Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPORTING INFORMATION

Ground and Excited State Properties of Furanoflavylium Derivatives. The Effect of the Furano Bridge.

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NMR spectra

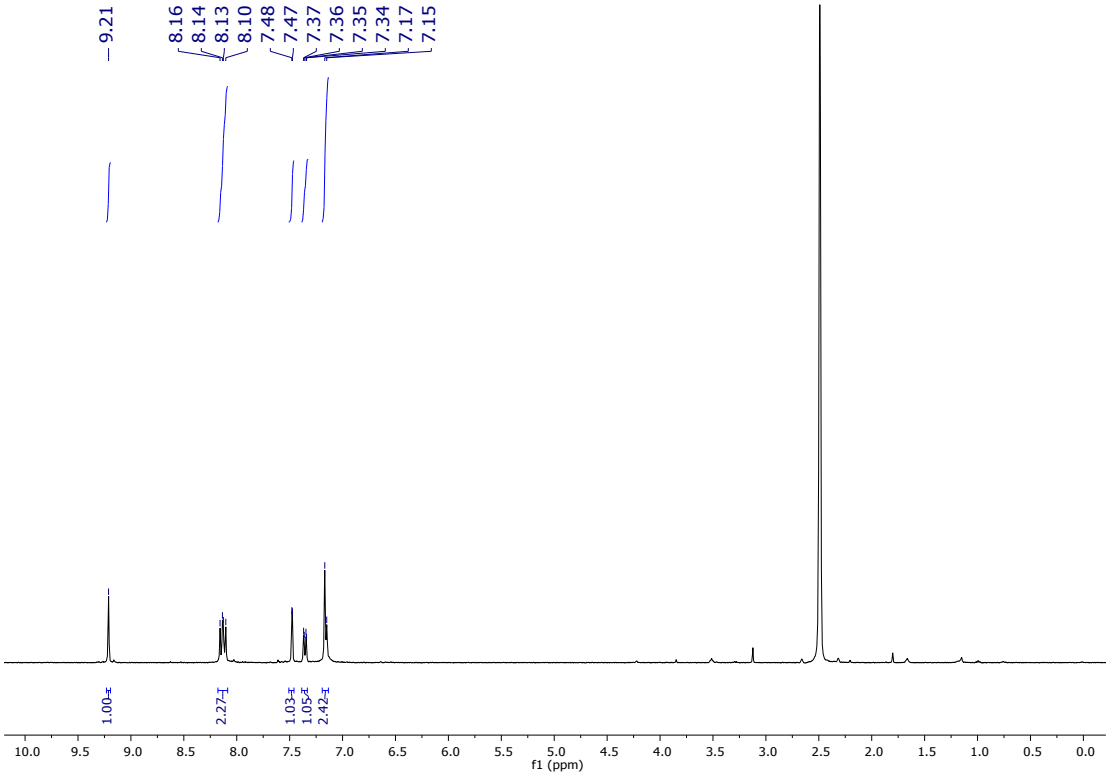


Figure S1. ^{1}H NMR of compound **4** in DMSO:TFA-d_1 (4:1)

