# Supplementary Material

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

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## Table of Contents



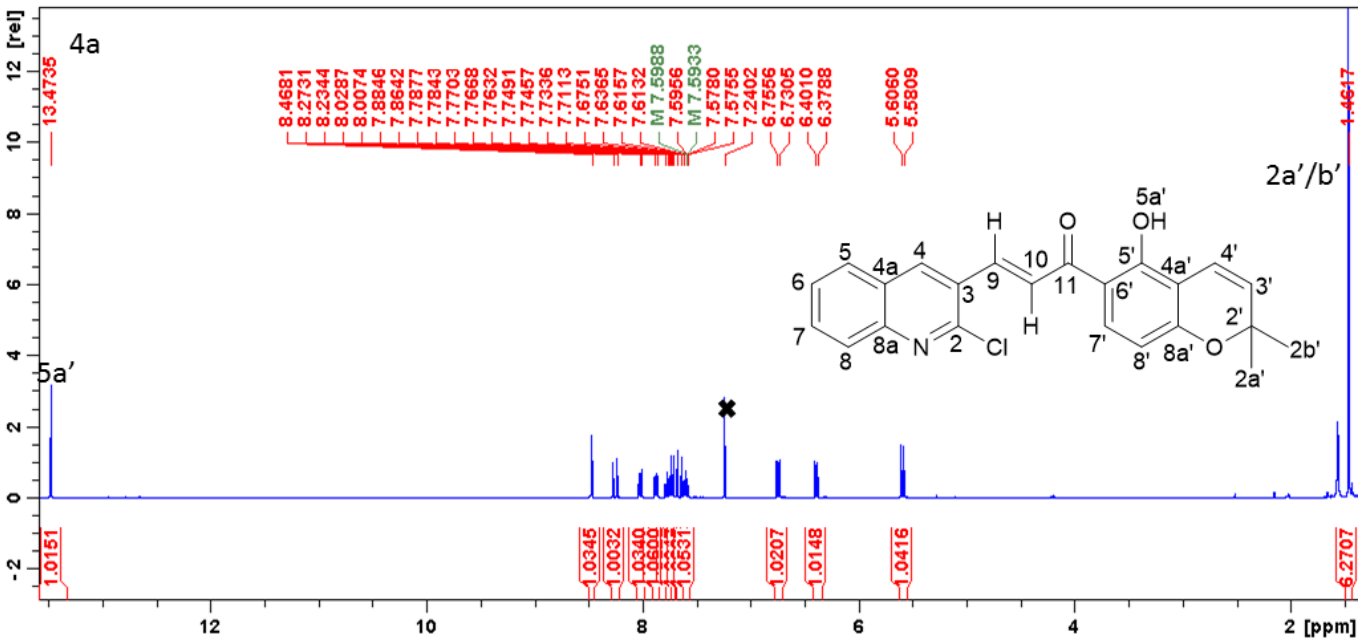



**Figure S1** $^{1}$H NMR spectrum of **4a**

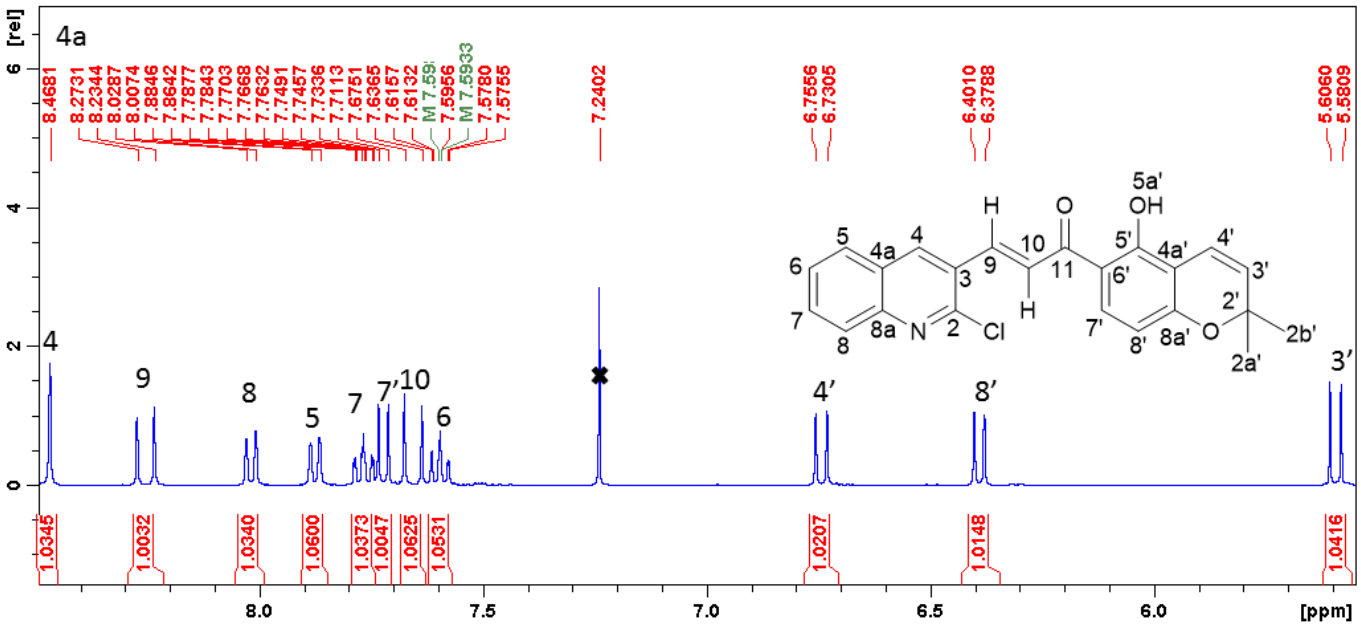



**Figure S2** $^{1}$H NMR spectrum (expansion 1) of **4a**

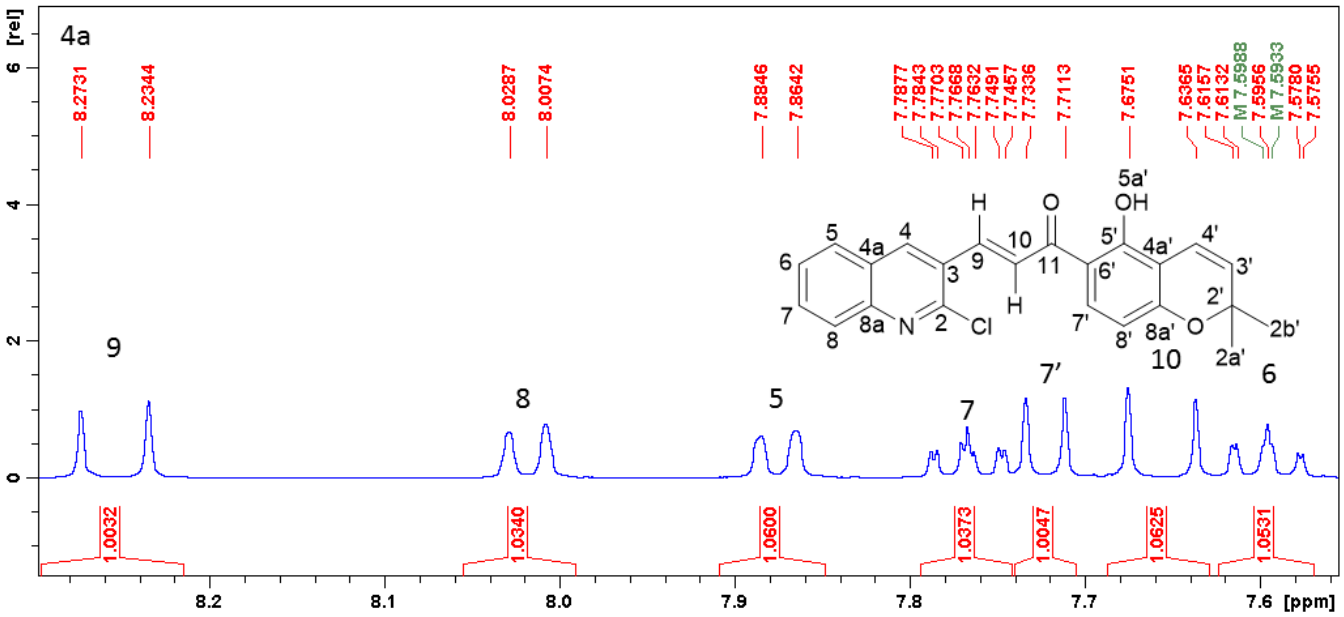



**Figure S3** $^{1}$H NMR spectrum (expansion 2) of **4a**

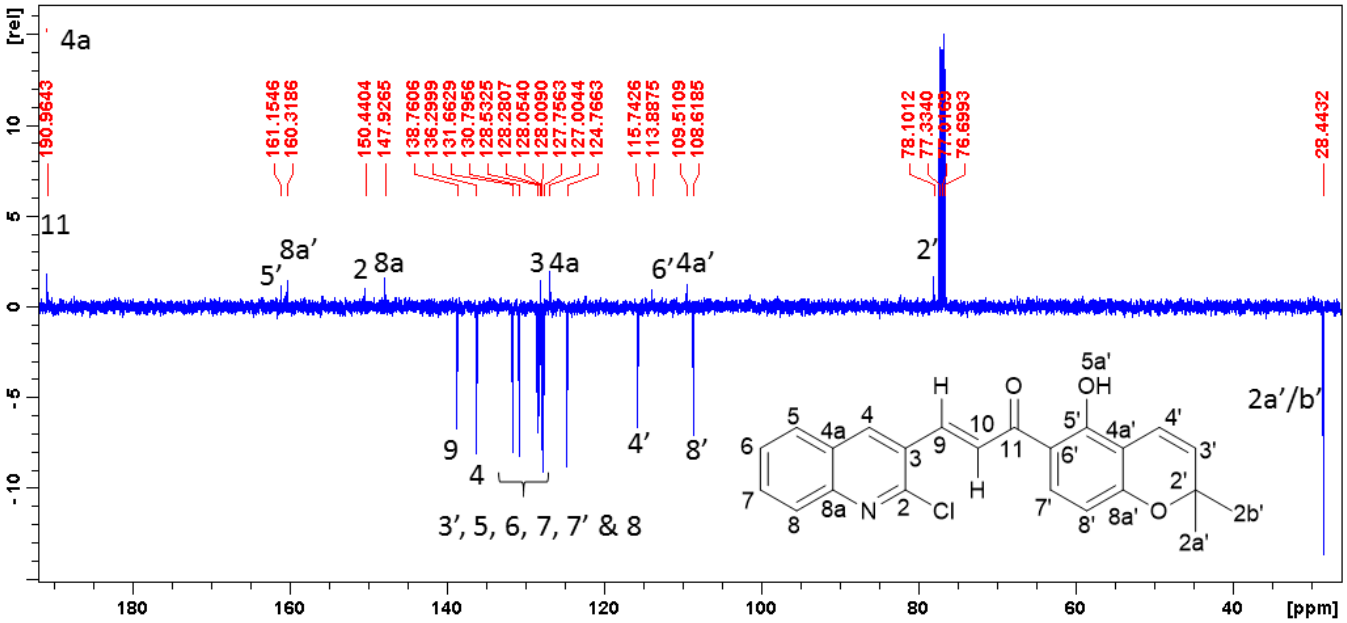



