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SUPPLEMENTARY MATERIAL TO

Experimental and theoretical study on solvent and substituent effects on the intramolecular charge transfer in 3-[(4--substituted)phenylamino]isobenzofuran-1(3*H*)-ones

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TABLE S-I. Solvent parameters used in the Kamlet–Taft equation[1,2]

Solvent	π	β	α
1,2-Dichloroethane	0.81	0.10	0.00
Decan-1-ol	0.45	0.82	0.70
Dichloromethane	0.82	0.10	0.13
1,4-Dioxane	0.27	0.49	0.00
Ethane-1,2-diol	0.9	0.52	0.90
Ethanol	0.54	0.75	0.86
Water	1.09	0.47	1.17
Hexane	0.00	0.00	–0.04
2-Methylpropan-1-ol	0.40	0.84	0.79
Propan-2-ol	0.48	0.84	0.76
Methanol	0.60	0.66	0.98
Butan-1-ol	0.47	0.84	0.84
Propan-1-ol	0.52	0.90	0.84
Butan-2-ol	0.40	0.80	0.69
2-Methylpropan-2-ol	0.41	0.93	0.41
Tetrahydrofuran	0.58	0.55	0.00

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TABLE S-II. Solvent parameters used in Catalán equation[3]

Solvent	SP	SdP	SA	SB
1,2-Dichloroethane	0.77	0.74	0.03	0.13
Decan-1-ol	0.72	0.38	0.26	0.91
Dichloromethane	0.76	0.77	0.04	0.18
1,4-Dioxane	0.62	0.32	0.66	0.00
Ethane-1,2-diol	0.78	0.91	0.72	0.53
Ethanol	0.63	0.78	0.40	0.66
Water	0.68	0.99	1.06	0.03
Hexane	0.62	0.00	0.00	0.06
2-Methylpropan-1-ol	0.66	0.68	0.31	0.83
Propan-2-ol	0.63	0.80	0.28	0.83
Methanol	0.60	0.90	0.60	0.54
Butan-1-ol	0.67	0.65	0.34	0.80
Propan-1-ol	0.65	0.75	0.37	0.78
Butan-2-ol	0.66	0.70	0.22	0.89
2-Methylpropan-2-ol	0.63	0.73	0.16	0.93
Tetrahydrofuran	0.71	0.63	0.00	0.59

RESULTS OF THE CHARACTERIZATION

*3-(Phenylamino)isobenzofuran-1(3*H*)-one (**1**)*. Yield: 0.55 g (74 %); colourless needles; m.p.: 179–180 °C; Anal. Calcd. for $C_{14}H_{11}NO_2$: C, 74.65; H, 4.92; N, 6.22; O, 14.21 %. Found: C, 74.69; H, 4.91; N, 6.17; O, 14.23 %; IR (ATR, cm^{-1}): 3334*m* (N–H), 3038*w* (C–H, Ar), 1734*s* (C=O), 1605*m* (N–H), 1285*w* (C–N), 1206*w* (C–O–C), 1098*m* (C–O–C); ^{1}H-NMR (200 MHz, DMSO-d_6, δ / ppm): 6.54 (1H, *d*, J = 8.0 Hz, H-8), 6.83 (2H, *dd*, J_1 = 8 Hz & J_2 = 2 Hz, H-2′ & H-6′), 6.95–7.00 (1H, *m*, H-4′), 7.13 (1H, *d*, J = 8.0 Hz, H-3), 7.24 (2H, *dd*, J_1 = 8 Hz & J_2 = 2 Hz, H-3′ & H-5′), 7.70–7.76 (2H, *m*, H-5 & H-6), 7.84––7.92 (2H, *m*, H-4 & H-7). ^{13}C-NMR (50 MHz DMSO-d_6, δ / ppm): 88.53, 114.39, 114.84, 119.84, 124.62, 125.43, 129.64, 131.04, 134.91, 145.67, 146.38, 169.70.

*3-[(4-Methylphenyl)amino]isobenzofuran-1(3*H*)-one (**2**).* Yield: 0.58 g (78 %); colourless needles; m.p.: 183–185 °C, Anal. Calcd. for $C_{15}H_{13}NO_2$: C, 75.30; H, 5.48; N, 5.85; O, 13.37 %. Found: C, 75.31; H, 5.48; N, 5.80; O, 13.41 %; IR (ATR, cm^{-1}): 3345*m* (N–H), 3020*w* (C–H, Ar), 1736*s* (C=O), 1615*m* (N–H), 1285*m* (C–N), 1218*w* (C–O–C), 1097*m* (C–O–C); ^{1}H-NMR (200 MHz, DMSO--d_6, δ / ppm): 2.23 (3H, *s*, CH_3), 6.46 (1H, *d*, J = 8.0 Hz, H-8), 6.87–7.05 (4H, *m*, H-2′, H-3′, H-5′ & H-6′), 7.13 (1H, *d*, J = 8.0 Hz, H-3), 7.66–7.75 (2H, *m*, H-5 & H-6), 7.81–7.91 (2H, *m*, H-4 & H-7); ^{13}C-NMR (50 MHz, DMSO-d_6, δ / ppm): 169.39, 159.48, 146.15, 142.96, 134.51, 130.68, 129.78, 129.71, 128.15, 127.79, 124.87, 124.31, 114.70, 88.75, 20.33.

