

Reinvestigating the synthesis and characterization of ethyl 3-[5-(2-ethoxycarbonyl-1-methylvinyl)-1-methyl-1H-indol-3-yl]-but-2-enoate (MIBE)

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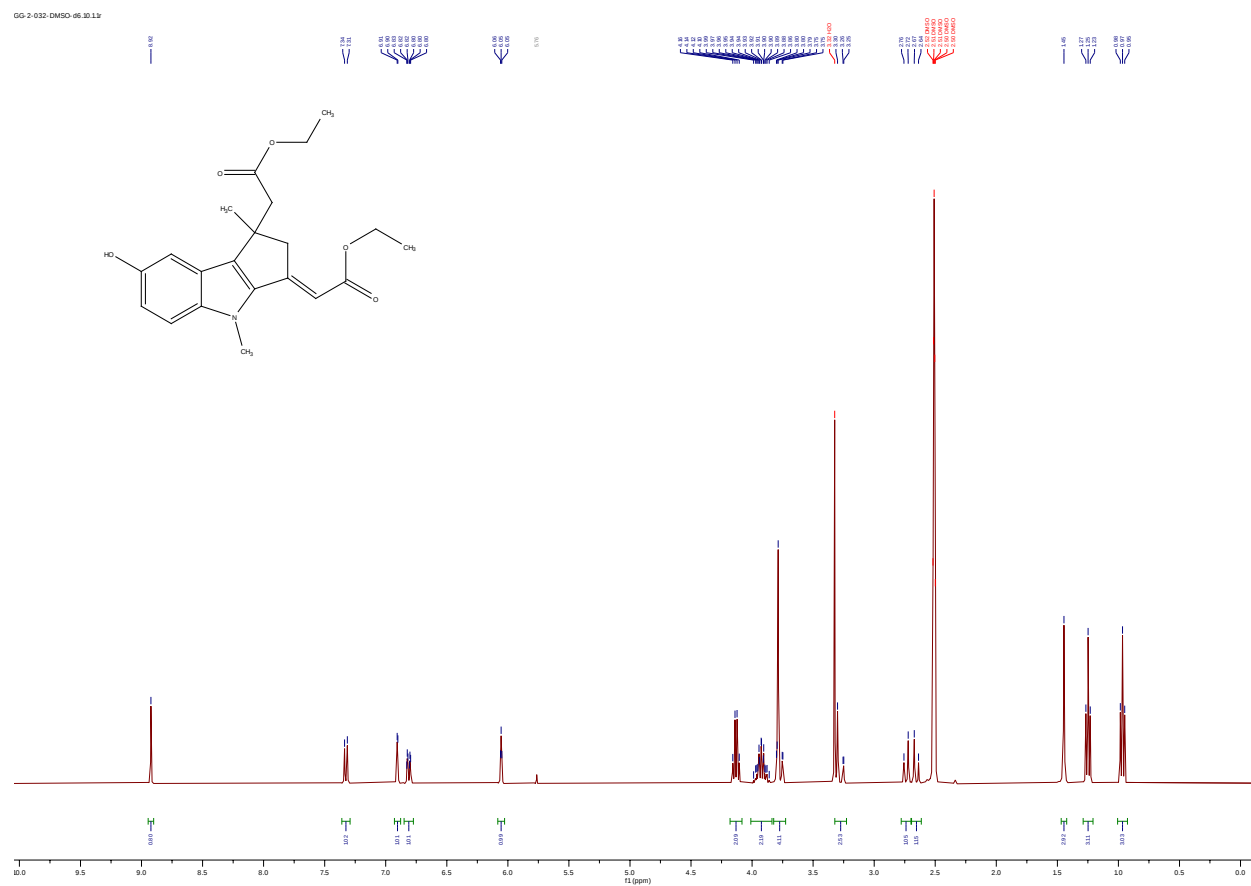
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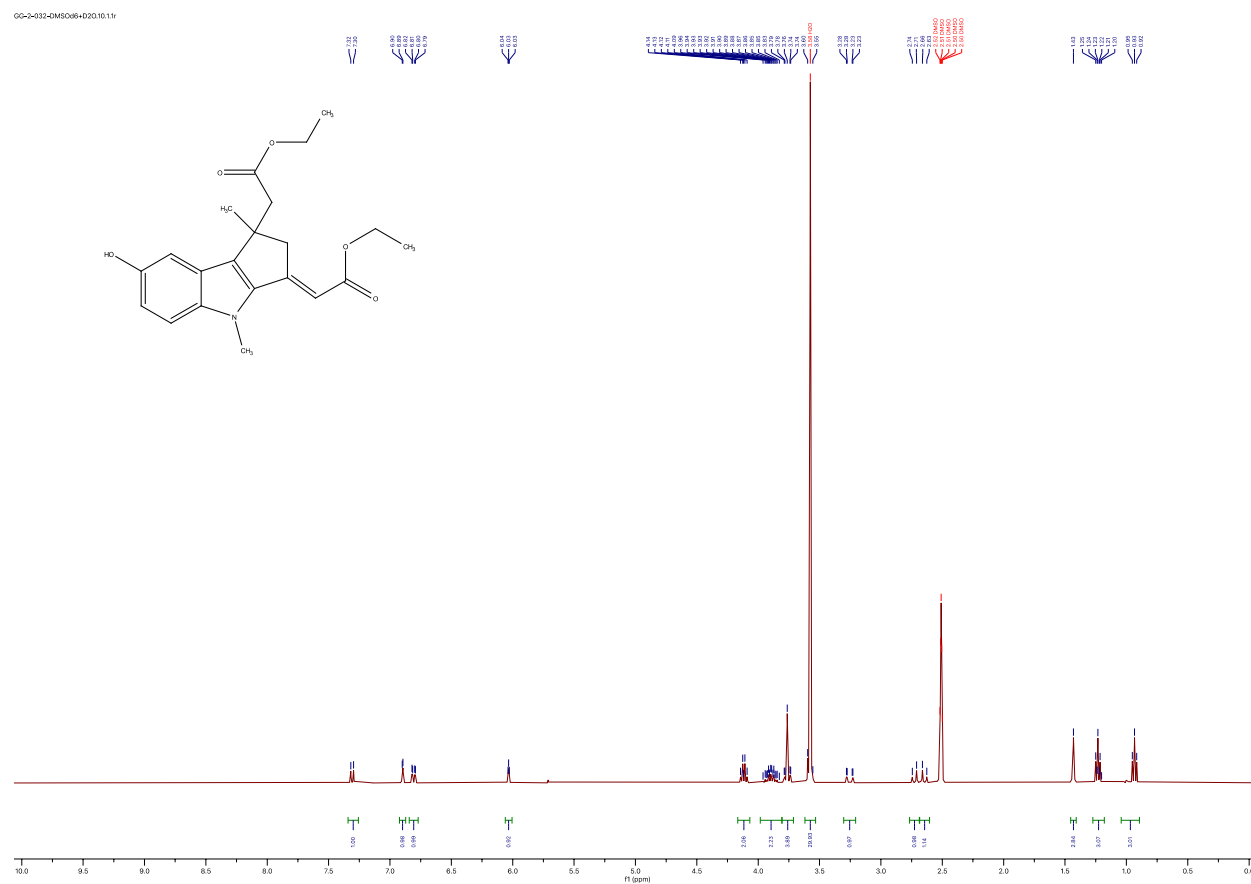
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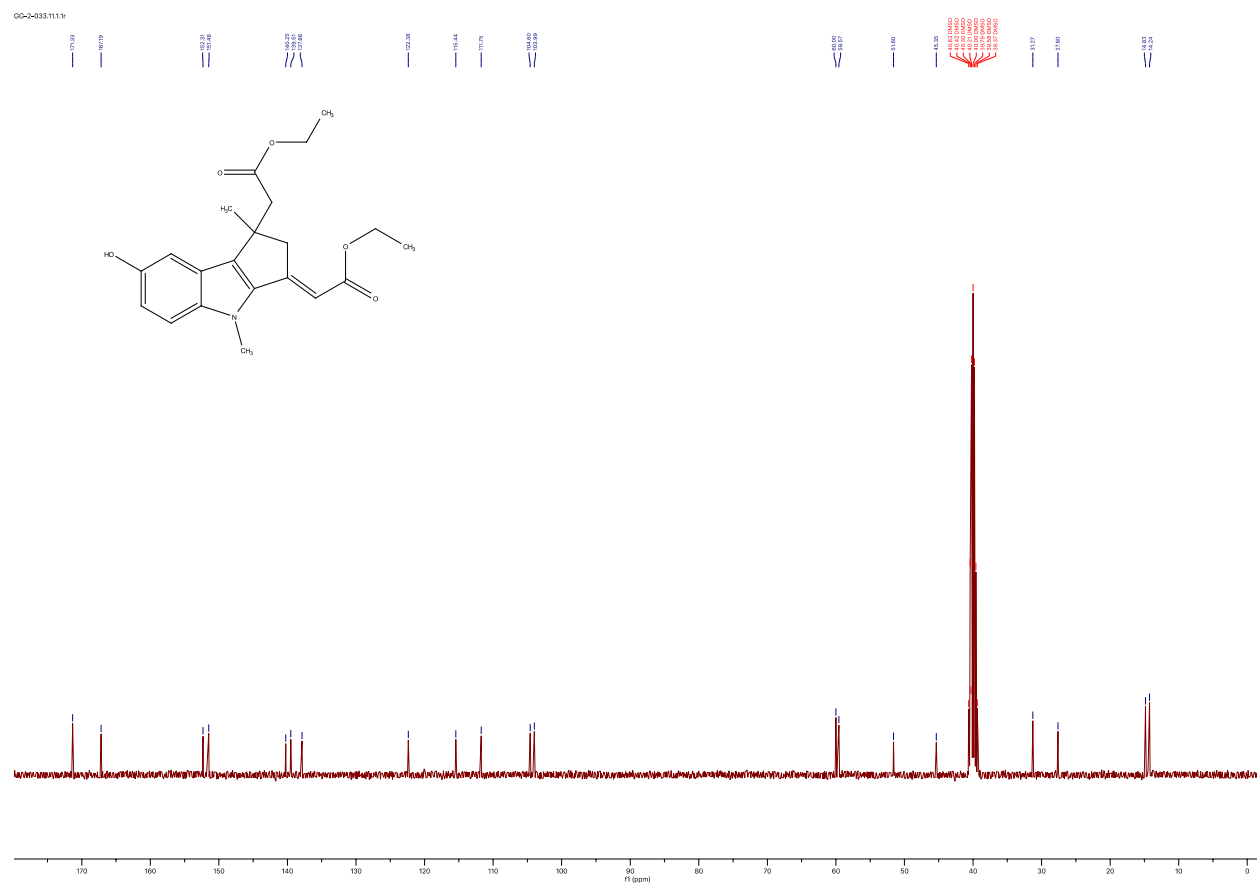
¹H NMR of **2a** in DMSO-d₆



