Electronic Supplementary Material (ESI) for CrystEngComm.


**Electronic Supplementary Information**

# Relationship Between Crystal Structures and Photochromic Properties of *N*-Salicylideneaminopyridine Derivatives

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Table S1 The difference of pKa (conjugate acid of base) and pKa (acid).

| Compound name | pKa | ΔpKa |
|---|---|---|
| SAP2 | 5.63 | |
| 4-Chlorobenzoic acid (c) | 3.97 | 1.66 |
| SAP3 | 5.63 | |
| Benzoic acid (a) | 4.25 | 1.43 |
| 2-Hydroxybenzoic acid (b) | 3.01 | 2.62 |
| 4-Chlorobenzoic acid (c) | 3.97 | 1.66 |
| 3,5-Dihydroxybenzoic acid (d) | 3.96 | 1.67 |
| 3,4-Dihydroxybenzoic acid (e) | 4.45 | 1.18 |
| 3,5-Dichlorobenzoic acid (f) | 3.46 | 2.17 |
| SAP12 | 5.43 | |
| 3,5-Dinitrobenzoic acid (g) | 2.77 | 2.68 |

The pKa values were calculated by Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02

Table S2 Crystal data and experimental details.

| Identification code | SAP4 | SAP5_III | SAP7 | SAP9 |
|---|---|---|---|---|
| Chemical formula | $C_{13}H_{12}N_2O$ | $C_{13}H_{12}N_2O_2$ | $C_{14}H_{14}N_2O_2$ | $C_{12}H_{10}N_2O_2$ |
| Formula weight | 212.25 | 228.25 | 242.27 | 214.22 |
| Temp/K | 173(2) | 293(2) | 293(2) | 293(2) |
| wavelength/Å | 0.71075 | 1.54186 | 0.71075 | 1.54186 |
| cryst syst | Monoclinic | Triclinic | Orthorhombic | Monoclinic |
| space group | $P2_1/n$ | $P$-1 | $Fdd2$ | $P2_1/c$ |
| $a$ / Å | 14.5415(18) | 6.1596(4) | 41.659(5) | 13.1386(3) |
| $b$ / Å | 5.0163(6) | 7.4634(4) | 24.658(3) | 7.1572(2) |
| $c$ / Å | 14.8807(18) | 12.7106(6) | 4.8420(6) | 11.8627(2) |
| $\alpha$ / deg | 90 | 77.175(3) | 90 | 90 |
| $\beta$ / deg | 100.551(2) | 81.457(3) | 90 | 116.8000(10) |
| $\gamma$ / deg | 90 | 78.821(3) | 90 | 90. |
| Vol / Å$^3$ | 1067.1(2) | 555.53(5) | 4973.8(10) | 995.69(4) |
| $Z$ | 4 | 2 | 16 | 4 |
| calcd density / g·cm$^{-3}$ | 1.321 | 1.365 | 1.294 | 1.429 |
| abs coeff / mm$^{-1}$ | 0.086 | 0.767 | 0.088 | 0.819 |
| $F$(000) | 448 | 240 | 2048 | 448 |
| cryst size / mm$^3$ | 0.316 × 0.221 × 0.216 | 0.140 × 0.110 × 0.050 | 0.210 × 0.080 × 0.080 | 0.130 × 0.050 × 0.030 |
| $\theta$ range for data collection | 3.602 to 27.475° | 3.588 to 68.211° | 3.305 to 27.476° | 3.769 to 68.198° |
| index ranges | $-18 \le h \le 18$ | $-7 \le h \le 7$ | $-53 \le h \le 54$ | $-15 \le h \le 15$ |
| | $-6 \le k \le 6$ | $-8 \le k \le 8$ | $-31 \le k \le 32$ | $-8 \le k \le 8$ |
| | $-19 \le l \le 19$ | $-14 \le l \le 15$ | $-6 \le l \le 6$ | $-14 \le l \le 14$ |
| reflns collected | 10577 | 6023 | 12219 | 6505 |
| indep reflns | 2453 | 1988 | 2798 | 1762 |
| $R_{int}$ | 0.0328 | 0.0657 | 0.0680 | 0.0405 |
| completeness to $\theta$ | 99.8 % | 98.1 % | 99.8 % | 97.4 % |
| abs correction | Semi-empirical from equivalents | | | |
| max and min transm | 0.982 and 0.821 | 0.962 and 0.721 | 0.993 and 0.411 | 0.976 and 0.774 |
| refinement meth | Full-matrix least-squares on $F^2$ | | | |
| data / restraints / params | 2453 / 0 / 147 | 1988 / 0 / 156 | 2798 / 1 / 169 | 1762 / 0 / 151 |
| goodness-of-fit on $F^2$ | 1.043 | 1.062 | 1.007 | 1.086 |
| final $R$ indices [$I > 2\sigma(I)$] | $R_1 = 0.0426$ | $R_1 = 0.0618$ | $R_1 = 0.0474$ | $R_1 = 0.0399$ |
| | $wR_2 = 0.1112$ | $wR_2 = 0.1638$ | $wR_2 = 0.1018$ | $wR_2 = 0.1143$ |
| $R$ indices (all data) | $R_1 = 0.0543$ | $R_1 = 0.0807$ | $R_1 = 0.0767$ | $R_1 = 0.0435$ |
| | $wR_2 = 0.1185$ | $wR_2 = 0.1998$ | $wR_2 = 0.1202$ | $wR_2 = 0.1191$ |
| largest diff peak, hole, | 0.176 and -0.187 | 0.240 and -0.345 | 0.260 and -0.197 | 0.192 and -0.212 |
| CCDC number | 1814043 | 1814047 | 1814048 | 1814049 |

| Identification code | SAP10 | SAP11 | SAP12 |
|---|---|---|---|
| Chemical formula | $C_{20}$ $H_{26}$ $N_2$ O | $C_{12}$ $H_8$ $Cl_2$ $N_2$ O | $C_{12}$ $H_8$ $Br_2$ $N_2$ O |
| Formula weight | 310.43 | 267.10 | 356.02 |
| Temp/K | 297(2) | 293(2) | 293(2) |
| wavelength/Å | 0.71075 | 1.54186 | 1.54186 |
| cryst syst | Monoclinic | Monoclinic | Monoclinic |
| space group | $P2_1$ | $C\,2/c$ | $P2_1/n$ |
| $a$ / Å | 6.1462(6) | 26.1636(6) | 14.6532(3) |
| $b$ / Å | 18.7572(19) | 3.80910(10) | 4.52630(10) |
| $c$ / Å | 16.1025(16) | 34.4455(6) | 18.6301(4) |
| $\alpha$ / deg | 90 | 90 | 90 |
| $\beta$ / deg | 95.859(2) | 137.464(1) | 92.499(2) |
| $\gamma$ / deg | 90 | 90 | 90 |
| Vol / Å$^3$ | 1846.7(3) | 2320.77(10) | 1234.46(5) |
| $Z$ | 4 | 8 | 4 |
| calcd density / g·cm$^{-3}$ | 1.117 | 1.529 | 1.916 |
| abs coeff / mm$^{-1}$ | 0.069 | 4.900 | 8.209 |
| $F$(000) | 672 | 1088 | 688 |
| cryst size / mm$^3$ | 0.150 × 0.120 × 0.060 | 0.190 × 0.150 × 0.050 | 0.138 × 0.092 × 0.088 |
| $\theta$ range for data collection | 3.332 to 27.480° | 3.380 to 68.135° | 3.759 to 68.215° |
| index ranges | $-6 \le h \le 7$ | $-29 \le h \le 30$ | $-17 \le h \le 17$ |
| | $-24 \le k \le 24$ | $-4 \le k \le 4$ | $-5 \le k \le 5$ |
| | $-20 \le l \le 20$ | $-41 \le l \le 41$ | $-22 \le l \le 22$ |
| reflns collected | 17821 | 11218 | 12010 |
| indep reflns | 8298 | 2131 | 2256 |
| $R_{int}$ | 0.0566 | 0.0959 | 0.0865 |
| completeness to $\theta$ | 99.7 % | 99.9 % | 99.8 % |
| abs correction | Semi-empirical from equivalents | | |
| max and min transm | 0.996 and 0.196 | 0.783 and 0.513 | 0.532 and 0.336 |
| refinement meth | Full-matrix least-squares on $F^2$ | | |
| data / restraints / params | 8298 / 181 / 491 | 2131 / 0 / 154 | 2256 / 0 / 155 |
| goodness-of-fit on $F^2$ | 1.030 | 1.097 | 1.038 |
| final $R$ indices [$I > 2\sigma(I)$] | $R_1 = 0.0686$ | $R_1 = 0.0455$ | $R_1 = 0.0384$ |
| | $wR_2 = 0.1397$ | $wR_2 = 0.1208$ | $wR_2 = 0.0988$ |
| $R$ indices (all data) | $R_1 = 0.1515$ | $R_1 = 0.0603$ | $R_1 = 0.0471$ |
| | $wR_2 = 0.1736$ | $wR_2 = 0.1312$ | $wR_2 = 0.1027$ |
| largest diff peak, hole, | 0.179 and -0.205 | 0.401 and -0.275 | 0.621 and -0.417 |
| CCDC number | 1814050 | 1814051 | 1814052 |

