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Supplementary Information

Efficient Synthesis of Novel Pyranoquinoline Derivatives from Simple Acetanilide Derivatives: Experimental and Theoretical Study of their Physicochemical Properties using DFT Calculations

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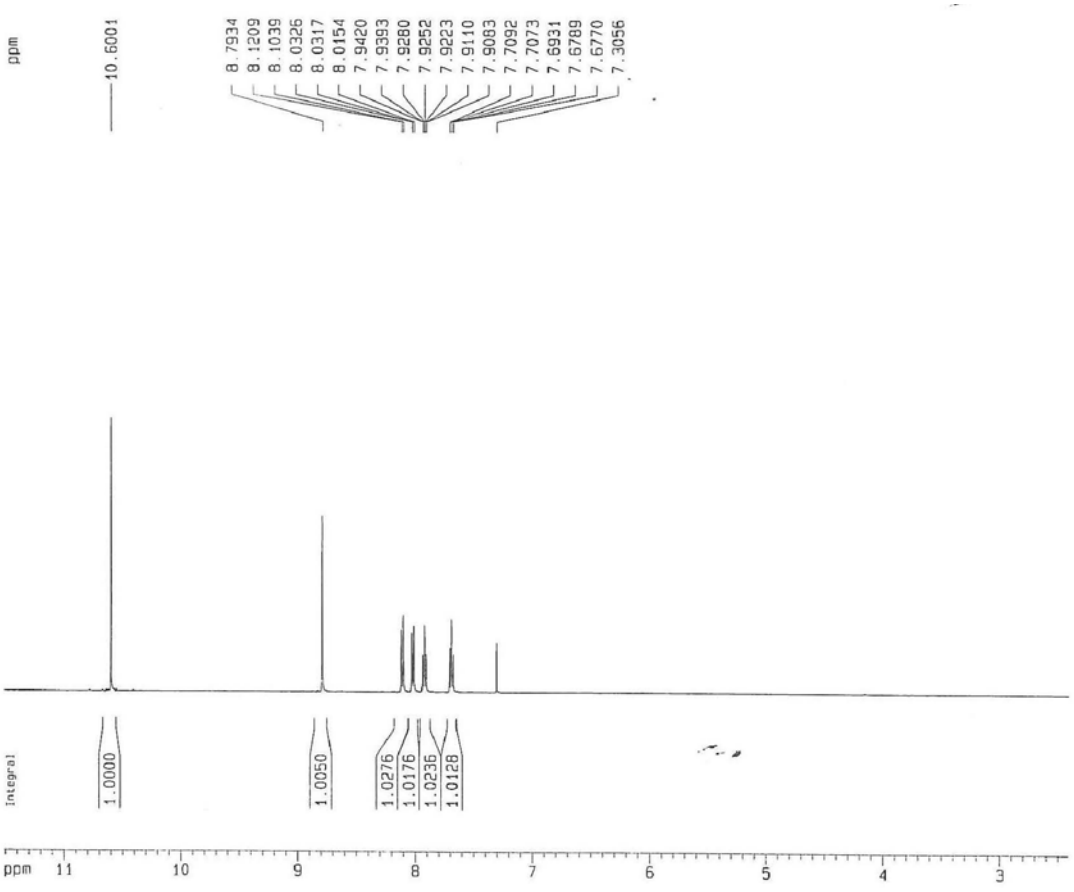

Figure S1. ^{1}H NMR of spectrum **3a** ($CDCl_3$, 500 MHz).

*e-mail: h_porkaleh@yahoo.com

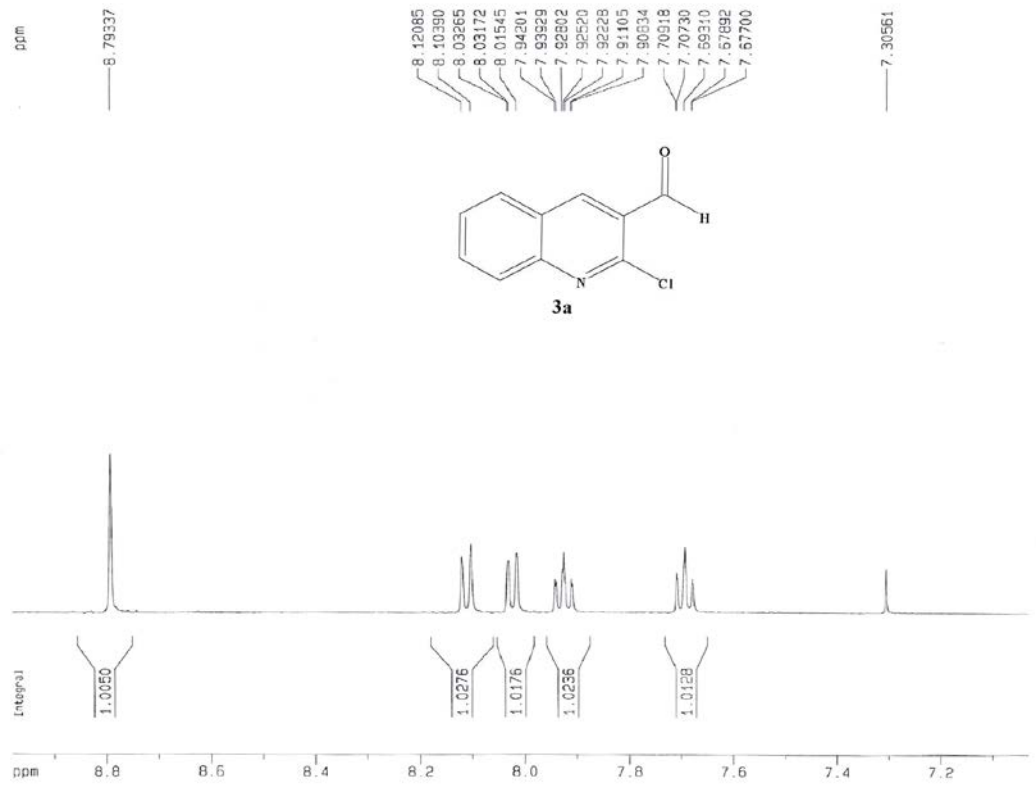

Figure S2. ^{1}H NMR spectrum of **3a** ($CDCl_3$, 500 MHz).

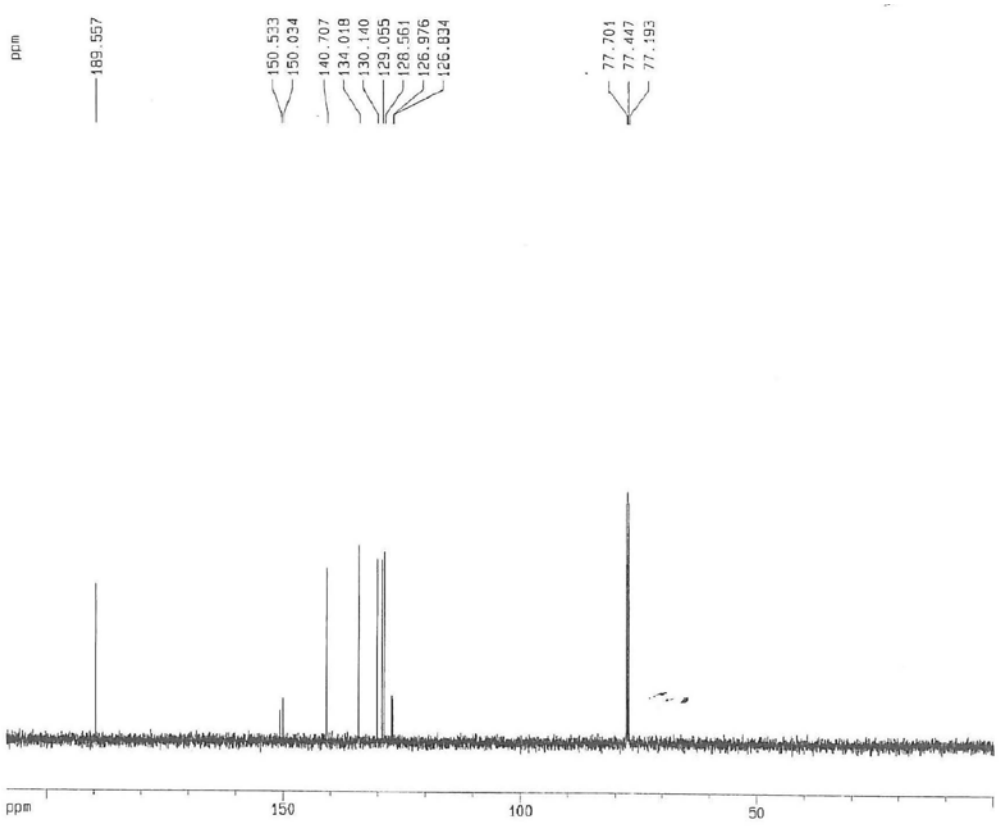

Figure S3. ^{13}C NMR spectrum of **3a** ($CDCl_3$, 125 MHz).

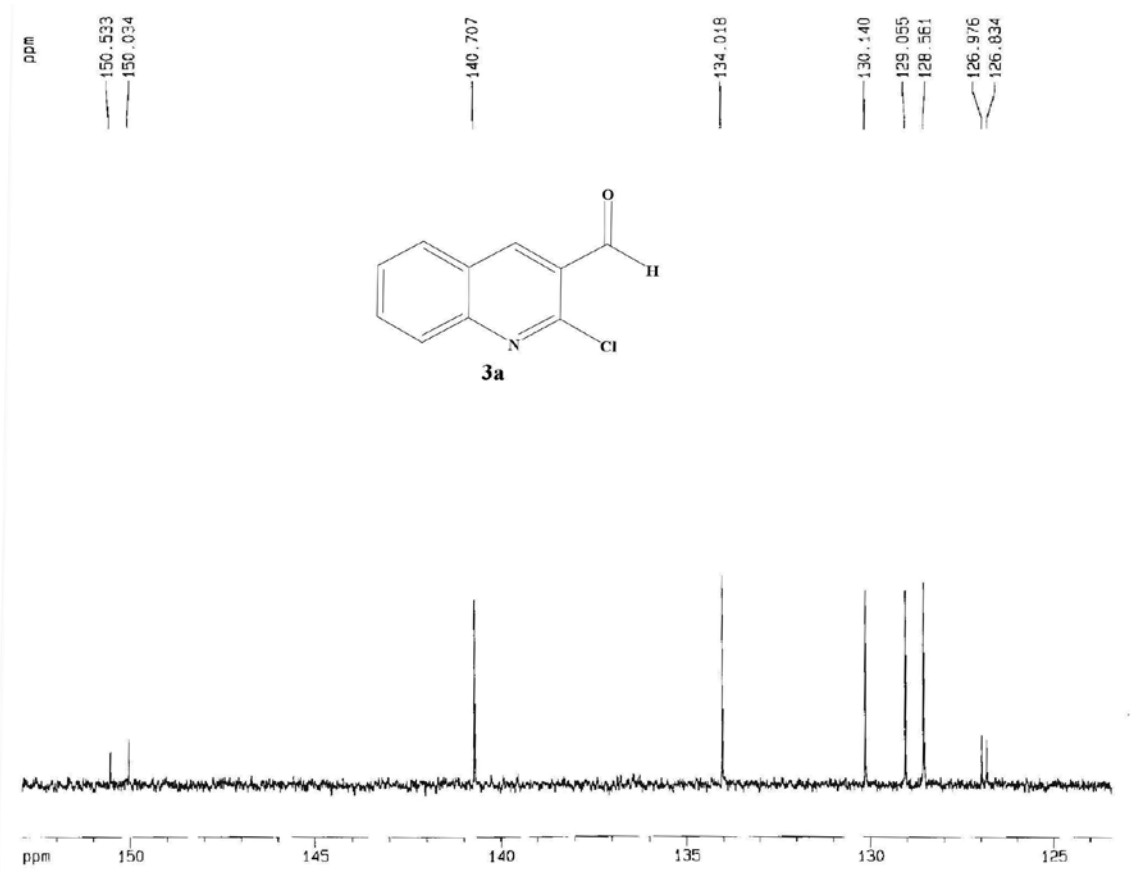

Figure S4. ^{13}C NMR spectrum of **3a** ($CDCl_3$, 125 MHz).

