

Electronic Supplementary Information

Synthesis of 4-styrylcoumarins *via* FeCl₃-promoted cascade reactions of propargylamines with β -keto esters

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X-Ray Crystallography Structures of Compounds **3ad**.

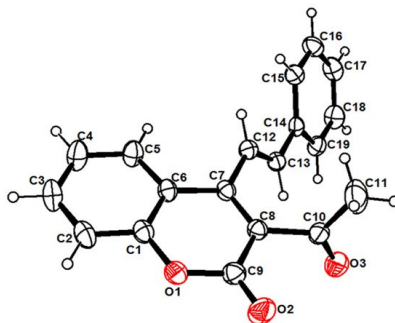
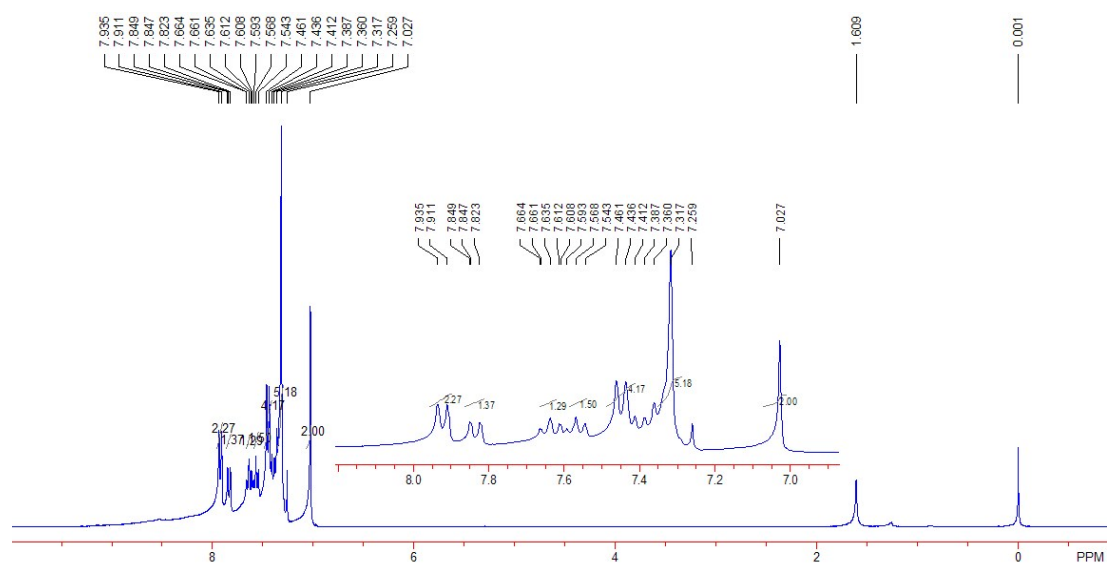
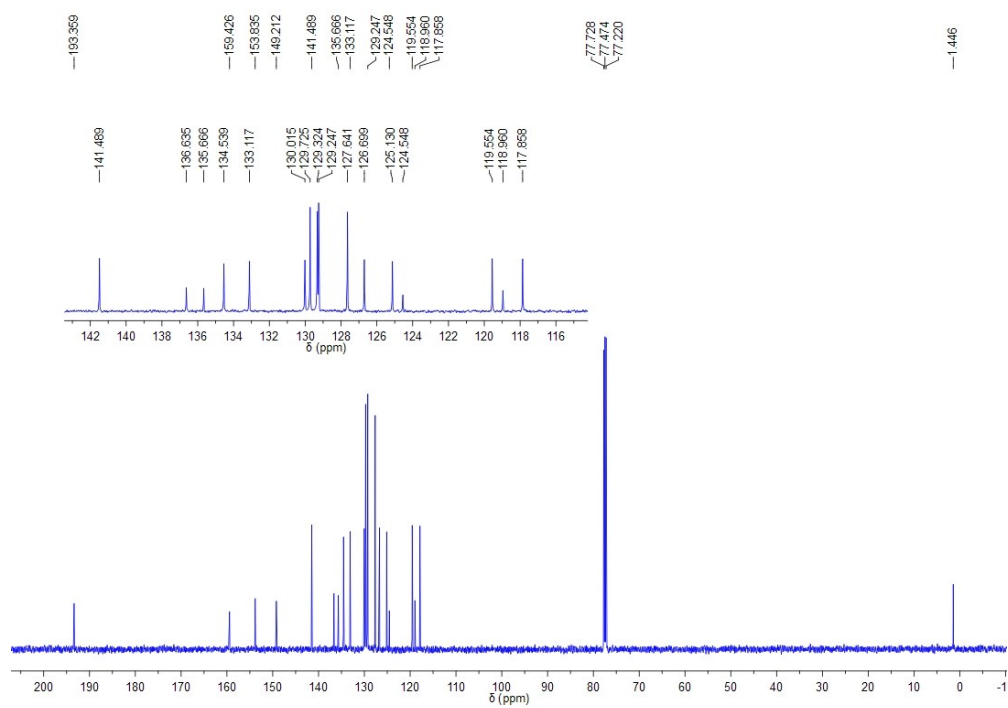


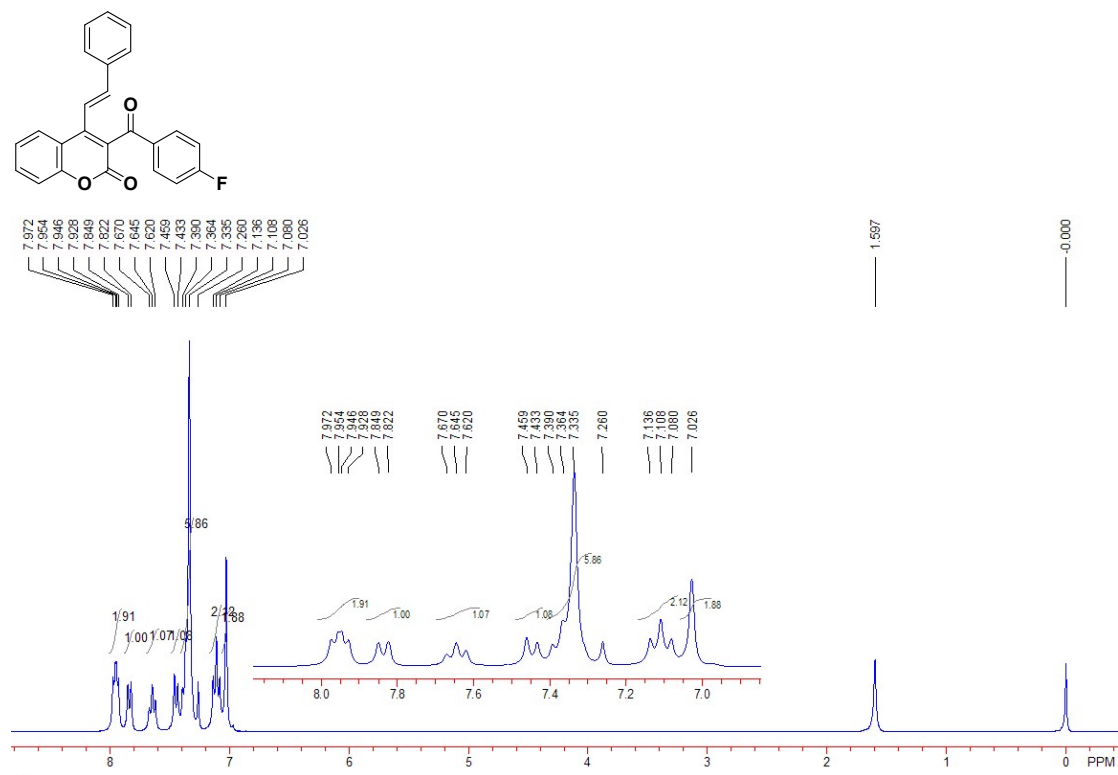
Figure S1. X-ray crystal structure of compound **3ad**.

Crystal data for **3ad**: $C_{19}H_{14}O_3$, $M_r = 290.30$, Monoclinic, $a = 8.5355$ (3) Å, $b = 9.9613$ (3) Å, $c = 17.9321$ (5) Å, $\alpha = 90^\circ$, $\beta = 100.199$ (2) $^\circ$, $\gamma = 90^\circ$, $V = 1500.58$ (8) Å³, $T = 273$ (2) K, space group P2(1)/n, $Z = 4$, 15425 reflections collected, 3318 unique ($R_{\text{int}} = 0.0338$) which were used in all calculation. The ellipsoid contour probability level in the caption is 30%.

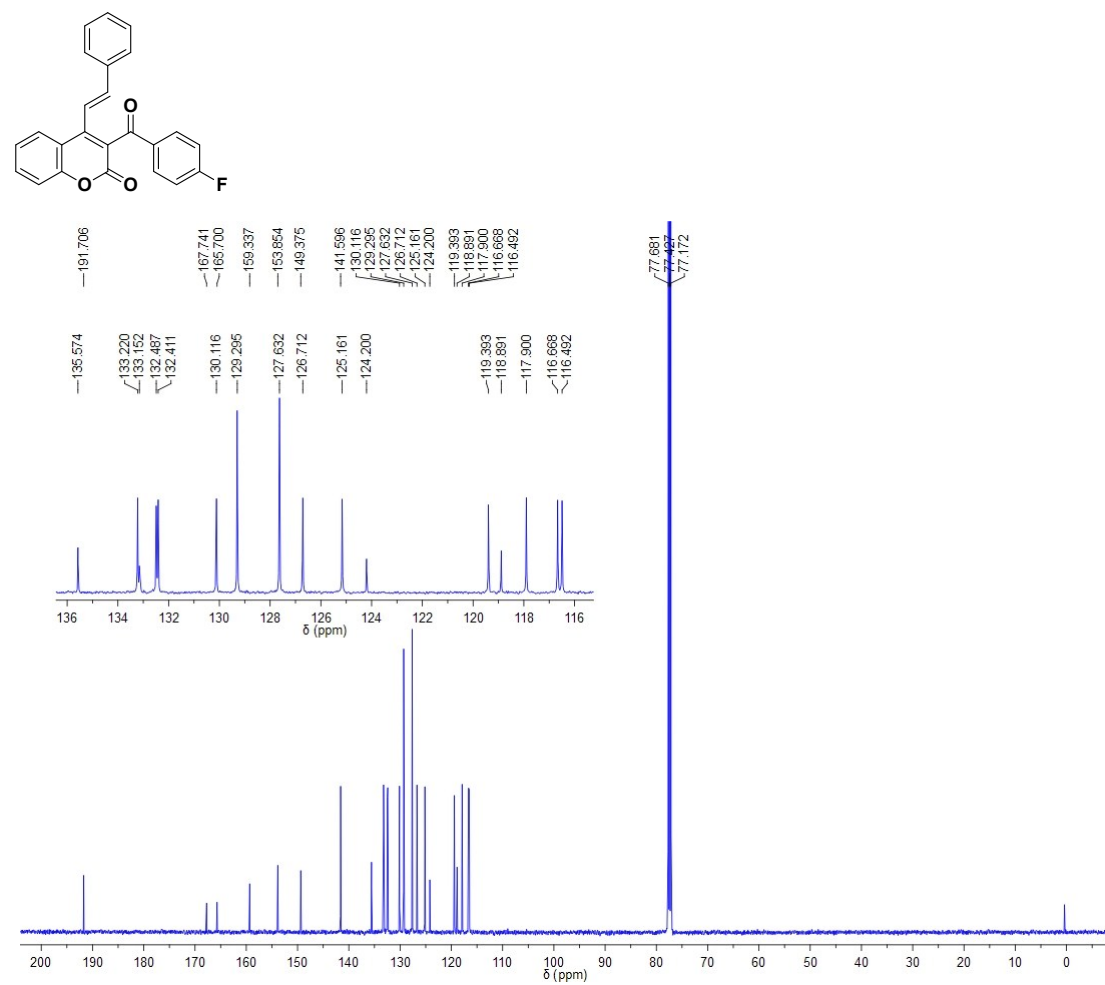
Crystallographic data for compound **3ad** reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. **CCDC-1868191**.

O=C1C(=O)c2ccccc2C(=O)C1=Cc3ccccc3
O=C1C(=O)c2ccccc2C(=C1)C(=C3C=CC(=C3)c4ccccc4)

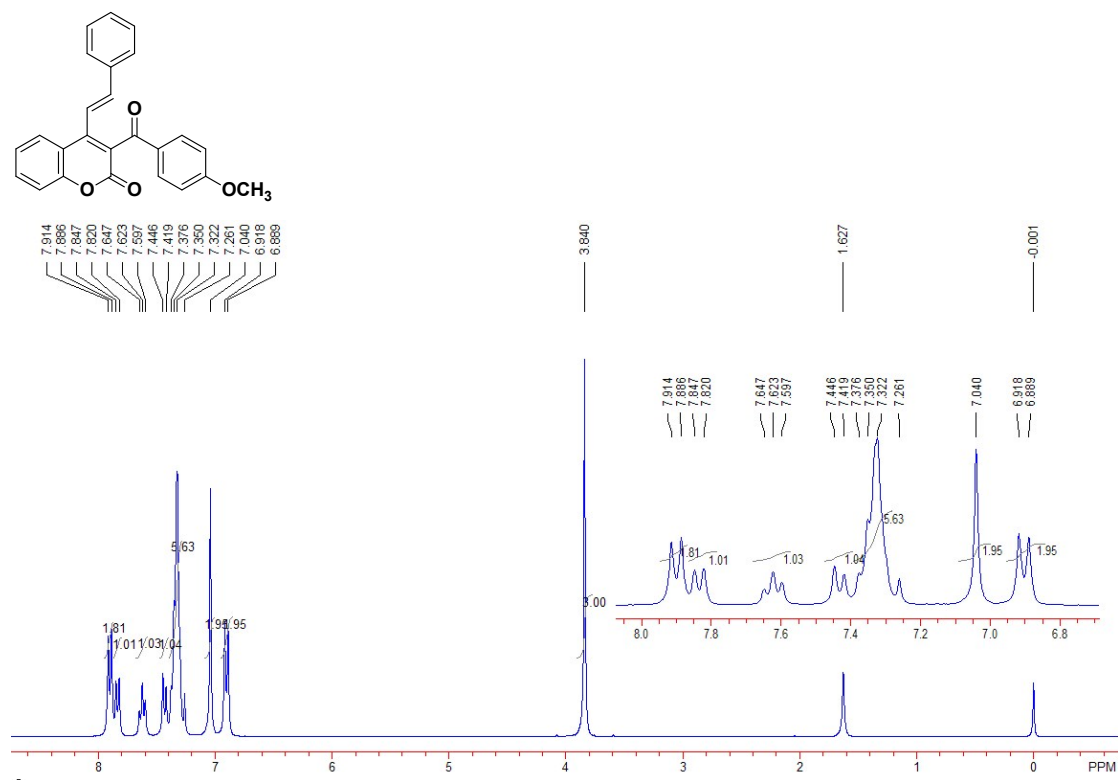
¹H NMR and ¹³C NMR Spectra of Compound 3ab



