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

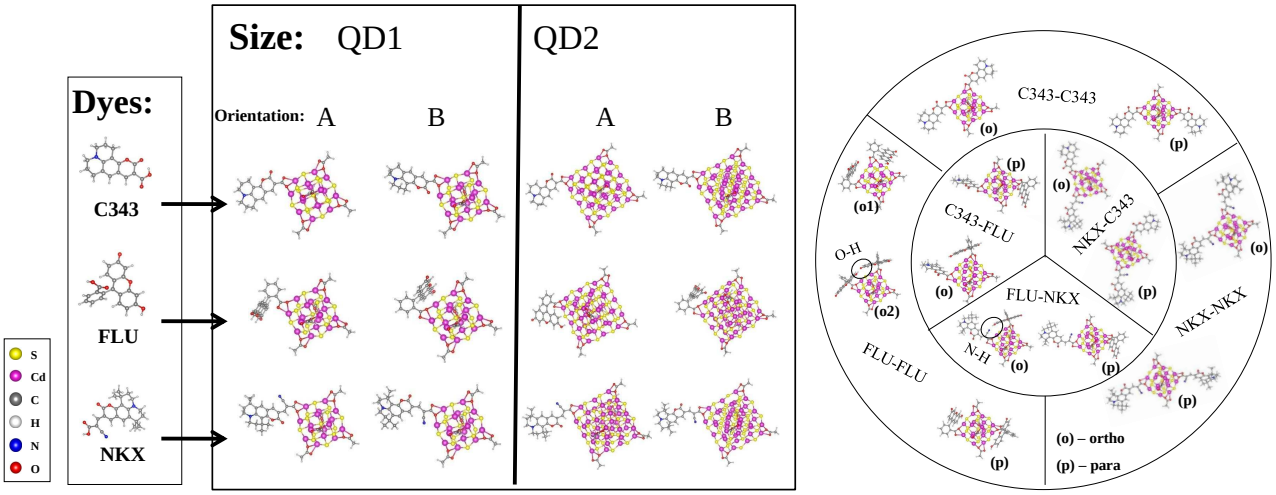

FIG. S1: Optimised structures of the model QDs sensitized with (a) one dye and (b) two dye molecules.

TABLE S1: Interaction energy of the single-dye-sensitized QDs.

System		Energy of composite (E′)eV	Calculted Energy* (E″)eV	Interaction Energy (E = E′-E″)eV
C343-QD1	A	-82112.39	-82112.74	0.35
	B	-82113.27	-82112.74	-0.53
C343-QD2	A	-120461.60	-120461.96	0.36
	B	-120462.48	-120461.96	-0.52
FLU-QD1	A	-86766.05	-86765.82	-0.23
	B	-86766.10	-86765.82	-0.28
FLU-QD2	A	-125115.39	-125115.04	-0.35
	B	-125115.90	-125115.04	-0.86
NKX-QD1	A	-91006.39	-91006.38	-0.01
	B	-91006.65	-91006.38	-0.27
NKX-QD2	A	-129355.61	-129355.60	-0.01
	B	-129355.86	-129355.60	-0.26

* E″ is the energy given by (QD#) - (acetic acid) + (dye molecule).

Energy of Ligated QD1= -61834.38 eV

Energy of Ligated QD2= -100183.60 eV

Energy of acetic acid= -6233.05 eV

Energy of C343 dye= -26511.41 eV

Energy of FLU dye= -31164.49 eV

Energy of NKX dye= -35405.05 eV

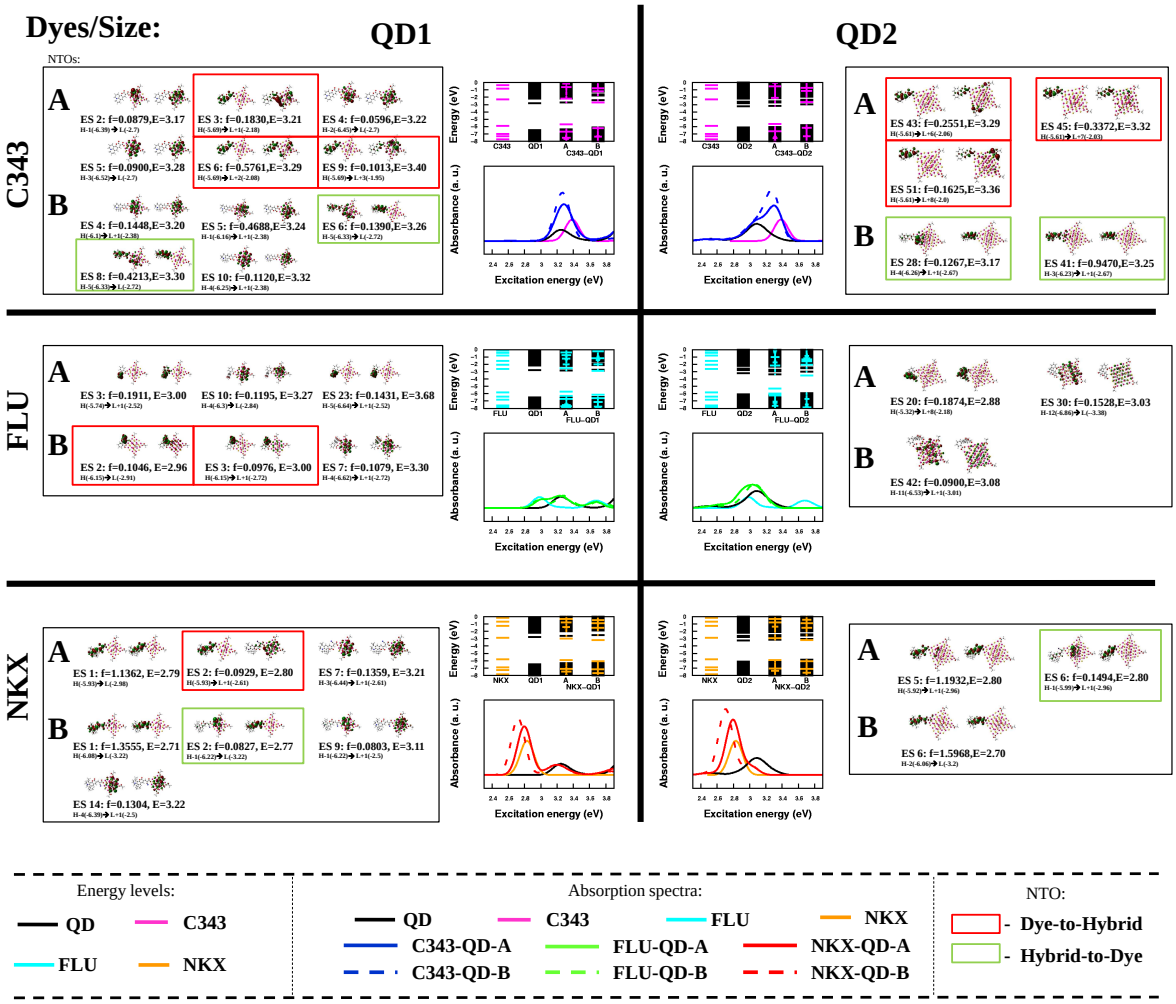

FIG. S2: Energy levels, absorption spectra and NTOs for the model single dye-sensitized QDs, sensitized with three different dyes C343, FLU and NKX and 2 different sizes of QD- QD1 and QD2. Legends for energy level diagrams, absorption spectra and charge transfers are indicated in the respective boxes given at the bottom of the figure. Nature of charge transfers shown above is presented in tabular form in Table S2.

TABLE S2: Nature of charge transfer in single-dye-sensitized QDs.