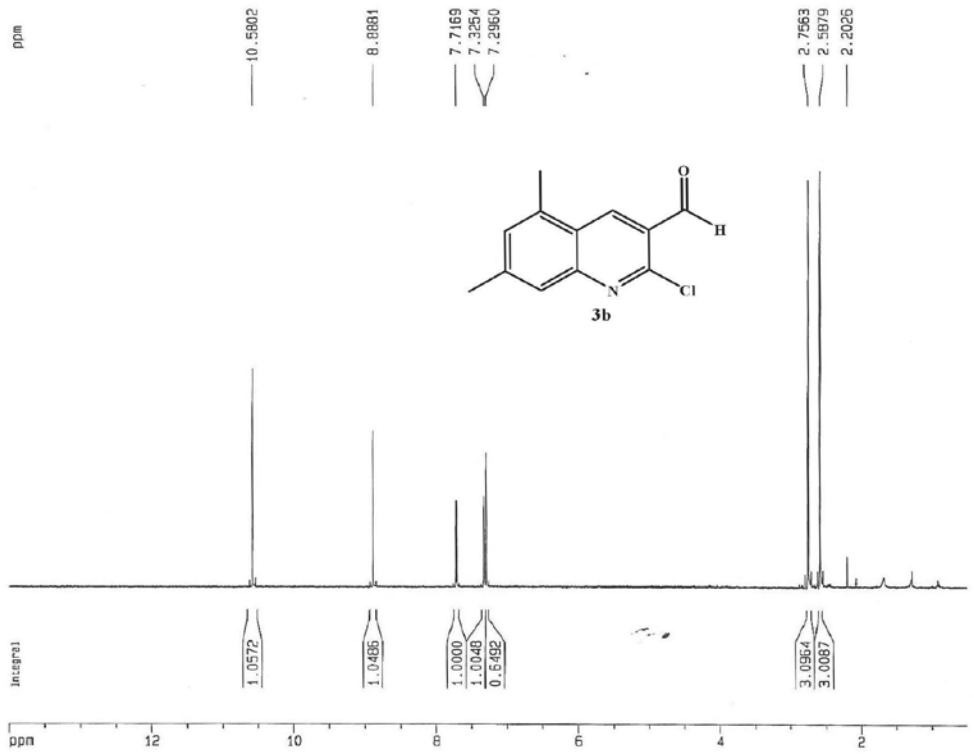

Figure S5. ^{1}H NMR spectrum of **3b** ($CDCl_3$, 500 MHz).

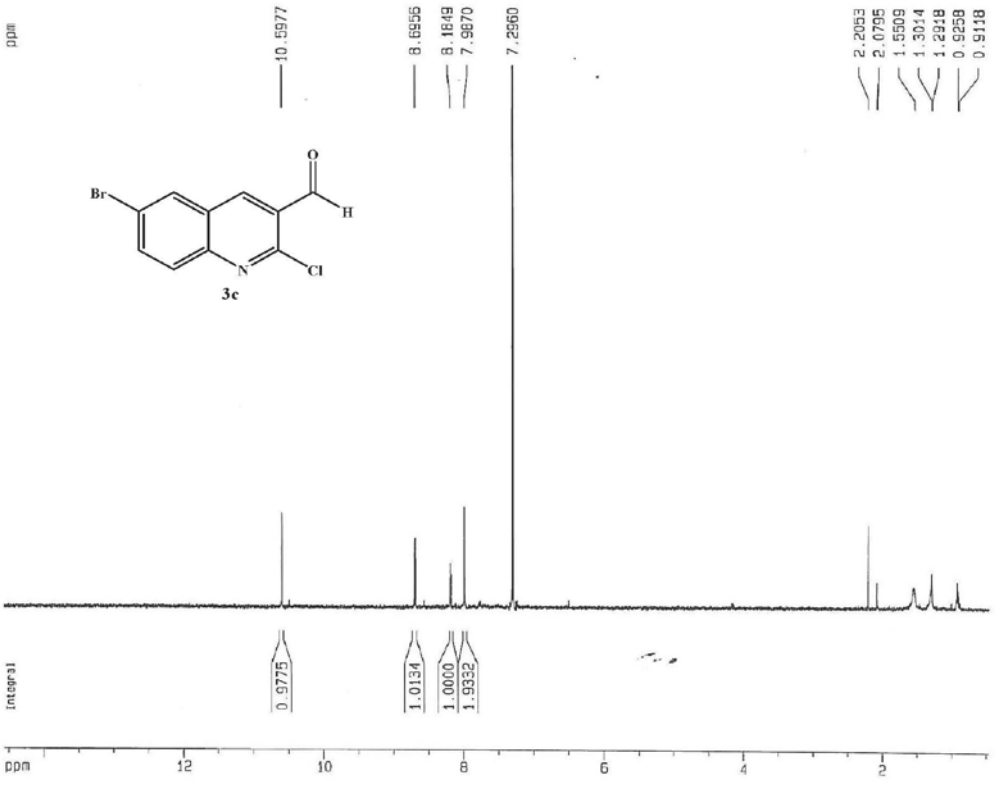

Figure S6. ^{1}H NMR spectrum of **3c** ($CDCl_3$, 500 MHz).

Figure S7. ^{1}H NMR spectrum of **3d** ($CDCl_3$, 500 MHz).

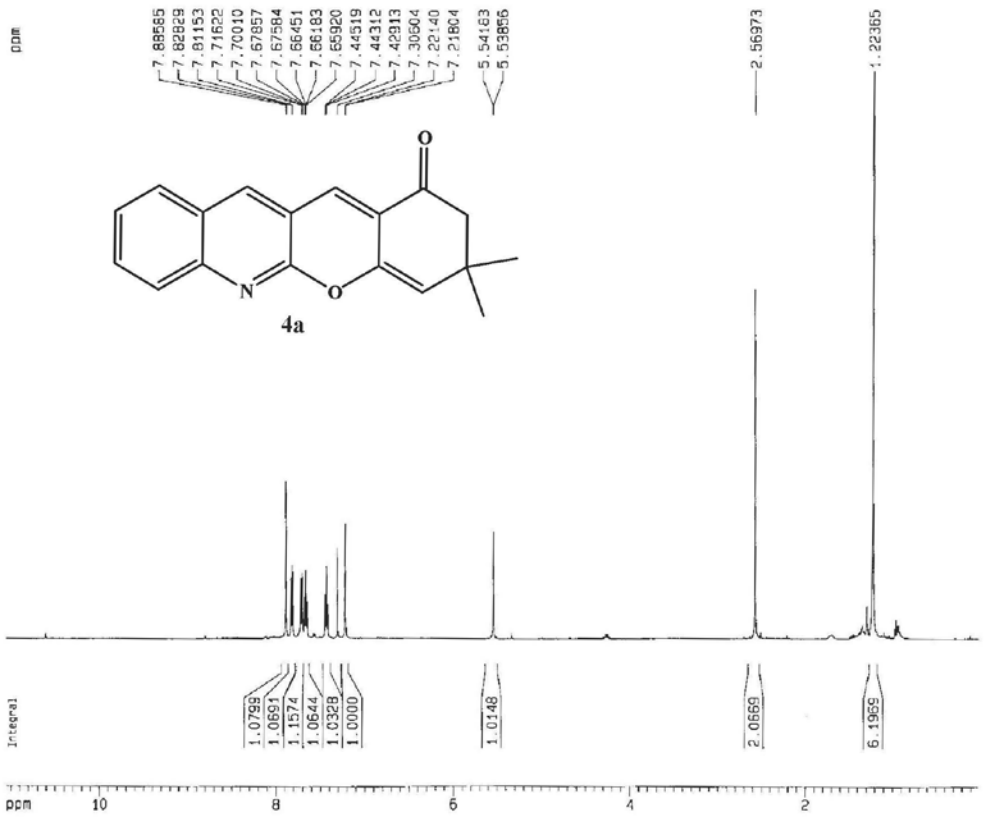

Figure S8. ^{1}H NMR spectrum of **4a** ($CDCl_3$, 500 MHz).

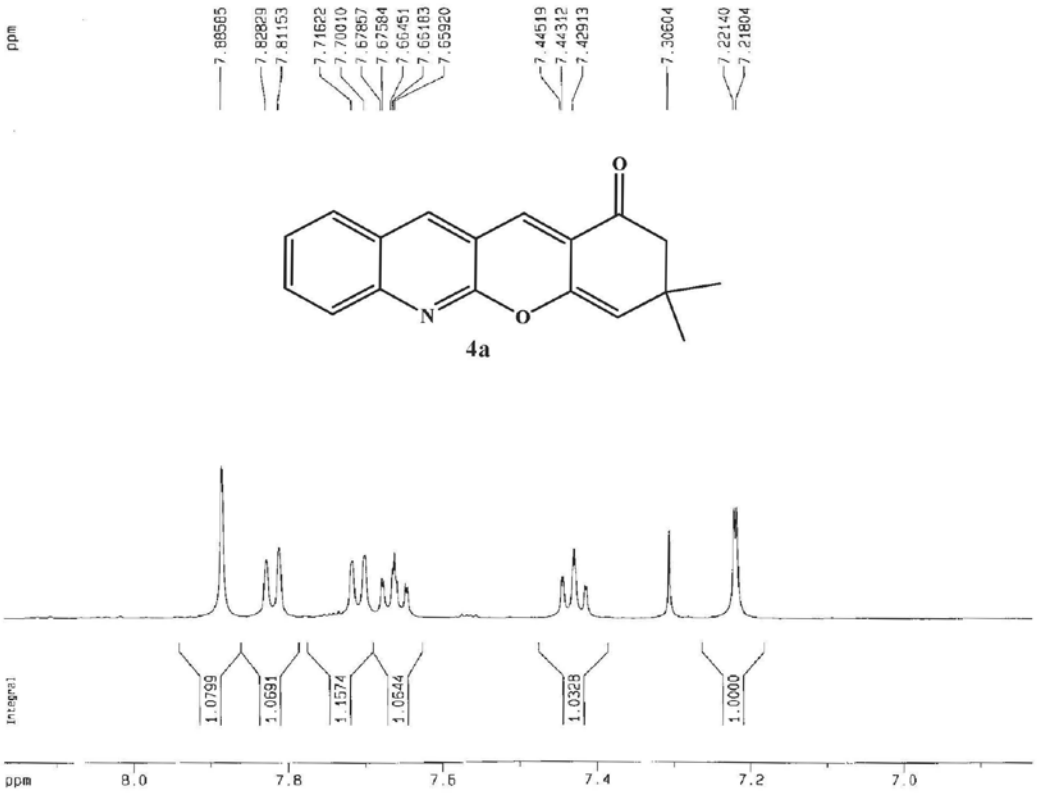

Figure S9. ^{1}H NMR spectrum of **4a** ($CDCl_3$, 500 MHz).

