SUPPLEMENTARY INFORMATION FOR

Switchable polarity solvent (SPS) systems: probing solvatoswitching with a spiropyran (SP) - merocyanine (MC) photoswitch

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Contents:

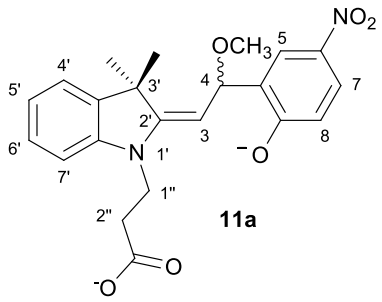
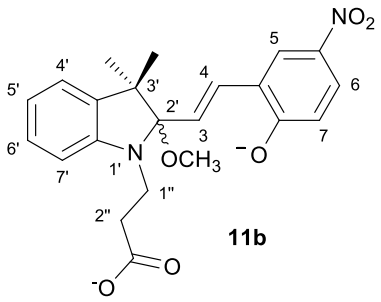


Table S1: Table of experimental[a] and calculated[b] ^{1}H NMR spectroscopic parameters for the 1,4-methoxide addition product, ***11a*.**[1]

Proton	Experimental	Calculated
H-3	[c]	5.45, d, J = 6.2
H-4	5.91. br s.	4.81, d, J = 6.2
H-5	8.10, d, J = 2.8	8.25, d, J = 1.5
H-7	8.03, d, d, H = 8.7, 2.8	7.99, d, d, J = 7.5, 1.5
H-8	6.79, d, J = 8.7	6.34, d, J = 7.5
H-4’	7.1, m[d]	7.08, d,d, J = 7.5, 1.5
H-5’	[d]	6.69, m, J = 7.5, 7.5, 1.5
H-6’	[d]	7.05, m, J = 7.5, 7.5, 1.5
H-7’	[d]	6.23, d, d, J = 7.5, 1.5
CH_3O-4	[c]	3.30, s
CH_3-3’	1.49, 1.69, s	1.69, s
H-1’’	[c]	3.39, t, J = 7.1
H-2’’	[c]	2.63, t, J=7.1

[a]Recorded on a Bruker AVANCE-300 spectrometer (300.01 MHz), CD_3OD/CD_3ONa. Chemical shifts (δ are listed in parts per million (ppm) and coupling constants (J) are given in Hertz (Hz).
[b]ChemNMR ^{1}H Estimation from ChemDraw program using additivity rules for chemical shifts.
[c]Not observed either due to exchange with the medium or overlap with more intense signals of other species in solution.
[d]Unresolved multiplet overlaps other aromatic ring proton signals.



11b

Table S2: Table of experimental[a] and calculated[b] ^{1}H NMR spectroscopic parameters for the 1,2-methoxide addition product, ***11b*.**[1]

Proton	Experimental	Calculated
H-3	[c]	6.50, d, J = 15.1
H-4	7.1, m[d]	6.76, d, J = 15.1
H-5	8.41, d, J = 3.1	7.93, d, J = 1.5
H-7	7.96, d, d, H = 9.3, 3.1	7.94, d, d, J = 7.5, 1.5
H-8	6.55, d, J = 9.3	6.36, d, J = 7.5
H-4’	7.1, m[d]	7.06, d,d, J = 7.5, 1.5
H-5’	[d]	6.71, m, J = 7.5, 7.5, 1.5
H-6’	[d]	7.07, m, J = 7.5, 7.5, 1.5
H-7’	[d]	6.56, d, d, J = 7.5, 1.5
CH_3O-4	[c]	3.30, s
CH_3-3’	1.17, 1.27, s	1.40, s
H-1’’	[c]	3.68, t, J = 7.1
H-2’’	[c]	2.63, t, J=7.1

[a]Recorded on a Bruker AVANCE-300 spectrometer (300.01 MHz), CD_3OD/CD_3ONa. Chemical shifts (δ are listed in parts per million (ppm) and coupling constants (J) are given in Hertz (Hz).

