Electronic Supporting Information

Synthesis of 2-aroylfuro[3,2-*c*]quinolines from quinolone-based chalcones and evaluation of their antioxidant and anticholinesterase activities

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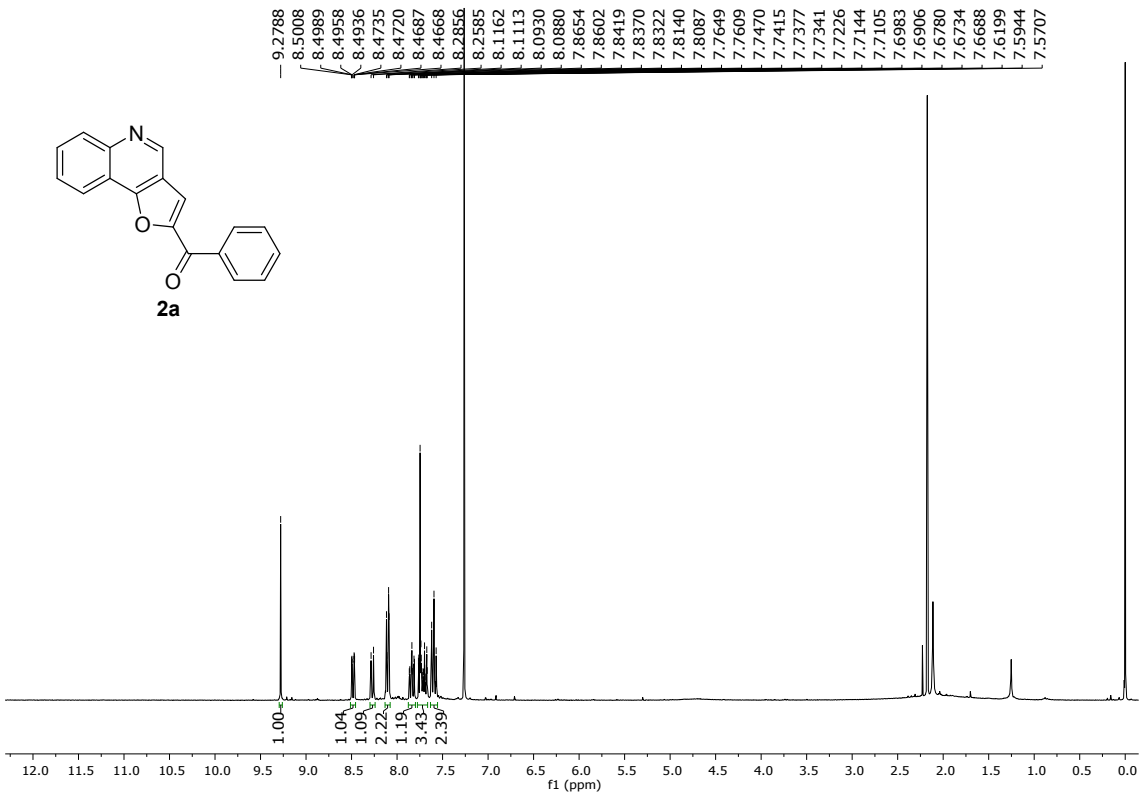

Figure S1. ^{1}H NMR spectrum of compound **2a** (300.13 MHz, $CDCl_3$)

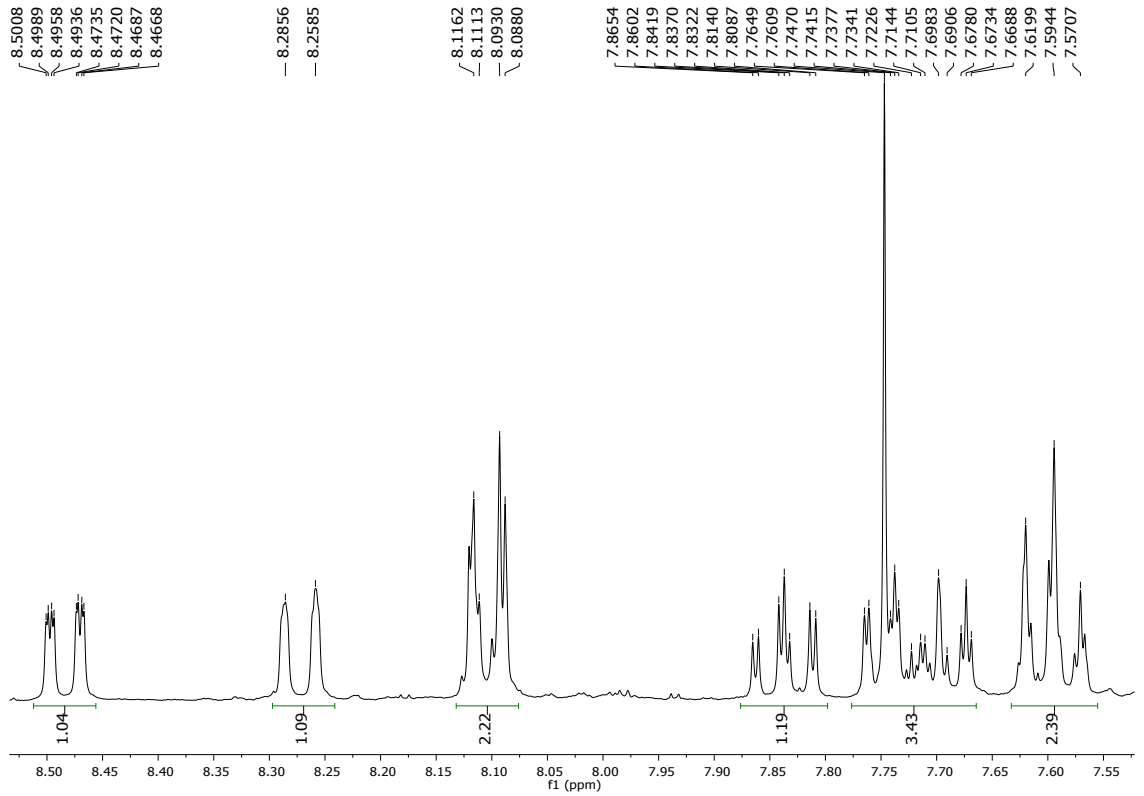

Figure S2. Expansion of ^{1}H NMR spectrum of compound **2a** (300.13 MHz, $CDCl_3$)