| Identification code | MSAP1 | MSAP2 | MSAP3 |
|---|---|---|---|
| Chemical formula | $C_{17}H_{20}N_2O$ | $C_{13}H_{11}ClN_2O$ | $C_{13}H_{11}BrN_2O$ |
| Formula weight | 268.35 | 246.69 | 291.15 |
| Temp/K | 293(2) | 293(2) | 566(2) |
| wavelength/Å | 0.71075 | 0.71075 | 0.71075 |
| cryst syst | Orthorhombic | Triclinic | Triclinic |
| space group | $P2_12_12_1$ | $P$-1 | $P$-1 |
| $a$ / Å | 6.0801(5) | 5.8388(13) | 5.8531(9) |
| $b$ / Å | 15.1860(13) | 7.4762(17) | 7.5224(12) |
| $c$ / Å | 16.4018(14) | 13.369(3) | 13.598(2) |
| $\alpha$ / deg | 90 | 93.793(7) | 94.526(7) |
| $\beta$ / deg | 90 | 93.656(7) | 93.369(7) |
| $\gamma$ / deg | 90. | 99.044(7) | 99.310(7) |
| Vol / Å$^3$ | 1514.4(2) | 573.4(2) | 587.41(16) |
| $Z$ | 4 | 2 | 2 |
| calcd density / g·cm$^{-3}$ | 1.177 | 1.429 | 1.646 |
| abs coeff / mm$^{-1}$ | 0.074 | 0.316 | 3.482 |
| $F$(000) | 576 | 256 | 292 |
| cryst size / mm$^3$ | 0.335 x 0.234 x 0.187 | 0.235 x 0.235 x 0.187 | 0.290 x 0.200 x 0.140 |
| $\theta$ range for data collection | 3.574 to 27.483°. | 3.058 to 27.482°. | 3.014 to 27.478° |
| index ranges | $-7 \le h \le 7$ | $-7 \le h \le 7$ | $-7 \le h \le 7$ |
| | $-19 \le k \le 19$ | $-9 \le k \le 9$ | $-9 \le k \le 9$ |
| | $-21 \le l \le 21$ | $-17 \le l \le 17$ | $-17 \le l \le 17$ |
| reflns collected | 16034 | 6067 | 6173 |
| indep reflns | 3465 | 2634 | 2698 |
| $R_{int}$ | 0.0364 | 0.0164 | 0.0350 |
| completeness to $\theta$ | 99.7 % | 99.9 % | 99.9 % |
| abs correction | Semi-empirical from equivalents | | |
| max and min transm | 0.986 and 0.793 | 0.943 and 0.830 | 0.641 and 0.331 |
| refinement meth | Full-matrix least-squares on $F^2$ | | |
| data / restraints / params | 3465 / 0 / 186 | 2634 / 0 / 156 | 2698 / 0 / 156 |
| goodness-of-fit on $F^2$ | 1.052 | 1.055 | 1.011 |
| final $R$ indices [$I > 2\sigma(I)$] | $R_1 = 0.0473$ | $R_1 = 0.0418$ | $R_1 = 0.0341$ |
| | $wR_2 = 0.1150$ | $wR_2 = 0.1126$ | $wR_2 = 0.0766$ |
| $R$ indices (all data) | $R_1 = 0.0573$ | $R_1 = 0.0518$ | $R_1 = 0.0496$ |
| | $wR_2 = 0.1221$ | $wR_2 = 0.1196$ | $wR_2 = 0.0825$ |
| largest diff peak, hole, | 0.183 and -0.260 | 0.168 and -0.303 | 0.324 and -0.473 |
| CCDC number | 1814053 | 1814054 | 1814055 |

| Identification code | 3a | 3b | 3c | 3d |
|---|---|---|---|---|
| Chemical formula | $C_{19}H_{15}BrN_2O_3$ | $C_{19}H_{15}BrN_2O_4$ | $C_{19}H_{14}BrClN_2O_3$ | $C_{19}H_{15}BrN_2O_5$ |
| Formula weight | 399.24 | 415.24 | 433.68 | 431.24 |
| Temp/K | 173(2) | 173(2) | 296(2) | 298(2) |
| wavelength/Å | 1.54186 | 1.54186 | 0.71075 | 0.71075 |
| cryst syst | Monoclinic | Monoclinic | Monoclinic | Triclinic |
| space group | *C*2/*c* | $P2_1/c$ | *C*2/*c* | *P*-1 |
| *a* / Å | 32.6081(14) | 3.82640(10) | 33.0322(16) | 8.5222(14) |
| *b* / Å | 6.1424(3) | 20.7111(7) | 6.2046(3) | 10.9876(18) |
| *c* / Å | 17.8481(8) | 21.2587(8) | 18.5200(8) | 11.5925(19) |
| *α* / deg | 90 | 90 | 90 | 106.506(6). |
| *β* / deg | 106.922(3) | 93.890(2) | 109.2160(10) | 103.783(4). |
| *γ* / deg | 90 | 90 | 90 | 112.254(10). |
| Vol / Å$^3$ | 3420.0(3) | 1680.85(10) | 3584.2(3) | 878.2(3) |
| *Z* | 8 | 4 | 8 | 2 |
| calcd density / g·cm$^{-3}$ | 1.551 | 1.641 | 1.607 | 1.631 |
| abs coeff / mm$^{-1}$ | 3.456 | 3.589 | 2.465 | 2.375 |
| *F*(000) | 1616 | 840 | 1744 | 436 |
| cryst size / mm$^3$ | 0.196 x 0.176 x 0.030 | 0.109 x 0.035 x 0.032 | 0.170 x 0.150 x 0.090 | 0.070 × 0.050 × 0.030 |
| *θ* range for data collection | 5.131 to 68.264° | 2.982 to 68.235° | 3.023 to 27.426° | 3.184 to 27.431° |
| index ranges | $-38 \le h \le 38$ | $-4 \le h \le 4$ | $-4\ 2 \le h \le 42$ | $-11 \le h \le 11$ |
| | $-7 \le k \le 7$ | $-24 \le k \le 24$ | $-6 \le k \le 8$ | $-14 \le k \le 14$ |
| | $-21 \le l \le 21$ | $-25 \le l \le 25$ | $-23 \le l \le 23$ | $-14 \le l \le 14$ |
| reflns collected | 18693 | 15638 | 16182 | 8609 |
| indep reflns | 3128 | 3090 | 4063 | 3953 |
| $R_{int}$ | 0.0651 | 0.0542 | 0.0365 | 0.0758 |
| completeness to *θ* | 99.8 % | 99.9 % | 99.8 % | 99.7 % |
| abs correction | Semi-empirical from equivalents | | | |
| max and min transm | 0.903 and 0.687 | 0.894 and 0.773 | 0.801 and 0.475 | 0.931 and 0.455 |
| refinement meth | Full-matrix least-squares on $F^2$ | | | |
| data / restraints / params | 3128 / 0 / 232 | 3090 / 0 / 242 | 4063 / 0 / 237 | 3953 / 0 / 250 |
| goodness-of-fit on $F^2$ | 1.072 | 1.101 | 1.093 | 0.963 |
| final *R* indices [$I > 2\sigma(I)$] | $R_1 = 0.0416$ | $R_1 = 0.0312$ | $R_1 = 0.0452$ | $R_1 = 0.0643$ |
| | $wR_2 = 0.1075$ | $wR_2 = 0.0809$ | $wR_2 = 0.1144$ | $wR_2 = 0.1234$ |
| *R* indices (all data) | $R_1 = 0.0499$ | $R_1 = 0.0337$ | $R_1 = 0.0691$ | $R_1 = 0.1663$ |
| | $wR_2 = 0.1145$ | $wR_2 = 0.0834$ | $wR_2 = 0.1468$ | $wR_2 = 0.1605$ |
| largest diff peak, hole, | 0.718 and -0.504 | 0.482 and -0.263 | 0.387 and -0.797 | 0.367 and -0.465 |
| CCDC number | 1814057 | 1814058 | 1814059 | 1814060 |