*3-[(4-Methoxyphenyl)amino]isobenzofuran-1(3*H*)-one (**3**)*. Yield: 0.64 g (83 %); colourless needles, m.p.: 143–144 °C; Anal. Calcd. for $C_{15}H_{13}NO_3$: C, 70.58; H, 5.13; N, 5.49; O, 18.80 %. Found C 70.51, H 5.17, N 5.51, O 18.81 %. IR

(ATR, cm^{-1}): 3321*m* (N–H), 3031*w* (C–H, Ar), 1740*s* (C=O), 1597*w* (N–H), 1255*m* (C–N), 1113*w* (C–O–C), 1076*m* (C–O–C); ^{1}H-NMR (200 MHz, DMSO-d_6, δ / ppm): 3.70 (3H, *s*, CH_3), 6.52 (1H, *d*, J = 8.0 Hz, H-8), 6.88–7.05 (4H, *m*, H-2′, H-3′, H-5′ & H-6′), 7.13 (1H, *d*, J = 8.0 Hz, H-3), 7.66–7.73 (2H, *m*, H-5 & H-6), 7.85–7.91 (2H, *m*, H-4 & H-7); ^{13}C-NMR (50 MHz DMSO-d_6, δ / ppm): 169.34, 159.80, 153.33, 146.03, 139.19, 139.04, 134.34, 130.66, 128.05, 124.95, 124.50, 116.14, 115.06, 114.76, 89.50.

*3-[(4-Hydroxyphenyl)amino]isobenzofuran-1(3*H*)-one (**4**)*. Yield: 0.65 g (87 %); colourless needles; m.p.: 180–183 °C; Anal. Calcd. for $C_{14}H_{11}NO_3$: C, 69.70; H, 4.60; N, 5.81; O, 19.90 %. Found: C, 69.80; H, 4.57; N, 5.79; O, 19.84 %; IR (ATR, cm^{-1}): 3352*m* (N–H), 3177*m* (O–H), 3177*w* (C–H, Ar), 1710*s* (C=O), 1616*w* (N–H), 1258*m* (C–N), 1208*s* (C–O–C), 1108*m* (C–O–C); ^{1}H-NMR (200 MHz, DMSO-d_6, δ / ppm): 6.48 (1H, *d*, J = 8.0 Hz, H-8), 6.67–6.71 (2H, *m*, H-2′ & H-6′), 6.84–6.89 (2H, *m*, H-3′ & H-5′), 7.63 (1H, *d*, J = 8.0 Hz, H-3), 7.66–7.90 (4H, *m*, H-4, H-5, H-6 & H-7); ^{13}C-NMR (50 MHz, DMSO-d_6, δ / ppm) 169.30, 159.09, 151.75, 145.34, 138.13, 134.10, 130.59, 128.48, 125.66, 125.24, 124.80, 117.04, 116.21, 89.74.

*3-[(4-Fluorophenyl)amino]isobenzofuran-1(3*H*)-one (**5**)*. Yield: 0.59 g (79 %); colourless needles; m.p.: 188–189 °C; Anal. Calcd. for $C_{14}H_{10}FNO_2$: C, 69.13; H, 4.14; F, 7.81; N, 5.76; O, 13.16 %. Found: C, 69.01; H, 4.20; F, 7.76; N, 5.86; O, 13.17 %; IR (ATR, cm^{-1}): 3330*m* (N–H), 3044*w* (C–H, Ar), 1728*s* (C=O), 1610*w* (N–H), 1229*m* (C–N), 1208*s* (C–O–C), 1108*w* (C–O–C); ^{1}H-NMR (200 MHz, DMSO-d_6, δ / ppm): 6.52 (1H, *d*, J = 8.0 Hz, H-8), 6.94–7.01 (2H, *m*, H-3 & H-5′), 7.05–7.09 (2H, *m*, H-2′ & H-6′), 7.15 (1H, *d*, J = 8.0 Hz, H-3), 7.67–7.92 (4H, *m*, H-4, H-5, H-6 & H-7); ^{13}C-NMR (50 MHz, DMSO-d_6, δ / ppm) 169.32, 158.81, 154.14, 145.98, 141.92, 134.60, 130.77, 127.67, 124.92, 124.30, 116.00, 115.80, 115.64, 88.62.

