

Supplementary Materials for

Förster Resonance Energy Transfer between Fluorescent
Proteins: Efficient Transition Charge-Based Study

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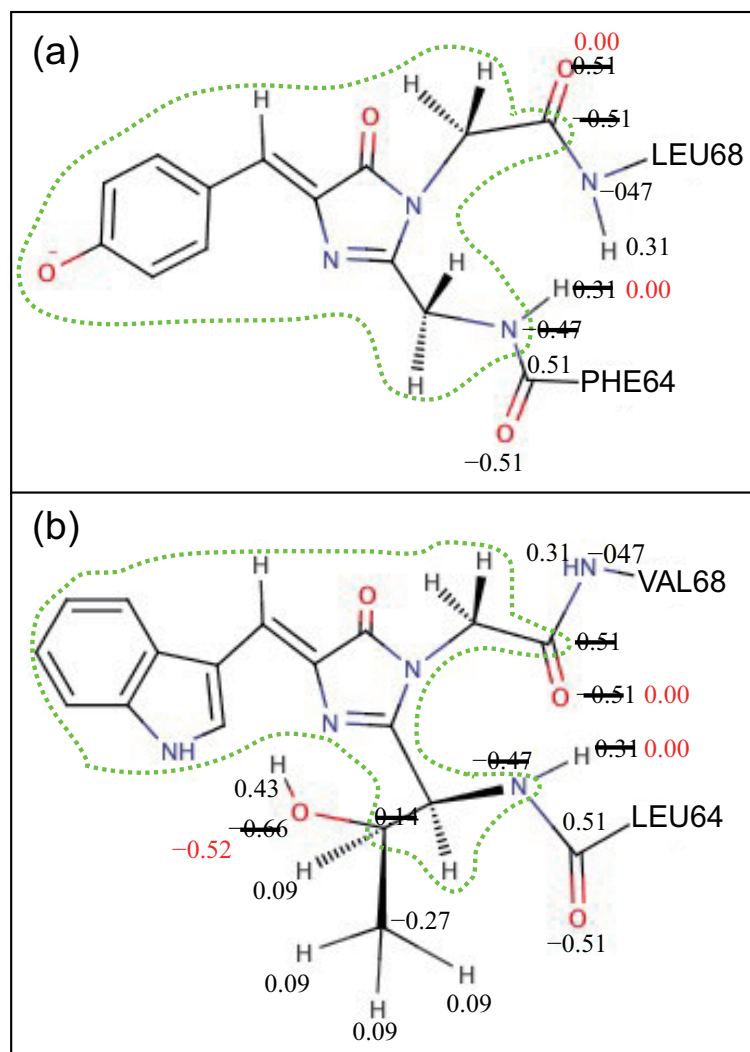


Figure S1 The atomic point charges of the QM/MM border amino acids for (a) donor and (b) acceptor molecules.

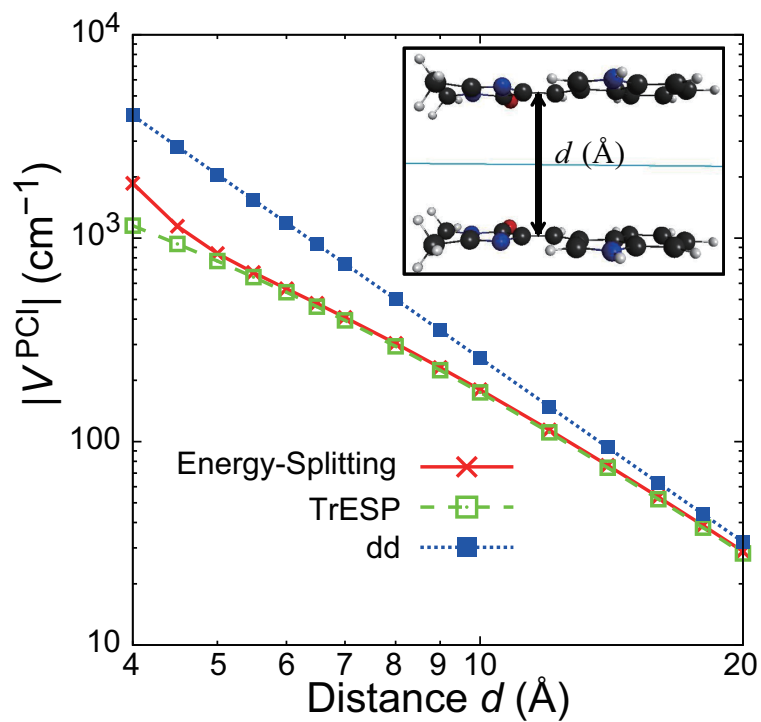


Figure S2 Distance-dependence of the absolute PCI values from the energy splitting (red cross), TrESP (green open square), and the dd-approximation (blue closed square) obtained for the face-to-face eclipsed homo-dimer of D molecules.

Table S 1: Gas-phase optimized geometry, reference transition charges for Frozen-TrESP, and van der Waals radii for Poisson-TrESP of the acceptor molecule (YFP fluorophore).

	X (Å)	Y (Å)	Z (Å)	$q_i^{\text{Frozen-TrESP}} (\times 10^{-2} \text{ a.u.})$	R_i^A (Å)
C	2.761487	-3.044931	0.000000	5.87449	2.0600
C12	2.311303	-1.619962	0.000000	-11.26203	1.8000
N11	1.068127	-1.229050	0.000000	0.78721	1.8500
N13	3.212754	-0.559191	0.000000	2.98042	1.8500
C14	2.468857	0.645682	0.000000	-3.67885	1.8000
O15	2.987350	1.775399	0.000000	-10.01148	1.7000
C10	1.088774	0.175650	0.000000	-5.35572	1.8000
C	4.655055	-0.602842	0.000000	3.44515	2.0600
C8	0.000000	1.039602	0.000000	-0.67771	2.0900
C1	-1.393233	0.808716	0.000000	-2.80020	1.9924
C7	-2.005544	-0.490190	0.000000	12.82064	1.9924
C2	-2.283852	1.933089	0.000000	3.74810	1.9924
C6	-3.368546	-0.643833	0.000000	-2.82512	1.9924
C3	-3.648761	1.796225	0.000000	-0.46239	1.9924
C4	-4.290172	0.487703	0.000000	6.31231	1.9924
O5	-5.541396	0.343774	0.000000	10.97774	1.7000
H	-1.353617	-1.357898	0.000000	-1.36763	1.3582
H	-1.844363	2.931026	0.000000	1.37001	1.3582
H	-3.817025	-1.635121	0.000000	1.64380	1.3582
H	-4.302142	2.665817	0.000000	0.70440	1.3582
H	4.999204	0.435246	0.000000	-1.29471	1.3200
H	5.048274	-1.108581	-0.891484	-1.68436	1.3200
H	5.048274	-1.108581	0.891484	-1.68436	1.3200
H	3.368203	-3.284693	-0.884184	-3.10017	1.3200
H	3.368203	-3.284693	0.884184	-3.10017	1.3200
H	1.877190	-3.685567	0.000000	-2.79834	1.3200
H9	0.301803	2.087904	0.000000	1.43897	1.3200
Center	-0.110428	0.063887	0.000000		

Table S 2: Same as Table S1, but for donor molecule (CFP fluorophore).

