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Supplementary material

Solvent and substituent effect on intramolecular charge transfer in 5-arylidene-3-substituted-2.4-thiazolidinediones: experimental and theoretical study

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1. Introduction

Table S1. Solvent parameters (Kamlet et al., 1983; Marcus, 1993) used in Kamlet–Taft equation.

	Solvent[a]	π^*	β	α
1	Ethanol (EtOH)	0.54	0.75	0.86
2	Methanol (MeOH)	0.6	0.66	0.98
3	1-Propanol (1-PrOH)	0.48	0.84	0.76
4	2-Propanol (2-PrOH)	0.48	0.95	0.76
5	1-Butanol (1-BuOH)	0.47	0.84	0.84
6	2-Methylpropan-1-ol (iBuOH)	0.4	0.84	0.79
7	2-Metoxyethanol (2ME)	0.71	0	0
8	2-Chloroethanol (2CE)	0.46	0.53	1.28
9	Diethyl ether (Et_2O)	0.27	0.47	0
10	Diisopropyl ether (iPr_2O)	0.27	0.49	0
11	Cyclohexane (Ch)	0	0	0
12	Heptane (Hp)	-0.08	0	0
13	Pentane (Pen)	-0.08	0	0
14	*trans*-1,2-Dichloroethene (1,2-DCE)	0.44	0	0
15	Dioxane	0.55	0.37	0
16	Acetonitrile (AcN)	0.75	0.4	0.19
17	*N,N*-Dimethylformamide (DMF)	0.88	0.69	0
18	Dimethyl sulfoxide (DMSO)	1	0.76	0
19	Formamide (FA)	0.97	0.48	0.71

[a] Solvent abbreviation was taken from www.chemnetbase

Table S2. Solvent parameters (Catalán, 2009) used in Catalán equation[a].

	Solvent	*SP*	*SdP*	*SA*	*SB*
1	Ethanol	0.633	0.783	0.4	0.658
2	Methanol	0.608	0.904	0.605	0.545
3	1-Propanol	0.658	0.748	0.367	0.782
4	2-Propanol	0.633	0.808	0.283	0.83
5	1-Butanol	0.674	0.655	0.341	0.809
6	Isobutanol	0.657	0.684	0.311	0.828
7	2-Metoxyethanol	0.6996	0.8952	0.36	0.56
8	2-Chloroethanol	0.7704	0.9736	0.56	0.38
9	Diethyl ether	0.617	0.385	0	0.562
10	Diisopropyl ether	0.625	0.324	0	0.657
11	Cyclohexane	0.683	0	0	0.073
12	Heptane	0.635	0	0	0.083
13	Pentane	0.593	0	0	0.073
14	Dioxane	0.737	0.312	0	0.444
15	Acetonitrile	0.645	0.974	0.044	0.286
16	*N*,*N*-Dimethylformamide	0.759	0.977	0.031	0.613
17	Dimethyl sulfoxide	0.83	1	0.072	0.647
18	Formamide	0.814	1.006	0.549	0.414

[a] Catalán parameters for *trans*-1,2-dichloroethene are not available

Table S3. Hammett substituent parameters (Hansch, 1995).

Supstituent	σ_p
H	0
Br	0.23
F	0.06
Cl	0.23
NO_2	0.78
CH_3	-0.17
OCH_3	-0.27
NMe_2	-0.83
3,4-di-OCH_3	-0.15

2. Experimental

2.1. Materials

Chloroacetic acid, thiourea, *conc*. hydrochloric acid, ethanol, potassium hydroxide, chloroform, calcium sulphate, phenylisothiocyanate, aniline, glacial acetic acid, benzaldehyde, 4-methylbenzaldehyde, 4-methoxybenzaldehyde, 4-brombenzaldehyde, 4-chlorobnzaldehyde, 4-fluorobenzaldehyde, 4-(dimethylamino)benzaldehyde, 4-nitrobenzaldehyde and 3,4-diemthoxybenzaldehyde, all p.a. grade, were purchased from Sigma Aldrich. All used solvents were of spectroscopic quality (Table S1).

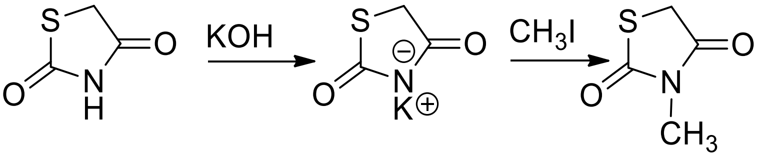
2.2. Synthesis of 2,4-thiazolidinedione, 3-methyl-2,4-thiazolidinedione, diphenylthiourea and 3-phenyl-2,4-thiazolidinedione

Synthesis of 2,4-thiazolidinedione (Jain et al., 2012; Brown, 1961)

In a 250 ml three-necked flask, a solution containing 56.4 g (0.6 mol) of chloroacetic acid in 60 ml of water and 45.6 g (0.6 moles) of thiourea dissolved in 60 ml of water were added. The mixture was stirred for 15 min until white precipitates occured. Afterwards, 60 ml of concentrated hydrochloric acid was slowly added form dropping funnel to the flask until dissolution of the precipitate and, then, the reaction mixture was stirred and refluxed for 11 h at 100-110 °C. On cooling the content of the flask solidify to a mass of clusters of white needles. The product was filtered and washed with water to remove traces of hydrochloric acid, recrystallized from ethanol and dried (yield: 85%. m.p: 123-125 °C).

Synthesis of 3-methyl-2,4-thiazolidinedione (Macháček et al., 1981)

In a 100 ml flask, 16 g of 2,4-thiazolidinedione dissolved in 25 ml of warm ethanol and 8.4 g of potassium hydroxide, dissolved in 20 ml of ethanol, was added. After addition of 10 ml freshly distilled methyl iodide, the reaction mixture was refluxed for 4 h, and poured into 50 ml of MilliQ water. Separated oily phase of 3-methyl-2,4-thiazolidinedione was extracted with chloroform (2 x 100 ml), washed by water and the exstract was dried with calcium-sulphate. Chloroform was removed by distilation and the product was crystalized after adding small amount of ether into residue after distillation (yield 48 %, m.p. 41-43 ^{0}C).



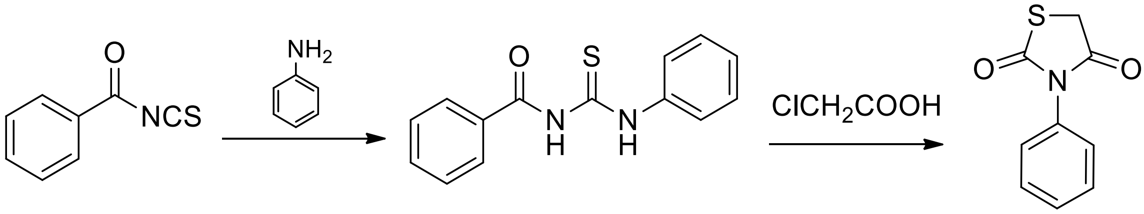
Scheme S1. *Synthesis of 3-methyl-2,4-thiazolidinedione*

Synthesis of N-benzoyl-N'-phenylthiourea (Yamin et al., 2003)

In a 100 ml flask was firstly added 13.5 g of benzoylisothiocyanate dissolved in 20 ml of ethanol, and dropwise addition of 9.3 g of aniline for 10 min at room temperature was performed. Reaction mixture was heated for 15 min and poured into 200 ml of cold MilliQ water, raw product was recrystallized from methanol (yield 96%, m.p. 151^{0}C.

Synthesis of 3-phenyl-2,4-thiazolidinedione (Singh et al., 1981)

N-benzoyl-*N*'-phenylthiourea (22.8 g, 0.1 mol) was dissolved in 40 ml of glacial acetic acid and then, cloroacetic acid was added (9.45 g, 0.1 mol) and reaction mixer was refluxed for 5 h. After cooling the mixture to room temperature, water was added to the flask and the product was filtered and recrystallized from ethanol (yield 52%, m.p. 142-143 ^{o}C).



Scheme S2. *Synthesis of 3-phenyl-2,4-thiazolidinedione*

2.4. Characterization methods

The ^{1}H and ^{13}C NMR spectral measurements were done on a Varian Gemini 200. The spectra were recorded at room temperature in deuterated chloroform ($CDCl_3$) at ambient temperature. The chemical shifts are expressed in ppm values referenced to TMS (δ_H=0 ppm) in ^{1}H NMR spectra, and the residual solvent signal (δ_C=39.5 ppm,) in ^{13}C NMR spectra. The chemical shifts were assigned by the complementary use of DEPT–, two dimensional ^{1}H–^{13}C correlation HETCOR and by selective INEPT long-range experiments. Fourier-transform infrared (FTIR) spectra were recorded by using FTIR BOMEM MB 100 in the form of KBr pellets in the transmission mode between 400 i 4000 cm^{-1} with a resolution of 4 cm^{-1}. Elemental analysis (C, H, N) was performed using a VARIO EL III Elemental analyzer, and O, F, Cl, and Br content was calculated as substraction. The UV absorption spectra were measured in a range 200-600 nm by using Shimadzu 1700 UV/Vis spectrophotometer. The UV/Vis spectra were taken in spectro quality solvents (Fluka) at a concentration of 1×10^{-5} mol dm^{-3}. Three measurements were performed and mean value was presented.

2.5. Theoretical calculations

Geometries of all molecular species were optimized by the MP2 method using 6-31G(d,p) basis set. In order to find the global minimum on the potential energy surface,multiple geometry optimizations were performed for every compound, with varying rotatable torsion angle (θ, Scheme 1) for increment of 30° and minimizing the energy with respect to all geometrical parameters.The nature of the lowest energy minimum was further confirmed with frequency calculations; no negative frequencies was found.