| Identification code | 3e | 3f | 2c | 12g |
|---|---|---|---|---|
| Chemical formula | $C_{50}H_{39}Br_3N_6O_{11}$ | $C_{19}H_{13}BrCl_2N_2O_3$ | $C_{19}H_{14}Cl_2N_2O_3$ | $C_{19}H_{12}Br_2N_4O_7$ |
| Formula weight | 1139.60 | 468.12 | 389.22 | 568.15 |
| Temp/K | 296(2) | 293(2) | 296(2) | 296(2) |
| wavelength/Å | 1.54186 | 1.54186 | 0.71075 | 0.71075 |
| cryst syst | Triclinic | Monoclinic | Monoclinic | Monoclinic |
| space group | *P*1 | *C*2/*c* | *C*2/*c* | *C*2 |
| *a* / Å | 8.2123(2) | 34.7332(18) | 32.818(8) | 37.206(3) |
| *b* / Å | 12.3360(2) | 3.8928(2) | 6.2380(15) | 7.3594(6) |
| *c* / Å | 13.0008(2) | 28.2337(15) | 18.465(5) | 7.5694(6) |
| *α* / deg | 65.6550(10) | 90 | 90 | 90 |
| *β* / deg | 78.6480(10) | 99.982(2) | 109.440(4) | 91.589(2) |
| *γ* / deg | 83.5680(10) | 90 | 90 | 90 |
| Vol / Å$^3$ | 1175.78(4) | 3759.7(3) | 3564.7(15) | 2071.8(3) |
| *Z* | 1 | 8 | 8 | 4 |
| calcd density / g·cm$^{-3}$ | 1.609 | 1.654 | 1.450 | 1.821 |
| abs coeff / mm$^{-1}$ | 3.768 | 5.799 | 0.386 | 3.964 |
| *F*(000) | 574 | 1872 | 1600 | 1120 |
| cryst size / mm$^3$ | 0.100 × 0.040 × 0.040 | 0.140 × 0.030 × 0.020 | 0.090 × 0.060 × 0.050 | 0.110 × 0.100 × 0.020 |
| *θ* range for data collection | 3.785 to 68.250° | 3.179 to 68.250° | 3.043 to 27.367° | 3.219 to 27.415° |
| index ranges | $-9 \le h \le 9$ | $-33 \le h \le 33$ | $-42 \le h \le 42$ | $-48 \le h \le 47$ |
| | $-14 \le k \le 14$ | $-4 \le k \le 4$ | $-8 \le k \le 6$ | $-9 \le k \le 9$ |
| | $-15 \le l \le 15$ | $-33 \le l \le 33$ | $-23 \le l \le 23$ | $-9 \le l \le 9$ |
| reflns collected | 13821 | 19294 | 16488 | 10066 |
| indep reflns | 7248 | 3386 | 4021 | 4666 |
| $R_{int}$ | 0.0299 | 0.1032 | 0.0458 | 0.0663 |
| completeness to *θ* | 98.4 % | 99.7 % | 99.8 % | 99.7 % |
| abs correction | Semi-empirical from equivalents | | | |
| max and min transm | 0.860 and 0.733 | 0.893 and 0.578 | 0.981 and 0.603 | 0.925 and 0.52 |
| refinement meth | Full-matrix least-squares on $F^2$ | | | |
| data / restraints / params | 7248 / 3 / 640 | 3386 / 0 / 246 | 4021 / 0 / 237 | 4666 / 1 / 291 |
| goodness-of-fit on $F^2$ | 1.123 | 1.194 | 1.055 | 1.082 |
| final *R* indices [$I > 2\sigma(I)$] | $R_1 = 0.0464$ | $R_1 = 0.0982$ | $R_1 = 0.0456$ | $R_1 = 0.0473$ |
| | $wR_2 = 0.1011$ | $wR_2 = 0.2357$ | $wR_2 = 0.1141$ | $wR_2 = 0.1044$ |
| *R* indices (all data) | $R_1 = 0.0650$ | $R_1 = 0.1411$ | $R_1 = 0.0810$ | $R_1 = 0.0967$ |
| | $wR_2 = 0.1303$ | $wR_2 = 0.2972$ | $wR_2 = 0.1481$ | $wR_2 = 0.1427$ |
| largest diff peak, hole, | 0.575 and -0.338 | 0.937 and -0.945 | 0.273 and -0.244 | 0.682 and -0.402 |
| CCDC number | 1814061 | 1814062 | 1814063 | 1814064 |

| Identification code | 3h | 3i | 3j |
|---|---|---|---|
| Chemical formula | $C_{15}$ $H_{11}$ Br I $N_2$ O | $C_{18}$ $H_{13}$ Br I $N_2$ O | $C_{15}$ $H_{11}$ Br I $N_2$ O |
| Formula weight | 442.07 | 480.11 | 442.07 |
| Temp/K | 173(2) | 93(2) | 93(2) |
| wavelength/Å | 1.54186 | 0.71075 | 0.6998 |
| cryst syst | Monoclinic | Monoclinic | Orthorhombic |
| space group | $P2_1/c$ | $P2_1/c$ | *Pnma* |
| *a* / Å | 33.7985(6) | 37.851(2) | 6.1651(12) |
| *b* / Å | 6.91740(10) | 6.9901(4) | 66.924(13) |
| *c* / Å | 6.17460(10) | 6.168(3) | 6.8330(13) |
| $\alpha$ / deg | 90 | 90 | 90 |
| $\beta$ / deg | 92.7900(10) | 90.041(2) | 90 |
| $\gamma$ / deg | 90 | 90 | 90 |
| Vol / Å$^3$ | 1441.90(4) | 1631.9(8) | 2819.2(9) |
| *Z* | 4 | 4 | 8 |
| calcd density / g·cm$^{-3}$ | 2.036 | 1.954 | 2.083 |
| abs coeff / mm$^{-1}$ | 20.669 | 4.416 | 4.878 |
| *F*(000) | 844 | 924 | 1688 |
| cryst size / mm$^3$ | 0.040 × 0.040 × 0.020 | 0.040 × 0.040 × 0.020 | 0.120 × 0.100 × 0.030 |
| $\theta$ range for data collection | 3.928 to 68.224°. | 3.107 to 25.350°. | 1.198 to 27.026°. |
| index ranges | $-40 \le h \le 40$, , | $-45 \le h \le 45$ | $-8 \le h \le 8$ |
| | $-8 \le k \le 8$ | $-8 \le k \le 8$ | $-83 \le k \le 83$ |
| | $-7 \le l \le 6$ | $-7 \le l \le 7$ | $-8 \le l \le 8$ |
| reflns collected | 12885 | 12155 | 16830 |
| indep reflns | 2584 | 2976 | 3207 |
| $R_{int}$ | 0.0570 | 0.0837 | 0.0634 |
| completeness to $\theta$ | 98.0 % | 99.5 % | 99.6 % |
| abs correction | Semi-empirical from equivalents | | |
| max and min transm | 0.683 and 0.536 | 0.917 and 0.433 | 0.867 and 0.419 |
| refinement meth | Full-matrix least-squares on $F^2$ | | |
| data / restraints / params | 2584 / 0 / 181 | 2976 / 0 / 208 | 3207 / 0 / 185 |
| goodness-of-fit on $F^2$ | 1.094 | 1.050 | 1.060 |
| final *R* indices [$I > 2\sigma(I)$] | $R_1 = 0.0316$ | $R_1 = 0.0377$ | $R_1 = 0.0294$ |
| | $wR_2 = 0.0757$ | $wR_2 = 0.0813$ | $wR_2 = 0.0768$ |
| *R* indices (all data) | $R_1 = 0.0340$ | $R_1 = 0.0417$ | $R_1 = 0.0339$ |
| | $wR_2 = 0.0786$ | $wR_2 = 0.0838$ | $wR_2 = 0.0797$ |
| largest diff peak, hole, | 2.339 and -0.481 | 1.491 and -0.784 | 1.047 and -1.626 |
| CCDC number | 1814065 | 1814066 | 1814067 |

