SUPPLEMENTARY MATERIAL

Assembly of New Merocyanine Chromophores with a 1,8-Naphthalimide Core by a New Method for the Synthesis of the Methine Function

Aleksey A. Vasilev,[A,F] Stanislav Baluschev,[B] Diana Cheshmedzhieva,[A] Sonia Ilieva,[A] Obis D. Castaño,[C] Juan J. Vaquero,[D] Silvia E. Angelova,[C,E] Katharina Landfester [B]

[A]Department of Pharmaceutical and Applied Organic Chemistry, Faculty of Chemistry and Pharmacy, University of Sofia, James Bourchier 1, 1164 Sofia, Bulgaria

[B] Max Planck Institute for Polymer Research, 55021 Mainz, Germany

[C]Departamento de Química Analítica, Química Física e Ingeniería Química, Universidad de Alcalá, 28871 Alcalá de Henares, Madrid, Spain

[D]Departamento de Química Orgánica, Universidad de Alcalá, 28871 Alcalá de Henares, Madrid, Spain

[E]Institute of Organic Chemistry with Centre of Phytochemisty, Bulgarian Academy of Sciences, 1113, Sofia, Bulgaria (permanent address)

[F]Corresponding author: Email: ohtavv@chem.uni-sofia.bg

Analytical and spectral characterization data

Table S1-A. Absorption Maxima and Molar Absorptivities (ε (l. $mol^{-1}.cm^{-1}$)) of Dyes **7a-7k** in various solvents with different polarity (ε_r).

Dye №	CCl$_4$ (ε_r = 2.24)	1,4-dioxane (ε_r = 2.25)	benzene (ε_r = 2.27)	toluene (ε_r = 2.4)	CHCl$_3$ (ε_r = 4.7)	EtAc (ε_r = 6.02)
7a	-	519 (1106) 374; 343	520 (1003); 379; 348	519 (1433); 379; 347	533 (1521); 381; 348	531 (1860); 384; 350
7b	523 (25118); 344	525; 342	526 (26819); 345	524 (13667); 343	544(20433); 349	540(27137); 347
7c	523(9097); 394; 346; 334	530(15982); 428; 410; 344	527(12191); 394; 348	525(10864); 389; 348	548(9039); 430; 399; 347	545(2111); 390; 347
7d	523(2118);	524(1446);	526(2665);	525(1752);	543(2115);	540(1742);

	381; 345	378; 346	385; 340	382; 346	388; 348	358; 347
7e				516(6267); 347	533(6374); 349	
7f			529 (29952) 335; 283	528 (35512)	544 (26466)	540 (33210)
7g	515 (5748); 391	516; 394;331	516 (4958); 394	515 (5477); 392; 348	530 (6967); 388	528 (6126); 382
7h				523(3871); 381; 342	542(8100); 377; 341	542(5216); 378; 341
7i			572(4767); 391; 314	569(5344); 391; 314	597(42113); 398; 316	600(7016); 398; 316
7j	566.5 (10600); 390	566.5 (19600); 388	569 (18052); 390	567.5 (30920); 389.5; 294	593 (33378); 392; 284	577 (10662);
7k	567 (4570); 384;317	569 (38400); 387; 312	574 (31683); 391; 316	575 (16951); 389; 314	594 (39035); 392; 316	584 (18646); 389; 314

Table S1-B. Absorption Maxima and Molar Absorptivities (ε (l. mol^{-1}.cm^{-1})) of Dyes **7a-7k** in various solvents with different polarity (ε_r).

| Dye №	acetone ($\varepsilon_r = 20.7$)	EtOH ($\varepsilon_r = 24.9$)	MeOH ($\varepsilon_r = 33$)	AcCN ($\varepsilon_r = 36$)	DMF ($\varepsilon_r = 38.3$)	DMSO ($\varepsilon_r = 48$)
7a	521 (1600); 377; 346	541 (1716); 380; 347	540 (1570); 379; 347	526 (1564); 385; 345	533 (1512); 381; 350	541 (1906); 381; 347
7b	529(24984); 344	Not soluble	548; 344	533(26813); 344	535(26015); 345	546(3272); 350
7c	535(3074); 425; 405; 345	551(12446); 425; 401; 346	552(11106); 423; 397; 346	540(4776); 384;346	546(4179); 428;408;347	553(4109); 430;408;347
7d	529(1409); 379; 347	548(1422); 381; 346	547(1829); 380; 346	532(1516); 381;345	538(1863); 384;350	546(1978); 382;346
7e	521(5764); 343	538(5510); 346	538(5510); 346	524(8925); 346	531(9579); 350	539(10999); 346
7f	529 (33437) 339; 276			532 (26419)	535 (31432)	545 (30697)
7g		534 (6132); 389; 349	531; 388; 331	523 (4772); 385	530 (4631); 395; 349	535 (6273); 397; 333
7h	532(5032); 371; 339	535(3667); 373; 338	535; 321	533(2663); 375; 340	543(7451); 373; 340	546 (6208); 377; 341
7i	591(31742); 398	587 (10571)	586 (47713)	592 (31598)	603 (46985); 404;317	610 (34388); 407; 319
7j	589 (29860); 392	610 (21095); 394	608 (8940); 393; 281	588 (14100); 391; 282	605 (36784); 395	614 (41290); 399; 282
7k	592 (16380); 390	Not soluble	Not soluble	591 (3661); 388; 341	608 (35407); 394; 315	619 (19844); 395; 315
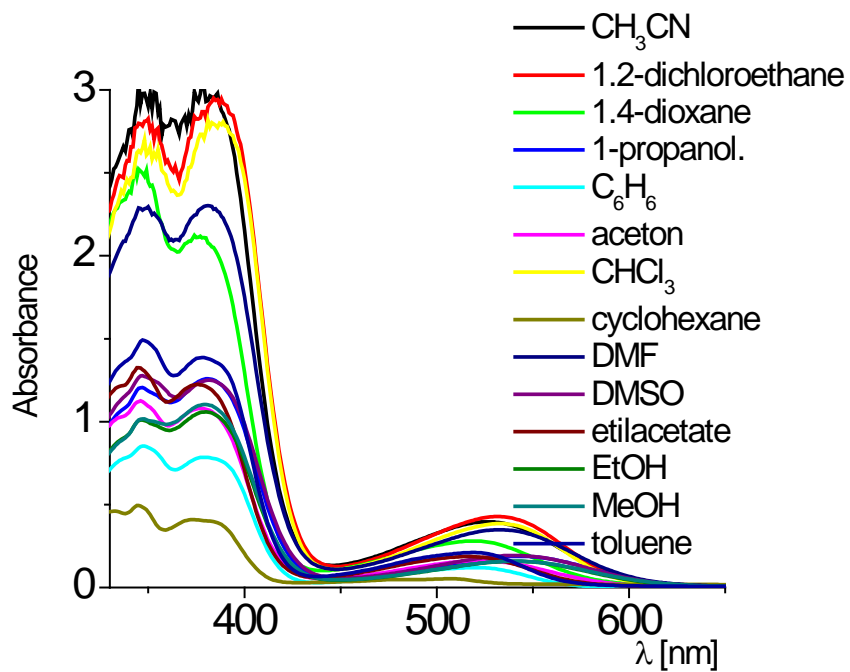
Figure S1. Absorption spectra for dye **7a** in solvents with different polarity.
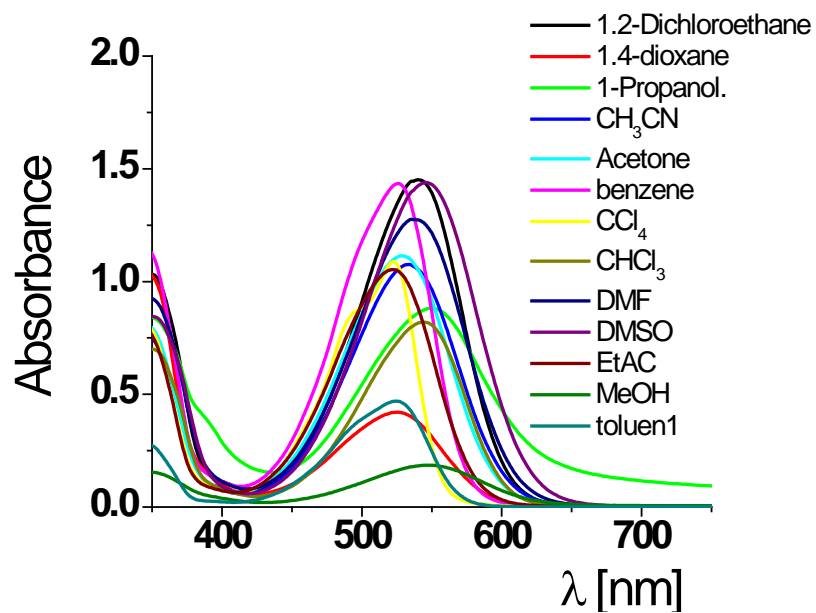

