Supplementary Material

Synthesis, structural elucidation, intramolecular hydrogen bonding and DFT studies of quinoline-chalcone-chromene hybrids

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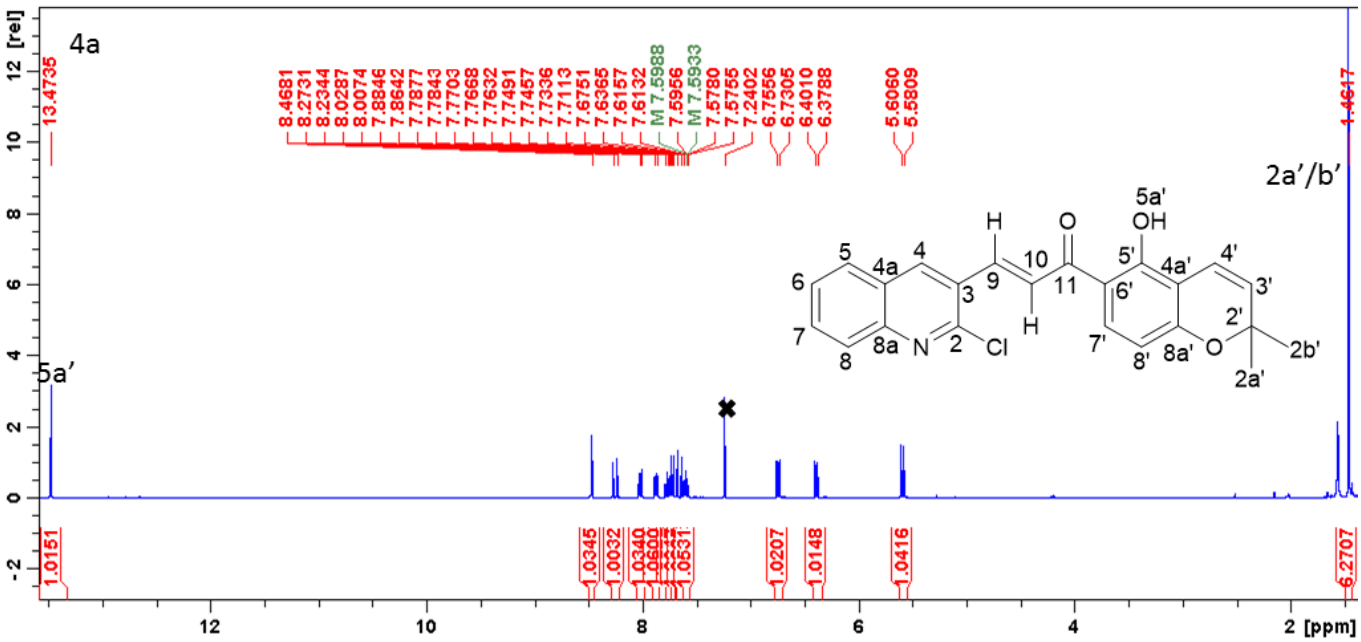