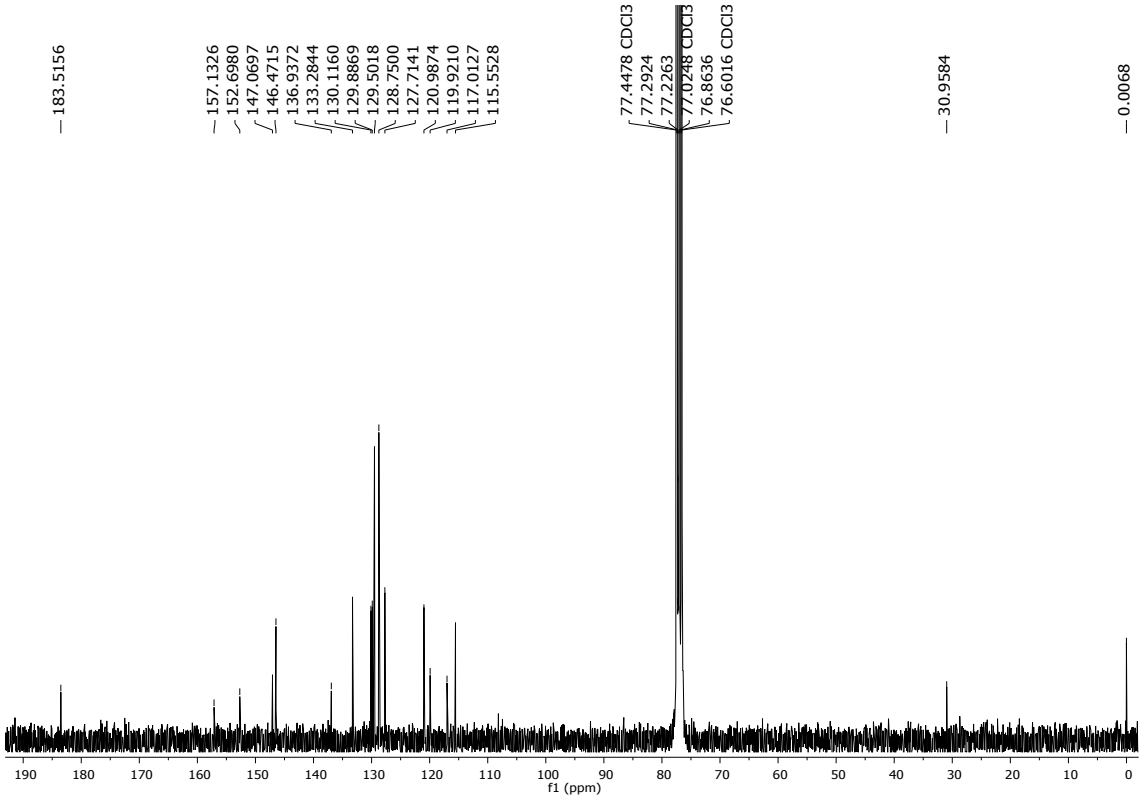

Figure S3. ^{13}C NMR spectrum of compound **2a** (75.47 MHz, $CDCl_3$)

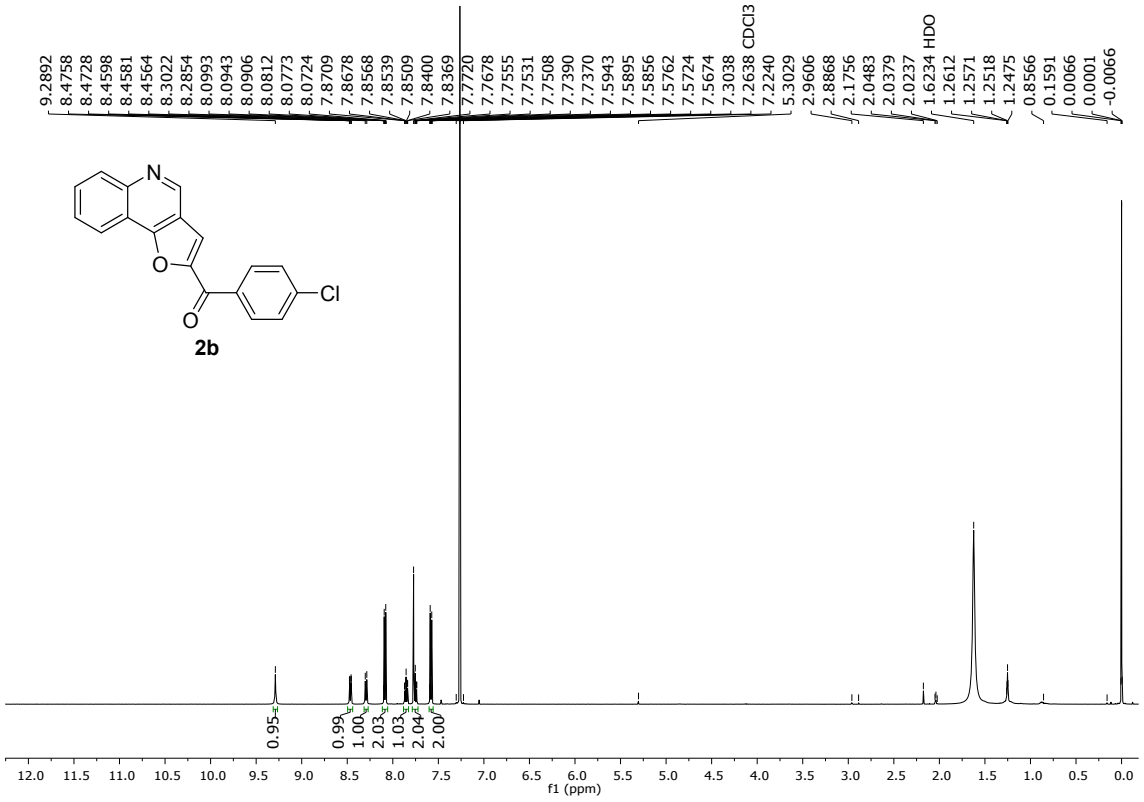

Figure S4. ^{1}H NMR spectrum of compound **2b** (300.13 MHz, $CDCl_3$)

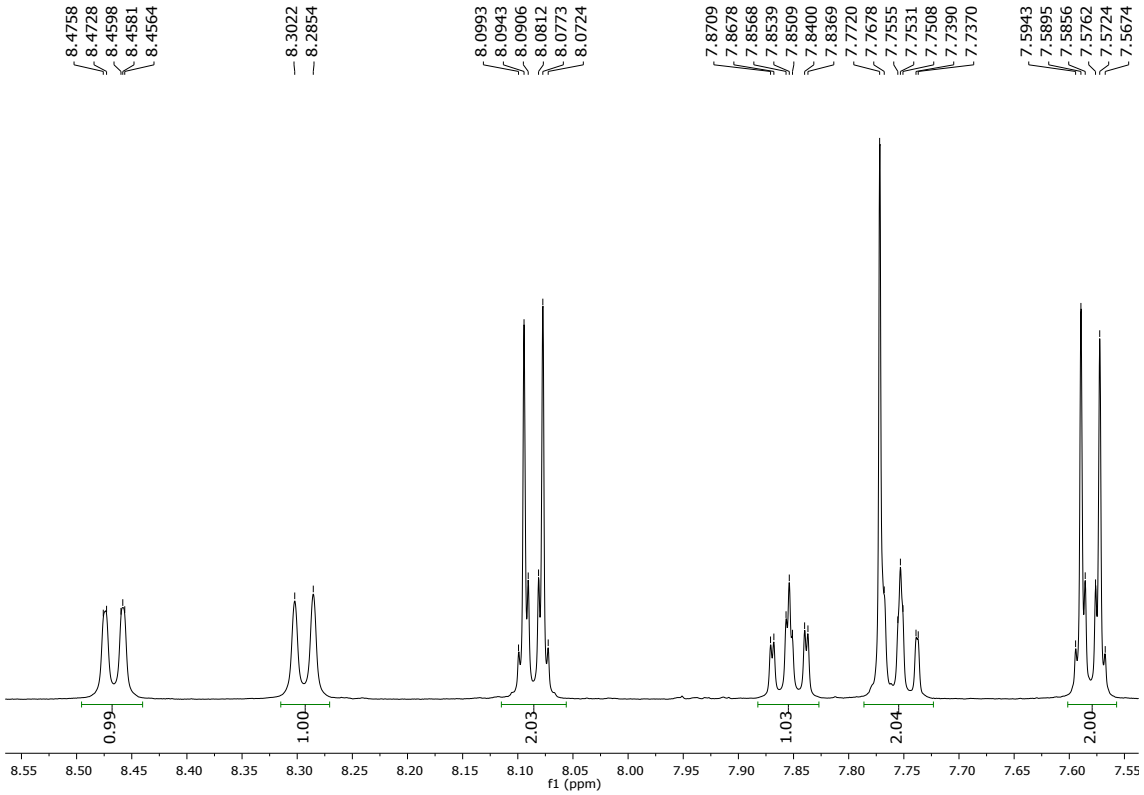

Figure S5. Expansion of ^{1}H NMR spectrum of compound **2b** (300.13 MHz, $CDCl_3$)

