Supplementary Materials (ESI) for RSC Advances

Red-shifted optical absorption induced by donor-acceptor-donor π-extended dibenzalacetone derivatives

Vitória M. R. Vasconcelos,[a] Bruna B. Postacchini,[b] Hélcio S. dos Santos,[c] Francisco F. M. Cajazeiras,[c] Valder N. Freire,[d] Clodomiro Alves Junior,[f] Cláudia Pessoa,[e] Roner F. da Costa,[f] Igor F. Vasconcelos,[a] and Eveline M. Bezerra*[f]

*Corresponding author. Email: eveline.bezerra@ufersa.edu.br

This PDF file includes: Tables S1 to S9

Table S1 Preparation of solutions containing dibenzalacetone derivatives (DBAd) in solvents employed.

	Stock Solution	**Concentration** $\times 10^{-5}\,\mathrm{mol\cdot L^{-1}}$				
DBAd	$\mathrm{mol\cdot L^{-1}}$	1st	2nd	3rd	4th	5th
DBA	1.7×10^{-3}	0.55 (3)	1.11 (5)	1.67 (6)	2.25 (5)	2.83 (5)
DBC	2.1×10^{-3}	0.66 (9)	1.34 (9)	2.03 (9)	2.72 (9)	3.42 (5)
DEP	1.6×10^{-3}	0.53 (4)	1.07 (6)	1.62 (9)	2.17 (9)	2.72 (9)
DMA	1.9×10^{-3}	0.63 (5)	1.27 (9)	1.91 (9)	2.57 (9)	3.22 (9)

[a]Toluene ($\kappa = 2.37$); [b]Dichloromethane ($\kappa = 8.93$); [c]Acetonitrile ($\kappa = 35.67$);

Table S2 Molar absorption coefficients of the dibenzalacetone derivatives (DBAd) in solvents employed, determined by linear regression.

	Molar absorption coefficients $\times 10^4\ \mathrm{L\cdot mol^{-1}\cdot cm^{-1}}$			
Solvent	**DBA**	**DBC**	**DEP**	**DMA**
Dichloromethane	6.59 (1)	3.27 (5)	4.83 (7)	4.63 (8)
Toluene	4.71 (3)	3.24 (3)	4.05 (4)	4.09 (2)
Acetonitrile	7.44 (8)	4.44 (3)	5.96 (5)	6.75 (4)

[a]Toluene ($\kappa = 2.37$); [b]Dichloromethane ($\kappa = 8.93$); [c]Acetonitrile ($\kappa = 35.67$);

Table S3 Optimized geometric parameters (bond length) for the two chalcone compounds: DBA ($C_{17}H_{14}O$), and DBC ($C_{17}H_{12}Cl_2O$). The atom labels are presented in Fig.3

DBA				DBC			
Lig.	Å	Lig.	°	Lig.	Å	Lig.	°
C1-C2	1.399	C2-C1-C3	118.7	C1-C2	1.399	C2-C1-C3	118.5
C1-C3	1.402	C2-C1-C7	118.4	C1-C3	1.401	C2-C1-C7	118.5
C1-C7	1.469	C1-C2-C4	120.9	C1-C7	1.469	C1-C2-C4	121.3
C2-C4	1.391	C1-C2-H	119.2	C2-C4	1.389	C1-C2-H	119.5
C2-H	1.085	C3-C1-C7	122.9	C2-H	1.084	C3-C1-C7	123.0
C3-C5	1.387	C1-C3-C5	120.4	C3-C5	1.386	C1-C3-C5	120.9
C3-H	1.084	C1-C3-H	120.3	C3-H	1.083	C1-C3-H	120.6
C4-C6	1.391	C1-C7-C8	126.4	C4-C6	1.387	C1-C7-C8	126.4
C4-H	1.083	C1-C7-H	114.9	C4-H	1.082	C1-C7-H	114.9
C5-C6	1.395	C4-C2-H	119.9	C5-C6	1.391	C4-C2-H	119.2
C5-H	1.084	C2-C4-C6	119.9	C5-H	1.082	C2-C4-C6	118.7
C6-H	1.084	C2-C4-H	119.9	C6-Cl1	1.745	C2-C4-H	120.9
C7-C8	1.340	C5-C3-H	119.3	C7-C8	1.339	C5-C3-H	118.6
C7-H	1.087	C3-C5-C6	120.3	C7-H	1.087	C3-C5-C6	119.1
C8-C9	1.482	C3-C5-H	119.7	C8-C9	1.482	C3-C5-H	120.7
C8-H	1.085	C6-C4-H	120.2	C8-H	1.085	C6-C4-H	120.4
C9-C10	1.482	C4-C6-C5	119.8	C9-C10	1.483	C4-C6-C5	121.5
C9-O1	1.222	C4-C6-H	120.2	C9-O1	1.222	C4-C6-Cl1	119.4
C10-C11	1.340	C6-C5-H	120.0	C10-C11	1.340	C6-C5-H	120.1
C10-H	1.085	C5-C6-H	120.1	C10-H	1.085	C5-C6-Cl1	119.1
C11-C12	1.469	C8-C7-H	118.6	C11-C12	1.469	C8-C7-H	118.7
C11-H	1.087	C7-C8-C9	124.0	C11-H	1.087	C7-C8-C9	123.9
C12-C15	1.402	C7-C8-H	121.7	C12-C15	1.401	C7-C8-H	121.8
C12-C17	1.399	C9-C8-H	113.9	C12-C17	1.399	C9-C8-H	113.9
C13-C14	1.395	C8-C9-C10	121.4	C13-C14	1.392	C8-C9-C10	121.4
C13-C15	1.387	C8-C9-O1	119.3	C13-C15	1.386	C8-C9-O1	119.3
C13-H	1.084	C10-C9-O1	119.2	C13-H	1.082	C10-C9-O1	119.3
C14-C16	1.391	C9-C10-C11	124.1	C14-C16	1.387	C9-C10-C11	124.0
C14-H	1.084	C9-C10-H	113.8	C14-Cl2	1.746	C9-C10-H	113.8
C15-H	1.084	C11-C10-H	121.6	C15-H	1.083	C11-C10-H	121.8
C16-C17	1.391	C10-C11-C12	126.2	C16-C17	1.389	C10-C11-C12	126.3
C16-H	1.083	C10-C11-H	118.7	C16-H	1.082	C10-C11-H	118.8
C17-H	1.085	C12-C11-H	115.1	C17-H	1.084	C12-C11-H	114.9
		C11-C12-C15	122.7			C11-C12-C15	123.0
		C11-C12-C17	118.6			C11-C12-C17	118.5
		C15-C12-C17	118.7			C15-C12-C17	118.5
		C12-C15-C13	120.5			C12-C15-C13	120.9
		C12-C15-H	120.2			C12-C15-H	120.5
		C12-C17-C16	120.8			C12-C17-C16	121.3
		C12-C17-H	119.3			C12-C17-H	119.5
		C14-C13-C15	120.3			C14-C13-C15	119.1
		C14-C13-H	120.0			C14-C13-H	120.1
		C13-C14-C16	119.8			C13-C14-C16	121.5
		C13-C14-H	120.1			C13-C14-C*l*2	119.2
		C15-C13-H	119.7			C15-C13-H	120.8
		C13-C15-H	119.3			C13-C15-H	118.6
		C16-C14-H	120.2			C16-C14-C*l*2	119.4
		C14-C16-C17	119.9			C14-C16-C17	118.7
		C14-C16-H	120.2			C14-C16-H	120.4
		C17-C16-H	119.9			C17-C16-H	120.9
		C16-C17-H	119.9			C16-C17-H	119.3