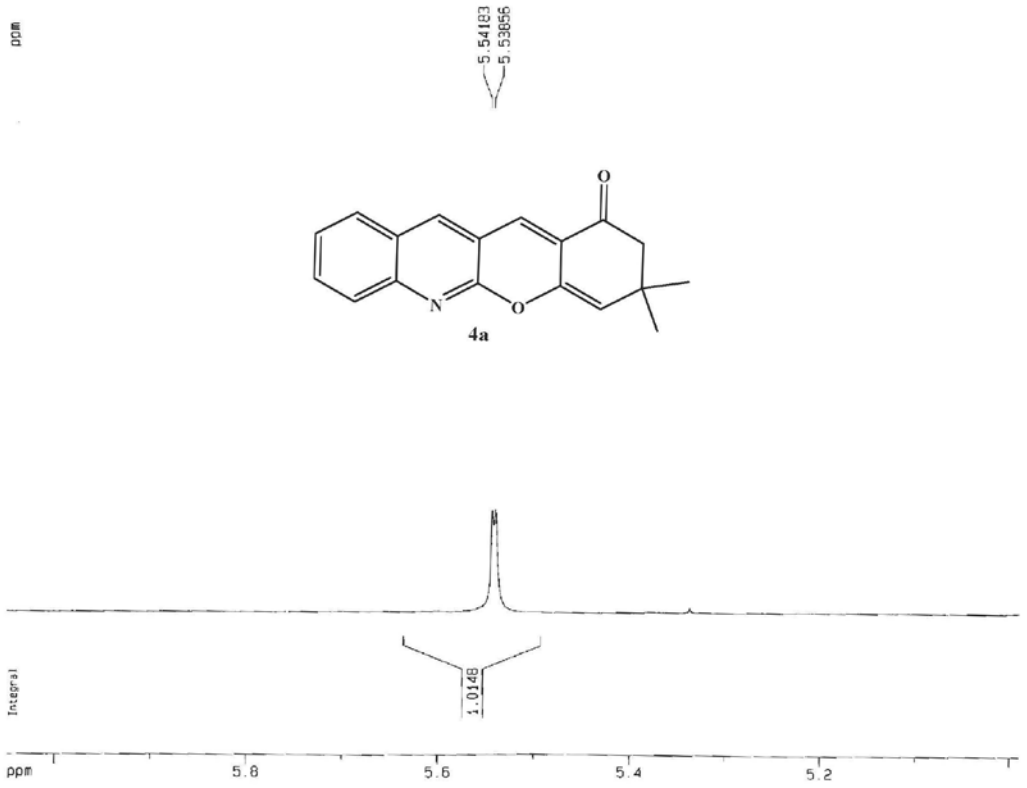

Figure S10. ^{1}H NMR spectrum of **4a** ($CDCl_3$, 500 MHz).

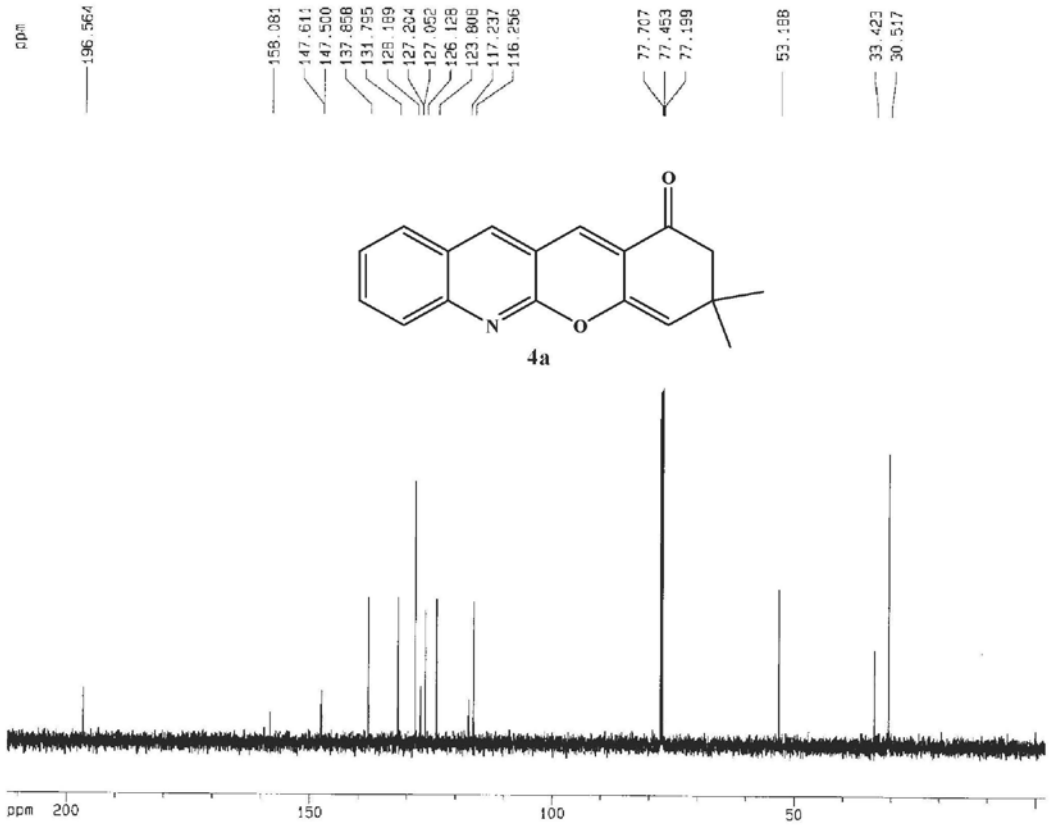

Figure S11. ^{13}C NMR spectrum of **4a** ($CDCl_3$, 125 MHz).

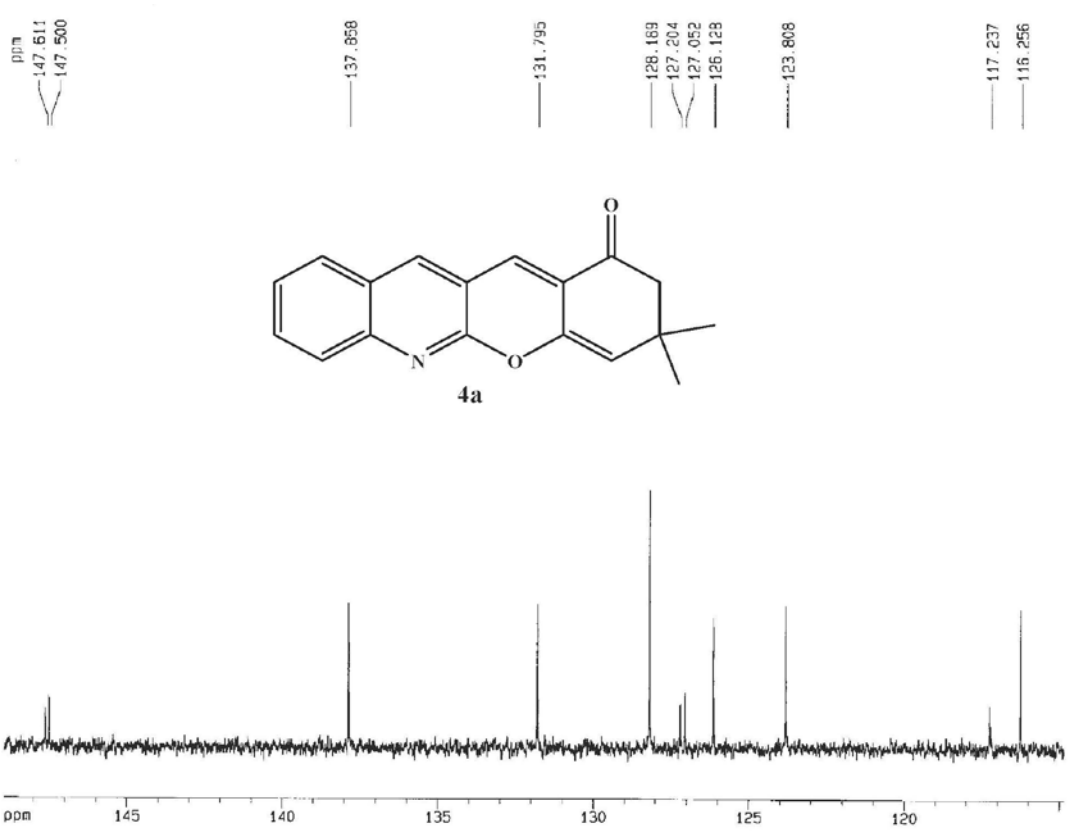

Figure S12. ^{13}C NMR spectrum of **4a** ($CDCl_3$, 125 MHz).