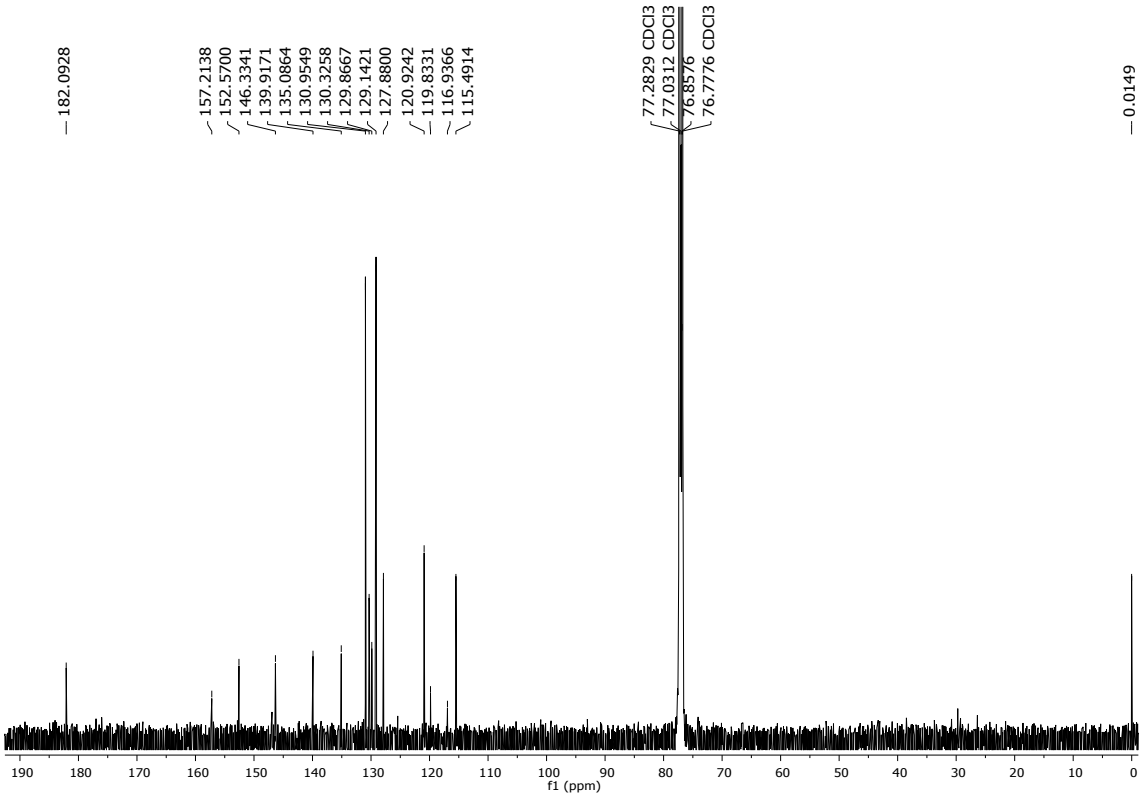

Figure S6. ^{13}C NMR spectrum of compound **2b** (75.47 MHz, $CDCl_3$)

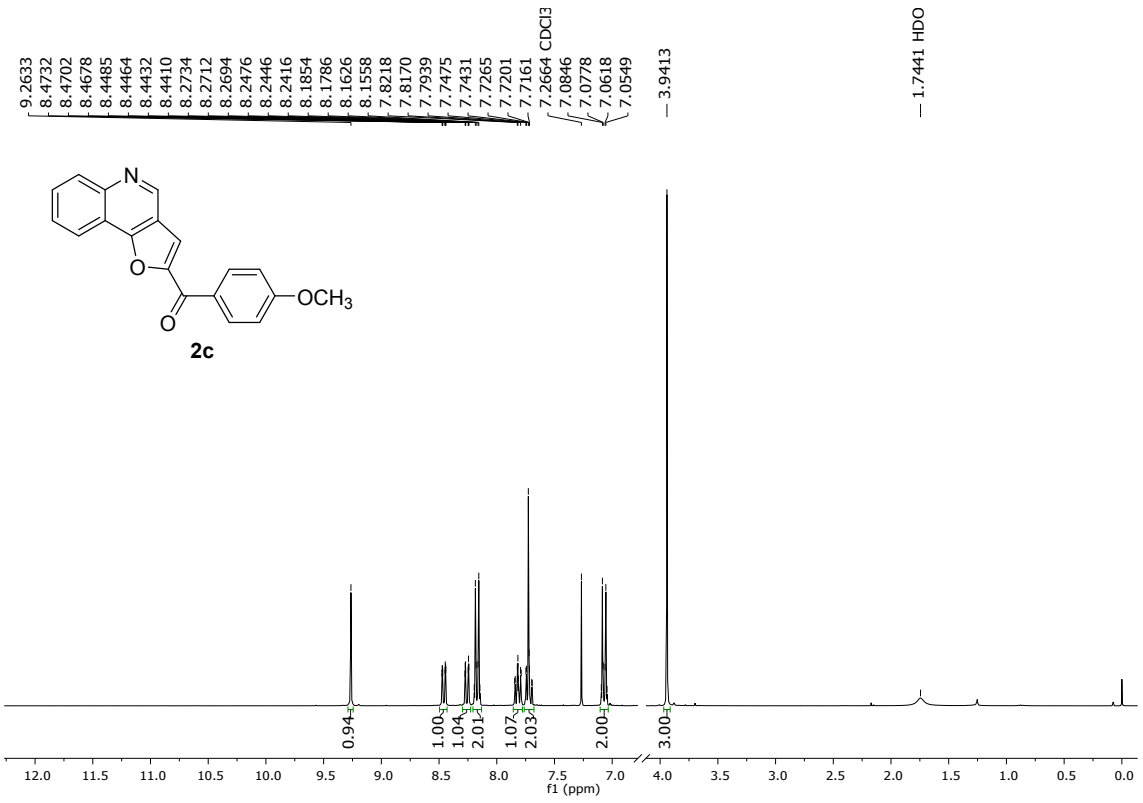

Figure S7. ^{1}H NMR spectrum of compound **2c** (300.13 MHz, $CDCl_3$)