Theoretical absorption spectra and ground/excited state propereties are calculated on MP2/6-31G(d,p) optimized geometries using time-dependant (TD) density functional theory (DFT) method. The TD-DFT calculations were done in acetonitrile with CAM-B3LYP long range corrected functional (Yanai et al., 2004) and 6-311G(d,p) basis set. Qualitative charge transfer indices: the charge-transfer distance (D_{CT}), amount of transferred charge (Q_{CT}), and the value of variation of dipole moment between the ground and excited states (μ_{CT}) were evaluated according to method proposed by Le Bahers *et al*. (Le Bahers et al., 2011).

NMR chemical shifts were calculated on the MP2 optimized structures using GIAO calculations in chloroform as a solvent, with the specially parameterized WP04 functional using aug-cc-pVDZ basis set. This method was proven to give best accuracy/cost ratio in NMR chemical shift prediction (Jain et al., 2009). The calculated values of ^{13}C chemical shifts are scaled relative to ^{13}C chemical shift of TMS, calculated with the same method. Solvents in NMR and TD-DFT calculations were simulated with Polarizable Continuum model (PCM). All quantum chemical calculations were carried out using the Gaussian09 program package (Frisch et al., 2009).

3. Results and discussion

3.1. Results of the characterization of series 1 and series 2

5-benzylidene-3-methyl-2,4-thiazolidinedione (1a) (Yang et al., 2005). White solid; Yield: 79%, Melting point (m.p.): 130-131 °C (lit. m.p. 133 ^{o}C); ^{1}H NMR: 3.2 (3H, s, N-CH$_3$); 7.4 (2H, d, Ph); 7.5 (2H, d, Ph); 7.3 (H, s, Ph) 7.9 (1H, s, =CH-); ^{13}C NMR: 27.9 (CH3, N-CH$_3$); 130.2 (C3`, C5`, Ph); 129.2 (C2', C6', Ph); 121.4 (C5, TZD); 133.7 (C6, =CH-); 133.2 (C1', Ph); 128.6 (C4', Ph); 166.4 (C4, 4-C=O); 167.9 (C2, 2-C=O); IR (KBr, cm^{-1}): 3036 (C-H stretching of phenyl group); 1742 (C=O stretching); 1672 (amide band I – C2=O and C4=O stretching);

Elemental Analysis:

Calculated: %C, 60.26; %H, 4.14; %N, 6.39; %O, 14.59; %S, 14.62

Found: %C, 60.20; %H, 4.17; %N, 6.40 %O, 14.60; %S, 14.63

5-(4-methylbenzylidene)-3-methyl-2,4-thiazolidinedione (1b) (Chandrappa et al., 2008)**.** White solid; Yield: 73%, m.p.: 148-150 °C (lit. m.p. 125-127 ^{o}C); ^{1}H NMR: 2.4 (3H, s, Ph-CH$_3$); 3.2 (3H, s, N-CH$_3$); 7.3 (2H, d, Ph); 7.9 (1H, s, =CH-); 7.4 (2H, d, Ph); ^{13}C NMR: 21.5 (CH$_3$, Ph); 27.8 (CH$_3$, N-CH$_3$); 130.3 (C3', C5',Ph); 129.9 (C2', C6', Ph); 120.2 (C5, TZD); 141.2 (C6, =CH-); 130.4 (C1', Ph); 133.8 (C4', Ph); 166.5 (C4, 4-C=O); 168.1 (C2, 2-C=O); IR (KBr, cm^{-1}): 3013 (C-H stretching of phenyl group); 1732 (C=O stretching); 1685 (amide band I – C2=O and C4=O stretching); Elemental Analysis:

Calculated: %C, 61.78; %H, 4.75; %N, 6.00; %O, 13.72; %S, 13.74

Found: %C, 61.79; %H, 4.67; %N, 6.06; %O, 13.80; %S, 13.68

5-(4-methoxybenzylidene)-3-methyl-2,4-thiazolidinedione (1c) (Yang et al., 2005). Yellow solid; Yield: 88%, m.p.: 148-150 °C (lit. m.p. 145-147 ^{o}C); ^{1}H NMR: 2.9 (3H, s, OCH$_3$); 3.1 (3H, s, N-CH$_3$); 6.9 (2H, d, Ph); 7.2 (4H, dd, Ph); 7.9 (1H, s, =CH-); ^{13}C NMR: 27.9 (CH$_3$, N-CH$_3$); 55.7 (CH$_3$, OCH$_3$); 113.9; 115.2 (C3', C5', Ph); 118.4 (C5, TZD); 125.7 (C1`, Ph); 130.8 (C6, =CH-); 132.5; 132.9 (C2', C6', Ph); 159.3 (C4', Ph); 166.2 (C4, 4-C=O); 173.8 (C2, 2-C=O); IR (KBr, cm^{-1}): 3015 (C-H stretching of phenyl group); 1731 (C=O stretching); 1677 (amide band I – C2=O and C4=O stretching);

Elemental Analysis:

Calculated: %C, 57.82; %H, 4.45; %N, 5.62; %O, 19.25; %S, 12.86

Found: %C, 57.80; %H, 4.46; %N, 5.59; %O, 19.21; %S, 12.94

5-(4-nitrobenzylidene)-3-methyl-2,4-thiazolidinedione (1h) (Romagnoli et al., 2013) 12]**.** Yellow solid; Yield: 75%, m.p.: 220-222 °C (lit m.p. 222-224 ^{o}C); ^{1}H NMR: 3.1 (3H, s, N-CH_3); 7.9 (2H, d, Ph); 8.0 (1H, s, =CH-); 8.3 (2H, d, Ph); ^{13}C NMR: 28.2 (CH_3, N-CH_3); 124.6 (C3', C5', Ph); 130.1; 131.2 (C2', C6', Ph); 126.0 (C5, TZD); 134 (C6, =CH-); 139.5 (C1', Ph); 147.8 (C4', Ph); 166.3 (C4, 4-C=O); 172.6 (C2, 2-C=O); IR (KBr, cm^{-1}): 3029 (C-H stretching of phenyl group); 1744 (C=O stretching); 1678 (amide band I – C2=O and C4=O stretching);

Elemental Analysis:

Calculated: %C, 50.00; %H, 3.05; %N, 10.60; %O, 24.22; %S, 12.13

Found: %C, 50.04; %H, 2.99; %N, 10.63; %O, 24.19; %S, 12.15

5-benzylidene-3-phenyl-2,4-thiazolidinedione (2a) (Yang et al., 2008). White solid; Yield: 89%, m.p.: 209-209.8 °C (lit m.p. 208-209 ^{o}C); ^{1}H NMR: 7.3 (H, s, N-Ph); 7.4 (H, s, Ph); 7.4 (2H, s, Ph); 7.5 (4H, m, N-Ph); 7.6 (2H, m, Ph); 8.0 (1H, s, =CH-); ^{13}C NMR: 121.0 (C5, TZD); 127.3 (C3", C5", N-Ph); 129.3 (C2', C3', C5', C6', Ph); 129.4 (C4', Ph; C4", C5", C6" N-Ph); 132.6 (C1', N-Ph); 130.4 (C1', Ph); 134.6 (C6, =CH-), 165.7 (C2, 2-C=O), 167.3 (C4, 4-C=O); IR (KBr, cm^{-1}): 3066 (C-H stretching of phenyl group); 1754 (C=O stretching); 1696 (amide band I – C2=O i C4=O stretching);

Elemental Analysis:

Calculated: %C, 68.31; %H, 3.94; %N, 4.98; %O, 11.37; %S, 11.40

Found: %C, 68.29; %H, 3.95; %N, 5.04; %O, 11.40; %S, 11.32

5-(4-methylbenzylidene)-3-phenyl-2,4-thiazolidinedione (2b) (Yang et al., 2008). Yellow solid; Yield: 80%, m.p.: 190-191 °C (lit m.p. 190-191 ^{o}C); ^{1}H NMR: 2.4 (3H, s, CH_3-Ph); 7.2-7.4 (4H, m, Ph); 7.4-7.6 (5H, m, N-Ph); 8.0 (1H, s, =CH-); ^{13}C NMR: 21.6 (CH_3, Ph); 119.8 (C5, TZD); 127.3 (C2", C4 ", C6", *N*-Ph); 129.3 (C3', C5', Ph; C3", C5", *N*-Ph); 130.4 (C1', Ph); 132.7 (C1", N-Ph); 134.6 (C4’, Ph); 141.5 (C6, =CH-); 165.8 (C4, 4-C=O); 167.4 (C2, 2-C=O); IR (KBr, cm^{-1}): 3045 (C-H stretching of phenyl group); 1743 (C=O stretching); 1671 (amide band I – C2=O i C4=O stretching);

Elemental Analysis:

Calculated: %C, 69.13; %H, 4.44; %N, 4.74; %O, 10.83; %S, 10.86

Found: %C, 69.23; %H, 4.42; %N, 4.75; %O, 10.77; %S, 10.83

5-(4-methoxybenzylidene)-3-phenyl-2,4-thiazolidinedione (2c) (Yang et al., 2008). White solid; Yield: 79%, m.p.: 199-201 °C (lit m.p. 200-202 ^{o}C); ^{1}H NMR: 3.9 (3H, s, OCH_3); 7.0 (2H, d, Ph); 7.3 (1H, s, *N*-Ph); 7.4 (2H, dd, Ph); 7.4-7.6 (4H, m, *N*-Ph); 7.9 (1H, s, =CH-); ^{13}C NMR: 55.5 (OCH_3, Ph); 114.8 (C3’, C5’, Ph); 117.9 (C5, TZD);