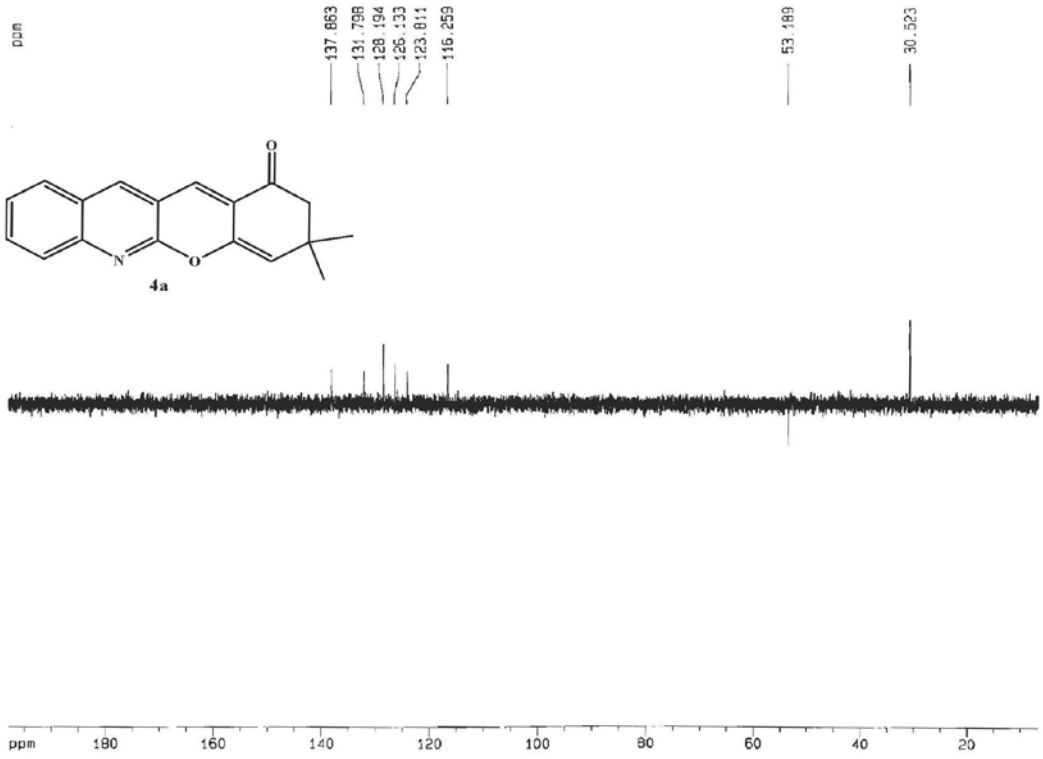

Figure S13. ^{13}C NMR (DEPT 135) spectrum of **4a** ($CDCl_3$, 125 MHz).

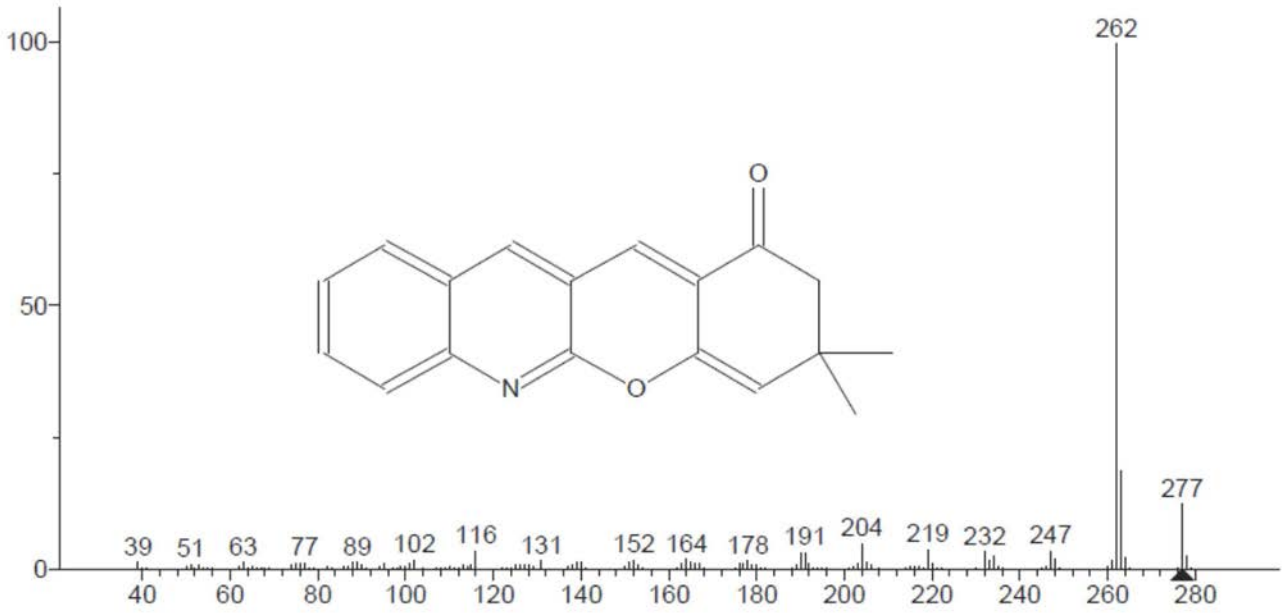

Figure S14. EI-MS spectrum of **4a**.

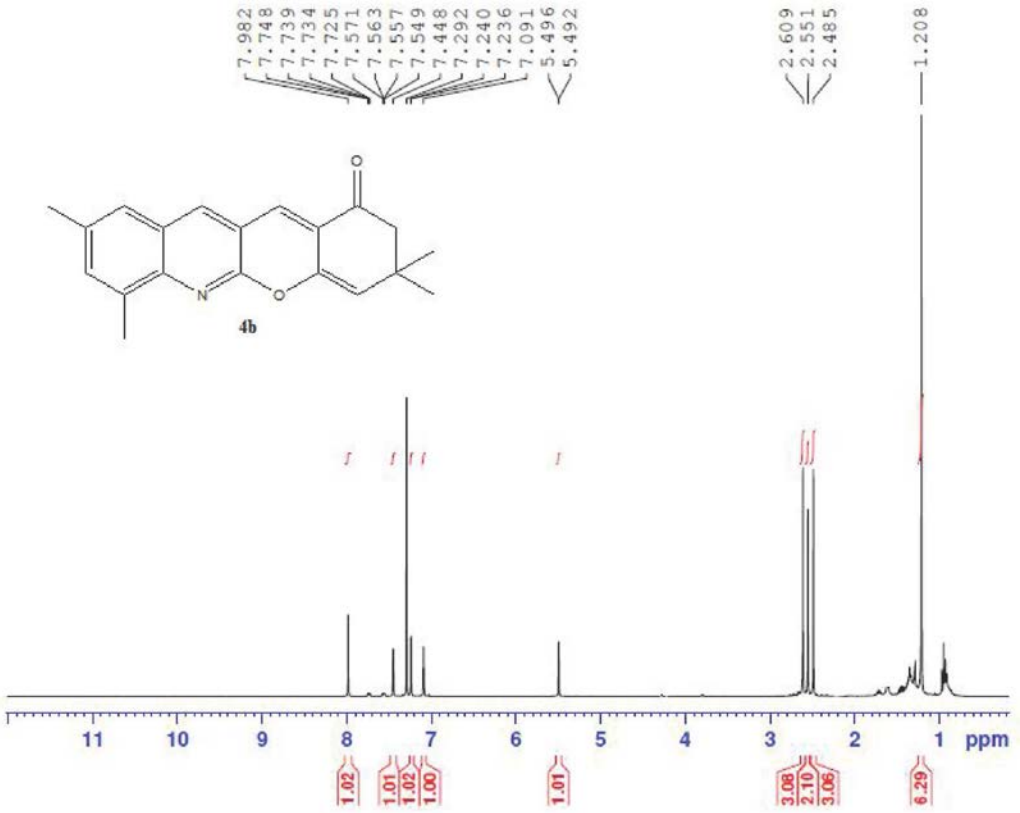

Figure S15. ^{1}H NMR spectrum of **4b** ($CDCl_3$, 400 MHz).

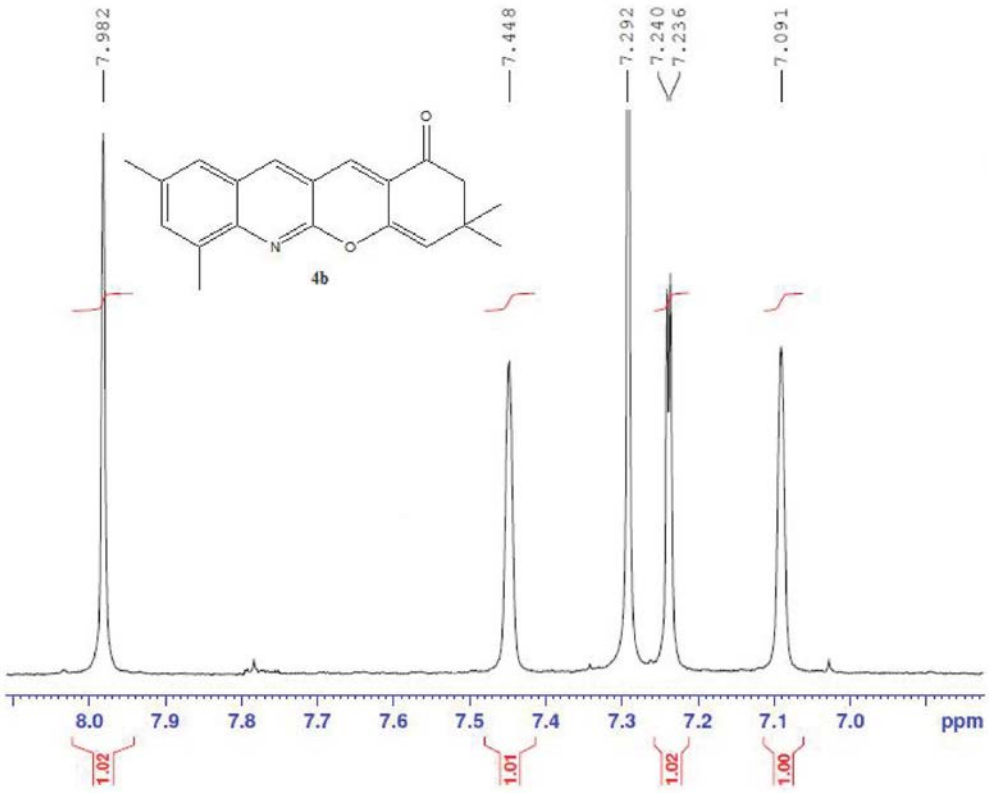

Figure S16. ^{1}H NMR spectrum of **4b** ($CDCl_3$, 400 MHz).