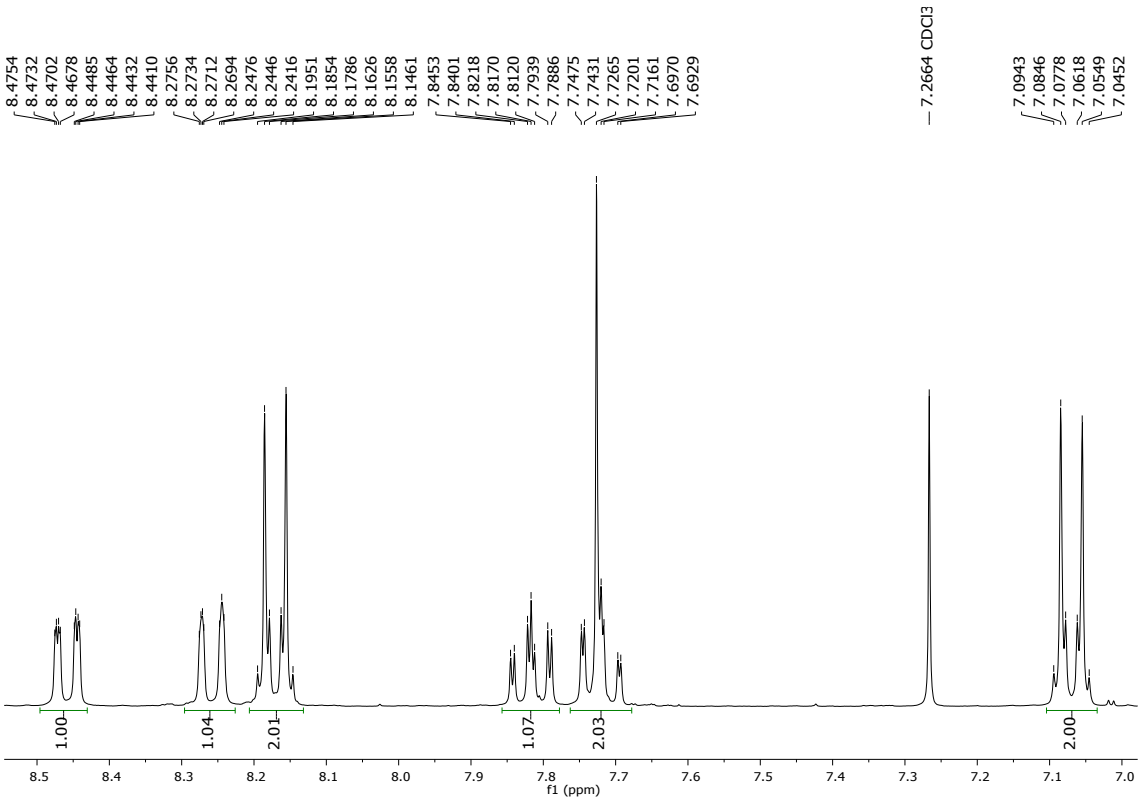

Figure S8. Expansion of ^{1}H NMR spectrum of compound **2c** (300.13 MHz, $CDCl_3$)

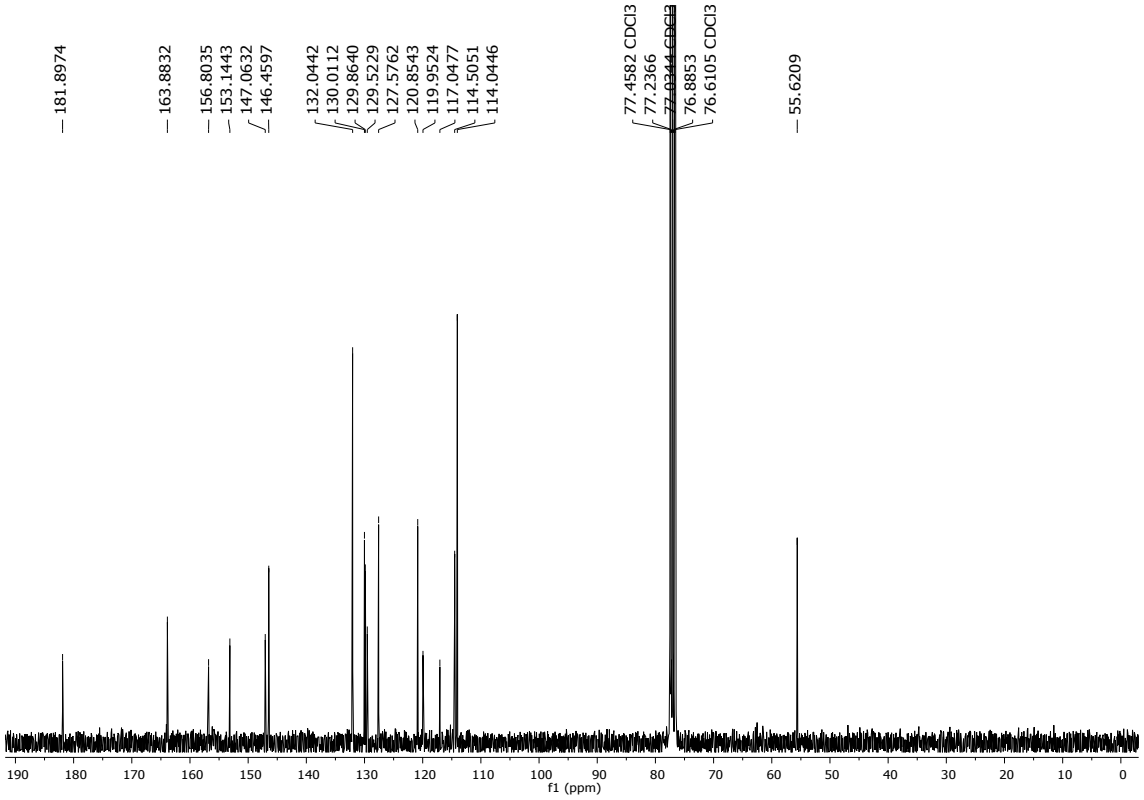

Figure S9. ^{13}C NMR spectrum of compound **2c** (75.47 MHz, $CDCl_3$)