Figure S2. Absorption spectra for dye **7b** in solvents with different polarity
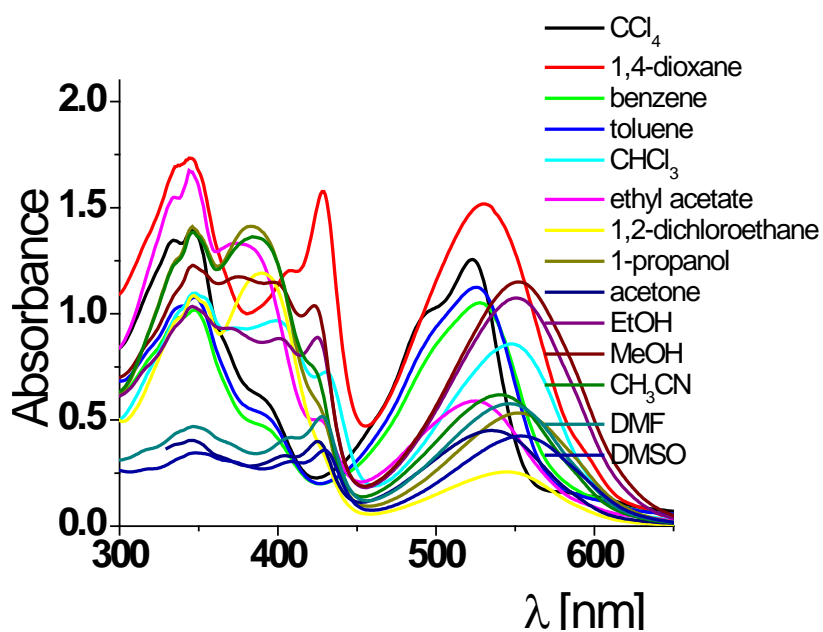
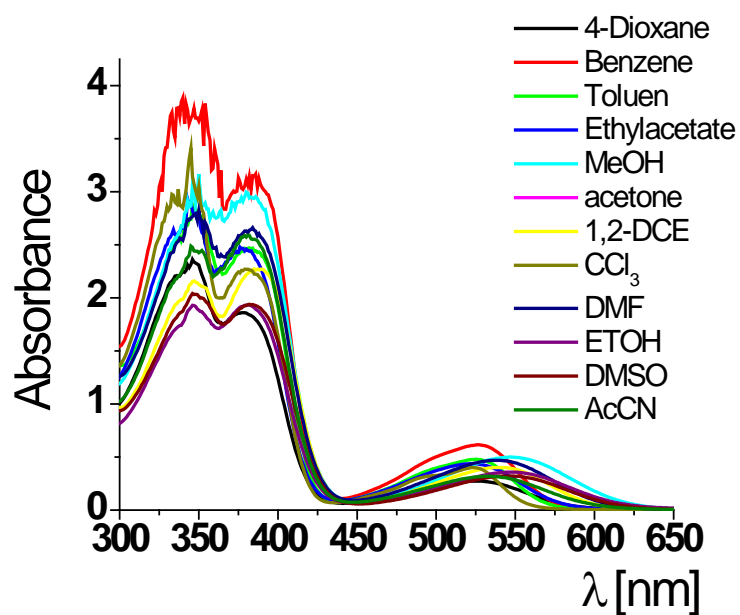**Figure S3.** Absorption spectra for dye **7c** in solvents with different polarity

Figure S4. Absorption spectra for dye **7d** in solvents with different polarity.
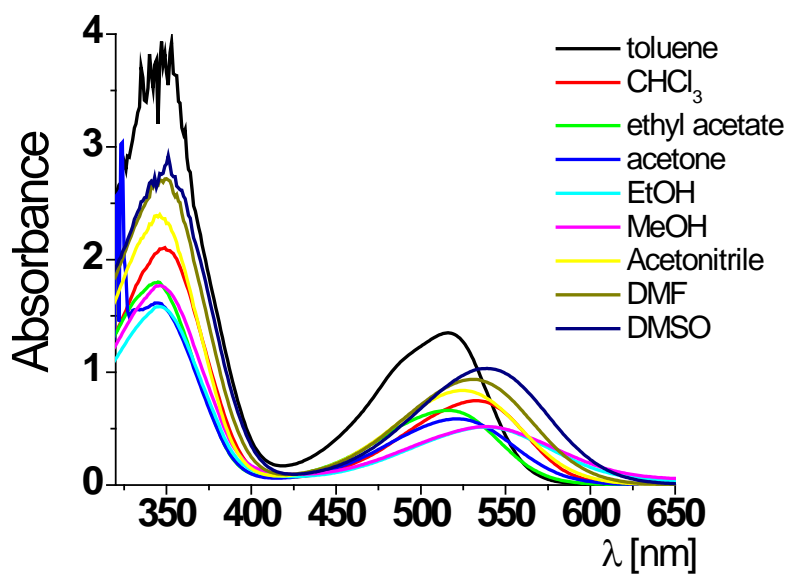
Figure S5. Absorption spectra for dye **7e** in solvents with different polarity.

Figure S6. Absorption spectra for dye **7f** in solvents with different polarity.

Figure S7. Absorption spectra for dye **7g** in solvents with different polarity.

Figure S8. Absorption spectra for dye **7h** in solvents with different polarity.

Figure S9. Absorption spectra for dye **7i** in solvents with different polarity.
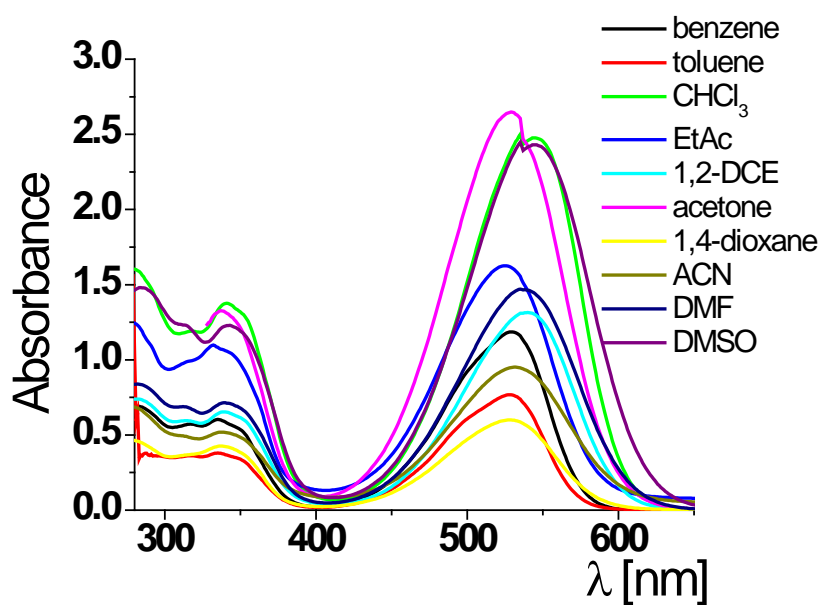

Figure S10. Absorption spectra for dye **7j** in solvents with different polarity.

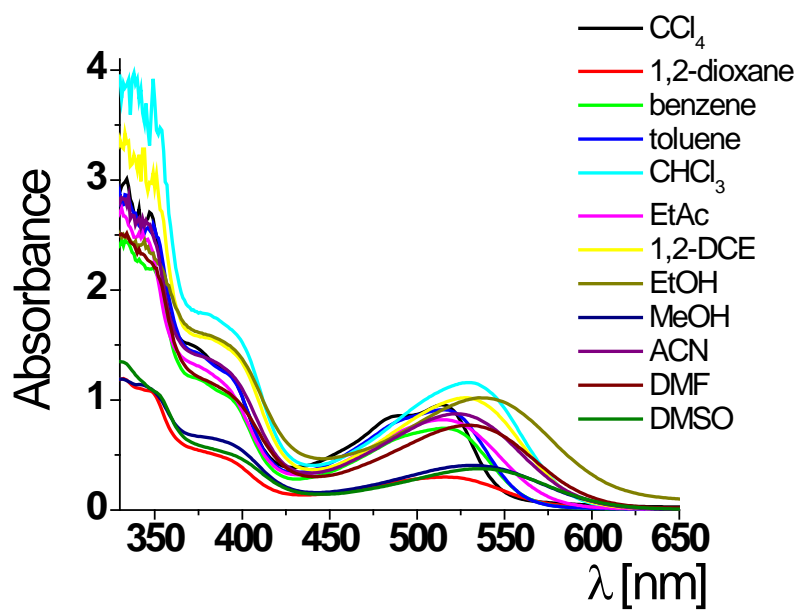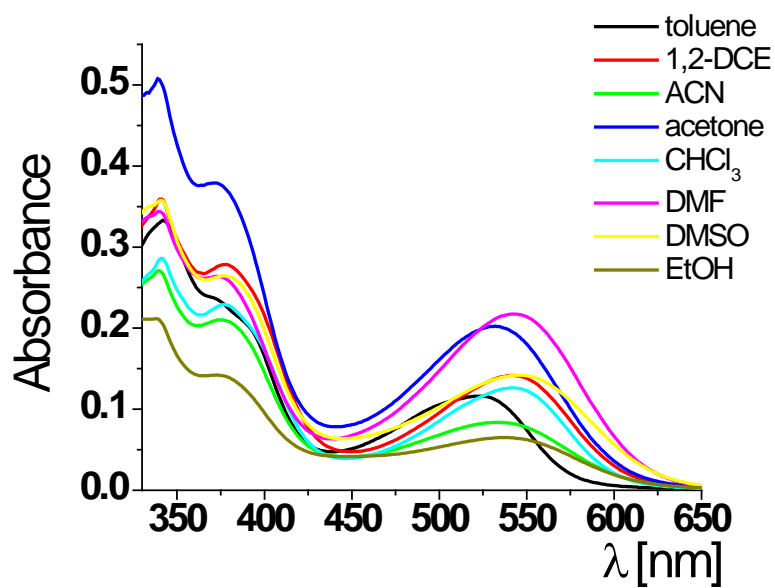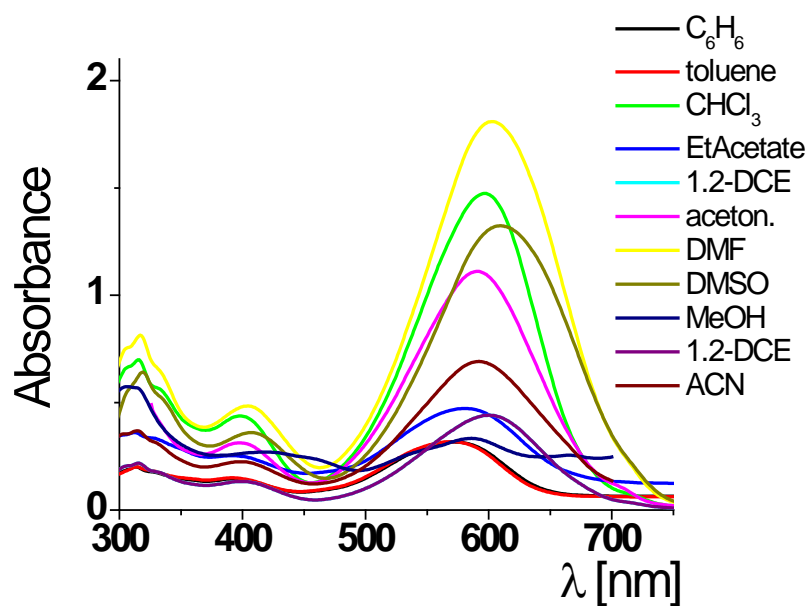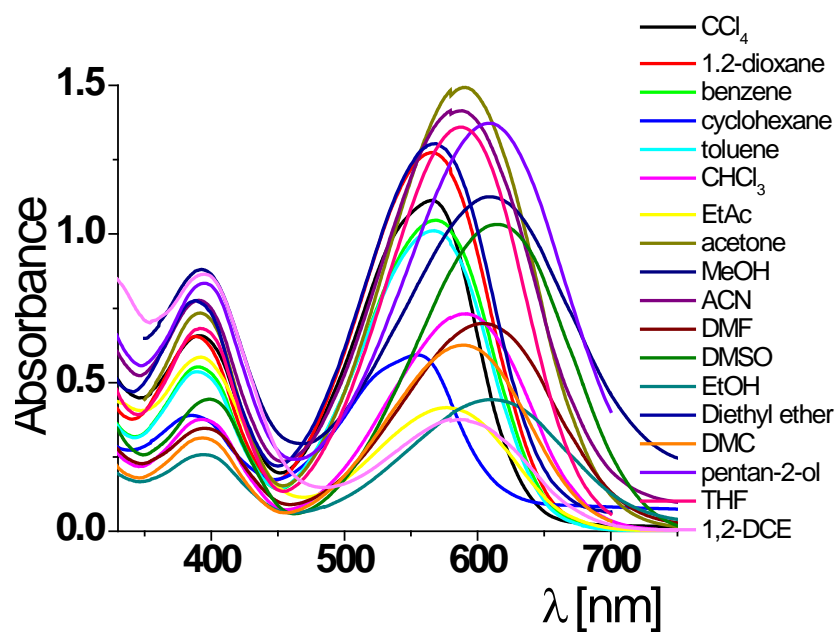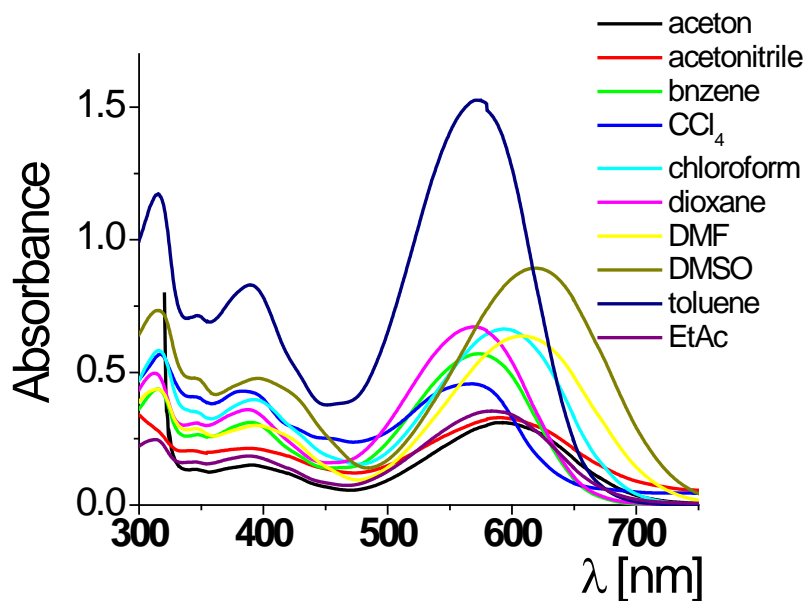**Figure S11.** Absorption spectra for dye **7k** in solvents with different polarity.