[a]Toluene ($\kappa = 2.37$); [b]Dichloromethane ($\kappa = 8.93$); [c]Acetonitrile ($\kappa = 35.67$);

Table S4 Optimized geometric parameters (bond length) for the two chalcone compounds: DEP ($C_{21}H_{22}O_3$), and DMA ($C_{21}H_{18}O$). The atom labels are presented in Fig. 3

DEP				DMA			
Lig.	Å	Lig.	°	Lig.	Å	Lig.	°
C1-C2	1.403	C2-C1-C3	117.9	C1-C2	1.402	C2-C1-C3	118.5
C1-C3	1.398	C2-C1-C7	119.1	C1-C3	1.400	C2-C1-C19	122.8
C1-C7	1.465	C1-C2-C4	121.3	C1-C19	1.468	C1-C2-C4	120.6
C2-C4	1.382	C1-C2-H	119.3	C2-C4	1.388	C1-C2-H	120.2
C2-H	1.085	C3-C1-C7	122.9	C2-H	1.084	C3-C1-C19	118.8
C3-C5	1.389	C1-C3-C5	121.5	C3-C5	1.391	C1-C3-C5	120.9
C3-H	1.084	C1-C3-H	120.1	C3-H	1.085	C1-C3-H	119.2
C4-C6	1.399	C1-C7-C8	126.2	C4-C6	1.395	C1-C19-C18	126.2
C4-H	1.083	C1-C7-H	115.2	C4-H	1.084	C1-C19-H	115.2
C5-C6	1.399	C4-C2-H	119.4	C5-C6	1.391	C4-C2-H	119.2
C5-H	1.081	C2-C4-C6	120.0	C5-H	1.084	C2-C4-C6	120.3
C6-O2	1.352	C2-C4-H	121.2	C6-H	1.084	C2-C4-H	119.7
C7-C8	1.342	C5-C3-H	118.4	C7-C8	1.343	C5-C3-H	119.8
C7-H	1.087	C3-C5-C6	119.6	C7-H	1.086	C3-C5-C6	120.0
C8-C9	1.480	C3-C5-H	119.2	C8-C9	1.481	C3-C5-H	119.8
C8-H	1.085	C6-C4-H	118.8	C8-H	1.086	C6-C4-H	120.0
C9-C10	1.480	C4-C6-C5	119.6	C9-C10	1.481	C4-C6-C5	119.6
C9-O1	1.225	C4-C6-O2	116.1	C9-O1	1.224	C4-C6-H	120.1
C10-C11	1.342	C6-C5-H	121.2	C10-C11	1.343	C6-C5-H	120.2
C10-H	1.086	C5-C6-O2	124.3	C10-H	1.086	C5-C6-H	120.2
C11-C12	1.465	C6-O2-C18	118.4	C21-C12	1.469	C18-C19-H	118.6
C11-H	1.087	O2-C18-C19	107.4	C11-H	1.086	C19-C18-C7	124.0
C12-C15	1.398	O2-C18-H	109.3	C12-C15	1.400	C19-C18-H	120.1
C12-C17	1.404	O2-C18-H	109.3	C12-C17	1.402	C7-C18-H	115.8
C13-C14	1.399	C19-C18-H	111.1	C13-C14	1.391	C18-C7-C8	125.3
C13-C15	1.389	C19-C18-H	111.1	C13-C15	1.391	C18-C7-H	115.8
C13-H	1.081	C18-C19-H	110.5	C13-H	1.084	C8-C7-H	118.8
C14-C16	1.399	C18-C19-H	110.5	C14-C16	1.394	C7-C8-C9	124.4
C14-O3	1.352	C18-C19-H	110.5	C14-H	1.083	C7-C8-H	120.9
C15-H	1.084	H-C18-H	108.6	C15-H	1.085	C9-C8-H	114.3
C16-C17	1.382	H-C19-H	108.9	C16-C17	1.388	C8-C9-C10	121.3
C16-H	1.083	H-C19-H	108.9	C16-H	1.084	C8-C9-O1	119.4
C17-H	1.085	H-C19-H	108.9	C17-H	1.084	C10-C9-O1	119.3
O2-C18	1.428	C8-C7-H	118.6	C21-C12	1.469	C9-C10-C11	124.4
C18-C19	1.512	C7-C8-C9	124.1	C19-C18	1.342	C9-C10-H	114.2
C20-C21	1.512	C7-C8-H	121.3	C20-C21	1.342	C11-C10-H	120.9
C18-H	1.095	C9-C8-H	114.1	C18-H	1.086	C10-C11-C20	125.5
C18-H	1.095	C8-C9-C10	121.4			C10-C11-H	118.8
C19-H	1.091	C8-C9-O1	119.3	C19-H	1.088	C20-C11-H	115.7
C19-H	1.091	C10-C9-O1	119.3			C11-C20-C21	124.2
C19-H	1.091	C9-C10-C11	124.2			C11-C20-H	115.6
O3-C20	1.428	C9-C10-H	113.9	C18-C7	1.461	C21-C20-H	120.1
C20-C21	1.512	C11-C10-H	121.4	C11-C20	1.461	C20-C21-C12	126.4
C20-H	1.095	C10-C11-C12	126.5	C20-H	1.085	C20-C21-H	118.6
C20-H	1.095	C10-C11-H	118.5			C12-C21-H	115.0
C21-H	1.091	C12-C11-H	114.9			C21-C12-C15	118.6
C21-H	1.091	C11-C12-C15	123.3	C21-H	1.088	C21-C12-C17	122.9
C21-H	1.091	C11-C12-C17	118.8			C15-C12-C17	118.4
		C15-C12-C17	117.9			C12-C15-C13	121.0
		C12-C15-C13	121.5			C12-C15-H	119.2
		C12-C15-H	120.2			C12-C17-C16	120.6
		C12-C17-C16	121.4			C12-C17-H	120.2
		C12-C17-H	119.2			C14-C13-C15	120.0
		C14-C13-C15	119.6			C14-C13-H	120.1
		C14-C13-H	121.1			C13-C14-C16	119.7
		C13-C14-C16	119.6			C13-C14-H	120.2
		C13-C14-O3	124.3			C15-C13-H	119.9
		C15-C13-H	119.2			C13-C15-H	119.8
		C13-C15-H	118.3			C16-C14-H	120.1
		C16-C14-O3	116.1			C14-C16-C17	120.4
		C14-C16-C17	120			C14-C16-H	120.0
		C14-C16-H	118.8			C17-C16-H	119.7
		C14-O3-C20	118.5			C16-C17-H	119.2
		C17-C16-H	121.3				
		C16-C17-H	119.4				
		O3-C20-C21	107.5				
		O3-C20-H	109.2				
		O3-C20-H	109.2				
		C21-C20-H	111.0				
		C21-C20-H	111.0				
		C20-C21-H	110.8				
		C20-C21-H	110.8				
		C20-C21-H	110.8				
		H-C20-H	108.5				
		H-C21-H	108.8				
		H-C21-H	108.8				
		H-C21-H	108.8				