Table S3 Structure number and compound name or refcode

| Structure | Name / CSD REFCODE | Reference |
|---|---|---|
| 1 | SAP1 / SLCPYA | 38 |
| 2 | SAP2 / QOXVOP | 38 |
| 3 | SAP3 / SOPFAG | 21 |
| 4 | SAP4 | |
| 5 | SAP5_I / SLCPYB | 39 |
| 6 | SAP5_II / EDEQAG01 | 24 |
| 7 | SAP5_III | |
| 8 | SAP6 | |
| 9 | SAP7 | |
| 10 | SAP8 | |
| 11 | SAP9 | |
| 12 | SAP10 | |
| 13 | SAP11 | |
| 14 | SAP12 | |
| 15 | MSAP1 | |
| 16 | MSAP2 | |
| 17 | MSAP3 | |
| 19 | 3a | |
| 20 | 3b | |
| 21 | 3c | |
| 22 | 3d | |
| 23 | 3e | |
| 24 | 3f | |
| 25 | 2c | |
| 26 | 12g | |
| 27 | 3h | |
| 28 | 3i | |
| 29 | 3j | |

| Structure | Name / CSD REFCODE | Reference |
|---|---|---|
| 31 | KIPTOU | 22 |
| 32 | RUDLOT | 22 |
| 33 | RUDMAG | 22 |
| 34 | RUDMEK | 22 |
| 35 | RUDMIO | 22 |
| 36 | RUDLIN | 22 |
| 38 | CHLSAN01 | 18 |
| 39 | FAXWIM | 18 |
| 40 | FAXWOS | 18 |
| 41 | FAXWUY | 18 |
| 42 | FAXXAF | 18 |
| 43 | FAXXIN | 18 |
| 44 | FAXXUZ | 18 |
| 45 | IVOHIL01 | 18 |
| 47 | NEZXAT | 19 |
| 48 | NEZXEX | 19 |
| 49 | NEZWIB | 19 |
| 50 | NEZXOH | 19 |
| 51 | NEZXUN | 19 |
| 52 | NEZYAU | 19 |
| 53 | WIGFOJ | 19 |
| 54 | WIGFUP | 19 |
| 55 | WIGGAW | 19 |
| 56 | WIGGEA | 19 |
| 57 | WIGGIE | 19 |
| 59 | BSALAP | 21 |
| 60 | UNICUR | 21 |

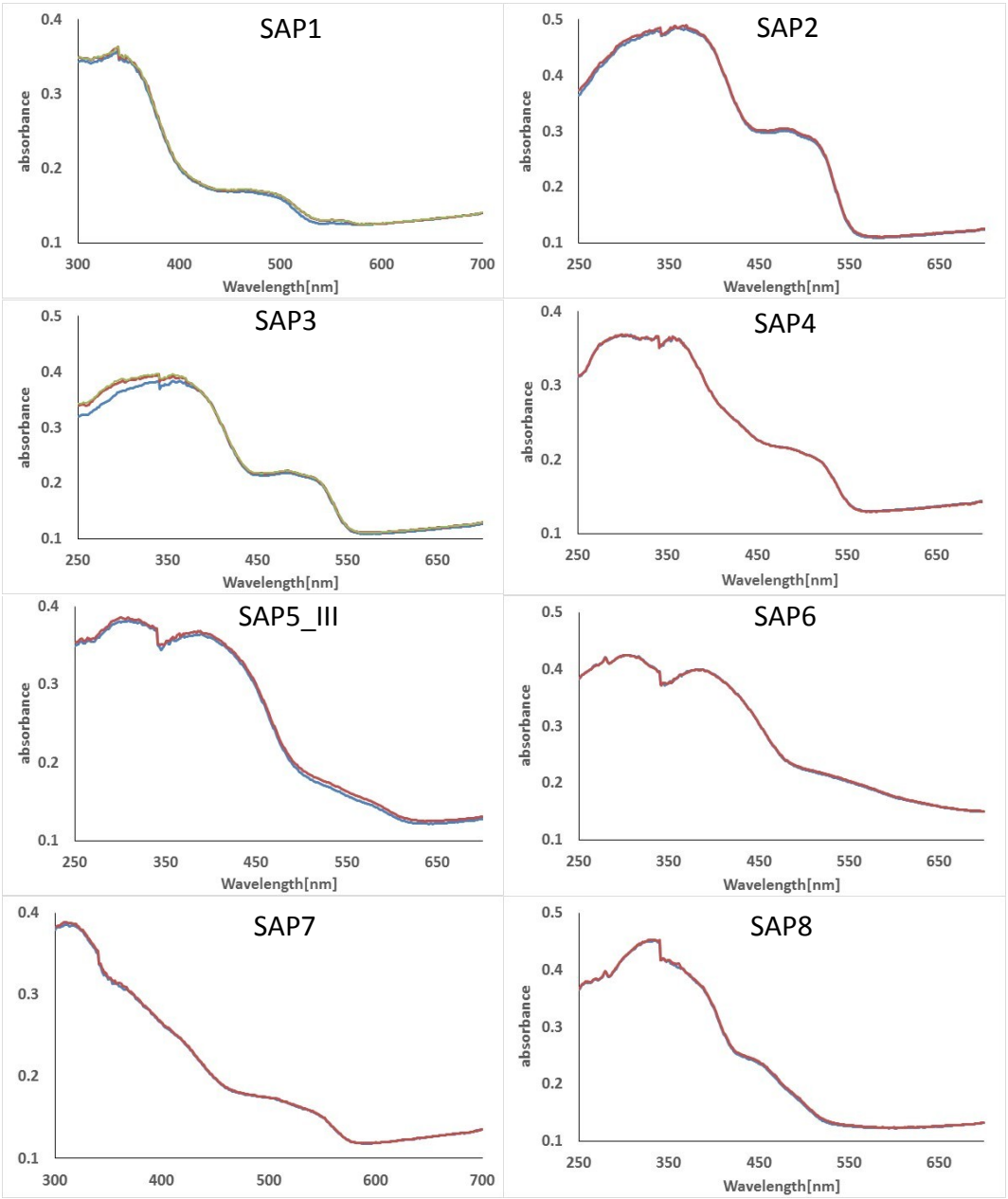


Figure S1: UV-Vis. spectra [before (blue line) and after (red line) UV irradiation, and after visible light exposure to colored sample (green line)] of SAP derivatives, SAP1-SAP8.

