**Supporting Information**

**for**

# Excited State Electron Transfer from Donor-π System-Acceptor Dyes to ZnO Nanocrystals

Rachel Swedin,[a] Deepak Badgurjar,[a] Andrew Healy,[a] Robin Harkins,[a] Amanda Oehrlein,[a] Lindsey Greenlund,[a] Mohammed Alshebber,[a] Nathan Ripp,[a] Nathaniel T. Anderson,[b] Benjamin R. Honzay,[b] Ted M. Pappenfus,[b] Daron E. Janzen,[c] David A. Blank,[a] and Wayne L. Gladfelter[a]

[a] Department of Chemistry, University of Minnesota-Twin Cities, Minneapolis, Minnesota 55455, United States

[b] Division of Science and Mathematics, University of Minnesota, Morris, Minnesota 56267, United States

[c] Department of Chemistry and Biochemistry, St. Catherine University, St. Paul, Minnesota 55105, United States

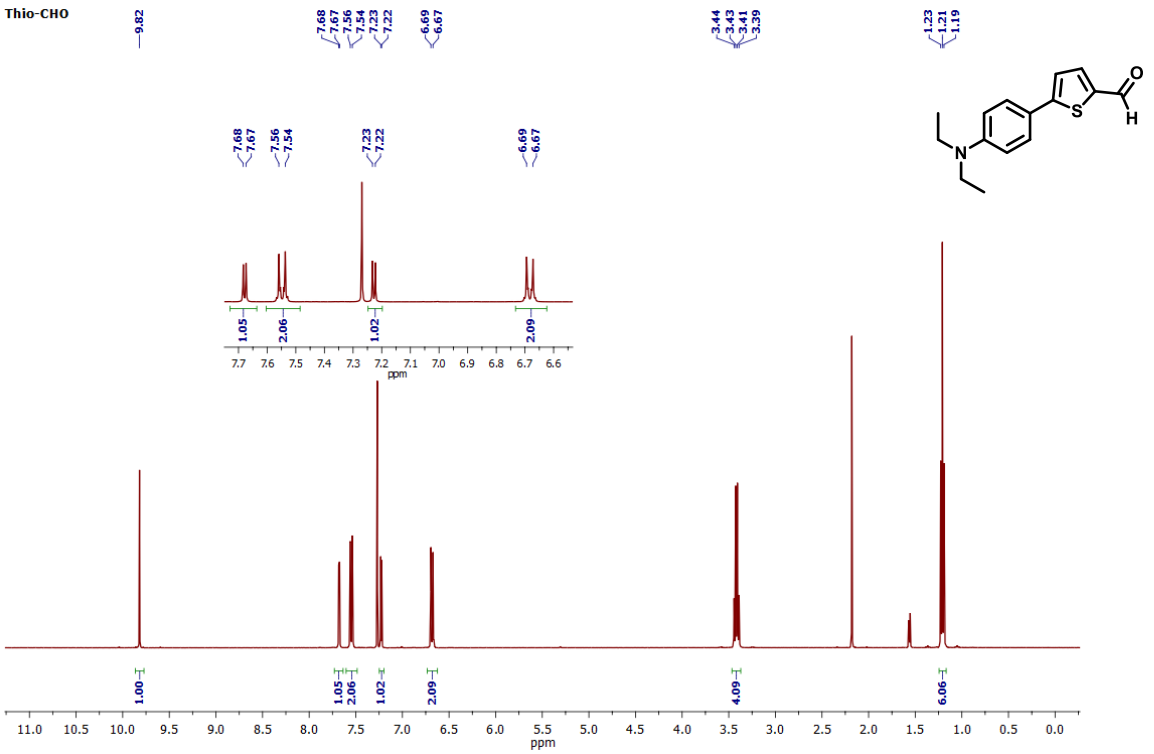


**Figure S1.** $^{1}$H NMR spectrum of 5-(4-(diethylamino)phenyl)thiophene-2-carbaldehyde **(3)** in $CDCl_3$.

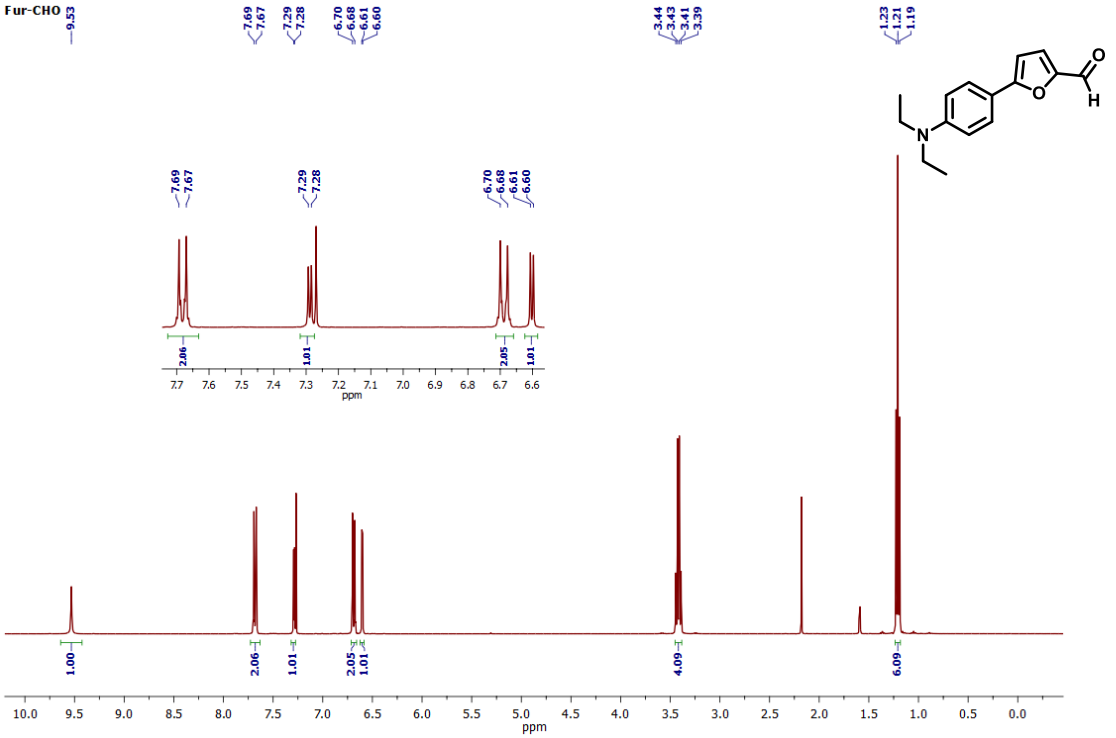


**Figure S2** $^{1}$H NMR spectrum of 5-(4-(diethylamino)phenyl)furan-2-carbaldehyde **(4)** in $CDCl_3$.

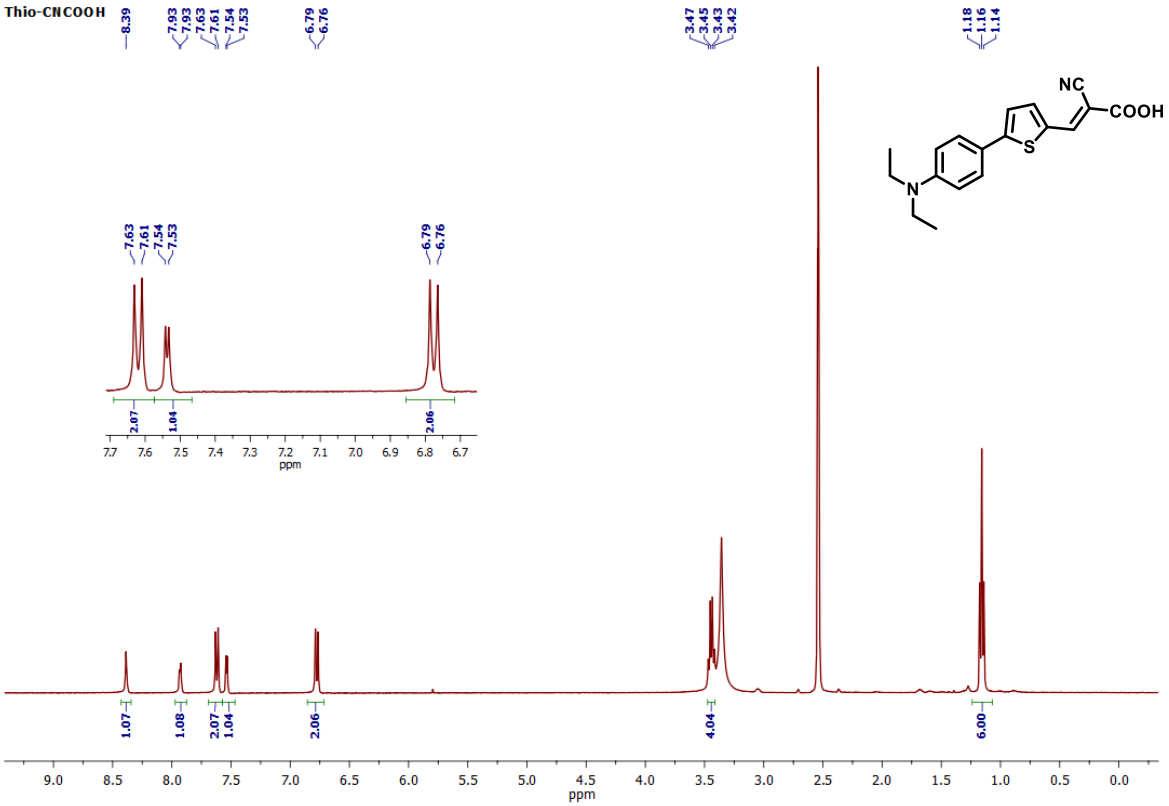


**Figure S3** $^{1}$H NMR spectrum of (*E*)-2-cyano-3-(5-(4-(diethylamino)phenyl)thiophen-2-yl)acrylic acid **(1)** in *d*6-DMSO.