[b]ChemNMR ^{1}H Estimation from ChemDraw program using additivity rules for chemical shifts.

[c]Not observed either due to exchange with the medium or overlap with more intense signals of other species in solution.

[d]Unresolved multiplet overlaps other aromatic ring proton signals.

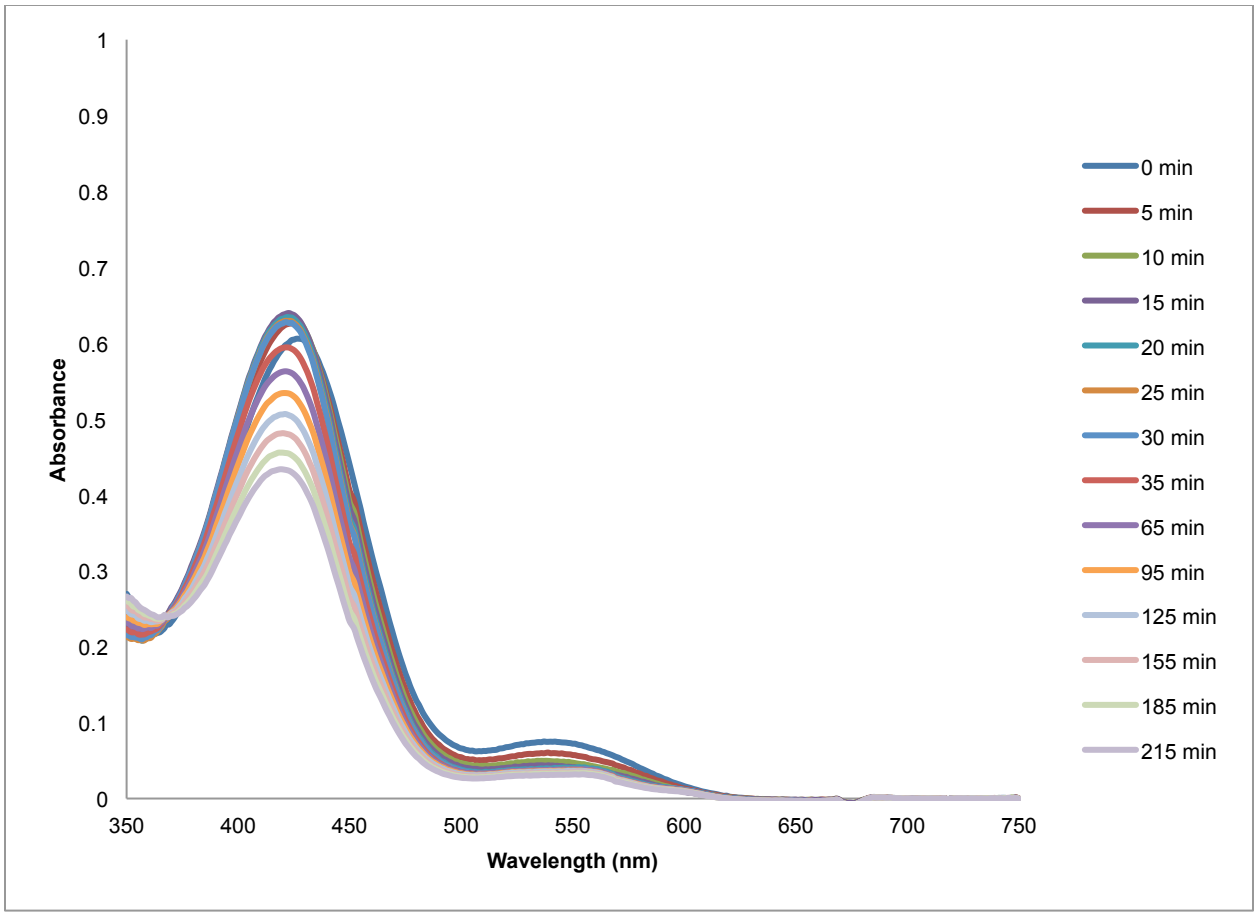


Figure S1: MC, ***2***, in PrOH with 1,1,3,3-tetramethylguanidine (TMG) (0.01:1 v/v). With the addition of TMG absorbance for MC is reduced and the species at 420 nm is observed.