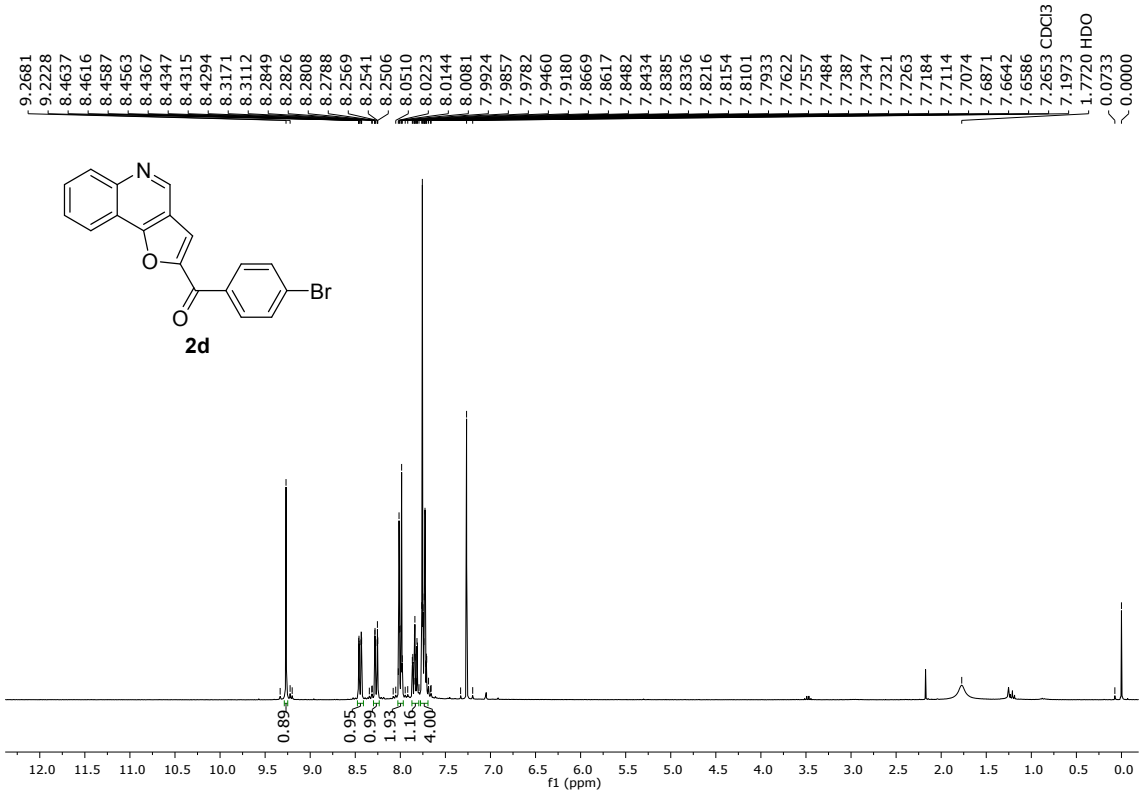

Figure S10. ^{1}H NMR spectrum of compound **2d** (300.13 MHz, $CDCl_3$)

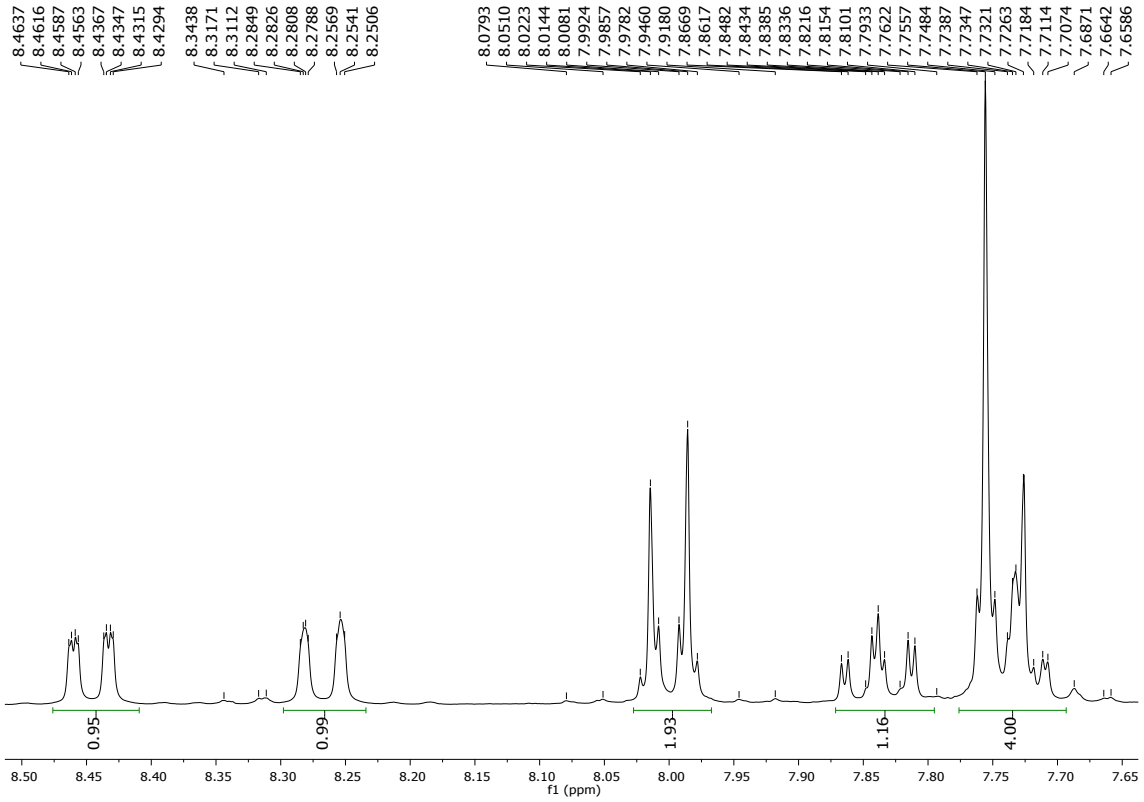

Figure S11. Expansion of ^{1}H NMR spectrum of compound **2d** (300.13 MHz, $CDCl_3$)

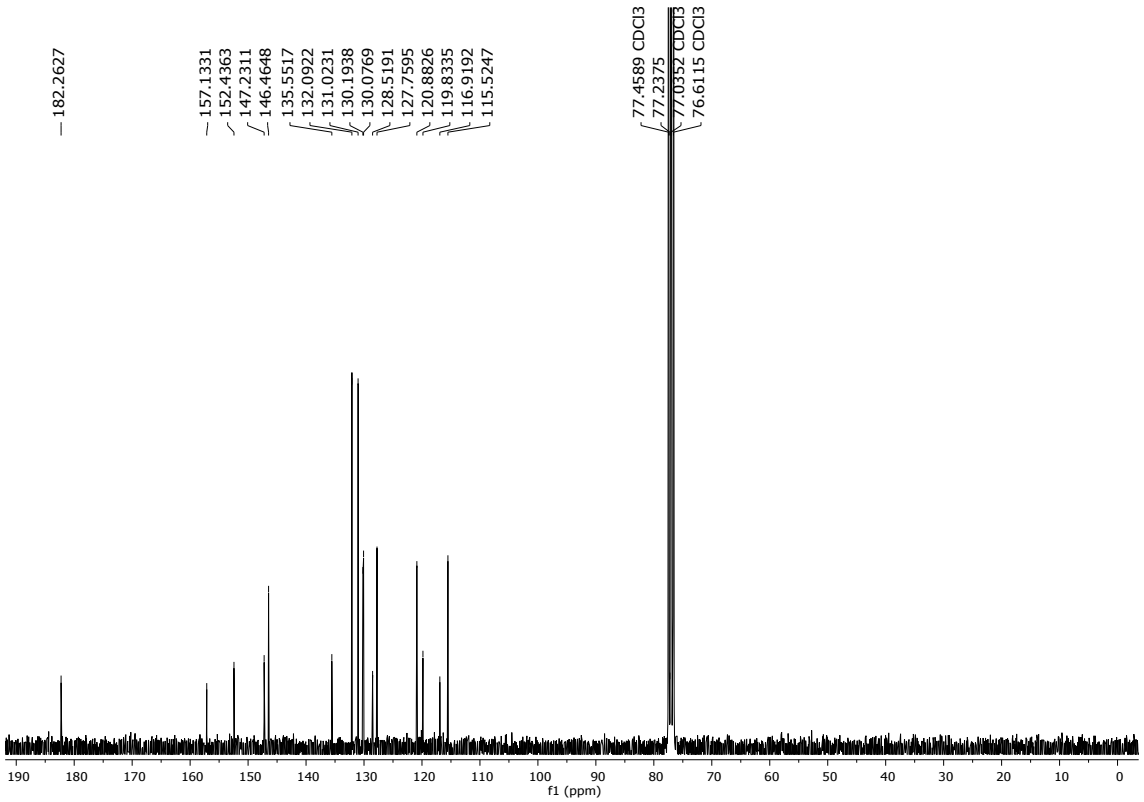

Figure S12. ^{13}C NMR spectrum of compound **2d** (75.47 MHz, $CDCl_3$)

