

Electronic Supporting Information

Influence of substituent on nitrogen atom
of 3-[2-(4-aminophenyl)benzoxazol-5-yl]alanine derivatives
on their photophysical properties - solvatochromic studies

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Synthesis

1 4-(*N*-Phenylamino)benzaldehyde and 4-(*N*-methyl-*N*-phenylamino)benzaldehyde - *general procedure*

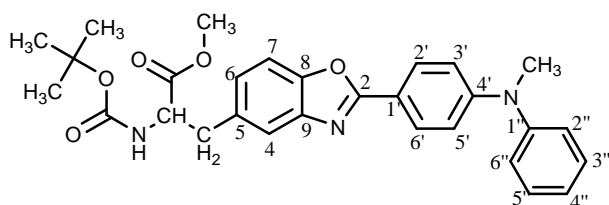
A magnetically stirred solution of the appropriate amine (diphenylamine or *N*-methyl-*N*-phenylamine, 1 mmol) in 1,2-dichlorobenzene (3.5 mL) was cooled in an ice bath and 1.2 mmol of 1,1-dichloromethyl methyl ether and 1.4 mmol of TiCl₄ were subsequently added. The reaction was continued for 1 h in the ice bath. Then the reaction mixture was allowed to warm to room temp. and poured onto ice (35 g) and concentrated HCl (2.5 mL). The organic layer was diluted with dichloromethane, washed with a 5% aqueous solution of HCl and with water and dried with anhydrous MgSO₄. After evaporation the residue was purified by column chromatography (Merck, Silica gel 60, 0.040–0.063 mm), giving the desired compound which was used in the next step of the synthesis.

2 3-(2-Benzoxazol-5-yl)alanine derivatives – *general procedure*

A mixture of *N*-Boc-3-nitro-*L*-tyrosine methyl ester and 10% palladium on active charcoal in methanol was stirred under a hydrogen atmosphere at room temperature for about 90 min. (TLC monitoring, Merck silica-gel plates (Kieselgel 60 *F*₂₅₄), (CH₂Cl₂/MeOH/AcOH 100:10:1), *R*_f = 0.9 (*N*-Boc-3-nitro-*L*-tyrosine methyl ester), *R*_f = 0.72 (*N*-Boc-3-amino-*L*-tyrosine methyl ester)). The catalyst was filtered off and the solvent was evaporated to give a brownish oily product, which was dissolved in anhydrous ethanol and mixed with the solution of the appropriate aldehyde (1 eq) in anhydrous ethanol. The mixture was stirred at room temp. overnight (TLC monitoring (AcOEt/petroleum ether 1:3). After this time, the solvent was removed by evaporation, the Schiff base obtained was dissolved in DMSO, and lead tetraacetate (1.5 eq) was added. The mixture was stirred at room temp. for about 2 h (TLC

monitoring (AcOEt/petroleum ether 1:3) and then dissolved in AcOEt and washed in turns with a saturated aqueous solution of NaCl (1×), a 5% aqueous solution of NaHCO₃ (2×), a saturated aqueous solution of NaCl (3×), and dried with anhydrous MgSO₄. The solvent was evaporated and the product was isolated by means of column chromatography (Merck, Silica gel 60, 0.040–0.063 mm), using a mixture of AcOEt/petroleum ether 1:3 (compounds **1** and **3**) or AcOEt/petroleum ether 1:2 (compound **2**) as an eluent. The crude product **2** was recrystallized from a mixture of AcOEt/petroleum ether, giving a colorless solid with 48 % yield. In the cases of compounds **1** and **3**, an additional purification by means of RP-HPLC was necessary (gradient 50-100% B over 120 min (A = 0.01% water solution of trifluoroacetic acid, B = 80% of acetonitrile in A), Kromasil column, C-8, 5 μm, 250mm long, i.d. = 20 mm). Compounds **1** and **3** were obtained as colorless solids with 18 % and 3 % yield, respectively. The purity of the obtained compounds was checked by means of analytical RP-HPLC (Kromasil column, C-8, 5 μm, 250mm long, i.d. = 4.5 mm) with detection at λ = 223 nm. The mobile phase was a gradient running from 0 to 100% of B over 60 min plus 100% of B over 10 min (t_R = 61.5 min (**1**), t_R = 50.3 min (**2**), t_R = 57.8 min (**3**)). The identification of the products was based on the ¹H NMR (Varian, Unity 500 plus spectrometer (500 MHz) in CDCl₃ and mass spectra (Bruker Biflex III (MALDI-TOF)).

Compound **1**:



¹H NMR: δ_H/ppm = 1.44 (s, 9H, (CH₃)₃), 3.16-3.29 (m, 2H, C^βH₂), 3.43 (s, 3H, CH₃), 3.75 (s, 3H, OCH₃), 4.65 (d, 1H, C^αH, J=7.33 Hz), 5.04 (d, 1H, NH, J=7.81 Hz), 6.91