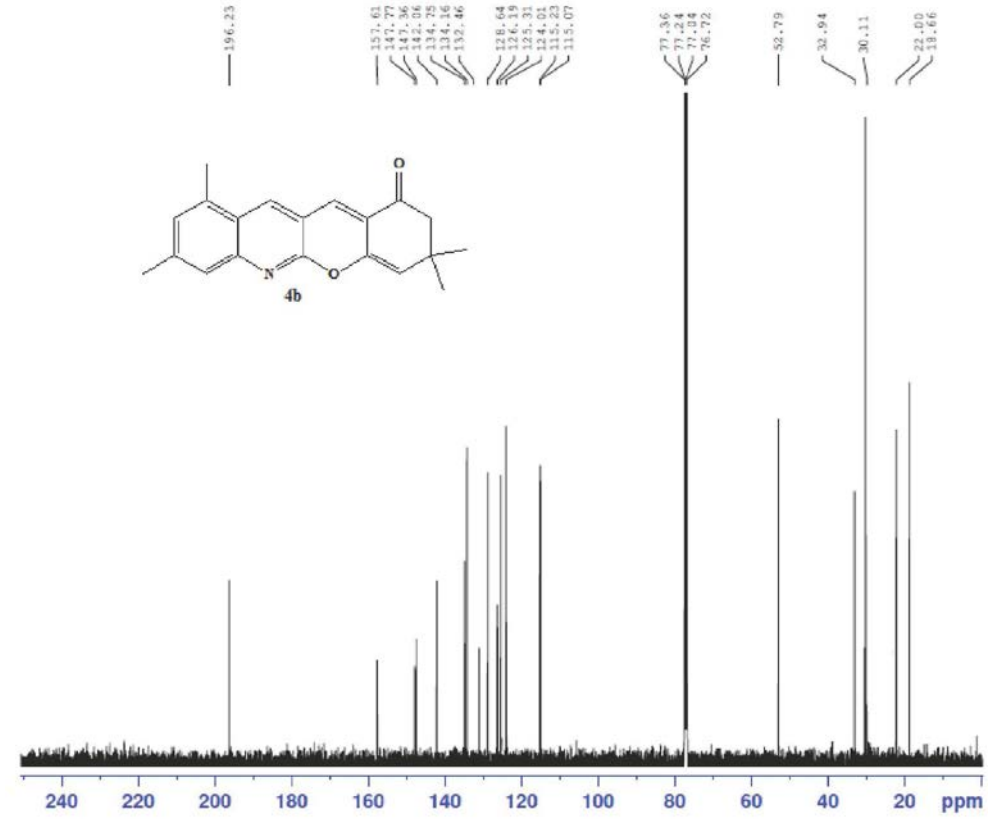

Figure S17. ^{13}C NMR spectrum of **4b** ($CDCl_3$, 100 MHz).

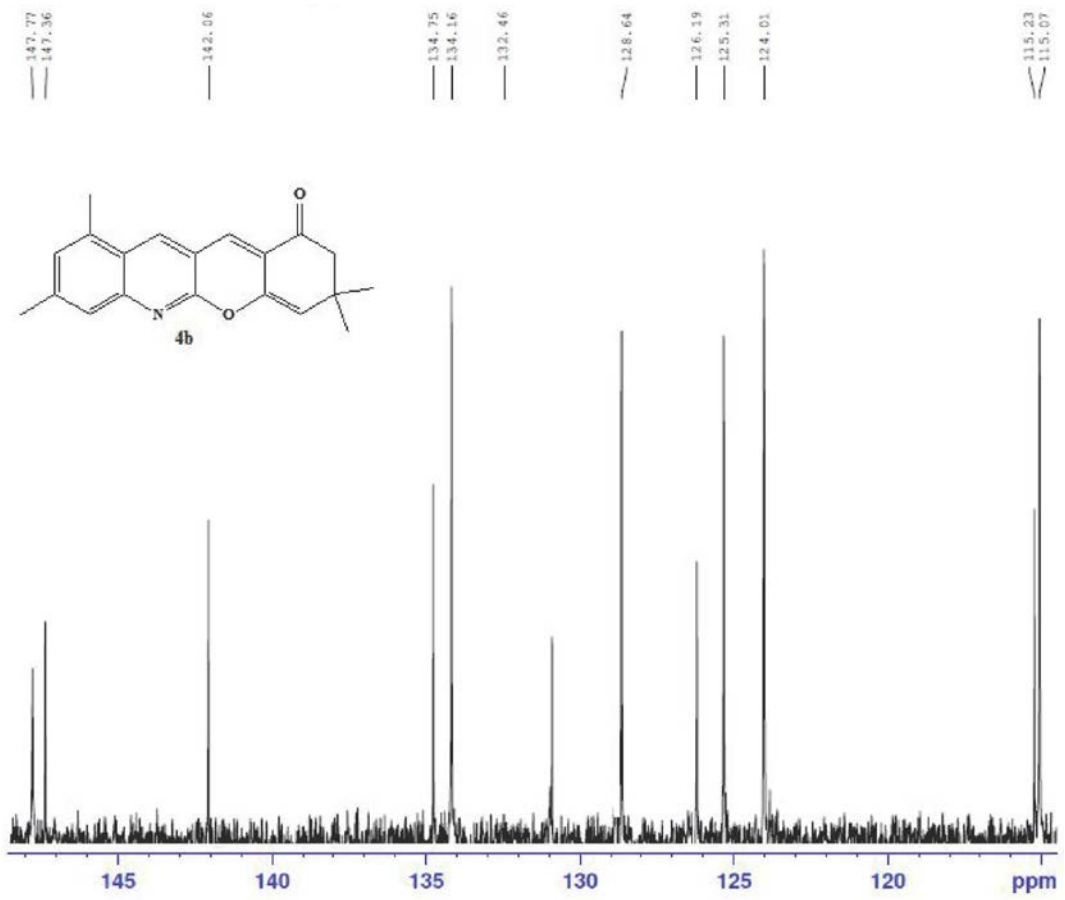

Figure S18. ^{13}C NMR spectrum of **4b** ($CDCl_3$, 100 MHz).

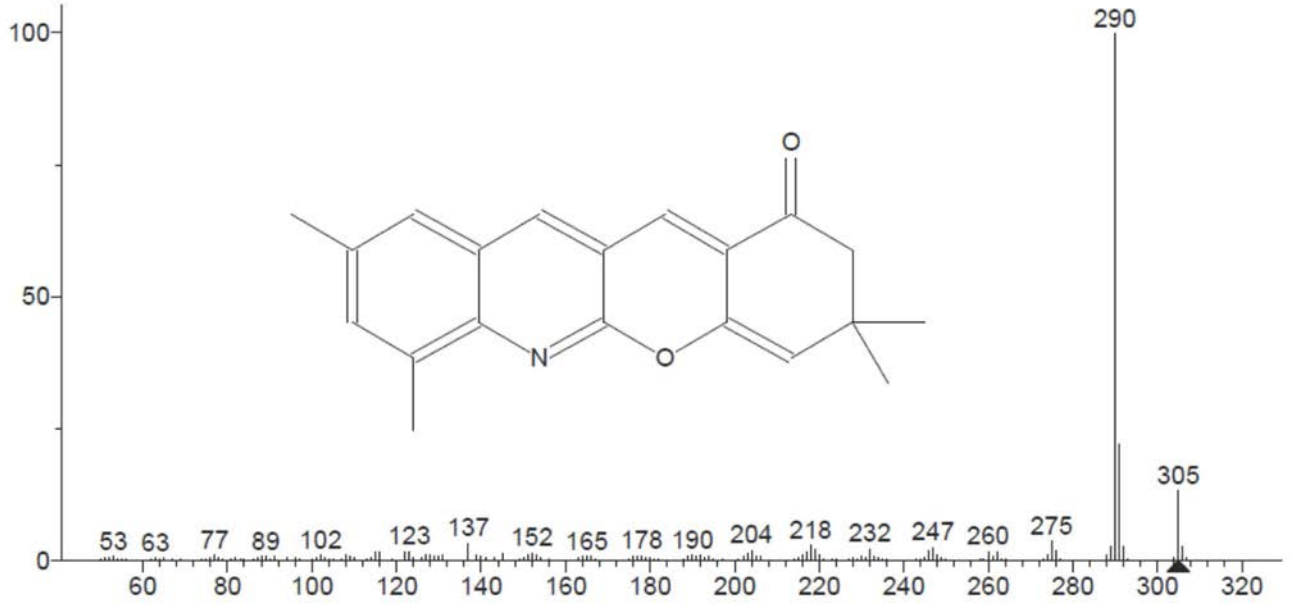

Figure S19. EI-MS spectrum of **4b**.

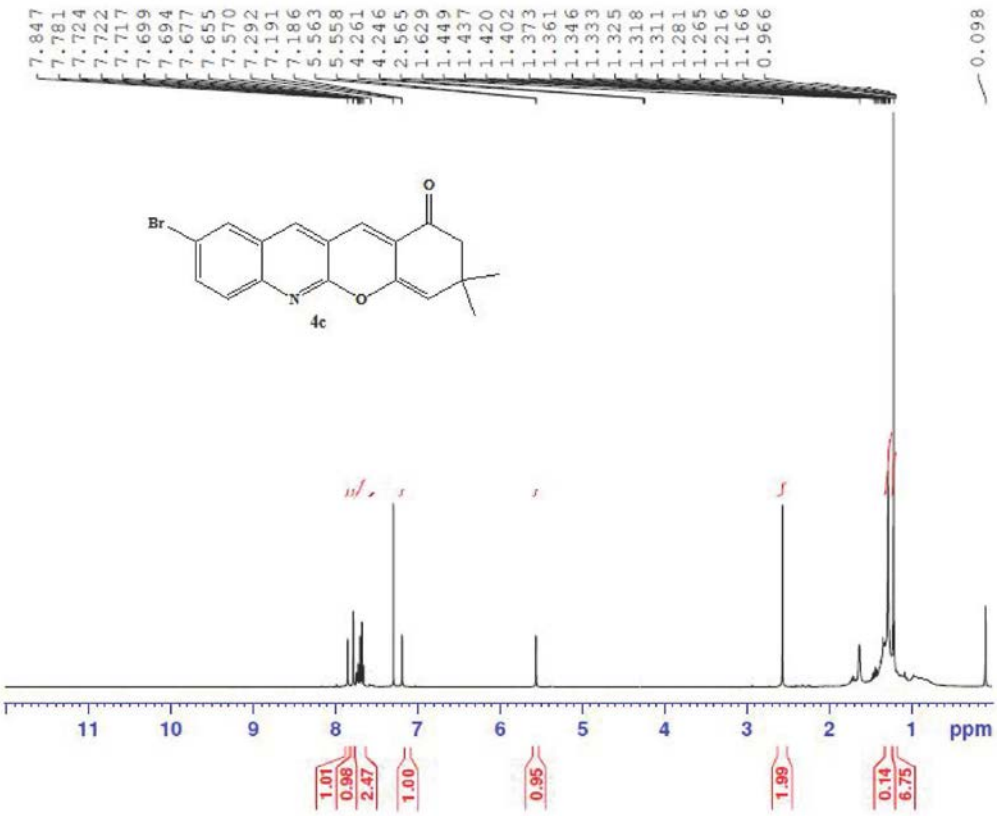

Figure S20. ^{1}H NMR spectrum of **4c** ($CDCl_3$, 400 MHz).

