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Electronic Supplementary Information

Structure–Property Relationship in Contrasting Aggregation-Induced Enhancement/Quenching of Emission in Rigid Aromatic Molecules

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Table S1. Summary of photophysical properties for **1**–**6** solutions and crystals

		Φ^a	τ^b / ns	error^b / ns	$\chi^{2\,b}$	$k_r{}^c$ / ns^{-1}	$k_{nr}{}^c$ / ns^{-1}
1	in DCM	0.009	0.066	$\pm 3.1 \times 10^{-4}$	1.30	0.14	15
	in Toluene	0.008	0.073	$\pm 3.9 \times 10^{-4}$	2.35	0.11	14
	in EtOAc	0.003	0.039	$\pm 5.7 \times 10^{-4}$	2.87	0.077	26
	in MeCN	0.007	0.082	$\pm 3.6 \times 10^{-4}$	2.47	0.085	12
	Crystal	0.21	1.36	$\pm 6.4 \times 10^{-4}$	0.99	0.15	0.58
2	in DCM	0.049	0.33	$\pm 9.7 \times 10^{-4}$	6.23	0.15	2.9
	Crystal	0.12	1.53^d	$\pm 3.3 \times 10^{-2}$	1.93	0.078	0.58
3	in DCM	0.004	≤0.02	—	—	≥0.18	≥45
	Crystal	0.11	0.41^d	$\pm 4.8 \times 10^{-3}$	1.38	0.27	2.2
4	in DCM	0.32	0.86	$\pm 4.3 \times 10^{-4}$	1.03	0.37	0.79
	Crystal	0.59	1.76	$\pm 8.7 \times 10^{-3}$	1.03	0.34	0.23
5	in DCM	0.90	2.37	$\pm 2.0 \times 10^{-2}$	1.04	0.38	0.042
	Crystal	0.20	1.87	$\pm 1.7 \times 10^{-3}$	1.17	0.11	0.43
6	in DCM	0.98	2.56	$\pm 8.4 \times 10^{-3}$	0.97	0.38	0.0078
	Crystal	0.45	2.39	$\pm 6.1 \times 10^{-3}$	1.01	0.19	0.23

[a]Relative quantum yield for solutions using quinine sulfate (0.60 in 0.05 M H_2SO_4) as a standard, or absolute quantum yield for crystals measured using an integrating sphere. [b]Fluorescent lifetime τ, its error, and χ^2 obtained by a single exponential fitting of the decay curves upon excitation at 365 or 368 nm. [c]Calculated according to $k_r = \Phi / \tau$ and $k_{nr} = (1 - \Phi) / \tau$. [d]Area-weighted averaged lifetimes obtained by a biexponential fitting.

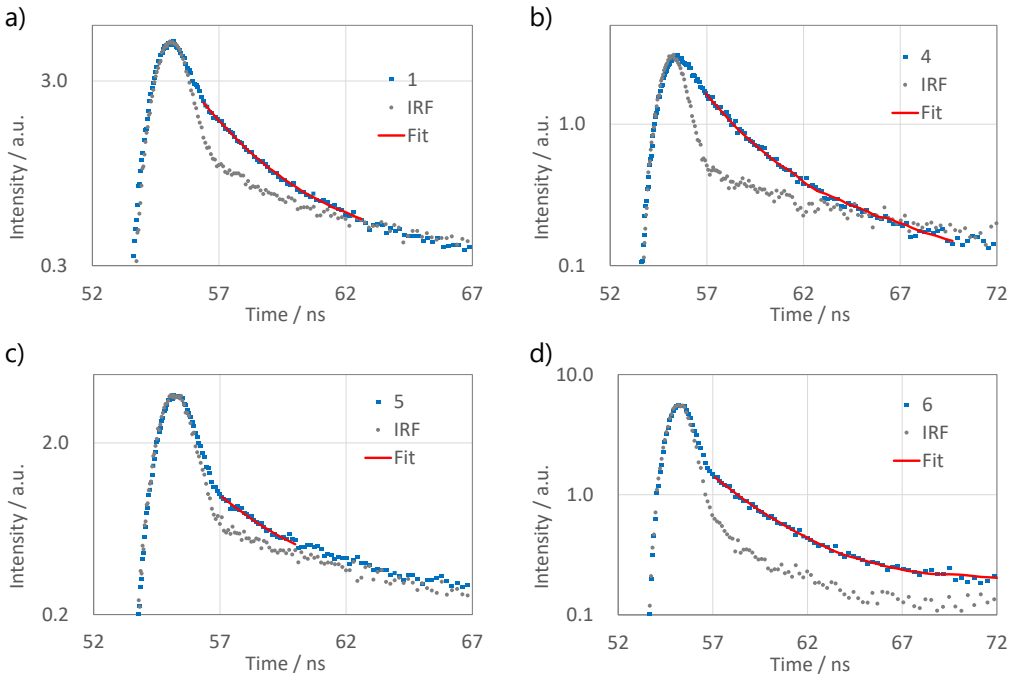

Figure S1. Fluorescence decay curves (blue dots) of **1** and **4**–**6** crystals in semi-log scale. Red lines denote the fitting curves.