[a]Toluene ($\kappa = 2.37$); [b]Dichloromethane ($\kappa = 8.93$); [c]Acetonitrile ($\kappa = 35.67$);

Table S5 Calculated global reactivity descriptors for the dibenzalacetone derivatives (DBAd): DBA ($C_{17}H_{14}O$), DBC ($C_{17}H_{12}Cl_2O$), DEP ($C_{21}H_{22}O_3$), and DMA ($C_{21}H_{18}O$) in toluene ($\kappa_{TOL} = 2.37$), dichloromethane ($\kappa_{DMC} = 8.93$) and acetonitrile ($\kappa_{ACN} = 35.67$).

Descriptor	**DBA**			**DBC**		
	TOL	DCM	ACN	TOL	DCM	ACN
$\mathbf{E_{HOMO}}$	−7.999	−8.011	−8.017	−8.020	−7.989	−7.981
$\mathbf{E_{LUMO}}$	−1.522	−1.595	−1.622	−1.710	−1.718	−1.724
[a]**IP**	7.999	8.011	8.017	8.020	7.989	7.981
[b]**EA**	1.522	1.595	1.622	1.710	1.718	1.724
[c]$\mathbf{E_F}$	6.477	6.416	6.395	6.310	6.271	6.257
[d]$\mathbf{E_B}$	2.865	2.734	2.687	2.708	2.601	2.563
[e]χ	4.761	4.803	4.819	4.865	4.854	4.852
[f]η	3.238	3.208	3.198	3.155	3.135	3.129
[g]**S**	0.309	0.312	0.313	0.317	0.319	0.320
[h]μ	−4.761	−4.803	−4.819	−4.865	−4.854	−4.852
[i]ω	36.702	37.000	37.136	37.330	36.936	36.831
Descriptor	**DEP**			**DMA**		
	TOL	DCM	ACN	TOL	DCM	ACN
$\mathbf{E_{HOMO}}$	−7.367	−7.396	−7.434	−7.544	−7.553	−7.541
$\mathbf{E_{LUMO}}$	−1.292	−1.415	−1.458	−1.728	−1.795	−1.834
[a]**IP**	7.367	7.396	7.434	7.544	7.553	7.541
[b]**EA**	1.292	1.415	1.458	1.728	1.795	1.834
[c]$\mathbf{E_F}$	6.075	5.981	5.976	5.817	5.758	5.707
[d]$\mathbf{E_B}$	2.407	2.243	2.214	2.287	2.149	2.072
[e]χ	4.329	4.406	4.446	4.636	4.674	4.687
[f]η	3.037	2.991	2.988	2.908	2.879	2.854
[g]**S**	0.329	0.334	0.335	0.344	0.347	0.350
[h]μ	−4.329	−4.406	−4.446	−4.636	−4.674	−4.687
[i]ω	28.465	29.022	29.532	31.251	31.453	31.344

[a]Ionization Potential (**IP**); [b]Electron Affinity (**EA**); [c]Fundamental Gap Energy ($\mathbf{E_F}$); [d]Binding Energy of the Electron-Hole Pair ($\mathbf{E_B}$); [e]Electronegativity (χ); [f]Chemical Hardness (η); [g]Chemical Softness (**S**); [h]Electronic Chemical Potential (μ); [i]Electrophilicity Index (ω);

Table S6 Excited states, energies (E in eV), oscillator strengths (O Str), vertical transition and propability (%) of DBA chalcone TD-DFT calculated at M06-2X/6-311G(d,p) level in toluene ($\kappa_{TOL} = 2.37$), dichloromethane ($\kappa_{DCM} = 8.93$) and acetonitrile ($\kappa_{ACN} = 35.67$).

