

SYNTHESIS AND STRUCTURAL CHARACTERIZATION OF THREE NOVEL 23,24-DINORCHOLANE BRASSINOSTEROID ANALOGS BEARING BENZOATE GROUPS AND HALOGEN SUBSTITUENTS.

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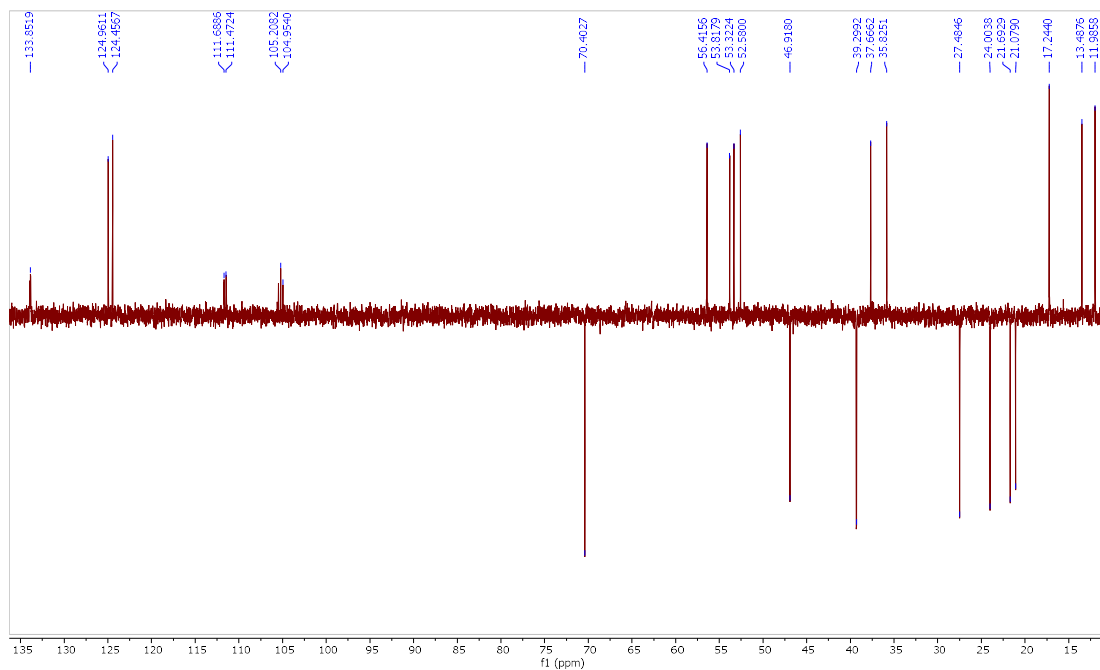


Fig. S3. ^{13}C DEPT-135 NMR Spectrum of 6-Oxo-23,24-dinor-5 α -Cholan-2-en-22-yl-(2,4-difluoro)-benzoate (22).

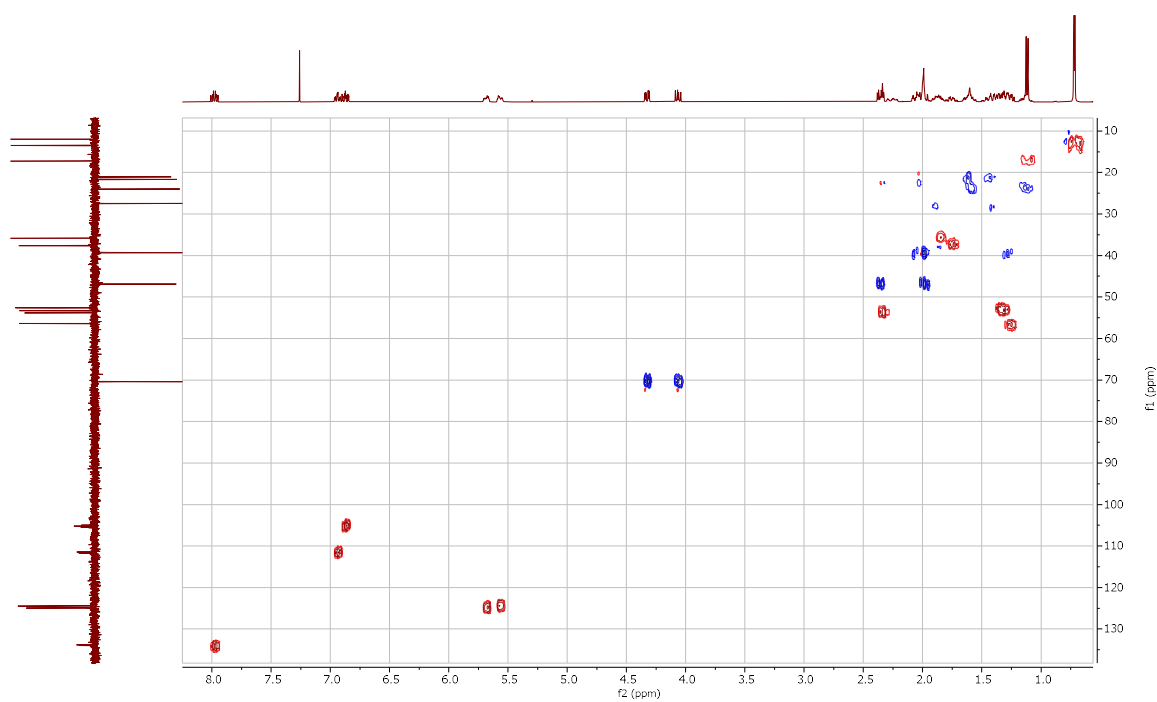


Fig. S4. 2D ^1H - ^{13}C HSQC Spectrum of 6-Oxo-23,24-dinor-5 α -Cholan-2-en-22-yl-(2,4-difluoro)-benzoate (22).

