Supporting Information for

Gold-catalyzed synthesis of 1*H*-isochromene-4-carbaldehydes *via* oxidative cascade cyclization†

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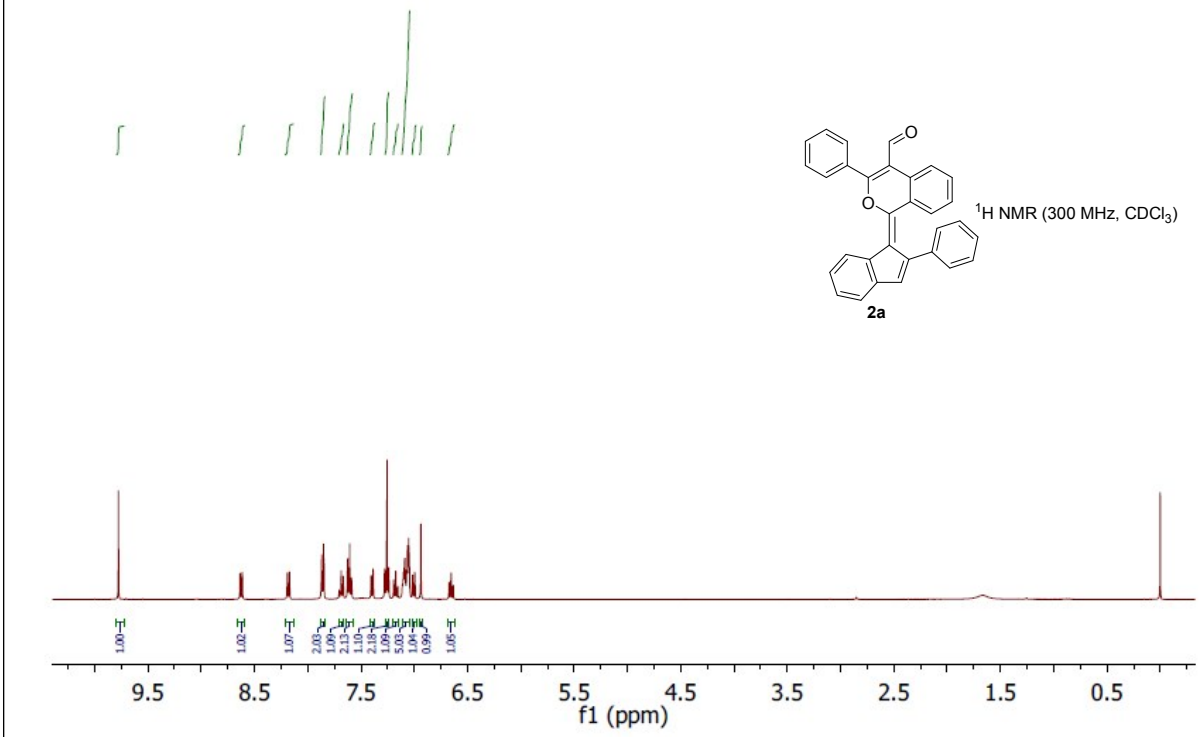
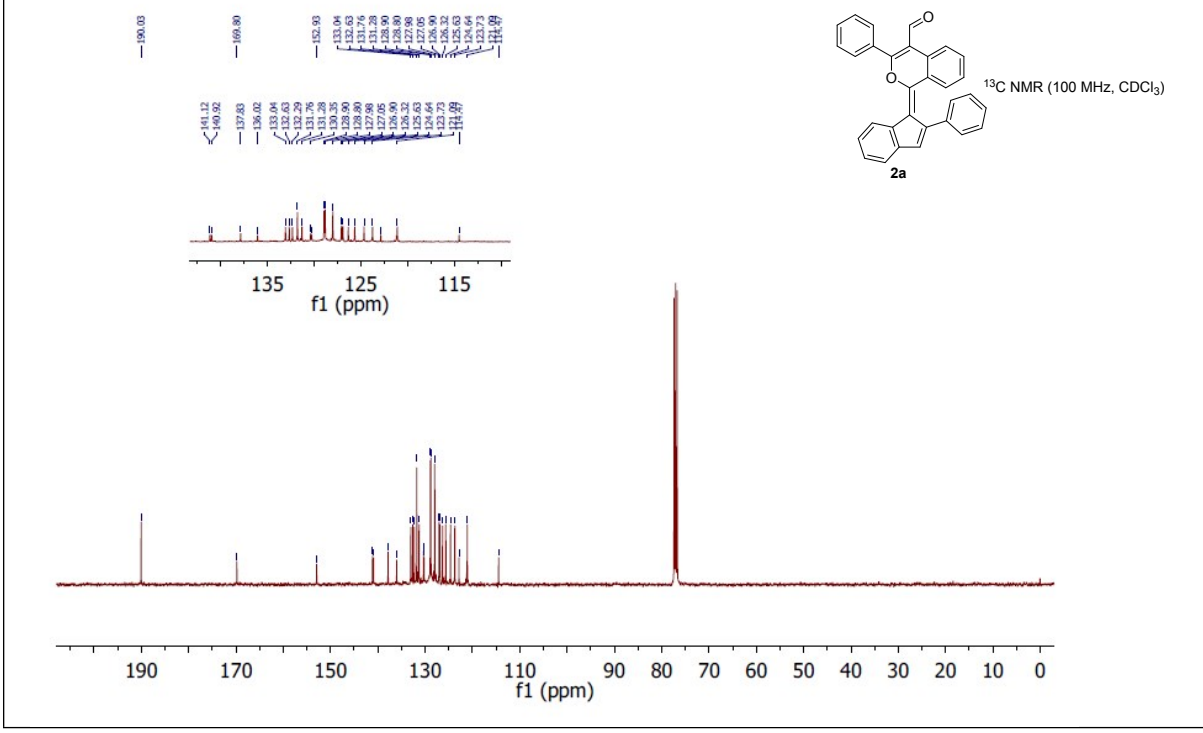
Contents:

Electronic Supplementary Material (ESI) for Chemical Communications

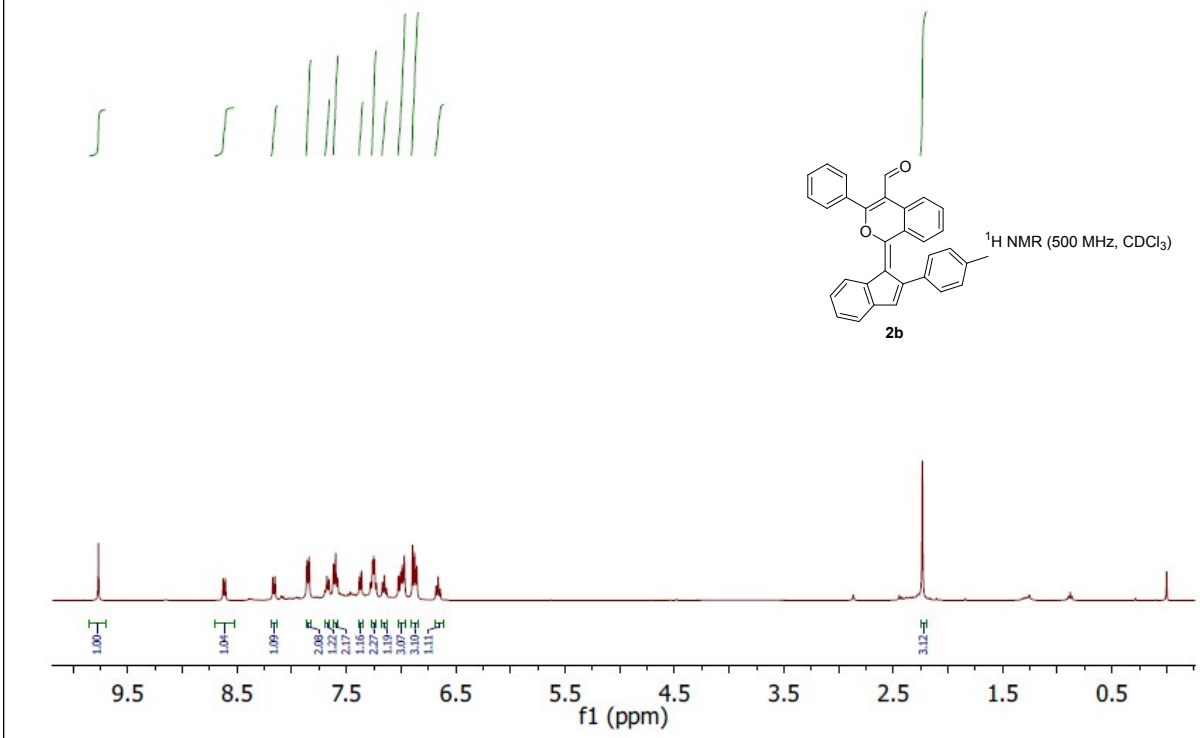
1. Copies of ^{1}H and ^{13}C NMR spectra (2a-2r)

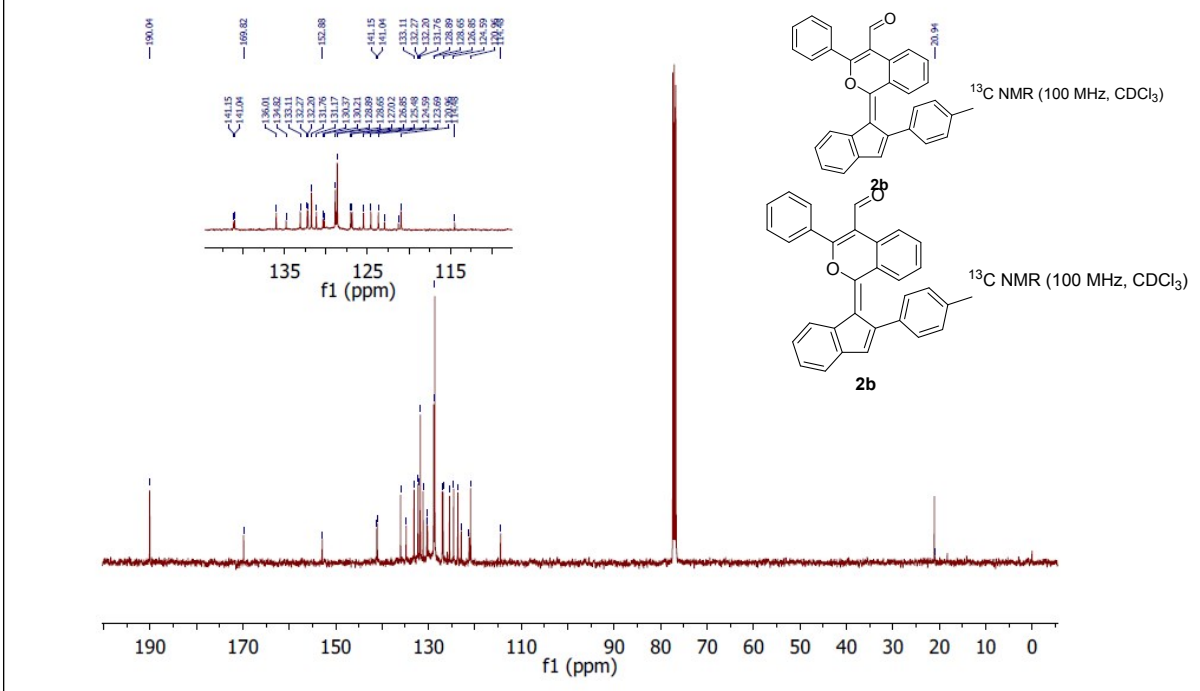
(*E*)-3-Phenyl-1-(2-phenyl-1*H*-inden-1-ylidene)-1*H*-isochromene-4-carbaldehyde-2a



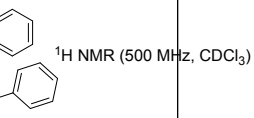


(*E*)-3-Phenyl-1-(2-(*p*-tolyl)-1*H*-inden-1-ylidene)-1*H*-isochromene-4-carbaldehyde-2b