Table S2. Table Kamlet – Taft parameters for solvents with different polarities (α, β, π^*).

solvents	dielectric constant	Kamlet - Taft		
		α	β	π^*
cyclohexane	2.02	0.00	0.00	0.00
CCl4	2.24	0.00	0.10	0.28
1,4-dioxane	2.25	0.00	0.37	0.55
benzene	2.27	0.00	0.10	0.59
toluene	2.4	0.00	0.11	0.49
diethyl ether	4.33	0.00	0.47	0.27
$CHCl_3$	4.70	0.20	0.10	0.69
ethylacetate	6.02	0.00	0.45	0.55
tetrahydrofurane	7.58	0.00	0.55	0.58
dichloromethane	8.93	0.13	0.10	0.82
1,2-dichloroethan	10.50	0.00	0.10	0.81
aceton	20.70	0.08	0.48	0.62
2-propanol	22.50	0.76	0.84	0.48
ethanol	24.90	0.86	0.75	0.54
methanol	33.00	0.98	0.66	0.6
acetonitrile	37.50	0.19	0.40	0.66
DMF	38.30	0.00	0.69	0.88
DMSO	48.00	0.00	0.76	1.00
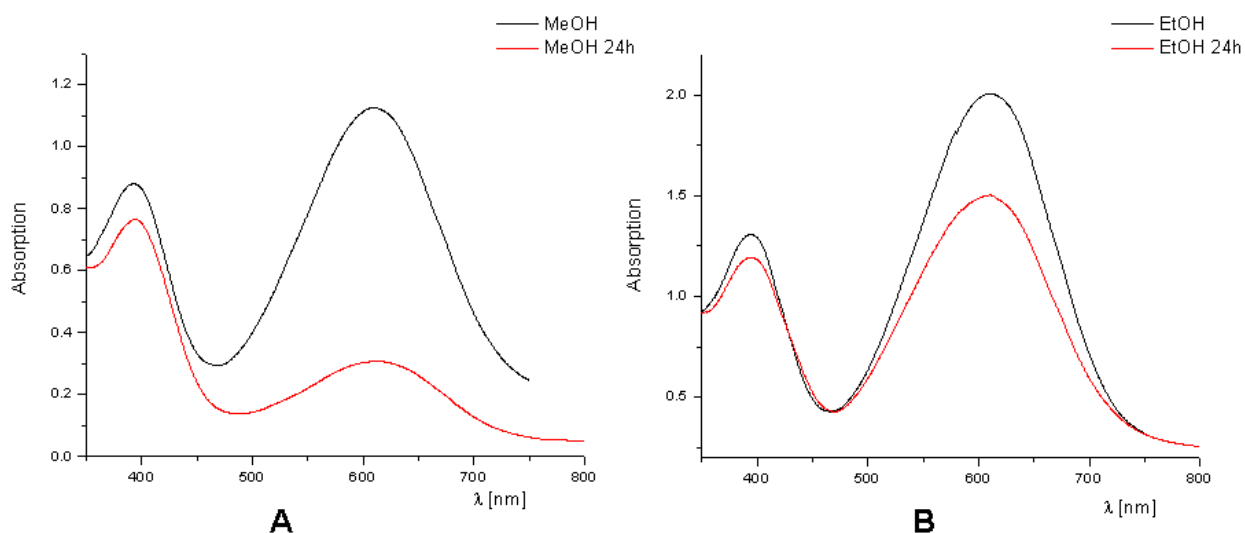
Figure S12. Change of the absorption intensity with time for dye **7j** in methanol (A) and ethanol (B).

Figure S13. The change of the absorption of dye **7j** after one day is seen even with naked eye (green –in MeOH; blue - in EtOH).
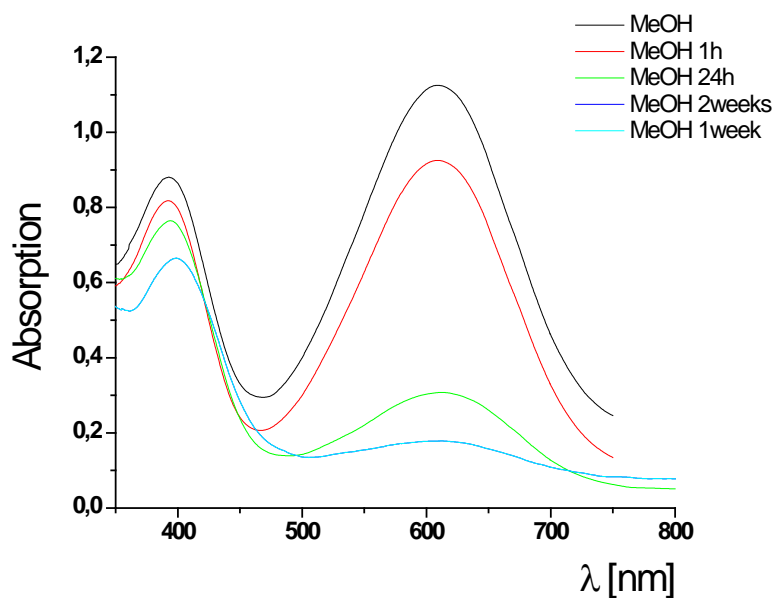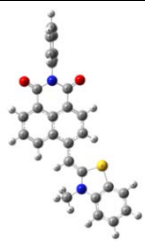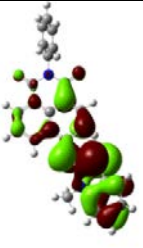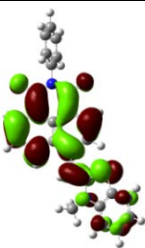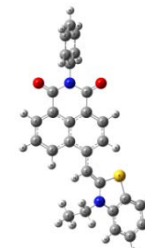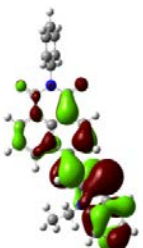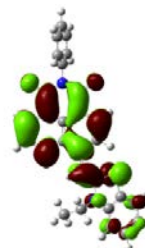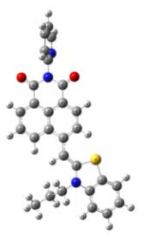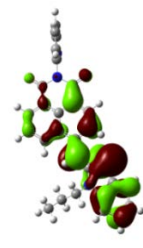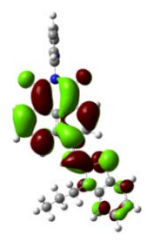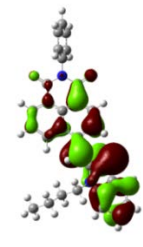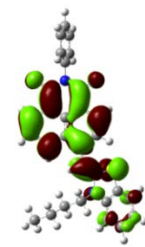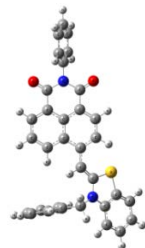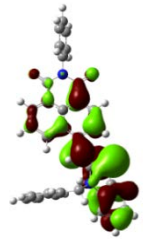
Figure S14. The change with time of the absorption for dye 7j in MeOH.

