Electronic Supplementary Information (ESI) for Physical Chemistry Chemical Physics

A computationally-derived model for the solvatochromism of p-phenolates with high predictive power

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1 Molecular structures of negative-, inverted- and positivesolvatochromic dyes studied.



Figure 1: Molecular structures of all negative-solvatochromic dyes studied in this work.

The experimental data of negative-solvatochromic dyes 1, 6–16 can be found in: 1 [14], 6 [8], 7 [6], 8 [5], 9 [12], 10 [18], 11 [15], 12 [2], 13 [19] 14 [10] 15 [10] and 16 [9]

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Figure 2: Molecular structures of all inverted-solvatochromic dyes studied in this work.

The experimental data of negative-solvatochromic dyes 2 and 13–20 can be found in: 2 [1], 17 [3,7], 18 [13], 19 [16], 20 [17], 21 [1] and 22 [1],



Figure 3: Molecular structures of all positive-solvatochromic dyes studied in this work.

The experimental data of negative-solvatochromic dyes **3** and **21–26** can be found in: **3** [11], **23–26** [4], and **26** [11].

2 Cartesian coordinates for the all the dyes's optimized structures at def2-TZVP level of theory.

XYZ coordinates of negative-solvatochromic dye 1

С	1.7580044	1.1176970	-0.4456669
С	3.1423867	1.1193537	-0.4072581
С	3.8908465	-0.0000057	0.0000287
С	3.1424078	-1.1193376	0.4073086
С	1.7580071	-1.1177166	0.4457223
С	-0.3710359	-0.0000497	0.0000089
С	-1.0743474	1.0913526	0.5377776
С	-2.4562229	1.1404370	0.5252106
С	-3.2371561	-0.0000010	-0.0000119
С	-2.4562288	-1.1404897	-0.5252080
С	-1.0743413	-1.0913616	-0.5377267
Η	3.6434035	1.9975781	-0.8111933
Η	3.6434233	-1.9975661	0.8112471
Η	-0.5160670	1.9094454	0.9939160
Η	-0.5160620	-1.9095059	-0.9938784
С	1.0467236	2.2648102	-1.0588837
С	0.1211620	2.0886483	-2.1035761
С	1.3438724	3.5661633	-0.6244887
С	-0.4899168	3.1921713	-2.6917324
Η	-0.1337949	1.0837002	-2.4394895
С	0.7236276	4.6703845	-1.2137358
Η	2.0414578	3.7090120	0.2023157
С	-0.1966923	4.4866824	-2.2464723
Η	-1.2099535	3.0408169	-3.4961749
Η	0.9503665	5.6737584	-0.8516831
Η	-0.6950369	5.3456328	-2.6965530
С	1.0467476	-2.2648433	1.0589263
С	1.3439027	-3.5661819	0.6245294
С	0.1211857	-2.0886996	2.1036308
С	0.7236757	-4.6704145	1.2137670
Η	2.0414864	-3.7090346	-0.2022818
С	-0.4898769	-3.1922301	2.6917741

Η	-0.1337631	-1.0837504	2.4395486
С	-0.1966419	-4.4867340	2.2465052
Η	0.9504261	-5.6737798	0.8517051
Н	-1.2099193	-3.0408995	3.4962276
Н	-0.6949558	-5.3456991	2.6965806
С	-3.1320998	-2.3536693	-1.0234554
С	-2.5685815	-3.6196898	-0.7590351
С	-4.3294366	-2.3022611	-1.7642351
С	-3.1625384	-4.7876470	-1.2357319
Н	-1.6710464	-3.6877503	-0.1410981
С	-4.9195779	-3.4729544	-2.2415106
Н	-4.7913890	-1.3362742	-1.9549897
С	-4.3415051	-4.7199241	-1.9838071
Н	-2.7103924	-5.7550730	-1.0092483
Н	-5.8428419	-3.4106808	-2.8202496
Η	-4.8115182	-5.6322860	-2.3544450
С	-3.1321228	2.3536087	1.0234759
С	-4.3294414	2.3022328	1.7642043
С	-2.5685421	3.6196717	0.7590692
С	-4.9196055	3.4728805	2.2415180
Н	-4.7914185	1.3362192	1.9549311
С	-3.1625286	4.7875773	1.2358138
Η	-1.6710263	3.6877135	0.1411440
С	-4.3414727	4.7199005	1.9838252
Η	-5.8428620	3.4106382	2.8202038
Η	-2.7103182	5.7550306	1.0093447
Η	-4.8114930	5.6322299	2.3544980
С	5.3598476	0.0000194	0.0000208
С	6.0855646	-1.1927042	-0.1969920
С	6.0855630	1.1927258	0.1970220
С	7.4788985	-1.1917072	-0.1967260
Η	5.5518830	-2.1250703	-0.3860299
С	7.4789009	1.1917432	0.1967390
Η	5.5518829	2.1250993	0.3860672
С	8.1834327	0.0000089	0.0000010
Η	8.0189955	-2.1250641	-0.3607357
Η	8.0189974	2.1250941	0.3607329
Η	9.2738341	0.0000173	-0.0000029
Ν	1.0501429	-0.0000117	0.0000213

XYZ coordinates of negative-solvatochromic dye 4

22

С	-1.7994634	-1.1400172	-0.3158570
С	-3.1779309	-1.1570619	-0.2988729
С	-3.9081511	-0.0001570	0.0002613
С	-3.1780948	1.1570820	0.2989601
С	-1.7996059	1.1402655	0.3155036
С	0.3242714	0.0001409	0.0000604
С	1.0464426	-1.1896304	0.2902131
С	2.4171230	-1.1935080	0.2995505
С	3.2060398	-0.0000583	0.0000160
С	2.4172910	1.1935289	-0.2993223
С	1.0465808	1.1898768	-0.2899487
Η	-1.2105491	-1.9976156	-0.6238915
Η	-3.6793208	-2.0885498	-0.5599194
Η	-4.9960041	-0.0003393	0.0005291
Η	-3.6795734	2.0884763	0.5599169
Η	-1.2108005	1.9981066	0.6231044
Η	0.5082227	-2.0943359	0.5810507
Η	2.9708534	-2.0931916	0.5708004
Η	2.9710328	2.0932432	-0.5704364
Η	0.5085807	2.0947475	-0.5805457
Ο	4.4557600	-0.0001738	-0.0000717
Ν	-1.0797041	0.0001709	-0.0001009

С	0.3101602	1.1997541	-0.0648442
С	1.6957161	1.1854061	-0.0992112
С	2.4453431	-0.0000525	-0.0000032
С	1.6956559	-1.1854720	0.0992137
С	0.3100975	-1.1997527	0.0648620
С	-1.8189924	0.0000595	0.0000155
С	-2.5287270	-0.7103078	0.9956397
С	-3.9023695	-0.7001014	1.0119195
С	-4.6888716	0.0000462	-0.0000526
С	-3.9023278	0.7001973	-1.0119899
С	-2.5286862	0.7104216	-0.9956429
Η	2.1942239	2.1513243	-0.1566053
Η	2.1941175	-2.1514141	0.1566005
Η	-1.9721209	-1.2431143	1.7688586
Η	-4.4556099	-1.2128019	1.7998308
Η	-4.4555356	1.2128734	-1.7999403
Η	-1.9720491	1.2432186	-1.7688461
С	-0.4016201	2.4978120	0.0045012
С	-0.0887397	3.5052229	-0.9214697
С	-1.3287514	2.7730172	1.0261638
С	-0.6936623	4.7610391	-0.8347631
Η	0.6140415	3.2921595	-1.7287710
С	-1.9230139	4.0284201	1.1128729
Η	-1.5966495	1.9950830	1.7405320
С	-1.6128754	5.0260189	0.1811021
Η	-0.4520457	5.5281756	-1.5713473
Η	-2.6421505	4.2260853	1.9079848
Η	-2.0946593	6.0022327	0.2442168
С	-0.4017535	-2.4977730	-0.0044756
С	-0.0888791	-3.5052198	0.9214595
С	-1.3289742	-2.7729049	-1.0260783
С	-0.6938985	-4.7609913	0.8347816
Η	0.6139696	-3.2922183	1.7287184
С	-1.9233396	-4.0282609	-1.1127544
Η	-1.5968732	-1.9949455	-1.7404184
С	-1.6132092	-5.0258919	-0.1810159