Figure S1 ^{1}H NMR spectrum of **4a**

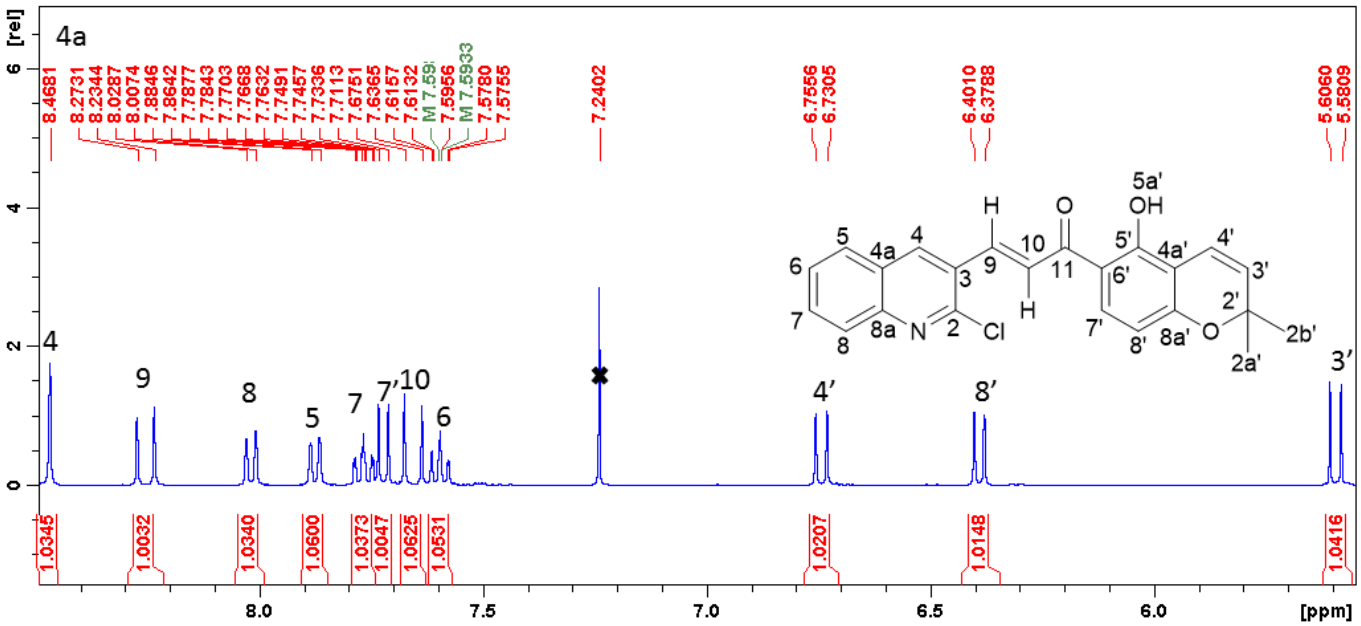


Figure S2 ^{1}H NMR spectrum (expansion 1) of **4a**

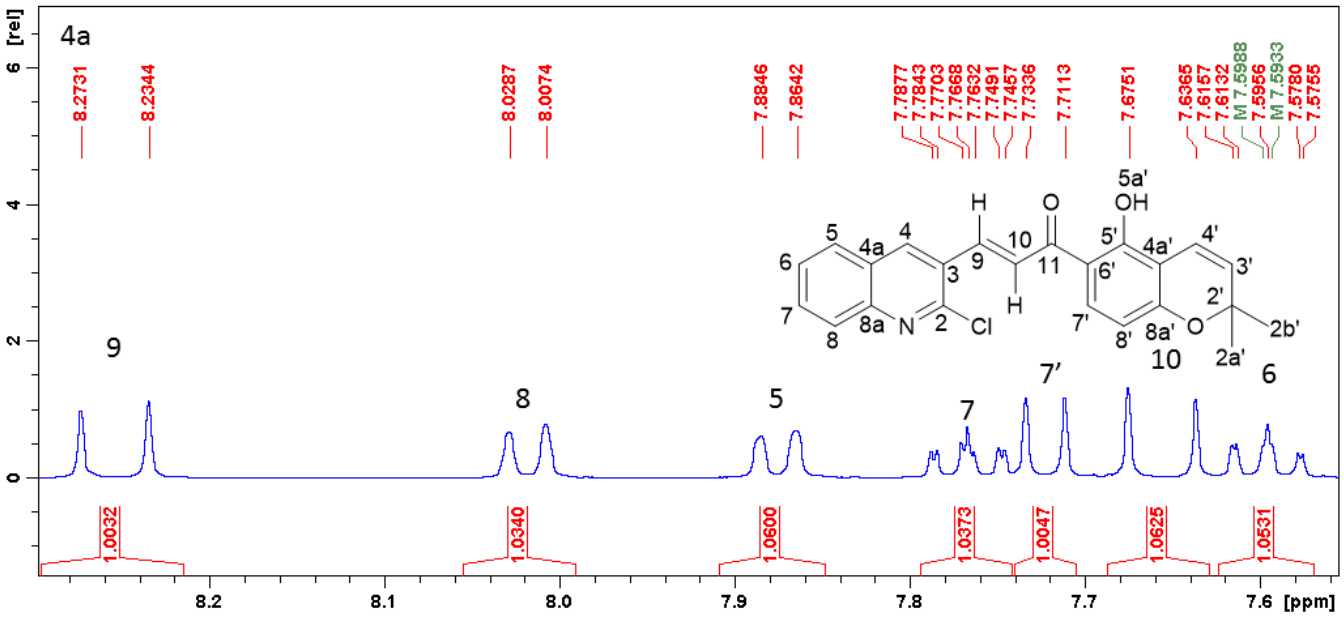


Figure S3 ^{1}H NMR spectrum (expansion 2) of **4a**

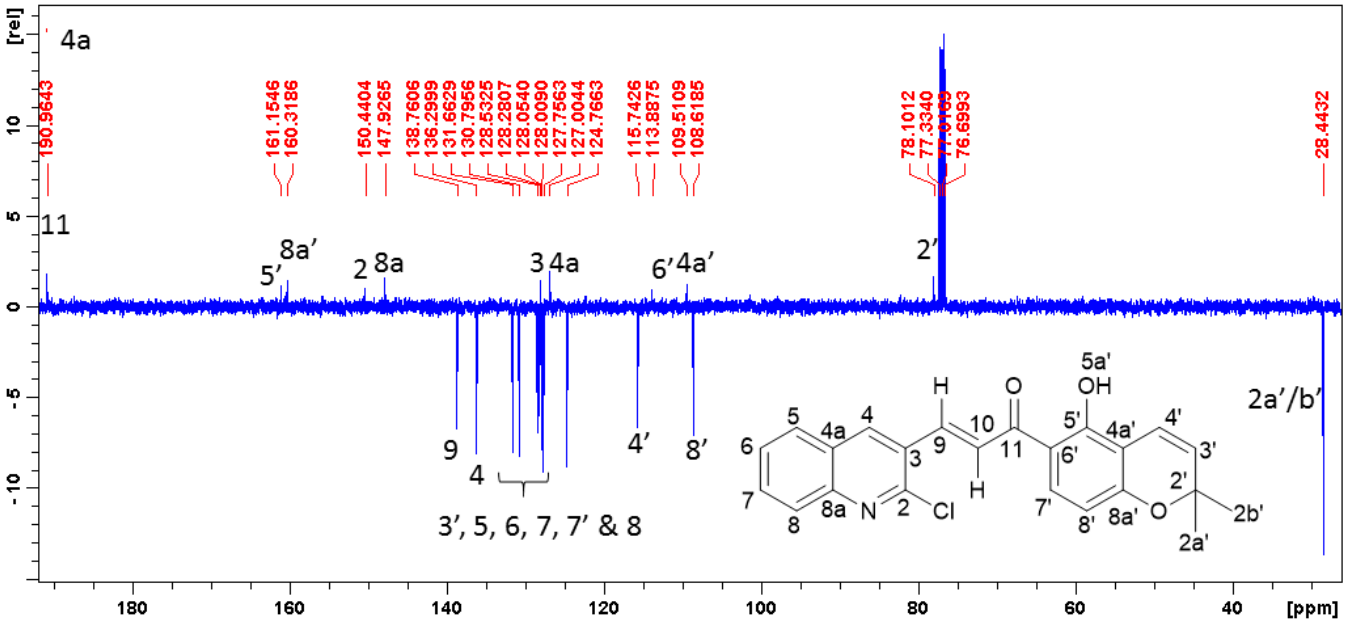


Figure S4 ^{13}C NMR spectrum of **4a**

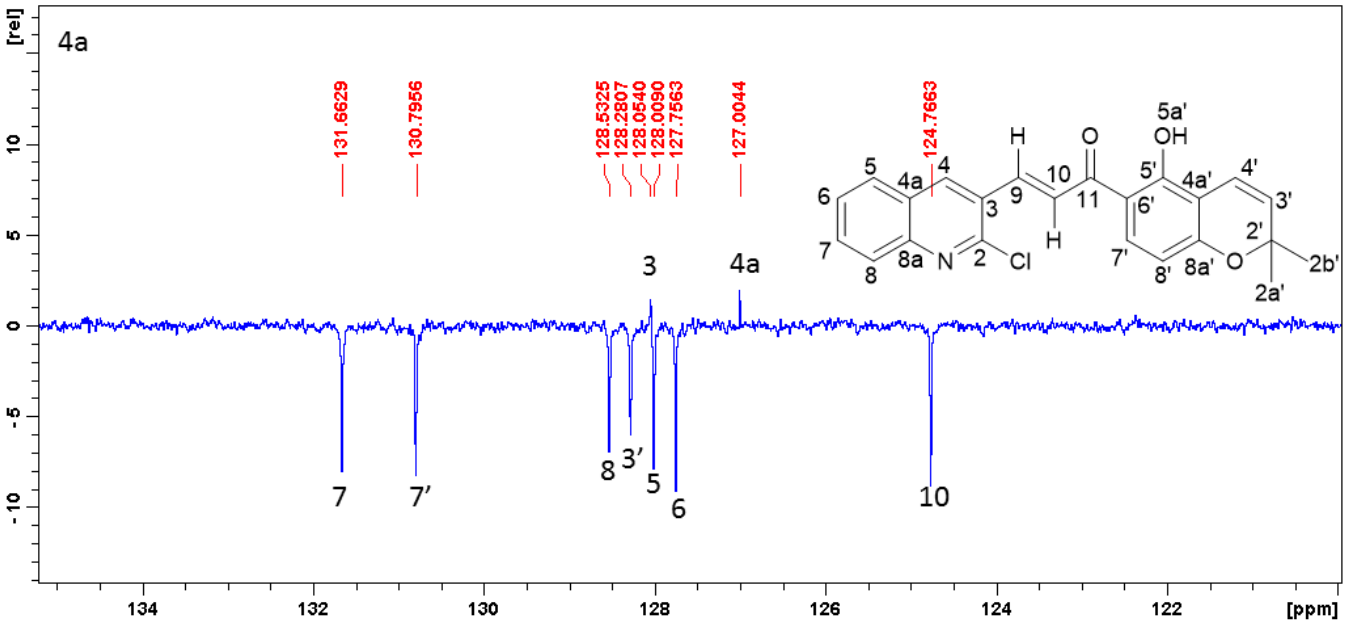


Figure S5 ^{13}C NMR spectrum (expanded) of **4a**

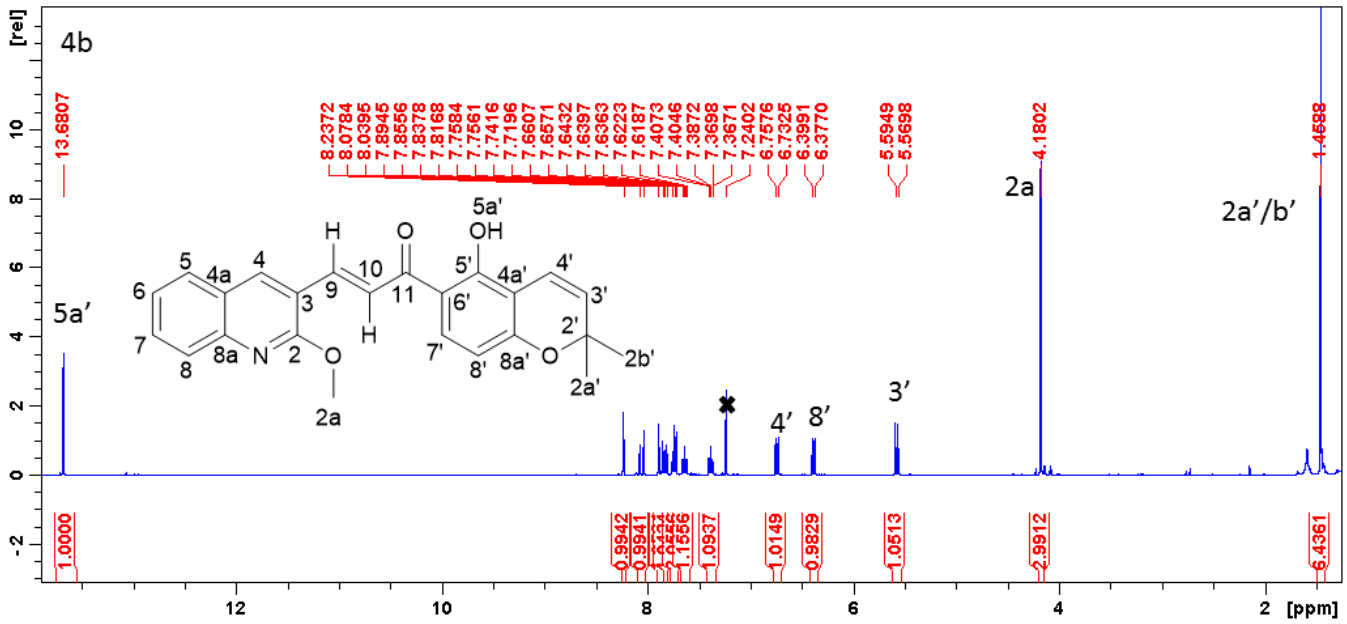


Figure S6 ^{1}H NMR of **4b**

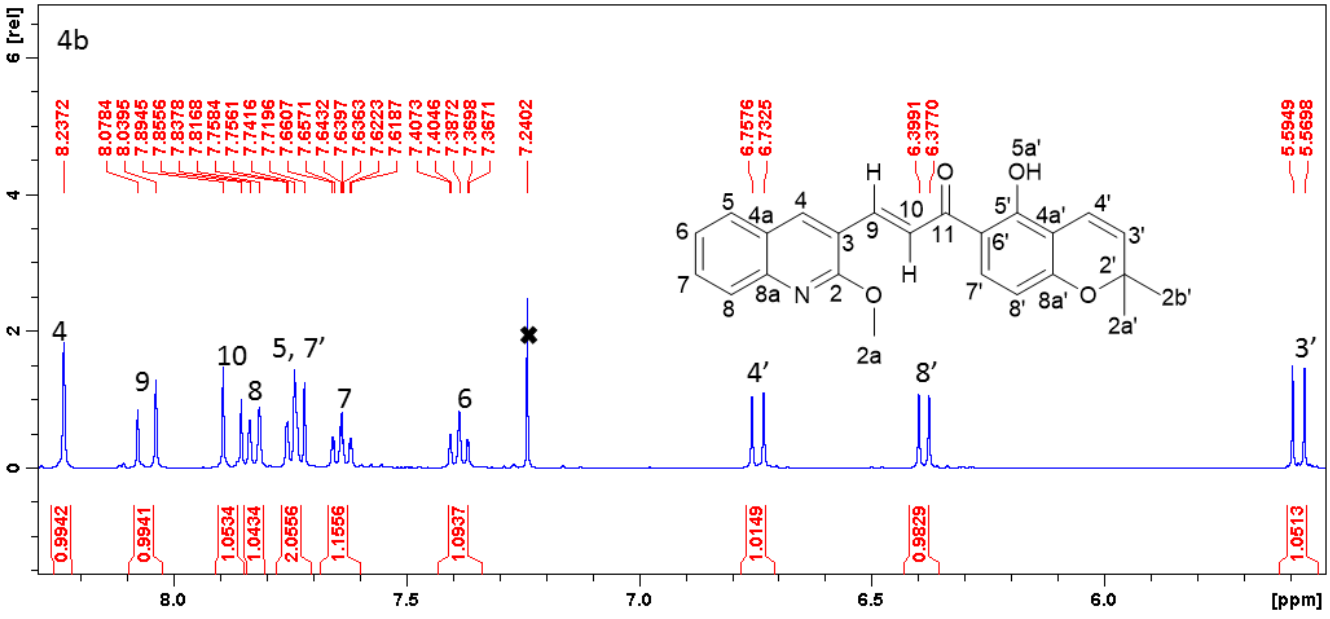


Figure S7 ^{1}H NMR spectrum (expanded) of **4b**

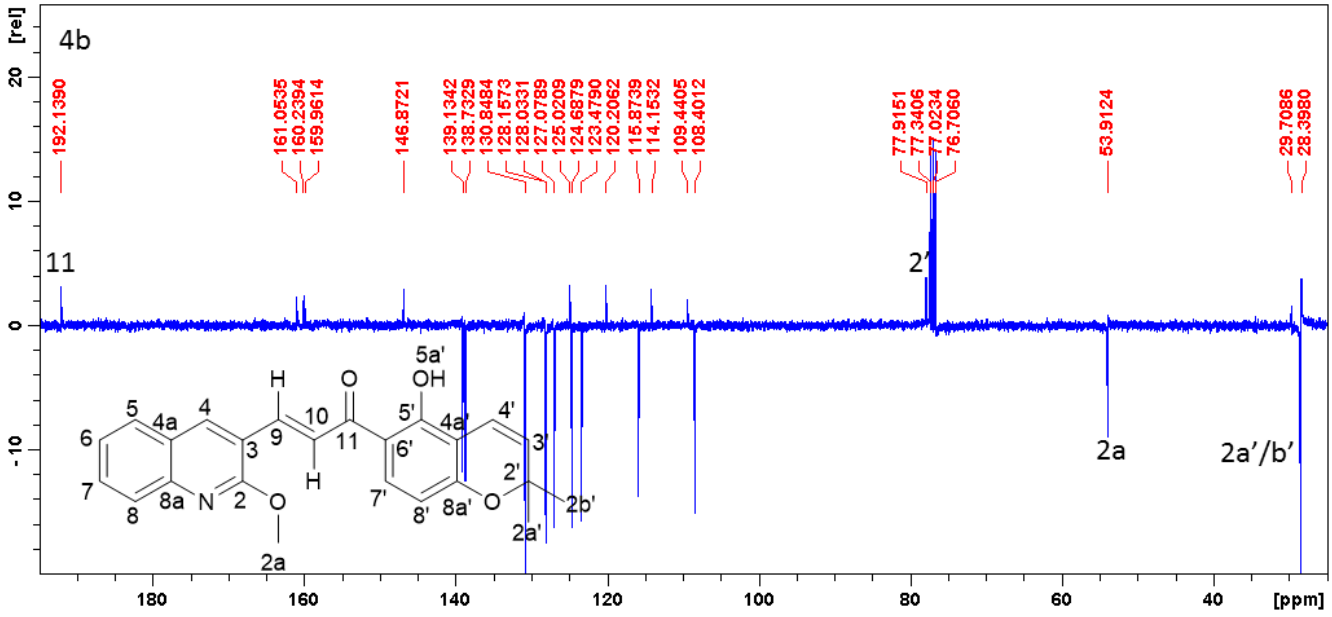


Figure S8 ^{13}C NMR spectrum of **4b**

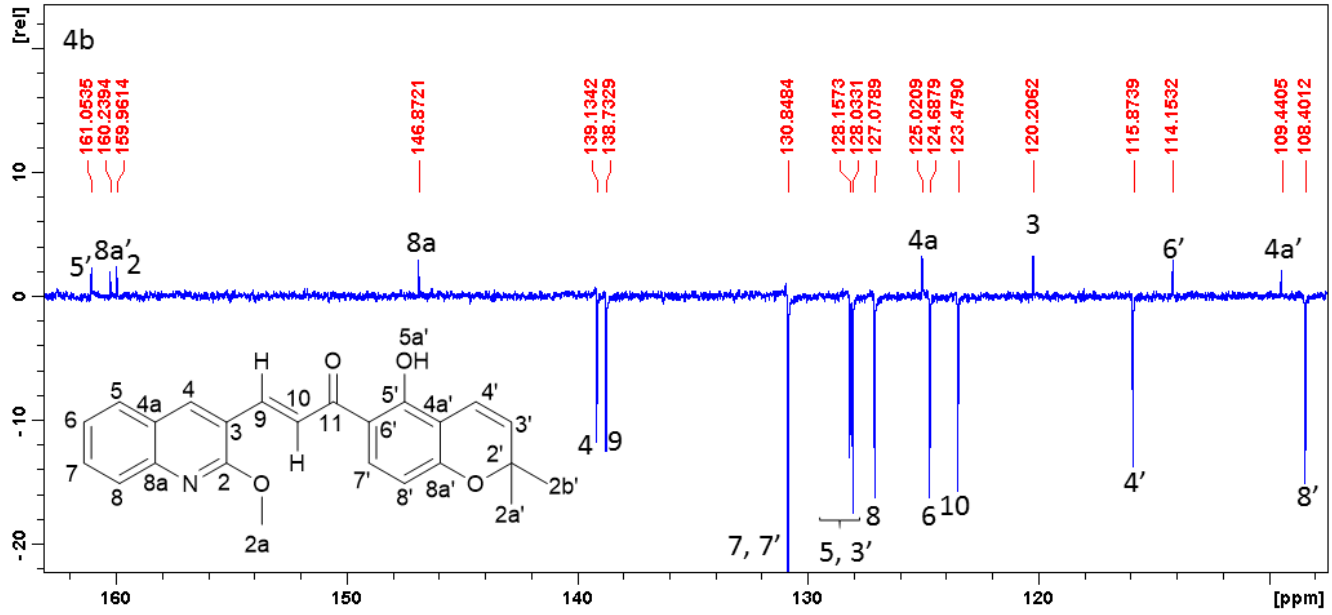
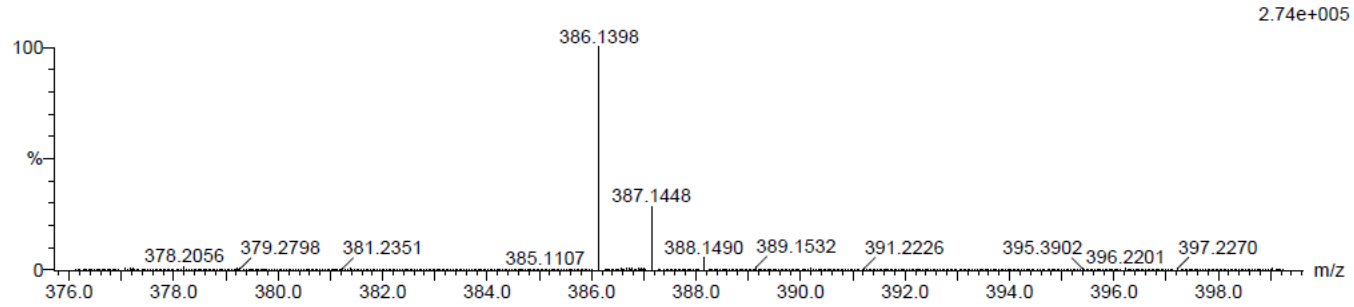


Figure S9 ^{13}C NMR spectrum (expanded) of **4b**

Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
11 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 20-25 H: 20-25 N: 0-5 O: 0-5
4b 29 (0.945) Cm (1:61)
TOF MS ES-



Minimum:				-1.5			
Maximum:		5.0	5.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
386.1398	386.1392	0.6	1.6	15.5	595.4	0.0	C24 H20 N O4

Figure S10 HRMS of **4b**

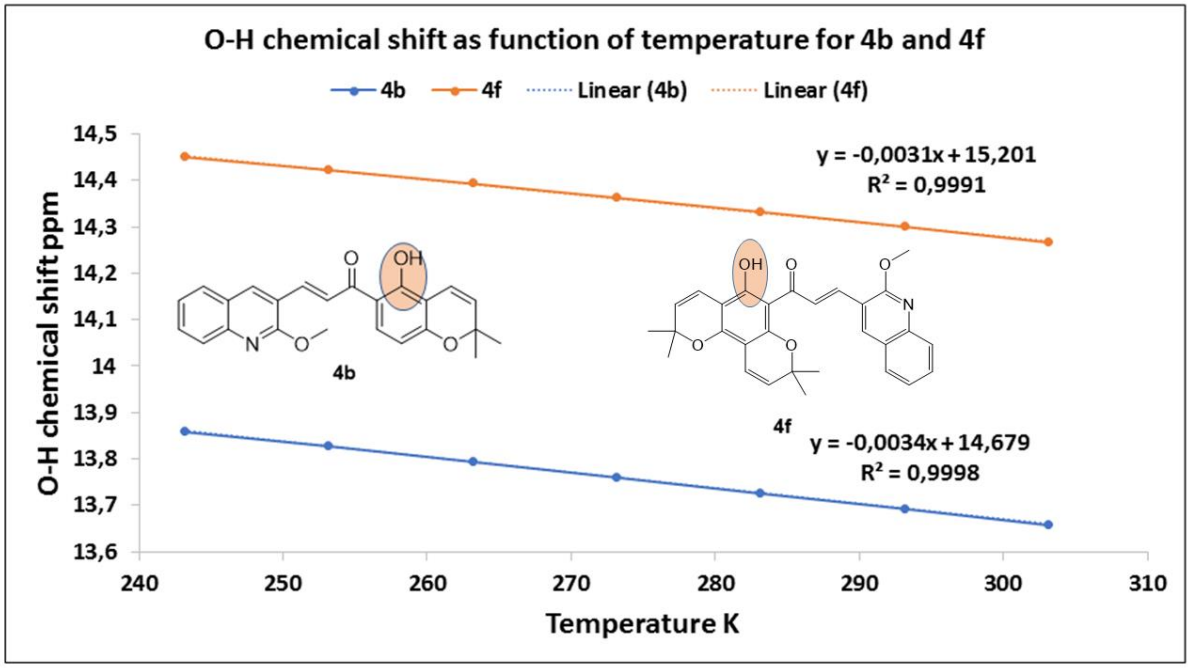


Figure S11 OH ^{1}H NMR chemical shift of **4b** and **4f** as function of temperature