Computations

	Charge		HOMO	LUMO
7a	0			
7b	0			
7c	0			
7d	0			
7e	0			
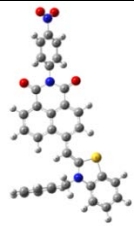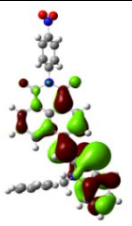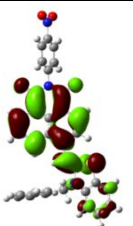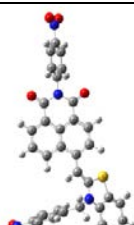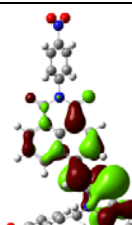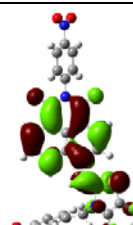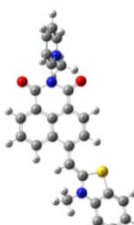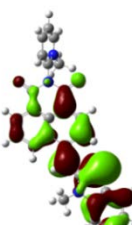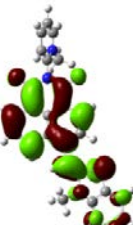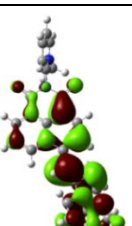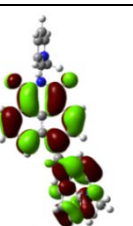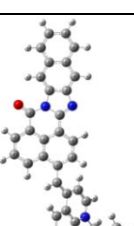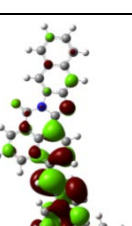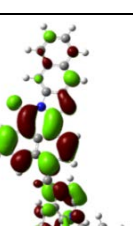
7f	0			
7g	0			
7h	1			
7i	1			
7j	0			
7k	0			

Figure S15. PBE0/6-311G(d,p) optimized structures and HOMO and LUMO of the compounds.

PBE0/6-311G(d,p) optimized geometries of compounds 7a-7k:

7a

6	6.003772000	-0.729428000	1.268062000
6	5.357772000	-0.597039000	0.047065000
6	6.002439000	-0.938711000	-1.133181000
6	7.303994000	-1.419435000	-1.089377000
6	7.958619000	-1.552180000	0.129248000
6	7.307229000	-1.205346000	1.306774000
1	5.486610000	-0.452942000	2.179671000
1	5.480313000	-0.834795000	-2.077314000
1	7.807409000	-1.691316000	-2.011013000
1	8.976550000	-1.926183000	0.161232000
1	7.814453000	-1.305128000	2.260465000
6	3.809156000	1.252639000	0.290209000
6	2.993841000	-1.024199000	-0.313891000
6	2.410993000	1.736711000	0.248186000
6	1.621618000	-0.495067000	-0.345348000
6	2.166543000	3.060715000	0.537705000
6	1.349848000	0.862373000	-0.073027000
6	0.852842000	3.544606000	0.531155000
6	0.013604000	1.351295000	-0.109594000
6	-0.194935000	2.708109000	0.221021000
1	-1.204955000	3.098861000	0.255073000
6	0.581405000	-1.344180000	-0.655981000
6	-1.058242000	0.450869000	-0.451965000
6	-0.731094000	-0.876226000	-0.715840000
1	3.008240000	3.699816000	0.779634000

1	0.659964000	4.581744000	0.782878000
1	-1.504688000	-1.564165000	-1.036045000
1	0.812382000	-2.380369000	-0.877702000
7	4.009032000	-0.103882000	0.005034000
8	3.260829000	-2.182310000	-0.546380000
8	4.740643000	1.978034000	0.558354000
6	-2.412737000	0.945244000	-0.547522000
6	-3.565806000	0.251923000	-0.340752000
16	-3.696027000	-1.406664000	0.249395000
6	-5.873185000	-0.014479000	-0.065557000
6	-5.438004000	-1.267375000	0.379339000
1	-2.532682000	1.995478000	-0.780571000
6	-7.228387000	0.298813000	-0.026244000
6	-8.123461000	-0.660700000	0.435576000
6	-6.329573000	-2.221988000	0.836012000
6	-7.685567000	-1.910095000	0.860467000
1	-8.398619000	-2.643883000	1.218074000
1	-5.975980000	-3.190061000	1.172713000
1	-9.180519000	-0.421043000	0.468402000
1	-7.589523000	1.272357000	-0.335277000
7	-4.830876000	0.781451000	-0.511287000
6	-5.019974000	2.099840000	-1.063326000
1	-4.812592000	2.884474000	-0.326442000
1	-4.357740000	2.233375000	-1.921844000
1	-6.047313000	2.201487000	-1.409531000

7b

6	6.416416000	-0.187168000	0.993692000
6	5.554318000	-0.569255000	-0.024253000
6	5.995908000	-1.389064000	-1.052935000

6	7.311709000	-1.831526000	-1.060498000
6	8.181937000	-1.450780000	-0.046087000
6	7.732804000	-0.627579000	0.979428000
1	6.054860000	0.457061000	1.786984000
1	5.306859000	-1.681584000	-1.836881000
1	7.657189000	-2.475816000	-1.861931000
1	9.210462000	-1.795990000	-0.054684000
1	8.408836000	-0.326459000	1.772558000
6	3.962120000	1.233586000	-0.323822000
6	3.197418000	-1.053025000	0.309209000
6	2.551595000	1.682112000	-0.307500000
6	1.813503000	-0.555706000	0.327792000
6	2.276786000	2.992252000	-0.630681000
6	1.510224000	0.788956000	0.026951000
6	0.951738000	3.443613000	-0.642081000
6	0.162316000	1.246029000	0.048036000
6	-0.076543000	2.589420000	-0.315110000
1	-1.094761000	2.957223000	-0.358977000
6	0.792703000	-1.421561000	0.656715000
6	-0.889727000	0.328643000	0.409419000
6	-0.530301000	-0.983766000	0.705242000
1	3.104263000	3.646066000	-0.882119000
1	0.734654000	4.469345000	-0.919532000
1	-1.286594000	-1.683009000	1.041307000
1	1.047442000	-2.446892000	0.901723000
7	4.192474000	-0.111853000	-0.012029000
8	3.490931000	-2.202220000	0.553990000
8	4.878664000	1.978063000	-0.591349000
6	-2.253942000	0.795913000	0.492129000
6	-3.396374000	0.073142000	0.326119000

16	-3.488230000	-1.610220000	-0.200224000
6	-5.698802000	-0.277643000	0.110527000
6	-5.235746000	-1.533844000	-0.293107000
1	-2.391735000	1.851662000	0.685377000
6	-7.064677000	-0.009331000	0.103356000
6	-7.940721000	-1.015380000	-0.291465000
6	-6.108126000	-2.534498000	-0.683492000
6	-7.473852000	-2.266212000	-0.680066000
1	-8.172425000	-3.036448000	-0.985862000
1	-5.733426000	-3.505031000	-0.988807000
1	-9.005935000	-0.812440000	-0.299329000
1	-7.446495000	0.963371000	0.390106000
7	-4.675201000	0.573205000	0.491715000
6	-4.927518000	1.919036000	0.972001000
1	-4.144425000	2.165369000	1.693250000
1	-5.863457000	1.892768000	1.536484000
6	-4.998224000	2.952995000	-0.142609000
1	-4.066771000	2.981700000	-0.713077000
1	-5.809117000	2.722737000	-0.837973000
1	-5.177083000	3.947517000	0.274619000

7c

6	6.542845000	-0.435748000	1.108555000
6	5.743757000	-0.504480000	-0.023365000
6	7.415014000	-1.341710000	-1.296206000
6	8.308083000	-1.319300000	-0.233460000
6	7.858710000	-0.855464000	0.995657000
1	6.136417000	-0.065043000	2.041481000
1	7.728032000	-1.697974000	-2.274358000
1	9.328994000	-1.657724000	-0.369095000

1	8.522071000	-0.820928000	1.853318000
6	4.102279000	1.248516000	-0.287119000
6	3.423406000	-1.051341000	0.398888000
6	2.676319000	1.642727000	-0.289469000
6	2.020740000	-0.611744000	0.391981000
6	2.352128000	2.933862000	-0.641026000
6	1.669104000	0.713741000	0.055988000
6	1.010135000	3.330832000	-0.673273000
6	0.303842000	1.116690000	0.054302000
6	0.014449000	2.441708000	-0.338800000
1	-1.017525000	2.766121000	-0.400644000
6	1.031645000	-1.509837000	0.730077000
6	-0.715182000	0.165545000	0.422841000
6	-0.308265000	-1.124577000	0.752598000
1	3.155015000	3.614924000	-0.900024000
1	0.754223000	4.340868000	-0.974213000
1	-1.041192000	-1.845878000	1.093906000
1	1.324149000	-2.518470000	1.001059000
7	4.372293000	-0.079015000	0.050919000
8	3.773807000	-2.173739000	0.690626000
8	5.000242000	2.016156000	-0.552990000
6	-2.098746000	0.577570000	0.476691000
6	-3.206346000	-0.195349000	0.301260000
16	-3.215970000	-1.888128000	-0.202628000
6	-5.487025000	-0.648205000	0.050557000
6	-4.963083000	-1.888619000	-0.326736000
1	-2.284215000	1.629404000	0.650601000
6	-6.862942000	-0.439944000	0.016575000
6	-7.687629000	-1.488724000	-0.377680000
6	-5.784334000	-2.931650000	-0.717090000