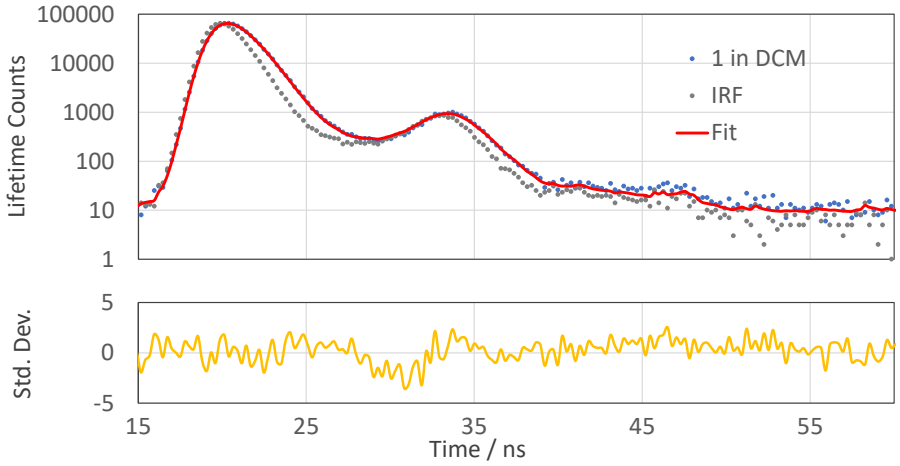

Figure S2. Top: Decay curve (blue dots) of the fluorescence intensity at 430 nm for **1** in dichloro-methane in semi-log scale. Red lines denote the fitting curves. Bottom: Residue of the fit.

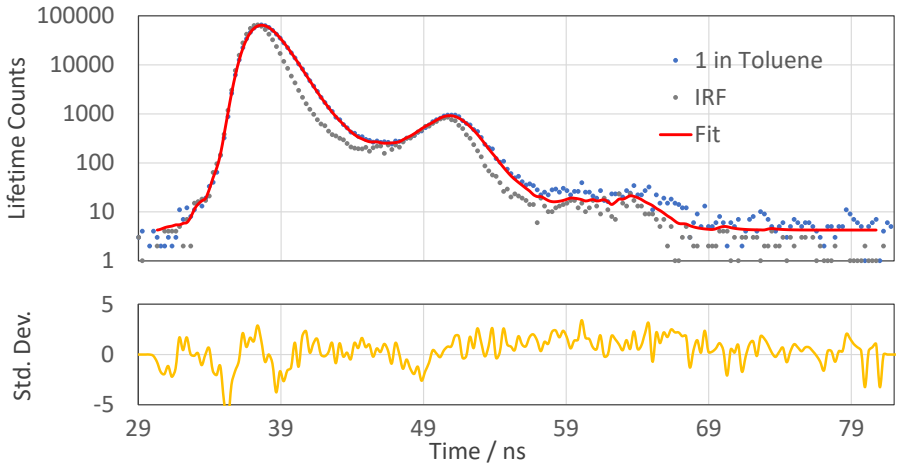

Figure S3. Top: Decay curve (blue dots) of the fluorescence intensity at 460 nm for **1** in toluene in semi-log scale. Red lines denote the fitting curves. Bottom: Residue of the fit.