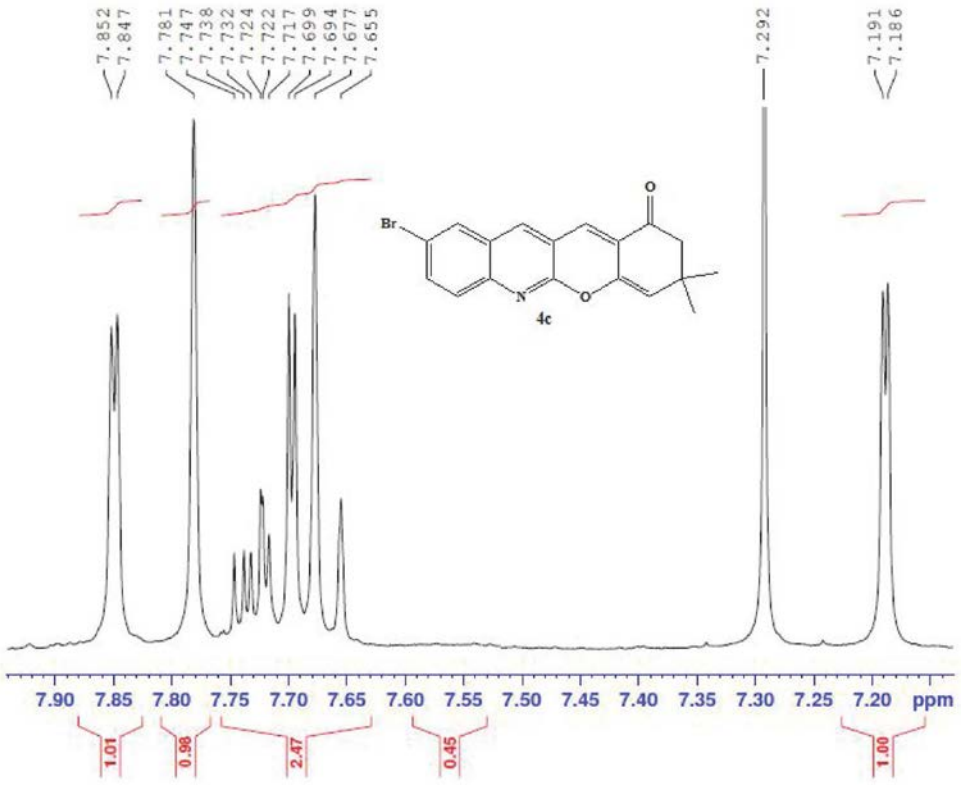

Figure S21. ^{1}H NMR spectrum of **4c** ($CDCl_3$, 400 MHz).

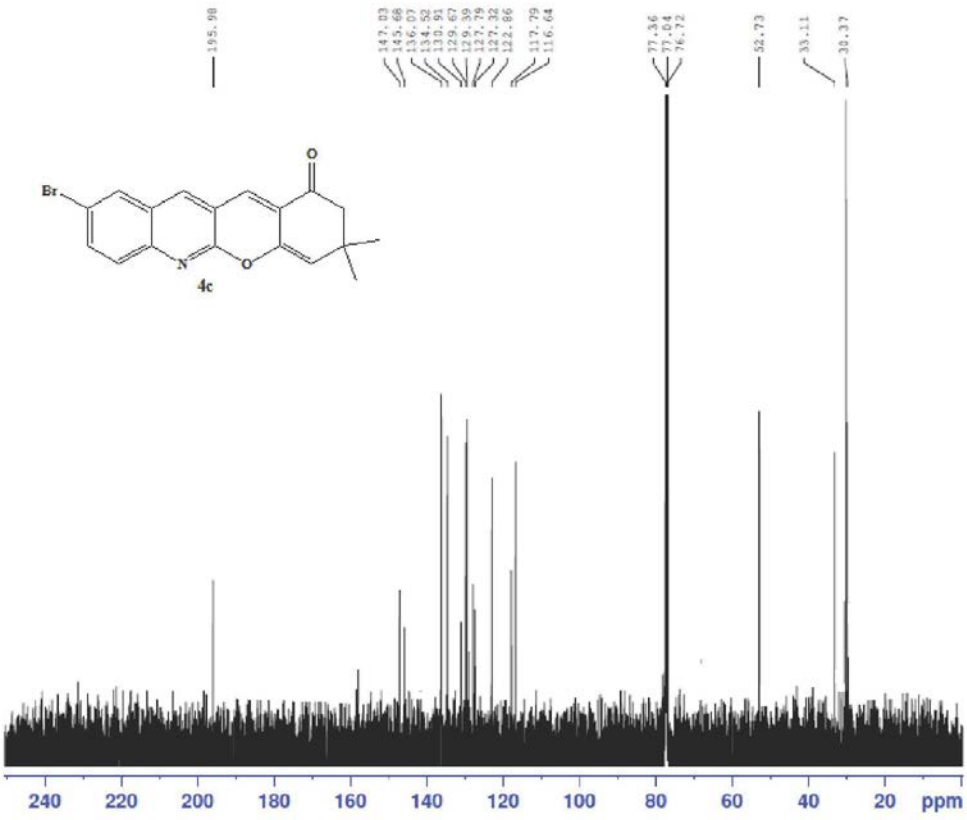

Figure S22. ^{13}C NMR spectrum of **4c** ($CDCl_3$, 100 MHz).

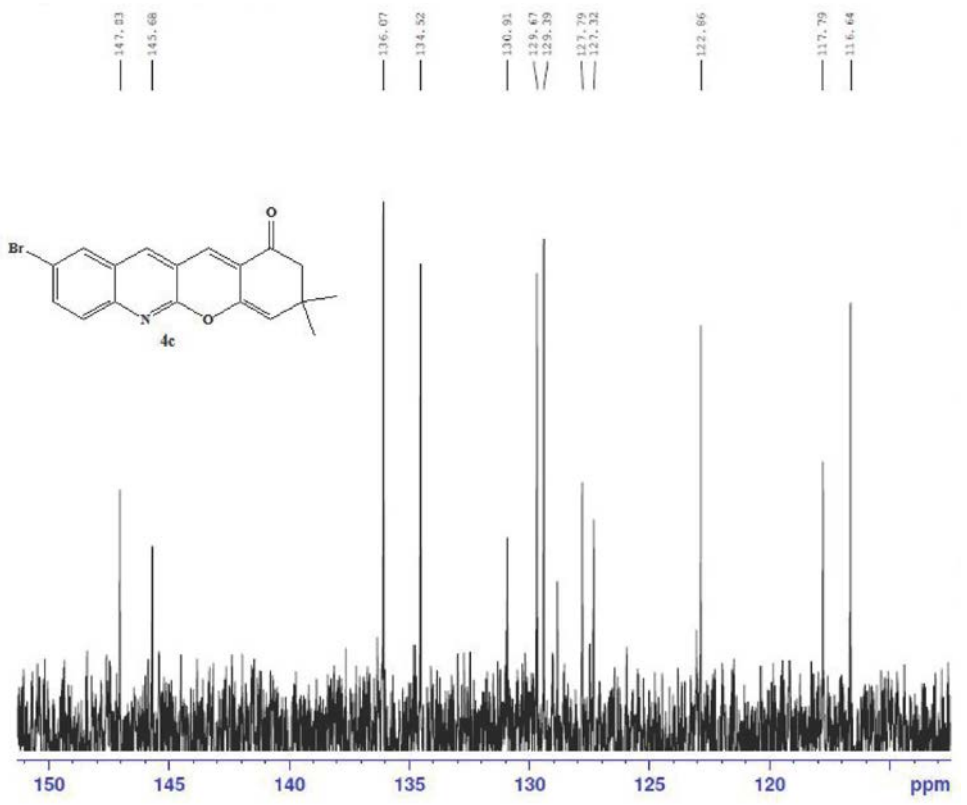

Figure S23. ^{13}C NMR spectrum of **4c** ($CDCl_3$, 100 MHz).

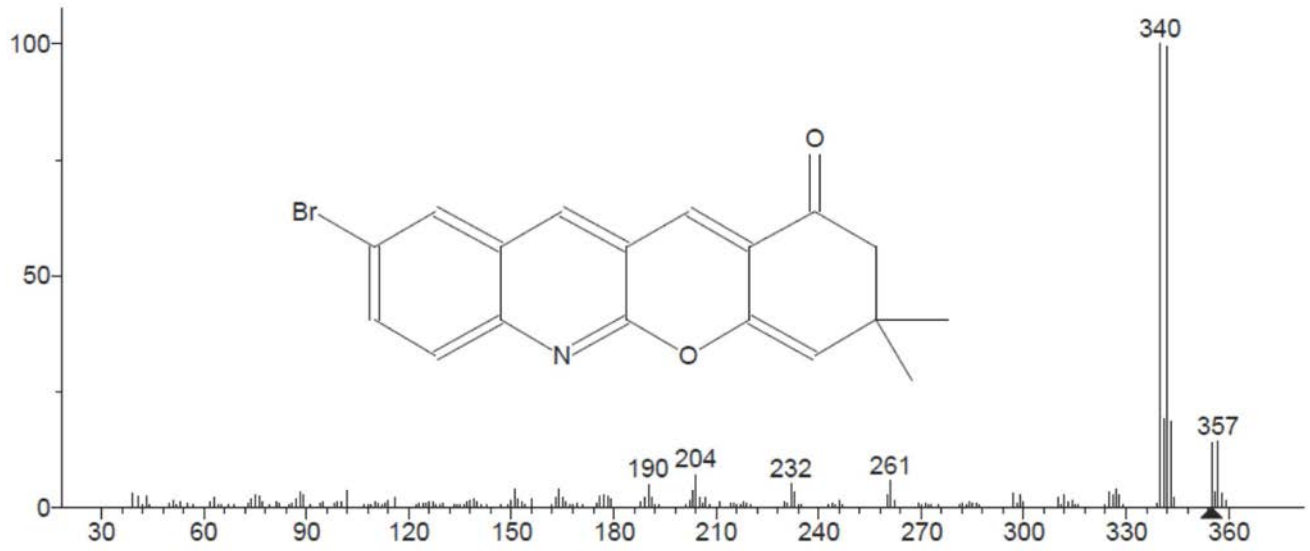

Figure S24. EI-MS spectrum of **4c**.