6	-7.160318000	-2.723279000	-0.740219000
1	-7.819440000	-3.527407000	-1.046389000
1	-5.362558000	-3.888977000	-1.002013000
1	-8.760367000	-1.332584000	-0.406208000
1	-7.290920000	0.519357000	0.282606000
7	-4.508125000	0.251751000	0.436395000
6	-4.826168000	1.587671000	0.900731000
1	-4.067095000	1.877765000	1.633136000
1	-5.771406000	1.530325000	1.449599000
6	-4.923105000	2.618367000	-0.219671000
1	-3.981407000	2.628890000	-0.778851000
1	-5.695545000	2.300838000	-0.928443000
6	-5.237267000	4.007682000	0.314981000
1	-5.305075000	4.735852000	-0.496468000
1	-6.190798000	4.022851000	0.852618000
1	-4.462909000	4.354108000	1.006943000
7	6.149034000	-0.942057000	-1.200603000

7d

6	6.789015000	0.064234000	0.951820000
6	5.946665000	-0.404456000	-0.046606000
6	6.440737000	-1.202136000	-1.069065000
6	7.788487000	-1.534321000	-1.089843000
6	8.638825000	-1.065684000	-0.095602000
6	8.137176000	-0.265246000	0.923554000
1	6.387617000	0.690152000	1.740445000
1	5.767832000	-1.565462000	-1.837053000
1	8.174388000	-2.161724000	-1.886219000
1	9.692249000	-1.324590000	-0.114861000
1	8.796739000	0.104801000	1.701255000

6	4.210877000	1.272383000	-0.279577000
6	3.636245000	-1.090606000	0.266406000
6	2.768949000	1.604328000	-0.243105000
6	2.217081000	-0.707819000	0.305478000
6	2.388645000	2.900222000	-0.512809000
6	1.804104000	0.618194000	0.057285000
6	1.031898000	3.243880000	-0.502719000
6	0.423755000	0.963587000	0.098272000
6	0.076869000	2.297273000	-0.209316000
1	-0.967272000	2.585572000	-0.236356000
6	1.271195000	-1.665366000	0.603144000
6	-0.549680000	-0.050164000	0.422647000
6	-0.082557000	-1.339030000	0.669284000
1	3.159833000	3.627796000	-0.739286000
1	0.731911000	4.259396000	-0.737220000
1	-0.777147000	-2.110614000	0.978810000
1	1.609518000	-2.675038000	0.808773000
7	4.552205000	-0.060951000	-0.019613000
8	4.021114000	-2.221283000	0.467404000
8	5.061536000	2.099811000	-0.520054000
6	-1.946995000	0.299540000	0.517188000
6	-3.028514000	-0.510209000	0.340392000
16	-2.987613000	-2.188715000	-0.206136000
6	-5.295959000	-1.041037000	0.125270000
6	-4.735649000	-2.252350000	-0.291912000
1	-2.172064000	1.336407000	0.728719000
6	-6.679147000	-0.883598000	0.125406000
6	-7.473117000	-1.953267000	-0.275231000
6	-5.526298000	-3.316519000	-0.688513000
6	-6.909102000	-3.159156000	-0.677162000

1	-7.544966000	-3.980368000	-0.987133000
1	-5.075995000	-4.250922000	-1.004213000
1	-8.551252000	-1.836715000	-0.276914000
1	-7.136356000	0.052468000	0.423433000
7	-4.342516000	-0.114369000	0.511157000
6	-4.699885000	1.203506000	0.999429000
1	-3.942289000	1.508573000	1.727009000
1	-5.635045000	1.105333000	1.558998000
6	-4.846099000	2.243408000	-0.106310000
1	-3.913954000	2.292678000	-0.681373000
1	-5.620376000	1.912408000	-0.808715000
6	-5.196086000	3.622401000	0.438671000
1	-6.120823000	3.557550000	1.026203000
1	-4.415605000	3.945826000	1.139085000
6	-5.361648000	4.664874000	-0.658036000
1	-5.609174000	5.645075000	-0.242596000
1	-4.442402000	4.773442000	-1.241994000
1	-6.161304000	4.385239000	-1.350867000

7e

6	-7.021203000	0.086984000	-0.903741000
6	-6.174494000	-0.377245000	0.093080000
6	-6.675844000	-1.111064000	1.158902000
6	-8.035455000	-1.383651000	1.225039000
6	-8.890037000	-0.918949000	0.232594000
6	-8.380941000	-0.182540000	-0.830219000
1	-6.613788000	0.663077000	-1.726484000
1	-5.999573000	-1.471738000	1.925165000
1	-8.427335000	-1.961153000	2.055516000
1	-9.952671000	-1.130875000	0.287407000

1	-9.043802000	0.184343000	-1.606615000
6	-4.365740000	1.233100000	0.215124000
6	-3.902694000	-1.173850000	-0.239615000
6	-2.912816000	1.501276000	0.135383000
6	-2.469237000	-0.854004000	-0.324333000
6	-2.470638000	2.788947000	0.343711000
6	-1.997264000	0.463100000	-0.142239000
6	-1.100482000	3.072290000	0.295111000
6	-0.605337000	0.747671000	-0.225451000
6	-0.191607000	2.075378000	0.022449000
1	0.864977000	2.317183000	0.023130000
6	-1.571263000	-1.864008000	-0.595391000
6	0.314663000	-0.319273000	-0.527740000
6	-0.206410000	-1.597837000	-0.703923000
1	-3.204585000	3.558533000	0.554785000
1	-0.751949000	4.081776000	0.483847000
1	0.452531000	-2.409595000	-0.989151000
1	-1.956086000	-2.866623000	-0.746409000
7	-4.767933000	-0.094987000	0.019938000
8	-4.338312000	-2.294839000	-0.382899000
8	-5.176449000	2.104638000	0.436775000
6	1.722318000	-0.029857000	-0.672079000
6	2.772841000	-0.861665000	-0.443373000
16	2.697132000	-2.492819000	0.228107000
6	5.033245000	-1.427027000	-0.205215000
6	4.445909000	-2.589791000	0.304105000
1	1.985838000	0.984558000	-0.942224000
6	6.418490000	-1.296260000	-0.210425000
6	7.190129000	-2.349988000	0.268776000
6	5.214939000	-3.637126000	0.780489000

6	6.600839000	-3.511413000	0.756036000
1	7.219231000	-4.320913000	1.126309000
1	4.745317000	-4.534431000	1.167602000
1	8.270249000	-2.254193000	0.267082000
1	6.893939000	-0.387713000	-0.561067000
7	4.096042000	-0.511462000	-0.656883000
6	4.446288000	0.709595000	-1.344979000
1	3.766324000	0.823314000	-2.196423000
1	5.445482000	0.570686000	-1.768037000
6	4.413668000	1.959523000	-0.492036000
6	4.310469000	3.203115000	-1.114309000
6	4.511026000	1.902259000	0.895194000
6	4.312903000	4.371037000	-0.363127000
1	4.223250000	3.258206000	-2.196355000
6	4.509309000	3.071095000	1.647882000
1	4.577366000	0.939856000	1.392056000
6	4.412975000	4.307570000	1.022272000
1	4.230365000	5.331955000	-0.860152000
1	4.580532000	3.012785000	2.728877000
1	4.410288000	5.218453000	1.611310000

7f

6	-6.196048000	0.552350000	-0.893378000
6	-5.353330000	-0.078172000	0.015776000
6	-5.870018000	-0.930950000	0.985525000
6	-7.234192000	-1.158213000	1.049248000
6	-8.059509000	-0.519725000	0.136788000
6	-7.562022000	0.334327000	-0.835090000
1	-5.780868000	1.219792000	-1.637637000
1	-5.201409000	-1.422240000	1.680667000

1	-7.668659000	-1.816656000	1.789869000
1	-8.245390000	0.810213000	-1.526030000
6	-3.491866000	1.470493000	0.140158000
6	-3.110325000	-0.963378000	-0.284615000
6	-2.031095000	1.679969000	0.084916000
6	-1.670107000	-0.694377000	-0.356209000
6	-1.543447000	2.951325000	0.297312000
6	-1.152522000	0.605534000	-0.173867000
6	-0.163545000	3.181038000	0.271831000
6	0.250014000	0.837176000	-0.237921000
6	0.709772000	2.148323000	0.014890000
1	1.774502000	2.350105000	0.032503000
6	-0.805398000	-1.738853000	-0.611338000
6	1.135175000	-0.264356000	-0.525983000
6	0.568186000	-1.524654000	-0.703268000
1	-2.250037000	3.749781000	0.493749000
1	0.221104000	4.176283000	0.465173000
1	1.198774000	-2.362218000	-0.976988000
1	-1.224072000	-2.727717000	-0.762842000
7	-3.942475000	0.152486000	-0.046594000
8	-3.589216000	-2.067515000	-0.420976000
8	-4.275501000	2.371745000	0.338611000
6	2.550720000	-0.024621000	-0.655565000
6	3.573564000	-0.896801000	-0.441806000
16	3.445064000	-2.537113000	0.194082000
6	5.813728000	-1.538980000	-0.217129000
6	5.189364000	-2.693831000	0.264699000
1	2.852276000	0.985242000	-0.900171000
6	7.202586000	-1.453068000	-0.221273000
6	7.939338000	-2.542129000	0.232208000