	X (Å)	Y (Å)	Z (Å)	$q_i^{\text{Frozen-TrESP}} (\times 10^{-2} \text{ a.u.})$	$\mathbf{R}_i^{\text{D}}$ (Å)
C	-4.499164	-1.251270	0.000000	-3.39829	2.0600
C14	-3.350779	-0.298511	0.000000	10.87673	1.8000
N13	-2.095120	-0.651423	0.000000	-4.69281	1.8500
N15	-3.548295	1.078861	0.000000	-5.16982	1.8500
C16	-2.284133	1.697523	0.000000	1.75159	1.8000
O17	-2.087639	2.908144	0.000000	11.74998	1.7000
C12	-1.356107	0.542282	0.000000	19.29571	1.8000
C	-4.801205	1.809593	0.000000	0.52226	2.0600
C10	0.000000	0.669411	0.000000	-21.39427	2.0900
C1	0.985053	-0.372961	0.000000	9.66061	1.9924
C9	0.768695	-1.747327	0.000000	-23.50930	1.9924
C2	2.427583	-0.191001	0.000000	10.37502	1.8000
C7	3.012553	-1.483453	0.000000	-7.26591	1.8000
N8	1.971089	-2.401975	0.000000	1.44757	1.8500
C3	3.271658	0.932250	0.000000	-5.74484	1.9924
C6	4.395746	-1.687724	0.000000	2.17881	1.9924
C4	4.650735	0.739927	0.000000	-0.81145	1.9924
C5	5.208205	-0.556242	0.000000	-2.29154	1.9924
H	-0.173204	-2.274871	0.000000	2.96178	1.3582
H	2.859465	1.937240	0.000000	0.52202	1.3582
H	5.311691	1.601692	0.000000	-1.08944	1.3582
H	4.822721	-2.686851	0.000000	-1.73008	1.3582
H	6.287755	-0.674008	0.000000	-0.51156	1.3582
H	-5.133416	-1.111008	-0.883565	2.13869	1.3200
H	-5.133416	-1.111008	0.883565	2.13869	1.3200
H	-4.548436	2.872134	0.000000	0.03995	1.3200
H	-5.394817	1.584548	-0.892463	0.64665	1.3200
H	-5.394817	1.584548	0.892463	0.64665	1.3200
H	-4.112500	-2.271257	0.000000	2.37471	1.3200
H	2.079716	-3.404414	0.000000	-0.93188	0.2245
H11	0.363624	1.694885	0.000000	-0.78620	1.3200
Center	0.064026	0.017544	0.000000		

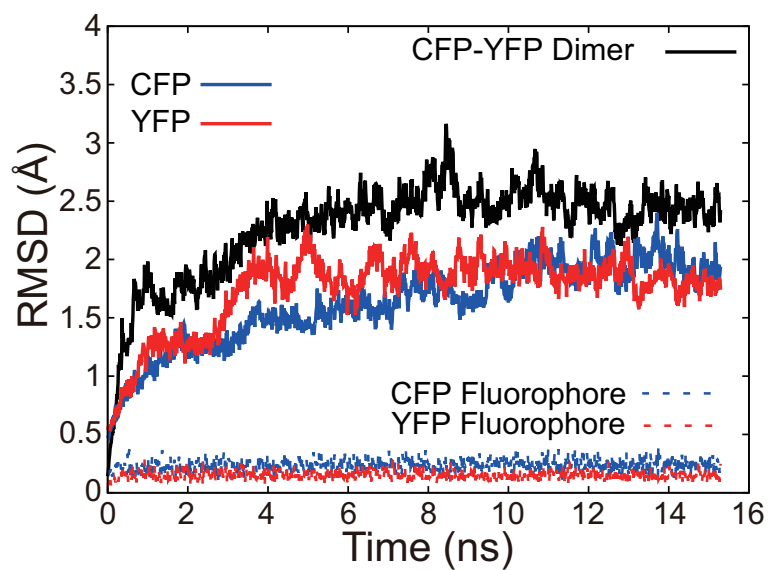


Figure S3 Root-mean-square deviations (RMSDs) from the corresponding starting structures for CFP-YFP dimer, CFP, YFP, CFP fluorophore, and YFP fluorophore during the entire MD simulations.

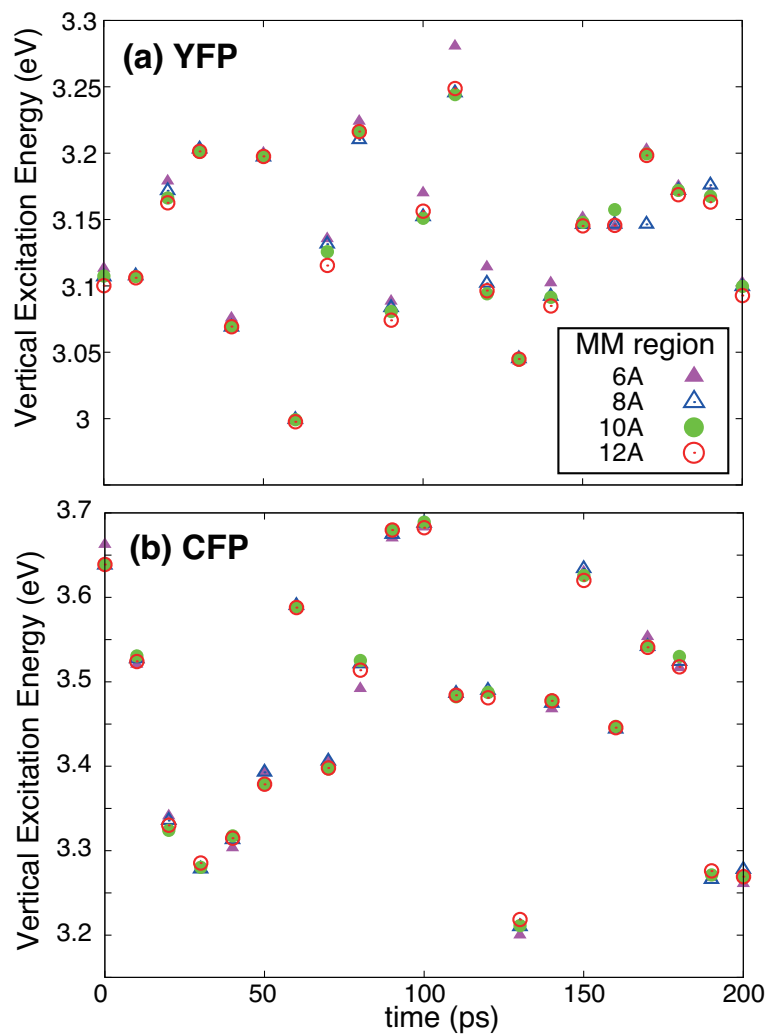


Figure S4 Time-dependence of the vertical excitation energies of (a) YFP and (b) CFP calculated for the first 200 ps long trajectory. In the QM/MM calculations performed at each snapshot, the counter ions and water molecules were removed when they were 6 (closed triangle), 8 (open triangle), 10 (closed circle), and 12 Å (open circle) away from the protein, respectively.