*3-[(4-Chlorophenyl)amino]isobenzofuran-1(3*H*)-one (**6**)*. Yield: 0.54 g (72 %); colourless needles; m.p.: 180–182 °C; Anal. Calcd. for $C_{14}H_{10}ClNO_2$: C, 64.75; H, 3.88; Cl, 13.65; N, 5.39; O, 12.32 %. Found: C, 64.61; H, 3.74; Cl, 13.69; N, 5.43; O, 12.53 %; IR (ATR, cm^{-1}): 3341*m* (N–H), 3020*w* (C–H, Ar), 1732*s* (C=O), 1560*m* (N–H), 1303*m* (C–N), 1206*m* (C–O–C), 1090*m* (C–O–C); ^{1}H-NMR (200 MHz, DMSO-d_6, δ / ppm): 6.52 (1H, *d*, J = 8.0 Hz, H-8), 6.88 (2H, *dd*, J_1 = 8 Hz & J_2 = 2 Hz, H-2′ & H-6′), 7.14 (1H, *d*, J = 8.0 Hz, H-3), 7.28 (2H, *dd*, J_1 = 8 Hz & J_2 = 2 Hz, H-3′ & H-5′), 7.71–7.76 (2H, *m*, H-5 & H-6), 7.82–7.92 (2H, *m*, H-4 & H-7); ^{13}C-NMR (50 MHz, DMSO-d_6, δ / ppm): 169.26, 159.45, 145.86, 144.47, 134.68, 130.83, 129.10, 127.55, 124.96, 124.32, 123.08, 116.09, 116.03, 87.72.

*3-[(4-Acetylphenyl)amino]isobenzofuran-1(3*H*)-one (**7**)*. Yield, 0.50 g (66 %); colourless needles; m.p.: 246–247 °C; Anal. Calcd. for $C_{16}H_{13}NO_3$: C, 71.90; H, 4.90; N, 5.24; O, 17.96 %. Found: C, 71.93; H, 4.86; N, 5.28; O, 17.93

%; IR (ATR, cm^{-1}): 3340*s* (N–H), 3020*w* (C–H, Ar), 1760*s* (C=O), 1596*s* (N–H), 1284*m* (C–N), 1220*m* (C–O–C), 1107*w* (C–O–C); ^{1}H-NMR (200 MHz, DMSO-d_6, δ / ppm): 2.50 (3H, *s*, CH_3), 6.55 (1H, *d*, J = 8.0 Hz, H-8), 7.04 (2H, *dd*, J_1 = 8 Hz, J_2 = 2 Hz, H-2′ & H-6′), 7.25 (1H, *d*, J = 8.0 Hz, H-3), 7.69–7.73 (2H, *m*, H-3′ & H-5′), 7.85–7.95 (4H, *m*, H-4, H-5, H-6 & H-7); ^{13}C-NMR (50 MHz DMSO-d_6, δ / ppm): 196.18, 169.18, 159.16, 150.02, 145.70, 134.81, 130.92, 130.49, 128.62, 127.35, 125.04, 124.37, 113.67, 113.56, 86.53, 26.49.

*3-[(4-Nitrophenyl)amino]isobenzofuran-1(3*H*)-one (**8**)*. Yield: 0.48 g (64 %); colourless needles; m.p.: 241–243 °C, Anal. Calcd. for $C_{14}H_{10}N_2O_4$: C, 62.22; H, 3.73; N, 10.37; O, 23.68 %. Found: C, 62.18; H, 3.69; N, 10.40; O, 23.73 %; IR (ATR, cm^{-1}): 3330*m* (N–H), 3044*w* (C–H, Ar), 1728*s* (C=O), 1610*s* (N–H), 1229*w* (C–N), 1208*m* (C–O–C), 1083*m* (C–O–C); ^{1}H-NMR (200 MHz, DMSO-d_6, δ / pm): 6.58 (1H, *d*, J = 8.0 Hz, H-8), 7.10 (2H, *dd*, J_1 = 8 Hz & J_2 = = 2 Hz, H-2′ & H-6 ′), 7.26 (1H, *d*, J = 8.0 Hz, H-3), 7.71–7.96 (4H, *m*, H-4, H-5, H-6 & H-7), 8.17 (2H, *dd*, J_1 = 4 Hz & J_2 = 2 Hz, H-3′ & H-5′); ^{13}C-NMR (50 MHz, DMSO-d_6, δ / ppm): 168.99, 159.69, 152.04, 145.35, 139.47, 134.94, 131.09, 127.12, 126.11, 125.14, 124.43, 113.83, 113.72, 85.70.

*3-(2-Pyridynylamino)isobenzofuran-1(3*H*)-one (**9**)*. Yield: 0.43 g (57 %); Colourless needles; m.p.: 206–207 °C; Anal. Calcd. for $C_{13}H_{10}N_2O_2$: C, 69.02; H, 4.46; N, 12.38; O, 14.14 %. Found: C, 69.00; H, 4.39; N, 12.44; O, 14.17 %; IR (ATR, cm^{-1}): 3329*w* (N–H), 3040*w* (C–H, Ar), 1751*s* (C=O), 1594*s* (N–H), 1262*s* (C–N), 1225*w* (C–O–C), 1063*s* (C–O–C); ^{1}H-NMR (200 MHz, DMSO--d_6, δ / ppm): 6.92 (1H, *d*, J = 8.0 Hz, H-8), 7.47 (1H, *d*, J = 8.0 Hz, H-3), 7.85––7.89 (1H, *m*, H-4′), 7.97–8.03 (2H, *m*, H-5′ & H-6′), 7.67–7.89 (4H, *m*, H-4, H-5, H-6 & H-7). 8.48 (1H, *dd*, J_1 = 4 Hz & J_2 = 2 Hz, H-3′); ^{13}C-NMR (50 MHz DMSO-d_6, δ / ppm): 169.34, 161.31, 159.95, 158.60, 146.31, 134.58, 130.46, 127.46, 124.77, 124.05, 113.72, 113.60, 84.58.