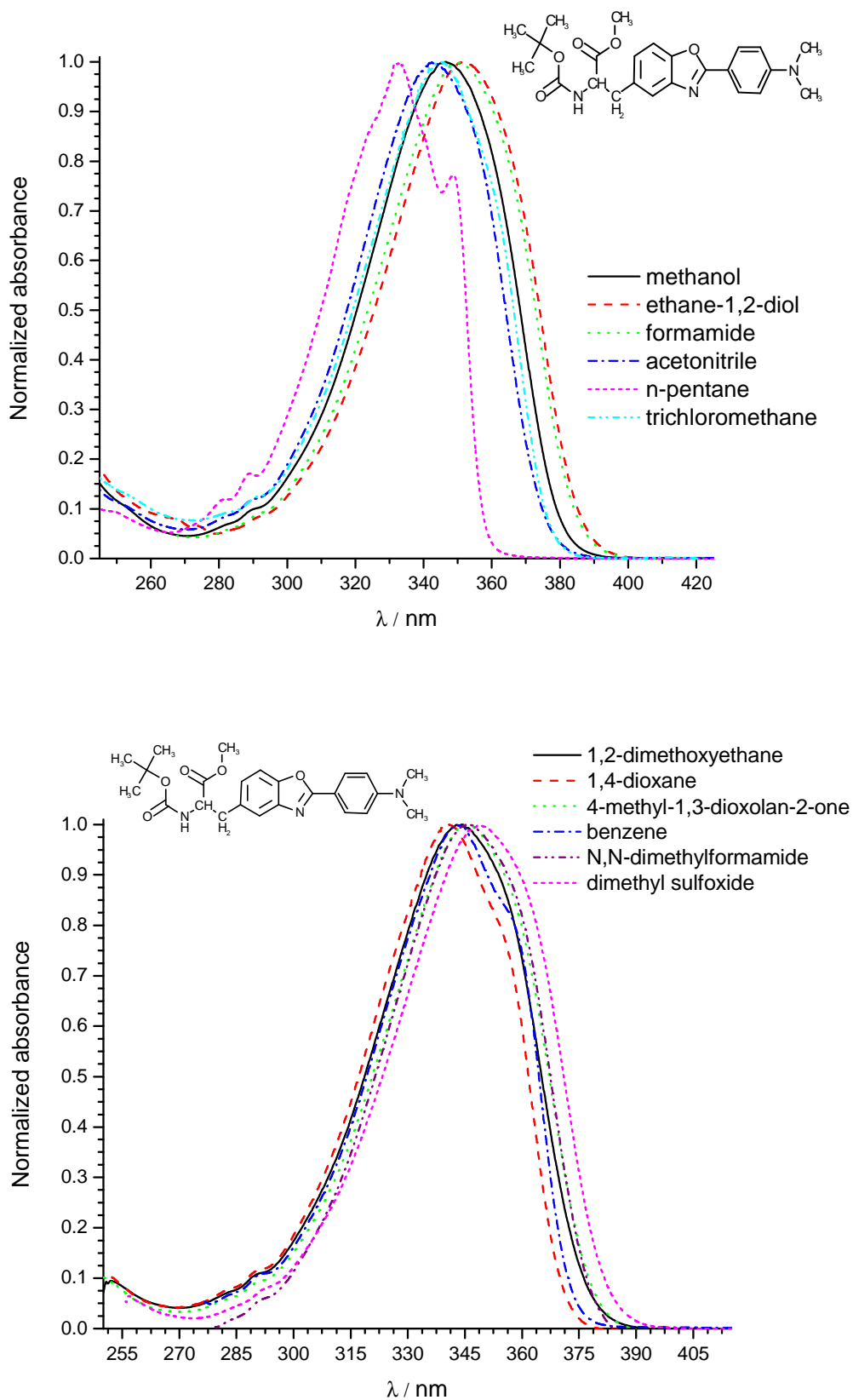


Fig. 1S Normalized UV absorption spectra of **2** in 12 selected solvents.

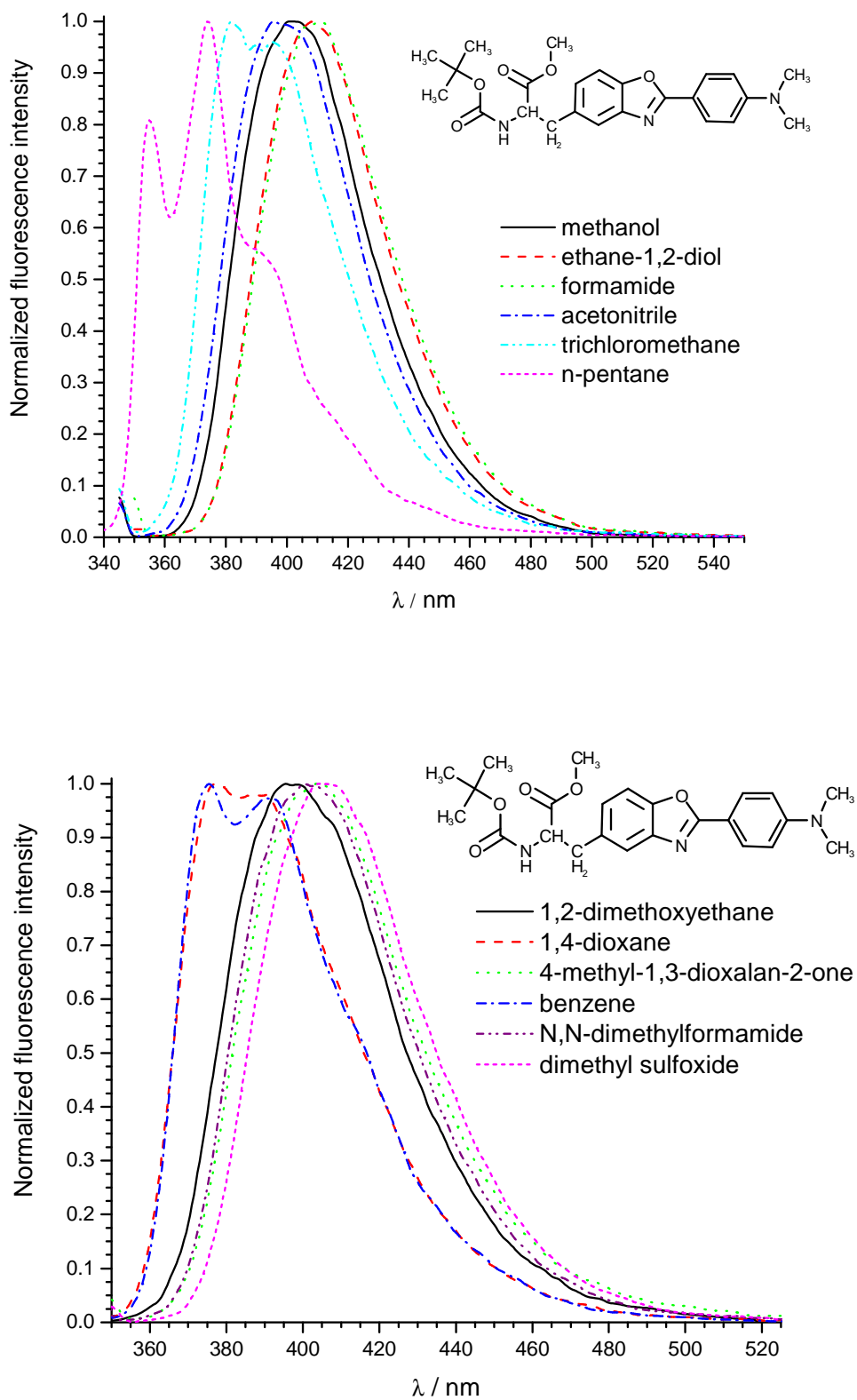


Fig 2S Normalized fluorescence spectra of **2** in 12 selected solvents.

Table 1S Spectroscopic and photophysical properties of **2** in 36 solvents studied.

solvent	$\tilde{\nu}_a / \text{cm}^{-1}$	$\tilde{\nu}_f / \text{cm}^{-1}$	QY	τ / ns	α	χ_R^2	$\Delta\tilde{\nu} / \text{cm}^{-1}$	$k_f / 10^8 \text{ s}^{-1}$	$k_{nr} / 10^7 \text{ s}^{-1}$	
1	methanol	28860	24783	0.81	1.26	1.00	1.02	4077	6.43	15.10
2	ethanol	28852	24814	0.98	1.35	1.00	0.99	4038	7.26	1.48
3	1-butanol	28910	25031	0.99	1.29	1.00	0.97	3879	7.67	0.77
4	2-methylpropan-1-ol	29028	25221	1.00	1.29	1.00	1.13	3807	7.75	0
5	2-propanol	29078	25189	1.00	1.30	1.00	0.92	3889	7.69	0
6	1-pentanol	29180	25740	1.00	1.25	1.00	0.92	3440	8.00	0
7	1-hexanol	28935	25126	1.00	1.32	1.00	0.99	3827	7.57	0
8	cyclohexanol	28860	25063	0.91	1.28	1.00	1.01	3797	7.11	7.03
9	1-heptanol	28927	25221	1.00	1.29	1.00	1.10	3706	7.75	0
10	ethane-1,2-diol	28417	24480	0.76	1.13	1.00	1.07	3937	6.72	21.23
11	propane-1,2-diol	28612	24480	0.99	1.32	1.00	1.09	4132	7.50	0.76
12	formamide	28620	24301	0.71	1.14	1.00	0.99	4319	6.23	25.43
13	acetone	29146	25349	1.00	1.26	1.00	0.97	3797	7.94	0
14	acetonitrile	29121	25284	0.95	1.32	1.00	0.97	3837	7.20	3.79
15	trichloromethane	29019	26178	0.68	0.79	1.00	1.14	2841	8.61	40.50
16	dichloromethane	29028	25773	1.00	1.23	1.00	1.03	3255	8.13	0
17	n-pentane	30039	26738	0.95	1.12	1.00	1.02	3301	8.48	4.46
18	3-methyl-pentane	30030	26702	0.92	1.02	1.00	0.99	3328	9.02	7.84
19	cyclohexane	29842	26525	1.00	1.06	1.00	1.00	3317	9.43	0
20	n-hexane	29976	26667	0.93	1.04	1.00	1.10	3309	8.94	6.73
21	2,2,4-trimethylpentane	30030	26667	0.95	1.02	1.00	1.03	3363	9.31	4.90
22	n-nonane	29860	26596	1.00	1.08	1.00	1.06	3264	10.10	0
23	n-decane	29860	26525	0.93	1.09	1.00	1.16	3335	8.53	6.427
24	1,2-dimethoxyethane	29078	25284	0.70	0.88	1.00	1.04	3794	7.95	34.09
25	1,4-dioxane	29343	26525	1.00	1.21	1.00	1.17	2818	8.26	0
26	tetrahydrofuran	29257	25543	0.88	1.21	1.00	0.97	3714	7.27	9.92
27	2-methyl-tetrahydrofuran	29507	26008	1.00	1.15	1.00	0.96	3499	8.69	0
28	diethyl ether	29568	26350	0.99	1.24	1.00	0.86	3218	7.98	0.81
29	di-i-propyl ether	29455	25806	1.00	1.20	1.00	0.94	3649	8.33	0
30	4-methyl-1,3-dioxolan-2-one	28977	24752	1.00	1.41	1.00	1.84	4225	7.23	0
				1.38	1.00					
				6.14	0.00	1.15				
31	benzene	29155	26631	0.97	1.08	1.00	0.93	2524	8.98	2.78
32	methylbenzene	29240	26702	0.90	1.04	1.00	0.90	2538	8.65	9.61
33	1,2-dimethylbenzene	29291	26810	0.99	1.07	1.00	0.87	2481	9.25	9.34
34	ethyl acetate	29438	26212	1.00	1.19	1.00	0.95	3226	8.40	0
35	N,N-dimethylformamide	28860	24969	0.92	1.28	1.00	1.15	3891	7.19	6.25
36	dimethyl sulfoxide	28694	24480	1.00	1.26	1.00	1.09	4214	7.93	0