Excited state	Energy eV	Oscillator strength	Transition	Hole transfer (In valance band)	Electron transfer (In conduction band)	Direction of electron transfer
C343-QD1-B			N=40, E*=3.93			
S4	3.20	0.1448	QD$\Longrightarrow$ QD (H$\rightarrow$L+1)	$\times$	$\longrightarrow$ Dye	QD to Dye.
S5	3.24	0.4688	QD$\Longrightarrow$ QD (H-1$\rightarrow$L+1)	$\times$	$\longrightarrow$ Dye	QD to Dye.
S6	3.26	0.1390	Hybrid$\Longrightarrow$ Dye (H-5$\rightarrow$L)	QD $\sim$	$\times$	QD to Dye(Direct).
S8	3.30	0.4213	Hybrid$\Longrightarrow$ Dye (H-5$\rightarrow$L)	QD $\sim$	$\times$	QD to Dye(Direct).
S10	3.32	0.1120	QD$\Longrightarrow$ QD (H-4$\rightarrow$L+1)	Dye or QD $\longleftarrow$	$\longrightarrow$ Dye	Multiple case.
C343-QD2-A			N=55, E*=3.39			
S43	3.29	0.2551	Dye$\Longrightarrow$ Hybrid (H$\rightarrow$L+6)	$\times$	$\sim$ QD	Dye to QD(Direct).
S45	3.32	0.3372	Dye$\Longrightarrow$ Hybrid (H$\rightarrow$L+7)	$\times$	$\sim$ QD	Dye to QD(Direct).
S51	3.36	0.1625	Dye$\Longrightarrow$ Hybrid (H$\rightarrow$L+8)	$\times$	$\sim$ QD	Dye to QD(Direct).
C343-QD2-B			N=55, E*=3.41			
S28	3.17	0.1267	Hybrid$\Longrightarrow$ Dye (H-4$\rightarrow$L+1)	QD or Dye $\sim$	$\longrightarrow$ QD	Multiple case.
S41	3.29	0.9470	Hybrid$\Longrightarrow$ Dye (H-3$\rightarrow$L+1)	QD $\sim$	$\longrightarrow$ QD	Energy transfer.
FLU-QD1-A			N=25, E*=3.73			
S3	3.00	0.1911	Dye$\Longrightarrow$ Dye (H$\rightarrow$L+1)	$\times$	$\longrightarrow$ QD	Dye to QD.
S10	3.27	0.1195	QD$\Longrightarrow$ QD (H-4$\rightarrow$L)	Dye $\longleftarrow$	$\times$	Dye to QD.
S23	3.68	0.1431	Dye$\Longrightarrow$ Dye (H-5$\rightarrow$L+1)	Dye or QD $\longleftarrow$	$\longrightarrow$ QD	Multiple case.
FLU-QD1-B			N=55, E*=3.22			
S2	2.96	0.1046	Dye$\Longrightarrow$ Hybrid (H$\rightarrow$L)	$\times$	$\times$	Dye to Hybrid(Direct).
S3	3.00	0.0976	Dye$\Longrightarrow$ Hybrid (H$\rightarrow$L+1)	$\times$	$\sim$ Hybrid	Dye to Hybrid(Direct).
S7	3.30	0.1079	QD$\Longrightarrow$ QD (H-4$\rightarrow$L+1)	Dye or QD $\longleftarrow$	$\longrightarrow$ Hybrid	Multiple case.
FLU-QD2-A			N=55, E*=3.22			
S20	2.88	0.1874	Dye$\Longrightarrow$ Dye (H$\rightarrow$L+8)	$\times$	$\longrightarrow$ QD	Dye to QD.
S30	3.03	0.1528	QD$\Longrightarrow$ QD (H-12$\rightarrow$L)	Dye $\longleftarrow$	$\times$	Dye to QD.
FLU-QD2-B			N=60, E*=3.20			
S42	3.08	0.0900	QD$\Longrightarrow$ QD (H-11$\rightarrow$L+1)	$\times$	$\longrightarrow$ Dye	QD to Dye.
NKX-QD1-B			N=50, E*=3.92			
S1	2.71	1.3555	Dye$\Longrightarrow$ Dye (H$\rightarrow$L)	$\times$	$\times$	No transfer.
S2	2.77	0.0827	Hybrid$\Longrightarrow$ Dye (H-1$\rightarrow$L)	Dye $\sim$	$\times$	Energy transfer.
S9	3.11	0.0803	QD$\Longrightarrow$ QD (H-1$\rightarrow$L+1)	Dye $\longleftarrow$	$\longrightarrow$ Dye	Energy transfer.
S14	3.22	0.1304	QD$\Longrightarrow$ QD (H-4$\rightarrow$L+1)	Dye $\longleftarrow$	$\longrightarrow$ Dye	Energy transfer.
NKX-QD2-A			N=20, E*=3.04			
S5	2.80	1.1932	Dye$\Longrightarrow$ Dye (H$\rightarrow$L+1)	$\times$	$\longrightarrow$ QD	Dye to QD.
S6	2.80	0.1494	Hybrid$\Longrightarrow$ Dye (H-1$\rightarrow$L+1)	Dye $\sim$	$\longrightarrow$ QD	Energy transfer.
NKX-QD2-B			N=30, E*=3.09			
S6	2.70	1.5968	Dye$\Longrightarrow$ Dye (H-2$\rightarrow$L)	QD $\longleftarrow$	$\times$	QD to Dye.

E* is the maximum energy obtained in each case by using the maximum number of states given, N.

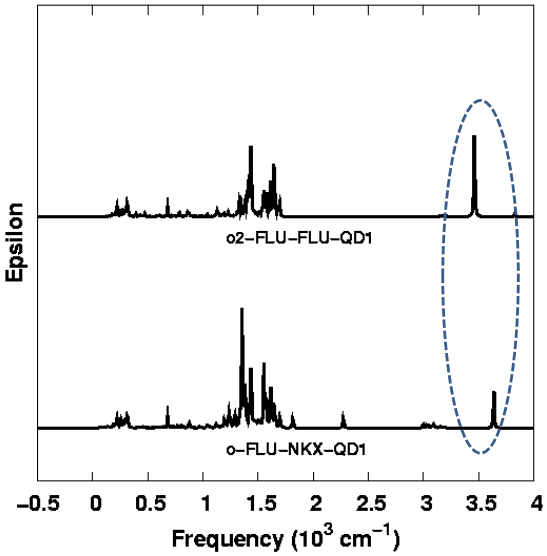

FIG. S3: IR absorption spectrum of o2-FLU-FLU-QD1 and o-FLU-NKX-QD1. The appearance of additional absorption peaks (shown on dotted oval) is due to inter molecular hydrogen bonding between dye molecules.