Table S 3: Average transition charges $\langle q_i^{\text{TrESP}} \rangle$ (in $\times 10^{-2}$ a.u.) and their standard deviations $\delta\{q_i^{\text{TrESP}}\}$ (in $\times 10^{-2}$ a.u.) obtained from the no-embedding (NE) and QM/MM calculations for the MD configurations of the acceptor molecule. The reference transition charges for the Frozen-TrESP method, $q_i^{\text{Frozen-TrESP}}$ (in $\times 10^{-2}$ a.u.), are also listed.

	$\langle q_i^{\text{TrESP(NE)}} \rangle$	$\delta\{q_i^{\text{TrESP(NE)}}\}$	$\langle q_i^{\text{TrESP(QM/MM)}} \rangle$	$\delta\{q_i^{\text{TrESP(QM/MM)}}\}$	$q_i^{\text{Frozen-TrESP}}$
C1	-4.24	3.98	-6.13	4.44	-2.80020
C2	4.88	3.39	6.46	3.62	3.74810
C3	0.12	3.69	-1.95	3.78	-0.46239
C4	5.60	3.09	7.46	3.42	6.31231
O5	10.7	0.796	10.4	0.818	10.97774
C6	-1.15	3.89	-2.34	4.17	-2.82512
C7	10.8	3.89	12.6	4.50	12.82064
C8	2.66	3.28	3.93	3.81	-0.67771
H9	0.46	0.603	0.60	0.650	1.43897
C10	-6.95	2.36	-7.36	2.66	-5.35572
N11	0.06	1.14	0.01	1.42	0.78721
C12	-8.18	1.63	-7.48	1.83	-11.26203
N13	0.85	1.42	0.20	1.69	2.98042
C14	-2.75	1.36	-3.31	1.46	-3.67885
O15	-9.95	0.576	-10.2	0.620	-10.01148

Table S 4: Same as Table S3, but for donor molecule (CFP fluorophore). The reference transition charges obtained for the relaxed S₁-state geometry, $q_i^{\text{Frozen-TrESP(S1)}}$ (in $\times 10^{-2}$ a.u.), were also listed.

	$\langle q_i^{\text{TrESP(NE)}} \rangle$	$\delta\{q_i^{\text{TrESP(NE)}}\}$	$\langle q_i^{\text{TrESP(QM/MM)}} \rangle$	$\delta\{q_i^{\text{TrESP(QM/MM)}}\}$	$q_i^{\text{Frozen-TrESP}}$	$q_i^{\text{Frozen-TrESP(S1)}}$
C1	11.7	3.64	11.1	4.65	9.66061	7.59619
C2	6.24	3.23	5.93	3.94	10.37502	11.36138
C3	-2.85	2.38	-3.13	3.02	-5.74484	-5.96726
C4	-3.27	1.96	-2.93	2.37	-0.81145	-0.85924
C5	0.14	1.81	-0.23	2.18	-2.29154	-2.48781
C6	-1.05	2.12	-0.81	2.41	2.17881	2.31375
C7	-3.33	2.69	-3.20	3.07	-7.26591	-7.69697
N8	-0.41	2.73	-1.05	3.06	1.44757	1.17845
C9	-21.6	3.38	-19.2	4.07	-23.50930	-22.34691
C10	-21.9	3.65	-23.4	4.77	-21.39427	-23.09721
H11	-0.33	0.885	-0.40	1.15	-0.78620	0.01060
C12	16.5	2.51	15.9	3.26	19.29571	18.42081
N13	-3.83	1.26	-3.70	1.62	-4.69281	-5.84635
C14	9.43	1.61	9.59	1.91	10.87673	12.10679
N15	-4.13	1.35	-4.56	1.87	-5.16982	-5.84635
C16	4.06	1.49	5.08	1.95	1.75159	2.58137
O17	10.7	0.650	11.5	0.651	11.74998	12.07285

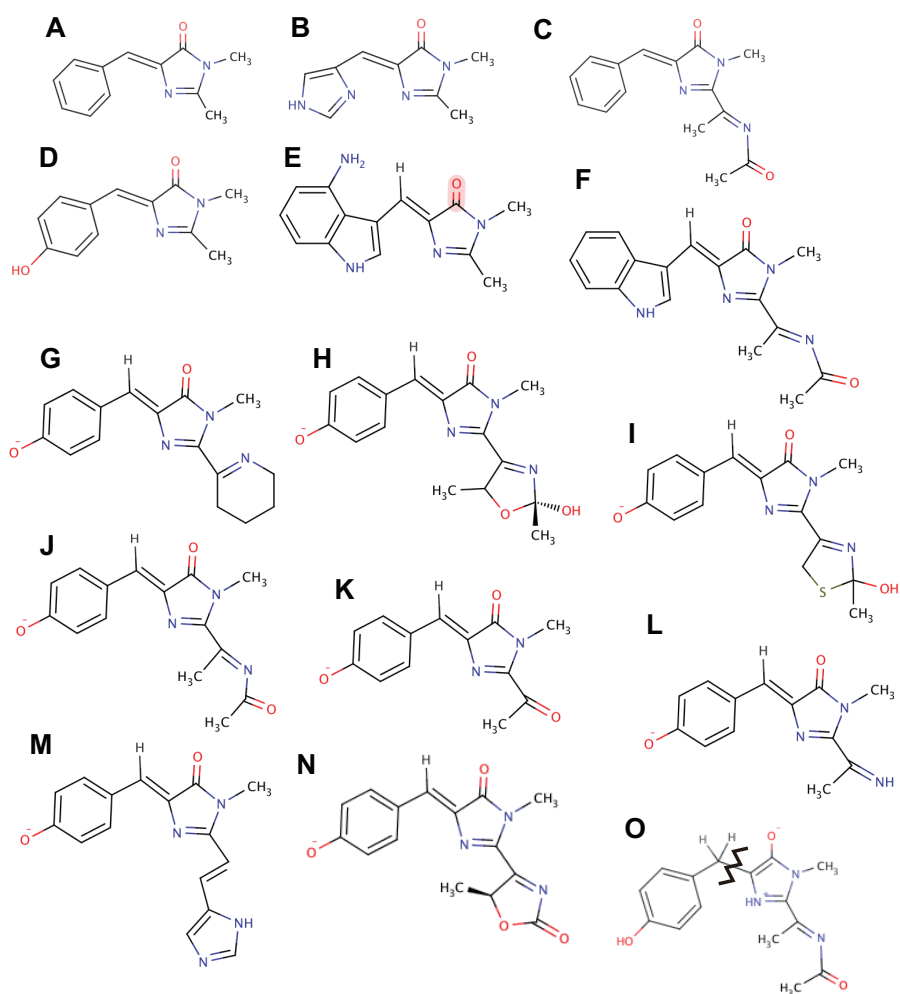


Figure S 5: Chemical structures of fluorophore models of various fluorescent proteins.