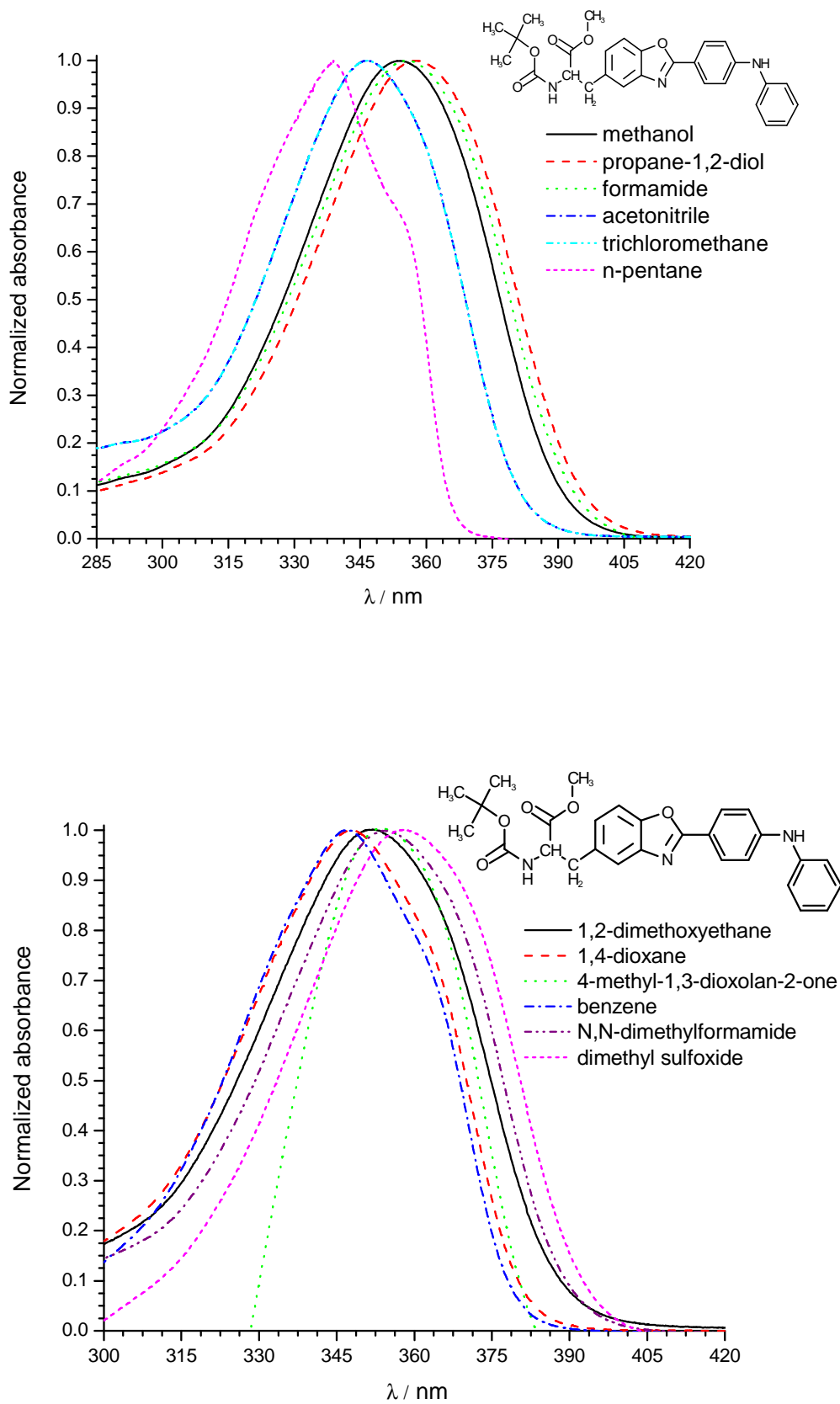


Fig. 3S Normalized UV absorption spectra of **3** in 12 selected solvents.

