Electronic Supplementary Material (ESI) for Dalton Transactions.
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Supplementary Material

Structural and electrochemical studies of TiO_2 complexes with (4,4'-((1E,1'E)-(2,5-bis(octyloxy)-1,4-phenylene)bis(ethene-2,1-diyl))bis-(E)-N-(2,5-bis(octyloxy)benzylidene)) imine derivatives bases towards organic devices

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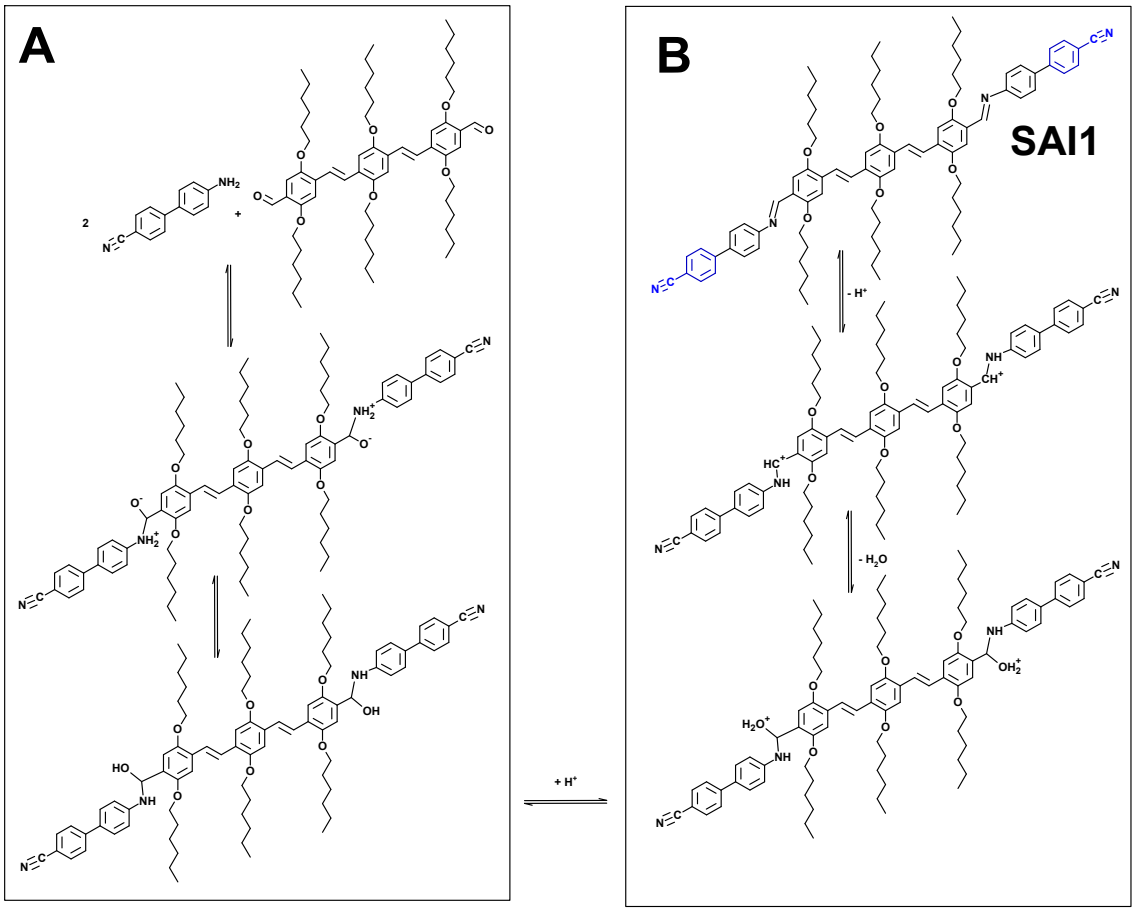
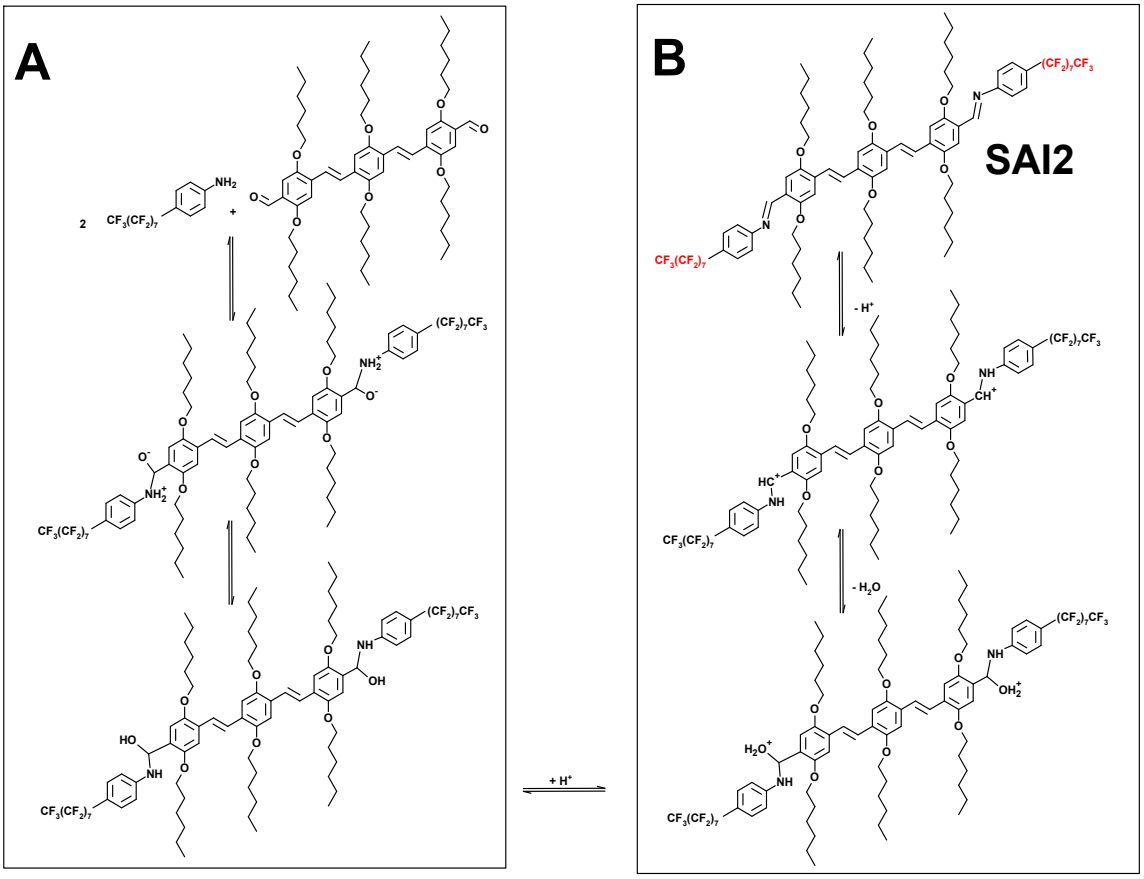