6	5.923804000	-3.776952000	0.715629000
6	7.312644000	-3.695175000	0.692811000
1	7.904779000	-4.532607000	1.043255000
1	5.425543000	-4.667496000	1.081858000
1	9.021974000	-2.481785000	0.231326000
1	7.707673000	-0.553093000	-0.552096000
7	4.905789000	-0.582496000	-0.644491000
6	5.294227000	0.644582000	-1.302987000
1	4.631377000	0.790466000	-2.162885000
1	6.296887000	0.491158000	-1.711910000
6	5.273607000	1.876451000	-0.424270000
6	5.145847000	3.132176000	-1.016515000
6	5.407241000	1.789740000	0.958656000
6	5.159567000	4.283776000	-0.240100000
1	5.030843000	3.210063000	-2.094545000
6	5.416695000	2.941748000	1.736368000
1	5.493285000	0.817336000	1.432746000
6	5.295497000	4.190881000	1.140394000
1	5.058191000	5.254607000	-0.713796000
1	5.516479000	2.860867000	2.813625000
1	5.301804000	5.088659000	1.749154000
7	-9.507464000	-0.755755000	0.201862000
8	-10.205831000	-0.185604000	-0.611309000
8	-9.915194000	-1.506192000	1.064781000

7g

6	-6.630557000	0.740037000	-0.916009000
6	-5.826691000	0.114006000	0.030687000
6	-6.394699000	-0.588756000	1.087950000
6	-7.772063000	-0.671480000	1.201041000

6	-8.557980000	-0.040475000	0.249624000
6	-8.008938000	0.666860000	-0.808397000
1	-6.175286000	1.291056000	-1.728936000
1	-5.757459000	-1.078017000	1.813288000
1	-8.246279000	-1.211988000	2.009613000
1	-8.662949000	1.143752000	-1.526530000
6	-3.816568000	1.469701000	-0.045804000
6	-3.692706000	-1.019385000	-0.226327000
6	-2.344575000	1.523206000	-0.159407000
6	-2.234140000	-0.907565000	-0.355870000
6	-1.727928000	2.753712000	-0.096476000
6	-1.584924000	0.344669000	-0.323372000
6	-0.333590000	2.839220000	-0.182105000
6	-0.169287000	0.424538000	-0.443012000
6	0.424467000	1.702398000	-0.346572000
1	1.503656000	1.795903000	-0.379246000
6	-1.487412000	-2.055199000	-0.519130000
6	0.591350000	-0.785174000	-0.626809000
6	-0.102005000	-1.991741000	-0.661467000
1	-2.344866000	3.635959000	0.031236000
1	0.151927000	3.805935000	-0.107836000
1	0.434410000	-2.912365000	-0.858629000
1	-2.006643000	-3.006456000	-0.558008000
7	-4.402091000	0.192323000	-0.084854000
8	-4.279937000	-2.078108000	-0.240038000
8	-4.498554000	2.461588000	0.078173000
6	2.023769000	-0.714234000	-0.801024000
6	2.947512000	-1.660004000	-0.480830000
16	2.648384000	-3.171420000	0.379351000
6	5.107299000	-2.521819000	-0.179410000

6	4.365609000	-3.516712000	0.463332000
1	2.422129000	0.215112000	-1.188095000
6	6.495717000	-2.596972000	-0.206210000
6	7.114309000	-3.689975000	0.392286000
6	4.982216000	-4.603690000	1.058317000
6	6.370685000	-4.686282000	1.015223000
1	6.871572000	-5.529163000	1.477075000
1	4.394950000	-5.371362000	1.549382000
1	8.196386000	-3.756275000	0.376344000
1	7.091962000	-1.816315000	-0.664308000
7	4.304102000	-1.535386000	-0.735049000
6	4.823304000	-0.482459000	-1.570822000
1	4.116809000	-0.323373000	-2.392936000
1	5.746737000	-0.847996000	-2.030309000
6	5.093884000	0.829510000	-0.867314000
6	5.460529000	1.938589000	-1.632849000
6	5.001510000	0.954056000	0.516459000
6	5.737000000	3.154186000	-1.030973000
1	5.529954000	1.851354000	-2.713233000
6	5.273278000	2.166940000	1.134085000
1	4.709216000	0.100337000	1.117488000
6	5.638383000	3.247746000	0.349594000
1	6.023684000	4.026822000	-1.603732000
1	5.206785000	2.288318000	2.207724000
7	-10.019793000	-0.124470000	0.366330000
8	-10.682960000	0.440469000	-0.479089000
8	-10.472137000	-0.753726000	1.300740000
7	5.928333000	4.535455000	0.998253000
8	6.244261000	5.461673000	0.281076000
8	5.832423000	4.585768000	2.206238000

7h

6	-5.943374000	0.028014000	-1.230464000
6	-5.151660000	-0.434537000	-0.192153000
6	-6.916644000	-1.794259000	0.549826000
6	-7.727346000	-1.375365000	-0.475742000
6	-7.236220000	-0.437483000	-1.377870000
1	-5.516666000	0.749254000	-1.914068000
1	-7.236392000	-2.517180000	1.288377000
1	-8.728842000	-1.777420000	-0.557877000
1	-7.853430000	-0.082525000	-2.195212000
6	-3.645216000	1.388106000	0.222205000
6	-2.797328000	-0.951249000	-0.309669000
6	-2.253533000	1.831053000	0.279710000
6	-1.454431000	-0.432091000	-0.264814000
6	-2.009219000	3.157482000	0.587616000
6	-1.192646000	0.929077000	0.024466000
6	-0.696545000	3.616155000	0.665601000
6	0.149259000	1.404235000	0.064663000
6	0.350597000	2.753882000	0.413092000
1	1.358885000	3.137058000	0.507843000
6	-0.391104000	-1.289185000	-0.527744000
6	1.246199000	0.495301000	-0.223989000
6	0.914316000	-0.840024000	-0.509998000
1	-2.852020000	3.813462000	0.773951000
1	-0.496820000	4.647639000	0.931199000
1	1.690293000	-1.539778000	-0.790316000
1	-0.612058000	-2.322323000	-0.773171000
7	-3.828947000	0.001112000	-0.030006000
8	-3.130297000	-2.096456000	-0.550208000

8	-4.617025000	2.090792000	0.385266000
6	2.583196000	0.979678000	-0.244745000
6	3.764163000	0.268757000	-0.196231000
16	3.947653000	-1.447016000	0.106606000
6	6.080057000	0.014811000	-0.099417000
6	5.689610000	-1.305478000	0.134095000
1	2.713228000	2.051601000	-0.281090000
6	7.431716000	0.347898000	-0.098899000
6	8.361547000	-0.659965000	0.117712000
6	6.617420000	-2.312804000	0.346573000
6	7.964706000	-1.977578000	0.335421000
1	8.709572000	-2.746808000	0.501949000
1	6.298349000	-3.333836000	0.521236000
1	9.416377000	-0.410247000	0.120635000
1	7.764632000	1.367187000	-0.251395000
7	4.995125000	0.856212000	-0.314874000
6	5.139936000	2.260371000	-0.633602000
1	4.458039000	2.525404000	-1.443930000
1	4.935877000	2.891048000	0.237670000
1	6.155963000	2.446298000	-0.974331000
6	-4.860829000	-1.793617000	1.833252000
1	-4.183174000	-2.571056000	1.480796000
1	-4.290693000	-0.960448000	2.239850000
1	-5.538029000	-2.177883000	2.592520000
7	-5.662856000	-1.317179000	0.697143000

7i

6	5.877491000	0.444530000	1.282287000
6	5.175647000	-0.228143000	0.294548000
6	7.085598000	-1.505469000	-0.191849000

6	7.809732000	-0.875980000	0.789573000
6	7.198091000	0.126980000	1.534692000
1	5.359137000	1.209870000	1.843628000
1	7.500402000	-2.289779000	-0.810767000
1	8.838089000	-1.167597000	0.959273000
1	7.744653000	0.646918000	2.313103000
6	3.542071000	1.382185000	-0.406667000
6	2.870462000	-0.938652000	0.402847000
6	2.122922000	1.692510000	-0.551242000
6	1.493324000	-0.547525000	0.259411000
6	1.775558000	2.942334000	-1.035240000
6	1.133981000	0.742529000	-0.199865000
6	0.432283000	3.271031000	-1.200610000
6	-0.239308000	1.096132000	-0.319114000
6	-0.546842000	2.362004000	-0.852878000
1	-1.584416000	2.627009000	-1.017540000
6	0.491312000	-1.453134000	0.604974000
6	-1.269183000	0.150163000	0.069895000
6	-0.843666000	-1.116948000	0.511609000
1	2.565630000	3.639597000	-1.290426000
1	0.156119000	4.235829000	-1.609737000
1	-1.581189000	-1.822500000	0.872201000
1	0.788524000	-2.424221000	0.986318000
7	3.829716000	0.059420000	0.031474000
8	3.290814000	-2.011684000	0.795980000
8	4.459715000	2.137348000	-0.638756000
6	-2.635571000	0.551201000	0.092937000
1	-2.800326000	1.614257000	0.205931000
6	5.097383000	-1.870688000	-1.529286000
1	4.480878000	-2.657001000	-1.094337000

1	4.468700000	-1.157876000	-2.059518000
1	5.839242000	-2.281823000	-2.210002000
7	5.802236000	-1.172315000	-0.444915000
6	-3.773279000	-0.236985000	-0.009796000
6	-5.100885000	0.295650000	0.301969000
6	-3.766448000	-1.575389000	-0.500647000
6	-5.278984000	1.565916000	0.875113000
6	-6.264006000	-0.479866000	0.067044000
6	-4.917354000	-2.264243000	-0.708611000
1	-2.841737000	-2.044291000	-0.804777000
6	-6.526566000	2.072015000	1.166768000
1	-4.407679000	2.160420000	1.119125000
6	-7.532784000	0.043306000	0.361307000
1	-4.903396000	-3.263437000	-1.126632000
6	-7.661354000	1.306490000	0.897382000
1	-6.623379000	3.054883000	1.613220000
1	-8.421383000	-0.544109000	0.172374000
1	-8.649082000	1.694456000	1.119890000
6	-7.325701000	-2.573878000	-0.695908000
1	-7.880214000	-2.753106000	0.228945000
1	-7.983533000	-2.089575000	-1.422095000
1	-7.008145000	-3.532865000	-1.101242000
7	-6.146905000	-1.762656000	-0.444927000