**Figure S4** $^{13}$C NMR spectrum of **4a**

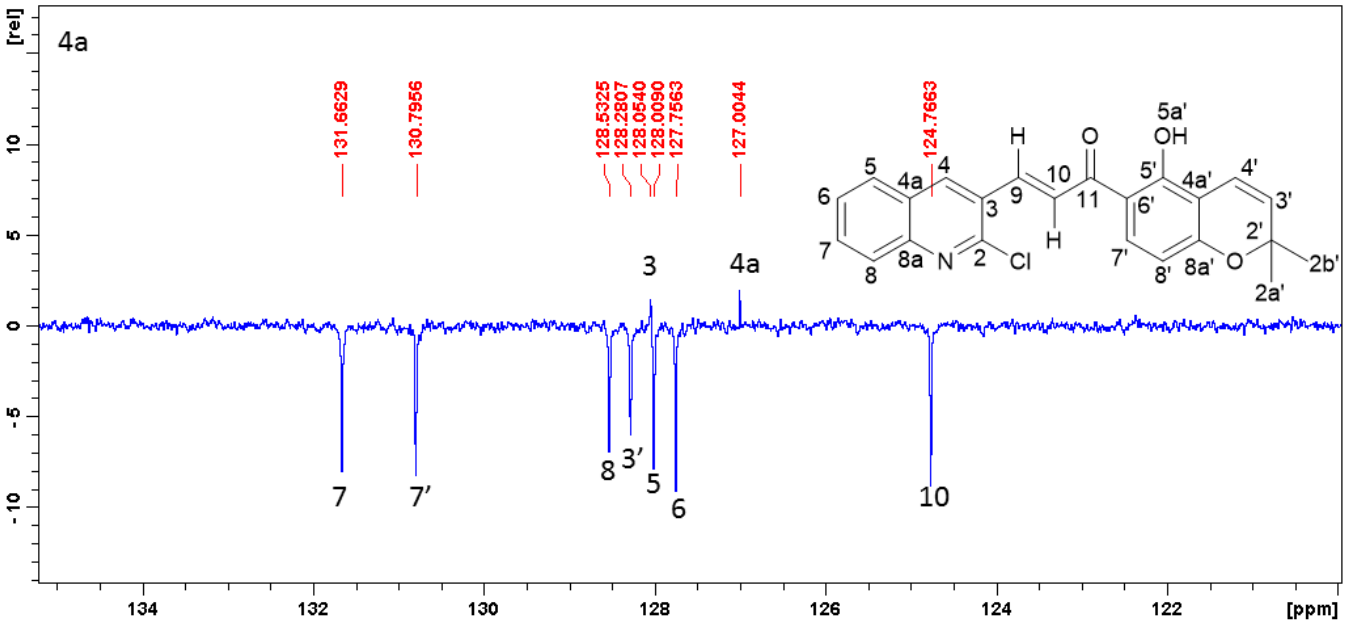



**Figure S5** $^{13}$C NMR spectrum (expanded) of **4a**

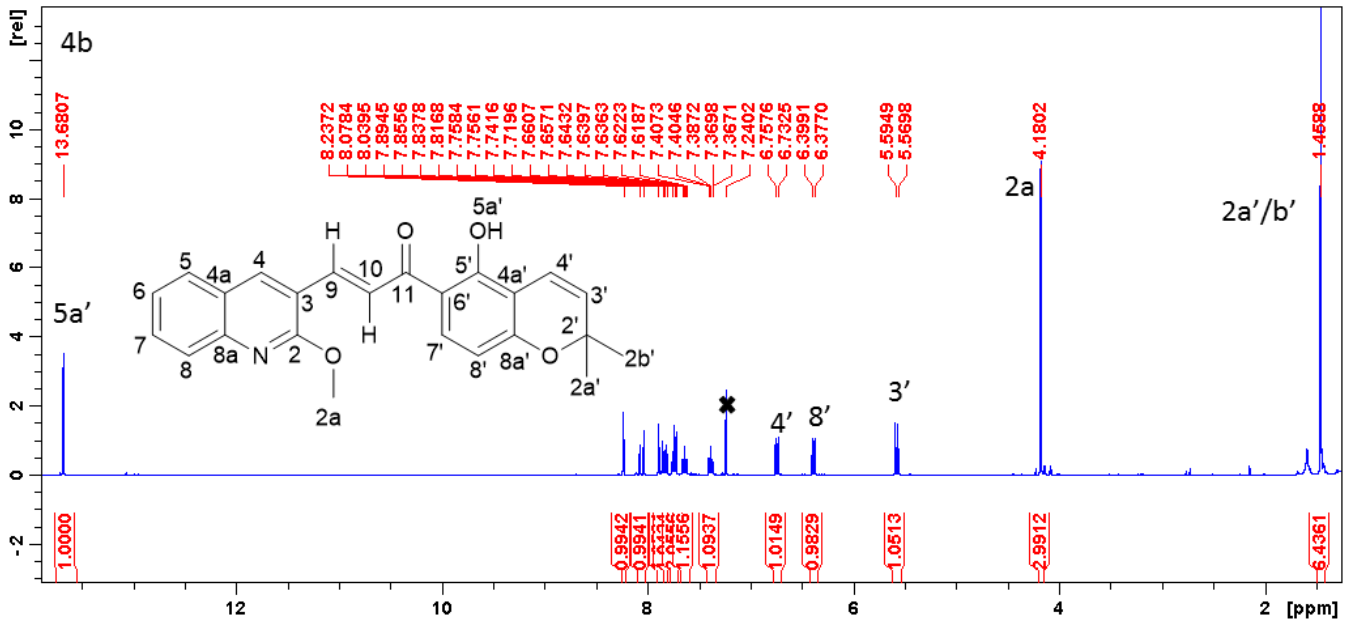



**Figure S6** $^{1}$H NMR of **4b**

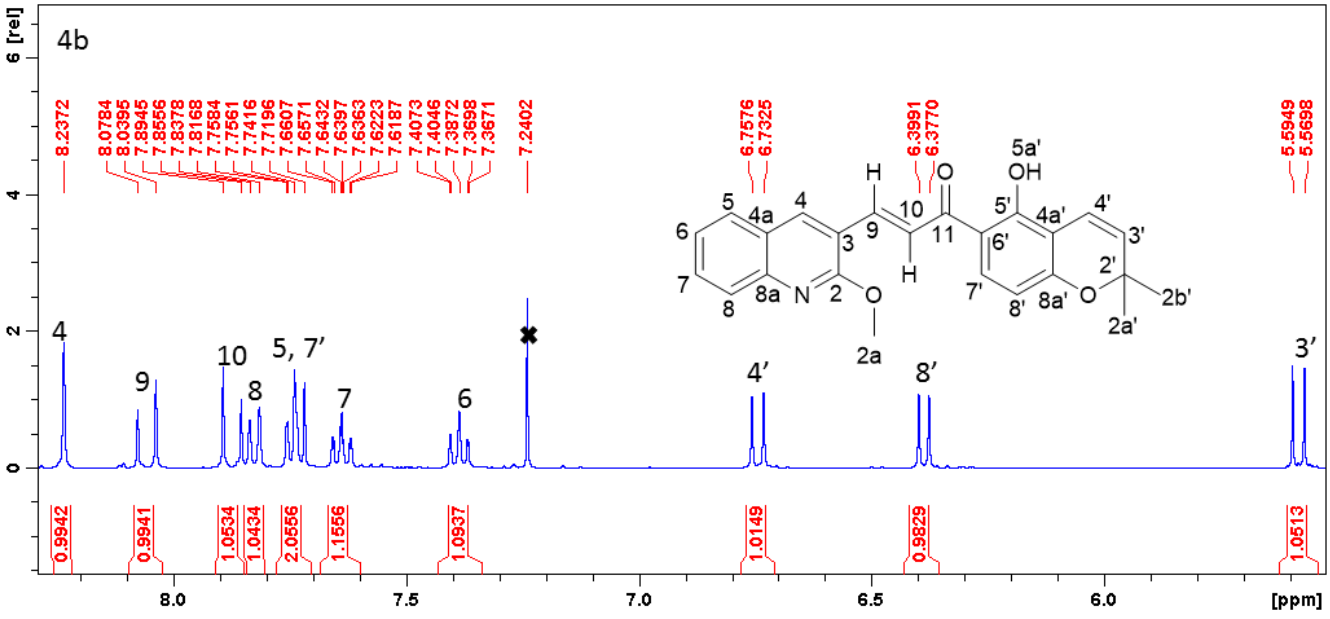



**Figure S7** $^{1}$H NMR spectrum (expanded) of **4b**

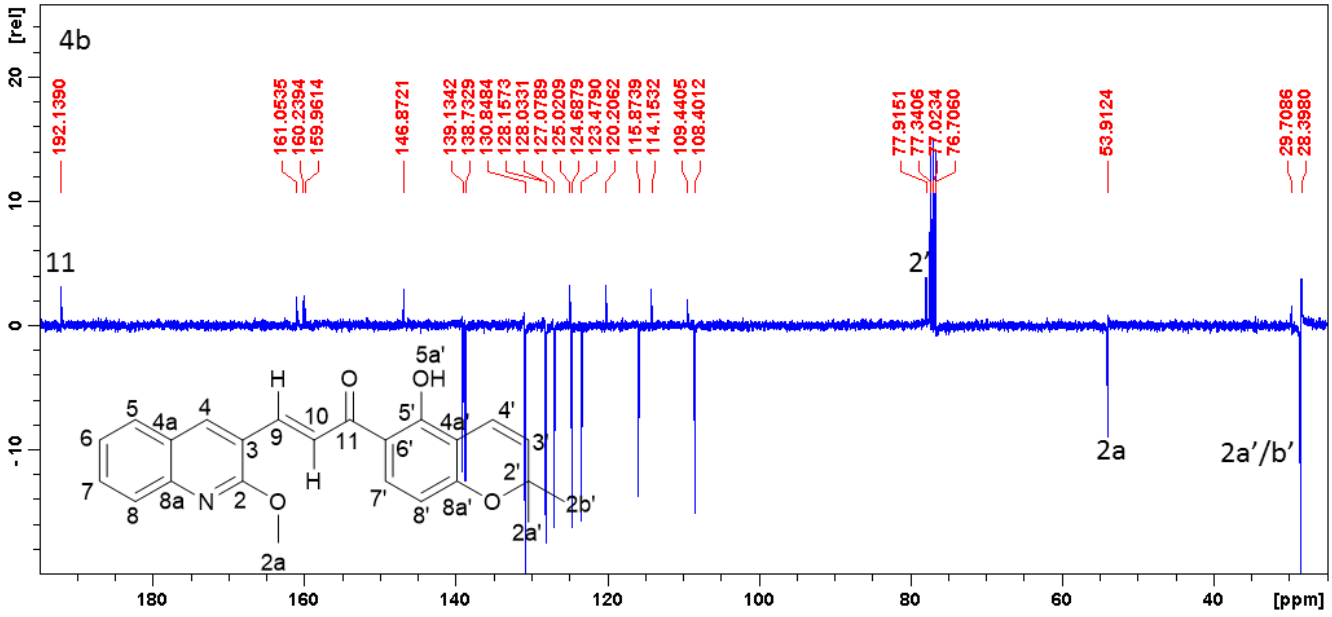



**Figure S8** $^{13}$C NMR spectrum of **4b**

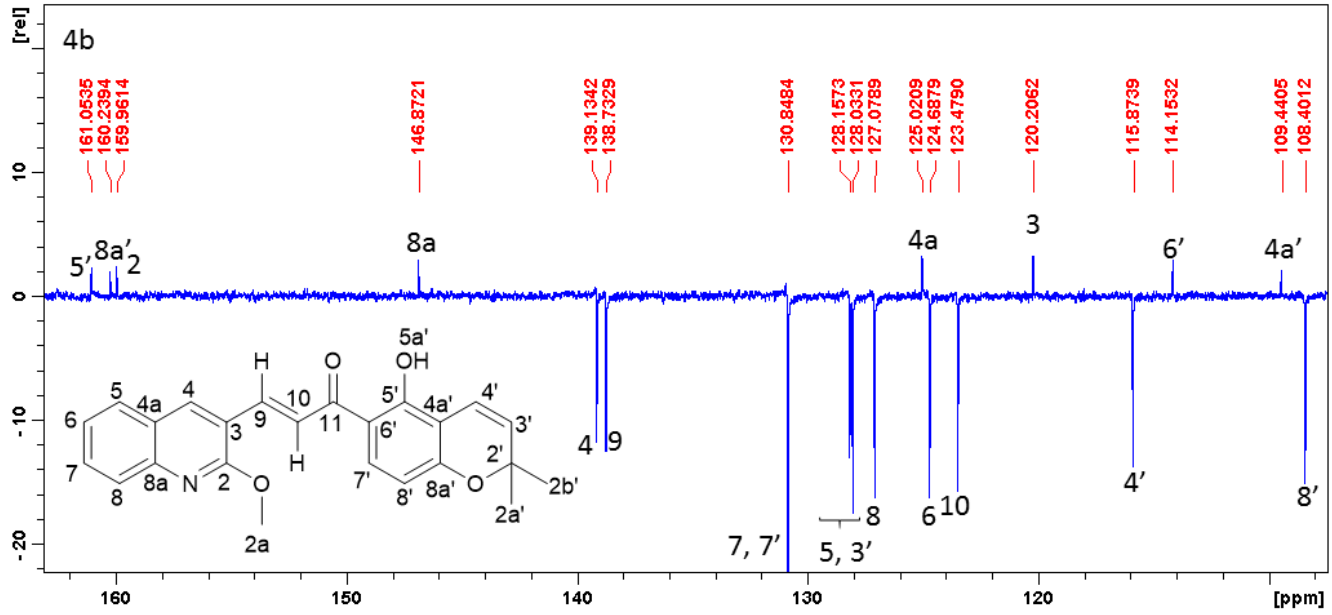
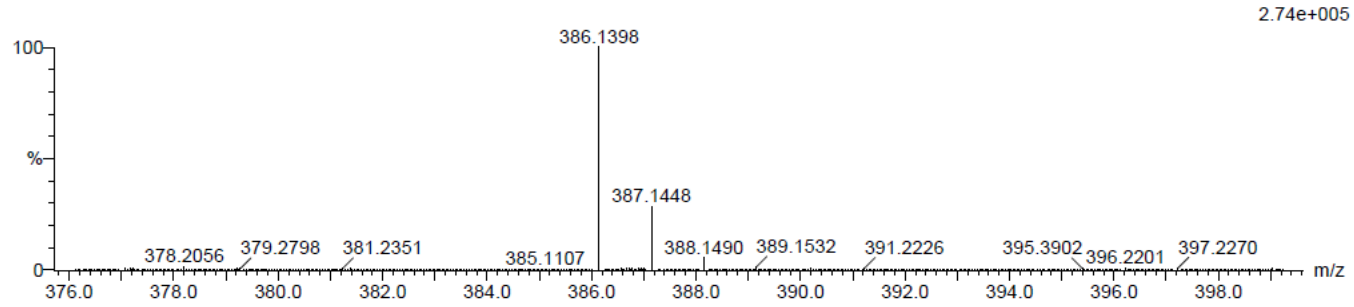