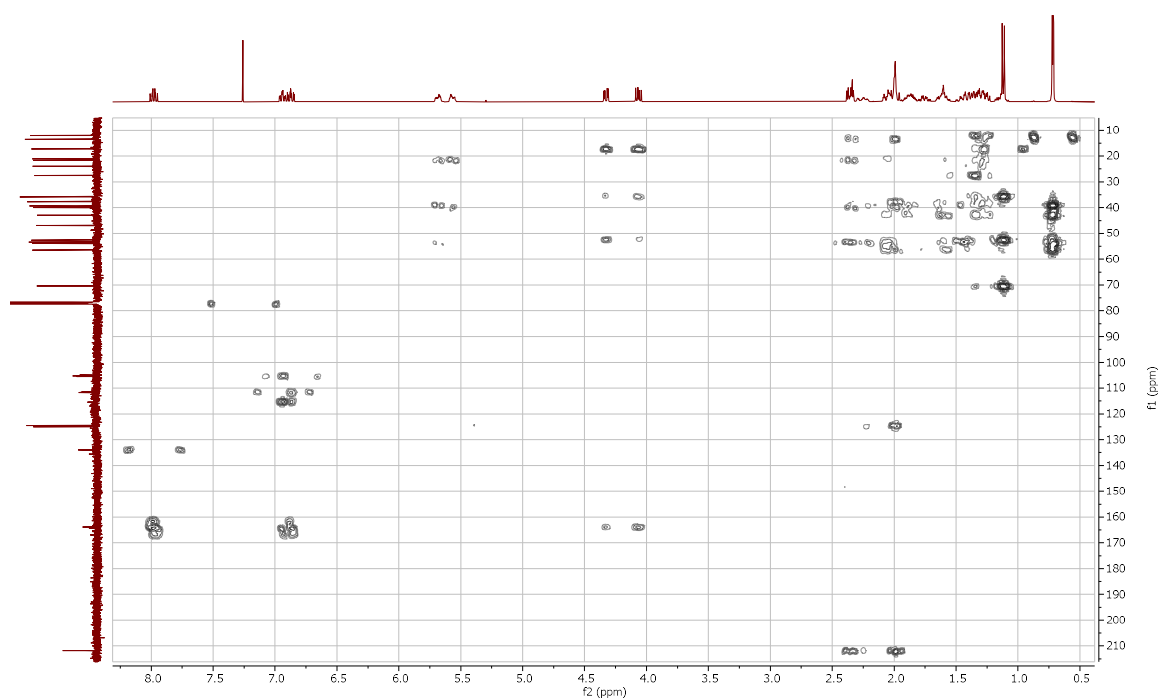


Fig. S5. 2D ^1H - ^{13}C HMBC Spectrum of 6-Oxo-23,24-dinor-5 α -Cholan-2-en-22-yl-(2,4-difluoro)-benzoate (**22**).

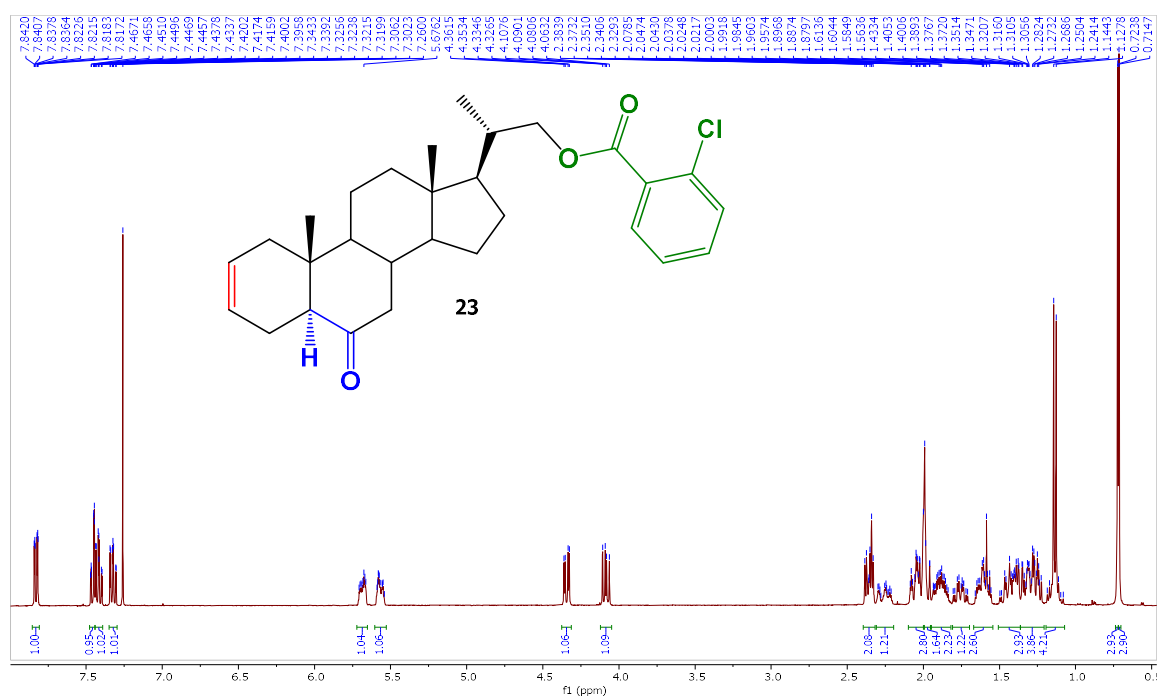


Fig. S6. ^1H NMR Spectrum of 6-Oxo-23,24-dinor-5 α -Cholan-2-en-22-yl-(2-chloro)-benzoate (**23**).

