Supplementary Material

**Solvent, Substituents and pH Effects towards the Spectral Shifts of some highly colored Indicators**

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The Chemical structures and the corresponding abbreviations of the six studied indicators are given below:



Fig. S-1. Structure of the investigated indicators and their abbreviations

*The pH effect on the absorption spectra:*

A representative example for the effect of pH on the absorption spectra of AYGG is given below



Fig. S-2. Effect of pH on the electronic absorption spectra of 1 × 10-4 M of AYGG

*The solvent parameters*:

TABLE S-I. The Physical parameters for the solvents

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Solvent | Dioxane | Ethanol | DMF | DMSO | Acetone | Acetonitrile | H2O |
| n | 1.422 | 1.361 | 1.427 | 1.478 | 1.359 | 1.344 | 1.333 |
| D | 2.2 | 24.3 | 36.7 | 48.9 | 20.7 | 37.5 | 78.5 |
| K | 0.223 | 0.470 | 0.480 | 0.485 | 0.465 | 0.48 | 0.491 |
| M | 0.203 | 0.181 | 0.204 | 0.221 | 0.180 | 0.175 | 0.171 |
| N | 0.031 | 0.665 | 0.666 | 0.658 | 0.648 | 0.712 | 0.757 |
| E | 36.0 | 51.9 | 43.8 | 45.0 | 42.2 | 46.0 | 63.1 |
| J | 0.286 | 0.886 | 0.922 | 0.941 | 0.868 | 0.924 | 0.963 |
| H | 0.254 | 0.221 | 0.257 | 0.283 | 0.220 | 0.212 | 0.206 |
| β | 0.37 | 0.77 | 0.69 | 0.76 | 0.48 | 0.31 | 0.47 |
| α | 0.00 | 0.83 | 0.00 | 0.00 | 0.08 | 0.19 | 1.17 |
| π\* | 0.55 | 0.54 | 0.87 | 1.00 | 0.71 | 0.75 | 1.09 |

*The regression data for the indicators:*

TABLE S-II. Regression analysis data for Y1 and Y2 bands for SO indicator

|  |
| --- |
| Y1 |
| Parameters | a0 | a1 | a2 | a3 | a4 | MCC | P |
| *K* | 314.092 | -10.037 |  |  |  | 0.281 | 0.358 |
| *M* | 292.304 | 89.085 |  |  |  | 0.585 | 0.132 |
| *N* | 312.171 | -4.339 |  |  |  | 0.334 | 0.307 |
| *E* | 323.149 | -0.300 |  |  |  | 0.621 | 0.113 |
| *K,M* | 297.235 | -7.851 | 81.069 |  |  | 0.752 | 0.248 |
| *K,N* | 287.678 | 115.606 | -49.984 |  |  | 0.614 | 0.386 |
| *K,E* | 325.008 | 6.196 | -0.401 |  |  | 0.657 | 0.343 |
| *M,N* | 296.353 | 77.102 | -3.104 |  |  | 0.745 | 0.255 |
| *M,E* | 307.574 | 58.557 | -0.208 |  |  | 0.816 | 0.184 |
| *N,E* | 325.651 | 1.880 | -0.379 |  |  | 0.640 | 0.360 |
| *K,M,N* | 338.248 | -411.615 | 297.965 | 162.954 |  | 0.925 | 0.345 |
| *K,M,E* | 307.498 | -9.85E-02 | 58.732 | -0.206 |  | 0.816 | 0.529 |
| *K,N,E* | 304.406 | 85.937 | -33.453 | -0.294 |  | 0.780 | 0.575 |
| *M,N,E* | 307.699 | 58.381 | 5.84E-02 | -0.211 |  | 0.816 | 0.529 |
| Y2 |
| *K* | 416.508 | -9.860 |  |  |  | 0.009 | 0.844 |
| *M* | 317.234 | 498.397 |  |  |  | 0.787 | 0.008 |
| *N* | 416.989 | -8.196 |  |  |  | 0.039 | 0.672 |
| *E* | 451.818 | -0.847 |  |  |  | 0.490 | 0.080 |
| *K,M* | 303.480 | 18.850 | 526.797 |  |  | 0.816 | 0.034 |
| *K,N* | 227.867 | 882.599 | -349.177 |  |  | 0.896 | 0.011 |
| *K,E* | 444.992 | 52.666 | -1.199 |  |  | 0.649 | 0.123 |
| *M,N* | 306.622 | 533.118 | 6.765 |  |  | 0.810 | 0.036 |
| *M,E* | 351.369 | 405.771 | -0.352 |  |  | 0.845 | 0.024 |
| *N,E* | 457.490 | 18.886 | -1.206 |  |  | 0.609 | 0.153 |
| *K,M,N* | 243.283 | 639.102 | 177.567 | -250.122 |  | 0.916 | 0.040 |
| *K,M,E* | 349.573 | 47.246 | 388.287 | -0.689 |  | 0.943 | 0.008 |
| *K,N,E* | 269.565 | 741.252 | -286.940 | -0.340 |  | 0.919 | 0.038 |
| *M,N,E* | 356.298 | 409.369 | 19.379 | -0.716 |  | 0.969 | 0.009 |
| *K,M,N,E* | 329.412 | 187.900 | 325.422 | -58.246 | -0.597 | 0.974 | 0.051 |