125.9 (C1', Ph); 127.3 (C2", C4", C6", N-Ph); 129.2 (C3", C5", *N*-Ph); 129.4 (C2', C6', Ph); 132.4 (C1", *N*-Ph); 134.4 (C6, =CH-); 161.6 (C4', Ph); 165.9 (C4, 4-C=O); 167.5 (C2, 2-C=O); IR (KBr, cm^{-1}): 3062 (C-H stretching of phenyl group); 1750 (C=O stretching); 1694 (amide band I – C2=O i C4=O stretching);

Elemental Analysis:

Calculated: %C, 65.58; %H, 4.21; %N, 4.50; %O, 15.42; %S, 10.30

Found: %C, 65.60; %H, 4.23; %N, 4.47; %O, 15.46; %S, 10.24

5-(4-nitrobenzylidene)-3-phenyl-2,4-thiazolidinedione (2h) (Yang et al., 2008)**.** Orange solid; Yield: 80%, m.p.: 249-250°C (lit m.p. 238-240°C); ^{1}H NMR: 7.3 (1H, s, *N*-Ph); 7.4 (4H, m, *N*-Ph); 7.7 (2H, d, Ph); 8.0 (1H, s, =CH-); 8.4 (2H, d, Ph); ^{13}C NMR: 124.5 (C3', C5', Ph); 127.2 (C2", C4", C6", N-Ph); 129.6 (C2', C6', Ph, C3", C5", N-Ph); 130.7 (C1", N-Ph); 131.2 (C1', Ph); 131.4 (C6, =CH-); 132.3 (C5, Ph); 139.3 (C1', Ph); 166.4 (C4, 4-C=O); 172.6 (C2, 2-C=O); IR (KBr, cm^{-1}): 3022 (C-H stretching of phenyl group); 1744 (C=O stretching); 1695 (amide band I – C2=O i C4=O stretching);

Elemental Analysis:

Calculated: %C, 58.89; %H, 3.09; %N, 8.58; %O, 19.61; %S, 9.83

Found: %C, 58.91; %H, 2.97; %N, 8.65; %O, 19.64; %S, 9.84

5-(3,4-dimetoxybenzylidene)-3-phenyl-2,4-thiazolidinedione (2i) (Yang et al., 2008)**.** Yellow solid; Yield: 85%, m.p.: 208-209 °C (lit m.p. 209-210°C); ^{1}H NMR: 3.9 (3H, s, Ph-OCH$_3$); 3.9 (3H, s, Ph-OCH$_3$); 7.0 (H, t, CH (C3')); 7.0 (H, d, CH (C2')); 7.2 (H, d, CH (C6')); 7.3 (2H, m, N-Ph); 7.5 (3H, m, N-Ph); 7.9 (1H, s, =CH-); ^{13}C NMR: 55.9, 56.0 (OCH$_3$, Ph); 111.4 (C6', Ph); 126.1 (C3', Ph); 126.1 (C4", N-Ph); 124.8 (C2", C6", N-Ph); 127.3 (C3", C5", N-Ph); 129.4 (C5, Ph); 132.7 (C1', Ph); 134.5 (C1'', N-Ph); 134.6 (C2', Ph); 149.3 (C4', Ph); 149.4 (C5', Ph); 151.3 (C6, =CH-); 166.8 (C4, 4-C=O); 167.3 (C2, 2-C=O); IR (KBr, cm^{-1}): 3052 (C-H stretching of phenyl group); 1736 (C=O stretching); 1694 (amide band I – C2=O i C4=O stretching);

Elemental Analysis:

Calculated: %C, 63.33; %H, 4.43; %N, 4.10; %O, 18.75; %S, 9.39

Found: %C, 63.30; %H, 4.39; %N, 4.14; %O, 18.79; %S, 9.38

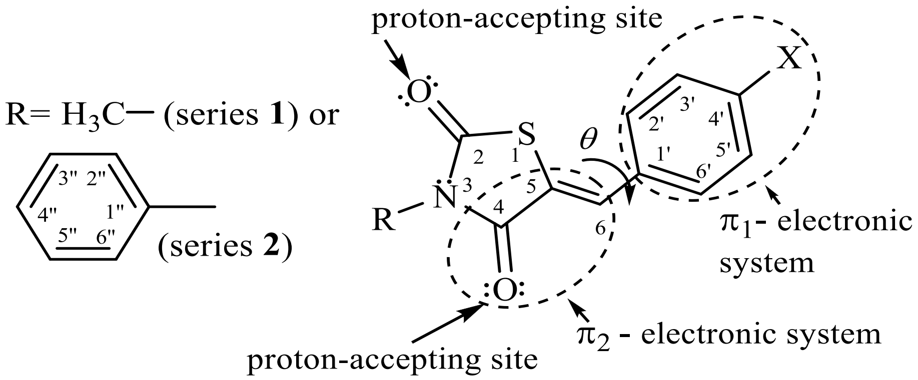


Fig. S1. Electronic structure of 5-arylidene-3-substituted-2,4-thiazolidinediones with *π*-electronic units and marked sites responsible for solute/solvent interactions

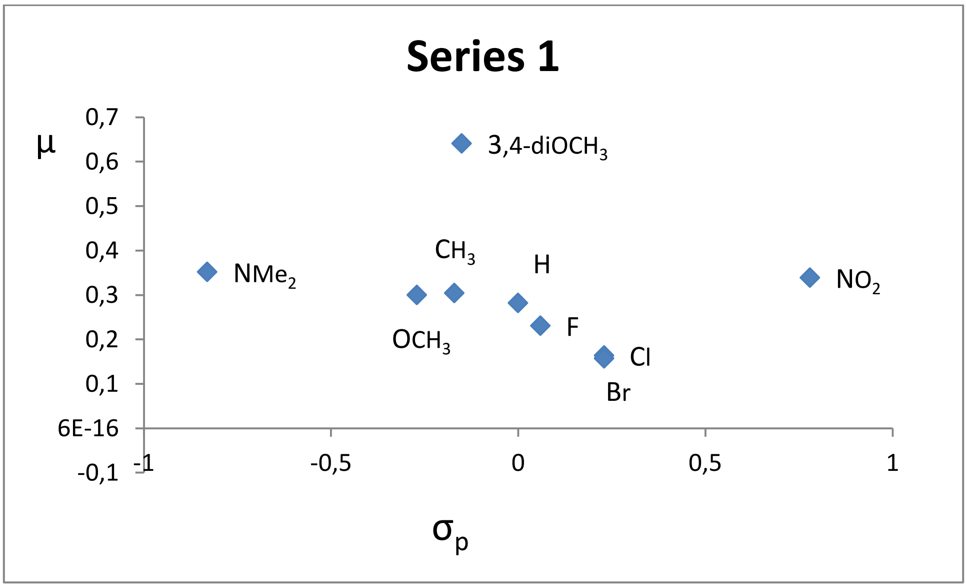


Fig. S2. Correlation od calculated dipole moment *vs* substituent parameters for compounds **1a-1i**

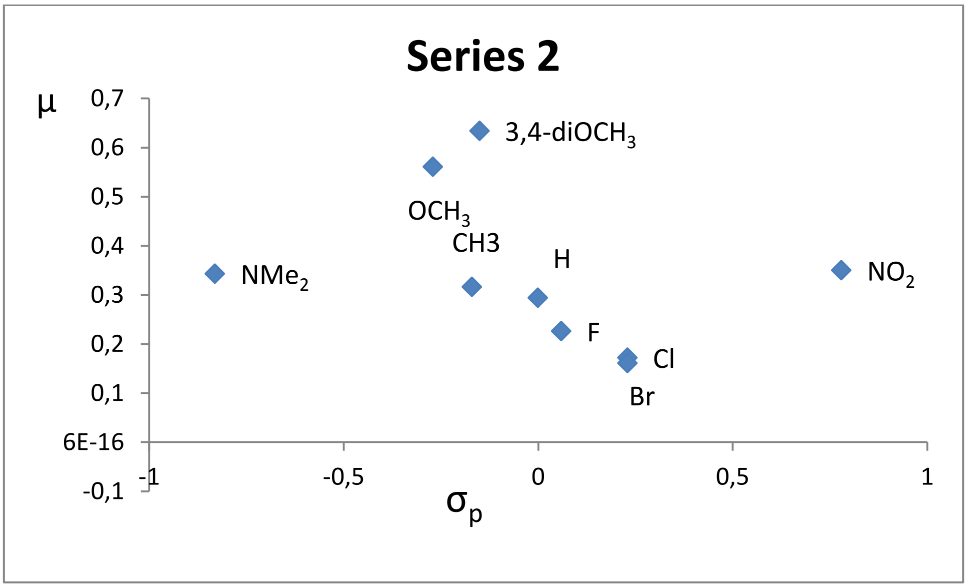


Fig. S3. Correlation od calculated dipole moment vs substituent parameters for compounds **2a-2i**

Table S4. Calculated NMR chemical shifts for compounds **1a-1i**.