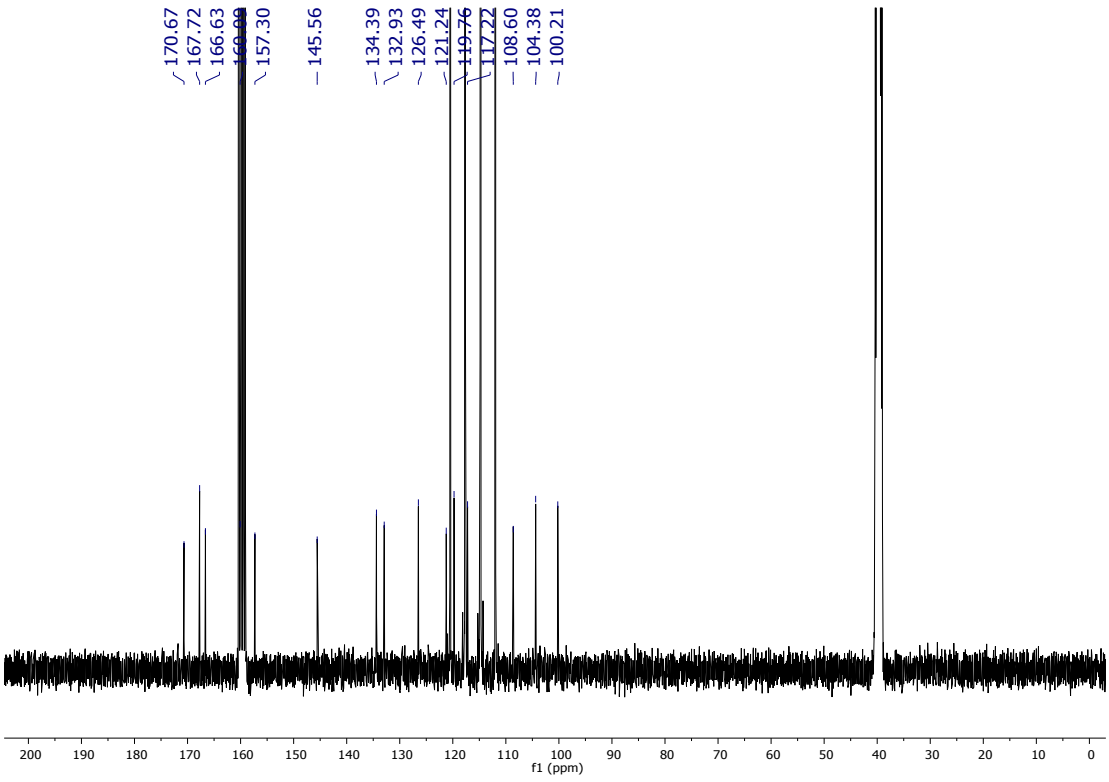


Figure S2. ^{13}C NMR of compound **4** in DMSO:TFA-d_1 (4:1)

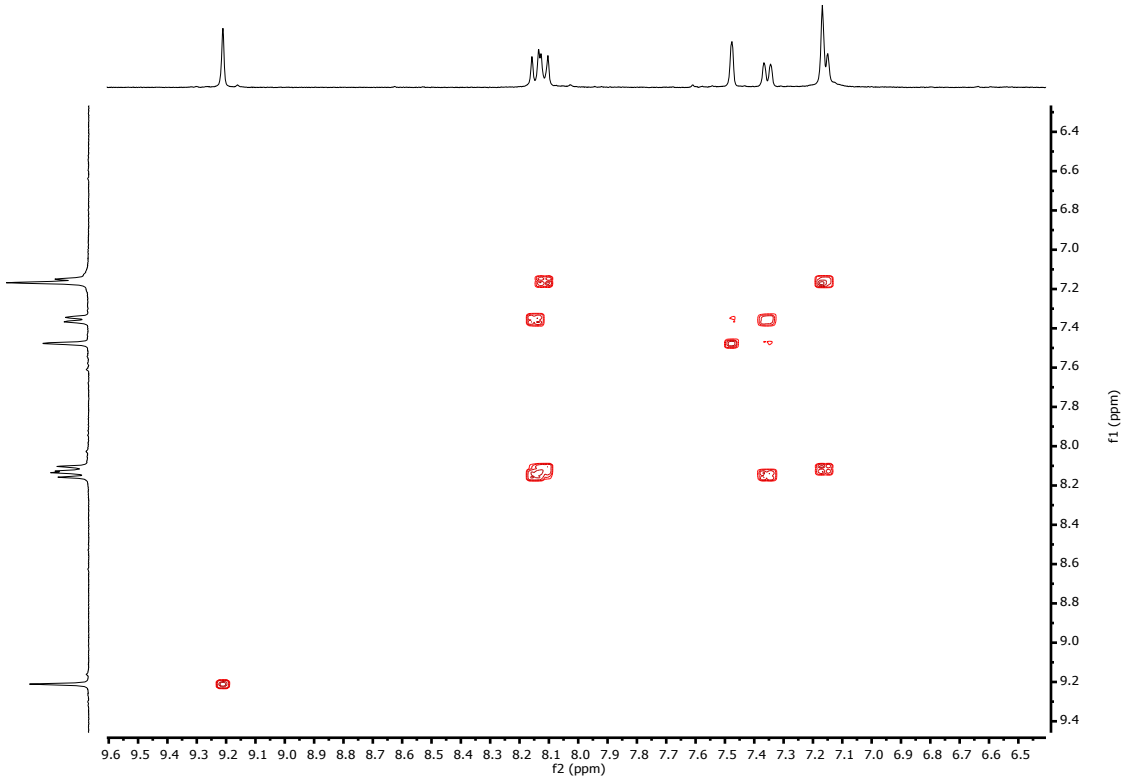


Figure S3. ^{1}H-^{1}H-COSY of compound **4** in DMSO:TFA-d_1 (4:1)