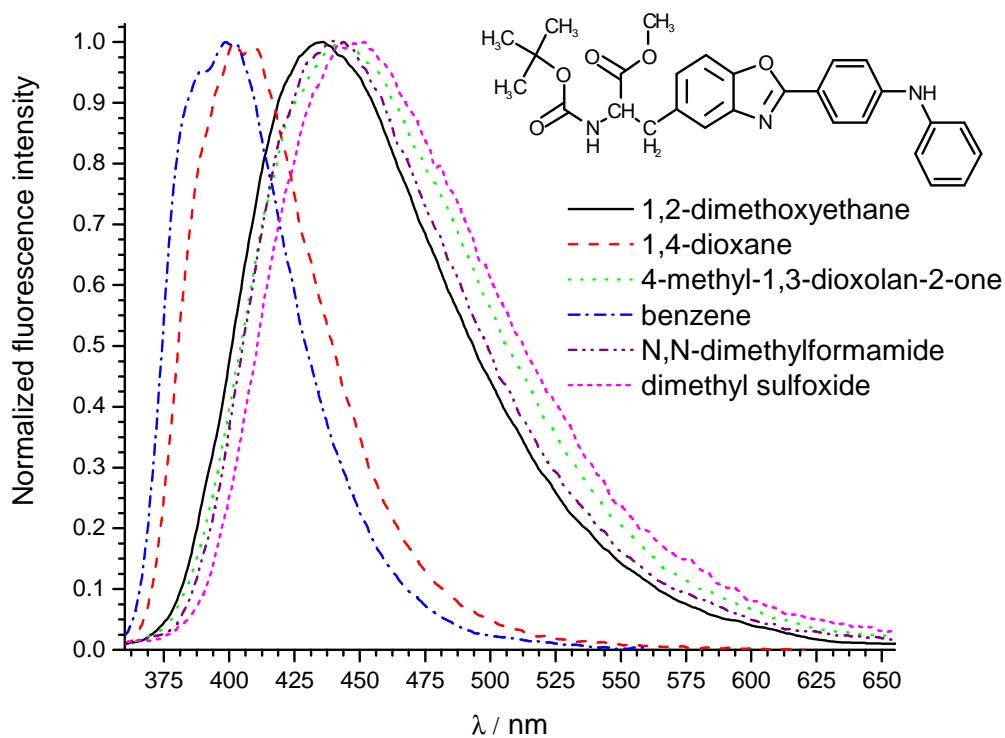
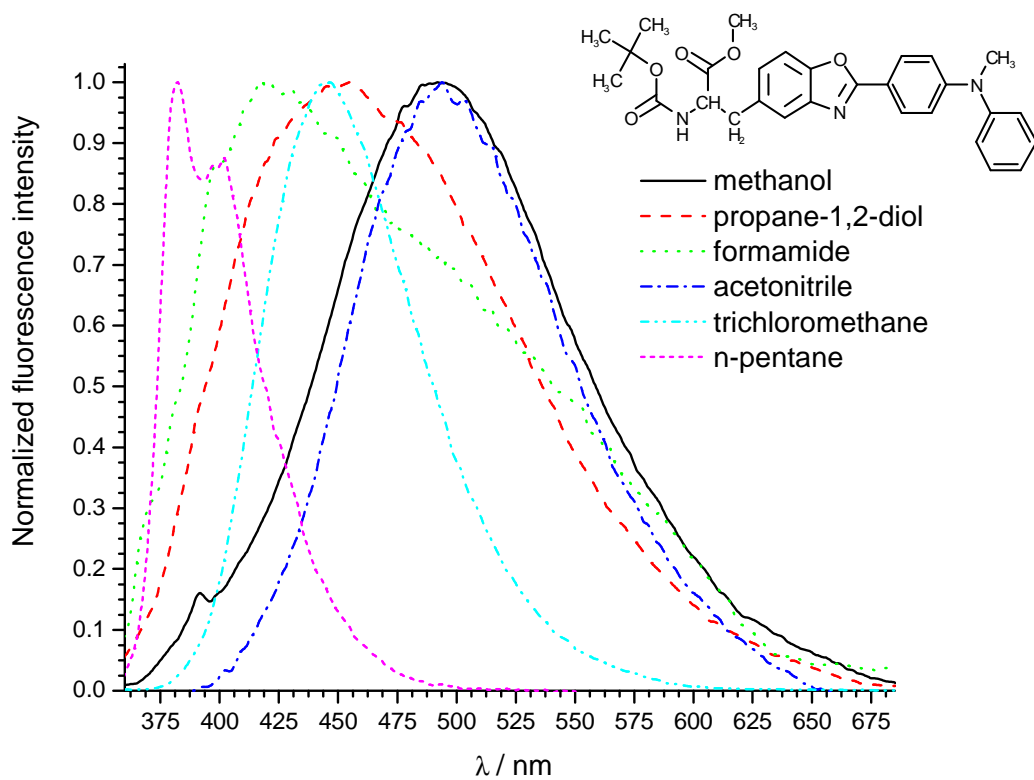


Fig. 4S Normalized fluorescence spectra of **3** in 12 selected solvents.

Table 2S. Spectroscopic and photophysical properties of **3** in 36 solvents studied.

	solvent	$\tilde{\nu}_{\text{abs}}/\text{cm}^{-1}$	$\tilde{\nu}_{\text{fluo}}/\text{cm}^{-1}$	QY	τ/ns	α	χ_{R}^2	$\Delta\tilde{\nu}/\text{cm}^{-1}$
1	methanol	28288	21882	0.01	0.43	1.00	14.98	6346
					0.29	0.98	1.18	
					1.76	0.02		
2	ethanol	28074	22051	0.05	0.800	1.00	4.90	6023
					0.40	0.72	1.18	
					1.04	0.28		
3	1-butanol	27939	22650	0.76	2.00	1.00	15.77	5289
					2.27	0.32	0.97	
					0.20	0.69		
4	2-methyl-propan-1-ol	27941	22831	0.78	2.23	1.00	8.95	5110
					2.40	0.29	1.00	
					0.21	0.71		
5	2-propanol	28129	22701	0.69	2.43	1.00	7.43	5428
					2.51	0.47	1.05	
					0.29	0.53		
6	1-pentanol	28137	23585	0.61	2.89	1.00	3.23	4552
					2.98	0.46	0.99	
					0.27	0.54		
7	1-hexanol	27840	23310	0.48	2.41	1.00	12.37	4530
					2.73	0.30	0.96	
					0.35	0.70		
8	cyclohexanol	28003	22727	0.29	2.23	1.00	15.86	5276
					2.52	0.32	1.05	
					0.35	0.68		
9	1-heptanol	27816	23015	0.50	2.23	1.00	11.94	4801
					2.49	0.33	1.00	
					0.36	0.66		
10	ethane-1,2-diol	27941	22573	0.03	2.95	1.00	17.11	5368
					0.17	0.99	1.37	
					1.52	0.01		
11	propane-1,2-diol	28106	22831	0.09	0.54	1.00	24.43	5275
					0.38	0.99	3.24	
					4.59	0.01		
12	formamide	28106	22371	0.01	1.70	1.00	105.77	5735
					0.33	0.95	3.44	
					4.98	0.05		
13	acetone	28694	22753	0.62	2.96	1.00	1.12	5941
					0.17	0.96	1.15	
					2.21	0.03		
14	acetonitrile	28868	22124	0.34	2.26	1.00	1.15	6744
					0.17	0.96	1.15	
					2.21	0.03		
15	trichloromethane	28802	23809	0.79	2.26	1.00	5.22	4993
					2.46	0.54	1.11	
					0.60	0.46		

16	dichloromethane	28935	24067	0.69	3.10	1.00	1.74	4868
					3.18	0.74		
					0.58	0.26	0.97	
17	n-pentane	29507	26178	1.00	1.14	1.00	1.46	3329
					1.10	0.98		
					2.79	0.02	1.02	
18	3-methyl-pentane	29472	26111	1.00	1.03	1.00	1.02	3361
19	cyclohexane	29308	26178	0.99	1.23	1.00	2.46	3130
					1.06	0.94		
					0.44	0.06	1.10	
20	n-hexane	29507	26076	1.00	1.02	1.00	1.02	3431
21	2,2,4-trimethylpentane	29507	26042	1.00	1.01	1.00	1.07	3465
22	n-nonane	29386	26008	0.98	1.06	1.00	1.07	3378
23	n-decane	29412	25974	1.00	1.09	1.00	1.17	3438
24	1,2-dimethoxyethane	28417	22727	0.08	0.90	1.00	2.42	5690
					0.41	0.47		
					0.99	0.53	1.21	
25	1,4-dioxane	28789	24360	1.00	1.83	1.00	1.12	4429
26	tetrahydrofuran	28498	23866	0.62	2.68	1.00	2.42	4632
					0.51	0.33		
					2.78	0.67	1.00	
27	2-methyl-tetrahydrofuran	28727	23529	0.55	2.75	1.00	5.96	5198
					2.06	0.79		
					4.08	0.21	0.96	
28	diethyl ether	28868	24420	0.67	2.27	1.00	1.92	4448
					0.59	0.26		
					2.35	0.74	1.08	
29	di-i-propyl ether	28571	23474	0.69	2.48	1.00	2.72	5097
					2.58	0.62		
					0.41	0.38	1.04	
30	4-methyl-1,3-dioxolan-2-one	28257	21858	0.31	1.98	1.00	2.05	6399
					2.95	0.17		
					1.68	0.83	1.03	
31	benzene	28827	25094	0.95	1.42	1.00	1.08	3733
32	methylbenzene	28852	24907	0.85	1.34	1.00	1.09	3945
33	1,2-dimethylbenzene	28868	24907	0.92	1.35	1.00	1.06	3961
34	ethyl acetate	28852	24272	0.71	2.46	1.00	0.97	4580
35	N,N-dimethylformamide	28233	22346	0.62	2.45	1.00	1.28	5887
					2.47	0.80		
					0.32	0.20	1.08	
36	dimethyl sulfoxide	27941	21763	0.41	1.92	1.00	1.54	6178
					1.30	0.33		
					2.09	0.67	1.14	

