Electronic Supplementary Material (ESI) for New Journal of Chemistry.

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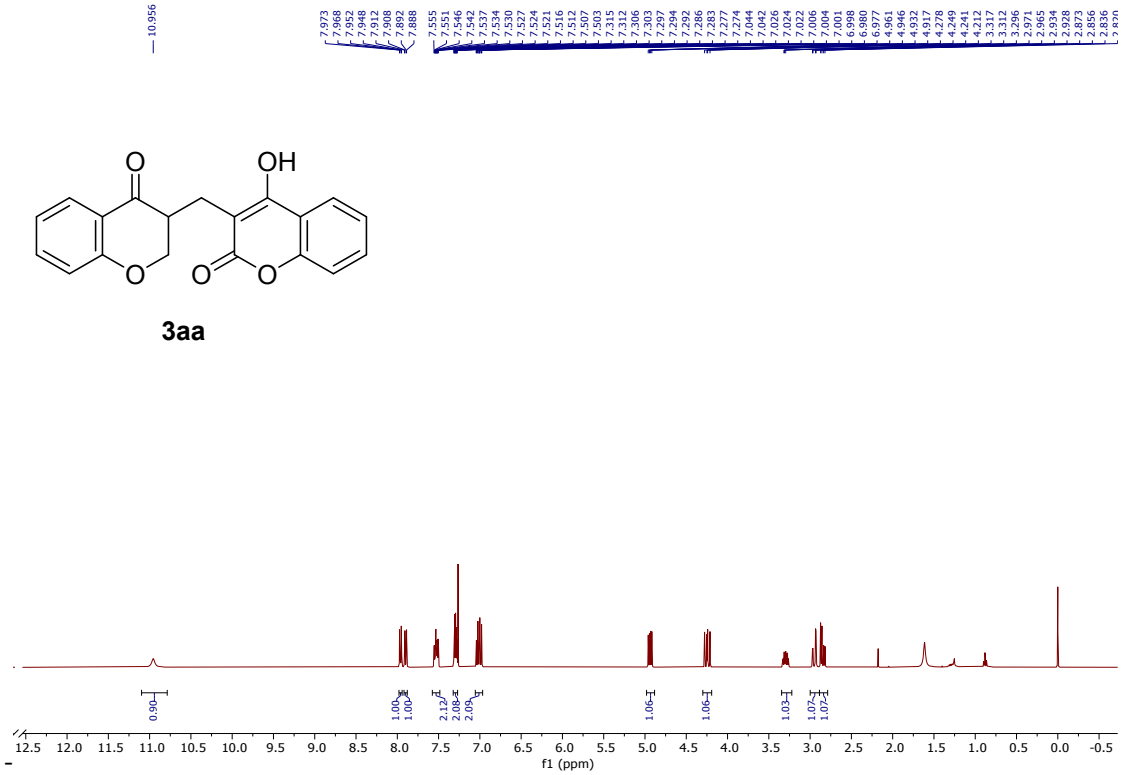
^{1}H-NMR (400 MHz, $CDCl_3$)



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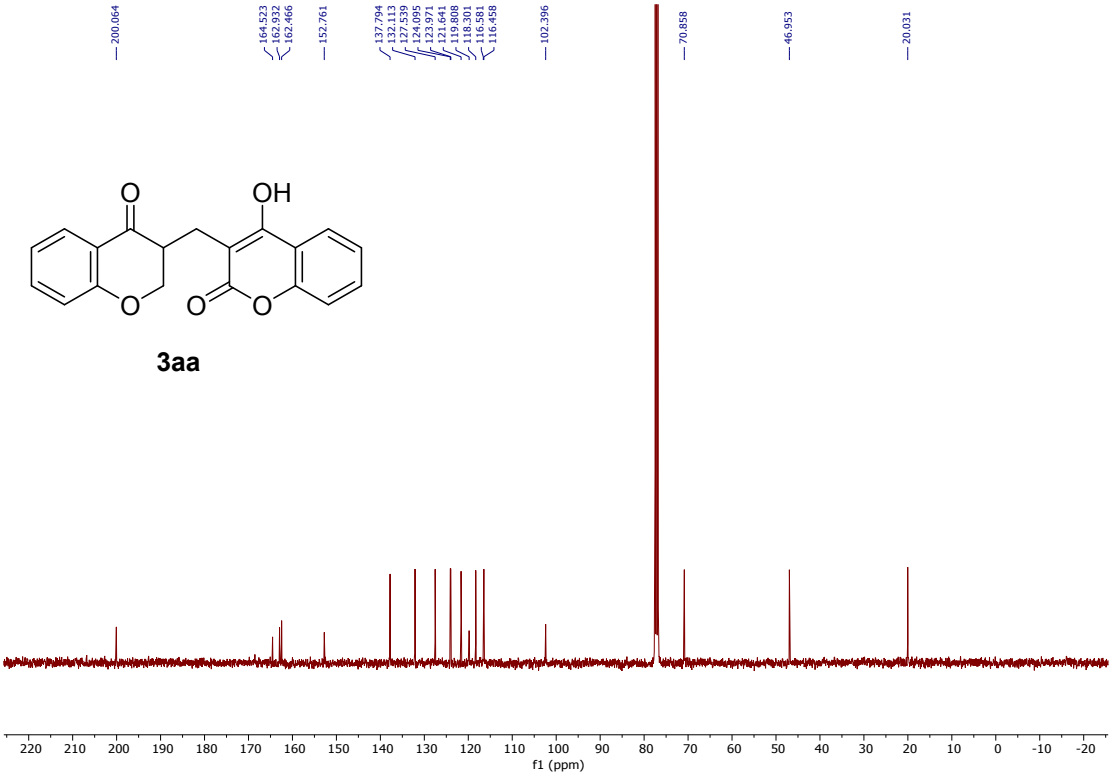
^{13}C-NMR (100 MHz, $CDCl_3$)



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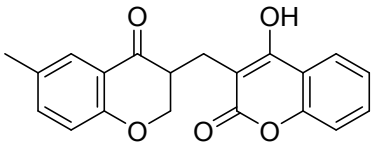

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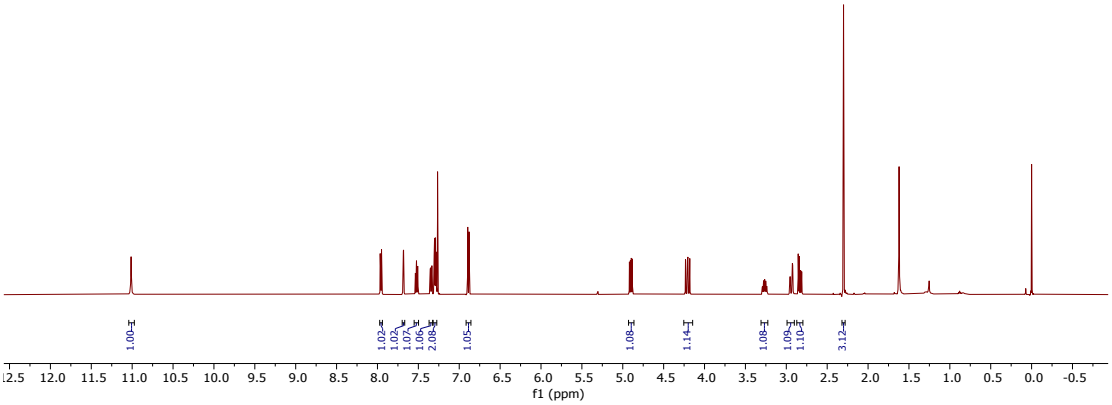

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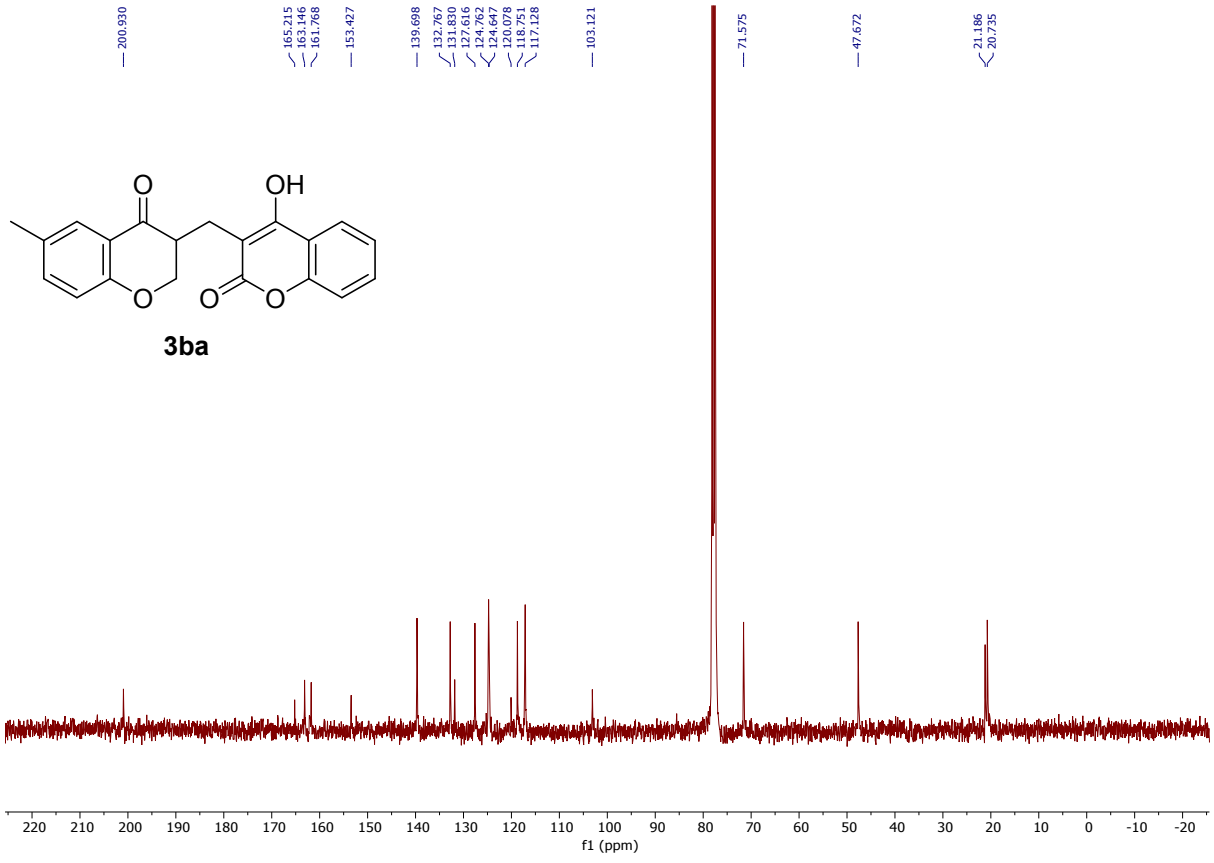

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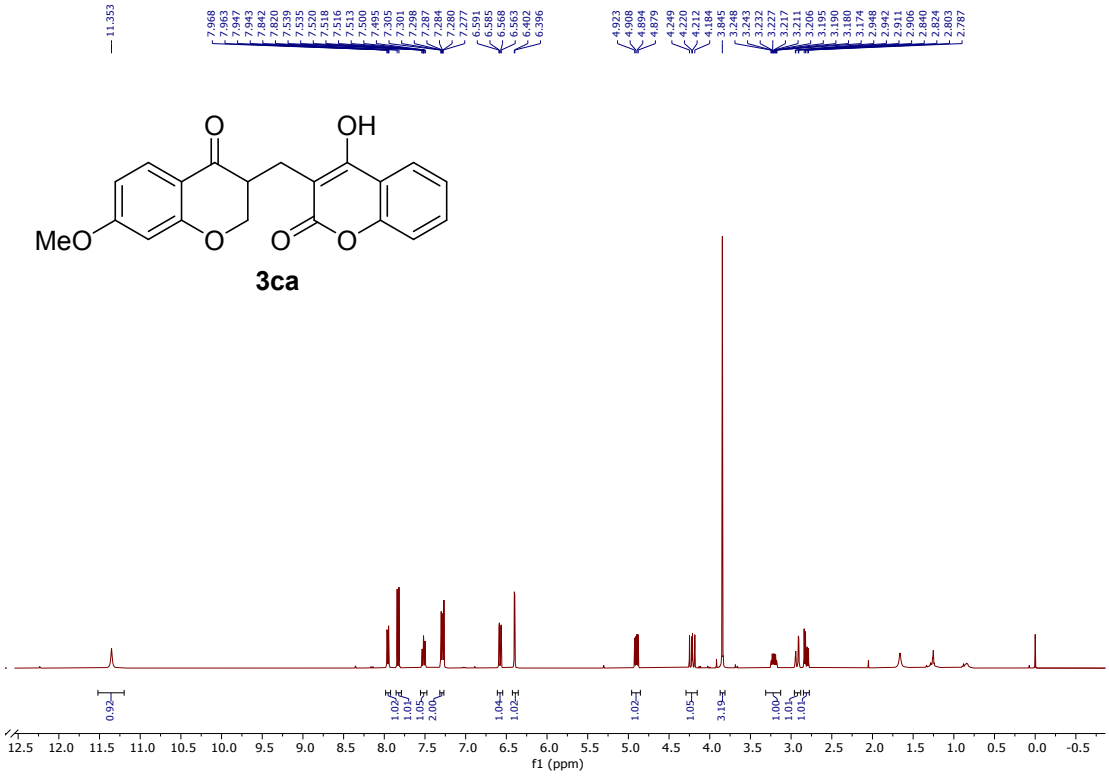

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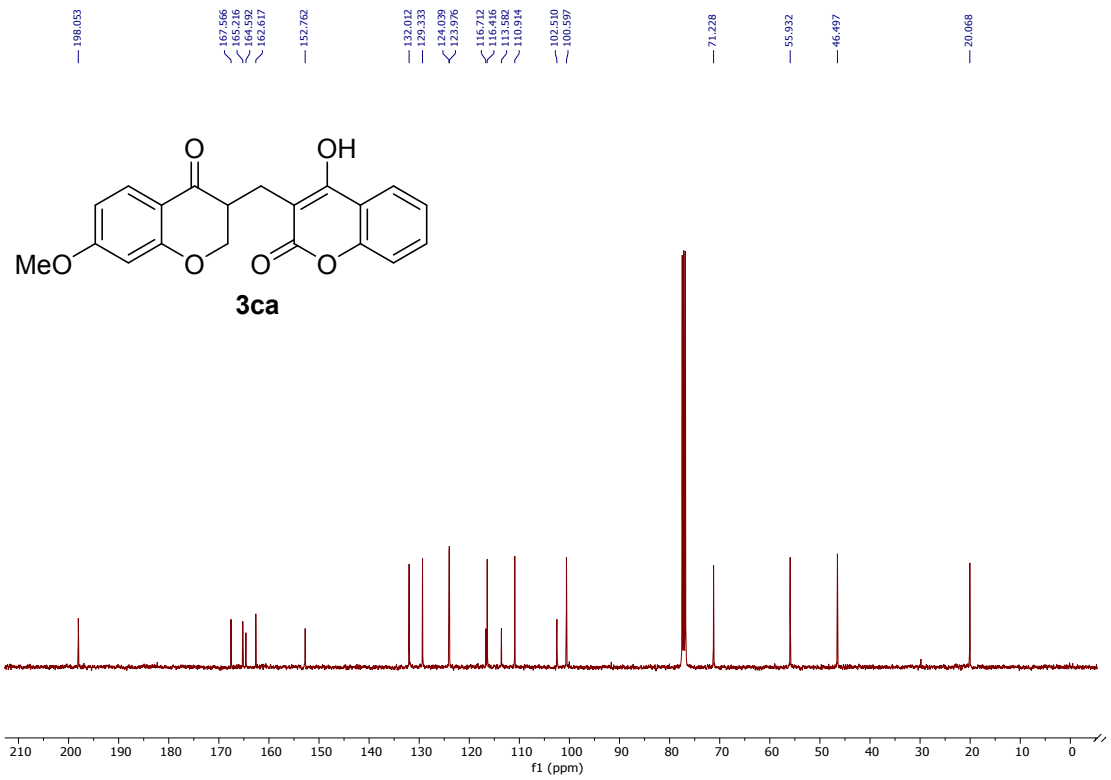

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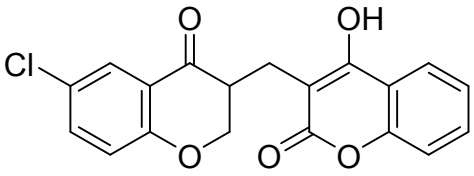

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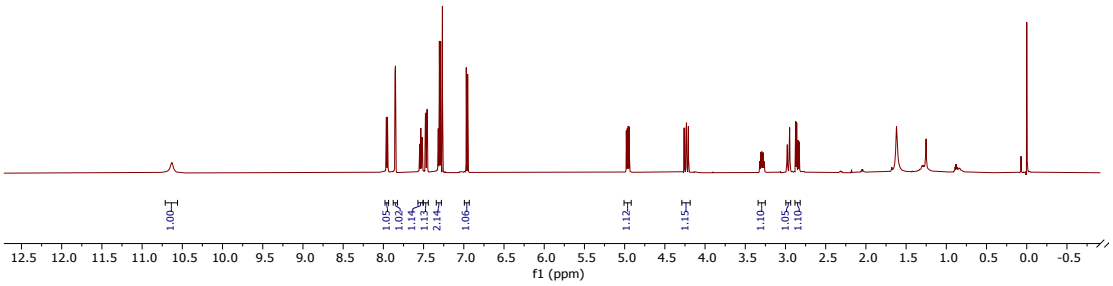

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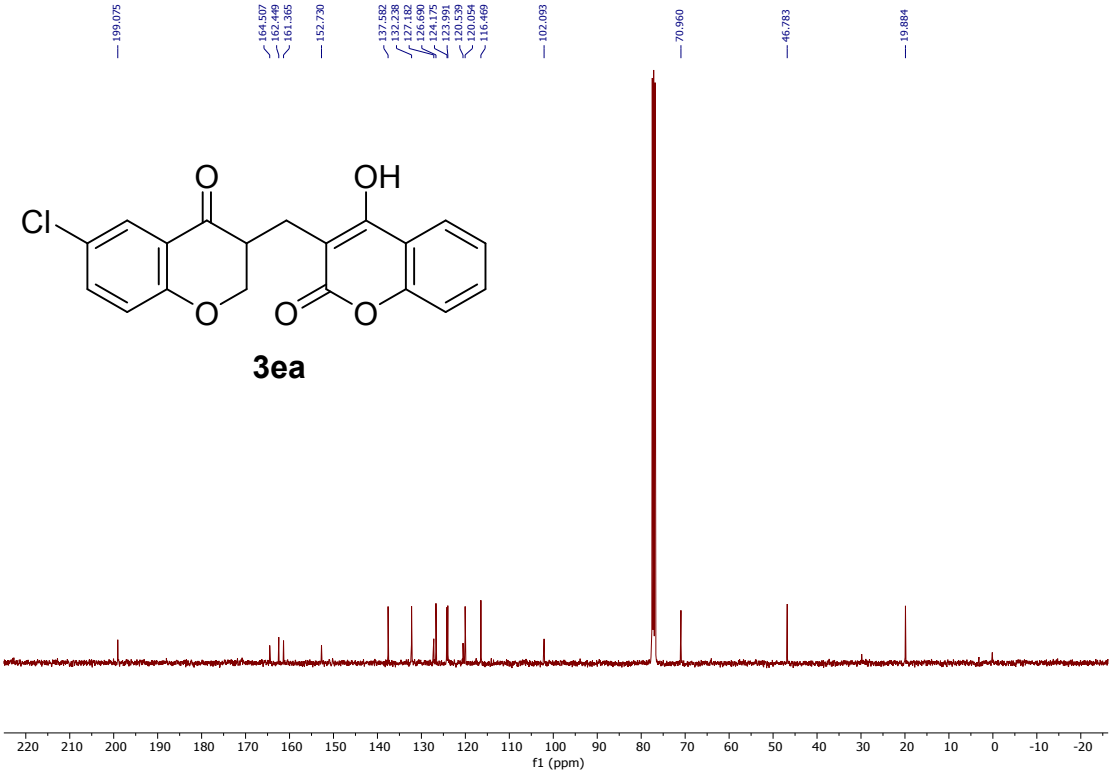

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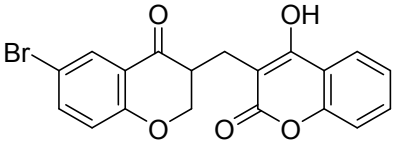