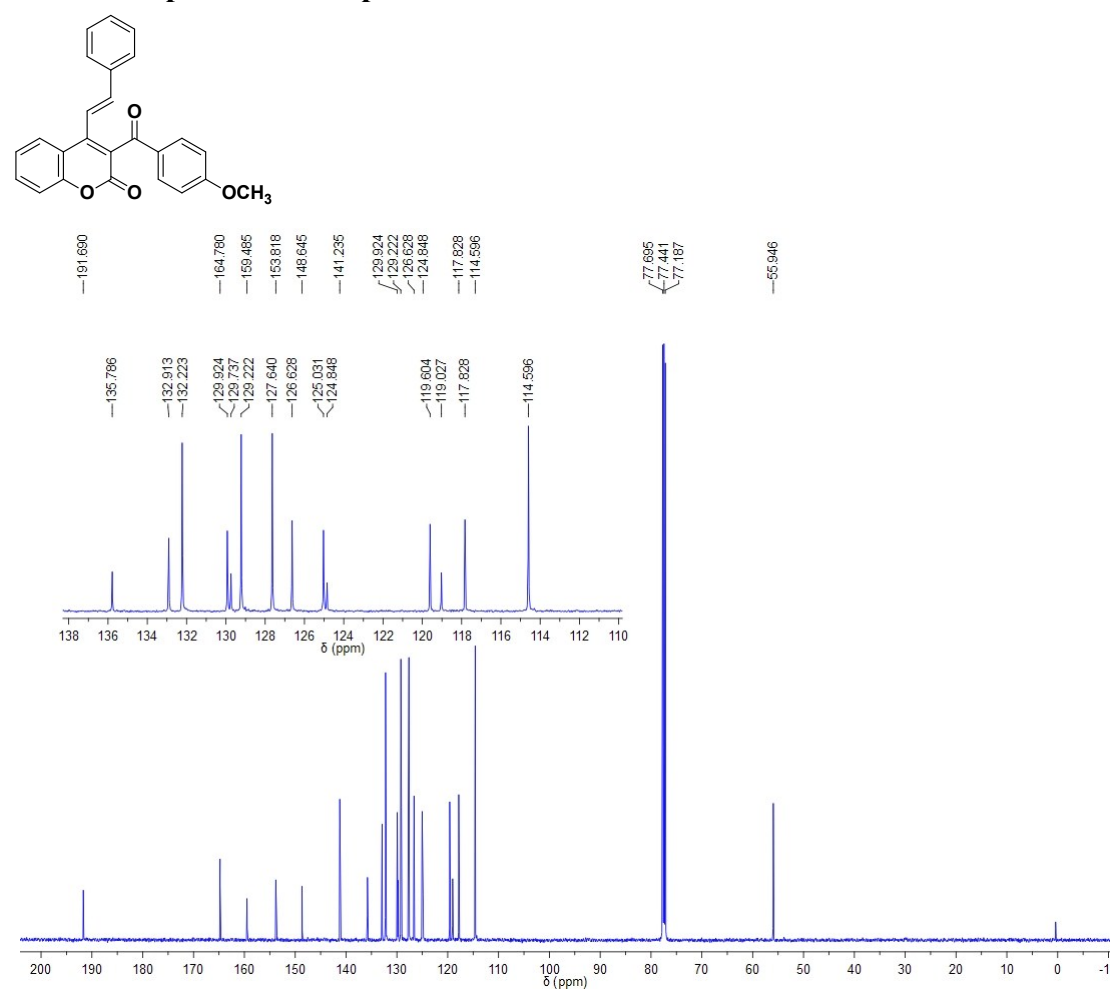
¹³C NMR Spectra of Compound 3ab



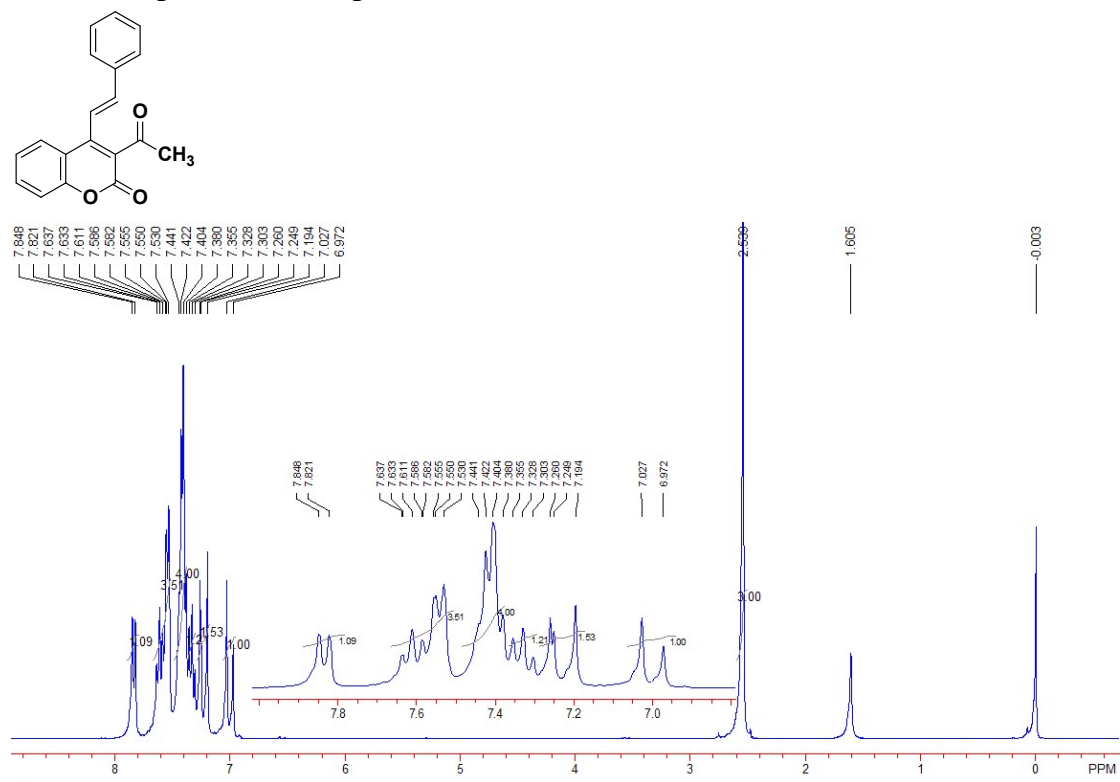
¹H NMR Spectra of Compound 3ac



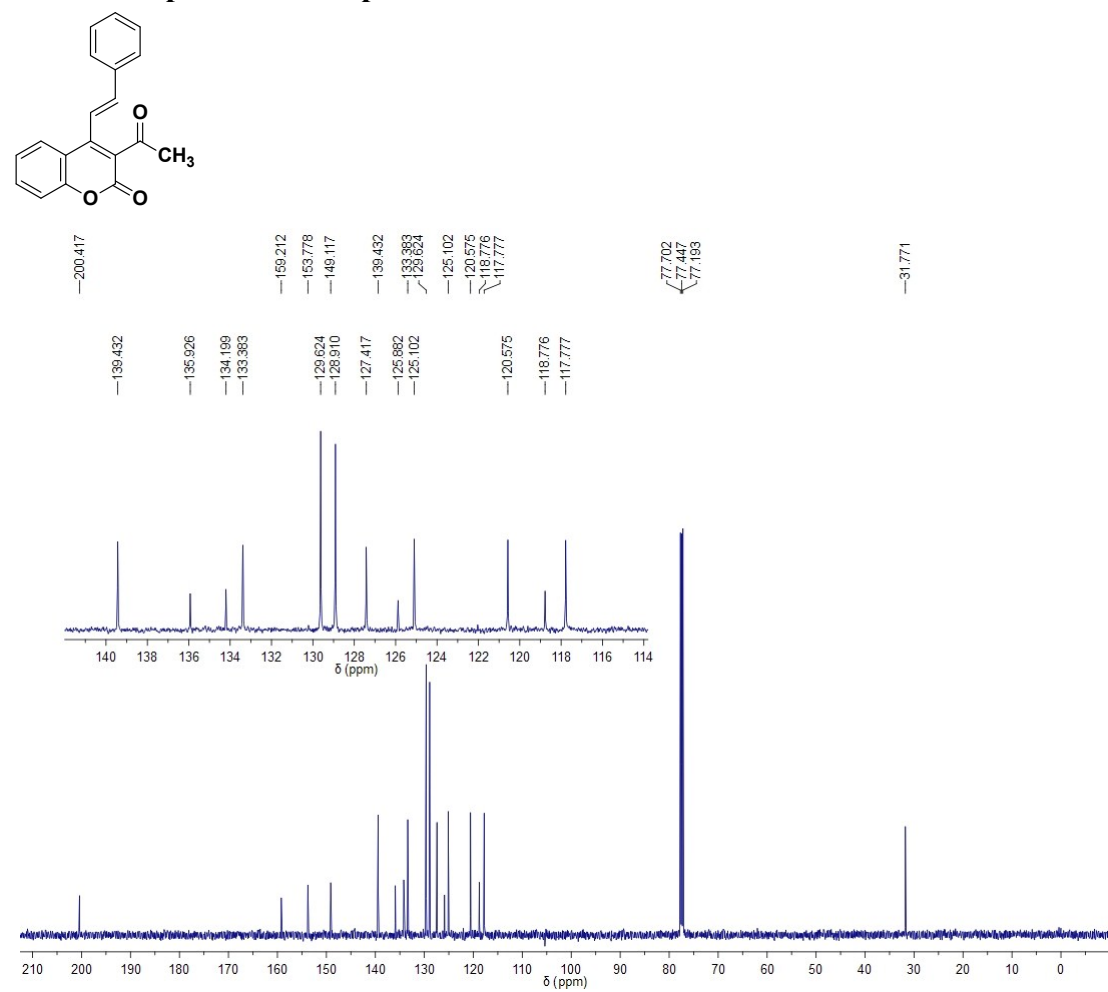
¹³C NMR Spectra of Compound 3ac



¹H NMR Spectra of Compound 3ad



¹³C NMR Spectra of Compound 3ad



O=C1C(=O)c2ccccc2Oc3cc(Cl)ccc3C=Cc4ccccc4

Chemical structure of the compound: 2-chloro-3-oxo-3-phenyl-5-phenyl-2,3-dihydro-1H-benzofuran-4-ylidene-1-phenyl-1H-imidazole.

¹H NMR spectrum (CDCl₃) showing peaks in the aromatic region (6.8-8.0 ppm) and a reference peak at 0.001 ppm. Integration values are provided for several peak groups.

Peak list (ppm): 7.916, 7.891, 7.778, 7.771, 7.598, 7.590, 7.589, 7.580, 7.556, 7.468, 7.442, 7.416, 7.403, 7.373, 7.327, 7.261, 7.054, 7.000, 6.978, 6.924.

Integration values: 2.02, 1.00, 2.41, 1.01, 2.35, 2.02, 1.00, 2.21, 1.96, 1.11, 5.84, 2.35.

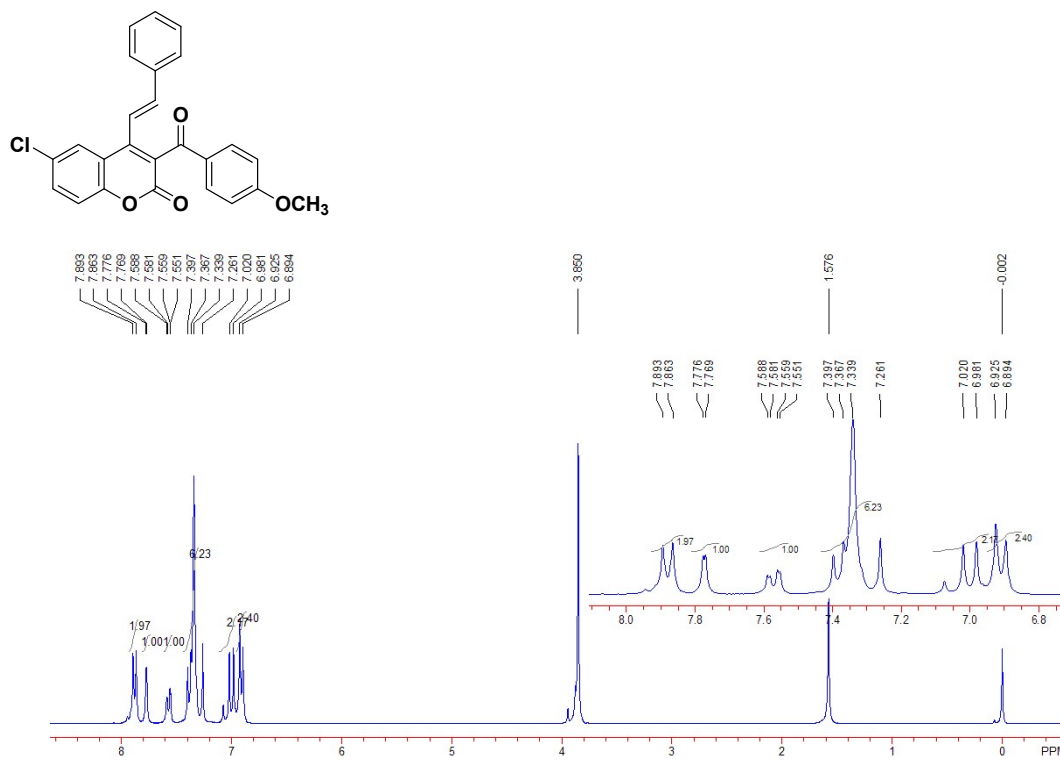
O=C1C(=O)c2ccccc2Oc3cc(Cl)ccc3C=Cc4ccccc4

Chemical structure of 2-chloro-3-phenyl-4-oxo-4-phenyl-2,3-dihydro-1H-benzofuran-5-carboxylic acid is shown above the spectrum.

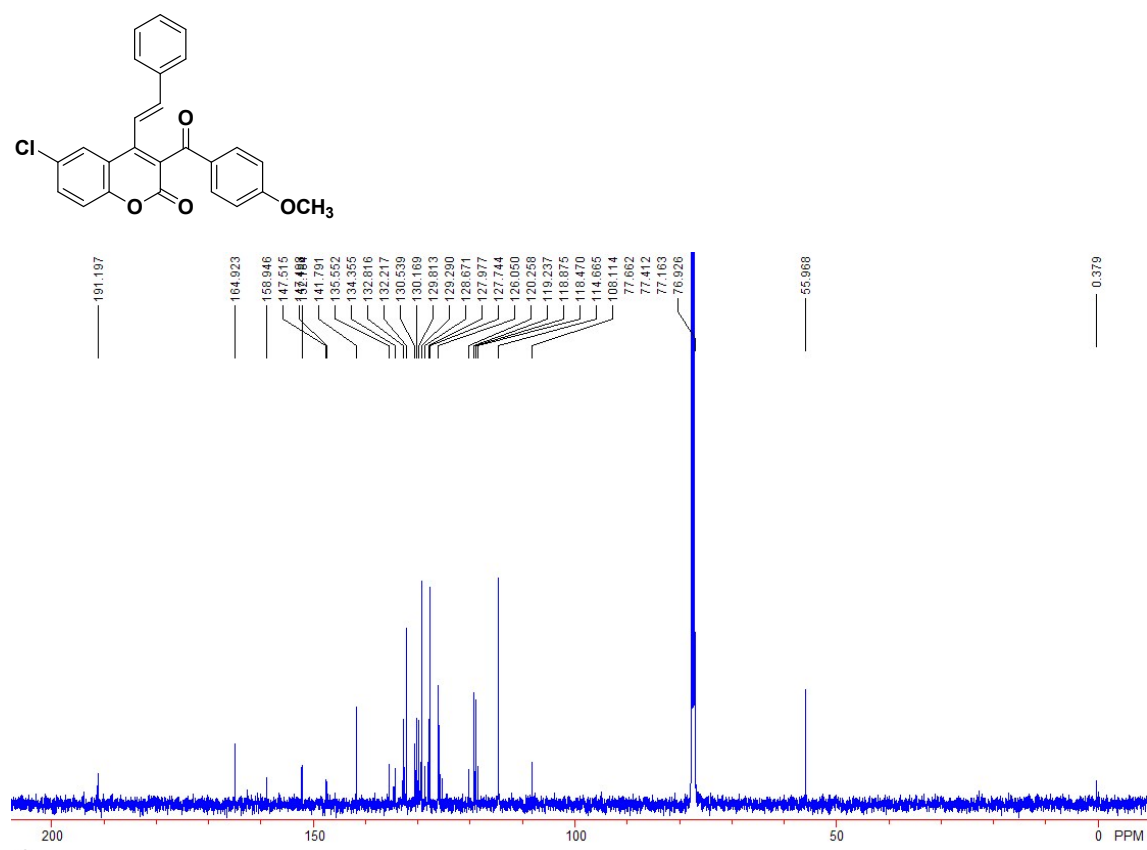
¹³C NMR peaks (ppm):

- 192.832
- 158.827
- 152.200
- 148.046
- 142.025
- 134.672
- 130.225
- 129.287
- 125.443
- 120.190
- 119.256
- 118.819
- 136.409
- 135.432
- 134.672
- 132.974
- 130.601
- 130.225
- 129.686
- 129.368
- 127.717
- 126.095
- 125.443
- 120.190
- 119.256
- 118.819
- 77.680
- 77.435
- 77.181
- 0