**Figure S9** $^{13}$C NMR spectrum (expanded) of **4b**

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**

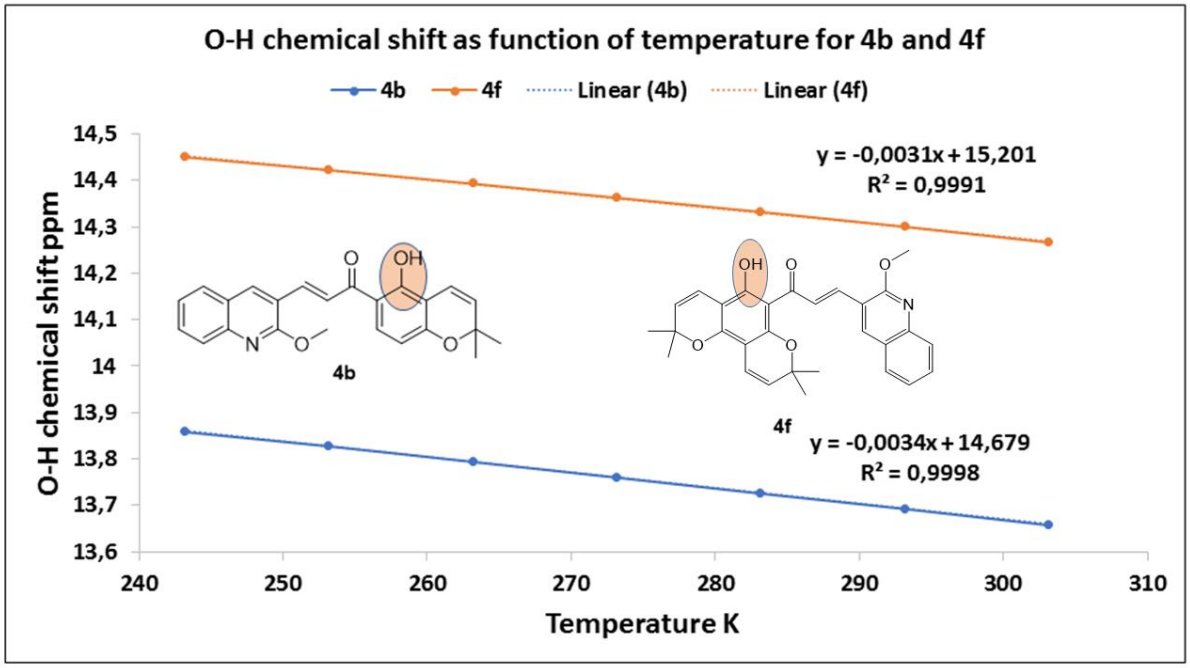



**Figure S11** OH $^{1}$H NMR chemical shift of **4b** and **4f** as function of temperature

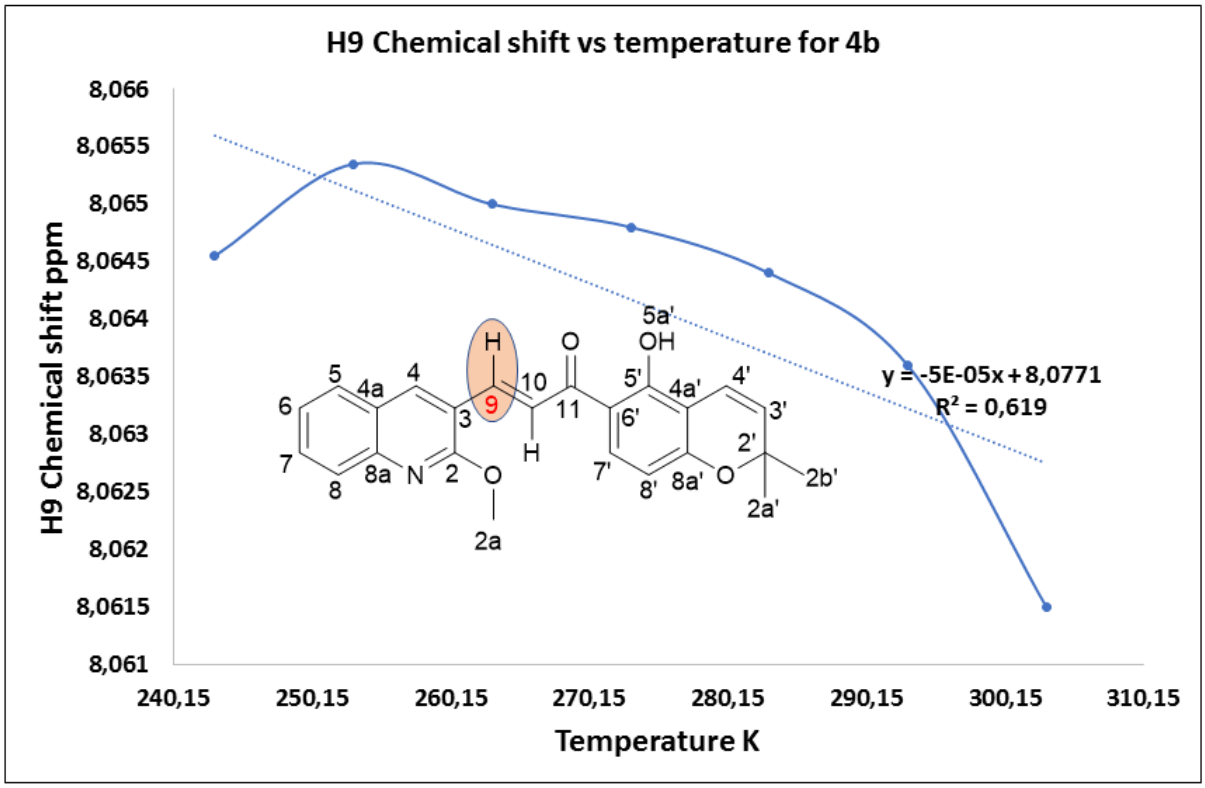



**Figure S12** H-9 $^{1}$H NMR chemical shift of **4b** as function of temperature

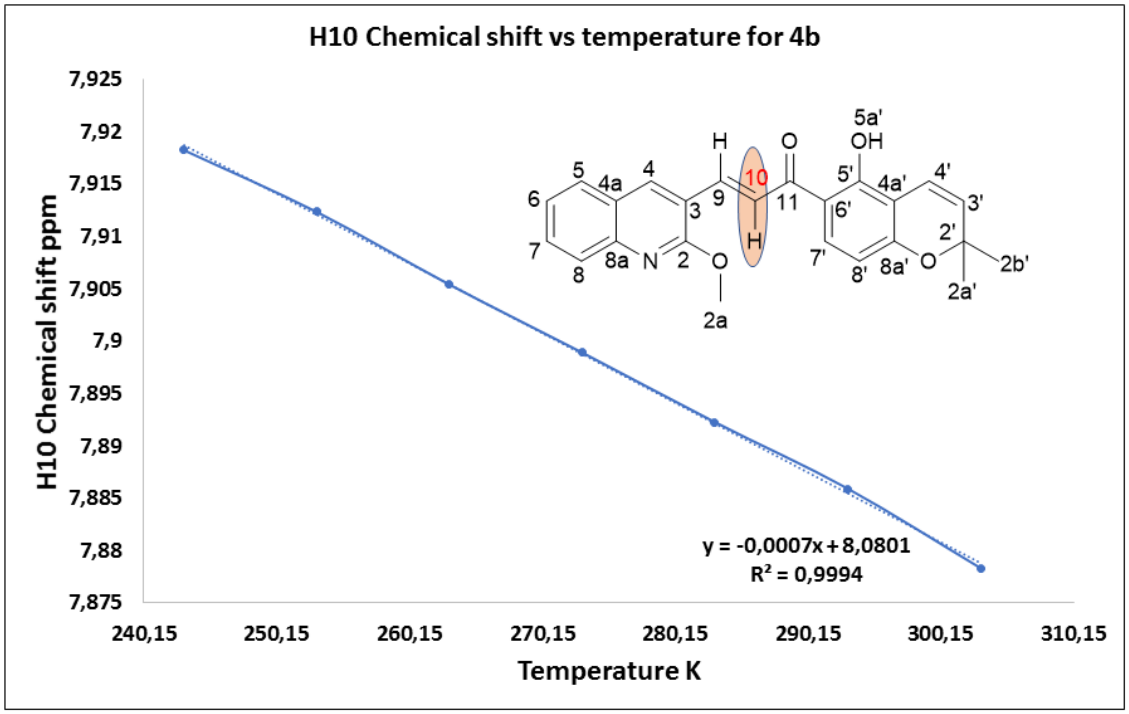



**Figure S13** H-10 $^{1}$H NMR chemical shift of **4b** as function of temperature

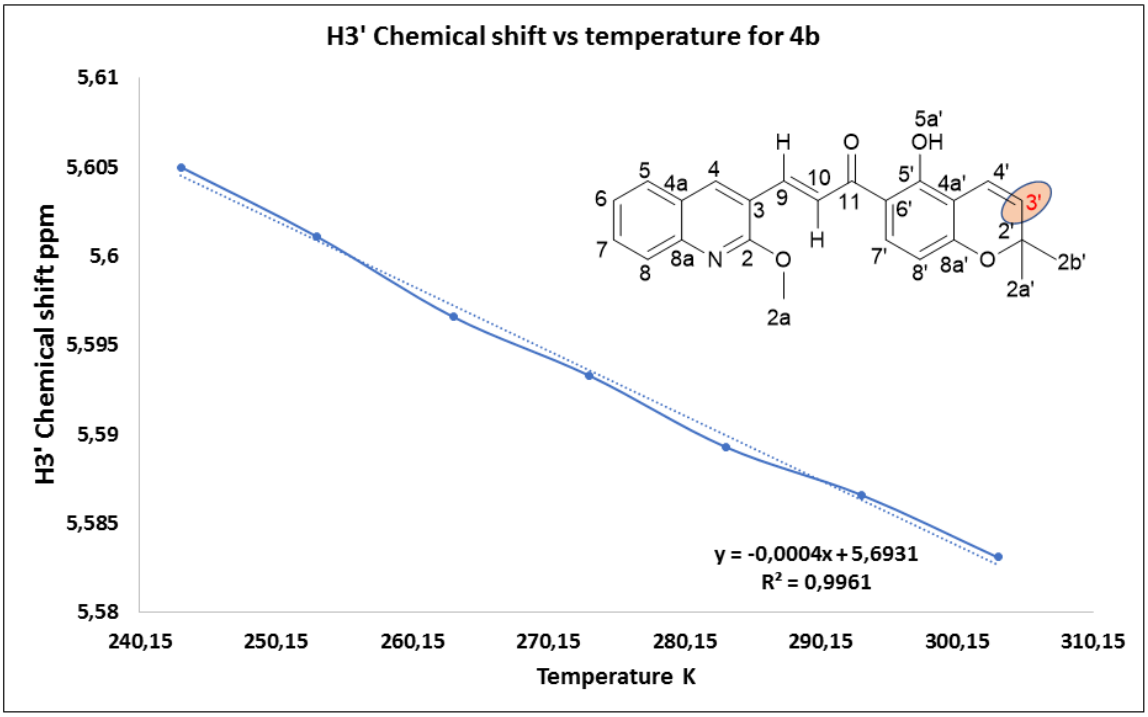



**Figure S14** H-3' $^{1}$H NMR chemical shift of **4b** as function of temperature

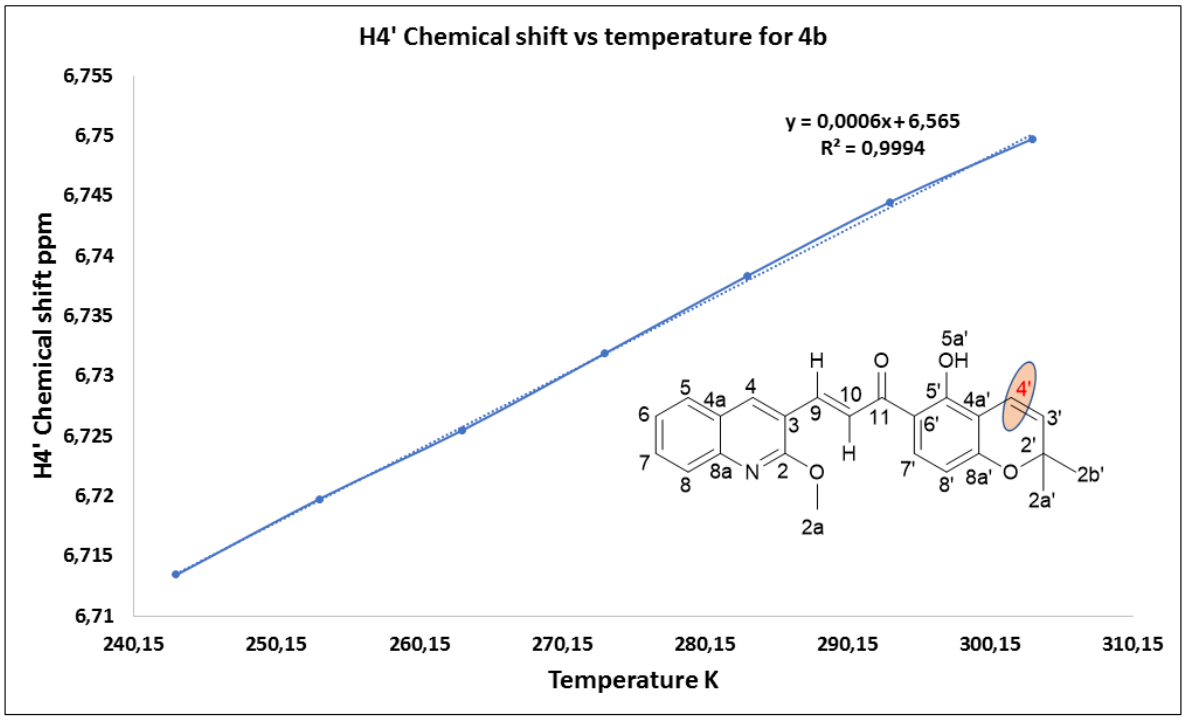



**Figure S15** H-4' $^{1}$H NMR chemical shift of **4b** as function of temperature

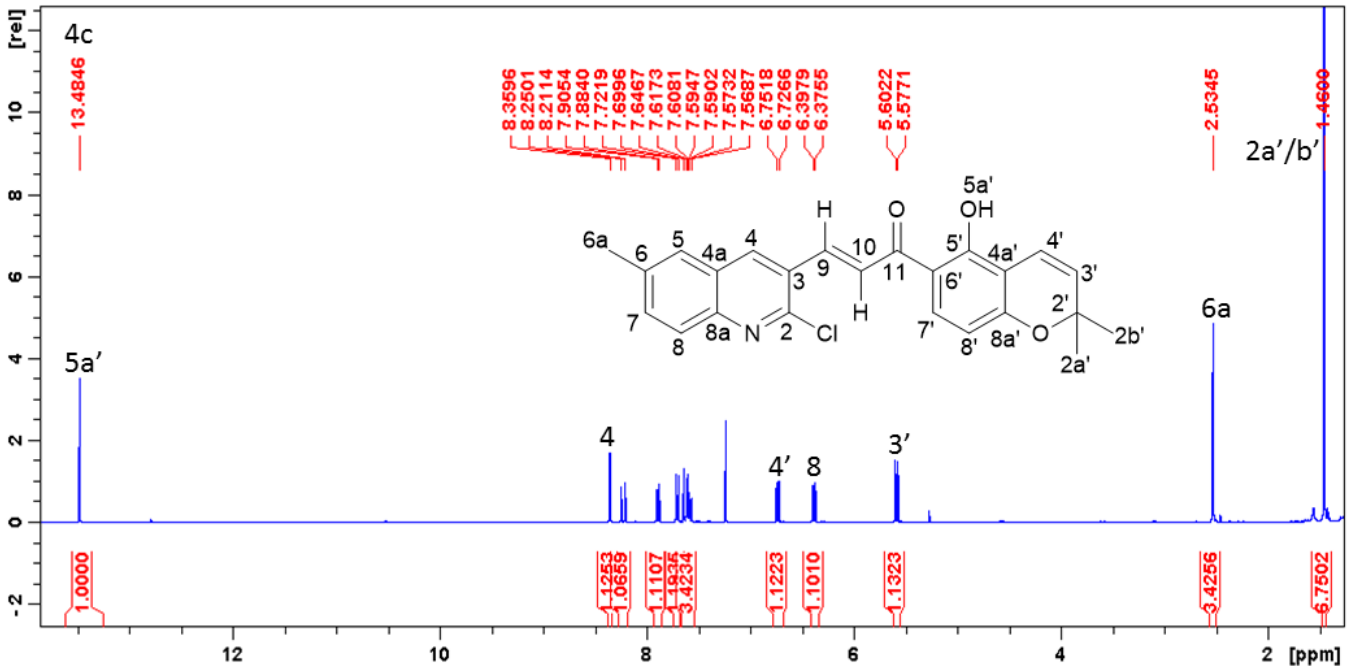