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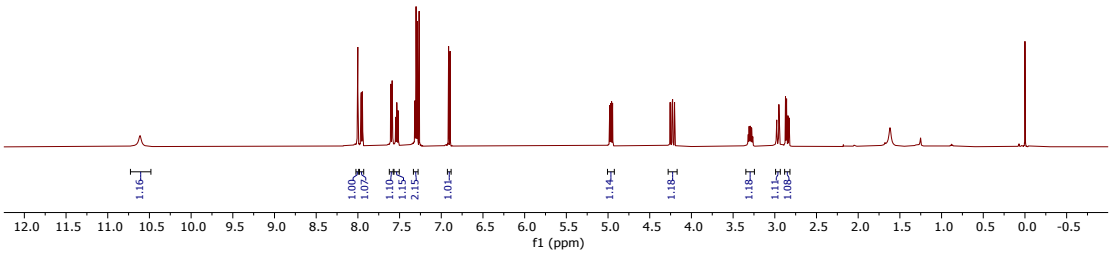

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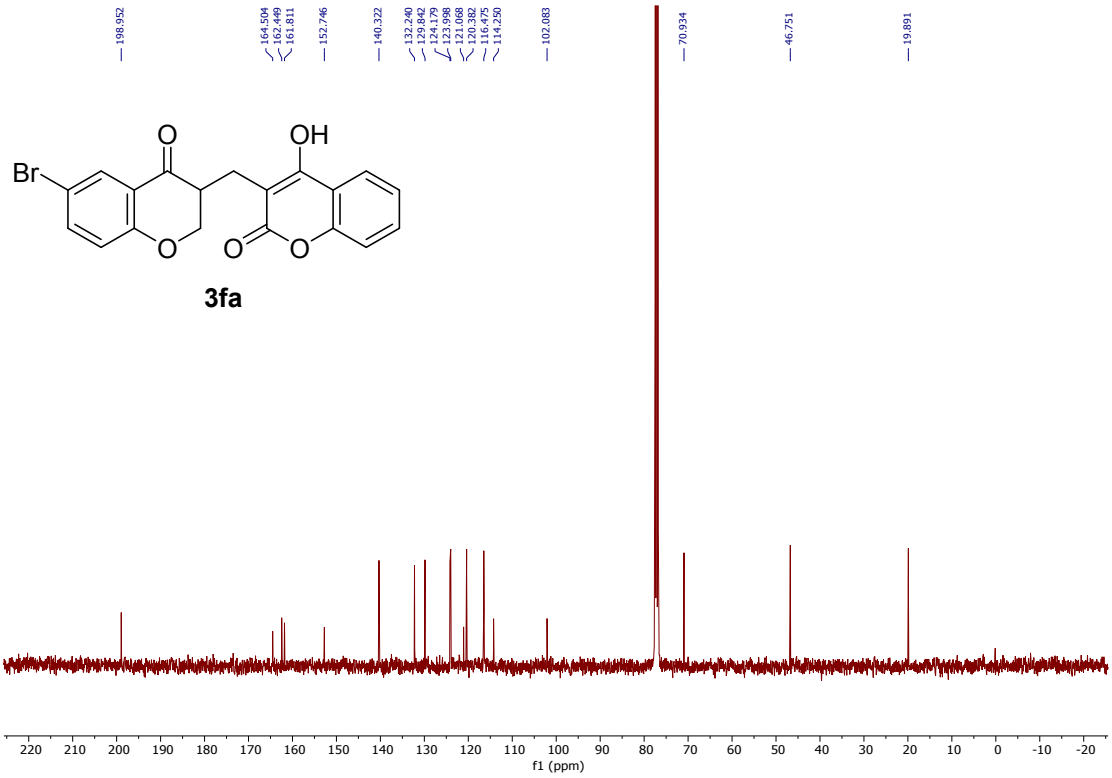

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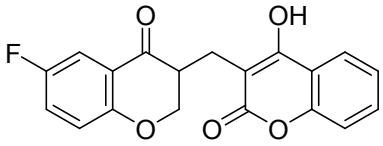

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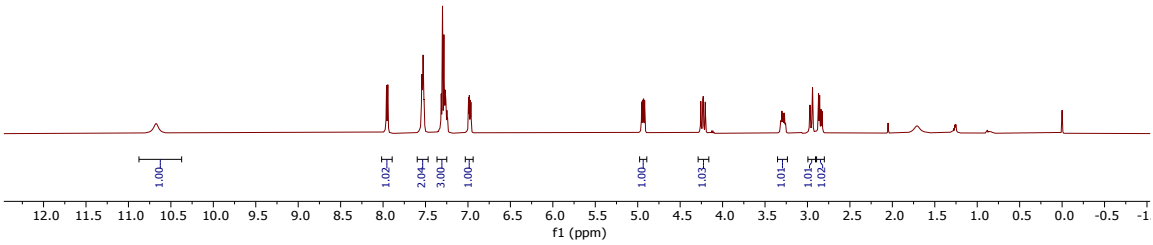

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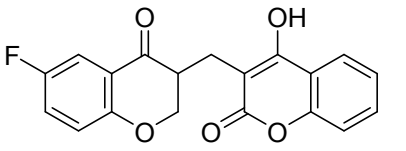

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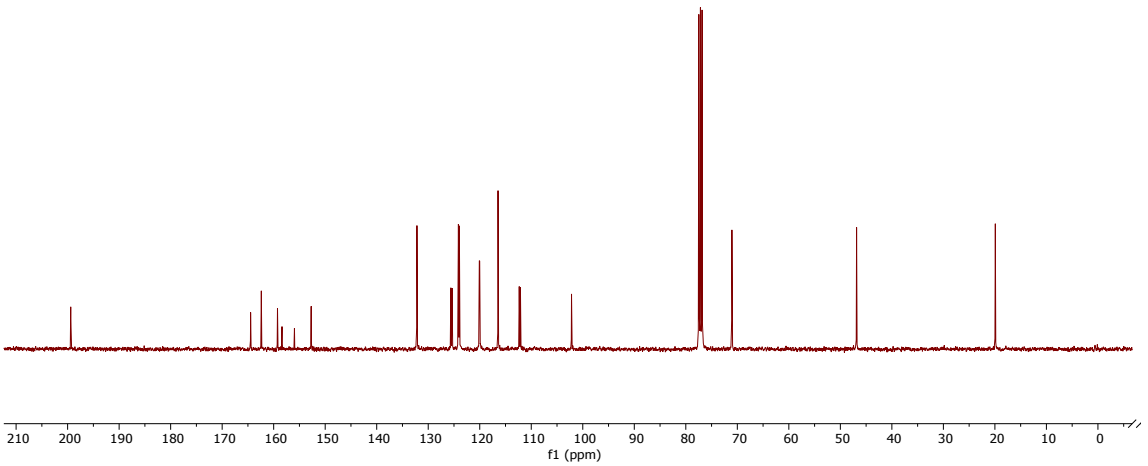

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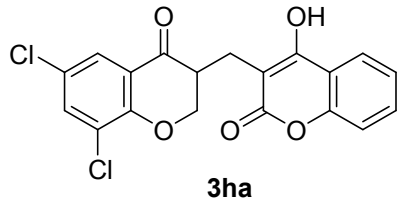

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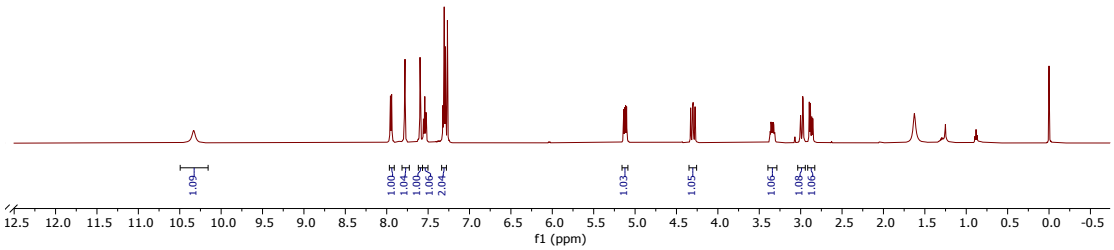

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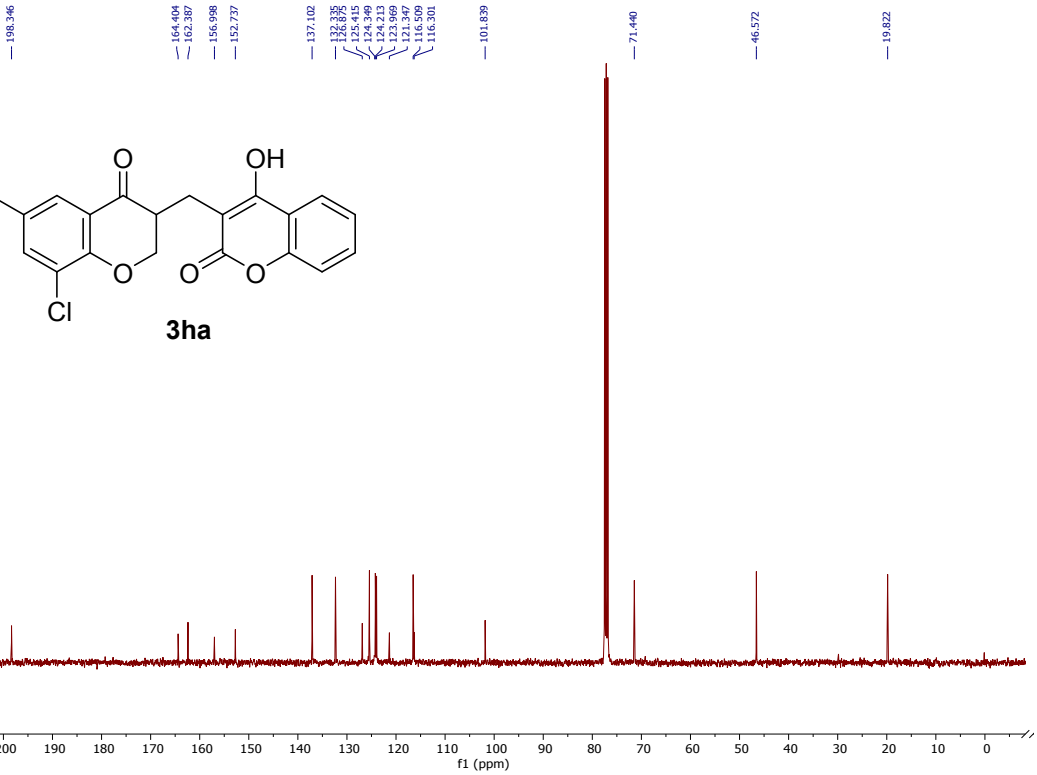

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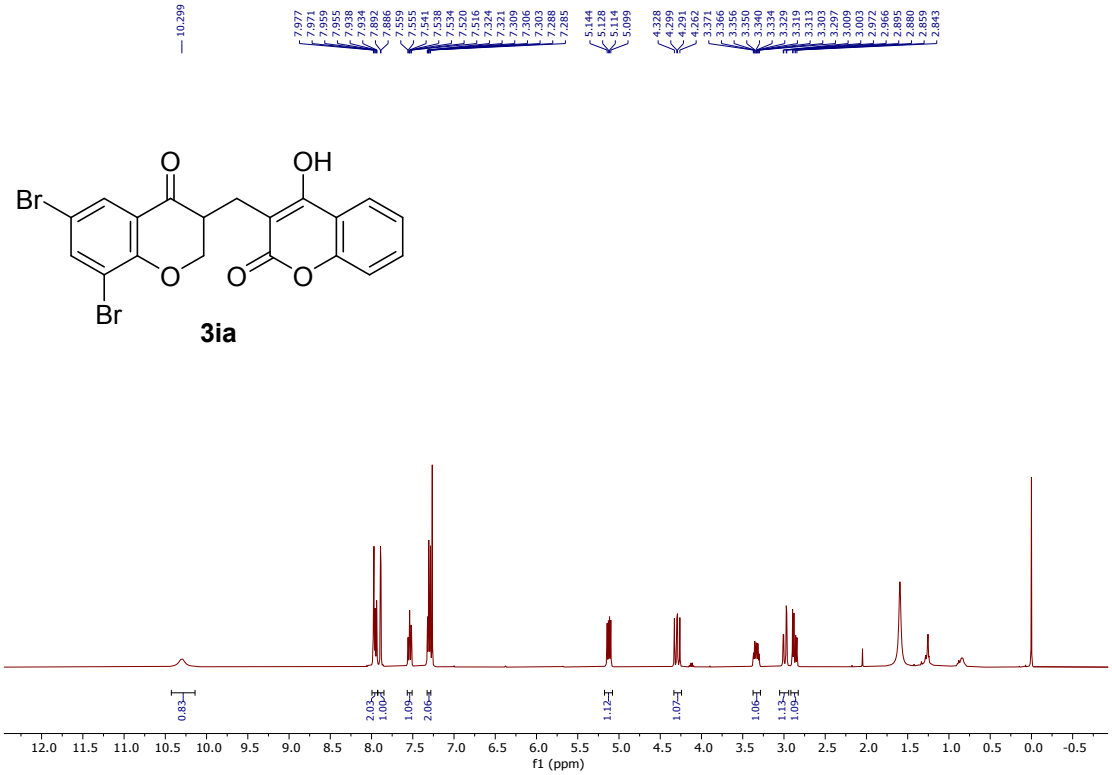

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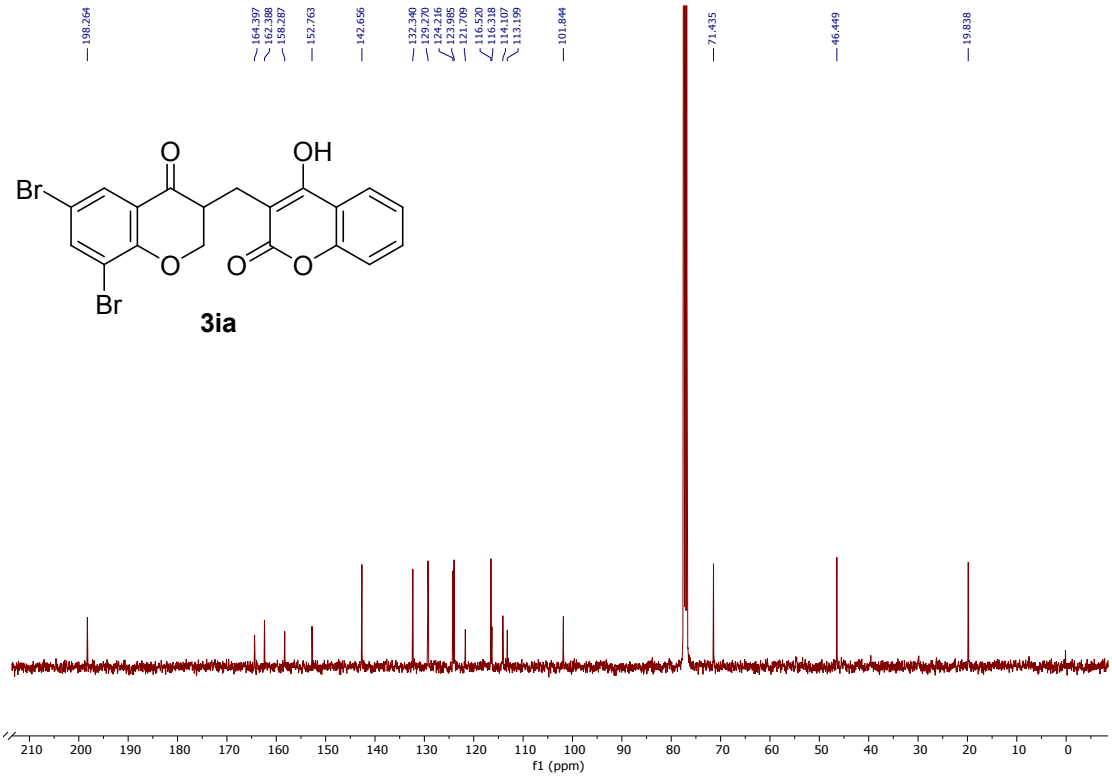

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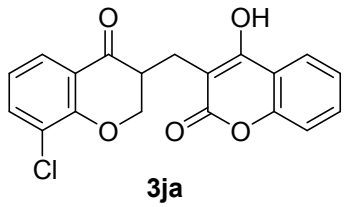

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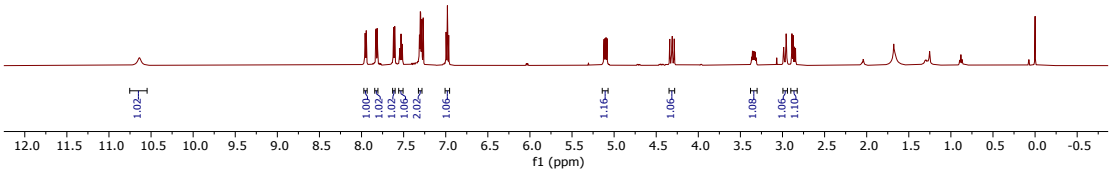

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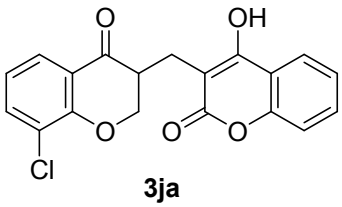

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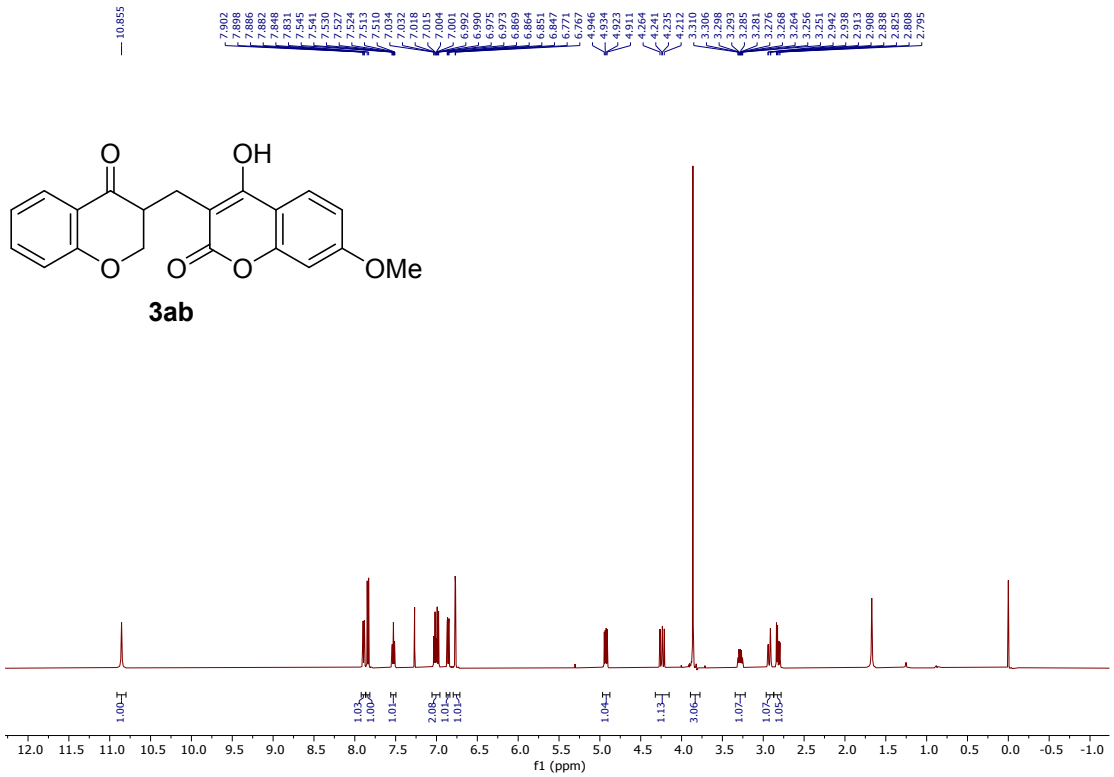