Η	-0.4522865	-5.5281526	1.5713416
Н	-2.6425594	-4.2258583	-1.9078078
Н	-2.0950781	-6.0020660	-0.2440990
С	3.9175825	-0.0000889	-0.0000146
С	4.6445525	-1.1082890	-0.4813230
С	4.6446142	1.1080764	0.4812810
С	6.0380373	-1.1066942	-0.4823743
Η	4.1135525	-1.9689811	-0.8897181
С	6.0380990	1.1064142	0.4823096
Η	4.1136628	1.9687950	0.8896833
С	6.7433525	-0.0001573	-0.0000378
Η	6.5768662	-1.9723181	-0.8699464
Η	6.5769761	1.9720124	0.8698719
Η	7.8338423	-0.0001838	-0.0000465
Ν	-0.3971325	0.0000207	0.0000150
0	-5.9419795	0.0000414	-0.0000816

XYZ coordinates of negative-solvatochromic dye 6

С	-0.0879184	-0.2626738	-0.0060352
С	-0.9822659	-1.3829518	-0.0041173
С	-2.3365754	-1.2172241	0.0001232
С	-2.9956506	0.1030286	0.0030988
С	-2.0217654	1.2185363	0.0009652
С	-0.6688116	1.0486431	-0.0032684
Η	-0.5592580	-2.3891212	-0.0060744
Η	-0.0251917	1.9278264	-0.0044917
С	1.2969583	-0.4961375	-0.0100192
Η	1.5821427	-1.5530294	-0.0109816
С	2.3242556	0.4511022	-0.0122158
Η	2.0537630	1.5095042	-0.0126265
С	3.6992219	0.1750081	-0.0136741
С	4.6619262	1.2442469	-0.0165185
С	4.2845133	-1.1420769	-0.0155083
С	6.0050717	1.0116279	-0.0190115

Η	4.3154501	2.2776055	-0.0205745
\mathbf{C}	5.6356460	-1.3244427	-0.0175868
Η	3.6564777	-2.0306917	-0.0196060
Η	6.7392992	1.8153893	-0.0182715
Η	6.0891841	-2.3143573	-0.0160092
\mathbf{C}	7.9587537	-0.4889620	0.0703634
Η	8.2948664	-0.4512119	1.1179260
Η	8.2079613	-1.4704715	-0.3490840
Η	8.4909698	0.2790330	-0.5045104
Ν	6.5178825	-0.2675513	-0.0283358
Ο	-4.2191826	0.2632504	0.0069521
Br	-3.4843279	-2.7375005	0.0025523
Br	-2.7613959	2.9746019	0.0045399

XYZ coordinates of negative-solvatochromic dye 7

С	-0.500228	1.256926	-0.071666
С	0.187157	2.457139	-0.128980
С	-0.449219	3.711555	-0.046729
С	-1.853672	3.658501	0.048092
С	-2.565887	2.470714	0.040230
С	-2.610613	0.027431	0.062742
С	-2.391465	-0.961018	-0.914680
С	-3.101140	-2.139852	-0.866235
С	-4.085888	-2.462377	0.178006
С	-4.235551	-1.374481	1.156747
С	-3.543040	-0.186220	1.095140
Η	1.270616	2.379271	-0.169967
Η	-2.449465	4.567730	0.060716
Η	-1.680280	-0.790083	-1.721727
Η	-3.702785	0.573726	1.859046
С	0.256831	-0.015152	-0.000652
С	1.231140	-0.288448	-0.972695
С	0.067663	-0.923071	1.056335
С	1.996782	-1.453957	-0.898129

Η	1.367052	0.403507	-1.805565
С	0.840040	-2.078501	1.131342
Η	-0.696202	-0.729548	1.809344
С	1.802483	-2.351518	0.152468
Η	2.737810	-1.663779	-1.670170
Η	0.683559	-2.776009	1.954578
Η	2.392391	-3.266880	0.207328
С	-4.045638	2.502263	-0.032779
С	-4.767066	3.278048	0.887503
С	-4.740311	1.823851	-1.050535
С	-6.158245	3.365869	0.801584
Η	-4.235934	3.790084	1.691651
С	-6.125786	1.921507	-1.136964
Η	-4.194076	1.206963	-1.763814
С	-6.840796	2.687158	-0.208640
Η	-6.708420	3.956065	1.535194
Η	-6.652434	1.388620	-1.929035
Η	-7.927868	2.745543	-0.270402
С	0.299350	4.981410	-0.058140
С	-0.364245	6.227728	-0.042705
С	1.711163	5.002006	-0.079462
С	0.344202	7.426694	-0.048870
Η	-1.452533	6.272822	-0.030658
С	2.419486	6.200917	-0.081579
Η	2.275989	4.070788	-0.087194
С	1.741708	7.423025	-0.066911
Η	-0.199946	8.371897	-0.038862
Η	3.509920	6.179831	-0.093893
Η	2.296276	8.361780	-0.069212
Cl	-2.850590	-3.334500	-2.102686
Cl	-5.348340	-1.643066	2.463699
Ο	-4.716713	-3.529558	0.227835
Ν	-1.889153	1.254736	0.007519

XYZ coordinates of negative-solvatochromic dye 8

С	-0.683749	1.407937	-0.690973
С	0.032830	2.585802	-0.682509
С	-0.444666	3.713547	-0.002634
С	-1.661596	3.581918	0.678385
С	-2.340673	2.382063	0.689382
С	-2.588233	0.062932	0.001154
С	-1.897684	-1.164791	-0.113616
С	-2.557518	-2.372764	-0.104773
С	-4.030799	-2.393824	0.005297
С	-4.730124	-1.096633	0.111949
С	-3.996787	0.068205	0.117290
Η	0.962496	2.621222	-1.249611
Η	-2.083384	4.411791	1.244528
Η	-0.808551	-1.148715	-0.129691
Η	-4.513821	1.026955	0.131423
0	-4.667124	-3.477798	0.007892
Ν	-1.876087	1.275430	-0.000268
Η	0.106520	4.651605	-0.003040
Η	-0.381910	0.544002	-1.273969
Η	-3.240910	2.224821	1.274291
С	-1.790501	-3.699834	-0.171681
С	-2.075536	-4.537239	1.098027
С	-2.232111	-4.487396	-1.429627
С	-0.268131	-3.489746	-0.262746
Η	-1.749489	-3.994941	1.998397
Η	-3.144464	-4.758132	1.187013
Η	-1.519798	-5.486590	1.051589
Η	-2.016425	-3.910170	-2.341429
Η	-1.677787	-5.436930	-1.487605
Η	-3.304892	-4.704353	-1.395206
Η	0.228479	-4.468894	-0.318752
Η	0.018114	-2.925239	-1.163882
Η	0.132954	-2.968847	0.620430
С	-6.262668	-1.072766	0.179044
С	-6.855225	-1.733266	-1.088709
С	-6.735327	-1.838213	1.439212
С	-6.820517	0.359479	0.265950
Η	-6.540334	-1.187207	-1.990788
Η	-6.527639	-2.774762	-1.174729

Η	-7.954960	-1.710014	-1.042094
Н	-6.336487	-1.365543	2.349479
Η	-7.834667	-1.816774	1.497083
Н	-6.401925	-2.880770	1.407975
Н	-7.917550	0.316611	0.321858
Н	-6.466991	0.886821	1.165748
Η	-6.560578	0.961054	-0.618749

XYZ coordinates of negative-solvatochromic dye 9

С	-9.068144	-0.061201	-0.073029
С	-7.541850	-0.057440	-0.057099
0	-9.617166	0.731168	0.737366
0	-9.595486	-0.856659	-0.895432
С	-6.824631	1.143163	0.091348
С	-6.815111	-1.254120	-0.190278
С	-5.437248	1.153041	0.091150
С	-4.696610	-0.049084	-0.030508
С	-5.428087	-1.255624	-0.163820
С	-3.241924	-0.045419	-0.024469
С	-2.483201	1.015579	0.525653
С	-2.476966	-1.098354	-0.579188
С	-1.101833	1.010123	0.551527
Ν	-0.393591	-0.039703	-0.022142
С	-1.094614	-1.086071	-0.607946
С	1.042884	-0.033964	-0.007276
С	1.736782	1.046803	-0.562297
С	1.747063	-1.101130	0.562290
С	3.136879	-1.129610	0.572416
С	3.123925	1.088638	-0.576395
С	3.911856	-0.044224	-0.059476
0	5.167849	-0.066001	-0.123513
С	-0.360091	-2.145775	-1.338749
С	0.589440	-1.836743	-2.329058
С	-0.658225	-3.492084	-1.078216