	1a		1b		1c		1d		1e		1f		1h		1g		1i
C2	176.6	**C2**	176.8	**C2**	176.7	**C2**	176.3	**C2**	176.3	**C2**	176.4	**C2**	176.6	**C2**	175.4	**C2**	175.5
C4	166.4	**C4**	166.2	**C4**	166.1	**C4**	166.4	**C4**	166.3	**C4**	166.3	**C4**	165.8	**C4**	166.5	**C4**	166.3
C5	128.4	**C5**	127.3	**C5**	125.9	**C5**	129.5	**C5**	129.2	**C5**	128.7	**C5**	122.3	**C5**	134.7	**C5**	126.3
C6	133.6	**C6**	133.4	**C6**	132.9	**C6**	131.8	**C6**	131.7	**C6**	131.9	**C6**	132.9	**C6**	130.2	**C6**	134.0
C(CH3)	27.3	**C(CH3)**	27.3	**C(CH3)**	27.6	**C(CH3)**	27.9	**C(CH3)**	27.6	**C(CH3)**	27.4	**C(CH3)**	27.1	**C(CH3)**	27.9	**C(CH3)**	27.5
C1'	132.0	**C1'**	129.4	**C1'**	125.1	**C1'**	131.2	**C1'**	130.7	**C1'**	129.5	**C1'**	119.4	**C1'**	139.5	**C1'**	128.5
C2'	127.9	**C2'**	127.6	**C2'**	128.7	**C2'**	128.6	**C2'**	128.6	**C2'**	129.6	**C2'**	129.2	**C2'**	128.3	**C2'**	122.0
C3'	124.2	**C3'**	124.9	**C3'**	113.4	**C3'**	127.3	**C3'**	124.7	**C3'**	112.3	**C3'**	108.9	**C3'**	120.7	**C3'**	118.9
C4'	126.0	**C4'**	140.9	**C4'**	159.7	**C4'**	144.3	**C4'**	143.1	**C4'**	161.7	**C4'**	150.8	**C4'**	148.0	**C4'**	149.4
C5'	123.7	**C5'**	125.0	**C5'**	108.1	**C5'**	127.8	**C5'**	125.0	**C5'**	112.3	**C5'**	110.6	**C5'**	121.6	**C5'**	150.5
C6'	123.0	**C6'**	122.2	**C6'**	125.3	**C6'**	123.9	**C6'**	123.8	**C6'**	124.8	**C6'**	124.5	**C6'**	123.7	**C6'**	108.4
H(CH3)	3.2	**H(CH3)**	3.2	**H(CH3)**	3.2	**H(CH3)**	3.2	**H(CH3)**	3.2	**H(CH3)**	3.2	**H(CH3)**	3.2	**H(CH3)**	3.3	**H(CH3)**	3.2
H6	8.3	**H6**	8.3	**H6**	8.3	**H6**	8.3	**H6**	8.3	**H6**	8.3	**H6**	8.2	**H6**	8.4	**H6**	8.2
H2'	7.6	**H2'**	7.5	**H2'**	7.6	**H2'**	7.5	**H2'**	7.6	**H2'**	7.7	**H2'**	7.6	**H2'**	7.8	**H2'**	7.2
H3'	7.6	**H3'**	7.4	**H3'**	7.0	**H3'**	7.5	**H3'**	7.4	**H3'**	7.3	**H3'**	6.8	**H3'**	8.6	**H3'**	7.2
H4'	7.6	**H5'**	7.4	**H5'**	7.0	**H5'**	7.6	**H5'**	7.5	**H5'**	7.3	**H5'**	6.9	**H5'**	8.6	**H6'**	7.1
H5'	7.6	**H6'**	7.7	**H6'**	7.7	**H6'**	7.6	**H6'**	7.7	**H6'**	7.8	**H6'**	7.6	**H6'**	7.9	**C(OCH$_3$)meta**	53.1
H6'	7.7	**C(Me)**	20.9	**C(OMe)**	53.4							**C1(NMe2)**	38.1			**C(OCH$_3$)para**	56.0
		H(Me)	2.3	**H(OMe)**	3.8							**C2(NMe2)**	36.6			**H(OCH3)meta**	3.9
												H1(NMe2)	2.9			**H(OCH3)para**	3.8
												H2(NMe2)	2.9				

Table S5. Calculated NMR chemical shifts for compounds **2a**-**2i**.

2a		**2b**		**2c**		**2d**		**2e**		**2f**		**2h**		**2g**		**2i**	
C2	179.7	**C2**	179.7	**C2**	179.6	**C2**	179.1	**C2**	179.2	**C2**	179.3	**C2**	179.7	**C2**	178.5	**C2**	179.2
C4	171.8	**C4**	171.8	**C4**	171.7	**C4**	171.8	**C4**	171.8	**C4**	171.6	**C4**	171.2	**C4**	171.9	**C4**	171.9
C5	131.3	**C5**	129.8	**C5**	127.8	**C5**	132.2	**C5**	132.1	**C5**	131.5	**C5**	124.6	**C5**	137.8	**C5**	129.2
C6	141.6	**C6**	141.6	**C6**	140.7	**C6**	139.9	**C6**	139.8	**C6**	139.9	**C6**	140.6	**C6**	138.2	**C6**	141.3
C1'	138.4	**C1'**	135.6	**C1'**	130.8	**C1'**	137.5	**C1'**	137.1	**C1'**	135.4	**C1'**	127.2	**C1'**	146.1	**C1'**	135.1
C2'	135.8	**C2'**	136.1	**C2'**	138.7	**C2'**	136.9	**C2'**	137.1	**C2'**	138.1	**C2'**	137.9	**C2'**	136.7	**C2'**	130.1
C3'	131.6	**C3'**	132.3	**C3'**	113.4	**C3'**	135.9	**C3'**	132.9	**C3'**	119.5	**C3'**	116.0	**C3'**	128.4	**C3'**	127.0
C4'	133.9	**C4'**	148.1	**C4'**	168.4	**C4'**	150.5	**C4'**	150.0	**C4'**	172.7	**C4'**	158.2	**C4'**	156.1	**C4'**	158.5
C5'	131.9	**C5'**	132.8	**C5'**	121.6	**C5'**	135.8	**C5'**	132.8	**C5'**	119.5	**C5'**	116.4	**C5'**	128.6	**C5'**	160.5
C6'	131.2	**C6'**	130.8	**C6'**	132.6	**C6'**	132.1	**C6'**	132.3	**C6'**	133.3	**C6'**	132.4	**C6'**	132.0	**C6'**	113.9
C1"	138.3	**C1"**	138.4	**C1"**	138.4	**C1''**	138.1	**C1''**	138.2	**C1"**	138.4	**C1"**	138.9	**C1''**	137.9	**C1"**	138.7
C2"	129.6	**C2"**	129.6	**C2"**	129.6	**C2"**	129.6	**C2"**	129.6	**C2"**	129.9	**C2"**	129.9	**C2"**	129.5	**C2"**	129.8
C3"	131.2	**C3"**	131.1	**C3"**	131.1	**C3"**	131.2	**C3"**	131.2	**C3"**	131.3	**C3"**	131.0	**C3"**	131.4	**C3"**	131.1
C4"	131.4	**C4"**	131.3	**C4"**	131.2	**C4"**	131.6	**C4"**	131.6	**C4"**	131.5	**C4"**	131.0	**C4"**	132.0	**C4"**	131.1
C5"	131.2	**C5"**	131.2	**C5"**	131.2	**C5"**	131.3	**C5"**	131.3	**C5"**	131.2	**C5"**	131.0	**C5"**	131.5	**C5"**	131.0
C6"	129.9	**C6"**	129.9	**C6"**	129.9	**C6"**	129.9	**C6"**	129.9	**C6"**	129.9	**C6"**	129.9	**C6"**	129.9	**C6"**	129.9
H6	8.0	**H6**	8.0	**H6**	7.9	**H6**	7.9	**H6**	7.9	**H6**	8.0	**H6**	7.8	**H6**	8.0	**H6**	7.9
H2'	7.4	**H2'**	7.2	**H2'**	7.3	**H2'**	7.3	**H2'**	7.3	**H2'**	7.4	**H2'**	7.2	**H2'**	7.5	**H2'**	7.0
H3'	7.3	**H3'**	7.1	**H3'**	6.7	**H3'**	7.3	**H3'**	7.2	**H3'**	7.0	**H3'**	6.6	**H3'**	8.3	**H3'**	6.9
H4'	7.3	**H5'**	7.2	**H5'**	6.9	**H5'**	7.4	**H5'**	7.3	**H5'**	7.0	**H5'**	6.6	**H5'**	8.4	**H6'**	7.0
H5'	7.3	**H6'**	7.4	**H6'**	7.4	**H6'**	7.4	**H6'**	7.4	**H6'**	7.5	**H6'**	7.3	**H6'**	7.6	**H2''**	7.3
H6'	7.5	**H2''**	7.3	**H2''**	7.2	**H2''**	7.2	**H2''**	7.2	**H2''**	7.3	**H2''**	7.3	**H2''**	7.2	**H3"**	7.3
H2''	7.3	**H3"**	7.3	**H3"**	7.3	**H3"**	7.3	**H3"**	7.3	**H3"**	7.3	**H3"**	7.3	**H3"**	7.3	**H4"**	7.2
H3"	7.3	**H4"**	7.2	**H4"**	7.2	**H4"**	7.2	**H4"**	7.2	**H4"**	7.2	**H4"**	7.2	**H4"**	7.3	**H5"**	7.3
H4"	7.2	**H5"**	7.3	**H5"**	7.3	**H5"**	7.3	**H5"**	7.3	**H5"**	7.3	**H5"**	7.2	**H5"**	7.3	**H6"**	7.3
H5"	7.3	**H6"**	7.3	**H6"**	7.2	**H6"**	7.2	**H6"**	7.2	**H6"**	7.2	**H6"**	7.2	**H6"**	7.2	**C(OCH$_3$)meta**	55.9
H6"	7.3	**C(Me)**	21.2	**C(OMe)**	56.0							**C1(NMe2)**	40.1			**C(OCH$_3$)para**	59.9
		H(Me)	2.1	**H(OMe)**	3.4							**C2(NMe2)**	40.1			**H(OCH3)meta**	3.6
												H1(NMe2)	2.6			**H(OCH3)para**	3.4
												H2(NMe2)	2.6				