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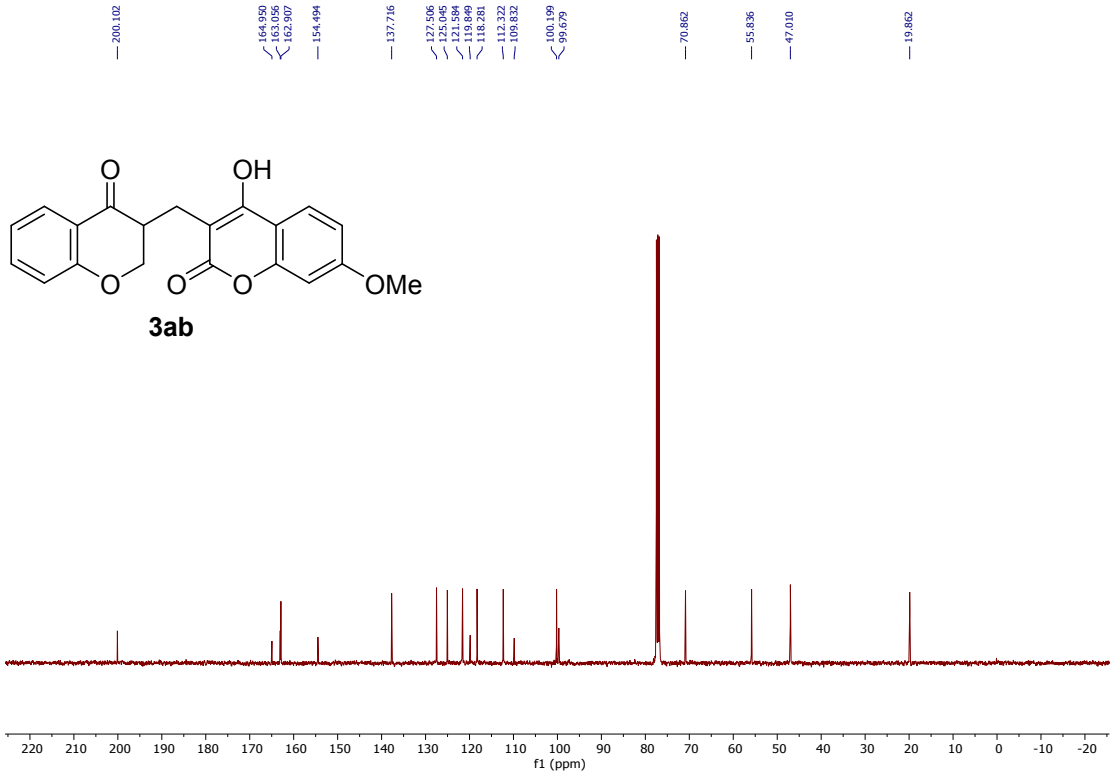

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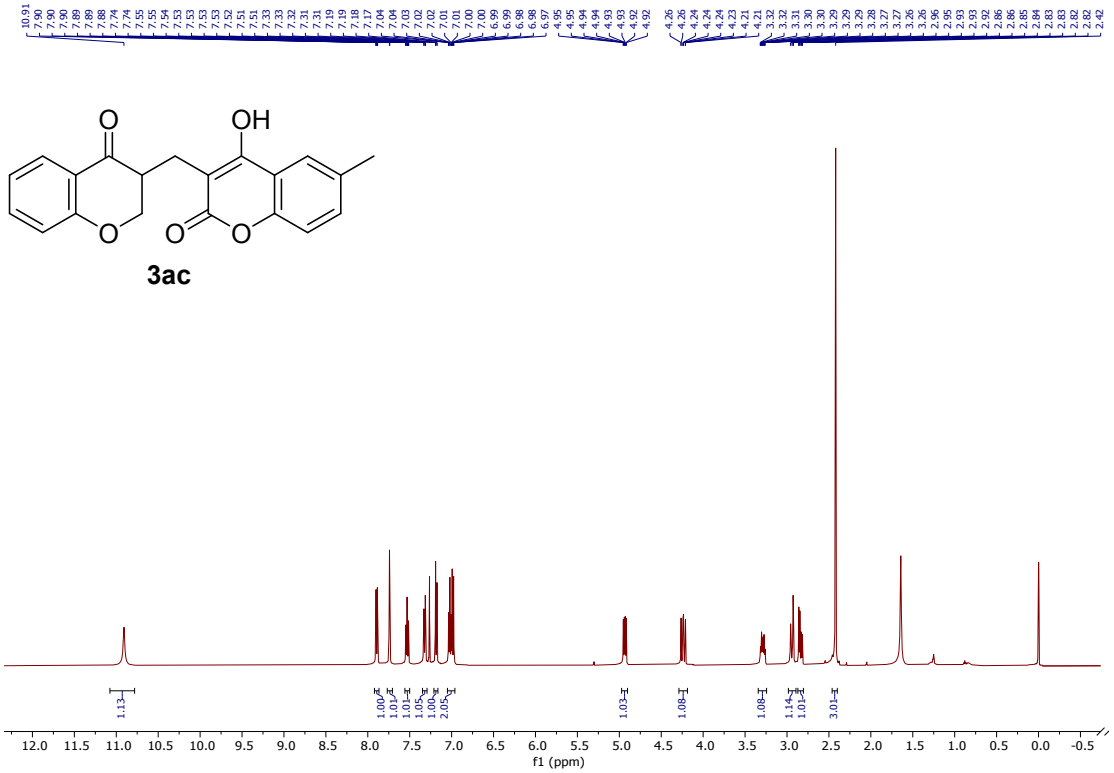

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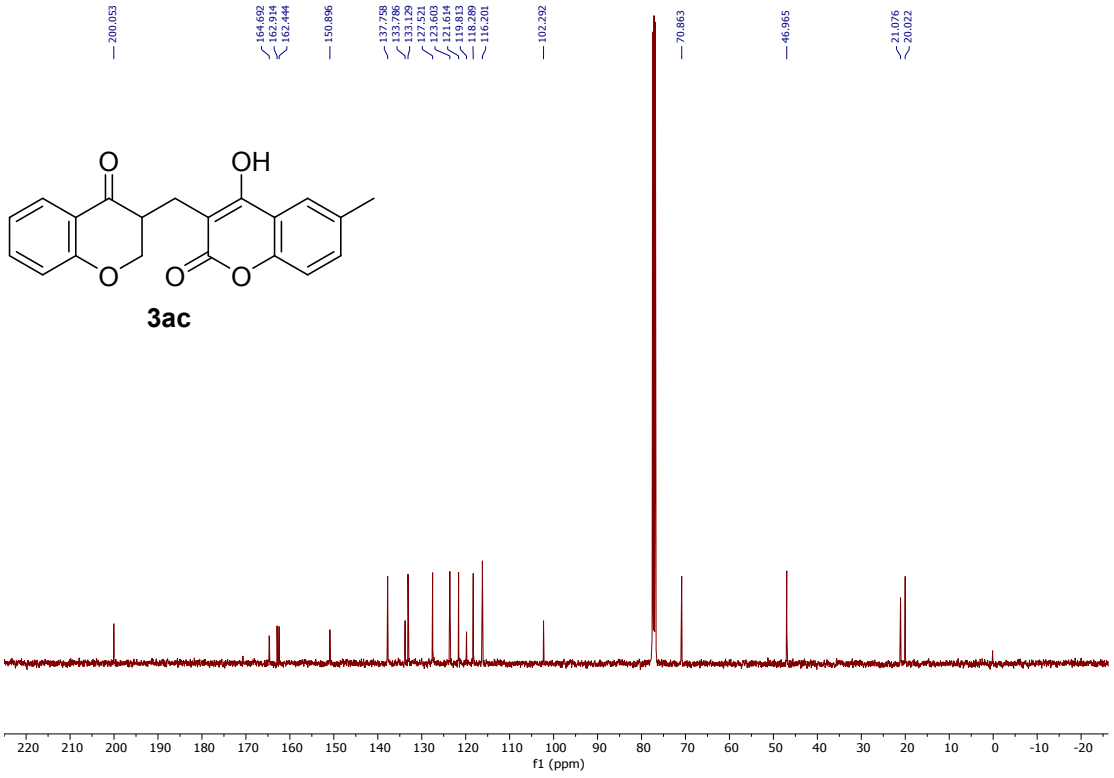

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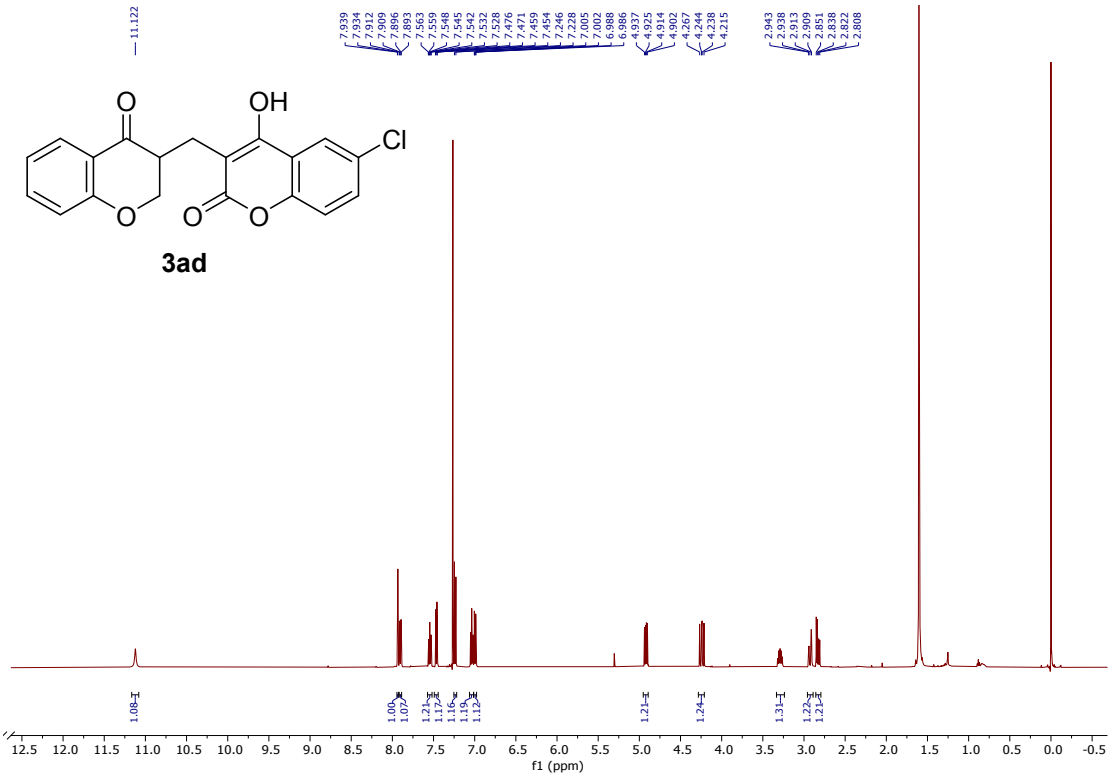

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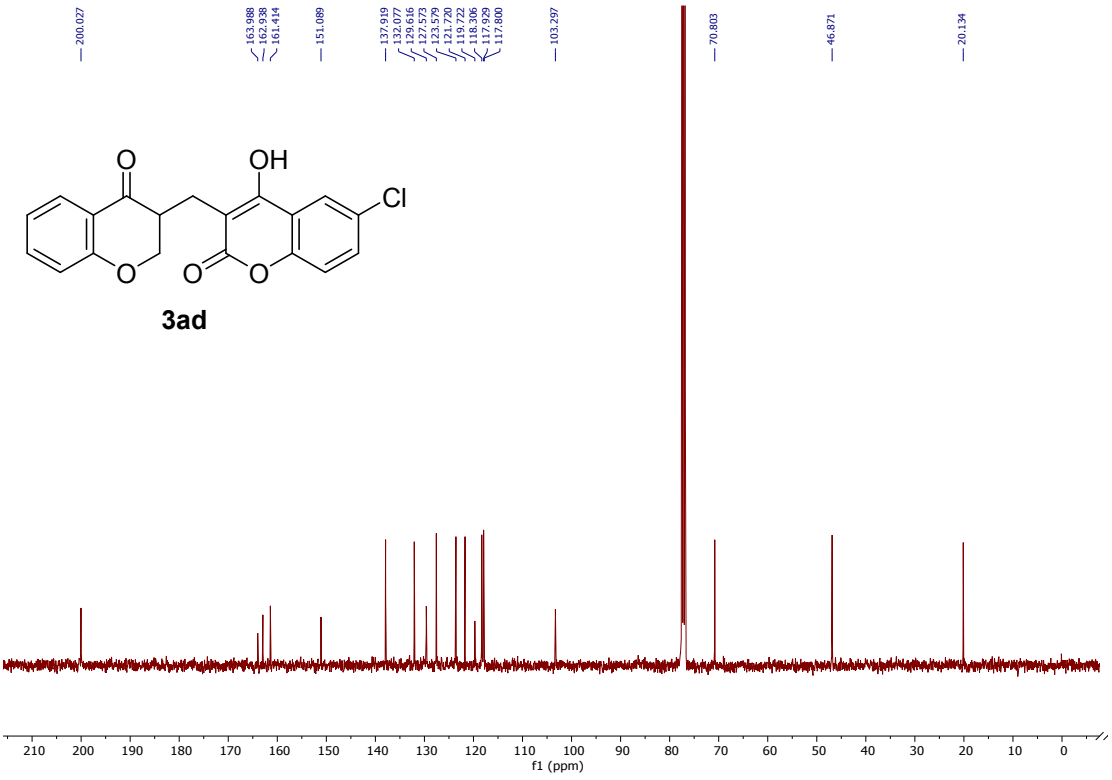

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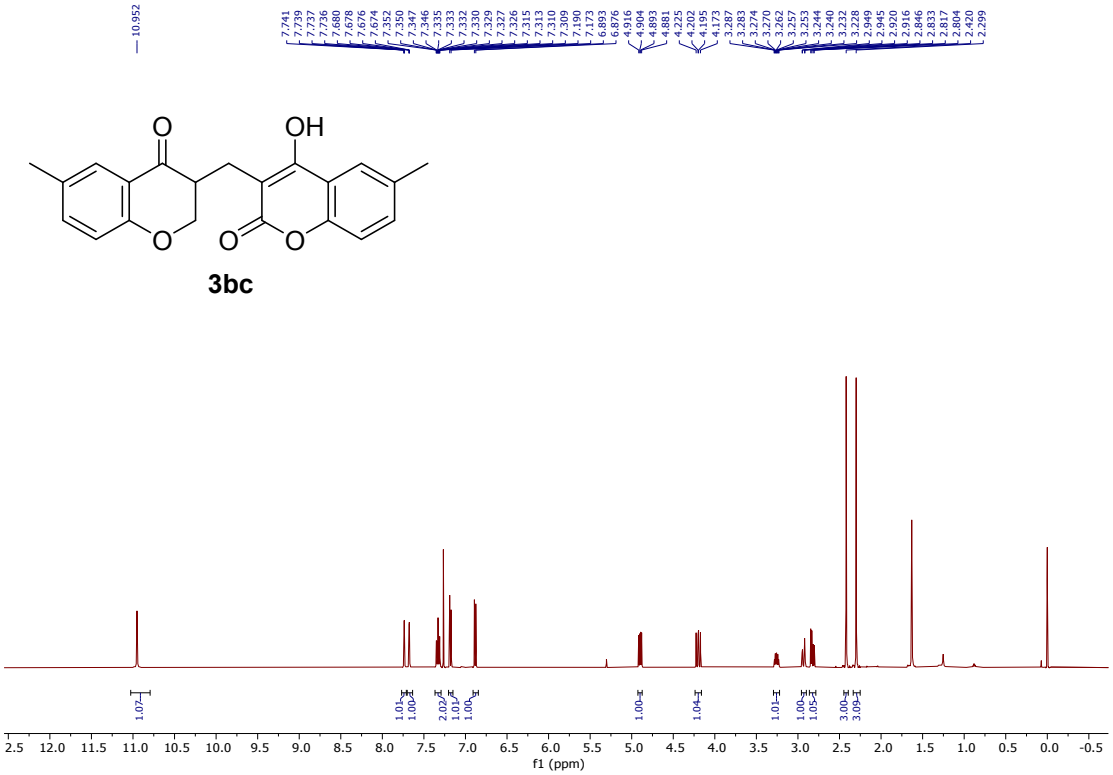

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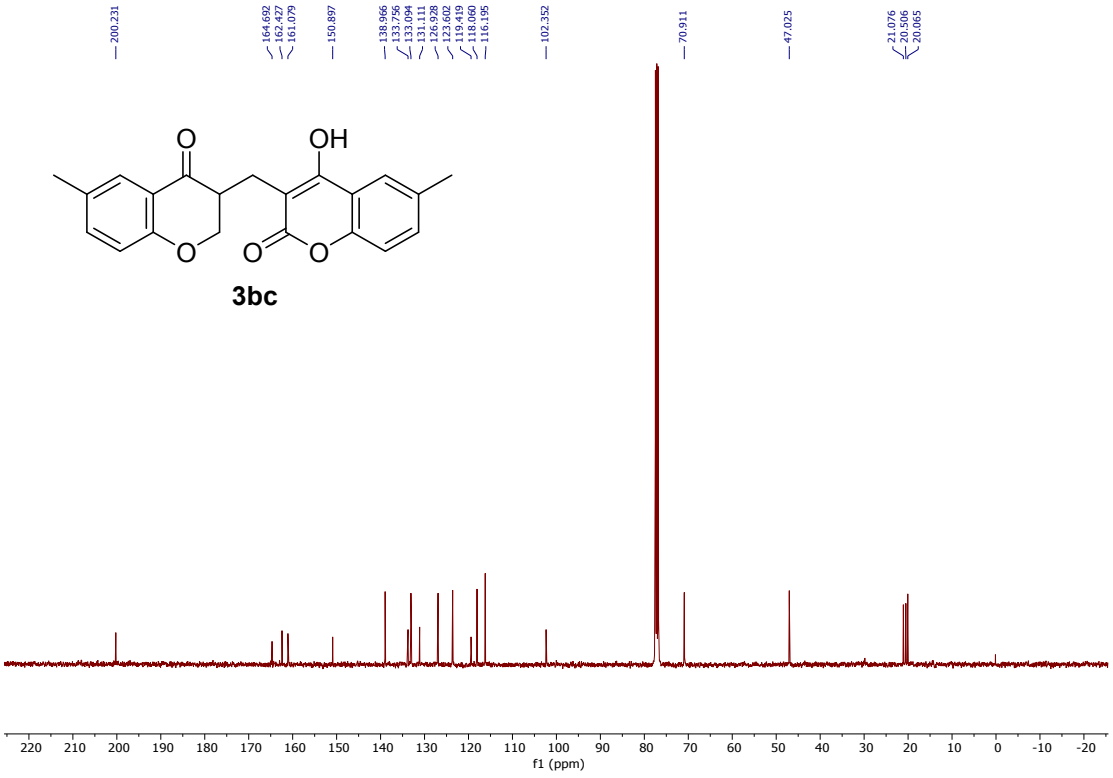

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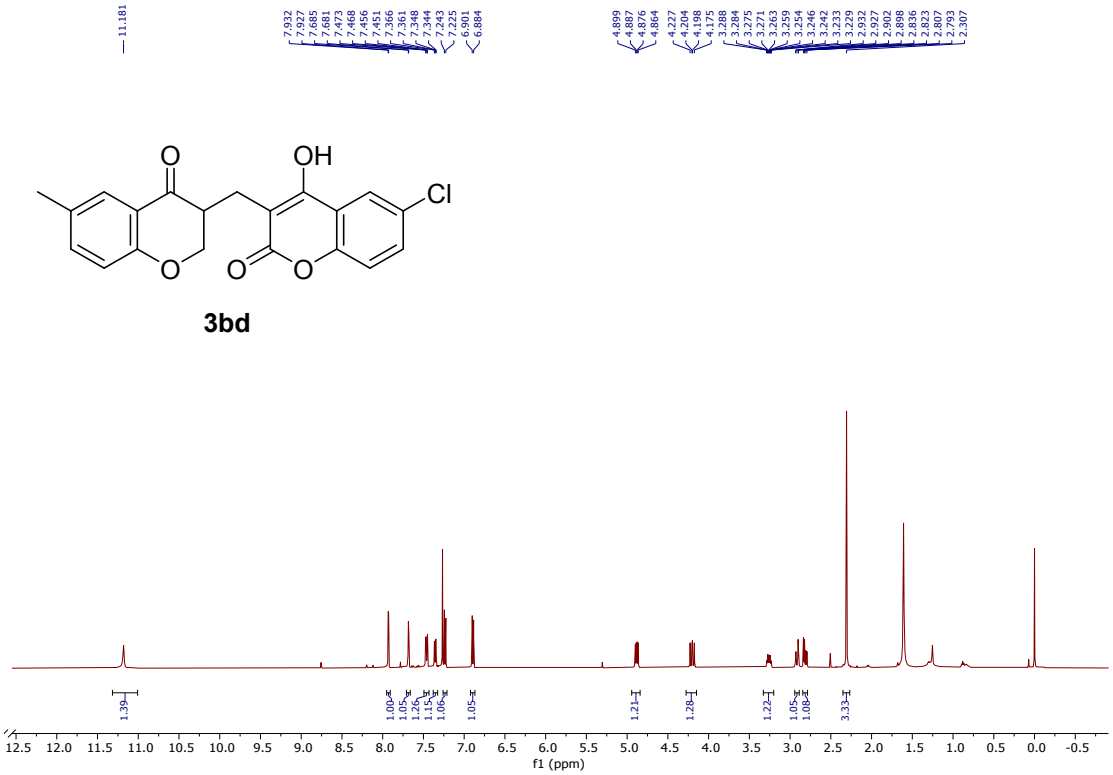