С	-0.013594	-4.511018	-1.782594
С	0.932287	-4.196108	-2.759209
С	1.226084	-2.855233	-3.032538
С	-0.366178	2.100570	1.236819
С	-0.635260	3.431186	0.882146
С	0.578864	1.840955	2.244908
С	1.244044	2.891420	2.870767
С	0.981490	4.216065	2.501712
С	0.037074	4.482857	1.509562
С	3.829140	-2.250799	1.239564
С	3.308551	-2.809727	2.425543
С	5.016498	-2.810046	0.722118
С	5.633772	-3.890160	1.354305
С	3.927006	-3.889375	3.056689
С	5.096315	-4.439131	2.522752
С	3.791253	2.295175	-1.102325
С	3.247295	3.570145	-0.836979
С	4.968375	2.230123	-1.875632
С	5.554219	3.390719	-2.382835
С	4.993445	4.645816	-2.125125
С	3.836082	4.728593	-1.344682
Η	-7.394978	2.064899	0.217048
Η	-4.912485	2.108298	0.157708
Η	-4.895741	-2.207319	-0.220302
Η	-7.377568	-2.179278	-0.326729
Η	-2.971845	-1.918600	-1.095214
Η	-2.981318	1.842415	1.028164
Η	-1.351104	3.636762	0.084888
Η	-0.168320	5.510506	1.206978
Η	1.520375	5.034596	2.980335
Η	1.984284	2.673501	3.641192
Η	0.812855	0.811526	2.514101
Η	0.841762	-0.796525	-2.531820
Η	-1.380475	-3.738441	-0.298413
Η	-0.244385	-5.552594	-1.555317
Η	1.446393	-4.990675	-3.301518
Η	1.964921	-2.599491	-3.792789
Η	2.416070	-2.368279	2.873663
Η	3.502246	-4.293149	3.978044

Η	5.588484	-5.278538	3.017344
Η	6.548819	-4.307668	0.928842
Н	5.449340	-2.375725	-0.175661
Η	1.186430	-1.938955	0.982109
Н	1.169449	1.863535	-1.012673
Н	2.367552	3.651120	-0.194313
Н	5.417573	1.257185	-2.061205
Н	6.461397	3.314136	-2.986146
Н	5.460317	5.550487	-2.519183
Η	3.397072	5.702046	-1.116168

XYZ coordinates of negative-solvatochromic dye $10\,$

С	6.327456	-0.662801	-0.000193
С	5.039765	-1.111030	-0.000180
С	6.642742	0.767177	-0.000021
С	5.482029	1.665365	0.000160
С	4.202916	1.196859	0.000161
С	3.912698	-0.214455	-0.000009
С	2.613898	-0.740732	-0.000019
С	1.403760	-0.036008	0.000058
С	0.119356	-0.598625	0.000059
Ο	7.813299	1.196545	-0.000024
С	-0.153653	-2.014946	0.000072
С	-1.048198	0.224159	0.000048
С	-2.341031	-0.254393	0.000030
С	-1.422001	-2.487373	0.000066
Ν	-2.536606	-1.653009	0.000041
С	-3.541580	0.586506	-0.000007
С	-4.831119	-0.018295	-0.000019
С	-3.805472	-2.212510	0.000033
С	-4.925613	-1.453876	0.000006
С	-3.464359	1.992886	-0.000037
С	-4.612265	2.776868	-0.000072
С	-5.880043	2.177319	-0.000081

С	-5.983243	0.793231	-0.000055
Η	7.174616	-1.350408	-0.000330
Η	4.835419	-2.186315	-0.000310
Η	5.698004	2.735125	0.000297
Η	3.374001	1.908025	0.000308
Η	1.443193	1.056175	0.000095
Η	2.561511	-1.834933	-0.000122
Η	0.657398	-2.740598	0.000102
Η	-0.903753	1.302772	0.000043
Η	-2.495086	2.488876	-0.000034
Η	-4.521570	3.863287	-0.000095
Η	-6.778909	2.794678	-0.000109
Η	-6.963492	0.313406	-0.000064
Η	-5.900484	-1.938446	-0.000000
Η	-3.824990	-3.300591	0.000050
Η	-1.650951	-3.551363	0.000084

XYZ coordinates of negative-solvatochromic dye $11\,$

С	-2.848954	1.181235	0.161047
\mathbf{C}	-1.464961	1.186081	0.199560
Ν	-0.757324	0.000000	-0.000014
\mathbf{C}	-1.464986	-1.186006	-0.199579
\mathbf{C}	-2.849039	-1.181100	-0.161027
\mathbf{C}	-3.597793	0.000058	0.000028
\mathbf{C}	0.663060	-0.000025	-0.000010
\mathbf{C}	1.362815	0.945134	-0.771253
\mathbf{C}	1.362745	-0.945201	0.771236
\mathbf{C}	2.739259	-0.988356	0.786521
С	2.739291	0.988265	-0.786490
\mathbf{C}	3.503487	-0.000048	0.000022
\mathbf{C}	3.483989	2.055719	-1.595894
\mathbf{C}	3.483893	-2.055844	1.595917
Ο	4.763060	-0.000068	0.000045
С	-0.739012	-2.428491	-0.555942

С	-0.985340	-3.604375	0.168323
С	0.171603	-2.462596	-1.627242
С	0.826278	-3.646573	-1.952460
С	0.590293	-4.812386	-1.213866
С	-0.320459	-4.789246	-0.157134
С	-0.738863	2.428540	0.555917
С	-0.985204	3.604381	-0.168427
С	-0.320203	4.789313	0.156969
С	0.590624	4.812389	1.213699
С	0.826546	3.646560	1.952330
С	0.171742	2.462633	1.627140
С	-5.066815	0.000125	0.000053
С	-5.793143	1.125485	-0.441210
С	-7.186527	1.124581	-0.440519
С	-7.891244	0.000121	0.000181
С	-7.186537	-1.124240	0.440768
С	-5.793181	-1.125312	0.441405
Н	-7.726670	-2.003004	0.795718
Η	-5.259845	-1.998096	0.820629
Н	-8.981683	0.000172	0.000212
Η	-7.726634	2.003309	-0.795407
Η	-5.259808	1.998335	-0.820484
Η	-3.349463	-2.125690	-0.369254
Η	-3.349361	2.125841	0.369294
Η	0.386196	1.551349	2.185209
Η	1.535701	3.657614	2.780291
Η	1.122538	5.731978	1.459218
Η	-0.503929	5.690171	-0.429436
Η	-1.673141	3.577825	-1.015134
Η	0.785527	1.645302	-1.371627
Η	0.785444	-1.645360	1.371586
Η	-0.504219	-5.690181	0.429285
Η	1.122161	-5.732007	-1.459457
Η	1.535417	-3.657625	-2.780452
Η	0.386055	-1.551326	-2.185264
Η	-1.673292	-3.577781	1.015076
С	2.518162	-2.997011	2.339499
С	4.407105	-1.391912	2.643209
С	4.322583	-2.922450	0.624175

С	2.518308	2.996899	-2.339519
С	4.407203	1.391732	-2.643145
С	4.322697	2.922318	-0.624166
Η	1.903748	2.459045	-3.078164
Η	3.100351	3.753406	-2.885511
Η	1.846901	3.529126	-1.647595
Η	3.665833	3.413467	0.110060
Η	4.854988	3.705659	-1.186007
Η	5.055311	2.307745	-0.089900
Η	3.815287	0.790214	-3.349836
Η	5.141083	0.740886	-2.155691
Η	4.940975	2.164846	-3.217616
Η	3.665702	-3.413536	-0.110076
Η	4.854834	-3.705842	1.186001
Η	5.055230	-2.307886	0.089945
Η	1.903608	-2.459140	3.078136
Η	3.100152	-3.753560	2.885492
Η	1.846753	-3.529189	1.647542
Η	3.815187	-0.790401	3.349906
Η	5.141010	-0.741064	2.155797
Η	4.940851	-2.165064	3.217668

XYZ coordinates of negative-solvatochromic dye $12\,$

С	-3.706095	1.021516	0.606325
С	-2.321435	1.015918	0.641950
Ν	-1.613661	-0.001780	-0.000068
С	-2.319235	-1.021016	-0.642065
С	-3.703866	-1.029583	-0.606375
С	-4.452891	-0.004871	0.000001
С	-5.922100	-0.006523	0.000076
С	-6.648811	1.201489	0.025377
С	-8.042169	1.198730	0.025211
С	-8.745001	-0.009740	0.000239
С	-8.039422	-1.216602	-0.024818