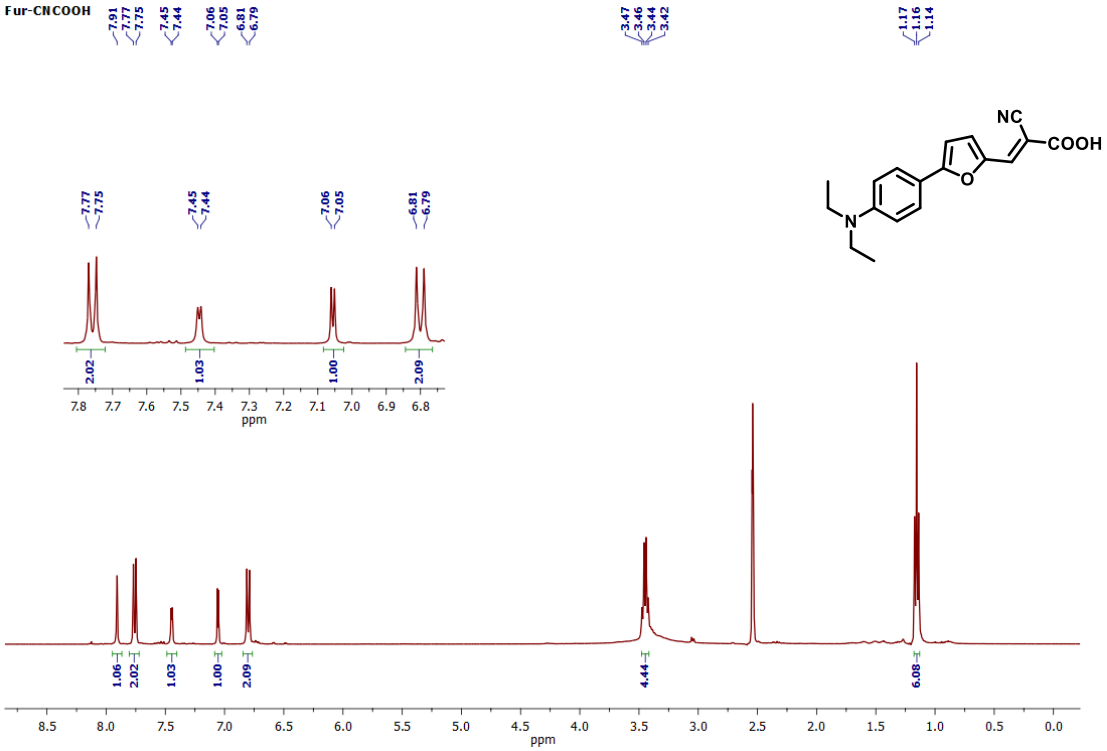


**Figure S4** $^{1}$H NMR spectrum of (*E*)-2-cyano-3-(5-(4-(diethylamino)phenyl)furan-2-yl)acrylic acid **(2)** in *d*6-DMSO.

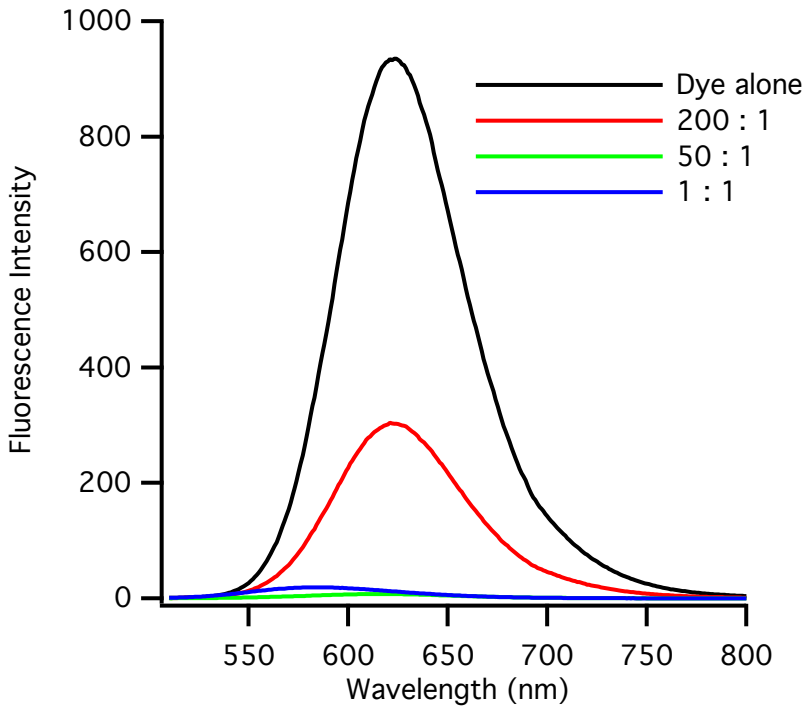


**Figure S5**. Fluorescence quenching of **1** by ZnO NCs. The ratios shown in the figure indicate molar ratios of dyes to ZnO NC.