¹H NMR of **2a** in DMSO-d6 + D2O

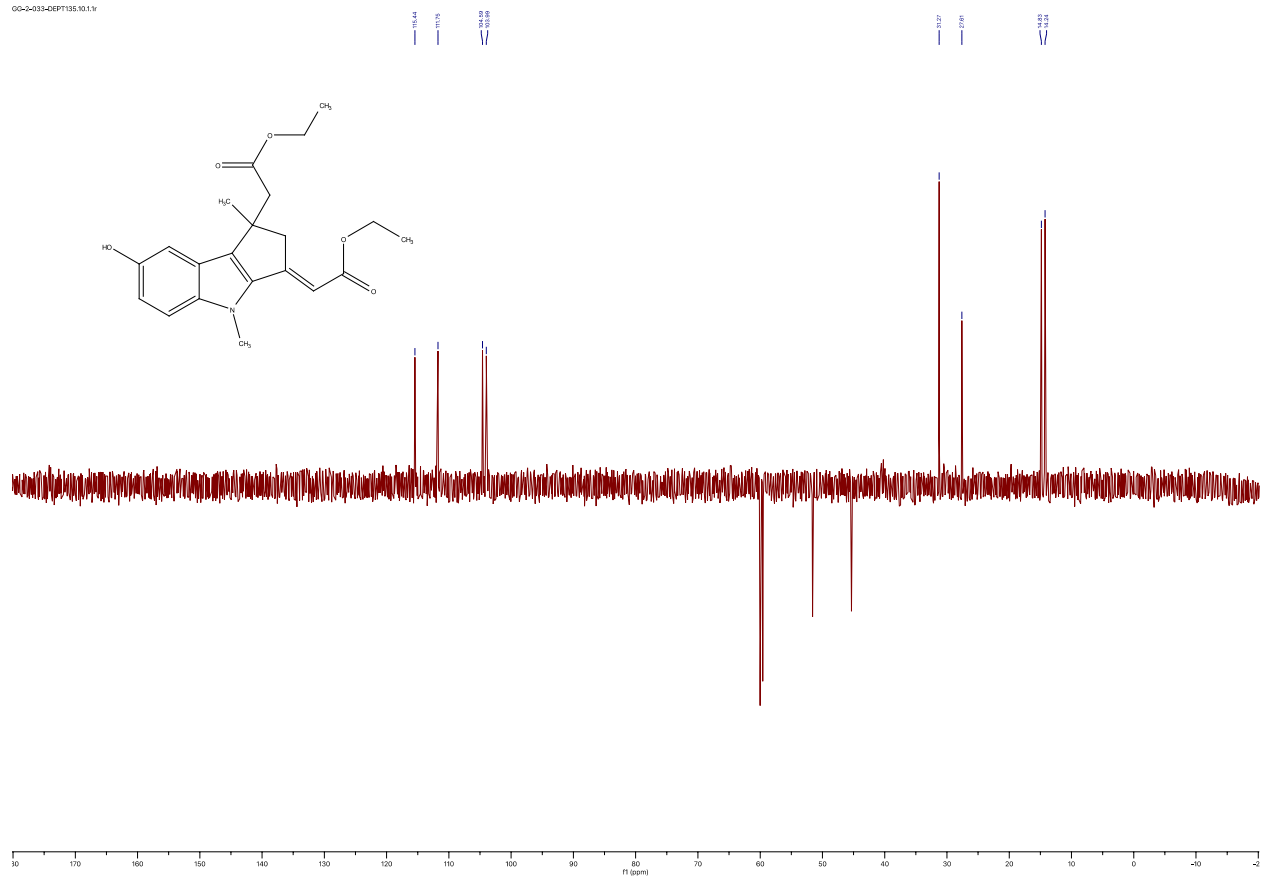


¹³C NMR of 2a in DMSO-d6

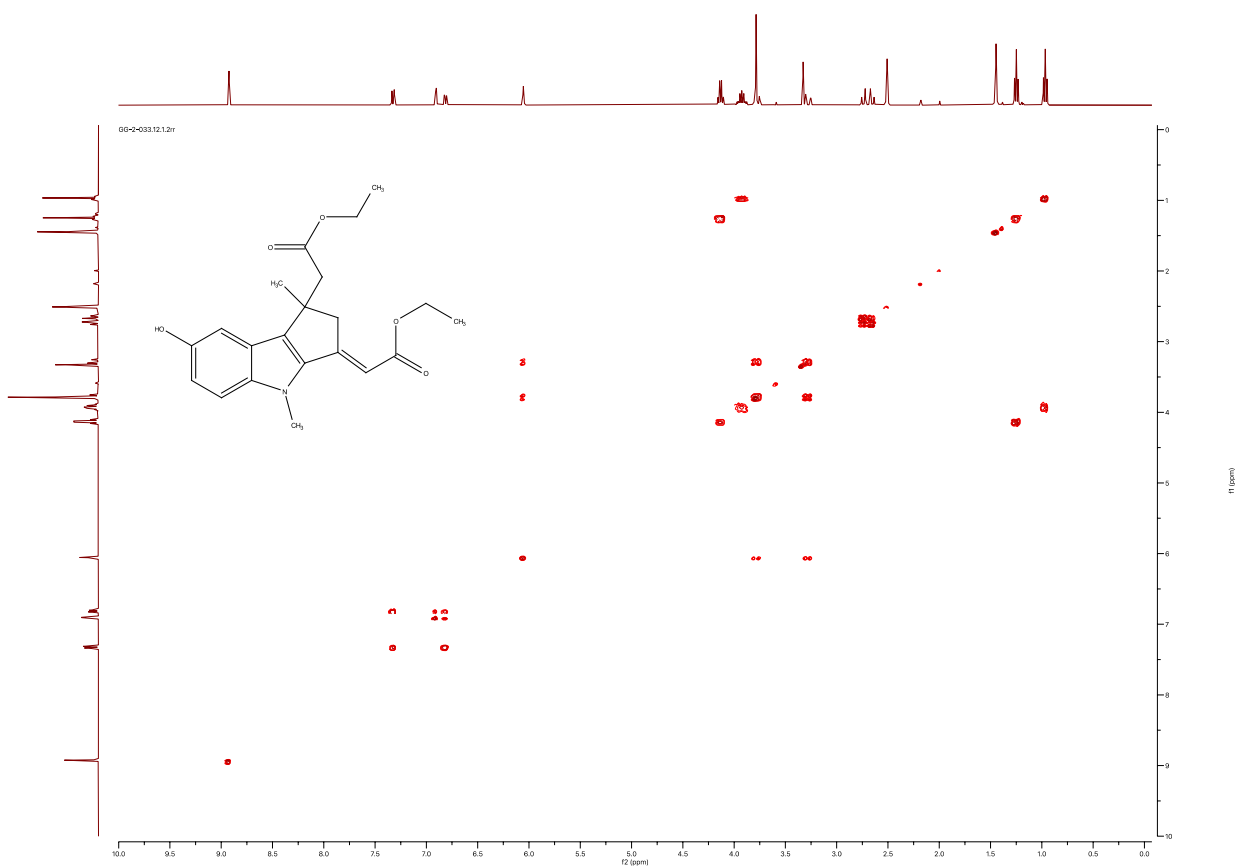


DEPT135 of **2a**

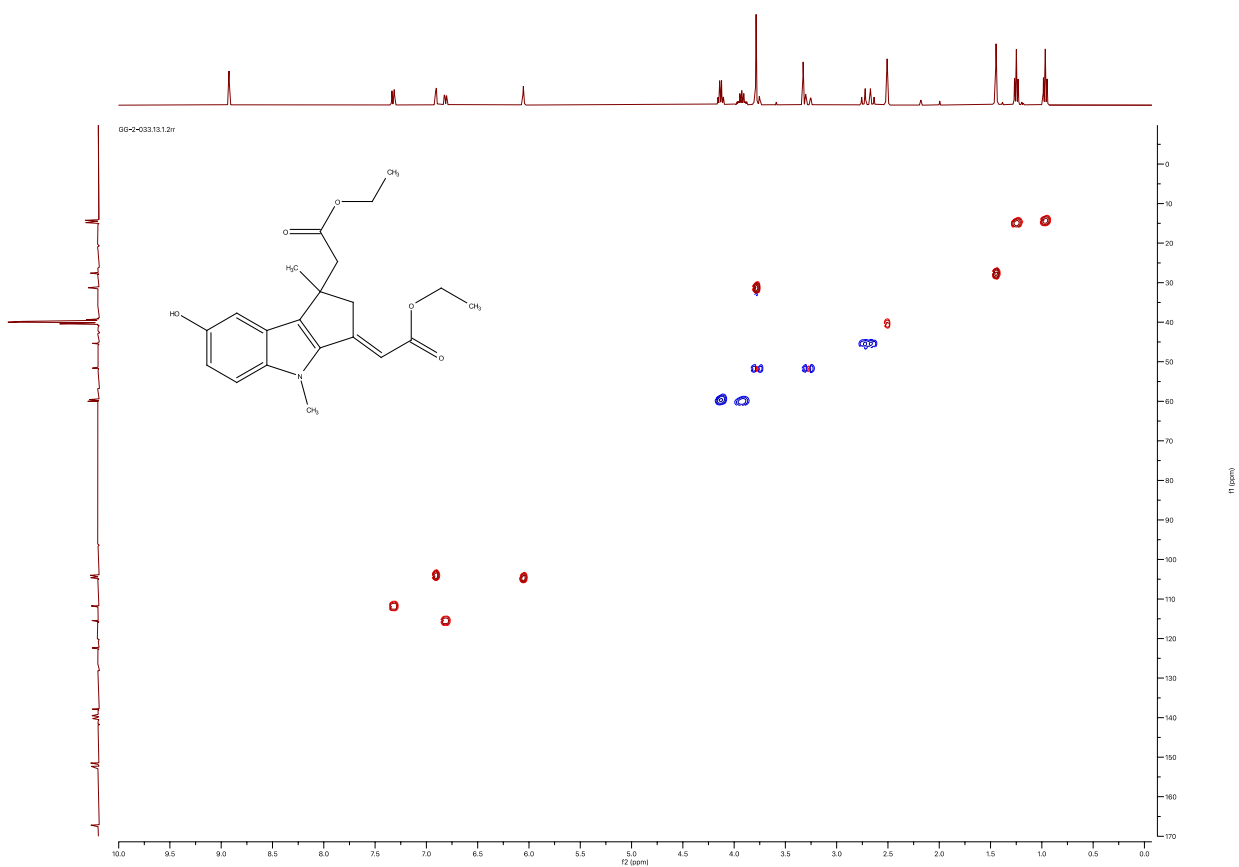
06-2-033-DEPT135, 50.1 %



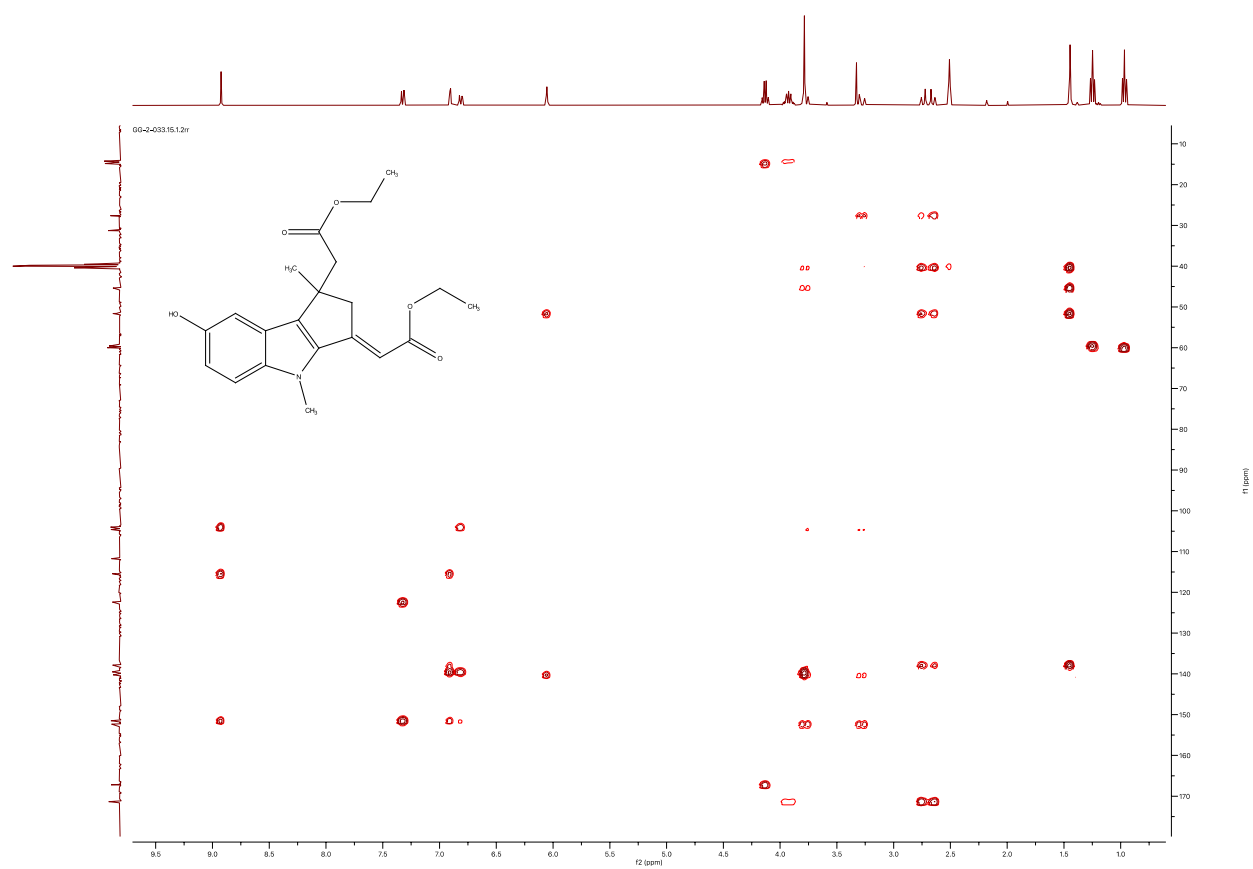
COSY of 2a