С	-6.646077	-1.216180	-0.025152
С	-0.192150	-0.000206	-0.000124
С	0.509811	1.170414	-0.330946
С	0.512431	-1.169252	0.330699
С	1.894853	-1.214316	0.302752
С	1.892114	1.218543	-0.303100
С	2.674974	0.002979	-0.000233
0	3.926742	0.004383	-0.000319
С	-1.606999	-2.042215	-1.447939
С	-1.914693	-3.398867	-1.257853
С	-0.668959	-1.688187	-2.435184
С	-0.057573	-2.672251	-3.206788
С	-1.294054	-4.383346	-2.030538
С	-0.362294	-4.023753	-3.005112
С	-1.611382	2.038632	1.447838
С	-1.922069	3.394635	1.257881
С	-1.303534	4.380417	2.030656
С	-0.370930	4.022783	3.005158
С	-0.063262	2.671926	3.206675
С	-0.672524	1.686574	2.435024
Η	-2.629506	3.678632	0.477266
Η	-1.542156	5.430302	1.856849
Η	0.126874	4.791344	3.596906
Η	0.667559	2.384538	3.962771
Η	-0.404767	0.640471	2.581622
Η	-0.047189	2.057729	-0.632970
С	2.560003	2.507713	-0.558185
Η	-0.042560	-2.057783	0.632800
С	2.565635	-2.501957	0.557898
Η	-0.403508	-0.641514	-2.581853
Η	0.672565	-2.383354	-3.962925
Η	0.137156	-4.791273	-3.596798
Η	-1.530330	-5.433746	-1.856648
Η	-2.621474	-3.684355	-0.477161
Η	-4.204911	-1.818833	-1.164455
Η	-4.208831	1.809677	1.164440
Η	-6.116222	2.153343	0.010536
Η	-8.583423	2.145625	0.034798
Η	-9.835382	-0.011000	0.000296

Η	-8.578480	-2.164750	-0.034360
Η	-6.111283	-2.166788	-0.010381
С	2.005161	-3.674159	0.058644
С	2.576914	-4.944778	0.306882
С	3.778517	-5.026084	1.089867
С	3.771442	-2.594904	1.316183
С	4.348264	-3.817937	1.575858
С	2.003331	-6.143602	-0.198319
С	2.580774	-7.369352	0.062997
С	3.762466	-7.449713	0.840635
С	4.347099	-6.302140	1.339800
С	1.996981	3.678601	-0.058745
С	2.565888	4.950529	-0.306875
С	3.767245	5.034576	-1.089996
С	4.339618	3.827777	-1.576197
С	3.765518	2.603416	-1.316597
С	1.989724	6.148016	0.198561
С	2.564437	7.375078	-0.062654
С	3.745867	7.458157	-0.840412
С	4.332970	6.311938	-1.339813
Η	1.105847	3.625595	0.570840
Η	5.256212	3.884424	-2.167775
Η	4.225003	1.688280	-1.683021
Η	1.078705	6.075188	0.797365
Η	2.111699	8.286941	0.330210
Η	4.192084	8.433266	-1.041753
Η	5.246057	6.374604	-1.936061
Η	1.113859	-3.623178	-0.570856
Η	5.265030	-3.872527	2.167333
Η	1.092094	-6.072880	-0.797010
Η	2.129998	-8.282277	-0.329660
Η	4.210854	-8.423809	1.042060
Η	5.260374	-6.362729	1.935977
Η	4.228917	-1.678684	1.682480

XYZ coordinates of negative-solvatochromic dye 13

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С	-2.437953	-1.117199	-0.416946
С	-1.055395	-1.115561	-0.454199
Ν	-0.346983	0.000001	0.000046
С	-1.055416	1.115562	0.454240
С	-2.437940	1.117197	0.416960
С	-3.189280	0.000005	0.000012
С	-4.652776	0.000019	0.000014
С	-5.382498	-1.206615	0.105593
С	-6.770540	-1.213317	0.105138
С	-7.455823	0.000048	-0.000008
С	-6.770538	1.213389	-0.105102
С	-5.382493	1.206652	-0.105563
С	1.071808	-0.000025	0.000049
С	1.773627	-1.094574	0.535490
С	1.773671	1.094550	-0.535427
С	3.154577	1.139528	-0.532577
С	3.154619	-1.139592	0.532582
С	3.933930	-0.000038	-0.000020
Ο	5.183400	-0.000056	-0.000043
С	-0.339519	2.254206	1.078301
С	-0.615565	3.559973	0.644379
С	0.573843	2.061934	2.130608
С	1.196349	3.155110	2.726342
С	0.016437	4.653584	1.240898
С	0.925850	4.454205	2.280551
С	-0.339501	-2.254163	-1.078270
С	-0.615590	-3.559952	-0.644361
С	0.016417	-4.653546	-1.240916
С	0.925842	-4.454152	-2.280539
С	1.196346	-3.155077	-2.726304
С	0.573891	-2.061879	-2.130592
Η	-1.305386	-3.714323	0.186852
Η	-0.193212	-5.660919	-0.879915
Η	1.431259	-5.305254	-2.737552
Η	1.905201	-2.992066	-3.538391
Η	0.809580	-1.052634	-2.468027
Η	1.214116	-1.912075	0.990682

С	3.834579	-2.339044	1.054604
Η	1.214092	1.912061	-0.990572
С	3.834572	2.338964	-1.054616
Η	0.809547	1.052681	2.468085
Η	1.905204	2.992083	3.538377
Η	1.431274	5.305300	2.737558
Η	-0.193145	5.660934	0.879848
Н	-1.305341	3.714399	-0.186886
Н	-2.934884	1.992275	0.832193
Н	-2.934891	-1.992255	-0.832215
Н	-4.854216	-2.152567	0.224663
Η	-7.336416	-2.138520	0.196461
Ν	-8.929511	0.000202	-0.000091
Η	-7.336356	2.138594	-0.196383
Η	-4.854189	2.152576	-0.224613
С	3.286544	3.614050	-0.801773
С	3.886565	4.767380	-1.305314
С	5.053428	4.674341	-2.069682
С	5.019423	2.261751	-1.812804
С	5.614731	3.417807	-2.317323
С	3.286553	-3.614104	0.801768
С	3.886538	-4.767459	1.305279
С	5.053440	-4.674443	2.069698
С	5.614735	-3.417854	2.317343
С	5.019415	-2.261832	1.812777
Η	2.398755	-3.700591	0.171878
Н	6.528340	-3.336660	2.908544
Н	5.466980	-1.288022	1.998172
Η	2.398762	3.700527	-0.171885
Η	6.528395	3.336606	-2.908494
Н	3.449390	-5.743602	1.087914
Н	5.527885	-5.575468	2.461294
Η	3.449379	5.743554	-1.087933
Η	5.527918	5.575408	-2.461317
Η	5.466941	1.287955	-1.998215
0	-9.503851	-1.093640	0.076585
0	-9.503793	1.093762	-0.076819

\mathbf{XYZ} coordinates of negative-solvatochromic dye $\mathbf{14}$

\mathbf{C}	-1.711031	0.407426	0.077499
С	-0.265917	0.380727	0.192954
С	0.434212	1.560515	0.261283
С	-1.532516	2.843789	0.109740
С	-2.322296	1.722413	0.038542
С	-2.491111	-0.796760	0.003439
С	-2.091952	-1.894086	-0.812897
С	-2.819381	-3.054677	-0.932488
С	-4.059254	-3.214911	-0.148371
С	-4.461026	-2.093286	0.722897
С	-3.698109	-0.949696	0.744981
Η	1.513700	1.580251	0.400271
Η	-1.949154	3.847224	0.036805
Н	-1.212110	-1.756277	-1.438621
Н	-3.968390	-0.148057	1.430053
С	0.614348	4.010239	0.378549
Η	0.129838	4.831809	-0.162767
Η	0.699541	4.281604	1.441821
Η	1.618292	3.862918	-0.036208
С	-2.374412	-4.183198	-1.873369
С	-3.462910	-4.439245	-2.942089
С	-1.064211	-3.845534	-2.608039
С	-2.130418	-5.474343	-1.054395
Η	-4.409094	-4.726651	-2.470737
Η	-3.629105	-3.533697	-3.545154
Η	-3.143445	-5.246674	-3.619499
Η	-0.230531	-3.679323	-1.908547
Η	-0.786675	-4.687364	-3.258814
Η	-1.164843	-2.954484	-3.246664
Н	-1.795804	-6.284533	-1.721363
Н	-1.346857	-5.308638	-0.299119
Η	-3.047758	-5.788793	-0.545521
С	-5.716926	-2.232725	1.594266
С	-5.978030	-0.977195	2.446440