A
B
SAI1
+ H+
- H+
- H2O


A
B
SAI2
2
+ H+
- H+
- H2O

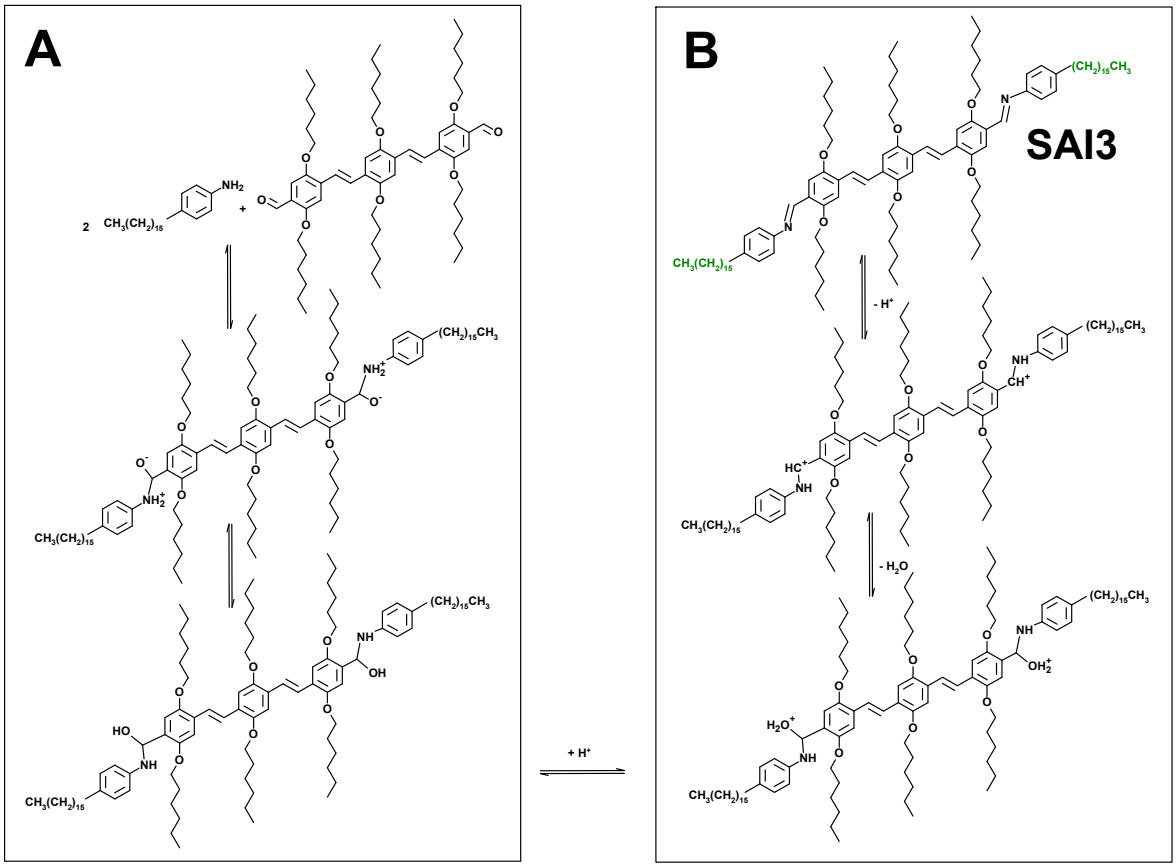
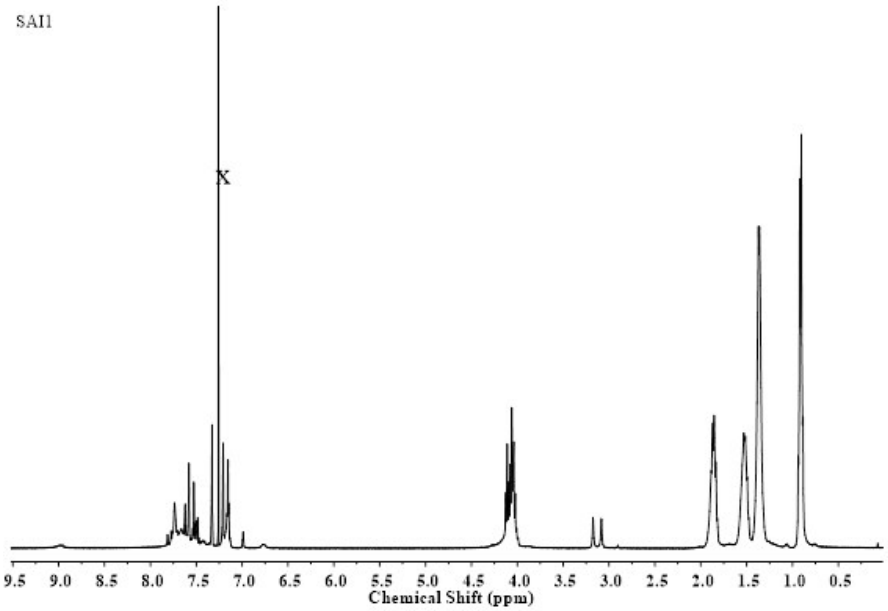
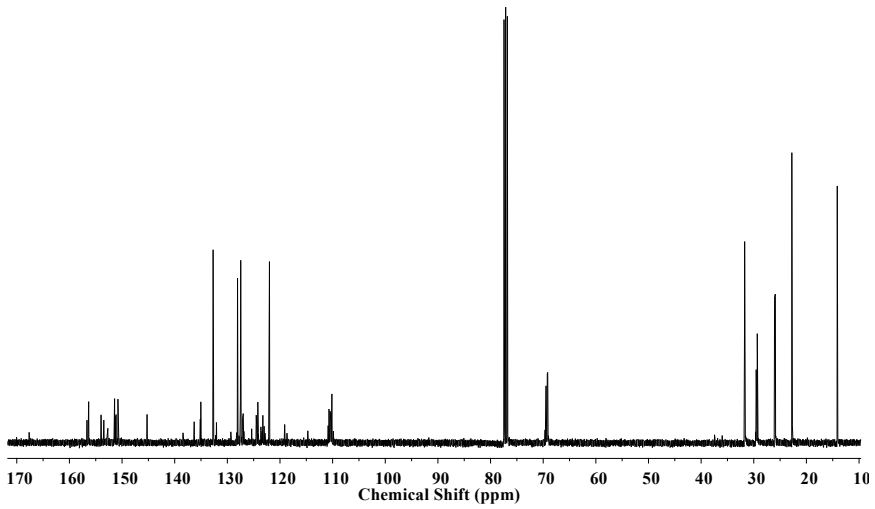