**Figure S16** $^{1}$H NMR spectrum of **4c**

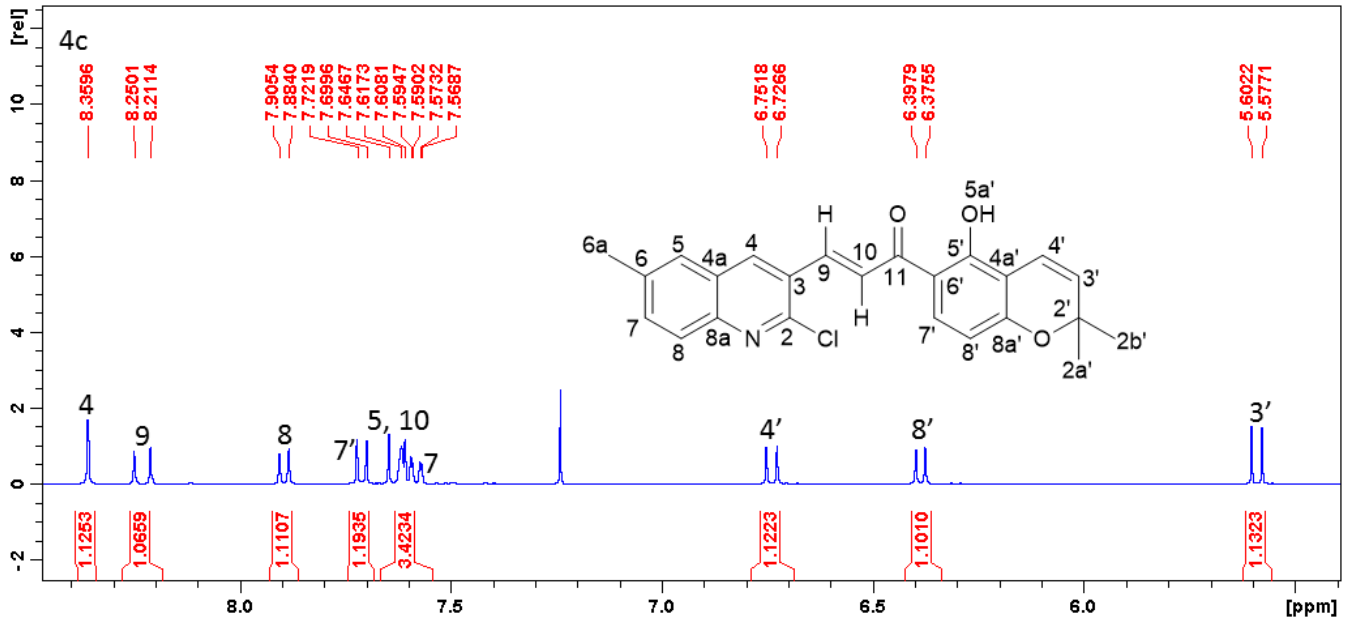



**Figure S17** $^{1}$H NMR spectrum (expanded) of **4c**

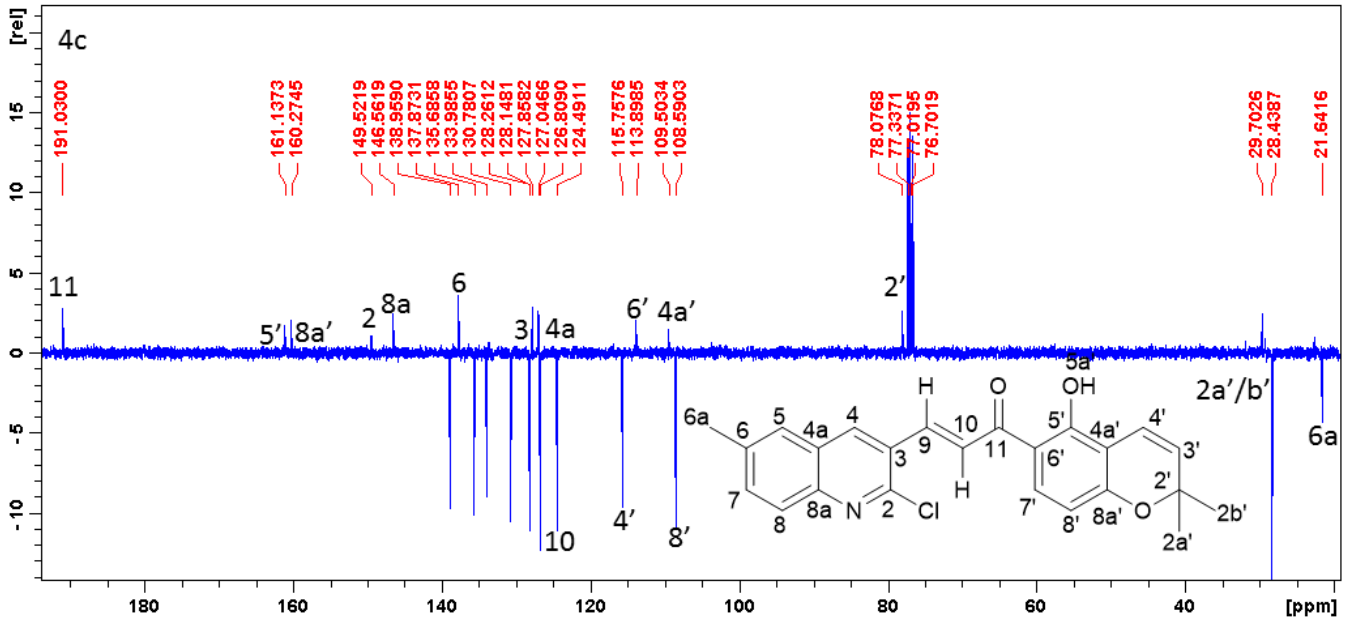



**Figure S18** $^{13}$C NMR spectrum of **4a**

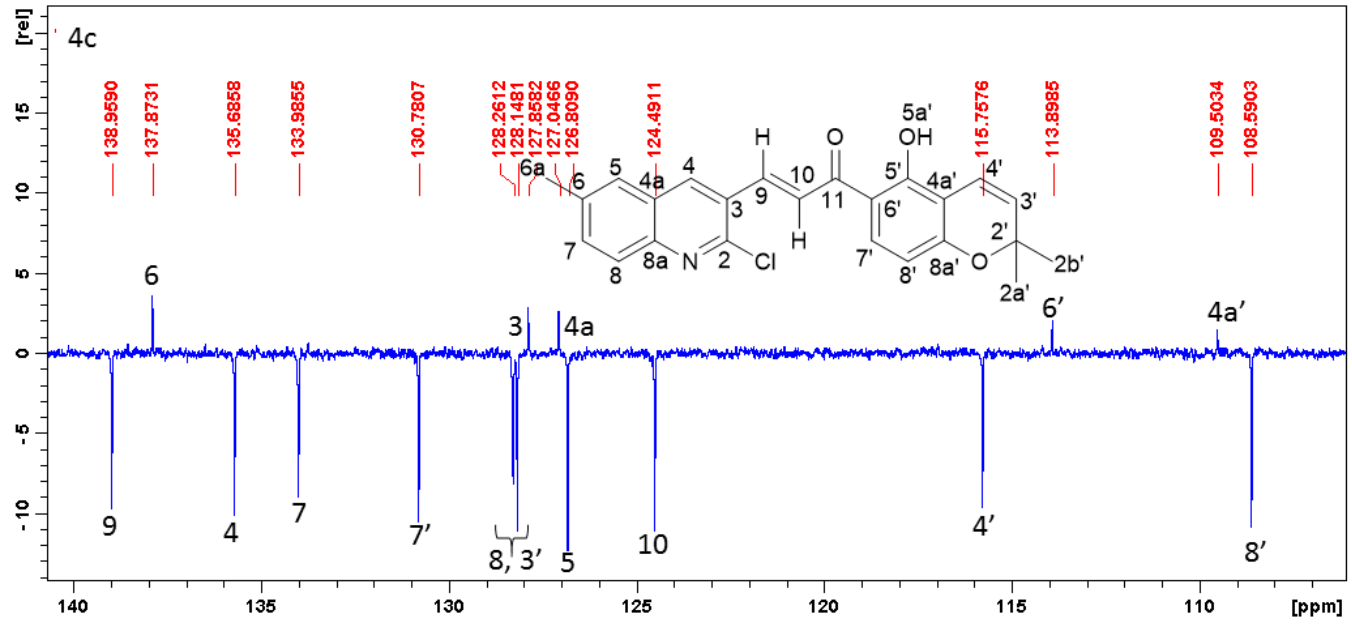
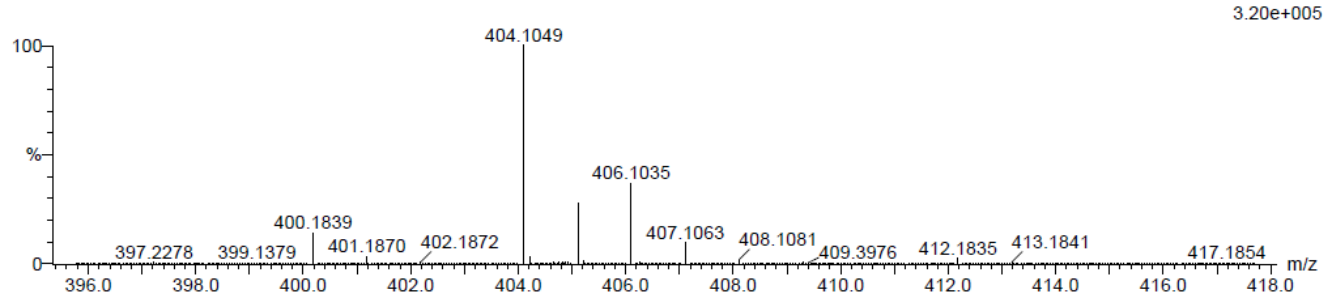



**Figure S19** $^{13}$C NMR spectrum (expanded) of **4c**

**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**

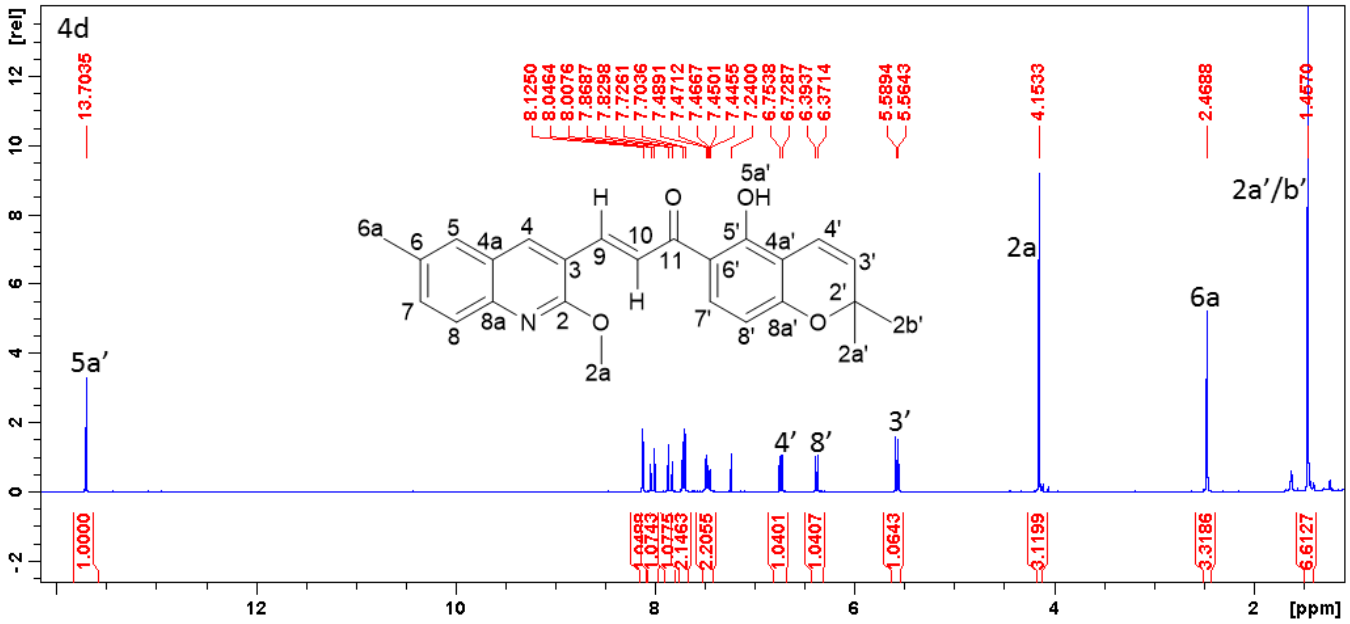



**Figure S21** $^{1}$H NMR spectrum of **6d**

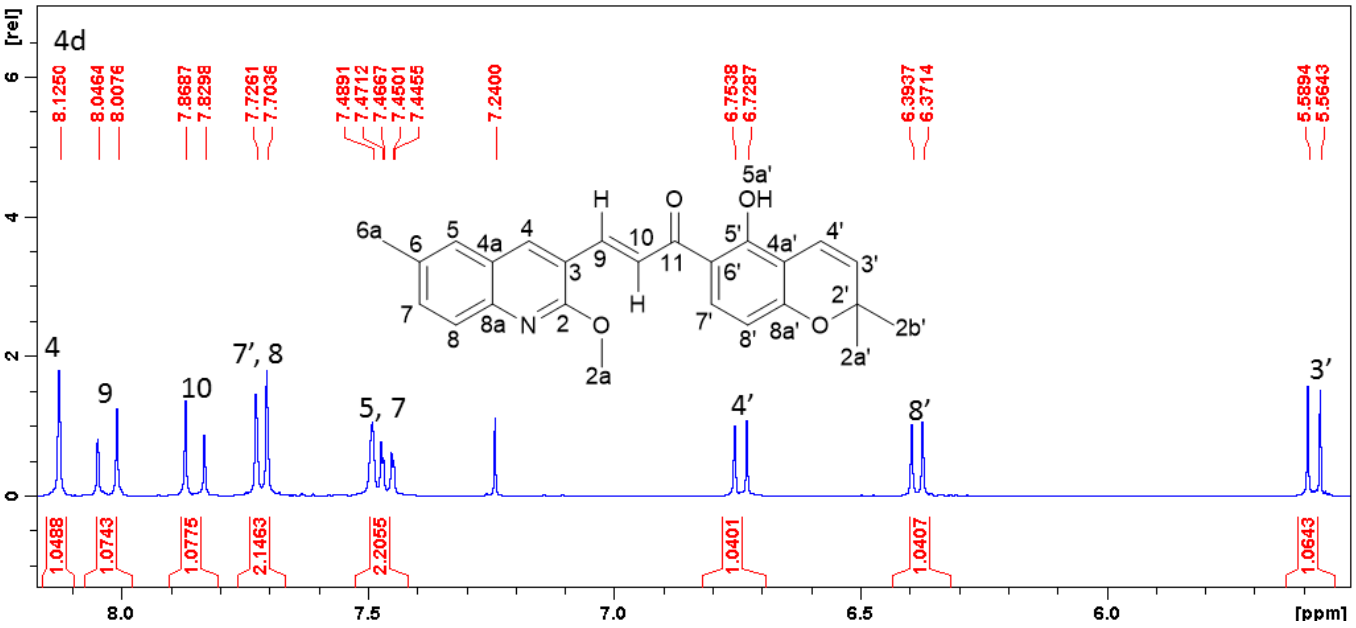



**Figure S22** $^{1}$H NMR spectrum (expanded) of **4d**

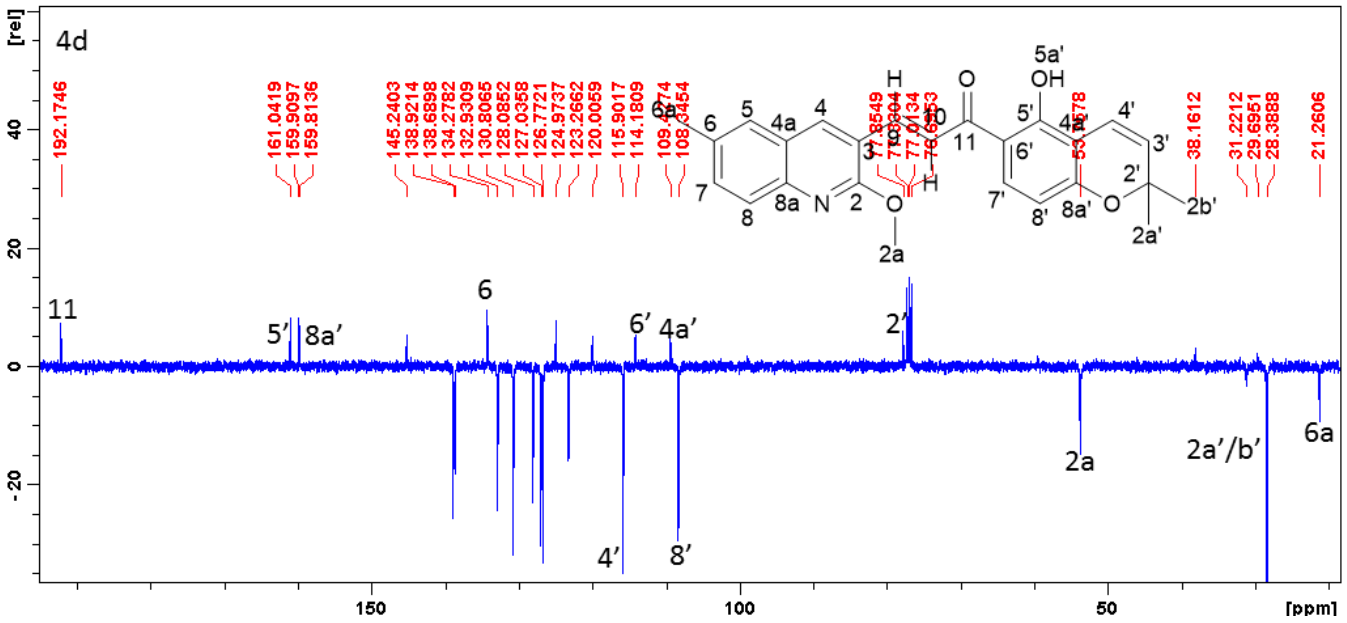



**Figure S23** $^{13}$C NMR spectrum of **4d**

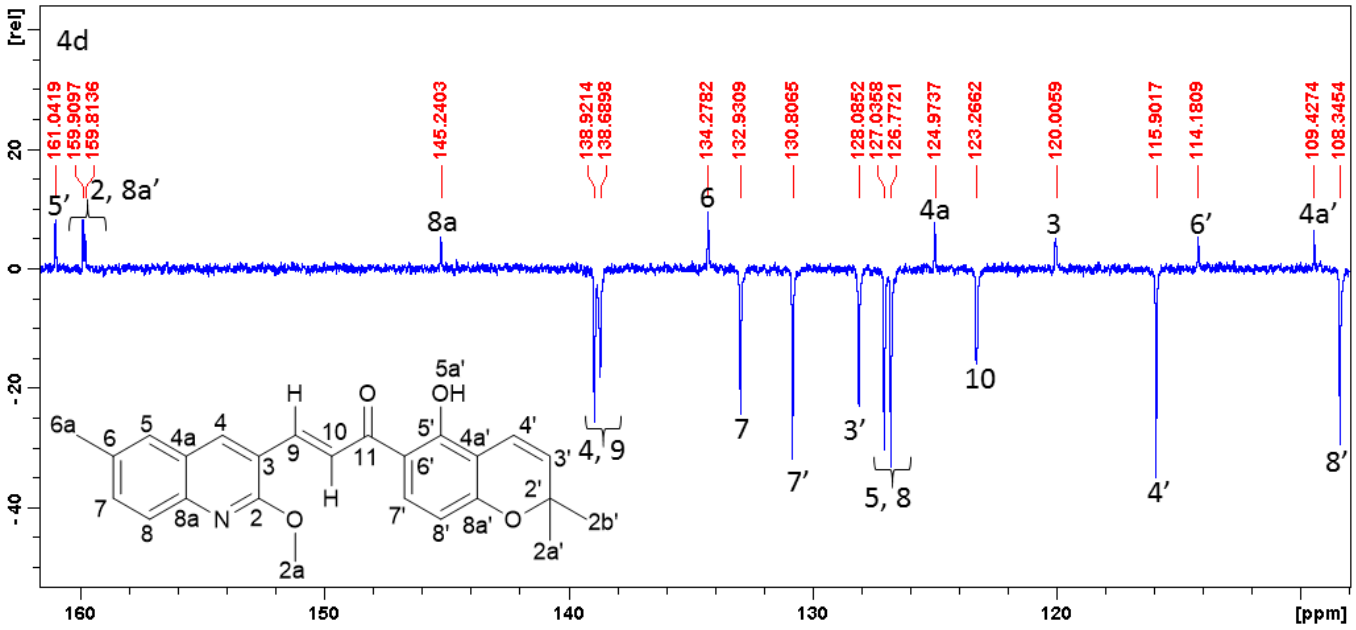
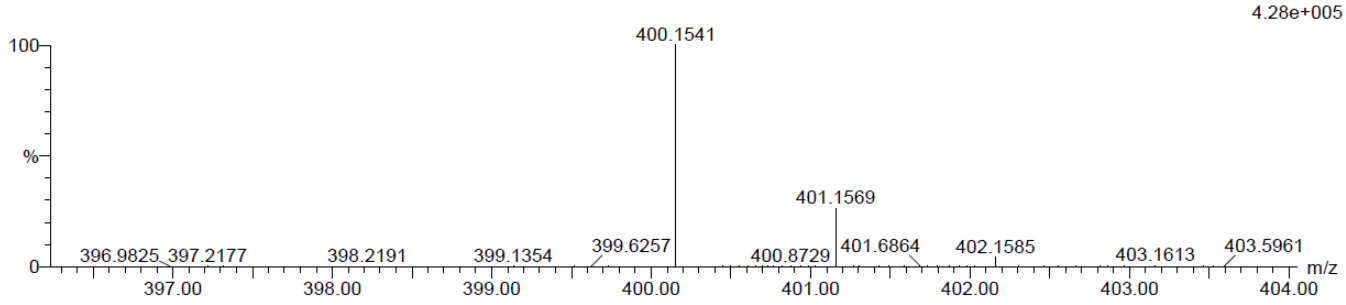



