Supplementary Materials: Power Conversion Efficiency of Arylamine Organic Dyes for Dye-Sensitized Solar Cells (DSSCs) Explicit to Cobalt Electrolyte: Understanding the Structural Attributes Using a Direct QSPR Approach

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Table S1. The complete list of computed descriptors for the study.

Quantum-Chemical Descriptors		
Methods/Software	**Symbol**	**Definition**
DFT B3LYP/6-31g(d,p)	SP	The number of sp hybridized carbon atoms
	SP^2	The number of sp^2 hybridized carbon atoms
	SPA	$(SP+SP^2)/N_A$
	SP/SP^2	Ratio of sp and sp^2 hybridized carbon atoms
	$n Csp^3$	The number of sp^3 hybridized carbon atoms
	E_T	Total energy
	E_H	Energy of HOMO [a]
	E_{H-1}	Energy of HOMO – 1 [b]
	E_L	Energy of LUMO [c]
	E_{L+1}	Energy of LUMO + 1 [d]
	E_{gHL}	$E_{HOMO} - E_{LUMO}$
	BLD	Band level difference [= $E_L - E_{CB}$ [e]]
	ECP	Electronic chemical potentials [= $(E_H + E_L)/2$]
	MEN	Mullikan electro-negativity [= $-(E_H + E_L)/2$]
	AH	Absolute hardness [= $-(E_H - E_L)/2$]
	RI	Refractive index (= $MEN^2/2\times AH$)
	VB	Valence band maxima (= ECP − 0.5 × E_{gHL})
	CB	Conduction band minima (= ECP + 0.5 × E_{gHL})
	D_g	Dipole moment for ground state
	N_A	Total atoms
	N_V	Total number of valence electrons
TD-DFT CAM-B3LYP/6-31g(d,p)	$(E_T)_{Ex}$	Total energy for the excited state
	$(E_H)_{Ex}$	Energy of HOMO for the first excited state
	$(E_{H-1})_{Ex}$	Energy of HOMO − 1 for the first excited state
	$(E_L)_{Ex}$	Energy of LUMO for the first excited state
	$(E_{L+1})_{Ex}$	Energy of LUMO + 1 for the first excited state
	$(E_{gHL})_{Ex}$	$(E_H)_{Ex} - (E_L)_{Ex}$ for the first excited state
	$(BLD)_{Ex}$	Band level difference [= $(E_L)_{Ex} - E_{CB}$]
	E_{max}	Maximum absorption energy of the dye sensitizer
	D_{Ex}	Dipole moment
	Wavelength	Excitation wavelength corresponding to E_{max}
	f	Oscillator strength corresponding to E_{max}
DRAGON Descriptors		
Constitutional indices Ring descriptors Functional group counts Atom-type E-state	MW-O% *n*CIC-D/Dtr12 *n*Cp-*n*HAcc $SsCH_3$-NaaS	See the following link for complete description: http://www.talete.mi.it/products/dragon_molecular_descriptor_list.pdf

[a] HOMO = highest occupied molecular orbital; [b] LUMO = lowest unoccupied molecular orbital; [c] HOMO − 1 = second highest occupied molecular orbital; [d] LUMO + 1 = second lowest unoccupied molecular orbital; and [e] E_{CB} = conduction band minimum energy of semiconductor TiO_2 in vacuum [1,2].

Table S2. Computed λ_{max} in reported experimental solvents at the TD CAM-B3LYP/6-31G (d, p) level of theory along with the experimental λ_{max} of the dyes.

Dye ID	λ_{max} (Expt.)	λ_{max} (Computed)
1	517	516.10 [a]
3	497	483.45 [a]
4	504	479.95 [a]
5	503	479.95 [a]
6	429	426.11 [a]
7	514	505.48 [a]
8	511	478.49 [a]
17	488	554.50 [b]
18	520	461.00 [c]
19	501	465.48 [c]
20	498	458.89 [c]
21	500	509.48 [c]

[a] Acetonitrile; [b] Dimethylformamide; [c] Dichloromethane.

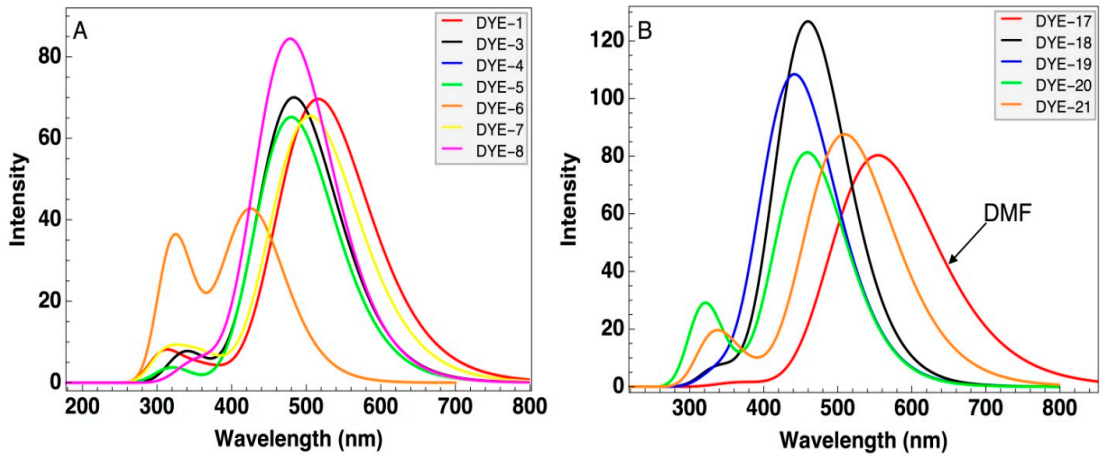

Figure S1. Simulated absorption spectra for the investigated dyes calculated at the TD CAM-B3LYP/6-31G (d, p) level of theory in reported experimental solvents: (**A**) Acetonitrile; (**B**) dichloromethane, except Dye-17 in Dimethylformamide (DMF).

References

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2. Katoh, R.; Furube, A.; Yoshihara, T.; Hara, K.; Fujihashi, G.; Takano, S.; Murata, S.; Arakawa, H.; Tachiya, M. Efficiencies of electron injection from excited N3 dye into nanocrystalline semiconductor (ZrO_2, TiO_2, ZnO, Nb_2O_5, SnO_2, In_2O_3) films. *J. Phys. Chem. B* **2004**, *108*, 4818–4822.