	Toluene ($\kappa_{TOL} = 2.37$)				**dichloromethane** ($\kappa_{DCM} = 8.93$)				**Acetonitrile** ($\kappa_{ACN} = 35.67$)			
Excited State	E eV	[c]**O Str**	**Electronic Transition**	[d](%)	E eV	[c]**O Str**	**Electronic Transition**	[d](%)	E eV	[c]**O Str**	**Electronic Transition**	[d](%)
1	3.61	0.006	H-4 ⟶ L	76.3	3.68	0.007	H-4 ⟶ L	77.1	3.71	0.007	H-4 ⟶ L	77.3
			H-4 ⟶ L+9	5.6			H-4 ⟶ L+9	5.8			H-4 ⟶ L+9	5.5
			H-1 ⟶ L	3.9			H-1 ⟶ L	4.0			H-1 ⟶ L	3.9
			H-4 ⟶ L+12	3.7			H-4 ⟶ L+12	2.4			H-4 ⟶ L+7	2.3
											H-4 ⟶ L+12	2.2
2	4.27	0.839	H ⟶ L	87.5	4.22	0.824	H ⟶ L	88.8	4.21	0.810	H ⟶ L	89.3
			H-1 ⟶ L+1	9.3			H-1 ⟶ L+1	8.0			H-1 ⟶ L+1	7.4
3	4.60	0.490	H-1 ⟶ L	87.2	4.57	0.474	H-1 ⟶ L	88.1	4.58	0.454	H-1 ⟶ L	88.6
			H ⟶ L+1	5.9			H ⟶ L+1	4.9			H ⟶ L+1	4.3
			H-4 ⟶ L	3.6			H-4 ⟶ L	3.5			H-4 ⟶ L	3.4
4	4.98	0.014	H-3 ⟶ L	27.5	4.96	0.019	H-2 ⟶ L	32.9	4.95	0.019	H-3 ⟶ L	26.8
			H-3 ⟶ L+1	20.9			H-3 ⟶ L+1	19.7			H-2 ⟶ L	23.4
			H-2 ⟶ L	18.0			H-3 ⟶ L	16.1			H-3 ⟶ L+1	20.4
			H-1 ⟶ L+4	9.4			H ⟶ L+2	10.1			H ⟶ L+2	9.1
			H ⟶ L+2	6.0			H-1 ⟶ L+3	5.2			H-1 ⟶ L+3	8.6
			H ⟶ L+2	4.0			H-1 ⟶ L+4	4.9				
			H ⟶ L+4	2.5			H ⟶ L+1	2.2				
			H ⟶ L+1	2.2								
5	4.98	0.011	H-2 ⟶ L	27.4	4.96	0.012	H-3 ⟶ L	33.1	4.95	0.013	H-2 ⟶ L	26.6
			H-2 ⟶ L+1	21.1			H-2 ⟶ L+1	20.0			H-3 ⟶ L	23.6
			H-3 ⟶ L	18.0			H-2 ⟶ L	16.0			H-2 ⟶ L+1	20.7
			H ⟶ L+4	10.6			H-1 ⟶ L+2	8.6			H ⟶ L+3	10.1
			H-1 ⟶ L+3	5.4			H ⟶ L+3	7.1			H-1 ⟶ L+2	7.6
			H-1 ⟶ L+2	3.3			H ⟶ L+4	4.5				
			H-1 ⟶ L+4	2.3								
			H-1 ⟶ L+1	2.2								
6	5.29	0.077	H-1 ⟶ L+1	79.3	5.30	0.084	H-1 ⟶ L+1	81.5	5.31	0.086	H-1 ⟶ L+1	81.5
			H ⟶ L	6.8			H ⟶ L	5.8			H ⟶ L	5.4
			H-3 ⟶ L	3.1			H-3 ⟶ L	2.7			H-3 ⟶ L	2.4
7	5.33	0.019	H ⟶ L+1	81.6	5.31	0.024	H ⟶ L+1	82.9	5.31	0.027	H ⟶ L+1	82.9
			H-1 ⟶ L	4.4			H-1 ⟶ L	3.6			H-1 ⟶ L	3.1
			H-2 ⟶ L	3.4			H-2 ⟶ L	3.2			H-2 ⟶ L	2.9
8	5.77	0.004	H-4 ⟶ L+1	86.3	5.86	0.006	H-4 ⟶ L+1	85.1	5.90	0.009	H-4 ⟶ L+1	82.8
							H-4 ⟶ L+13	3.1			H-4 ⟶ L+13	3.1
											H ⟶ L+3	2.2
9	5.96	0.145	H ⟶ L+4	29.8	5.95	0.115	H-1 ⟶ L+2	25.6	5.96	0.099	H ⟶ L+3	27.7
			H-3 ⟶ L	24.6			H-3 ⟶ L	25.1			H-1 ⟶ L+2	21.1
			H-1 ⟶ L+3	17.9			H ⟶ L+3	17.4			H-3 ⟶ L	23.9
			H-1 ⟶ L+2	11.7			H ⟶ L+4	11.9			H-2 ⟶ L	9.1
			H-2 ⟶ L	8.9			H-2 ⟶ L	8.2			H-4 ⟶ L+1	3.9
10	5.98	0.319	H-2 ⟶ L	25.3	5.97	0.267	H ⟶ L+2	30.5	5.97	0.236	H ⟶ L+2	30.9
			H-1 ⟶ L+4	25.0			H-2 ⟶ L	26.3			H-2 ⟶ L	25.9
			H ⟶ L+3	19.2			H-1 ⟶ L+3	12.7			H-1 ⟶ L+3	22.7
			H ⟶ L+2	13.9			H-1 ⟶ L+4	11.1			H-3 ⟶ L	9.2
			H-3 ⟶ L	8.9			H-3 ⟶ L	8.3			H ⟶ L+1	2.3
			H ⟶ L+1	2.4			H ⟶ L+1	2.3				

[a] κ, is the dielectric constant for the solvent; [b]H=HOMO, L=LUMO. [c]O Str, oscillator strength; [d]Probability;

Table S7 Excited states, energies (E in eV), oscillator strengths (O Str), vertical transition and propability (%) of DBC chalcone TD-DFT calculated at M06-2X/6-311G(d,p) level in toluene ($\kappa_{TOL} = 2.37$), dichloromethane ($\kappa_{DCM} = 8.93$) and acetonitrile ($\kappa_{ACN} = 35.67$).