Table S 5: Gas-phase optimized geometry and the reference transition charges of fluorophore Fig. S5 A for Frozen-TrESP.

	X (Å)	Y (Å)	Z (Å)	$q_i^{\text{Frozen-TrESP}} (\times 10^{-2} \text{ a.u.})$
C	3.558732	1.377307	0.000000	-2.31139
C	2.067187	1.372859	0.000000	12.08352
N	1.333721	0.295386	0.000000	-5.03221
N	1.336525	2.558331	0.000000	-9.43394
C	-0.026405	2.222974	0.000000	8.76899
O	-0.955693	3.019168	0.000000	11.54989
C	0.000000	0.730846	0.000000	15.00805
C	1.832215	3.922444	0.000000	1.02320
C	-1.137226	-0.011478	0.000000	-31.58866
C	-1.313691	-1.456046	0.000000	27.67704
C	-0.240937	-2.376599	0.000000	-22.36798
C	-2.632225	-1.961912	0.000000	-15.31797
C	-0.491898	-3.747282	0.000000	10.59254
C	-2.877134	-3.334027	0.000000	9.29403
C	-1.805546	-4.232600	0.000000	-19.32076
H	0.774834	-1.999521	0.000000	2.50296
H	-3.465947	-1.264230	0.000000	0.68868
H	0.342124	-4.443597	0.000000	-1.68546
H	-3.899346	-3.701338	0.000000	-1.34068
H	0.959414	4.578857	0.000000	-0.25995
H	2.432409	4.127583	-0.892499	0.67997
H	2.432409	4.127583	0.892499	0.67997
H	3.954319	1.892242	-0.883599	1.88812
H	3.954319	1.892242	0.883599	1.88812
H	3.914870	0.346532	0.000000	1.89172
H	-2.052550	0.578455	0.000000	1.50237
H	-1.991471	-5.303097	0.000000	0.93981
Center	-0.068799	-0.007856	0.000000	

Table S 6: Same as Table S5, but for Fig. S5**B** fluorophore.

	X (Å)	Y (Å)	Z (Å)	$q_i^{\text{Frozen-TrESP}}$ ($\times 10^{-2}$ a.u.)
C	2.142038	0.729608	0.000000	11.87862
N	1.231195	-0.198109	0.000000	-4.52018
C	0.000000	0.470388	0.000000	10.45620
C	0.238838	1.945356	0.000000	9.80951
O	-0.539101	2.892605	0.000000	11.98769
N	1.634726	2.033222	0.000000	-8.79871
C	3.610408	0.468955	0.000000	-2.51473
C	2.367003	3.284961	0.000000	0.23949
C	-1.257487	-0.038247	0.000000	-26.95330
C	-1.712444	-1.405577	0.000000	14.03514
N	-0.908190	-2.537352	0.000000	-3.26433
C	-1.728869	-3.556520	0.000000	-5.05654
N	-3.045352	-3.156744	0.000000	-3.05312
C	-3.049614	-1.785966	0.000000	-12.17773
H	-3.960952	-1.207171	0.000000	-0.31746
H	-1.444800	-4.599884	0.000000	-0.43795
H	1.626663	4.087733	0.000000	-0.17014
H	2.995080	3.379233	-0.892046	0.65674
H	2.995080	3.379233	0.892046	0.65674
H	4.092354	0.903968	-0.883757	2.01554
H	4.092354	0.903968	0.883757	2.01554
H	3.772697	-0.609398	0.000000	1.81654
H	-2.044815	0.713635	0.000000	1.32355
H	-3.856752	-3.757017	0.000000	0.37293
Center	-0.081548	-0.031772	0.000000	

Table S 7: Same as Table S5, but for Fig. S5C fluorophore.

	X (Å)	Y (Å)	Z (Å)	$q_i^{\text{Frozen-TrESP}} (\times 10^{-2} \text{ a.u.})$
C	5.357324	-1.129426	1.235767	1.56145
C	4.556200	-1.046243	-0.045892	-2.76301
O	4.924458	-1.527259	-1.105570	3.02082
N	3.402957	-0.254067	0.048081	4.16933
C	2.206659	-0.694866	-0.090625	-2.80196
C	1.816965	-2.142843	-0.265620	0.31985
C	1.093015	0.280659	-0.064183	14.88668
N	-0.153690	-0.123320	-0.038223	-11.12755
N	1.244265	1.663960	-0.059563	-6.23355
C	-0.044580	2.222541	-0.028126	3.94313
O	-0.305481	3.417433	-0.021580	10.02336
C	-0.936658	1.028275	-0.011807	13.65876
C	2.441607	2.494728	-0.124085	3.58667
C	-2.294037	1.134115	0.020677	-28.62244
C	-3.316657	0.103706	0.037668	24.61329
C	-3.034193	-1.281918	0.020495	-19.02015
C	-4.668439	0.513984	0.072524	-13.98681
C	-4.071753	-2.210253	0.038333	7.72539
C	-5.702274	-0.419670	0.090008	7.44129
C	-5.406578	-1.786619	0.073099	-15.55316
H	5.705310	-0.130127	1.518733	0.04448
H	-4.898443	1.576246	0.085534	0.79529
H	-2.001478	-1.607495	-0.007390	2.75921
H	-6.734891	-0.084192	0.116493	-1.33181
H	-3.841581	-3.271855	0.024384	-1.53356
H	3.055825	2.367145	0.769102	-0.16208
H	2.091439	3.526830	-0.190800	-0.98171
H	1.057940	-2.419987	0.470107	1.45252
H	2.685619	-2.796096	-0.181622	0.41063
H	4.735021	-1.499304	2.058307	0.43228
H	6.213787	-1.788365	1.086657	0.58180
H	3.041479	2.245814	-1.001344	-0.17497
H	1.367780	-2.287076	-1.253504	0.99673
H	-2.654113	2.161841	0.034667	1.33848
H	-6.209841	-2.517815	0.086413	0.53133
Center	-0.025246	0.045416	-0.025152	

Table S 8: Same as Table S5, but for Fig. S5D fluorophore.