С	-6.953842	-2.447664	0.688778
С	-5.559365	-3.433209	2.556907
Η	-5.154049	-0.773369	3.147718
Η	-6.134652	-0.082322	1.824626
Η	-6.889279	-1.127826	3.043445
Η	-6.838785	-3.354724	0.085934
Η	-7.859929	-2.542519	1.307737
Η	-7.089752	-1.588923	0.013615
Η	-6.459225	-3.533532	3.183940
Η	-5.414020	-4.362807	1.995908
Η	-4.694942	-3.282090	3.221258
С	0.539893	-0.903659	0.381072
С	1.368417	-0.874190	1.678025
С	1.431571	-1.205693	-0.835195
Η	-0.182634	-1.723265	0.484084
Η	0.737004	-0.637487	2.545535
Η	1.832041	-1.856266	1.849505
Η	2.182094	-0.133765	1.634756
Η	0.849266	-1.243546	-1.765832
Η	2.208526	-0.434959	-0.957500
Η	1.936289	-2.174304	-0.711190
С	-3.810764	1.948367	-0.221717
С	-4.048450	2.814628	-1.471636
С	-4.524832	2.543663	1.003607
Η	-4.252930	0.965294	-0.427840
Η	-3.524900	2.401978	-2.344925
Η	-5.122710	2.852180	-1.702558
Η	-3.709427	3.852470	-1.329096
Η	-4.379940	1.923555	1.898612
Η	-4.146989	3.552674	1.231051
Η	-5.605359	2.624042	0.817624
Ν	-0.168995	2.787669	0.212848
Ο	-4.746906	-4.266788	-0.219526

XYZ coordinates of inverted-solvatochromic dye 2

С	4.0346253	1.1211234	-0.0158028
С	2.7032922	1.4230098	-0.0126810
С	1.7033345	0.3951509	-0.0120867
С	2.2099586	-0.9506062	-0.0170868
С	3.5484300	-1.1996226	-0.0213280
Ν	4.4814114	-0.1811010	-0.0293602
Η	4.8091472	1.8862035	-0.0130883
Η	2.4065125	2.4720500	-0.0141794
Η	1.5004529	-1.7760612	-0.0215383
Η	3.9581682	-2.2086474	-0.0230719
С	0.3288350	0.6885352	-0.0097578
Η	0.0447105	1.7529132	-0.0086745
С	5.9059470	-0.4884972	0.0665818
Η	6.2038175	-0.6690439	1.1109667
Η	6.1326241	-1.3820381	-0.5285333
Η	6.4903331	0.3495114	-0.3307529
С	-1.8910120	-0.1320313	-0.0033403
С	-2.6895744	-1.3325211	-0.0065968
С	-2.5927540	1.1326673	0.0069336
С	-4.0510982	-1.2996204	-0.0008295
Η	-2.1401077	-2.2766136	-0.0140146
С	-3.9532893	1.1827004	0.0128266
Η	-2.0208563	2.0626267	0.0103572
С	-4.7840464	-0.0315992	0.0092776
Η	-4.6496820	-2.2117885	-0.0033457
Η	-4.4916706	2.1323010	0.0206936
Ν	-0.5626902	-0.3035389	-0.0095366
Ο	-6.0285560	0.0260678	0.0148185

XYZ coordinates of inverted-solvatochromic dye $15\,$

294.0615492 С 1.1646973-0.01954851.3751076-0.0146515С 2.7157848 С 1.76726570.2900293 -0.0128516 С -0.01770502.3773865 -1.0187615

С	3.7302064	-1.1787256	-0.0221845
Η	4.7825503	1.9805469	-0.0179827
Н	2.3526726	2.4028597	-0.0163175
Η	1.7638448	-1.9174948	-0.0226029
Н	4.2000173	-2.1612196	-0.0227978
С	6.0392241	-0.3055749	0.0730079
Η	6.5633321	0.4797793	-0.4861056
Н	6.3700336	-0.2788433	1.1231327
Η	6.3091117	-1.2760566	-0.3600659
С	0.3911186	0.5407470	-0.0095453
Η	0.0997792	1.5939572	-0.0076765
С	-0.6236042	-0.4273445	-0.0085007
Η	-0.3149525	-1.4784556	-0.0122585
С	-2.0078775	-0.2226881	-0.0027208
С	-2.8876650	-1.3634322	-0.0030953
С	-2.6283193	1.0785238	0.0041425
С	-4.2450017	-1.2382442	0.0025870
Η	-2.4291842	-2.3571043	-0.0082223
С	-3.9827155	1.2252555	0.0099138
Η	-1.9944328	1.9679831	0.0048604
С	-4.8945157	0.0743909	0.0095948
Η	-4.9012553	-2.1099710	0.0021764
Η	-4.4503385	2.2116000	0.0151134
0	-6.1337861	0.2101553	0.0149844
Ν	4.5973465	-0.1071126	-0.0339205

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С	3.3552066	-1.2877543	-0.0000107
С	1.9833052	-1.4427793	-0.0000495
С	1.0867697	-0.3314034	-0.0000461
С	1.6906967	0.9638702	-0.0000124
С	3.0606385	1.1302913	0.0000265
С	3.9108929	0.0059869	0.0000321
Η	4.0254941	-2.1456998	-0.0000080
Н	1.5588635	-2.4496864	-0.0000787
Η	1.0573864	1.8517140	-0.0000133
Η	3.5104559	2.1221291	0.0000566
С	-0.3228891	-0.5638096	-0.0000640
Η	-0.6215774	-1.6162391	-0.0000783
С	-1.3169973	0.3964969	-0.0000422
Η	-0.9991533	1.4454988	-0.0000237
С	-2.7248599	0.2136893	-0.0000189
С	-3.5841465	1.3571991	-0.0000100
С	-3.3683105	-1.0653081	-0.0000383
С	-4.9526199	1.2545375	0.0000206
Η	-3.1135913	2.3466464	-0.0000667
С	-4.7333969	-1.1906489	-0.0000058
Η	-2.7507010	-1.9675197	-0.0001165
С	-5.6290773	-0.0360243	0.0000547
Η	-5.5876505	2.1434594	0.0000276
Η	-5.2095929	-2.1742294	-0.0000153
Ν	5.3365522	0.1785844	0.0000893
Ο	5.8010552	1.3433805	0.0001319
0	6.0648995	-0.8419215	0.0000947
0	-6.8820356	-0.1525289	0.0000402

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XYZ coordinates of inverted-solvatochromic dye $17\,$

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 $C \qquad 1.0447780 \qquad 0.2436146 \qquad -0.2042347$

С	0.1711992	1.3536410	-0.1319900
С	-1.2032405	1.2266373	-0.0280061
С	-1.7318586	-0.0969845	0.0393132
С	-0.9141277	-1.1905655	-0.1050309
Ν	0.4443818	-1.0218251	-0.3351124
Η	0.6298250	2.3403316	-0.1054853
Η	-2.7792997	-0.2649670	0.2818925
С	1.1749337	-2.1000632	-1.0279121
Η	1.9710760	-1.6377824	-1.6218785
Η	1.6304834	-2.8223191	-0.3412105
Η	0.4756286	-2.6330358	-1.6823961
С	-1.4450490	-2.5656119	0.0190091
С	-0.8379822	-3.4940041	0.8841828
С	-2.5956259	-2.9491513	-0.6897666
С	-1.3698748	-4.7731456	1.0336643
Η	0.0402855	-3.1968475	1.4591133
С	-3.1250527	-4.2318142	-0.5396171
Η	-3.0607026	-2.2383765	-1.3743935
С	-2.5131852	-5.1478251	0.3197530
Η	-0.8953950	-5.4789871	1.7162943
Η	-4.0146903	-4.5184698	-1.1014468
Η	-2.9252846	-6.1509909	0.4346121
С	-2.0910476	2.4006091	0.0785039
С	-3.4016797	2.3523216	-0.4346099
С	-1.6580589	3.5955345	0.6849300
С	-4.2432119	3.4613725	-0.3558034
Η	-3.7540348	1.4454733	-0.9283899
С	-2.5012879	4.7021066	0.7666974
Η	-0.6615706	3.6475325	1.1253911
С	-3.7973251	4.6414408	0.2455356
Η	-5.2506755	3.4050740	-0.7700412
Η	-2.1480490	5.6140045	1.2497361
Η	-4.4568819	5.5074417	0.3117307
С	2.4605250	0.3814675	-0.1388851
С	3.2985348	-0.6184235	0.4579083
С	3.1091729	1.5734765	-0.6065527
С	4.6501118	-0.4532856	0.5788713
Η	2.8332517	-1.5031225	0.8972255
С	4.4631239	1.7416598	-0.5233103