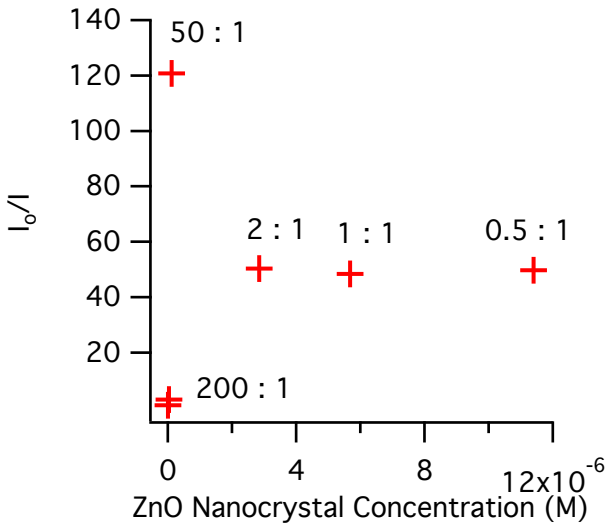


**Figure S6.** Stern Volmer graph for compound **1**. The ratios indicate the dye to ZnO NC values.

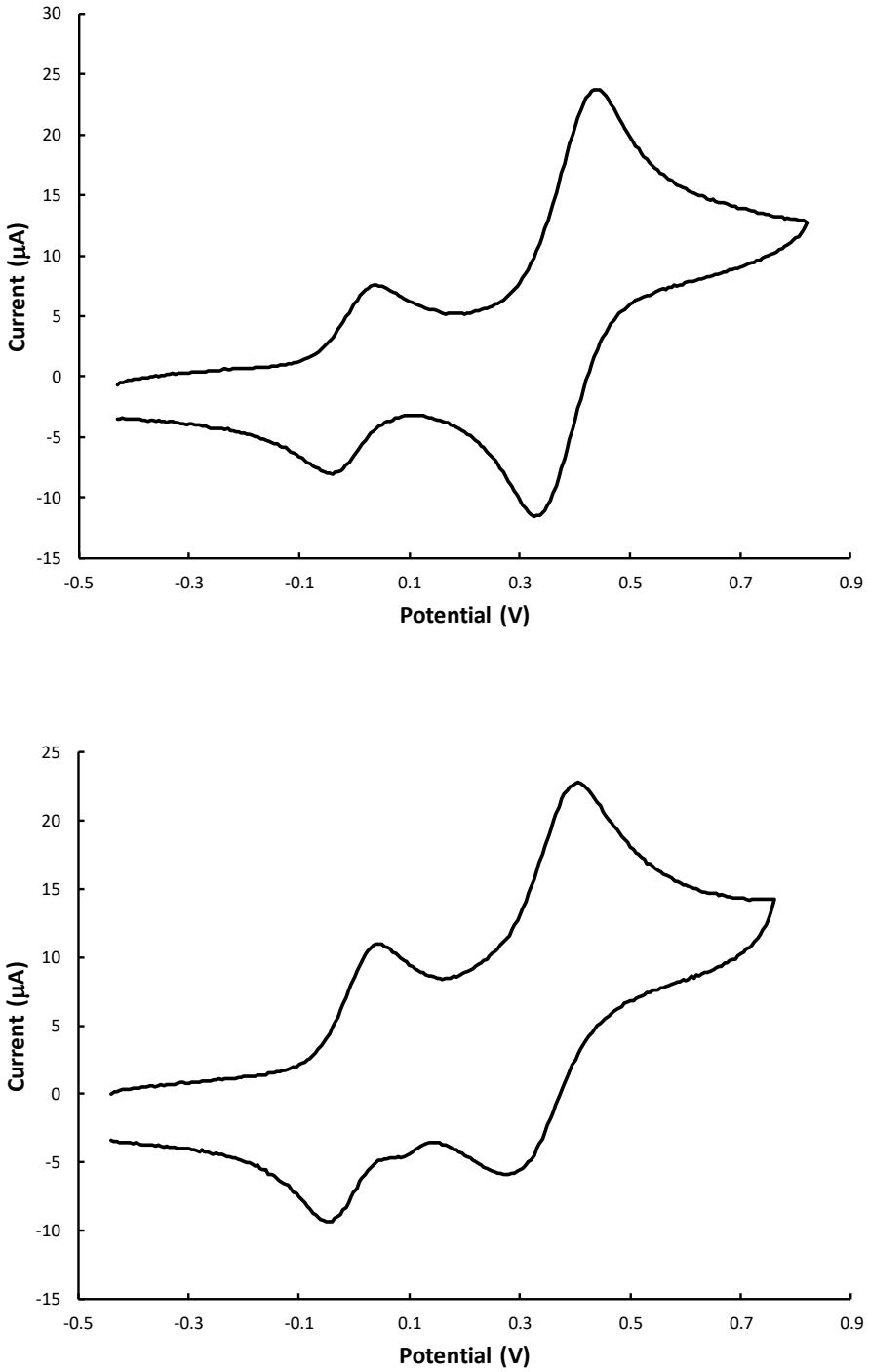


**Figure S7.** Cyclic voltammograms of for **1** (top) and **2** (bottom) with ferrocene as an internal standard (0 V). Experiments conducted in 0.1 M $TBAPF_6/CH_2Cl_2$ solutions at a carbon electrode ($\nu$ = 100 mV/s).

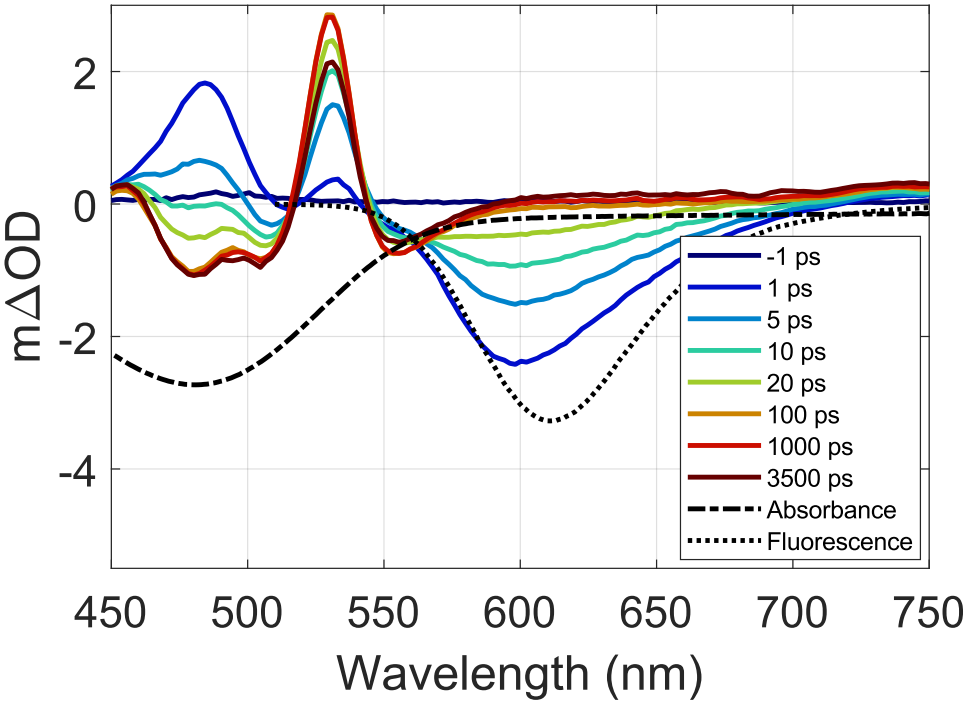


**Figure S8.** Pump-probe spectra of furan dye in a 1 to 1 concentration ratio with 3.4 nm ZnO nanocrystals in dichloromethane pumped at 500 nm with 100 µW of power. Associated fit is found in **Table 2**.