7j

6	-5.404212000	1.248334000	0.279039000
6	-4.374535000	-0.957033000	-0.216401000
6	-4.036235000	1.810348000	0.258443000
6	-3.049687000	-0.391497000	-0.238395000
6	-3.888500000	3.157758000	0.510565000

6	-2.902681000	0.997348000	-0.002970000
6	-2.613159000	3.733738000	0.526965000
6	-1.606431000	1.585071000	-0.017023000
6	-1.501526000	2.962622000	0.275382000
1	-0.517592000	3.415313000	0.322052000
6	-1.931532000	-1.163784000	-0.489669000
6	-0.454538000	0.768701000	-0.292531000
6	-0.662322000	-0.589089000	-0.521417000
1	-4.778534000	3.745560000	0.706112000
1	-2.501494000	4.789149000	0.749899000
1	0.185626000	-1.210314000	-0.786518000
1	-2.067014000	-2.221441000	-0.687960000
7	-5.466913000	-0.123424000	0.034944000
8	-6.405232000	1.896073000	0.489947000
6	0.860682000	1.369939000	-0.412193000
1	0.875309000	2.348467000	-0.877884000
6	2.054472000	0.843326000	-0.000984000
6	3.348983000	1.471784000	-0.324569000
6	2.154044000	-0.323523000	0.837602000
6	3.443246000	2.566139000	-1.194425000
6	4.556765000	0.964259000	0.214728000
6	3.334018000	-0.742677000	1.334820000
1	1.258678000	-0.841428000	1.151463000
6	4.648232000	3.164880000	-1.505149000
1	2.540346000	2.947083000	-1.655590000
6	5.779468000	1.568093000	-0.112998000
1	3.392906000	-1.589891000	2.007835000
6	5.823334000	2.661762000	-0.954675000
1	4.676126000	4.008650000	-2.185417000
1	6.705144000	1.160853000	0.272119000

1	6.780668000	3.110385000	-1.196801000
6	5.741619000	-0.657611000	1.666208000
1	6.300501000	0.166056000	2.123931000
1	5.427420000	-1.303494000	2.491619000
7	4.530974000	-0.138504000	1.061497000
7	-4.716043000	-2.199535000	-0.405459000
6	-6.091503000	-2.223307000	-0.280180000
6	-6.966372000	-3.302187000	-0.388956000
6	-6.595018000	-0.937805000	-0.003512000
6	-8.320007000	-3.059020000	-0.215911000
1	-6.583631000	-4.293580000	-0.602190000
6	-7.947555000	-0.682197000	0.171964000
6	-8.801187000	-1.772527000	0.059608000
1	-9.024374000	-3.880461000	-0.294894000
1	-8.304426000	0.316084000	0.384496000
1	-9.867620000	-1.621785000	0.188887000
6	6.644138000	-1.440052000	0.736749000
6	7.994568000	-1.576567000	1.054322000
6	6.150440000	-2.063835000	-0.405481000
6	8.837059000	-2.332243000	0.249563000
1	8.391257000	-1.086011000	1.939676000
6	6.993999000	-2.816773000	-1.213615000
1	5.103949000	-1.952983000	-0.670651000
6	8.337457000	-2.955376000	-0.888158000
1	9.886336000	-2.429592000	0.507954000
1	6.598652000	-3.294752000	-2.103775000
1	8.994341000	-3.542193000	-1.521295000

7k

6	-4.319321000	1.903246000	0.282585000

6	-3.492022000	-0.391021000	-0.197684000
6	-2.906086000	2.340153000	0.259621000
6	-2.122535000	0.053438000	-0.221528000
6	-2.636777000	3.669914000	0.503070000
6	-1.851404000	1.425941000	0.002770000
6	-1.314363000	4.128183000	0.515085000
6	-0.507704000	1.894234000	-0.017820000
6	-0.277739000	3.258500000	0.266332000
1	0.743240000	3.619907000	0.309455000
6	-1.078552000	-0.819050000	-0.466395000
6	0.565277000	0.975388000	-0.291301000
6	0.236471000	-0.361333000	-0.505782000
1	-3.470203000	4.336407000	0.695528000
1	-1.107306000	5.170287000	0.732372000
1	1.024265000	-1.058049000	-0.768532000
1	-1.309434000	-1.861758000	-0.655435000
7	-4.504399000	0.544275000	0.046571000
8	-5.258185000	2.640803000	0.488600000
6	1.925799000	1.459436000	-0.424415000
1	2.019646000	2.432383000	-0.892303000
6	3.075658000	0.837110000	-0.020522000
6	4.413159000	1.358111000	-0.358068000
6	3.088385000	-0.328267000	0.825081000
6	4.587628000	2.428320000	-1.245669000
6	5.580225000	0.768750000	0.186993000
6	4.234782000	-0.829184000	1.326294000
1	2.157588000	-0.775222000	1.144832000
6	5.833608000	2.929828000	-1.566279000
1	3.715110000	2.868002000	-1.713051000
6	6.844243000	1.275175000	-0.149039000

1	4.230804000	-1.672132000	2.007247000
6	6.968497000	2.349616000	-1.007200000
1	5.923735000	3.757966000	-2.260206000
1	7.737506000	0.806868000	0.242947000
1	7.956303000	2.722242000	-1.255669000
6	6.641435000	-0.909984000	1.668593000
1	7.252363000	-0.119274000	2.117641000
1	6.278827000	-1.520182000	2.501234000
7	5.472791000	-0.317889000	1.048055000
7	-3.939463000	-1.598187000	-0.380345000
6	-5.314771000	-1.505126000	-0.260657000
6	-6.264710000	-2.492639000	-0.367567000
6	-5.705996000	-0.162371000	0.010115000
6	-7.623196000	-2.149698000	-0.203656000
1	-5.972967000	-3.516461000	-0.574336000
6	-7.009912000	0.216865000	0.176789000
6	-7.996900000	-0.791109000	0.069761000
1	-7.277627000	1.244854000	0.381759000
6	7.494309000	-1.765828000	0.757210000
6	8.831449000	-1.984898000	1.084536000
6	6.965936000	-2.375375000	-0.377156000
6	9.626331000	-2.807357000	0.297058000
1	9.255482000	-1.506334000	1.963739000
6	7.762176000	-3.195001000	-1.168248000
1	5.930045000	-2.201315000	-0.649920000
6	9.092276000	-3.415317000	-0.833210000
1	10.665818000	-2.968661000	0.562865000
1	7.340424000	-3.660986000	-2.052619000
1	9.712386000	-4.053944000	-1.453145000
6	-8.647767000	-3.126313000	-0.303082000

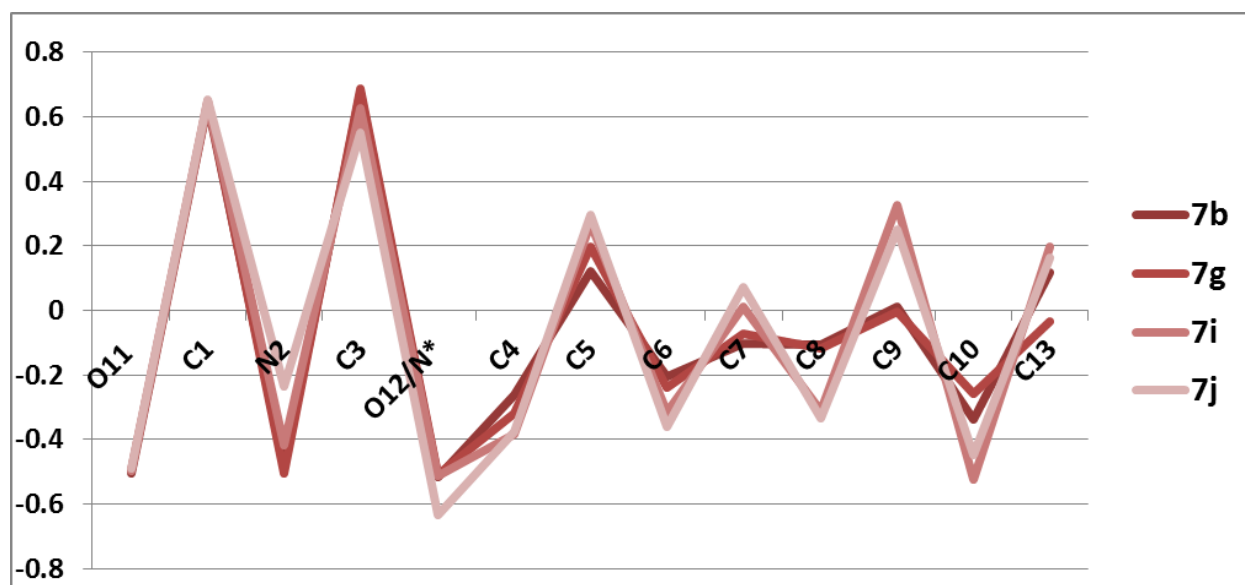|			
6	-9.964863000	-2.791643000	-0.143256000
1	-8.363265000	-4.153664000	-0.510391000
1	-10.733104000	-3.553727000	-0.223254000
6	-10.331525000	-1.454439000	0.126296000
6	-9.371286000	-0.484109000	0.229121000
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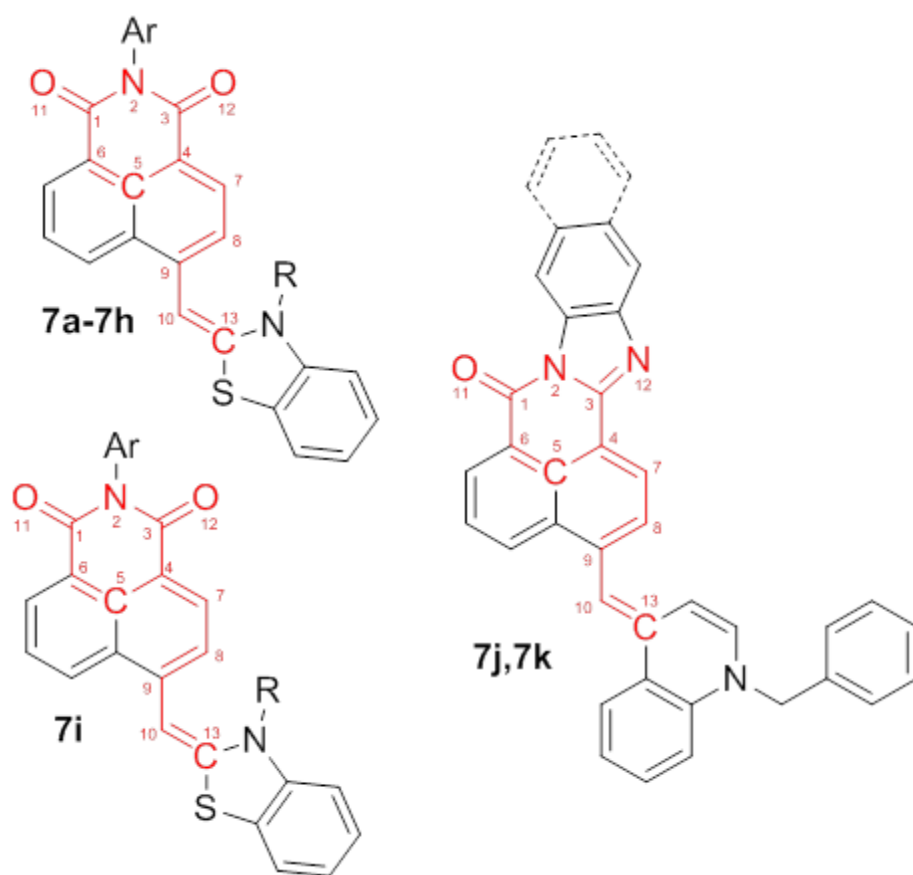
Figure S2. ESP charges of the selected atoms for the compounds **7b, 7g, 7i** and **7j**