	X (Å)	Y (Å)	Z (Å)	$q_i^{\text{Frozen-TrESP}} (\times 10^{-2} \text{ a.u.})$
C	2.989499	-2.810810	0.000000	2.95963
C	2.446932	-1.421711	0.000000	-11.78728
N	1.178189	-1.124736	0.000000	4.95929
N	3.288420	-0.312153	0.000000	7.73375
C	2.484046	0.838567	0.000000	-6.82354
O	2.893404	1.992855	0.000000	-11.49027
C	1.105039	0.276990	0.000000	-15.33720
C	4.739018	-0.281853	0.000000	0.02507
C	0.000000	1.068444	0.000000	27.20106
C	-1.405382	0.710322	0.000000	-24.41142
C	-1.879593	-0.623909	0.000000	21.96556
C	-2.362145	1.747245	0.000000	14.56600
C	-3.239750	-0.898994	0.000000	-8.51617
C	-3.727486	1.479149	0.000000	-7.37859
C	-4.169538	0.150611	0.000000	11.86985
O	-5.493973	-0.185867	0.000000	4.06180
H	-1.160720	-1.434531	0.000000	-2.75365
H	-2.025126	2.780464	0.000000	-0.68917
H	-3.603982	-1.921192	0.000000	1.30330
H	-4.445831	2.295985	0.000000	1.08820
H	-6.040365	0.611265	0.000000	0.65236
H	5.034922	0.769174	0.000000	-0.14965
H	5.147395	-0.767288	-0.892319	-0.88270
H	5.147395	-0.767288	0.892319	-0.88270
H	3.612282	-2.994221	-0.883567	-2.10225
H	3.612282	-2.994221	0.883567	-2.10225
H	2.157032	-3.515198	0.000000	-2.13678
H	0.219154	2.135062	0.000000	-0.94224
Center	-0.066179	0.050223	0.000000	

Table S 9: Same as Table S5, but for Fig. S5**E** fluorophore.

	X (Å)	Y (Å)	Z (Å)	$q_i^{\text{Frozen-TrESP}} (\times 10^{-2} \text{ a.u.})$
C	-4.881449	0.163139	0.000000	3.03695
C	-3.491602	0.705896	0.000000	-9.69144
N	-2.409970	-0.023908	0.000000	2.95499
N	-3.244756	2.075255	0.000000	4.41665
C	-1.850744	2.262698	0.000000	-2.68510
O	-1.279271	3.350014	0.000000	-8.89690
C	-1.334546	0.876499	0.000000	-12.42709
C	-4.204566	3.162768	0.000000	0.63676
C	0.000000	0.589099	0.000000	9.15053
C	0.641474	-0.693210	0.000000	-8.67933
C	-0.029405	-1.914744	0.000000	26.43103
C	2.068431	-1.014968	0.000000	-6.96369
C	2.170101	-2.429726	0.000000	3.08223
N	0.876110	-2.932934	0.000000	-2.94025
C	3.272483	-0.260881	0.000000	1.45906
C	3.377032	-3.137398	0.000000	3.73131
C	4.487687	-0.967548	0.000000	6.45022
C	4.537458	-2.369394	0.000000	-1.65872
H	-1.095288	-2.085748	0.000000	-3.72652
H	5.417161	-0.403294	0.000000	-0.02199
H	3.405883	-4.222366	0.000000	0.62213
H	5.506942	-2.859166	0.000000	0.72722
H	-5.439702	0.495737	-0.883493	-1.85299
H	-5.439702	0.495737	0.883493	-1.85299
H	-3.631411	4.092495	0.000000	-0.38676
H	-4.839092	3.135003	-0.892277	-0.89658
H	-4.839092	3.135003	0.892277	-0.89658
H	-4.835440	-0.926725	0.000000	-2.06328
H	0.641670	-3.913623	0.000000	0.90970
H	0.617898	1.481105	0.000000	1.75683
N	3.288641	1.118674	0.000000	-1.07424
H	4.166520	1.609500	0.000000	0.77043
H	2.453506	1.673242	0.000000	0.57847
Center	0.058377	-0.012715	0.000000	

Table S 10: Same as Table S5, but for Fig. S5F fluorophore.

	X (Å)	Y (Å)	Z (Å)	$q_i^{\text{Frozen-TrESP}} (\times 10^{-2} \text{ a.u.})$
C	6.301392	-0.968517	1.196192	-1.09873
C	5.437327	-0.996559	-0.047030	2.96282
O	5.769437	-1.549777	-1.084467	-3.35409
N	4.273773	-0.223484	0.047667	-5.17600
C	3.081285	-0.688847	-0.057690	3.78994
C	2.721670	-2.151620	-0.175300	-0.72323
C	1.950979	0.261131	-0.051751	-15.21749
N	0.708013	-0.163722	-0.030422	8.56196
N	2.070019	1.647234	-0.064532	4.14623
C	0.767188	2.180028	-0.049708	0.14032
O	0.484936	3.372775	-0.058863	-9.24378
C	-0.091415	0.973476	-0.026906	-12.40348
C	3.247963	2.503829	-0.124820	-3.46343
C	-1.458494	1.021578	-0.009382	18.57258
H	6.650265	0.053686	1.378545	-0.22759
H	3.860948	2.392901	0.771766	0.40987
H	2.874205	3.527504	-0.195597	0.70081
H	1.954098	-2.410471	0.557815	-1.42372
H	3.600336	-2.783756	-0.046335	-0.48771
H	5.724578	-1.273785	2.076336	-0.59695
H	7.158155	-1.629772	1.059346	-0.81324
H	3.858768	2.267141	-0.998075	0.43092
H	2.298596	-2.347946	-1.165854	-0.97996
H	-1.874981	2.026973	-0.008112	0.02979
C	-2.385438	-0.064811	0.004219	-12.20784
C	-2.100086	-1.429521	-0.007675	20.01113
C	-3.836807	0.043485	0.029060	-2.29844
N	-3.264610	-2.141197	0.008654	3.53795
H	-1.133865	-1.910120	-0.028789	-2.86633
C	-4.353651	-1.276260	0.031242	-0.12592
C	-4.736416	1.121725	0.049642	2.40505
H	-3.322785	-3.148231	0.001576	-0.09849
C	-5.723354	-1.553707	0.052653	1.22447
C	-6.103535	0.857283	0.070893	2.21512
H	-4.377237	2.146778	0.048831	0.36048
C	-6.592932	-0.465615	0.072432	0.72228
H	-6.097654	-2.573587	0.053559	0.99384
H	-6.808140	1.683429	0.086536	0.77665
H	-7.664689	-0.639014	0.089090	0.81420
Center	-0.040897	0.028028	-0.022362	

Table S 11: Same as Table S5, but for Fig. S5G fluorophore.