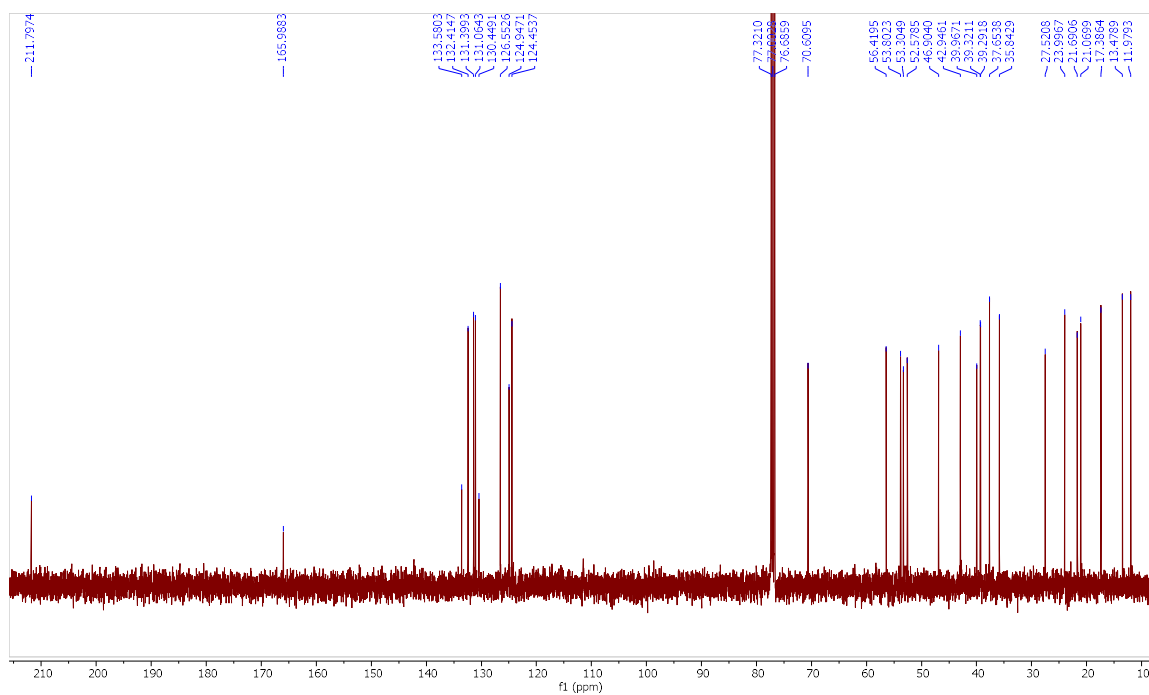


Fig. S7. ^{13}C NMR Spectrum of 6-Oxo-23,24-dinor-5 α -Cholan-2-en-22-yl-(2-chloro)-benzoate (**23**).

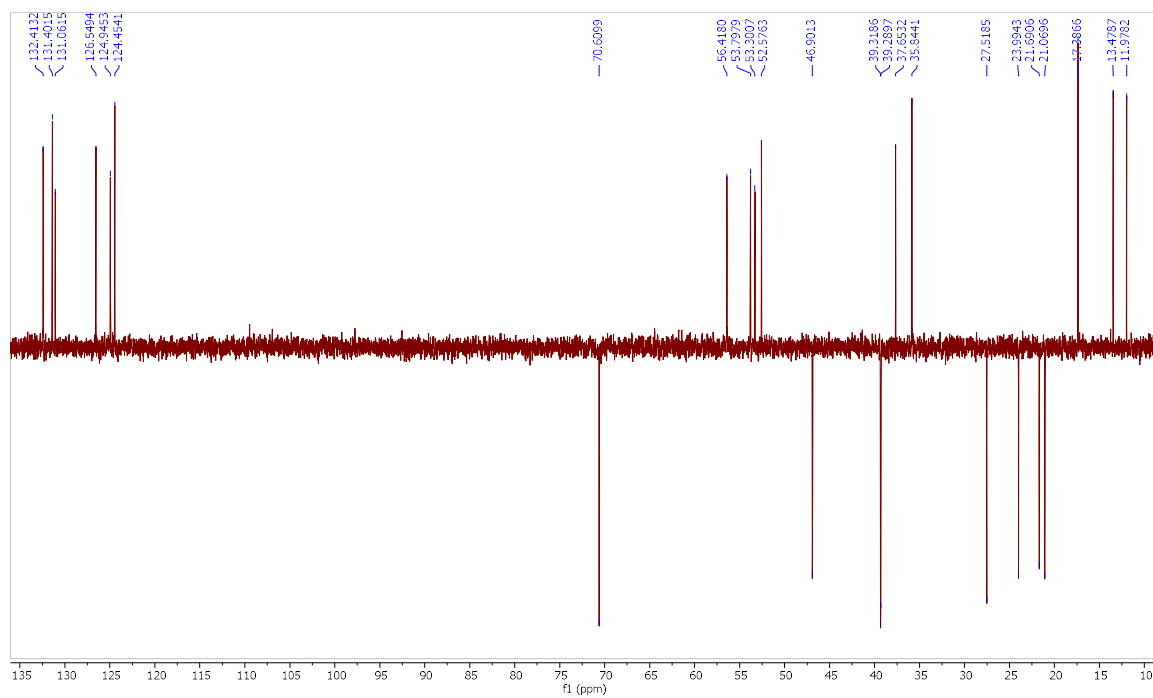


Fig. S8. ^{13}C DEPT-135 NMR Spectrum of 6-Oxo-23,24-dinor-5 α -Cholan-2-en-22-yl-(2-chloro)-benzoate (**23**).