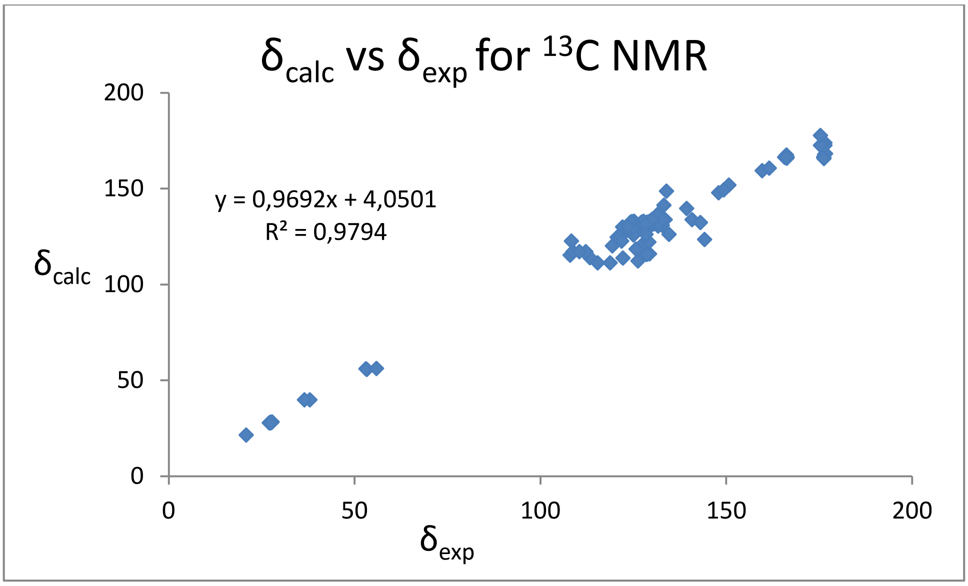


Fig. S4. Correlation od calculated *vs* experimental ^{13}C NMR chemical shifts for compounds **1a-1i**

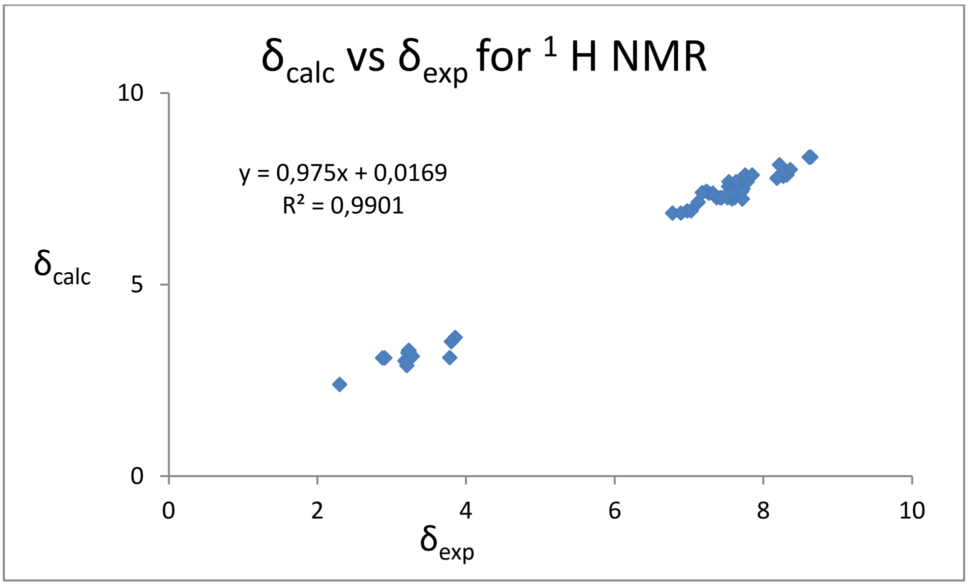


Fig. S5. Correlation od calculated *vs* experimental ^{1}H NMR chemical shifts for compounds **1a-1i**

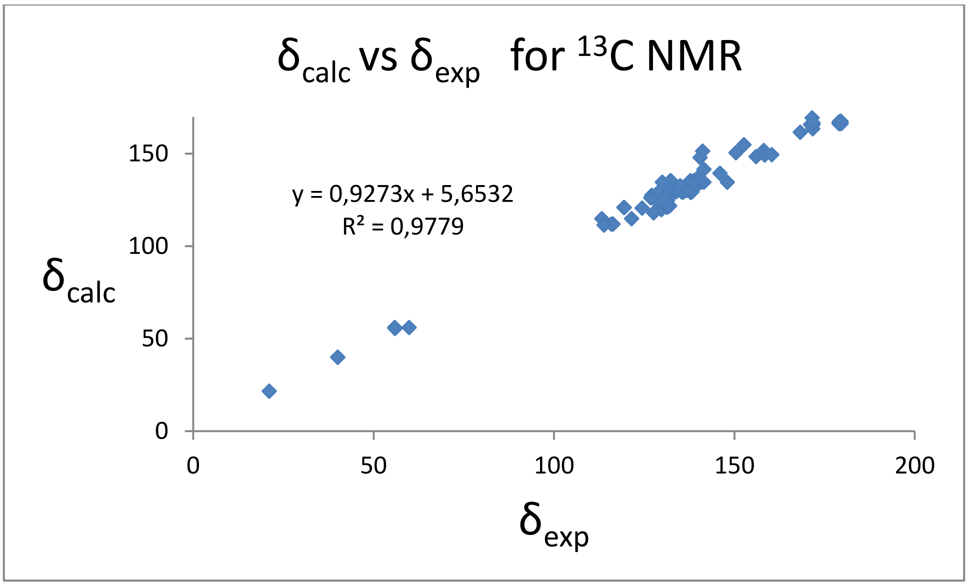


Fig. S6. Correlation od calculated *vs* experimental ^{13}C NMR chemical shifts for compounds **2a-2i**

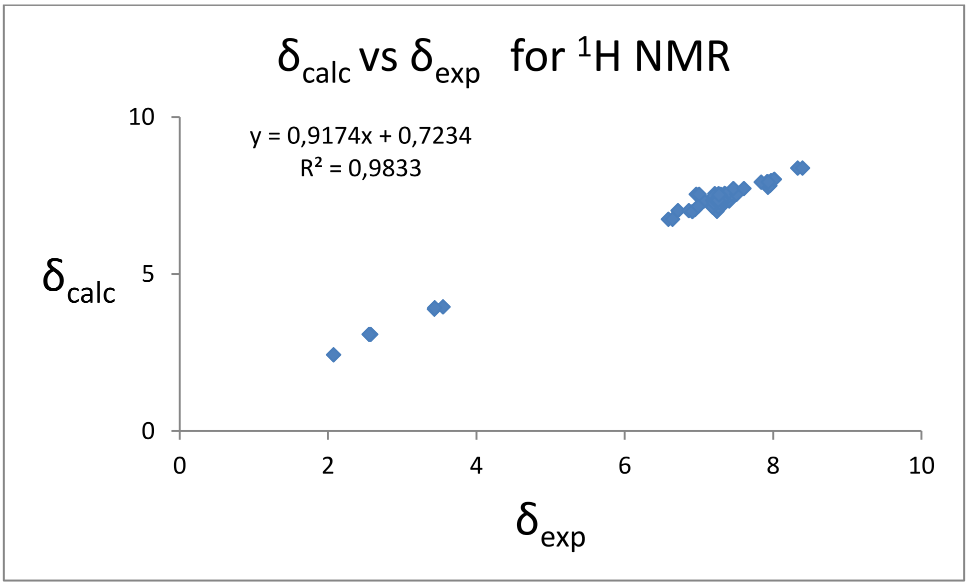


Fig. S7. Correlation od calculated *vs* experimental ^{1}H NMR chemical shifts for compounds **2a-2i**

Table S6. Correlations of the *SCS* values for investigated compounds with SSP equation for C5[*], C6[*] and C1' carbon atoms of 5-arylidene-2,4-thiazolidinediones (Rančić et al., 2013)

Atom		ρ	h	R	F	sd
C5	σ_p	10.46±0.84	–0.45±0.37	0.972	156	1.17
	σ_p^+	6.30±0.67	1.06±0.56	0.952	88	1.53
C6	σ_p	–1.73±0.32	–0.15±0.14	0.872	28	0.46
	σ_p^+	–1.02±0.22	–0.39±0.18	0.842	22	0.50
C1’	σ_p	13.43±1.31	–2.86±0.58	0.960	106	1.83
	σ_p^+	8.45±0.54)	–0.75±0.45	0.982	246	1.23

[*] C5 and C6 are equivalent to C_β and C_α, respectively, used in a previous study (Rančić et al., 2013)

Table S7. Correlation results of the *SCS* values with the DSP (Reynolds) equation for C5, C6 and C1' carbon atoms of 5-arylidene-2,4-thiazolidinediones (Rančić et al., 2013)

Atom	ρ_F	ρ_R	R	F	sd	$\lambda=\rho_R/\rho_F$
C5	8.15±1.75	17.03±1.65	0.977	84	2.09	2.09
C6	–1.65±0.85	–2.41±0.80	0.827	9	0.55	1.46
C1’	6.35±1.52	24.76±1.43	0.990	193	0.99	3.90

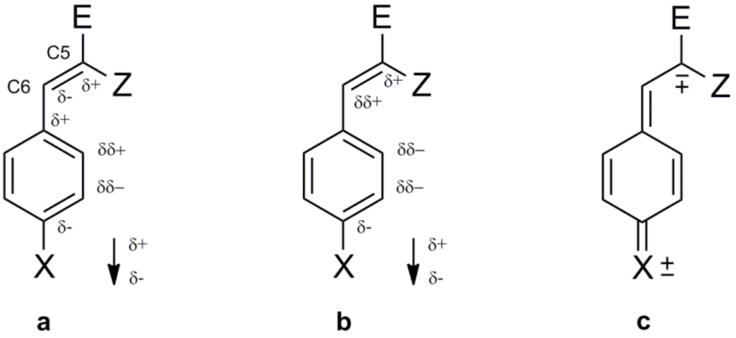


Fig. S8. Mechanisms of the transmission of substituent effect in electron-acceptor substituted compound: a) localized π-polarization b) extended π-polarization, and c) resonance interaction (Craik and Brownlee, 1983; Reynolds et al., 1983).