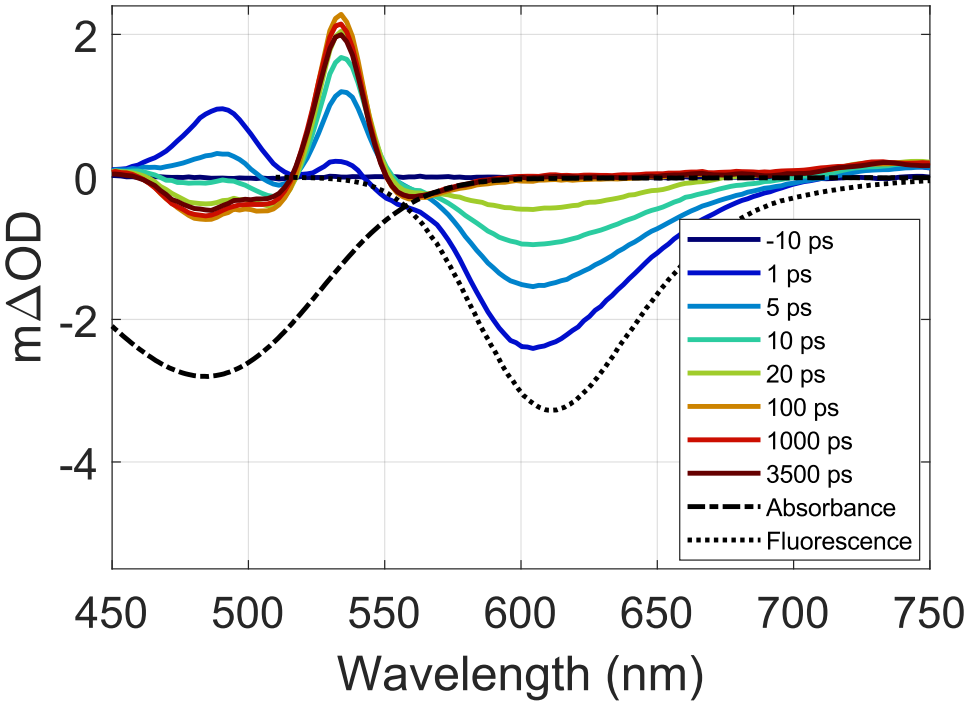


**Figure S9.** Pump-probe spectra of furan dye in a 1 to 1 concentration ratio with 4.7 nm ZnO nanocrystals in dichloromethane pumped at 500 nm with 100 µW of power. Associated fit is found in **Table 2**.

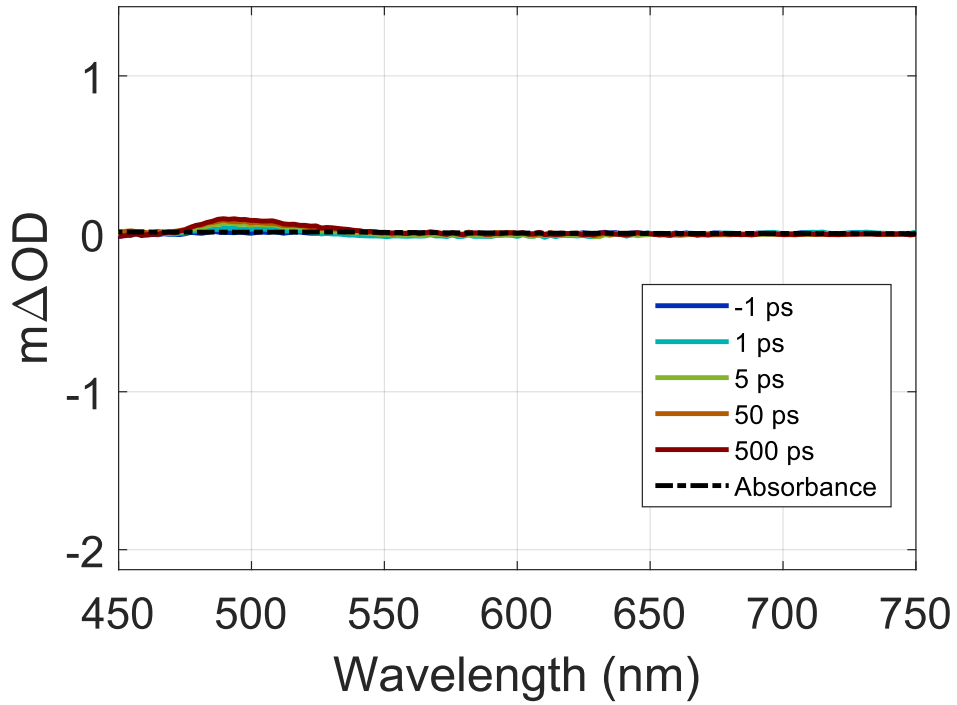


**Figure S10.** Pump-probe spectra of 5.2 nm ZnO nanocrystals pumped at 500 nm with 100 µW of power in dichloromethane.

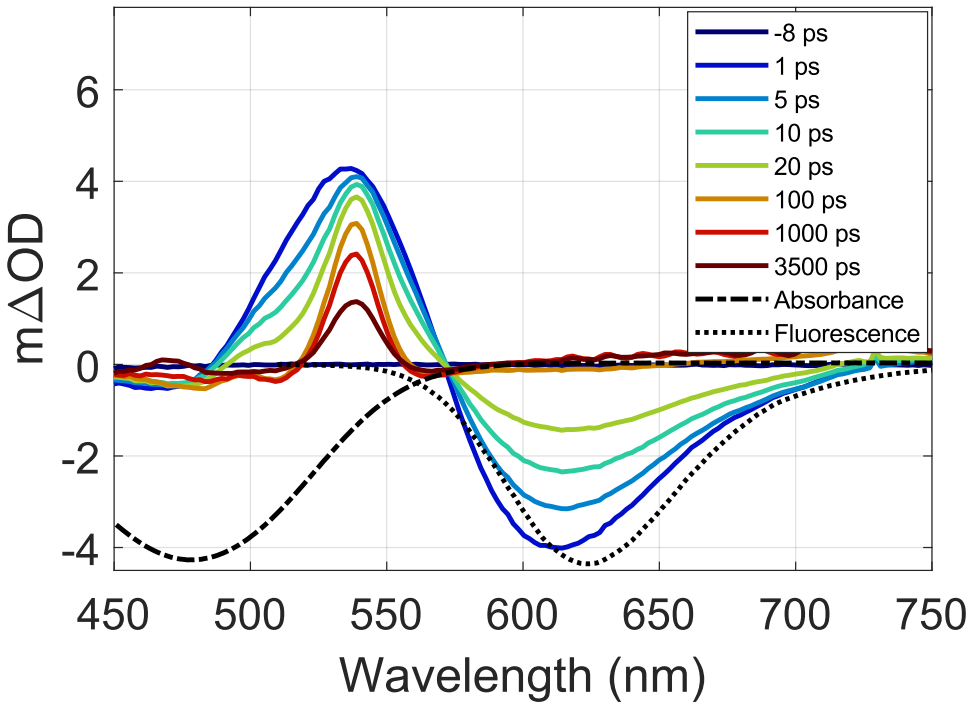


**Figure S11.** Pump-probe spectra of thiophene dye in a 1 to 1 concentration ratio with 3.15 nm ZnO nanocrystals in dichloromethane pumped at 500 nm with 100 µW of power. Associated fit is found in **Table 2**.