Table 3S. The values of the estimated coefficients (y_0 and a) and their standard errors as well as the regression coefficients (r) obtained from the linear fit of the photophysical properties $\{\tilde{\nu}_{abs}, \tilde{\nu}_{fluo}, \Delta\tilde{\nu}$ and $QY\}$ of **1** versus E^N_T solvent polarity scale. $Np.$ denotes a number of solvents used in the analysis.

		Compound 1			
		equation $y=y_0 + a \cdot E^N_T$		r	$Np.$
		y_0	a		
$(\tilde{\nu}_{abs}) / \text{cm}^{-1}$	all solvents	29020±70	-(990±160)	0.7474	32
	aprotic	29100±90	-(1590±340)	0.7387	22
	protic	29230±330	-(1240±510)	0.6293	10
$(\tilde{\nu}_{fluo}) / \text{cm}^{-1}$	all solvents ^a	23880±350	-(6940±820)	0.8475	31
	aprotic	24790±230	-(12740±910)	0.9571	21
	protic	23920±1540	-(6030±2440)	0.6582	10
$\Delta\tilde{\nu} / \text{cm}^{-1}$	all solvents ^a	5130±330	5970±780	0.8223	31
	aprotic	4320±250	11140±980	0.9368	21
	protic	5200±550	4980±2460	0.5817	10
QY	all solvents ^b	0.85±0.05	-(1.23±0.10)	0.9072	30
	aprotic	0.97±0.04	-(1.96±0.16)	0.9474	20
	protic	0.61±0.09	-(0.73±0.15)	0.8670	10

^a without formamide

^b without formamide and 1,2-dimethoxyethane

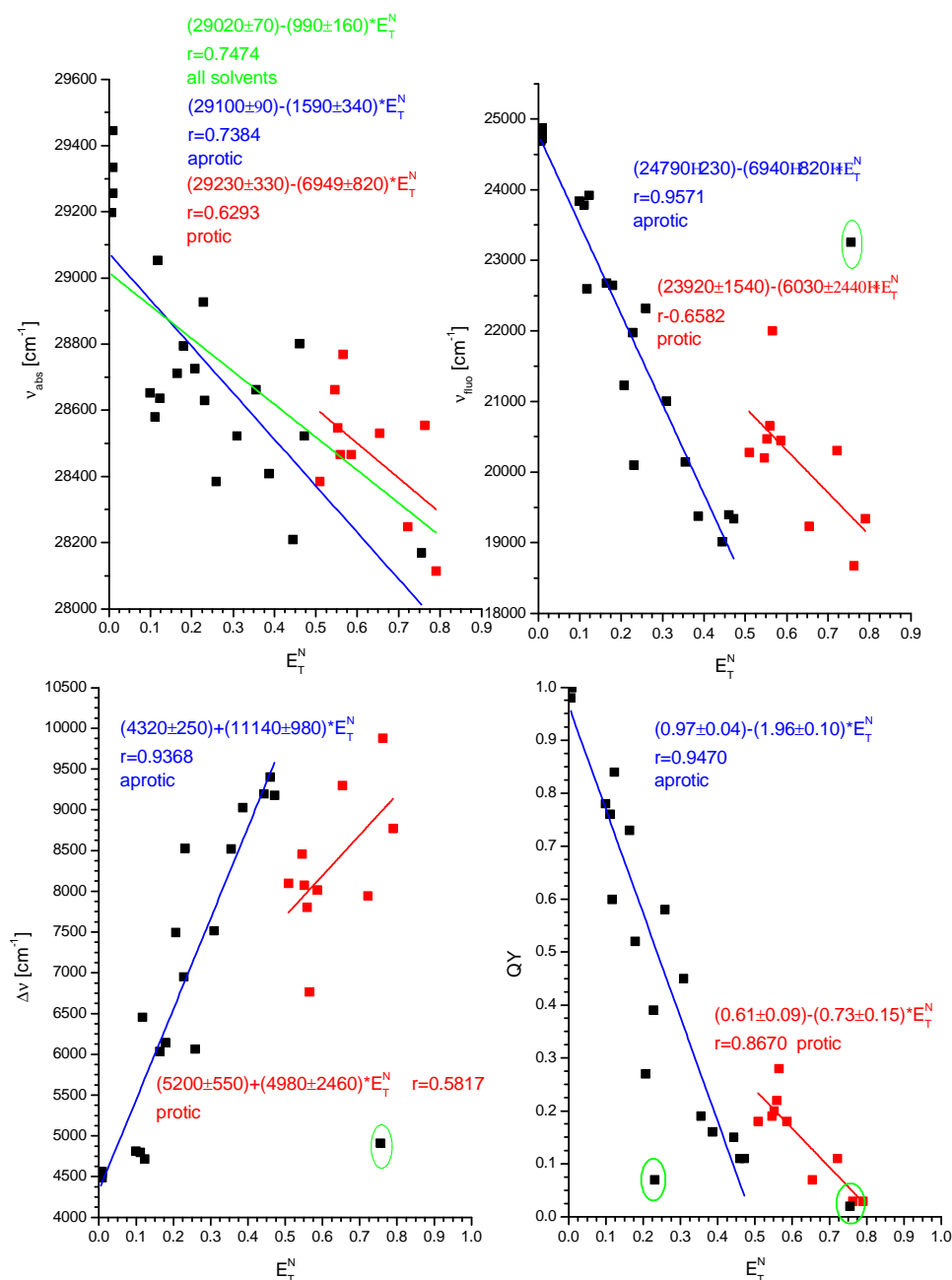


Fig. 5S Plot of dependence of absorption maximum position (top left), fluorescence maximum position (top right), Stokes shift (bottom left), and fluorescence quantum yield (bottom right) of **1** as a function of the solvent polarity parameter E_T^N for all solvents (green), aprotic solvents (blue), and protic solvents (red). The point(s) in green circle denotes these which were not included in the regression analysis.

Table 4S. The values of estimated coefficients (y_0 and a) and their standard errors as well as regression coefficients (r) obtained from the linear fit of photophysical properties $\{\tilde{\nu}_{abs}, \tilde{\nu}_{fluo}, \Delta\tilde{\nu}, \tau, \text{ and } QY\}$ of **2** versus the E^N_T solvent polarity scale. N_p denotes a number of solvents used in the analysis.