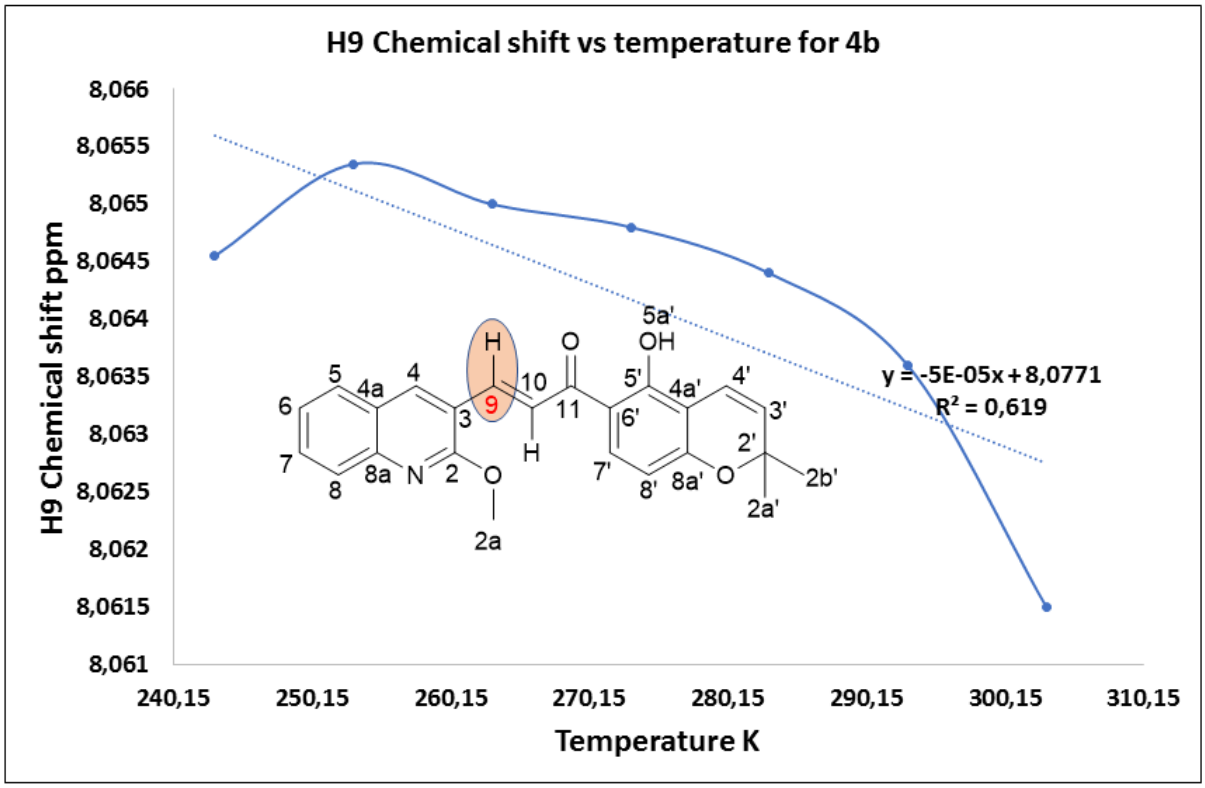


Figure S12 H-9 ^{1}H NMR chemical shift of **4b** as function of temperature

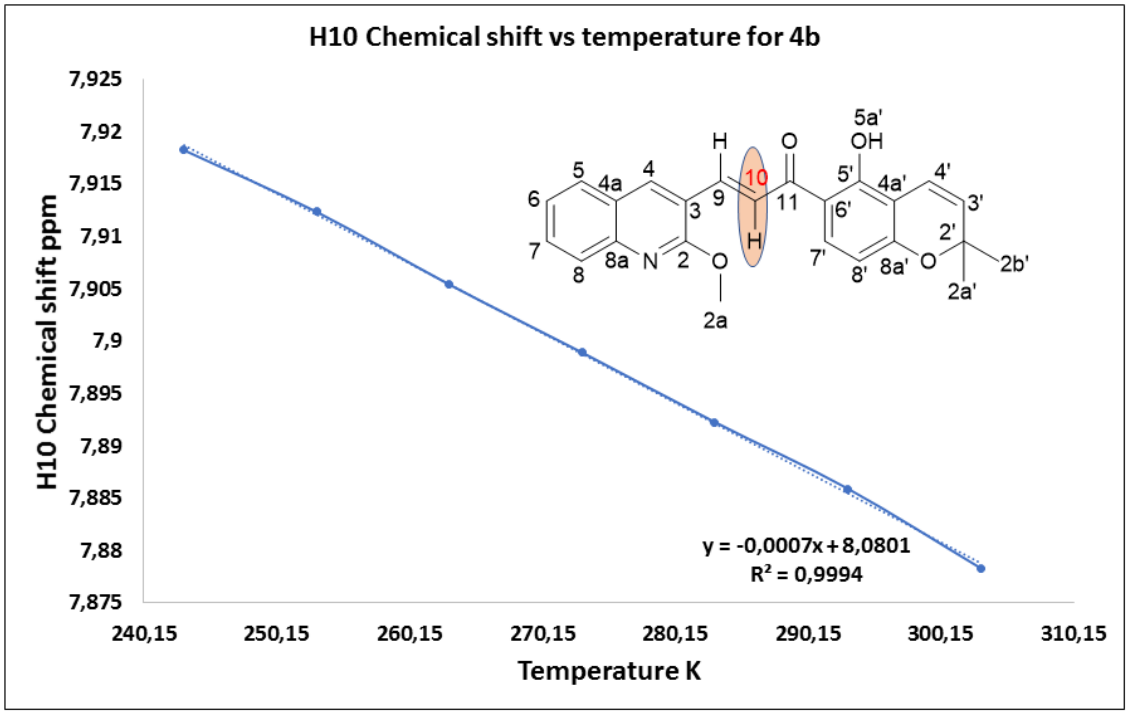


Figure S13 H-10 ^{1}H NMR chemical shift of **4b** as function of temperature

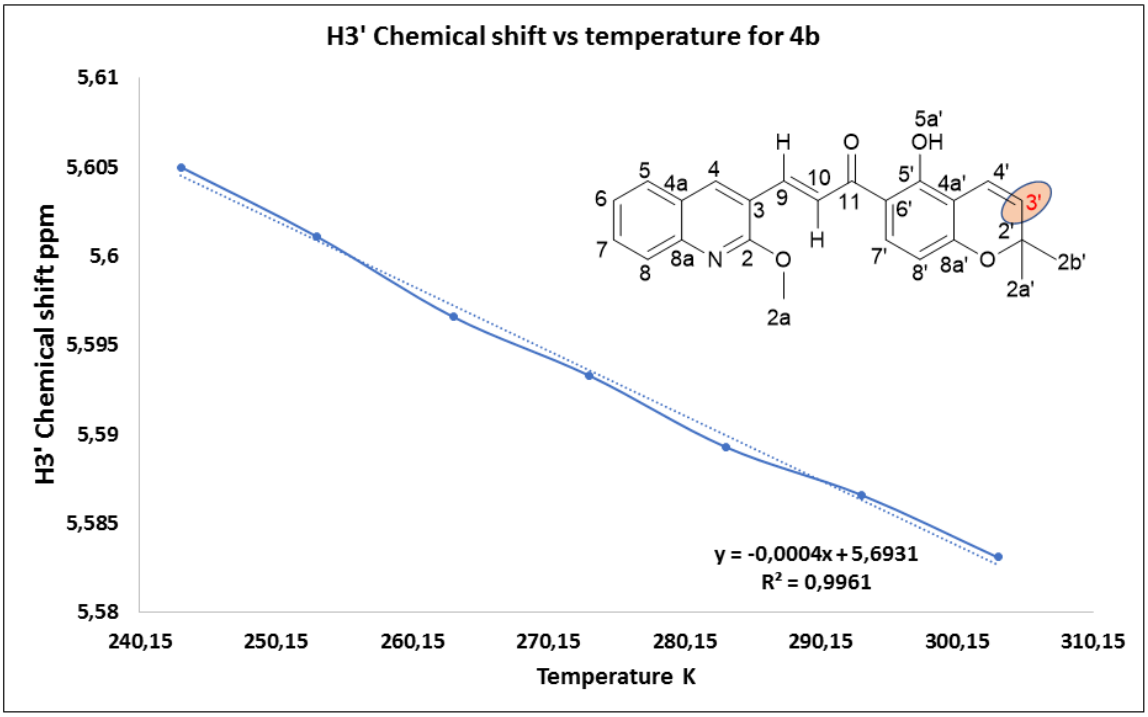


Figure S14 H-3' ^{1}H NMR chemical shift of **4b** as function of temperature

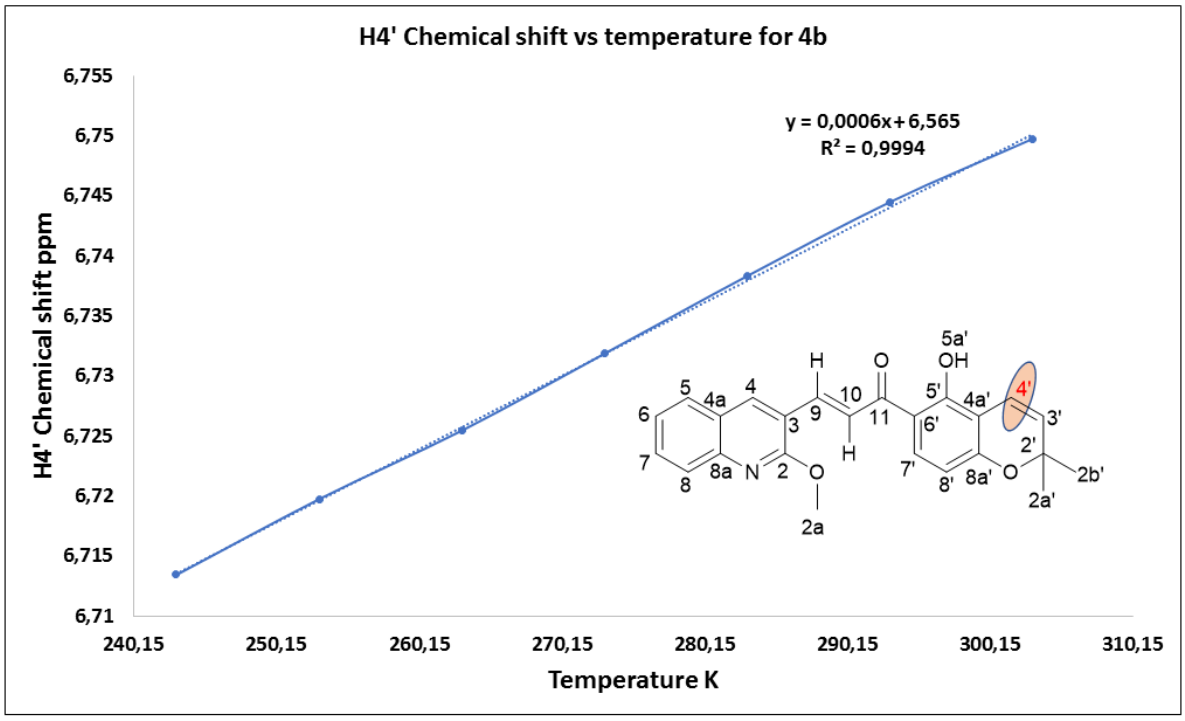


Figure S15 H-4' ^{1}H NMR chemical shift of **4b** as function of temperature

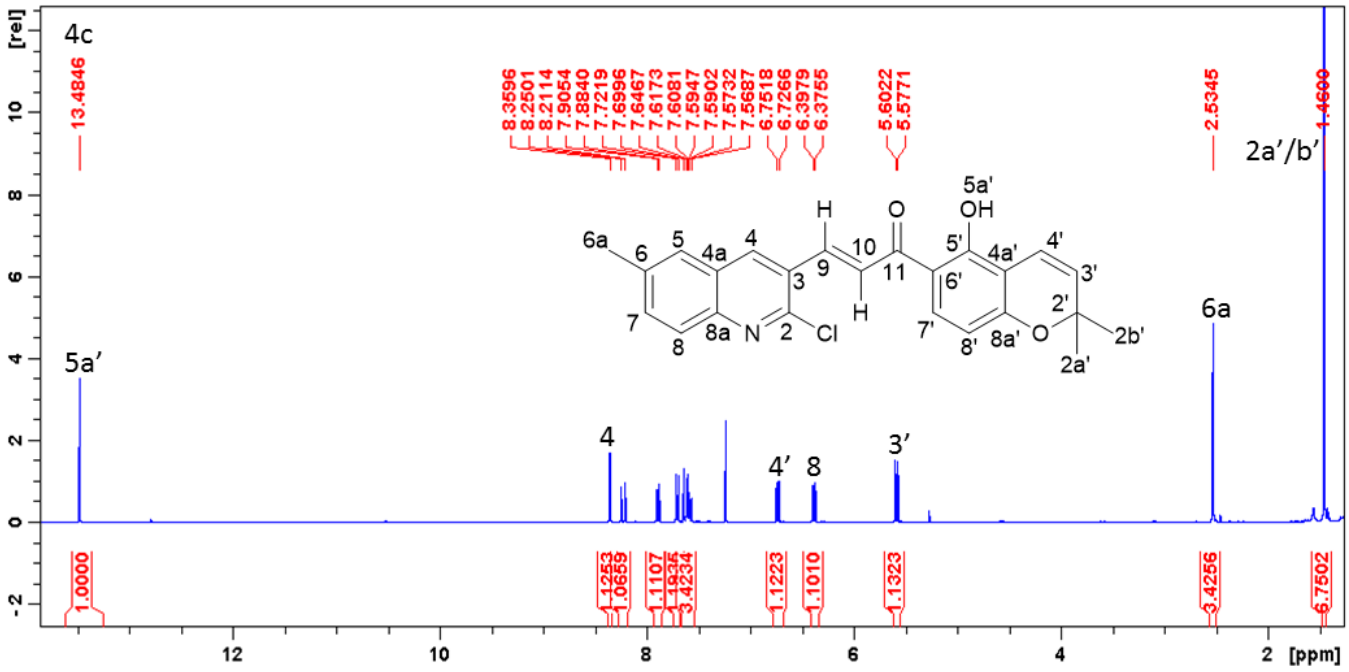


Figure S16 ^{1}H NMR spectrum of **4c**

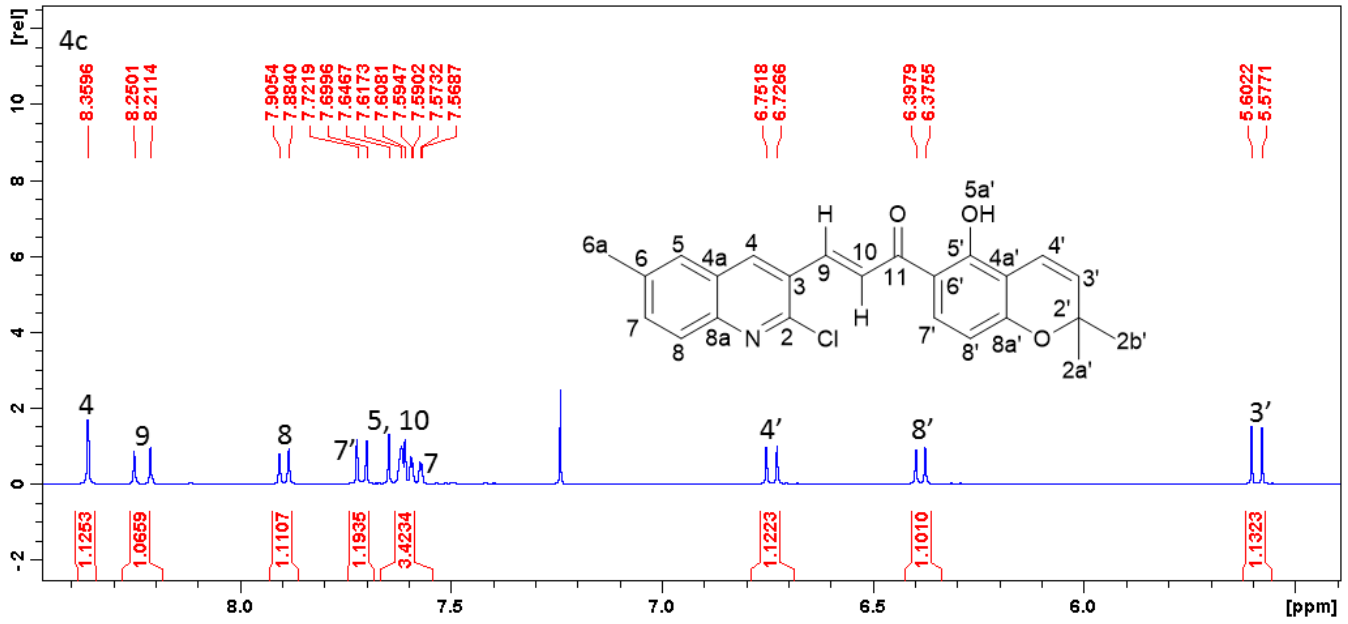


Figure S17 ^{1}H NMR spectrum (expanded) of **4c**

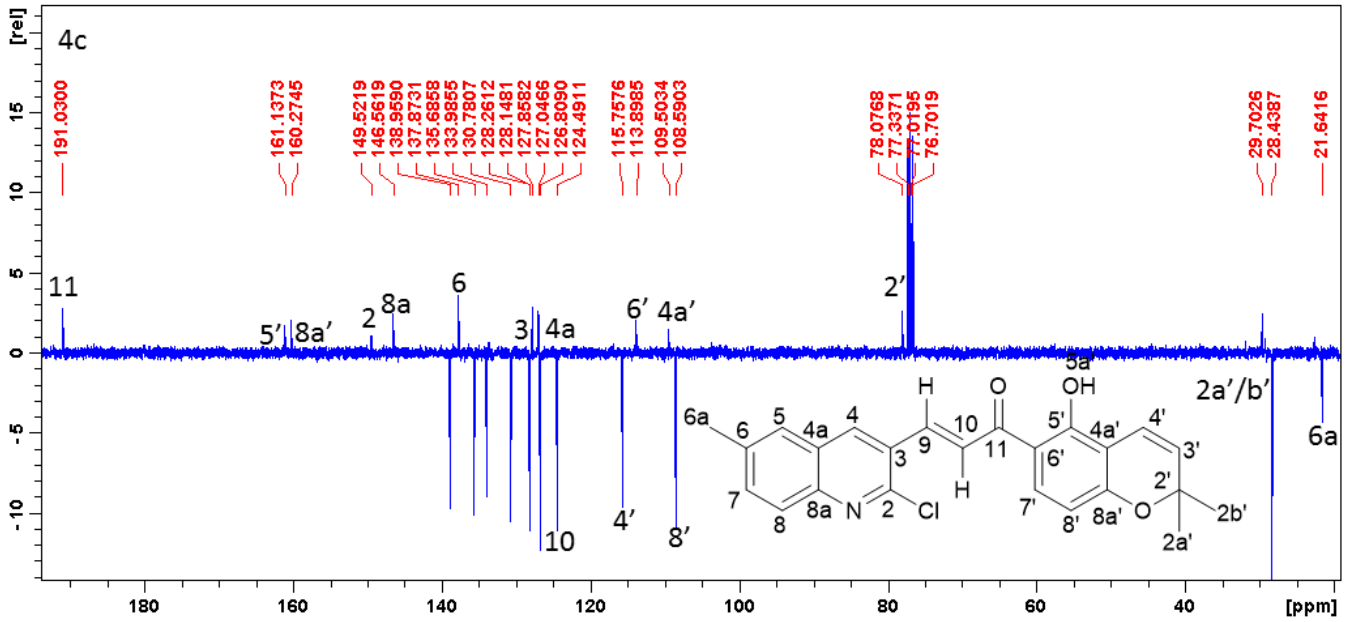


Figure S18 ^{13}C NMR spectrum of **4a**

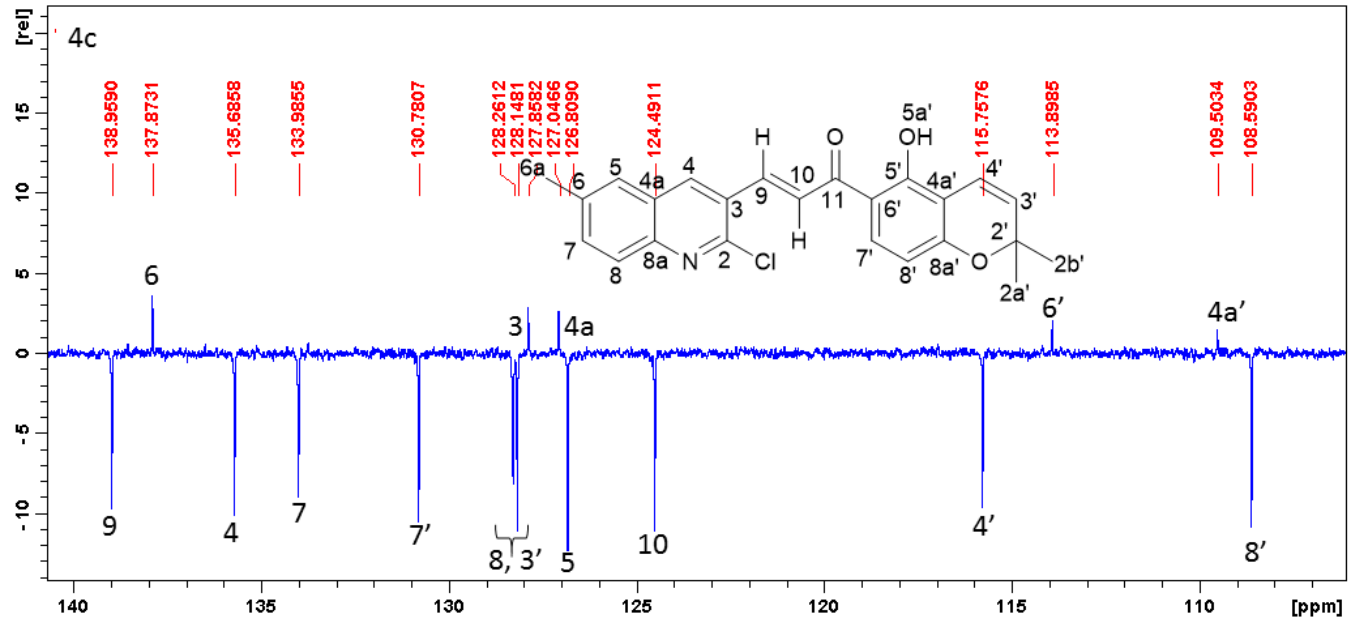
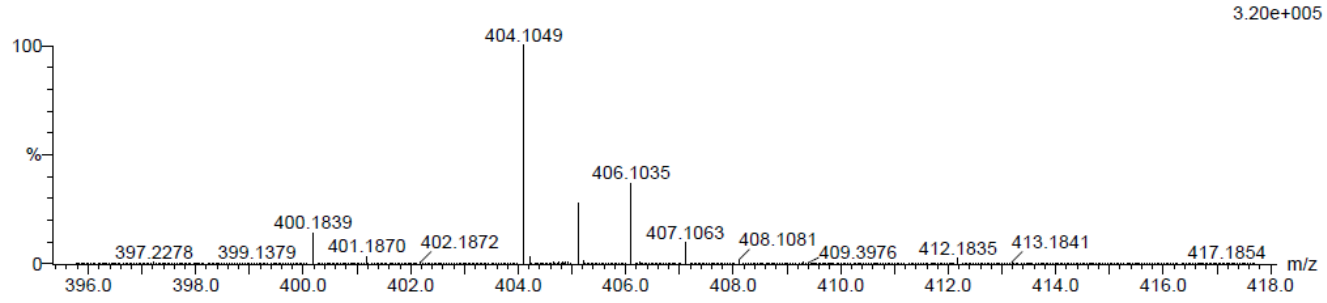


Figure S19 ^{13}C NMR spectrum (expanded) of **4c**

Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
43 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 20-25 H: 15-25 N: 0-5 O: 0-5 Cl: 0-1
4c 3 (0.068) Cm (1:61)
TOF MS ES-



Minimum:				-1.5			
Maximum:		5.0	5.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
404.1049	404.1053	-0.4	-1.0	15.5	598.3	0.0	C24 H19 N O3 Cl