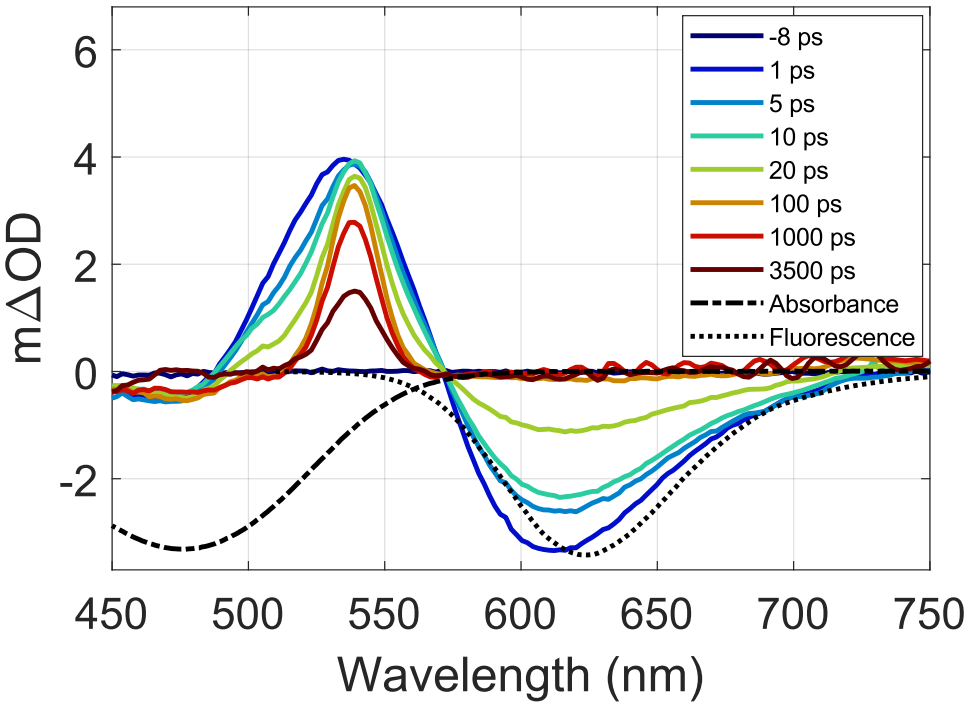


**Figure S12.** Pump-probe spectra of thiophene dye in a 1 to 1 concentration ratio with 4.0 nm ZnO nanocrystals in dichloromethane pumped at 500 nm with 100 μW of power. Associated fit is found in **Table 2**.