	X (Å)	Y (Å)	Z (Å)	$q_i^{\text{Frozen-TrESP}} (\times 10^{-2} \text{ a.u.})$
N	-3.903361	-0.085067	0.079943	6.06594
C	-2.672138	-0.474725	0.018033	-1.41627
C	-2.212694	-1.927823	-0.069529	-0.77071
C	-3.325016	-2.911136	0.307337	-0.04338
C	-4.629795	-2.482843	-0.369263	-0.02383
C	-4.988446	-1.060035	0.079094	-1.72128
C	-1.597105	0.517825	0.016809	12.92529
N	-0.324955	0.166319	0.012571	-2.26717
O	6.039232	-2.171043	-0.001342	-9.77524
C	4.206893	0.950862	-0.008096	-2.84137
C	5.267523	0.084622	-0.006613	-1.61310
C	5.077575	-1.361890	-0.002774	-2.57854
C	3.683750	-1.799881	-0.001102	-2.78304
C	2.634035	-0.920586	-0.002262	-6.78767
C	2.841215	0.502712	-0.005431	0.60319
C	1.809550	1.458760	-0.006373	-1.07152
C	0.418555	1.330690	-0.000978	1.16826
C	-0.479064	2.487404	-0.005845	-1.77943
O	-0.261555	3.709459	-0.017848	7.20328
N	-1.760633	1.904785	0.006702	-0.90620
C	-2.966868	2.711037	0.000208	0.95991
H	4.388419	2.025649	-0.011060	-1.10614
H	1.611053	-1.282221	-0.001401	0.21219
H	6.292876	0.446646	-0.008331	-0.67887
H	3.513035	-2.874128	0.000911	-0.64736
H	-3.588509	2.487013	-0.870743	-0.06435
H	-2.633784	3.752004	-0.030995	0.23292
H	-1.323689	-2.053024	0.553116	1.39791
H	-1.873764	-2.114041	-1.098052	1.21321
H	-3.466046	-2.915028	1.397907	0.29819
H	-3.040766	-3.931333	0.022480	1.36086
H	-5.455213	-3.167098	-0.131769	1.05843
H	-4.497656	-2.505384	-1.460490	0.54328
H	-5.399190	-1.090587	1.102182	2.28186
H	-5.794461	-0.652600	-0.546780	1.56285
H	-3.568114	2.533233	0.895556	-0.22891
H	2.129215	2.501355	-0.012826	0.01680
Center	0.150583	0.058734	0.001334	

Table S 12: Same as Table S5, but for Fig. S5**H** fluorophore.

	X (Å)	Y (Å)	Z (Å)	$q_i^{\text{Frozen-TrESP}} (\times 10^{-2} \text{ a.u.})$
C	5.157594	-1.113877	1.472759	0.75346
C	4.327070	-1.050467	0.197150	-7.39082
O	5.241299	-1.119527	-0.878339	3.33587
N	3.519208	0.155092	0.117583	9.50234
C	2.271699	-0.189134	0.033145	-0.21223
C	2.076262	-1.700871	0.027903	-4.13873
C	1.408107	-2.275930	-1.221034	1.14485
O	3.425310	-2.171094	0.144811	3.72869
C	1.159369	0.723476	-0.018496	13.57764
N	-0.097136	0.302912	0.002211	-1.08188
N	1.250326	2.114763	-0.058533	-2.13362
C	-0.057526	2.628683	-0.066842	-0.98725
O	-0.343205	3.834610	-0.104881	5.81825
C	-0.893295	1.423264	-0.022321	-3.66439
C	2.425532	2.964799	-0.097686	2.19847
C	-2.294118	1.485718	-0.007047	2.41899
C	-3.275079	0.486292	0.041791	-1.61071
C	-3.000075	-0.926712	0.098316	-5.19353
C	-4.662509	0.871860	0.036335	-3.05389
C	-4.005506	-1.852003	0.140427	-2.96220
C	-5.679445	-0.040678	0.077997	-1.81075
C	-5.419547	-1.477116	0.131929	-2.23685
O	-6.340086	-2.327619	0.169258	-9.42922
H	5.842946	-0.263604	1.511707	0.51095
H	-1.961499	-1.239875	0.109444	-0.21279
H	-4.892265	1.936258	-0.004099	-0.96767
H	-3.786443	-2.916207	0.183764	-0.85461
H	-6.720939	0.270842	0.072292	-0.74184
H	2.057082	3.992799	-0.140690	0.10566
H	3.046233	2.823231	0.790820	-0.64049
H	1.925105	-1.938448	-2.126355	-0.13990
H	1.452913	-3.369292	-1.187323	1.23269
H	1.514145	-2.011451	0.918645	2.08225
H	0.365190	-1.956141	-1.269171	1.08255
H	4.496730	-1.087109	2.342665	0.72308
H	5.731161	-2.045016	1.483854	1.61942
H	4.745946	-0.942455	-1.690433	0.34889
H	-2.660975	2.511955	-0.040106	-0.16667
H	3.040146	2.750366	-0.976586	-0.55401
Center	-0.084707	0.020899	0.000150	

Table S 13: Same as Table S5, but for Fig. S5I fluorophore.

	X (Å)	Y (Å)	Z (Å)	$q_i^{\text{Frozen-TrESP}} (\times 10^{-2} \text{ a.u.})$
C	5.203193	-0.781106	1.287954	-0.62263
C	4.369798	-0.833774	0.009793	12.48476
O	5.283424	-0.696358	-1.057782	-4.38678
N	3.374279	0.203807	-0.016616	-11.55355
C	2.139957	-0.184330	-0.008501	2.40993
C	1.020258	0.726211	-0.013115	-13.72644
C	1.828760	-1.678237	0.017659	0.09132
S	3.447160	-2.501927	-0.144802	-6.79624
N	-0.229795	0.287419	-0.010040	2.11207
C	-1.042381	1.395019	-0.009362	2.16568
C	-0.224689	2.613519	-0.013220	1.95928
O	-0.528416	3.815571	-0.015294	-5.71677
C	-2.444501	1.435227	-0.004472	-1.28930
C	-3.408483	0.418900	0.003319	1.53930
C	-3.109719	-0.990683	0.009391	4.80638
C	-4.802244	0.781881	0.006453	2.92351
C	-4.100048	-1.932848	0.017422	3.29360
C	-5.803947	-0.147939	0.014324	1.99486
C	-5.520158	-1.581000	0.020264	1.89929
O	-6.426606	-2.447065	0.027475	9.42250
N	1.091297	2.119444	-0.014331	1.68953
C	2.250462	2.992012	-0.018044	-2.79258
H	-2.066006	-1.286718	0.007693	0.10384
H	-5.049270	1.843168	0.002220	0.95934
H	-3.863852	-2.994253	0.022114	0.82502
H	-6.850469	0.146266	0.016488	0.74938
H	1.861934	4.013553	-0.020525	0.01440
H	2.871808	2.828981	0.866721	0.87009
H	5.710817	0.187430	1.339976	-0.93479
H	4.770062	-0.664057	-1.877763	-0.20962
H	1.335979	-1.946977	0.956108	-1.31175
H	-2.827798	2.455949	-0.006635	-0.09876
H	2.870828	2.823933	-0.902437	0.92352
H	5.950853	-1.579280	1.280485	-2.00337
H	4.560812	-0.900326	2.162879	-0.74849
H	1.154516	-1.945825	-0.797958	-1.04651
Center	-0.062318	-0.017243	-0.018033	

Table S 14: Same as Table S5, but for Fig. S5J fluorophore.