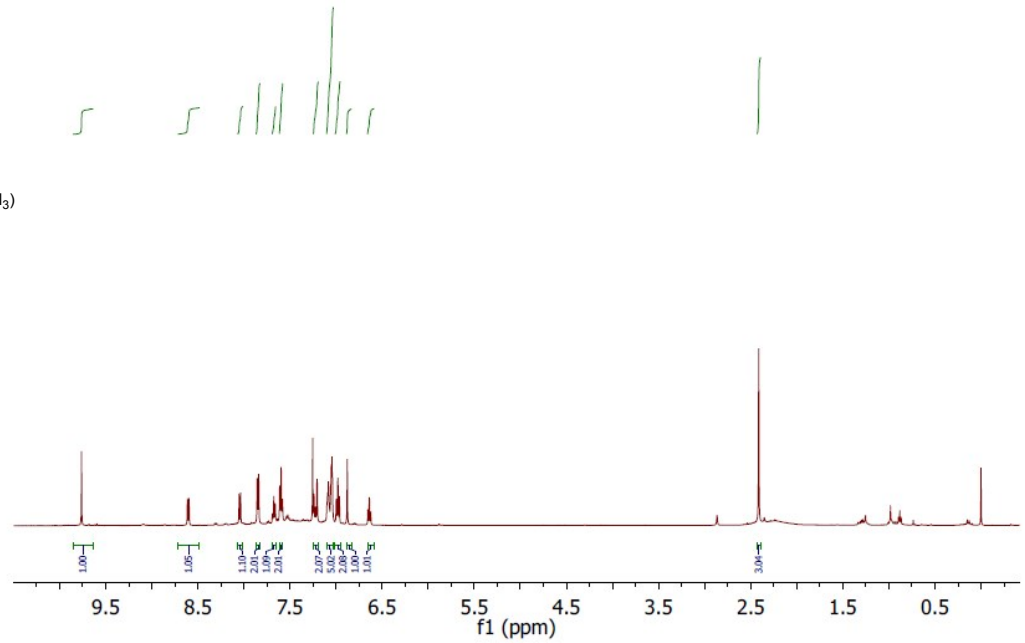


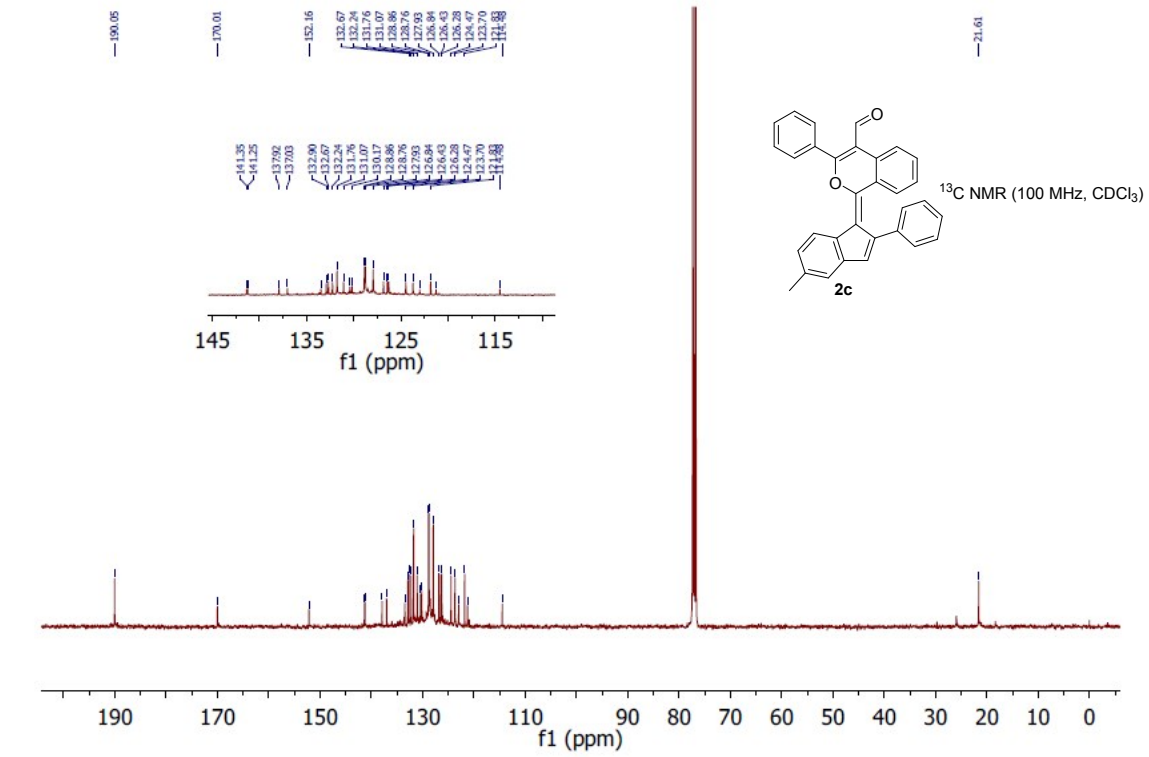


(*E*)-1-(5-Methyl-2-phenyl-1*H*-inden-1-ylidene)-3-phenyl-1*H*-isochromene-4-carbaldehyde-2c



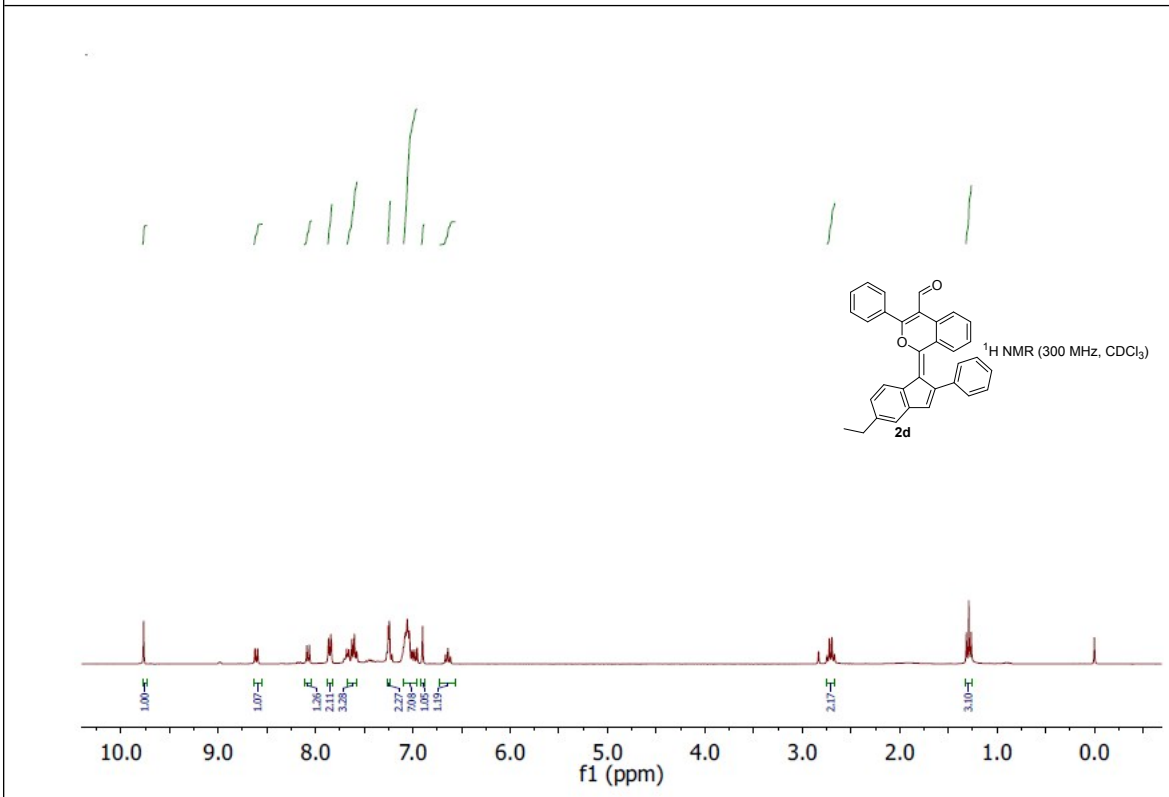
^{1}H NMR (500 MHz, $CDCl_3$)

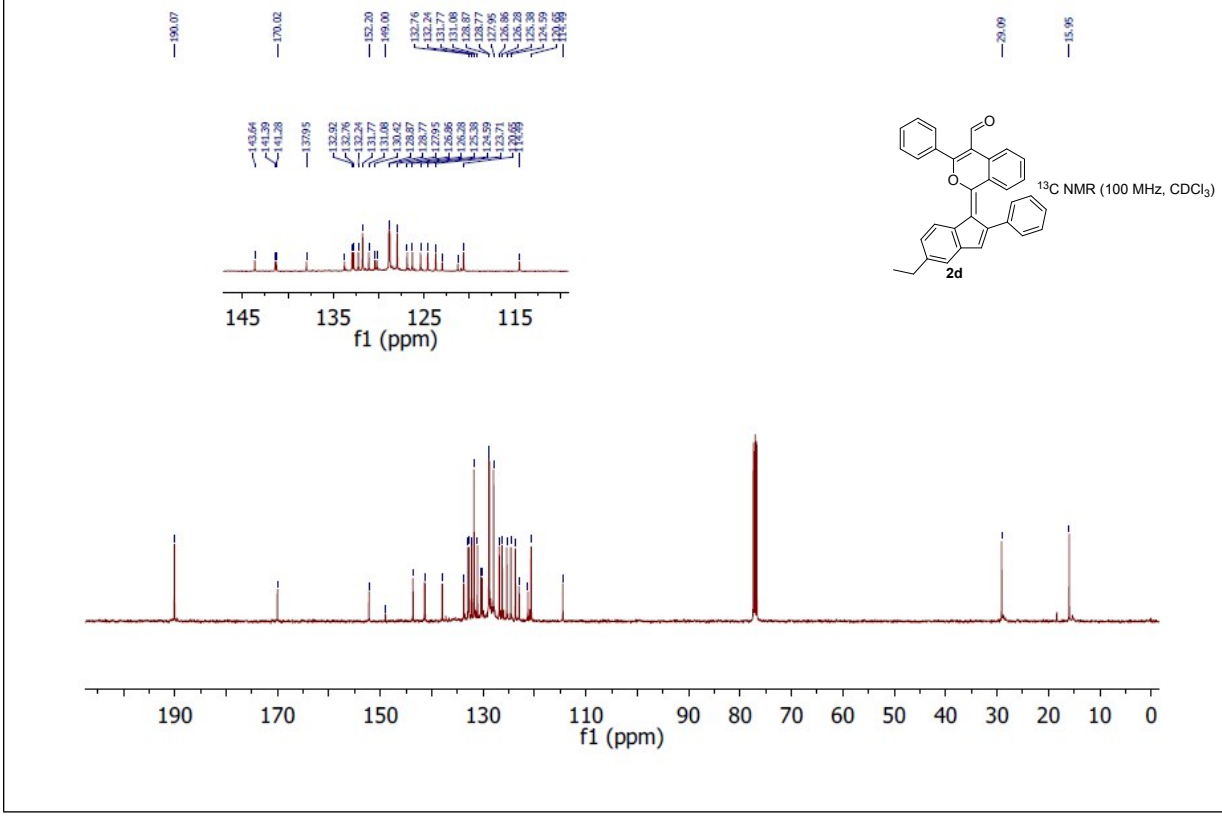




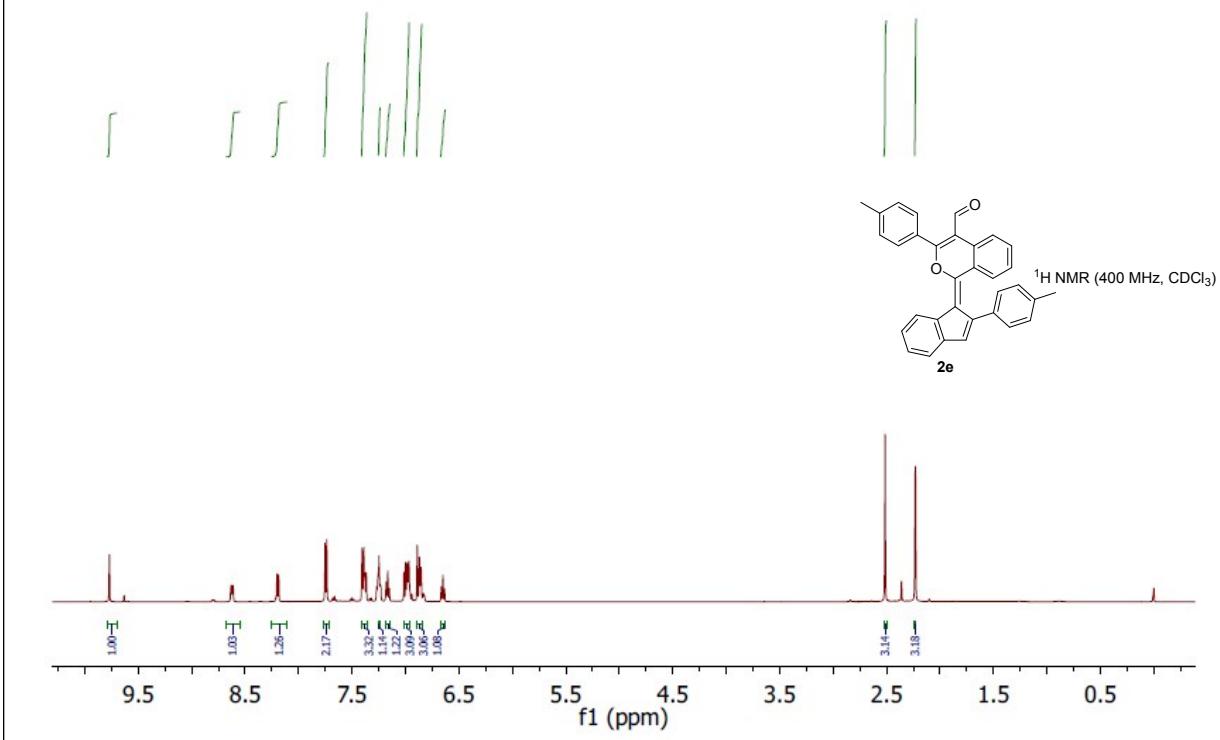
^{13}C NMR (100 MHz, $CDCl_3$)

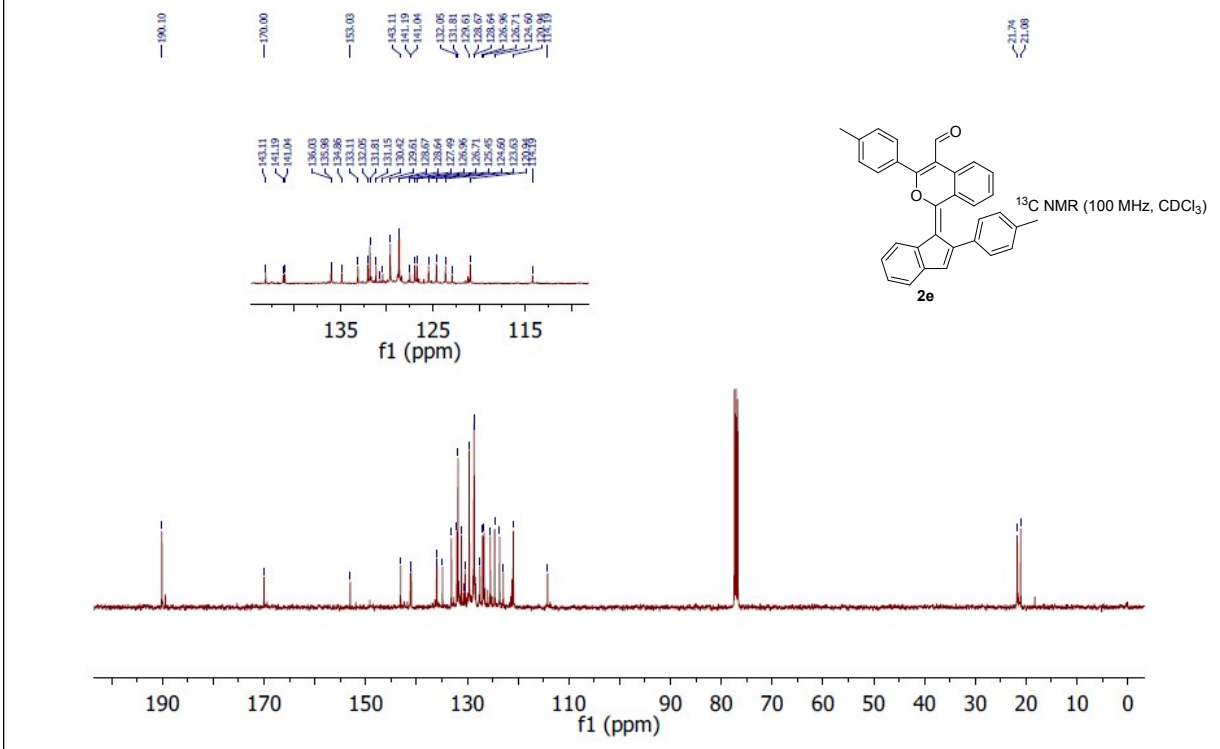
(*E*)-1-(5-Ethyl-2-phenyl-1*H*-inden-1-ylidene)-3-phenyl-1*H*-isochromene-4-carbaldehyde -2d