Figure S20 HRMS of **4c**

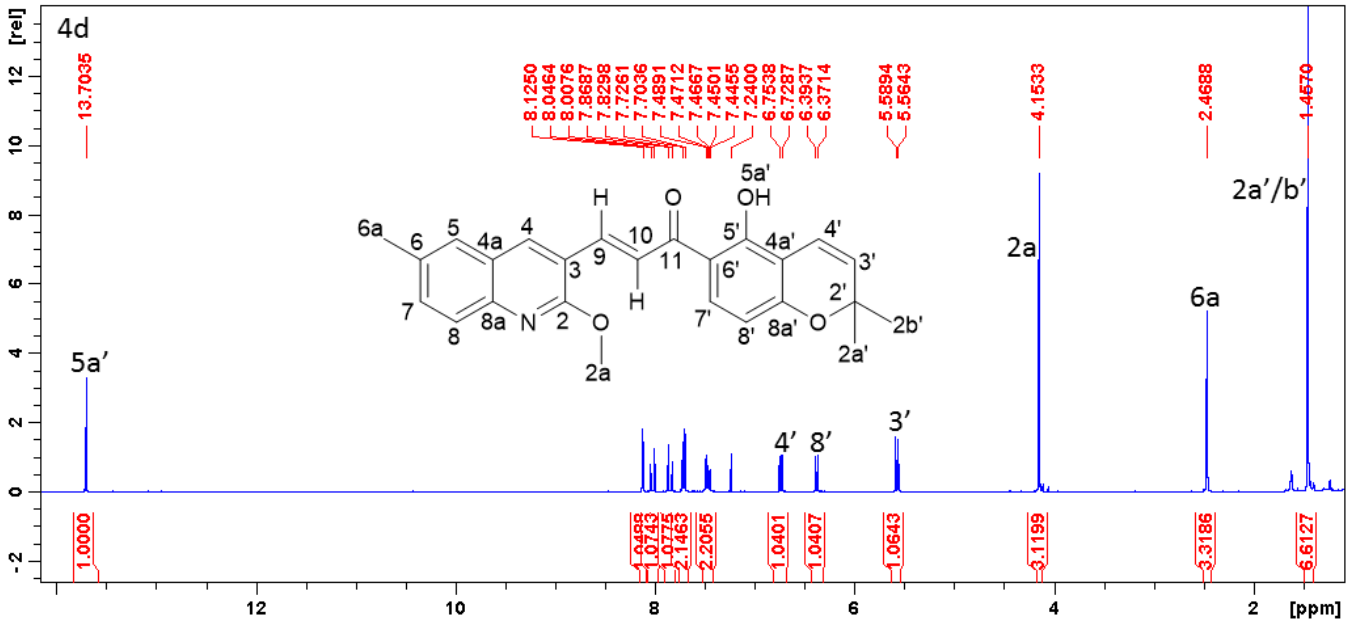


Figure S21 ^{1}H NMR spectrum of **6d**

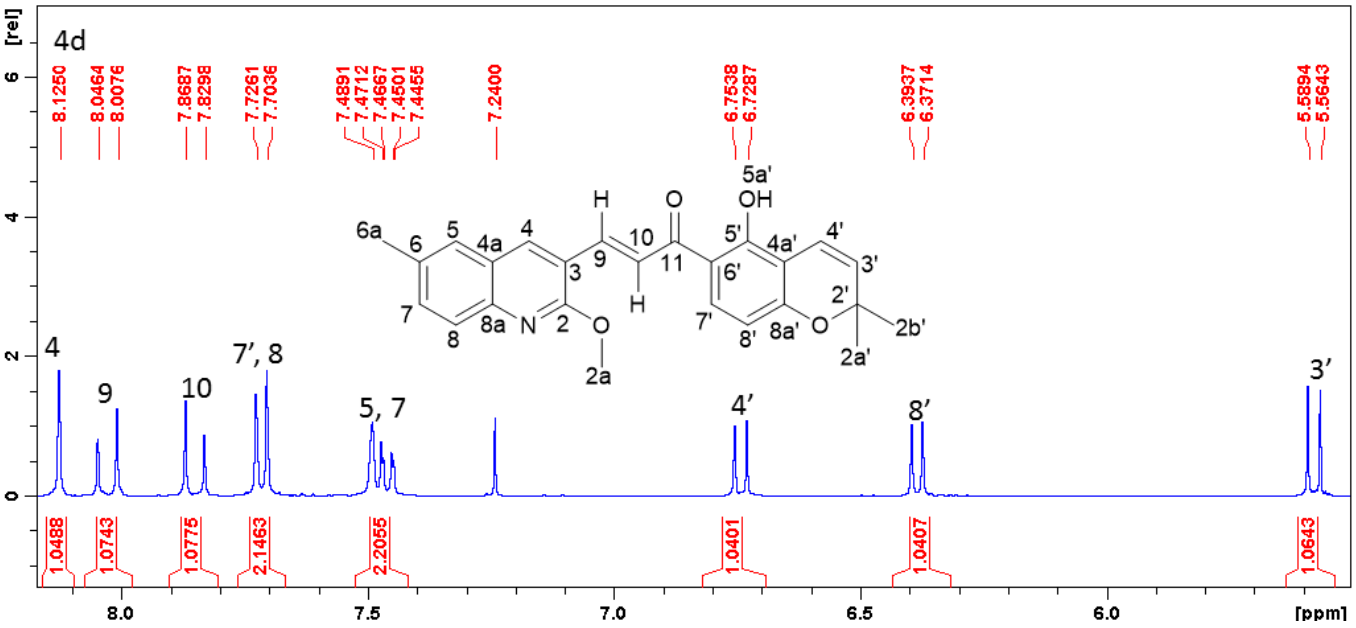


Figure S22 ^{1}H NMR spectrum (expanded) of **4d**

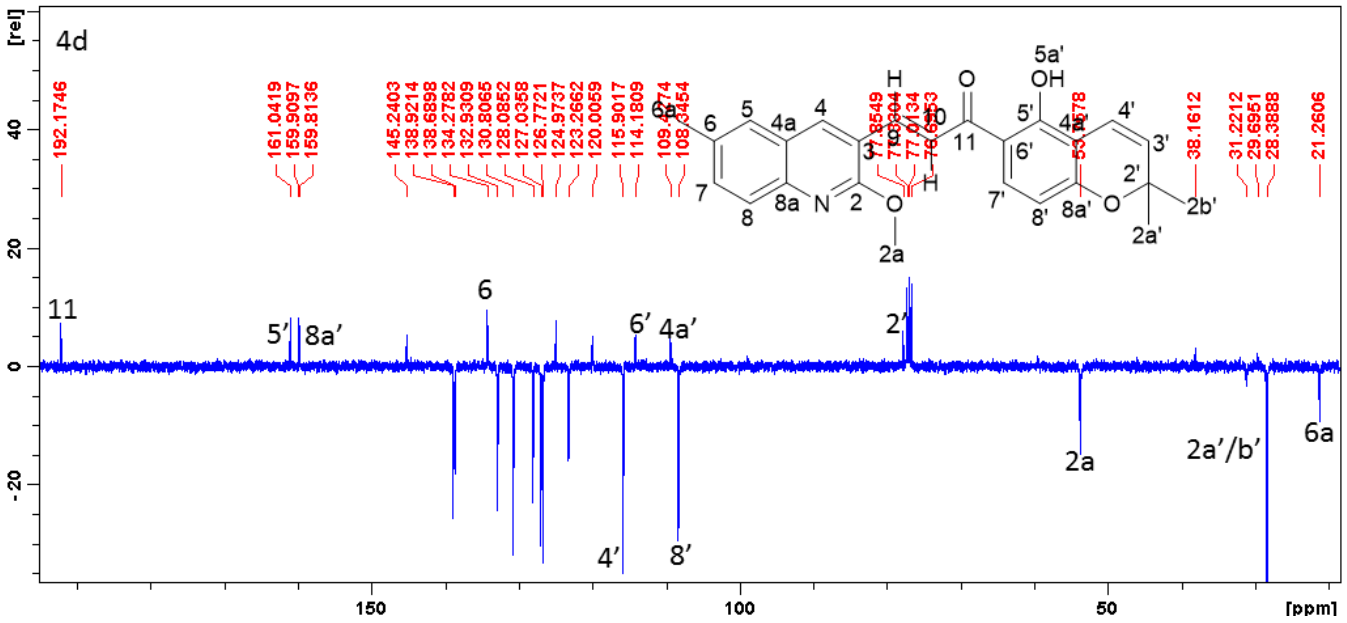


Figure S23 ^{13}C NMR spectrum of **4d**

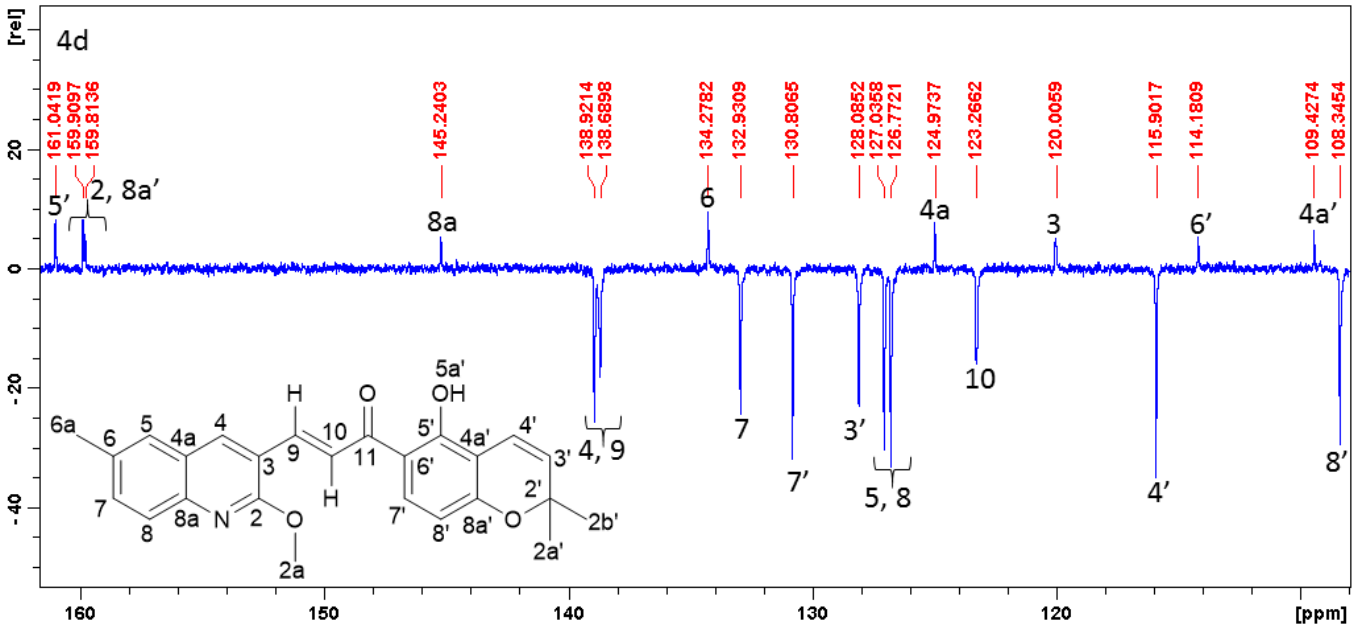
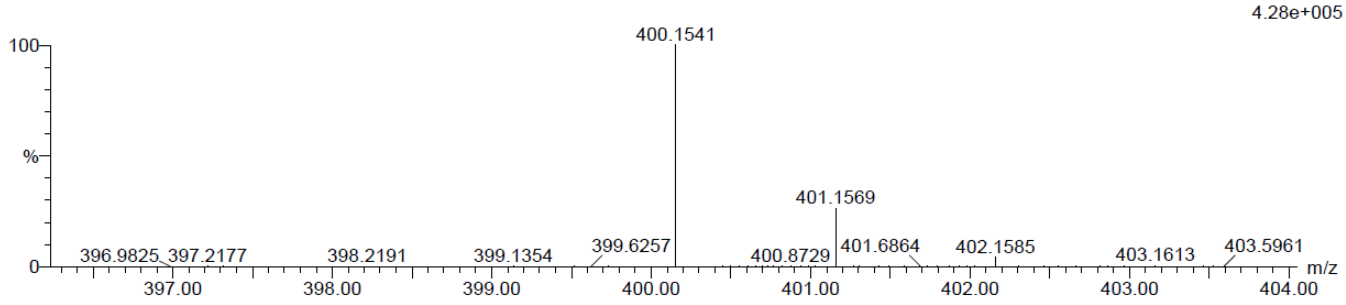


Figure S24 ^{13}C NMR spectrum of **4d**

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
12 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 20-25 H: 20-25 N: 0-5 O: 0-5
4d 25 (0.810) Cm (1:61)
TOF MS ES-



Minimum:				-1.5			
Maximum:		5.0	5.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
400.1541	400.1549	-0.8	-2.0	15.5	580.9	0.0	C25 H22 N O4