	Toluene ($\kappa_{TOL} = 2.37$)				**dichloromethane** ($\kappa_{DCM} = 8.93$)				**Acetonitrile** ($\kappa_{ACN} = 35.67$)			
Excited State	E eV	[c]**O Str**	**Electronic Transition**	[d](%)	E eV	[c]**O Str**	**Electronic Transition**	[d](%)	E eV	[c]**O Str**	**Electronic Transition**	[d](%)
1	3.60	0.007	H-4 ⟶ L	74.0	3.67	0.008	H-4 ⟶ L	74.7	3.69	0.008	H-4 ⟶ L	74.8
			H-4 ⟶ L+10	5.0			H-4 ⟶ L+6	5.8			H-4 ⟶ L+6	6.2
			H-4 ⟶ L+6	4.3			H-1 ⟶ L	3.9			H-1 ⟶ L	3.9
			H-1 ⟶ L	3.8			H-4 ⟶ L+10	3.4			H-4 ⟶ L+10	2.9
											H-5 ⟶ L	2.1
2	4.18	1.014	H ⟶ L	85.0	4.14	0.992	H ⟶ L	86.4	4.14	0.975	H ⟶ L	87.0
			H-1 ⟶ L+1	10.9			H-1 ⟶ L+1	9.4			H-1 ⟶ L+1	8.8
			H-6 ⟶ L	2.5			H-6 ⟶ L	2.6			H-6 ⟶ L	2.7
3	4.51	0.549	H-1 ⟶ L	83.8	4.50	0.535	H-1 ⟶ L	85.1	4.51	0.544	H-1 ⟶ L	85.8
			H ⟶ L+1	8.8			H ⟶ L+1	7.4			H ⟶ L+1	6.6
			H-4 ⟶ L	3.0			H-4 ⟶ L	3.0			H-4 ⟶ L	2.9
							H-5 ⟶ L	2.0			H-5 ⟶ L	2.1
4	4.96	0.000	H-2 ⟶ L	19.4	4.95	0.002	H-2 ⟶ L	26.3	4.95	0.003	H-2 ⟶ L	27.5
			H-1 ⟶ L+3	18.4			H ⟶ L+2	18.7			H ⟶ L+2	18.2
			H ⟶ L+2	18.2			H-1 ⟶ L+3	18.3			H-1 ⟶ L+3	17.8
			H-3 ⟶ L+1	14.9			H-3 ⟶ L+1	15.5			H-3 ⟶ L+1	15.7
			H ⟶ L+1	8.6			H ⟶ L+1	8.9			H ⟶ L+1	8.6
			H-3 ⟶ L	7.4			H-3 ⟶ L	3.4			H-3 ⟶ L	3.5
5	4.96	0.001	H ⟶ L+3	21.1	4.96	0.002	H-3 ⟶ L	26.8	4.96	0.002	H-3 ⟶ L	28.1
			H-3 ⟶ L	19.3			H ⟶ L+3	21.3			H ⟶ L+3	20.7
			H-1 ⟶ L+2	16.1			H-1 ⟶ L+2	16.5			H-2 ⟶ L+1	16.2
			H-2 ⟶ L+1	15.1			H-2 ⟶ L+1	15.9			H-1 ⟶ L+2	16.1
			H-1 ⟶ L+1	8.7			H-1 ⟶ L+1	7.8			H-1 ⟶ L+1	7.2
			H-2 ⟶ L	7.3			H-2 ⟶ L	3.5			H-2 ⟶ L	3.4
6	5.21	0.100	H-1 ⟶ L+1	70.4	5.23	0.110	H-1 ⟶ L+1	72.5	5.23	0.035	H ⟶ L+1	71.1
			H ⟶ L	7.0			H ⟶ L	6.1			H-2 ⟶ L	7.6
			H-3 ⟶ L	6.1			H-3 ⟶ L	5.7			H-1 ⟶ L1	3.6
			H-2 ⟶ L+1	2.8			H-2 ⟶ L+1	2.7			H-1 ⟶ L	3.6
											H-3 ⟶ L+1	3.0
											H-5 ⟶ L	2.2
7	5.24	0.026	H ⟶ L+1	72.1	5.23	0.030	H ⟶ L+1	72.7	5.85	0.039	H-1 ⟶ L+1	71.1
			H-2 ⟶ L	6.8			H-2 ⟶ L	6.9			H-3 ⟶ L	6.3
			H-1 ⟶ L	5.1			H-1 ⟶ L	4.2			H ⟶ L	5.4
			H-3 ⟶ L+1	3.6			H-3 ⟶ L+1	3.5			H ⟶ L+1	3.6
			H-5 ⟶ L	2.4			H-5 ⟶ L	2.3			H-2 ⟶ L+1	2.1
8	5.72	0.005	H-4 ⟶ L+1	84.2	5.82	0.015	H-4 ⟶ L+1	79.1	5.85	0.039	H-4 ⟶ L+1	63.5
							H-3 ⟶ L	3.3			H-3 ⟶ L	10.8
							H-4 ⟶ L+12	2.9			H ⟶ L+3	7.8
							H ⟶ L+3	2.4			H-1 ⟶ L+2	5.9
											H-4 ⟶ L+2	2.7
9	5.86	0.146	H-3 ⟶ L	38.2	5.87	0.121	H-3 ⟶ L	35.7	5.88	0.088	H-3 ⟶ L	28.8
			H ⟶ L+3	24.8			H ⟶ L+3	24.7			H-4 ⟶ L+1	22.0
			H-1 ⟶ L+2	24.6			H-1 ⟶ L+2	23.5			H ⟶ L+3	19.8
			H-2 ⟶ L+1	4.9			H-4 ⟶ L+1	6.6			H-1 ⟶ L+2	19.1
			H-2 ⟶ L	3.0			H-2 ⟶ L+1	2.6				
							H-2 ⟶ L	2.1				
10	5.88	0.390	H-2 ⟶ L	38.0	5.88	0.359	H-2 ⟶ L	38.6	5.90	0.333	H-2 ⟶ L	39.3
			H ⟶ L+2	28.6			H ⟶ L+2	30.1			H ⟶ L+2	30.3
			H-1 ⟶ L+3	21.1			H-1 ⟶ L+3	21.7			H-1 ⟶ L+3	21.4
			H-3 ⟶ L+1	4.5			H-3 ⟶ L+1	2.7				
			H-3 ⟶ L	2.9			H-3 ⟶ L	2.2				