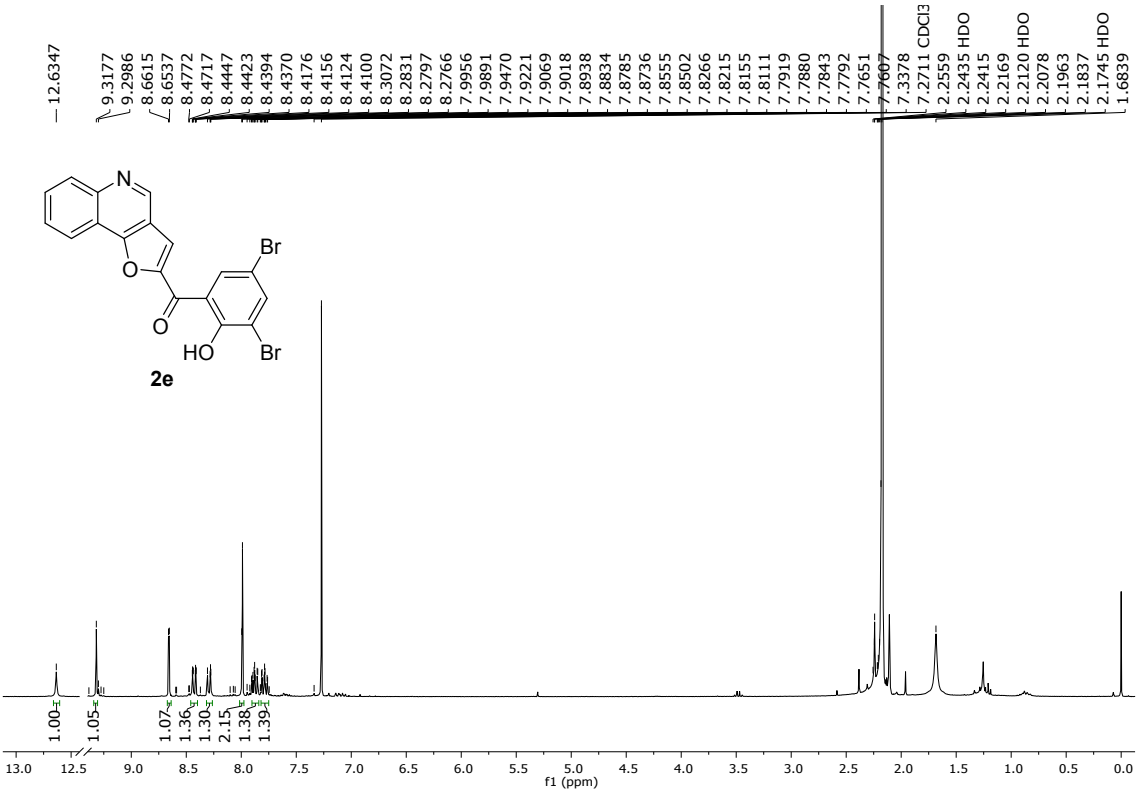

Figure S13. ^{1}H NMR spectrum of compound **2e** (300.13 MHz, $CDCl_3$)

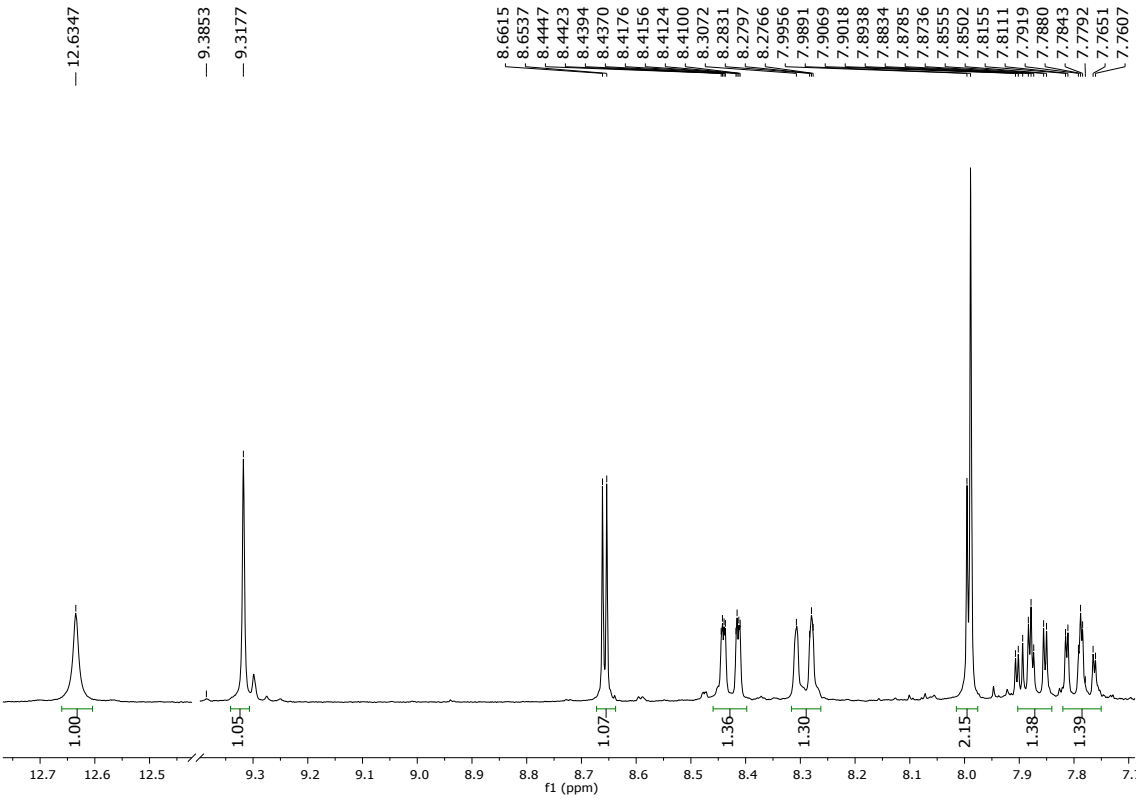

Figure S14. Expansion of ^{1}H NMR spectrum of compound **2e** (300.13 MHz, $CDCl_3$)