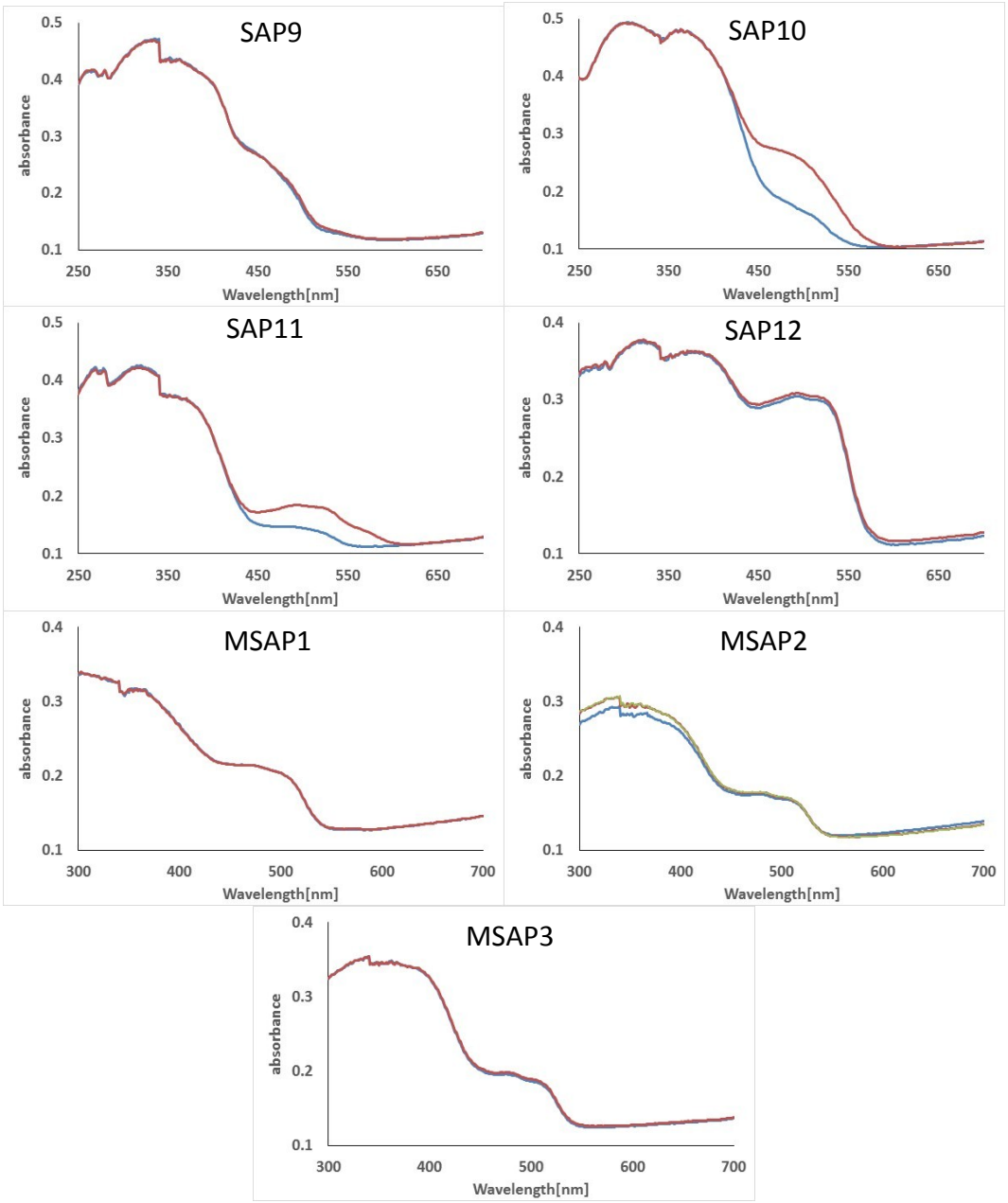


Figure S2: UV-Vis. spectra [before (blue line) and after (red line) UV irradiation, and after visible light exposure to colored sample (green line)] of SAP derivatives, SAP9-MSAP3.

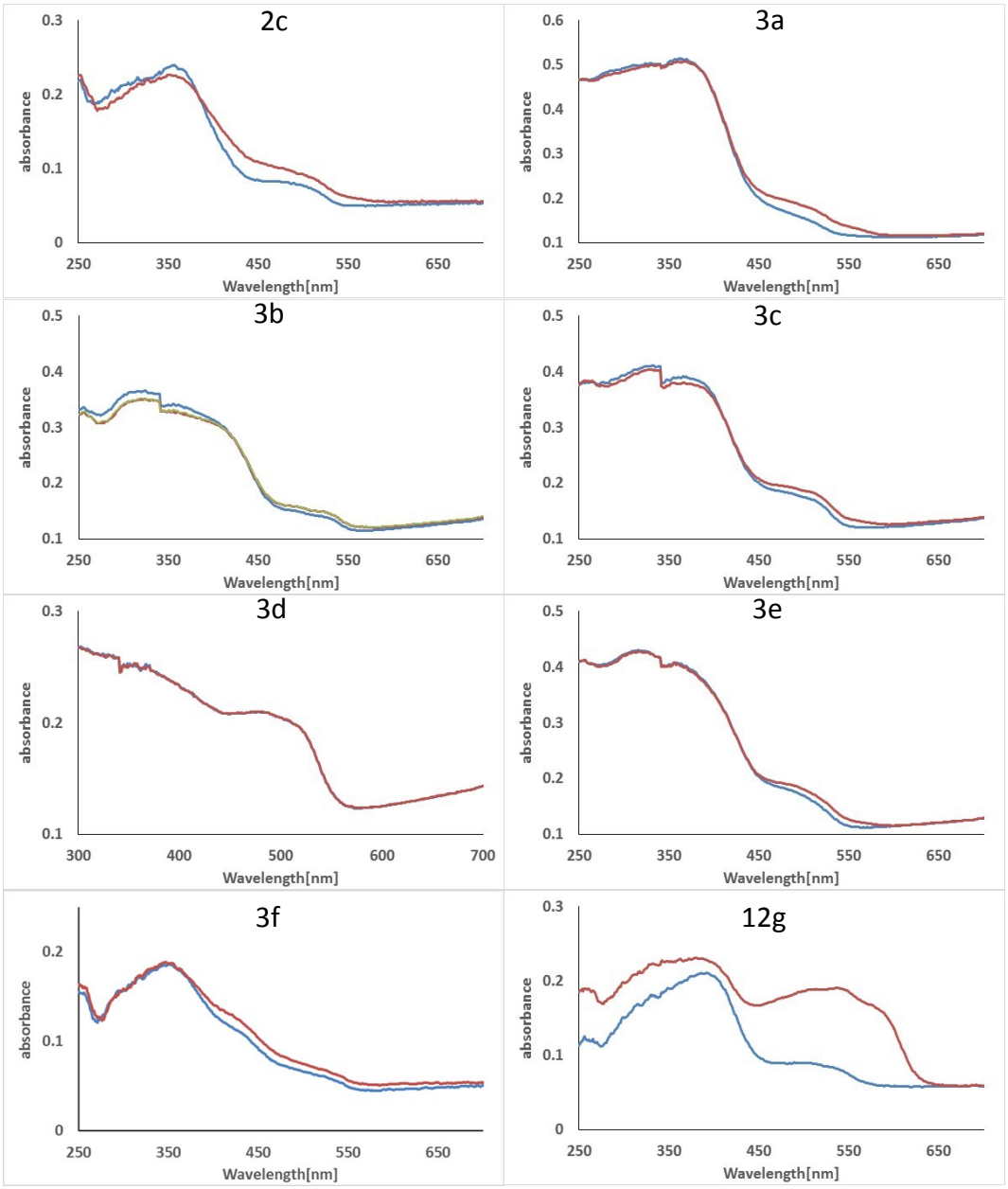


Figure S3: UV-Vis. spectra [before (blue line) and after (red line) UV irradiation, and after visible light exposure to colored sample (green line)] of co-crystals, 3a-12g