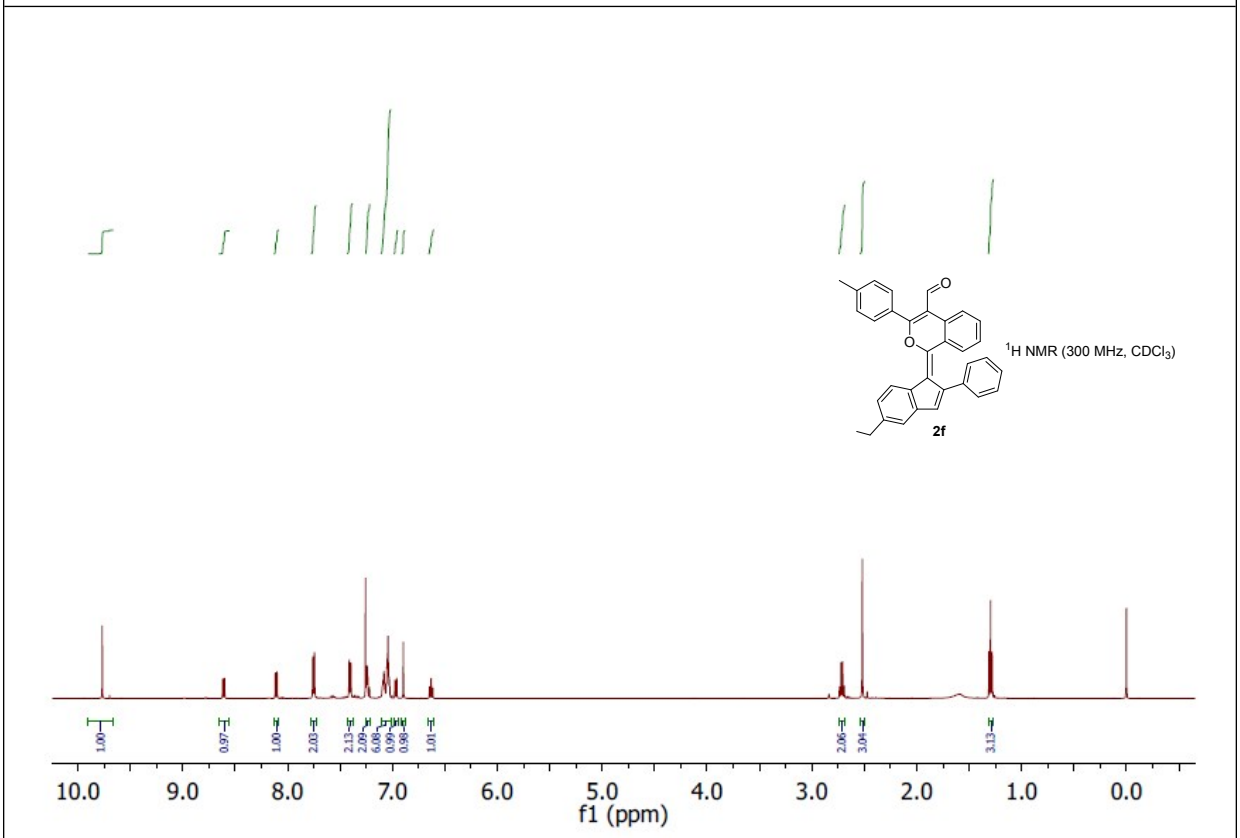


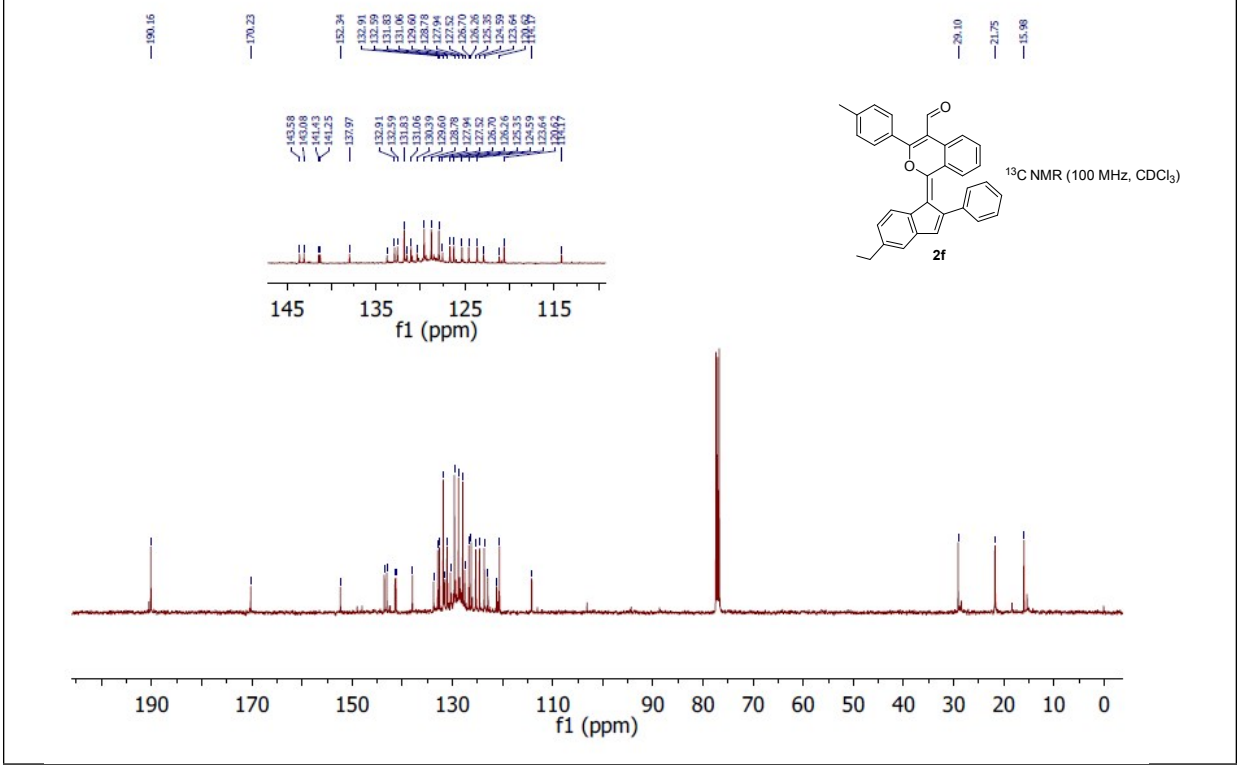
(*E*)-3-(*p*-Tolyl)-1-(2-(*p*-tolyl)-1*H*-inden-1-ylidene)-1*H*-isochromene-4-carbaldehyde-2e



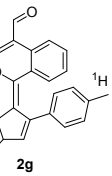


(*E*)-1-(5-Ethyl-2-phenyl-*1H*-inden-1-ylidene)-3-(*p*-tolyl)-*1H*-isochromene-4-carbaldehyde -2f



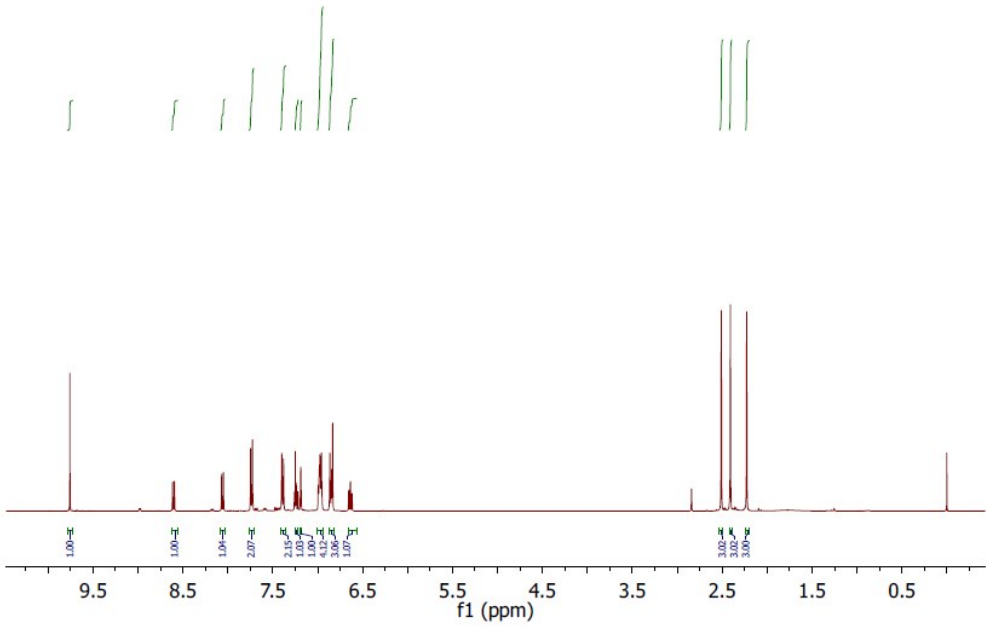


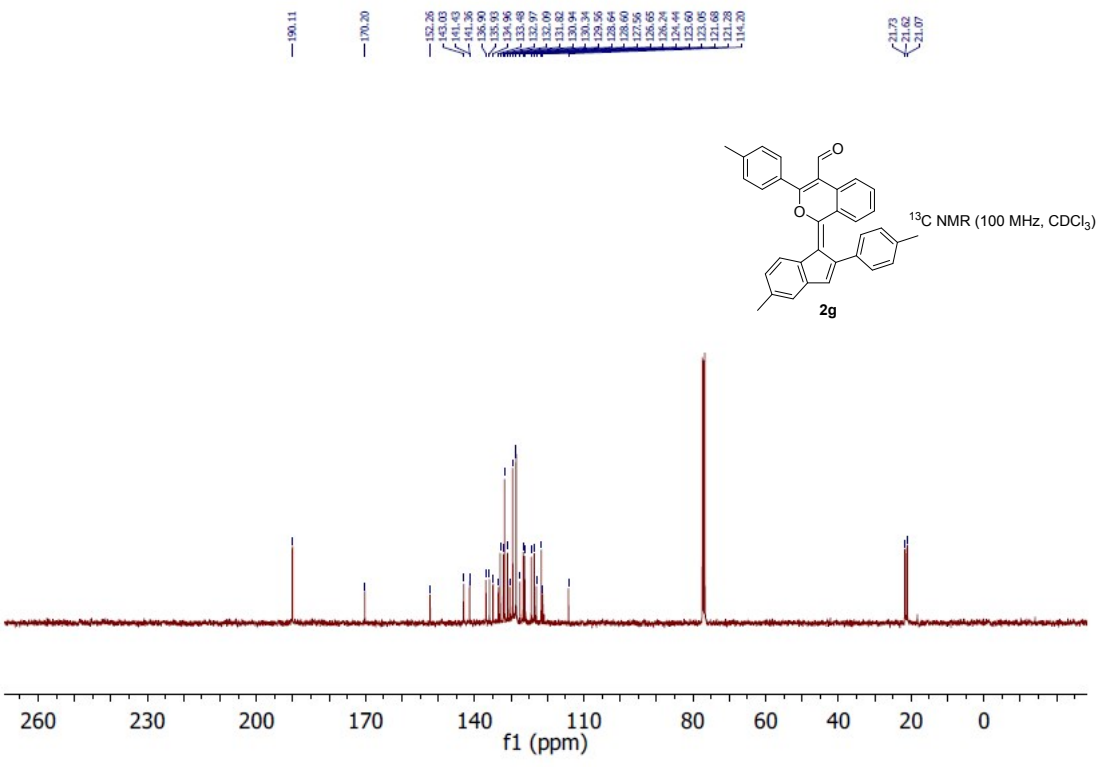
(*E*)-1-(5-Methyl-2-(*p*-tolyl)-*1H*-inden-1-ylidene)-3-(*p*-tolyl)-*1H*-isochromene-4-carbaldehyde-2g