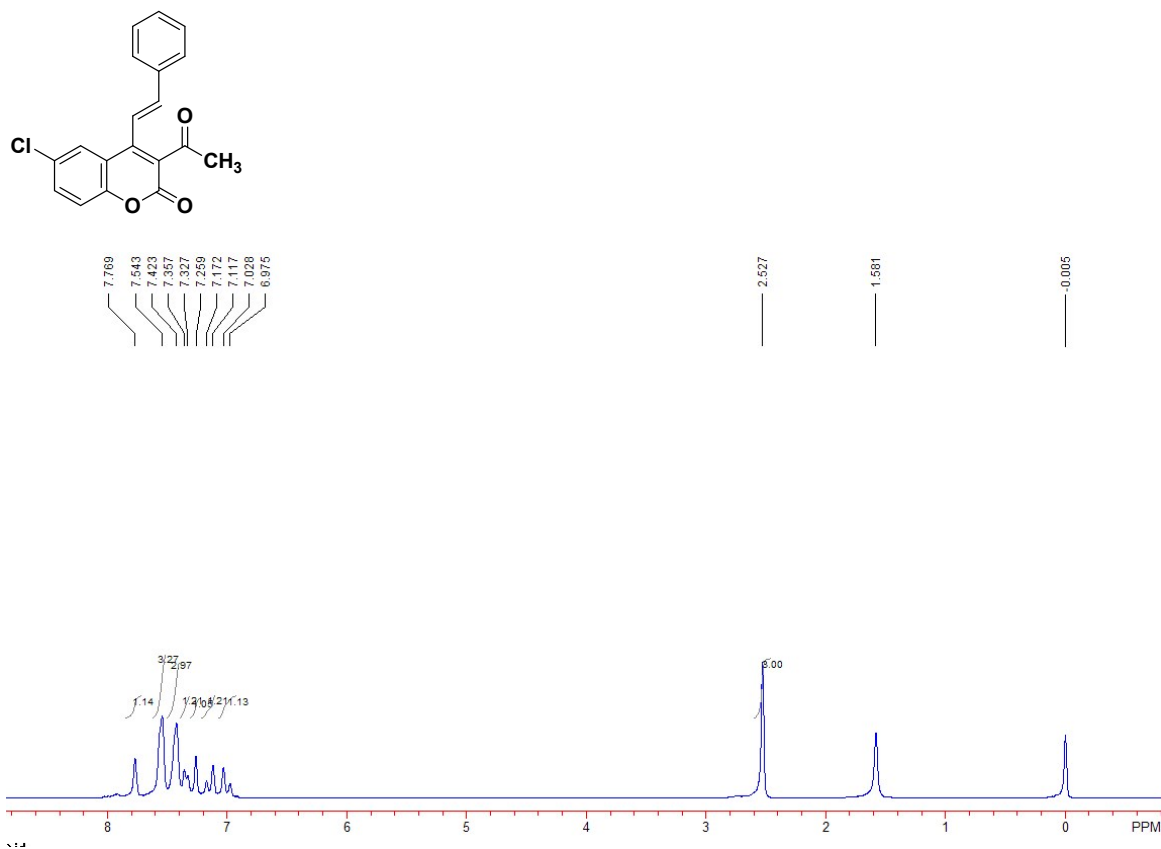
¹H NMR Spectra of Compound 3bc



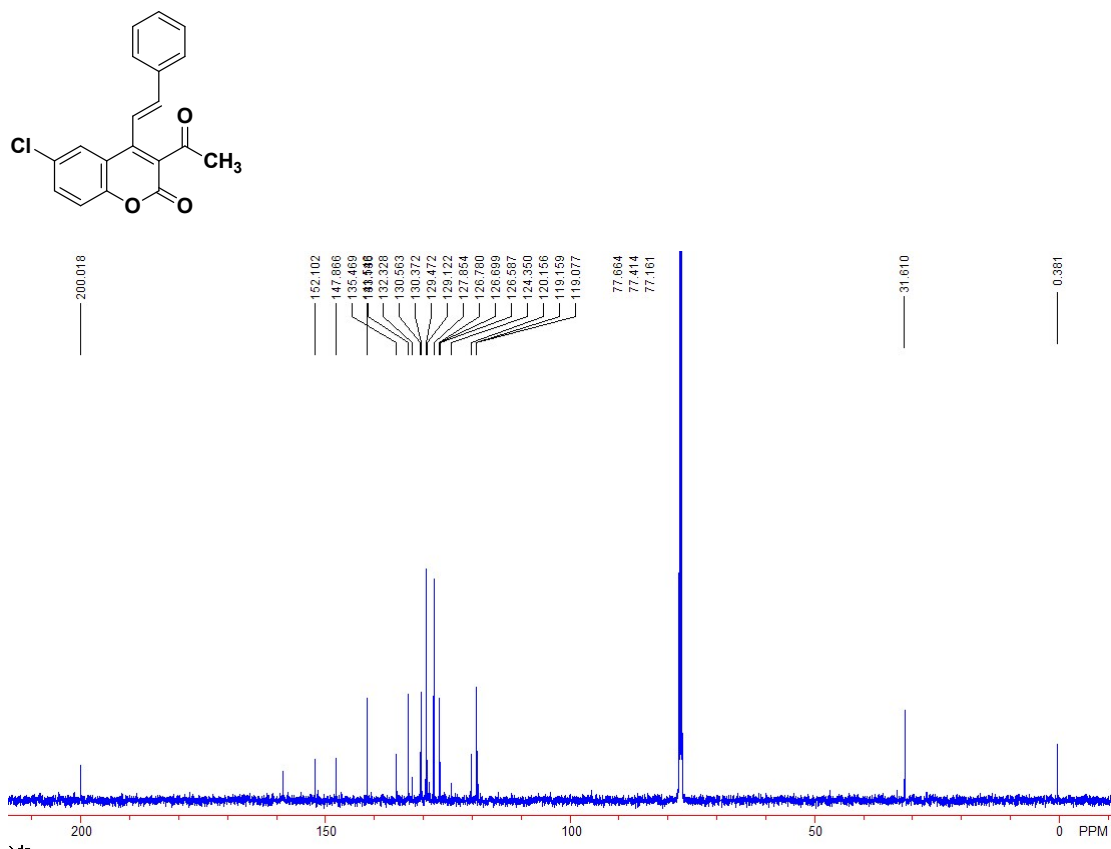
¹³C NMR Spectra of Compound 3bc



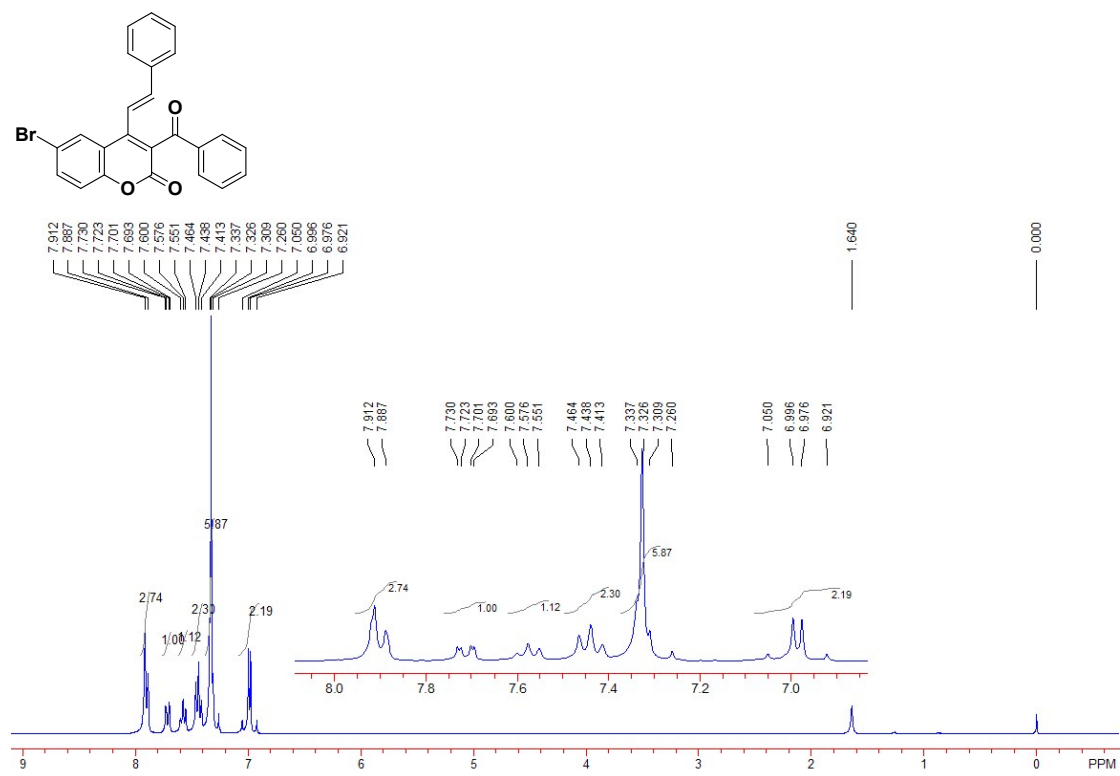
¹H NMR Spectra of Compound 3bd



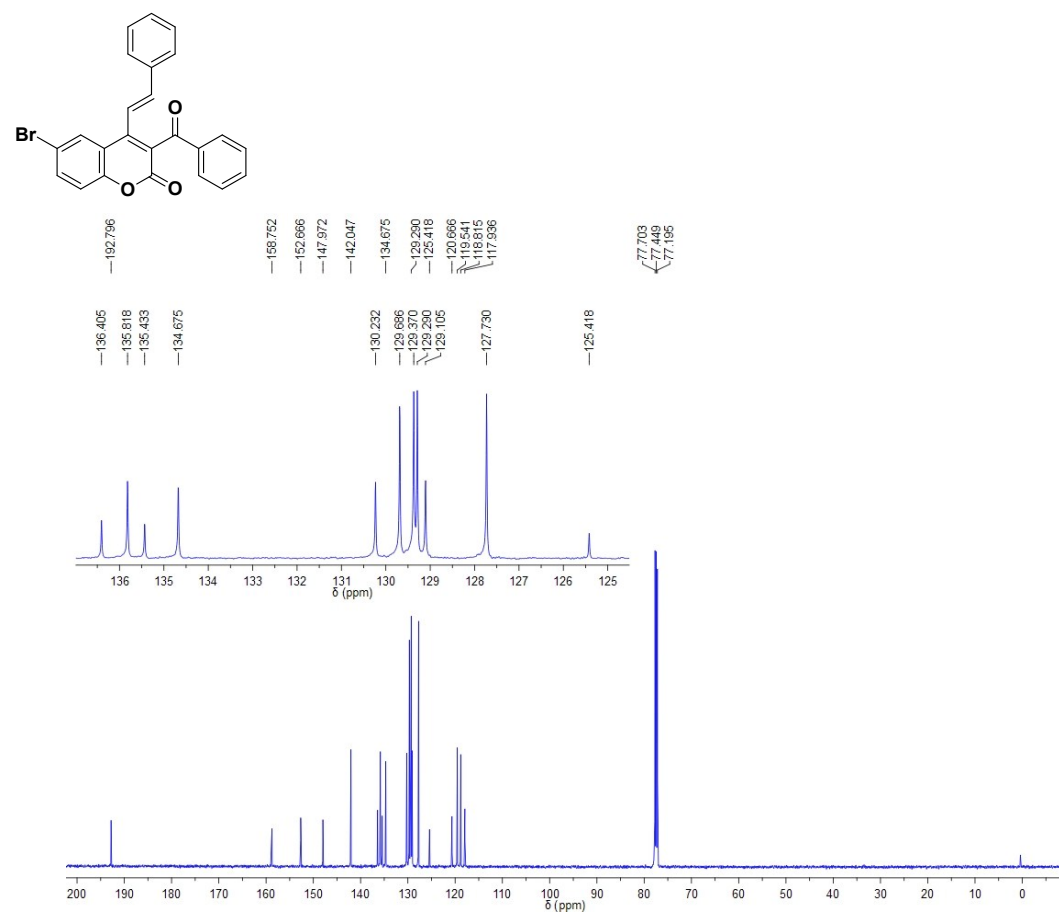
¹³C NMR Spectra of Compound 3bd



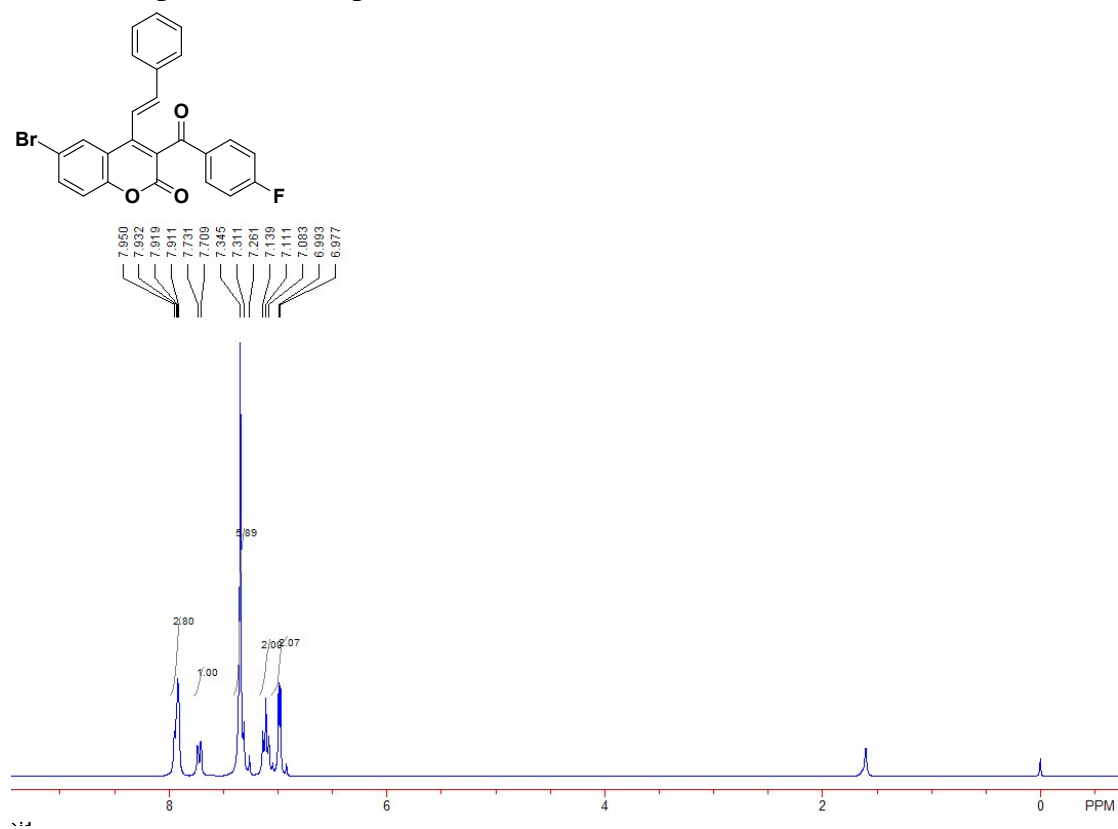
¹H NMR Spectra of Compound 3ca



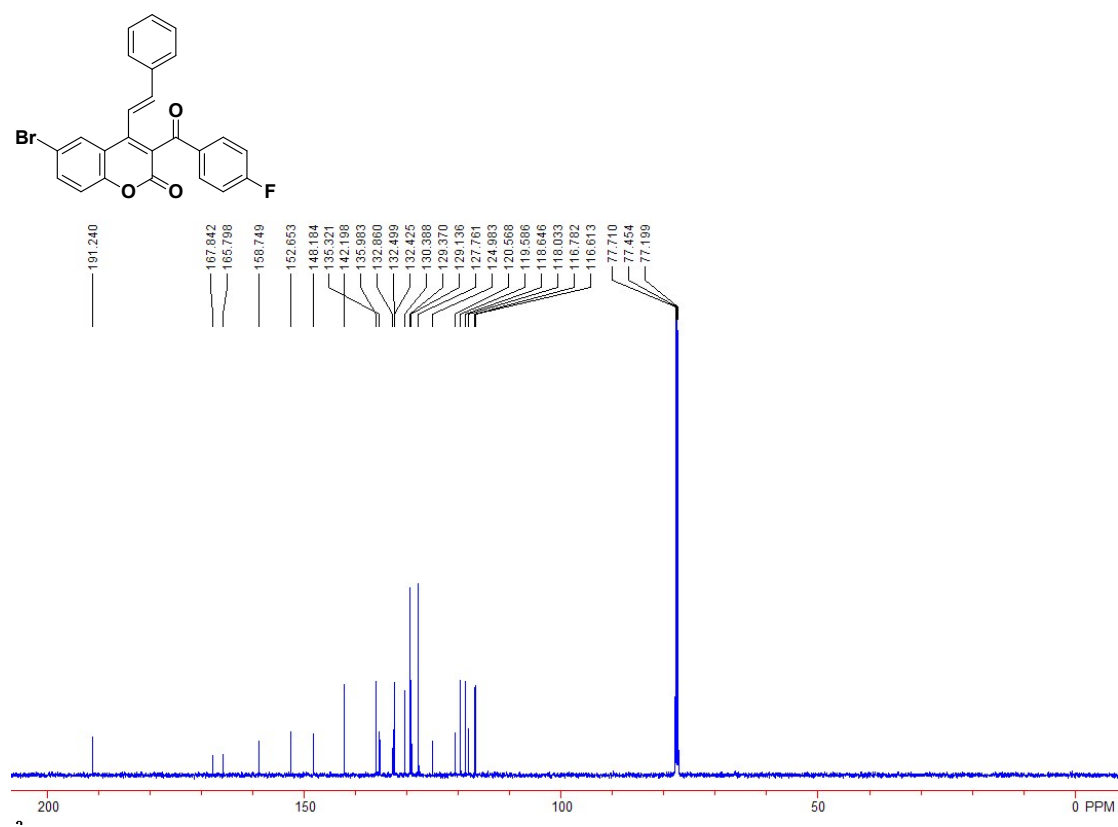
¹³C NMR Spectra of Compound 3ca



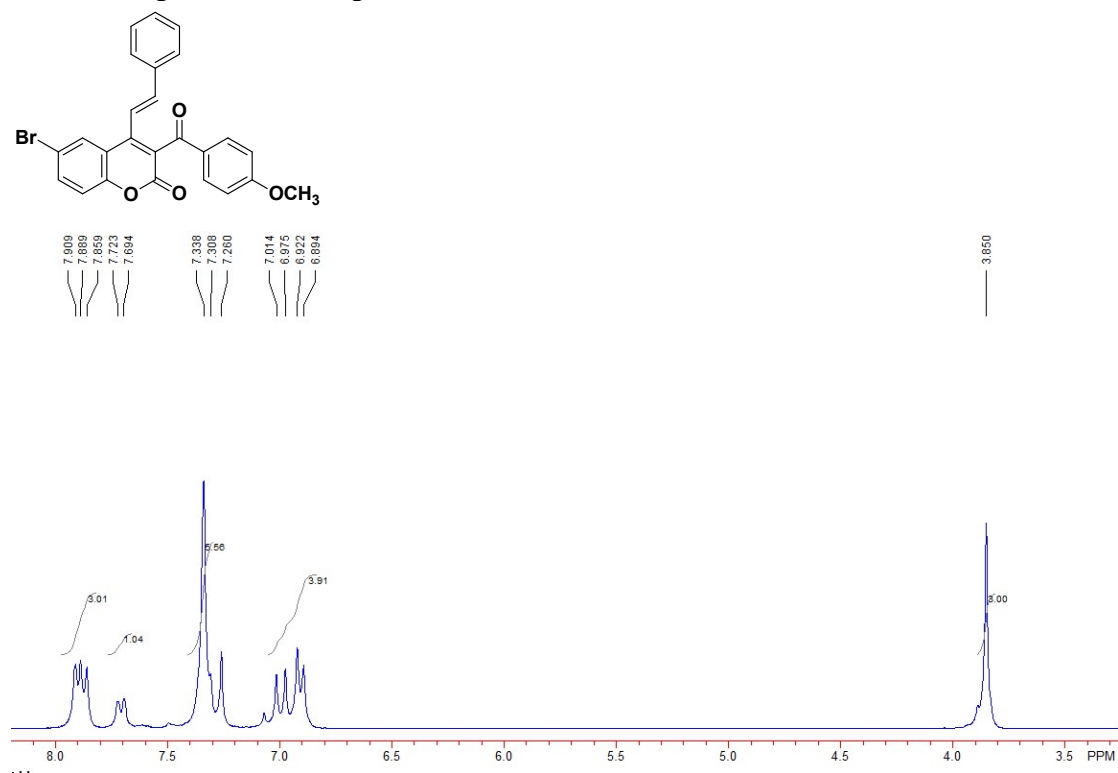
¹H NMR Spectra of Compound 3cb



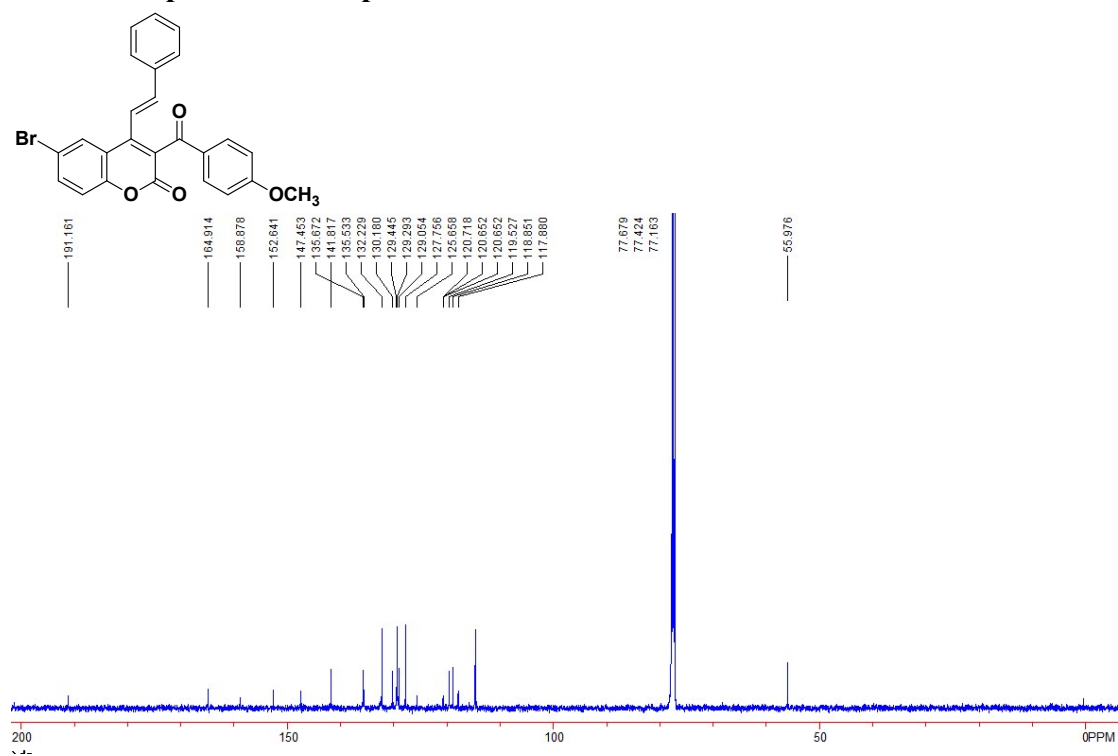
¹³C NMR Spectra of Compound 3cb



¹H NMR Spectra of Compound 3cc



¹³C NMR Spectra of Compound 3cc



CC(=O)C(=Cc1ccc(Br)cc1OC(=O)c2ccccc2)C(=O)c3ccccc3

Chemical Structure: 2-bromo-4-(benzylidene)-6-oxo-1,2,3,4-tetrahydronaphthalen-1-ylidene-benzene

¹H NMR Data (CDCl₃):

Chemical Shift (ppm)	Integration
7.911, 7.904, 7.708, 7.679, 7.671, 7.565, 7.535, 7.441, 7.420, 7.417, 7.293, 7.284, 7.261, 7.252, 7.166, 7.111, 7.101, 6.972	1.00, 0.96, 2.33, 3.08, 1.49, 1.09, 0.99
2.523	2.96

Chemical structure of compound 10: CC(=O)C(=Cc1ccccc1)c2cc(Br)ccc2O

¹³C NMR spectrum (top): CDCl₃. Peaks (ppm): 200.006, 152.549, 147.765, 141.578, 138.603, 152.549, 147.765, 141.578, 136.450, 135.972, 135.450, 130.362, 129.473, 128.689, 126.751, 120.614, 127.865, 119.438, 117.885, 126.751, 120.614, 119.040, 117.895.

¹³C NMR spectrum (bottom): DMSO-d₆. Peaks (ppm): 200.006, 152.549, 147.765, 141.578, 138.603, 152.549, 147.765, 141.578, 136.450, 135.972, 135.450, 130.362, 129.473, 128.689, 126.751, 120.614, 127.865, 119.438, 117.885, 126.751, 120.614, 119.040, 117.895, 31.636.

Chemical structure of 2-methyl-6-phenyl-2H-chromene-3-carboxylic acid is shown above the spectrum. The structure includes a chromene core with a methyl group at position 2, a phenyl group at position 6, and a carboxylic acid group at position 3. Protons are labeled with numbers corresponding to the integration values.

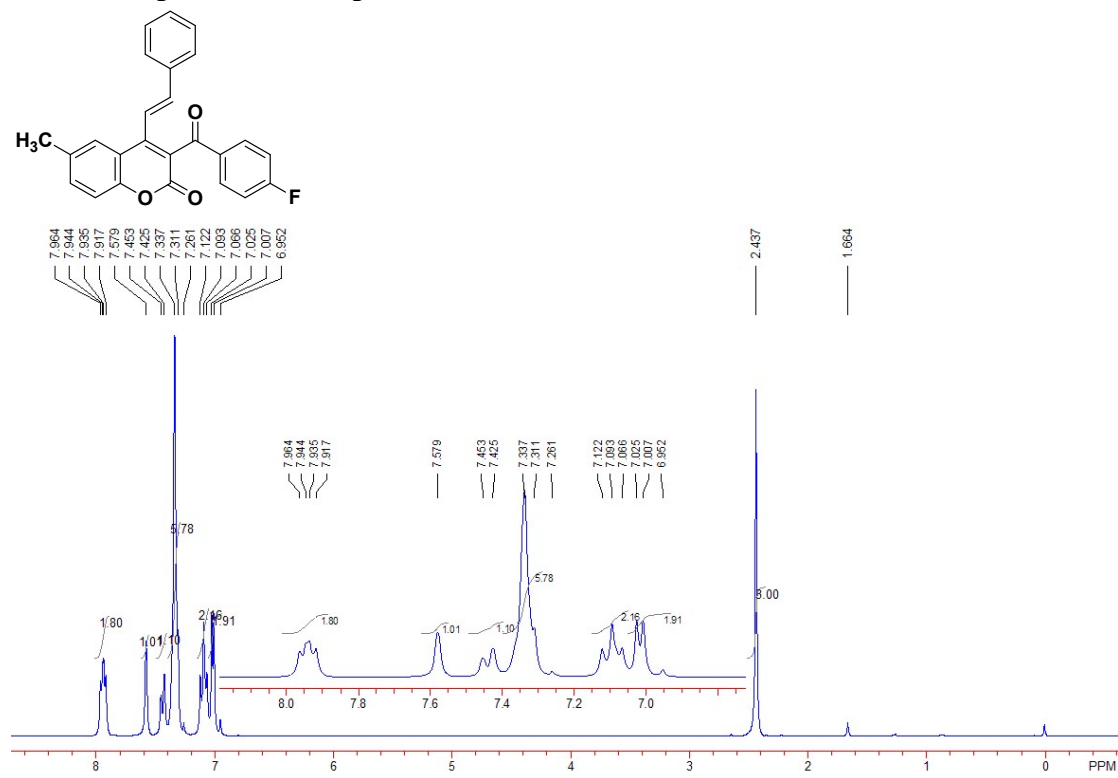
¹H NMR spectrum (CDCl₃) showing peaks in the aromatic region (6.5-8.0 ppm) and aliphatic region (1.5-2.5 ppm). The spectrum is integrated, showing values such as 1.80, 2.15, 3.05, 1.94, 3.00, 1.579, and 0.001.

Chemical structure of 6-methyl-2-phenyl-2H-chromene-3-carbonyl is shown above the ^{13}C NMR spectrum. The spectrum displays two regions of peaks, with chemical shifts (ppm) labeled above the peaks.