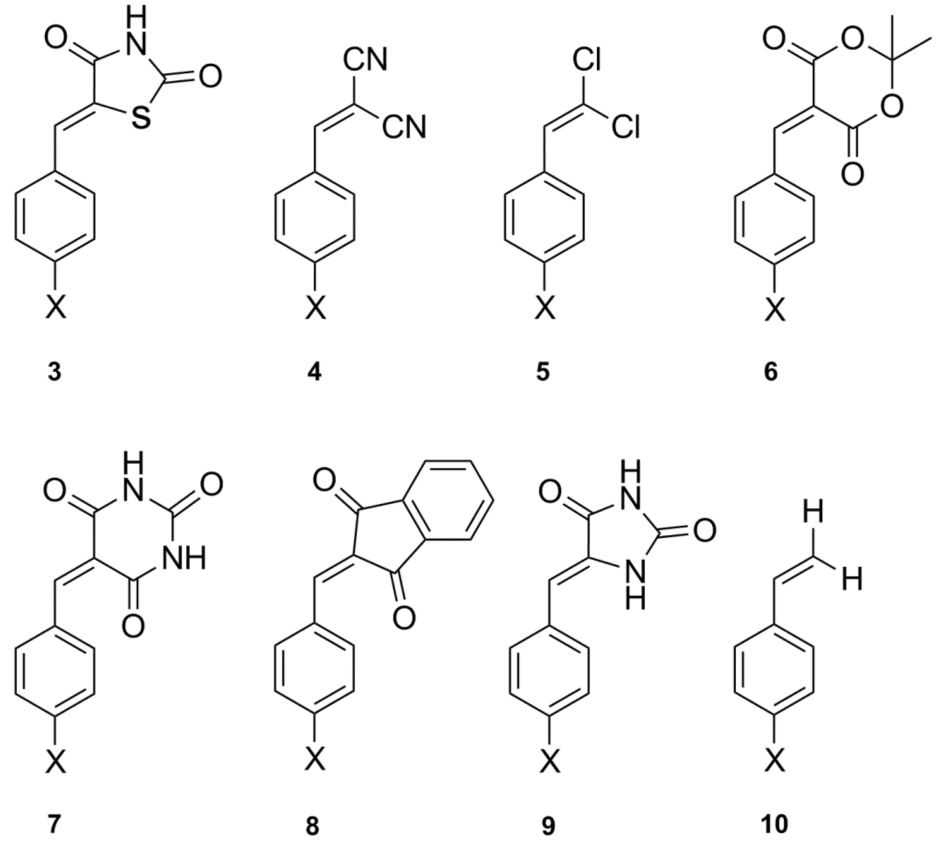


Fig. S9. Styrene series **3** – **10** used in comparative analysis (Rančić et al., 2013)

Table S8. Correlation results for series **3**–**10** with SSP equation for C5[*] carbon (Rančić et al., 2013)

Series		ρ	h	R	F	sd
3	σ_p	10.46±0.84	–0.45±0.37	0.972	156	1.17
	σ_p^+	6.30±0.67	1.06±0.56	0.952	88	1.53
4	σ_p	10.74±1.84	2.02±0.82	0.946	34	1.79
	σ_p^+	8.32±0.46	–0.47±0.25	0.994	322	0.61
5	σ_p	9.52±0.76	1.52±0.39	0.984	155	1.03
	σ_p^+	6.16±0.13	0.21±0.10	0.999	2176	0.28
6	σ_p	10.18±1.65	–1.88±0.70	0.940	38	1.85
	σ_p^+	6.43±0.56	–0.46±0.43	0.981	132	1.04
7	σ_p	7.52±0.84	–1.38±0.39	0.959	80	1.16
	σ_p^+	5.02±0.22	–0.16±0.16	0.994	544	0.46
8	σ_p	5.91±0.48	–0.70±0.20	0.980	149	0.56
	σ_p^+	3.66±0.10	–0.13±0.07	0.998	1218	0.20
9	σ_p	4.33±0.28	–0.60±0.14	0.988	236	0.40
	σ_p^+	2.78±0.13	0.16±0.11	0.993	436	0.30
10	σ_p	5.78±0.36	–0.21±0.17	0.987	258	0.51
	σ_p^+	3.59±0.35	0.80±0.27	0.968	105	0.78

[*] C5 is equivalent to C_β used in a previous study (Rančić et al., 2013)

Table S9. Correlation results for series **3**–**10** with SSP equation for C6* carbon

Series		ρ	h	R	F	sd
3	σ_p	–1.73±0.32	–0.15±0.14	0.872	28	0.46
	σ_p^+	–1.02±0.22	–0.39±0.18	0.842	22	0.50
4	σ_p	–1.51±0.32	–0.36±0.14	0.925	24	0.31
	σ_p^+	–1.03±0.35	–0.60±0.19	0.828	9	0.46
5	σ_p	–0.94±0.74	–1.57±0.39	0.490	2	1.00
	σ_p^+	–0.44±0.51	–1.72±0.41	0.360	1	1.07
6	σ_p	–1.81± 0.50	–0.78±0.22	0.849	13	0.57
	σ_p^+	–0.97± 0.38	–0.98±0.29	0.753	7	0.71
7	σ_p	–2.32±0.66	–1.12±0.31	0.800	12	0.90
	σ_p^+	–1.28±0.52	–1.46±0.37	0.683	6	1.10
8	σ_p	–2.74±0.59	–0.82±0.24	0.885	22	0.68
	σ_p^+	–1.48±0.48	–1.15±0.34	0.785	10	0.91
9	σ_p	–3.34±0.22	–0.45±0.11	0.987	235	0.31
	σ_p^+	–2.06±0.27	–1.02±0.23	0.952	58	0.60
10	σ_p	–1.10±0.28	–0.81±0.13	0.824	15	0.40
	σ_p^+	–0.59±0.22	–0.99±0.17	0.707	7	0.50

* C6 is equivalent to C_α used in a previous study (Rančić et al., 2013)

Table S10. The correlation results for the C5 atom in series **3**–**10** obtained by the use of the DSP Reynolds model (Rančić et al., 2013)

Series	ρ_F	ρ_R	R	$\lambda=\rho_R/\rho_F$
3	8.15±1.75	17.03±1.65	0.977	2.09
4	6.21± 2.31	18.59±2.92	0.981	2.99
5	7.38± 3.48	14.70±3.27	0.961	1.99
6	5.87±0.29	18.04±0.24	0.925	3.07
7	4.93±0.53	12.45±2.71	0.933	2.53
8	4.54±0.19	10.07±1.30	0.974	2.22
9	2.67±0.72	7.52±0.69	0.988	2.82
10	5.25± 0.14	8.52±0.13	0.999	1.62

Table S11. The correlation results for the C6 atom in series **3**–**10** obtained by the use of the DSP Reynolds model (Rančić et al., 2013)

Series	ρ_F	ρ_R	R	$\lambda=\rho_R/\rho_F$
3	–1.65±0.85	–2.41±0.80	0.827	1.46
4	–2.36±0.23	–0.59±0.33	0.990	0.25
5	–3.61±1.53	–0.58±0.27	0.787	0.16
6	–3.44±0.47	–1.53±0.49	0.975	0.44
7	–4.60±0.92	–1.49±0.29	0.934	0.32
8	–4.72±0.65	–2.54±0.71	0.971	0.54
9	–3.84±0.57	–4.38±0.55	0.988	1.14
10	–2.62±0.15	–0.17±0.15	0.993	0.06

Table S12. Elements of the optimized geometries of 5-arylidene-2,4-thiazolidinedione compounds obtained by the use of *ab initio* MP2 method (Rančić et al., 2013)

Comp./ substituent	Interatomic distance (Å)							Torsion angle θ (^{o})
	C2–N3	N3–C4	C4–C5	C5–C6	C6–C7	C4=O	C2=O	
1/H	1.3867	1.3909	1.4925	1.3505	1.4573	1.2224	1.2138	27.36
2/CH$_3$	1.3867	1.3912	1.4919	1.3507	1.4560	1.2225	1.2140	26.60
3/iPr	1.3866	1.3913	1.4918	1.3508	1.4558	1.2225	1.2140	26.42
4/OCH$_3$	1.3862	1.3918	1.4904	1.3513	1.4536	1.2229	1.2142	23.89
5/OC$_2$H$_5$	1.3862	1.3919	1.4903	1.3513	1.4534	1.2229	1.2143	23.79
6/OH	1.3863	1.3916	1.4908	1.3511	1.4542	1.2228	1.2141	24.52
7/NH$_2$	1.3857	1.3926	1.4891	1.3517	1.4521	1.2230	1.2145	22.52
8/N(CH$_3$)$_2$	1.3855	1.3931	1.4882	1.3524	1.4501	1.2233	1.2148	20.99
9/Cl	1.3866	1.3906	1.4931	1.3510	1.4557	1.2222	1.2133	25.96
10/Br	1.3866	1.3905	1.4933	1.3510	1.4558	1.2222	1.2133	26.04
11/CN	1.3867	1.3898	1.4949	1.3515	1.4560	1.2220	1.2127	26.57
12/NO$_2$	1.3867	1.3897	1.4949	1.3519	1.4558	1.2221	1.2126	26.53