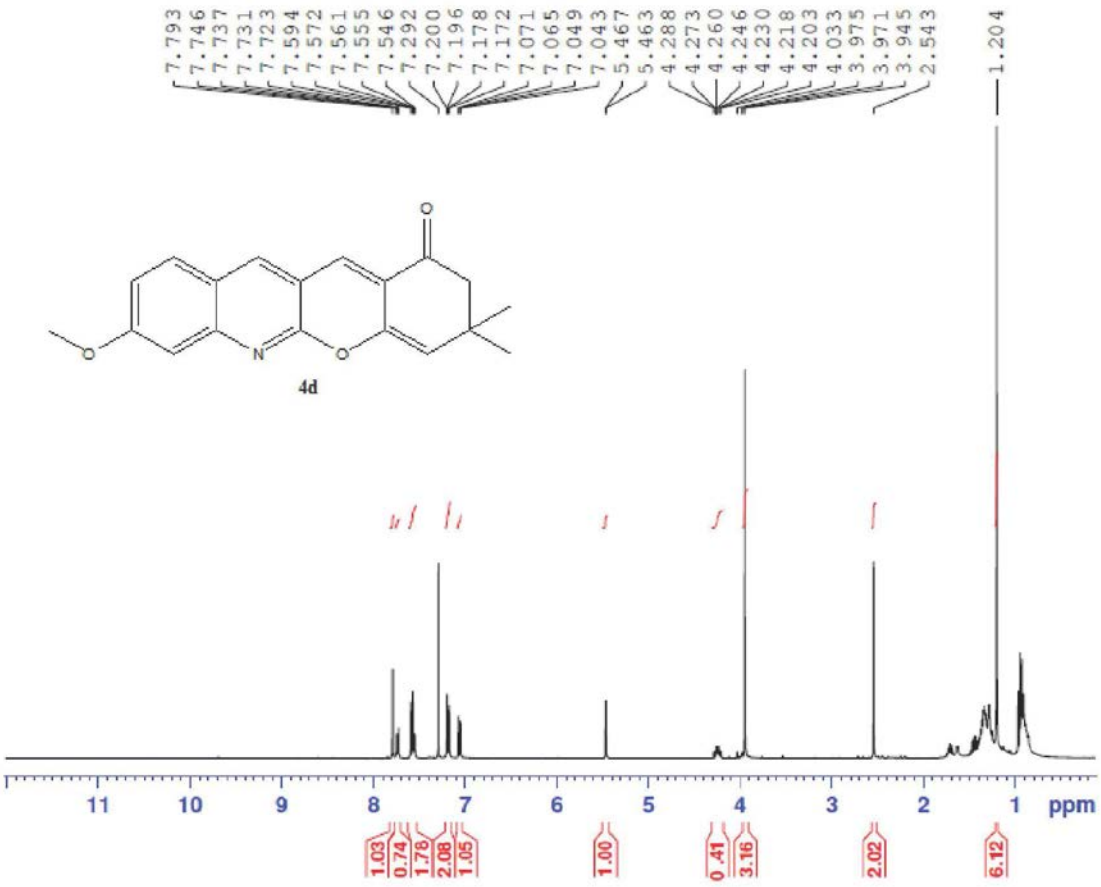

Figure S25. ^{1}H NMR spectrum of **4d** ($CDCl_3$, 400 MHz).

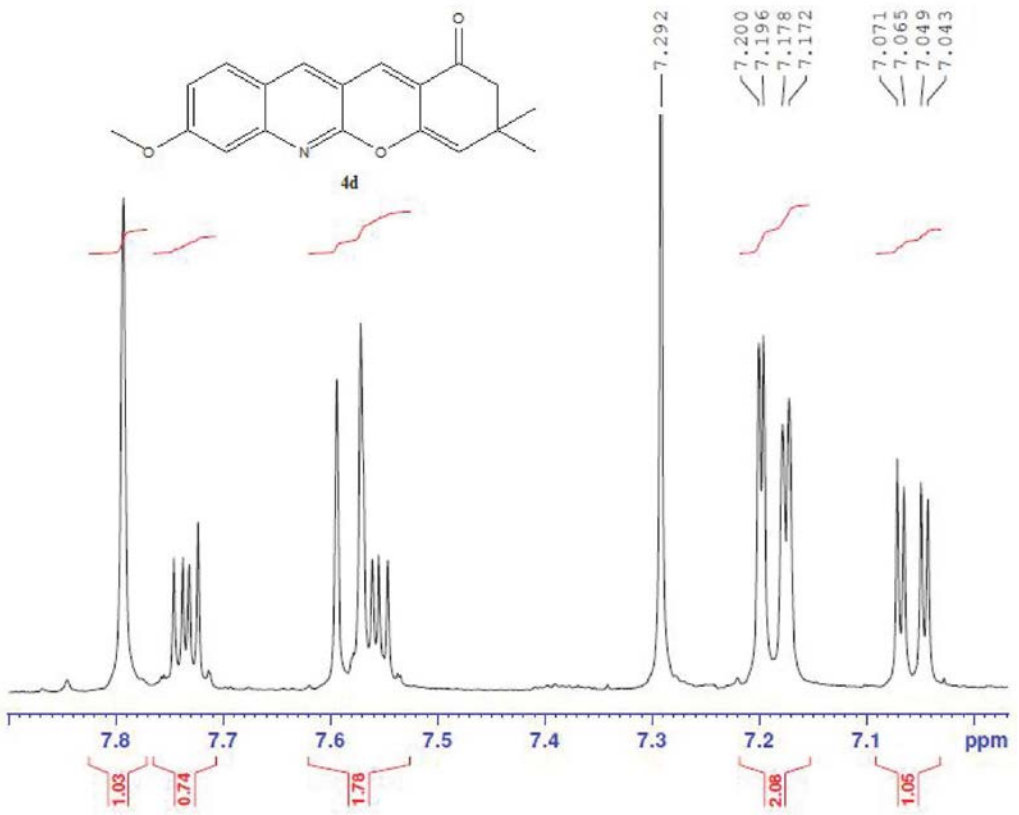

Figure S26. ^{1}H NMR spectrum of **4d** ($CDCl_3$, 400 MHz).

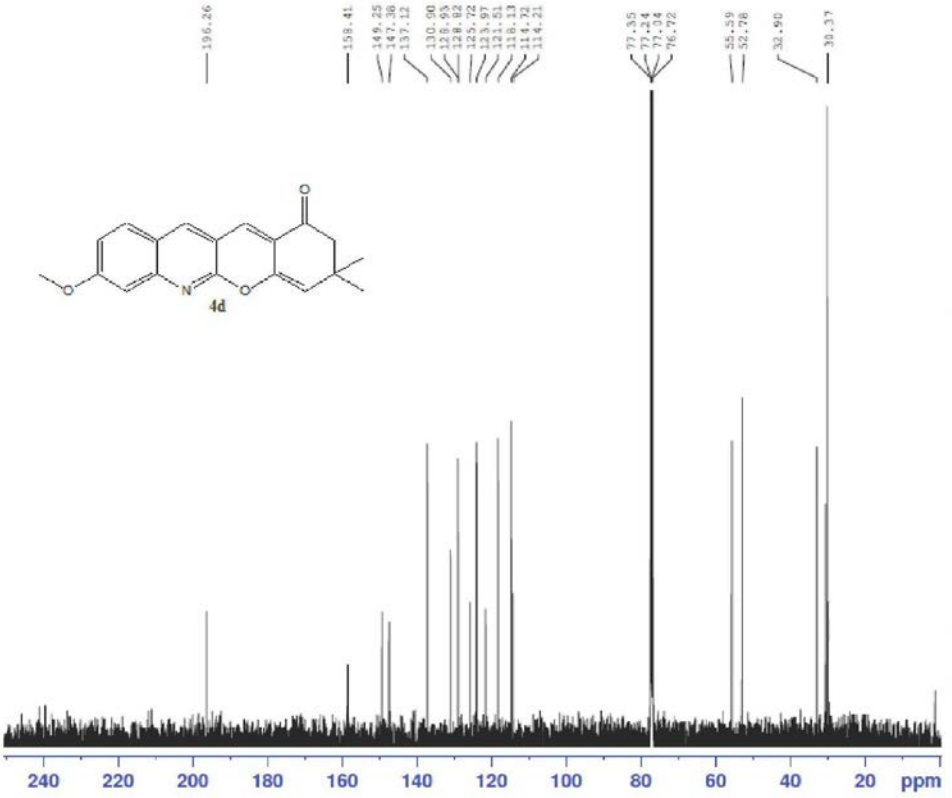

Figure S27. ^{13}C NMR spectrum of **4d** ($CDCl_3$, 100 MHz).

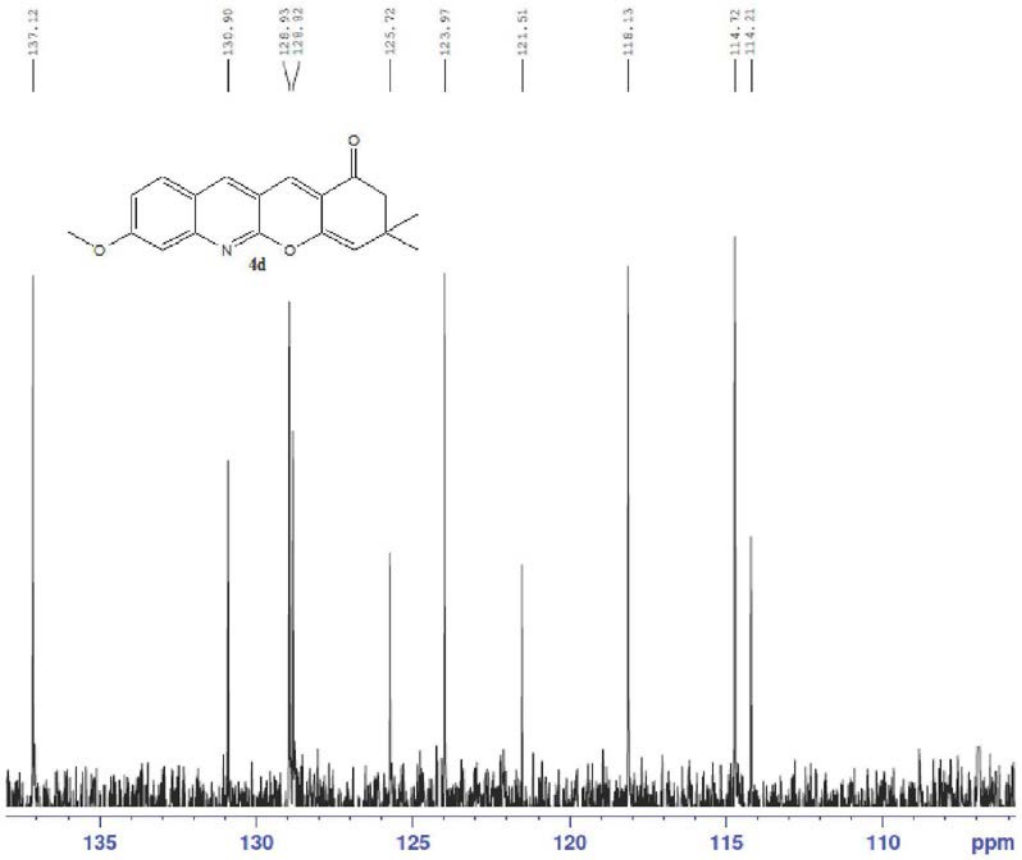

Figure S28. ^{13}C NMR spectrum of **4d** ($CDCl_3$, 100 MHz).