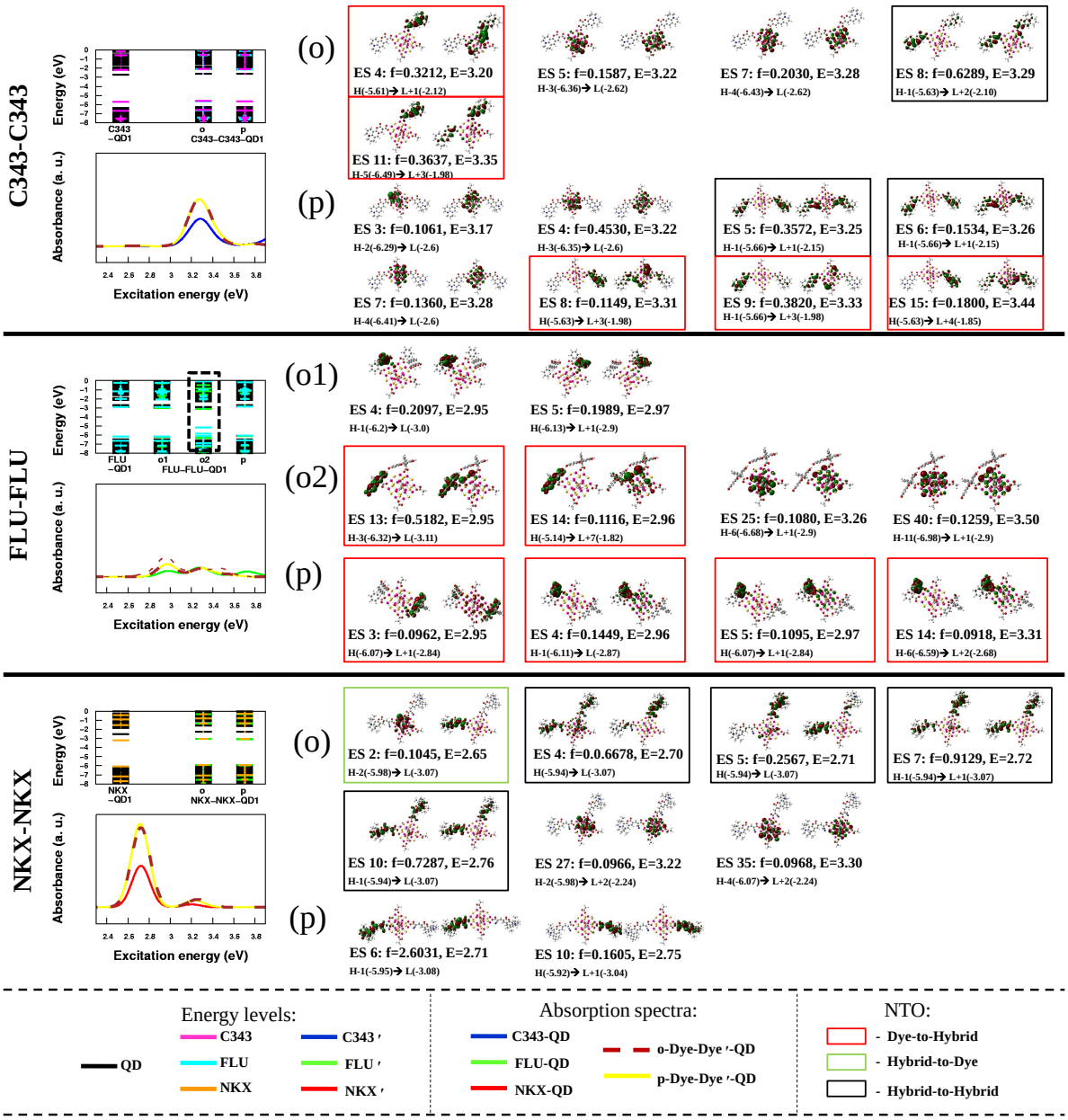

FIG. S4: Energy levels, absorption spectra and NTOs for the model 2-dye-sensitized QDs sensitized with dyes of different species. Legends for energy level diagrams, absorption spectra and charge transfers are indicated in the respective boxes given at the bottom of the figure. Nature of charge transfers shown above is presented in tabular form in Table S3.

TABLE S3: Nature of charge transfer in 2-dye-sensitized-QD1 sensitized with same species of dye molecules.

Excited state	Energy eV	Oscillator strength	Transition	Hole transfer (In valance band)	Electron transfer (In conduction band)	Direction of electron transfer
C343-C343-QD-o			N=40, E*=3.88			
S4	3.20	0.3212	Dye$\Longrightarrow$ Hybrid1 (H$\rightarrow$L+1)	$\times$	$\sim$ QD	Dye to QD.
S5	3.22	0.1587	QD$\Longrightarrow$ QD (H-3$\rightarrow$L)	Dye $\longleftarrow$	$\times$	Dye to QD.
S7	3.28	0.2030	QD$\Longrightarrow$ QD (H-4$\rightarrow$L)	Dye $\longleftarrow$	$\times$	Dye to QD.
S8	3.29	0.6289	Hybrid3$\Longrightarrow$ Hybrid2 (H-1$\rightarrow$L+2)	Dye $\sim$	$\sim$ QD	Dye to QD.
S11	3.35	0.3637	Dye$\Longrightarrow$ Hybrid2 (H-5$\rightarrow$L+3)	Dye or QD $\longleftarrow$	$\sim$ Dye or QD	Multiple case.
C343-C343-QD-p			N=40, E*=3.89			
S3	3.17	0.1061	QD$\Longrightarrow$ QD (H-2$\rightarrow$L)	Dye $\longleftarrow$	$\times$	Dye to QD.
S4	3.22	0.4530	QD$\Longrightarrow$ QD (H-3$\rightarrow$L)	Dye $\longleftarrow$	$\times$	Dye to QD.
S5	3.25	0.3572	Hybrid3$\Longrightarrow$ Hybrid2 (H-1$\rightarrow$L+1)	Dye $\sim$	$\sim$ QD	Dye to QD.
S6	3.26	0.1534	Hybrid3$\Longrightarrow$ Hybrid2 (H-1$\rightarrow$L+1)	Dye $\sim$	$\sim$ QD	Dye to QD.
S7	3.28	0.1360	QD$\Longrightarrow$ QD (H-4$\rightarrow$L)	Dye1 $\longleftarrow$	$\times$	Dye1 to QD.
S8	3.31	0.1149	Dye$\Longrightarrow$ Hybrid2 (H$\rightarrow$L+3)	$\times$	$\sim$ QD	Dye to QD.
S9	3.33	0.3820	Hybrid3$\Longrightarrow$ Hybrid1 (H-1$\rightarrow$L+3)	Dye1 $\sim$	$\sim$ QD	Dye to QD.
S15	3.44	0.1800	Dye$\Longrightarrow$ Hybrid2 (H$\rightarrow$L+4)	$\times$	$\sim$ QD or Dye	Multiple case.
FLU-FLU-QD-o1			N=40, E*=3.64			
S4	2.95	0.2097	Dye$\Longrightarrow$ Dye (H-1$\rightarrow$L)	Dye$'$ $\longleftarrow$	$\times$	Dye$'$ to Dye.
S5	2.97	0.1989	Dye$'\Longrightarrow$ Dye$'$ (H$\rightarrow$L+1)	$\times$	$\longrightarrow$ Dye	Dye$'$ to Dye.
FLU-FLU-QD-o2			N=40, E*=3.50			
S13	2.95	0.5182	Dye$\Longrightarrow$ Hybrid1 (H-3$\rightarrow$L)	Dye$'$ $\longleftarrow$	$\times$	Dye$'$ to Hybrid1.
S14	2.96	0.1116	Dye$\Longrightarrow$ Hybrid1 (H$\rightarrow$L+7)	$\times$	$\sim$ Hybrid1	Dye to Hybrid1.
S25	3.26	0.1080	QD$\Longrightarrow$ QD (H-6$\rightarrow$L+1)	Dye $\longleftarrow$	$\longrightarrow$ Hybrid1	Dye to Hybrid1.
S40	3.50	0.1259	QD$\Longrightarrow$ QD (H-11$\rightarrow$L+1)	Dye $\longleftarrow$	$\longrightarrow$ Hybrid1	Dye to Hybrid1.
FLU-FLU-QD-p			N=40, E*=3.64			
S3	2.95	0.0962	Dye$'\Longrightarrow$ Hybrid1 (H$\rightarrow$L+1)	$\times$	$\sim$ Dye	Dye$'$ to Dye.
S4	2.96	0.1449	Dye$\Longrightarrow$ Hybrid1 (H-1$\rightarrow$L)	Dye$'$ $\longleftarrow$	$\times$	Dye$'$ to Hybrid1.
S5	2.97	0.1095	Dye$\Longrightarrow$ Hybrid1 (H$\rightarrow$L+1)	$\times$	$\sim$Dye$'$	Dye to Dye$'$.
S14	3.31	0.0918	Dye$\Longrightarrow$ Hybrid1 (H-6$\rightarrow$L+2)	Dye$'$ $\longleftarrow$	$\sim$ Hybrid1	Dye$'$ to Hybrid1.
NKX-NKX-QD-o			N=40, E*=3.36			
S2	2.65	0.1045	Hybrid1 $\Longrightarrow$ Dye1 (H-2$\rightarrow$L)	Hybrid2 $\sim$	$\times$	Hybrid2 to Dye1.
S4	2.70	0.6678	Hybrid2$\Longrightarrow$ Hybrid3 (H$\rightarrow$L)	$\times$	$\times$	Hybrid2 to Hybrid3.
S5	2.71	0.2567	Hybrid2$\Longrightarrow$ Hybrid3 (H$\rightarrow$L)	$\times$	$\times$	Hybrid2 to Hybrid3.
S7	2.72	0.9129	Hybrid2$\Longrightarrow$ Hybrid3 (H-1$\rightarrow$L+1)	$\times$	$\times$	Hybrid2 to Hybrid3.
S10	2.76	0.7287	Hybrid2$\Longrightarrow$ Hybrid3 (H-1$\rightarrow$L)	$\times$	$\times$	Hybrid2 to Hybrid3.
S27	3.22	0.0966	QD $\Longrightarrow$ QD (H-2$\rightarrow$L+2)	Hybrid2 $\longleftarrow$	$\longrightarrow$ Hybrid3	Hybrid2 to Hybrid3.
S35	3.30	0.0968	QD $\Longrightarrow$ QD (H-4$\rightarrow$L+2)	Hybrid2 $\longleftarrow$	$\longrightarrow$ Hybrid3	Hybrid2 to Hybrid3.
NKX-NKX-QD-p			N=40, E*=3.36			
S6	2.71	2.6031	Dye $\Longrightarrow$ Dye (H-1$\rightarrow$L)	Dye$'$ $\longleftarrow$	$\times$	Dye$'$ to Dye.
S10	2.75	0.1605	Dye$'$ $\Longrightarrow$ Dye$'$ (H$\rightarrow$L+1)	$\times$	$\longrightarrow$ Dye	Dye$'$ to Dye.