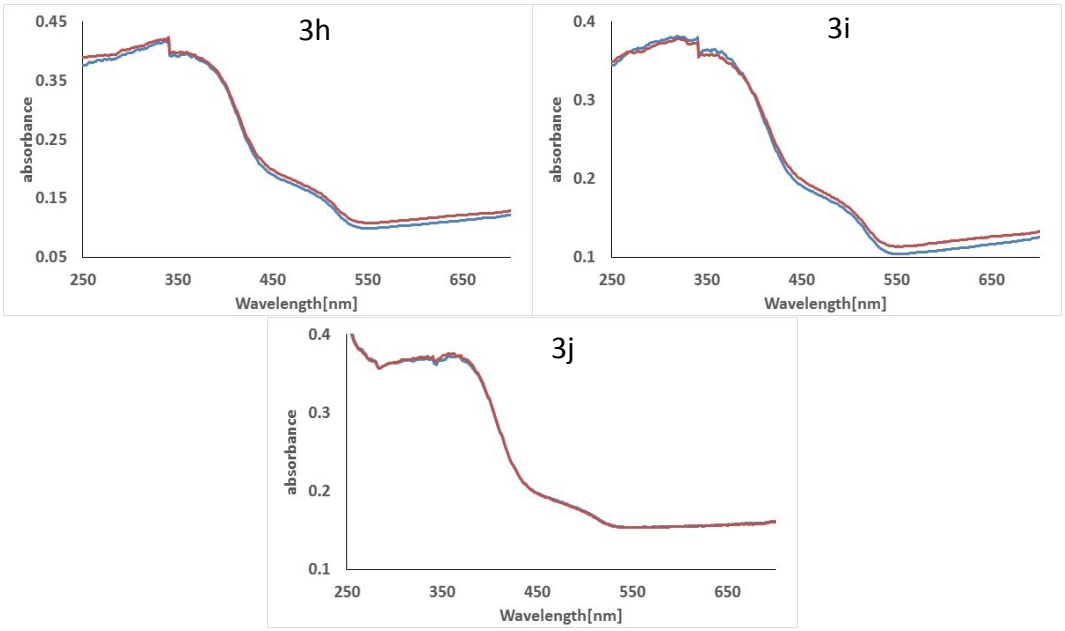


Figure S4: UV-Vis. spectra [before (blue line) and after (red line) UV irradiation, and after visible light exposure to colored sample (green line)] of co-crystals, 3h-3j

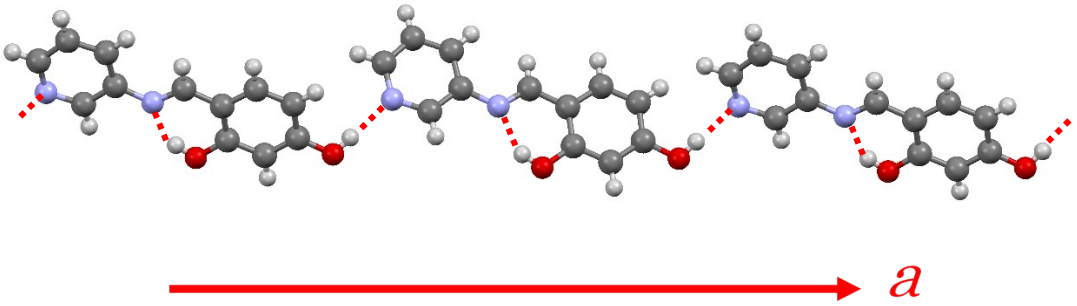


Figure S5: Chain motif along *a*-axis via intermolecular hydrogen bonding in the crystal structure of SAP9.

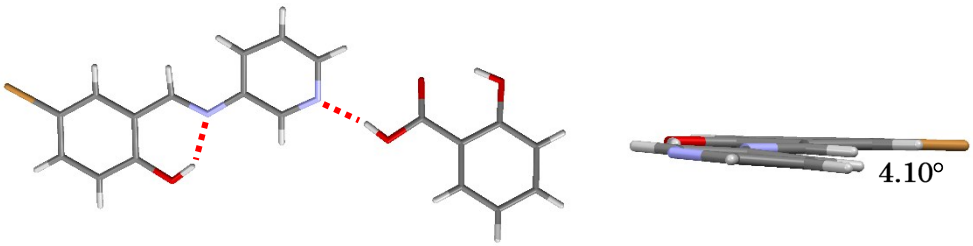


Figure S6: Crystal and molecular structure of 3b.

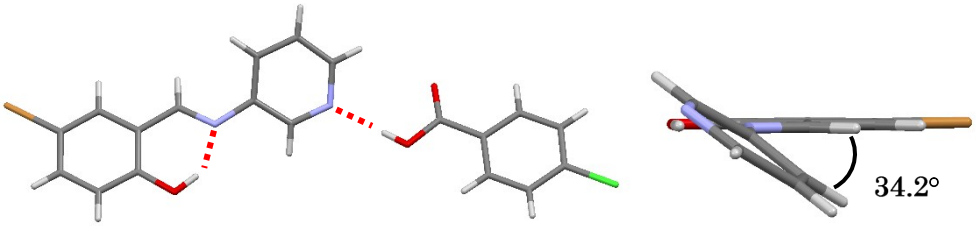


Figure S7: Crystal and molecular structure of 3c.

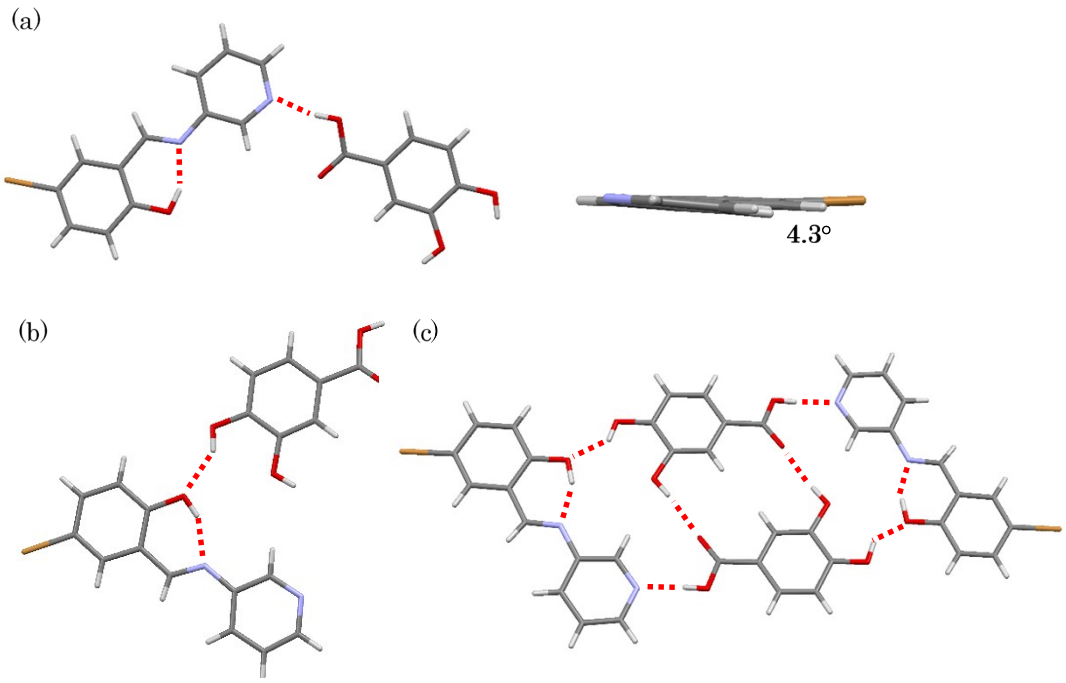


Figure S8: Crystal structure of 3d: (a) molecular structure of 3d; (b) intermolecular hydrogen bonds; (c) two-dimensional sheet-like structure.