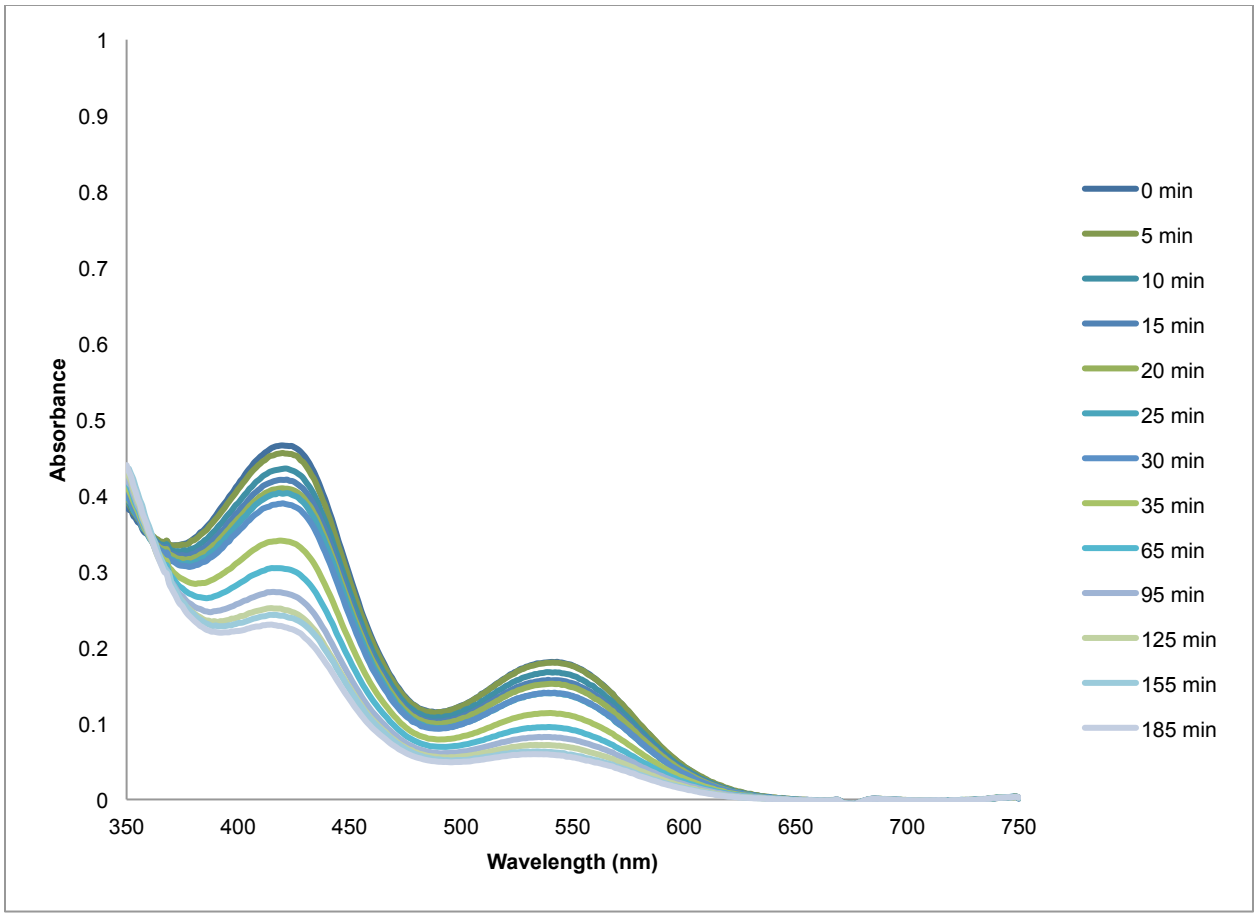


Figure S2: MC, ***2***, in PrOH with N-tert-butyl-N',N'-dimethylformamidine (BDF) (0.01:1 v/v). The BDF reduces the MC absorbance at 545 nm to a lesser extent than TMG or DBU.