E* is the maximum energy obtained in each case by using the maximum number of states given, N.

Hybrid1:Dye-QD,

Hybrid2:Dye-Dye$'$-QD,

Hybrid3:Dye-Dye$'$.

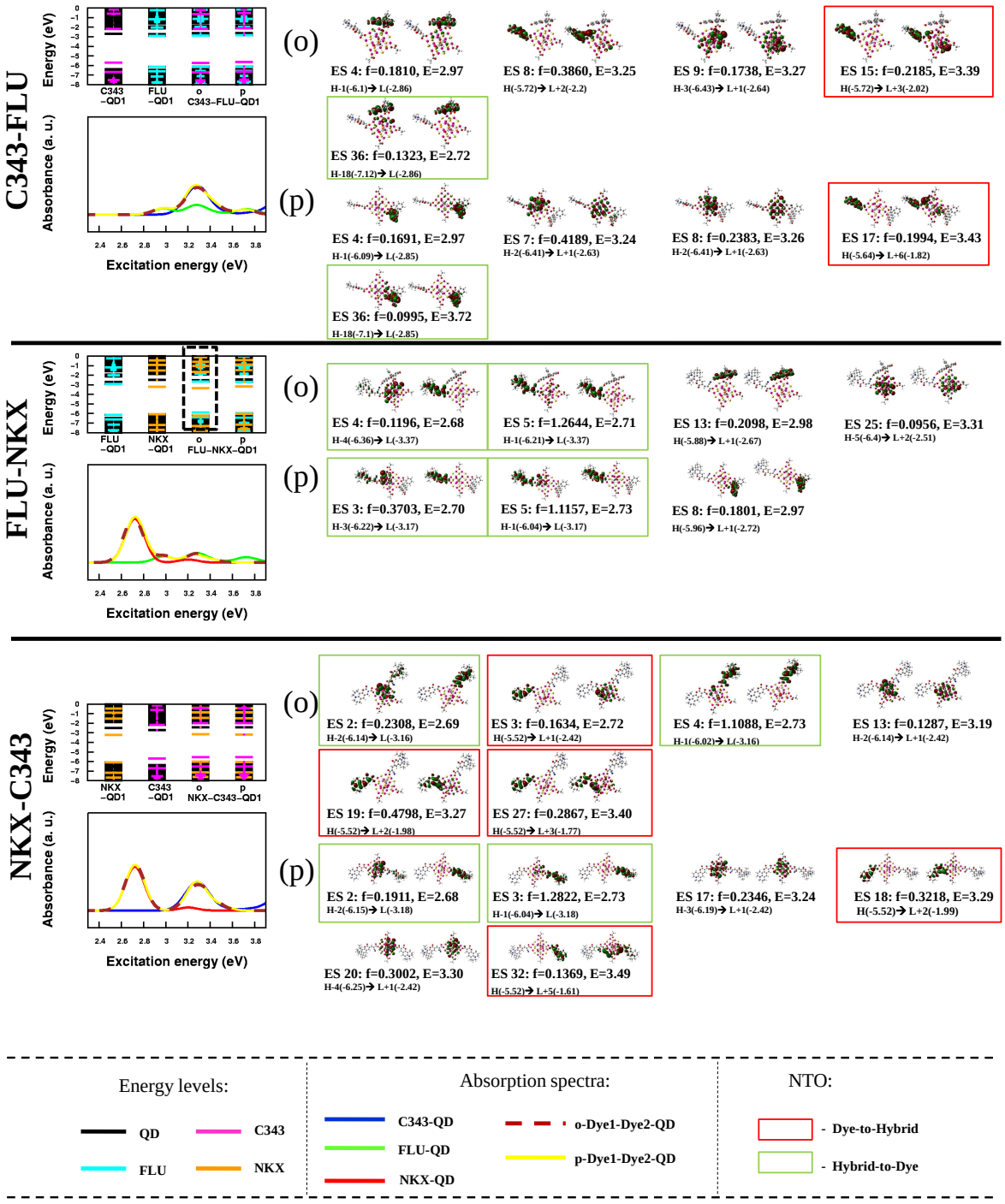

FIG. S5: Energy levels, Absorption spectra and NTOs for the model 2-dye-sensitized QDs sensitized with dyes of different species. Legends for energy level diagrams, absorption spectra and charge transfers are indicated in the respective boxes given at the bottom of the figure. Nature of charge transfers shown above is presented in tabular form in Table S4.

TABLE S4: Nature of charge transfer in 2-dye-sensitized-QD1 sensitized with different species of dye molecules.