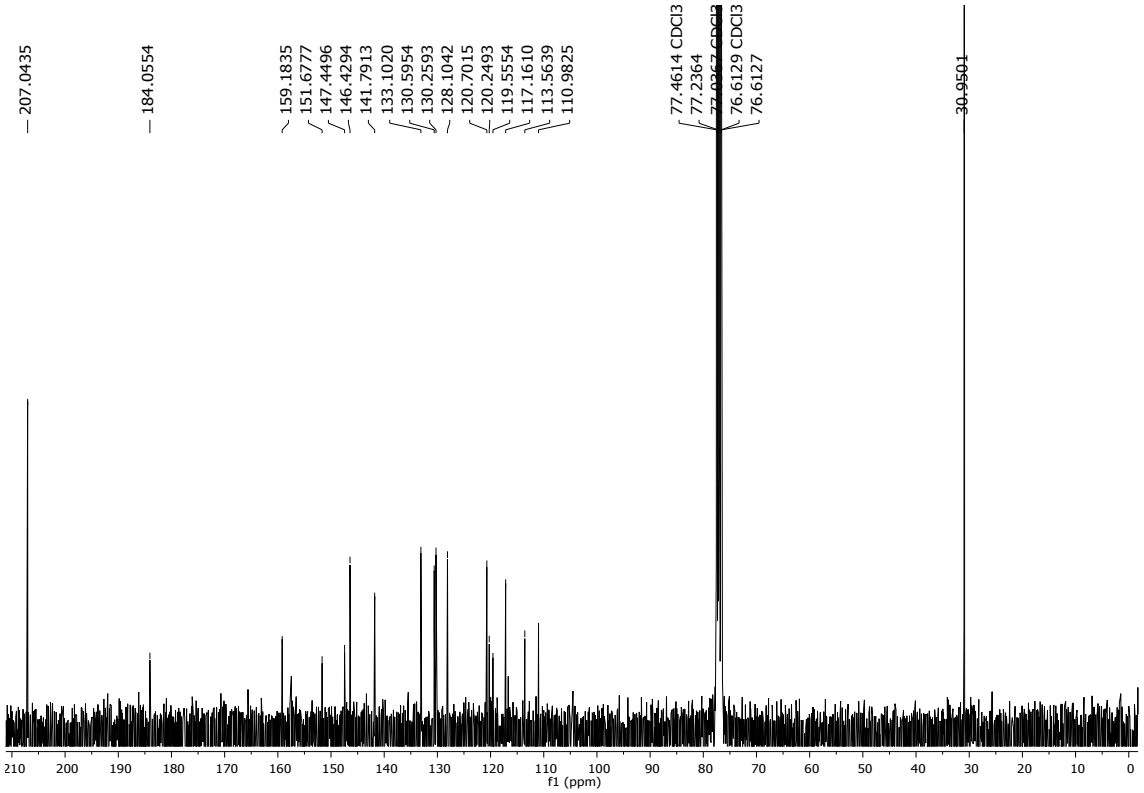

Figure S15. ^{13}C NMR spectrum of compound **2e** (75.47 MHz, $CDCl_3$)*

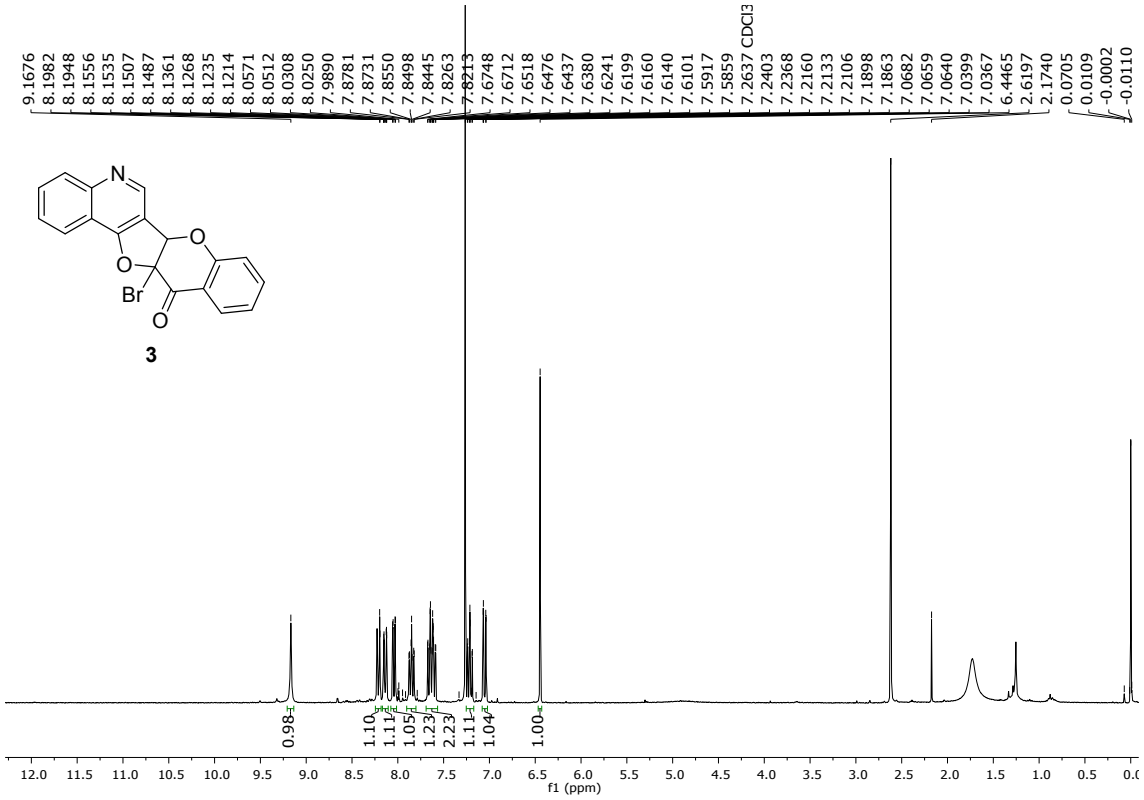

Figure S16. ^{1}H NMR spectrum of compound **3** (300.13 MHz, $CDCl_3$)

* Peaks at δ 30.9 ppm and 207.0 ppm are due to the presence of acetone since the spectrum was acquired before drying the compound in the vacuum pump.

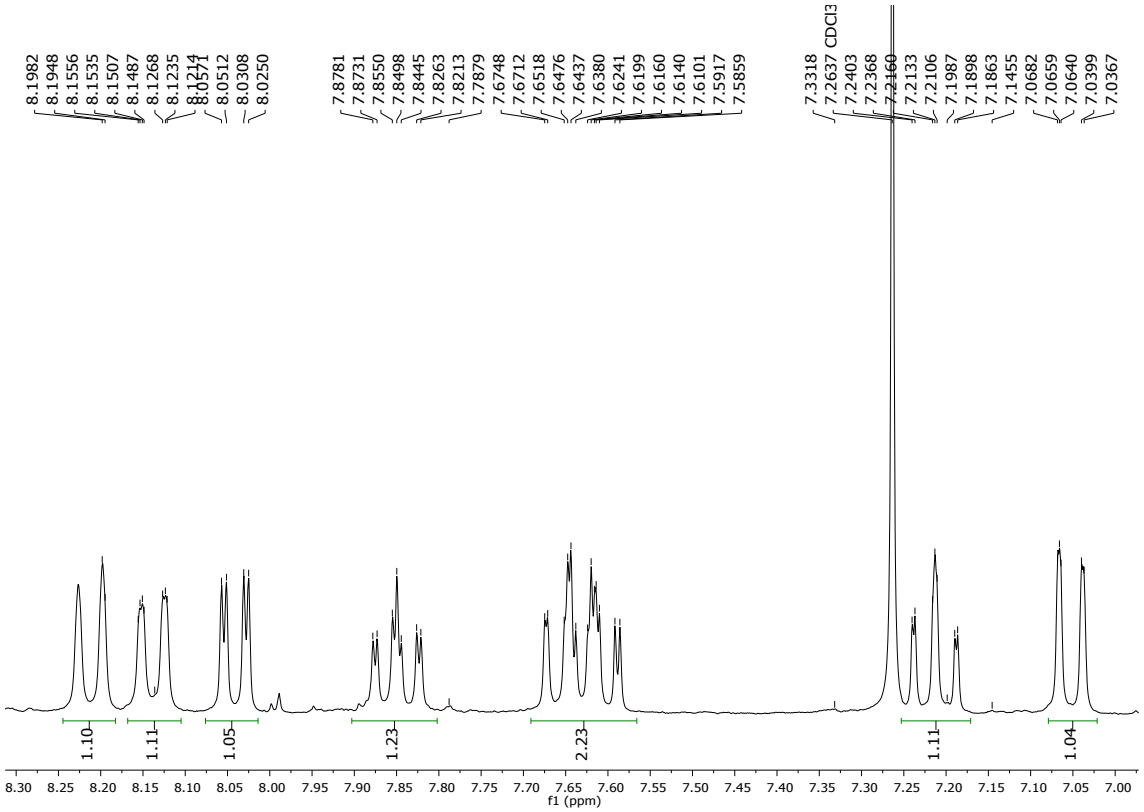

Figure S17. Expansion of ^{1}H NMR spectrum of compound **3** (300.13 MHz, $CDCl_3$)