2g

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

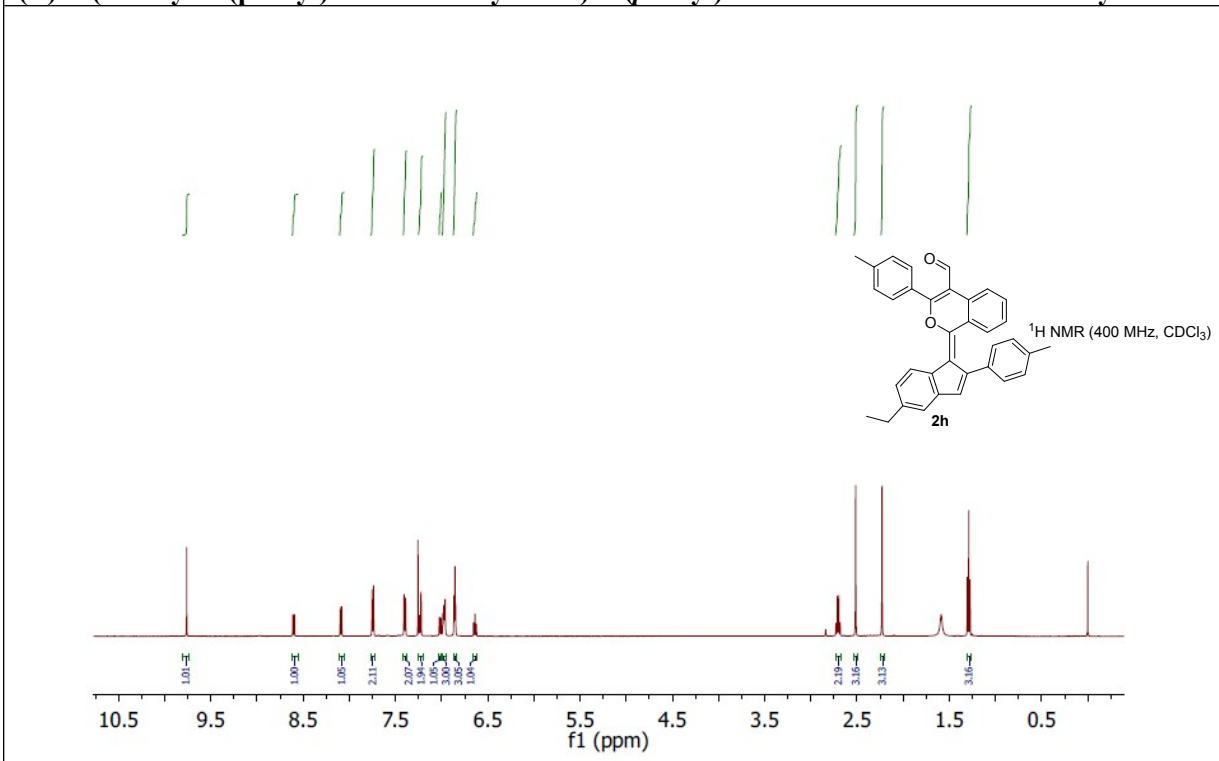


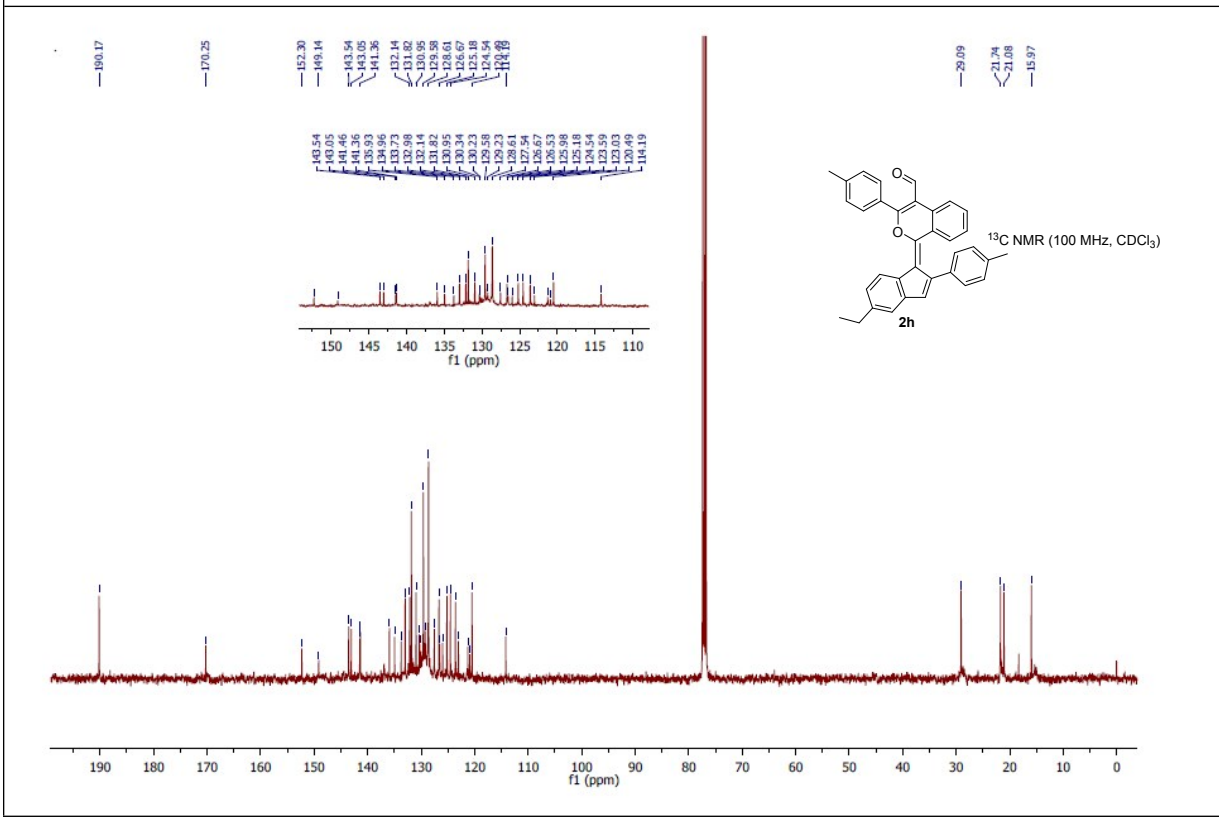


2g

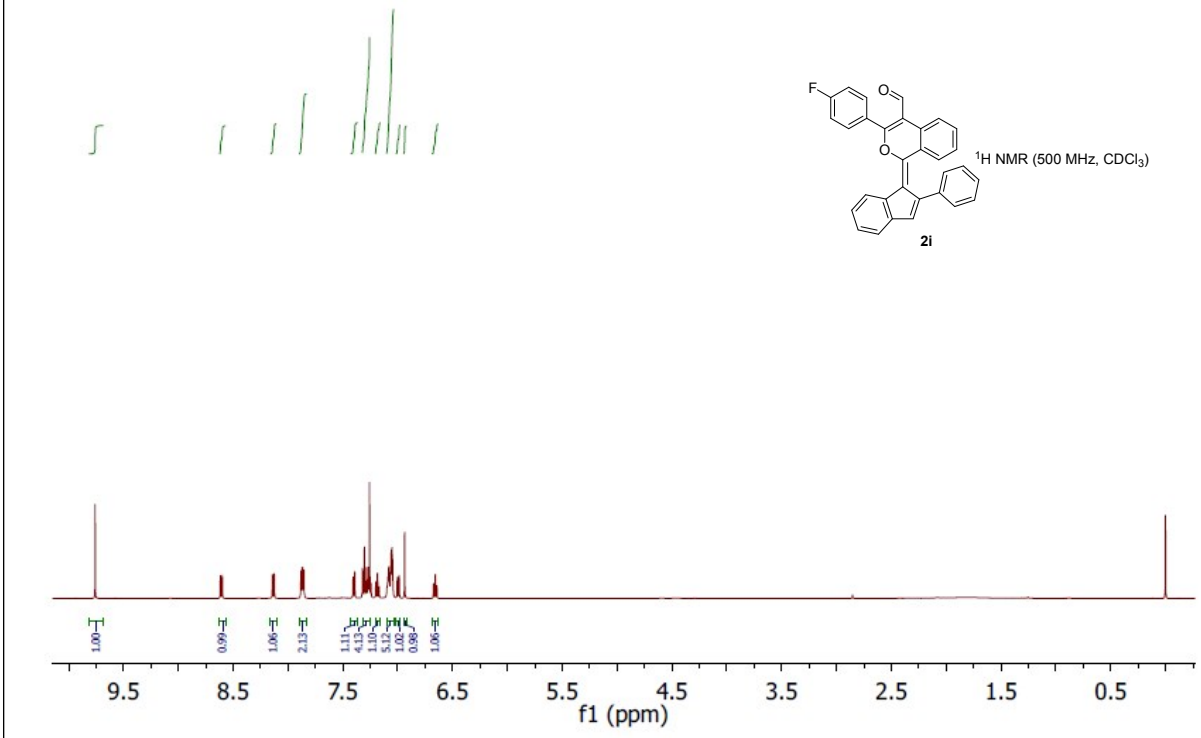
^{13}C NMR (100 MHz, $CDCl_3$)

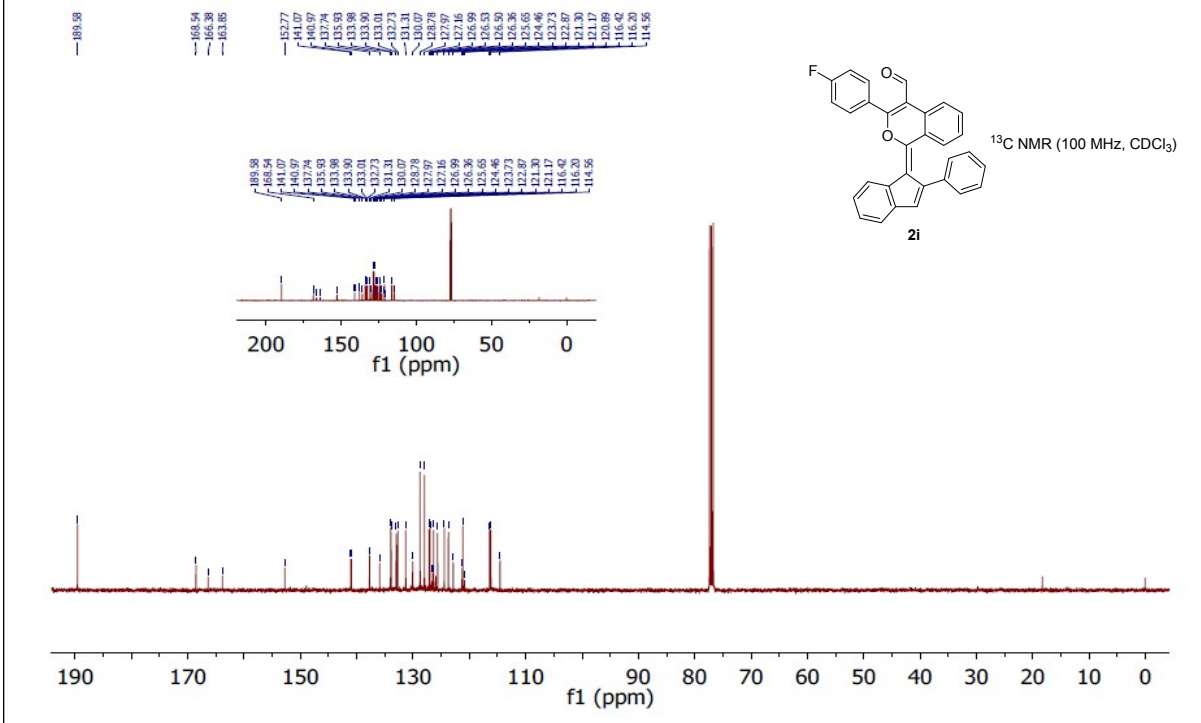
(*E*)-1-(5-Ethyl-2-(p-tolyl)-*1H*-inden-1-ylidene)-3-(*p*-tolyl)-*1H*-isochromene-4-carbaldehyde-2h