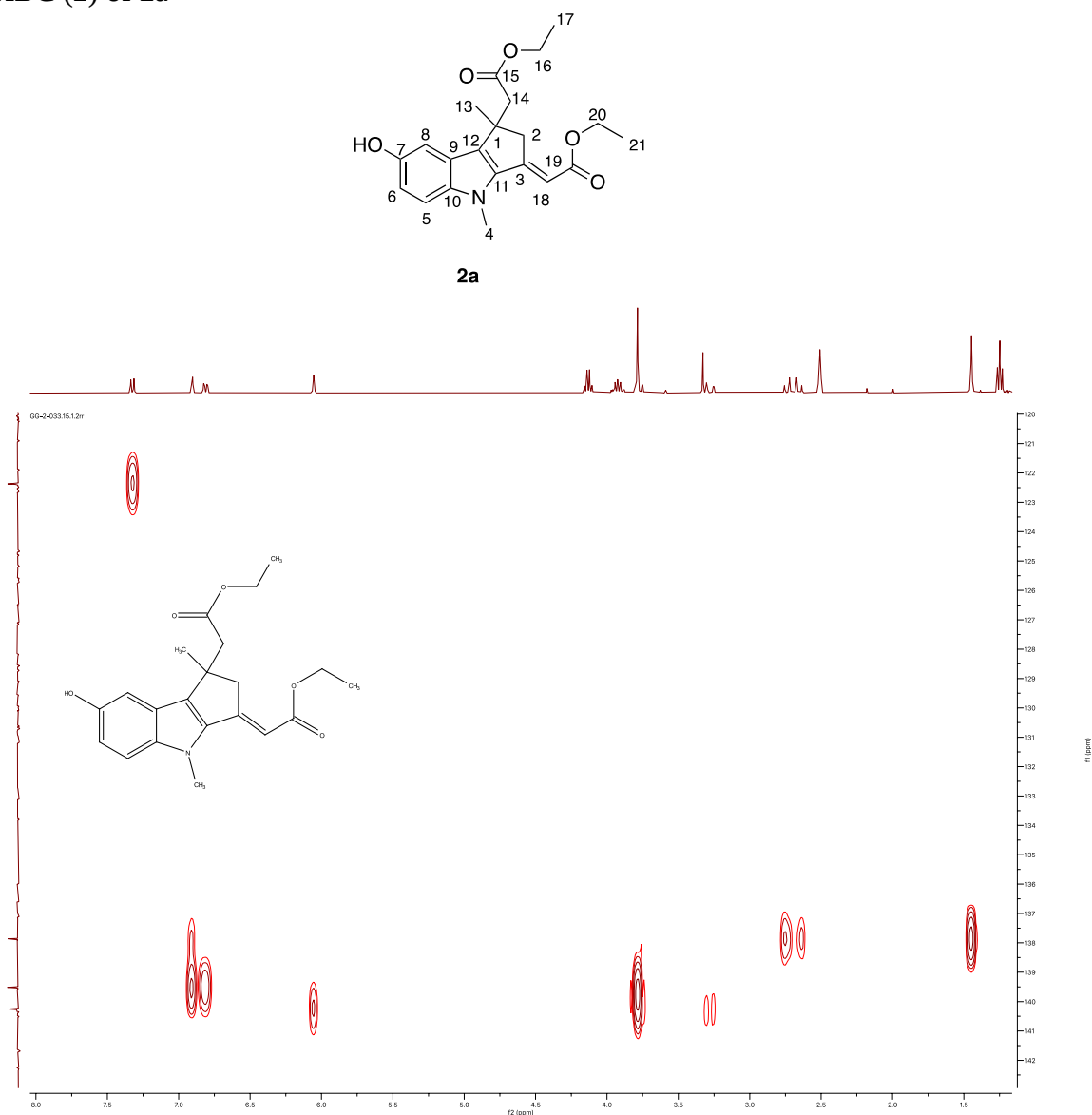
C-H HSQC of 2a



C-H HMBC of **2a**

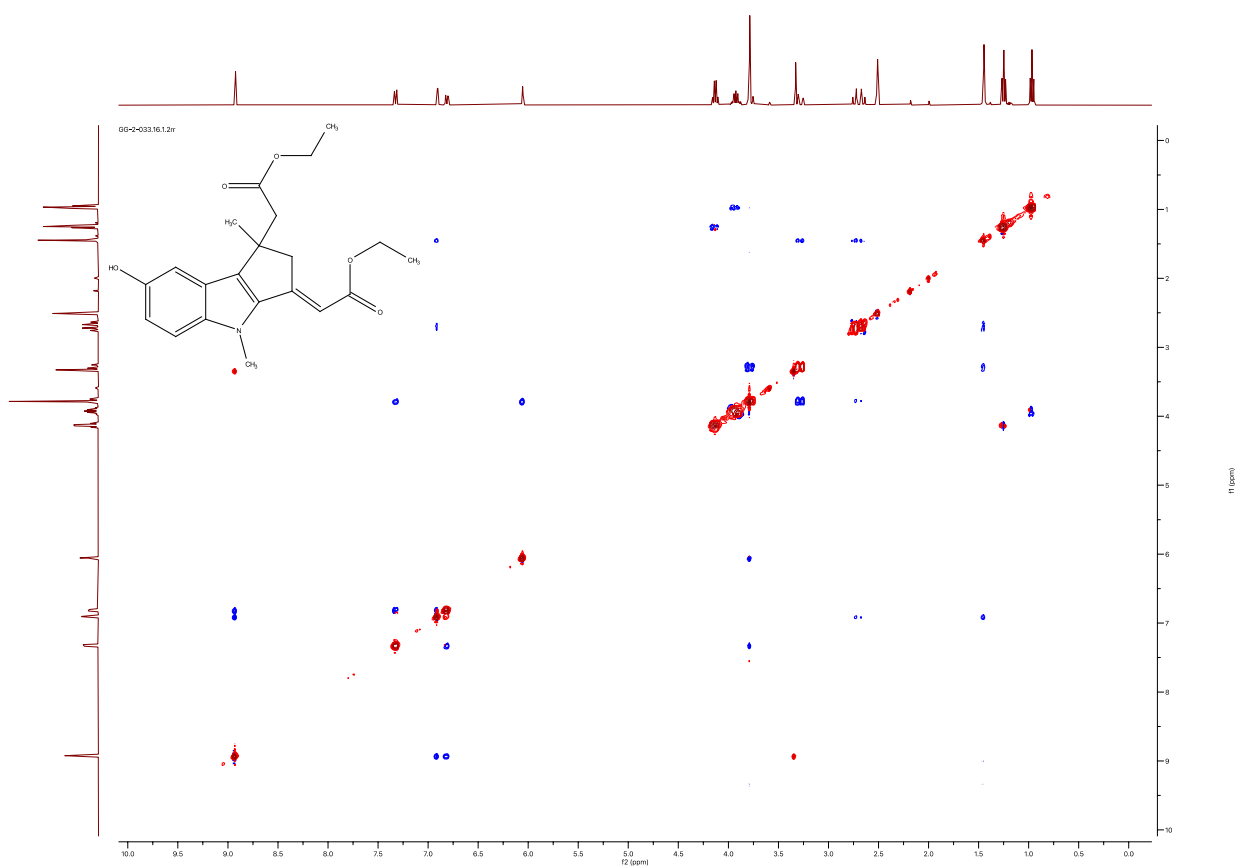


C-H HMBC (2) of **2a**

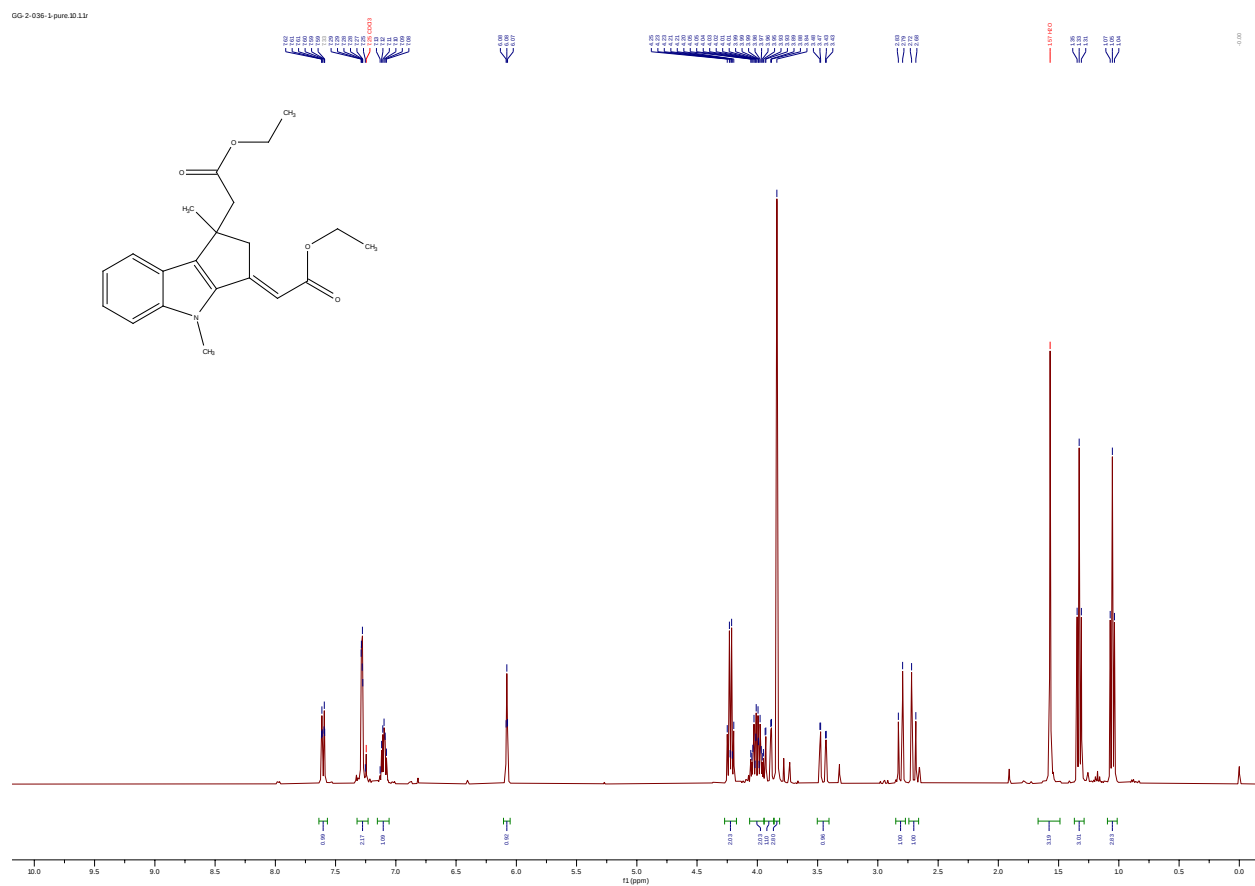


- For carbon δ 122.38 (9-C), a strong signal was observed with proton δ 7.32 (5-H) (three bonds distance between 9-C and 5-H).
- For carbon δ 137.86 (12-C), strong signals were observed with proton δ 6.90 (8-H), 2.74 (14-H), 2.65 (14-H) and 1.45 (13-Me) (three bonds distance between 12-C and 8-H, 11-C and 14-H, 12-C and 13-Me).
- For carbon δ 139.51 (10-C), strong signals were observed with protons δ 6.90 (8-H), 6.81 (6-H) and 3.78 (4-NCH₃) (three bonds distance between 10-C and 8-H, 10-C and 6-H, 10-H and 4-NCH₃).
- For carbon δ 140.25 (11-C), strong signals were observed with protons δ 6.08 – 6.03 (18-H) and 3.78 (4-NCH₃) (three bonds distance between 11-C and 18-H, 11-C and 4-NCH₃).