[a] κ, is the dielectric constant for the solvent; [b]H=HOMO, L=LUMO. [c]O Str, oscillator strength; [d]Probability;

Table S8 Excited states, energies (E in eV), oscillator strengths (O Str), vertical transition and propability (%) of DEP chalcone TD-DFT calculated at M06-2X/6-311G(d,p) level in toluene ($\kappa_{TOL} = 2.37$), dichloromethane ($\kappa_{DCM} = 8.93$) and acetonitrile ($\kappa_{ACN} = 35.67$).

	Toluene ($\kappa_{TOL} = 2.37$)				**dichloromethane** ($\kappa_{DCM} = 8.93$)				**Acetonitrile** ($\kappa_{ACN} = 35.67$)			
Excited State	E eV	[c]**O Str**	**Electronic Transition**	[d](%)	E eV	[c]**O Str**	**Electronic Transition**	[d](%)	E eV	[c]**O Str**	**Electronic Transition**	[d](%)
1	3.67	0.011	H-4 ⟶ L	72.7	3.74	0.016	H-4 ⟶ L	73.5	3.76	0.011	H-4 ⟶ L	74.0
			H-1 ⟶ L	3.6			H-1 ⟶ L	5.3			H-5 ⟶ L	5.1
			H-4 ⟶ L+16	3.52			H-5 ⟶ L	3.7			H-1 ⟶ L	3.5
			H-5 ⟶ L	2.7			H-4 ⟶ L+19	3.3			H-4 ⟶ L+19	2.4
			H-2 ⟶ L	2.6								
			H-4 ⟶ L+19	2.3								
2	3.97	1.065	H ⟶ L	85.5	3.90	1.053	H ⟶ L	87.2	3.91	1.048	H ⟶ L	87.2
			H-1 ⟶ L+1	10.5			H-1 ⟶ L+1	8.9			H-1 ⟶ L+1	8.6
			H-6 ⟶ L	2.3			H-6 ⟶ L	2.4			H-6 ⟶ L	2.5
3	4.32	0.451	H-1 ⟶ L	82.7	4.30	0.449	H-1 ⟶ L	82.0	4.28	0.424	H-1 ⟶ L	85.5
			H ⟶ L+1	10.4			H ⟶ L+1	9.5			H ⟶ L+1	7.5
			H-4 ⟶ L	2.6			H-4 ⟶ L	3.6			H-5 ⟶ L	2.3
							H-5 ⟶ L	2.2			H-4 ⟶ L	2.2
4	4.85	0.013	H ⟶ L+1	23.7	4.83	0.005	H ⟶ L+1	35.5	4.85	0.002	H ⟶ L+1	30.7
			H-1 ⟶ L+3	14.4			H-1 ⟶ L+2	20.6			H-1 ⟶ L+2	22.1
			H ⟶ L+4	13.7			H-2 ⟶ L	9.0			H ⟶ L+3	14.7
			H-3 ⟶ L	8.8			H ⟶ L+3	8.2			H-2 ⟶ L	6.9
			H-3 ⟶ L+1	6.3			H ⟶ L+4	7.6			H-3 ⟶ L	5.7
			H-1 ⟶ L+1	5.5			H-3 ⟶ L+1	5.6			H-3 ⟶ L+1	5.1
			H-1 ⟶ L+4	4.6			H-1 ⟶ L	5.4			H-1 ⟶ L	3.8
			H ⟶ L+2	4.2							H ⟶ L+4	2.6
			H-1 ⟶ L	4.2								
			H ⟶ L+3	3.4								
5	4.86	0.015	H ⟶ L+3	24.6	4.85	0.018	H ⟶ L+2	27.7	4.86	0.017	H ⟶ L+2	27.2
			H-1 ⟶ L+1	20.6			H-1 ⟶ L+1	27.3			H-1 ⟶ L+1	24.2
			H-1 ⟶ L+3	9.4			H-3 ⟶ L	11.1			H-1 ⟶ L+3	14.9
			H-1 ⟶ L+4	9.3			H-1 ⟶ L+3	8.6			H-3 ⟶ L	9.1