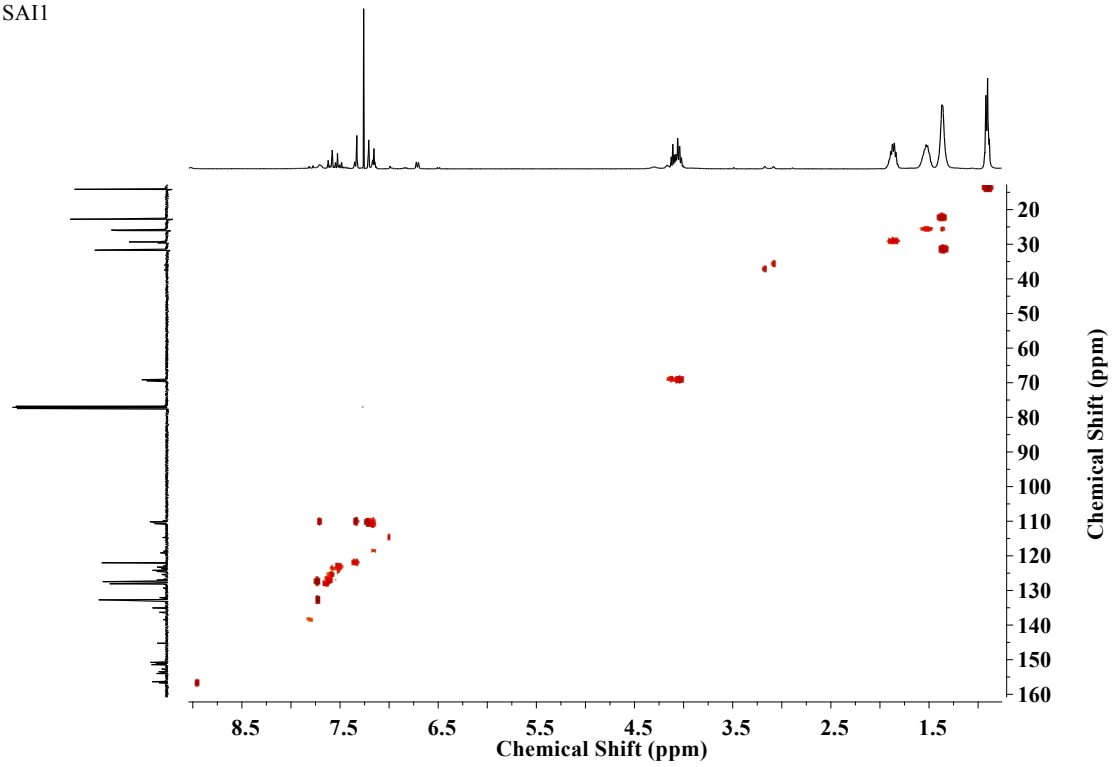
Fig. S1. Scheme of imine formation for SAI1-SAI3: A- aminocarbinol formation; B- imine formation.

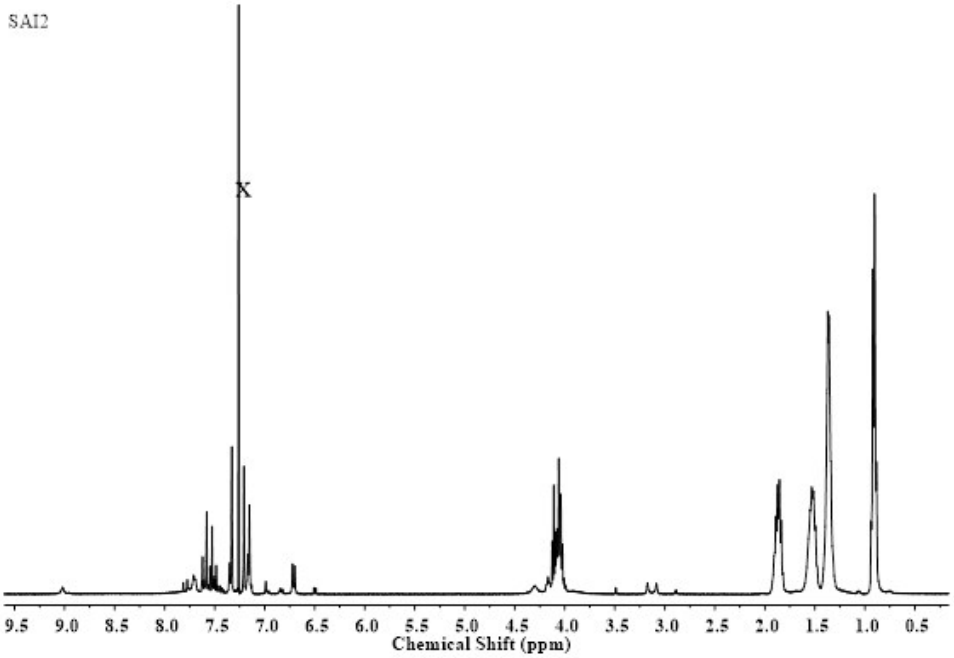


SAI1

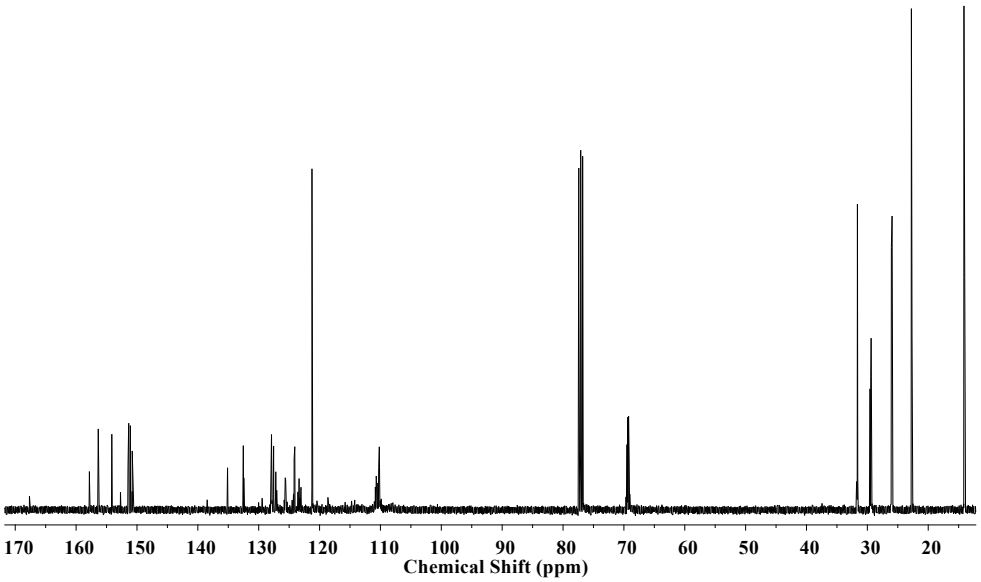

170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
Chemical Shift (ppm)