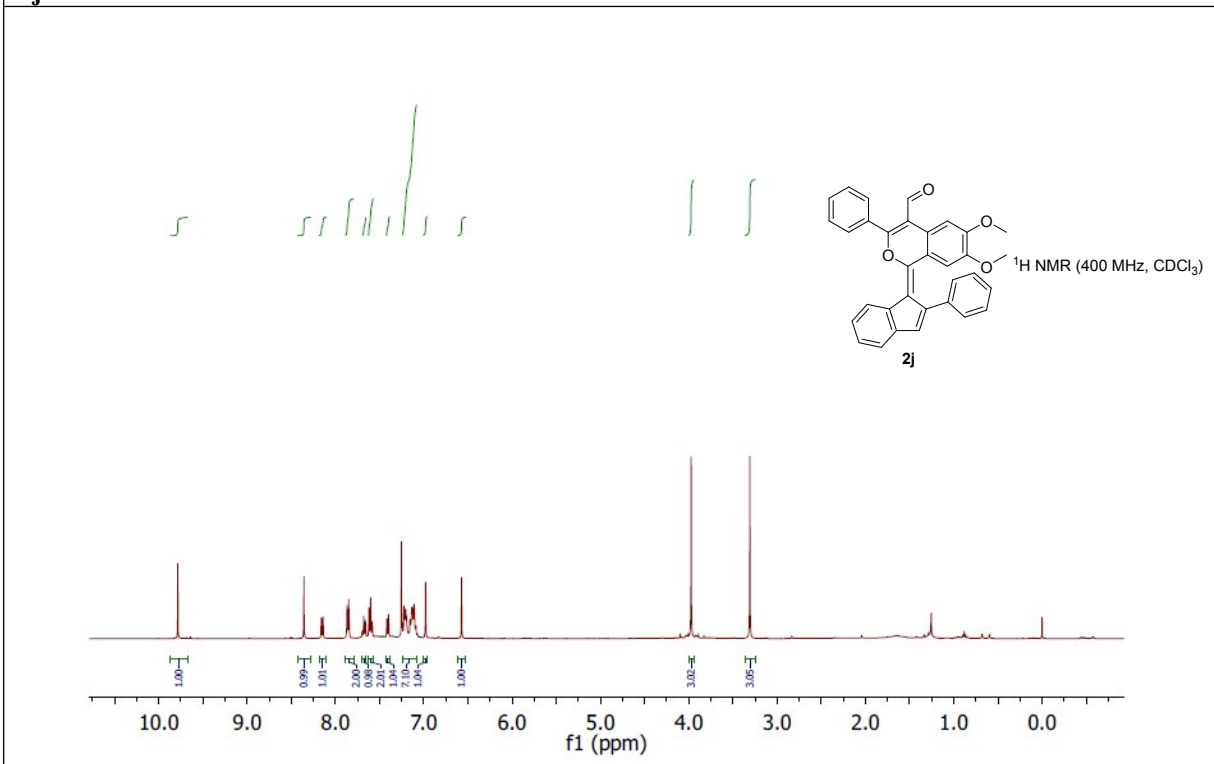


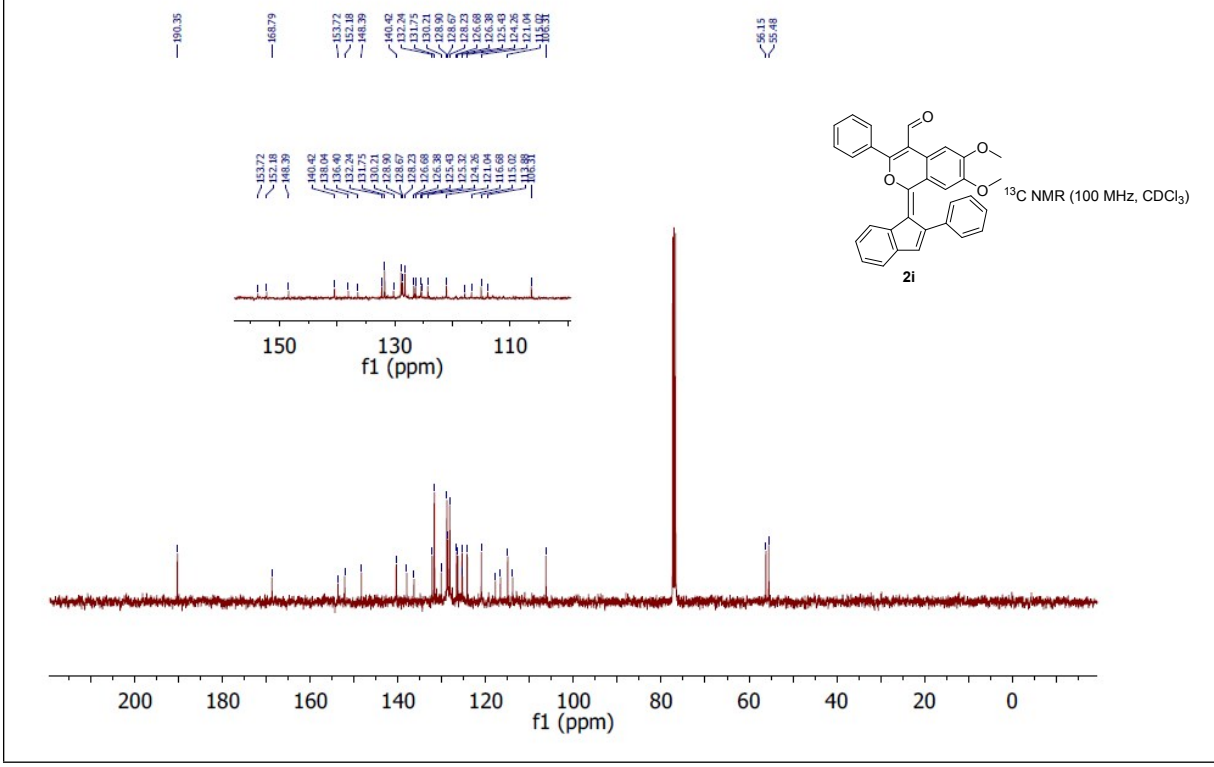
(*E*)-3-(4-Fluorophenyl)-1-(2-phenyl-*1H*-inden-1-ylidene)-*1H*-isochromene-4-carbaldehyde-2i



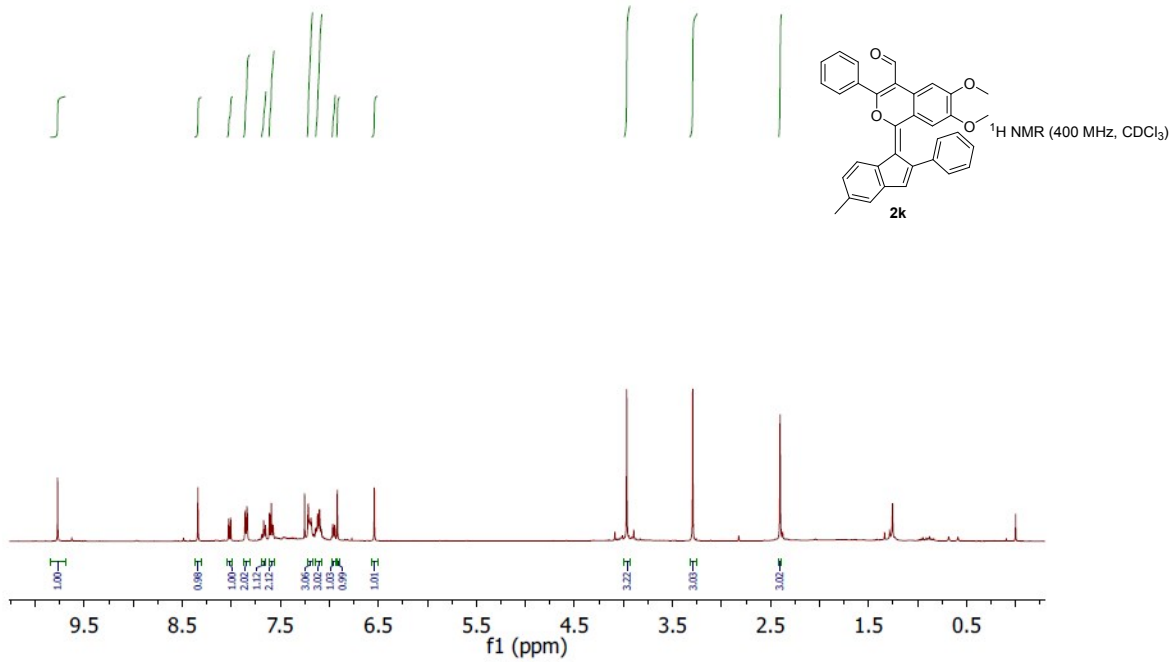


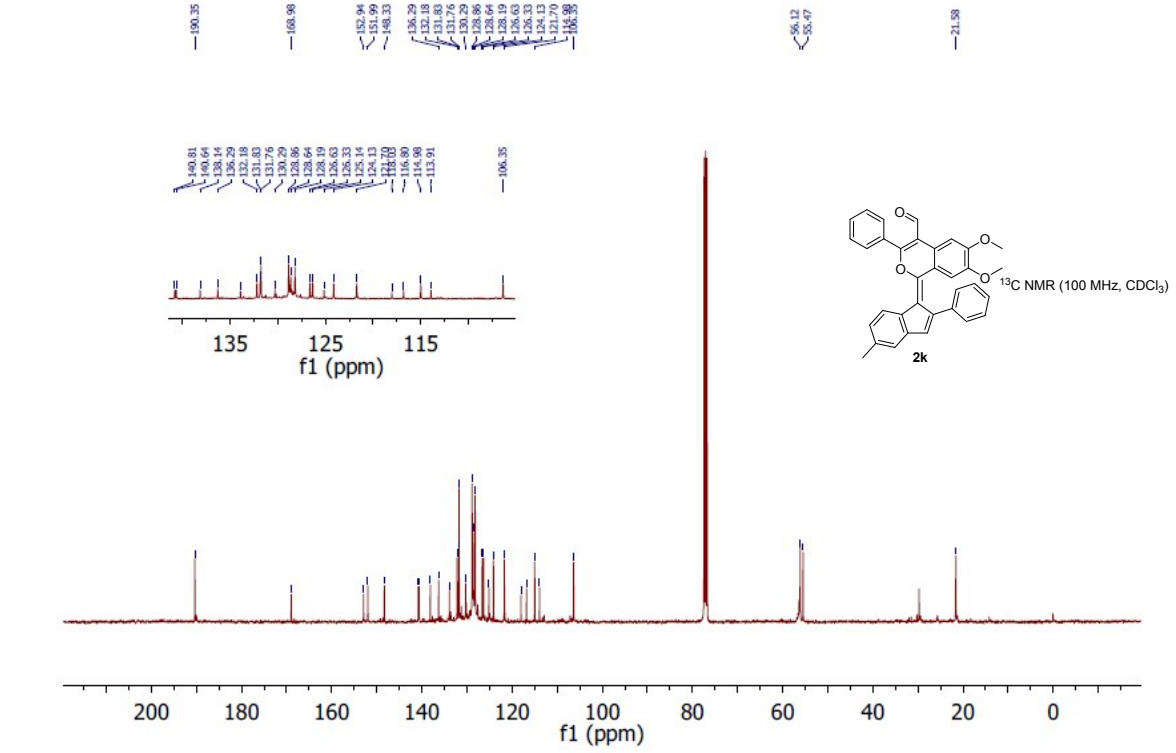
(*E*)-6,7-Dimethoxy-3-phenyl-1-(2-phenyl-*1H*-inden-1-ylidene)-*1H*-isochromene-4-carbaldehyde-2j



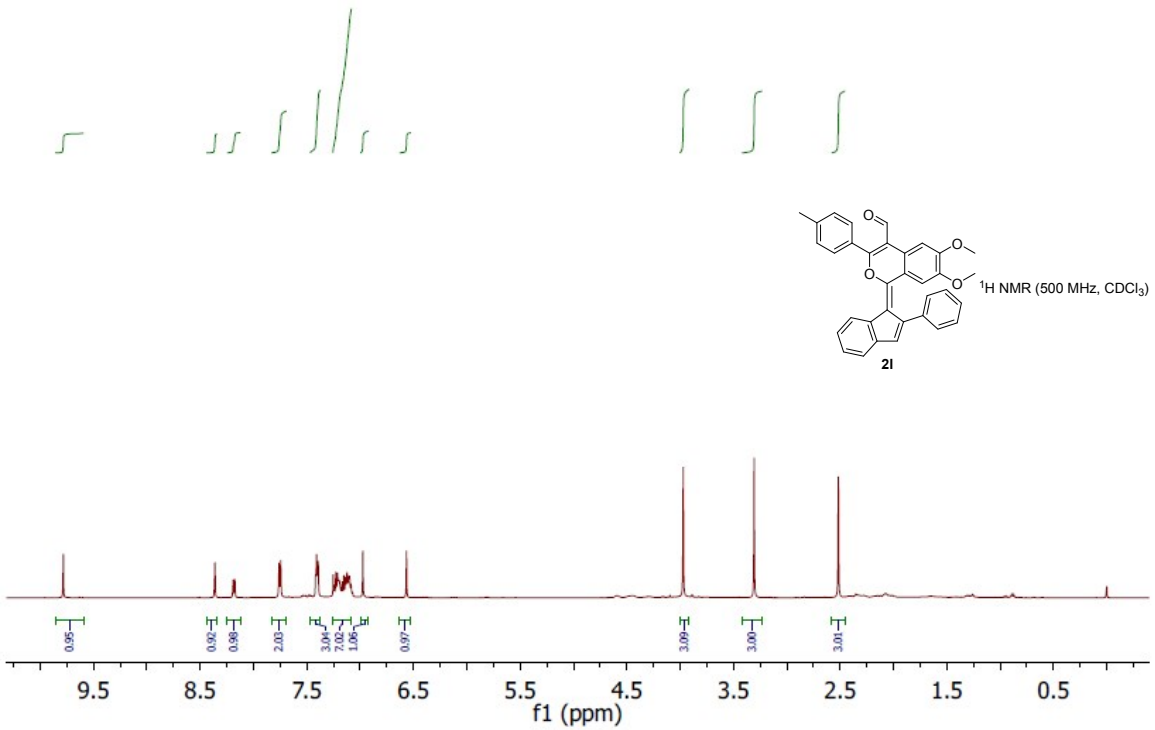


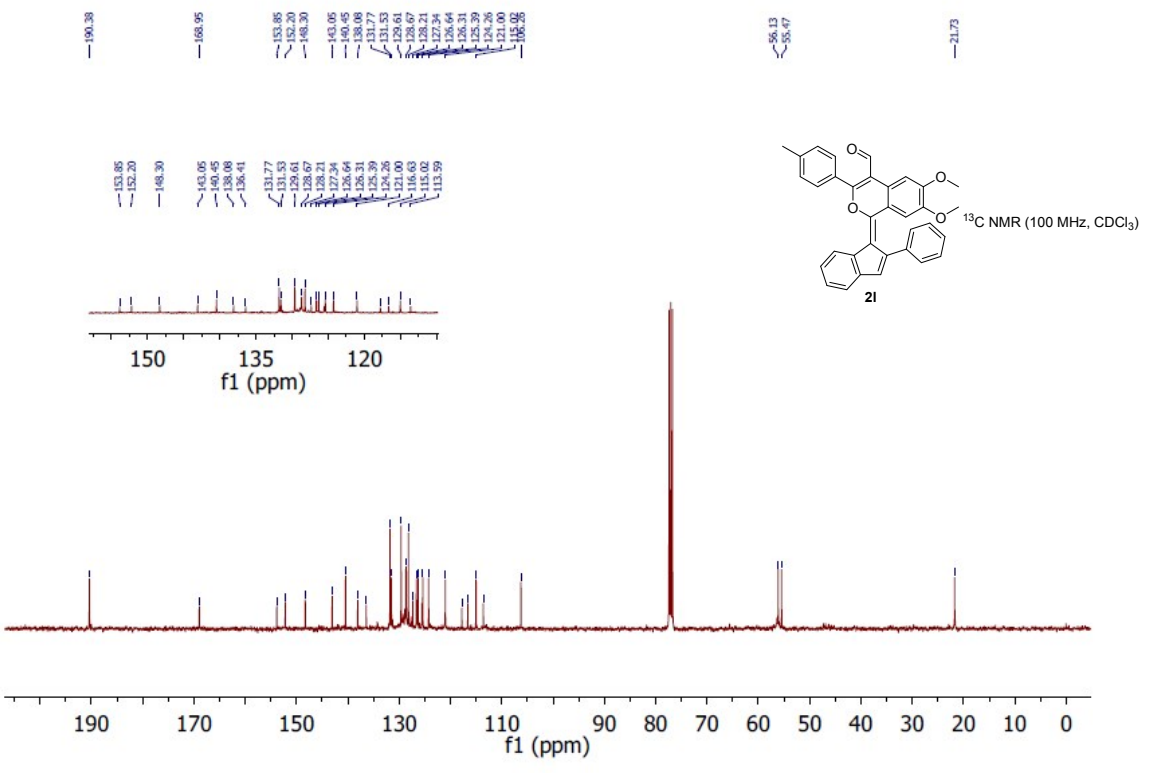
(*E*)-6,7-Dimethoxy-1-(5-methyl-2-phenyl-*1H*-inden-1-ylidene)-3-phenyl-*1H*-isochromene-4-carbaldehyde-2k