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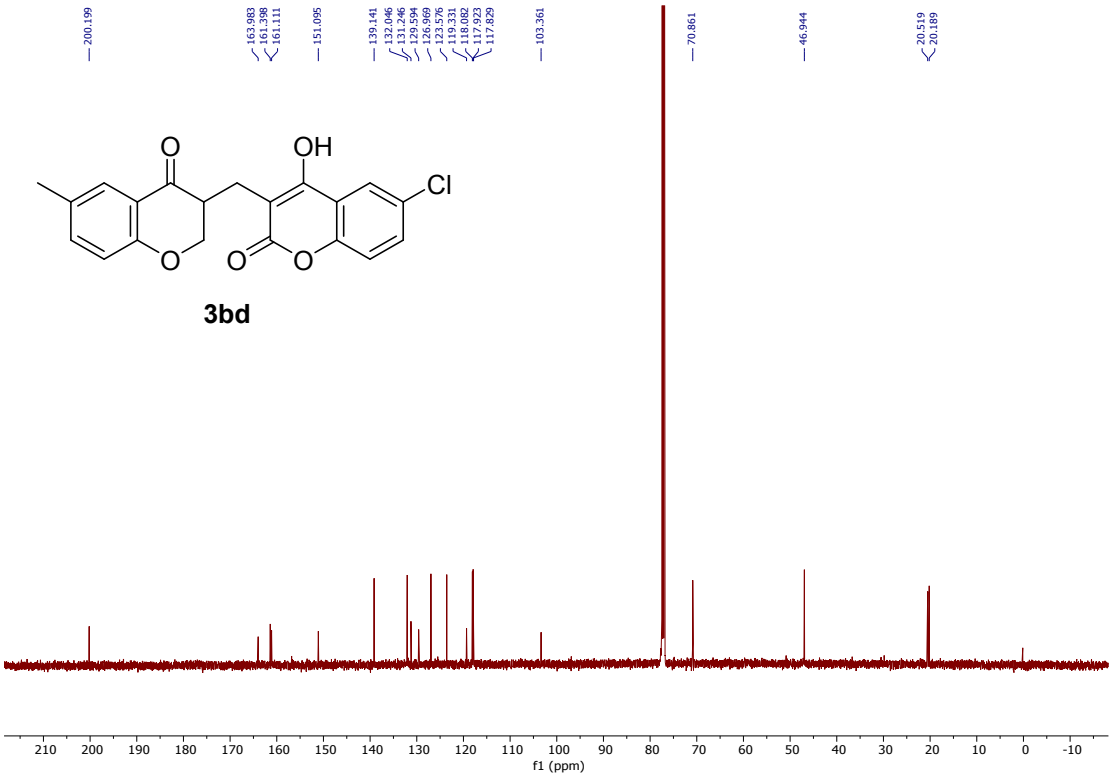

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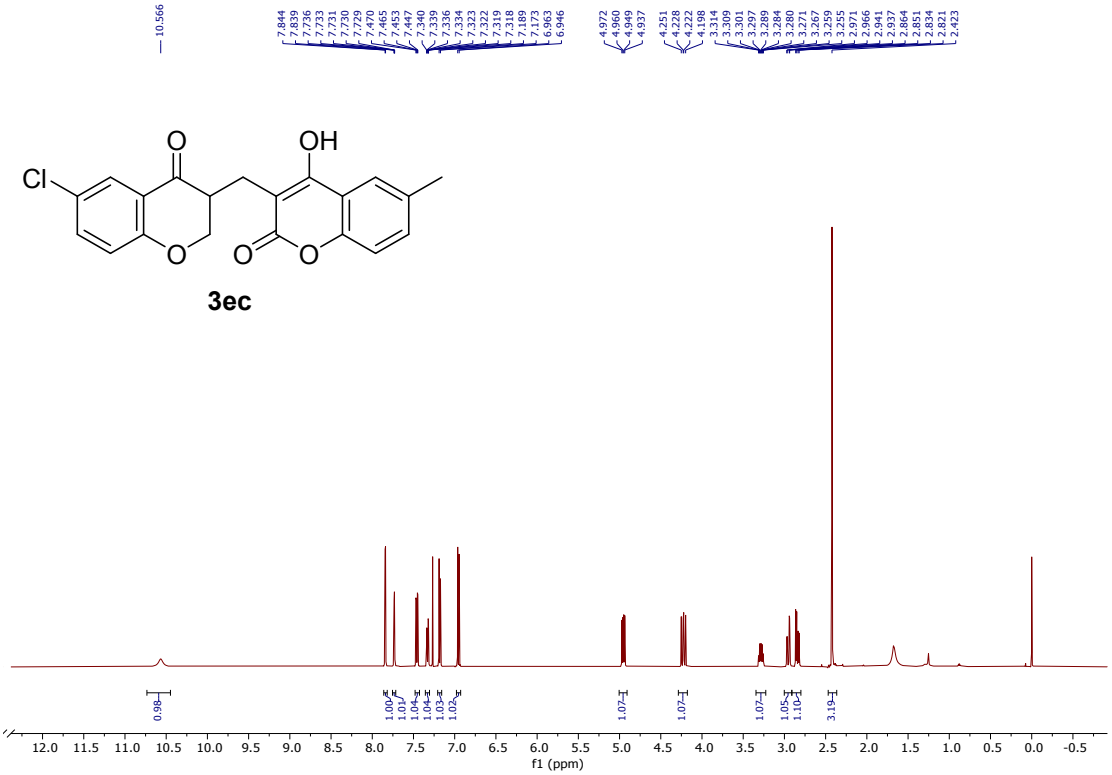

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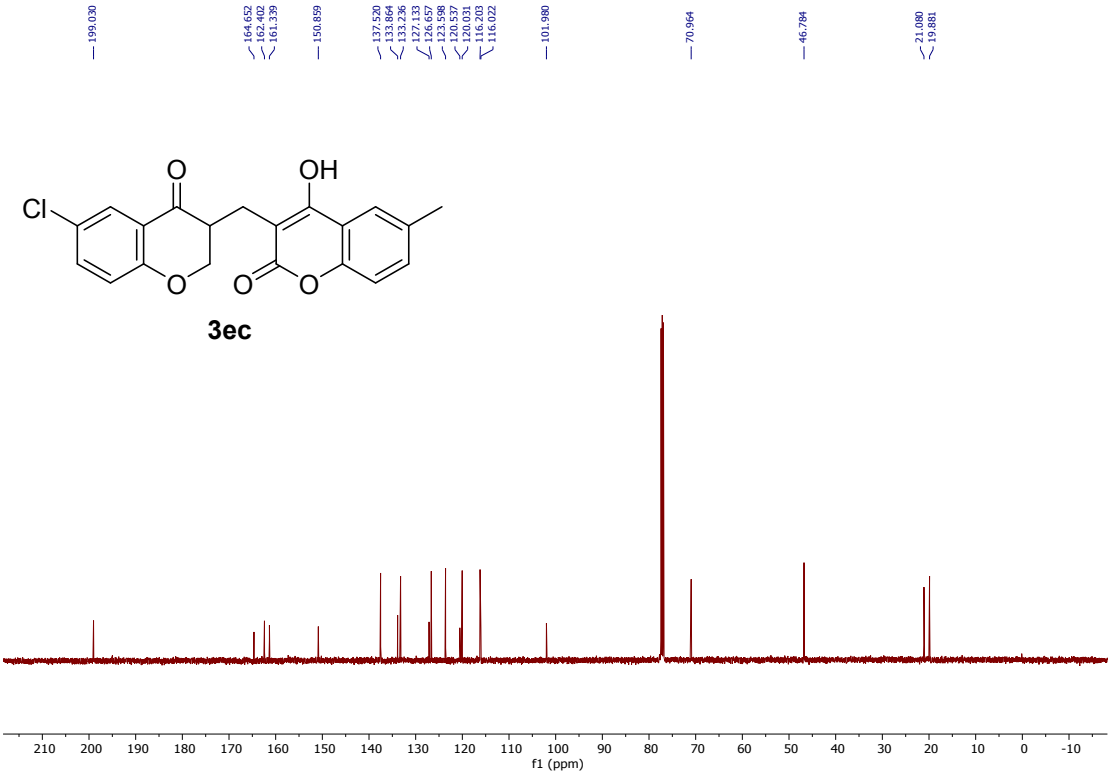

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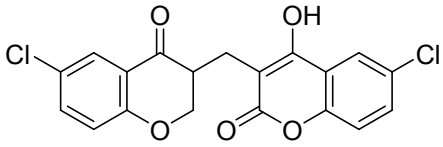

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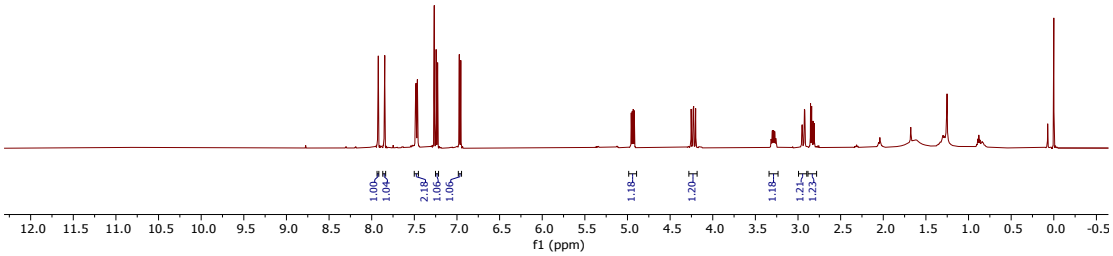

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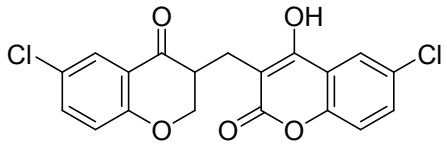

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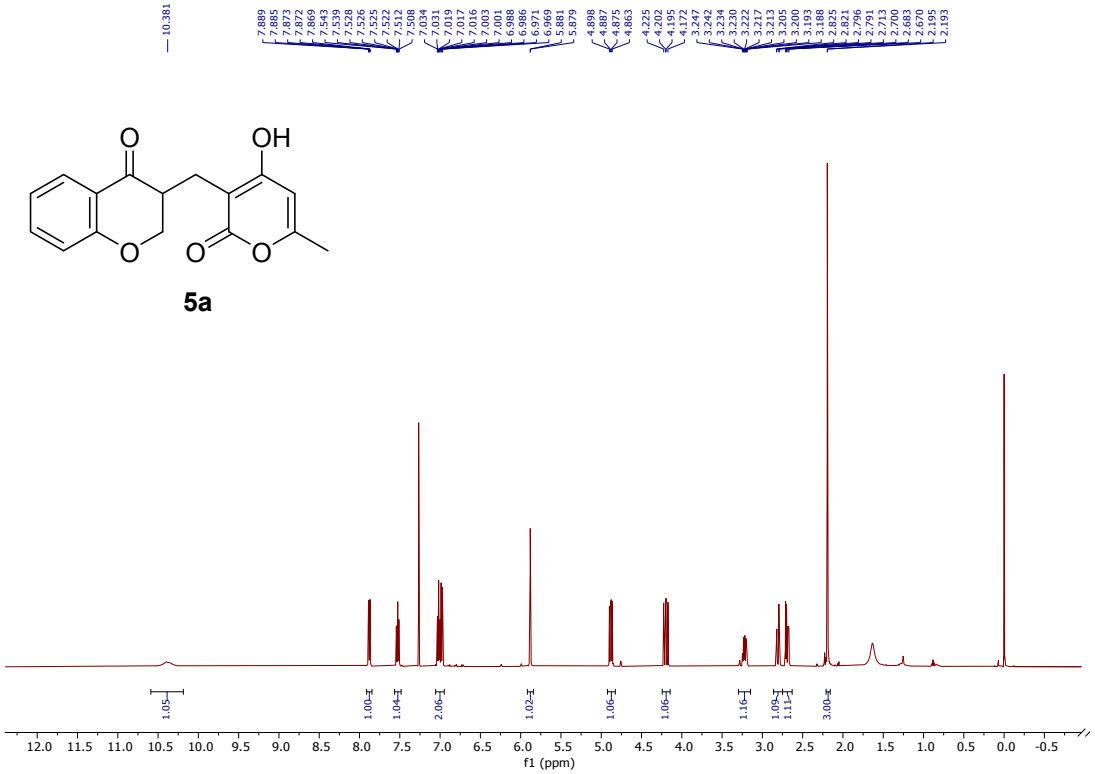

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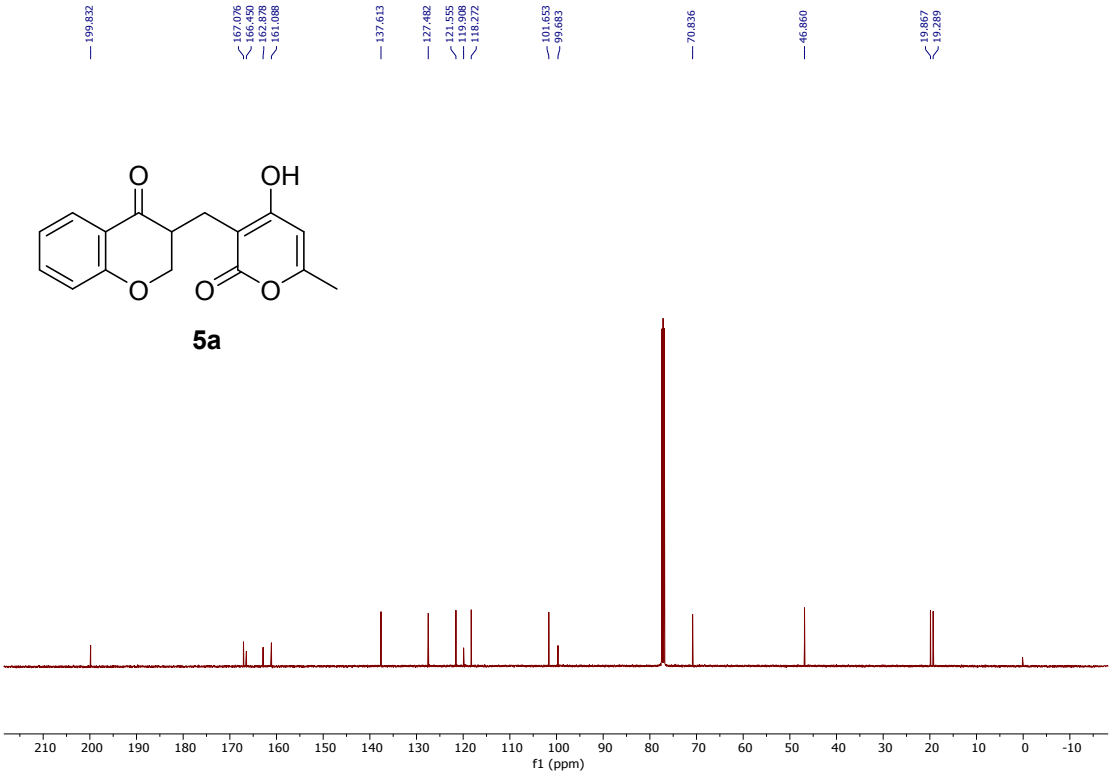

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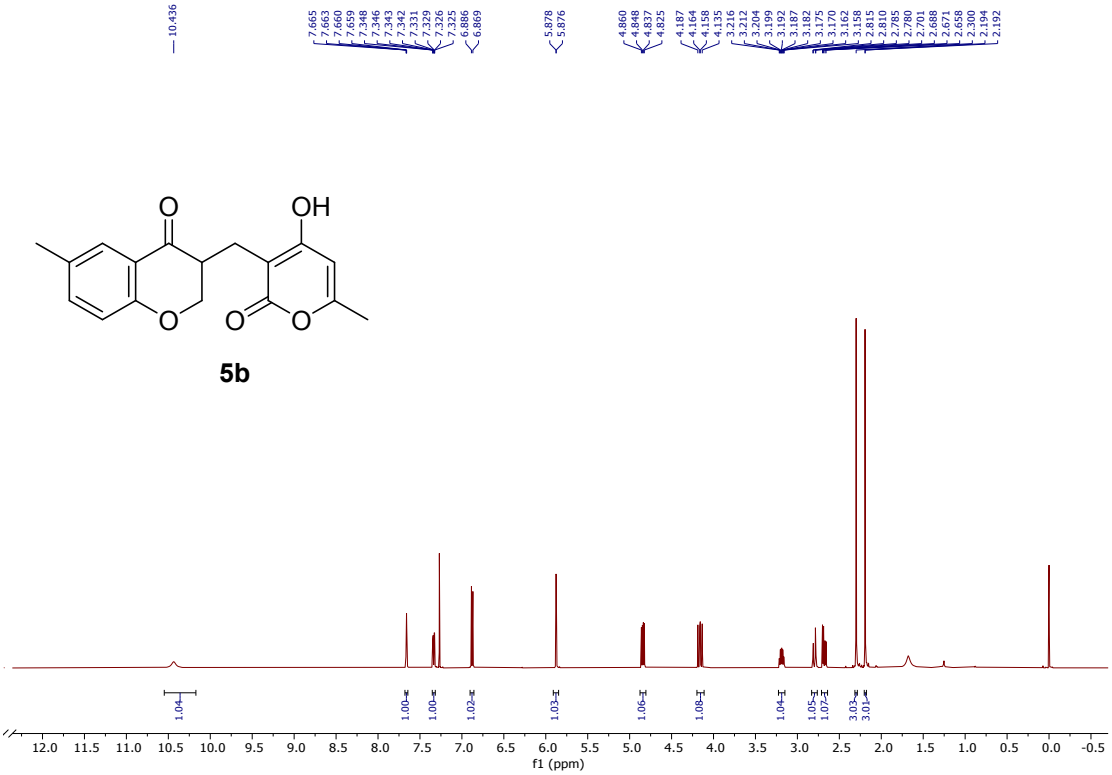

5b

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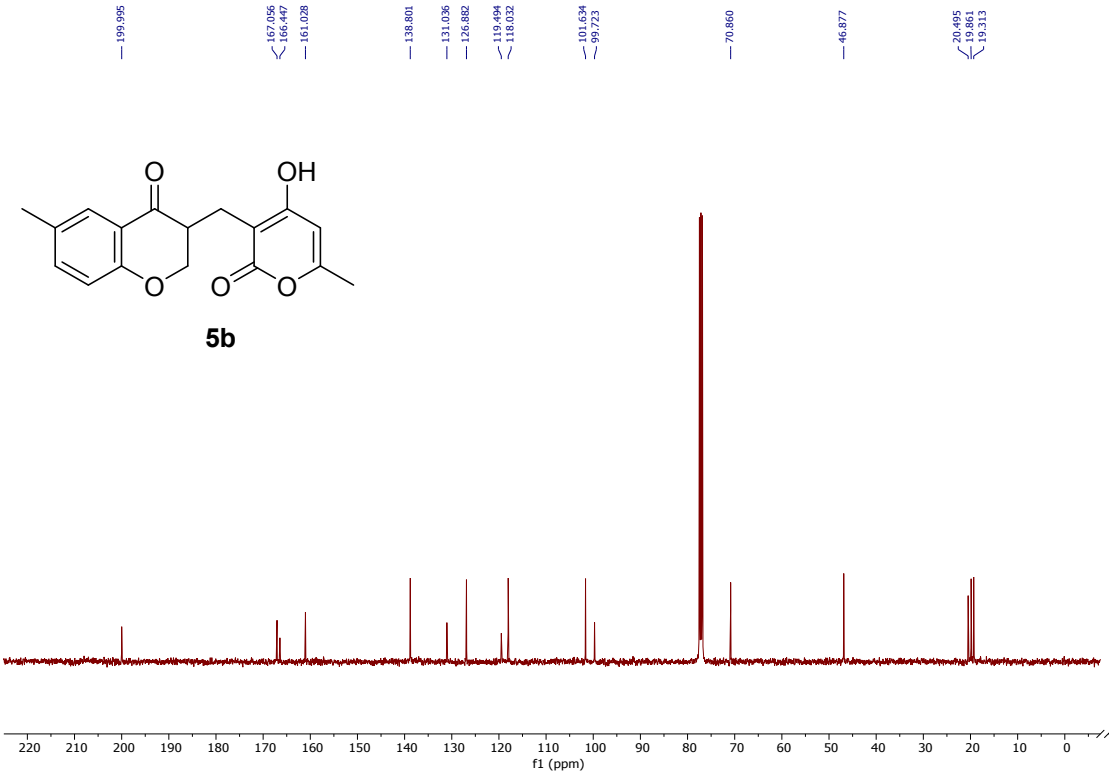