SAI1

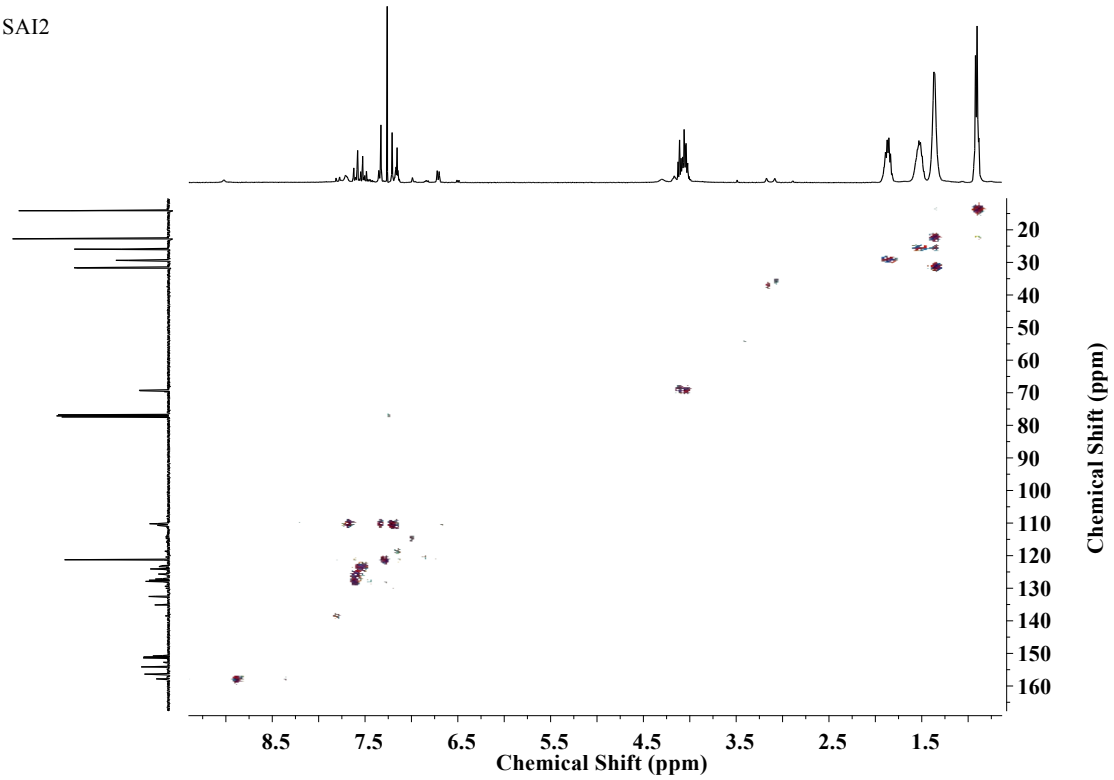

8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5
Chemical Shift (ppm)
20 30 40 50 60 70 80 90 100 110 120 130 140 150 160
Chemical Shift (ppm)


SAI2
X
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
Chemical Shift (ppm)

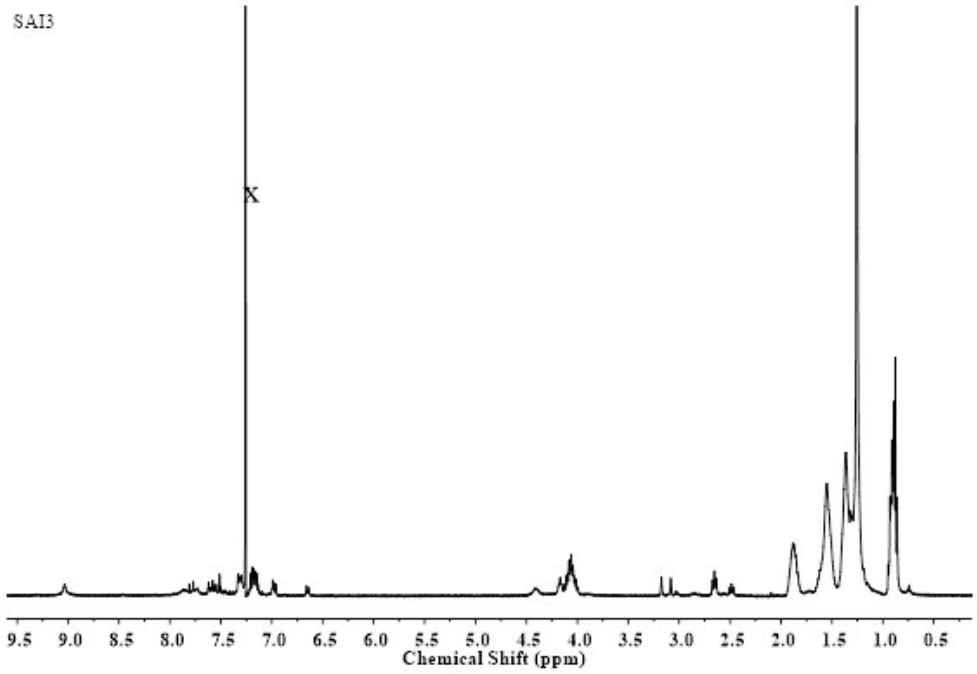
SAI2

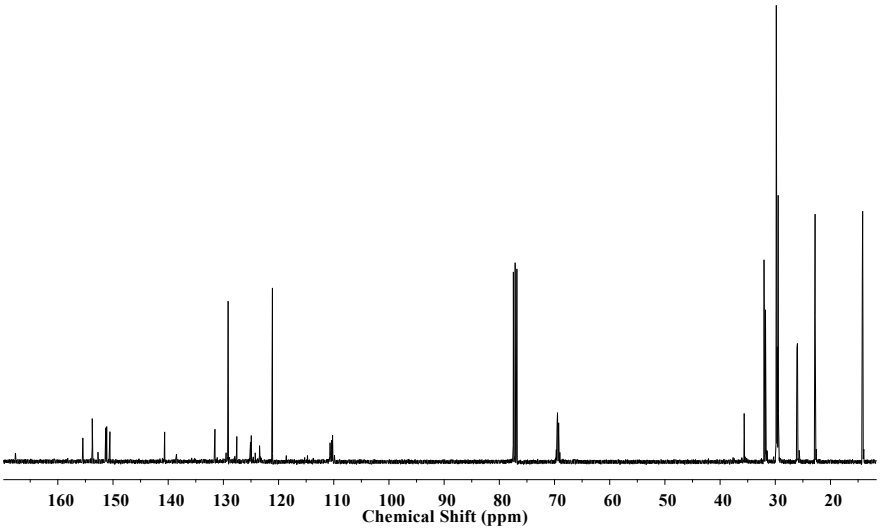

170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20
Chemical Shift (ppm)

SAI2


20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
Chemical Shift (ppm)
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
Chemical Shift (ppm)

SAI3


X
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
Chemical Shift (ppm)