Figure S25 HRMS of **4d**

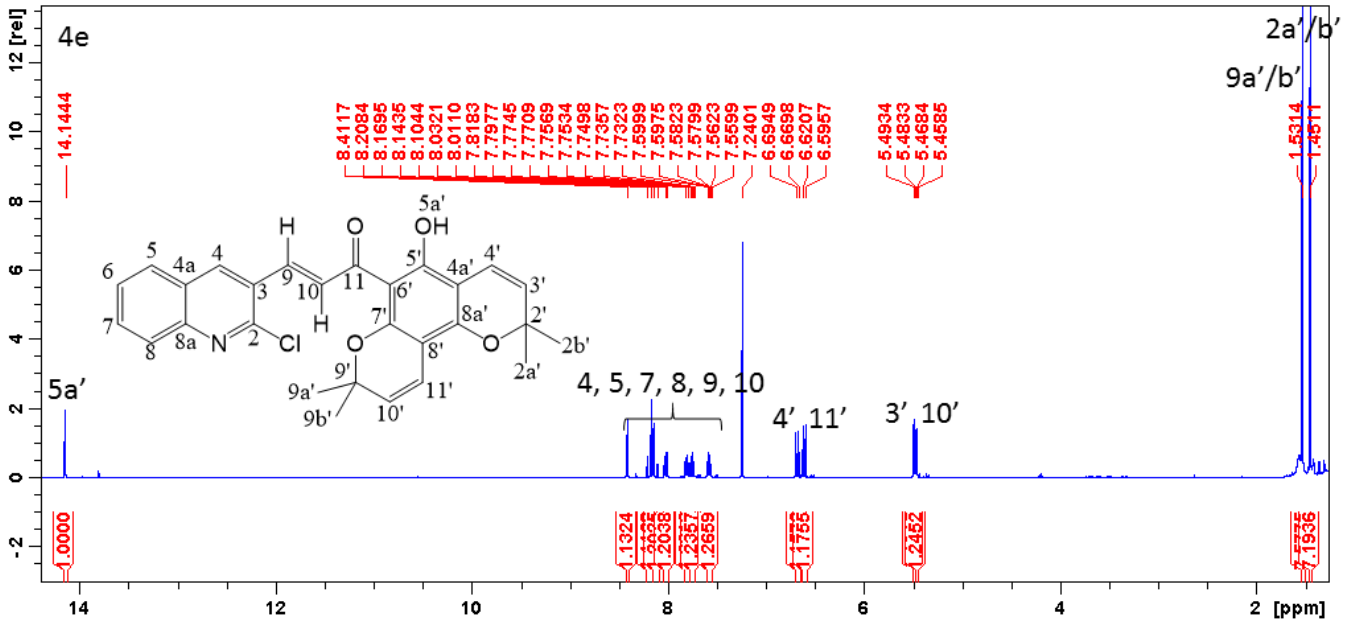


Figure S26 ^{1}H NMR spectrum of **4e**

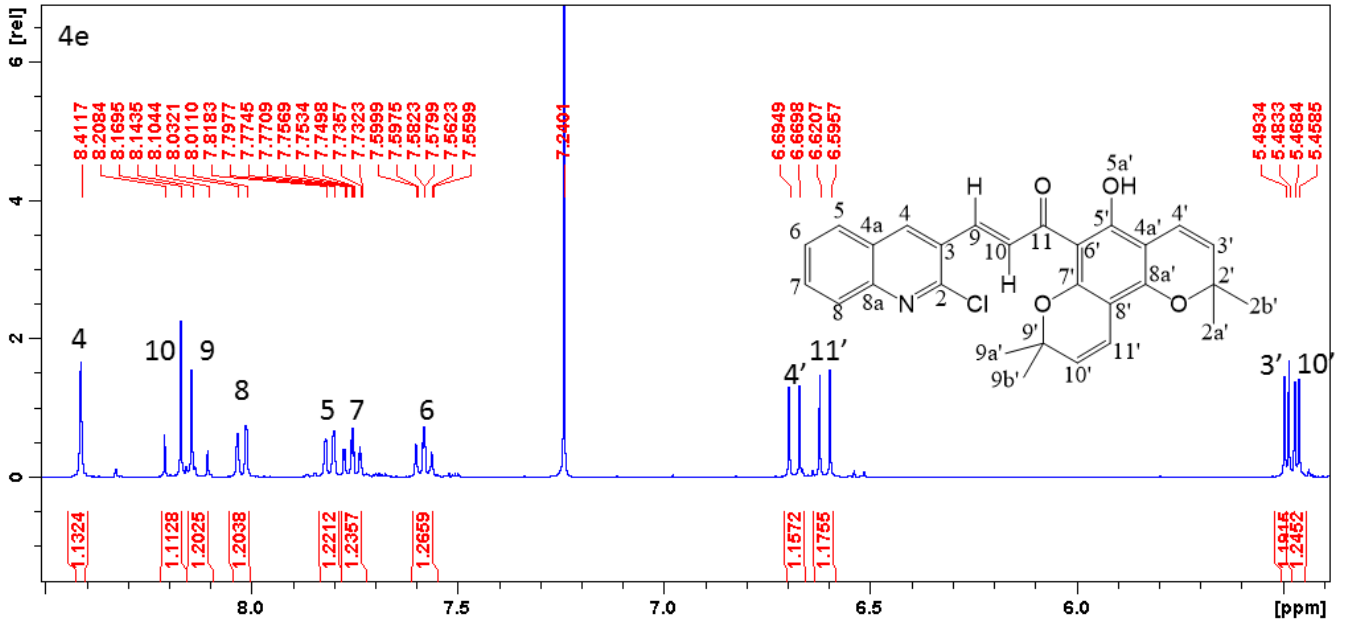


Figure S27 ^{1}H NMR spectrum (expanded) of **4e**

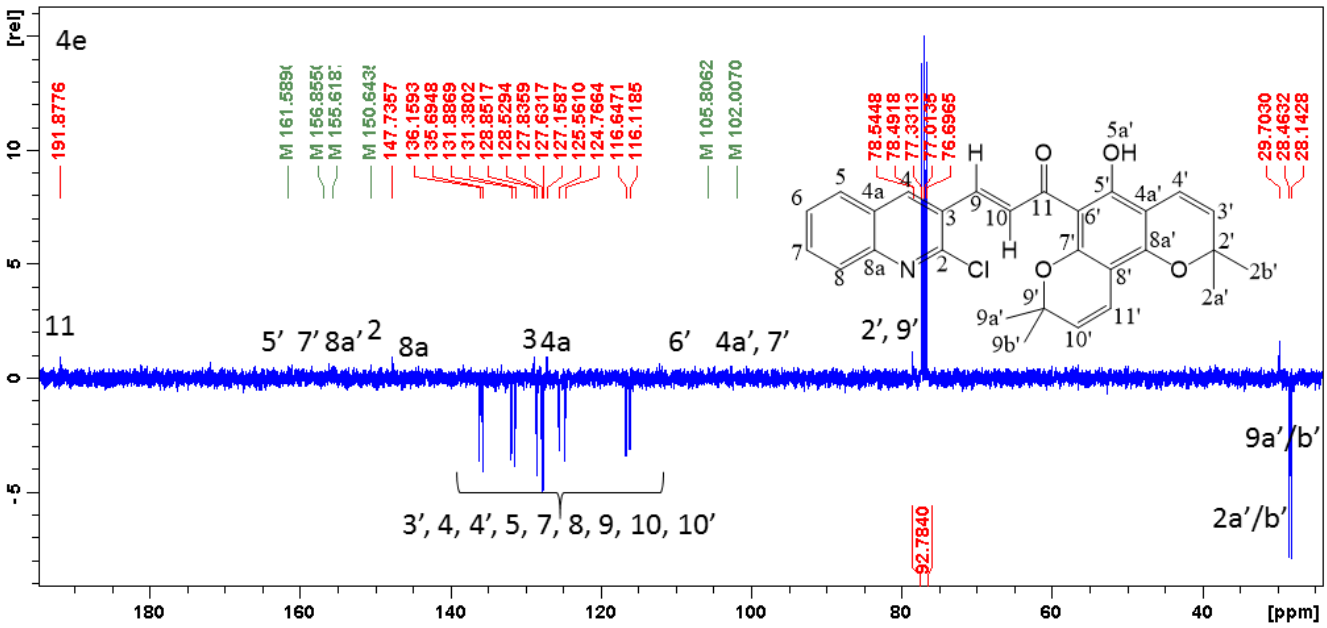


Figure S28 ^{13}C NMR spectrum of **4e**

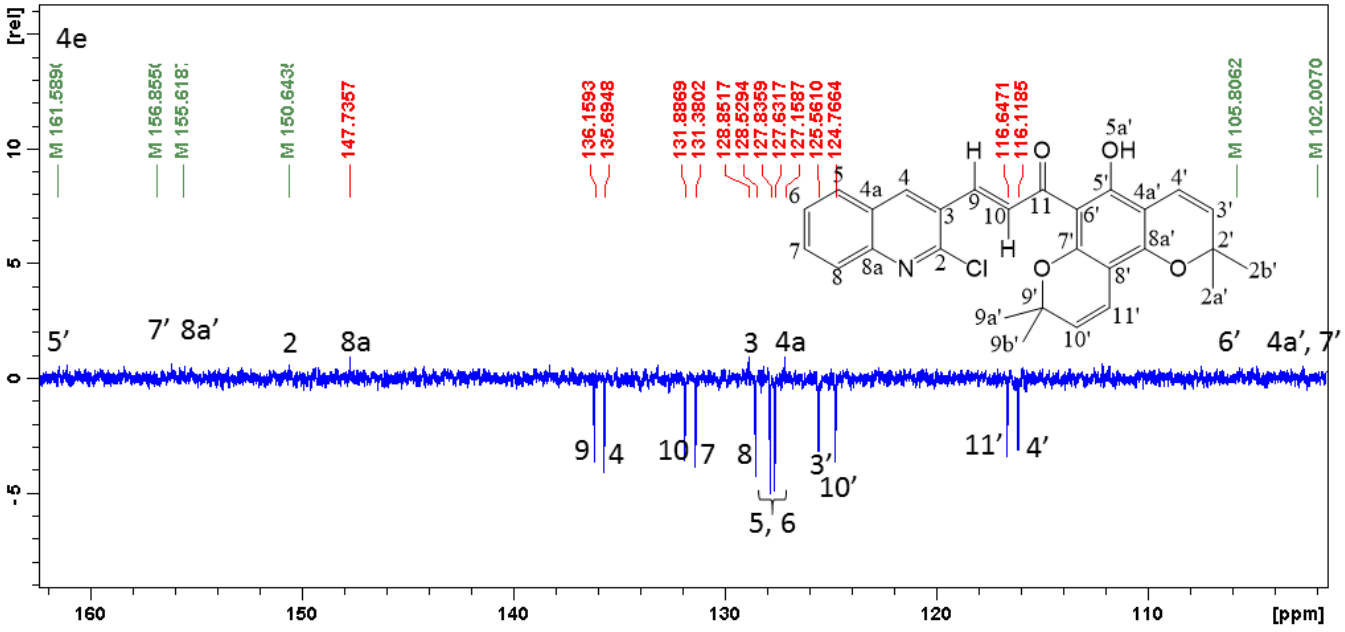
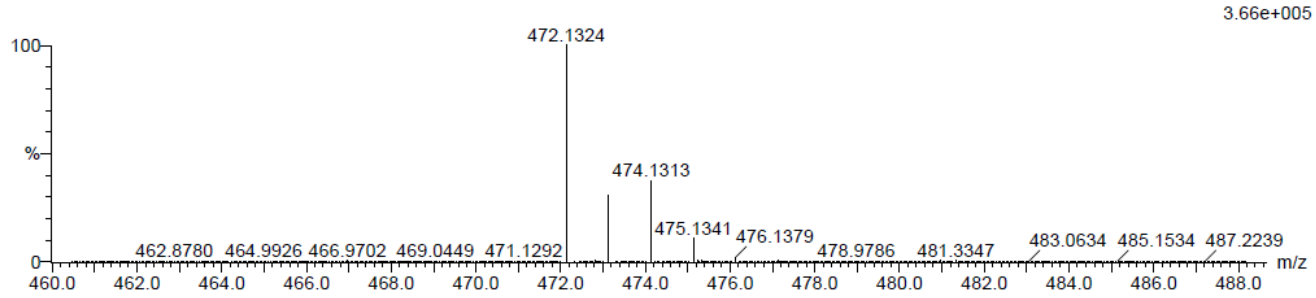


Figure S29 ^{13}C NMR spectrum (expanded) of **4e**

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
21 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 25-30 H: 20-25 N: 0-5 O: 0-5 Cl: 0-1
4e 16 (0.506) Cm (1:61)
TOF MS ES-



Minimum:				-1.5			
Maximum:		5.0	5.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
472.1324	472.1316	0.8	1.7	17.5	502.9	0.0	C28 H23 N O4 Cl

Figure S30 HRMS of **4e**

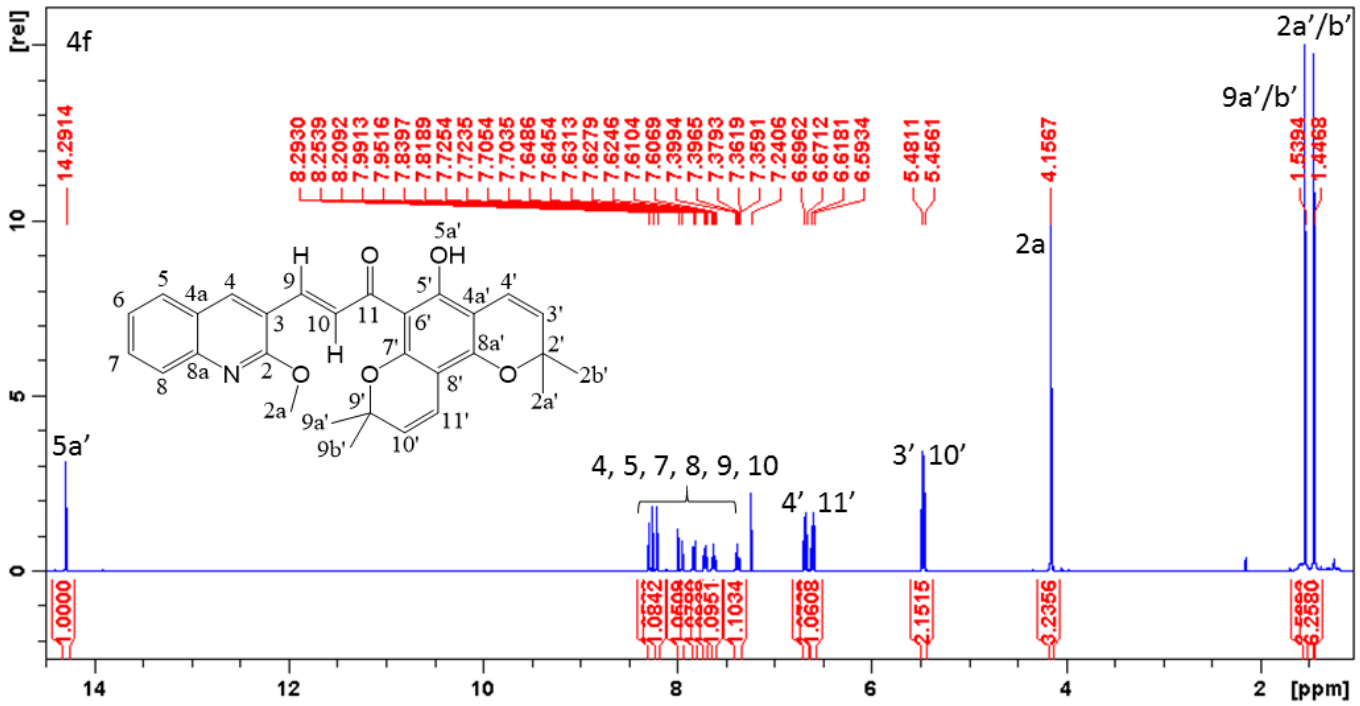


Figure S31 ^{1}H NMR spectrum (expanded) of **4f**

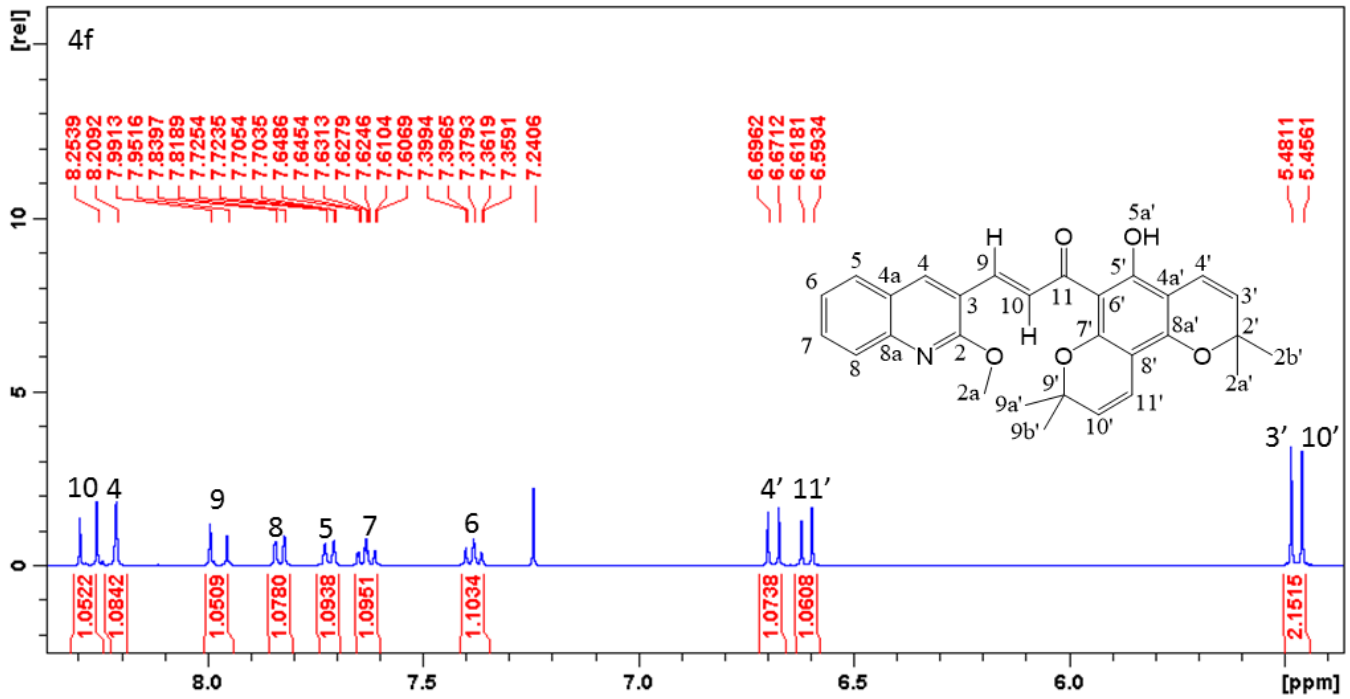


Figure S32 ^{1}H NMR spectrum (expanded) of **4f**

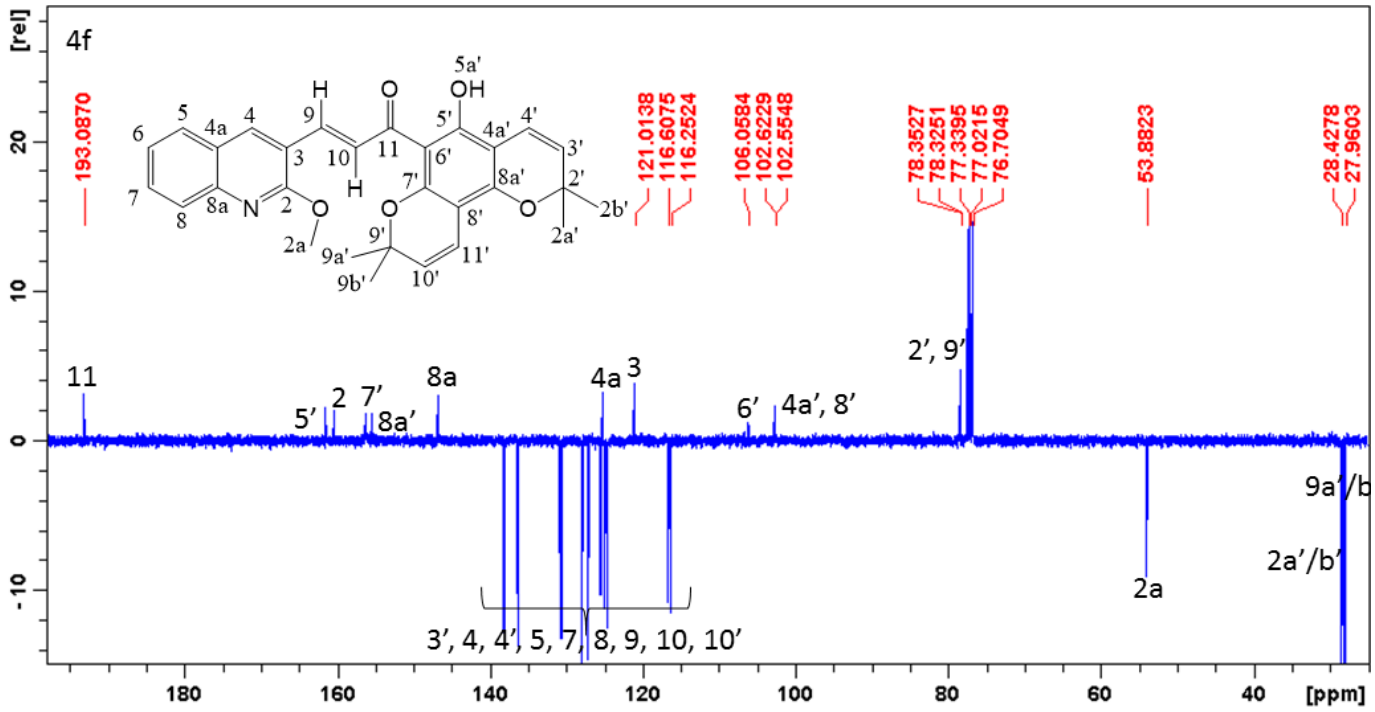


Figure S33 ^{13}C NMR spectrum of **4f**

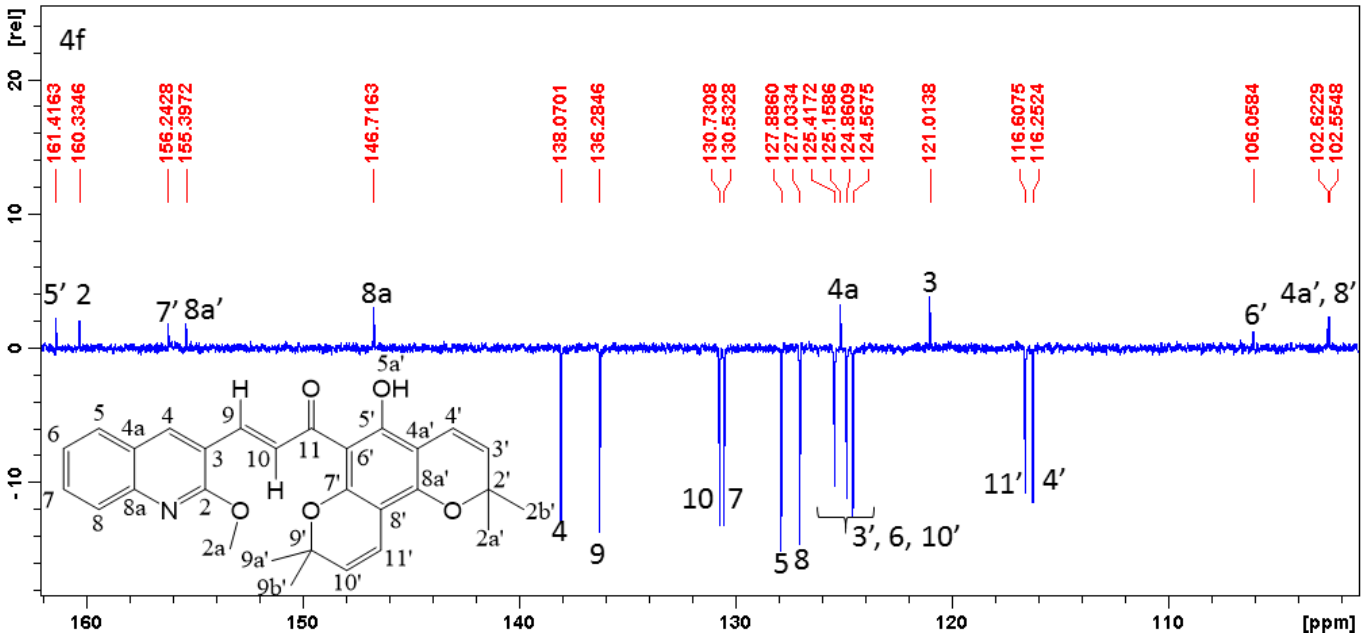
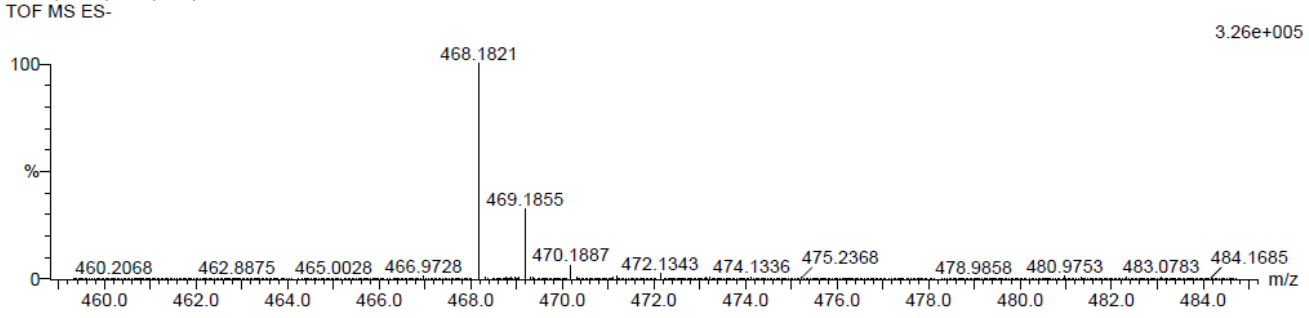


Figure S34 ^{13}C NMR spectrum (expanded) of **4f**

Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
21 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 25-30 H: 20-25 N: 0-5 O: 0-5 Cl: 0-1
4f 27 (0.877) Cm (1:61)
TOF MS ES-



Minimum:				-1.5			
Maximum:		5.0	5.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
468.1821	468.1824	-0.3	-0.6	22.5	576.7	0.0	C30 H22 N5 O