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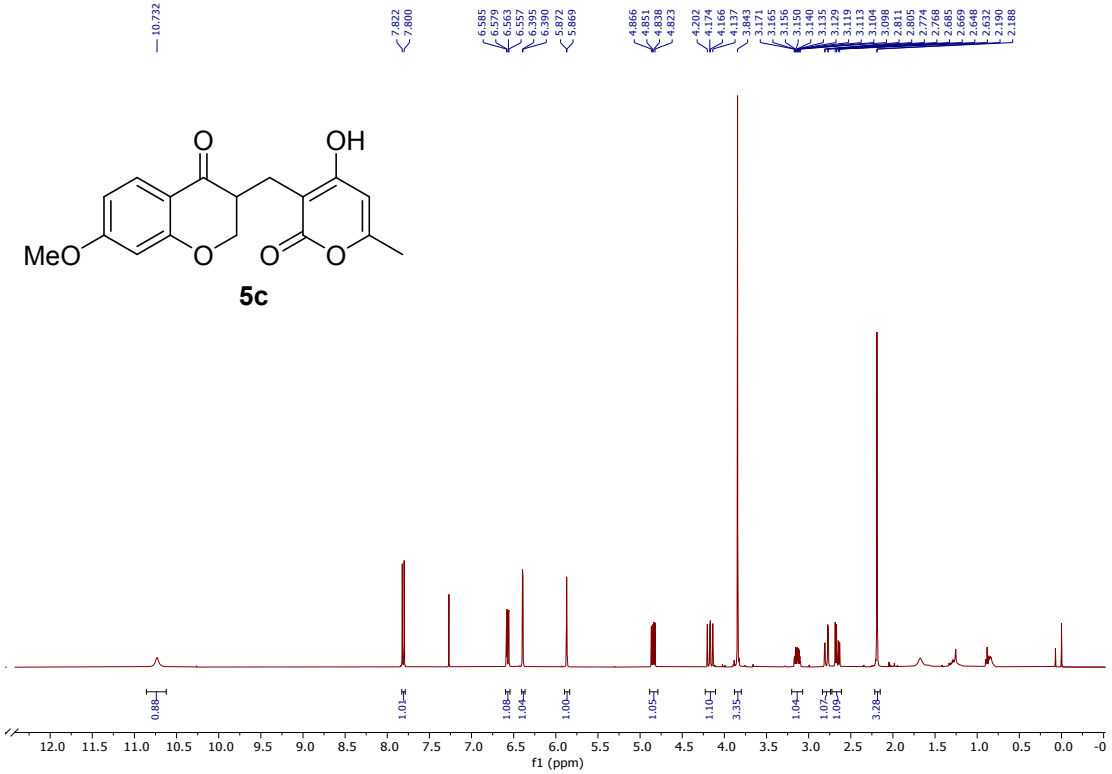

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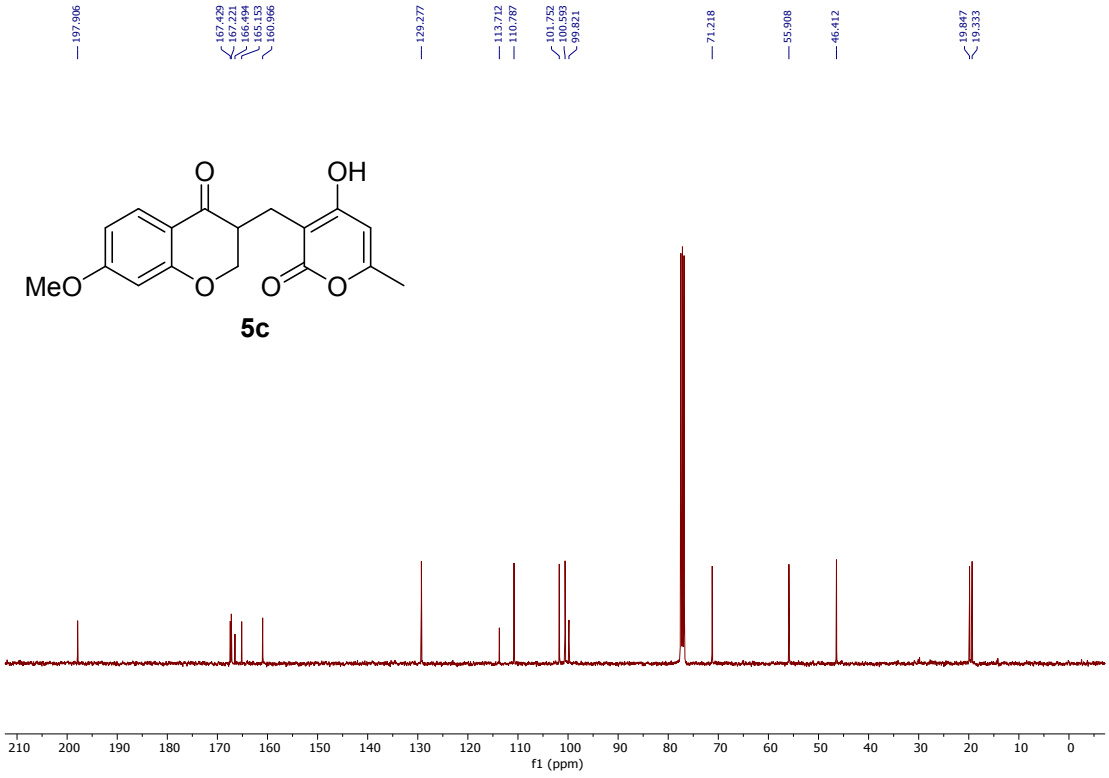

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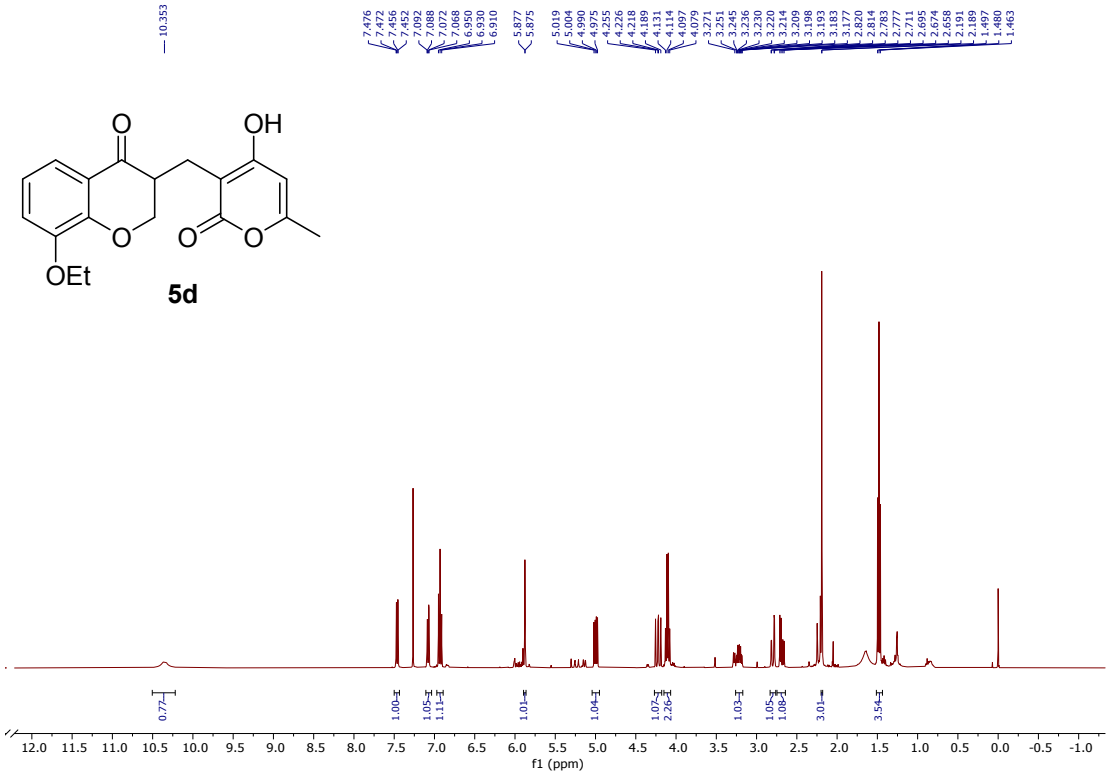

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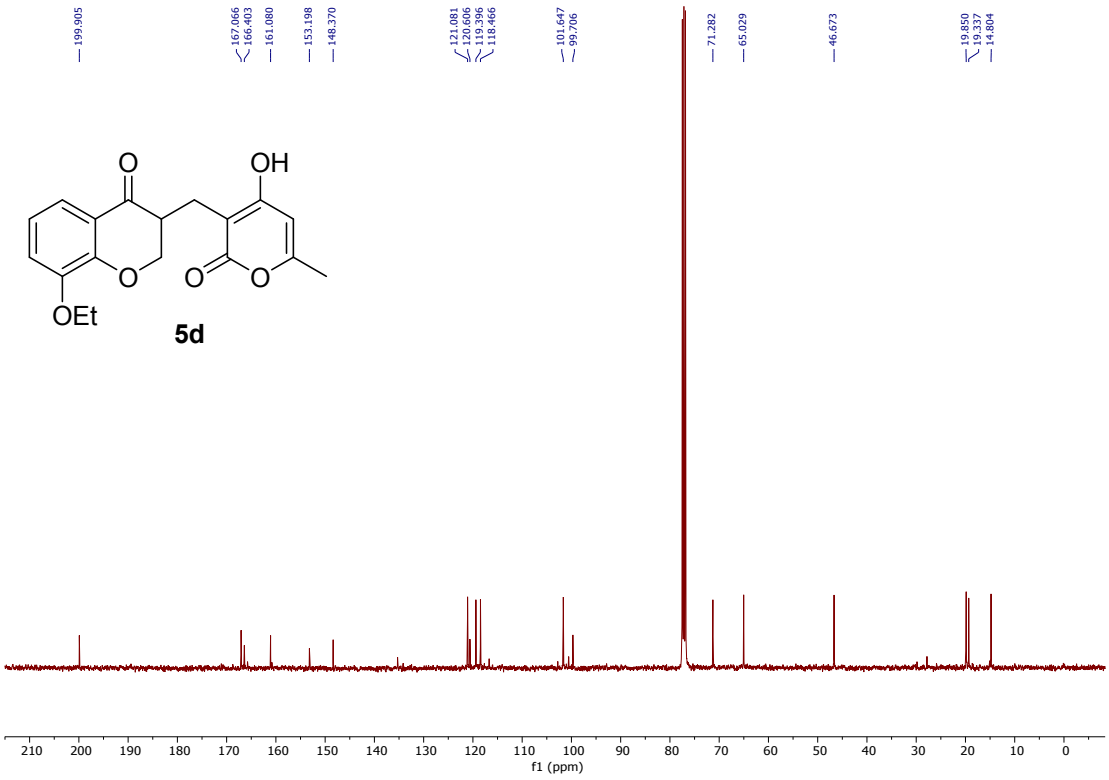

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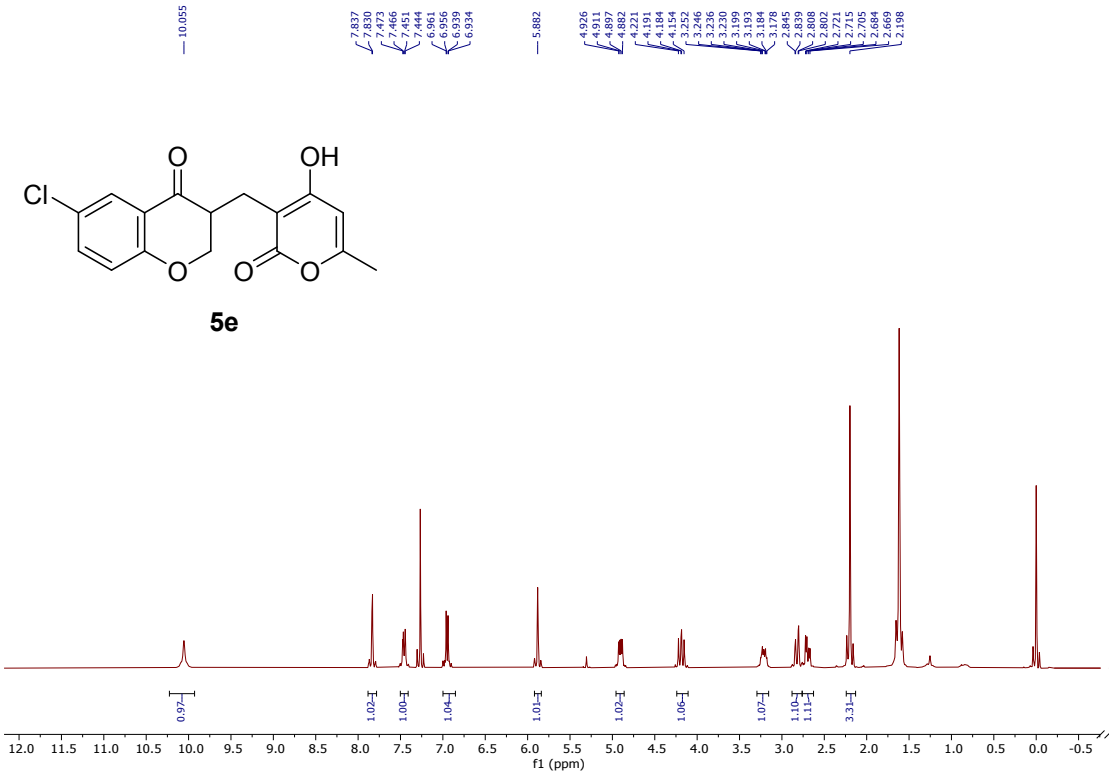

5e

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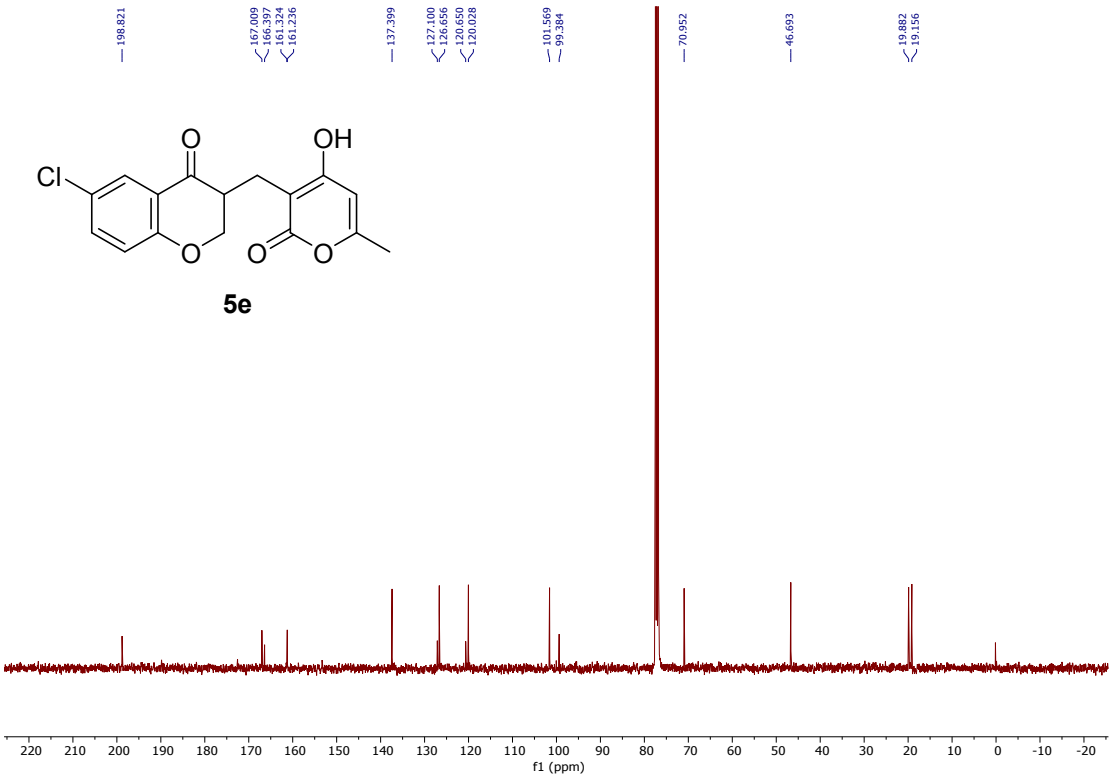

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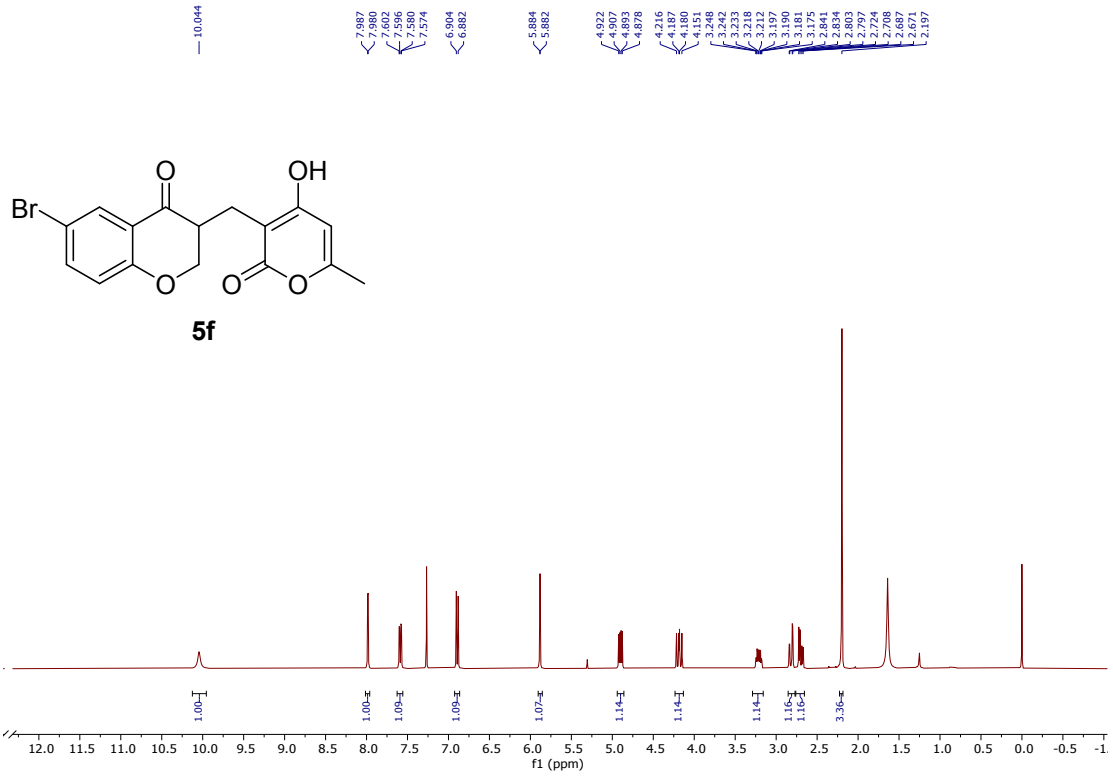