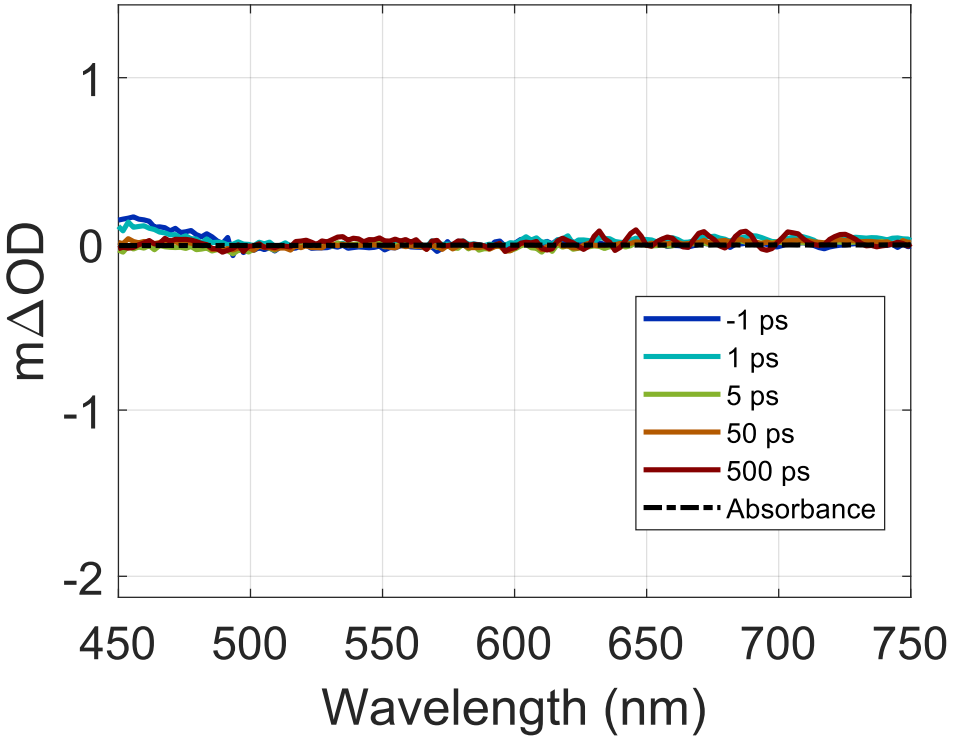


**Figure S13.** Pump-probe spectra of 3.15 nm ZnO nanocrystals pumped at 500 nm with 100 μW of power in dichloromethane.

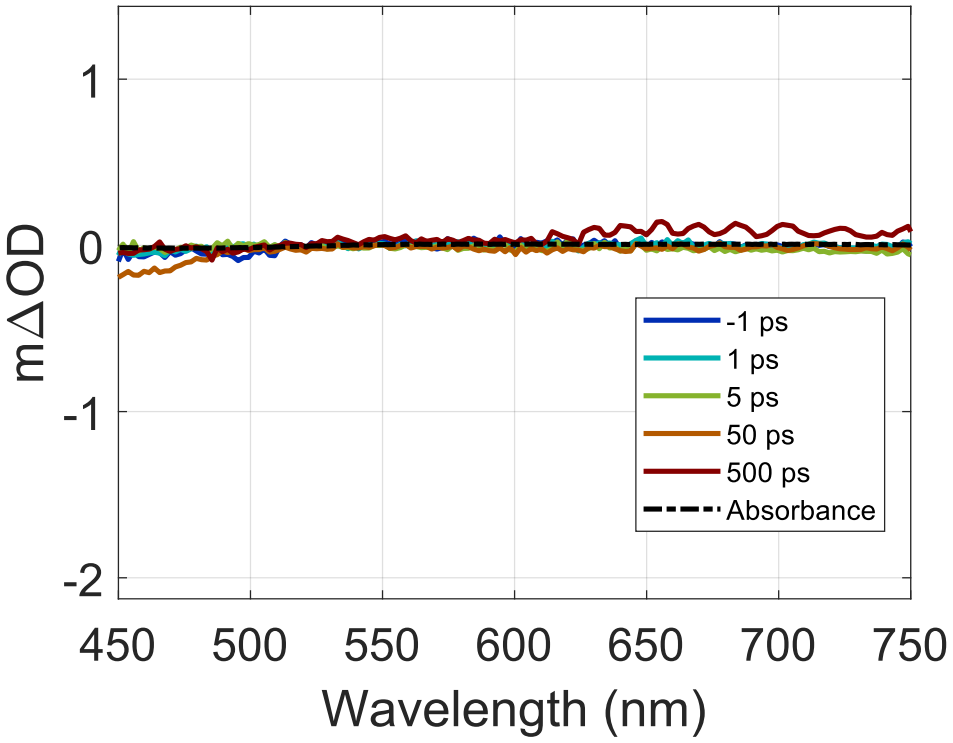


**Figure S14.** Pump-probe spectra of 4.0 nm ZnO nanocrystals pumped at 500 nm with 100 μW of power in dichloromethane.

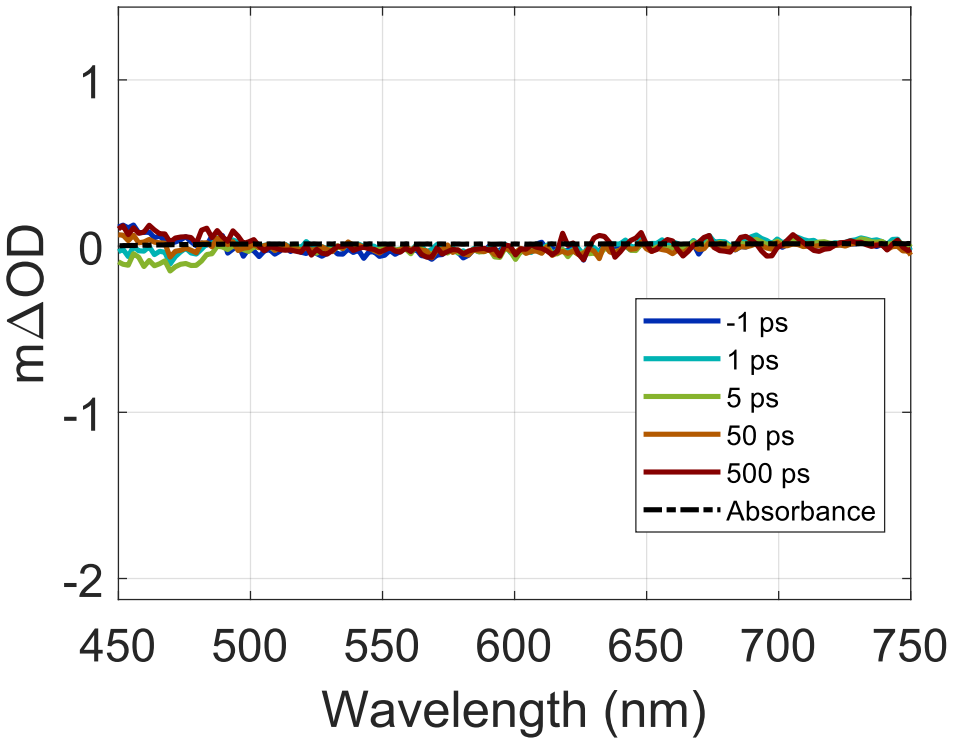


**Figure S15.** Pump-probe spectra of 5.0 nm ZnO nanocrystals pumped at 500 nm with 100 μW of power in dichloromethane.

**Table S1.** Computational details and Cartesian coordinates for calculated geometry of molecule **1**

# opt=tight freq b3lyp/6-31g(d,p) geom=connectivity int=ultrafine
Imaginary frequencies=0; Total energy= -1354.91057435

| Center # | Atomic # | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.851428 | 0.942801 | -0.551273 |
| 2 | 6 | 0 | -1.506599 | 0.616681 | -0.510859 |
| 3 | 6 | 0 | -1.061421 | -0.687102 | -0.219432 |
| 4 | 6 | 0 | -2.057730 | -1.649120 | 0.037727 |
| 5 | 6 | 0 | -3.406471 | -1.338804 | -0.000859 |
| 6 | 6 | 0 | -3.856238 | -0.029293 | -0.311418 |
| 7 | 1 | 0 | -3.119682 | 1.965633 | -0.780364 |
| 8 | 1 | 0 | -0.782788 | 1.397377 | -0.726985 |
| 9 | 1 | 0 | -1.770890 | -2.662056 | 0.302233 |
| 10 | 1 | 0 | -4.115973 | -2.123262 | 0.227555 |
| 11 | 7 | 0 | -5.201216 | 0.279332 | -0.391657 |
| 12 | 6 | 0 | -6.223794 | -0.733137 | -0.129881 |
| 13 | 6 | 0 | -6.524596 | -0.983759 | 1.354440 |
| 14 | 1 | 0 | -5.929570 | -1.669530 | -0.616676 |
| 15 | 1 | 0 | -7.137839 | -0.408340 | -0.636416 |
| 16 | 1 | 0 | -7.271655 | -1.777951 | 1.459171 |
| 17 | 1 | 0 | -5.625737 | -1.287728 | 1.897845 |
| 18 | 1 | 0 | -6.918772 | -0.083889 | 1.835074 |
| 19 | 6 | 0 | -5.645486 | 1.649738 | -0.649135 |
| 20 | 6 | 0 | -5.609301 | 2.583060 | 0.568814 |
| 21 | 1 | 0 | -6.668656 | 1.589801 | -1.031931 |
| 22 | 1 | 0 | -5.046507 | 2.072664 | -1.463565 |
| 23 | 1 | 0 | -5.923581 | 3.591616 | 0.279697 |
| 24 | 1 | 0 | -6.282065 | 2.231584 | 1.356227 |
| 25 | 1 | 0 | -4.603156 | 2.649017 | 0.991490 |
| 26 | 6 | 0 | 0.351199 | -1.035497 | -0.173475 |
| 27 | 6 | 0 | 0.925674 | -2.301385 | -0.228143 |
| 28 | 6 | 0 | 2.325589 | -2.281338 | -0.163081 |
| 29 | 1 | 0 | 0.345268 | -3.208532 | -0.342107 |
| 30 | 6 | 0 | 2.874564 | -1.005014 | -0.058225 |
| 31 | 1 | 0 | 2.946566 | -3.170019 | -0.203918 |
| 32 | 6 | 0 | 4.271364 | -0.748693 | 0.011253 |
| 33 | 6 | 0 | 4.969030 | 0.429440 | 0.102458 |
| 34 | 1 | 0 | 4.883245 | -1.646307 | -0.012211 |
| 35 | 6 | 0 | 4.335936 | 1.707491 | 0.144009 |
| 36 | 7 | 0 | 3.795382 | 2.738759 | 0.176115 |