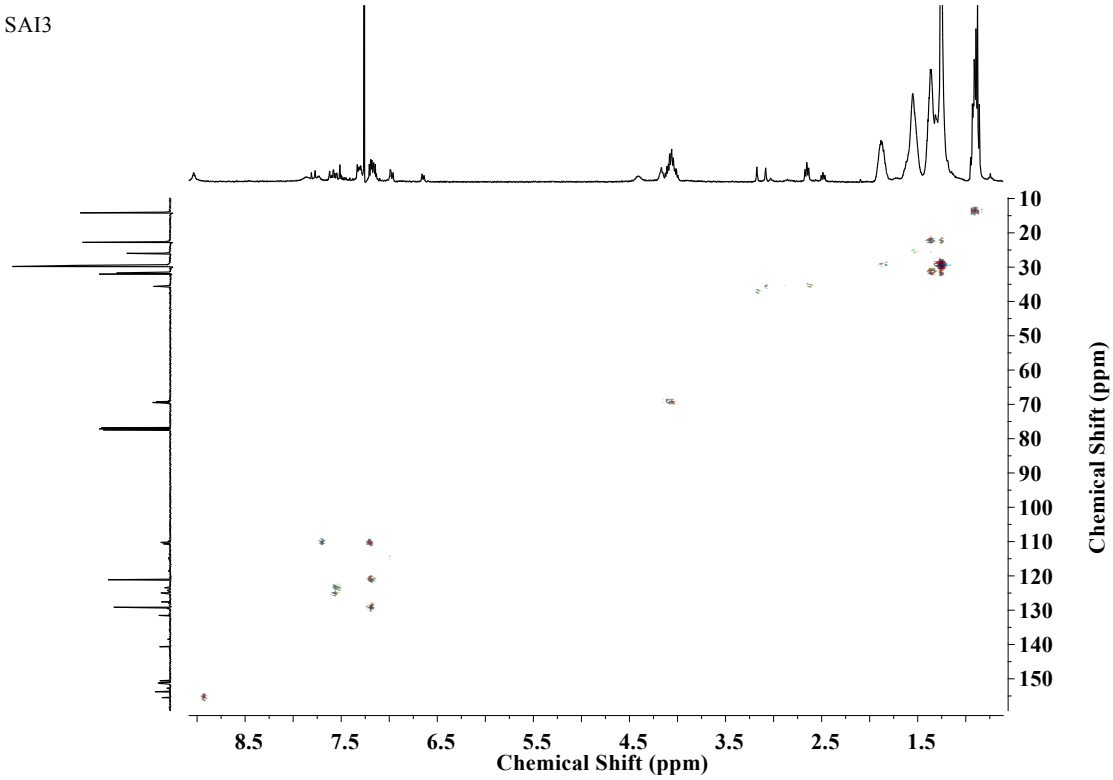


Fig. S2: ^{1}H, ^{13}C and ^{1}H-^{13}C HMQC NMR spectra of SAI1-SAI3 imines

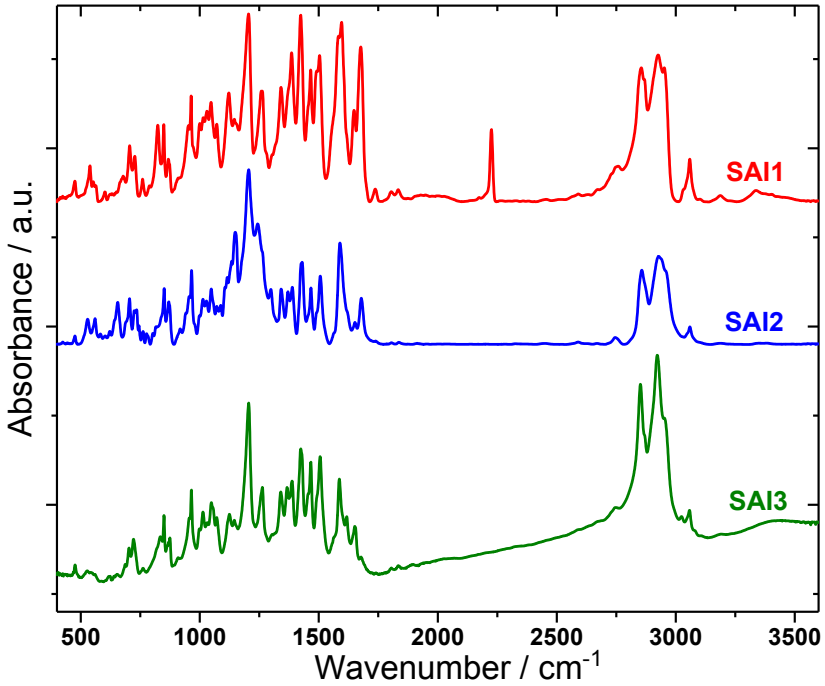


Fig. S3: Room temperature FT-IR spectra of SAI1-SAI3 imines

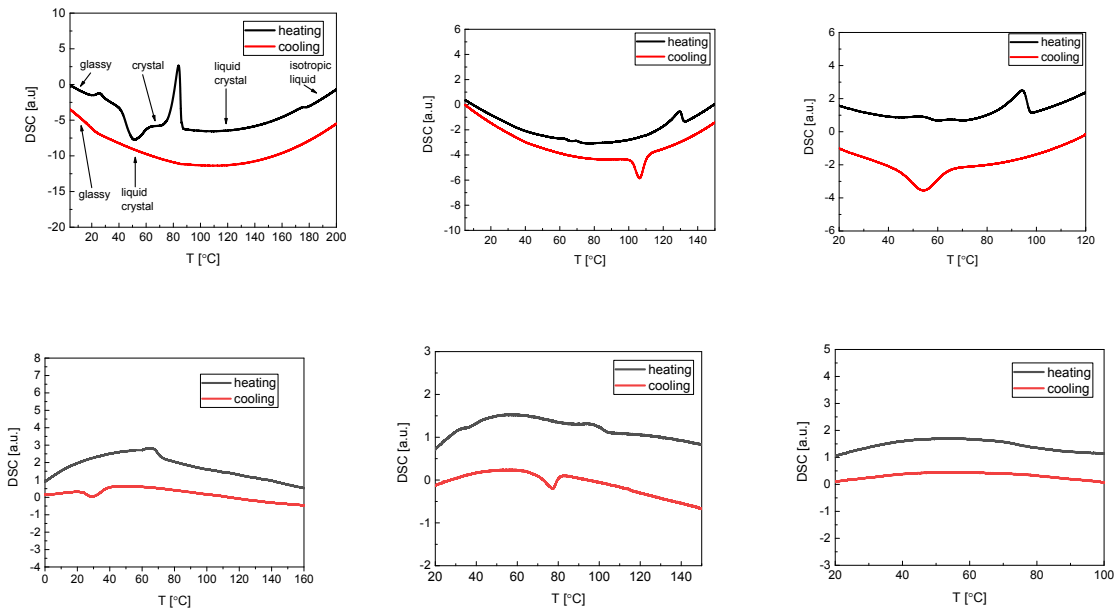


Fig. S4: DSC curves of the imines SAI1-SAI3 (from left to right, top) and SAI1-SAI3 with TiO_2 (from left to right, bottom) registered for heating and cooling cycles at rate10 °C/min