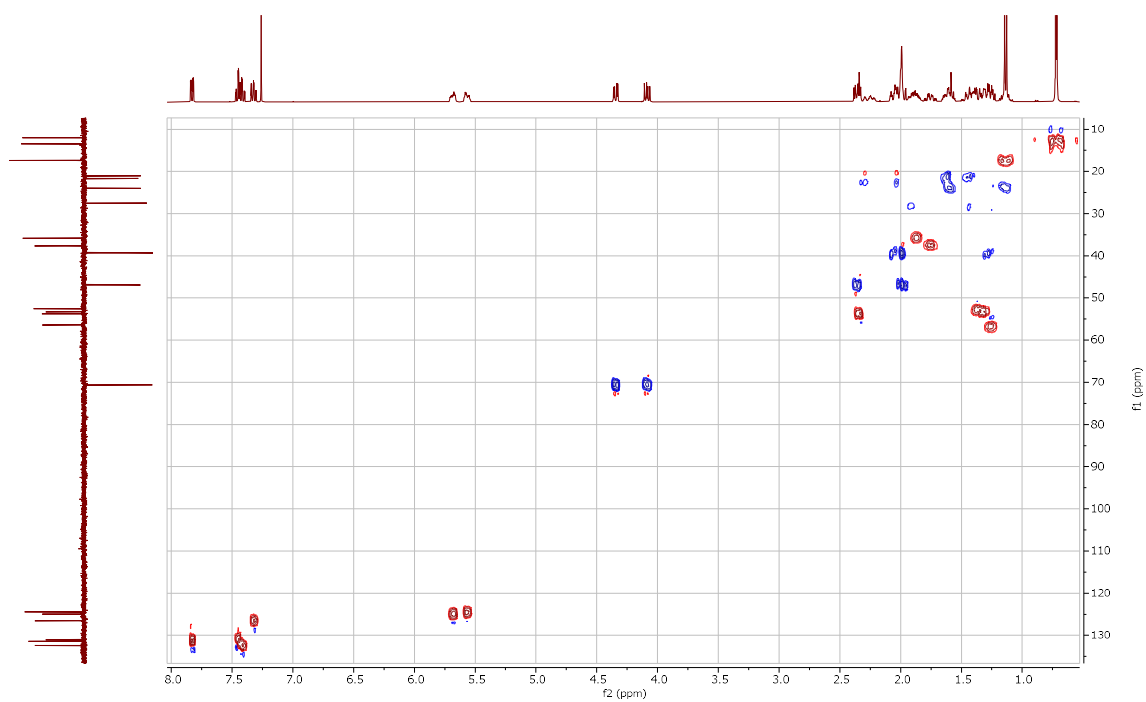


Fig. S9. 2D ^1H - ^{13}C HSQC NMR Spectrum of 6-Oxo-23,24-dinor-5 α -Cholan-2-en-22-yl-(2-chloro)-benzoate (23).

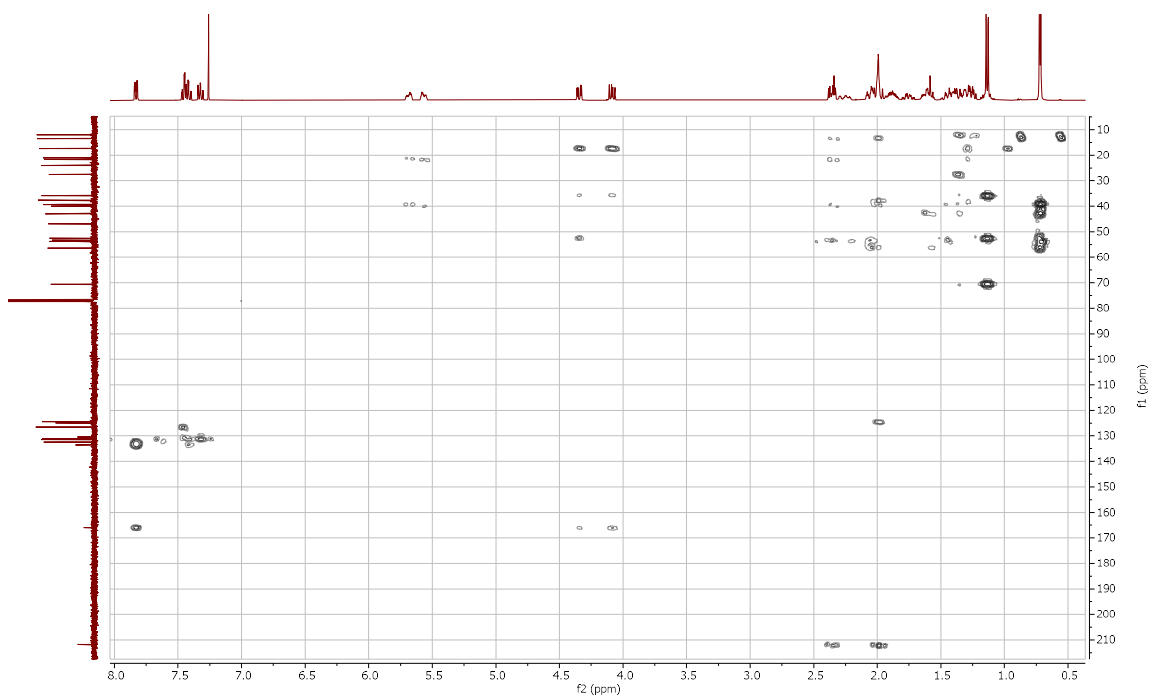


Fig. S10. 2D ^1H - ^{13}C HSQC NMR Spectrum of 6-Oxo-23,24-dinor-5 α -Cholan-2-en-22-yl-(2-chloro)-benzoate (23).

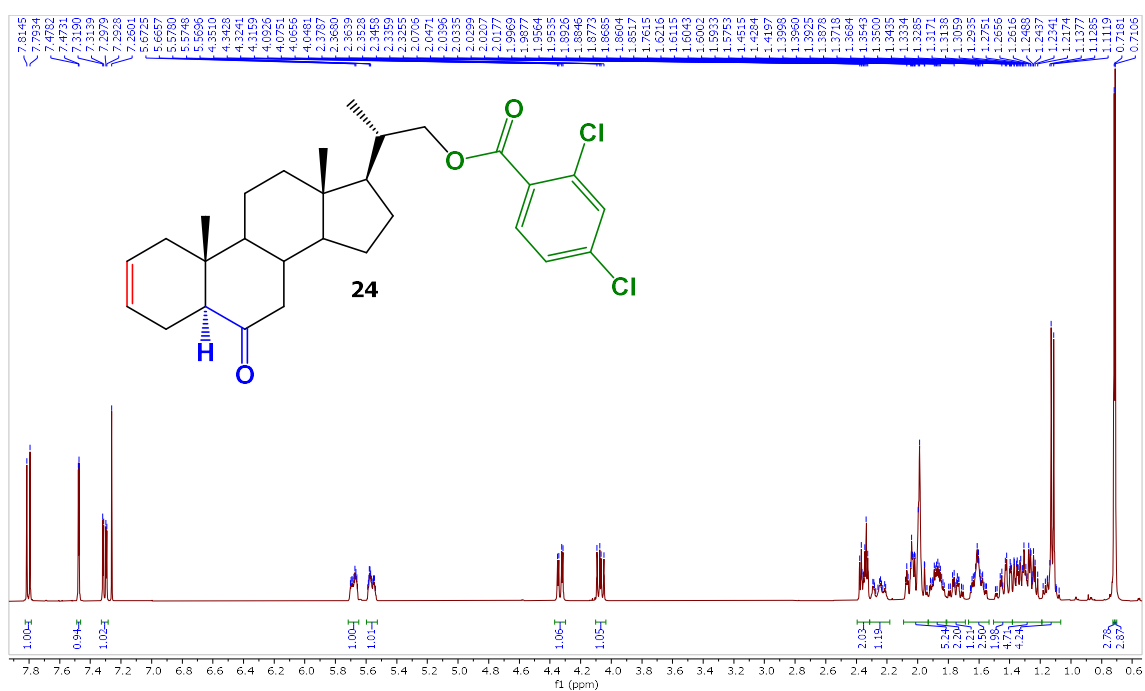


Fig. S11. ^1H NMR Spectrum of 6-Oxo-23,24-dinor-5 α -Cholan-2-en-22-yl-(2,4-dichloro)-benzoate (24).