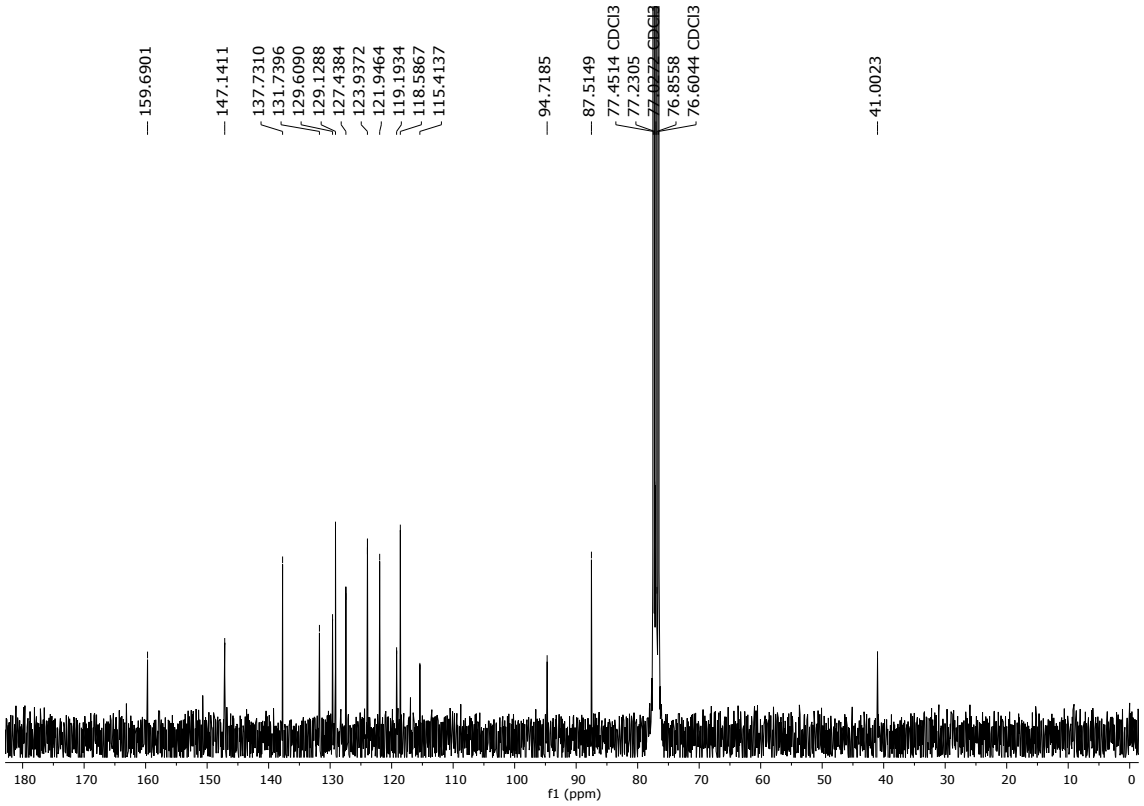

Figure S18. ^{13}C NMR spectrum of compound **3** (75.47 MHz, $CDCl_3$)[†]

[†] The peak at δ41.0 ppm was not assigned to the compound since no correlations were observed for this signal in the 2D HSQC or HMBC spectra.

2. Single-Crystal X-Ray Diffraction Studies

Experimental Section

Single crystals of compound 12a-bromo-6b,12a-dihydro-12*H*-chromeno[2',3':4,5]furo [3,2-*c*]quinolin-12-one (**3**) were manually harvested from an NMR tube and immersed in highly viscous FOMBLIN Y perfluoropolyether vacuum oil (LVAC 140/13, Sigma-Aldrich) to avoid degradation caused by the evaporation of the solvent.[1] Crystals were mounted on MiTeGen MicroLoops, typically with the help of a Stemi 2000 stereomicroscope equipped with Carl Zeiss lenses. X-ray diffraction data were collected at 150(2) K on a Bruker D8 QUEST equipped with Mo Kα sealed tube (λ = 0.71073 Å), a multilayer TRIUMPH X-ray mirror, a PHOTON 100 CMOS detector, and an Oxford Instruments Cryostrem 700+ Series low temperature device. Diffraction images were processed using the software package SAINT+,[2] and data were corrected for absorption by the multiscan semi-empirical method implemented in SADABS 2016/2.[3]

The structure was solved using the algorithm implemented in SHELXT-2014/5,[4] which allowed the immediate location of almost all of the heaviest atoms composing the molecular unit. The remaining missing and misplaced non-hydrogen atoms were located from difference Fourier maps calculated from successive full-matrix least-squares refinement cycles on F^2 using the latest SHELXL from the 2018/3 release.[5] All structural refinements were performed using the graphical interface ShelXle.[6]

Hydrogen atoms bound to carbon were placed at their idealized positions using appropriate *HFIX* instructions in SHELXL: *43* (aromatic carbon atoms) and *13* (tertiary carbon atoms). These hydrogen atoms were included in subsequent refinement cycles with isotropic thermal displacements parameters (U_{iso}) fixed at $1.2 \times U_{eq}$ of the parent carbon atoms.

The last difference Fourier map synthesis showed the highest peak (0.518 eÅ^{-3}) and the deepest hole (-0.348 eÅ^{-3}) located at 1.01 and 0.84 Å from Br1, respectively. Structural drawings have been created using the software package Crystal Impact Diamond.[7]

Crystal data for **3**: $C_{18}H_{10}BrNO_3$, $M = 368.18$, monoclinic, space group $P2_1/c$, $Z = 4$, $a = 15.6773(18)$ Å, $b = 6.7908(8)$ Å, $c = 15.3495(19)$ Å, $\beta = 118.405(4)^o$, $V = 1437.4(3)$ Å^3, μ(Mo-Kα) = 2.875 mm^{-1}, $D_c = 1.701$ g cm^{-3}, colourless plate with crystal size of 0.21×0.07×0.02 mm^3. Of a total of 25437 reflections collected, 2616 were independent ($R_{int} = 0.0464$). Final $R1 = 0.0251$ [$I > 2\sigma(I)$] and $wR2 = 0.0562$ (all data). Data completeness to theta = 25.24°, 99.7%. CCDC 1962713.

3. References

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2. SAINT+, *Data Integration Engine v. 8.37a*©, 1997-2015, Bruker AXS, Madison, Wisconsin, USA.
3. L. Krause, R. Herbst-Irmer, G. M. Sheldrick and D. Stalke, *J. Appl. Crystallogr.*, 2015, **48**, 3-10.
4. G. M. Sheldrick, *Acta Cryst. A*, 2015, **71**, 3-8.
5. G. M. Sheldrick, *Acta Cryst. C*, 2015, **71**, 3-8.
6. C. B. Hübschle, G. M. Sheldrick and B. Dittric, *J. Appl. Crystallogr.*, 2011, **44**, 1281-1284.
7. K. Brandenburg, *DIAMOND, Version 3.2f. Crystal Impact GbR, Bonn, Germany*, 1997-2010.