*3-(3-Pyridynylamino)isobenzofuran-1(3*H*)-one (**10**)*. Yield: 0.44 g (59 %); colourless needles; m.p.: 159–160 °C; Anal. Calcd. for $C_{13}H_{10}N_2O_2$: C, 69.02; H, 4.46; N, 12.38; O, 14.14 %. Found: C, 68.94; H, 4.45; N, 12.35; O, 14.26 %; IR (ATR, cm^{-1}): 3329*w* (N–H), 3042*w* (C–H, Ar), 1741*s* (C=O), 1583*m* (N–H), 1285*s* (C–N), 1215*m* (C–O–C), 1094*m* (C–O–C); ^{1}H-NMR (200 MHz, DMSO--d_6, δ / ppm): 6.64 (1H, *d*, J = 8.0 Hz, H-8), 7.18 (1H, *d*, J = 8.0 Hz, H-3), 7.44––7.48 (1H, *m*, H-6′), 7.51–7.56 (1H, *m*, H-5′), 7.69–7.94 (4H, *m*, H-4, H-5, H-6 & H-7), 8.06 (1H, *dd*, J_1 = 4.5 Hz & J_2 = 2 Hz, H-2′), 8.28 (1H, *d*, J = 4 Hz, H-4′); ^{13}C-NMR (50 MHz DMSO-d_6, δ / ppm): 169.21, 159.94, 145.81, 141.73, 140.81, 137.28, 134.75, 130.90, 127.47, 125.01, 124.34, 120.78, 87.30.

TABLE S-III. Structures and numbering of the synthesized 3-[(4-substituted)phenylamino]-isobenzofuran-1(3*H*)-ones

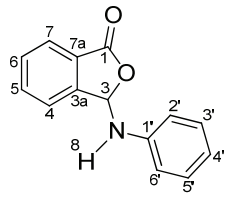
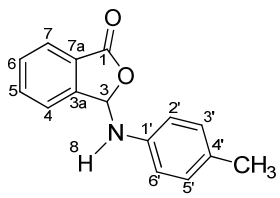
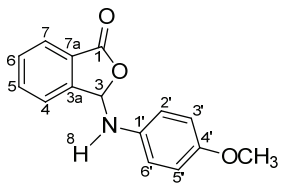
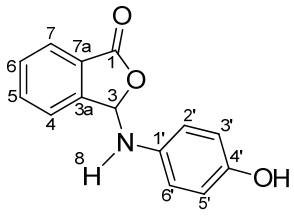
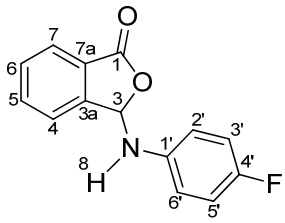
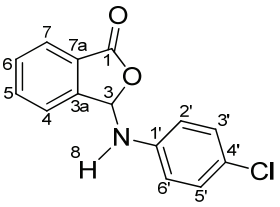
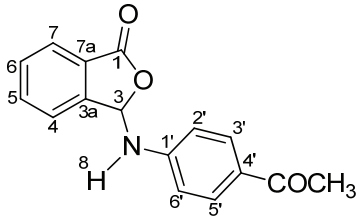
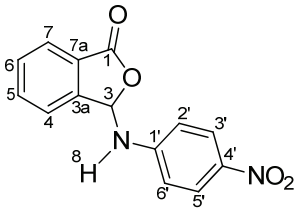
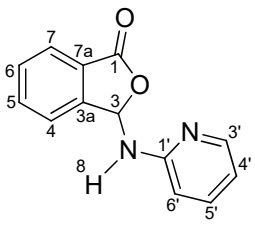
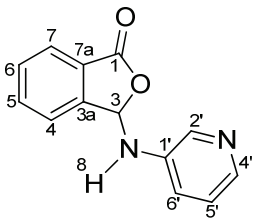
1 	2 	3 
4 	5 	6 
7 	8 	9 
10 		

TABLE S-IV. Results of the correlation analysis for the lower wavelength peak of the 3-[(4-substituted)phenylamino]isobenzofuran-1(3*H*)-ones according to the Kamlet–Taft equation