TABLE S-III. Regression analysis data for Y1 and Y2 bands for AYR indicator

|  |
| --- |
| Y1 |
| Parameters | a0 | a1 | a2 | a3 | a4 | MCC | P |
| *K* | 278.210 | 52.012 |  |  |  | 0.640 | 0.056 |
| *M* | 291.506 | 49.406 |  |  |  | 0.020 | 0.790 |
| *N* | 289.814 | 19.237 |  |  |  | 0.582 | 0.078 |
| *E* | 294.136 | 0.144 |  |  |  | 0.037 | 0.716 |
| *K,M* | 249.686 | 58.602 | 133.406 |  |  | 0.774 | 0.107 |
| *K,N* | 242.474 | 221.207 | -66.036 |  |  | 0.724 | 0.145 |
| *K,E* | 287.856 | 75.086 | -0.415 |  |  | 0.818 | 0.078 |
| *M,N* | 254.429 | 170.495 | 23.745 |  |  | 0.786 | 0.099 |
| *M,E* | 250.198 | 168.840 | 0.385 |  |  | 0.166 | 0.761 |
| *N,E* | 307.157 | 31.277 | -0.511 |  |  | 0.815 | 0.079 |
| *K,M,N* | 288.769 | -397.975 | 415.403 | 183.635 |  | 0.825 | 0.251 |
| *K,M,E* | 273.621 | 72.229 | 55.620 | -0.314 |  | 0.831 | 0.243 |
| *K,N,E* | 294.849 | 48.010 | 11.358 | -0.451 |  | 0.819 | 0.259 |
| *M,N,E* | 282.135 | 94.008 | 29.937 | -0.349 |  | 0.854 | 0.211 |
| *K,M,N,E* | 370.372 | -802.391 | 535.333 | 356.551 | -0.588 | 0.977 | 0.225 |
| Y2 |
| *K* | 379.351 | 28.895 |  |  |  | 0.398 | 0.129 |
| *M* | 415.873 | -124.617 |  |  |  | 0.268 | 0.234 |
| *N* | 384.916 | 12.222 |  |  |  | 0.471 | 0.089 |
| *E* | 379.131 | 0.278 |  |  |  | 0.287 | 0.215 |
| *K,M* | 398.304 | 24.081 | -88.336 |  |  | 0.522 | 0.229 |
| *K,N* | 424.896 | -186.579 | 84.305 |  |  | 0.680 | 0.103 |
| *K,E* | 376.264 | 22.118 | 0.130 |  |  | 0.158 | 0.315 |
| *M,N* | 399.884 | -72.301 | 10.193 |  |  | 0.548 | 0.204 |
| *M,E* | 397.919 | -75.898 | 0.185 |  |  | 0.354 | 0.417 |
| *N,E* | 382.270 | 10.453 | 7.880 |  |  | 0.484 | 0.266 |
| *K,M,N* | 436.429 | -368.745 | 132.843 | 158.411 |  | 0.741 | 0.205 |
| *K,M,E* | 397.034 | 23.298 | -84.520 | 1.899 |  | 0.044 | 0.472 |
| *K,N,E* | 458.156 | -299.326 | 133.949 | -0.271 |  | 0.760 | 0.184 |
| *M,N,E* | 400.555 | -73.974 | 10.364 | -9.684E-03 |  | 0.548 | 0.438 |
| *K,M,N,E* | 503.883 | -722.116 | 248.640 | 308.684 | -0.468 | 0.934 | 0.128 |