	X (Å)	Y (Å)	Z (Å)	$q_i^{\text{Frozen-TrESP}} (\times 10^{-2} \text{ a.u.})$
C	5.943355	-1.007438	0.892074	0.77462
C	4.777944	-1.288639	-0.046257	-4.17817
O	4.858566	-2.157385	-0.918309	6.14074
N	3.720474	-0.416874	0.118059	9.61740
C	2.463351	-0.765382	-0.012116	-1.95989
C	1.991852	-2.200497	-0.107399	3.44584
C	1.447901	0.258388	-0.030307	11.43052
N	0.147157	-0.026817	-0.021041	-1.63298
N	1.671207	1.640512	-0.049056	-0.75746
C	0.423479	2.278541	-0.058809	-2.51659
O	0.249493	3.505329	-0.083285	4.00863
C	-0.528648	1.159274	-0.035816	-3.92652
C	2.912470	2.391866	-0.104868	2.69772
C	-1.919327	1.364268	-0.023917	1.85801
C	-2.992740	0.468270	0.003891	-2.34929
C	-2.858356	-0.967393	0.024233	-4.57291
C	-4.335731	0.992179	0.016802	-2.06886
C	-3.950483	-1.787159	0.056383	-3.26453
C	-5.437420	0.185813	0.049019	-3.10586
C	-5.320251	-1.271022	0.072469	-1.02610
O	-6.320255	-2.024676	0.103983	-8.97684
H	6.383191	-0.033421	0.648742	0.89989
H	-4.456948	2.074802	0.000682	-1.03509
H	-1.855507	-1.380699	0.012741	-0.02317
H	-6.443086	0.598229	0.059100	-0.53198
H	-3.840180	-2.868695	0.071312	-0.89247
H	3.519587	2.221207	0.787294	-1.17001
H	2.626127	3.444807	-0.170524	0.17857
H	0.935142	-2.271660	0.147450	0.70262
H	2.588352	-2.844226	0.545175	0.40706
H	5.598686	-0.952012	1.930591	1.30394
H	6.701932	-1.785485	0.785866	1.26154
H	3.505189	2.109163	-0.978869	-1.27595
H	2.138700	-2.565100	-1.129198	0.31133
H	-2.179865	2.422785	-0.037497	0.22625
Center	-0.100299	0.012126	-0.017608	

Table S 15: Same as Table S5, but for Fig. S5**K** fluorophore.

	X (Å)	Y (Å)	Z (Å)	$q_i^{\text{Frozen-TrESP}}$ ($\times 10^{-2}$ a.u.)
C	-2.364126	3.046962	0.000000	0.89132
C	-3.098679	1.716615	0.000000	0.31604
C	-2.291781	0.502608	0.000000	-17.21137
N	-0.964595	0.504845	0.000000	3.67091
O	5.788889	1.047264	0.000000	9.54055
C	2.177097	0.766455	0.000000	3.36302
C	3.422814	1.329102	0.000000	3.78767
C	4.647357	0.528546	0.000000	1.69683
C	4.442941	-0.917927	0.000000	2.70933
C	3.190634	-1.465343	0.000000	1.53779
C	1.994449	-0.663012	0.000000	4.13416
C	0.749720	-1.304981	0.000000	-3.25095
C	-0.562172	-0.805956	0.000000	2.43713
C	-1.735442	-1.690579	0.000000	-1.12372
O	-1.837753	-2.926545	0.000000	-5.51459
N	-2.812827	-0.792974	0.000000	5.57174
C	-4.196118	-1.232947	0.000000	-2.32760
H	1.288933	1.389405	0.000000	0.51187
H	3.073873	-2.548720	0.000000	1.20687
H	3.549938	2.409036	0.000000	0.70036
H	5.334003	-1.540659	0.000000	0.52838
H	-4.726141	-0.869649	-0.884428	0.49872
H	-4.726141	-0.869649	0.884428	0.49872
H	-4.168977	-2.325721	0.000000	-0.52603
H	-2.675674	3.617537	-0.882134	-1.77647
H	-2.675674	3.617537	0.882134	-1.77647
H	-1.281341	2.923497	0.000000	-1.98654
H	0.775733	-2.395084	0.000000	0.40516
O	-4.338423	1.686112	0.000000	-8.51284
Center	0.086682	-0.046456	0.000000	

Table S 16: Same as Table S5, but for Fig. S5L fluorophore.

	X (Å)	Y (Å)	Z (Å)	$q_i^{\text{Frozen-TrESP}} (\times 10^{-2} \text{ a.u.})$
N	4.551912	1.201880	0.000000	10.52993
C	3.653852	-1.108736	0.000000	-1.90868
C	3.527300	0.406490	0.000000	-2.75373
C	2.172179	0.944113	0.000000	15.70880
N	1.100371	0.167833	0.000000	-2.97731
O	-4.060770	-4.234463	0.000000	-9.62602
C	-1.298152	-1.885880	0.000000	-6.51185
C	-1.978729	-3.073237	0.000000	-1.36568
C	-3.438692	-3.143479	0.000000	-3.33244
C	-4.118004	-1.851770	0.000000	-1.07908
C	-3.422680	-0.673021	0.000000	-2.68489
C	-1.985345	-0.621478	0.000000	-1.68909
C	-1.350513	0.631521	0.000000	3.35919
C	0.000000	0.996584	0.000000	-2.74355
C	0.434798	2.396324	0.000000	0.63968
O	-0.200281	3.462187	0.000000	6.27964
N	1.837341	2.299587	0.000000	-3.04984
C	2.688494	3.475733	0.000000	0.31970
H	-0.213322	-1.871544	0.000000	0.06406
H	-3.964085	0.272876	0.000000	-1.28860
H	-1.447653	-4.022377	0.000000	-1.15735
H	-5.205176	-1.867227	0.000000	-0.81499
H	3.332046	3.497765	-0.883020	-0.31534
H	3.332046	3.497765	0.883020	-0.31534
H	2.014452	4.336418	0.000000	0.88592
H	5.413701	0.649444	0.000000	1.08477
H	4.213364	-1.432275	-0.885934	1.64752
H	4.213364	-1.432275	0.885934	1.64752
H	2.677454	-1.592770	0.000000	2.18674
H	-2.012202	1.498327	0.000000	-0.73970
Center	-0.095329	-0.011763	0.000000	

Table S 17: Same as Table S5, but for Fig. S5M fluorophore.