Excited state	Energy eV	Oscillator strength	Transition	Hole transfer (In valance band)	Electron transfer (In conduction band)	Direction of electron transfer
C343-FLU-QD-o			N=40, E*=3.77			
S4	2.97	0.1810	FLU $\Longrightarrow$ FLU (H-1$\rightarrow$L)	C343 $\longleftarrow$	$\times$	C343 to FLU.
S8	3.25	0.3860	C343 $\Longrightarrow$ C343 (H$\rightarrow$L+2)	$\times$	$\longrightarrow$ QD or FLU	Multiple case.
S9	3.27	0.1738 $\longleftarrow$	QD $\Longrightarrow$ QD (H-3$\rightarrow$L+1)	FLU or C343	$\longrightarrow$ FLU	Multiple case.
S15	3.39	0.2185	C343 $\Longrightarrow$ Hybrid1 (H$\rightarrow$L+3)	$\times$	$\sim$ QD or FLU	Multiple case.
S36	3.72	0.1323	FLU $\Longrightarrow$ FLU (H-18$\rightarrow$L)	QD or FLU or C343 $\longleftarrow$	$\times$	Multiple case.
C343-FLU-QD-p			N=40, E*=3.78			
S4	2.97	0.1691	FLU $\Longrightarrow$ FLU (H-18$\rightarrow$L)	C343 $\longleftarrow$	$\times$	C343 to FLU.
S7	3.24	0.4189	QD $\Longrightarrow$ QD (H-2$\rightarrow$L+1)	FLU or C343 $\longleftarrow$	$\longrightarrow$ FLU	Multiple case.
S8	3.26	0.2383	QD $\Longrightarrow$ QD (H-2$\rightarrow$L+1)	FLU or C343 $\longleftarrow$	$\longrightarrow$ FLU	Multiple case.
S17	3.43	0.1994	C343 $\Longrightarrow$ Hybrid1 (H$\rightarrow$L+8)	$\times$	$\sim$ QD or FLU	Multiple case.
S36	3.72	0.0955	FLU $\Longrightarrow$ FLU (H-18$\rightarrow$L)	QD or FLU or C343 $\longleftarrow$	$\times$	Multiple case.
FLU-NKX-QD-o			N=40, E*=3.49			
S4	2.68	0.1196	Hybrid1 $\Longrightarrow$ NKX (H-4$\rightarrow$L)	NKX or FLU $\sim$	$\times$	Multiple case.
S5	2.71	1.2644	NKX $\Longrightarrow$ NKX (H-1$\rightarrow$L)	$\times$	FLU $\longleftarrow$	FLU to NKX.
S13	2.98	0.2098	FLU $\Longrightarrow$ FLU (H$\rightarrow$L+1)	$\times$	$\longrightarrow$ NKX	FLU to NKX.
S25	3.31	0.0956	QD $\Longrightarrow$ QD (H-5$\rightarrow$L+2)	FLU or NKX $\longleftarrow$	$\longrightarrow$ FLU or NKX	Multiple case.
FLU-NKX-QD-p			N=40, E*=3.54			
S3	2.70	0.3703	Hybrid1 $\Longrightarrow$ NKX (H-3$\rightarrow$L)	NKX or FLU $\sim$	$\times$	Multiple case.
S5	2.73	1.1157	Hybrid1 $\Longrightarrow$ NKX (H-1$\rightarrow$L)	FLU $\sim$	$\times$	FLU to NKX.
S8	2.97	0.1801	FLU $\Longrightarrow$ FLU (H$\rightarrow$L+1)	$\times$	$\longrightarrow$ NKX	FLU to NKX.
NKX-C343-QD-o			N=40, E*=3.64			
S2	2.69	0.2308	Hybrid1 $\Longrightarrow$ NKX (H-2$\rightarrow$L)	C343 $\sim$	$\times$	C343 to NKX.
S3	2.72	0.1634	C343 $\Longrightarrow$ Hybrid1 (H$\rightarrow$L+1)	$\times$	$\sim$ NKX	C343 to NKX.
S4	2.73	1.1088	NKX $\Longrightarrow$ NKX (H-1$\rightarrow$L)	C343 $\longleftarrow$	$\times$	C343 to NKX.
S13	3.19	0.1287	QD $\Longrightarrow$ QD (H-2$\rightarrow$L+1)	NKX or C343 $\longleftarrow$	$\longrightarrow$ NKX	Multiple case.
S19	3.27	0.4798	C343 $\Longrightarrow$ Hybrid1 (H$\rightarrow$L+2)	$\times$	$\sim$ QD or NKX	Multiple case.
S27	3.40	0.2867	C343 $\Longrightarrow$ Hybrid1 (H$\rightarrow$L+3)	$\times$	$\sim$ QD or NKX	Multiple case.
NKX-C343-QD-p			N=40, E*=3.64			
S2	2.68	0.1911	Hybrid1 $\Longrightarrow$ NKX (H-2$\rightarrow$L)	C343 or NKX $\sim$	$\times$	Multiple case.
S3	2.73	1.2822	Hybrid1 $\Longrightarrow$ NKX (H-1$\rightarrow$L)	C343 $\sim$	$\times$	C343 to NKX.
S17	3.24	0.2346	QD $\Longrightarrow$ QD (H-3$\rightarrow$L+1)	NKX or C343 $\longleftarrow$	$\longrightarrow$ NKX	Multiple case.
S18	3.29	0.3218	C343 $\Longrightarrow$ Hybrid1 (H$\rightarrow$L+2)	$\times$	$\sim$ QD or NKX	Multiple case.
S20	3.30	0.3002	QD $\Longrightarrow$ QD (H-4$\rightarrow$L+1)	NKX or C343 $\longleftarrow$	$\longrightarrow$ NKX	Multiple case.
S32	3.49	0.1369	C343 $\Longrightarrow$ Hybrid1 (H$\rightarrow$L+5)	$\times$	$\sim$ QD or NKX	Multiple case.

E* is the maximum energy obtained in each case by using the maximum number of states given, N.

TABLE S5: Nature of charge transfer in C343-QD1-A in solvents.

Excited state	Energy eV	Oscillator strength	Transition	Hole transfer (In valance band)	Electron transfer (In conduction band)	Direction of electron transfer
a	N=10, E*=3.63					
S2	3.19	0.9540	Dye$\Longrightarrow$ Dye (H$\rightarrow$L+1)	$\times$	$\longrightarrow$ QD	Dye to QD.
S3	3.35	0.1467	QD$\Longrightarrow$ QD (H-1$\rightarrow$L)	Dye $\longleftarrow$	$\times$	Dye to QD.
S4	3.39	0.1488	QD$\Longrightarrow$ QD (H-2$\rightarrow$L)	Dye $\longleftarrow$	$\times$	Dye to QD.
S5	3.44	0.2640	QD$\Longrightarrow$ QD (H-3$\rightarrow$L)	Dye $\longleftarrow$	$\times$	Dye to QD.
b	N=10, E*=3.67					
S2	3.20	0.9229	Dye$\Longrightarrow$ Dye (H$\rightarrow$L+1)	$\times$	$\longrightarrow$ QD	Dye to QD.
S3	3.39	0.1422	QD$\Longrightarrow$ QD (H-1$\rightarrow$L)	Dye $\longleftarrow$	$\times$	Dye to QD.
S4	3.44	0.1501	QD$\Longrightarrow$ QD (H-2$\rightarrow$L)	Dye $\longleftarrow$	$\times$	Dye to QD.
S5	3.48	0.2532	QD$\Longrightarrow$ QD (H-3$\rightarrow$L)	Dye $\longleftarrow$	$\times$	Dye to QD.
c	N=10, E*=3.71					
S1	3.14	0.3036	Dye$\Longrightarrow$ Hybrid (H$\rightarrow$L)	$\times$	$\times$	Dye to Hybrid(Direct).
S2	3.19	0.6420	Dye$\Longrightarrow$ Hybrid (H$\rightarrow$L+1)	$\times$	$\times$	Dye to Hybrid(Direct).
S3	3.46	0.1658	QD$\Longrightarrow$ QD (H-1$\rightarrow$L)	Dye $\longleftarrow$	$\times$	Dye to QD.
S4	3.50	0.1837	QD$\Longrightarrow$ QD (H-2$\rightarrow$L)	Dye $\longleftarrow$	$\times$	Dye to QD.
S5	3.53	0.2727	QD$\Longrightarrow$ QD (H-3$\rightarrow$L)	Dye $\longleftarrow$	$\times$	Dye to QD.
d	N=10, E*=3.58					
S1	3.18	0.8928	Dye$\Longrightarrow$ Dye (H$\rightarrow$L)	$\times$	$\times$	No transfer.
S7	3.56	0.1596	QD$\Longrightarrow$ QD (H-1$\rightarrow$L+1)	Dye $\longleftarrow$	$\longrightarrow$ Dye	Energy transfer.
S9	3.57	0.1955	QD$\Longrightarrow$ QD (H-2$\rightarrow$L+1)	Dye $\longleftarrow$	$\longrightarrow$ Dye	Energy transfer.
S10	3.58	0.1477	QD$\Longrightarrow$ QD (H-3$\rightarrow$L+1)	Dye $\longleftarrow$	$\longrightarrow$ Dye	Energy transfer.
e	N=10, E*=3.54					
S1	3.17	0.8394	Dye$\Longrightarrow$ Dye (H$\rightarrow$L)	$\times$	$\times$	No transfer.
S9	3.53	0.2028	QD$\Longrightarrow$ QD (H-1$\rightarrow$L+1)	Dye $\longleftarrow$	$\longrightarrow$ Dye	Energy transfer.
S10	3.54	0.1916	QD$\Longrightarrow$ QD (H-2$\rightarrow$L+1)	Dye $\longleftarrow$	$\longrightarrow$ Dye	Energy transfer.
f	N=10, E*=3.50					
S1	3.13	0.1890	Hybrid$\Longrightarrow$ Dye (H-1$\rightarrow$L)	Dye $\sim$	$\times$	Energy transfer.
S2	3.15	0.1984	Hybrid$\Longrightarrow$ Dye (H-2$\rightarrow$L)	Dye $\sim$	$\times$	Energy transfer.
S3	3.17	0.5122	Hybrid$\Longrightarrow$ Dye (H$\rightarrow$L)	$\times$	$\times$	Hybrid to Dye(Direct).
S10	3.50	0.2068	QD$\Longrightarrow$ QD (H-1$\rightarrow$L+1)	Dye $\longleftarrow$	$\longrightarrow$ Dye	Energy transfer.