Η	2.5076313	2.3434529	-1.0960533
С	5.3390455	0.7355758	0.0762538
Η	5.2657027	-1.2000992	1.0829973
Η	4.9443464	2.6384089	-0.9167625
Ο	6.5761542	0.8825204	0.1632736

XYZ coordinates of inverted-solvatochromic dye 18

С	2.2520449	-1.1561810	-0.1376050
С	0.9114946	-1.4349842	-0.0999401
С	-0.0991807	-0.4300238	0.0365980
С	0.3463101	0.9172955	0.2272376
С	1.6672313	1.2801330	0.2408271
С	2.7019099	0.2479918	0.0115566
Η	0.5849569	-2.4618048	-0.2588155
Η	-0.4103874	1.6647585	0.4569336
Ο	3.9177714	0.5471660	-0.0376433
С	3.3005254	-2.2554953	-0.3545497
С	4.0921951	-1.9756758	-1.6546375
С	4.2694203	-2.2931846	0.8526184
С	2.6633251	-3.6508758	-0.4846294
Η	3.4152090	-1.9633033	-2.5221409
Η	4.6084097	-1.0117429	-1.5970970
Η	4.8390636	-2.7684759	-1.8157138
Η	3.7194211	-2.5082799	1.7812042
Η	5.0165338	-3.0886331	0.7067244
Η	4.7900067	-1.3366341	0.9652083
Η	3.4571592	-4.3980652	-0.6272349
Η	2.1027663	-3.9342934	0.4195341
Η	1.9878926	-3.7191946	-1.3510137
С	2.1012995	2.7282139	0.5045714
С	3.0190798	2.7872436	1.7486092
С	2.8581908	3.2710438	-0.7324278
С	0.8997441	3.6553690	0.7624521
Η	2.4863044	2.4169454	2.6374811

Η	3.9188662	2.1812281	1.5997444
Η	3.3222536	3.8279132	1.9416942
Η	2.2088539	3.2501364	-1.6209079
Η	3.1620529	4.3147365	-0.5567138
Η	3.7516955	2.6718144	-0.9359706
Η	1.2636485	4.6779290	0.9377266
Η	0.2137201	3.6925489	-0.0976722
Η	0.3261910	3.3517033	1.6512681
С	-1.4753253	-0.7805439	0.0449875
С	-2.5584658	0.1301418	-0.3295764
С	-1.9056851	-2.0781539	0.4587221
С	-2.3403504	1.2959727	-1.0976672
С	-3.9147295	-0.1823019	0.0039060
С	-3.2140835	-2.3439409	0.7379730
Η	-1.1774107	-2.8554474	0.6779041
С	-3.3667120	2.1748567	-1.4159074
Η	-1.3348766	1.4897597	-1.4652626
С	-4.9470102	0.7287230	-0.2969917
Η	-3.5303199	-3.3053131	1.1385515
С	-4.6705216	1.9046607	-0.9834638
Η	-3.1564319	3.0638895	-2.0105052
Η	-5.9736938	0.5103840	-0.0113782
Η	-5.4828814	2.5948632	-1.2136285
С	-5.5765994	-1.7445654	0.9767833
Η	-5.9681425	-1.0153421	1.7005377
Η	-6.2397927	-1.7676169	0.0987331
Η	-5.5779656	-2.7343771	1.4440365
Ν	-4.2089811	-1.4099714	0.5949699

XYZ coordinates of inverted-solvatochromic dye 19

С	3.3547508	-1.1838488	0.0000548
С	2.0227097	-1.4931117	-0.0000054
С	0.9824152	-0.5064792	-0.0000451
С	1.3747693	0.8725647	-0.0000340

С	2.6805652	1.2747515	0.0000010
С	3.7536296	0.2447156	0.0000646
Н	1.7025254	-2.5367383	-0.0000124
Н	0.5865199	1.6239013	-0.0000934
0	4.9593119	0.5769837	0.0001088
С	-0.3531462	-0.9297050	-0.0001208
Н	-0.4892864	-2.0157530	-0.0001986
С	-1.5018069	-0.1235649	-0.0000753
Η	-1.3387351	0.9532993	0.0001761
С	-2.8257740	-0.5741504	-0.0002427
С	-3.9696024	0.3487726	-0.0000855
С	-3.1704047	-1.9656294	-0.0005460
С	-3.8127766	1.7506581	-0.0000396
С	-5.3086021	-0.1541314	0.0000453
С	-4.4625667	-2.3910538	-0.0004696
Η	-2.3945137	-2.7273335	-0.0008336
С	-4.8933688	2.6216128	0.0002085
Η	-2.8086950	2.1708571	-0.0002262
С	-6.4008578	0.7364456	0.0003330
Η	-4.7163270	-3.4497080	-0.0006609
С	-6.1957060	2.1100676	0.0004294
Η	-4.7238330	3.6983321	0.0002211
Η	-7.4195630	0.3550066	0.0004728
Η	-7.0542323	2.7820544	0.0006473
С	-6.8888861	-2.0684603	0.0000144
Η	-7.4411511	-1.7470792	0.8956724
Η	-7.4415027	-1.7466961	-0.8952862
Η	-6.8338396	-3.1618144	-0.0002353
Ν	-5.5330420	-1.5320762	-0.0001245
С	4.4441450	-2.2634821	0.0000813
С	5.3221091	-2.1207070	-1.2668454
С	5.3220455	-2.1207234	1.2670557
С	3.8498256	-3.6836993	0.0000588
Η	4.7099668	-2.2339047	-2.1742748
Η	5.8145087	-1.1429706	-1.2946869
Η	6.0940037	-2.9057871	-1.2759507
Η	4.7098349	-2.2338574	2.1744469
Η	6.0939062	-2.9058379	1.2762450
Η	5.8144949	-1.1430126	1.2948931

Η	4.6690545	-4.4171318	0.0000709
Η	3.2356595	-3.8743670	0.8932992
Η	3.2356895	-3.8743648	-0.8932032
С	3.0724612	2.7577077	-0.0000658
С	3.9010897	3.0798620	1.2672355
С	3.9011923	3.0797045	-1.2673486
С	1.8410289	3.6822775	-0.0001735
Η	3.3161829	2.8660356	2.1744800
Η	4.8217477	2.4877790	1.2943424
Η	4.1666761	4.1482596	1.2761557
Η	3.3164003	2.8656669	-2.1746177
Η	4.1667007	4.1481214	-1.2764346
Η	4.8219013	2.4876882	-1.2942737
Η	2.1774886	4.7291114	-0.0002203
Η	1.2149976	3.5369156	-0.8939427
Η	1.2149113	3.5370273	0.8935591

XYZ coordinates of inverted-solvatochromic dye 20

С	-2.6543163	-1.1425790	0.4030868
С	-1.2957144	-1.2291694	0.3097857
С	-0.4708290	-0.0557828	0.2833876
С	-1.1805140	1.1924173	0.3665947
С	-2.5384410	1.2261459	0.4596413
Ν	-3.2995622	0.0729955	0.4687895
Η	-3.2979328	-2.0205175	0.4240967
Η	-0.8397157	-2.2175882	0.2485323
Η	-0.6111400	2.1198709	0.3485208
Η	-3.0990655	2.1575215	0.5256127
С	-4.7434652	0.1395903	0.6737599
Η	-5.2209639	-0.7332980	0.2126781
Η	-4.9932313	0.1593704	1.7461135
Η	-5.1422280	1.0439960	0.1981764
С	0.9276174	-0.1323679	0.1756223
Η	1.3653950	-1.1413920	0.1160419

С	2.9991017	0.9972011	0.0331091
С	3.6154723	2.2912575	-0.0081519
С	3.8489759	-0.1587839	-0.0487545
С	4.9641454	2.4771280	-0.1282541
Η	2.9249667	3.1318605	0.0582807
С	5.2068246	-0.0667458	-0.1655995
Η	3.3802744	-1.1407331	-0.0139989
С	5.8403496	1.2830312	-0.2126775
С	5.5934421	3.8748236	-0.1848640
С	6.3365479	4.0585743	-1.5304146
С	4.5319918	4.9849000	-0.0798150
С	6.5842255	4.0577895	0.9900947
Η	7.1443043	3.3266511	-1.6375603
Η	5.6396916	3.9420206	-2.3740167
Η	6.7678423	5.0702887	-1.5819131
Η	3.9783551	4.9365748	0.8698515
Η	5.0291992	5.9646238	-0.1245426
Η	3.8075033	4.9422488	-0.9067173
Η	7.0159813	5.0701676	0.9573765
Η	6.0659709	3.9400000	1.9535537
Η	7.3978270	3.3267894	0.9366437
С	6.0992141	-1.3119472	-0.2473328
С	5.2785188	-2.6135632	-0.1904290
С	6.8851957	-1.3115028	-1.5810410
С	7.0873095	-1.3261342	0.9445052
Η	4.7189284	-2.7086665	0.7524941
Η	4.5686533	-2.6904524	-1.0280439
Η	5.9608269	-3.4731657	-0.2570285
Η	7.5340036	-0.4327797	-1.6542644
Η	7.5072779	-2.2176832	-1.6442596
Η	6.1934197	-1.3129570	-2.4366857
Η	7.7089073	-2.2337676	0.9000474
Η	7.7424432	-0.4491133	0.9217080
Η	6.5397441	-1.3342637	1.8988911
0	7.0800572	1.3989351	-0.3206613
Ν	1.6613873	0.9812112	0.1409758