		Compound 2		r	N_p
		equation $y=y_0 + a^*E^N_T$			
		y_0	a		
$(\tilde{\nu}_{abs}) / \text{cm}^{-1}$	all solvents	29645±64	-(1360±150)	0.8577	32
	aprotic	29700±70	-(1745±240)	0.8502	22
	protic	29935±320	-(1700±500)	0.7669	10
$(\tilde{\nu}_{fluo}) / \text{cm}^{-1}$	all solvents	26610±110	-(2840±260)	0.8916	32
	aprotic	26725±120	-(3681±414)	0.8935	22
	protic	26810±530	-(2906±840)	0.7753	10
$\Delta\tilde{\nu} / \text{cm}^{-1}$	all solvents	3080±110	1480±260	0.7229	32
	aprotic	2970±140	1936±474	0.6748	22
	protic	3128±340	1208±530	0.6248	10
τ / ns	all solvents ^a	1.12±0.02	0.25±0.06	0.6434	29
	aprotic ^a	1.07±0.02	0.54±0.07	0.8702	19
	protic	1.52±0.12	-(0.39±0.19)	0.5707	10
QY	all solvents ^a	0.99±0.02	-(0.11±0.05)	0.3645	29
	aprotic ^a	1.43±0.15	0.05±0.06	0.1896	19
	protic	1.43±0.15	-(0.79±0.24)	0.7449	10

^a without trichloromethane, 1,2-dimethoxyethane, and formamide

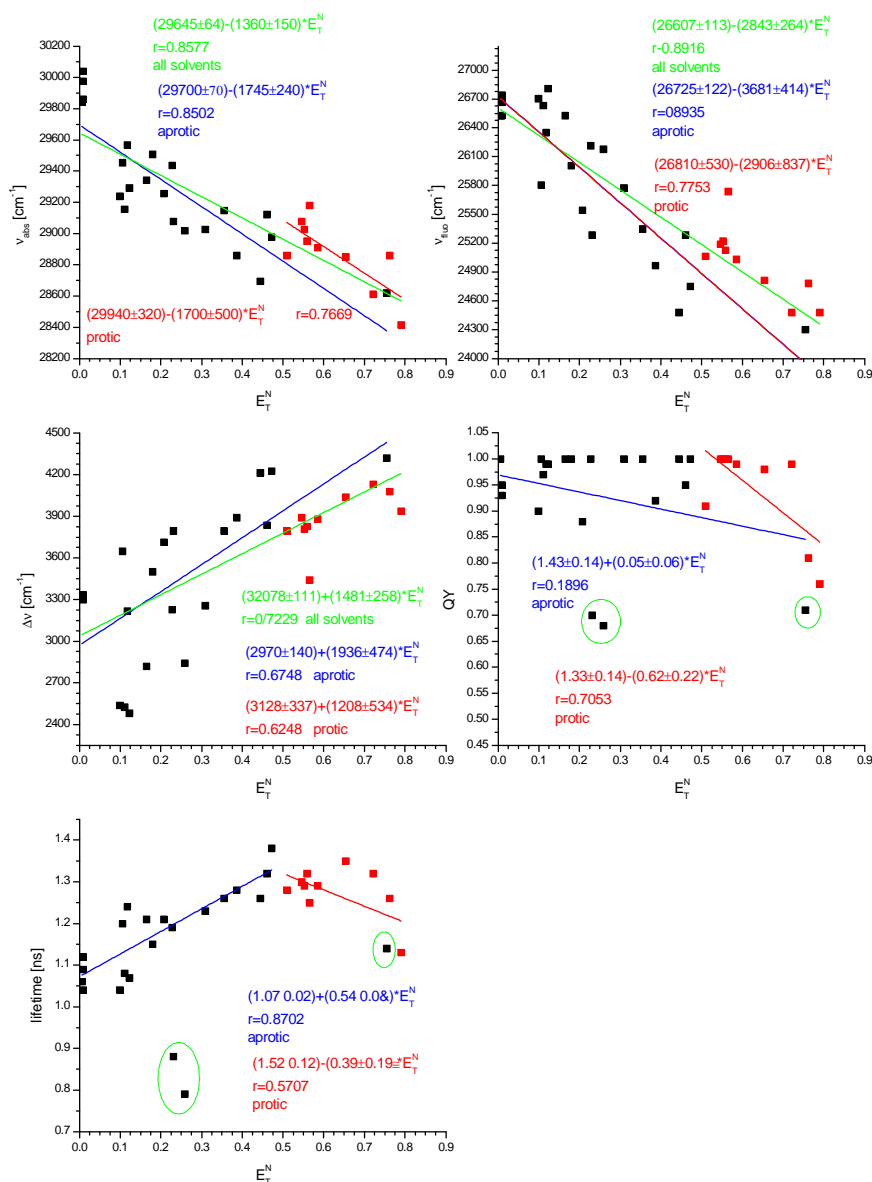


Fig. 6S Plot of dependence of absorption maximum position ($\tilde{\nu}_{abs}$) (top left), fluorescence maximum position ($\tilde{\nu}_{fluo}$) (top right), Stokes shift $\Delta\tilde{\nu}$ (middle left), fluorescence quantum yield (middle right), and fluorescence lifetime (bottom left) of **2** as a function of the solvent polarity parameter E_T^N for all solvents (green), aprotic solvents (blue), and protic solvents (red). The point(s) in green circle denotes these which were not included in the regression analysis.

Table 5S. The values of estimated coefficients (y_0 and a) and their standard errors as well as regression coefficients (r) obtained from the linear fit of photophysical properties $\{(\tilde{\nu}_{abs}), (\tilde{\nu}_{fluo}), \Delta\tilde{\nu}, \text{ and } QY\}$ of **1** versus the E_T^N solvent polarity scale. Np denotes a number of solvents used in the analysis.

		Compound 3		r	Np
		equation $y=y_0 + a \cdot E_T^N$			
		y_0	b		
$(\tilde{\nu}_{abs}) / \text{cm}^{-1}$	all solvents ^a	29130±80	-(1690±190)	0.8514	31
	aprotic ^a	29210±100	-(2020±400)	0.7544	21
	protic	27800±230	390±350	0.3453	10
$(\tilde{\nu}_{fluo}) / \text{cm}^{-1}$	all solvents ^a	25130±240	-(4430±560)	0.8204	31
	aprotic ^a	25790±200	-(8630±810)	0.9252	21
	protic	24380±840	-(2670±1310)	0.5619	10
$\Delta\tilde{\nu} / \text{cm}^{-1}$	all solvents ^a	4000±210	2730±500	0.7551	31
	aprotic ^a	3420±150	6610±590	0.9329	21
	protic	3410±930	3060±1440	0.5778	10
QY	all solvents ^b	0.98±0.05	-(1.08±0.13)	0.8816	31
	aprotic	0.99±0.04	-(1.28±0.13)	0.9153	21
	protic	1.93±0.45	-(2.48±0.72)	0.7757	10