TABLE S-IV. Regression analysis data for Y1 and Y2 bands for ATA indicator

|  |
| --- |
| Y1 |
| Parameters | a0 | a1 | a2 | a3 | a4 | MCC | P |
| *K* | 277.052 | 58.079 |  |  |  | 0.767 | 0.022 |
| *M* | 307.047 | -23.663 |  |  |  | 0.004 | 0.901 |
| *N* | 289.746 | 21.932 |  |  |  | 0.727 | 0.031 |
| *E* | 290.565 | 0.251 |  |  |  | 0.107 | 0.528 |
| *K,M* | 263.341 | 61.247 | 64.127 |  |  | 0.797 | 0.092 |
| *K,N* | 256.988 | 153.074 | -37.076 |  |  | 0.792 | 0.095 |
| *K,E* | 284.264 | 75.332 | -0.310 |  |  | 0.862 | 0.051 |
| *M,N* | 268.593 | 101.924 | 24.627 |  |  | 0.797 | 0.091 |
| *M,E* | 265.345 | 96.912 | 0.389 |  |  | 0.148 | 0.787 |
| *N,E* | 303.739 | 31.646 | -0.412 |  |  | 0.873 | 0.045 |
| *K,M,N* | 267.393 | 13.901 | 93.369 | 19.042 |  | 0.797 | 0.288 |
| *K,M,E* | 290.157 | 76.514 | -23.026 | -0.352 |  | 0.864 | 0.196 |
| *K,N,E* | 306.314 | -10.043 | 35.813 | 4.000 |  | 0.873 | 0.184 |
| *M,N,E* | 298.825 | 18.463 | 31.383 | -0.380 |  | 0.874 | 0.182 |
| *K,M,N,E* | 333.112 | -311.794 | 189.954 | 158.299 | -0.473 | 0.892 | 0.475 |
| Y2 |
| *K* | 395.774 | -2.715 |  |  |  | 0.004 | 0.888 |
| *M* | 381.445 | 68.929 |  |  |  | 0.102 | 0.486 |
| *N* | 395.625 | -1.782 |  |  |  | 0.012 | 0.812 |
| *E* | 409.108 | -0.310 |  |  |  | 0.445 | 0.102 |
| *K,M* | 380.618 | 1.135 | 70.639 |  |  | 0.102 | 0.806 |
| *K,N* | 364.235 | 146.492 | -58.378 |  |  | 0.172 | 0.686 |
| *K,E* | 406.428 | 20.673 | -0.448 |  |  | 0.610 | 0.152 |
| *M,N* | 381.167 | 69.841 | 0.178 |  |  | 0.102 | 0.807 |
| *M,E* | 413.732 | -18.680 | -0.333 |  |  | 0.450 | 0.303 |
| *N,E* | 411.825 | 9.050 | -0.482 |  |  | 0.628 | 0.138 |
| *K,M,N* | 359.967 | 213.910 | -49.164 | -85.804 |  | 0.183 | 0.875 |
| *K,M,E* | 412.932 | 21.042 | -26.467 | -0.483 |  | 0.620 | 0.349 |
| *K,N,E* | 438.568 | -105.482 | 52.570 | -0.606 |  | 0.671 | 0.287 |
| *M,N,E* | 416.029 | -17.003 | 9.030 | -0.503 |  | 0.633 | 0.333 |
| *K,M,N,E* | 461.618 | -318.611 | 125.339 | 140.654 | -0.705 | 0.726 | 0.473 |