File:A1 Ident:2_12 SMO(1,7) Acq:26-FEB-2013 14:15:56 +3:48 Cal:FD_3700-100T
ZAB-SEFPD FD+ Magnet BpI:18626514 TIC:4916225536
File Text:Kandinska
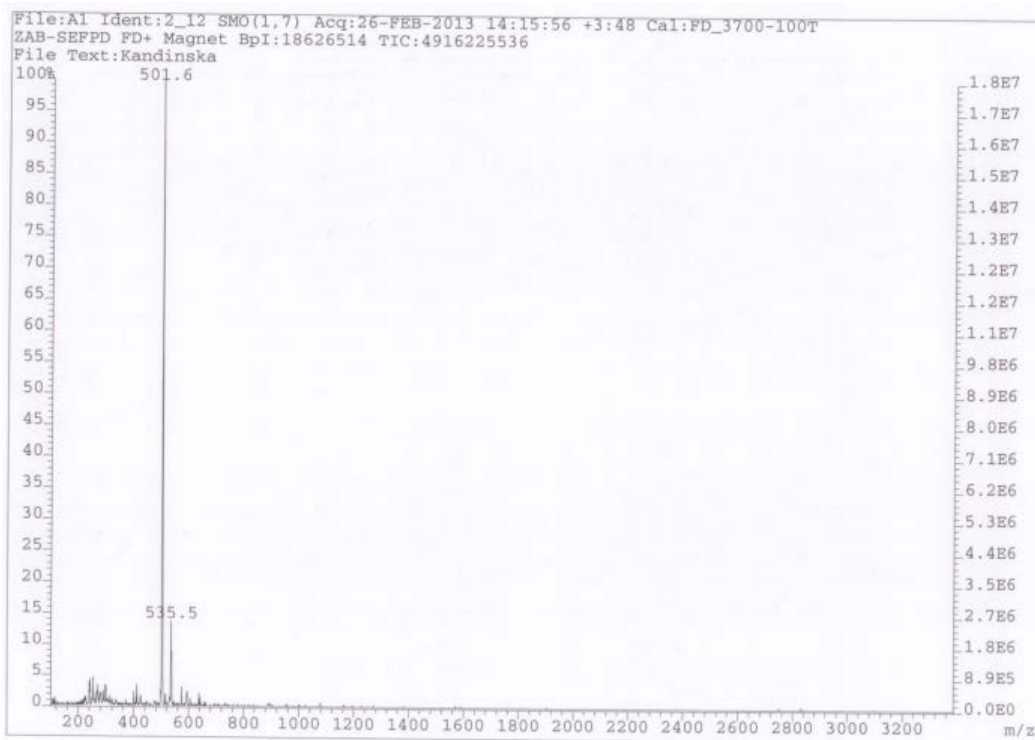
FD-MS (m/z (100%) [M$^+$], 8 kV) of dye **7j**.

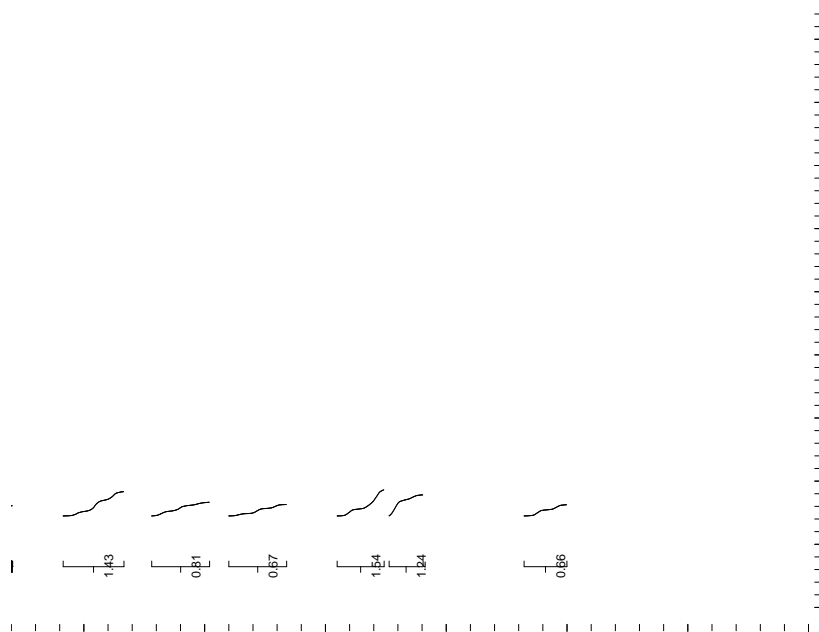**^{1}H-NMR (250 MHz) Spectra of dye 7a in DMSO-*d6***
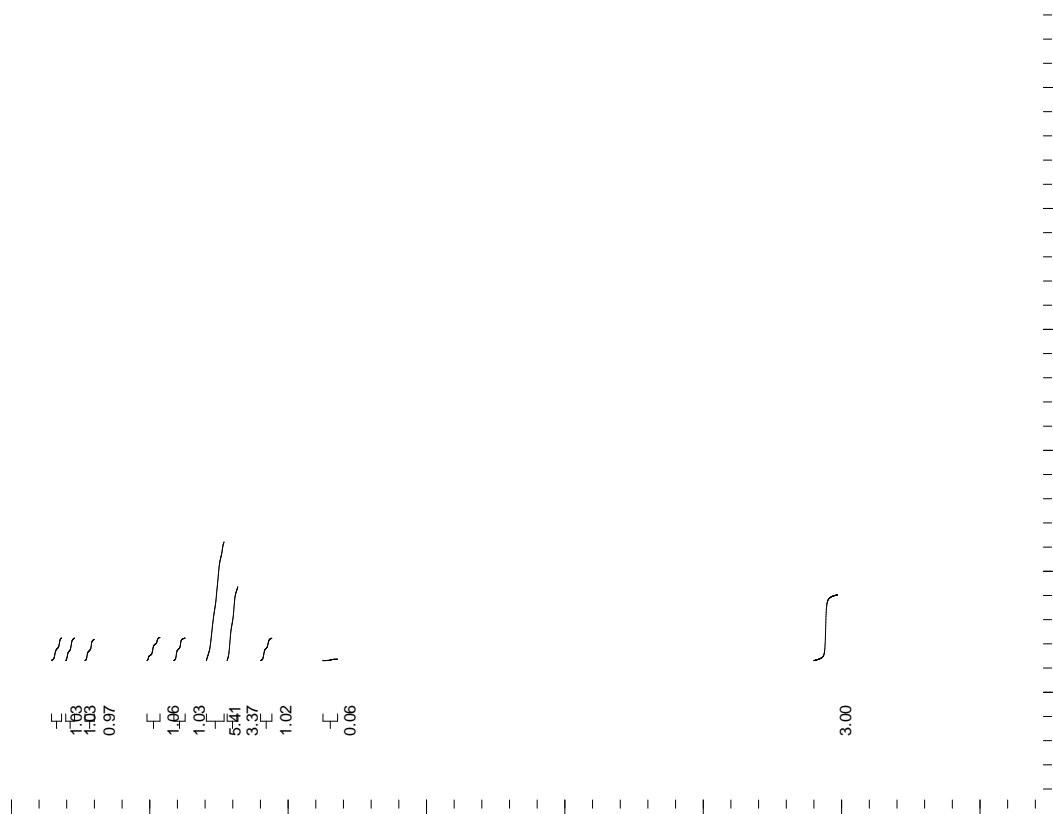
¹H-NMR Spectra of dye 7a in CDCl₃

¹H-NMR Spectra of the aromatic part in the molecule of dye 7a in CDCl₃

1.00
1.00
2.00
2.00
4.00
4.02
7.10
1.00
1.00
2.00

1.22
1.09
1.35
1.27
4.96
1.06
3.66
4.12
1.57
2.00
0.68
0.83
0.92

2.00

2.51
3.43
2.41

3.17
2.78
1.85

4.39
4.30

1.32

6.75

1.27

2.00