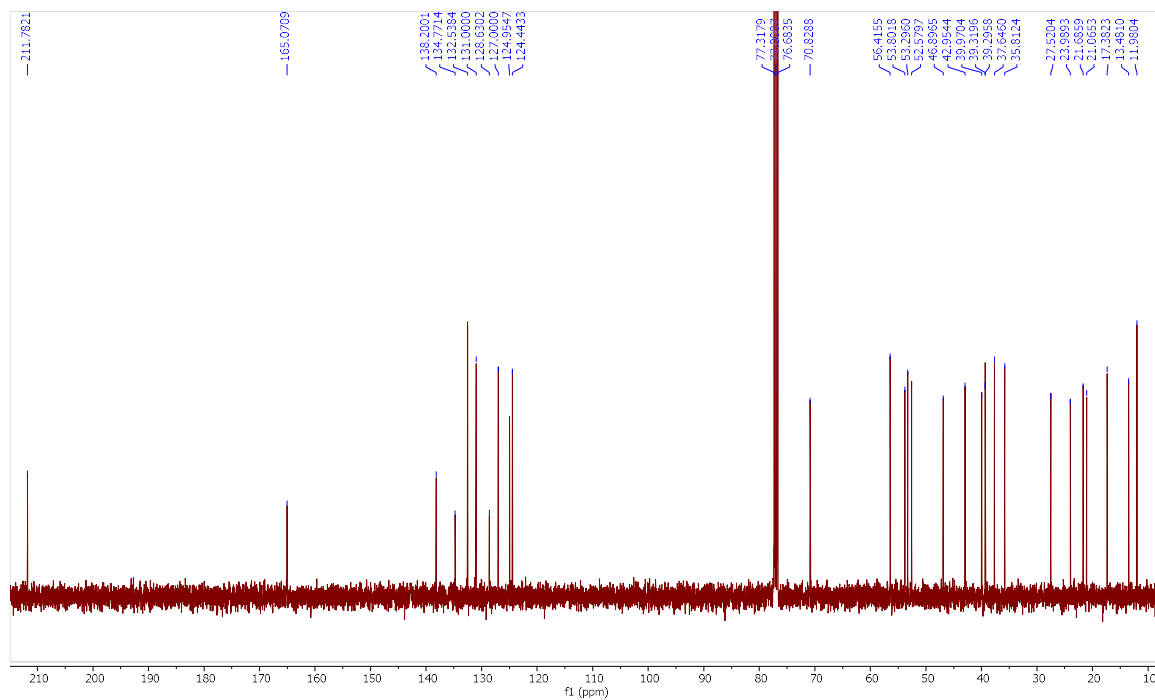


Fig. S12. ^{13}C NMR Spectrum of 6-Oxo-23,24-dinor-5 α -Cholan-2-en-22-yl-(2,4-dichloro)-benzoate (24).

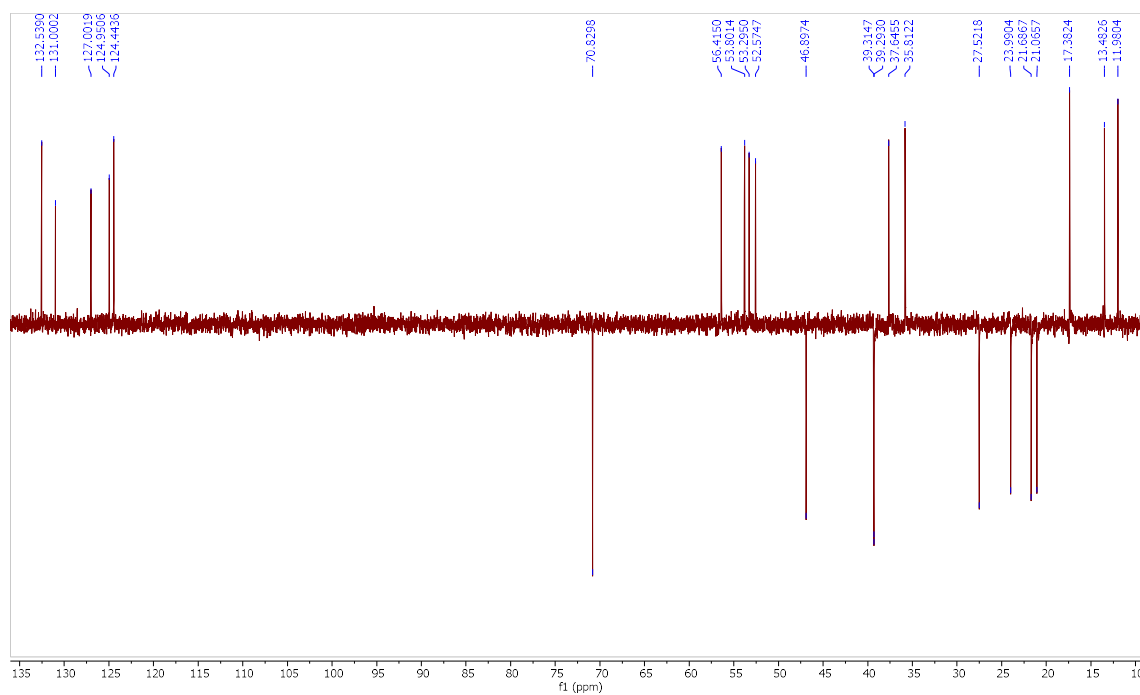


Fig. S13. ^{13}C DEPT-135 NMR Spectrum of 6-Oxo-23,24-dinor-5 α -Cholan-2-en-22-yl-(2,4-dichloro)-benzoate (24).