Figure S35 HRMS of **4f**

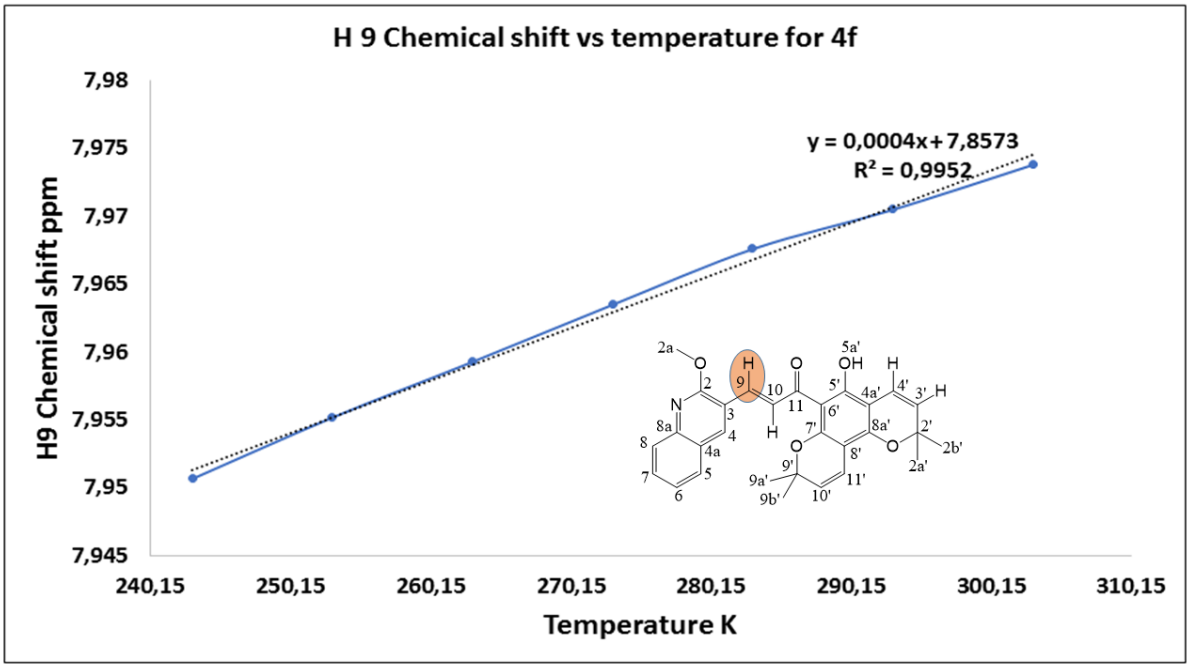


Figure S36 H-9 ^{1}H NMR chemical shift of **4f** as function of temperature

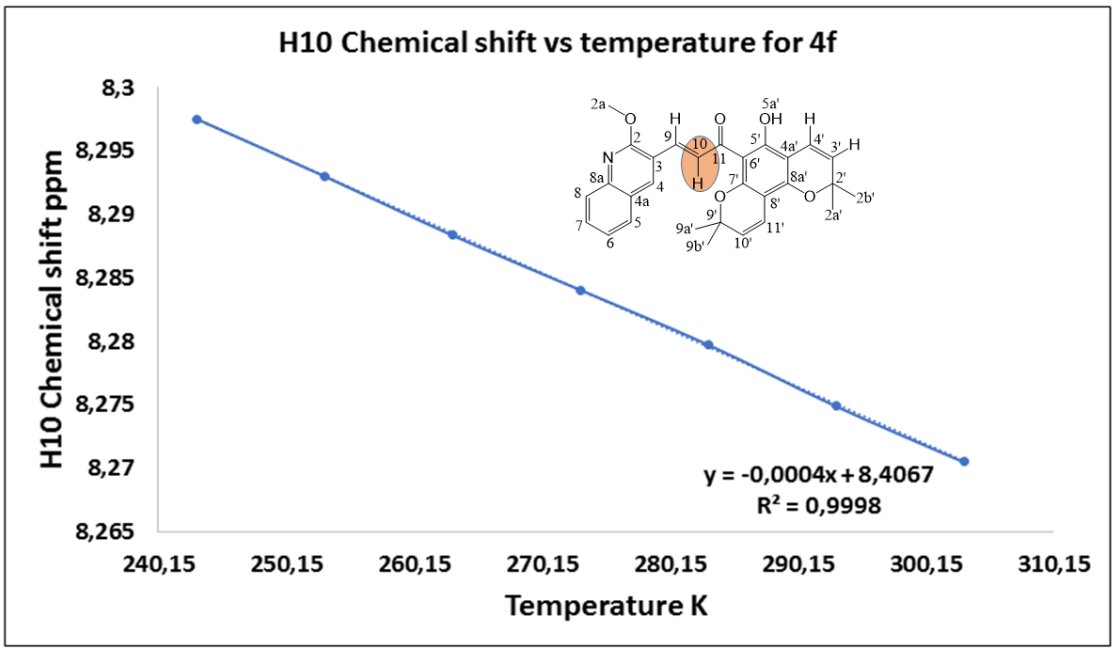


Figure S37 H-10 ^{1}H NMR chemical shift of **4f** as function of temperature

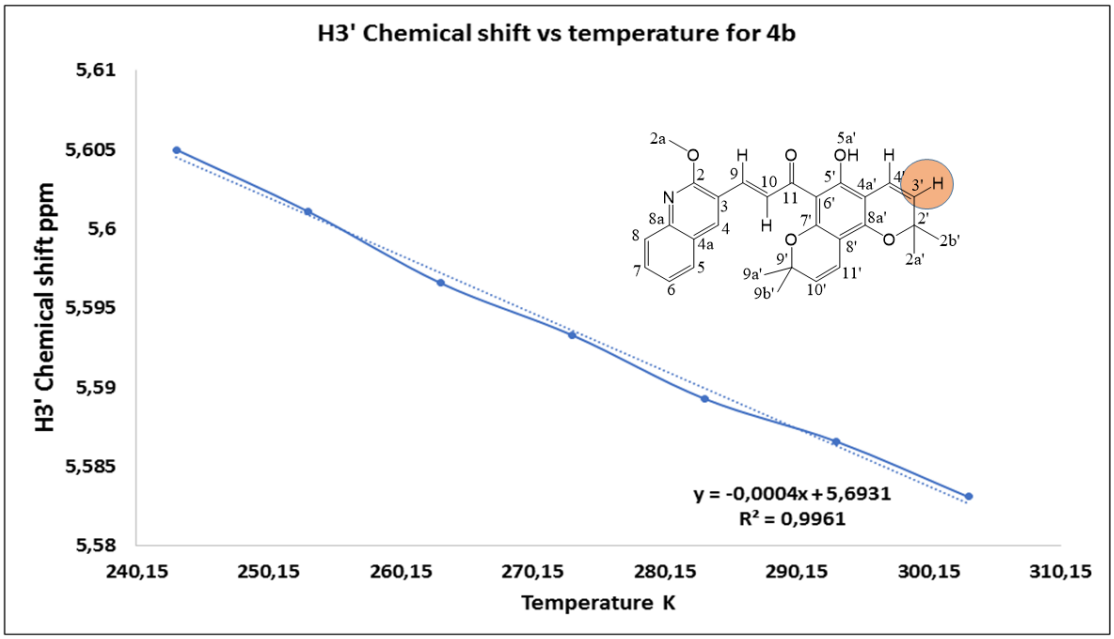


Figure S38 H-3' ^{1}H NMR chemical shift of **4f** as function of temperature

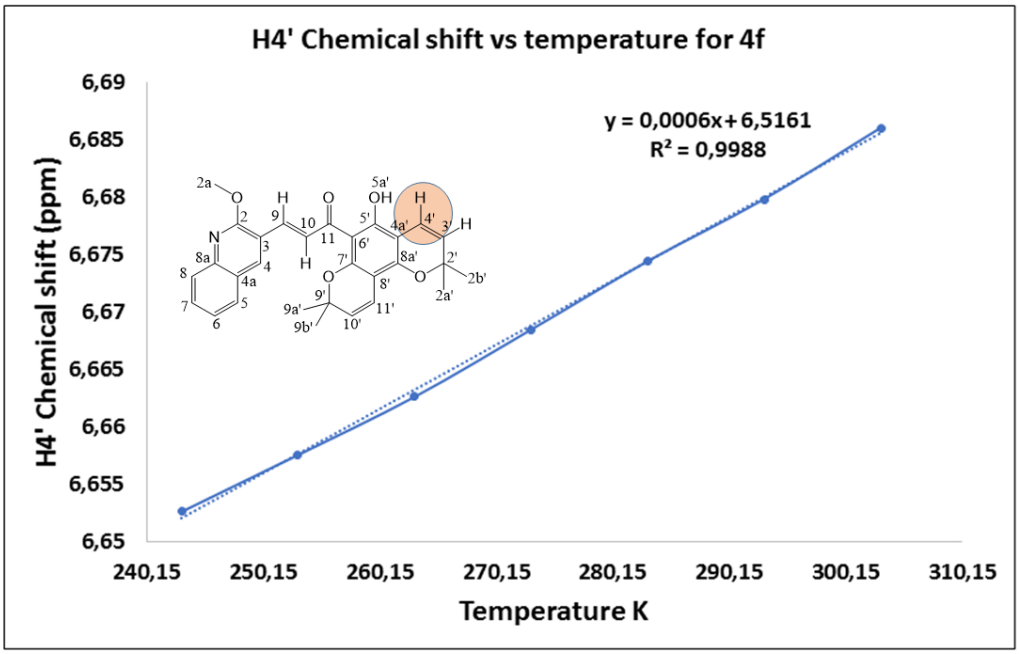


Figure S39 H-4' [1]HNMR chemical shift of **4f** as function of temperature

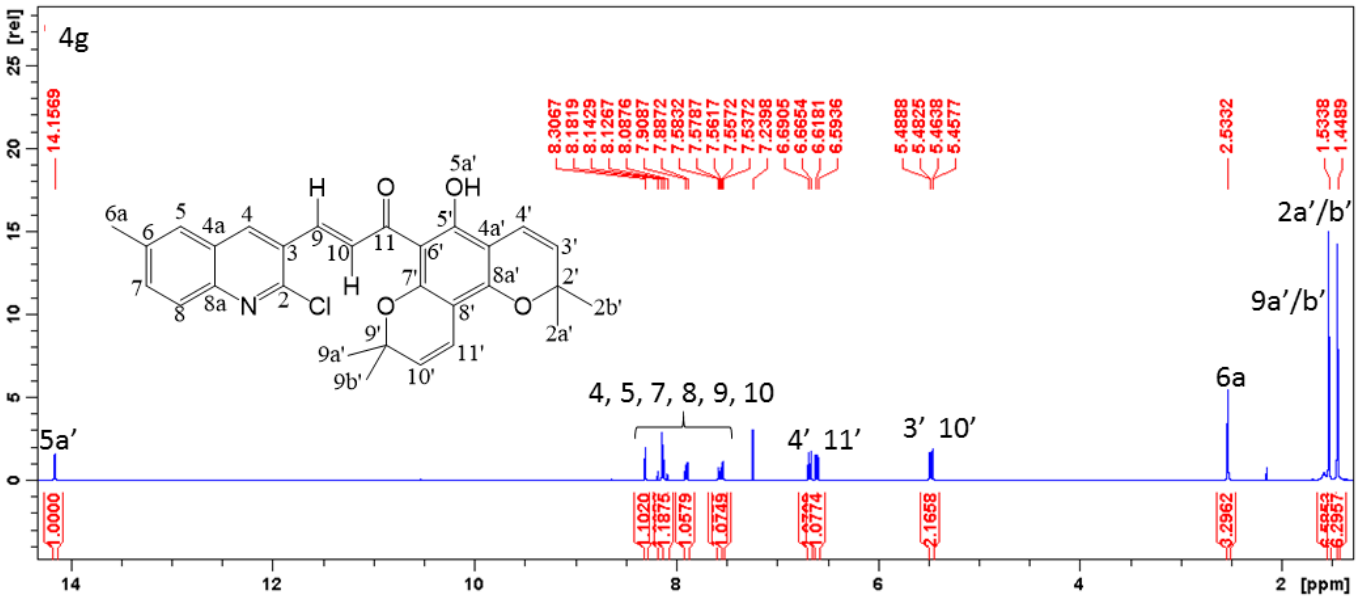


Figure S40 [1]H NMR spectrum of **4g**

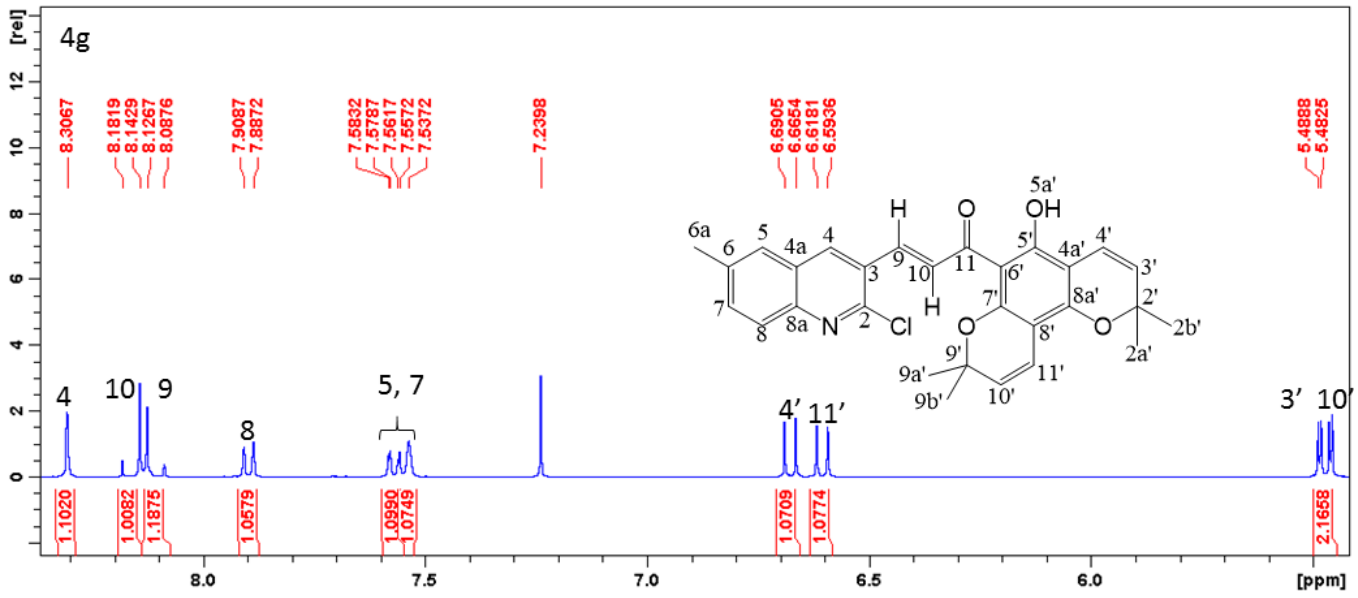


Figure S41 ^{1}H NMR spectrum (expanded) of **4g**

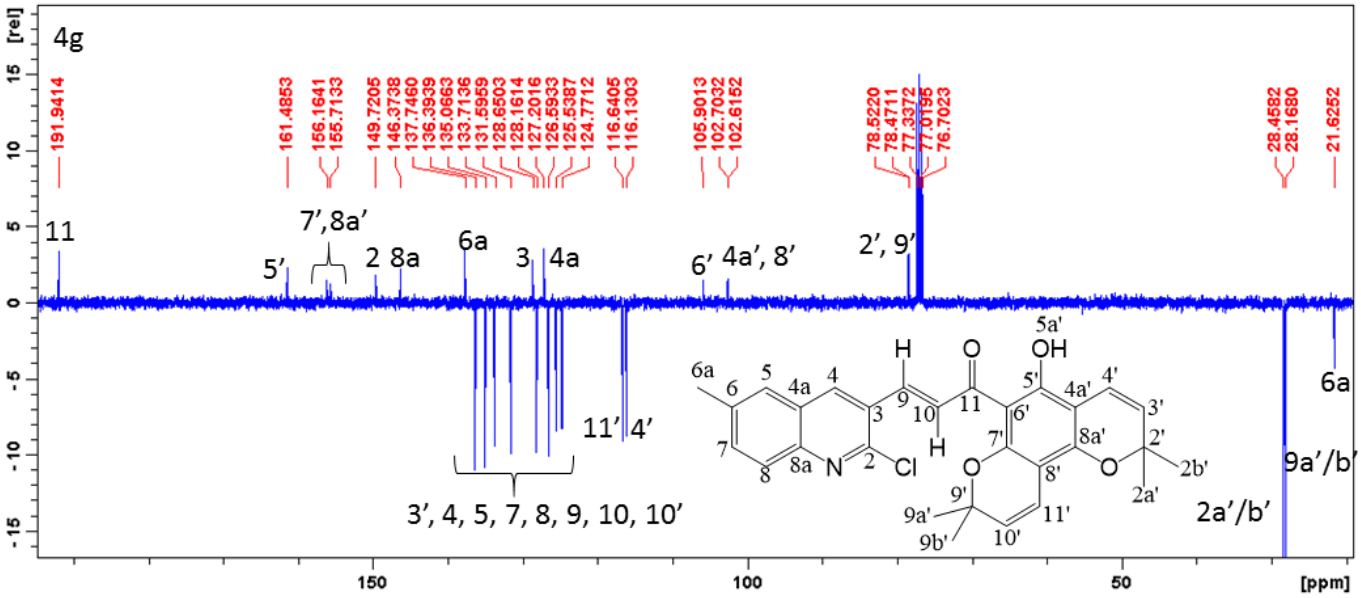


Figure S42 ^{13}C NMR spectrum of **4g**

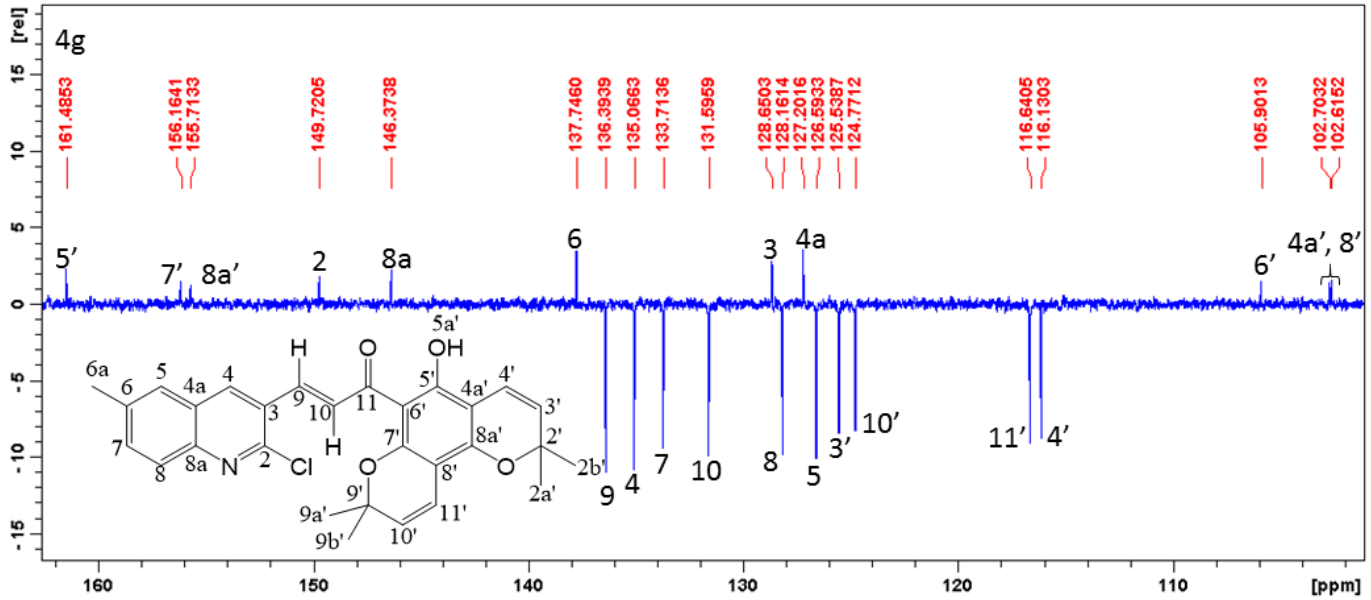


Figure S43 ^{13}C NMR spectrum (expanded) of **4g**

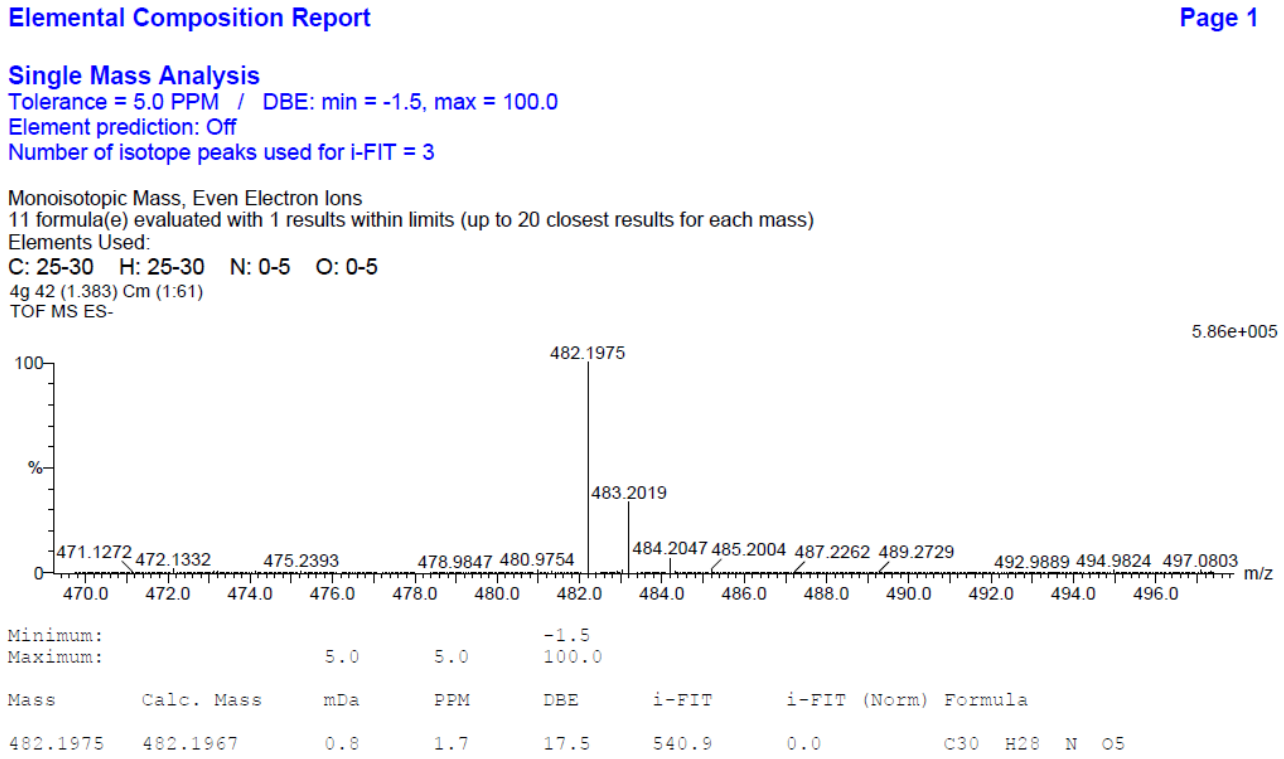


Figure S44 ^{1}H NMR spectrum of **4g**

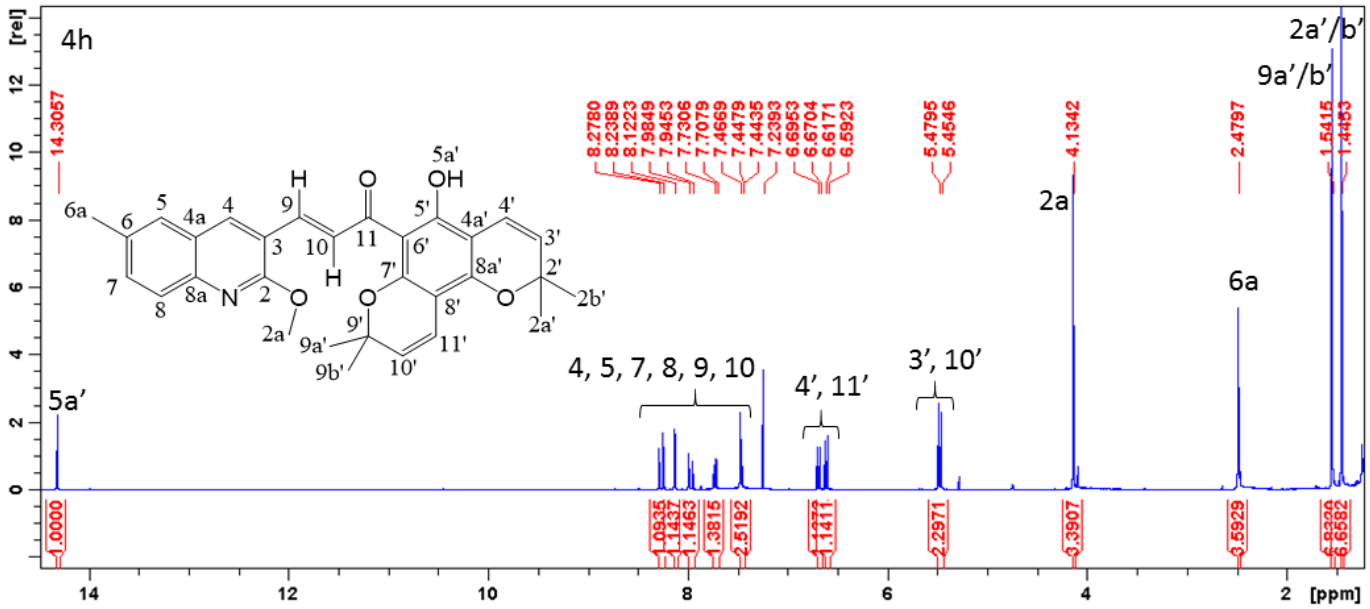


Figure S45 ^{1}H NMR spectrum of **4h**

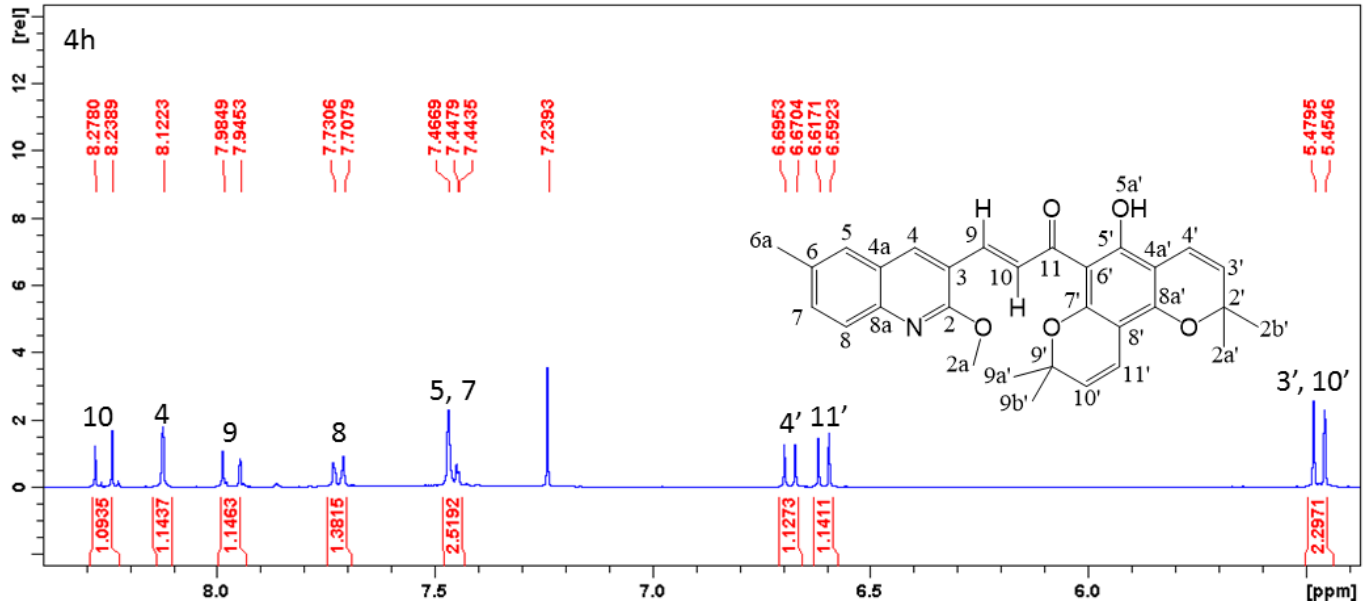


Figure S46 ^{1}H NMR spectrum (expanded) of **4h**

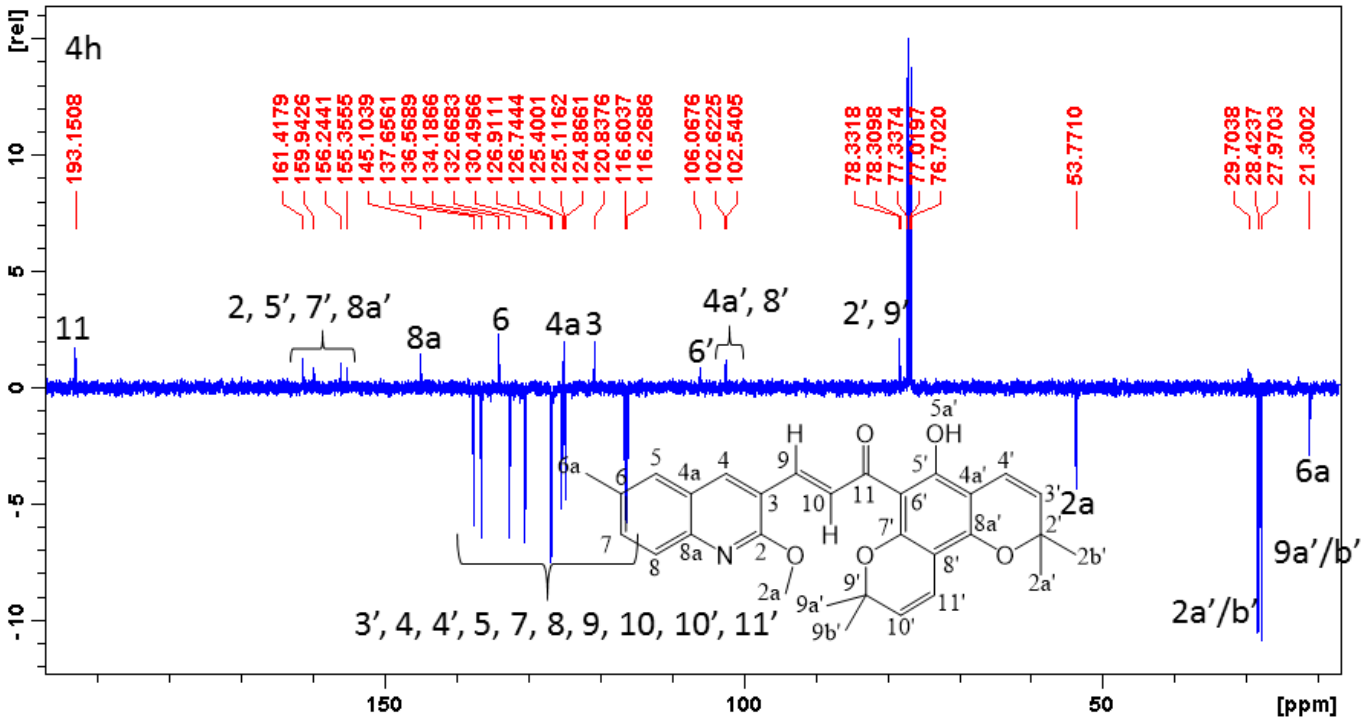


Figure S47 ^{13}C NMR spectrum of **4h**

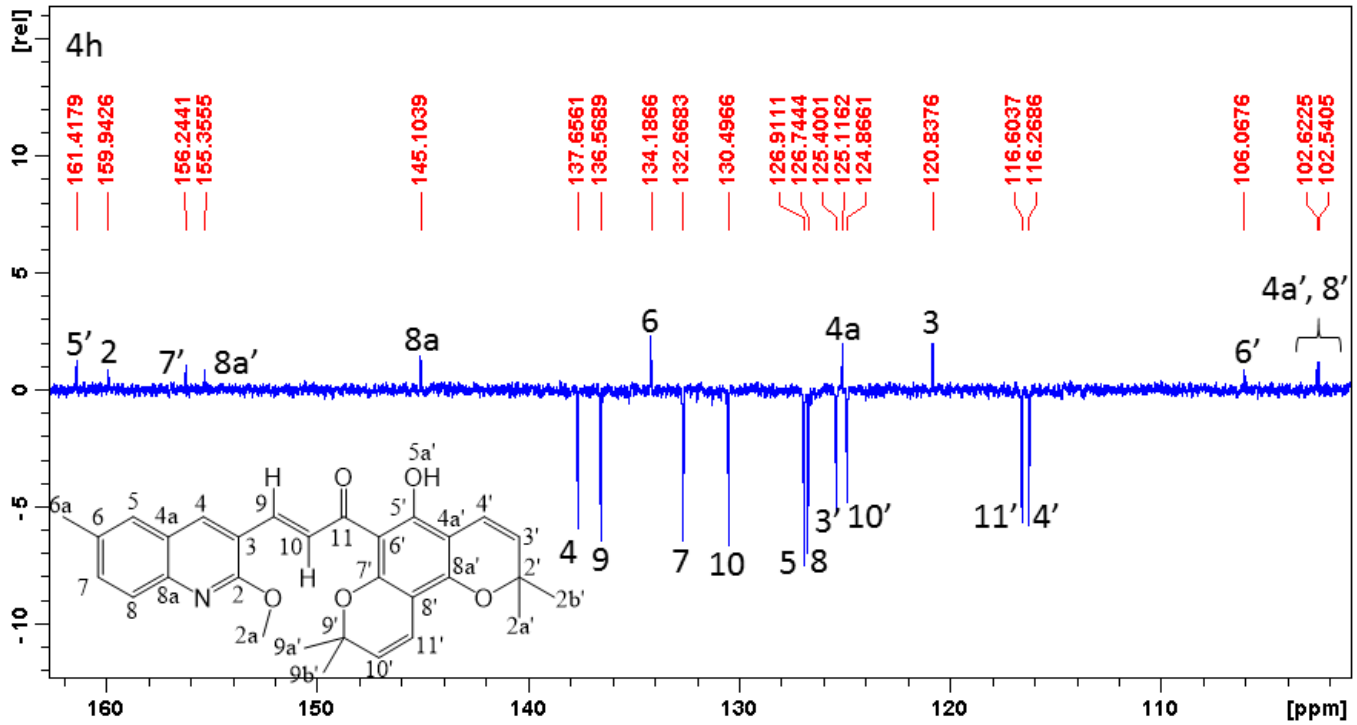
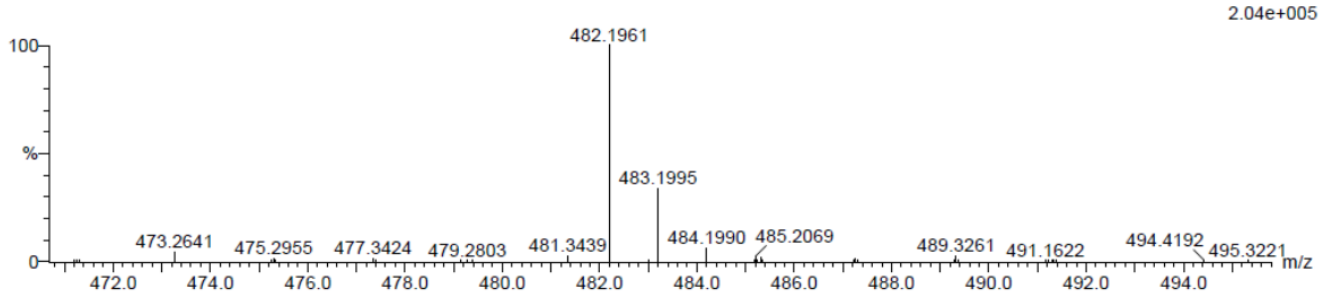


Figure S48 ^{13}C NMR spectrum (expanded) of **4h**

Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
11 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 25-30 H: 25-30 N: 0-5 O: 0-5
M2 19 (0.608) Cm (1:61)
TOF MS ES-



Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
482.1961	482.1967	-0.6	-1.2	17.5	25.0	0.0	C30 H28 N O5

Figure S49 HRMS of **4h**

Table S1 Single crystal data information of **4b** and **4f**

Compound	**4b**	**4f**
Empirical formula	$C_{24}H_{21}NO_4$	$C_{29}H_{27}NO_5$
Molecular weight	387.42	469.51
Temperature	100(2) K	100(2) K
Wavelength	0.71073 Å	0.71073 Å