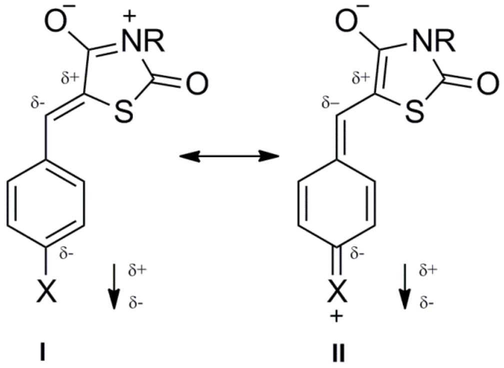


Fig. S9. Amide group participation (I) and extended resonance resonance interaction (II) in series **3** (Rančić et al., 2013)

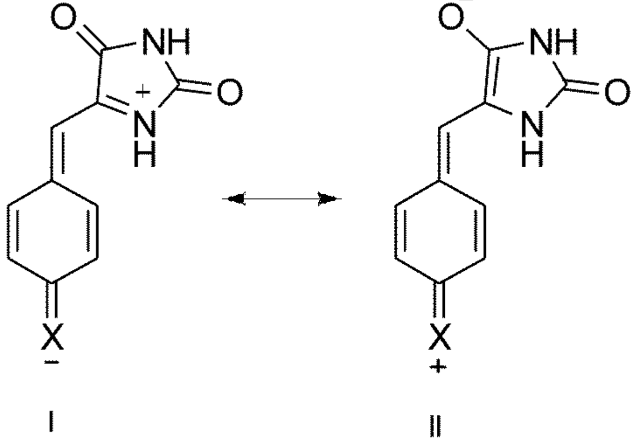
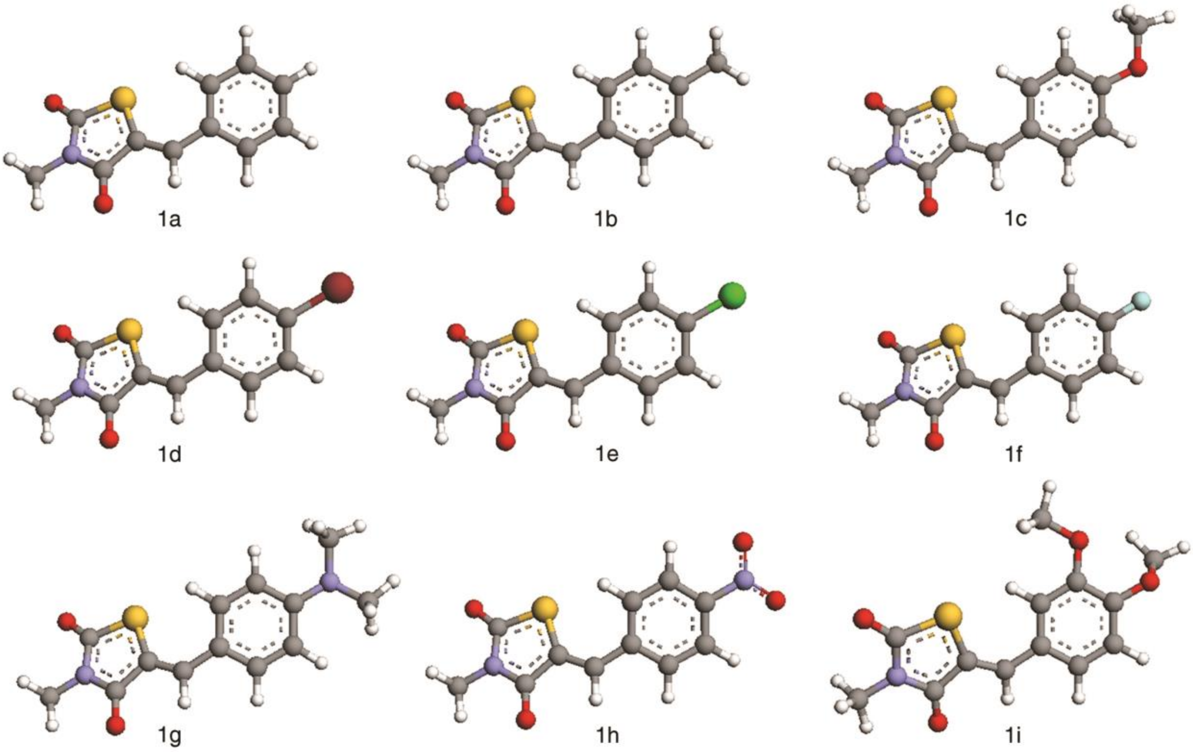


Fig. S10. Resonance structures of 5-arylidenehydantoins for electron-acceptor (I) and electron-donor substituent X (II) (Rančić et al., 2013)

Table S13. Energies of optimized structure of both series **1** and **2**.

Molecule	Isomer	Energy MP2	Energy (kcal)	Molecule	Isomer	Energy MP2	Energy (kcal)
1a	E	–1025.5962	0	**2a**	E	–1216.7453	0
	Z	–1025.6048	–5.3705		Z	–1216.7538	–5.3483
1b	E	–1064.7837	0	**2b**	E	–1255.9328	0
	Z	–1064.7924	–5.4361		Z	–1255.9413	–5.3420
1c	E	–1139.8016	0	**2c**	E	–1330.9507	0
	Z	–1139.8101	–5.3720		Z	–1330.9591	–5.2649
1d	E	–3595.0107	0	**2d**	E	–3786.1596	0
	Z	–3595.0188	–5.0675		Z	–3786.1678	–5.1514
1e	E	–1484.6208	0	**2e**	E	–1675.7697	0
	Z	–1484.6289	–5.0816		Z	–1675.7779	–5.1657
1f	E	–1124.6068	0	**2f**	E	–1315.7557	0
	Z	–1124.6149	–5.1254		Z	–1315.7640	–5.2122
1g	E	–1229.5977	0	**2g**	E	–1350.2973	0
	Z	–1159.1570	–5.4640		Z	–1350.3061	–5.4911
1h	E	–1254.0021	0	**2h**	E	–1420.7466	0
	Z	–1229.6052	–4.7251		Z	–1420.7543	–4.7979
1i	E	–1159.1482	0	**2i**	E	–1445.1513	0
	Z	–1254.0097	–4.7553		Z	–1445.1588	–4.6915



1a

1b

1c

1d

1e

1f

1g

1h

1i

Fig. S11. Optimized geometries of compounds **1a-1i**

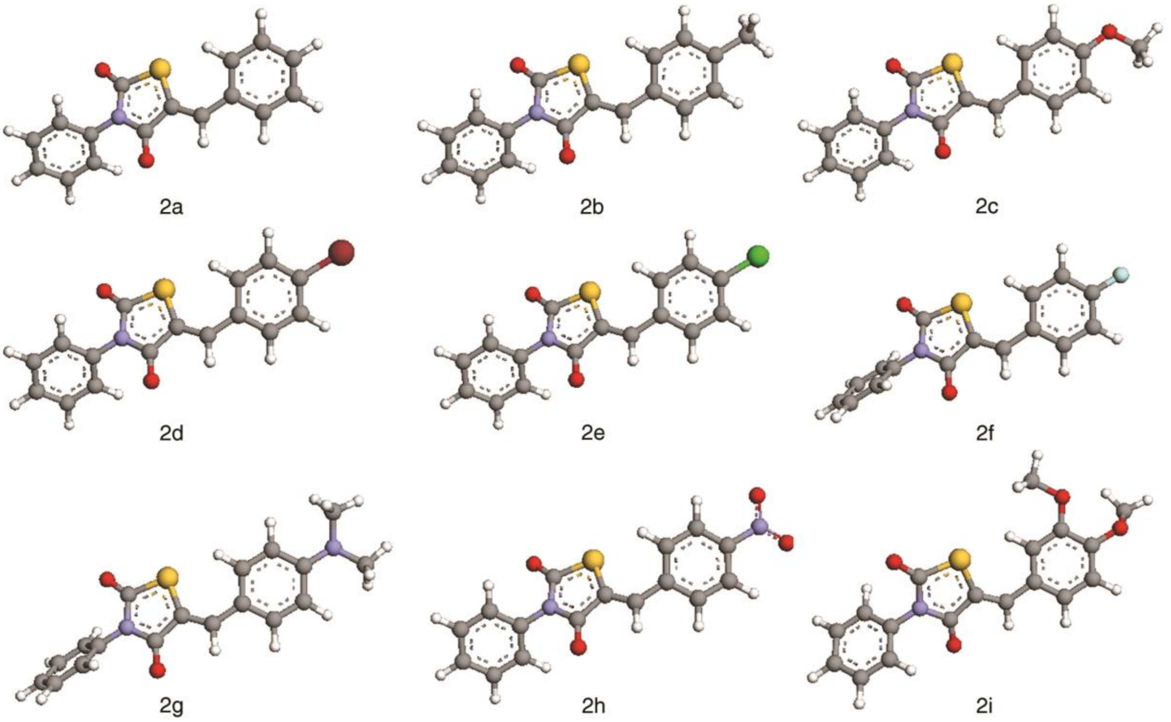


Fig. S12. Optimized geometries of compounds **2a-2i**

Table S14. Elements of the optimized geometries of series **1** obtained by MP2/6-31G(d,p) method.