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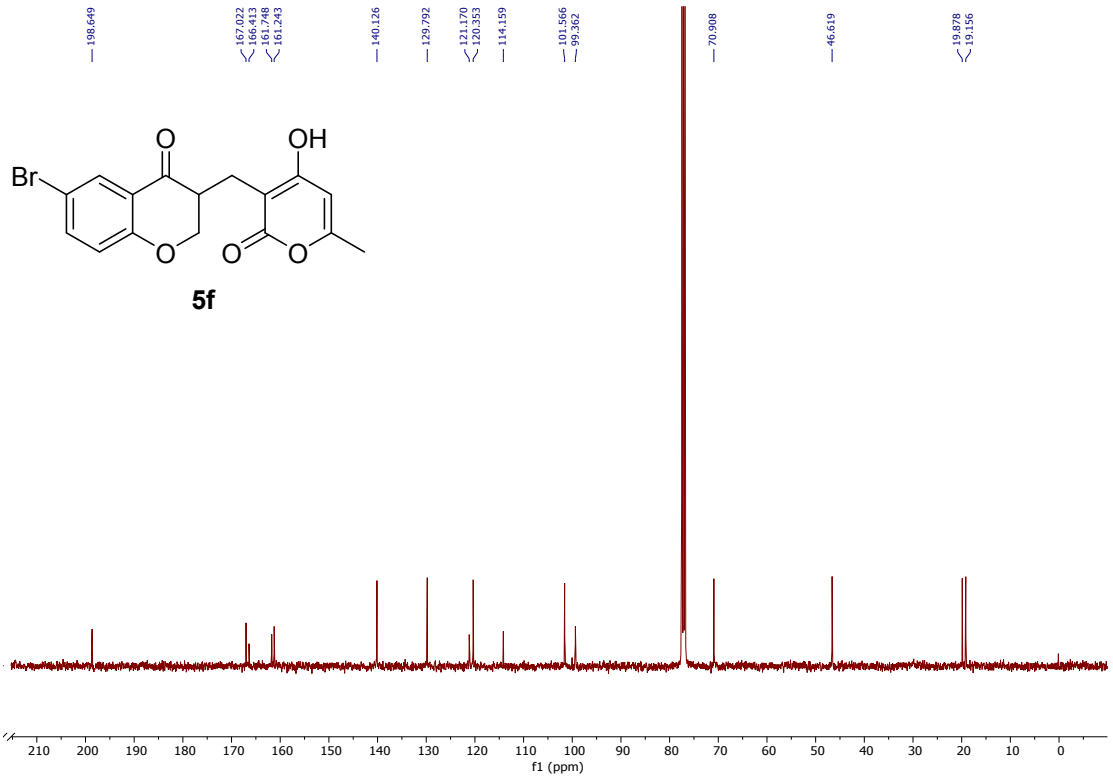

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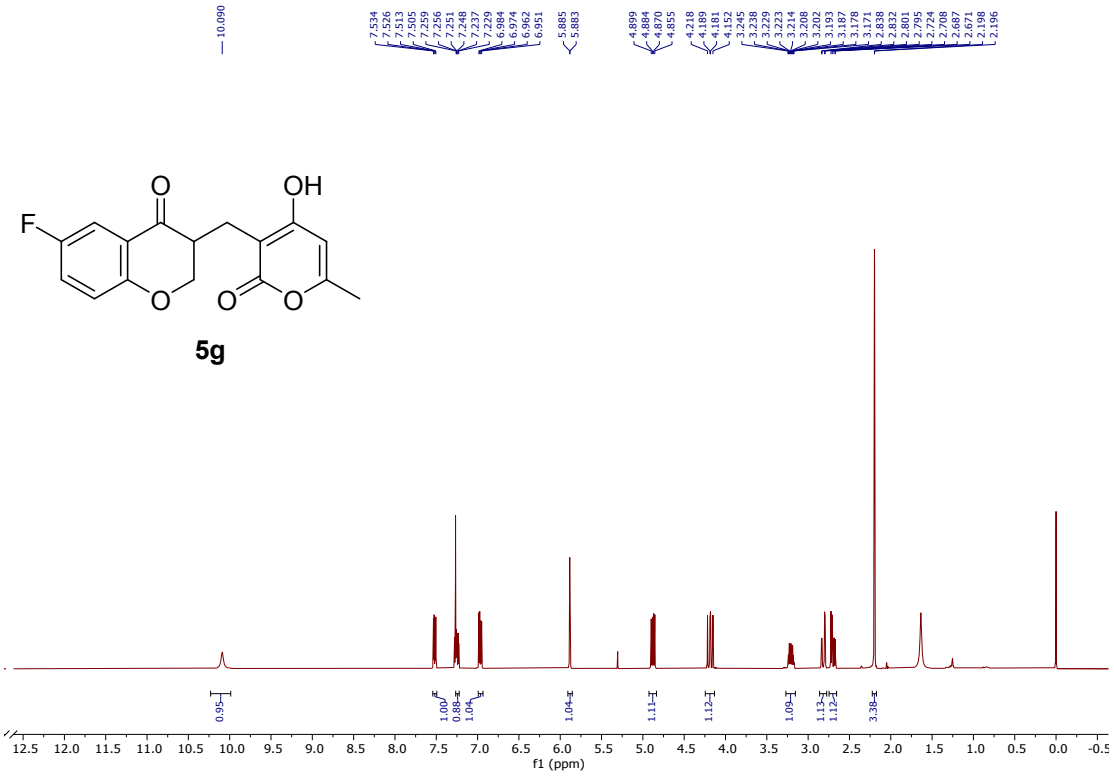

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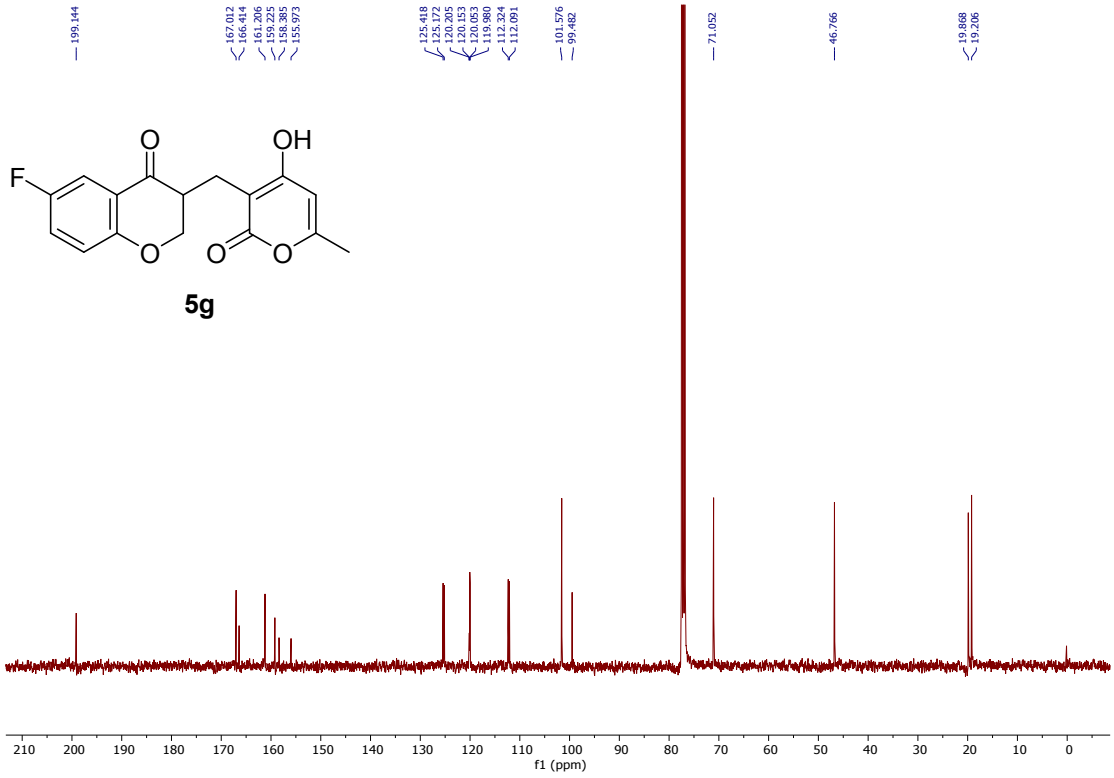
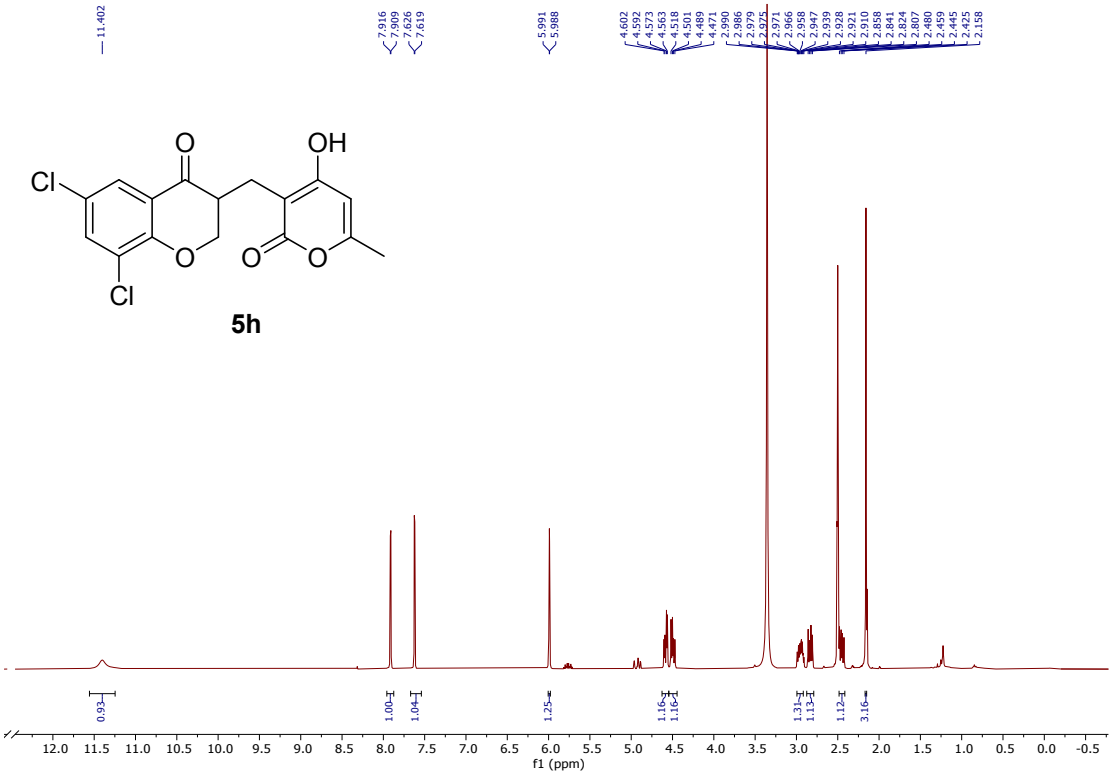


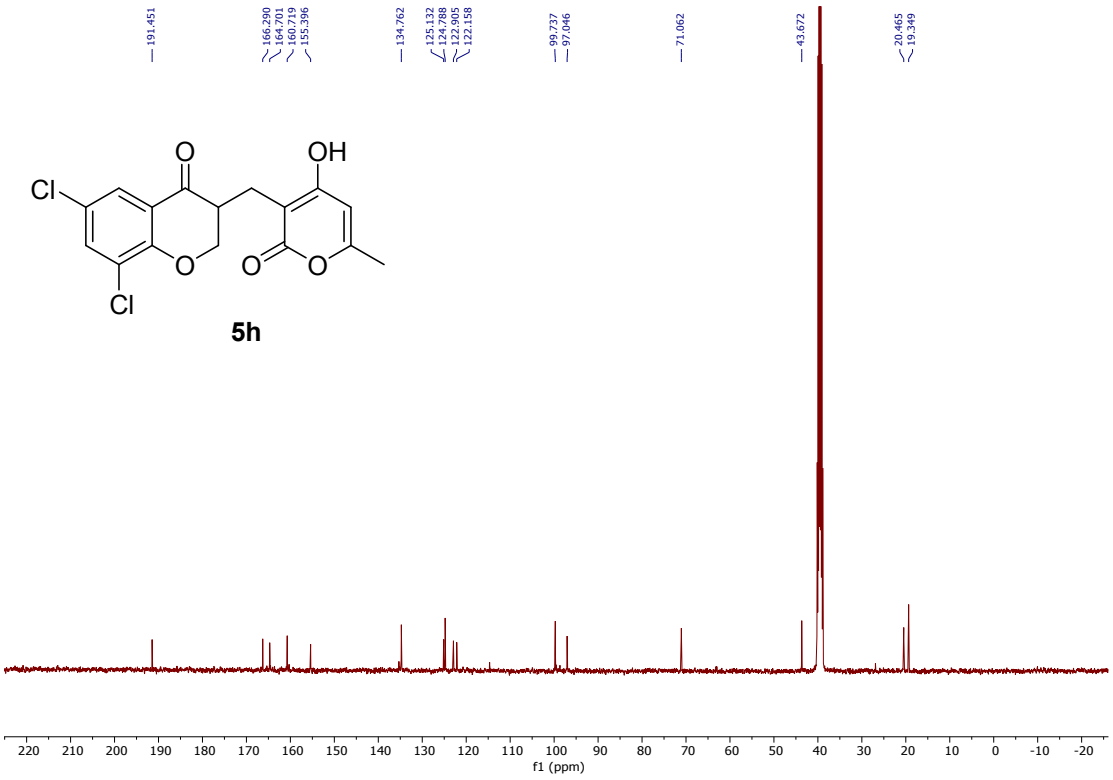
5g

^{1}H-NMR (400 MHz, DMSO-d_6)



5h

^{13}C-NMR (100 MHz, DMSO-d_6)



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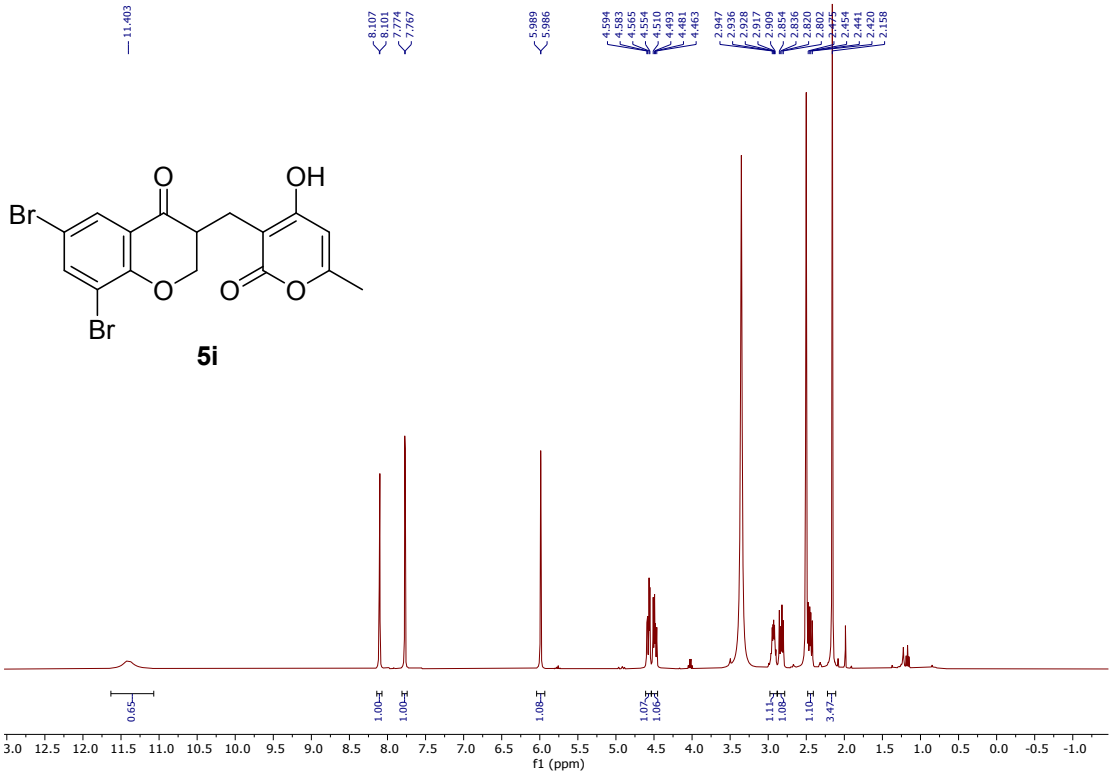
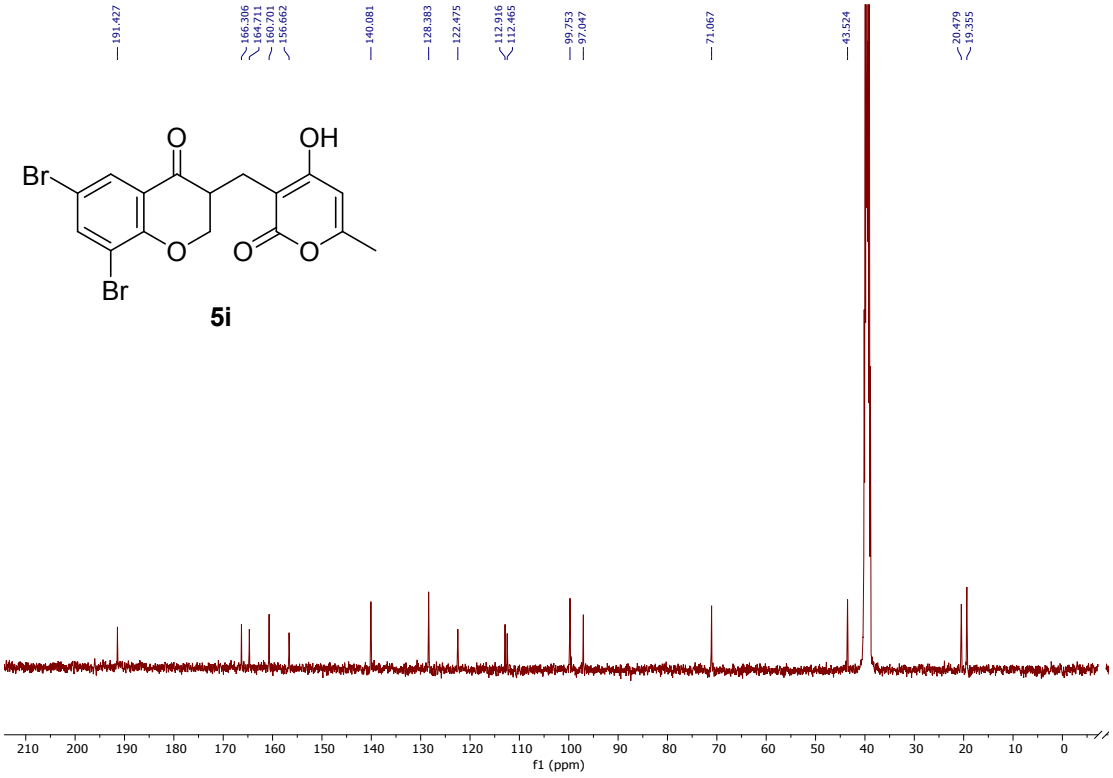
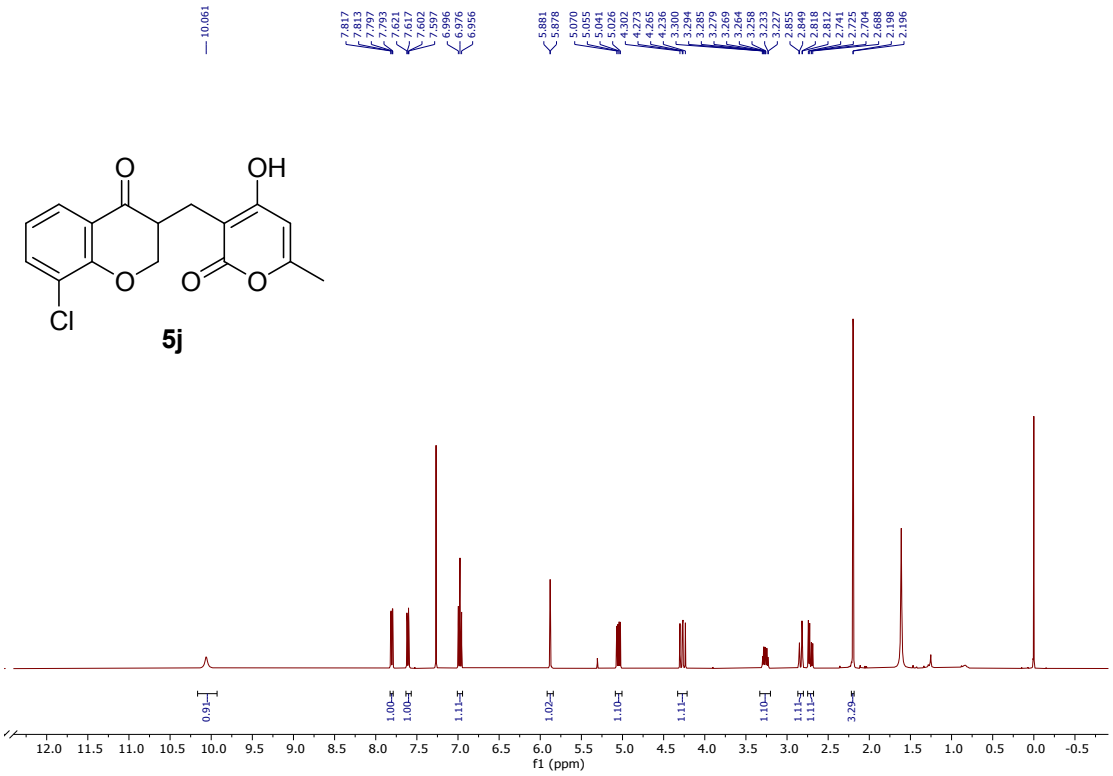
^{1}H-NMR (400 MHz, DMSO-d_6)