**Figure S24** $^{13}$C NMR spectrum of **4d**

**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**

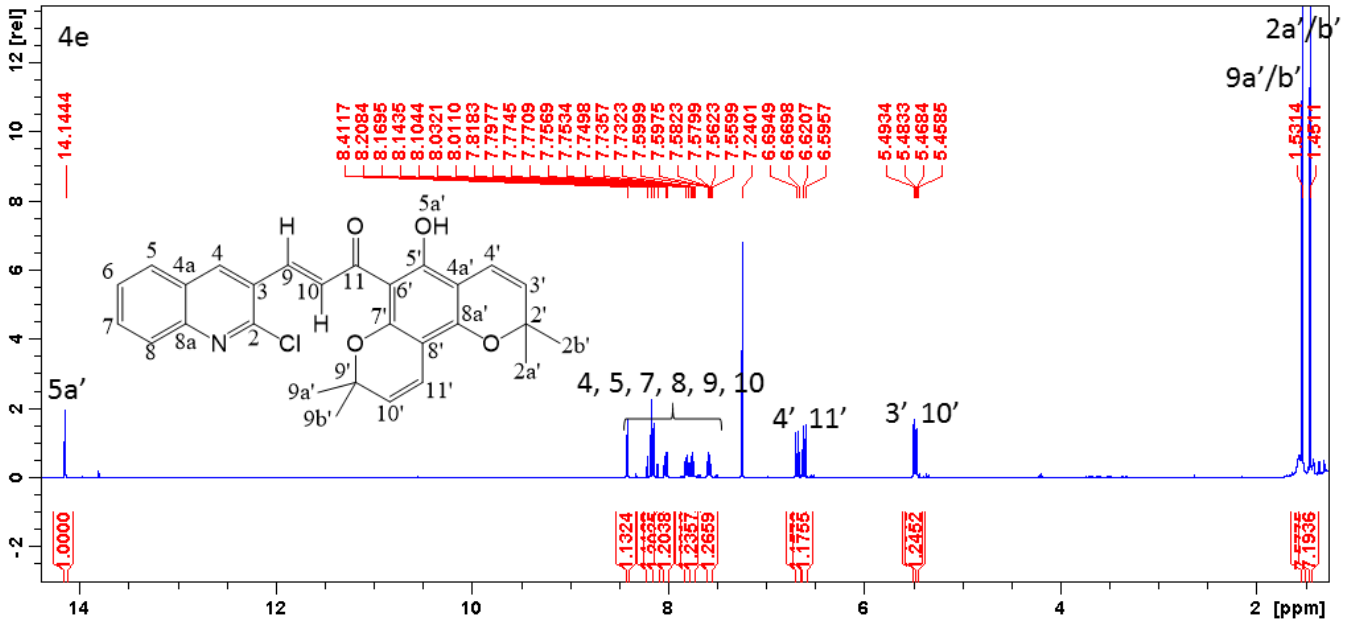



**Figure S26** $^{1}$H NMR spectrum of **4e**

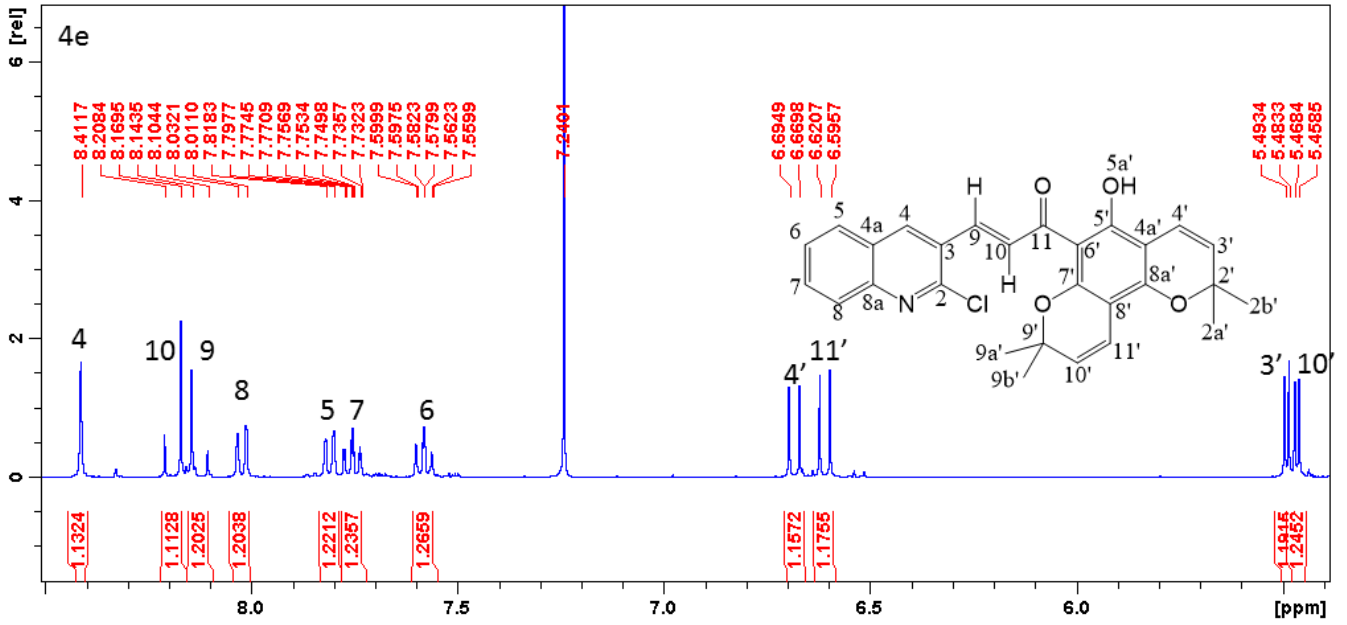



**Figure S27** $^{1}$H NMR spectrum (expanded) of **4e**

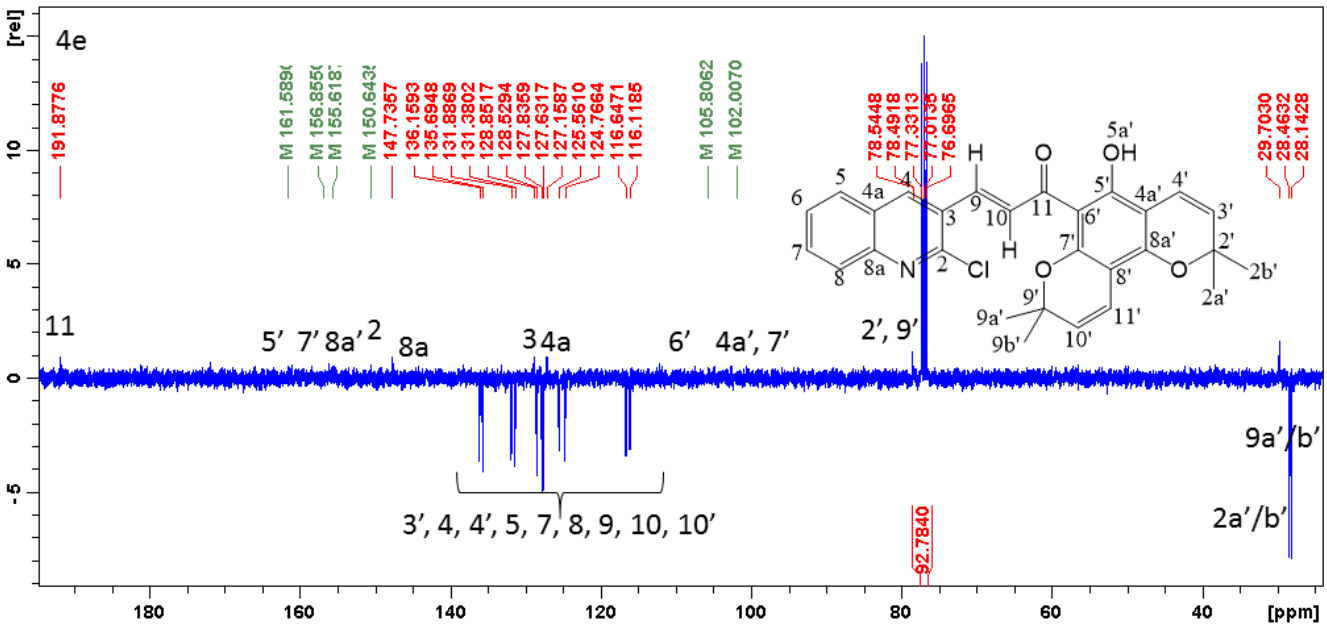



**Figure S28** $^{13}$C NMR spectrum of **4e**

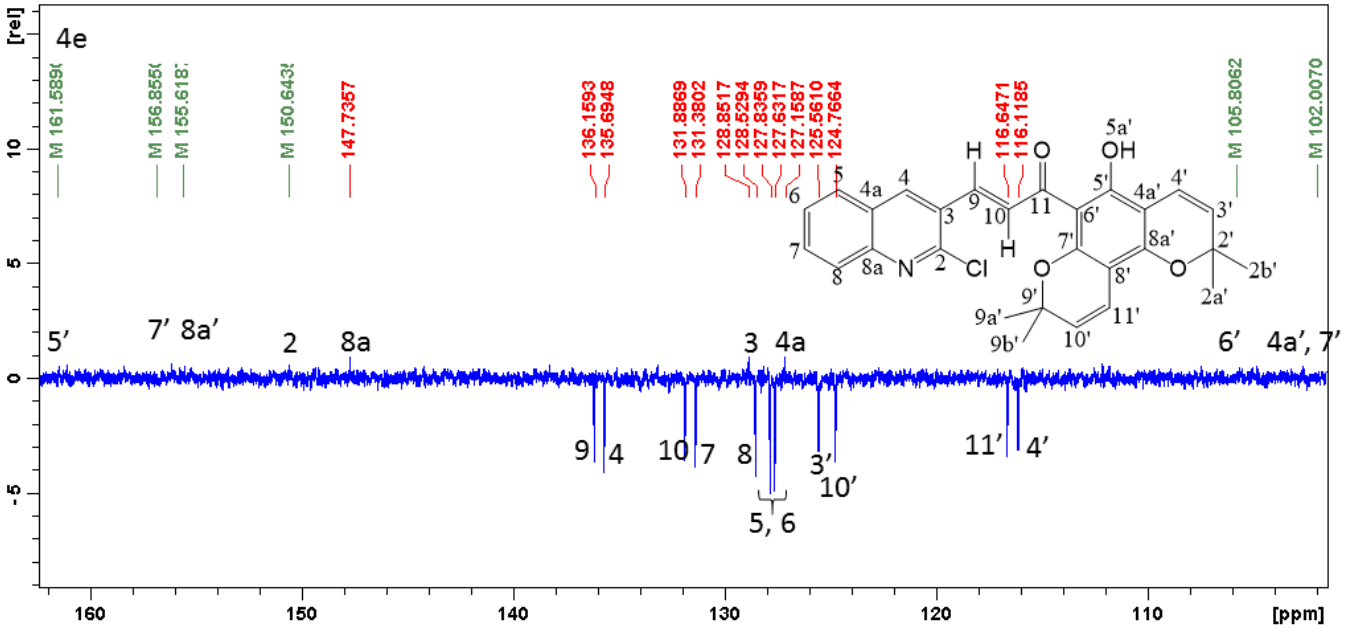
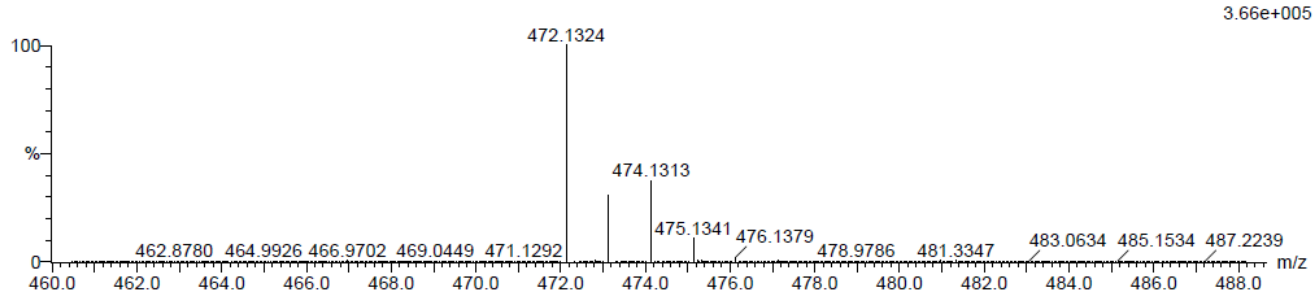