^a without formamide

^b without 1,2-dimethoxyethane

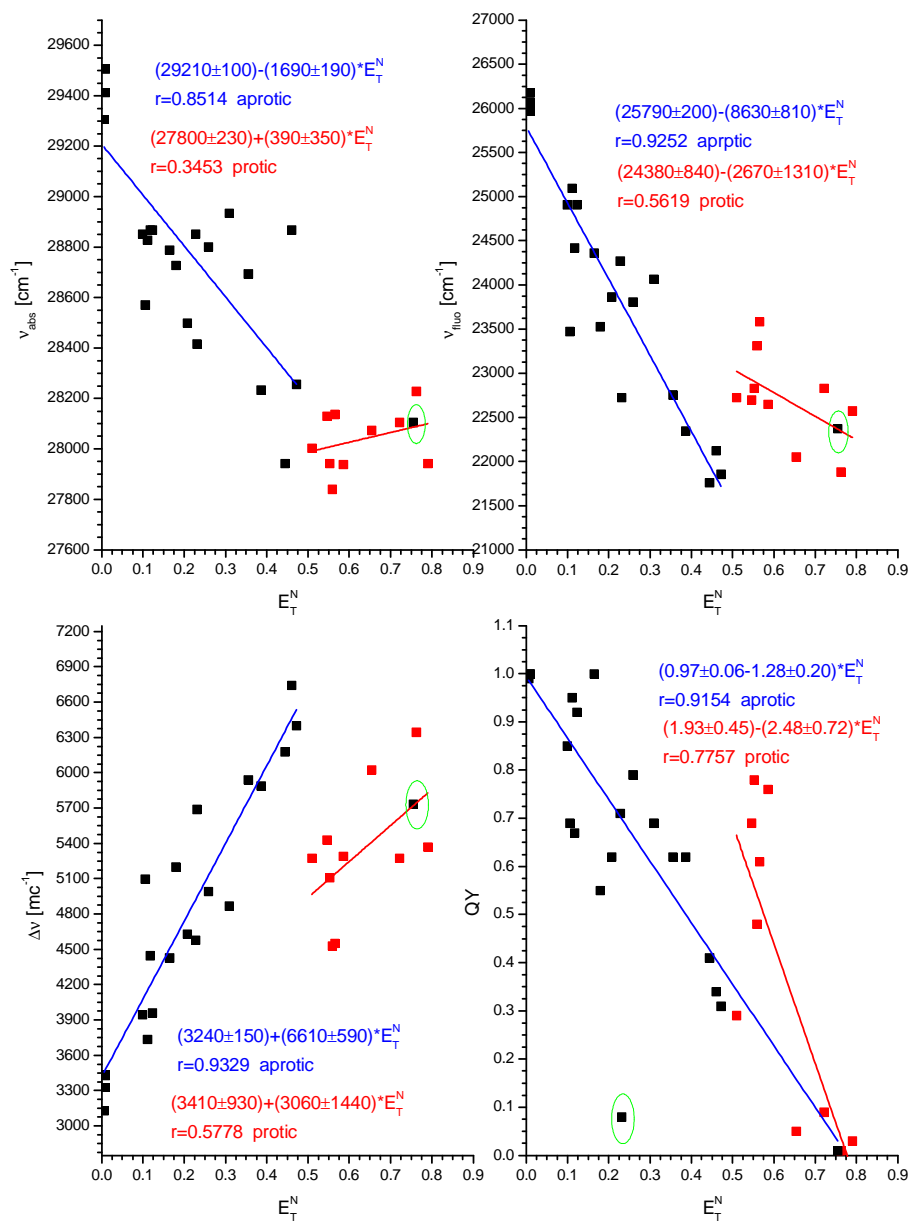


Fig. 7S Plot of dependence of absorption maximum position ($\tilde{\nu}_{abs}$) (top left), fluorescence maximum position ($\tilde{\nu}_{fluo}$) (top right), Stokes shift ($\Delta\tilde{\nu}$) (bottom left), and fluorescence quantum yield (bottom right) of **3** as a function of the solvent polarity parameter E_T^N for all solvents (green), aprotic solvents (blue), and protic solvents (red). The point in green circle denotes that which was not included in the regression analysis.

Table 6S The slopes (m_1 and m_2) of the linear fit of the Stokes shift ($\Delta\tilde{\nu}$) versus solvent polarity function f (Eq. 6) and ($\tilde{\nu}_{abs}+\tilde{\nu}_{flu}$) versus solvent polarity functions $f + 2g$ (Eq. 7) and the appropriate correlation coefficients.

compound	m_1	r	m_2	r
(1) ^a	5018±239	0,9665	6720±327	0.9652
(2)	1110±146	0.7936	3264±208	0.9371
(3) ^b	2549±239	0,8774	5181±375	0.9213

^a without 1,2-dimethoxyethane and formamide

^b without 1,2-dimethoxyethane

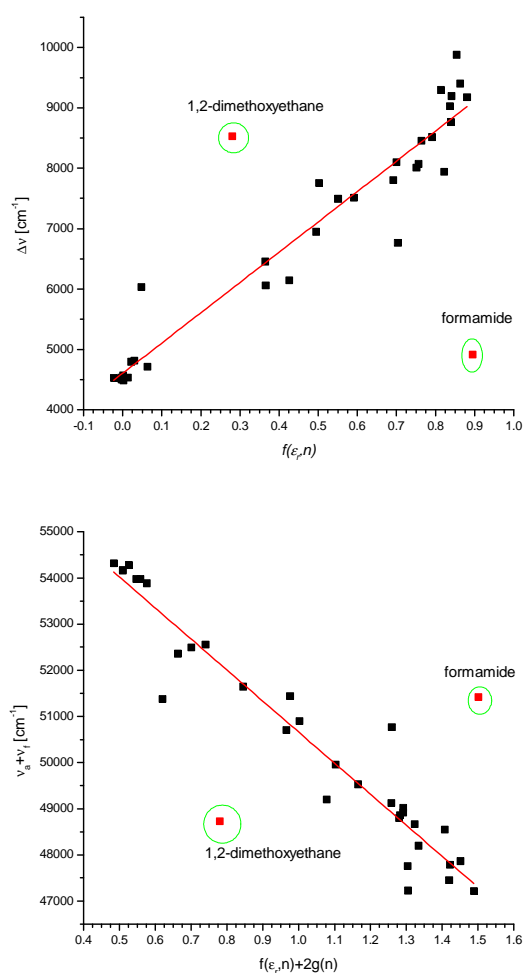


Fig. 8S The dependence of the Stokes shift ($\Delta\tilde{\nu}$) (top) and the sum of absorption and fluorescence wavenumber ($\tilde{\nu}_{abs}+\tilde{\nu}_{flu}$) (bottom) of **1** on two solvent polarity functions.

Table 7S . Estimated from eq. **3** coefficients (y_0 , a_{SPP} , b_{SA} , c_{SB});. their standard errors and correlation coefficients (r) for the multiple linear regression analysis of $\tilde{\nu}_{abs}$, $\tilde{\nu}_{fluo}$, QY, $\Delta\tilde{\nu}$ of **1** as function of the Catalán three-parameter solvent scale.

y	y_0	a_{SPP}	b_{SA}	c_{SB}	r
ν_a	30148±221	-(1863±329)	-(484±191)	-(97±158)	0.7441
	30110±205	-(1771±274)	-(463±177)		0.7382
ν_f	31511±850	-(11940±1267)	-(447±737)	-(1153±608)	0.8890
	31639±815	-(12131±1213)		-(1259±576)	0.8875
$\Delta\nu$	-(1333±1000)	10025±1490	-(262±850)	1426±703	0.8964
	-(1254±951)	9906±1416		1370±668	0.8960
QY	1.88±0.09	-(1.66±0.13)	-(0.32±0.07)	-(0.29±0.06)	0.9767

Table 8S. Estimated from eq. **2** coefficients (y_0 , a_{π^*} , b_α , c_β), their standard errors and correlation coefficients (r) for the multiple linear regression analysis of ν_{abs} , ν_{fluo} , QY, $\Delta\tilde{\nu}$, of **1** as a function of the Kamlet-Taft three-parameter solvent scale.

y	y_0	a_{π^*}	b_α	c_β	r
$\tilde{\nu}_{abs}/\text{cm}^{-1}$	29239±45	-(952±82)	-(260±79)	-(25±108)	0.8916
	29235±42	-(960±74)	-(272±57)		0.8914
$\tilde{\nu}_{fluo}/\text{cm}^{-1}$	24770±413	-(3042±750)	-(158±723)	-(3782±984)	0.7345
	24741±404	-(3061±733)		-(3634±706)	0.7340
$\Delta\tilde{\nu}/\text{cm}^{-1}$	4470±452	2087±773	-(417±745)	3757±1013	0.8026
	4493±418	2136±759		3387±731	0.8001
QY	0.97±0.03	-(0.55±0.06)	-(0.12±0.06)	-(0.58±0.08)	0.9629

Comparing the correlation coefficients obtained using four and three-parameter solvents scales, it should be noted that four-parameter solvent scale gives better results (higher correlation coefficient) than that of three-parameter solvent scale regardless of whether it is the old Catalán or Kamlet-Taft scale (Tables 7S and 8S).