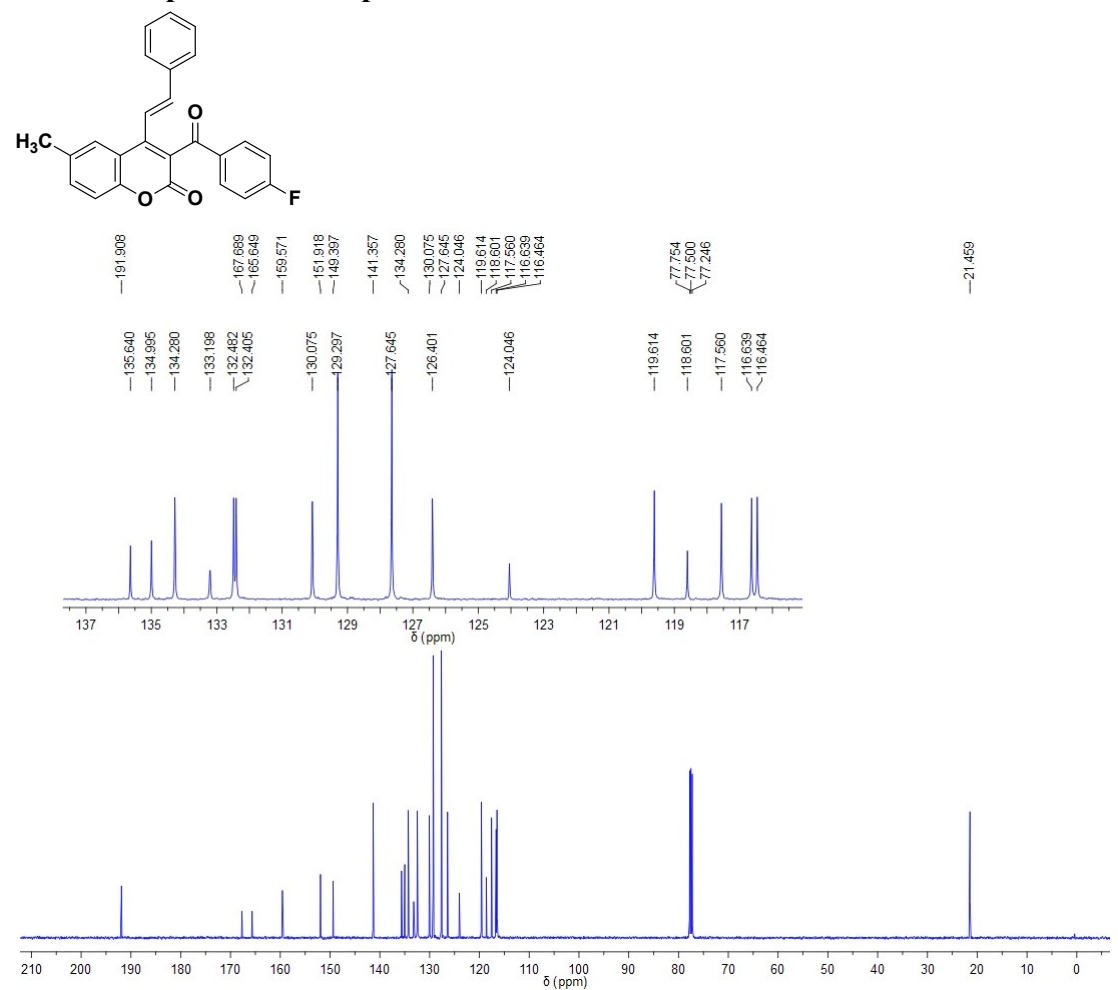
Top region peaks (ppm): 136.748, 135.763, 134.876, 134.434, 134.113, 133, 132, 131, 129.934, 129.700, 129.228, 129.276, 129.228, 127.624, 126.368, 124.509, 124.450.

Bottom region peaks (ppm): 200, 190, 180, 170, 160, 150, 140, 130, 120, 110, 100, 90, 80, 70, 60, 50, 40, 30, 20, 10, 0.