**Figure S29** $^{13}$C NMR spectrum (expanded) of **4e**

**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**

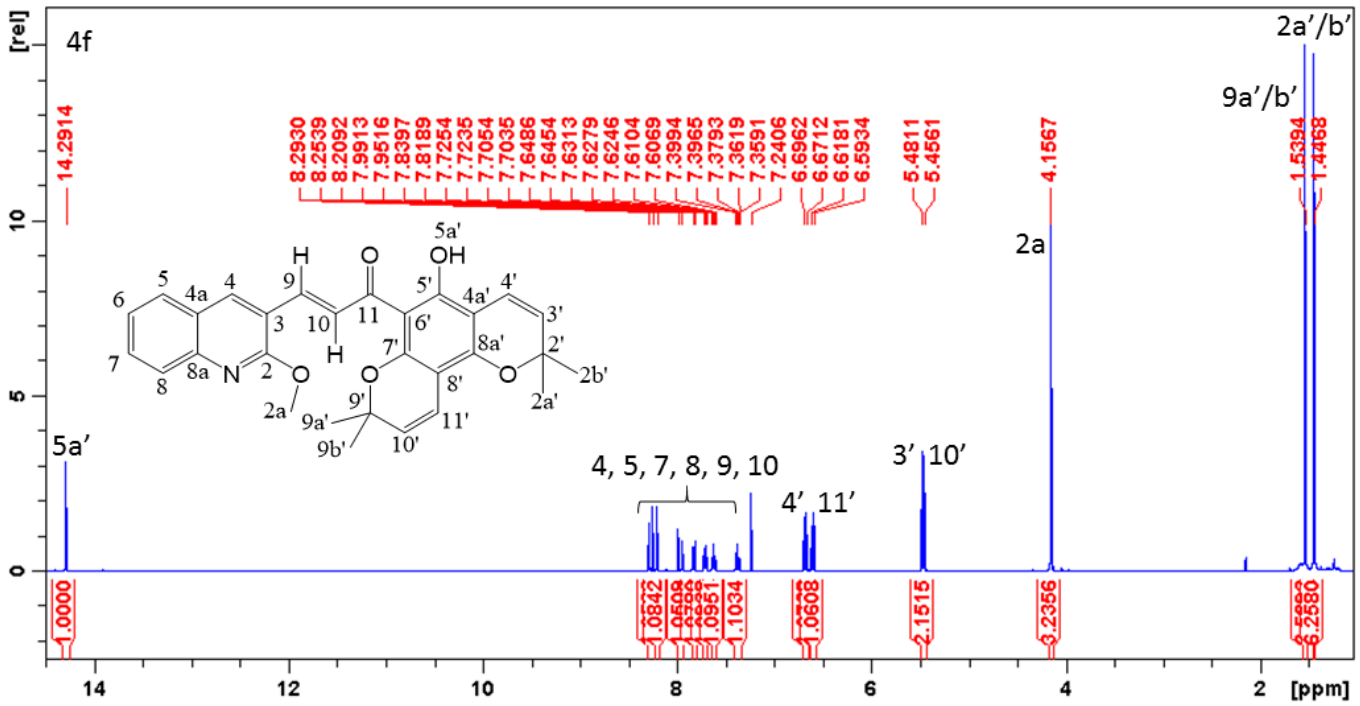



**Figure S31** $^{1}$H NMR spectrum (expanded) of **4f**

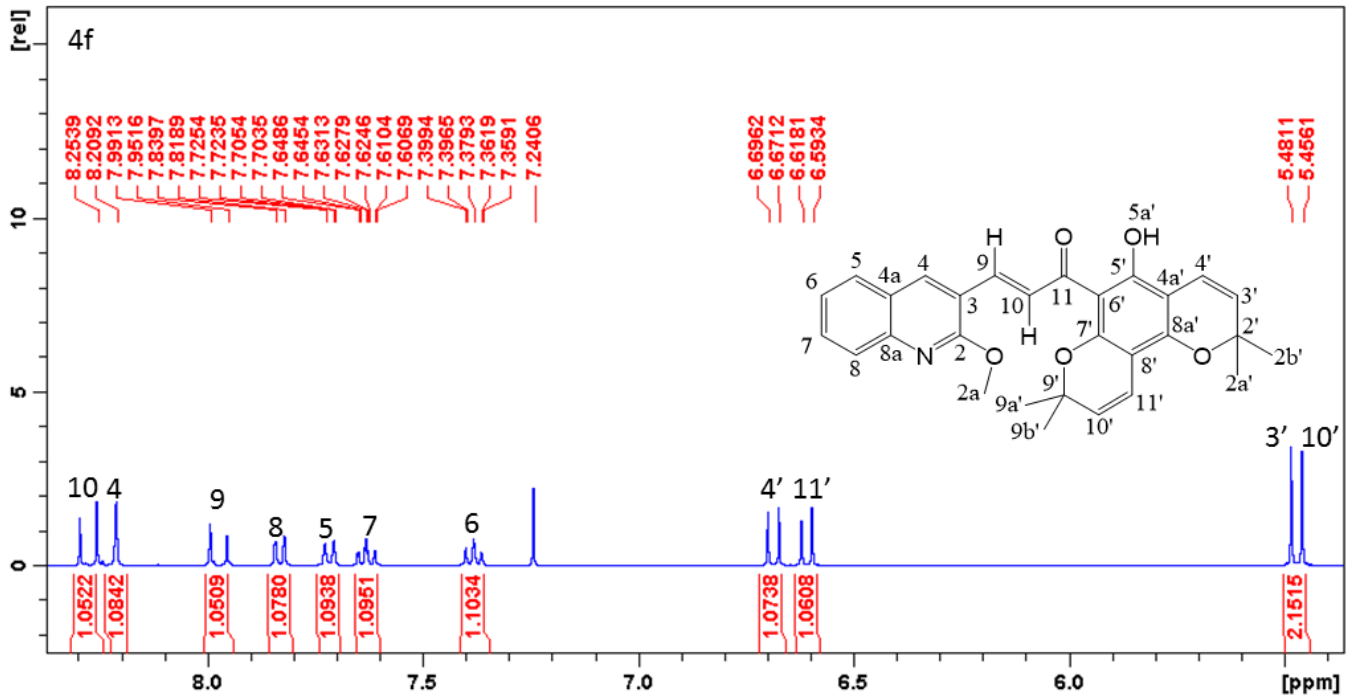



**Figure S32** $^{1}$H NMR spectrum (expanded) of **4f**

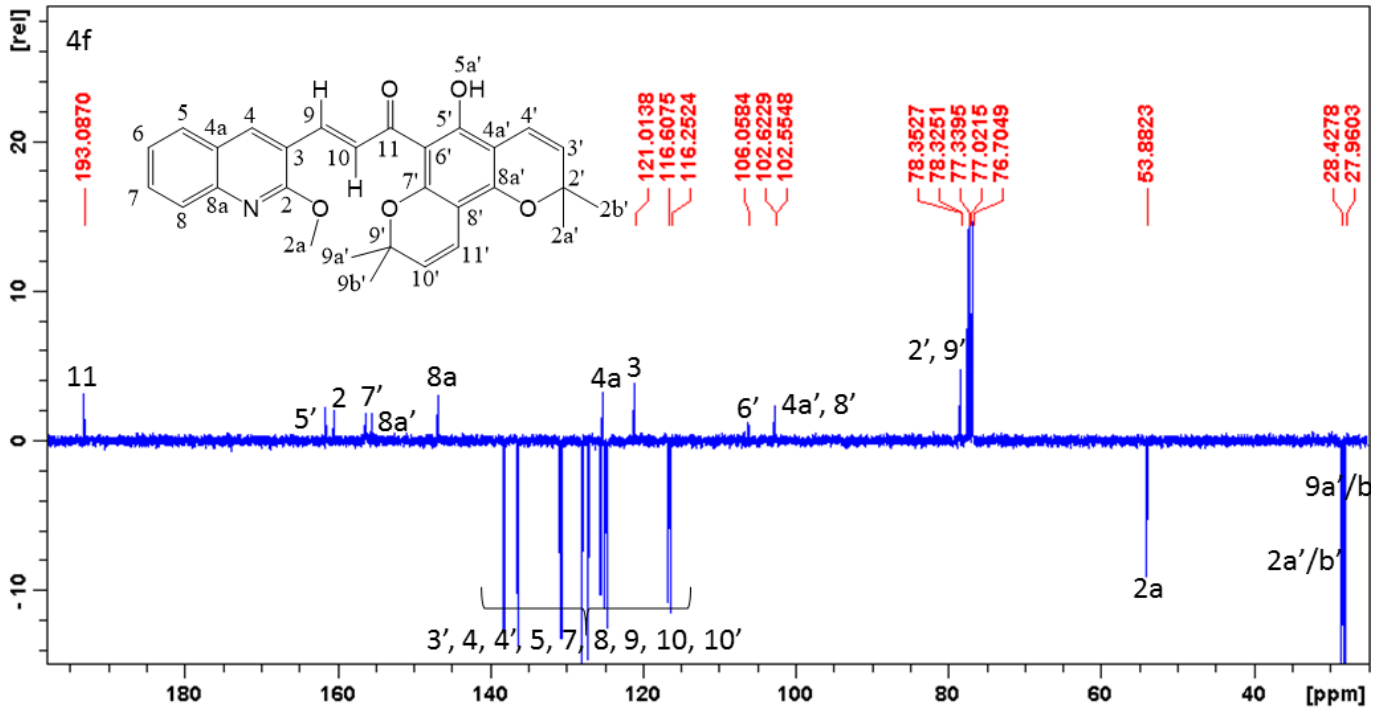



**Figure S33** $^{13}$C NMR spectrum of **4f**

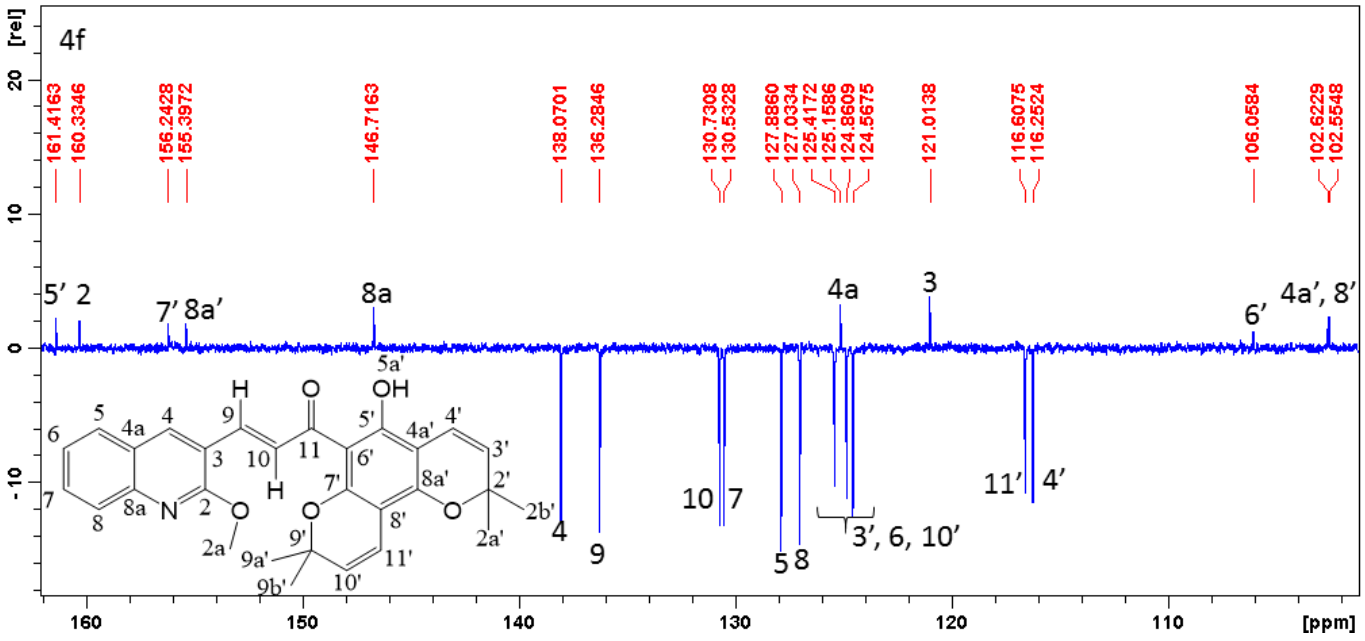
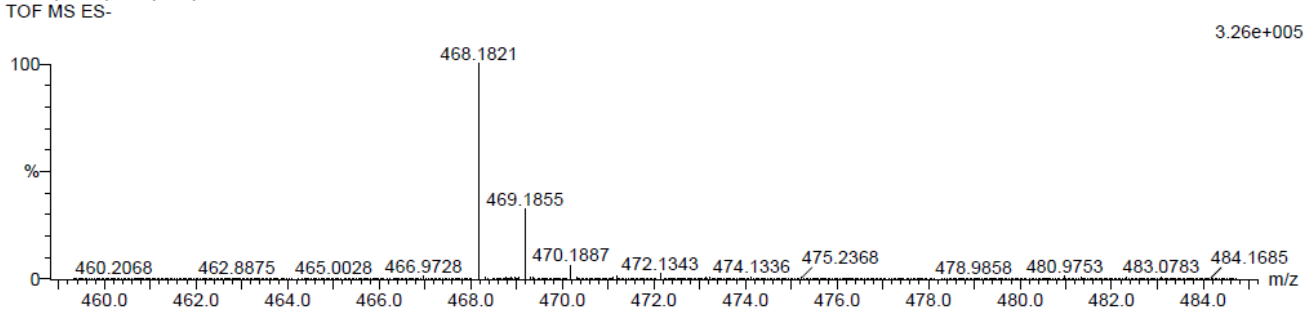