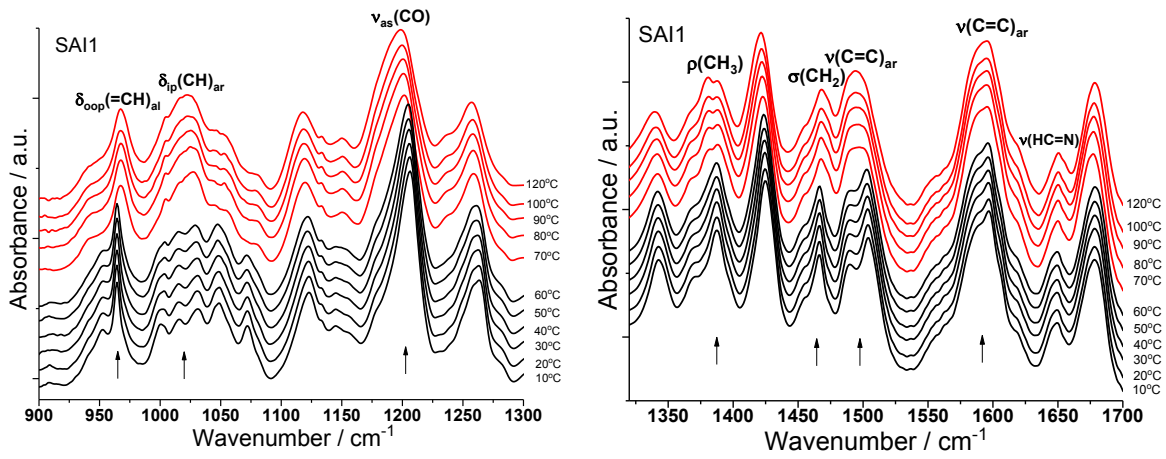


Fig. S5. Temperature evolution of the FT-IR spectrum of SAI1 obtained during cooling in the spectral range of 900–1300 cm^{-1} (left side) and of 1320–1700 cm^{-1} (right side). Crystalline solid and liquid phases are marked with black and red colour, respectively. The bands which change significantly at the phase transition are marked with arrows.

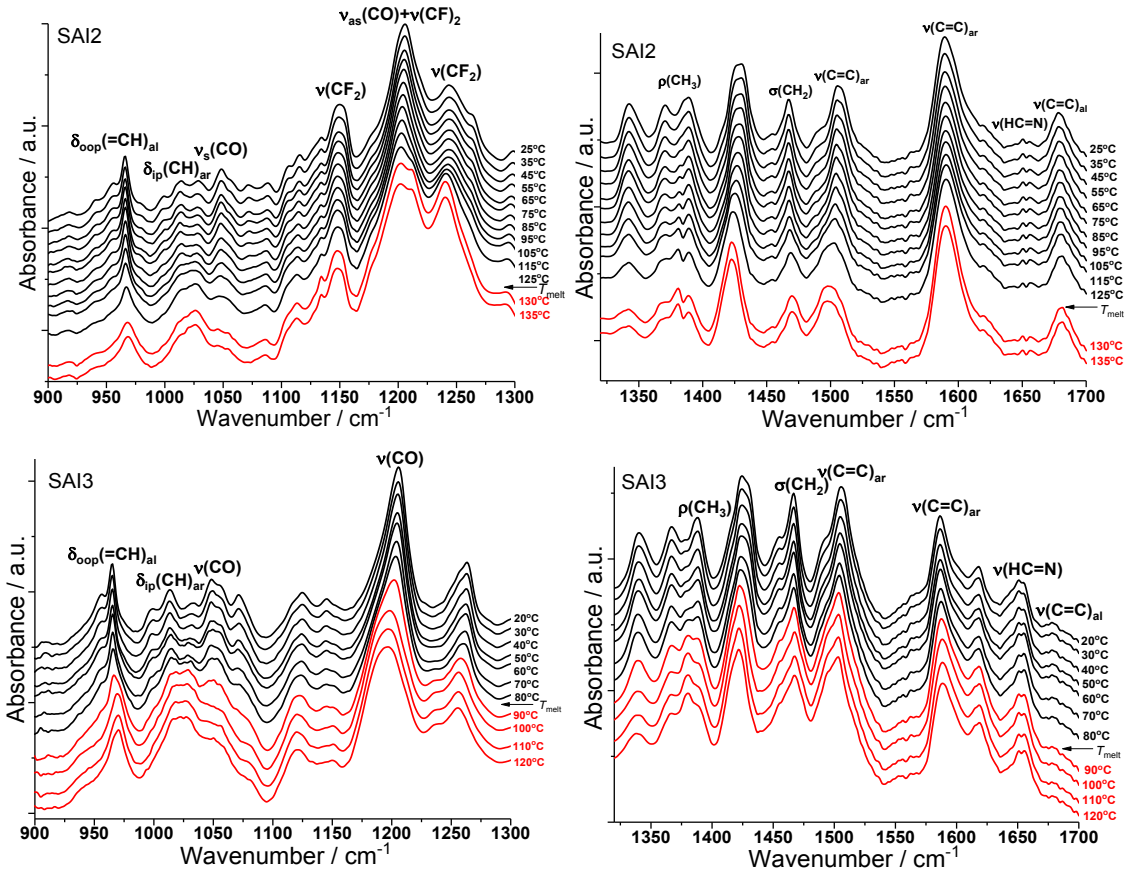


Fig. S6. Temperature evolution of the FT-IR spectra of SAI2 (top) and SAI3 (bottom) imines obtained during heating in the spectral range of 900–1300 cm^{-1} (left side) and of 1320–1700 cm^{-1} (right side). Crystalline solid and liquid phases are marked with black and red colour, respectively.