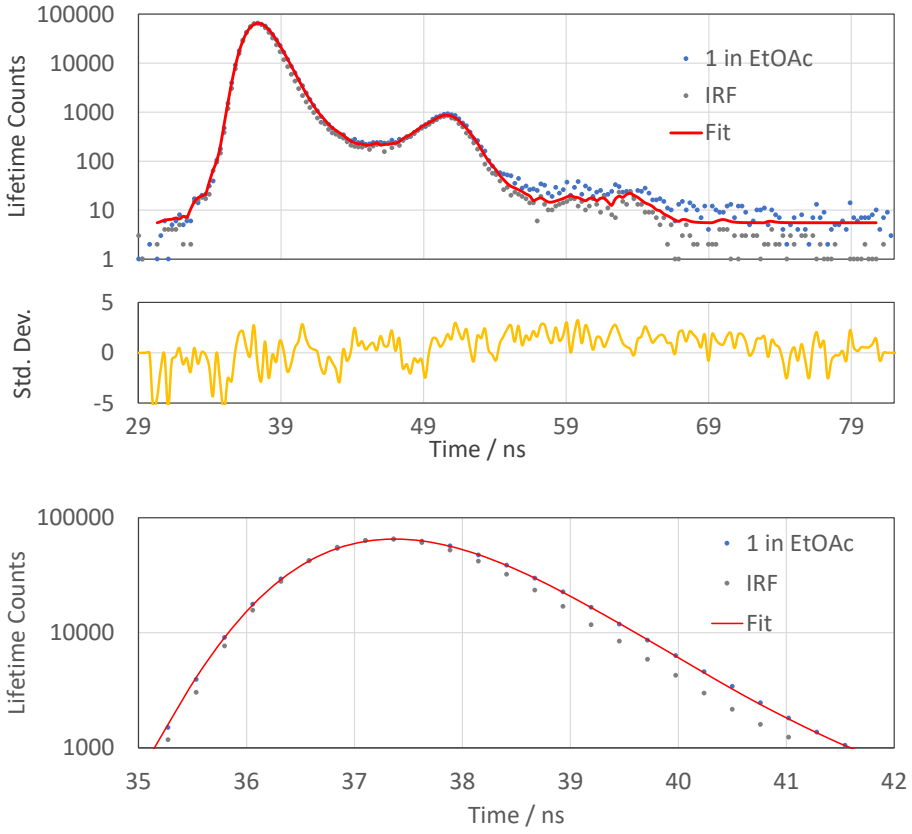

Figure S4. Top: Decay curve (blue dots) of the fluorescence intensity at 460 nm for **1** in ethyl acetate in semi-log scale. Red lines denote the fitting curves. Middle: Residue of the fit. Bottom: Enlarged graph near the peak top of the decay curve.

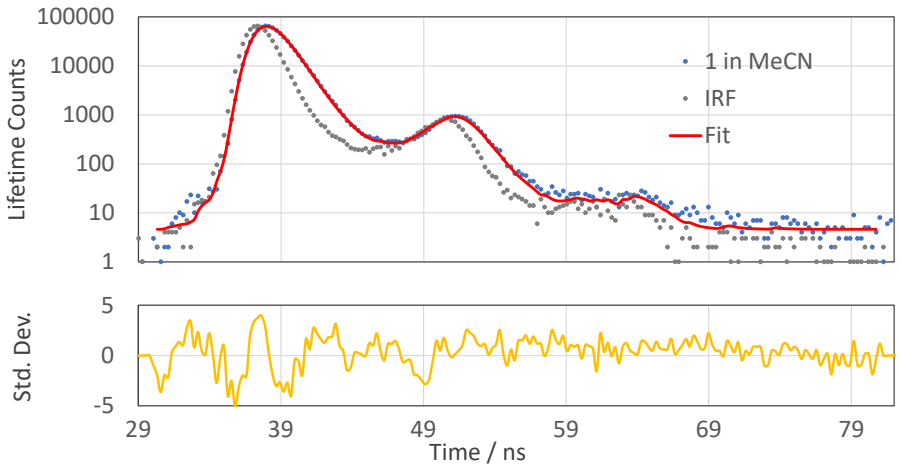

Figure S5. Top: Decay curve (blue dots) of the fluorescence intensity at 460 nm for **1** in acetonitrile in semi-log scale. Red lines denote the fitting curves. Bottom: Residue of the fit.

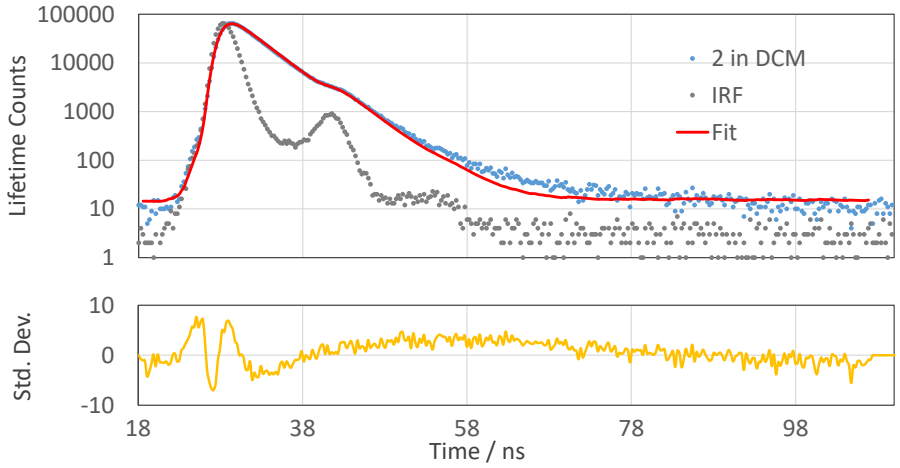

Figure S6. Top: Decay curve (blue dots) of the fluorescence intensity at 420 nm for **2** in dichloro-methane in semi-log scale. Red lines denote the fitting curves. Bottom: Residue of the fit.