Comp.	$\nu_0\times10^{-3}$ cm^{-1}	$s\times10^{-3}$ cm^{-1}	$b\times10^{-3}$ cm^{-1}	$a\times10^{-3}$ cm^{-1}	R^a	SD^b	F^c	Solvents excluded from the correlation
1	35.90 ±0.98	–1.71 ±0.75	–0.67 ±0.98	1.53 ±0.30	0.95	0.163	17.74	1,2-dichloroethane, dichloromethane, 1,4-dioxane, ethanol
2	43.3 ±0.19	–2.00 ±0.34	–0.46 ±0.28	1.12 ±0.24	0.91	0.18	13.57	1,2-dichloroethane, dichloromethane, 1,4-dioxane, water
3	43.23 ±0.17	–2.05 ±0.27	–0.32 ±0.23	1.12 ±0.22	0.93	0.17	18.97	1,2-dichloroethane, dichloromethane, 1,4-dioxane
4	40.13 ±0.45	2.67 ±0.57	3.42 ±0.70	–1.51 ±0.54	0.90	0.46	12.80	Butan-2-ol, 2-methyl propan-2-ol, tetrahydrofuran
5	43.48 ±0.22	–2.68 ±0.62	0.12 ±0.44	1.24 ±0.29	0.92	0.22	11.16	Dichloromethane, decan-1-ol, ethane-1,2-diol, hexane
6	50.80 ±2.35	–10.90 ±2.43	–6.87 ±2.06	3.08 ±0.92	0.91	0.52	8.48	1,2-Dichloroethane, 1,4-dioxane, ethanol, water, hexane, 2-methyl propan-1--ol, methanol
7	44.67 ±0.23	–1.83 ±0.37	0.10 ±0.38	0.11 ±0.33	0.91	0.28	11.86	Decan-1-ol, dichloro-methane, methanol, butan--1-ol, tetrahydrofuran
8	44.85 ±0.82	–4.47 ±1.26	2.52 ±1.54	–0.80 ±1.00	0.90	0.83	8.81	1,2-Dichloroethane, decan-1-ol, dichloro-methane, ethane-1,2-diol, ethanol, tetrahydrofuran
9	44.64 ±0.12	–1.61 ±0.16	–0.58 ±0.16	0.80 ±0.14	0.95	0.13	33.52	Dichloromethane, tetrahydrofuran
10	43.42 ±0.10	–0.60 ±0.14	–0.60 ±0.16	0.84 ±0.14	0.93	0.10	18.03	1,2-Dichloroethane, water, methanol, 2-methyl propan--2-ol, tetrahydrofuran

[a]Correlation coefficient; [b]standard deviation; [c]Fisher test of significance

TABLE S-V. Results of the correlation analysis for the higher wavelength peak of the 3-[(4--substituted)phenylamino]isobenzo-furan-1(3*H*)-ones according to the Kamlet–Taft equation

Comp.	$\nu_0\times10^{-3}$ cm^{-1}	$s\times10^{-3}$ cm^{-1}	$b\times10^{-3}$ cm^{-1}	$a\times10^{-3}$ cm^{-1}	R[a]	SD[b]	F[c]	Solvent excluded from the correlation
1	43.35 ±0.21	–2.35 ±0.38	–0.23 ±0.32	1.11 ±0.27	0.91	0.21	13.28	1,2-Dichloroethane, decan-1-ol, dichloromethane, 1,4-dioxane, ethanol, water
2	36.25 ±0.25	–2.53 ±0.35	0.02 ±0.34	0.84 ±0.28	0.94	0.26	20.43	Dichloromethane, 1,4-dioxane, ethane-1,2-diol, propan-1-ol
3	33.48 ±0.27	2.89 ±0.36	0.34 ±0.38	–2.12 ±0.30	0.96	0.28	37.63	1,2-Dichloroethane, dichloromethane, 1,4-dioxane, ethane-1,2-diol
4	35.30 ±1.23	–9.58 ±2.11	1.16 ±2.20	4.16 ±2.05	0.91	1.24	10.63	Decan-1-ol, dichloromethane, 1,4-dioxane, ethane-1,2-diol, water, tetrahydrofuran
5	34.28 ±0.27	0.48 ±0.39	2.33 ±0.37	–0.97 ±0.34	0.93	0.27	13.14	1,2-Dichloroethane, dichloro-methane, 2-methyl propan-1--ol, methanol, butan-1-ol, propan-1-ol
6	33.92 ±0.41	2.32 ±0.57	1.98 ±0.61	–3.23 ±0.55	0.90	0.42	13.68	Decan-1-ol, 1,4-dioxane, tetrahydrofuran
7	34.76 ±0.38	0.30 ±0.48	–1.32 ±0.49	–0.98 ±0.37	0.90	0.40	16.81	Ethane-1,2-diol
8	31.34 ±0.63	–2.00 ±0.81	–0.78 ±1.11	–1.05 ±0.80	0.90	0.64	7.41	Propan-2-ol, methanol, butan-1-ol, propan-1-ol, butan-2-ol, 2-methyl propan-2-ol, tetrahydrofuran
9	35.70 ±0.53	0.45 ±0.83	–2.16 ±1.09	–2.78 ±0.76	0.96	0.52	9.70	Decan-1-ol, ethanol, water, 2-methyl propan-1-ol, propan-2--ol, methanol, butan-1-ol, propan-1-ol, butan-2-ol, 2-methyl propan-2-ol
10	35.23 ±0.15	0.54 ±0.25	–0.74 ±0.23	–0.89 ±0.24	0.96	0.16	30.44	Decan-1-ol, 1,4-dioxane, ethane-1,2-diol, butan-1-ol, tetrahydrofuran

[a]Correlation coefficient; [b]standard deviation; [c]Fisher test of significance

TABLE S-VI. Results of the correlation analysis for the lower wavelength peak of the 3-[(4--substituted)phenylamino]isobenzo-furan-1(3*H*)-ones according to the Catalán equation