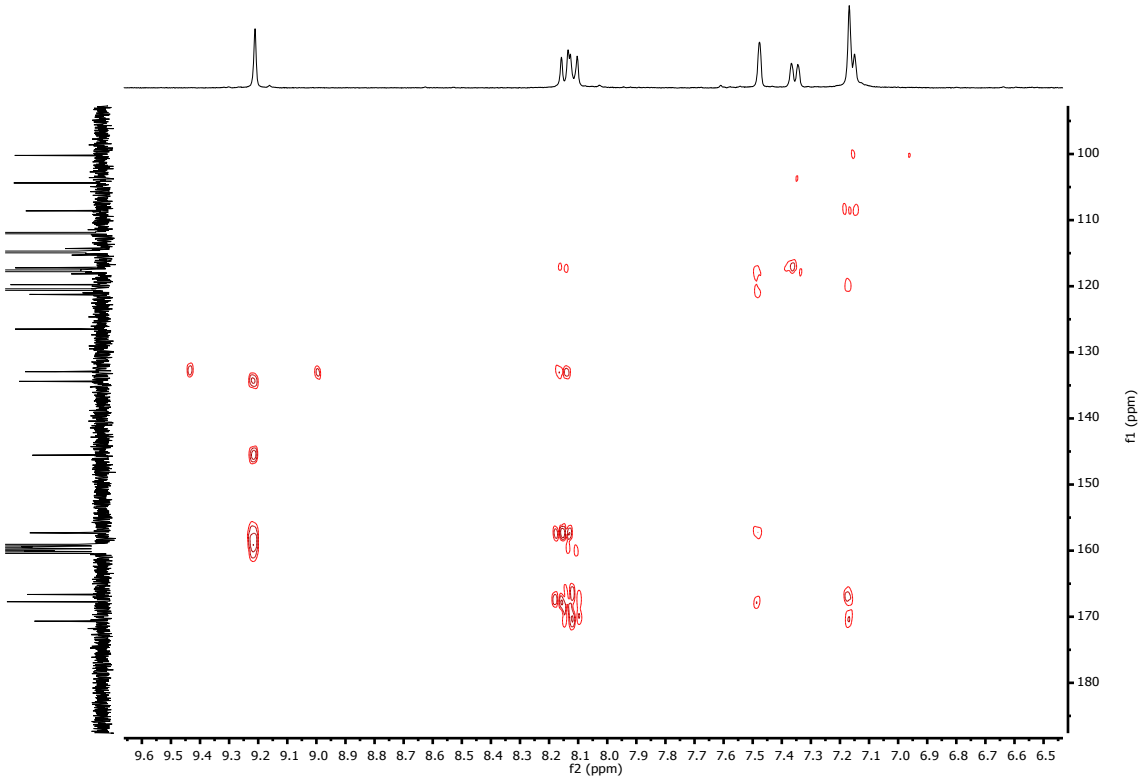
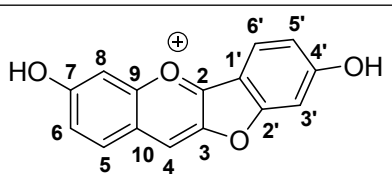


Figure S4. ^{1}H-^{13}C-HMBC of compound **4** in DMSO:TFA-d_1 (4:1)

Table S1 – ^{1}H-NMR and ^{13}C-NMR full peak assignment of compound **4** in DMSO:TFA-d_1 (4:1)

				
Position	**^{1}H δ/ppm (J/Hz)** DMSO:TFA-d_1 (4:1)	**^{13}C δ/ppm** DMSO:TFA-d_1 (4:1)	**HMBC** DMSO:TFA-d_1 (4:1)	**COSY** DMSO:TFA-d_1 (4:1)
1	-	-	-	-
2	-	160.1	4, 6’	-
3	-	145.6	4	-
4	9.21 (*s*)	132.9	2, 3, 5, 9	-
5	8.15 (*d*, 9.0)	139.4	4, 7, 9	6
6	7.35 (*dd*, 9.0, 2.2)	121.2	8, 10	5, 8
7	-	167.7	5, 8	-
8	7.48 (*d*, 2.2)	104.4	6, 10	6
9	-	157.3	4, 5, 8	-
10	-	117.2	6, 8	-
1’	-	108.6	3’, 5’	-
2’	-	166.3*	3’, 6’	-
3’	7.17 (*ov*)	100.2	1’, 2’, 4’, 5’	5’
4’	-	170.7*	3’, 6’	-
5’	7.17 (*ov*)	119.8	1’, 3’	3’, 6’
6’	8.12 (*d*, 9.1)	126.5	2, 2’, 4’	5’

*these signals may be interchangeables.