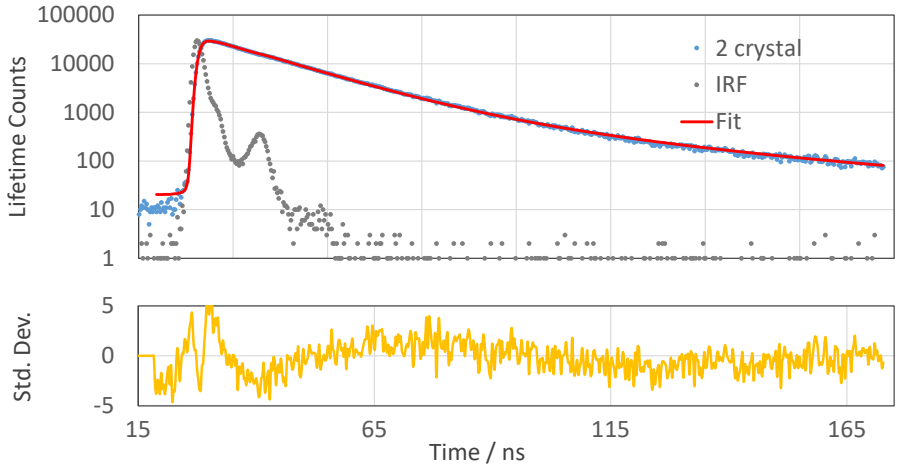

Figure S7. Top: Decay curve (blue dots) of the fluorescence intensity at 450 nm for **2** crystal in semi-log scale. Red lines denote the fitting curves. Bottom: Residue of the fit.

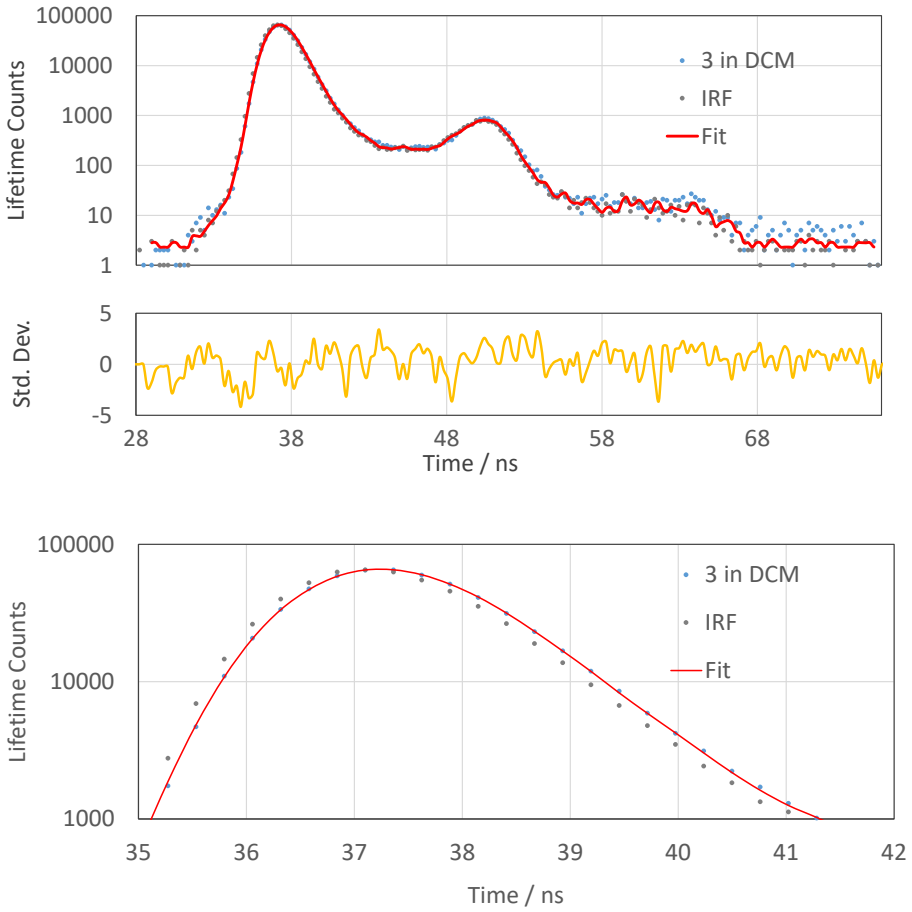

Figure S8. Top: Decay curve (blue dots) of the fluorescence intensity at 460 nm for **3** in dichloro-methane (2×10^{-5} M) in semi-log scale. Red lines denote the fitting curves. Middle: Residue of the fit. Bottom: Enlarged graph near the peak top of the decay curve. The fit provided $\tau = 4.9 \pm 5.8$ ps.