**Figure S34** $^{13}$C NMR spectrum (expanded) of **4f**

**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**

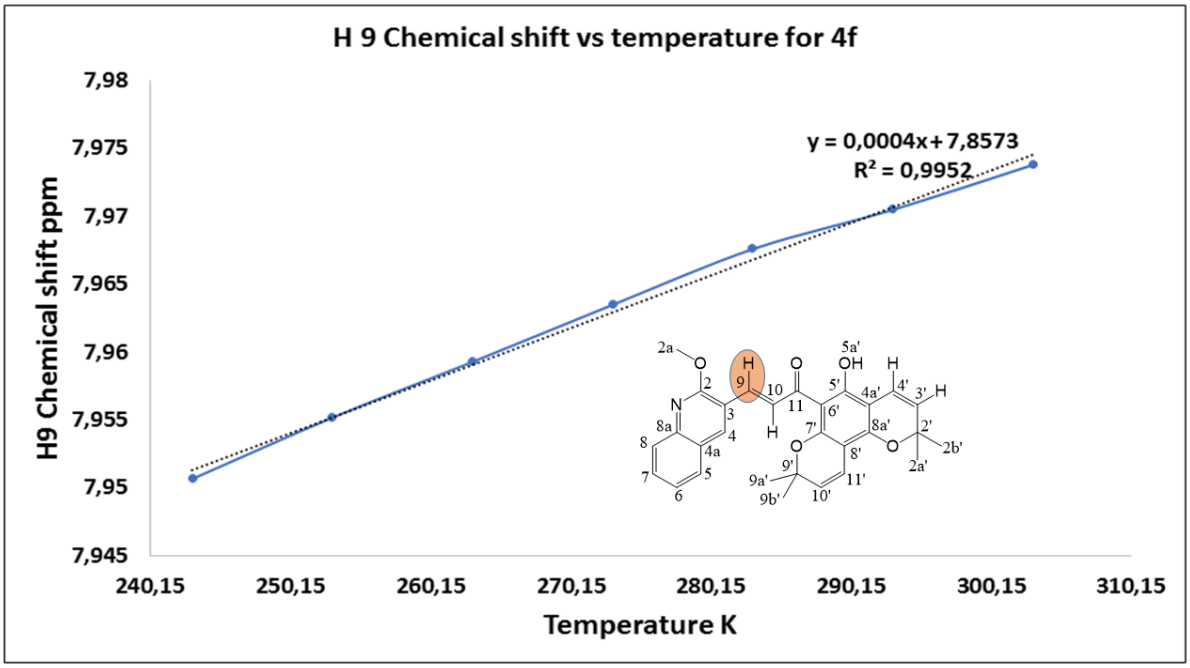



**Figure S36** H-9 $^{1}$H NMR chemical shift of **4f** as function of temperature

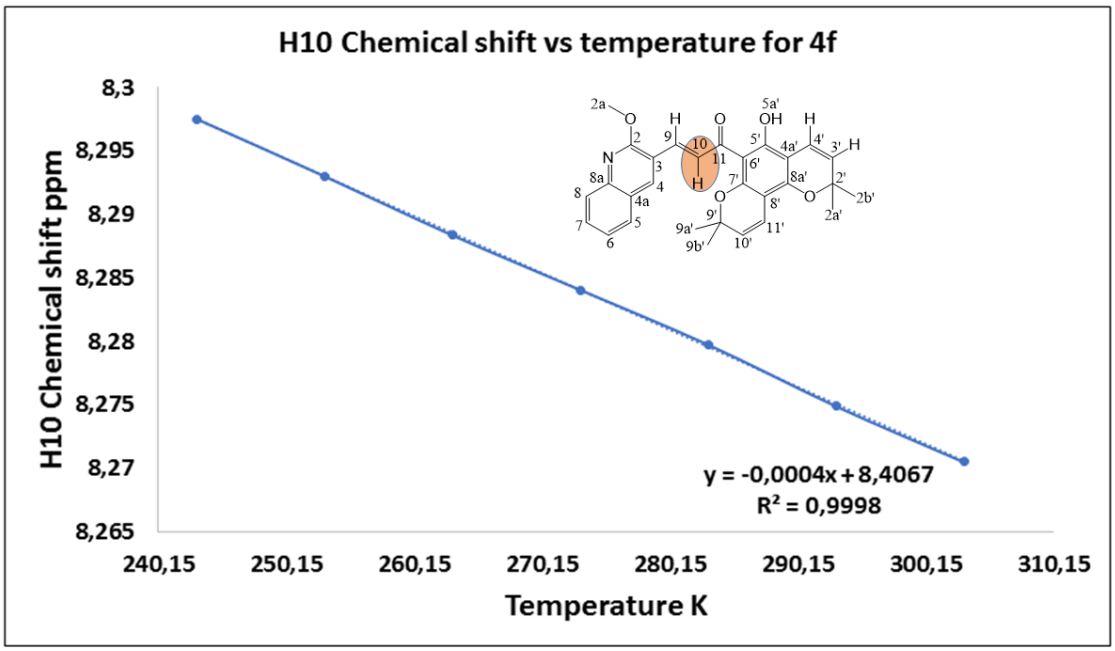



**Figure S37** H-10 $^{1}$H NMR chemical shift of **4f** as function of temperature

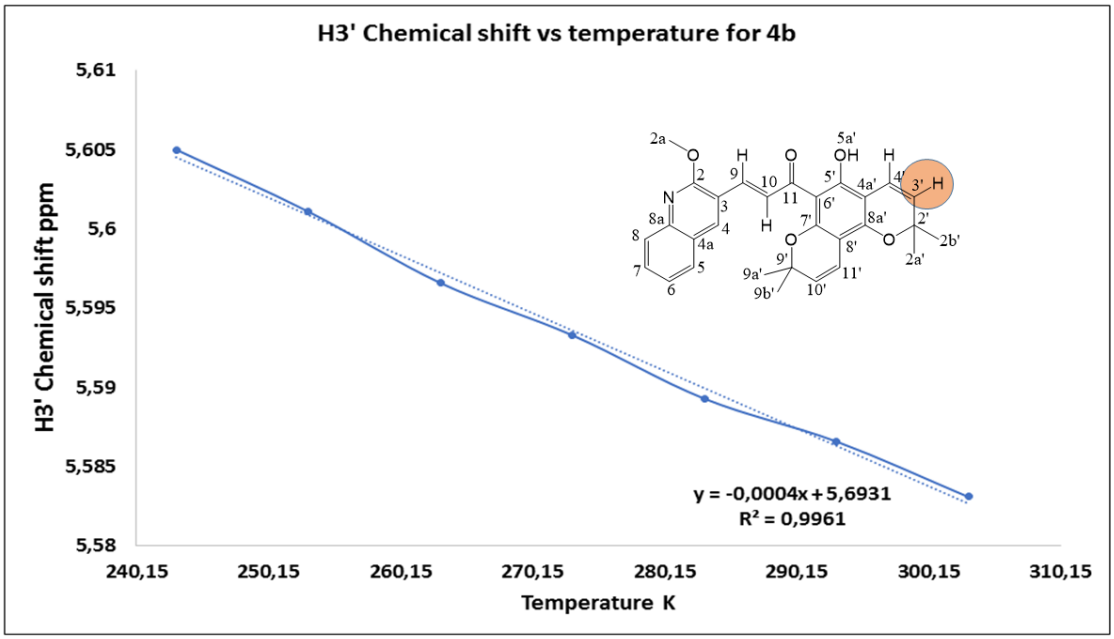



**Figure S38** H-3' $^{1}$H NMR chemical shift of **4f** as function of temperature

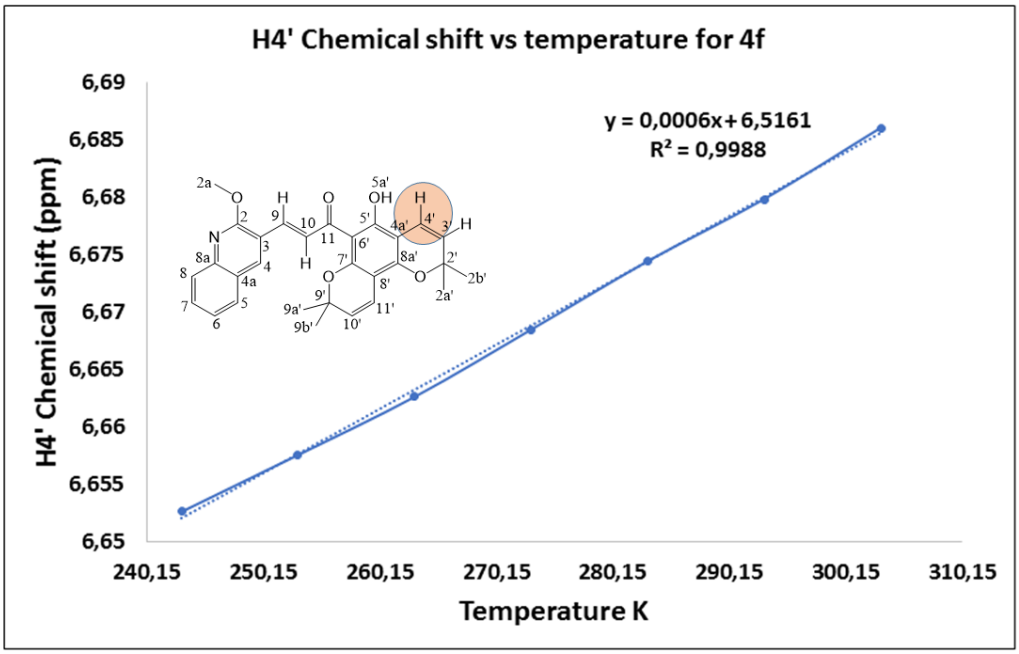



**Figure S39** H-4' [1]HNMR chemical shift of **4f** as function of temperature

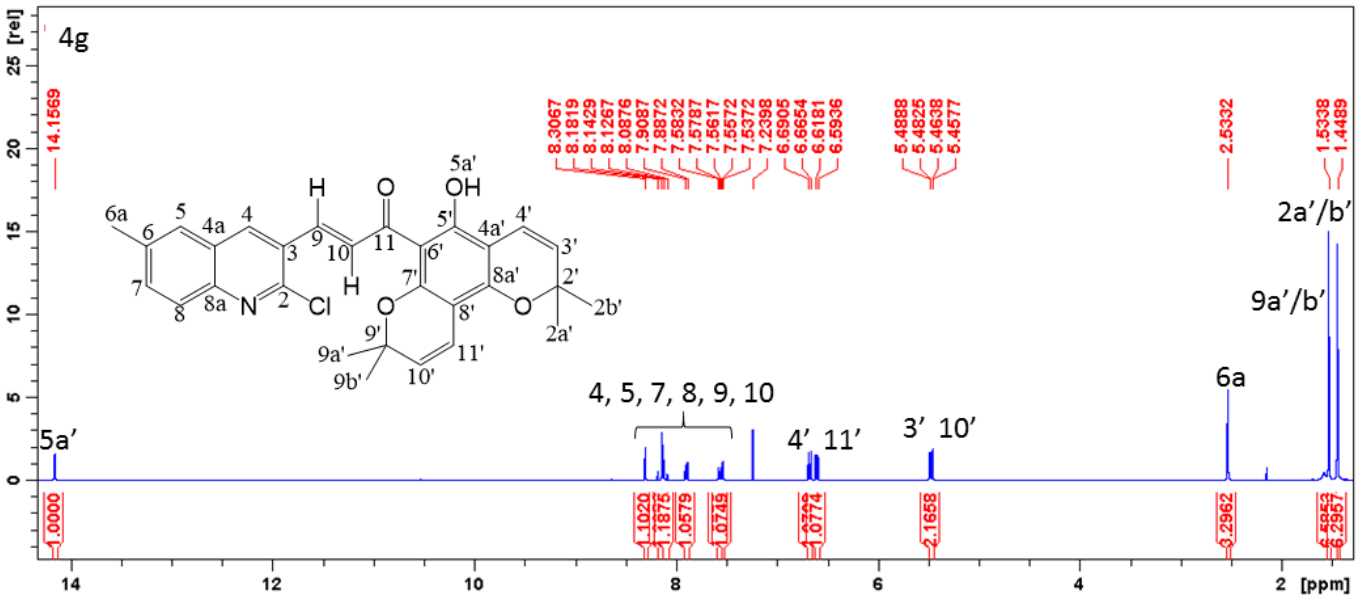



**Figure S40** [1]H NMR spectrum of **4g**

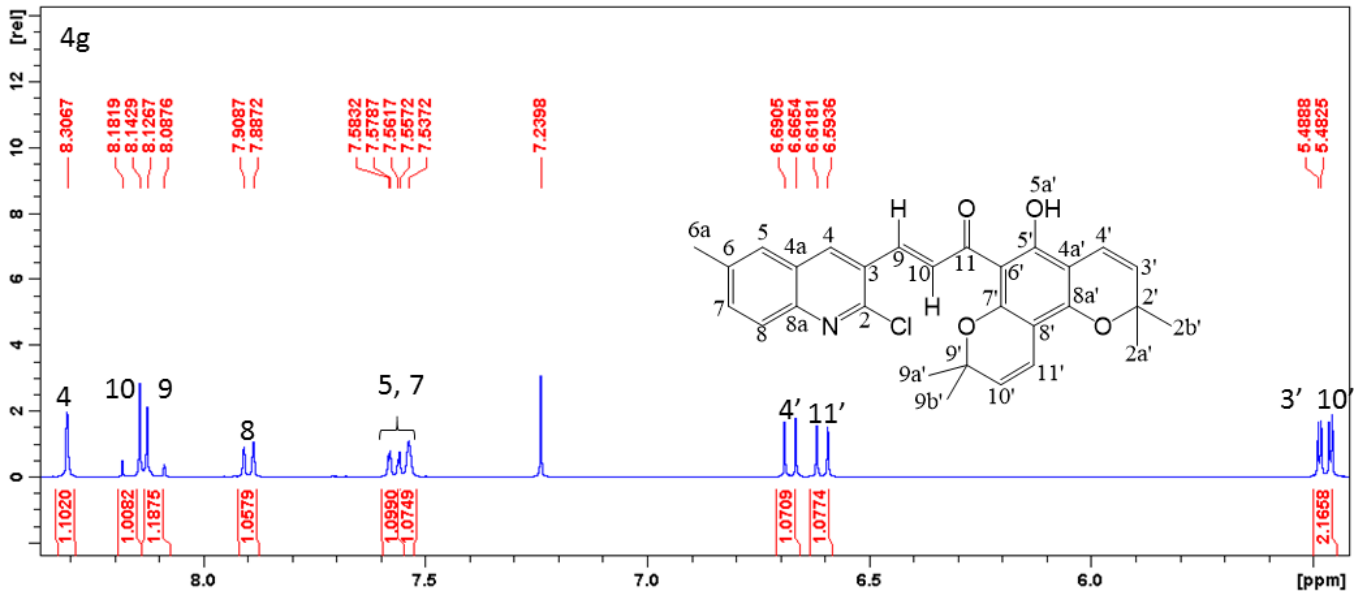