Comp.	$\nu_0\times10^{-3}$ cm^{-1}	$c\times10^{-3}$ cm^{-1}	$d\times10^{-3}$ cm^{-1}	$b\times10^{-3}$ cm^{-1}	$a\times10^{-3}$ cm^{-1}	R[a]	SD[b]	F[c]	Solvent excluded from the correlation
1	44.97 ±0.67	–2.55 ±0.99	–0.09 ±0.24	–0.85 ±0.31	–0.13 ±0.19	0.93	0.14	9.12	1,2-Dichloroethane, water, hexane, methanol, 2-methyl propan-2-ol, tetrahydofuran
2	46.70 ±0.67	–5.57 ±0.99	–1.11 ±0.23	1.19 ±0.30	0.22 ±0.19	0.96	0.14	20.1	Decan-1-ol, ethane-1,2-diol, water, methanol, butan-1-ol, 2-methyl propan-2-ol, tetrahydrofuran
3	44.16 ±0.41	–1.39 ±0.59	–0.28 ±0.17	–0.64 ±0.14	–[d]	0.94	0.11	16.0	Tetrahydrofuran
4	37.78 ±1.46	3.64 ±2.09	2.86 ±0.06	–0.85 ±0.51	1.42 ±0.36	0.93	0.40	13.80	–
5	45.57 ±0.42	–3.32 ±0.63	0.13 ±0.21	–0.60 ±0.19	–0.10 ±0.14	0.95	0.09	14.40	Decan-1-ol, dichloro-methane, water, tetrahydrofuran
6	42.95 ±6.75	–[d]	0.14 ±5.36	–4.44 ±2.12	0.53 ±2.05	0.93	0.64	3.25	1,2-Dichloroethane, decan-1-ol, dichloro-methane, ethane-1,2-diol, water, hexane, 2-methyl propan-1-ol, propan-2-ol, butan-2-ol, 2-methyl propan-2-ol, tetra-hydrofuran
7	48.23 ±1.07	–5.91 ±1.56	0.42 ±0.48	–1.50 ±0.43	–0.36 ±0.29	0.91	0.29	8.56	Dichloromethane, butan-1-ol, tetrahydrofuran
8	41.0.4 ±4.94	5.60 ±7.30	–3.34 ±2.11	1.77 ±1.80	4.67 ±1.30	0.90	1.28	5.70	Propan-1-ol, butan-2-ol, 2-methyl propan-2-ol, tetrahydofuran
9	46.79 ±0.18	–3.52 ±0.26	–0.84 ±0.08	0.11 ±0.07	0.13 ±0.05	0.99	0.04	124.88	1,2-Dichloroethane, 2-methyl propan-2-ol, tetrahydrofuran
10	43.48 ±0.36	–[d]	–0.84 ±0.15	0.25 ±0.12	–0.37 ±0.09	0.94	0.09	16.99	–

[a]Correlation coefficient; [b]standard deviation; [c]Fisher test of significance; [d]negligible values with high standard errors

TABLE S-VII. Results of the correlation analysis for the higher wavelength peak of the 3-[(4--substituted)phenylamino]isobenzofuran-1(3*H*)-ones according to the Catalán equation

Comp.	$\nu_0\times10^{-3}$ cm^{-1}	$c\times10^{-3}$ cm^{-1}	$d\times10^{-3}$ cm^{-1}	$b\times10^{-3}$ cm^{-1}	$a\times10^{-3}$ cm^{-1}	R^a	*SD*	F^c	Solvent excluded from correlation
1	69.13 ±9.45	–38.65 ±10.27	–9.13 ±2.60	1.30 ±0.93	–2.41 ±1.26	0.96	0.25	10.49	1,2-Dichloroethane, dichloromethane, ethane-1,2-diol, water, hexane
2	40.16 ±1.63	–6.54 ±2.37	–1.61 ±0.57	0.39 ±0.52	0.99 ±0.35	0.90	0.34	8.02	Dichloromethane, ethane-1,2-diol
3	33.91 ±1.46	–0.27 ±2.23	3.21 ±0.75	–2.94 ±0.58	–2.12 ±0.43	0.92	0.35	10.16	Decan-1-ol, dichloromethane, tetrahydrofuran
4	42.79 ±10.84	–12.64 ±16.81	–7.97 ±3.85	3.72 ±4.80	6.10 ±2.13	0.91	1.39	6.05	Decan-1-ol, dichloromethane, ethanol, water
5	35.45 ±2.42	–1.95 ±3.78	2.13 ±0.89	–1.60 ±0.74	0.55 ±0.55	0.94	0.30	8.21	1,2-Dichloroethane, decan-1-ol, ethane-1,2--diol, butan-1-ol, tetrahydofuran, propan-1-ol
6	34.14 ±1.09	–0.53 ±1.57	2.84 ±0.45	–3.40 ±0.54	–1.42 ±0.33	0.97	0.29	24.26	Water, 2-methyl propan-2-ol tetrahydrofuran
7	38.29 ±1.21	–5.42 ±1.73	0.77 ±0.50	–2.66 ±0.40	–2.04 ±0.30	0.95	0.33	22.42	–
8	37.87 ±2.17	–10.78 ±3.30	0.93 ±1.03	–3.18 ±0.72	–2.18 ±0.58	0.91	0.52	11.43	Decan-1-ol
9	50.69 ±1.16	–15.24 ±1.16	–3.99 ±0.57	–1.89 ±0.23	–2.38 ±0.27	0.99	0.17	75.75	2-Methylpropan-1-ol, propan-2-ol, hexane, tetrahydrofuran
10	29.24 ±1.34	9.80 ±1.96	–1.60 ±0.58	0.14 ±0.52	–0.01 ±0.36	0.90	0.35	8.60	1.2-Dihloroethane, tetrahydrofuran