Crystal system	monoclinic	Triclinic
Space group	P21/n	P -1
a	11.6463(2) Å	7.3903(3) Å
b	12.0584(2) Å	10.0787(3) Å
c	13.6163(3) Å	15.7008(5) Å
α	90°	97.851(2)°.
β	93.9760(10) °	93.122(2)°.
g	90°.	90.881(2)°.
Volume	1907.61(6) $Å^3$	1156.48(7) $Å^3$
Z	4	2
Density (calculated)	1.349 g cm^{-3}	1.348 g cm^{-3}
Absorption coefficient	0.092 mm^{-1}	0.092 mm^{-1}
F(000)	496	496
Crystal size	0.28×0.21×0.12 mm^3	0.285 x 0.185 x 0.143 mm^3
Theta range of data collection	2.226 to 28.332°	2.040 to 28.352°
Reflections collected	29697	13463
Independent reflections	4759 [R(int) = 0.0252]	5705 [R(int) = 0.0179]
Data / restraints / parameters	4759 / 0 /266	5705 / 0 / 322
Goodness-of-fit on F^2	1.052	1.020
Final R indices [I>2sigma(I)]	R1 = 0.0394, wR2 = 0.1021	R1 = 0.0427, wR2 = 0.1090
R indices (all data)	R1 = 0.0515, wR2 = 0.1098	R1 = 0.0593, wR2 = 0.1191
Largest diff. peak and hole	0.346 and -0.260 e.$Å^{-3}$	0.375 and -0.300 e.$Å^{-3}$

Table S2 Comparison of experimental and theoretical bond lengths of **4b**

Bond length	X-RAY	DFT (B3LYP)	Bond length	X-RAY	DFT (B3LYP)
C(1)-C(3)	1.5193	1.5370	C(15)-C(23)	1.4388	1.4485
C(2)-C(3)	1.5239	1.5301	C(16)-C(17)	1.4156	1.4148
C(3)-C(4)	1.5030	1.5123	C(17)-C(18)	1.4158	1.4182
C(3)-O(1)	1.4706	1.4673	C(17)-C(22)	1.4142	1.4277
C(4)-C(5)	1.3301	1.3389	C(18)-C(19)	1.3725	1.3780
C(5)-C(6)	1.4592	1.4592	C(19)-C(20)	1.405	1.4149
C(6)-C(7)	1.3949	1.4023	C(20)-C(21)	1.3703	1.3800
C(6)-C(11)	1.4015	1.4092	C(21)-C(22)	1.4123	1.4149
C(7)-C(8)	1.3993	1.4056	C(22)-N(5)	1.3722	1.3673
C(7)-O(1)	1.3558	1.3523	C(23)-O(4)	1.3482	1.3510
C(8)-C(9)	1.3768	1.3811	C(23)-N(5)	1.3028	1.3066
C(9)-C(10)	1.4094	1.4139	C(24)-O(4)	1.4348	1.4336
C(10)-C(11)	1.4188	1.4301	C(12)-O(3)	1.2514	1.2566
C(10)-C(12)	1.4654	1.4658	C(13)-C(14)	1.3421	1.3504
C(11)-O(2)	1.3447	1.3357	C(14)-C(15)	1.4569	1.4555
C(12)-C(13)	1.4733	1.4776	C(15)-C(16)	1.3749	1.3846