E* is the maximum energy obtained in each case by using the maximum number of states given, N.

TABLE S6: optimised coordinates of C343-QD1-A.

S	1.07443500	-0.02732100	0.04600200
S	0.25041000	-2.35467300	-3.70073300
S	2.30200900	3.57563600	-2.41248600
S	0.04082100	-3.59434500	2.57620100
S	1.68382500	2.41272800	3.78860900
S	4.28084300	-0.24287400	-3.10726600
S	3.91188700	-1.66740100	3.11210700
S	-1.82829400	1.45291900	-3.07204800
S	-2.13115800	0.43665400	3.15101800
S	3.12246600	-3.98197800	-0.49946200
S	5.05149700	1.99238600	0.56352500
S	-2.90546500	-2.05697200	-0.72955600
S	-1.04020100	3.87906100	0.72415500
Cd	-0.12244400	1.69189000	1.87894700
Cd	-1.45442300	-3.63553400	0.57524300
Cd	0.40391800	2.44818300	-3.59060200
Cd	5.49162700	-0.28088100	1.65239700
Cd	-0.82228100	-0.72880000	-1.90225200
Cd	1.04809400	4.69060000	-0.47934700
Cd	-0.94657200	-1.68051500	3.95335000
Cd	4.51337600	-2.21511300	-1.59268300
Cd	3.17162600	1.32912200	-1.24226900
Cd	1.21673500	-4.16474400	-2.20597900
Cd	2.51308700	0.08237600	4.21499100
Cd	-2.55444800	2.87177700	-1.05385600
Cd	2.04019400	-2.32039100	1.29518000
Cd	3.44993700	3.09418300	2.13184400
Cd	2.20990100	-0.91642200	-4.46085600
Cd	-3.25475700	-0.30868700	1.04959000
C	8.45392100	-2.53830800	-0.38127400
H	8.14694100	-3.58423100	-0.45478800
H	9.39828100	-2.46720800	0.15367300
H	8.57491300	-2.15460400	-1.39721100
C	7.38310700	-1.74842500	0.32670400
O	7.63915900	-1.11153300	1.37081300
O	6.19293900	-1.73796300	-0.16446900
C	1.38443600	1.87641600	-7.55233500
H	1.75160000	1.48960400	-8.50028900
H	1.87020000	2.82899800	-7.32770400
H	0.30908300	2.05835900	-7.61875700
C	1.65978500	0.89863300	-6.43853200
O	1.29564800	1.20394700	-5.24165100
O	2.23052800	-0.18902800	-6.66509900
C	3.54112000	7.21584400	1.86905700
H	3.33409700	7.05859700	2.93026900
H	3.35315900	8.25450400	1.60662700
H	4.59272900	6.97521700	1.69511800
C	2.67382400	6.29679100	1.04709100
O	1.88676500	6.75055100	0.19177100
O	2.75850400	5.02569800	1.24340900
C	0.25369800	-1.39539300	6.40152500
O	-0.85935100	-1.94305900	6.26049800
O	0.88811900	-0.94128400	5.37604900
C	-1.35483000	-7.38645200	-1.14930100
H	-1.22816700	-7.61865200	-0.08908100
H	-1.10808000	-8.25935400	-1.74949100
H	-2.40030900	-7.11147400	-1.30791700
C	-0.46784500	-6.22357800	-1.51576800

O	0.40980300	-6.33780100	-2.39538500
O	-0.63111400	-5.10330000	-0.90074600
C	0.88140200	-1.25145500	7.76422500
H	1.85049100	-1.75603400	7.77323000
H	0.23651200	-1.67794800	8.52922200
H	1.05450800	-0.19320900	7.97415500
O	-7.40786800	4.02610900	0.12983400
O	-8.89204500	2.37319500	0.08983800
O	-4.82623500	3.28041000	-0.97201100
O	-4.20776000	1.37273400	-0.06238500
N	-12.33035200	-0.92839100	0.06846000
C	-11.62739700	1.85454900	0.28305400
C	-12.96306500	1.43633200	-0.33110700
C	-13.38497500	0.07720200	0.21066600
C	-12.79893800	-2.31500800	0.10650800
C	-11.69334600	-3.29918100	0.46686900
C	-10.02179700	-1.60865100	-0.26477600
C	-10.47273400	-3.04128800	-0.41689400
C	-8.26573600	0.07725000	-0.21871700
C	-8.69404700	-1.25993000	-0.33619600
C	-6.91670900	0.49742800	-0.30583500
C	-6.55179000	1.81306700	-0.22186000
C	-7.56357600	2.84843200	-0.00580900
C	-9.25045700	1.06556300	-0.02180700
C	-10.60340900	0.76544300	0.07662500
C	-11.00352000	-0.58958800	-0.03658400
C	-5.13523100	2.20436500	-0.42119000
H	-11.26643200	2.78590900	-0.15471000
H	-11.75710400	2.05140000	1.35520700
H	-13.74327900	2.16876500	-0.10928700
H	-12.86683200	1.38150900	-1.42031600
H	-14.26581400	-0.28733900	-0.32825600
H	-13.67120000	0.16380700	1.26952000
H	-13.23652300	-2.58100400	-0.86706600
H	-13.60725000	-2.37396900	0.84351200
H	-12.06779600	-4.31846100	0.34199400
H	-11.41792800	-3.17663800	1.51936400
H	-9.65408700	-3.71966000	-0.16440500
H	-10.73793600	-3.24410600	-1.46308800
H	-7.94890200	-2.03265500	-0.49941000
H	-6.15108700	-0.25028200	-0.48754200

TABLE S7: optimised coordinates of C343-QD1-B.

S	-1.11343700	-0.00559300	-0.03291200
S	-1.00616500	0.03385000	4.42686600
S	-2.07108100	4.41096700	-0.09231600
S	-0.37389900	-4.46592200	-0.05589200
S	-0.91590500	0.01038100	-4.51732300
S	-4.63835700	1.72331500	2.16454400
S	-3.80641300	-2.87273600	-2.19296900
S	1.62343800	2.76459300	2.29410200
S	2.43731500	-1.59669400	-2.29008500
S	-3.75445600	-2.89595800	2.18394600
S	-4.66894600	1.64771300	-2.21244000
S	2.44875500	-1.54982500	2.30610300
S	1.60118000	2.76365100	-2.31528000
Cd	0.57698700	0.30391400	-2.22203600
Cd	0.92467500	-3.47005400	1.83655000
Cd	-0.50118700	3.98311800	1.80697900
Cd	-5.30855200	-0.81561200	-1.98133600
Cd	0.49999700	0.30955500	2.24148500
Cd	-0.47671200	4.20404900	-2.08455500
Cd	1.03641600	-3.69856900	-2.05089400
Cd	-4.98126500	-0.73760100	1.91382200
Cd	-3.11520500	1.94058300	-0.03074100
Cd	-2.06295800	-2.23439100	3.99573900
Cd	-2.03594900	-2.11171800	-3.78398600
Cd	2.69824900	2.79415400	-0.02367600
Cd	-2.25612900	-2.55561000	-0.01209800
Cd	-2.74017500	1.57613400	-3.80015800
Cd	-2.82529400	1.74856700	3.97938700
Cd	3.50754300	-1.24910400	-0.00574500
C	-8.75564500	-1.46892400	0.40986500
H	-8.59937800	-2.33540300	1.05689100
H	-9.61948800	-1.63695400	-0.22942000
H	-8.93230100	-0.60208300	1.05113200
C	-7.51900400	-1.23423700	-0.42008100
O	-7.57103000	-1.24853600	-1.66832800
O	-6.40211000	-1.01775100	0.18161000
C	-1.97542600	5.71049900	5.26855400
H	-2.48445100	5.90643500	6.20968100
H	-2.30726300	6.42547900	4.51188800
H	-0.89778300	5.83738300	5.39684100
C	-2.26175800	4.30837700	4.79255700
O	-1.73372100	3.91183200	3.68773000
O	-2.99574300	3.54398300	5.45282900
C	-2.37621600	5.21143800	-5.75753200
H	-2.06988700	4.51383900	-6.54068500
H	-2.10764900	6.22643200	-6.04189000
H	-3.46039400	5.13264100	-5.64682600
C	-1.71126600	4.83124100	-4.45843800
O	-0.97291300	5.63663500	-3.85530300
O	-1.92044900	3.65429000	-3.97969200
C	0.12764300	-4.75889900	-4.41909300
O	1.11124100	-5.22744700	-3.81026700
O	-0.50563900	-3.74084400	-3.94970300
C	0.17772500	-5.60185700	5.30804700
H	0.13241300	-6.39185800	4.55456300
H	-0.22726300	-5.96644200	6.24948400
H	1.22674300	-5.32535700	5.43818200
C	-0.60033700	-4.40368200	4.82451600
O	-1.56680700	-3.96003700	5.47889600