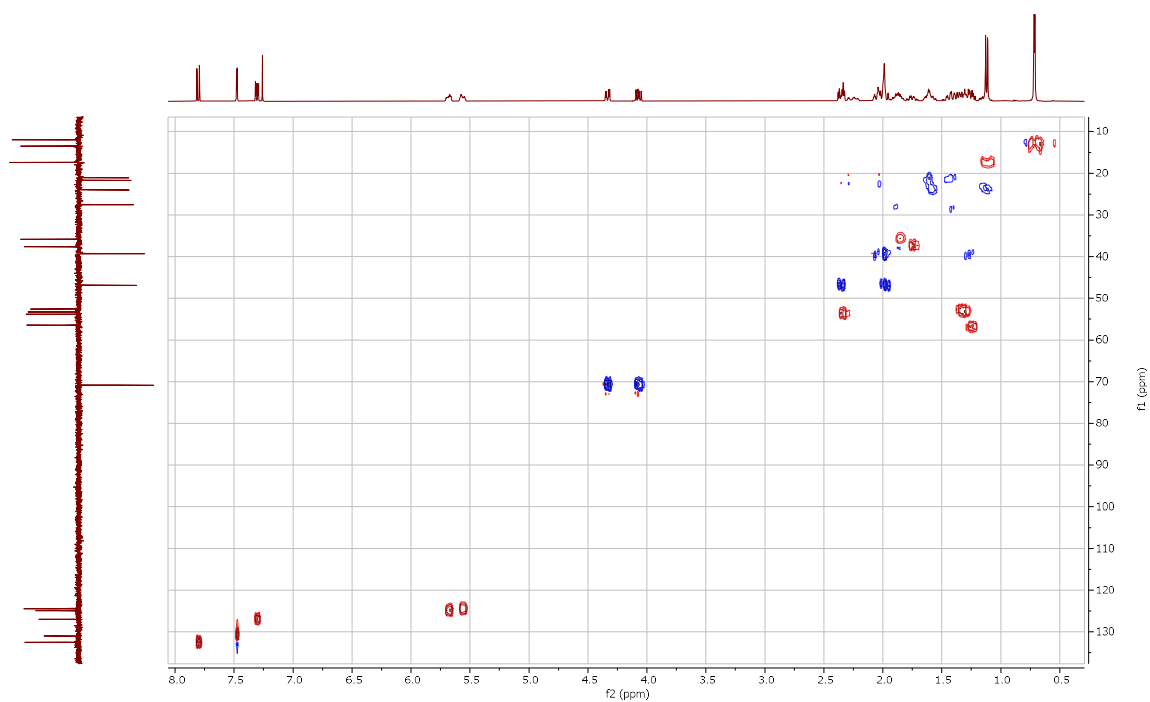


Fig. S14. 2D ^1H - ^{13}C HSQC NMR Spectrum of 6-Oxo-23,24-dinor-5 α -Cholan-2-en-22-yl-(2,4-dichloro)-benzoate (24).

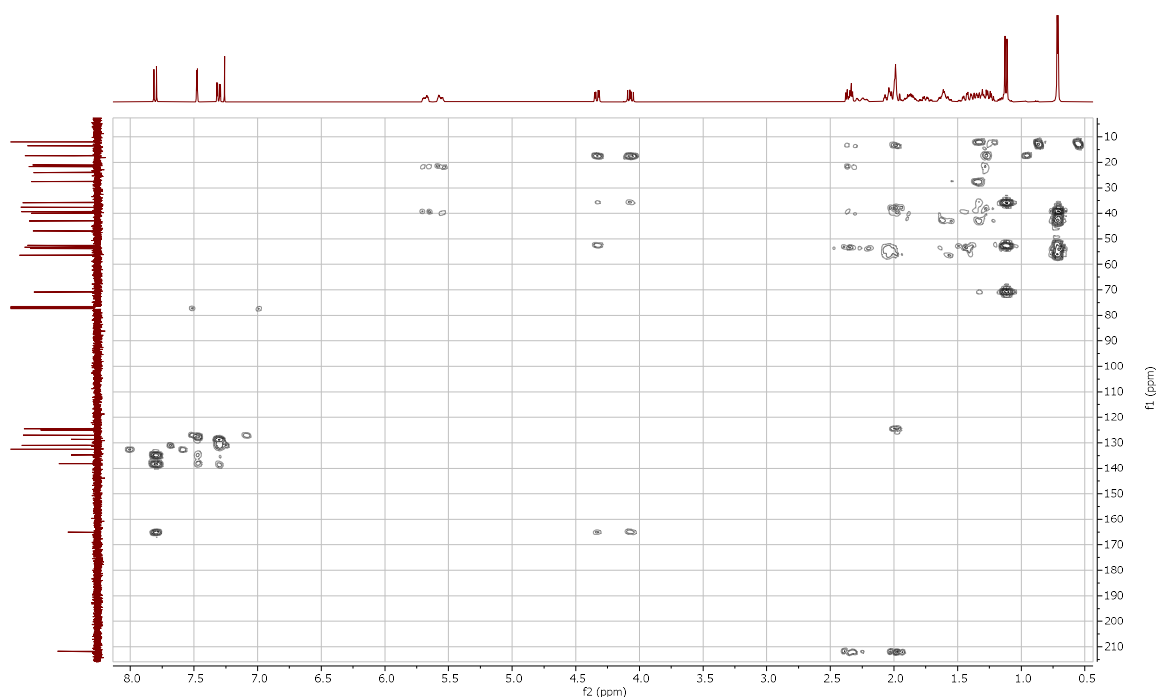


Fig. S15. 2D ^1H - ^{13}C HMBC NMR Spectrum of 6-Oxo-23,24-dinor-5 α -Cholan-2-en-22-yl-(2,4-dichloro)-benzoate (**24**).