^{13}C-NMR (100 MHz, DMSO-d_6)



^{1}H-NMR (400 MHz, $CDCl_3$)



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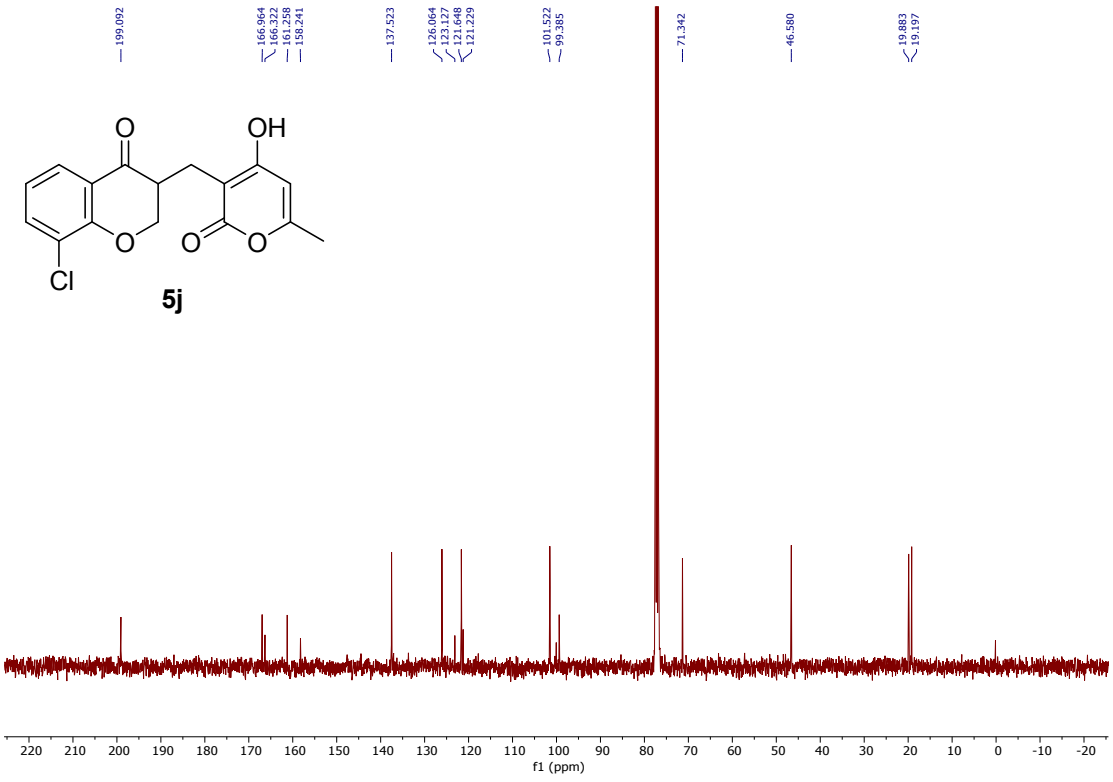
^{13}C-NMR (100 MHz, $CDCl_3$)



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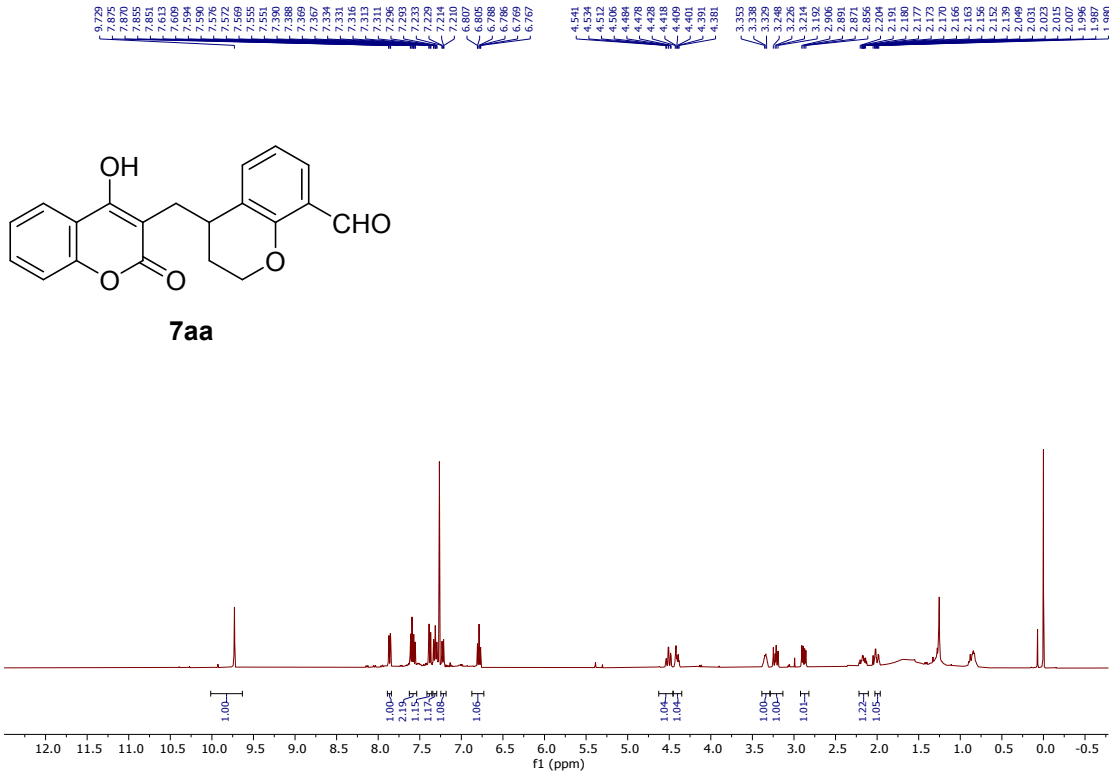
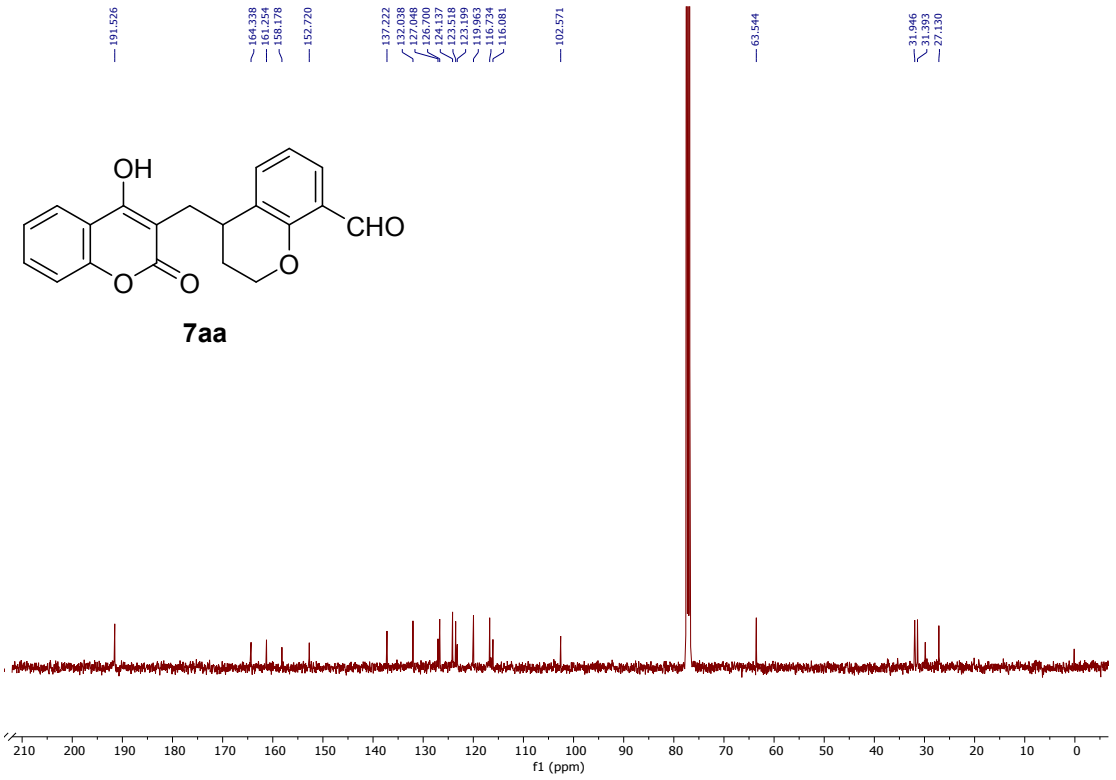
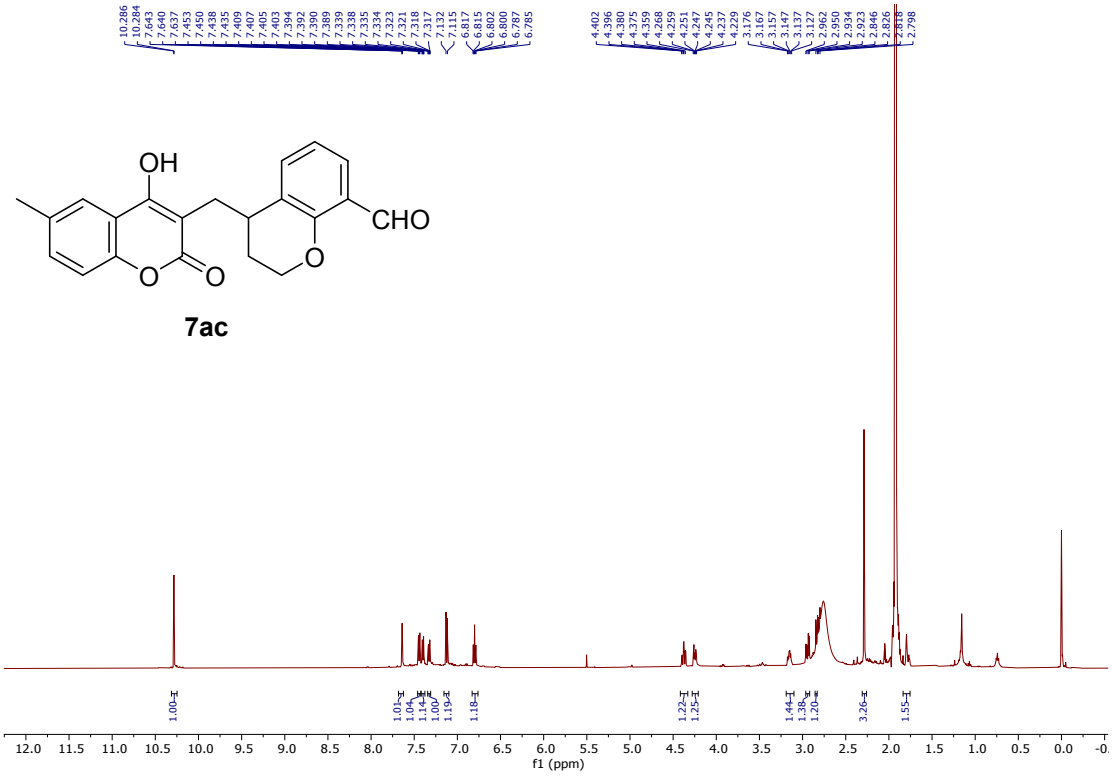
^{1}H-NMR (400 MHz, $CDCl_3$)



^{13}C-NMR (100 MHz, $CDCl_3$)



^{1}H-NMR (500 MHz, ACETONE-D_6)



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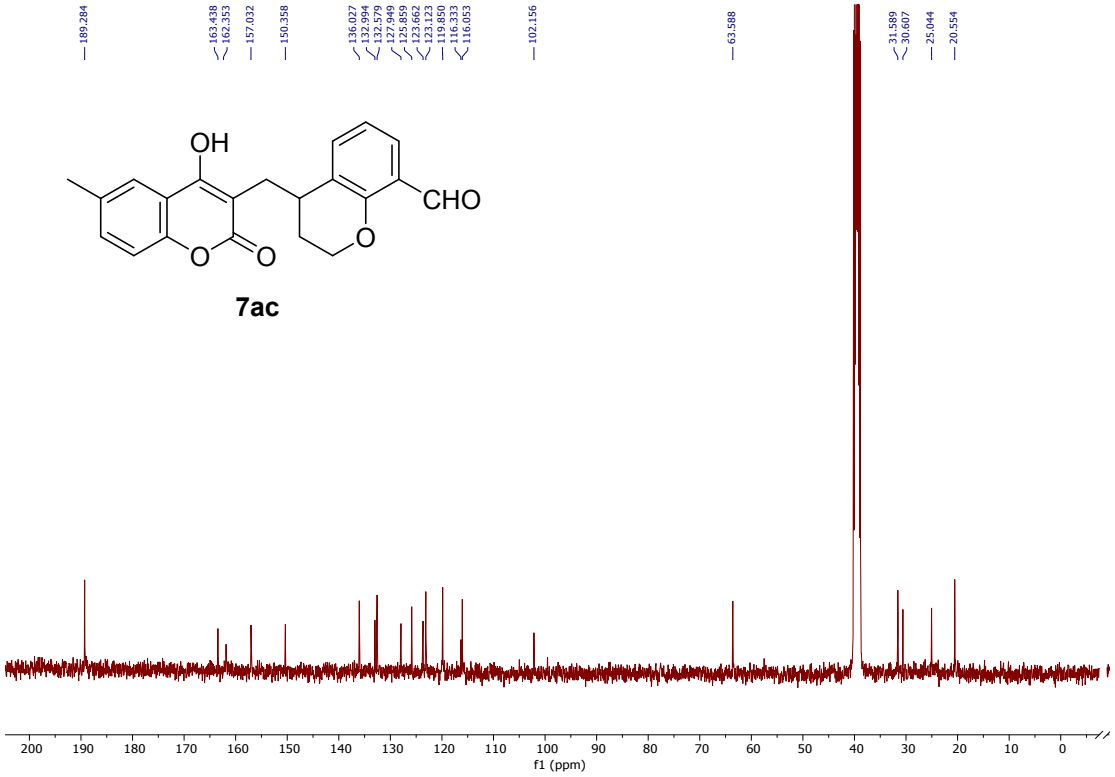

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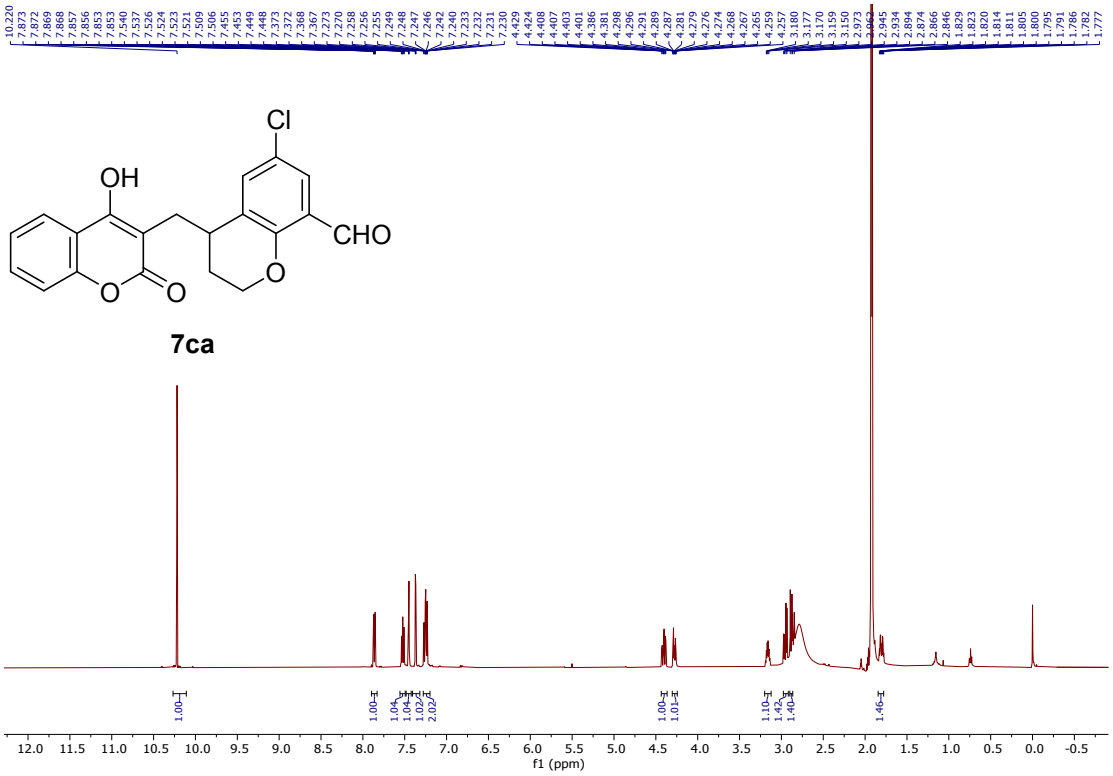
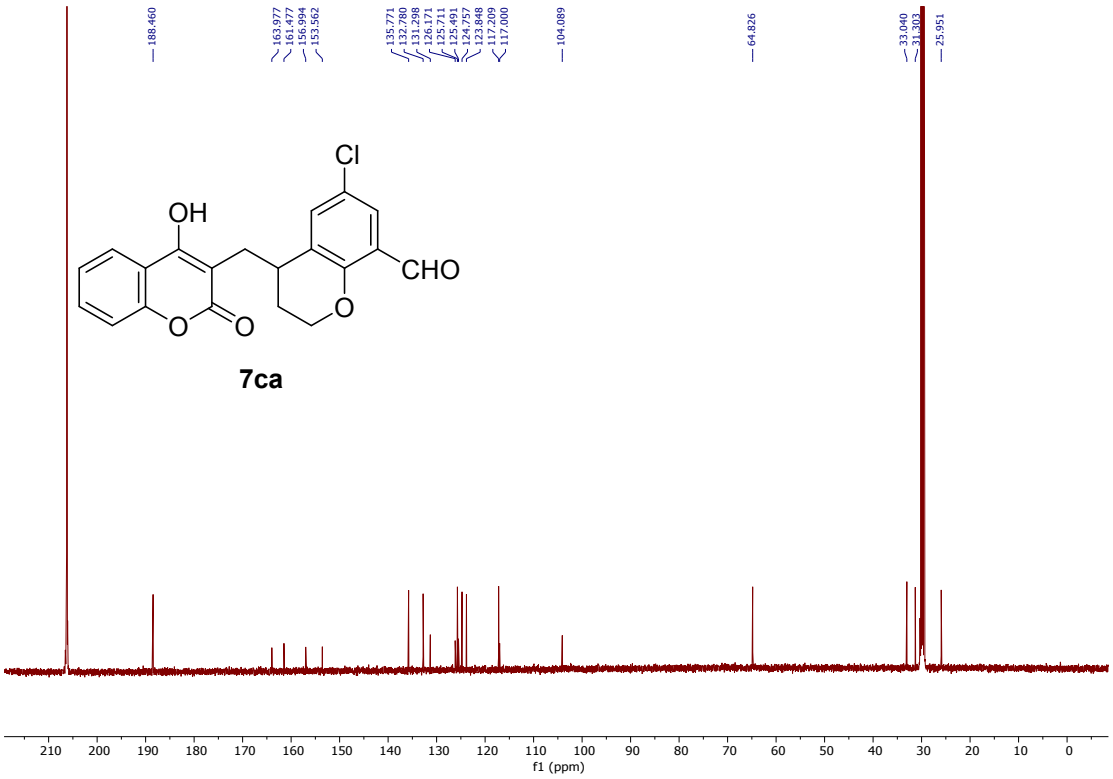
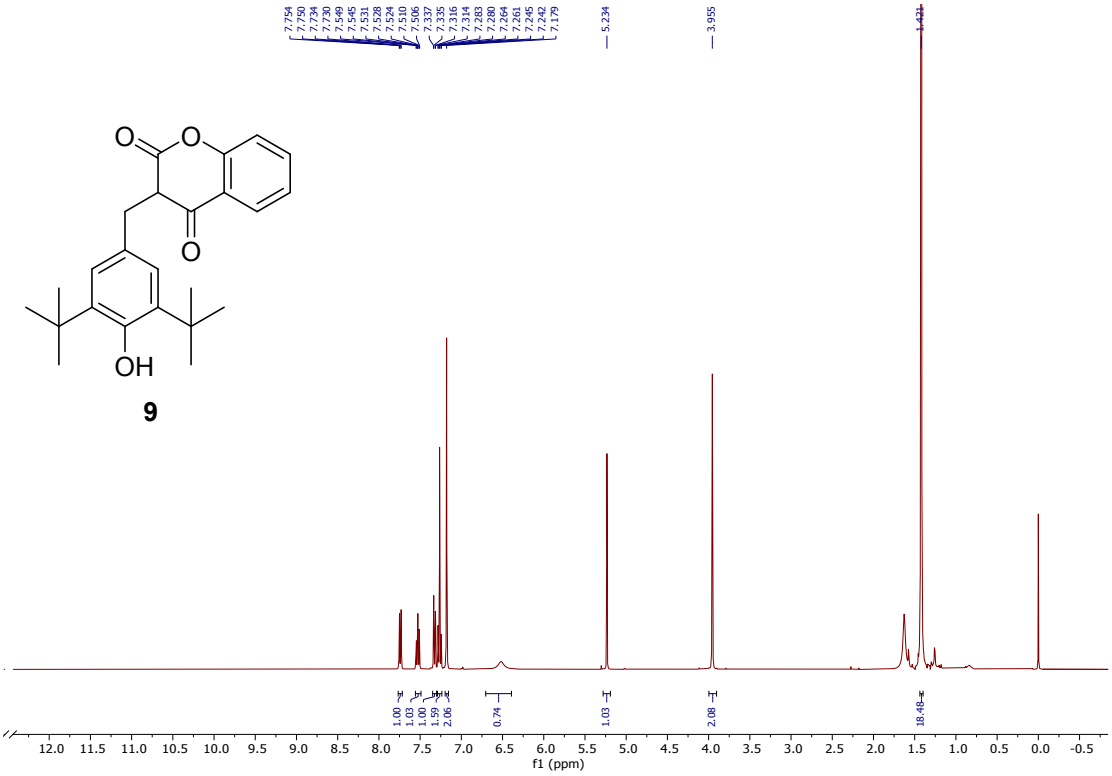