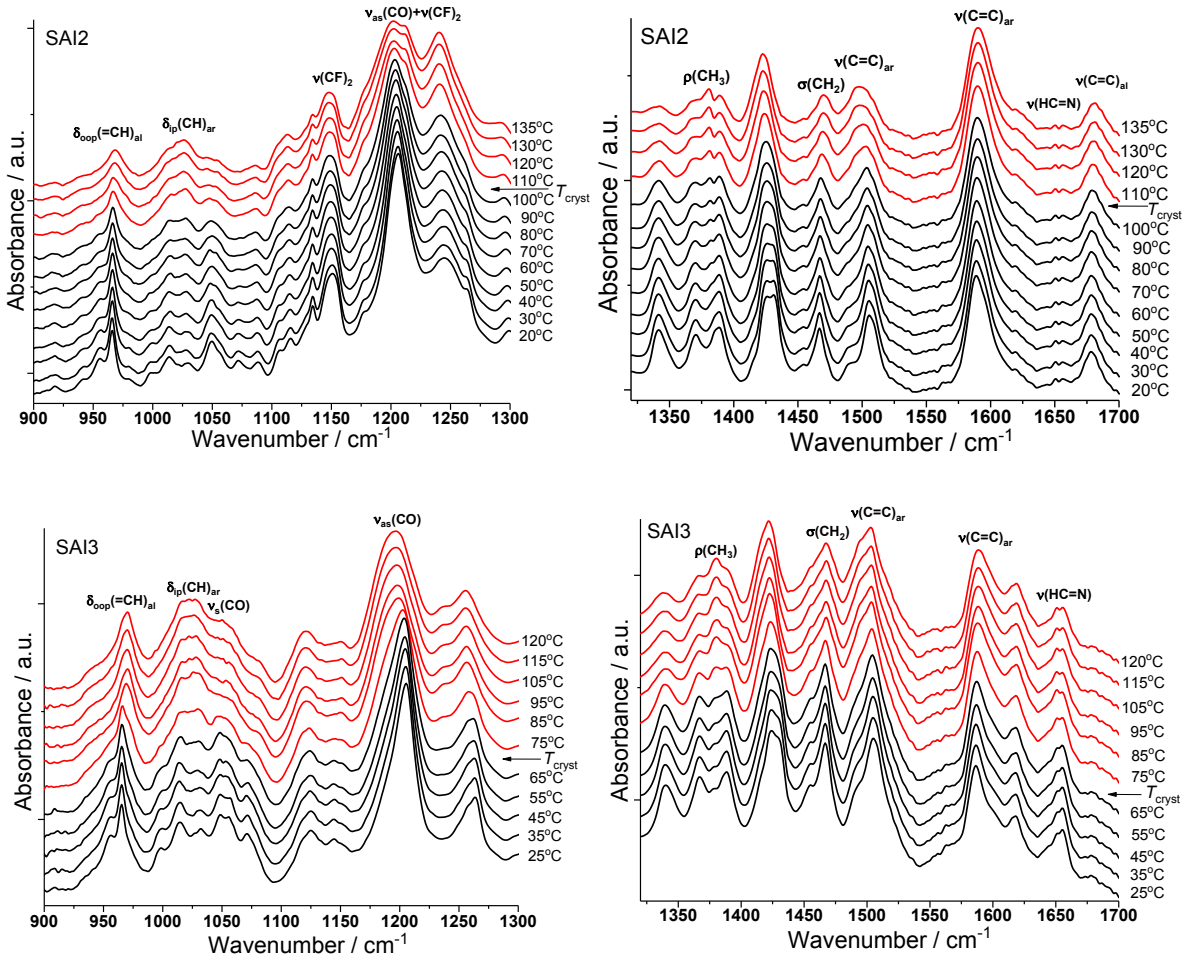


Fig. S7. Temperature evolution of the FT-IR spectra of SAI2 (top) and SAI3 (bottom) imines obtained during cooling in the spectral range of 900–1300 cm^{-1} (left side) and of 1320–1700 cm^{-1} (right side). Crystalline solid and liquid phases are marked with black and red colour, respectively

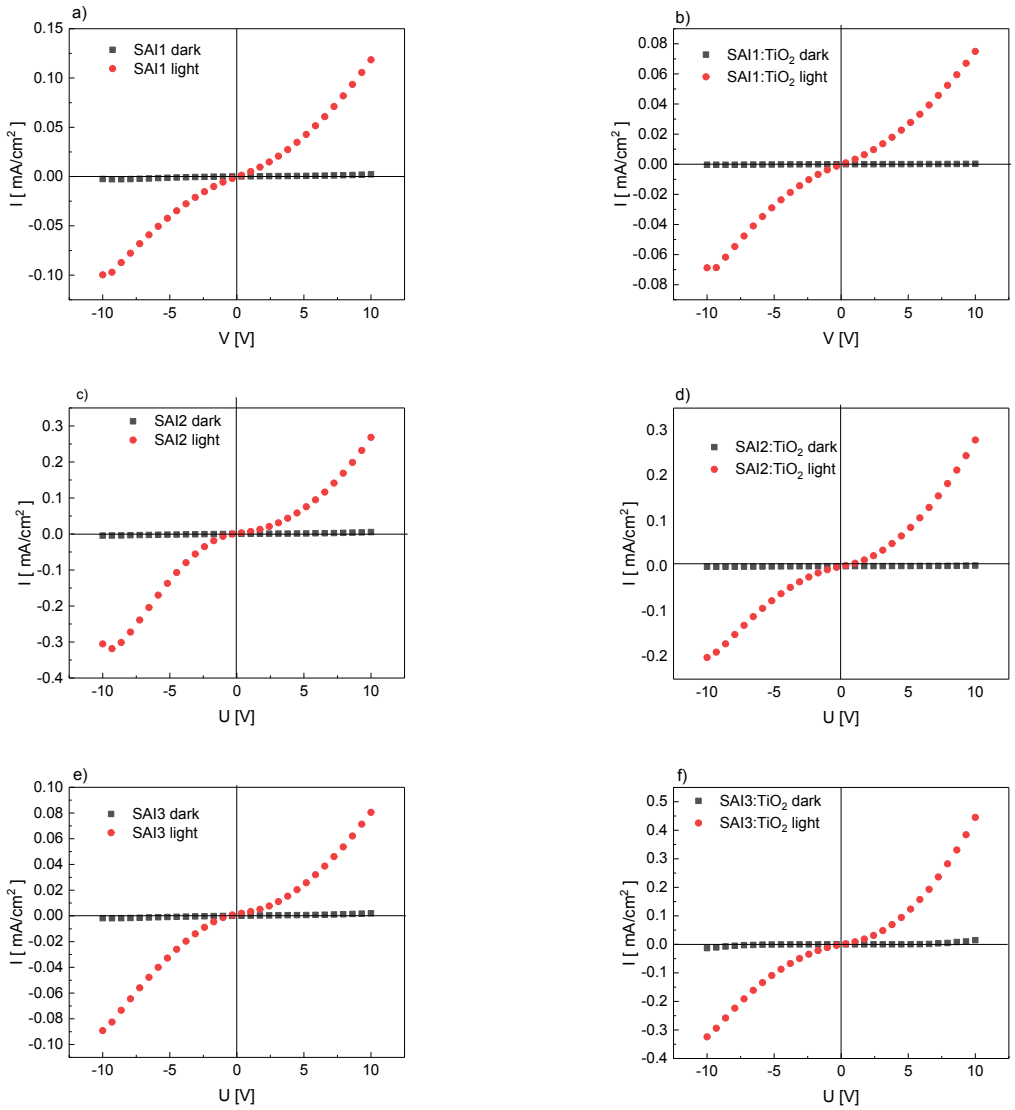


Fig. S8. I–V characteristics of the systems ITO/TiO_2/active layer/Au, Black squares show dark characteristics, red dots show characteristics collected under AM 1.5 solar simulator illuminated with 93 mW/cm^2 power density.