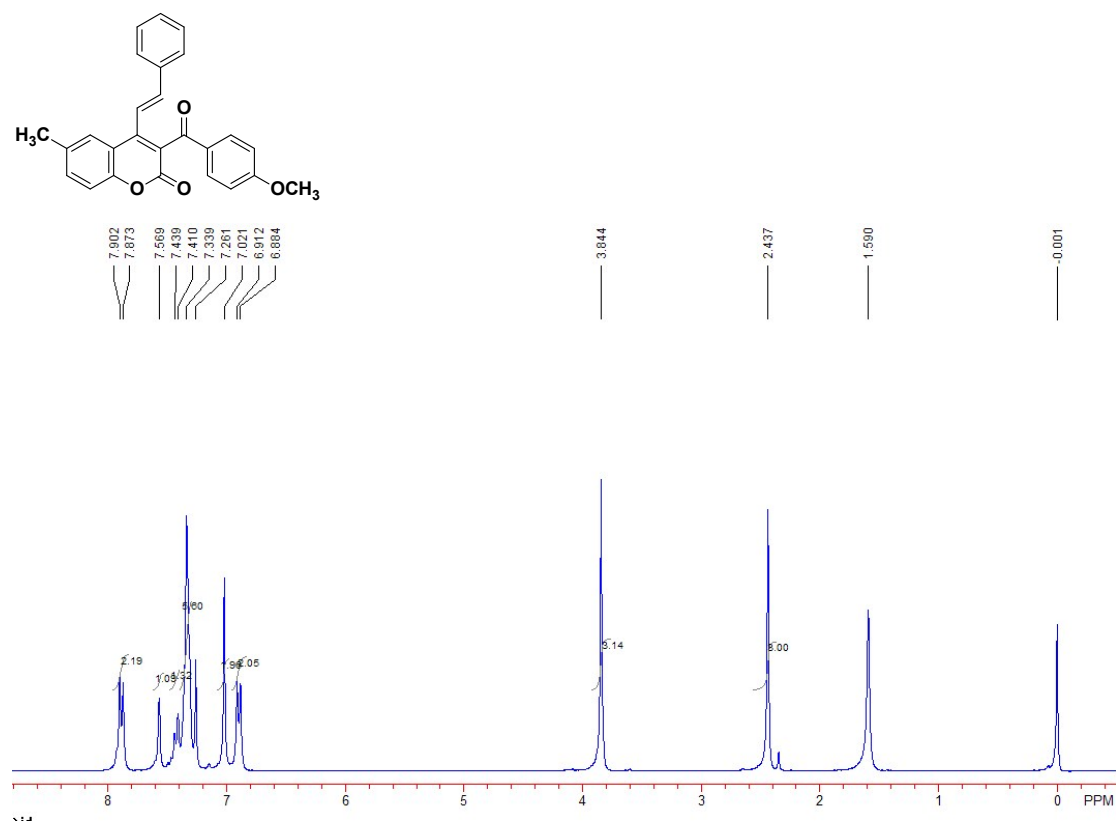
¹H NMR Spectra of Compound 3db



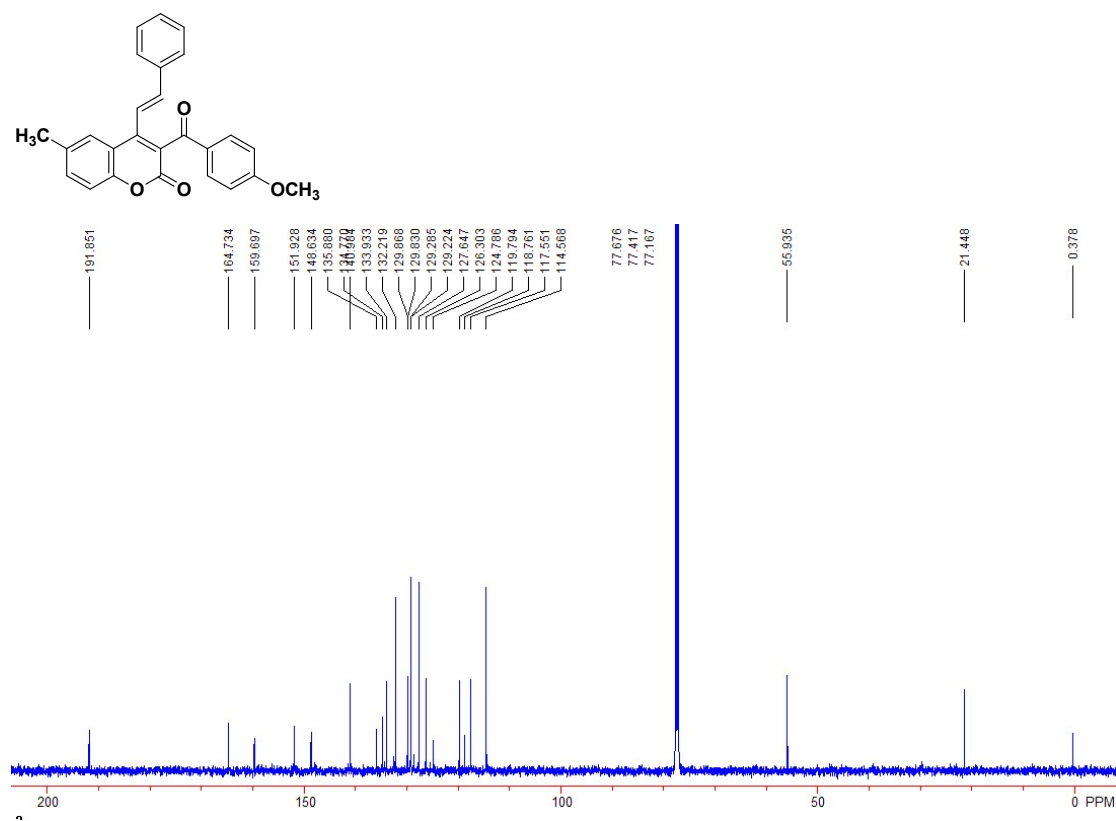
¹³C NMR Spectra of Compound 3db



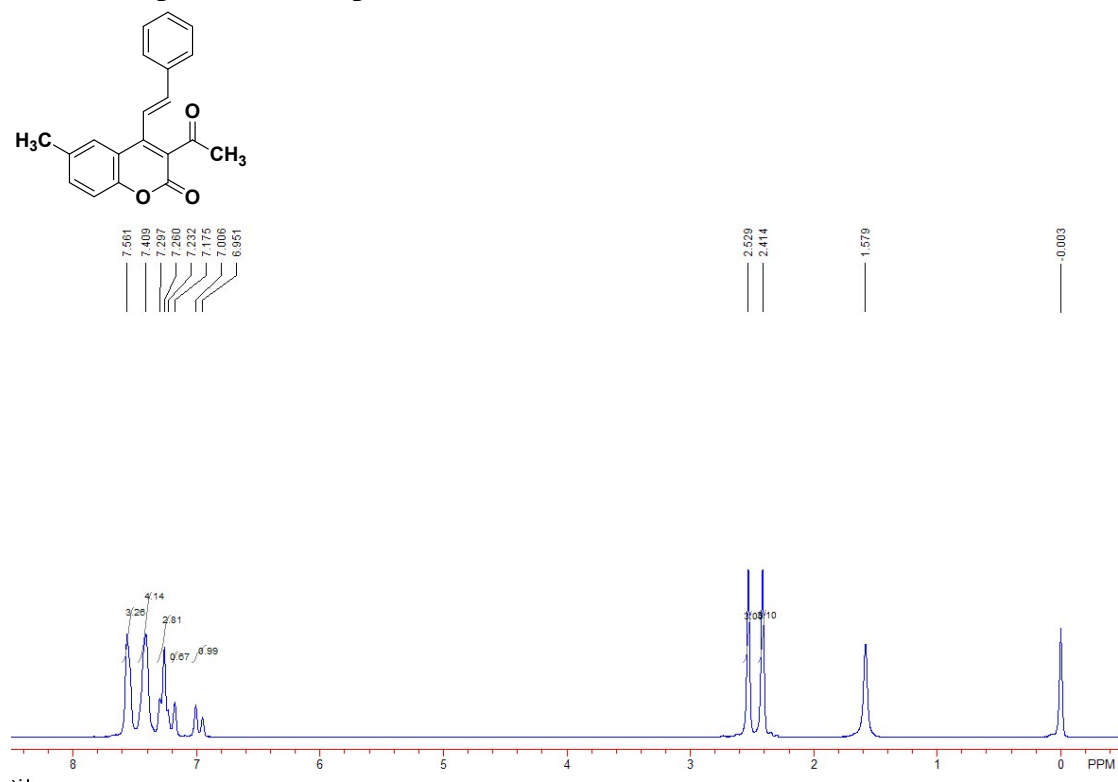
¹H NMR Spectra of Compound 3dc



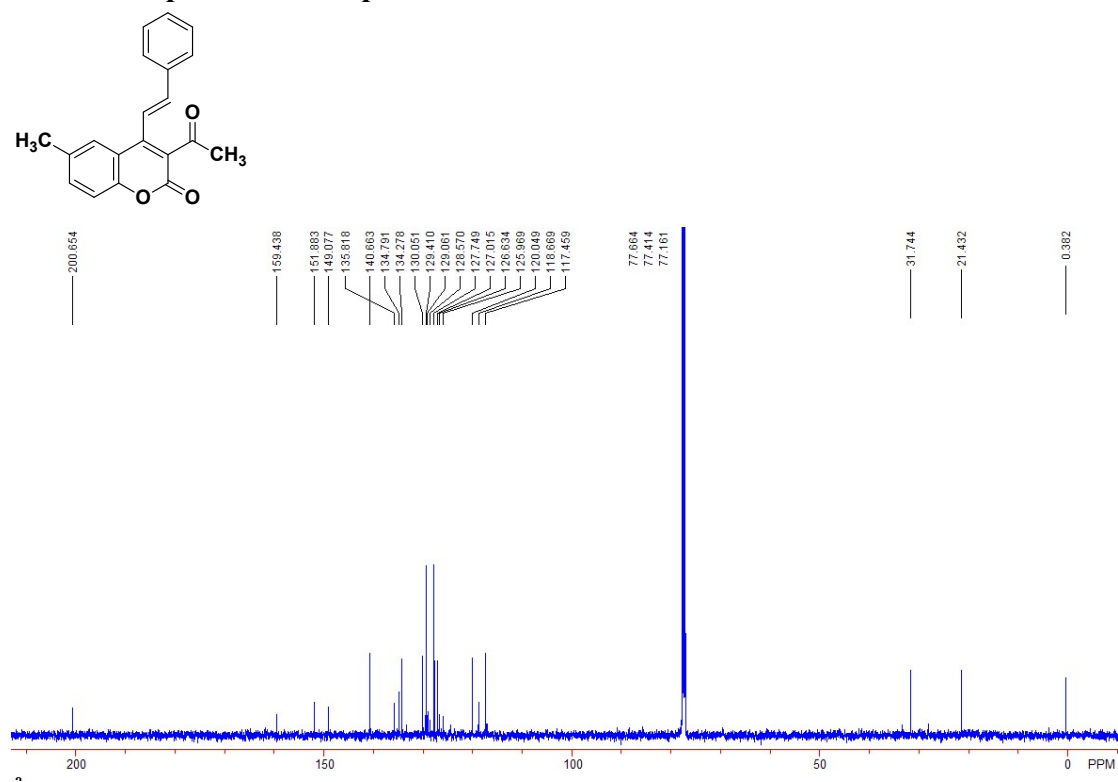
¹³C NMR Spectra of Compound 3dc



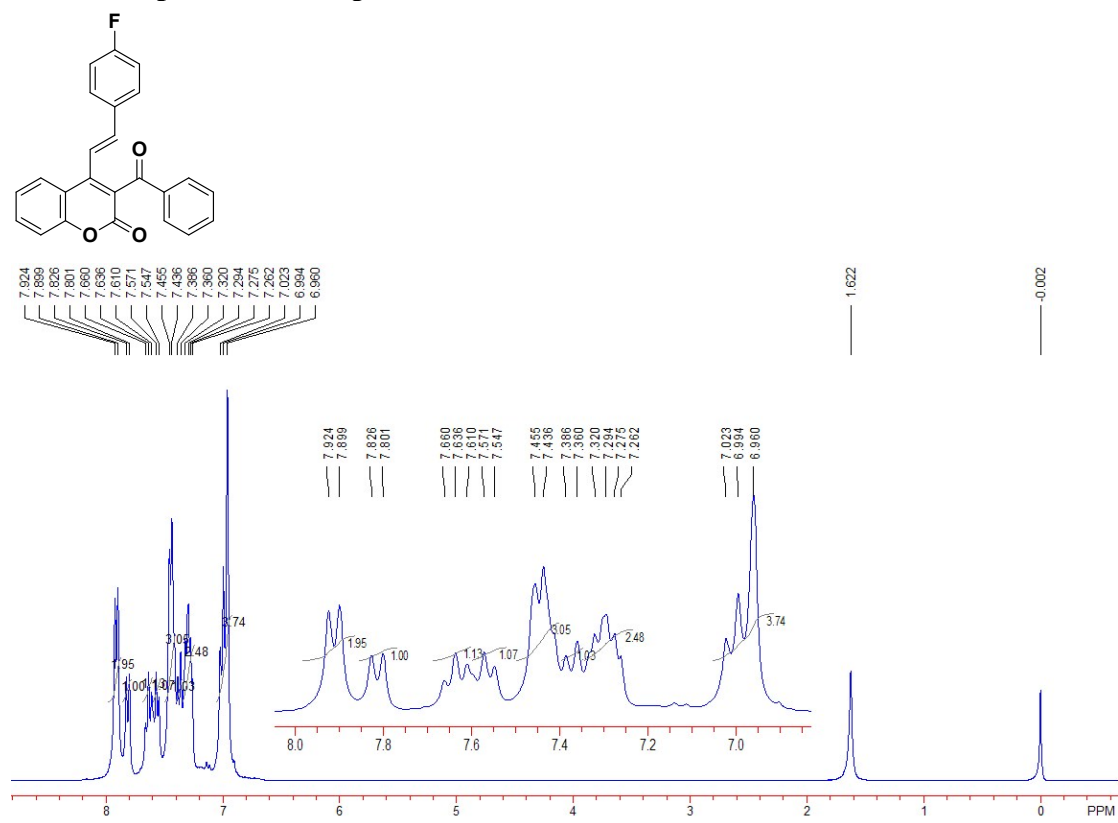
¹H NMR Spectra of Compound 3dd



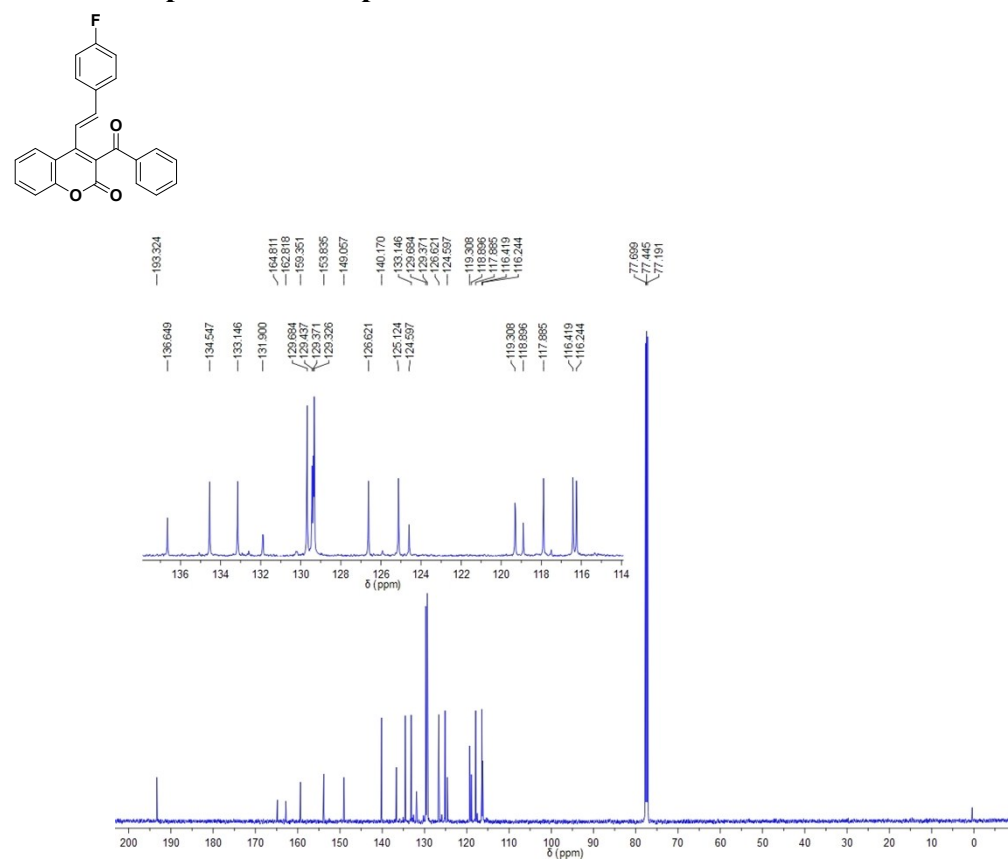
¹³C NMR Spectra of Compound 3dd



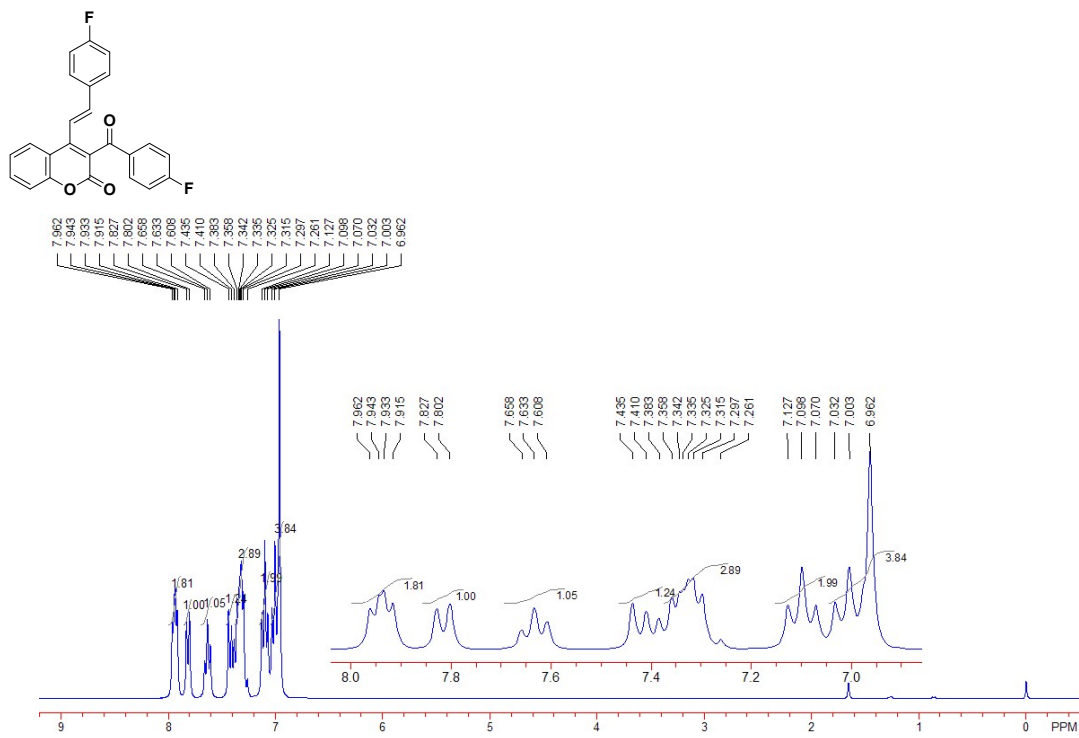
¹H NMR Spectra of Compound 3ea



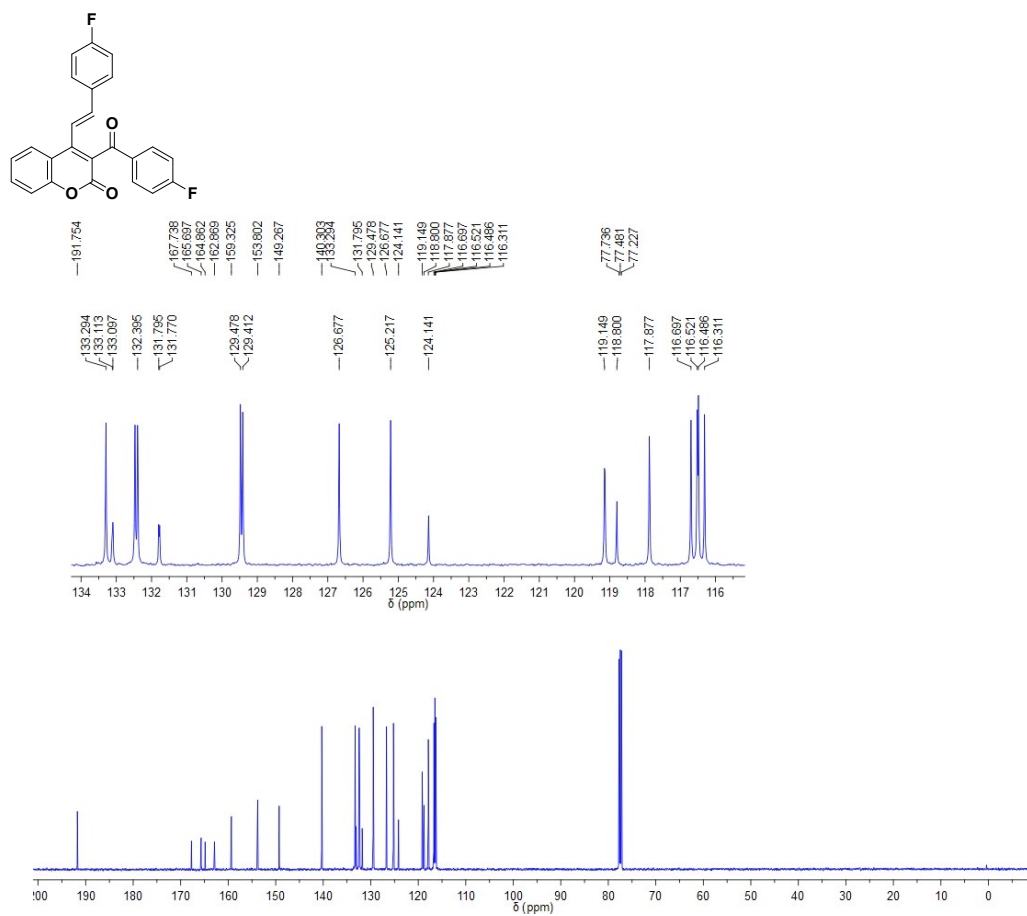
¹³C NMR Spectra of Compound 3ea



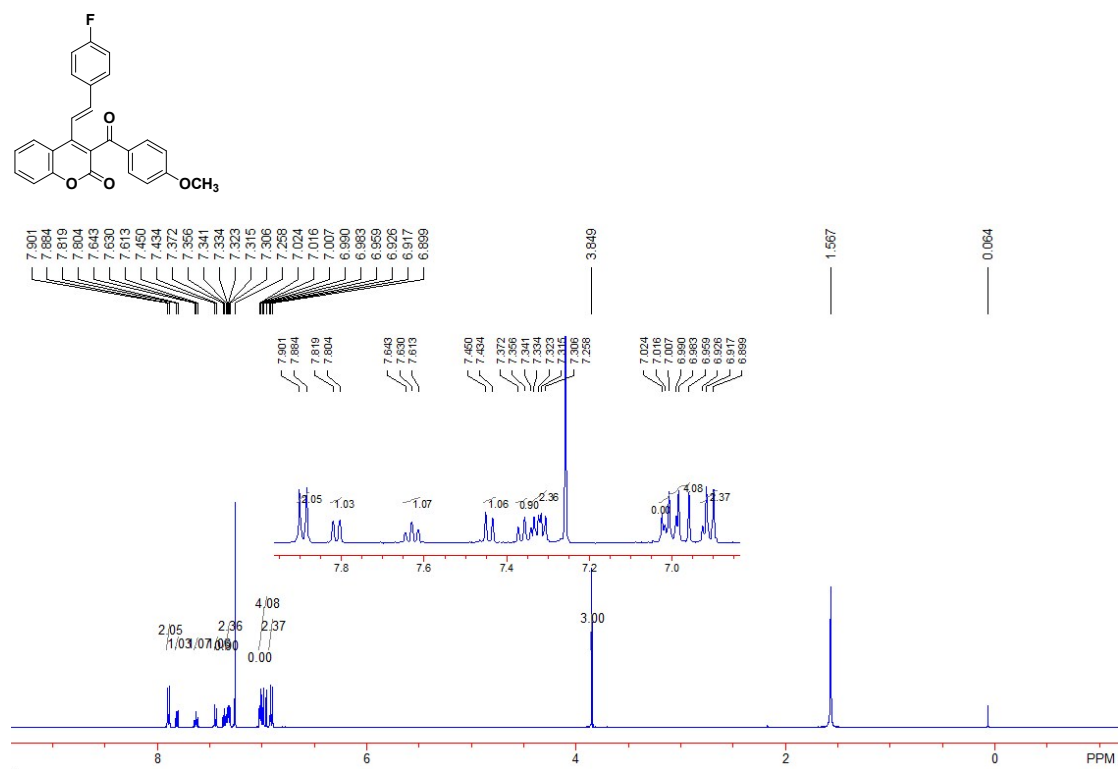
¹H NMR Spectra of Compound 3eb



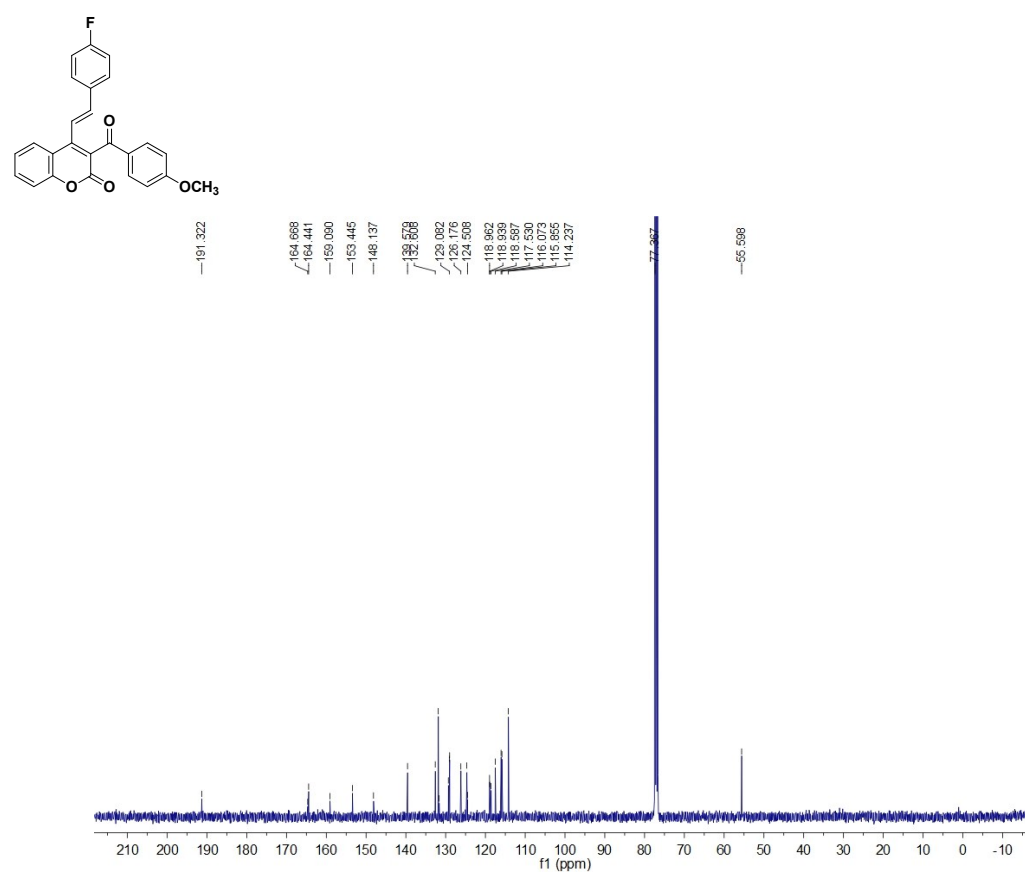
¹³C NMR Spectra of Compound 3eb



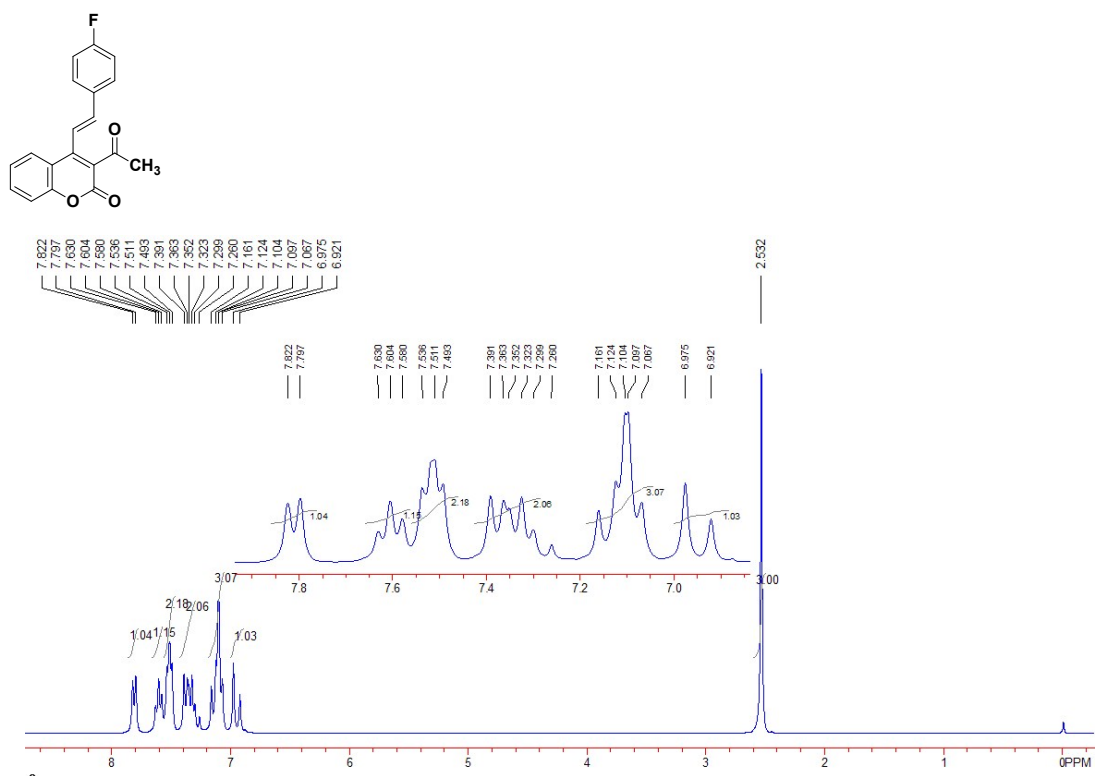