| 37 | 6 | 0 | 6.447219 | 0.454997 | 0.162840 |
| 38 | 8 | 0 | 7.120327 | 1.462038 | 0.242016 |
| 39 | 8 | 0 | 7.003000 | -0.787610 | 0.120474 |
| 40 | 1 | 0 | 7.961435 | -0.639752 | 0.166392 |
| 41 | 16 | 0 | 1.585594 | 0.194452 | -0.025449 |

**Table S2.** Computational details and Cartesian coordinates for calculated geometry of molecule **2**

# opt=tight freq b3lyp/6-31g(d,p) geom=connectivity int=ultrafine
Imaginary frequencies=0; Total energy= -1031.94038297

| Center # | Atomic # | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.680838 | 1.060684 | -0.124507 |
| 2 | 6 | 0 | 3.320592 | -0.021872 | -0.314918 |
| 3 | 7 | 0 | 4.593946 | -0.543500 | -0.442628 |
| 4 | 6 | 0 | -0.652551 | 1.606083 | -0.030662 |
| 5 | 6 | 0 | -2.859706 | 1.425507 | 0.065593 |
| 6 | 6 | 0 | -4.097383 | 0.747278 | 0.089822 |
| 7 | 1 | 0 | -4.965338 | 1.393746 | 0.164554 |
| 8 | 6 | 0 | -4.347002 | -0.603033 | 0.032395 |
| 9 | 6 | 0 | -5.726717 | -1.133212 | 0.070992 |
| 10 | 6 | 0 | -3.318351 | -1.589110 | -0.067100 |
| 11 | 7 | 0 | -2.475758 | -2.388571 | -0.148015 |
| 12 | 8 | 0 | -6.669687 | -0.153409 | 0.165915 |
| 13 | 8 | 0 | -6.022367 | -2.309941 | 0.024976 |
| 14 | 1 | 0 | -7.520287 | -0.620921 | 0.182493 |
| 15 | 6 | 0 | 4.790166 | -2.713778 | 0.841123 |
| 16 | 1 | 0 | 4.926986 | -3.790362 | 0.693629 |
| 17 | 1 | 0 | 5.591765 | -2.357204 | 1.494364 |
| 18 | 1 | 0 | 3.839998 | -2.560442 | 1.359664 |
| 19 | 6 | 0 | 4.812860 | -1.989295 | -0.511701 |
| 20 | 1 | 0 | 5.783158 | -2.145577 | -0.992749 |
| 21 | 1 | 0 | 4.070387 | -2.430084 | -1.185743 |
| 22 | 6 | 0 | 6.229788 | 0.765334 | 0.973171 |
| 23 | 1 | 0 | 5.434132 | 1.292566 | 1.506590 |
| 24 | 1 | 0 | 6.527782 | -0.094359 | 1.579972 |
| 25 | 1 | 0 | 7.090606 | 1.437961 | 0.892854 |
| 26 | 6 | 0 | 5.770557 | 0.325075 | -0.423943 |
| 27 | 1 | 0 | 5.575807 | 1.203835 | -1.048991 |
| 28 | 1 | 0 | 6.581264 | -0.218398 | -0.918507 |
| 29 | 6 | 0 | 2.171817 | -0.855440 | -0.296286 |
| 30 | 1 | 0 | 2.273011 | -1.931274 | -0.348734 |
| 31 | 6 | 0 | 0.894831 | -0.329790 | -0.209528 |
| 32 | 1 | 0 | 0.044760 | -1.004743 | -0.203371 |
| 33 | 6 | 0 | 1.814518 | 1.893969 | -0.126282 |
| 34 | 1 | 0 | 1.695012 | 2.971092 | -0.053861 |
| 35 | 6 | 0 | 3.094981 | 1.376642 | -0.212807 |
| 36 | 1 | 0 | 3.927211 | 2.067932 | -0.198901 |
| 37 | 6 | 0 | -1.159446 | 2.897468 | 0.060589 |
| 38 | 1 | 0 | -0.582228 | 3.809533 | 0.079638 |
| 39 | 6 | 0 | -2.559142 | 2.779518 | 0.121452 |
| 40 | 1 | 0 | -3.282126 | 3.579767 | 0.197428 |
| 41 | 8 | 0 | -1.683335 | 0.722009 | -0.027171 |