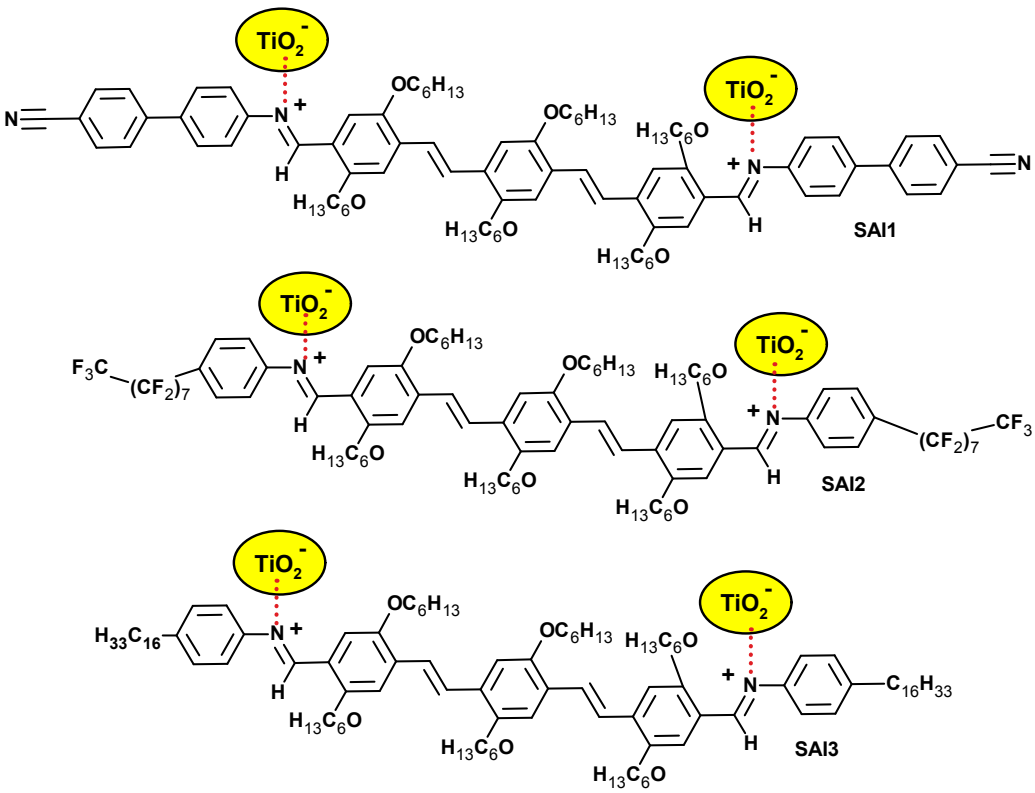
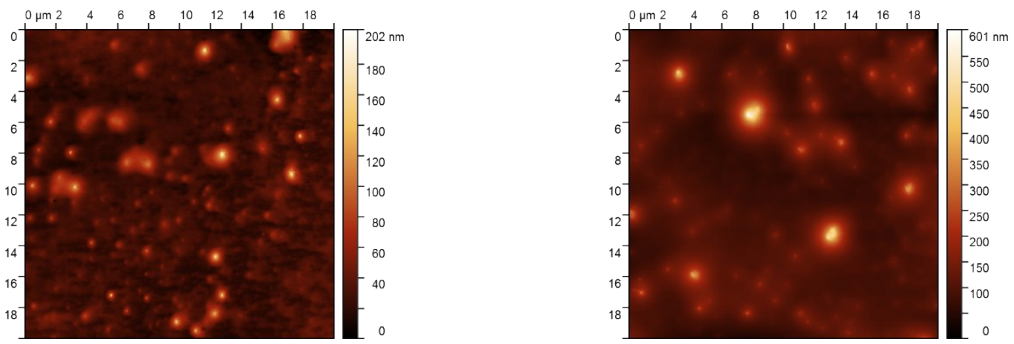


Fig. S9. Schematic illustration of interactions of the SAI1-SAI3 imines with TiO_2

AFM imaging of samples topography were measured at room temperature with the Agilent 5500 microscope working in non-contact mode. Set-point and gains were adjust to each measurement to obtain clear image without noises. Topography images were collected at several randomly chosen area. Samples for AFM measurements were prepared in form of thin films by spin – coating technique (1000 rpm, 40s).



(a)

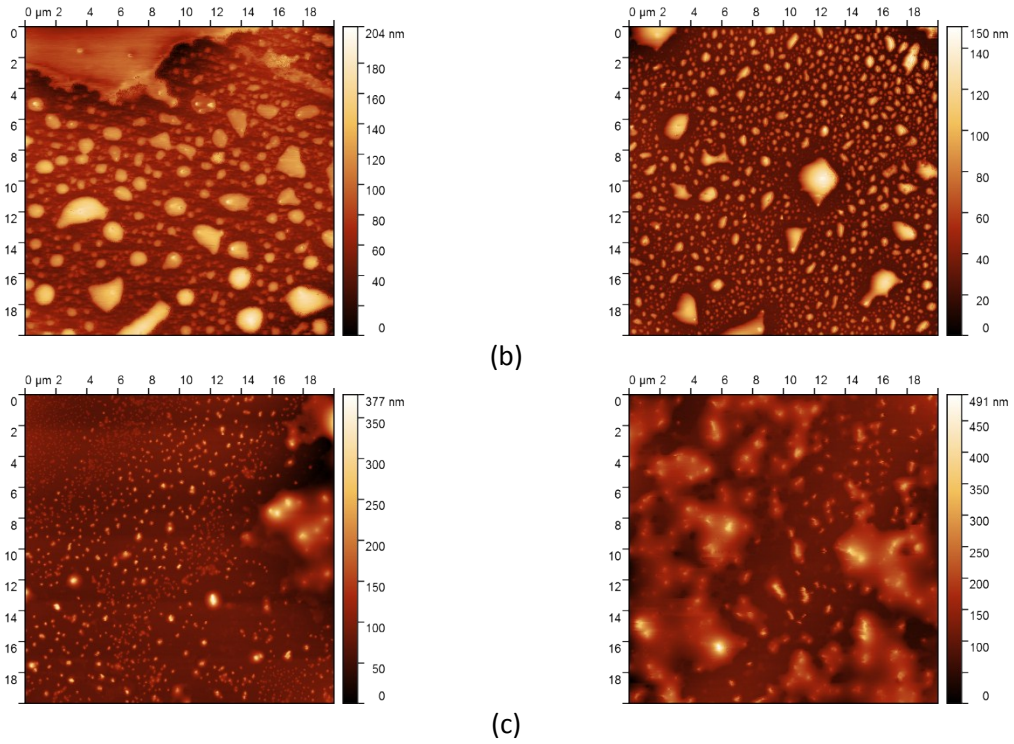


Figure S10. AFM topography images for SAI1 and SAI1:TiO_2 (3:2 w/w) (a), SAI2 and SAI2:TiO_2 (3:2 w/w) (b), SAI3 and SAI3:TiO_2 (3:2 w/w) (c), respectively from left to right

Synthesis of TiO_2

TiO_2 powder was prepared by sol-gel method using as a precursor titanium (IV) isopropoxide (TIPO). The 4.5 ml of TIPO was dissolved in the solution of 20 ml of ethanol and 3.5 ml of distilled water to create a titania sol. During the stirring of the titania sol about 4 h TiO_2 powder was obtained. The TiO_2 powder was first filtering and dried at room temperature and next heated at 500 ºC for one hour.