¹H NMR Spectra of Compound 3ec



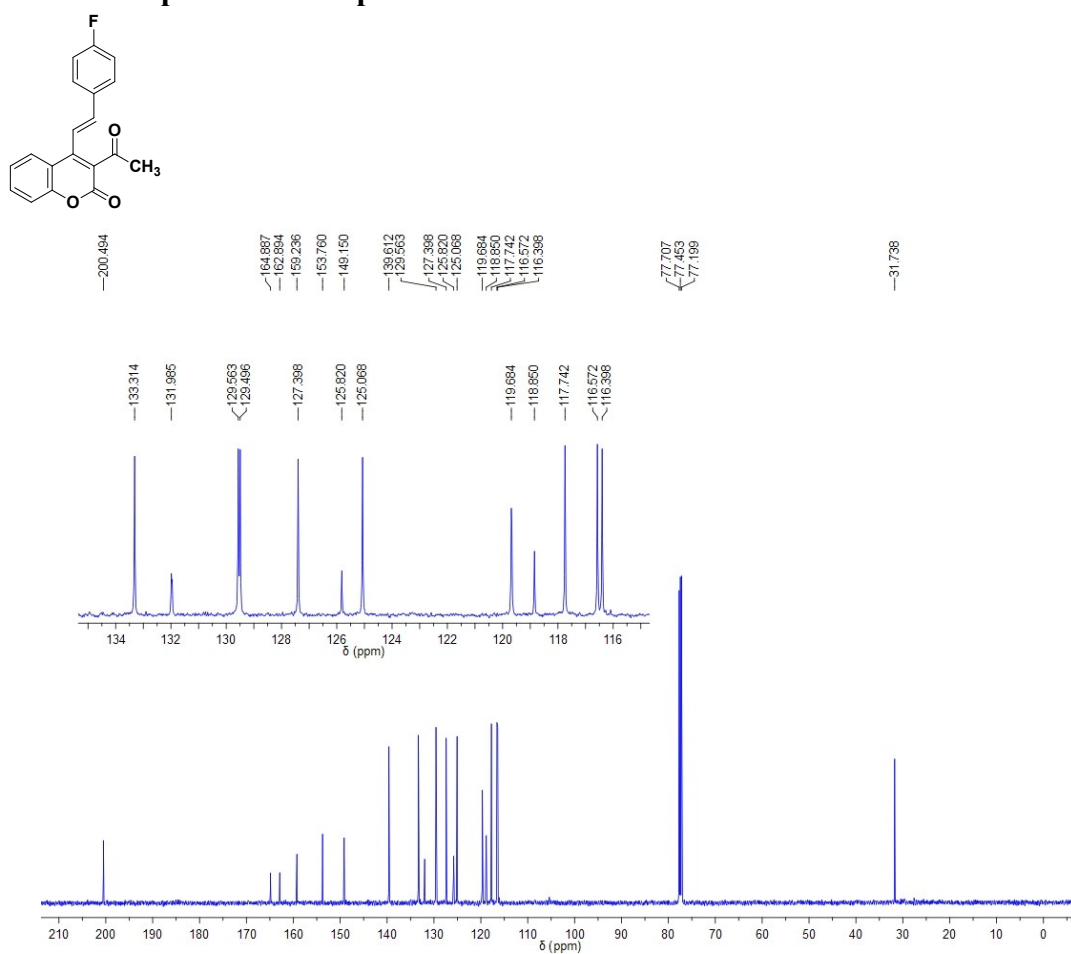
¹³C NMR Spectra of Compound 3ec



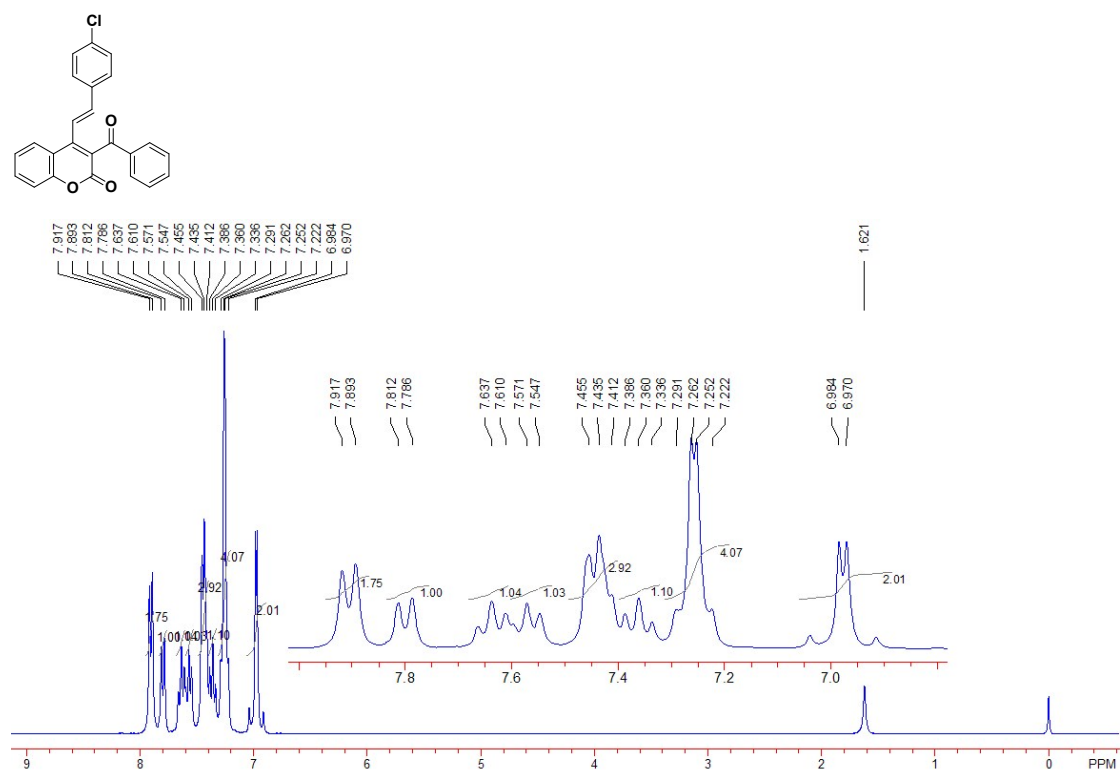
¹H NMR Spectra of Compound 3ed



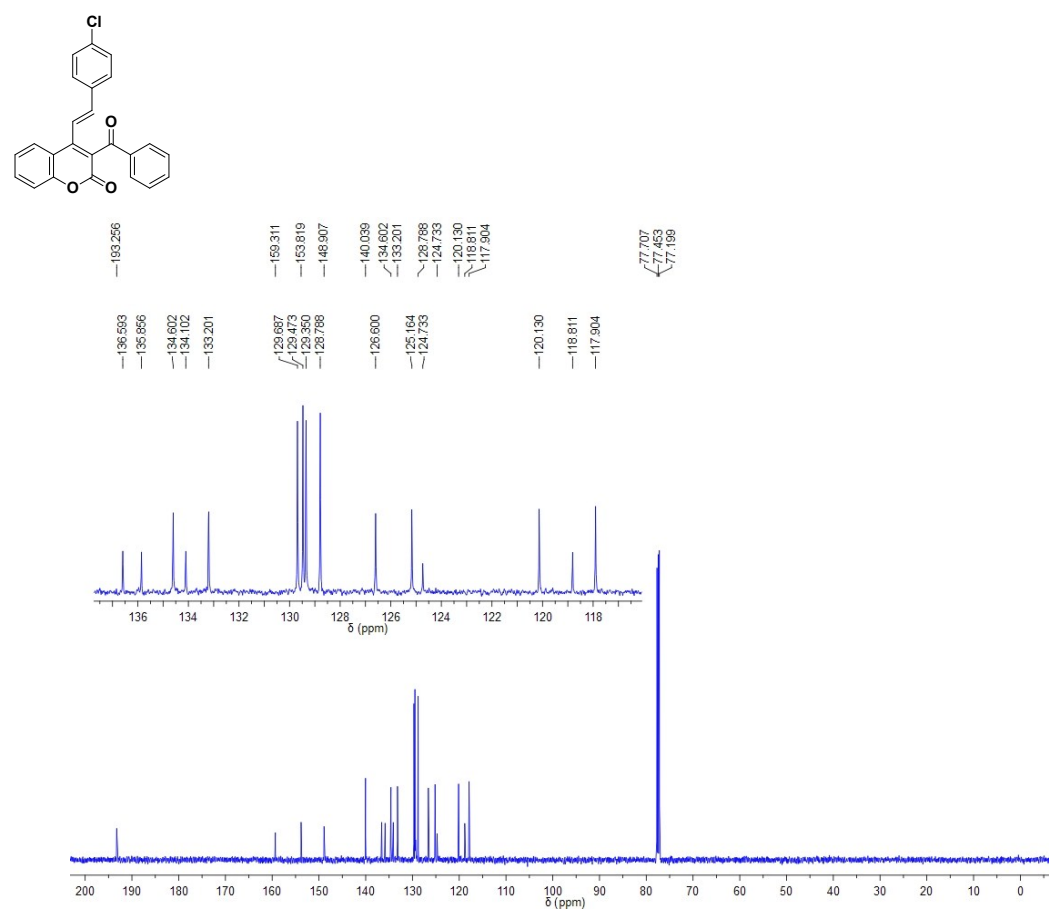
¹³C NMR Spectra of Compound 3ed



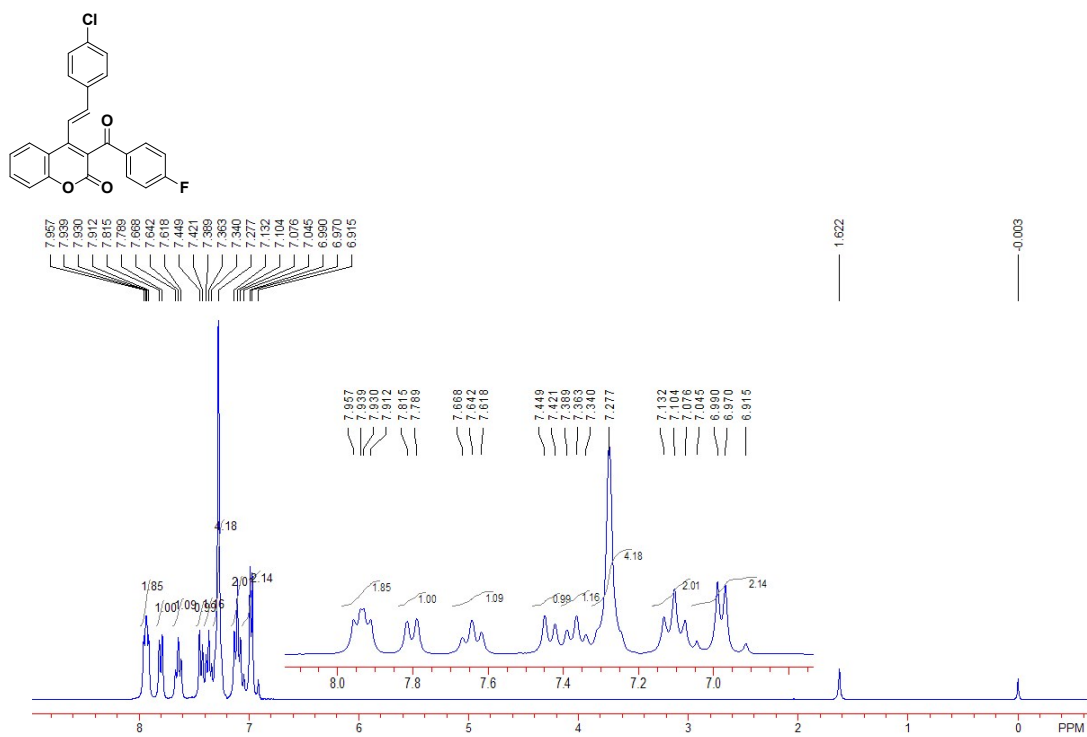
¹H NMR Spectra of Compound 3fa



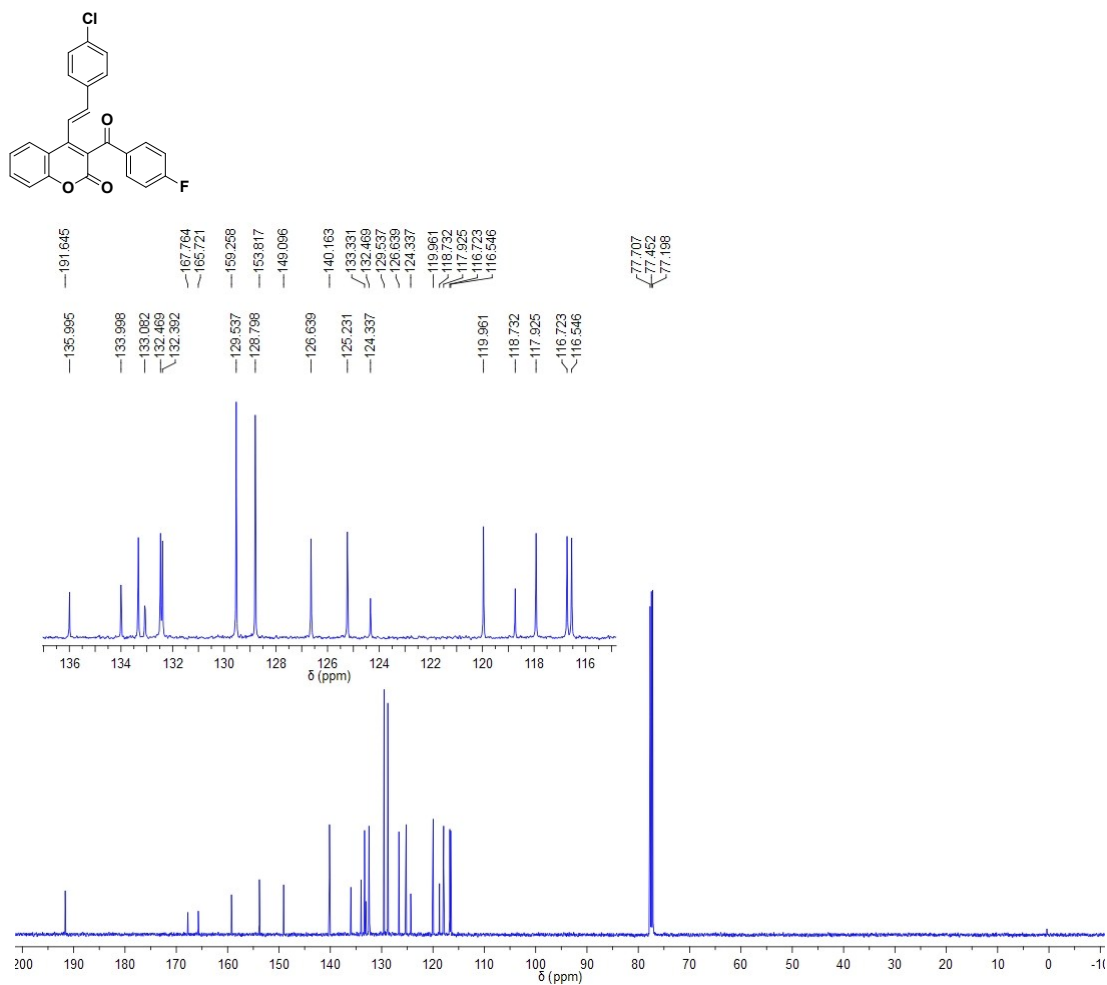
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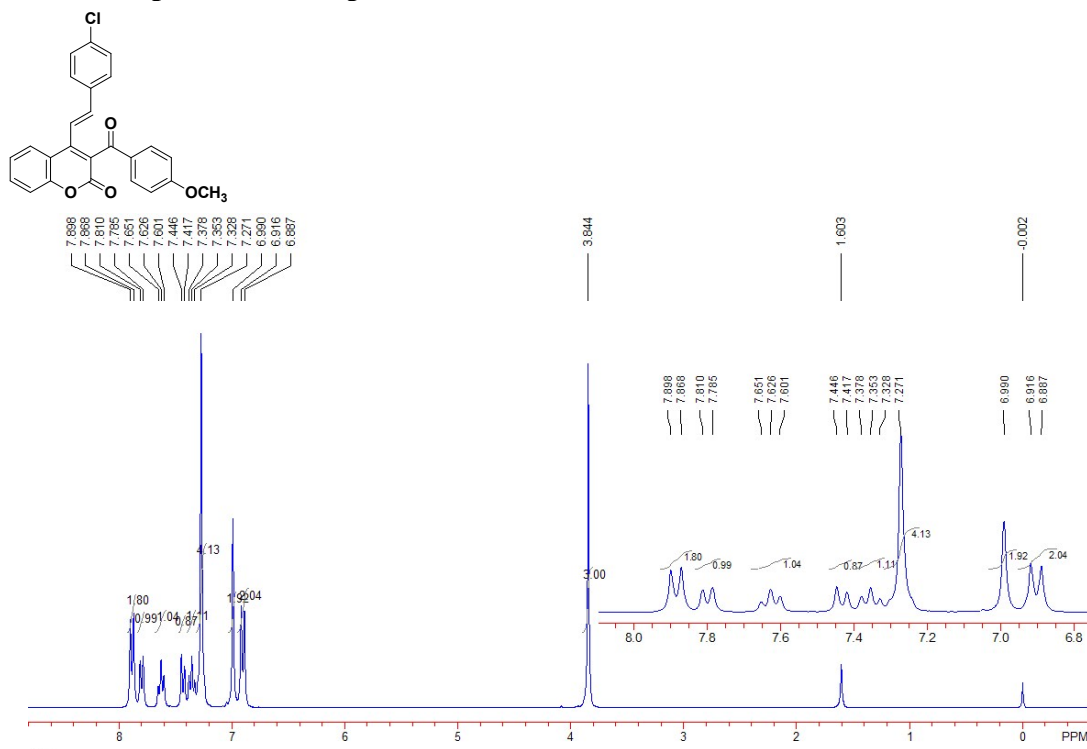
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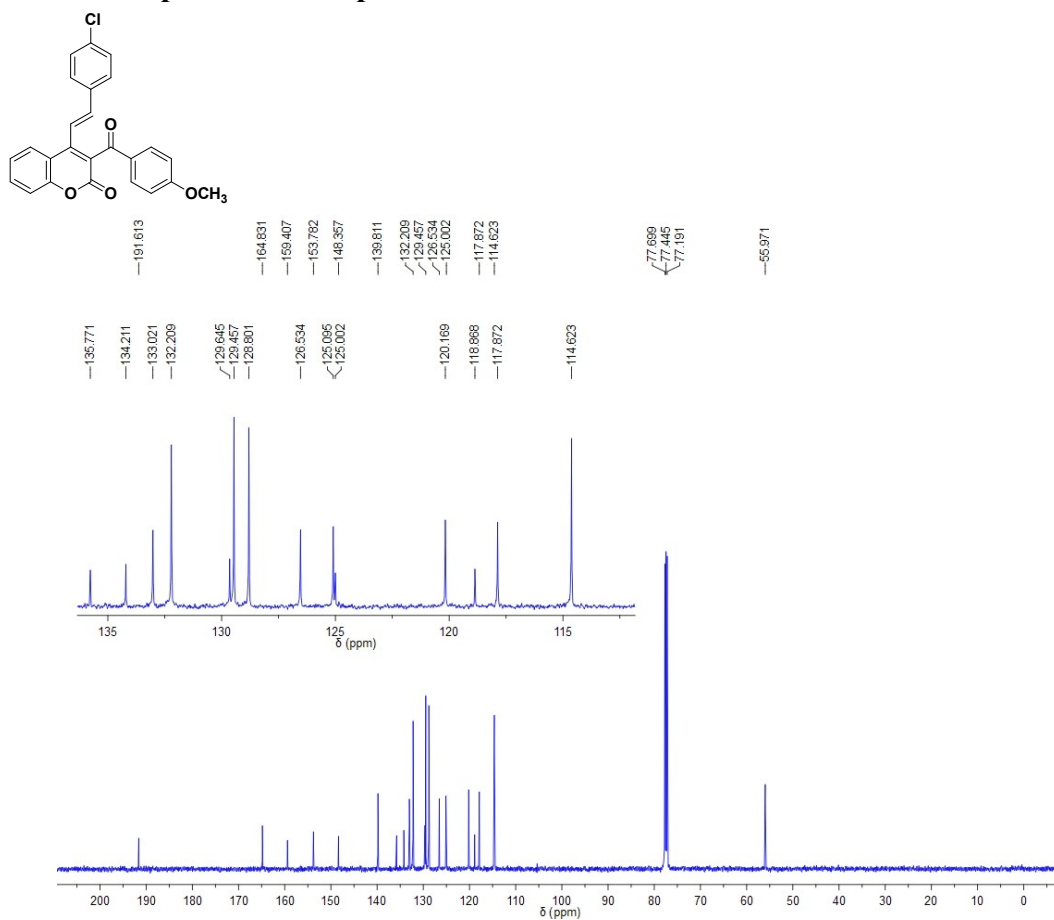
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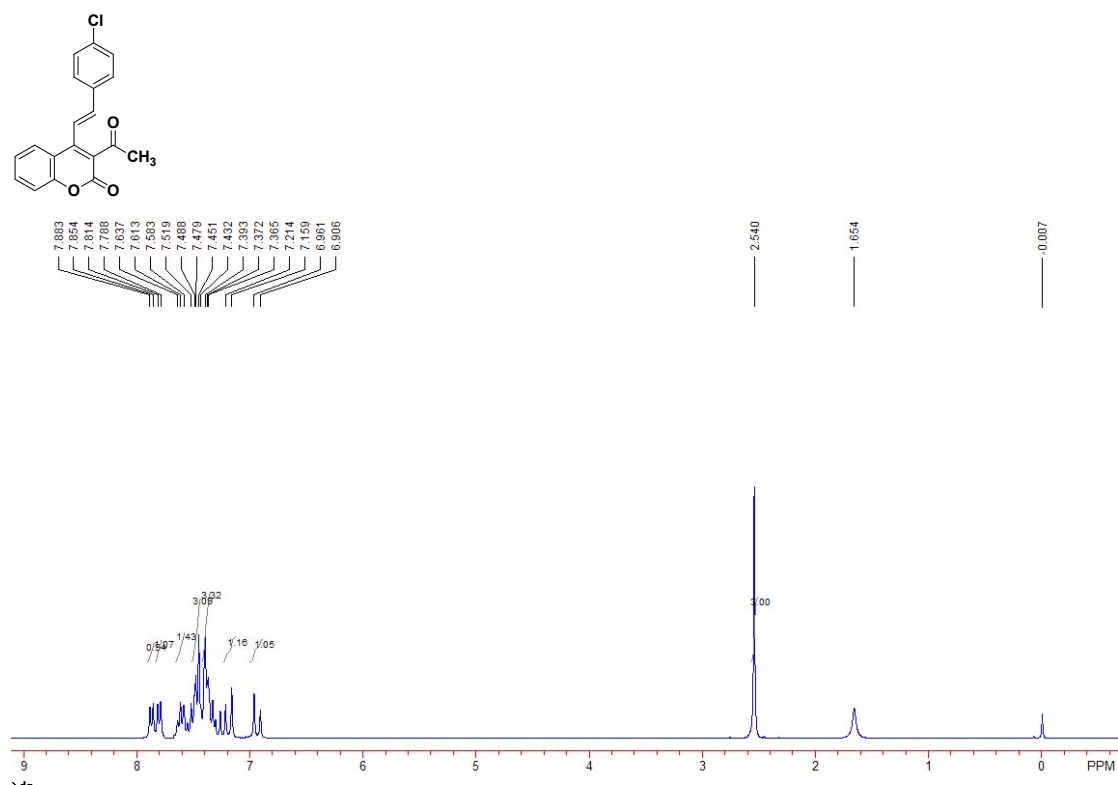
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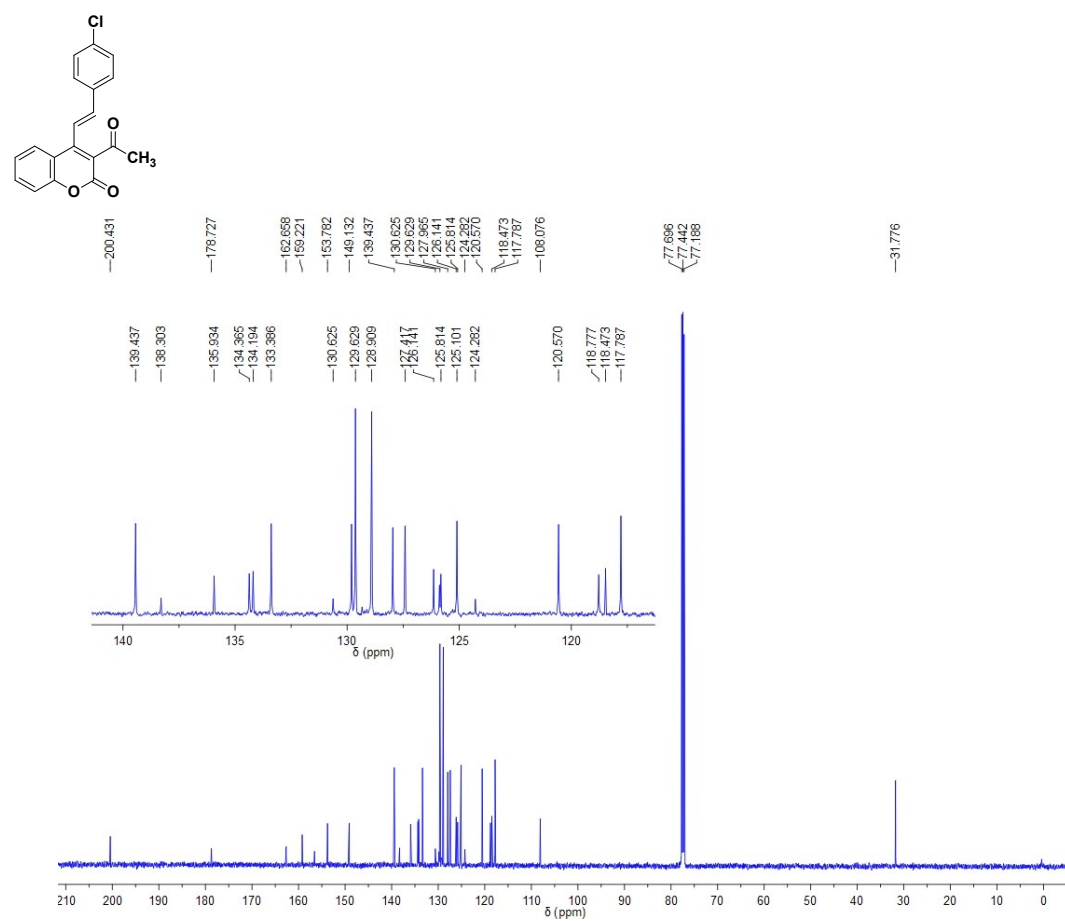
