964400	-4.71445800	-3.58816900
Cd	-4.99356400	-9.71709800	0.57348900
Cd	4.59455700	-8.33149400	4.27035100
Cd	-8.42039900	4.86782300	-4.98856100
S	9.04958500	-3.33702400	5.38859300
S	-4.68963100	9.65250000	-3.91799100
S	8.88432400	5.05376300	4.30382300
S	3.12862100	10.55945800	0.44237700
Cd	3.96571900	9.39647300	2.76644600
Cd	6.92791700	6.71827200	4.67494000
Cd	-2.46452900	-6.35718100	7.82610800
Cd	-12.05165600	0.65216700	4.16420600
Cd	3.12706800	7.75137600	6.73219400
S	1.31390100	7.27277000	8.50142900
S	-7.39787300	3.38937800	7.55083800
S	-1.96910600	-0.36768700	10.89560500
S	-10.85100600	0.26625600	-5.12728500
S	0.43924700	-11.10040200	3.05377500
Cd	10.85397800	2.07398600	1.63251800
Cd	3.40823800	10.25619200	-2.16753600
S	-3.52983200	-10.19429600	4.53178300
S	-11.36446400	-3.06702100	-2.19474800
Cd	9.43977900	-0.75951700	4.99619900
Cd	-0.91946800	10.97898000	-1.70989800
H	-0.92153400	2.53898900	12.57041300
N	4.57840600	-8.26674900	-7.62457800
H	4.10826400	-8.94716300	-7.03058100

H	4.79762900	-8.60921700	-8.55355900
H	5.35459800	-7.79793200	-7.16159300
N	6.75832300	-8.75480800	0.75792400
H	7.30040200	-9.03789400	-0.05275700
H	7.32222400	-8.28992200	1.46863700
N	5.94714900	-10.23805900	4.59949100
H	6.33737600	-9.99822500	5.55771400
H	5.39380600	-11.09400800	4.61050700
H	6.19718100	-9.51383600	1.13784500
H	6.70590000	-10.32370800	3.92511500
N	11.74988700	-1.15387100	4.57453300
H	11.99639700	-0.87252900	3.62515700
H	12.35111200	-0.71131900	5.26530600
N	11.66693000	3.66366500	3.12530600
H	12.15952500	3.18900000	3.88114600
H	12.29746700	4.31136200	2.65448200
H	10.84381200	4.16702800	3.51260900
H	11.73935500	-2.16828800	4.68278900
N	-4.56894900	-5.94926800	-8.73849300
H	-3.88767400	-6.50959800	-9.30639300
H	-5.53402800	-6.21539200	-8.92457000
H	-4.42308500	-4.94630700	-8.92318100
N	-5.95942100	8.14611100	5.69884300
H	-6.55324500	7.49587900	5.10872800
H	-5.36074900	8.67845600	5.02123600
H	-6.53836400	8.76730700	6.26560500
N	-0.88709000	9.06154000	6.54923900
H	-0.18904400	9.33148400	5.84224700
H	-0.37696200	8.50161100	7.26342200
H	-1.28490200	9.89635700	6.97949700
N	-1.86587600	2.31063200	12.90240700
H	-1.87870700	2.27011600	13.92082000
H	-2.09471300	1.38511400	12.50316500
N	-1.70810300	11.37093600	-3.86384300
H	-2.65289200	10.94050900	-3.87713200
H	-1.76559800	12.33325600	-4.19347500
N	3.40178300	12.30211900	-3.28134100
H	3.38069000	11.99976100	-4.29847900
H	2.57971700	12.85247600	-3.03972800
H	4.24890900	12.83082500	-3.07617800
H	-1.09107100	10.82007900	-4.46931900
N	-6.18619300	7.69150100	-7.39653300
H	-6.60113500	6.79750400	-7.68340700
H	-6.75345600	8.44854400	-7.79243800
H	-10.22745900	9.65810000	-1.87008800
N	6.93724700	-9.24088500	7.05875900

H	7.92341800	-9.41777200	7.23629800
H	6.38379900	-9.44306400	7.88863800
H	6.78365500	-8.26746700	6.75112900
N	-5.03492700	-1.89480400	11.20029100
H	-4.54661800	-1.91361700	12.09314600
H	-5.81755600	-2.54194400	11.17428400
H	-5.30808400	-0.93917000	10.96059800
N	11.34524400	3.15913200	-4.16950200
H	11.12424100	3.68784900	-3.32522500
H	11.80076700	3.74697800	-4.86295800
H	10.48281100	2.74910300	-4.54016100
N	4.08824800	7.20007200	-8.49798000
H	4.30931200	6.92353700	-9.45395200
H	4.72310800	6.72339700	-7.84240100
H	4.10670800	8.21045600	-8.37533100
N	7.53159700	3.66901900	7.59278000
H	6.83588200	4.41978800	7.56707700
H	8.25510000	3.86686800	6.89599600
H	7.90869000	3.47812700	8.53970700
N	10.13848900	-5.70018100	0.30169200
H	10.81655100	-5.52953400	-0.44081400
H	9.92872000	-6.69432700	0.37008100
H	10.50833400	-5.32196200	1.22536300
N	-10.43346300	-4.38127200	-5.78170800
H	-10.58239800	-5.26378600	-6.26864300
H	-11.31879300	-3.79785300	-5.74161600
H	-9.67440300	-3.85867600	-6.22346900
N	0.31390300	12.45670600	-0.34065500
H	0.60221500	13.35782000	-0.71828900
H	1.14500800	11.91364100	-0.03692600
H	-0.32065700	12.59770100	0.44662300
N	-4.64048800	-11.63903300	1.67042900
H	-5.36936000	-12.35040700	1.62080000
H	-3.72136700	-12.00773900	1.28651100
H	-4.47737200	-11.35192900	2.65604500
N	-6.57273200	-8.64414000	6.06655100
H	-7.46492600	-8.72575700	5.58710200
H	-6.24246500	-9.54298000	6.41306500
H	-6.58564200	-7.93029600	6.79102600
N	-2.05309300	-12.39421000	0.68445900
H	-1.41462200	-12.29514900	1.48260900
H	-1.83456800	-11.66961300	-0.00044700
H	-1.96459800	-13.31925300	0.26903700
N	-2.17695800	3.70682300	-10.75002100
H	-3.16531100	3.88377700	-10.90783000
H	-1.65303000	4.56949500	-10.60578000

N	-10.30485600	5.23073600	-6.29885800
H	-11.05018300	4.48487200	-6.19255600
H	-10.65099600	6.14383200	-6.00055100
H	-1.76844100	3.13853800	-11.48898000
H	-10.00534200	5.28803900	-7.27280200
N	-11.49318000	2.80409800	-2.74518600
H	-12.41744900	2.58384400	-2.37699300
H	-11.49004000	3.72786800	-3.17325700
N	-11.43926300	1.94001300	0.65531400
H	-12.11115600	2.72496800	0.79358300
H	-11.87062000	1.04365200	0.43474100
H	-11.18881100	2.07584700	-3.41374800
H	-10.90189200	1.84376800	1.52705300
N	2.75530800	-9.16046500	5.42470400
H	2.97825100	-9.92220900	6.06379300
H	2.39772300	-8.35593000	5.96374500
N	-0.50954700	-10.05198600	6.32530900
H	0.02706400	-10.44607200	5.54183100
H	-0.28634200	-10.52385100	7.20057000
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