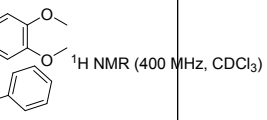


(*E*)-6,7-Dimethoxy-1-(2-phenyl-*1H*-inden-1-ylidene)-3-(*p*-tolyl)-*1H*-isochromene-4-carbaldehyde -2l

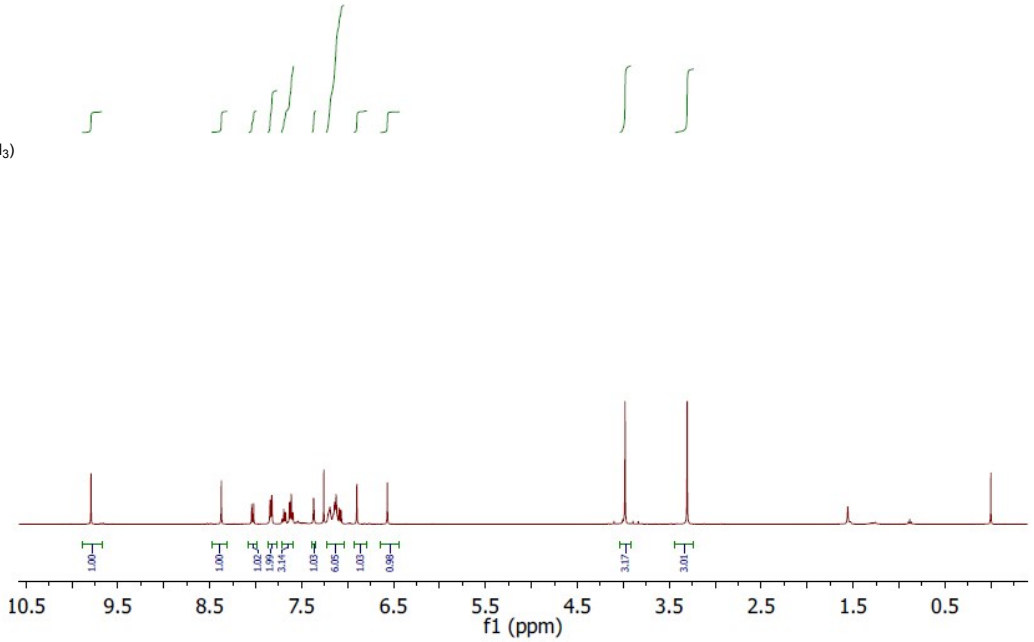


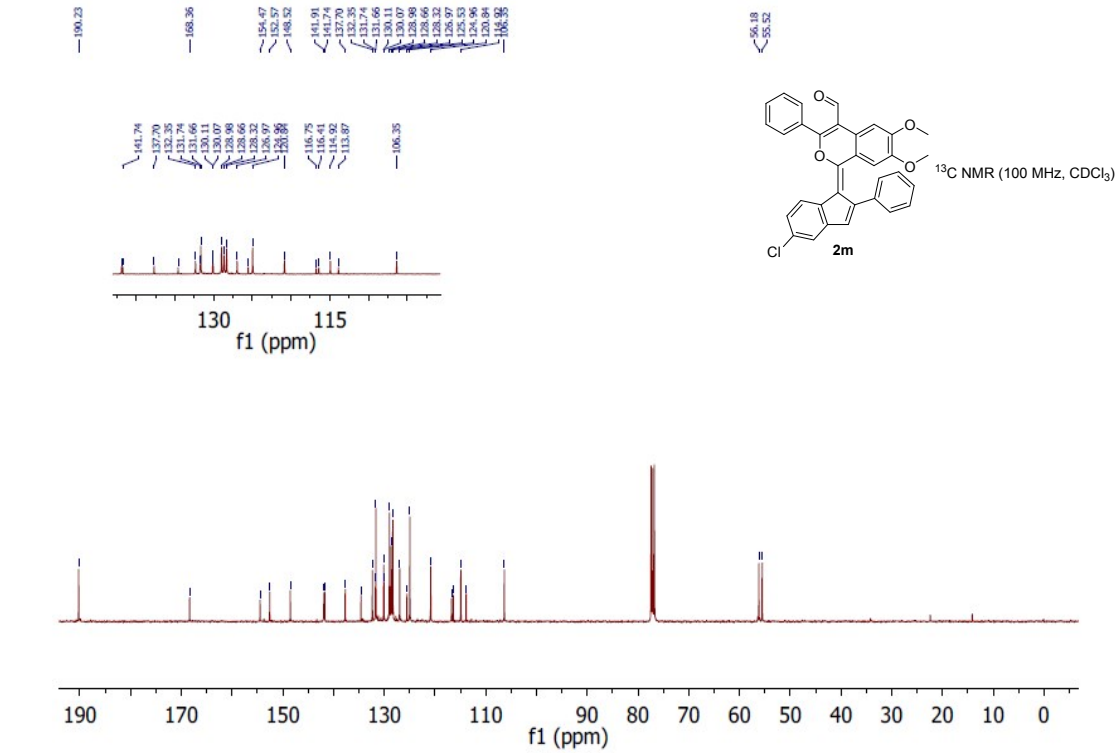


(*E*)-1-(5-Chloro-2-phenyl-*1H*-inden-1-ylidene)-6,7-dimethoxy-3-phenyl-*1H*-isochromene-4-carbaldehyde-2m



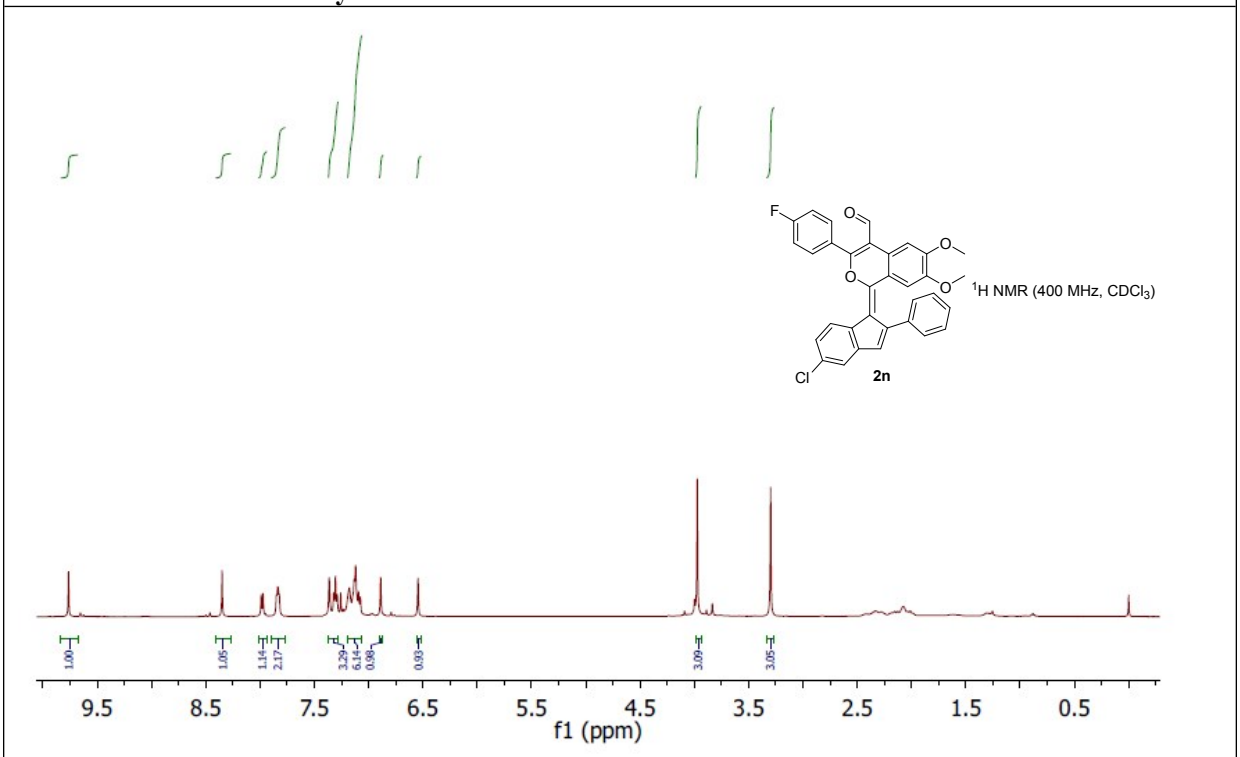
^{1}H NMR (400 MHz, $CDCl_3$)

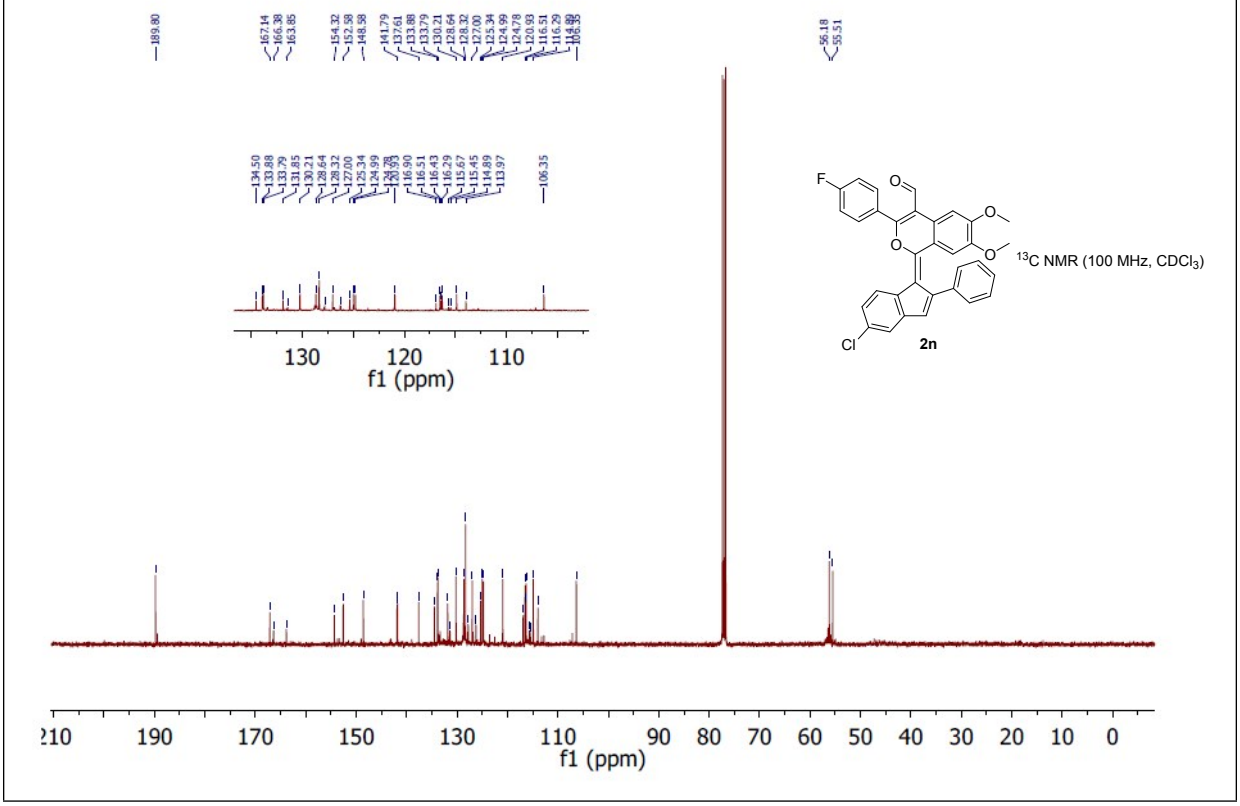




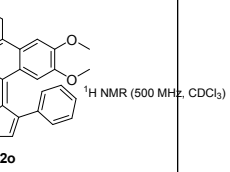
^{13}C NMR (100 MHz, $CDCl_3$)

