Supporting Information for:

Investigation into Solid and Solution Properties of Quinizarin

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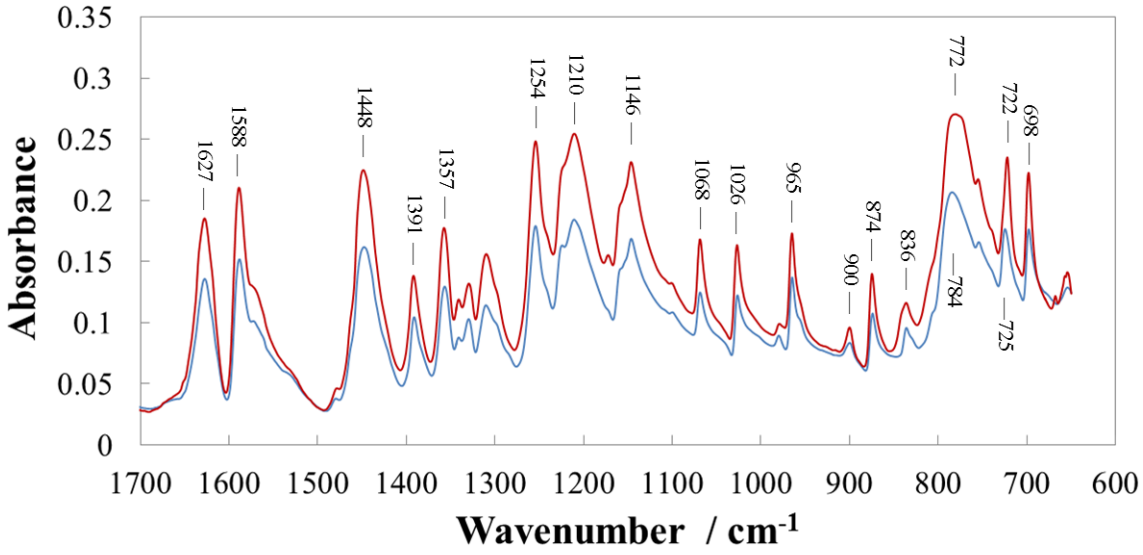

Figure S1. IR absorption spectra of quinizarin FI (blue) and FII (red).

Table S1. Crystal data and structure refinement for quinizarin FI and FII.

Compound	FI	FII
Empirical formula	$C_{14}H_8O_4$	$C_{14}H_8O_4$
Formula weight	240.20	240.20
Temperature	150.0(1) K	170.0(2) K
Wavelength	0.71073 Å	0.71073 Å
Crystal system	Monoclinic	Monoclinic
Space group	$P2_1/n$	Cc
Unit cell dimensions	a = 10.2390(8) Å	a = 20.0099(12) Å
	b = 6.0429(4) Å	b = 24.6219(9) Å
	c = 16.454(2) Å	c = 18.3201(11) Å
	β= 95.999(8)°	β= 116.274(8)°
Volume	1012.51(17) $Å^3$	8093.4(9) $Å^3$
Z, Z'	4, 1	32, 8
Density (calculated)	1.576 Mg/m^3	1.577 Mg/m^3
Absorption coefficient	0.117 mm^{-1}	0.117 mm^{-1}
F(000)	496	3968
Crystal size	0.65 x 0.16 x 0.10 mm^3	0.50 x 0.40 x 0.20 mm^3
Theta range for data collection	3.594 to 25.349°.	3.010 to 25.350°.
Index ranges	-12<=h<=7, -7<=k<=4,	-24<=h<=24, -29<=k<=25,
	-19<=l<=19	-14<=l<=22
Reflections collected	3895	15736
Independent reflections	1854 [R(int) = 0.0589]	10312 [R(int) = 0.0184]
Completeness to theta = 25.242°	99.8 %	99.8 %
Data / restraints / parameters	1854 / 0 / 171	10312 / 2 / 1297
Goodness-of-fit on F^2	0.984	1.033
Final R indices [I>2sigma(I)]	R1 = 0.0464, wR2 = 0.1213	R1 = 0.0440, wR2 = 0.1080
R indices (all data)	R1 = 0.0566, wR2 = 0.1314	R1 = 0.0672, wR2 = 0.1245
Largest diff. peak and hole	0.220 and -0.296 $e.Å^{-3}$	0.215 and -0.262 $e.Å^{-3}$