O	-0.24889100	-3.84450500	3.71993500
C	-0.34500600	-5.36876100	-5.71498000
H	-1.38128100	-5.69722200	-5.60482000
H	0.28197900	-6.21364900	-5.99117500
H	-0.31732200	-4.61324400	-6.50380600
O	5.84014700	-1.31930900	0.02033500
O	7.98712700	-0.91186000	0.04346100
O	5.09873500	2.89433100	-0.00011100
O	4.12465900	0.92371600	-0.01198700
N	12.73450000	-0.51882800	0.11808300
C	10.43969400	-2.25517400	0.07849700
C	11.74522400	-2.68147500	-0.59251500
C	12.92336700	-1.97146900	0.05966100
C	13.97304400	0.25140900	0.26873500
C	13.73104100	1.64653100	0.82895500
C	11.37407000	1.49195300	0.04633100
C	12.62698500	2.33392100	0.02572800
C	8.94872900	1.28518200	0.03544300
C	10.12680800	2.06360500	0.03936900
C	7.64114400	1.80391700	0.02108400
C	6.52529400	0.99791600	0.01581300
C	6.69362500	-0.43851500	0.02499600
C	9.09845700	-0.11590600	0.04711100
C	10.32971600	-0.75006900	0.07255900
C	11.49564300	0.06031100	0.08008200
C	5.18383300	1.64477900	0.00036100
H	9.57785000	-2.69139300	-0.42767000
H	10.41244800	-2.62964000	1.10977200
H	11.89039200	-3.76161900	-0.51552100
H	11.71114500	-2.43170400	-1.65773000
H	13.84074500	-2.16207700	-0.50621500
H	13.08689600	-2.35900900	1.07559100
H	14.48081100	0.31669700	-0.70416200
H	14.63384300	-0.31254100	0.93515100
H	14.66374400	2.21437300	0.78890200
H	13.43398100	1.57705200	1.88025900
H	12.41334500	3.32912900	0.42224800
H	12.96708800	2.47300400	-1.00885300
H	10.03439900	3.14474600	0.02936400
H	7.48036800	2.87633900	0.01227200

TABLE S8: optimised coordinates of NKX-QD1-A.

S	-1.68056800	-0.03175000	-0.03679600
S	-1.67715100	-0.31563500	4.43560900
S	-3.52084600	4.08361500	0.20595800
S	0.00757900	-4.18946600	-0.35694000
S	-1.47866700	0.38116900	-4.51536700
S	-5.53025300	0.74836200	2.17648400
S	-3.68629500	-3.21655000	-2.46244300
S	0.41576600	3.03308600	2.54441300
S	2.13252700	-0.62161300	-2.34103100
S	-3.68414100	-3.57043300	1.88635900
S	-5.49119200	1.01500800	-2.17583000
S	2.07420800	-0.95129500	2.32573500
S	0.43506900	3.39677500	-2.02096000
Cd	-0.12752700	0.81801600	-2.18307300
Cd	1.02631100	-3.13621000	1.66996500
Cd	-1.90446200	3.85044100	2.10087600
Cd	-5.59238400	-1.54019400	-2.15041200
Cd	-0.25759000	0.44749900	2.32843800
Cd	-1.89337900	4.38157700	-1.74934800
Cd	1.23288900	-3.00743000	-2.26664700
Cd	-5.34200400	-1.70475200	1.74010200
Cd	-4.05336200	1.46222400	0.05564000
Cd	-2.21196100	-2.71654600	3.80282200
Cd	-2.11243500	-1.98272900	-3.95916800
Cd	1.52270600	3.47142200	0.27881100
Cd	-2.25984700	-2.75258700	-0.22852500
Cd	-3.59550900	1.48818300	-3.73150600
Cd	-3.80339200	1.02795500	4.04846900
Cd	2.82513000	-0.23732600	0.03459100
C	-8.87186000	-3.06111200	0.07273500
H	-8.55284700	-3.91609200	0.67343700
H	-9.66719900	-3.36174700	-0.60558800
H	-9.24042800	-2.29257000	0.75654500
C	-7.69419500	-2.52072400	-0.69744300
O	-7.72299100	-2.44176600	-1.94396300
O	-6.65143500	-2.13769900	-0.04645400
C	-3.71622300	4.97490900	5.62048900
H	-4.27356900	5.00819600	6.55396400
H	-4.15347300	5.67327800	4.90289900
H	-2.68217000	5.28116800	5.79617500
C	-3.73489500	3.58297800	5.04167100
O	-3.12366000	3.36624800	3.92907900
O	-4.32952800	2.65291400	5.62524400
C	-3.92763500	5.25305900	-5.38423200
H	-3.46321300	4.71322100	-6.21304500
H	-3.88693200	6.32329100	-5.57398600
H	-4.96851400	4.92797800	-5.31593600
C	-3.21016500	4.91511800	-4.10201500
O	-2.65769500	5.80369300	-3.42210400
O	-3.17462600	3.68591200	-3.71756200
C	0.57828400	-4.04479100	-4.72070700
O	1.63624000	-4.33912600	-4.12703600
O	-0.25720500	-3.22059200	-4.18952200
C	0.68751900	-5.61067600	4.95284400
H	0.83394200	-6.33297200	4.14616400
H	0.35163700	-6.12402700	5.85102900
H	1.64709200	-5.12351100	5.14216100
C	-0.32332200	-4.57739700	4.52421000
O	-1.37512400	-4.40031200	5.17209300