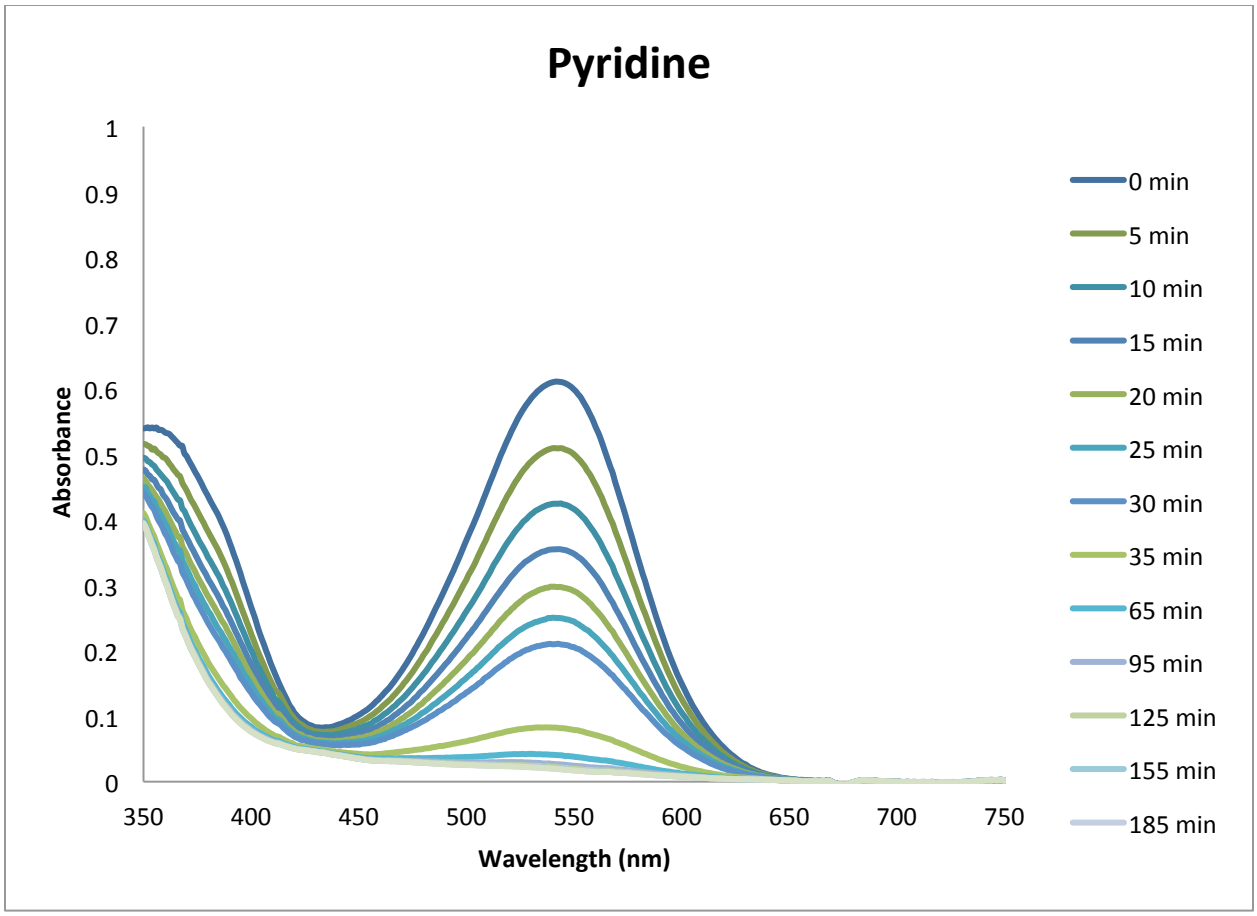


Figure S3: MC, ***2***, in PrOH with pyridine (0.01:1 v/v). The addition of pyridine has no effect on the absorbance of MC at 545 nm or on the rate of reversion back to SP.