[a]Correlation coefficient; [b]standard deviation; [c]Fisher test of significance

TABLE S-VIII. Results of energies of the molecules optimized by the DFT/B3LYP 6-31G(d,p) method

Compound	Energy, E_h
1	–745.3479
2	–784.6680
3	–859.8708
4	–820.5657
5	–844.5781
6	–1204.9419
7	–898.0002
8	–949.8508
9	–761.3929
10	–761.3810

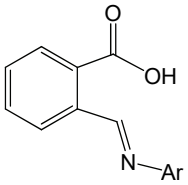
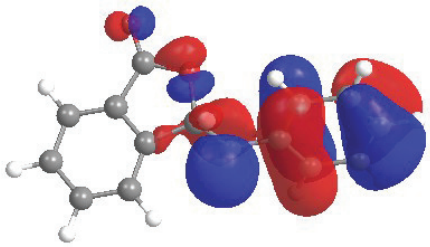
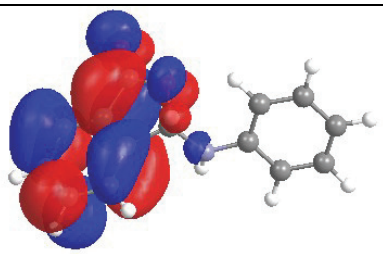
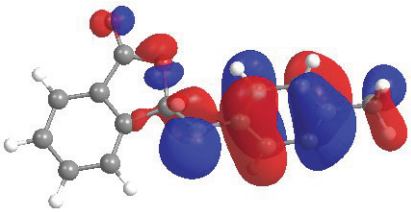
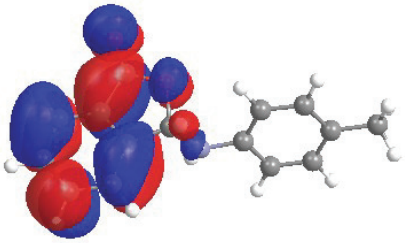
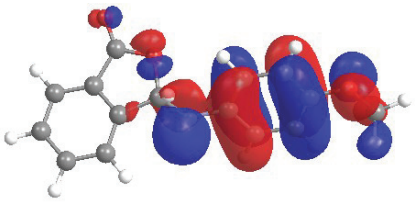
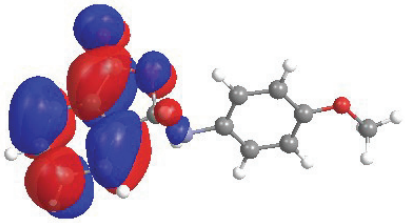
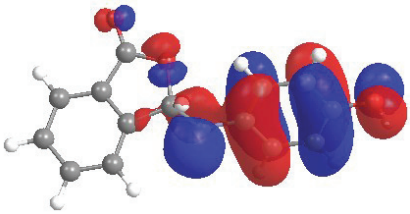
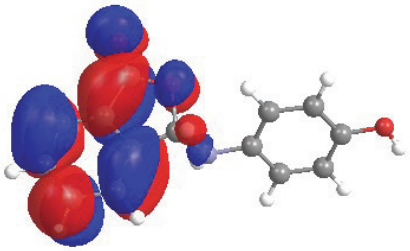
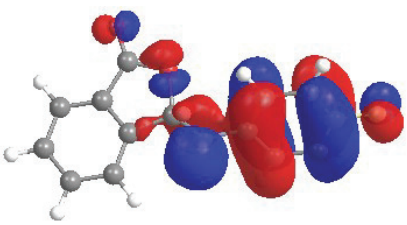
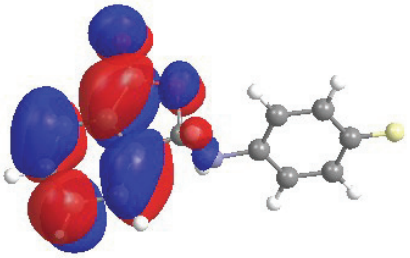