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XYZ coordinates of positive-solvatochromic dye 3

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С	3.5495610	-1.4229888	-0.3800914
С	4.9046012	-1.5067254	-0.3176120
С	5.7268726	-0.3572844	0.0739368
С	4.9821182	0.8635658	0.4093397
С	3.6258733	0.9348448	0.3269241
С	2.8298232	-0.1987911	-0.0914963
Н	2.9614696	-2.2971626	-0.6740034
Η	5.4343178	-2.4316740	-0.5510110
Η	5.5765758	1.7153043	0.7443326
Η	3.1267707	1.8551506	0.6237072
Ο	6.9677543	-0.4129063	0.1353326
С	1.4430695	-0.2243432	-0.2042216
Η	1.0352475	-1.2253241	-0.3936945
С	0.4641369	0.8097062	-0.1541623
С	0.8129558	2.2740765	-0.2791056
Η	-0.0074259	2.8385052	-0.7473979
Η	1.0087362	2.7392679	0.6998656
Η	1.7017081	2.4097173	-0.9070160
С	-0.8721403	0.4572303	-0.0287003
С	-3.4953934	0.5165213	-0.0100931
С	-3.1487064	-0.8437255	0.0888079
С	-4.8387598	0.9018362	-0.0715762
С	-4.1464758	-1.8241605	0.1221453
С	-5.8292213	-0.0801717	-0.0344398
Η	-5.1050094	1.9561405	-0.1505391
С	-5.4850158	-1.4337667	0.0611638
Н	-3.8798351	-2.8788540	0.1952233
Η	-6.8775772	0.2141654	-0.0825031
Η	-6.2660153	-2.1935726	0.0877264
\mathbf{S}	-1.4339775	-1.1941056	0.2076016
\mathbf{S}	-2.1590384	1.6515241	-0.0314434

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С	-3.2522648	-0.8380175	0.0001602
С	-2.9454891	0.5384856	0.0001612
С	-3.9703295	1.4898983	0.0002033
С	-5.2941471	1.0424165	0.0002475
С	-5.5960761	-0.3249192	0.0002573
С	-4.5749545	-1.2790831	0.0002148
С	-0.7839805	-0.3368593	0.0000388
Η	-3.7459923	2.5554085	0.0001917
Η	-6.1020842	1.7741771	0.0002718
Η	-6.6357399	-0.6516835	0.0002959
Η	-4.8042415	-2.3445554	0.0002219
С	2.6355125	0.2299243	-0.0001879
С	3.5260540	1.3680760	-0.0005325
С	3.2098163	-1.1002887	0.0002543
С	4.8743909	1.2109954	-0.0004470
Η	3.0638938	2.3576152	-0.0008664
С	4.5560620	-1.2671566	0.0003428
Η	2.5253478	-1.9482292	0.0005078
С	5.4884575	-0.1245297	-0.0000063
Η	5.5566644	2.0619731	-0.0007019
Η	5.0134222	-2.2582088	0.0006736
0	6.7193320	-0.2866950	0.0000647
С	-1.0841103	2.1784366	0.0002449
Η	0.0076676	2.1573204	0.0003001
Η	-1.4555091	2.6959707	-0.8961534
Η	-1.4556612	2.6958426	0.8966542
Ν	-1.5727329	0.7967306	0.0001160
\mathbf{S}	-1.7859022	-1.7878252	0.0000794
Ν	0.5140116	-0.5599269	-0.0000344
Ν	1.3337426	0.5094773	-0.0003024

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XYZ coordinates of positive-solvatochromic dye $\mathbf{22}$

С	2.2256254	1.9203544	0.0000000
С	1.8416879	0.5248018	0.0000000
С	2.8947684	-0.4991895	0.0000000
С	4.2539818	-0.1001261	0.0000000
С	4.6309730	1.3399503	0.0000000
С	3.5254840	2.3060968	-0.0000000
Η	1.5456033	-2.1804876	-0.0000000
Η	1.4196673	2.6540221	0.0000000
С	2.5911567	-1.8750366	0.0000000
С	5.2697998	-1.0698337	0.0000000
Η	3.8123304	3.3592018	-0.0000000
С	4.9540599	-2.4224207	0.0000000
С	3.6078166	-2.8222011	-0.0000000
Η	6.3036349	-0.7225641	-0.0000000
Η	5.7473107	-3.1711889	0.0000000
Η	3.3555580	-3.8838751	0.0000000
0	5.8108072	1.7161022	0.0000000
С	-1.5722357	0.5031478	-0.0000000
С	-3.8936309	0.4667939	-0.0000000
С	-3.6256977	-0.9180520	-0.0000000
С	-5.2078031	0.9420169	-0.0000000
С	-4.6702249	-1.8405620	-0.0000000
С	-6.2490494	0.0094786	0.0000000
Η	-5.4166559	2.0112882	-0.0000000
С	-5.9860626	-1.3656473	0.0000000
Η	-4.4628464	-2.9107696	-0.0000000
Η	-7.2801167	0.3631643	0.0000000
Η	-6.8121876	-2.0765443	0.0000000
\mathbf{S}	-1.8957864	-1.2393001	-0.0000000
С	-2.7433100	2.6911815	-0.0000000
Η	-3.2591576	3.0627585	0.8967157
Η	-1.7065649	3.0390477	-0.0000000
Η	-3.2591576	3.0627585	-0.8967157
Ν	-2.7319046	1.2338439	-0.0000000
Ν	0.5883980	0.1069555	0.0000000
Ν	-0.3813013	1.0498239	0.0000000

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XYZ coordinates of positive-solvatochromic dye $\mathbf{23}$

С	-2.2193494	-0.4114870	-2.3091989
С	-0.8334298	-0.5816083	-2.5084272
С	-0.0788733	0.4253397	-3.1188827
С	-0.7310004	1.5920477	-3.5265358
С	-2.1071299	1.7585136	-3.3278313
С	-2.8637588	0.7571188	-2.7129238
С	-1.3325962	-2.6274255	-1.5069258
Η	0.9916387	0.3041049	-3.2770664
Η	-0.1538129	2.3833216	-4.0051327
Η	-2.5970636	2.6754868	-3.6543108
Η	-3.9341084	0.8839910	-2.5523255
С	-0.2246661	-5.7567679	-0.5068046
С	1.0042660	-6.4976593	-0.5516819
С	-1.3911527	-6.3766058	0.0619144
С	1.1162235	-7.7704682	-0.0676733
Η	1.8576220	-6.0022629	-1.0193578
С	-1.3557558	-7.6526077	0.5473897
Η	-2.3067690	-5.7867492	0.1073555
С	-0.0787611	-8.4317265	0.5259842
С	2.4095075	-8.4851119	-0.1137662
С	2.4977148	-9.8503415	-0.4477171
С	3.6023872	-7.7872632	0.1553760
С	3.7390635	-10.4821745	-0.5290835
Η	1.5876668	-10.4124034	-0.6448141
С	4.8414454	-8.4221714	0.0792786
Η	3.5499887	-6.7392942	0.4563594
С	4.9154944	-9.7744534	-0.2660450
Η	3.7883901	-11.5380569	-0.8004610
Η	5.7507555	-7.8621228	0.3027679
Η	5.8830963	-10.2756910	-0.3220017
С	-2.5787418	-8.2817008	1.0876400
С	-3.8023489	-8.1221577	0.4104592
С	-2.5671496	-9.0214605	2.2848156
С	-4.9807030	-8.6665805	0.9203095
Η	-3.8186078	-7.5861452	-0.5400019