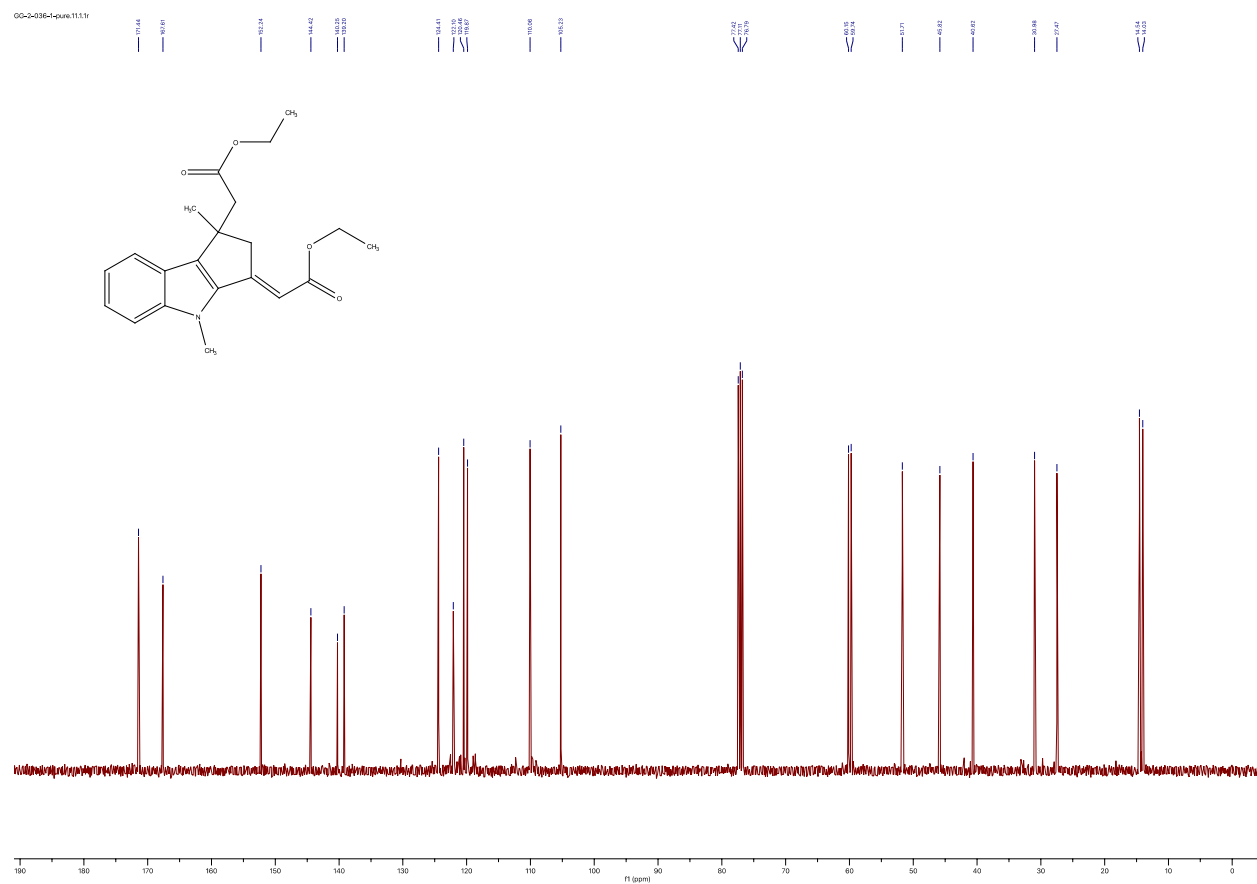
NOESY of **2a**



¹H NMR of **2b** in CDCl₃



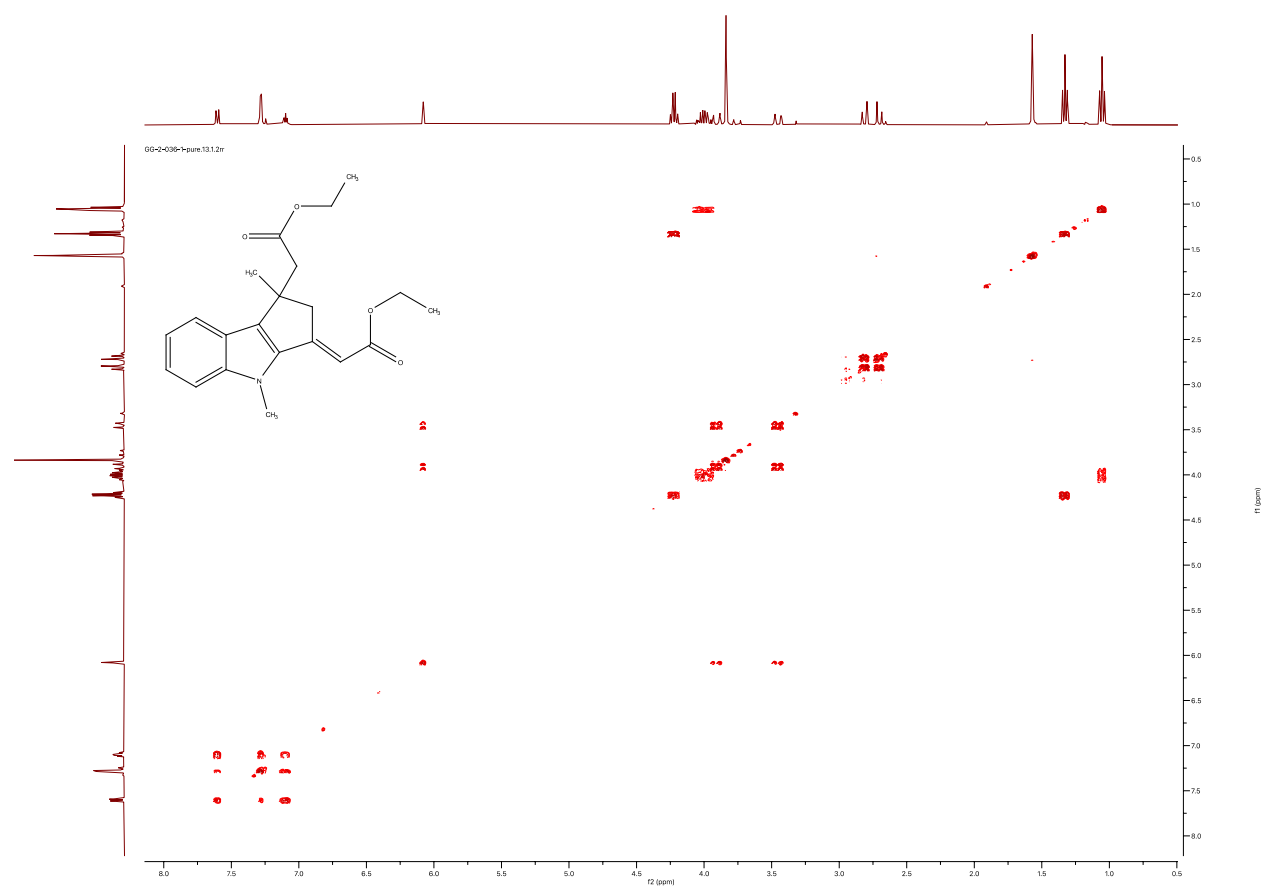
¹³C NMR of **2b** in CDCl₃