Table S3 Comparison of experimental and theoretical bond angles of **4b**

Bond angle	X-ray	DFT (B3LYP)	Bond angle	X-ray	DFT (B3LYP)
C(1)-C(3)-C(2)	111.38	111.35	C(16)-C(17)-C(18)	123.22	123.49
C(4)-C(3)-C(2)	110.21	110.21	C(22)-C(17)-C(16)	117.27	117.03
O(1)-C(3)-C(1)	105.09	104.40	C(22)-C(17)-C(18)	119.51	119.47
O(1)-C(3)-C(2)	107.77	107.24	C(19)-C(18)-C(17)	120.07	120.33
O(1)-C(3)-C(4)	110.20	111.11	C(18)-C(19)-C(20)	120.23	120.09
C(5)-C(4)-C(3)	121.22	212.59	C(21)-C(20)-C(19)	120.91	120.81
C(4)-C(5)-C(6)	119.01	120.06	C(20)-C(21)-C(22)	120.10	120.26
C(7)-C(6)-C(5)	118.48	118.09	C(21)-C(22)-C(17)	119.17	119.06
C(7)-C(6)-C(11)	118.34	118.91	N(5)-C(22)-C(17)	122.25	121.73
C(11)-C(6)-C(5)	123.01	122.89	N(5)-C(22)-C(21)	118.58	119.22
C(6)-C(7)-C(8)	121.76	121.38	O(4)-C(23)-C(15)	115.46	116.39
O(1)-C(7)-C(6)	120.89	121.48	N(5)-C(23)-C(15)	125.49	124.79
O(1)-C(7)-C(8)	117.29	117.09	N(5)-C(23)-O(4)	119.05	118.82
C(9)-C(8)-C(7)	119.00	119.12	C(7)-O(1)-C(3)	117.93	120.45
C(8)-C(9)-C(10)	121.97	122.15	C(23)-O(4)-C(24)	116.71	117.01
C(9)-C(10)-C(11)	117.59	117.71	C(23)-N(5)-C(22)	117.91	117.15
C(9)-C(10)-C(12)	123.37	123.59	O(3)-C(12)-C(13)	119.61	119.35
C(11)-C(10)-C(12)	119.05	118.70	C(14)-C(13)-C(12)	119.15	119.40
C(6)-C(11)-C(10)	121.34	120.72	C(13)-C(14)-C(15)	130.06	130.18
O(2)-C(11)-C(6)	116.96	117.74	C(16)-C(15)-C(14)	118.74	118.46
O(2)-C(11)-C(10)	121.70	121.54	C(16)-C(15)-C(23)	115.69	115.31
C(10)-C(12)-C(13)	120.55	121.54	C(23)-C(15)-C(14)	125.56	126.24
O(3)-C(12)-C(10)	119.84	120.44	C(15)-C(16)-C(17)	121.37	121.99

Table S4 Comparison of the experimental and theoretical dihedral angles of **4b**

Dihedral angles	X-ray	DFT (B3LYP)	Dihedral angles	X-ray	DFT (B3LYP)
C(1)-C(3)-C(4)-C(5)	-146.97	-131.43	C(15)-C(23)-O(4)-C(24)	178.31	179.83
C(1)-C(3)-O(1)-C(7)	161.28	151.86	C(15)-C(23)-N(5)-C(22)	-0.16	-0.02
C(2)-C(3)-C(4)-C(5)	88.44	95.80	C(16)-C(15)-C(23)-O(4)	180.00	179.94
C(2)-C(3)-O(1)-C(7)	-79.84	-89.90	C(16)-C(15)-C(23)-N(5)	-0.35	-0.02
C(3)-C(4)-C(5)-C(6)	5.26	4.03	C(16)-C(17)-C(18)-C(19)	-179.62	-179.99
C(4)-C(3)-O(1)-C(7)	40.45	31.38	C(16)-C(17)-C(22)-C(21)	178.85	179.99
C(4)-C(5)-C(6)-C(7)	12.51	9.71	C(16)-C(17)-C(22)-N(5)	-1.44	0.003
C(4)-C(5)-C(6)-C(11)	-172.42	-173.99	C(17)-C(18)-C(19)-C(20)	0.27	-0.01
C(5)-C(6)-C(7)-C(8)	175.01	175.57	C(17)-C(22)-N(5)-C(23)	1.09	0.03
C(5)-C(6)-C(7)-O(1)	-1.89	-1.67	C(18)-C(17)-C(22)-C(21)	-0.98	0.011
C(5)-C(6)-C(11)-C(10)	-174.45	-176.38	C(18)-C(17)-C(22)-N(5)	178.72	179.99
C(5)-C(6)-C(11)-O(2)	5.07	3.30	C(18)-C(19)-C(20)-C(21)	0.05	0.01
C(6)-C(7)-C(8)-C(9)	-0.21	1.07	C(19)-C(20)-C(21)-C(22)	-0.85	0.003
C(6)-C(7)-O(1)-C(3)	-26.11	-20.32	C(20)-C(21)-C(22)-C(17)	1.30	-0.012
C(7)-C(6)-C(11)-C(10)	0.63	-0.12	C(20)-C(21)-C(22)-N(5)	-178.42	-179.99
C(7)-C(6)-C(11)-O(2)	-179.85	-179.57	C(21)-C(22)-N(5)-C(23)	-179.20	-179.98
C(7)-C(8)-C(9)-C(10)	0.40	-0.26	C(22)-C(17)-C(18)-C(19)	0.21	-0.002
C(8)-C(7)-O(1)-C(3)	156.86	162.34	C(23)-C(15)-C(16)-C(17)	-0.05	0.05
C(8)-C(9)-C(10)-C(11)	-0.08	-069	O(1)-C(3)-C(4)-C(5)	-30.37	-23.34
C(8)-C(9)-C(10)-C(12)	179.91	179.98	O(1)-C(7)-C(8)-C(9)	176.79	178.442
C(9)-C(10)-C(11)-C(6)	-0.45	0.88	O(3)-C(12)-C(13)-C(14)	5.44	1.88
C(9)-C(10)-C(11)-O(2)	-179.95	-179.79	O(4)-C(23)-N(5)-C(22)	179.48	179.98
C(9)-C(10)-C(12)-C(13)	0.37	-2.17	N(5)-C(23)-O(4)-C(24)	-1.36	0.13
C(9)-C(10)-C(12)-O(3)	-179.28	-177.95	C(11)-C(10)-C(12)-C(13)	-179.65	-178.56
C(10)-C(12)-C(13)-C(14)	-174.20	-178.24	C(11)-C(10)-C(12)-O(3)	0.70	-1.32

C(11)-C(6)-C(7)-C(8)	-0.30	-0.88	C(12)-C(10)-C(11)-C(6)	179.56	179.80
C(11)-C(6)-C(7)-O(1)	-177.19	-178.11	C(12)-C(10)-C(11)-O(2)	0.07	0.53

Table S5 Comparison of experimental and theoretical bond lengths of **4f**

Bond length	X-RAY	DFT (B3LYP)	Bond length	X-RAY	DFT (B3LYP)
O(1)-C(3)	1.3578	1.3525	C(7)-O(5)	1.2510	1.2585
O(1)-C(2)	1.4736	1.4698	C(7)-C(8)	1.4739	1.4766
O(2)-C(5)	1.3412	1.3311	C(8)-C(9)	1.3325	1.3503
O(2)-H(2)	0.8400	1.0131	C(9)-C(10)	1.4629	1.4598
O(3)-C(11)	1.3513	1.3492	C(10)-C(18)	1.3671	1.3813
O(3)-C(22)	1.4341	1.4315	C(10)-C(11)	1.4394	1.4466
O(4)-C(24)	1.3588	1.3584	C(12)-C(13)	1.4096	1.4153
O(4)-C(28)	1.4748	1.4689	C(12)-C(19))	1.4162	1.4293
N(1)-C(11)	1.3028	1.3076	C(13)-C(14)	1.3733	1.3797
N(1)-C(12)	1.3749	1.3672	C(14)-C(21)	1.4024	1.4149
C(1)-C(2)	1.5228	1.5295	C(16)-C(17)	1.3310	1.3393
C(2)-C(16)	1.5012	1.5115	C(18)-C(19)	1.4146	1.4162
C(2)-C(15)	1.5193	1.5367	C(19)-C(20)	1.4119	1.4185
C(3)-C(4)	1.3915	1.3991	C(20)-C(21)	1.3692	1.3778
C(3)-C(25)	1.4014	1.4078	C(24)-C(25)	1.3939	1.4044
C(4)-C(5)	1.3950	1.407	C(25)-C(26)	1.4584	1.4557
C(4)-C(17)	1.4525	1.4551	C(26)-C(37)	1.3271	1.3385
C(5)-C(6)	1.4307	1.4398	C(37)-C(28)	1.4997	1.5095
C(6)-C(24)	1.4200	1.4247	C(28)-C(30)	1.5159	1.5362
C(6)-C(7)	1.4679	1.4728	C(28)-C(29)	1.5198	1.529

Table S6 Comparison of experimental and theoretical bond angles of **4f**

Bond angle	X-ray	DFT (B3LYP)	Bond angle	X-ray	DFT (B3LYP)
C(3)-O(1)-C(2)	119.91	120.224	N(1)-C(11)-O(3)	119.57	119.529
C(11)-O(3)-C(22)	116.11	117.142	N(1)-C(11)-C(10)	125.52	125.084
C(24)-O(4)-C(28)	119.97	120.247	O(3)-C(11)-C(10)	114.91	115.385
C(11)-N(1)-C(12)	117.70	118.549	N(1)-C(12)-C(13)	118.93	119.104
O(1)-C(2)-C(16)	111.17	110.799	N(1)-C(12)-C(19)	122.01	121.913
O(1)-C(2)-C(15)	104.16	104.261	C(13)-C(12)-C(19)	119.05	118.983
C(16)-C(2)-C(15)	112.18	111.041	C(14)-C(13)-C(12)	120.16	120.34
O(1)-C(2)-C(1)	107.27	107.226	C(13)-C(14)-C(21)	120.85	120.779
C(16)-C(2)-C(1)	110.77	111.041	C(17)-C(16)-C(2)	121.85	121.177
C(15)-C(2)-C(1)	111.01	111.377	C(16)-C(17)-C(4)	119.79	120.128
O(1)-C(3)-C(4)	121.69	121.185	C(10)-C(18)-C(19)	121.22	121.346
O(1)-C(3)-C(25)	115.93	116.748	C(20)-C(19)-C(18)	123.13	123.274
C(4)-C(3)-C(25)	122.24	121.988	C(20)-C(19)-C(12)	119.35	119.388
C(3)-C(4)-C(5)	118.31	118.734	C(18)-C(19)-C(12)	117.51	117.336
C(3)-C(4)-C(17)	118.50	118.178	C(21)-C(20)-C(19)	120.47	120.451
C(5)-C(4)-C(17)	122.85	122.941	C(20)-C(21)-C(14)	120.08	120.058
O(2)-C(5)-C(4)	116.51	116.948	O(4)-C(24)-C(25)	119.18	118.714
O(2)-C(5)-C(6)	121.11	121.207	O(4)-C(24)-C(6)	118.31	118.801
C(4)-C(5)-C(6)	122.37	121.845	C(25)-C(24)-C(6)	122.35	122.435
C(24)-C(6)-C(5)	116.26	116.425	C(24)-C(25)-C(3)	118.42	118.443
C(24)-C(6)-C(7)	125.67	126.195	C(24)-C(25)-C(26)	118.68	118.764
C(5)-C(6)-C(7)	118.08	117.347	C(3)-C(25)-C(26)	122.80	122.694
O(5)-C(7)-C(6)	119.69	119.423	C(37)-C(26)-C(25)	120.30	120.448
O(5)-C(7)-C(8)	117.55	117.835	C(26)-C(37)-C(28)	121.38	119.955
C(6)-C(7)-C(8)	122.75	122.704	O(4)-C(28)-C(37)	110.09	109.924
C(9)-C(8)-C(7)	121.21	120.061	O(4)-C(28)-C(30)	108.24	107.768
C(8)-C(9)-C(10)	123.42	125.772	C(37)-C(28)-C(30)	111.28	111.395
C(18)-C(10)-C(11)	115.94	115.766	O(4)-C(28)-C(29)	104.22	104.217
C(18)-C(10)-C(9)	123.29	124.225	C(37)-C(28)-C(29)	111.16	111.854
C(11)-C(10)-C(9)	120.77	120.003	C(30)-C(28)-C(29)	111.59	111.36

Table S7 Comparison of experimental and theoretical dihedral angles of **4f**

Dihedral angles	X-ray	DFT (B3LYP)	Dihedral angles	X-ray	DFT (B3LYP)
C(3)-O(1)-C(2)-C(16)	30.36	33.505	C(15)-C(2)-C(16)-C(17)	-141.77	-140.886
C(3)-O(1)-C(2)-C(15)	151.37	153.937	C(1)-C(2)-C(16)-C(17)	93.58	94.046
C(3)-O(1)-C(2)-C(1)	-90.88	-87.844	C(2)-C(16)-C(17)-C(4)	7.2	4.232
C(2)-O(1)-C(3)-C(4)	-17.28	-21.149	C(3)-C(4)-C(17)-C(16)	875	10.944
C(2)-O(1)-C(3)-C(25)	166.95	162.018	C(5)-C(4)-C(17)-C(16)	-178.06	-173.521
O(1)-C(3)-C(4)-C(5)	-177.15	-178.289	C(11)-C(10)-C(18)-C(19)	1.93	0.786
C(25)-C(3)-C(4)-C(5)	-1.65	-1.618	C(9)-C(10)-C(18)-C(19))	-177.79	-179.957
O(1)-C(3)-C(4)-C(17)	-3.65	-2.557	C(10)-C(18)-C(19)-C(20)	-178.38	-179.873
C(25)-C(3)-C(4)-C(17)	171.85	174.108	C(10)-C(18)-C(19)-C(12)	0.81	0.446
C(3)-C(4)-C(5)-O(2)	179.63	178.505	N(1)-C(12)-C(19)-C(20)	176.79	179.604
C(17)-C(4)-C(5)-O(2)	6.44	2.994	C(13)-C(12)-C(19)-C(20)	-2.03	-0.206
C(3)-C(4)-C(5)-C(6)	0.52	1.203	N(1)-C(12)-C(19)-C(18)	-2.44	-0.09
C(17)-C(4)-C(5)-C(6)	-172.68	-176.714	C(13)-C(12)-C(19)-C(18)	178.74	179.899
O(2)-C(5)-C(6)-C(24)	-177.59	-175.939	C(18)-C(19)-C(20)-C(21)	179.96	179.95
C(4)-C(5)-C(6)-C(24)	1.48	3.756	C(12)-C(19)-C(20)-C(21)	0.8	0.275
O(2)-C(5)-C(6)-C(7)	2.59	3.241	C(19)-C(20)-C(21)-C(14)	0.9	0.161
C(4)-C(5)-C(6)-C(7)	-178.33	-177.063	C(13)-C(14)-C(21)-C(20)	-1.3	-0.025
C(24)-C(6)-C(7)-O(5)	179.48	170.423	C(28)-O(4)-C(24)-C(25)	-28.73	-26.441
C(5)-C(6)-C(7)-O(5)	-0.72	-8.668	C(28)-O(4)-C(24)-C(6)	155.76	156.05
C(24)-C(6)-C(7)-C(8)	-1.8	-11.863	C(5)-C(6)-C(24)-O(4)	172.84	178.854
C(5)-C(6)-C(7)-C(8)	178.01	169.046	C(7)-C(6)-C(24)-O(4)	-7.36	-0.244
O(5)-C(7)-C(8)-C(9)	-20.75	-8.615	C(5)-C(6)-C(24)-C(25)	-2.52	-3.734
C(6)-C(7)-C(8)-C(9)	160.5	173.636	C(7)-C(6)-C(24)-C(25)	177.28	177.167
C(7)-C(8)-C(9)-C(10)	-179.92	-178.134	O(4)-C(24)-C(25)-C(3)	-173.8	-178.567
C(8)-C(9)-C(10)-C(18)	19.00	15.095	C(6)-C(24)-C(25)-C(3)	1.52	1.153
C(8)-C(9)-C(10)-C(11)	-160.75	-165.768	O(4)-C(24)-C(25)-C(26)	2.6	2.081
C(12)-N(1)-C(11)-O(3)	-178.40	-179.751	C(6)-C(24)-C(25)-C(26)	177.92	175.332
C(12)-N(1)-C(11)-C(10)	2.14	0.182	O(1)-C(3)-C(25)-C(24)	176.41	178.464
C(22)-O(3)-C(11)-N(1)	-0.90	-0.871	C(4)-C(3)-C(25)-C(24)	0.66	1.658
C(22)-O(3)-C(11)-C(10)	178.62	179.519	O(1)-C(3)-C(25)-C(26)	0.16	5.198
C(18)-C(10)-C(11)-N(1)	-3.62	-0.681	C(4)-C(3)-C(25)-C(26)	-175.58	-177.996
C(9)-C(10)-C(11)-N(1)	176.1	179.89	C(24)-C(25)-C(26)-C(37)	11.24	13.31
C(18)-C(10)-C(11)-O(3)	176.9	179.733	C(3)-C(25)-C(26)-C(37)	-172.53	-170.362
C(9)-C(10)-C(11)-O(3)	-3.38	-0.525	C(25)-C(26)-C(37)-C(28)	1.1	3.775
C(11)-N(1)-C(12)-C(13)	179.83	179.974	C(24)-O(4)-C(28)-C(37)	38.12	40.586
C(11)-N(1)-C(12)-C(19)	1.01	0.216	C(24)-O(4)-C(28)-C(30)	-83.71	-80.988
N(1)-C(12)-C(13)-C(14)	-177.21	-179.791	C(24)-O(4)-C(28)-C(29)	157.39	160.604
C(19)-C(12)-C(13)-C(14)	1.65	0.024	C(26)-C(37)-C(28)-O(4)	-23.97	-28.593
C(12)-C(13)-C(14)-C(21)	0.0	0.093	C(26)-C(37)-C(28)-C(30)	96.03	90.789
O(1)-C(2)-C(16)-C(17)	-25.59	-25.051	C(26)-C(37)-C(28)-C(29)	-138.93	-143.859