**Figure S41** $^{1}$H NMR spectrum (expanded) of **4g**

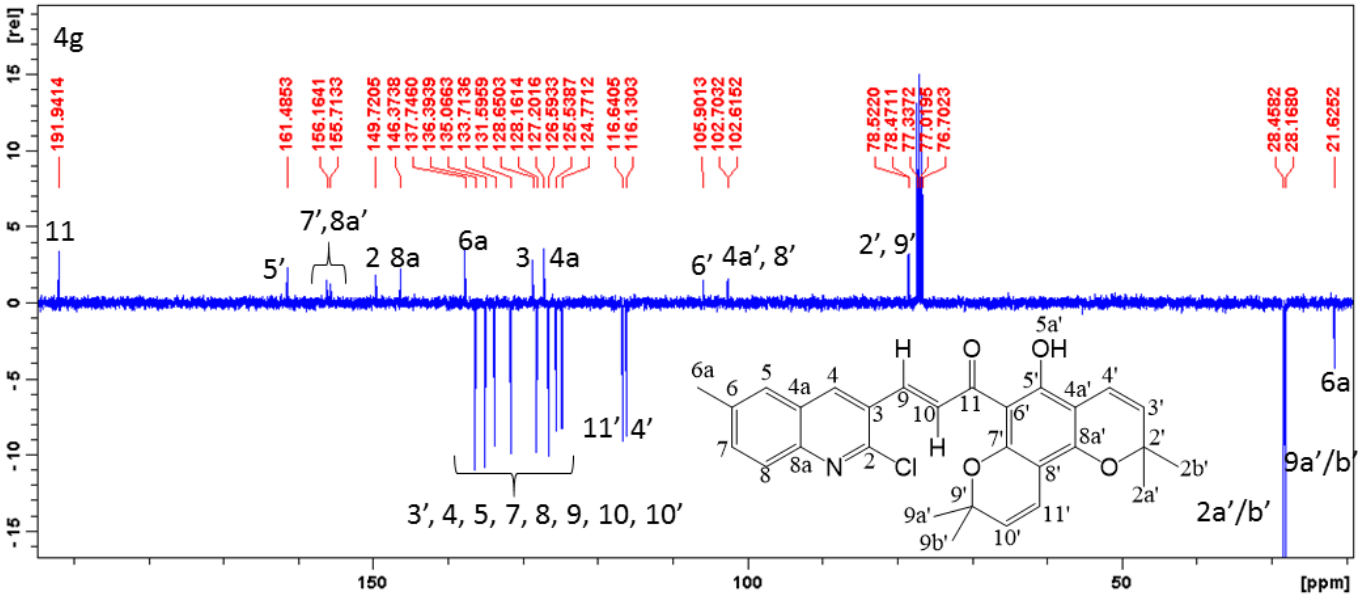



**Figure S42** $^{13}$C NMR spectrum of **4g**

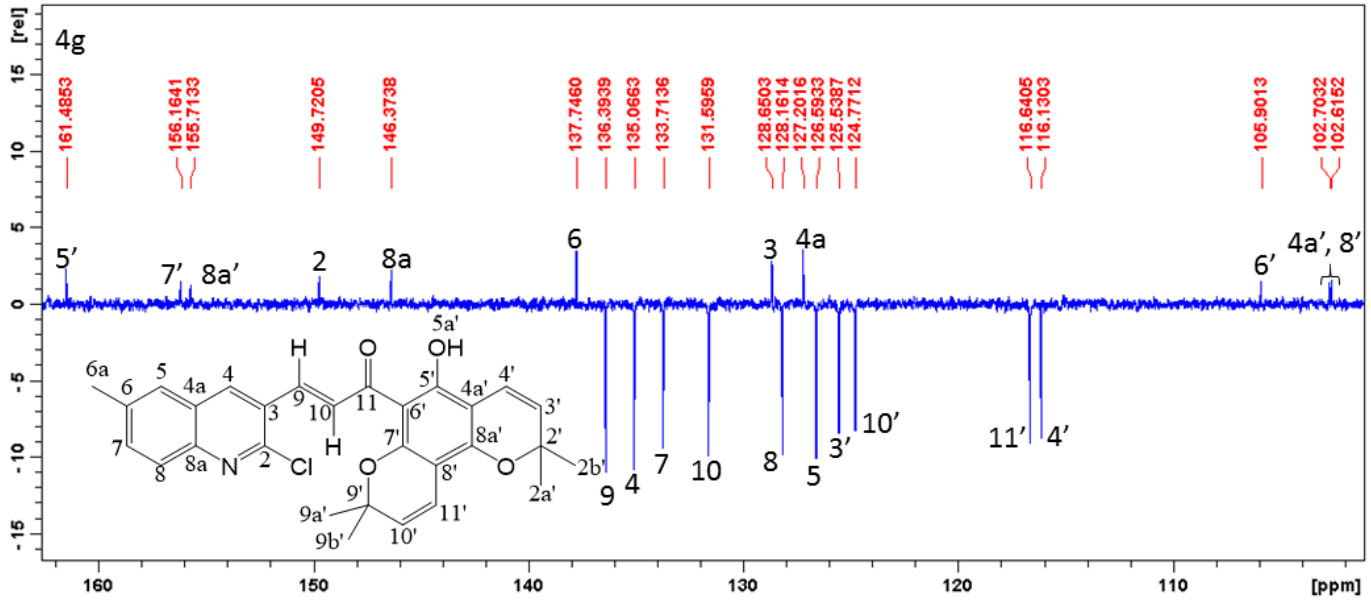



**Figure S43** $^{13}$C NMR spectrum (expanded) of **4g**

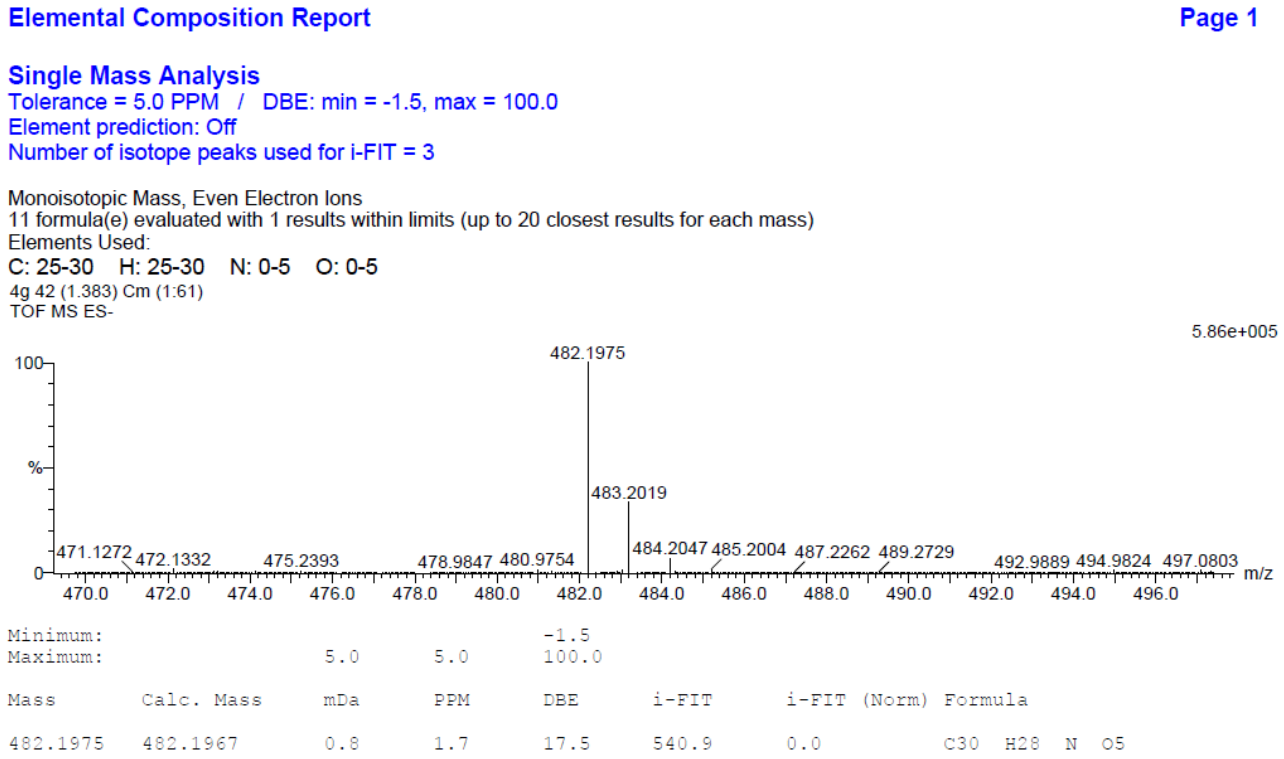



**Figure S44** $^{1}$H NMR spectrum of **4g**

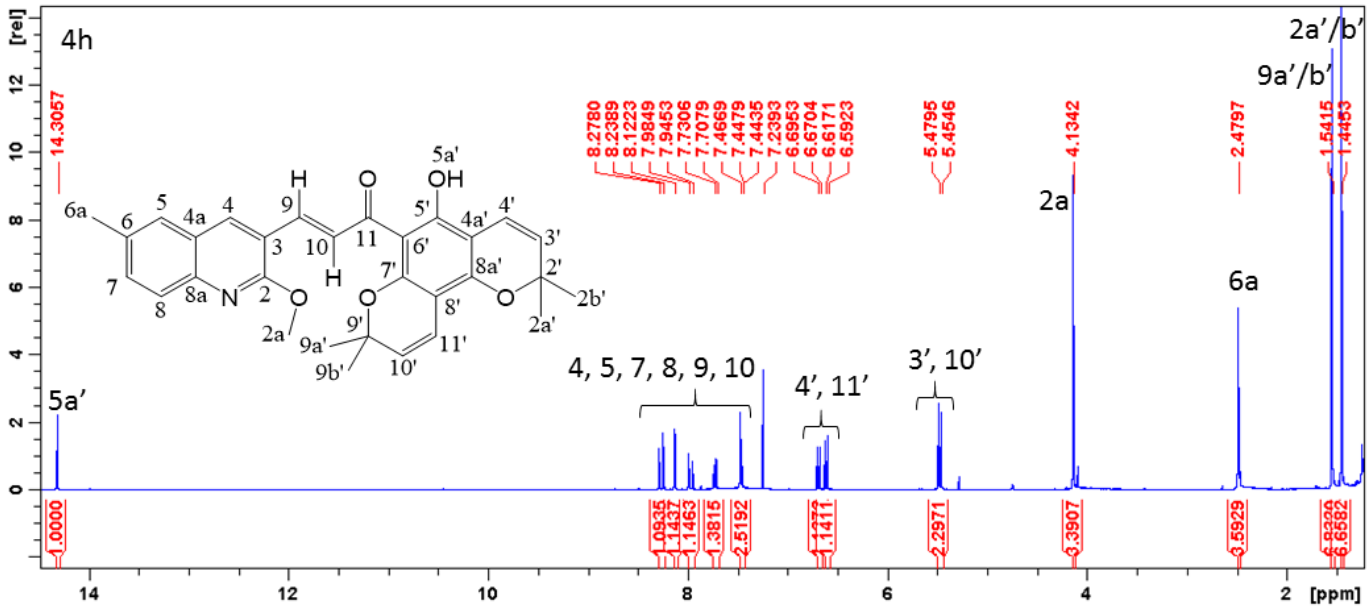



**Figure S45** $^{1}$H NMR spectrum of **4h**

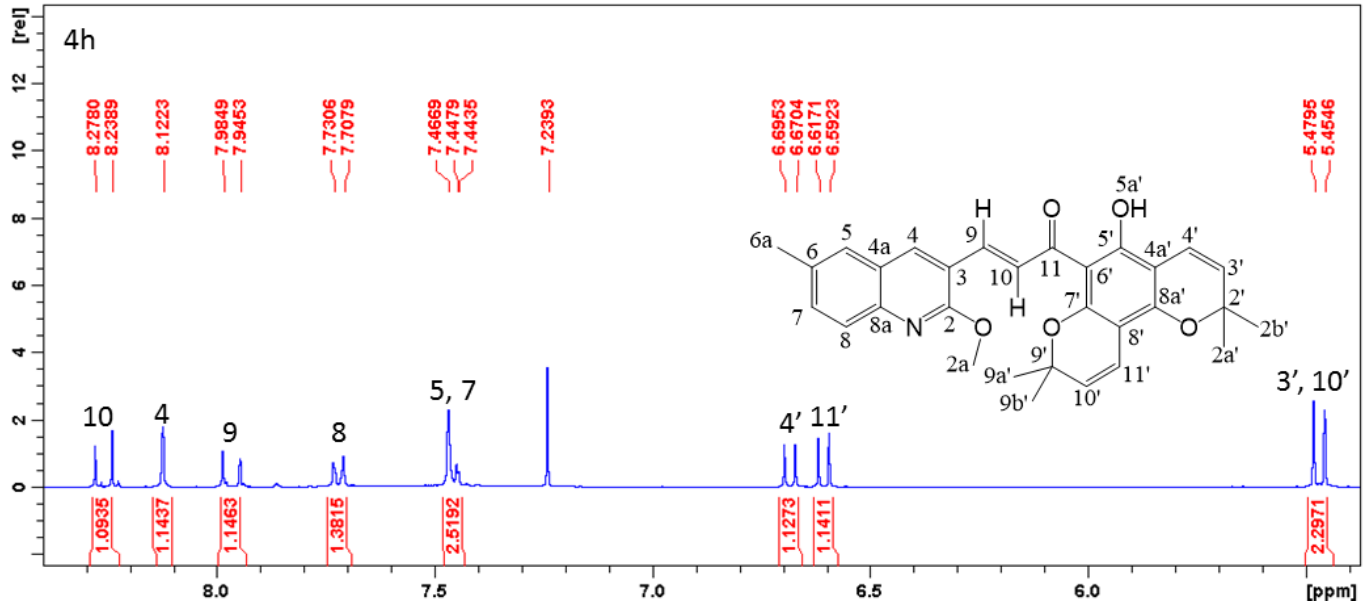



**Figure S46** $^{1}$H NMR spectrum (expanded) of **4h**

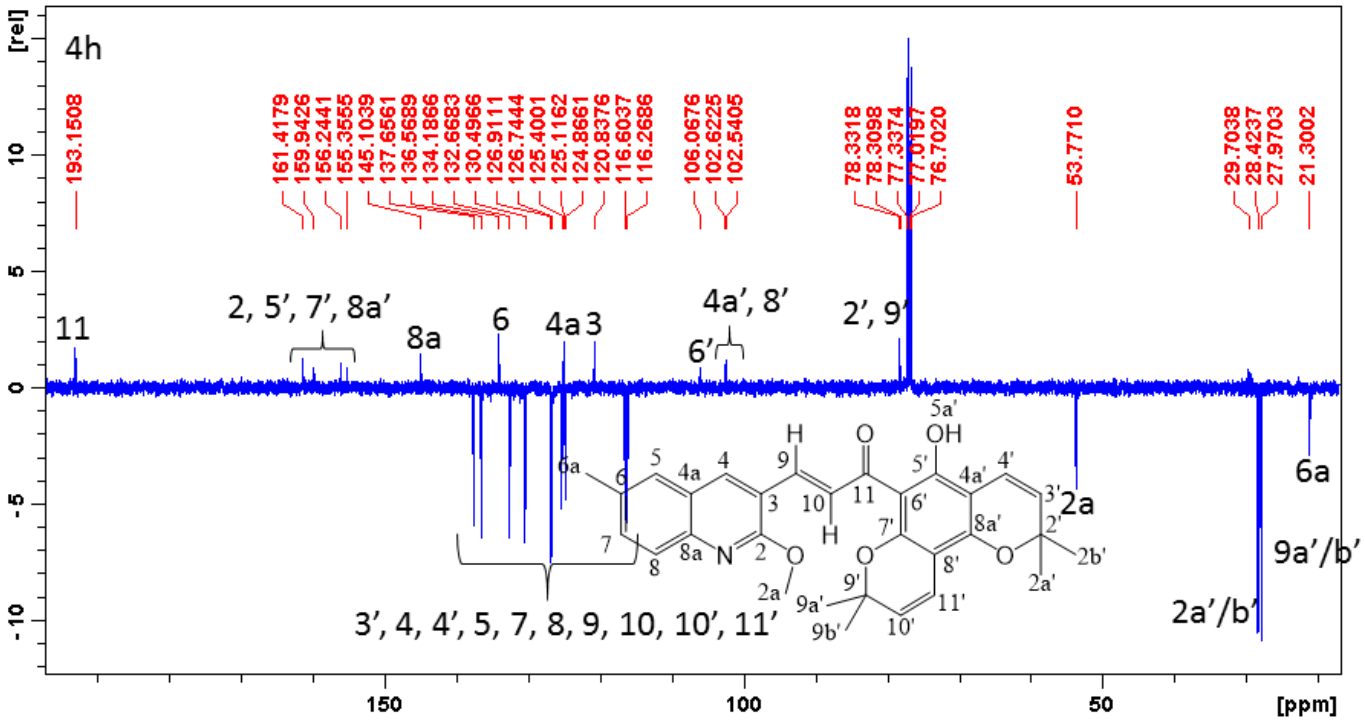



**Figure S47** $^{13}$C NMR spectrum of **4h**

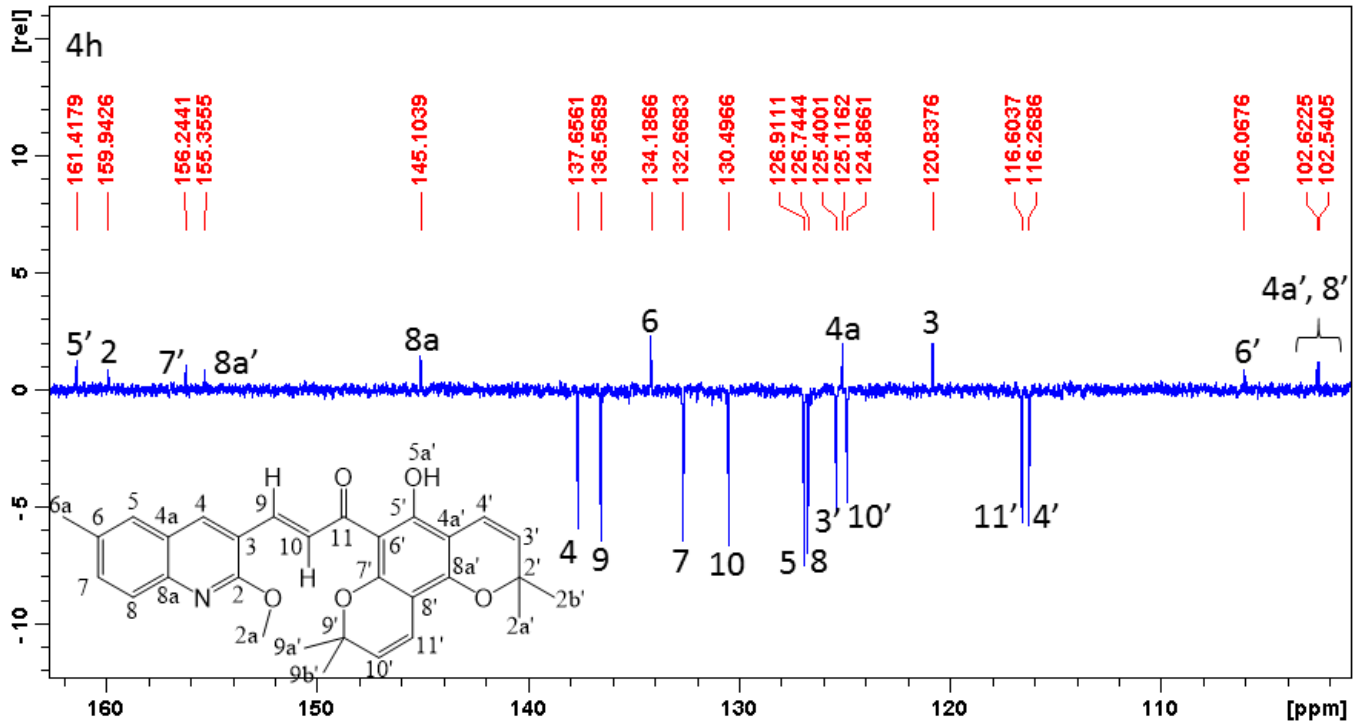
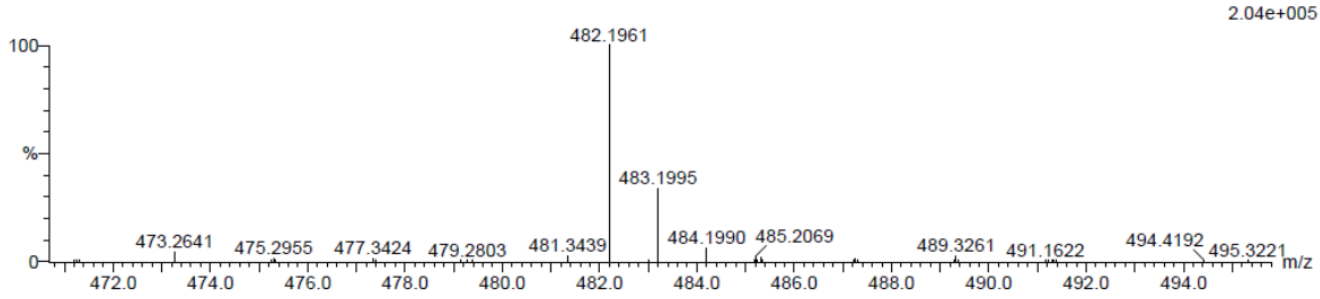



**Figure S48** $^{13}$C NMR spectrum (expanded) of **4h**

**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 |