TABLE S-V. Regression analysis data for Y1 and Y2 bands for AYGG indicator

|  |
| --- |
| Y1 |
| Parameters | a0 | a1 | a2 | a3 | a4 | MCC | P |
| *K* | 262.225 | -0.893 |  |  |  | 0.000 | 0.969 |
| *M* | 232.235 | 154.026 |  |  |  | 0.444 | 0.149 |
| *N* | 262.764 | -1.600 |  |  |  | 0.009 | 0.856 |
| *E* | 270.978 | -0.192 |  |  |  | 0.149 | 0.449 |
| *K,M* | 227.077 | 7.227 | 164.386 |  |  | 0.470 | 0.386 |
| *K,N* | 207.004 | 260.556 | -102.042 |  |  | 0.463 | 0.394 |
| *K,E* | 269.581 | 16.704 | -0.316 |  |  | 0.238 | 0.665 |
| *M,N* | 227.773 | 168.598 | 2.857 |  |  | 0.469 | 0.387 |
| *M,E* | 226.827 | 169.662 | 5.045 |  |  | 0.449 | 0.409 |
| *N,E* | 273.380 | 5.769 | -0.313 |  |  | 0.210 | 0.702 |
| *K,M,N* | 218.124 | 111.824 | 99.783 | -42.069 |  | 0.476 | 0.672 |
| *K,M,E* | 229.644 | 8.689 | 156.042 | -3.368 |  | 0.471 | 0.676 |
| *K,N,E* | 204.243 | 269.686 | -106.121 | 2.378 |  | 0.463 | 0.685 |
| *M,N,E* | 230.533 | 160.977 | 3.474 | -3.474 |  | 0.471 | 0.677 |
| *K,M,N,E* | 218.371 | 110.600 | 100.146 | -41.545 | -1.780 | 0.476 | 0.896 |
| Y2 |
| *K* | 374.040 | -39.781 |  |  |  | 0.159 | 0.376 |
| *M* | 388.693 | -169.431 |  |  |  | 0.104 | 0.481 |
| *N* | 364.214 | -13.167 |  |  |  | 0.115 | 0.457 |
| *E* | 360.080 | -7.793 |  |  |  | 0.005 | 0.883 |
| *K,M* | 427.655 | -53.400 | -249.885 |  |  | 0.366 | 0.402 |
| *K,N* | 468.745 | -487.830 | 175.300 |  |  | 0.414 | 0.343 |
| *K,E* | 367.186 | -54.827 | 0.288 |  |  | 0.201 | 0.639 |
| *M,N* | 421.536 | -276.889 | -20.937 |  |  | 0.353 | 0.419 |
| *M,E* | 429.300 | -279.617 | -0.419 |  |  | 0.197 | 0.645 |
| *N,E* | 354.093 | -19.934 | 0.301 |  |  | 0.156 | 0.713 |
| *K,M,N* | 466.733 | -456.053 | -23.173 | 162.373 |  | 0.415 | 0.608 |
| *K,M,E* | 431.245 | -260.674 | -51.188 | -5.367 |  | 0.367 | 0.667 |
| *K,N,E* | 532.935 | -705.420 | 271.109 | -0.523 |  | 0.477 | 0.529 |
| *M,N,E* | 424.142 | -283.381 | -20.275 | -3.759 |  | 0.353 | 0.684 |
| *K,M,N,E* | 557.250 | -930.240 | 132.215 | 364.024 | -0.628 | 0.488 | 0.762 |

TABLE S-VI. Regression analysis data for Y1 and Y2 bands for EBT indicator

|  |
| --- |
| Y1 |
| Parameters | a0 | a1 | a2 | a3 | a4 | MCC | P |
| *K* | 292.604 | -24.960 |  |  |  | 0.277 | 0.283 |
| *M* | 277.336 | 22.536 |  |  |  | 0.008 | 0.868 |
| *N* | 287.216 | -9.543 |  |  |  | 0.269 | 0.291 |
| *E* | 293.709 | -0.253 |  |  |  | 0.213 | 0.357 |
| *K,M* | 295.651 | -25.664 | -14.251 |  |  | 0.280 | 0.611 |
| *K,N* | 296.073 | -41.386 | 6.411 |  |  | 0.279 | 0.612 |
| *K,E* | 295.264 | -18.596 | -0.114 |  |  | 0.303 | 0.582 |
| *M,N* | 293.484 | -30.201 | -10.342 |  |  | 0.282 | 0.609 |
| *M,E* | 319.778 | -100.179 | -0.396 |  |  | 0.298 | 0.588 |
| *N,E* | 290.760 | -7.083 | -0.104 |  |  | 0.288 | 0.601 |
| *K,M,N* | 289.698 | 43.877 | -57.202 | -27.970 |  | 0.282 | 0.850 |
| *K,M,E* | 315.035 | -14.628 | -77.250 | -0.254 |  | 0.350 | 0.793 |
| *K,N,E* | 330.868 | -156.449 | 57.827 | -0.300 |  | 0.358 | 0.786 |
| *M,N,E* | 313.523 | -85.523 | -5.863 | -0.252 |  | 0.358 | 0.795 |
| *K,M,N,E* | 331.456 | -163.070 | 4.168 | 60.514 | -0.301 | 0.358 | 0.945 |
| Y2 |
| *K* | 406.647 | -16.443 |  |  |  | 0.254 | 0.308 |
| *M* | 398.778 | 3.728 |  |  |  | 0.000 | 0.970 |
| *N* | 403.180 | -6.528 |  |  |  | 0.254 | 0.308 |
| *E* | 425.142 | -0.581 |  |  |  | 0.789 | 0.018 |
| *K,M* | 410.305 | -17.088 | -17.440 |  |  | 0.262 | 0.634 |
| *K,N* | 404.526 | -6.353 | -4.017 |  |  | 0.254 | 0.644 |
| *K,E* | 428.191 | 12.975 | -0.778 |  |  | 0.857 | 0.054 |
| *M,N* | 408.474 | -25.851 | -7.038 |  |  | 0.271 | 0.622 |
| *M,E* | 441.902 | -67.092 | -0.666 |  |  | 0.898 | 0.032 |
| *N,E* | 432.249 | 6.086 | -0.819 |  |  | 0.877 | 0.043 |
| *K,M,N* | 387.182 | 181.010 | -109.178 | -80.219 |  | 0.319 | 0.820 |
| *K,M,E* | 447.011 | 14.899 | -73.530 | -0.900 |  | 0.986 | 0.021 |
| *K,N,E* | 458.665 | -109.310 | 50.698 | -0.911 |  | 0.951 | 0.072 |
| *M,N,E* | 448.921 | -66.859 | 6.059 | -0.903 |  | 0.985 | 0.022 |
| *K,M,N,E* | 444.832 | 31.449 | -80.942 | -6.781 | -0.895 | 0.986 | 0.174 |