	N3-CH$_3$	C2-N3	N3-C4	C4-C5	C5-C6	C6-C1'	C4=O	C2=O	θ	μ(D)
1a	1.4551	1.3870	1.3925	1.4910	1.3508	1.4575	1.2250	1.2165	27.64	0.282
1b	1.4550	1.3868	1.3929	1.4903	1.3510	1.4561	1.2251	1.2167	26.89	0.304
1c	1.4548	1.3863	1.3938	1.4889	1.3514	1.4542	1.2253	1.2169	25.50	0.300
1d	1.4555	1.3868	1.3921	1.4918	1.3514	1.4559	1.2248	1.2159	26.32	0.164
1e	1.4555	1.3868	1.3922	1.4917	1.3513	1.4559	1.2249	1.2160	26.25	0.157
1f	1.4553	1.3868	1.3924	1.4911	1.3508	1.4568	1.2249	1.2162	27.10	0.231
1g	1.4544	1.3859	1.3948	1.4867	1.3527	1.4504	1.2259	1.2175	22.57	0.339
1h	1.4560	1.3869	1.3911	1.4934	1.3522	1.4559	1.2247	1.2153	26.75	0.352
1i	1.4551	1.3857	1.3941	1.4889	1.3522	1.4537	1.2253	1.2167	24.07	0.641

Table S15. Elements of the optimized geometries of series **2** obtained by MP2/6-31G(d,p) method

	N3-Ph	C2-N3	N3-C4	C4-C5	C5-C6	C6-C1'	C4=O	C2=O	θ	μ(D)
2a	1.4285	1.3992	1.4028	1.4896	1.3513	1.4571	1.2231	1.2145	27.52	0.294
2b	1.4284	1.3991	1.4033	1.4889	1.3515	1.4557	1.2232	1.2147	26.40	0.316
2c	1.4282	1.3988	1.4040	1.4875	1.3521	1.4534	1.2235	1.2149	24.12	0.561
2d	1.4289	1.3989	1.4022	1.4904	1.3519	1.4556	1.2229	1.2139	26.21	0.172
2e	1.4289	1.3990	1.4022	1.4903	1.3517	1.4556	1.2230	1.2140	26.20	0.161
2f	1.4288	1.3988	1.4026	1.4897	1.3513	1.4565	1.2230	1.2142	27.08	0.226
2g	1.4277	1.3982	1.4057	1.4850	1.3533	1.4499	1.2238	1.2155	22.46	0.350
2h	1.4295	1.3986	1.4009	1.4922	1.3527	1.4555	1.2229	1.2133	26.52	0.343
2i	1.4285	1.3978	1.4047	1.4873	1.3528	1.4533	1.2233	1.2148	24.01	0.634

Table S16. Calculated energies of the HOMO and LUMO orbitals and energy gaps for investigated compounds in solvent acetonitrile

Comp.	HOMO (eV)	LUMO (eV)	Egap (eV)	Comp.	HOMO (eV)	LUMO (eV)	Egap (eV)
1a	–7.843	–1.261	6.582	**2a**	–7.865	–1.323	6.542
1b	–7.684	–1.212	6.472	**2b**	–7.703	–1.272	6.431
1c	–7.437	–1.157	6.280	**2c**	–7.443	–1.215	6.228
1d	–7.821	–1.384	6.437	**2d**	–7.841	–1.443	6.398
1e	–7.836	–1.375	6.461	**2e**	–7.858	–1.443	6.415
1f	–7.819	–1.267	6.552	**2f**	–7.842	–1.327	6.515
1g	–6.852	–1.076	5.776	**2g**	–6.866	–1.139	5.727
1h	–8.156	–2.132	6.024	**2h**	–8.179	–2.160	6.019
1i	–7.484	–1.268	6.216	**2i**	–7.501	–1.330	6.171

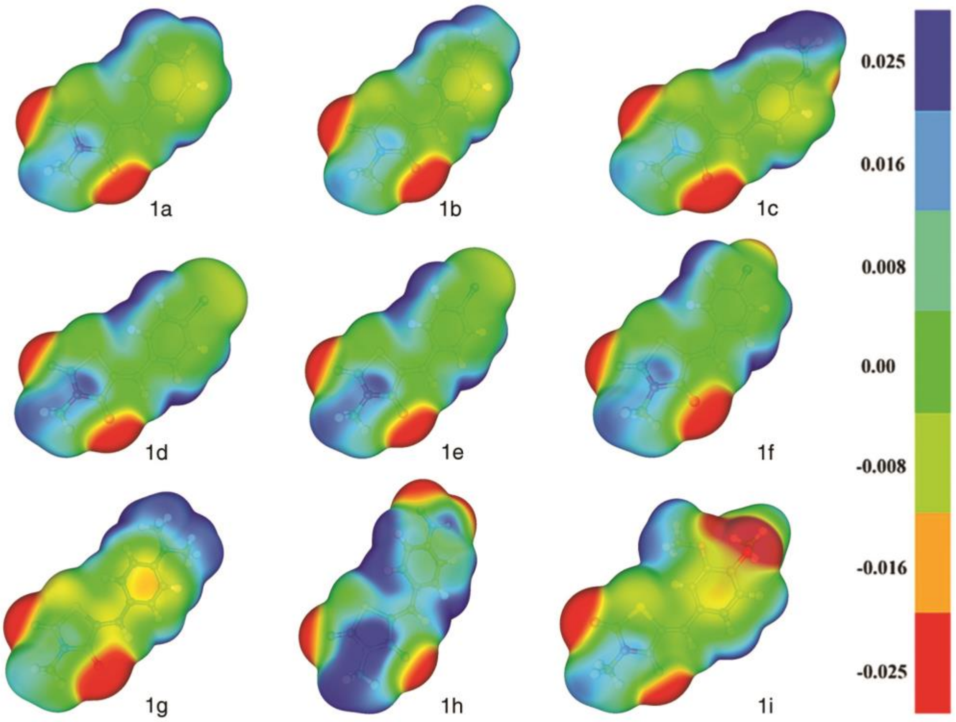


Fig. S13. MEP map of compounds **1a-1i** calculated by B3LYP/6-311G(d,p) method for ground state in acetonitrile

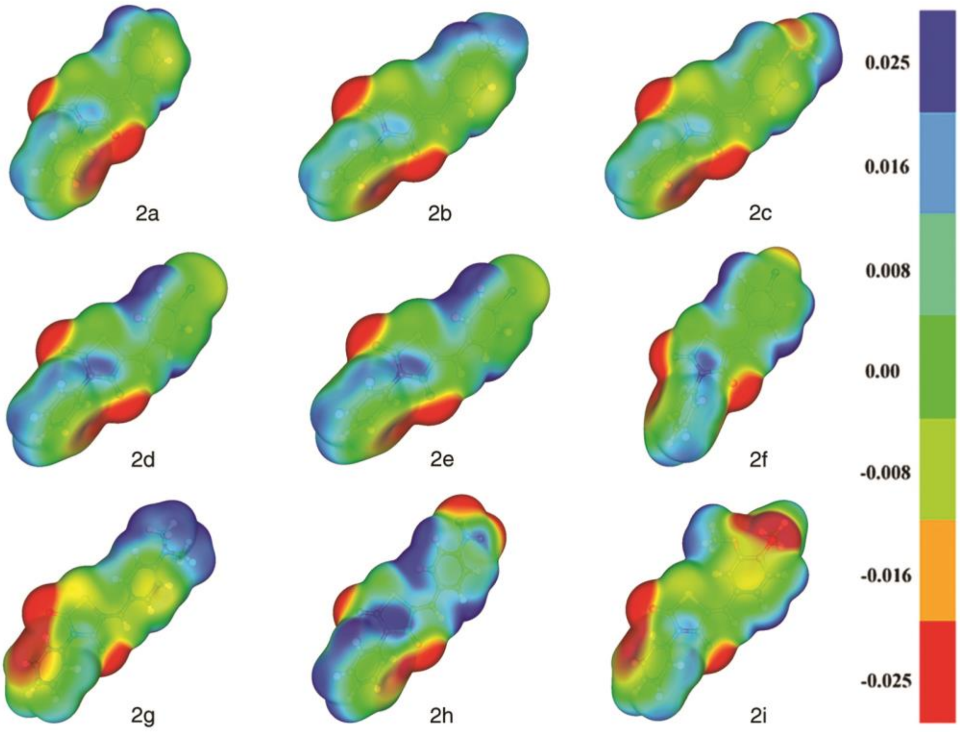


Fig. S14. MEP map of compounds **2a-2i** calculated by B3LYP/6-311G(d,p) method for ground state in acetonitrile

Table S17. Experimental and theoretical absorption maxima for investigated compounds in solvent acetonitrile

Comp.	*Experimental λ (nm)*	*Theoretical λ (nm)*
1a	318.17	306.97
1b	326.26	312.53
1c	339.44	322.09
1d	327.33	313.78
1e	325.95	312.72
1f	323.94	307.74
1g	395.73	349.72
1h	334.90	333.26
1i	338.87	323.77
2a	325.73	309.74
2b	332.12	315.44
2c	343.52	324.92
2d	333.89	316.55
2e	329.27	315.35
2f	330.36	310.34
2g	401.12	354.17
2h	351.99	334.60
2i	359.07	327.16

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