Table S2. Hydrogen-bonds geometry (Å and °) in the crystal structures of quinizarin FI and FII.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
FI				
O(4)-H(1O3)...O(1)#1	0.94(3)	1.73(3)	2.5716(15)	147(2)
O(4)-H(1O3)...O(1)#2	0.94(3)	2.39(3)	3.0811(17)	131(2)
O(3)-H(1O4)...O(2)#1	0.99(3)	1.70(2)	2.5735(16)	144.5(19)
O(3)-H(1O4)...O(2)#3	0.99(3)	2.29(2)	3.0464(17)	132.4(18)
FII				
O(1)-H(1)...O(3)	0.82	1.87	2.581(4)	144.6
O(1)-H(1)...O(28)#4	0.82	2.34	2.987(4)	136.8
O(2)-H(2O)...O(4)	0.82	1.86	2.577(4)	145.2
O(2)-H(2O)...O(27)#5	0.82	2.45	3.104(4)	137.9
O(5)-H(5O)...O(7)	0.82	1.87	2.580(4)	144.8
O(5)-H(5O)...O(12)#6	0.82	2.37	3.017(4)	137.0
O(6)-H(6O)...O(8)	0.82	1.86	2.575(4)	145.4
O(6)-H(6O)...O(11)	0.82	2.44	3.085(4)	136.9
O(9)-H(9)...O(8)	0.82	2.42	3.073(4)	137.9
O(9)-H(9)...O(11)	0.82	1.89	2.602(4)	144.2
O(10)-H(10)...O(7)#7	0.82	2.40	3.052(4)	137.5
O(10)-H(10)...O(12)	0.82	1.86	2.573(4)	145.1
O(13)-H(13)...O(15)	0.82	1.90	2.608(5)	144.0
O(13)-H(13)...O(20)#6	0.82	2.34	2.974(4)	134.5
O(14)-H(14)...O(16)	0.82	1.86	2.574(4)	145.4
O(14)-H(14)...O(19)	0.82	2.39	3.044(4)	137.0
O(17)-H(17O)...O(16)	0.82	2.33	2.983(5)	137.1
O(17)-H(17O)...O(19)	0.82	1.88	2.592(4)	143.8
O(18)-H(18)...O(15)#7	0.82	2.39	3.028(5)	134.7
O(18)-H(18)...O(20)	0.82	1.86	2.576(4)	144.6
O(21)-H(21)...O(23)	0.82	1.87	2.583(4)	144.4
O(21)-H(21)...O(31)#6	0.82	2.42	3.068(4)	136.5
O(22)-H(22)...O(24)	0.82	1.88	2.591(5)	144.1
O(22)-H(22)...O(32)	0.82	2.34	2.994(4)	137.0
O(25)-H(25O)...O(4)#8	0.82	2.42	3.073(4)	137.7
O(25)-H(25O)...O(27)	0.82	1.86	2.575(4)	144.8
O(26)-H(26O)...O(3)#9	0.82	2.37	3.026(4)	137.6
O(26)-H(26O)...O(28)	0.82	1.88	2.590(4)	144.6

O(29)-H(29)...O(23)#7	0.82	2.34	2.975(4)	135.0
O(29)-H(29)...O(31)	0.82	1.89	2.596(4)	144.1
O(30)-H(30O)...O(24)	0.82	2.40	3.068(4)	139.2
O(30)-H(30O)...O(32)	0.82	1.87	2.580(4)	143.7

Symmetry transformations used to generate equivalent atoms:

#1 x,y,z #2 -x+1,-y,-z+2 #3 -x+2,-y+2,-z+2 #4 x,y-1,z #5 x-1/2,y-1/2,z #6 x+1/2,y-1/2,z

#7 x-1/2,y+1/2,z #8 x+1/2,y+1/2,z #9 x,y+1,z