For last two scales, in the correlation of spectral and photophysical properties the same type of solvent parameters are important, although the values of corresponding coefficients are different (Tables 7S and 8S).

Table 9S. Estimated coefficients (y_0 , a_{SPP} , b_{SA} , c_{SB} ; see eq. 3), their standard errors and correlation coefficients (r) for the multiple linear regression analysis of $\tilde{\nu}_{abs}$, $\tilde{\nu}_{fluo}$, $\Delta\tilde{\nu}$, τ , and QY of **2** as a function of the Catalán three-parameter solvent scale.

y	y_0	a_{SPP}	b_{SA}	c_{SB}	r
$\tilde{\nu}_{abs}$	30980±175	-(2230±260)	-(743±154)	-(89±122)	0.8808
	30955±168	-(21661±227)	-(688±147)		0.8731
$\tilde{\nu}_{fluo}$	28804±318	-(3628±472)	-(1528±280)	-(299±222)	0.8968
	28945±323	-(4004±435)	-(1528±282)		0.8777
$\Delta\tilde{\nu}$	2177±400	1390±595	426±276	736±346	0.7570
τ	0.85±0.12	0.30±0.18	-(0.01±.11)	0.20±0.08	0.6627
	0.85±0.12	0.31±0.17		0.21±0.08	0.6625
QY	1.00±0.10	-(0.13±0.15)	-(0.19±0.08)	0.15±0.07	0.4644
	0.92±0.03		-(0.22±0.08)	0.12±0.06	0.4444

Table 10S. Estimated coefficients (y_0 , a_{π^*} , b_{α} , c_{β} ; see eq. 2) their standard errors and correlation coefficients (r) for the multiple linear regression analysis of $\tilde{\nu}_{abs}$, $\tilde{\nu}_{fluo}$, $\Delta\tilde{\nu}$, τ , and QY of **2** as a function of the Kamlet-Taft three-parameter solvent scale.

y	y_0	a_{π^*}	b_{α}	c_{β}	r
$\tilde{\nu}_{abs}$	29871±38	-(1058±68)	-(378±66)	-(129±90)	0.9447
$\tilde{\nu}_{fluo}$	26862±142	-(1309±254)	-(539±245)	-(972±323)	0.7935
$\Delta\tilde{\nu}$	3009±144	250±257	162±248	845±336	0.6800
	3066±119			1095±223	0.6629
τ	1.04±0.04	-(0.00±0.07)	-(0.04±0.06)	0.34±0.09	0.6978
	1.05±0.03			0.31±0.06	0.6937
QY	0.94±0.03	-(0.13±0.06)	-(0.12±0.06)	-(0.20±0.08)	0.5087

The correlation analysis of the spectral and photophysical properties of (**2**) applying a three-parameter solvent polarity scale reveals (Tables 9S and 10S, ESI) that the

Kamlet-Taft as well as the old Catalan scale give much lower correlation coefficients than that of four-parameter Catalán solvent polarity scale. Moreover, the contributions of various parameters characterizing the solvent in eqs. **2** and **3** are different. In the Kamlet-Taft correlation of the absorption and emission maxima all a_{π^*} , b_{α} and c_{β} coefficients have significant influence on the correlation, whereas in the Catalán correlation the solvent basicity has no impact. The differences also exist for the correlation of Stokes shift, fluorescence quantum yield and fluorescence lifetime (Tables 9S and 10S, ESI). It seems that this is the result of poor correlation, small values of estimates burdened with large standard errors.

Table 11S. Estimated coefficients (y_0 , a_{SPP} , b_{SA} , c_{SB} ; see eq. **3**), their standard errors and correlation coefficients (r) for the multiple linear regression analysis of $\tilde{\nu}_{abs}$, $\tilde{\nu}_{fluo}$, $\Delta\tilde{\nu}$, and QY of **3** as a function of the Catalán three-parameter solvent scale.

y	y_0	a_{SPP}	b_{SA}	c_{SB}	r
$\tilde{\nu}_{abs}$	33013±199	-(1345±261)	-(691±175)	-(935±139)	0.9033
$\tilde{\nu}_{fluo}$	32202±747	-(9887±1110)	-(518±660)	-(1352±522)	0.8822
	32373±710	-(10146±1053)		-(1457±501)	0.8795
$\Delta\tilde{\nu}$	18±587	6300±872	-(17±507)	72±405	0.8719
	-(12±506)	6377±644			0.8717
QY	1.61±0.23	-(1.19±0.34)	-(0.77±0.20)	0.02±0.16	0.8232
	1.60±0.22	-(1.16±0.29)	-(0.76±0.19)		0.8231

Table 12S. Estimated coefficients (y_0 , a_{π^*} , b_{α} , c_{β} ; see eq. **2**), their standard errors and correlation coefficients (r) for the multiple linear regression analysis of $\tilde{\nu}_{abs}$, $\tilde{\nu}_{fluo}$, $\Delta\tilde{\nu}$, and QY of **3** as a function of the Kamlet-Taft three-parameter solvent scale.

y	y_0	a_{π^*}	b_{α}	c_{β}	r
$\tilde{\nu}_{abs}$	29395±56	-(589±6)	-(254±3)	-(1050±132)	0.9211
$\tilde{\nu}_{fluo}$	26898±237	-(3447±423)	-(165±408)	-(3213±523)	0.8830
	26885±231	-(3457±416)		-(3064±407)	0.8824
$\Delta\tilde{\nu}$	3422±217	1917±383	-(225±374)	1424±507	0.8250
	3440±213	1931±383		1221±375	0.8226
QY	1.01±0.08	-(0.56±0.15)	-(0.31±0.14)	-(0.11±0.19)	0.7655
	0.99±0.07	-(0.59±0.14)	-(0.36±0.11)		0.7626

Comparing the correlation coefficients obtained using four and three-parameter solvents scales (Tables 11S and 12S, ESI), it should be noted that, as for previously described compounds, four-parameter solvent scale gives better results (higher correlation coefficient) than that of three-parameter solvent scale regardless of whether it is the old Catalán or Kamlet-Taft scale. For these two scales in the correlation of absorption and fluorescence maxima positions and fluorescence quantum yield the same type of solvent properties are important in the correlation although their values, also in this case, are different (Table 11S and 12S; ESI). Different solvent parameters are responsible for Stokes shift correlation. The correlation according to Kamlet-Taft equation shows that the acidity of the solvent can be omitted (the correlation coefficient $r=0.8226$ whereas for the original fit $r=0.8250$), while in the correlation using Catalán equation both the basicity and acidity of the solvent can be omitted, as in the case of a four-parameter correlation (the correlation coefficient $r=0.8717$ whereas for the original fit $r=0.8719$).