TABLE S-VII. Regression analysis data for Y1 and Y2 bands for TY indicator

|  |
| --- |
| Y1 |
| Parameters | a0 | a1 | a2 | a3 | a4 | MCC | P |
| *K* | 441.698 | -249.581 |  |  |  | 0.423 | 0.235 |
| *M* | 315.416 | 32.548 |  |  |  | 0.054 | 0.708 |
| *N* | 352.286 | -44.369 |  |  |  | 0.402 | 0.251 |
| *E* | 322.126 | -1.052 |  |  |  | 0.001 | 0.964 |
| *K,M* | 437.571 | -256.181 | 38.442 |  |  | 0.497 | 0.503 |
| *K,N* | 416.697 | -160.021 | -26.165 |  |  | 0.508 | 0.492 |
| *K,E* | 457.720 | -293.802 | 0.105 |  |  | 0.489 | 0.511 |
| *M,N* | 385.178 | -73.920 | -71.621 |  |  | 0.527 | 0.473 |
| *M,E* | 307.423 | 53.033 | 8.209 |  |  | 0.081 | 0.919 |
| *N,E* | 374.626 | -108.172 | 0.436 |  |  | 0.946 | 0.054 |
| *K,M,N* | -1108.976 | 7002.622 | -3050.621 | -1965.685 |  | 0.920 | 0.356 |
| *K,M,E* | 491.609 | -458.300 | 151.594 | 0.435 |  | 0.993 | 0.109 |
| *K,N,E* | 415.892 | -105.074 | -93.282 | 0.416 |  | 0.991 | 0.120 |
| *M,N,E* | 393.261 | -44.800 | -120.976 | 0.411 |  | 0.991 | 0.123 |
| Y2 |
| *K* | 280.821 | 266.019 |  |  |  | 0.094 | 0.555 |
| *M* | 355.899 | 278.413 |  |  |  | 0.558 | 0.088 |
| *N* | 437.009 | -41.882 |  |  |  | 0.058 | 0.645 |
| *E* | 403.565 | 9.798 |  |  |  | 0.011 | 0.841 |
| *K,M* | 280.611 | 161.641 | 266.772 |  |  | 0.591 | 0.261 |
| *K,N* | 125.796 | 811.188 | -155.246 |  |  | 0.502 | 0.351 |
| *K,E* | 266.602 | 303.183 | -7.385 |  |  | 0.098 | 0.856 |
| *M,N* | 311.567 | 338.076 | 48.338 |  |  | 0.610 | 0.244 |
| *M,E* | 303.972 | 399.963 | 0.597 |  |  | 0.870 | 0.047 |
| *N,E* | 483.512 | -168.709 | 0.829 |  |  | 0.331 | 0.548 |
| *K,M,N* | 670.455 | -1444.981 | 864.913 | 390.868 |  | 0.679 | 0.441 |
| *K,M,E* | 465.715 | -415.608 | 504.412 | 0.962 |  | 0.975 | 0.038 |
| *K,N,E* | 153.963 | 873.589 | -306.078 | 0.929 |  | 0.841 | 0.229 |
| *M,N,E* | 355.892 | 358.552 | -87.805 | 0.925 |  | 0.947 | 0.079 |
| *K,M,N,E* | 670.285 | -1269.805 | 821.065 | 216.230 | 0.905 | 1.000 | 0.011 |