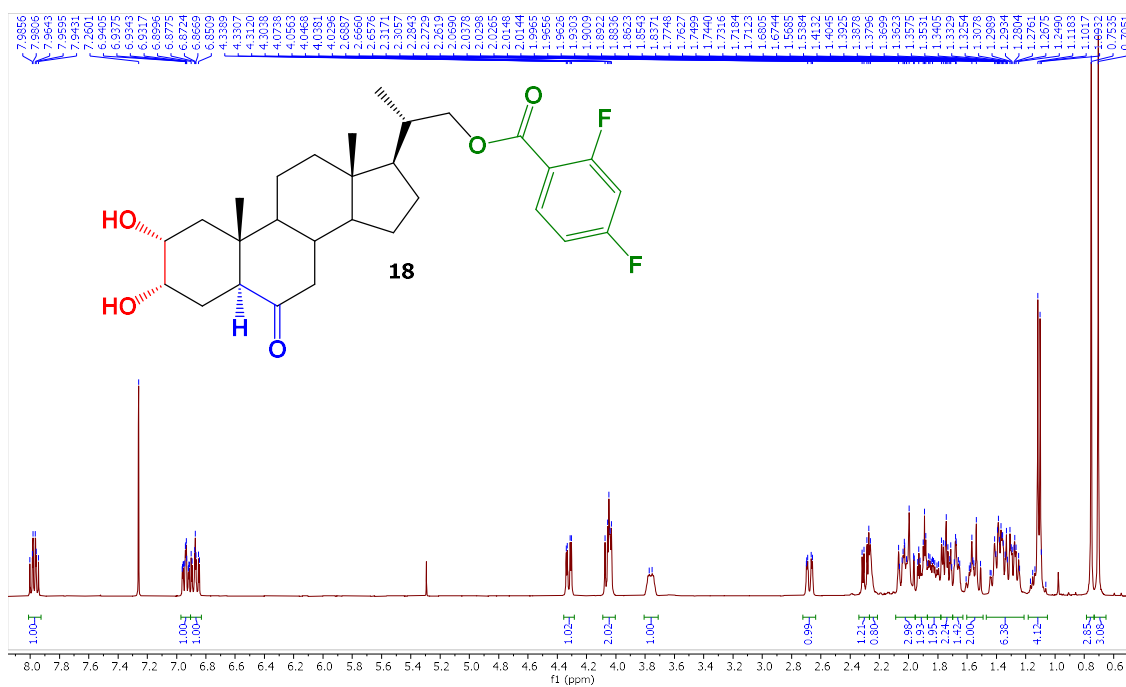


Fig. S16. ^1H NMR Spectrum of 2 α ,3 α -Dihydroxy-6-oxo-23,24-dinor-5 α -cholan-22-yl-(2,4-difluoro)-benzoate (**18**).

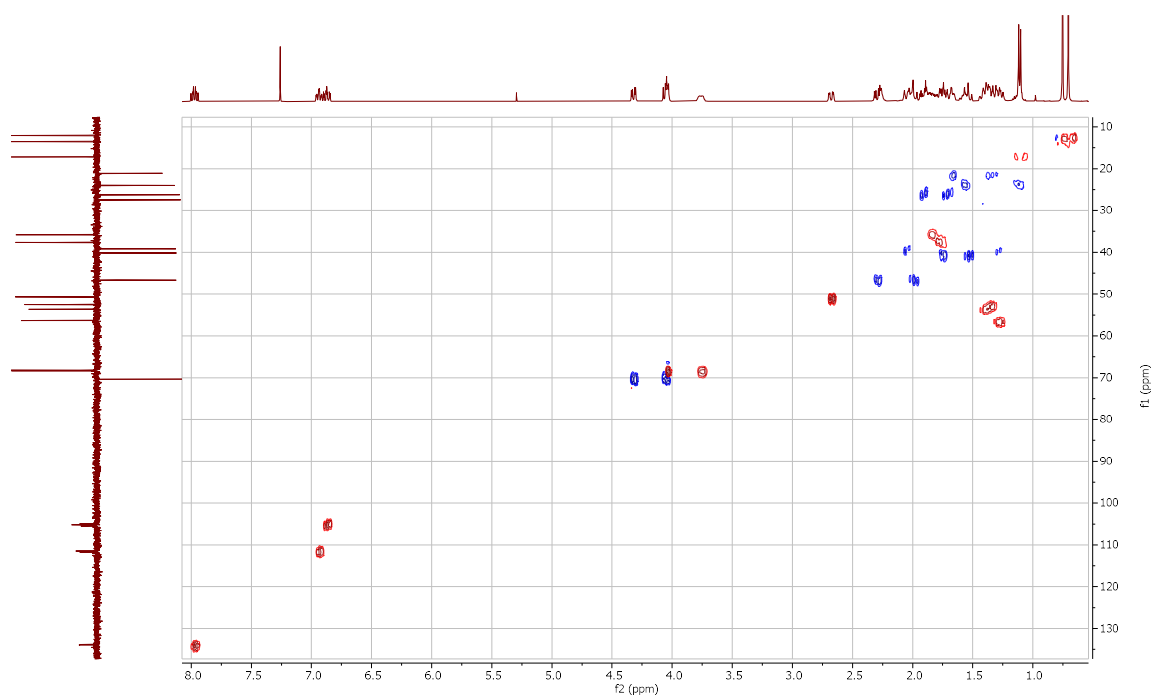


Fig. S19. 2D ^1H - ^{13}C HSQC NMR Spectrum of $2\alpha,3\alpha$ -Dihydroxy-6-oxo-23,24-dinor- 5α -cholan-22-yl-(2,4-difluoro)-benzoate (**18**).