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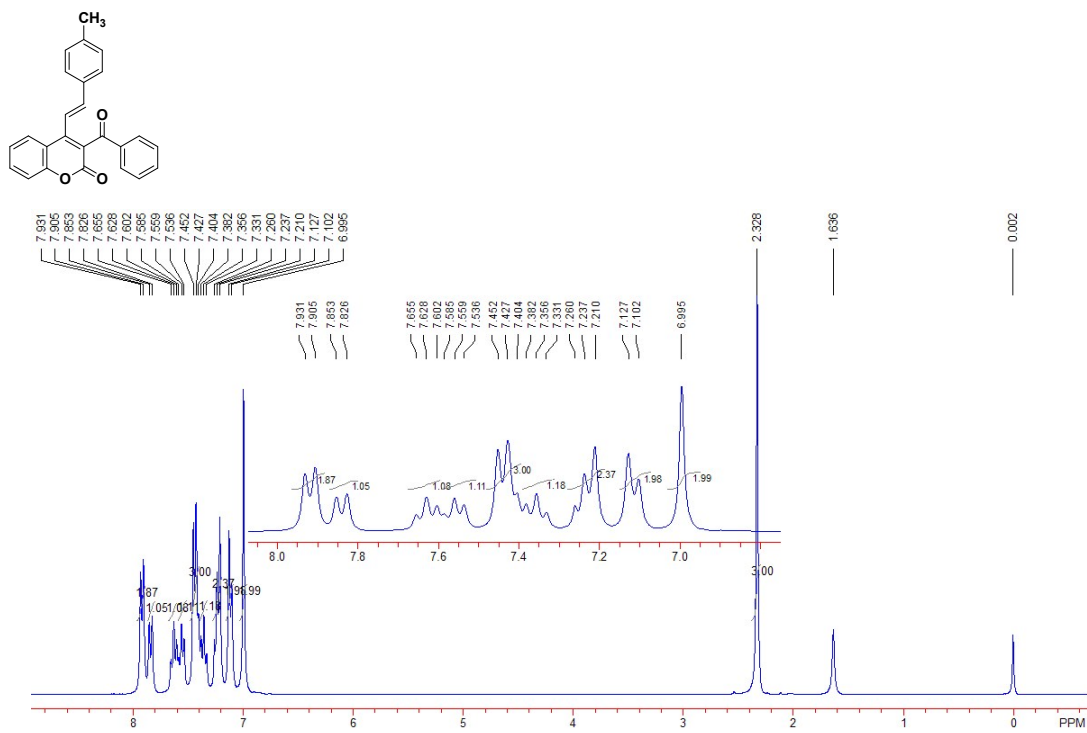
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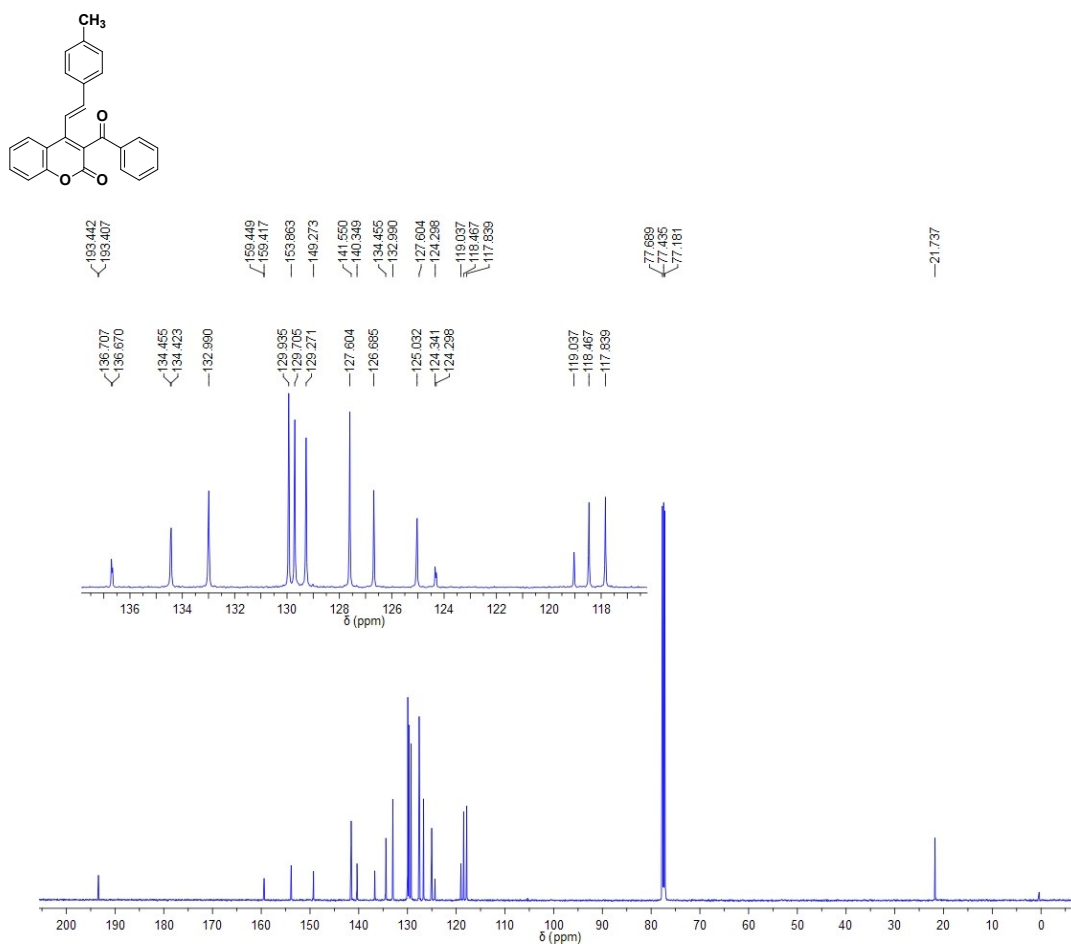
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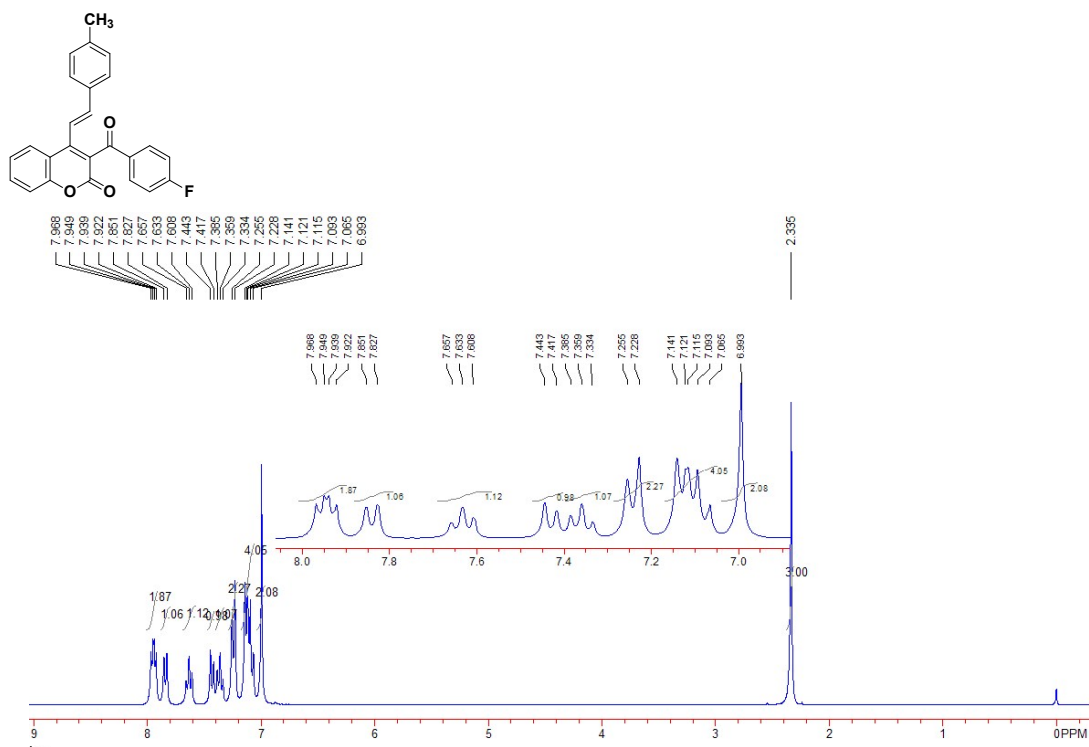
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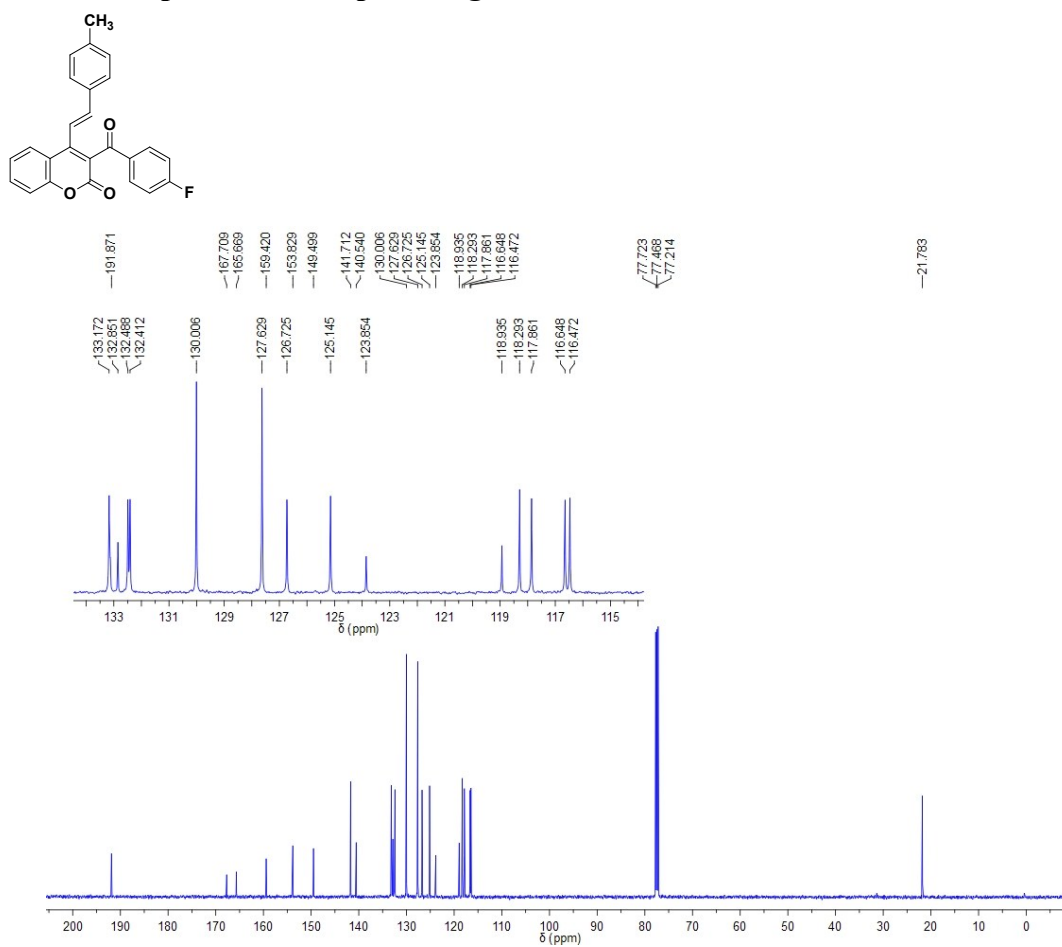
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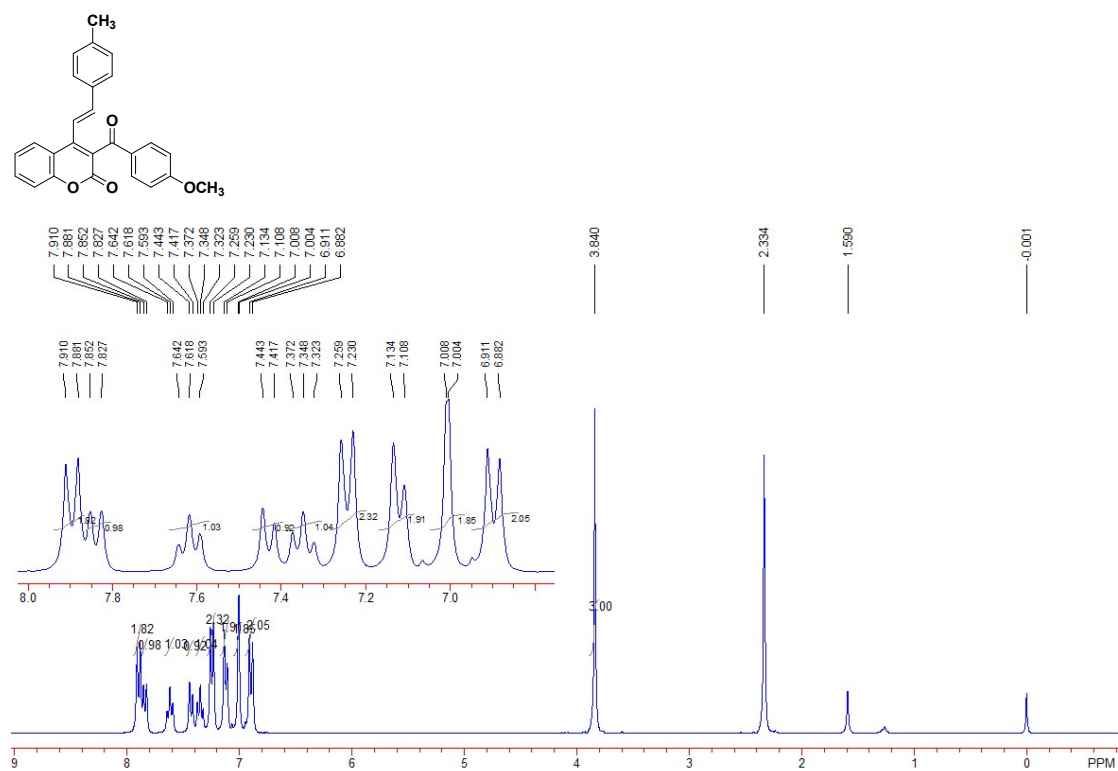
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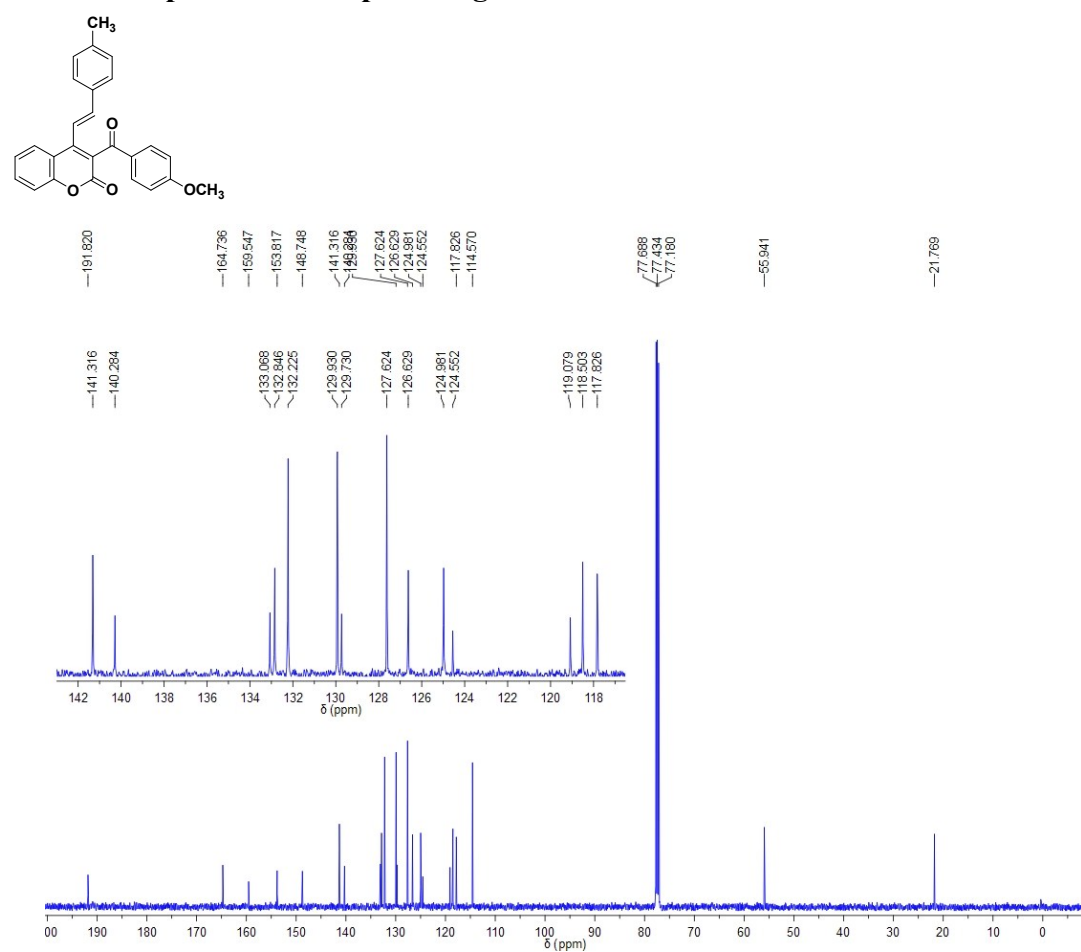
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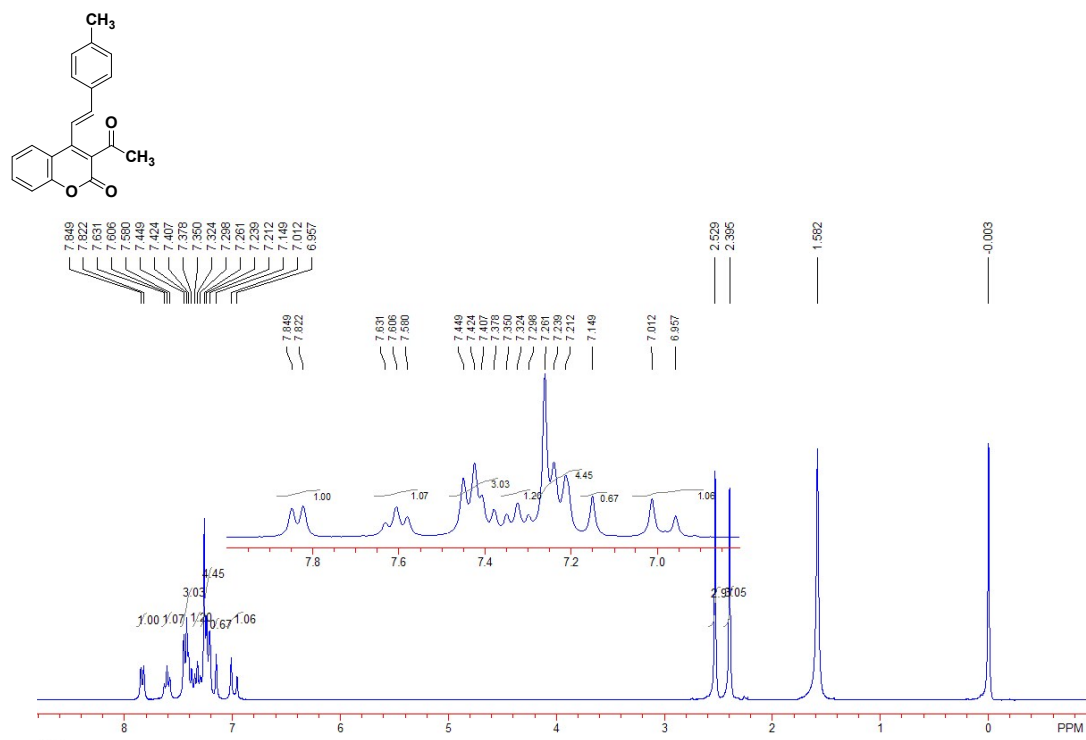
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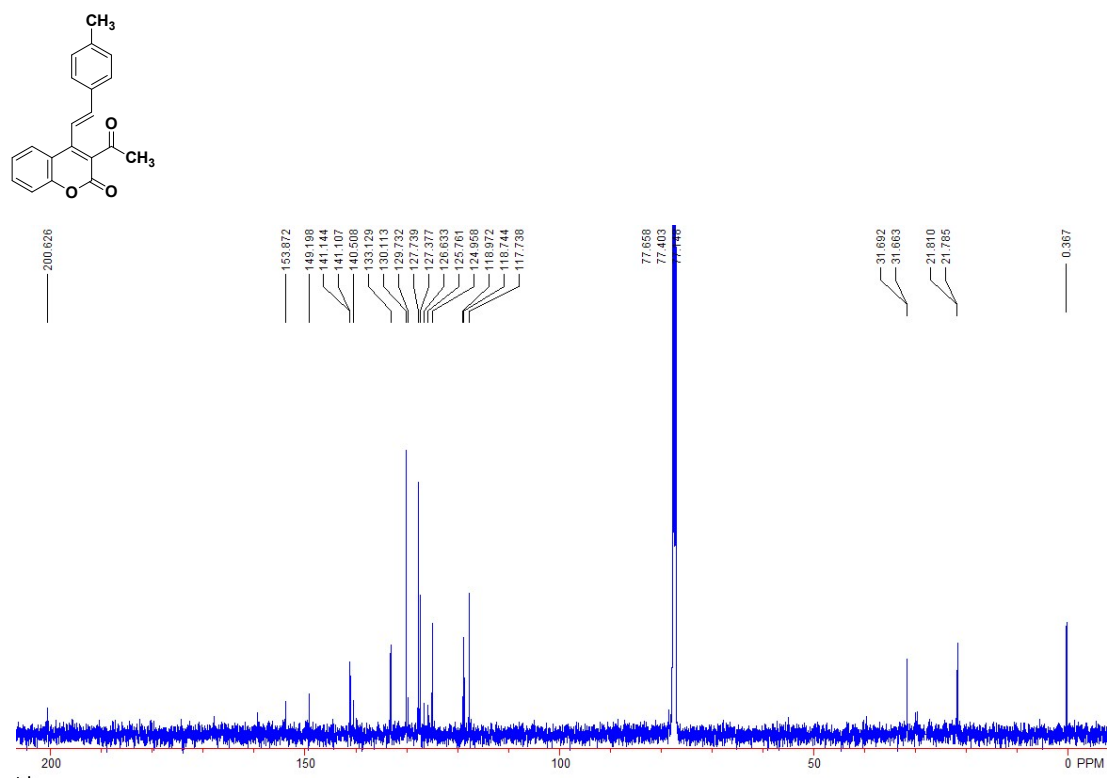
¹³C NMR Spectra of Compound 3gc