	X (Å)	Y (Å)	Z (Å)	$q_i^{\text{Frozen-TrESP}} (\times 10^{-2} \text{ a.u.})$
C	1.212453	1.084650	0.000000	10.82593
N	0.000000	0.563604	0.000000	-5.98267
C	-0.893581	1.617588	0.000000	0.25424
C	-0.166431	2.890857	0.000000	-4.31863
O	-0.541603	4.074063	0.000000	4.30605
N	1.179211	2.484920	0.000000	2.72569
C	2.281931	3.416052	0.000000	0.79872
C	2.449446	0.348418	0.000000	-9.46762
C	-2.290678	1.563204	0.000000	-1.21344
C	-3.187339	0.481174	0.000000	1.32403
C	-2.796623	-0.903621	0.000000	-6.36600
C	-4.600186	0.749890	0.000000	-3.50247
C	-3.723921	-1.910547	0.000000	-2.54328
C	-5.539453	-0.245438	0.000000	-2.32186
C	-5.163051	-1.655458	0.000000	-0.85471
O	-6.012084	-2.580971	0.000000	-8.47426
C	2.545592	-1.009919	0.000000	19.50907
C	3.764443	-1.775246	0.000000	-6.23472
N	5.049350	-1.244762	0.000000	-2.01592
C	3.977675	-3.149535	0.000000	6.49191
N	5.319986	-3.452141	0.000000	0.04624
C	5.937506	-2.287889	0.000000	7.39213
H	-4.918591	1.792301	0.000000	-0.65331
H	-1.735347	-1.129555	0.000000	0.75390
H	-6.603059	-0.019764	0.000000	-0.60959
H	-3.416354	-2.953723	0.000000	-1.05969
H	1.844314	4.418154	0.000000	-0.26646
H	2.910284	3.303106	-0.892912	-0.26805
H	2.910284	3.303106	0.892912	-0.26805
H	1.625058	-1.587001	0.000000	-1.46078
H	5.282983	-0.264112	0.000000	1.27961
H	3.223184	-3.923998	0.000000	0.90244
H	7.008551	-2.137654	0.000000	0.50230
H	-2.743922	2.554869	0.000000	0.10583
H	3.355571	0.953107	0.000000	0.66343
Center	-0.055484	-0.027645	0.000000	

Table S 18: Same as Table S5, but for Fig. S5N fluorophore.

	X (Å)	Y (Å)	Z (Å)	$q_i^{\text{Frozen-TrESP}} (\times 10^{-2} \text{ a.u.})$
C	0.350029	1.587363	0.017707	-10.29003
N	-0.722758	0.792436	0.011331	0.68927
C	-1.816253	1.604269	-0.019463	8.45866
C	-1.397863	3.017419	-0.027596	0.46050
O	-2.055897	4.065670	-0.047076	-3.16227
N	-0.000494	2.938177	-0.007485	0.43489
C	0.857513	4.110483	-0.000908	-0.98318
C	-3.174637	1.232372	-0.044602	-6.45023
C	-3.793895	-0.018504	-0.053356	6.40044
C	-3.089951	-1.278651	-0.045442	1.55297
C	-5.235539	-0.081424	-0.072214	0.38322
C	-3.756706	-2.469254	-0.052228	3.83641
C	-5.916658	-1.263543	-0.078679	3.13202
C	-5.219430	-2.549498	-0.068061	1.30386
O	-5.828411	-3.641989	-0.072963	8.78675
C	1.671915	1.065662	0.020576	-3.00314
N	2.776842	1.773054	-0.054439	-7.99929
C	1.964372	-0.426748	0.093833	3.63427
C	3.848080	0.872711	-0.081094	1.79083
H	-5.782713	0.860389	-0.080106	1.49810
H	-2.005732	-1.251390	-0.036403	1.36106
H	-7.002959	-1.293936	-0.092105	0.67176
H	-3.220101	-3.414651	-0.047350	0.93211
H	0.192368	4.977066	-0.013958	-0.55686
H	1.486078	4.132320	0.893310	0.60849
H	1.513060	4.122641	-0.874884	0.73323
H	-3.837657	2.097439	-0.059765	0.46081
O	3.397254	-0.438168	-0.023621	-2.92104
O	5.029241	1.131499	-0.152604	-5.41118
C	1.538021	-1.114805	1.389146	-0.33720
H	1.904751	-2.145866	1.397396	-1.60309
H	1.955568	-0.589750	2.254420	-0.04919
H	0.448489	-1.114785	1.462996	-1.78354
H	1.544014	-0.950312	-0.772163	-2.57939
Center	-1.607268	0.962736	0.065597	

Table S 19: Same as Table S5, but for Fig. S5O fluorophore.

	X (Å)	Y (Å)	Z (Å)	$q_i^{\text{Frozen-TrESP}} (\times 10^{-2} \text{ a.u.})$
C	4.116043	0.997155	0.700636	-0.65297
C	3.239467	0.034938	-0.074408	-3.82110
O	3.704076	-0.790548	-0.857280	6.54181
N	1.874793	0.247587	0.111905	10.74081
C	1.002674	-0.723353	0.092357	2.56452
C	1.355558	-2.202511	0.104700	-0.56866
C	-0.389203	-0.378963	0.076807	9.76601
N	-1.403803	-1.290708	0.061414	-9.80553
N	-0.997488	0.848844	0.049930	3.54954
C	-2.415198	0.712828	0.015436	-5.91572
O	-3.217328	1.654409	-0.009105	-6.65199
C	-2.628574	-0.706485	0.019848	-12.52255
C	-0.372829	2.166350	0.053157	6.60561
C	-3.925046	-1.432724	-0.015981	5.38871
H	3.963576	2.014769	0.323926	1.19776
H	0.240715	2.298611	0.945629	-2.50762
H	-1.194195	2.884910	0.040534	-0.50282
H	0.652500	-2.787090	0.707384	1.75780
H	2.354637	-2.352849	0.512216	0.06292
H	3.840605	1.004487	1.760795	1.78053
H	5.164497	0.719572	0.583743	1.55170
H	0.260449	2.294116	-0.826472	-2.87178
H	1.373023	-2.602352	-0.914903	0.99410
H	-4.027270	-2.063668	-0.908901	-4.30559
H	-4.072930	-2.070067	0.865789	-4.21147
H	-4.726727	-0.690495	-0.034469	-0.68182
H	-1.245218	-2.288064	0.054374	2.51779
Center	0.027232	-0.106185	0.039451	