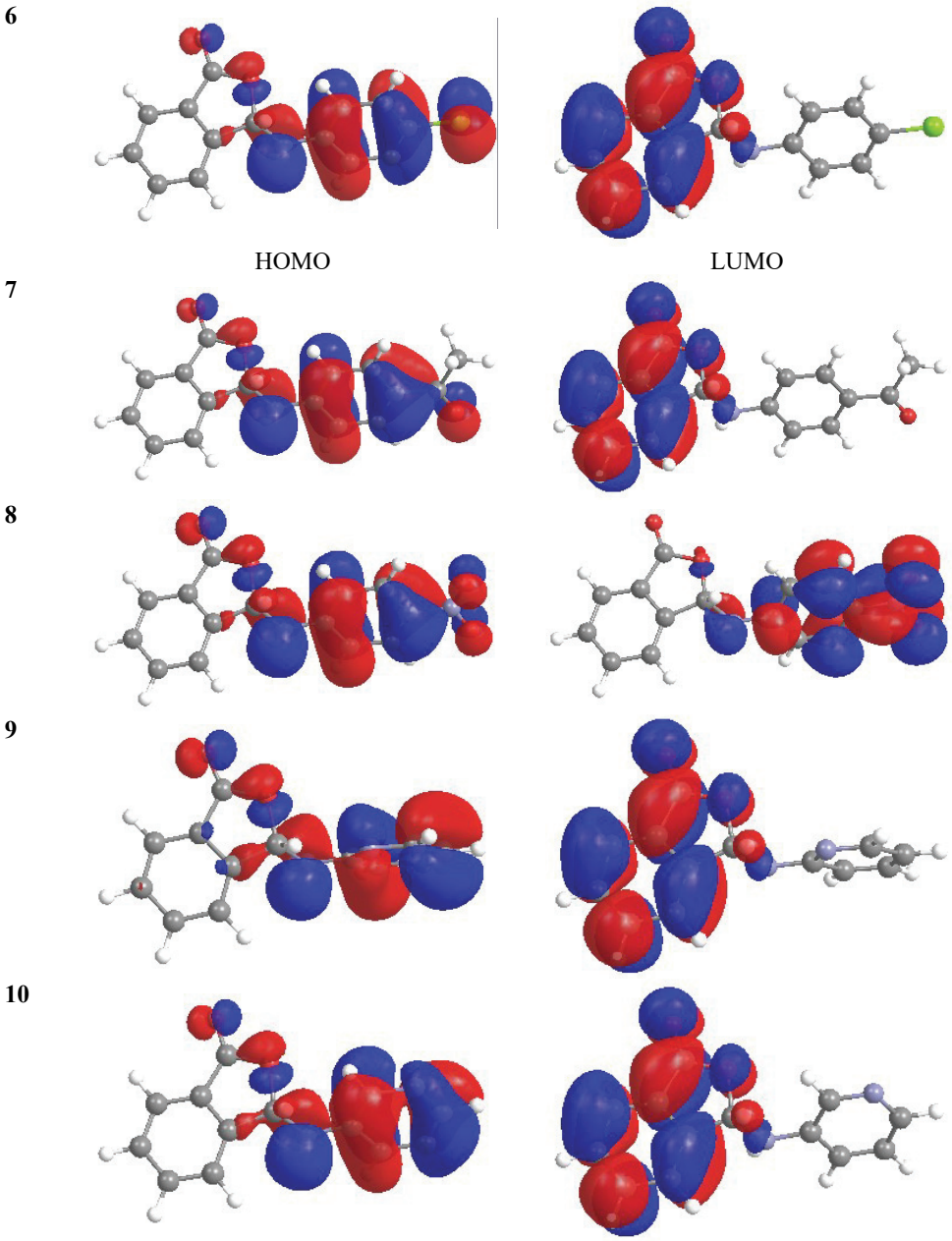
Fig. S-1. Open imine structure of the synthesized compounds.

TABLE S-IX. Elements of the optimized geometries of the investigated 3-((4-substituted)-phenylamino)isobenzofuran-1(3H)-ones **1**–**10** (Å), calculated by the MP2/6-31G(**) method

	C1–C7a	C1=O	C1–O2	C3–O2	C3–N	N–H	N–C1′	C1′–C2′	θ / °	μ / D
1	1.4872	1.2025	1.3727	1.4664	1.4158	1.0136	1.4141	1.4050	65.65	5.1602
2	1.4872	1.2026	1.3721	1.4675	1.4154	1.0137	1.4152	1.4046	65.64	5.0117
3	1.4871	1.2028	1.3719	1.4694	1.4149	1.0140	1.4196	1.4001	66.69	6.0281
4	1.4871	1.2027	1.3722	1.4689	1.4152	1.0141	1.4198	1.4024	66.71	6.2171
5	1.4868	1.2022	1.3738	1.4662	1.4165	1.0139	1.4136	1.4050	65.85	6.1120
6	1.4869	1.2019	1.3744	1.4643	1.4173	1.0138	1.4126	1.4048	65.29	6.3922
7	1.4869	1.2018	1.3749	1.4624	1.4178	1.0134	1.4067	1.4078	64.69	5.9823
8	1.4866	1.2011	1.3770	1.4591	1.4201	1.0133	1.4047	1.4067	64.29	9.4933
9	1.4874	1.2031	1.3713	1.4593	1.4259	1.0137	1.4048	1.4061	71.86	5.3511
10	1.4871	1.2017	1.3748	1.4611	1.4196	1.0137	1.4073	1.4031	65.23	7.0518

TABLE S-X. Molecular orbital surfaces for the HOMO and LUMO of compounds **1**–**10** calculated by the TD-DFT/ 6-31G(d,p) method in the solvent methanol

	HOMO	LUMO
1		
2		
3		
4		
5		



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