Supplementary Information

Kinetic and thermodynamic study of 2'-hydroxy-8-methoxyflavylium. Reaction networks interconverting flavylium cations and flavanones.

Vesselin Petrov [a,*], Ana Marta Diniz [a], Luís Cunha-Silva [b], A. Jorge Parola [a], Fernando Pina [a]

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1. Mole fraction distribution of species for the the equilibria descibed by K_a, $K^{\wedge}_a$ and K'_a

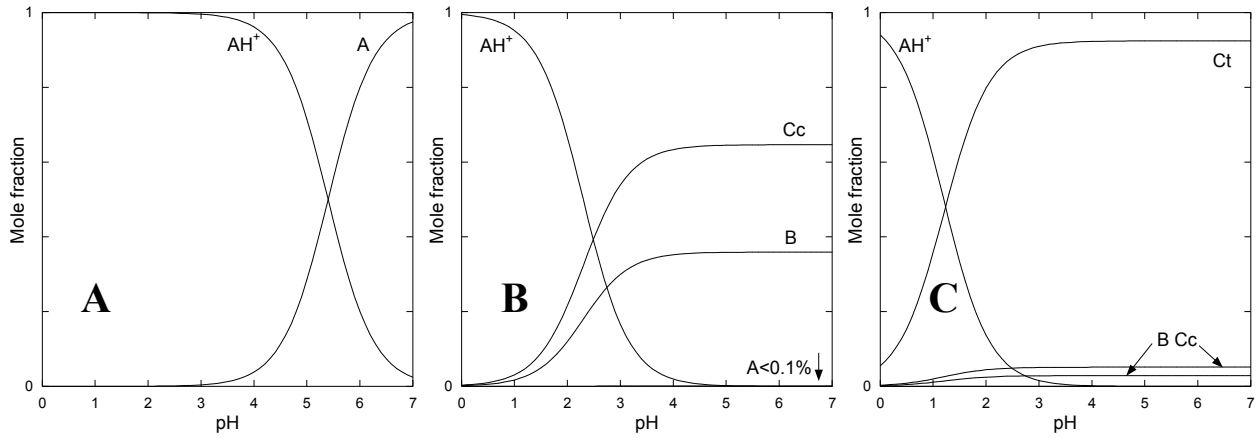
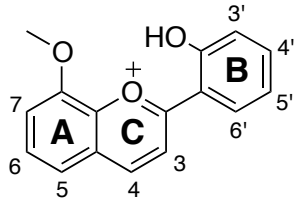
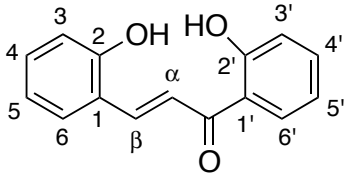
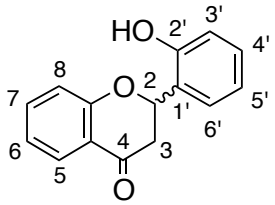


Figure S1. Mole fraction distribution of species corresponding to the equilibria described in Fig. 2 of the manuscript:
A - 4.5 ms after a pH jump from pH=0.6 to higher pH values (K_a);
B - The same as in A but after *ca.* 1 min after the pH jump ($K^{\wedge}_a$);
C - The same as in A after upon final thermodynamic equilibrium (*ca*. 8h; K'_a).

2. ^{1}H and ^{13}C NMR characterization of 2-(2'-hydroxyphenyl)-8-methoxy-1-benzopyrylium chloride (AH^{+}), *trans*-2,2'-dihydroxy-3-methoxychalcone (Ct) and 2'-hydroxy-3'-methoxyflavanone (F)

Table S1 – ^{1}H (δ/ppm, multiplicity, J/Hz) and ^{13}C (δ/ppm) NMR data for $\mathbf{AH^{+}}$ (D_2O/DCl, pD~1), **Ct** and **F** ($CDCl_3$).

	$\mathbf{AH^{+}}$		**Ct**		**F**	
						
Position	^{13}C	^{1}H	^{13}C	^{1}H	^{13}C	^{1}H
1			120.5			
2	173.8		163.8		74.9	5.87, dd, 12.7, 3.6
2OH				12.90, s		
3	121.0	8.64, d, 9.2	146.3		43.5	(a) 3.06, dd, 16.9, 12.7 (b) 2.98, dd, 16.9, 3.6
4	155.6	8.91, d, 9.2	112.5	6.92, dd, ~7, ~2	192.6	
4a	137.0				121.3	
5	119.0	7.46, d, 8.1	120.0	6.89, dd	127.3	7.95, dd, 7.8, 1.7
6	130.2	7.54, dd, 8.1, 8.1	122.4	7.20, dd, 5.6, 2.2	121.6	7.05, ddd, ~8, ~8, ~2
7	120.5	7.43, d, 8.1			136.1	7.50, ddd, ~7, ~7, 1.8
8	155.7				118.3	7.06, dd, ~8, ~2
8a	156.3				162.1	
α			121.9	7.92, d, 15.7		
β			141.0	8.13, d, 15.7		
1'	113.7		121.4		125.0	
2'	155.5		147.1		142.8	
2'OH				6.37, br s		5.89, br s
3'	118.0	6.70, d, 8.3	118.7	7.02, dd, ~7, 1.1	146.7	
4'	139.7	7.30, dd, 8.1, 8.1	136.3	7.48, ddd, ~7, ~7, 1.6	110.8	6.88, dd, ~8, 1.3
5'	121.5	6.76, dd, 8.1, 8.3	118.9	6.93, dd	120.2	6.94, dd
6'	130.6	7.79, d, 8.1	130.0	7.94, dd, 8.0, 1.6	118.9	7.18, dd, 5.1, 1.2
OCH_3	56.8	3.86, s	56.5	3.94, s	56.3	3.92, s
C=O			194.6			