			H-2 ⟶ L	7.7			H-1 ⟶ L+4	7.5			H-2 ⟶ L+1	5.9
			H-2 ⟶ L+1	6.9			H-2 ⟶ L+1	6.7			H-2 ⟶ L	5.0
			H ⟶ L+1	5.6			H ⟶ L	2.7			H ⟶ L	2.4
			H-3 ⟶ L	2.6							H-1 ⟶ L+4	2.3
			H ⟶ L	2.5								
6	5.12	0.073	H-1 ⟶ L+1	30.1	5.09	0.038	H ⟶ L+1	46.3	5.11	0.055	H ⟶ L+1	41.2
			H ⟶ L+1	23.5			H-2 ⟶ L	14.6			H-2 ⟶ L	13.3
			H-2 ⟶ L	9.7			H ⟶ L+3	7.4			H-1 ⟶ L+1	11.4
			H-2 ⟶ L+1	4.0			H ⟶ L+4	6.3			H ⟶ L+3	8.5
			H-1 ⟶ L+4	3.9			H-3 ⟶ L+1	6.0			H-2 ⟶ L+1	4.2
			H ⟶ L+3	3.9			H-1 ⟶ L+2	5.3			H-1 ⟶ L+2	2.9
			H ⟶ L+4	3.8			H-1 ⟶ L	2.8			H-1 ⟶ L+3	2.2
			H-1 ⟶ L+3	3.8							H-1 ⟶ L	2.0
			H ⟶ L	2.9								
			H-1 ⟶ L	2.0								
7	5.13	0.056	H ⟶ L+1	28.2	5.12	0.096	H-1 ⟶ L+1	55.2	5.13	0.075	H-1 ⟶ L+1	47.1
			H-1 ⟶ L+1	25.1			H-3 ⟶ L	11.4			H-3 ⟶ L	12.9
			H-3 ⟶ L	11.3			H-1 ⟶ L+3	4.8			H ⟶ L+1	11.2
			H ⟶ L+4	6.4			H-1 ⟶ L+4	4.6			H-1 ⟶ L+3	5.0
			H-1 ⟶ L+4	4.6			H ⟶ L+2	4.5			H-3 ⟶ L+1	3.4
			H-3 ⟶ L+1	4.5			H ⟶ L	4.3			H ⟶ L	3.3
			H ⟶ L	2.3			H-2 ⟶ L+1	4.0			H ⟶ L+2	2.7
8	5.75	0.006	H ⟶ L+2	54.7	5.74	0.136	H-3 ⟶ L	47.2	5.74	0.180	H-3 ⟶ L	37.1
			H-1 ⟶ L+5	15.5			H ⟶ L+2	20.7			H ⟶ L+2	20.8
			H ⟶ L+4	7.0			H-2 ⟶ L+1	8.3			H-2 ⟶ L	15.2
			H-3 ⟶ L	2.8			H-1 ⟶ L+3	6.9			H-1 ⟶ L+3	11.9
			H-1 ⟶ L+4	2.8			H-1 ⟶ L+4	6.7			H-2 ⟶ L+1	5.3
			H-1 ⟶ L+2	2.4			H-2 ⟶ L	4.4			H-1 ⟶ L+4	3.2
			H-1 ⟶ L+9	2.2							H-3 ⟶ L+1	2.3
9	5.77	0.147	H-3 ⟶ L	28.0	5.78	0.269	H ⟶ L+3	38.6	5.77	0.380	H-2 ⟶ L	38.1
			H ⟶ L+3	15.3			H-2 ⟶ L	31.8			H ⟶ L+3	19.0
			H-2 ⟶ L	13.5			H-1 ⟶ L+2	8.0			H-1 ⟶ L+2	16.1
			H-2 ⟶ L+1	10.6			H-1 ⟶ L+5	6.9			H-3 ⟶ L	14.8
			H-4 ⟶ L+1	9.8			H-3 ⟶ L+1	3.9			H-3 ⟶ L+1	3.4
			H-1 ⟶ L+4	7.9			H-3 ⟶ L	2.3			H ⟶ L+4	2.3
			H-3 ⟶ L+1	3.2							H-2 ⟶ L+1	2.3
10	5.78	0.032	H-1 ⟶ L+2	47.7	5.79	0.218	H ⟶ L+4	43.2	5.81	0.007	H ⟶ L+4	55.5
			H ⟶ L+5	24.2			H-2 ⟶ L	16.7			H-1 ⟶ L+5	18.2
			H-1 ⟶ L+4	5.9			H-1 ⟶ L+5	10.5			H ⟶ L+3	10.2
			H ⟶ L+2	3.1			H-1 ⟶ L+2	8.0				
			H ⟶ L+9	2.7			H ⟶ L+3	7.1				
			H-3 ⟶ L	2.1			H-3 ⟶ L	2.4				
							H-3 ⟶ L+1	2.3				