O	-0.08206600	-3.87502800	3.47145800
C	0.25103600	-4.64198300	-6.06563500
H	-0.69112000	-5.19139000	-5.99903700
H	1.04512500	-5.31055800	-6.39043400
H	0.11872100	-3.84111500	-6.79698100
O	6.61732200	-1.27671500	0.03111400
O	8.82231800	-1.10554300	0.00364300
O	3.75858000	4.11227600	0.34606200
O	3.42287700	1.93717300	0.19747900
N	13.59832600	-1.05064300	0.18388200
C	11.17854100	-2.66162300	-0.28408300
C	12.59393200	-3.09665800	-0.71097900
C	13.67982000	-2.50768200	0.16187300
C	14.86467700	-0.39407200	0.51561600
C	14.68549000	1.03149600	1.00326800
C	12.38693500	1.04843900	0.11623100
C	13.70878900	1.81872100	0.11053500
C	9.95258600	0.99780200	0.11456600
C	11.17927600	1.69411000	0.13892200
C	8.70320600	1.64200100	0.17108800
C	7.51460700	0.93866300	0.14085500
C	7.56233300	-0.52505000	0.05654500
C	9.99864900	-0.40896700	0.00883500
C	11.18329800	-1.13441200	-0.07507100
C	12.40303300	-0.39649600	0.07650000
C	4.21462000	2.94990600	0.26908900
H	12.65850600	-4.18807400	-0.68942600
H	12.76903500	-2.78371400	-1.74595700
H	14.66491400	-2.77753900	-0.22997400
H	13.62684800	-2.89896600	1.18759600
H	15.52166900	-0.42497300	-0.36332100
H	15.35468500	-0.99176200	1.29218900
H	15.66309900	1.52209000	1.02833700
H	14.29929200	1.02683800	2.02782000
H	11.13921400	2.77474200	0.18216800
H	8.68814700	2.72344400	0.23591200
C	5.68862200	2.73984300	0.25872100
C	6.18677200	1.47592600	0.17941100
C	6.50808400	3.90149000	0.33264700
N	7.22448200	4.80766000	0.39060500
H	5.43450700	0.70199300	0.13385200
C	13.57646000	3.24140500	0.67947400
H	12.95345200	3.88221800	0.05174200
H	13.15420900	3.23387700	1.68771100
H	14.56467900	3.70669600	0.73015300
C	14.24108700	1.91305900	-1.33966600
H	13.56458000	2.51499500	-1.95078200
H	15.22769800	2.38754200	-1.35731000
H	14.32459000	0.93341100	-1.81476600
C	10.76603300	-3.38099600	1.02066200
H	9.75416100	-3.09813100	1.31267500
H	10.78457700	-4.46586700	0.87429400
H	11.43451600	-3.13805800	1.85069500
C	10.23773900	-3.10536700	-1.43158500
H	9.18735400	-3.01317100	-1.17059800
H	10.42320300	-2.52001400	-2.33652300
H	10.43809300	-4.15527200	-1.66656500

TABLE S9: optimised coordinates of NKX-QD1-B.

S	-1.76599100	-0.01995700	-0.03876100
S	-1.84323700	-0.05152100	4.43254100
S	-2.92708100	4.35392300	-0.07218900
S	-0.82523400	-4.43923100	-0.08437500
S	-1.40730900	0.07093900	-4.51591900
S	-5.44928400	1.51657100	2.04391500
S	-4.23913200	-2.97461700	-2.33404900
S	0.74075800	2.83288100	2.42822300
S	1.92379400	-1.41522400	-2.19171900
S	-4.37212900	-3.05450200	2.03085300
S	-5.30947700	1.50172300	-2.32956500
S	1.75119100	-1.44305900	2.43830000
S	0.89500600	2.90524300	-2.17648600
Cd	-0.02538900	0.40773300	-2.16585300
Cd	0.33949200	-3.43488000	1.88929700
Cd	-1.41421100	3.97634700	1.88444300
Cd	-5.84305800	-0.99107300	-2.15915900
Cd	-0.28016300	0.33880100	2.30926200
Cd	-1.25217600	4.25306400	-2.00395200
Cd	0.61665300	-3.59196800	-2.02129600
Cd	-5.68842700	-0.95061200	1.73997700
Cd	-3.85705500	1.83817200	-0.08844200
Cd	-2.79544200	-2.35070800	3.92763900
Cd	-2.45453300	-2.11255500	-3.85562300
Cd	1.90164800	2.95358400	0.15592800
Cd	-2.79720500	-2.61446900	-0.09161100
Cd	-3.32720900	1.54568600	-3.85198400
Cd	-3.71439300	1.59236000	3.93206500
Cd	2.80579500	-1.08695400	0.15472900
C	-9.35813300	-1.84481700	0.06136200
H	-9.19114900	-2.71758100	0.69728100
H	-10.18438300	-2.03804100	-0.61915500
H	-9.60211400	-1.00115800	0.71126700
C	-8.09835500	-1.53808800	-0.70778300
O	-8.09106800	-1.54333600	-1.95712200
O	-7.02301300	-1.26959600	-0.05279400
C	-3.12230000	5.57710000	5.28905900
H	-3.68629600	5.73972200	6.20481900
H	-3.45117500	6.28171000	4.52144800
H	-2.05992000	5.75554700	5.47178300
C	-3.31531100	4.16705200	4.79098000
O	-2.71407700	3.80513400	3.71128600
O	-4.04219600	3.36152200	5.40862000
C	-3.01308000	5.19998700	-5.75959700
H	-2.63541800	4.51858800	-6.52581300
H	-2.77181900	6.22603900	-6.02823100
H	-4.09734800	5.07554400	-5.70796400
C	-2.40276700	4.84338400	-4.42771500
O	-1.72259200	5.67253400	-3.78994000
O	-2.59635900	3.66013500	-3.95641700
C	-0.13837800	-4.63562600	-4.44636900
O	0.84221600	-5.06992400	-3.80783100
O	-0.84138200	-3.66344200	-3.97799400
C	-0.49399800	-5.67158400	5.25615500
H	-0.47941400	-6.43921000	4.47859300
H	-0.92901500	-6.07814300	6.16647600
H	0.53835500	-5.36641000	5.44278300
C	-1.28936700	-4.48539300	4.77215800
O	-2.30519400	-4.09963700	5.38621400

O	-0.90123300	-3.87440900	3.70696400
C	-0.52604800	-5.23364700	-5.77516100
H	-1.54683400	-5.61884400	-5.71559400
H	0.15549200	-6.03680400	-6.04647100
H	-0.50765500	-4.45671700	-6.54314800
O	9.01951100	3.85768100	0.18243100
O	10.60940700	2.31619300	0.14991400
O	4.30557700	3.13229400	0.21829500
O	3.39369200	1.12229600	0.20272600
N	14.22230100	-0.77851400	-0.25172700
C	13.43070600	2.01718600	0.22560800
C	14.82906800	1.45496300	0.54715200
C	15.21240100	0.29116900	-0.33961800
C	14.74860900	-2.09941000	-0.60508200
C	13.66296400	-3.10178000	-0.95113300
C	11.96903700	-1.61947500	0.04679700
C	12.50094900	-3.05336400	0.05824300
C	10.13251700	-0.02399700	0.14295300
C	10.63054800	-1.34527800	0.12266600
C	8.76250600	0.28008000	0.17095300
C	8.28758500	1.57967100	0.18661800
C	9.25850200	2.68143800	0.17498500
C	11.06991200	1.03383500	0.14541700
C	12.44663900	0.83514900	0.12586900
C	12.90173100	-0.51584400	-0.02977500
C	4.42416300	1.89305100	0.21472100
H	15.57160800	2.25134100	0.44712300
H	14.85184000	1.12182900	1.59036300
H	16.17419400	-0.12336400	-0.02385300
H	15.32816500	0.60415400	-1.38652600
H	15.36751400	-2.46522800	0.22419300
H	15.41998200	-1.97015600	-1.46118000
H	14.10367900	-4.10271100	-0.98103300
H	13.26876600	-2.89229000	-1.95083400
H	9.91125100	-2.15307300	0.16257700
H	8.06734200	-0.55180800	0.17859200
C	5.76757700	1.23387100	0.21854300
C	6.91239800	1.97706100	0.20461400
C	5.67901300	-0.17987800	0.22711100
N	5.44217200	-1.31718300	0.23456500
H	6.74677800	3.05001900	0.20256700
C	11.44654000	-4.08775300	-0.36905000
H	10.62364000	-4.15923300	0.34579000
H	11.02869000	-3.85451400	-1.35188700
H	11.90840000	-5.07730000	-0.42486300
C	12.99283300	-3.40707400	1.48242500
H	12.15194400	-3.41615700	2.17977100
H	13.45455400	-4.39965100	1.49464700
H	13.72170500	-2.68729100	1.86074900
C	13.46172000	2.80665000	-1.10304500
H	12.48118700	3.23046500	-1.32161200
H	14.17829900	3.63118600	-1.03325700
H	13.75045800	2.17556700	-1.94753000
C	13.08485500	2.98239900	1.38631800
H	12.19483200	3.57257800	1.18753300
H	12.93608700	2.43240000	2.31985100
H	13.92225100	3.67109100	1.53529900