^{13}C-NMR (125 MHz, ACETONE-D_6)

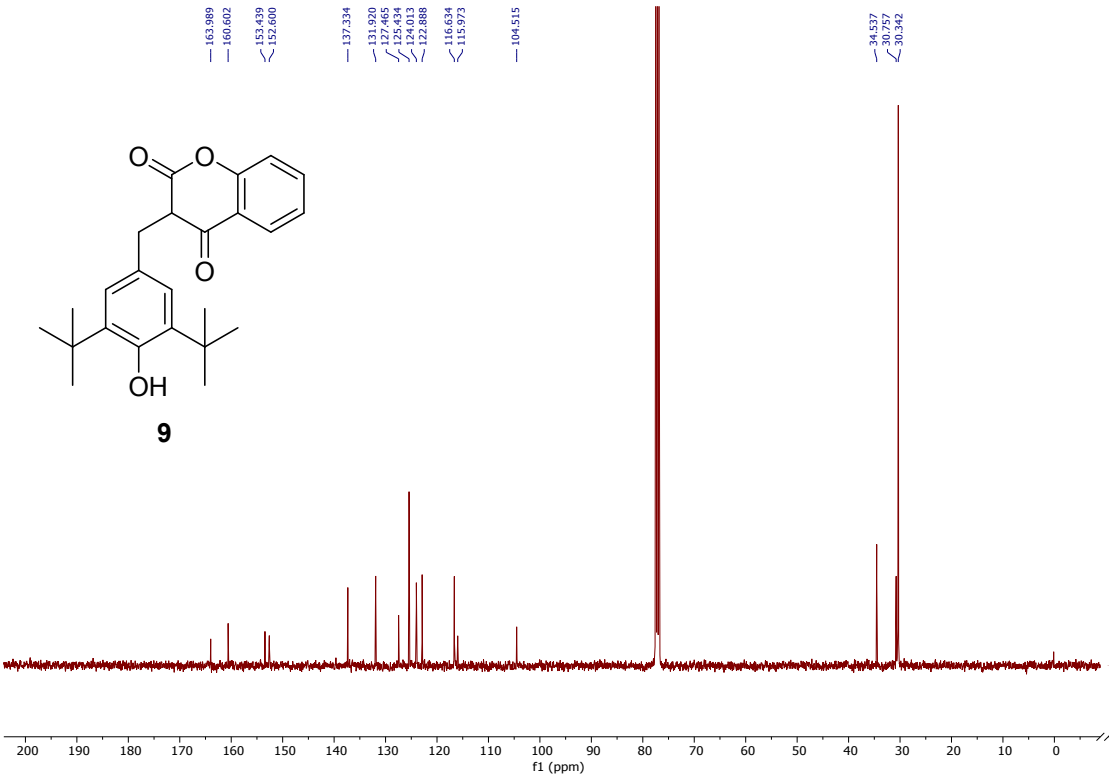


^{1}H-NMR (400 MHz, $CDCl_3$)



9

^{13}C-NMR (100 MHz, $CDCl_3$)



9

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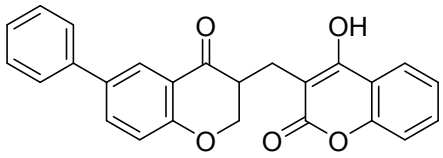

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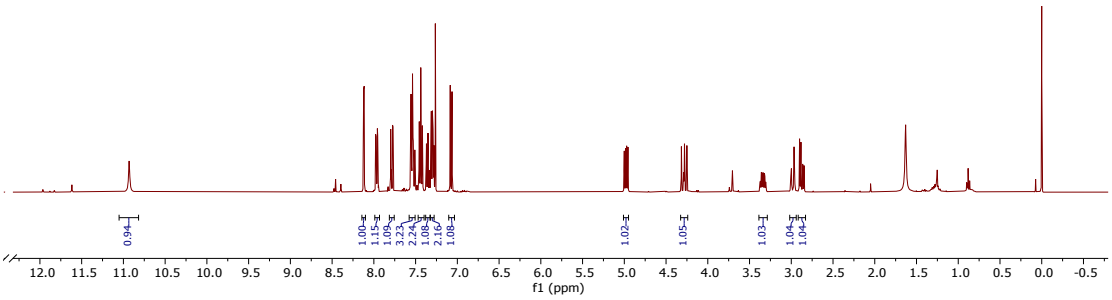
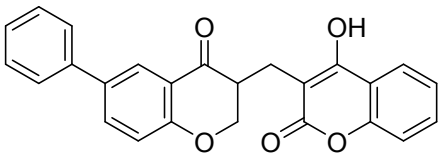


^{13}C-NMR (100 MHz, $CDCl_3$)



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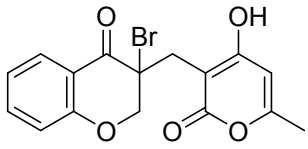

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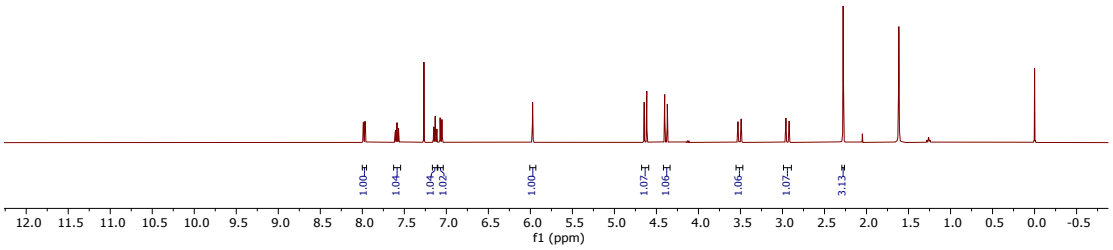
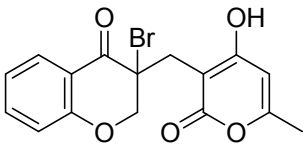


^{13}C-NMR (100 MHz, $CDCl_3$)



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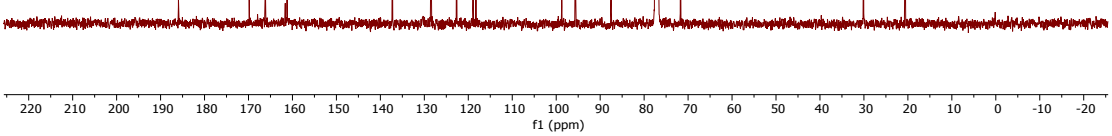
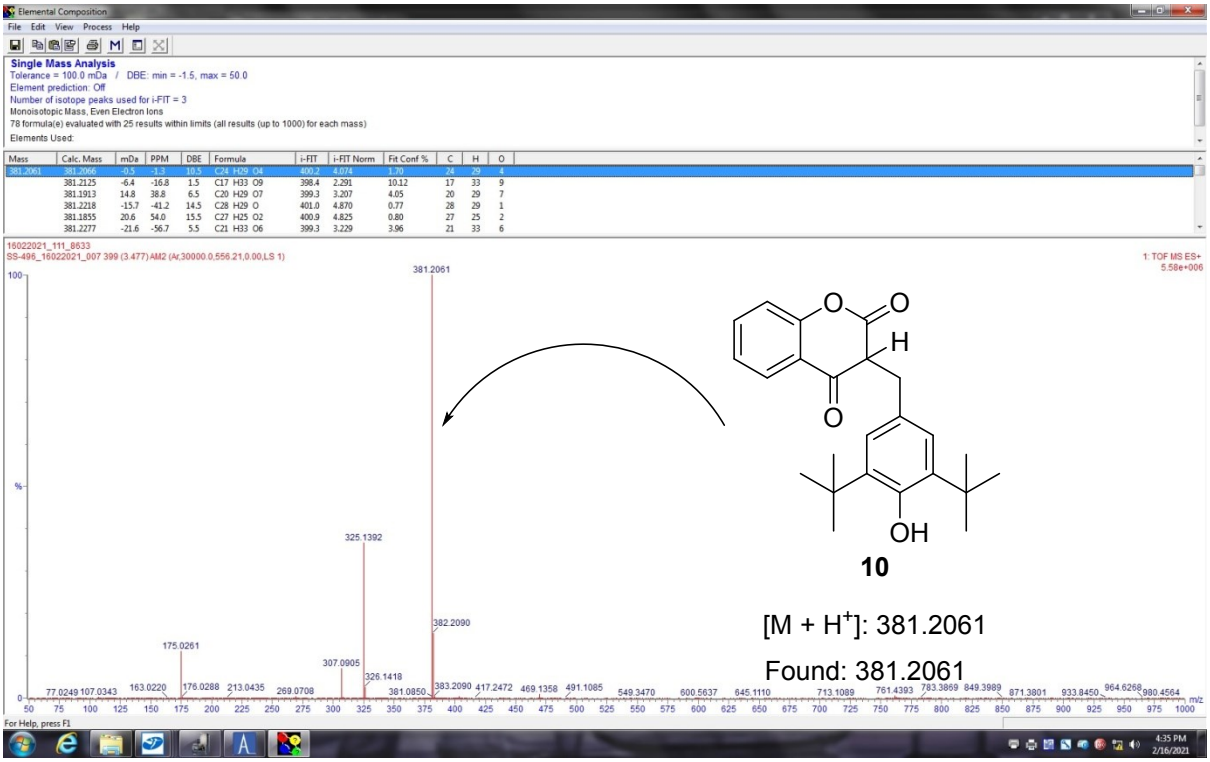
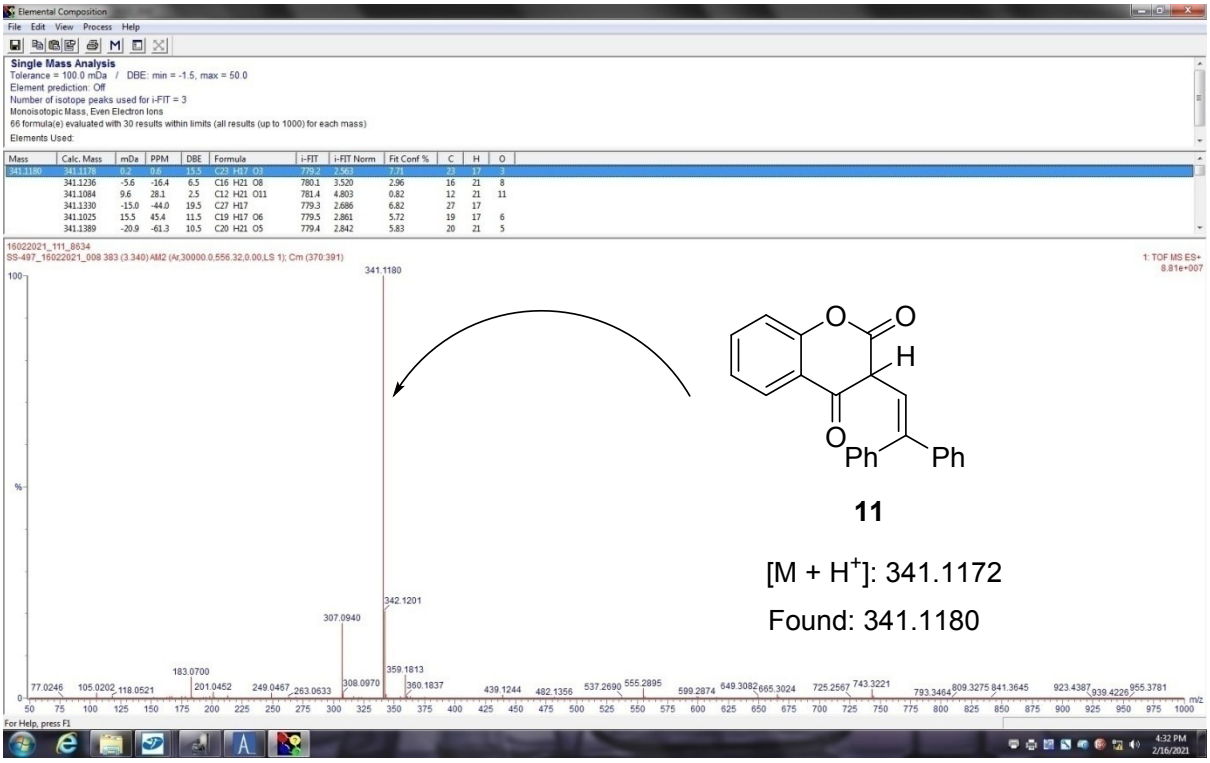



Elemental Composition
Single Mass Analysis
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
78 formula(e) evaluated with 25 results within limits (all results (up to 1000) for each mass)
Elements Used:
16022021_111_8633
SS-496_16022021_007 399 (3.477) AM2 (Ar,30000.0,556.21,0.00,LS 1)
1: TOF MS ES+
5.58e+006
381.2061
325.1392
382.2090
175.0261
307.0905
326.1418
O
O
H
O
OH
10
[M + H+]: 381.2061
Found: 381.2061


Elemental Composition
Single Mass Analysis
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
66 formula(e) evaluated with 30 results within limits (all results (up to 1000) for each mass)
Elements Used:
16022021_111_8634
SS-497_16022021_008 383 (3.340) AM2 (Ar,30000.0,556.32,0.00,LS 1); Cm (370:391)
1: TOF MS ES+
8.81e+007
341.1180
342.1201
307.0940
359.1813
183.0700
O
O
H
O
Ph
Ph
11
[M + H+]: 341.1172
Found: 341.1180

Crystallographic analysis:

Crystal structure is solved and refined in monoclinic space group *C*2/*c*, with one symmetry independent molecule in the lattice ORTEP with 50% probability ellipsoid is displayed in Fig 1. Details of Single crystal X-ray data collection method, crystal data parameter Table 1, CIF and CheckCIF report are available in ESI.

Table 1 Crystallographic parameters of the structure of compound **3ba**

Crystal data	compound **3ba**
Formula unit	$C_{20}H_{16}O_5$
Formula weight ($gmol^{-1}$)	336.33
Crystal system	Monoclinic
T [K]	100
a [Å]	28.45(6)
b [Å]	5.000(10)
c [Å]	24.77(6)
α [°]	90
β [°]	108.16(5)
γ [°]	90
Volume [$Å^3$]	3349(13)
Space group	*C*2/*c*
Z	8
D_{cal}[g/cm^3]	1.334
R_1, *w*R2	0.0554, 0.0928
Instrument	Bruker CCD Apex II
CCDC No	2074327

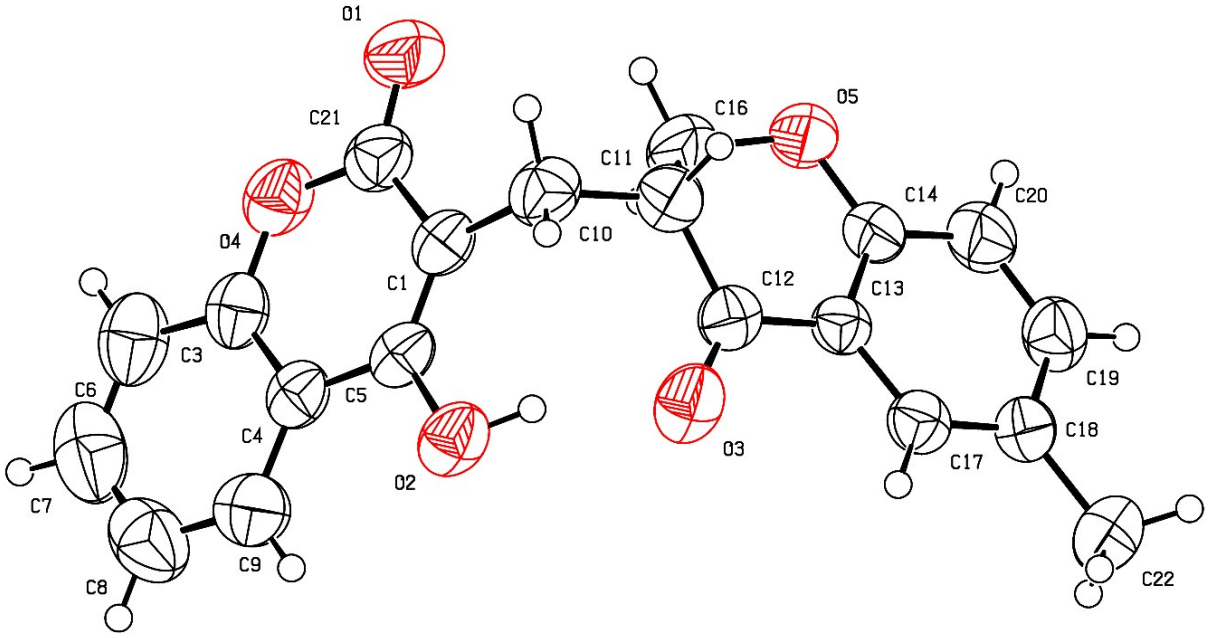


Figure 1: ORTEP of compound **3ba** with 50% probability ellipsoid

Single crystal X-ray diffraction: Single crystal X-ray diffractions were collected on a Bruker SMART APEX-II CCD diffractometer using Mo Kα (λ =0.71073 Å) radiation.[1] Bruker SAINT software has been employed for reducing the data and SADABS for correcting the intensities of absorption.[2]Structure was solved and refined using SHELXL with anisotropic displacement parameters for non-H atoms. In the crystal structure H-atoms are located experimentally, whereas C–H atoms were fixed geometrically using the HFIX command in SHELX-TL.[3] No any missed symmetry observed in the final check of CIF file using PLATON.[4,5] Information of crystallographic parameters for all structures is furnished in Table 1.

Reference

- SAINT Plus (v 6.14) Bruker AXS Inc., Madison, WI, 2008.
- Bruker AXS Inc., Madison, WI, 2008.
- G. M. Sheldrick, SHELXS and SHELXL97 Programs for structure refinement and solution, Göttingen, Germany, 1997.
- L. Spek, PLATON, A Multipurpose Crystallographic Tool Utrecht University, Utrecht, Netherland, 2002.
- L. Spek, J. Appl. Cryst., 2003, 36, 7–13.