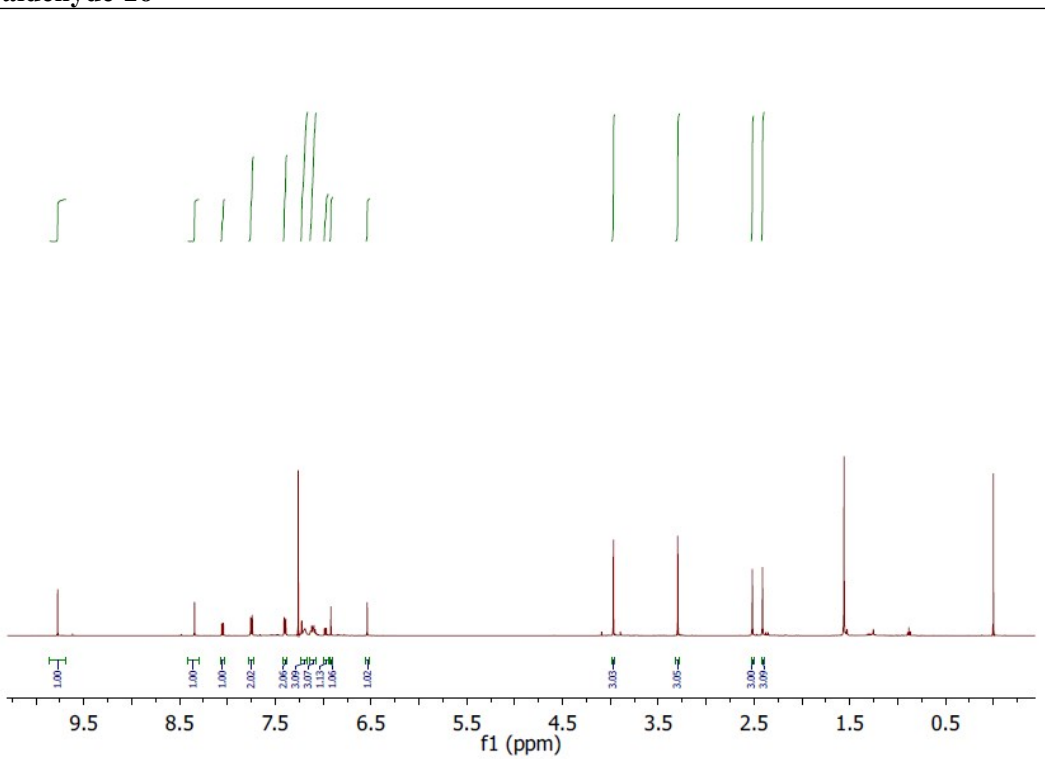
(*E*)-1-(5-Chloro-2-phenyl-1*H*-inden-1-ylidene)-3-(4-fluorophenyl)-6,7-dimethoxy-1*H*-isochromene-4-carbaldehyde-2n

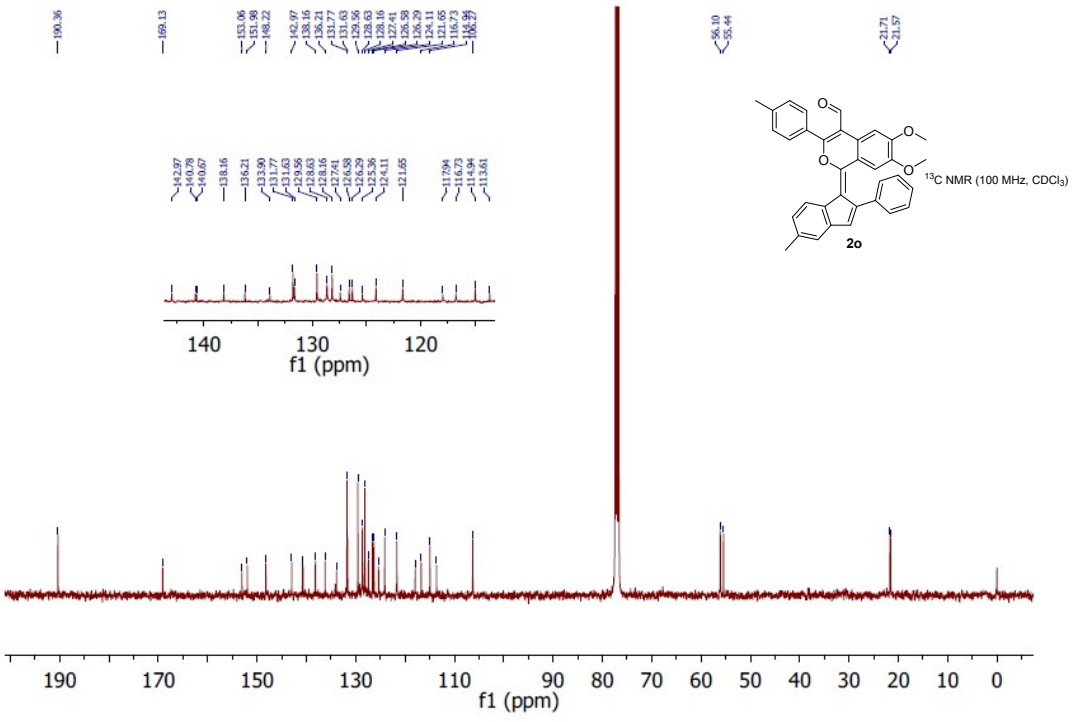




(*E*)-6,7-Dimethoxy-1-(5-methyl-2-phenyl-*1H*-inden-1-ylidene)-3-(*p*-tolyl)-*1H*-isochromene-4-carbaldehyde-2o







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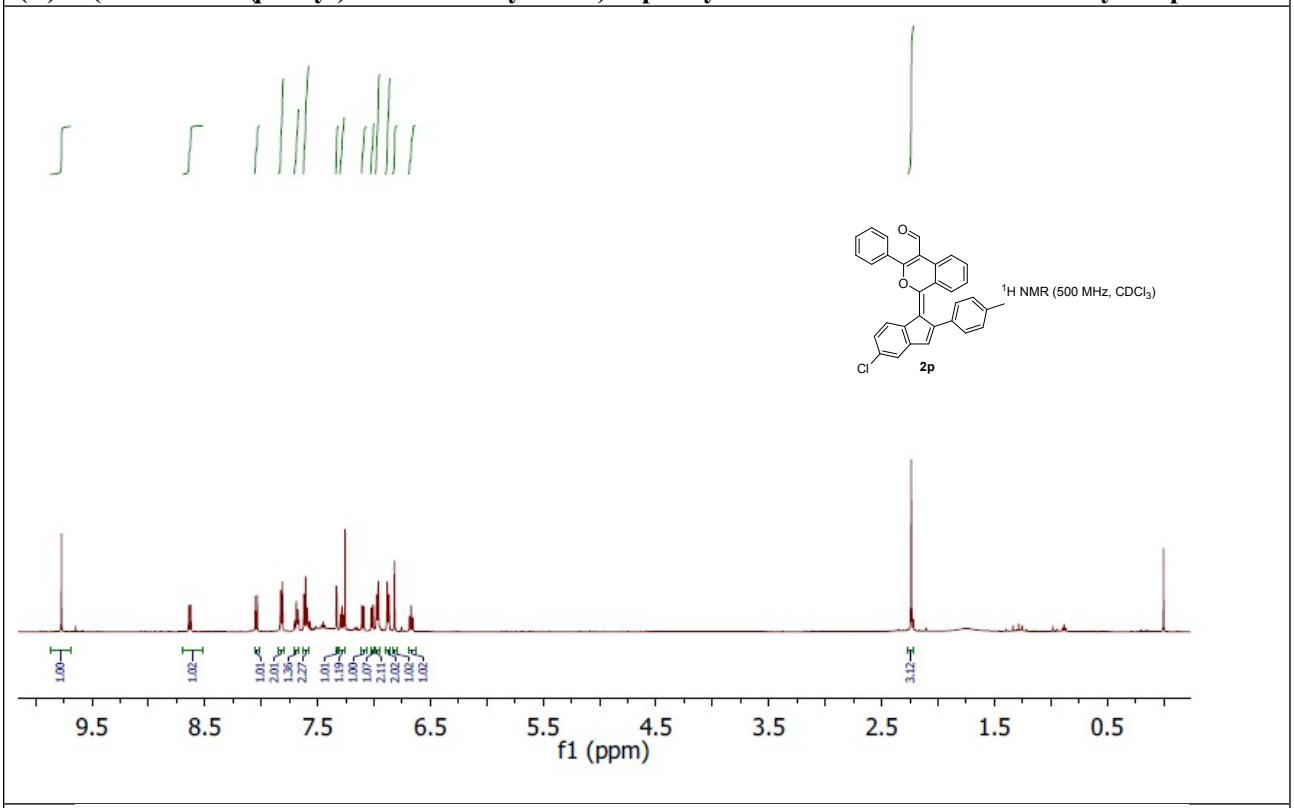

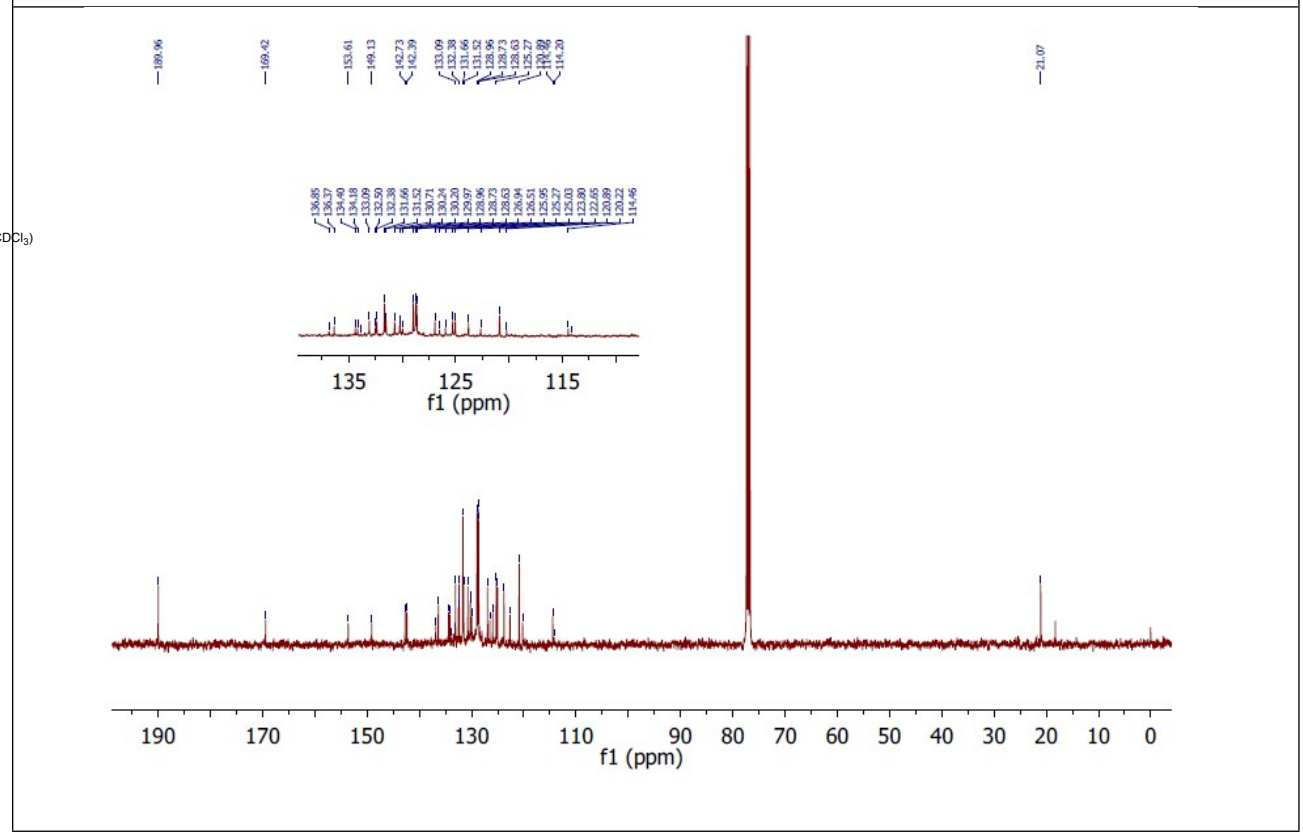

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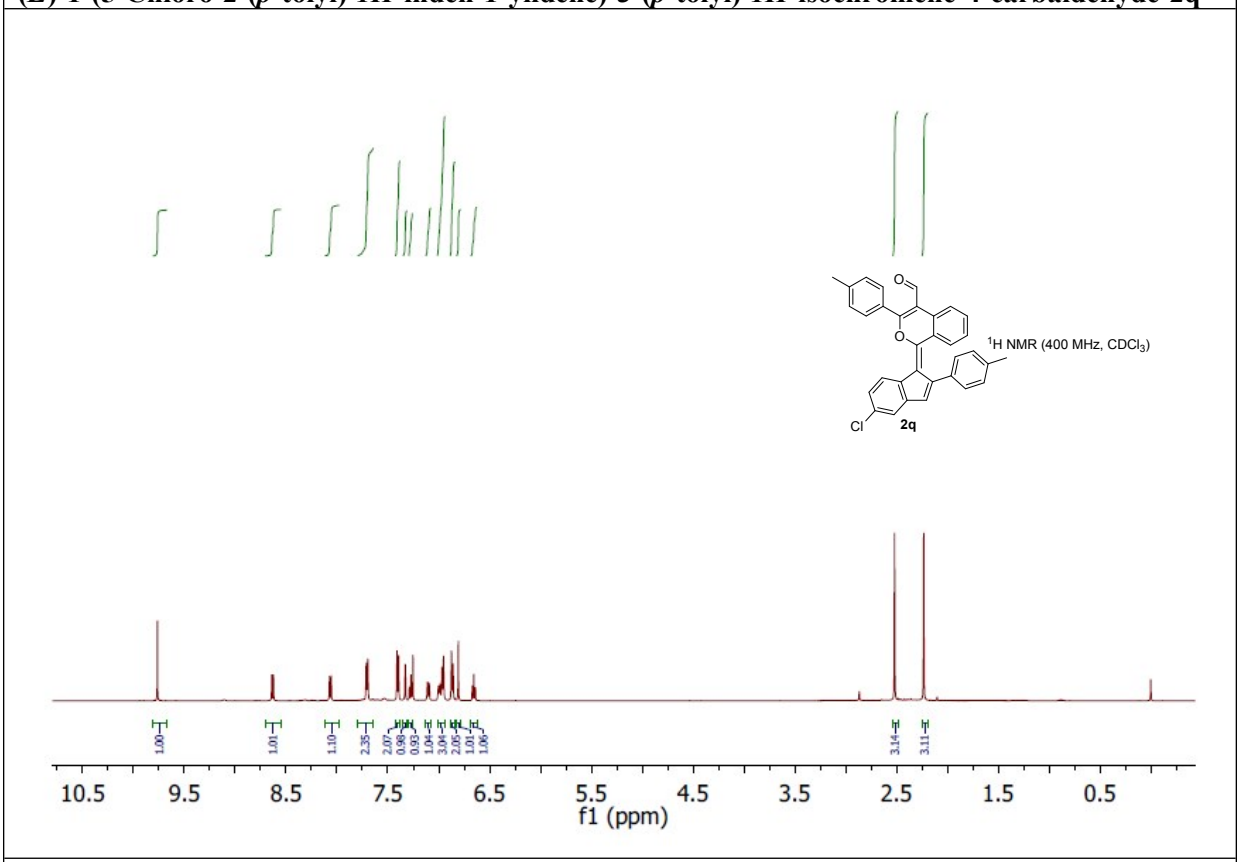