С	-3.7489886	-9.5547647	2.7986720
Η	-1.6273962	-9.1700743	2.8118138
С	-4.9594476	-9.3798973	2.1216726
Н	-5.9174977	-8.5412419	0.3751034
Η	-3.7233501	-10.1148249	3.7346578
Η	-5.8815855	-9.8021171	2.5236504
0	-0.0221905	-9.5795769	0.9862526
С	1.0753386	-2.1125566	-2.1073073
Η	1.2424745	-3.0879800	-1.6453357
Н	1.3991486	-2.1418352	-3.1582213
Η	1.6322828	-1.3263437	-1.5765878
Ν	-1.3366788	-3.8449389	-1.0034818
Ν	-0.1752215	-4.5260129	-1.0225911
Ν	-0.3570495	-1.8088846	-2.0434777
\mathbf{S}	-2.9022604	-1.8239679	-1.5391410

XYZ coordinates of positive-solvatochromic dye $\mathbf{24}$

-2.1957027	-0.1512168	-2.2356587
-0.8655101	-0.3200548	-2.6636091
-0.1686457	0.7439945	-3.2455632
-0.8106683	1.9738042	-3.3977577
-2.1341170	2.1428902	-2.9736872
-2.8334966	1.0845695	-2.3924693
-1.5698601	-2.6145864	-1.6114171
0.8625710	0.6117947	-3.5739509
-0.2721658	2.8066566	-3.8498547
-2.6259970	3.1081087	-3.0939658
-3.8630517	1.2168340	-2.0586425
-0.1663449	-5.9841349	-0.6385617
1.2068812	-6.4267081	-0.5138195
-1.1939521	-6.9758844	-0.4054684
1.5342577	-7.6965978	-0.1562591
1.9948294	-5.6927270	-0.7063325
-0.8816168	-8.2539540	-0.0608240
	$\begin{array}{r} -2.1957027\\ -0.8655101\\ -0.1686457\\ -0.8106683\\ -2.1341170\\ -2.8334966\\ -1.5698601\\ 0.8625710\\ -0.2721658\\ -2.6259970\\ -3.8630517\\ -0.1663449\\ 1.2068812\\ -1.1939521\\ 1.5342577\\ 1.9948294\\ -0.8816168\end{array}$	-2.1957027 -0.1512168 -0.8655101 -0.3200548 -0.1686457 0.7439945 -0.8106683 1.9738042 -2.1341170 2.1428902 -2.8334966 1.0845695 -1.5698601 -2.6145864 0.8625710 0.6117947 -0.2721658 2.8066566 -2.6259970 3.1081087 -3.8630517 1.2168340 -0.1663449 -5.9841349 1.2068812 -6.4267081 -1.1939521 -6.9758844 1.5342577 -7.6965978 1.9948294 -5.6927270 -0.8816168 -8.2539540

Η	-2.1398009	-4.2394397	1.5623522
С	0.5050959	-8.7075968	0.1076633
0	0.7850416	-9.8729340	0.4416136
\mathbf{S}	-2.9671554	-1.5557275	-1.5221819
\mathbf{S}	-0.1884926	-1.9246743	-2.4497365
С	-1.5835092	-3.8862286	-1.0552566
С	-0.3865307	-4.6544461	-0.9878430
Н	0.5280034	-4.0956970	-1.2223014
С	-2.8725182	-4.3500339	-0.4624824
С	-3.9716968	-4.6624385	-1.2776981
С	-2.9975586	-4.4725039	0.9303520
С	-5.1708324	-5.0993393	-0.7109012
Η	-3.8735516	-4.5756892	-2.3608849
С	-4.1961128	-4.9077899	1.4953057
С	-5.2847358	-5.2237976	0.6761443
Η	-6.0149213	-5.3502424	-1.3546400
Η	-4.2807185	-5.0039350	2.5784498
Η	-6.2198989	-5.5686057	1.1190567
Η	2.5726387	-8.0155954	-0.0547757
Η	-2.2380494	-6.6938873	-0.5278022
Н	-1.6582675	-9.0031658	0.1016179

3 TD-DFT UV-Vis spectrum of dye 7

Table 1: UV-Vis spectrum for dye 7 in N,N-dimethylformamide determined at the CAM-B3LYP/def2-TZVP level of theory with the PCM solvent model.

State	Wavelength (nm)	Oscilator Strength
1	448.3 0.549165455	
2	$347.3\ 0.000766181$	
3	$335.3\ 0.003086692$	
4	$272.9\ 0.048825963$	
5	$275.1\ 0.022940898$	
6	$242.2 \ 0.001160866$	
7	$220.6 \ 0.139547952$	
8	$216.6 \ 0.140970543$	
9	$202.1 \ 0.010964234$	
10	$207.3\ 0.000193735$	

4 FOD plots for all the negative-, inverted- and positivesolvatochromic dyes studied.





Figure 4: FOD plots of all negative-solvatochromic dyes 1, 6–10 studied in this work.









Figure 5: FOD plots of all negative-solvatochromic dyes 11-16 studied in this work. 43



Figure 6: FOD plots of all inverted-solvatochromic dyes 2, 17–22 studied in this work.



Figure 7: FOD plots of all inverted-solvatochromic dyes 3, 23–26 studied in this work.



Figure 8: FOD plots of related γ -pyridiniophenolate solvatochromic dyes 4–6.

5 D1 values for all solvatochromic dyes studied.

Negative dye	D1 / $\times 10^{-2}$	Inverted dye	D1 / $\times 10^{-2}$	Positive dye	D1 / $\times 10^{-2}$
1	8.29	2	6.03	3	5.88
6	7.05	17	6.32	23	5.89
7	7.07	18	6.68	24	6.03
8	6.94	19	7.24	25	5.59
9	6.71	20	6.68	26	6.11
10	7.28	21	6.31		
11	6.62	22	6.15		
12	6.61				
13	8.46				
14	8.13				
15	9.55				
16	7.21				
Average	7.49	Average	6.49	Average	5.89
σ	0.91	σ	0.41	σ	0.19

Table 2: D1 diagnostic values for all the negative-, inverted- and positive-solvatochromicdyes.

6 Absorption spectrum of negative solvatochromic dye 4 in dry DMF .

The negative solvatochromic dye 7 was synthesized according to the literature procedure reported by González *et al.*. [6] The UV-Vis spectrum in dry DMF at 25 °C is shown in Figure 9.



Figure 9: UV-VIs spectrum of dye 7 in dry N,N-dimethylformamide ([7] = 1.1×10^{-5} mol/L).

7 State-averaged NEVPT2 spectra calculations.

Table 3: Transition wavelenghts and oscillator strengths from an average-state calculation of the first four states for the *N*-phenolate dye **7** studied in this work. The letter "g" represents the ground state, while the excited states are numbered. Only singlet states are considered. The calculation was performed at the NEVPT2/def2-TZVP level of theory (see the methodological section of the main manuscript).

8 Molecular orbitals considered for the CASSCF calculations.



Figure 10: Molecular orbitals in the active space produced by a CASSCF(14,13)/def2-TZVP for the N-phenolate dye 7 studied in this work.

9 A tutorial for the calculation of the D1 diagnostic for molecular systems, and its statistical analysis.

The program package Turbomole (see citation in the main manuscript) is needed for the calculation of the D1 parameter, as it is the only electronic structure software, out the the ones familiar to the authors, that is able to obtain it. Refer to www.cosmologic.de (to which the authors are not affiliated) for information on how to obtain a copy. Details of each calculation can be found in the Turbomole manual and/or tutorial.

- 1. Prepare a geometry optimization of the system. We suggest BP86/def2-TZVP with a m4 integration grid and the RI approximation for compatibility with our results.
- 2. After the optimization has converged, without any further modification of the inputs, run a forces calculation (simply excecute "aoforce > aoforce.out"). Make sure that no negative frequencies are found.
- 3. Take the coord file from the previous calculation and prepare a RI-MP2/def2-QZVP calculation with the ricc2 module. Briefly, after defining coordinates, basis set and initial guess, select the "cc" option in the "defin" program. Select "freeze" for a frozen-core calculation. Select "cbas" for auxiliary basis sets for the RI-MP2 procedure. Select the ricc2 sub-menu and, from there, type the "model mp2" command. Exit the menus and the define program.
- 4. Edit the control file. Under the "\$ricc2" section, you will see a line that only contains white spaces and the text "mp2". Modify this line by adding "d1diag" after "mp2" ("mp2 d1diag").
- 5. Run a HF calculation by calling the program dscf (excecute "dscf > dscf.ou"). After it has converged, call the ricc2 program to perform the mp2 calculation (excecute "ricc2 > ricc2.out").
- 6. In the mp2 output file (ricc2.out in this example) you will find the value for the diagnostic.
- 7. use the provided program (next section the the supporting information and also available at github.com/rmera) with the obtained D1 value to determine whether your dye is expected to display positive, negative or inverted solvatochromism. Call the program with the "-help" option for instructions.

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