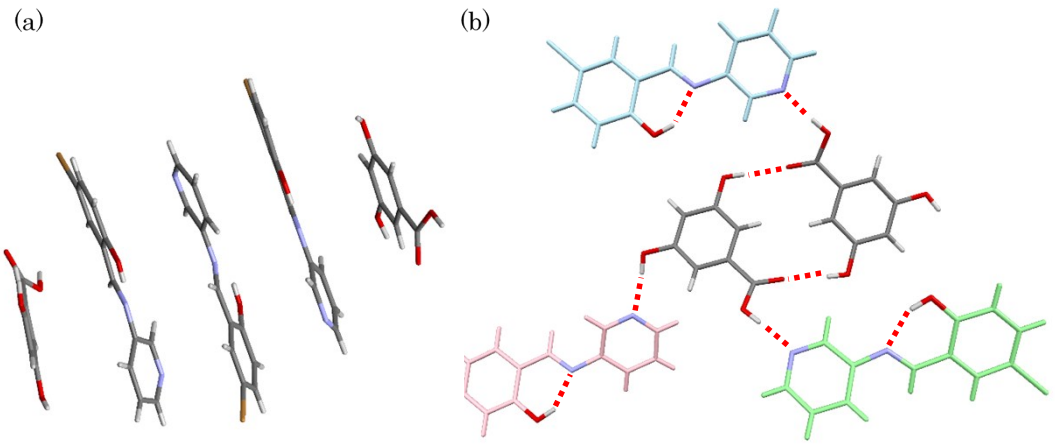


Figure S9: Crystal structure of 3e: (a) molecular packing of 3e; (b) two-dimensional sheet-like structure by intermolecular hydrogen bonding.

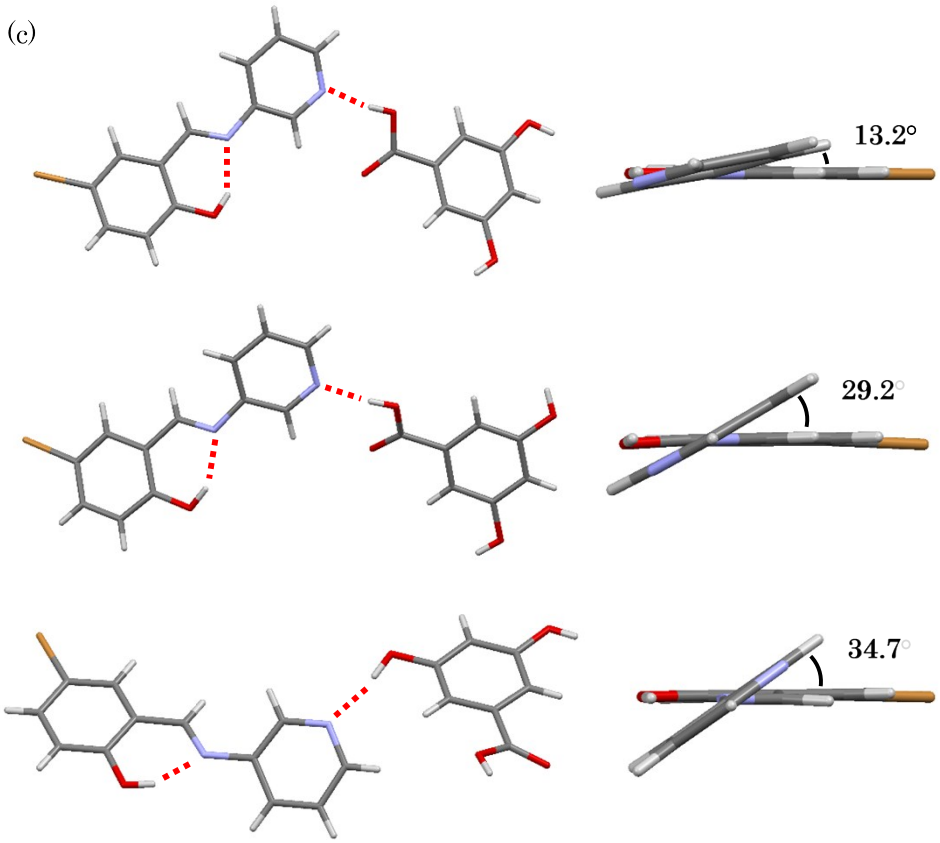


Figure S9:(c) Crystal and molecular structure of 3e.

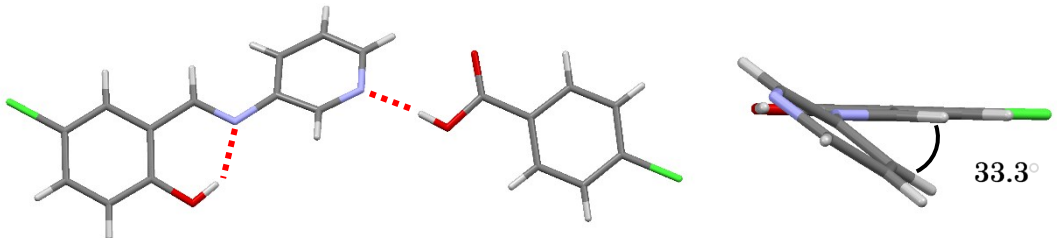


Figure S10: Crystal and molecular structure of 2c.

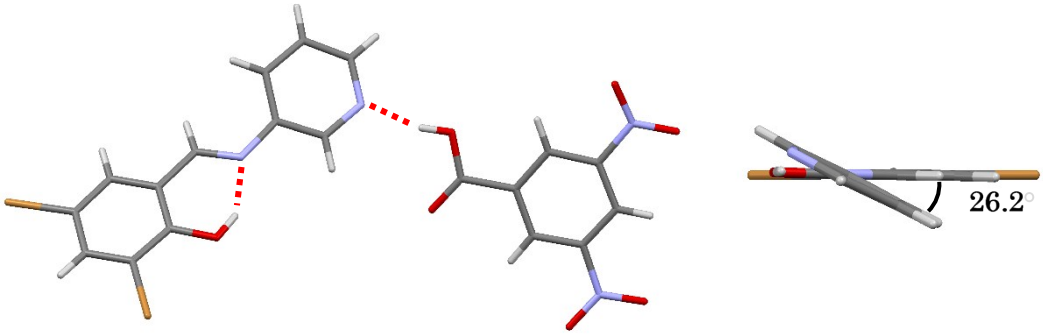


Figure S11: Crystal and molecular structure of 12g.

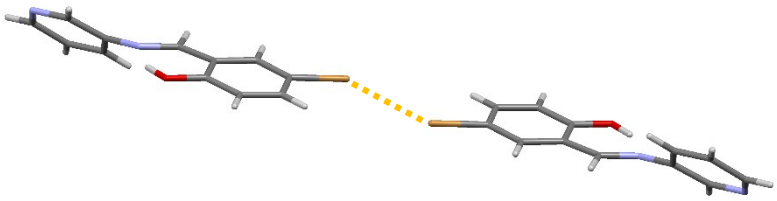

Figure S12: Halogen-halogen interaction in the crystal structure of 3h.

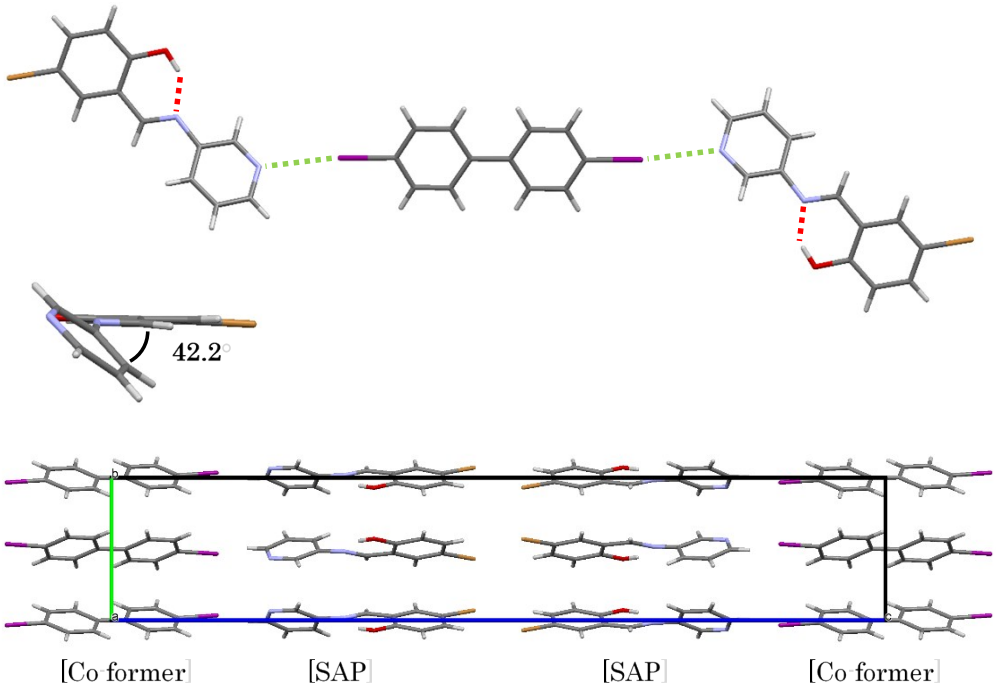


Figure S13: Crystal structure of 3i: (a) intermolecular interaction and molecular structure of 3i; (b) SAP and co-former molecules were arranged alternately via two different types of intermolecular interaction in the crystal structure.