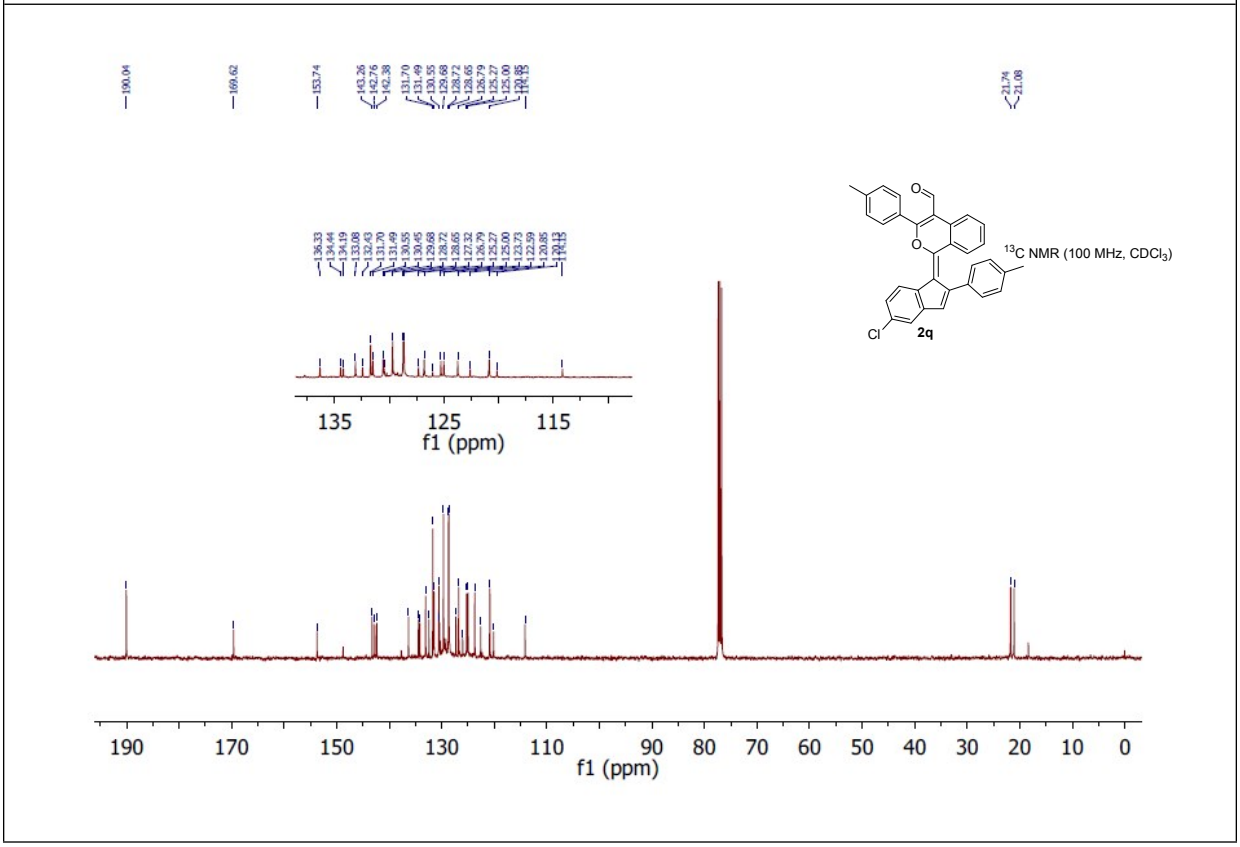

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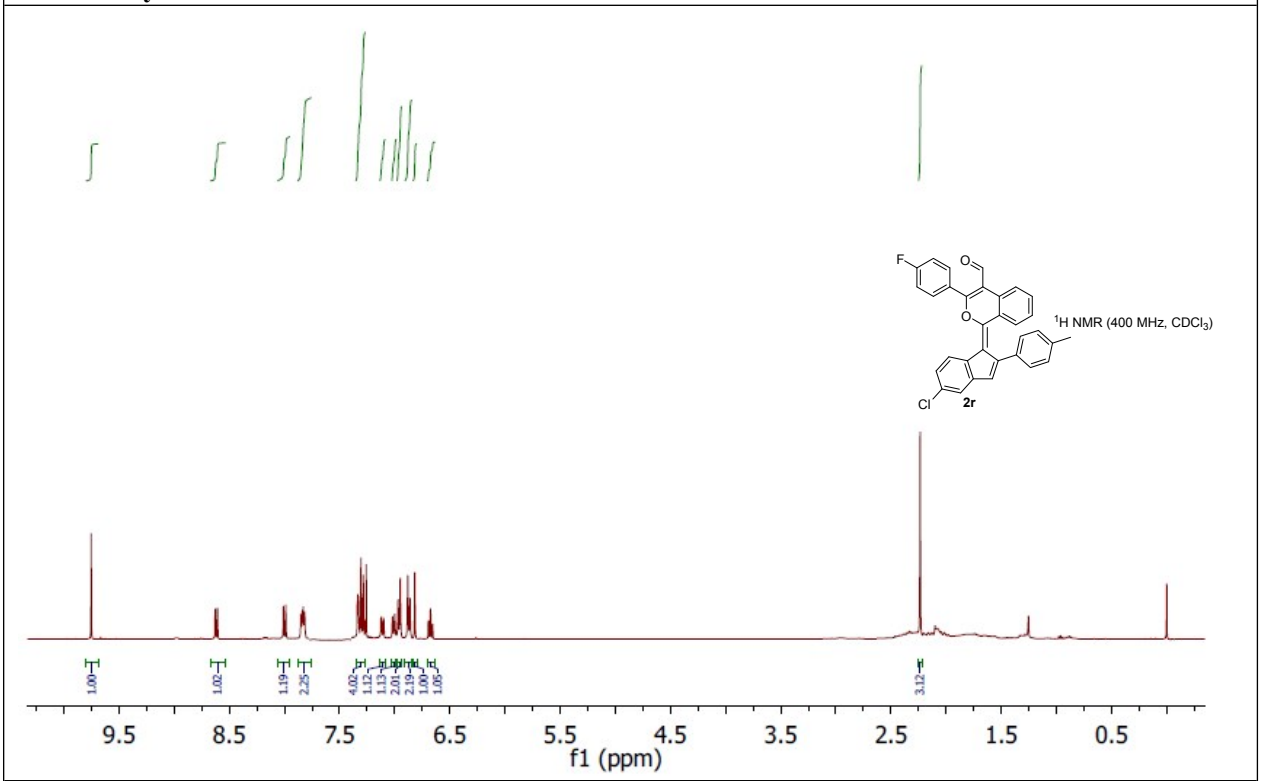

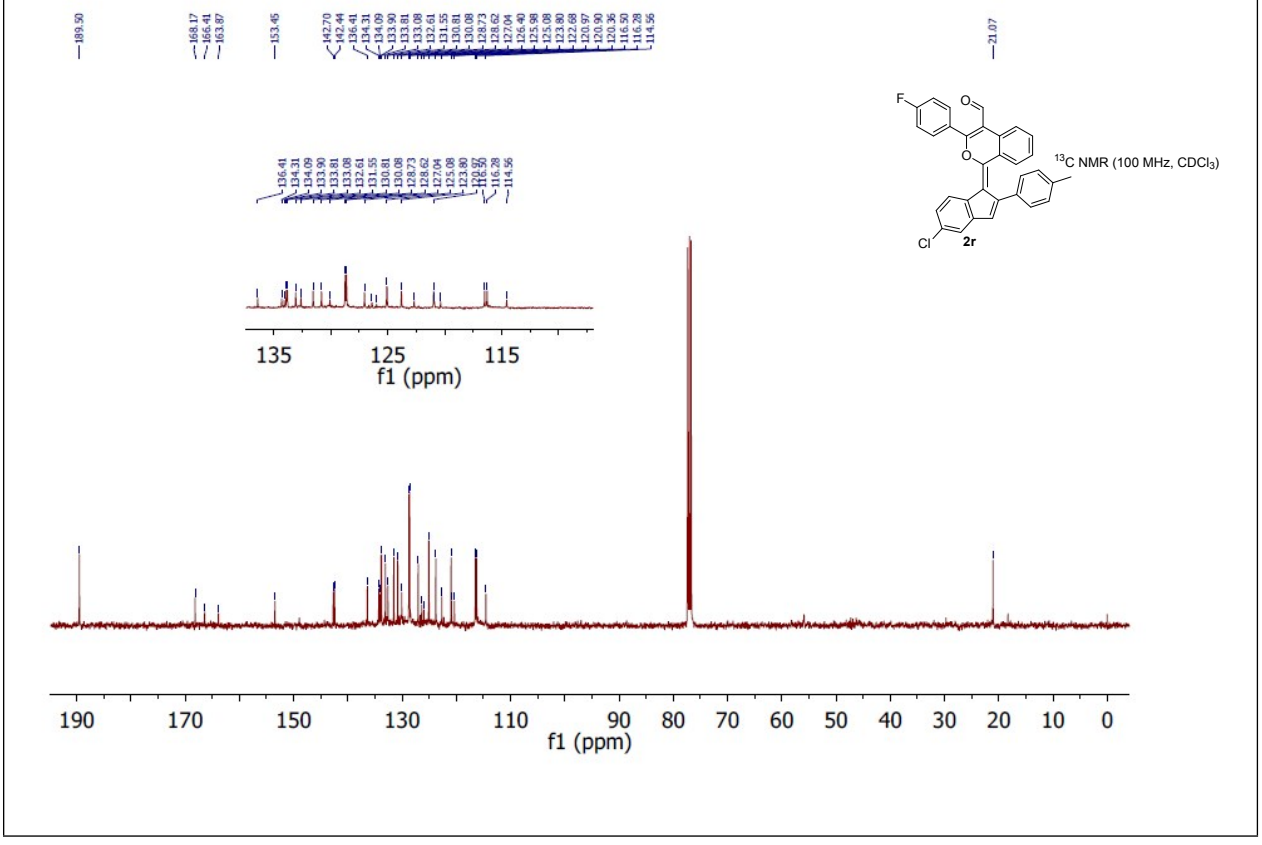

2. X-ray crystallography data of 2f.

X-ray data for the compound KA990was collected at room temperatureon a Bruker D8 QUEST instrument with an IμS Mo microsource (λ = 0.7107 A) and a PHOTON-100 detector. The raw data frames were reduced and corrected for absorption effects using the Bruker Apex 3 software suite programs.[1] The structure was solved using intrinsic phasing method [2] and further refined with the SHELXL[2] program and expanded using Fourier techniques. Anisotropic displacement parameters were included for all non-hydrogen atoms.All C bound H atoms were positioned geometrically and treated as riding on their parent C atoms [C-H = 0.93-0.97 Å, and $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H or $1.2U_{eq}(C)$ for other H atoms].

Crystal structure determination of [KA990_0m]

Crystal Data for 2f: $C_{34}H_{26}O_2$ (M =466.55 g/mol): monoclinic, space group $P2_1/c$ (no. 14), a = 12.1135(2) Å, b = 20.9493(4) Å, c = 10.1143(2) Å, β = 101.59(3)°, V = 2514.3(2) Å^3, Z = 4, T = 294.15 K, μ(MoKα) = 0.075 mm^{-1}, *Dcalc* = 1.232 g/cm^3, 30236 reflections measured (4.548° ≤ 2Θ ≤ 52.498°), 5070 unique (R_{int} = 0.0721, R_{sigma} = 0.0514) which were used in all calculations. The final R_1 was 0.0662 (I > 2σ(I)) and wR_2 was 0.1967 (all data). CCDC2042148 contains supplementary Crystallographic data for the structure. These data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html [or from the Cambridge Crystallographic Data Centre (CCDC), 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44(0) 1223 336 033; email: deposit@ccdc.cam.ac.uk].

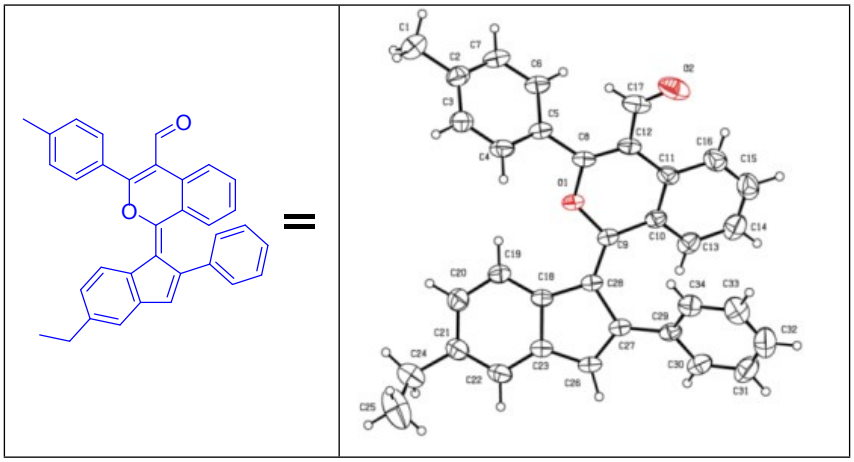

Figure 1. A view of **2f**, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are represented by circles of arbitrary radii.

References:

1. Bruker (2016). APEX3, SAINT and SADABS. Bruker AXS, Inc., Madison, Wisconsin, USA.
2. Sheldrick G. M. (2015**)** ActaCrystallogrC71:3-8.