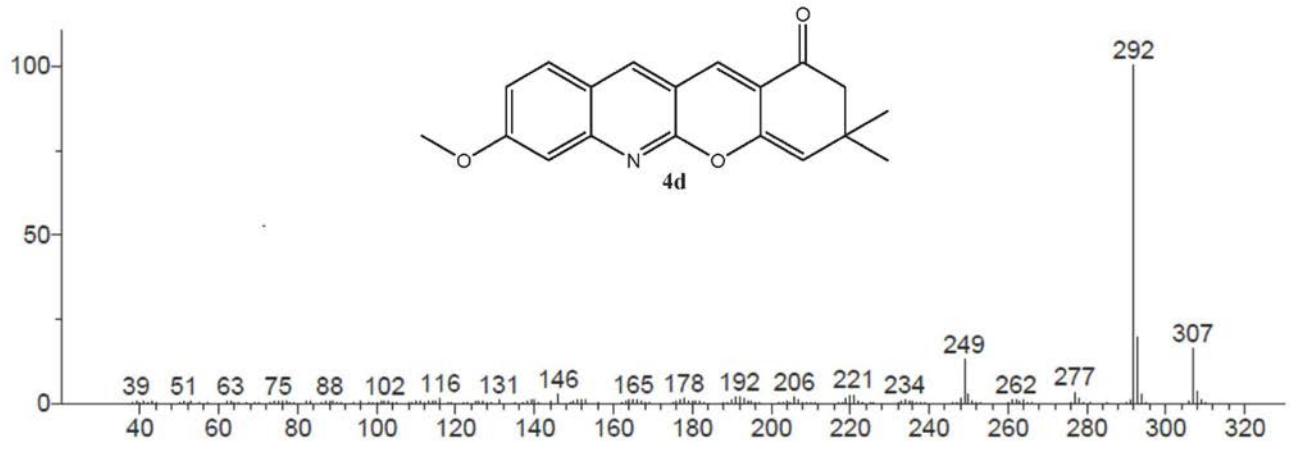

Figure S29. EI-MS spectrum of **4d**.

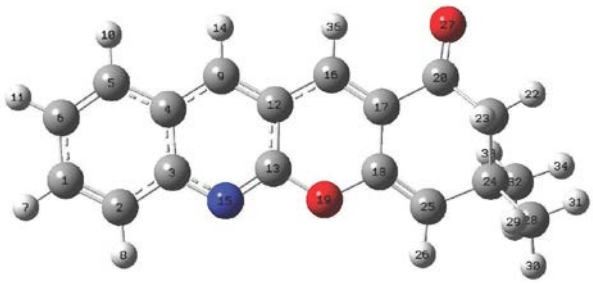

Figure S30. Atom numbering in accordance with molecular structure of pyranoquinoline **5a**.

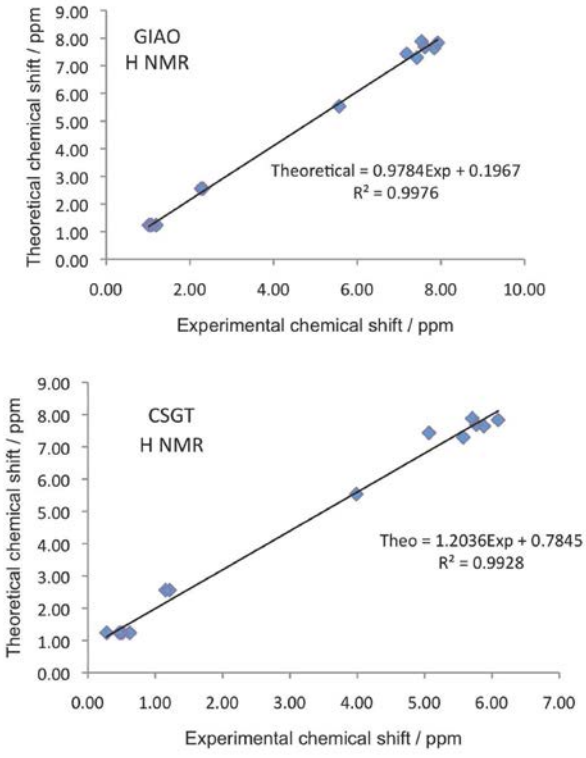

Figure S31. Correlation coefficient for ^{1}H NMR chemical shifts in GIAO and CSGT methods for pyranoquinoline **5a.**

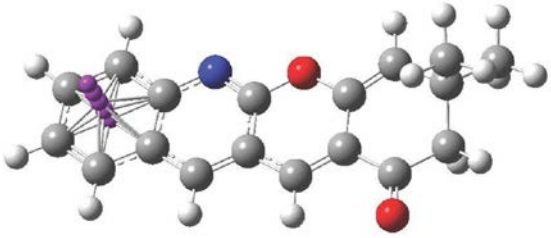

Figure S32. NMR calculations with molecular structure of pyranoquinoline **5a**.

Table S1. Symbolic Z-matrix: charge = 0, multiplicity = 1

C	5.58978	−1.00942	0.03819
C	4.33858	−1.57814	−0.01819
C	3.18587	−0.76528	−0.02234
C	3.34039	0.65245	0.03151
C	4.64035	1.20702	0.08847
C	5.74518	0.39132	0.09207
H	6.46684	−1.64214	0.04155
H	4.20461	−2.6495	−0.0592
C	2.16352	1.43239	0.0218
H	4.75061	2.28298	0.12902
H	6.73674	0.8196	0.13609
C	0.92876	0.82828	−0.03219
C	0.90737	−0.60511	-0.07651
H	2.23179	2.51264	0.05578
N	1.95798	−1.36227	−0.07596
C	−0.32426	1.53273	−0.06117
C	−1.48604	0.84859	−0.10623
C	−1.49516	−0.60227	−0.09691
O	−0.28019	−1.27097	−0.12881
C	−2.8002	1.55224	−0.17138
C	-3.98094	0.6916	−0.56567
H	−4.89626	1.2378	−0.34296
H	−3.91871	0.58645	−1.65479
C	−3.99208	−0.72161	0.06103
C	−2.61332	−1.33544	−0.02363
H	−2.52504	−2.41288	0.02598
O	−2.89644	2.7466	0.02855
C	−4.99623	−1.60222	−0.7036
H	−4.70869	−1.70921	−1.74999
H	−5.0479	−2.59967	−0.26455
H	−5.99685	−1.16871	−0.66713
C	−4.42511	−0.63359	1.54333
H	−3.76322	0.02019	2.1119
H	−5.44168	−0.24399	1.62466
H	−4.40191	−1.61836	2.01084
H	−0.34212	2.6144	−0.0548

Table S2. Computed B3LYP/6-31+G(d,p) ^{1}H and ^{13}C NMR chemical shifts (ppm) for pyranoquinoline **5a** and TMS

Atom	Pyranoquinoline **5a**		TMS	
	GIAO	CSGT	GIAO	CSGT
C1	65.5686	63.0161	191.3637	193.7630
C2	66.0551	63.6816	191.3637	193.7630
C3	46.5088	43.6895	191.3637	193.7630
C4	66.6606	64.7685	191.3637	193.7630
C5	68.7895	65.5050	191.3637	193.7630
C6	71.4025	68.8041	191.3637	193.7630
C9	59.9738	55.7594	191.3637	193.7630
C12	69.4734	73.4249	191.3637	193.7630
C13	37.4360	34.1288	191.3637	193.7630
C16	70.7957	65.3104	191.3637	193.7630
C17	66.0421	63.8793	191.3637	193.7630
C18	45.4116	41.1712	191.3637	193.7630
C20	0.5899	-1.0235	191.3637	193.7630
C21	137.8278	138.5408	191.3637	193.7630
C24	154.9028	159.3515	191.3637	193.7630
C25	79.5548	77.2708	191.3637	193.7630
C28	160.7181	161.6168	191.3637	193.7630
C32	162.3555	163.0471	191.3637	193.7630
H7	23.7831	23.5501	31.6210	29.4288
H8	23.7009	23.3384	31.6210	29.4288
H10	24.0046	23.6613	31.6210	29.4288
H11	24.1978	23.8558	31.6210	29.4288
H14	24.0849	23.7225	31.6210	29.4288
H22	29.3568	28.2171	31.6210	29.4288
H23	29.3125	28.2756	31.6210	29.4288
H26	26.0548	25.4430	31.6210	29.4288
H29	30.4356	28.9536	31.6210	29.4288
H30	30.4231	28.8072	31.6210	29.4288
H31	30.6055	28.9489	31.6210	29.4288
H33	30.5519	28.9604	31.6210	29.4288
H34	30.5932	29.1500	31.6210	29.4288
H35	30.5309	28.9178	31.6210	29.4288
H36	24.4410	24.3643	31.6210	29.4288

Table S3. Computed B3LYP/6-31+G(d,p) ^{1}H and ^{13}C NMR chemical shifts for pyranoquinoline **5a** relative to TMS

Atom	Chemical shifts / ppm	
	GIAO	CSGT
C1	125.80	130.75
C2	125.31	130.08
C3	144.85	150.07
C4	124.70	128.99
C5	122.57	128.26
C6	119.96	124.96
C9	131.39	138.00
C12	121.89	120.34
C13	153.93	159.63
C16	120.57	128.45
C17	125.32	129.88
C18	145.95	152.59
C20	190.77	194.79
C21	53.54	55.22
C24	36.46	34.41
C25	111.81	116.49
C28	30.65	32.15
C32	29.01	30.72
H7	7.84	5.88
H8	7.92	6.09
H10	7.62	5.77
H11	7.42	5.57
H14	7.54	5.71
H22	2.26	1.21
H23	2.31	1.15
H26	5.57	3.99
H29	1.19	0.48
H30	1.20	0.62
H31	1.02	0.48
H33	1.07	0.47
H34	1.03	0.28
H35	1.09	0.51
H36	7.18	5.06

Table S4. # B3LYP/6-31+G** NMR, Symbolic Z-matrix: charge = 0, multiplicity = 1 for **4c**

C	−4.27896	−0.14203	−0.01106
C	−4.03364	−1.53332	−0.05842
C	−2.73505	−1.99991	−0.09396
C	−1.64273	−1.09916	−0.08352
C	−1.90796	0.30717	−0.03557
C	−3.24821	0.77089	0.00051
N	−0.37312	−1.60563	−0.11793
C	0.62226	−0.76666	−0.1049
C	0.49238	0.66581	−0.06338
C	−0.78999	1.1788	−0.02878
O	1.85726	−1.34361	−0.14032
C	1.69403	1.46409	−0.07854
Br	−6.08609	0.46693	0.03666
C	2.9084	0.86213	−0.11168
C	3.02388	−0.58869	−0.098
C	4.19712	−1.24284	−0.0159
C	5.52774	−0.52397	0.08506
C	5.41827	0.88591	−0.5494
C	4.17154	1.65975	−0.16864
C	6.6087	−1.33045	−0.66321
O	4.17682	2.86742	0.02322
C	5.93189	−0.39816	1.5766
H	−4.86799	−2.22587	−0.06623
H	−2.52157	−3.06295	−0.13026
H	−3.4478	1.83686	0.03697
H	−0.94079	2.25508	0.00216
H	1.63219	2.54856	−0.07536
H	4.18774	−2.32839	0.03318
H	6.29258	1.50093	−0.31809
H	5.37583	0.7731	−1.64355
H	7.57637	−0.81828	−0.61685
H	6.34311	−1.46671	−1.717
H	6.7325	−2.32245	−0.21452
H	6.91875	0.0704	1.67024
H	5.97685	−1.38487	2.04927
H	5.21143	0.2079	2.13589
Bq	−2.96439	−0.57828	−0.04387
Bq	−2.9761	−0.63509	0.45275
Bq	−2.9761	−0.63509	0.95275
Bq	−2.9761	−0.63509	1.45275
Bq	−2.9761	−0.63509	1.95275