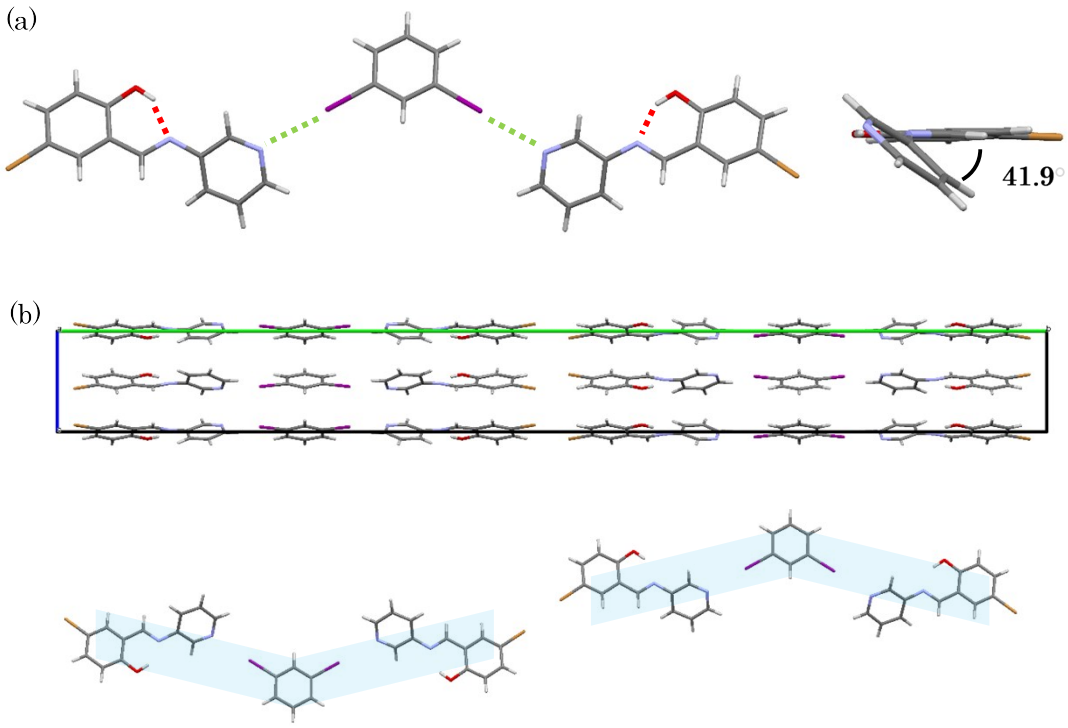


Figure S14: Crystal structure of 3j: (a) intermolecular interaction and molecular structure; (b) SAP molecules and co-formers were arranged alternately via two different types of intermolecular interaction in the crystal structure.


Figure S15: SA derivatives were also known to be thermochromic organic compounds.[23] As the temperature is lowered to 77 K, the crystal color changed from orange or yellow to pale yellow or colorless, respectively, because of the *cis*-keto to enol isomerization of SA. These pictures were taken at 296K (left) and at 77K (right).

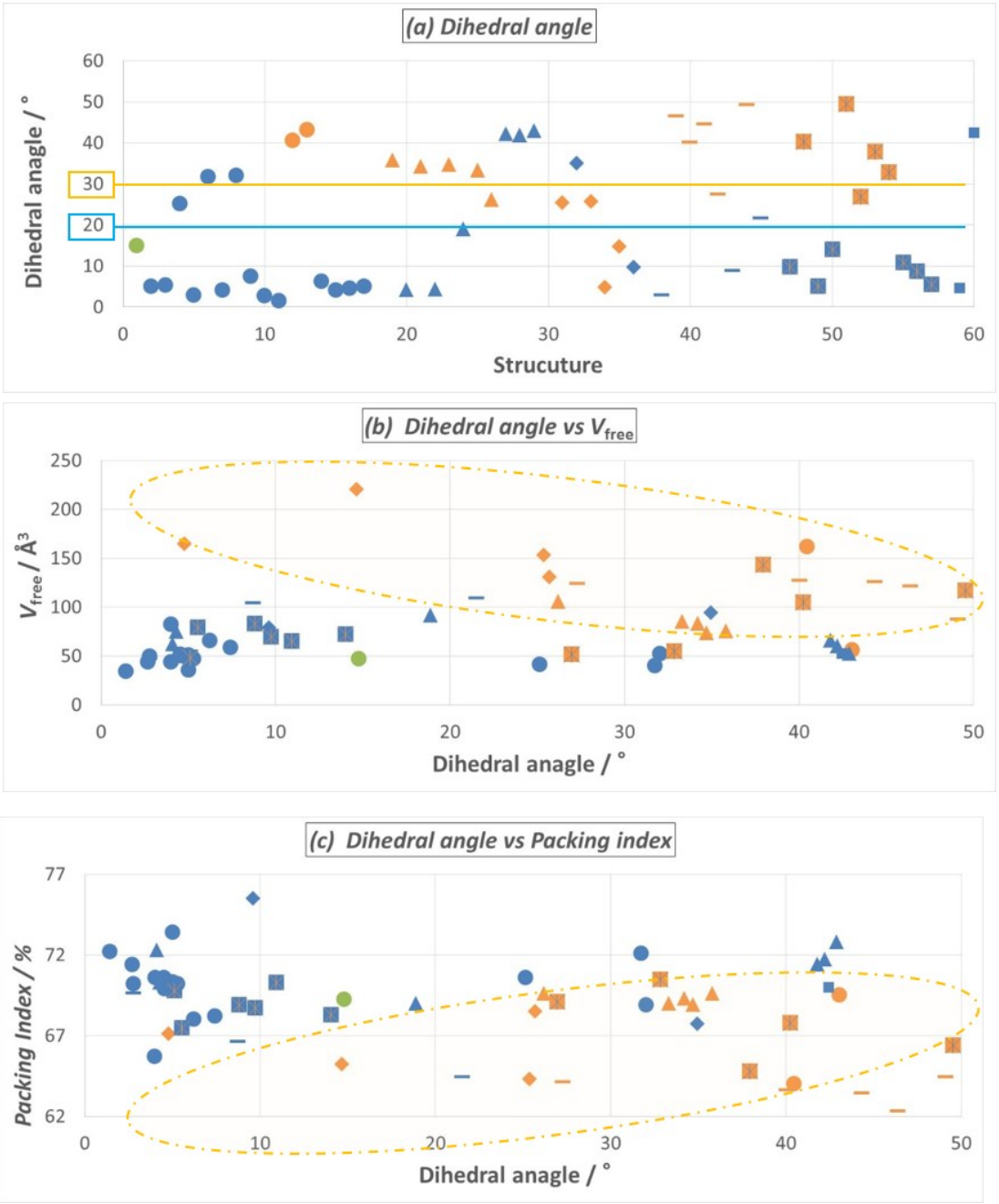


Figure S16: Structural factors and photochromic properties: (a) dihedral angle(°); combination plot: (b) Dihedral angle / $V_{free}$ and (c) Dihedral angle / packing index. Non-photochromic [blue] and photochromic [orange] crystals for SAP derivative [circle] and co-crystals [triangle] and recently reported SA related crystals [diamond: ref. 22], [bar: ref. 18], [square: ref. 19] and [small square: ref. 21]. The list in Table S3 includes all the SAP structures from the past study and present study.