[a] κ, is the dielectric constant for the solvent; [b]H=HOMO, L=LUMO. [c]O Str, oscillator strength; [d]Probability;

Table S9 Excited states, energies (E in eV), oscillator strengths (O Str), vertical transition and propability (%) of DMA chalcone TD-DFT calculated at M06-2X/6-311G(d,p) level in toluene ($\kappa_{TOL} = 2.37$), dichloromethane ($\kappa_{DCM} = 8.93$) and acetonitrile ($\kappa_{ACN} = 35.67$).

	Toluene ($\kappa_{TOL} = 2.37$)				**dichloromethane** ($\kappa_{DCM} = 8.93$)				**Acetonitrile** ($\kappa_{ACN} = 35.67$)			
Excited State	E eV	[c]**O Str**	**Electronic Transition**	[d](%)	E eV	[c]**O Str**	**Electronic Transition**	[d](%)	E eV	[c]**O Str**	**Electronic Transition**	[d](%)
1	3.53	0.002	H-4 ⟶ L	63.5	3.61	0.003	H-4 ⟶ L	57.4	3.64	0.034	H-4 ⟶ L	54.0
			H-5 ⟶ L	11.4			H-6 ⟶ L	18.0			H-6 ⟶ L	19.6
			H-4 ⟶ L+2	7.6			H-4 ⟶ L+2	7.1			H-4 ⟶ L+2	6.8
			H-4 ⟶ L+5	2.2			H-6 ⟶ L+2	2.5			H-6 ⟶ L+2	2.7
							H-4 ⟶ L+5	2.5			H-4 ⟶ L+5	2.4
											H ⟶ L	2.3
2	3.72	1.397	H-1 ⟶ L	77.6	3.68	1.376	H ⟶ L	79.6	3.65	1.336	H ⟶ L	75.7
			H ⟶ L+1	18.7			H-1 ⟶ L+1	16.6			H-1 ⟶ L+1	14.2
			H-6 ⟶ L	2.2			H-5 ⟶ L	2.1			H-1 ⟶ L	3.3
3	3.98	0.418	H ⟶ L	81.1	3.96	0.413	H-1 ⟶ L	82.4	3.95	0.402	H-1 ⟶ L	79.4
			H-1 ⟶ L+1	16.2			H ⟶ L+1	14.5			H ⟶ L+1	12.3
											H ⟶ L	3.5
4	4.76	0.078	H ⟶ L+1	70.7	4.74	0.049	H ⟶ L+1	48.1	4.71	0.032	H ⟶ L+1	54.4
			H-1 ⟶ L	15.0			H-1 ⟶ L+1	26.4			H-1 ⟶ L+1	21.3
			H-1 ⟶ L+2	4.8			H-1 ⟶ L	6.6			H-1 ⟶ L	11.8
			H-6 ⟶ L	2.8			H ⟶ L	5.7			H-1 ⟶ L+2	5.2
							H-1 ⟶ L+2	3.2				
							H ⟶ L+2	2.2				
5	4.77	0.014	H-1 ⟶ L+1	71.7	4.75	0.063	H-1 ⟶ L+1	47.5	4.72	0.088	H-1 ⟶ L+1	53.4
			H ⟶ L	13.2			H ⟶ L+1	26.9			H ⟶ L+1	22.2
			H ⟶ L+2	5.6			H ⟶ L	7.4			H ⟶ L	11.7
			H-5 ⟶ L	2.6			H-1 ⟶ L	5.1			H ⟶ L+2	5.1
							H ⟶ L+2	2.8			H-5 ⟶ L	2.1
							H-1 ⟶ L+2	2.4				
							H-5 ⟶ L	2.1				
6	4.93	0.011	H-3 ⟶ L	13.6	4.92	0.011	H-3 ⟶ L	24.5	4.90	0.010	H-3 ⟶ L	40.1
			H-3 ⟶ L+1	12.7			H-2 ⟶ L	12.6			H-3 ⟶ L+1	22.1
			H-2 ⟶ L	11.3			H-3 ⟶ L+1	12.3			H ⟶ L+3	6.7
			H ⟶ L+4	11.1			H-2 ⟶ L+1	11.4			H ⟶ L+5	6.1
			H-2 ⟶ L+1	10.9			H ⟶ L+5	7.8			H ⟶ L+2	3.5
			H-1 ⟶ L+5	6.8			H-1 ⟶ L+3	6.9			H-3 ⟶ L+2	3.2
			H-1 ⟶ L+2	5.5			H-1 ⟶ L+4	4.9			H-1 ⟶ L+3	2.6
							H ⟶ L+2	4.6				
							H-3 ⟶ L+2	2.2				
7	4.93	0.005	H-2 ⟶ L	23.8	4.92	0.005	H-2 ⟶ L	24.8	4.91	0.008	H-2 ⟶ L	36.2
			H-2 ⟶ L+1	12.7			H-3 ⟶ L	12.4			H-2 ⟶ L+1	25.0
			H-1 ⟶ L+4	11.5			H-2 ⟶ L+1	12.2			H-1 ⟶ L+3	7.5
			H-3 ⟶ L	11.2			H-3 ⟶ L+1	11.5			H-1 ⟶ L+5	5.3
			H-3 ⟶ L+1	11.0			H-1 ⟶ L+5	7.4			H-2 ⟶ L+2	3.3
			H ⟶ L+5	6.6			H ⟶ L+3	7.2			H ⟶ L+3	3.2
			H ⟶ L+2	4.5			H ⟶ L+4	5.1			H-1 ⟶ L+2	3.0
			H-1 ⟶ L+1	2.0			H-1 ⟶ L+2	3.8			H-2 ⟶ L+5	2.0
							H-2 ⟶ L+2	2.2				
8	5.50	0.002	H-4 ⟶ L+1	67.1	5.54	0.014	H-4 ⟶ L+1	36.6	5.55	0.020	H-5 ⟶ L	29.7
			H-6 ⟶ L	11.9			H-5 ⟶ L	26.8			H-4 ⟶ L+1	28.4
			H-4 ⟶ L+10	3.0			H ⟶ L+2	9.9			H ⟶ L+2	12.3
			H-1 ⟶ L+2	2.8			H-1 ⟶ L+3	3.4			H-1 ⟶ L+3	5.4
							H-3 ⟶ L	3.2			H-3 ⟶ L	4.0
							H-2 ⟶ L	2.3			H-2 ⟶ L	3.0
9	5.63	0.080	H-1 ⟶ L+2	21.6	5.66	0.014	H-1 ⟶ L+2	20.4	5.65	0.015	H ⟶ L+3	18.4
			H-5 ⟶ L+1	12.0			H ⟶ L+3	13.5			H-1 ⟶ L+2	16.4
			H-6 ⟶ L	11.2			H-2 ⟶ L	12.6			H-3 ⟶ L	14.7
			H-4 ⟶ L+1	10.6			H-6 ⟶ L	10.4			H-6 ⟶ L	8.1
			H ⟶ L+4	9.8			H-3 ⟶ L	9.5			H-2 ⟶ L	7.2
			H-3 ⟶ L	7.9			H ⟶ L+4	7.7			H ⟶ L+2	5.1
			H-2 ⟶ L	5.9			H-1 ⟶ L+5	4.7			H-1 ⟶ L+5	3.6
			H ⟶ L+10	2.5			H-5 ⟶ L+1	4.5			H-5 ⟶ L+1	3.2
			H ⟶ L+3	2.5			H-4 ⟶ L	3.6			H-4 ⟶ L	3.1
											H-4 ⟶ L+1	3.0
10	5.66	0.014	H ⟶ L+2	21.4	5.66	0.083	H-4 ⟶ L+1	31.9	5.67	0.079	H-4 ⟶ L+1	31.6
			H-1 ⟶ L+4	17.9			H ⟶ L+2	16.9			H ⟶ L+2	12.2
			H-2 ⟶ L	12.7			H-6 ⟶ L+1	10.9			H-1 ⟶ L+3	10.7
			H-5 ⟶ L	10.8			H-1 ⟶ L+3	7.8			H-2 ⟶ L	10.6
			H-3 ⟶ L	9.7			H-3 ⟶ L	6.9			H-6 ⟶ L+1	8.1
			H-6 ⟶ L+1	4.5			H-2 ⟶ L	5.0			H-1 ⟶ L+2	4.5
			H ⟶ L+5	3.7			H-1 ⟶ L+4	3.1			H-3 ⟶ L	2.2
			H-1 ⟶ L+3	3.2								
			H-3 ⟶ L+1	2.6								

[a] κ, is the dielectric constant for the solvent; [b]H=HOMO, L=LUMO. [c]O Str, oscillator strength; [d]Probability;