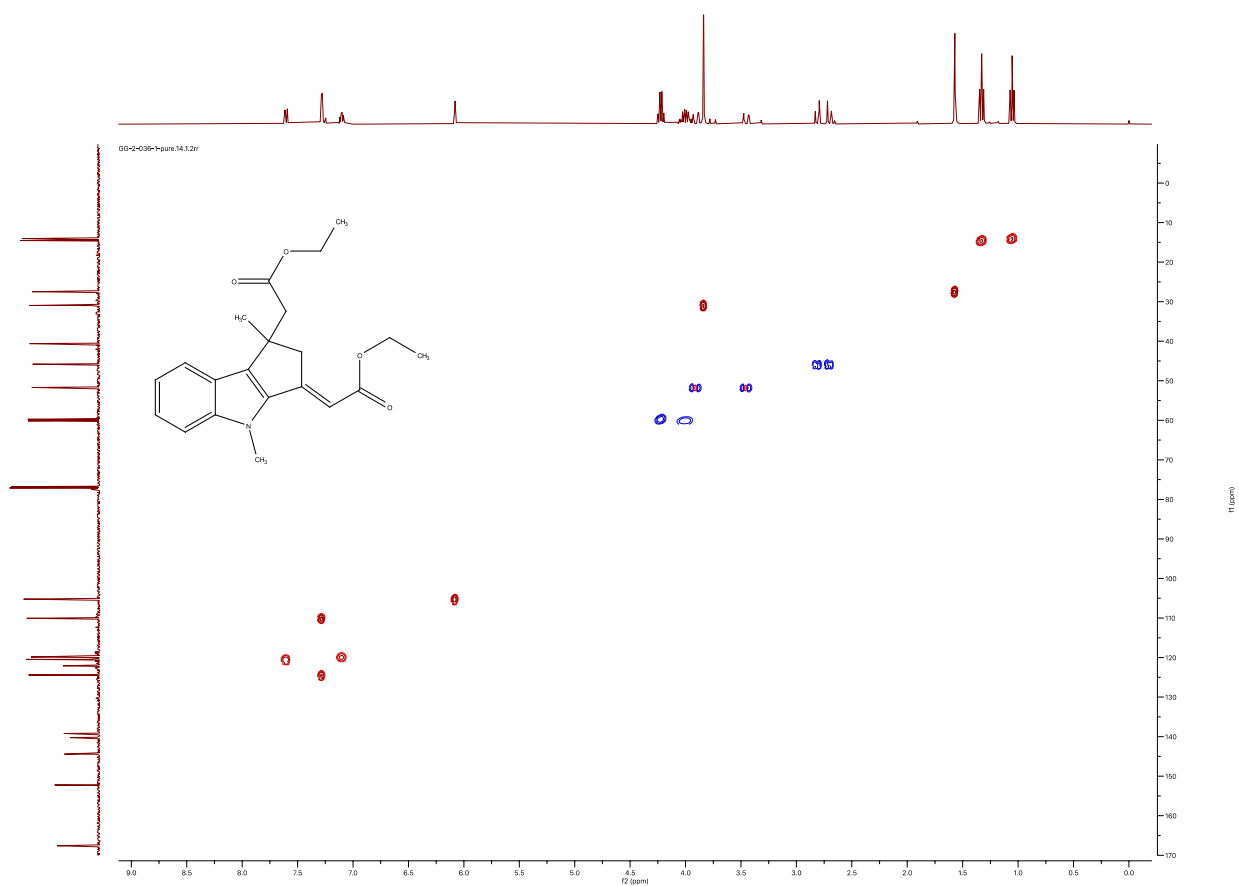
CC-2-036-1-pure.12.11r



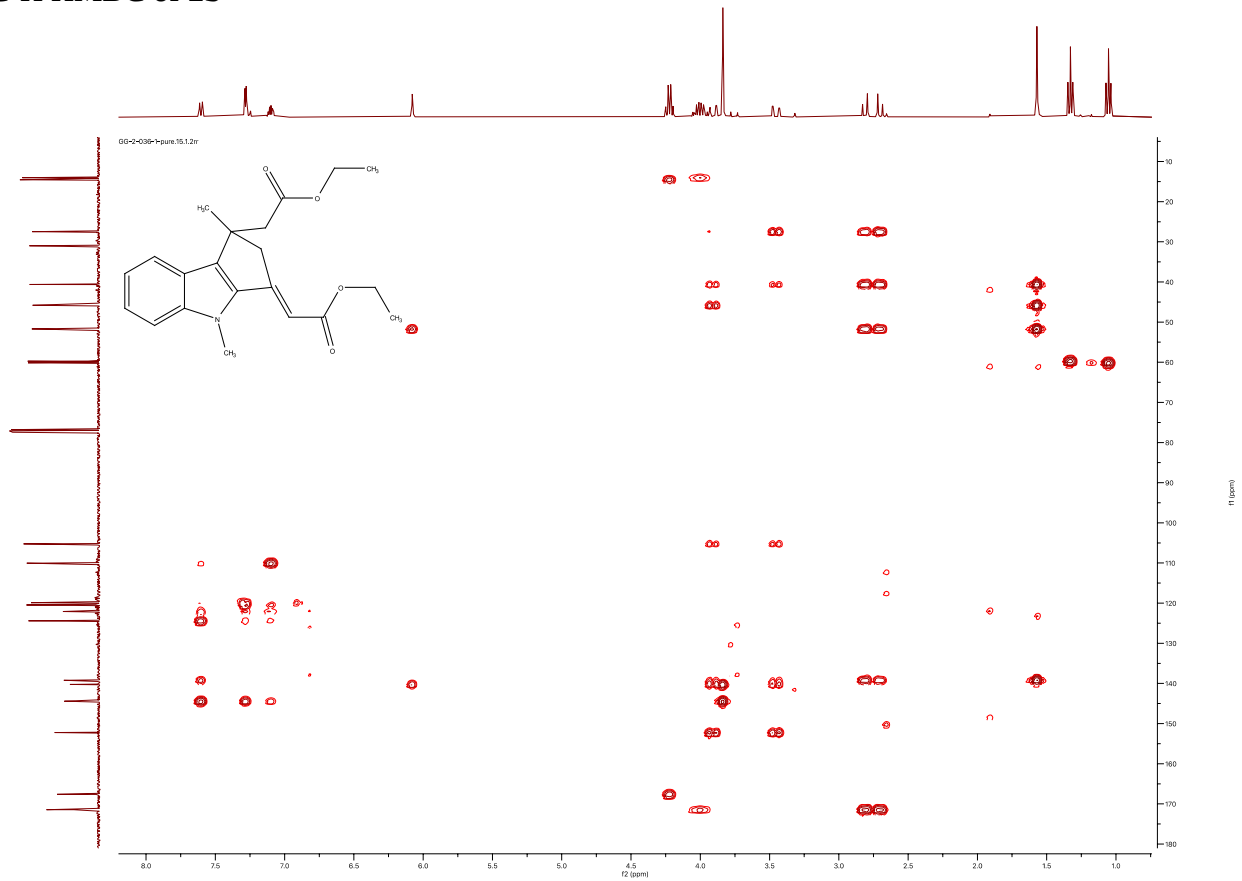
COSY of **2b**



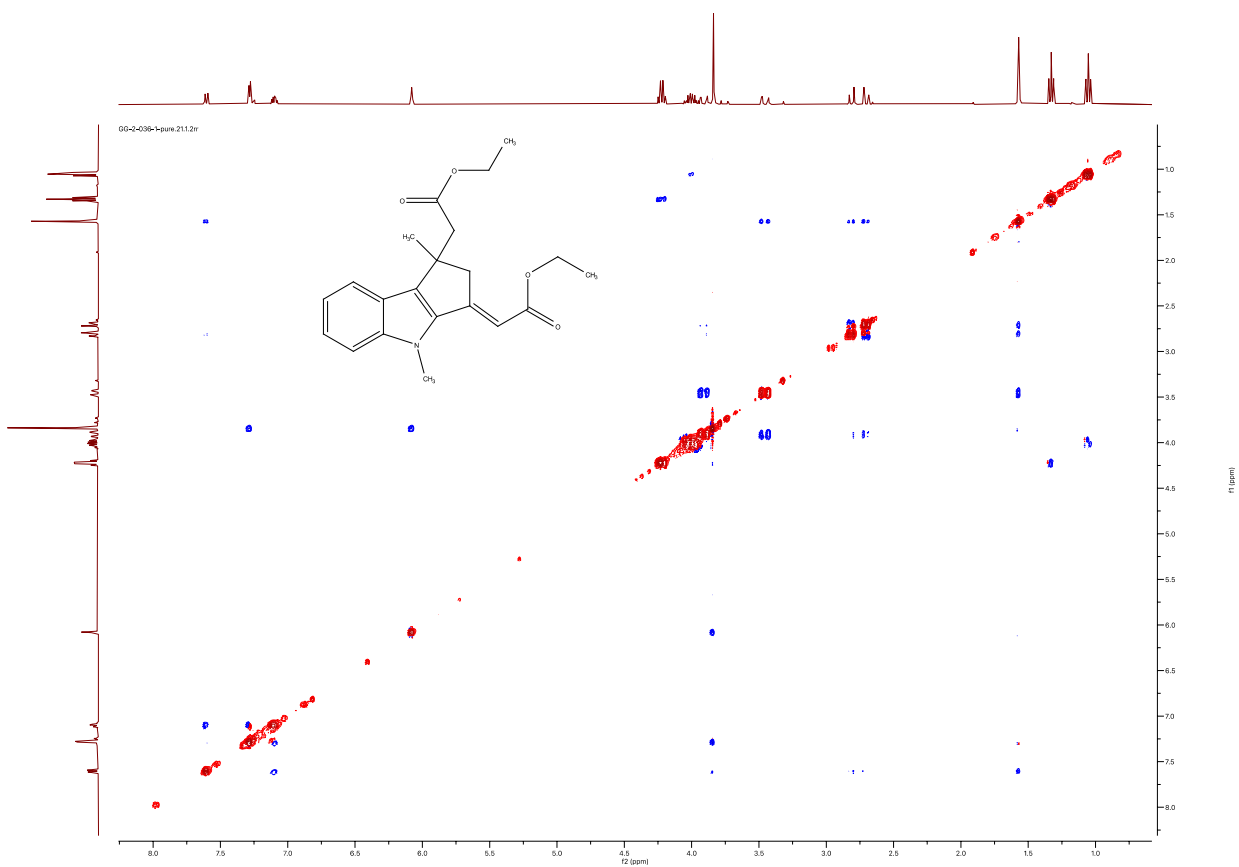
C-H HSQC of **2b**