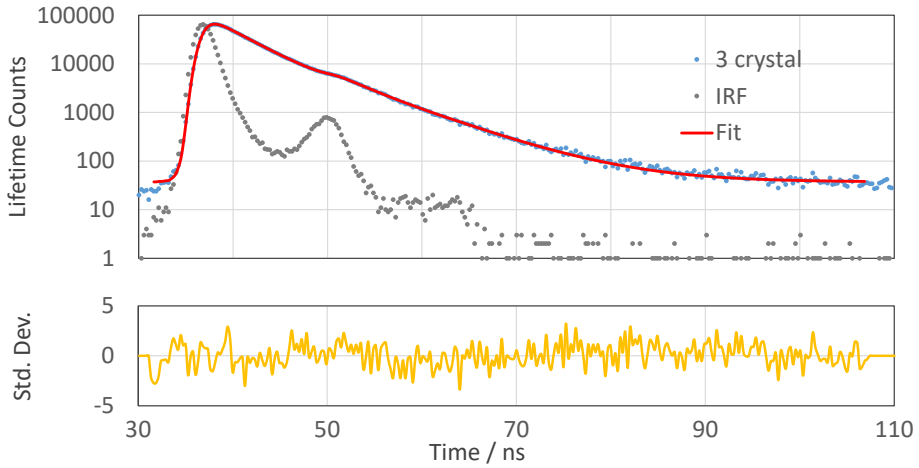

Figure S9. Top: Decay curve (blue dots) of the fluorescence intensity at 450 nm for **3** crystal in semi-log scale. Red lines denote the fitting curves. Bottom: Residue of the fit.

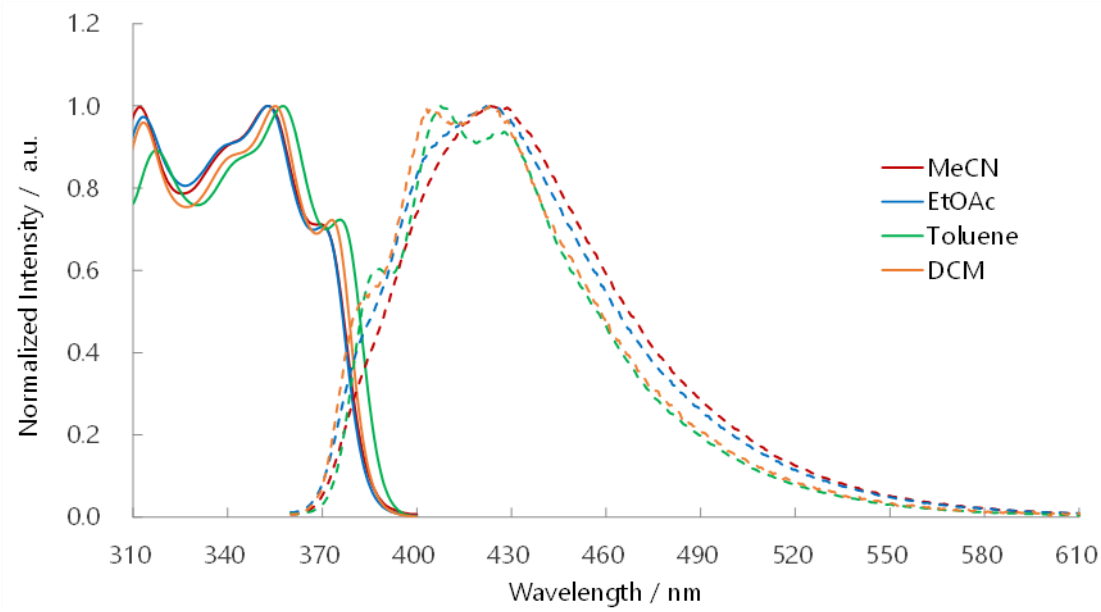

Figure S10. Normalized absorption (solid lines) and fluorescence (broken lines) spectra of **1** in acetonitrile (red), ethyl acetate (blue), toluene (green) and dichloromethane (orange).