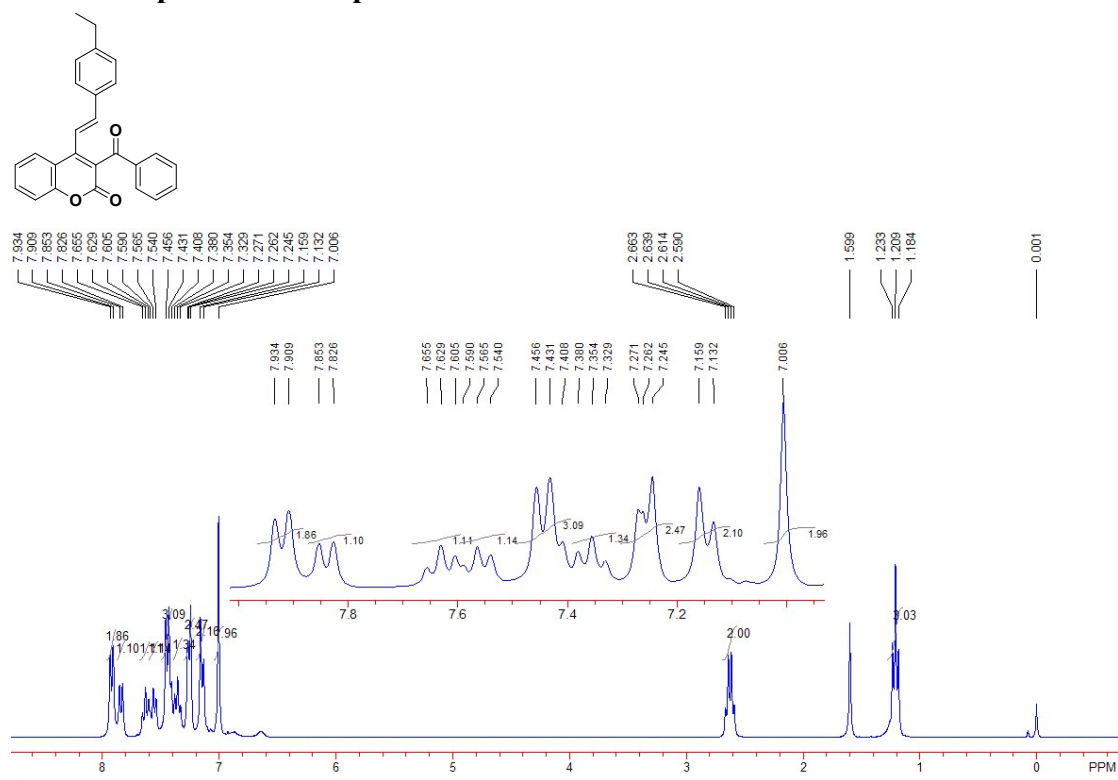
¹H NMR and ¹³C NMR Spectra of Compound 3gd



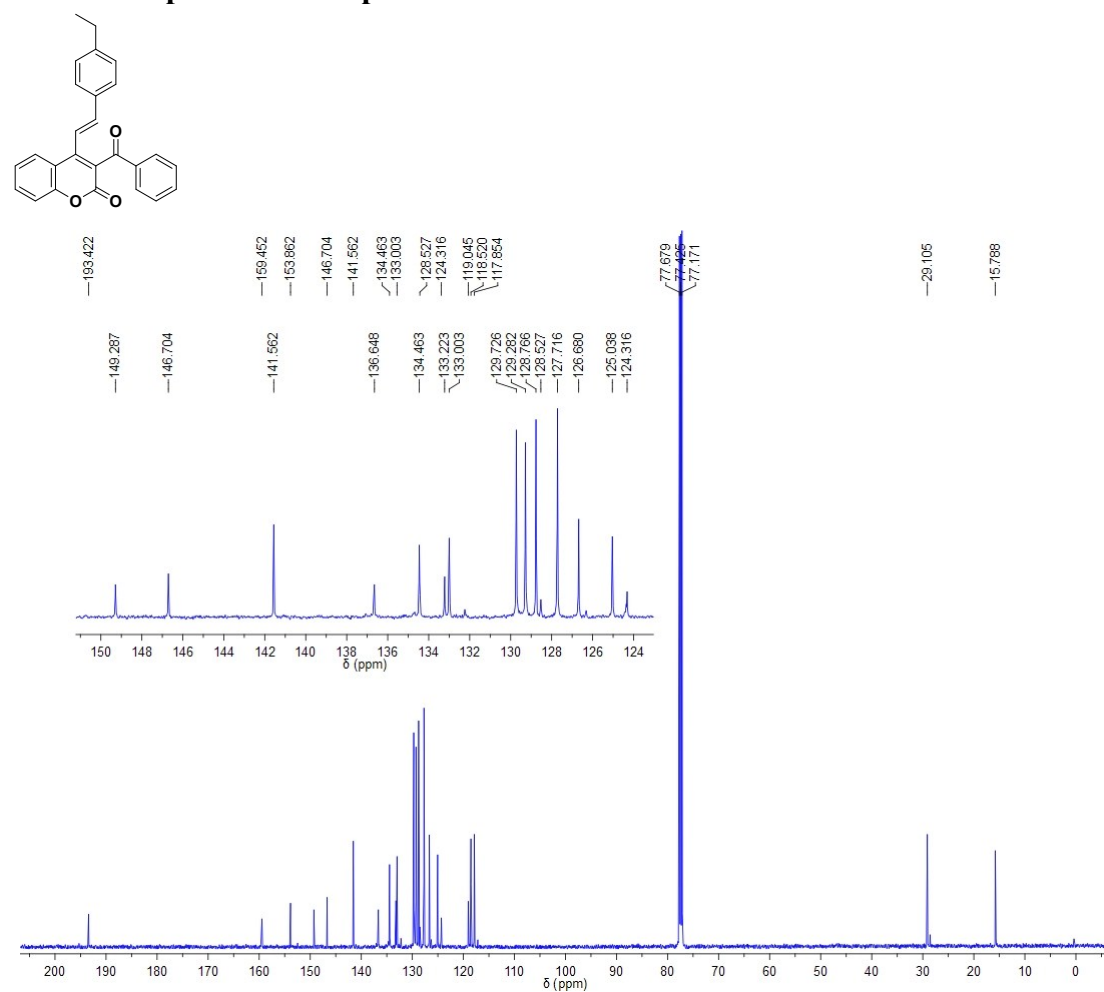
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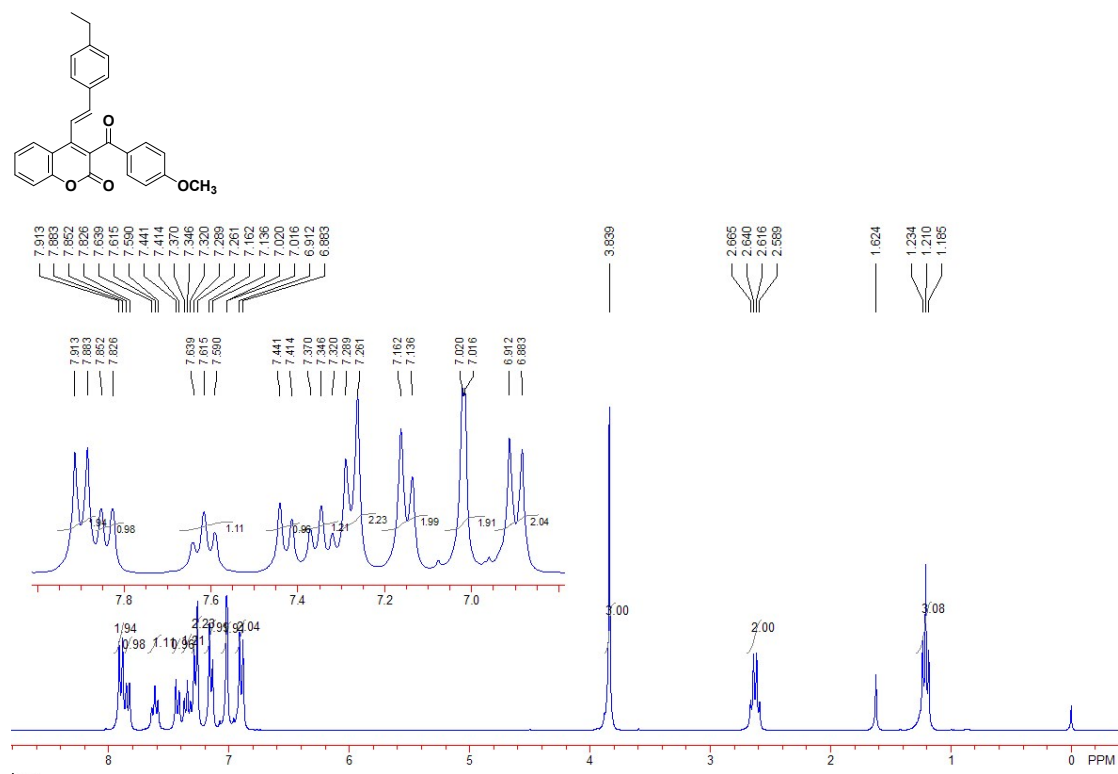
¹H NMR Spectra of Compound 3ha



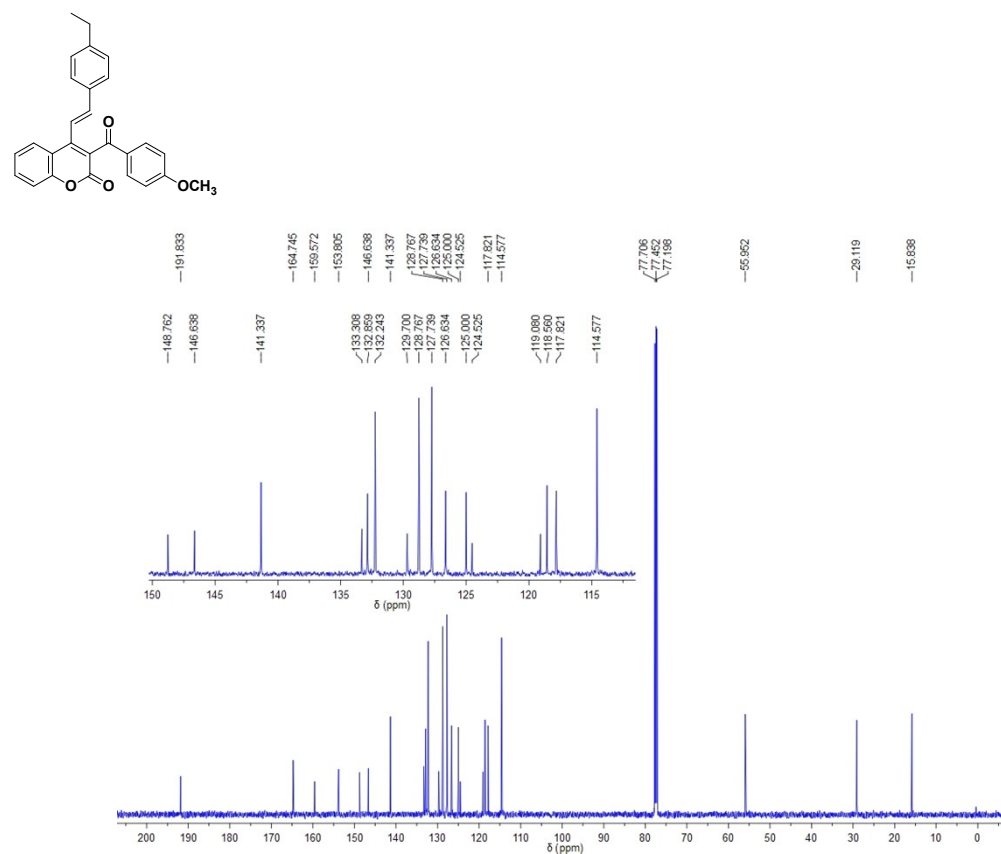
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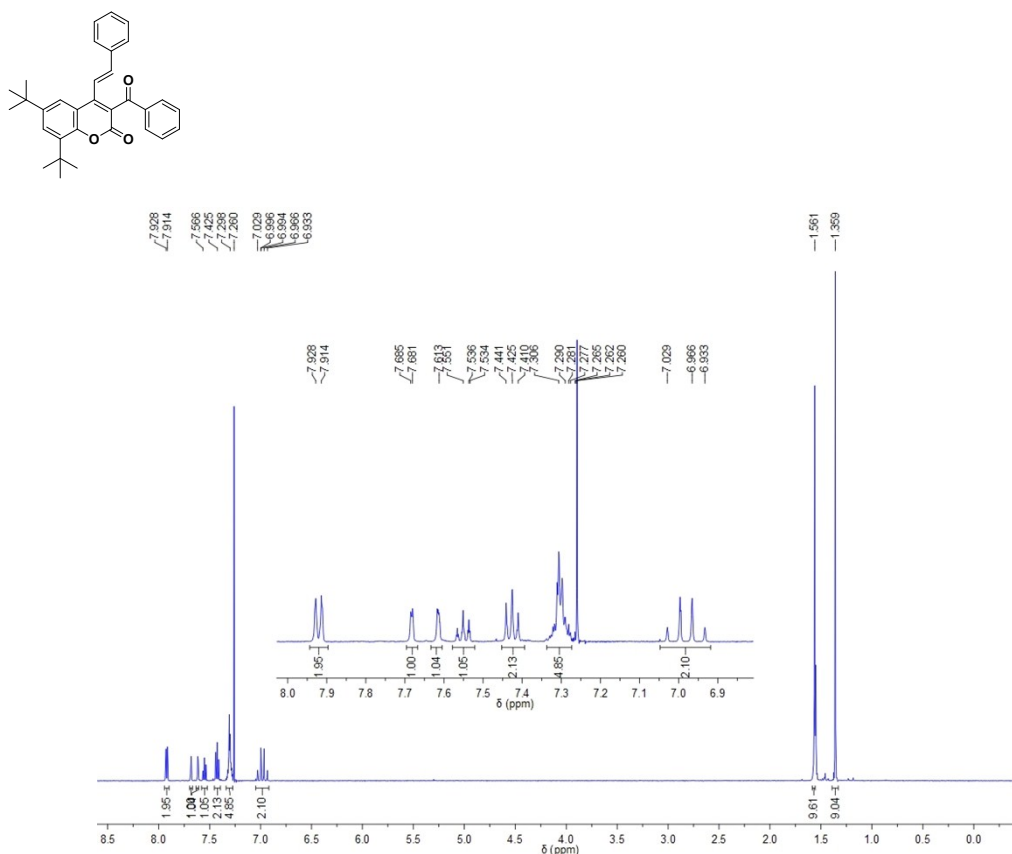
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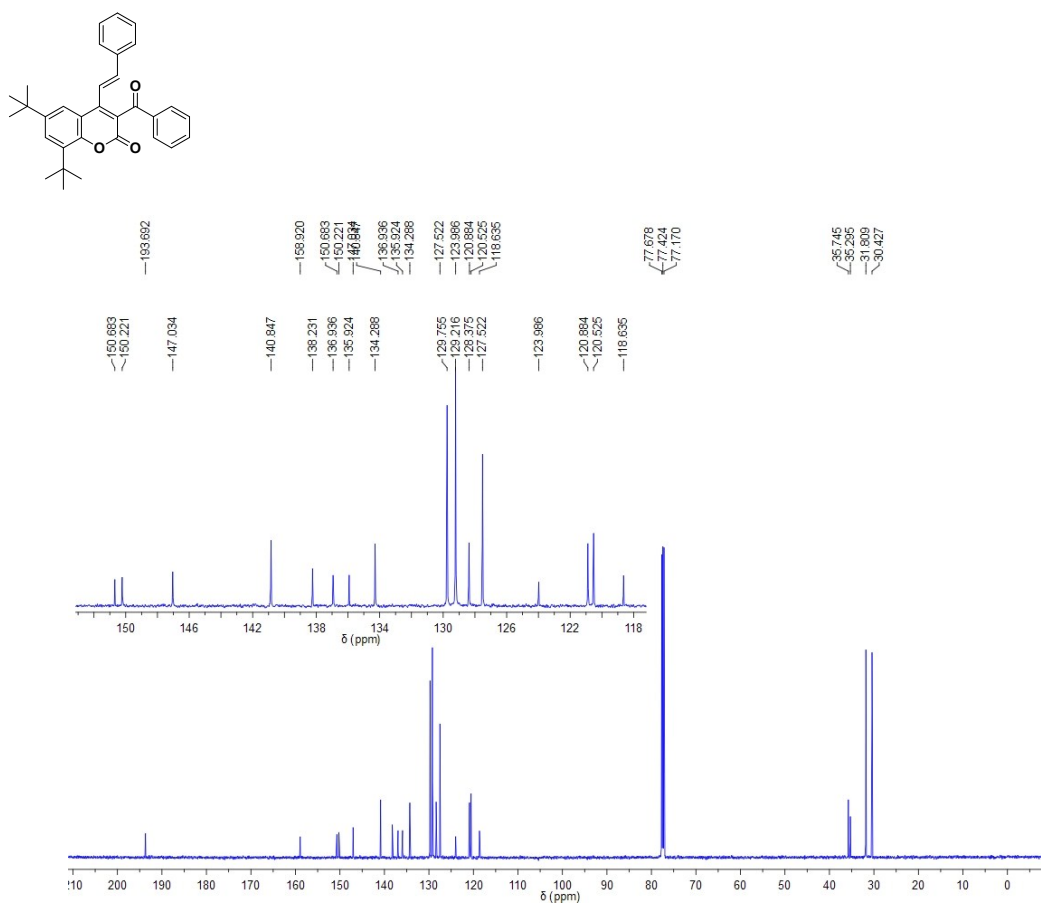
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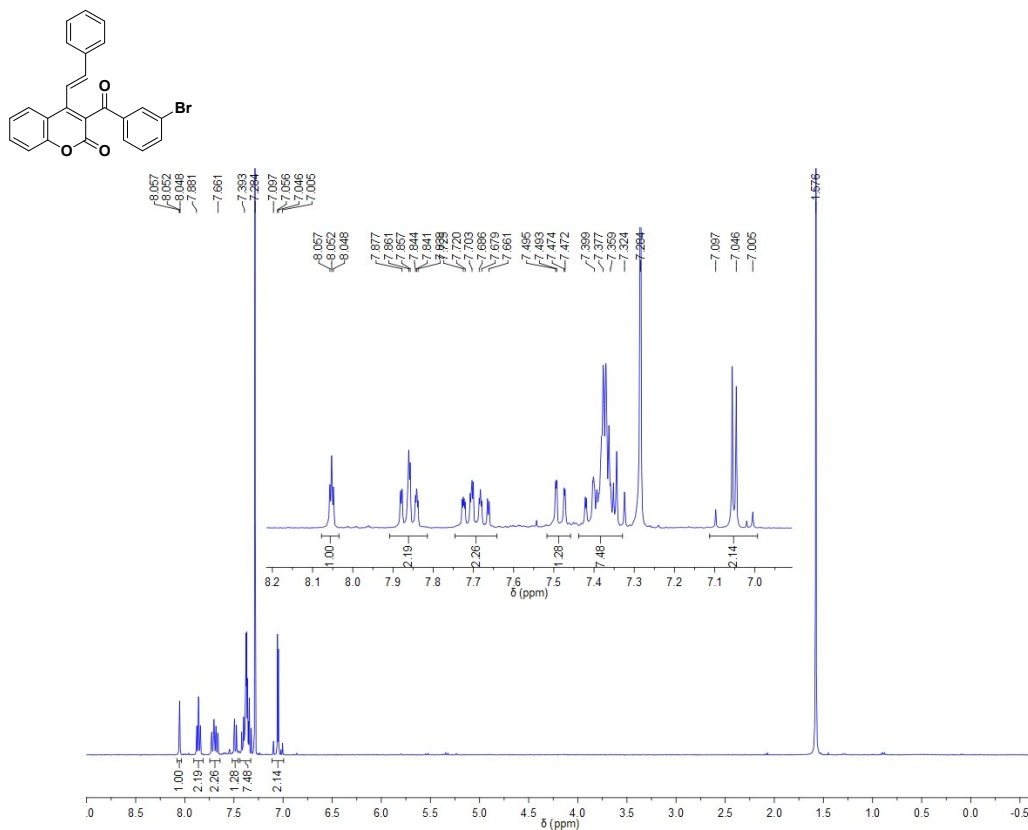
¹H NMR Spectra of Compound 3ia



¹³C NMR Spectra of Compound 3ia



¹H NMR Spectra of Compound 3ae



¹³C NMR Spectra of Compound 3ae