C-H HMBC of **2b**

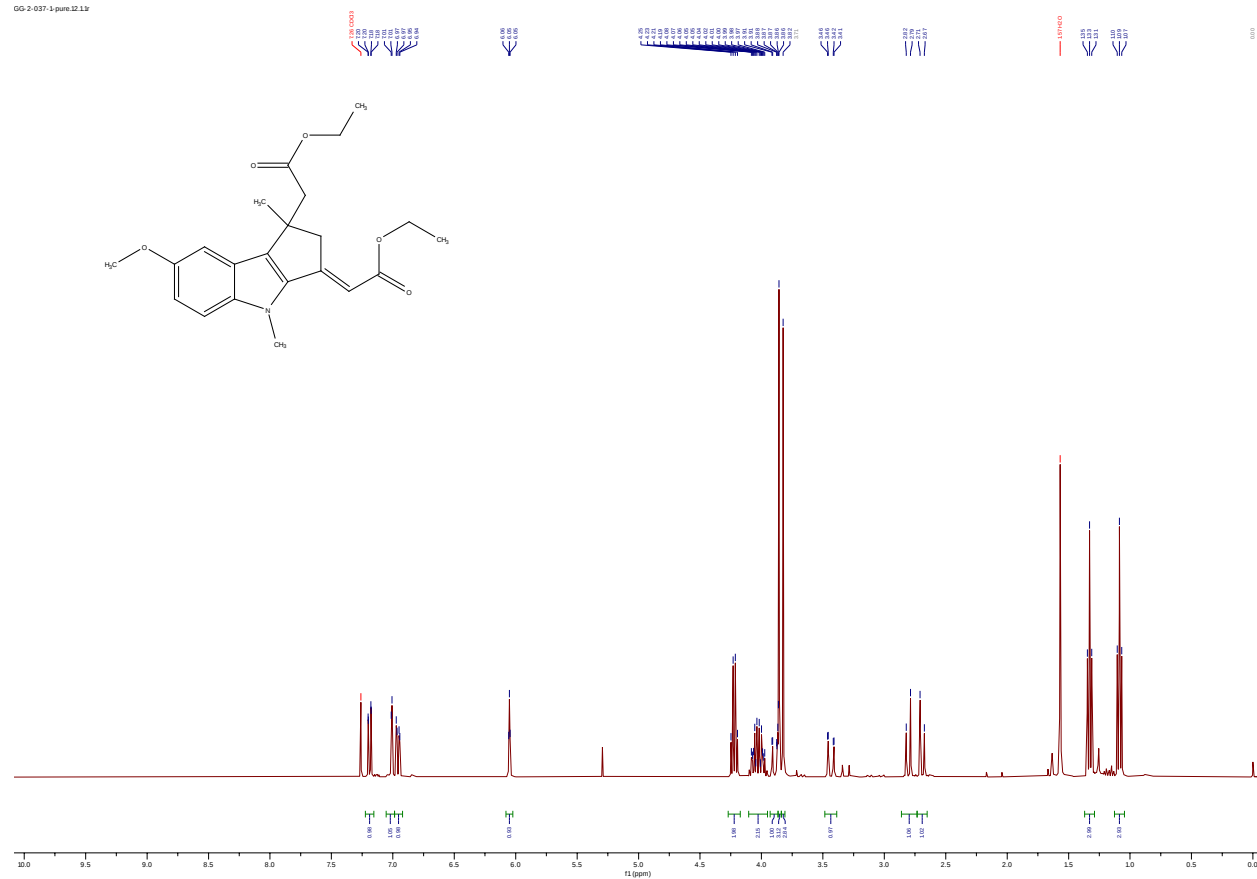


NOESY of **2b**



¹H NMR of **2c** in CDCl₃

GG-2-037-1-pure.12.119



¹³C NMR of **2c** in CDCl₃