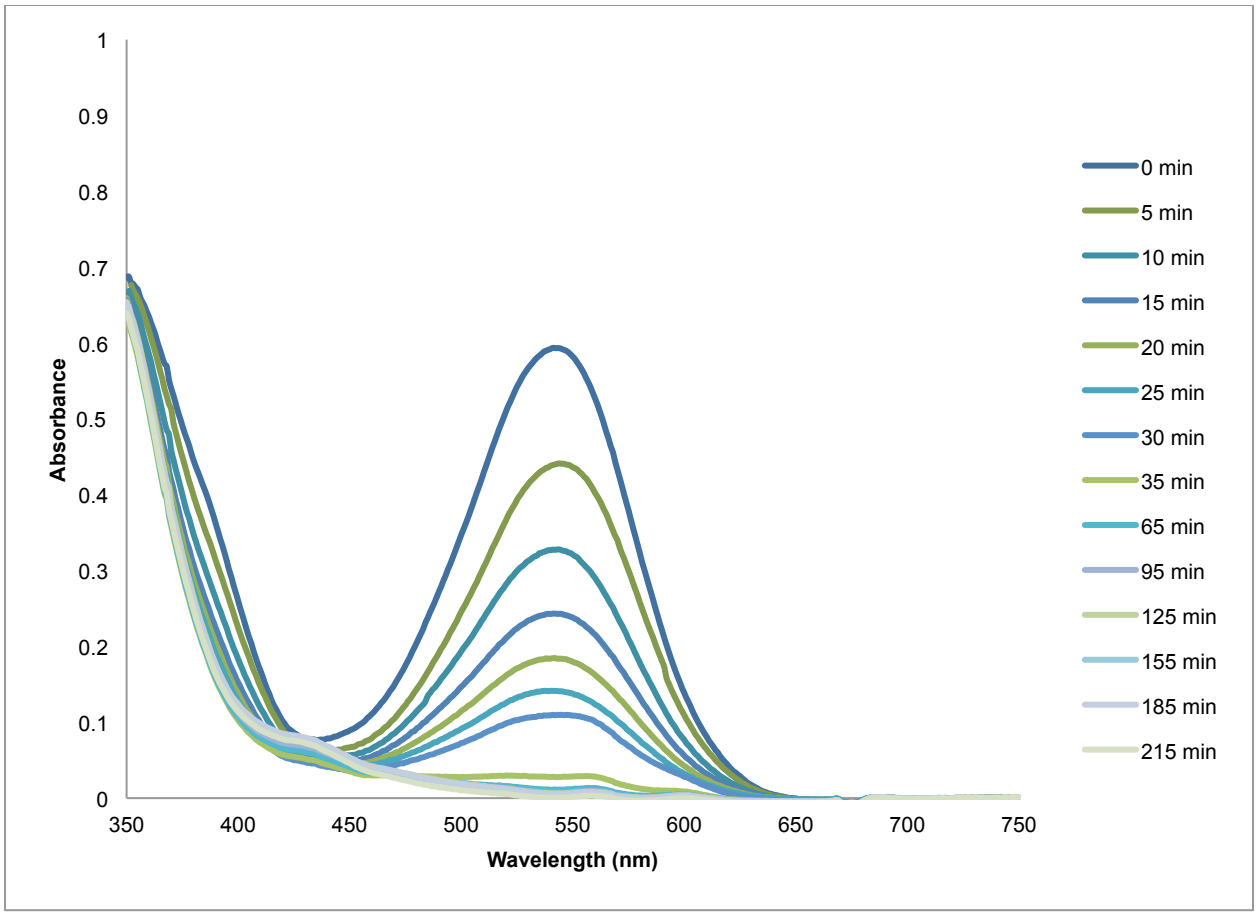


Figure S4: MC, ***2***, in PrOH with N-ethylbutylamine (0.01:1 v/v). The addition of the amine has no effect on the absorbance of MC at 545 nm or on the rate of reversion back to SP.

References

1. A. Wasey, Ph.D. Thesis, Queen's University, 2003.