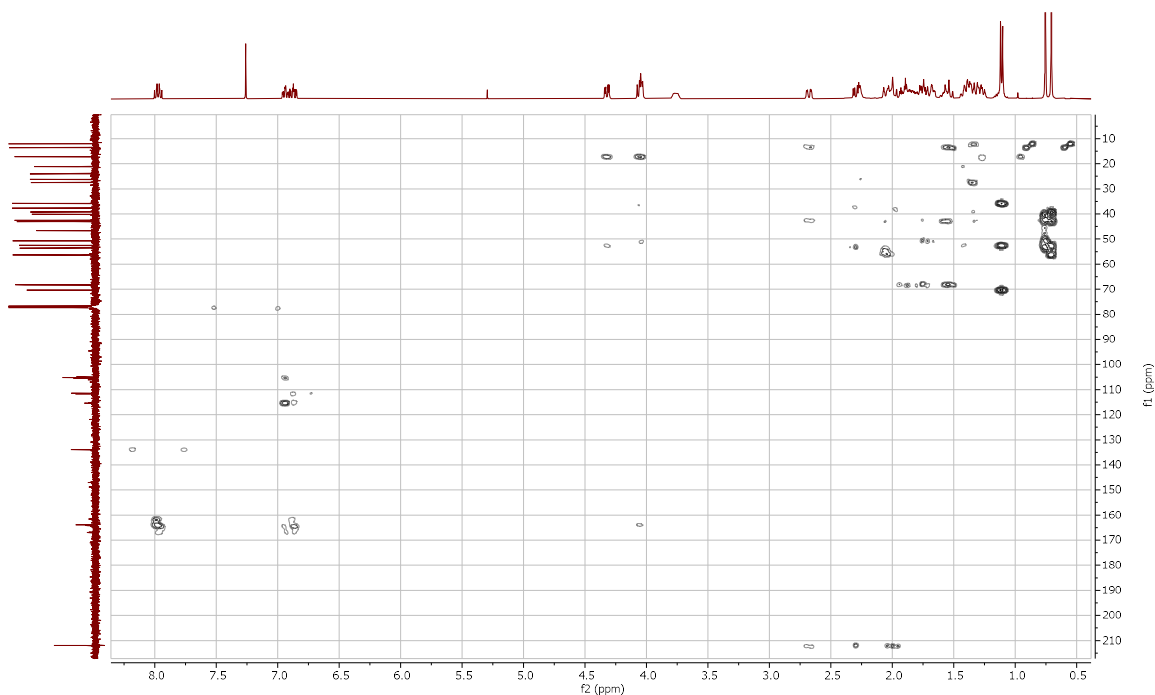


Fig. S20. 2D ^1H - ^{13}C HMBC NMR Spectrum of $2\alpha,3\alpha$ -Dihydroxy-6-oxo-23,24-dinor- 5α -cholan-22-yl-(2,4-difluoro)-benzoate (**18**).

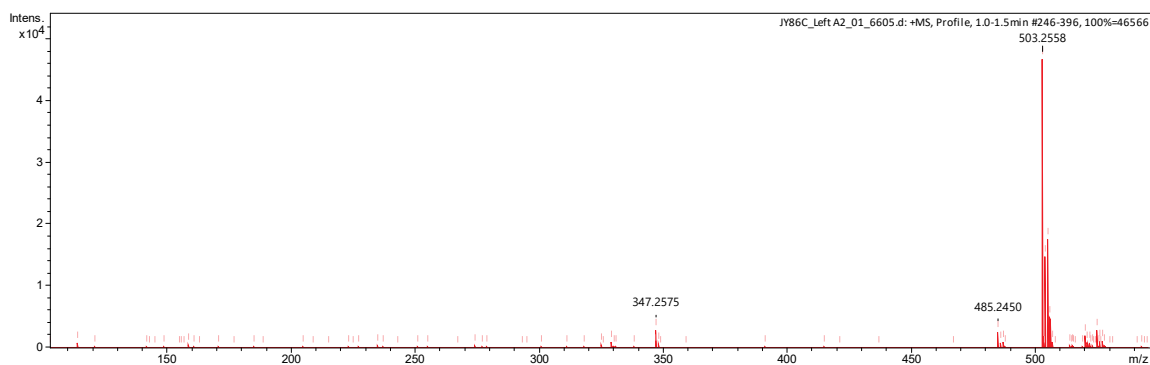


Fig. S21. HRMS spectrum of 2 α ,3 α -Dihydroxy-6-oxo-23,24-dinor-5 α -cholan-22-yl-(2,4-difluoro)-benzoate (18).

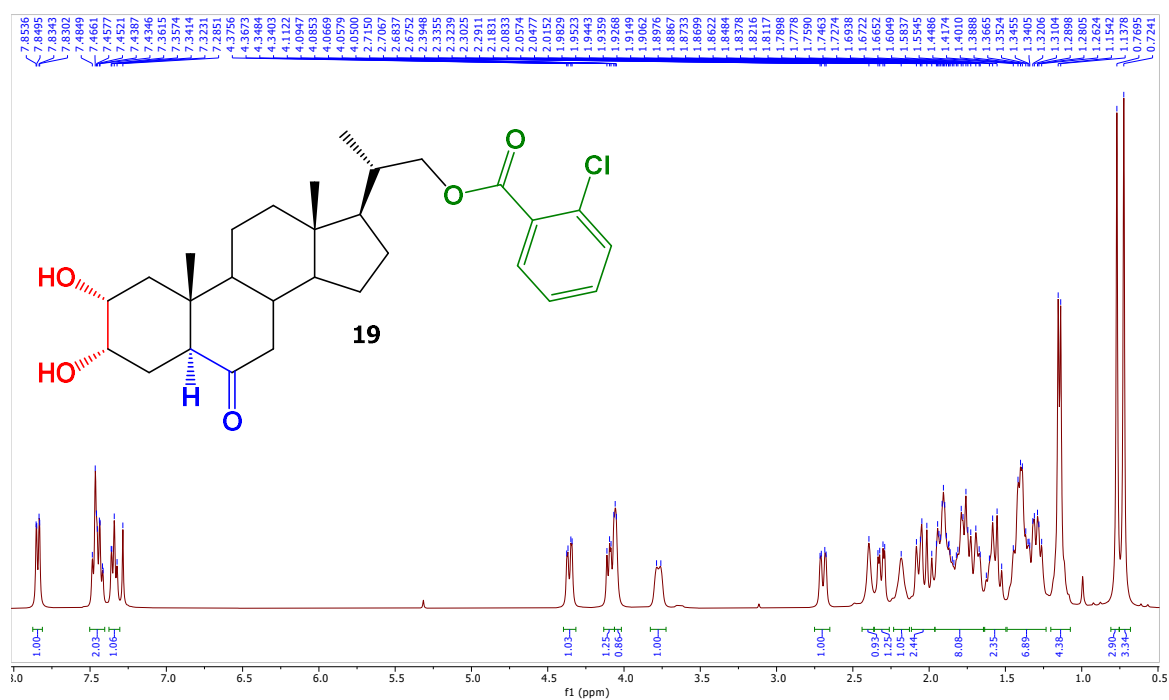


Fig. S22. ¹H NMR Spectrum of 2 α ,3 α -Dihydroxy-6-oxo-23,24-dinor-5 α -cholan-22-yl-(2-chloro)-benzoate (19).

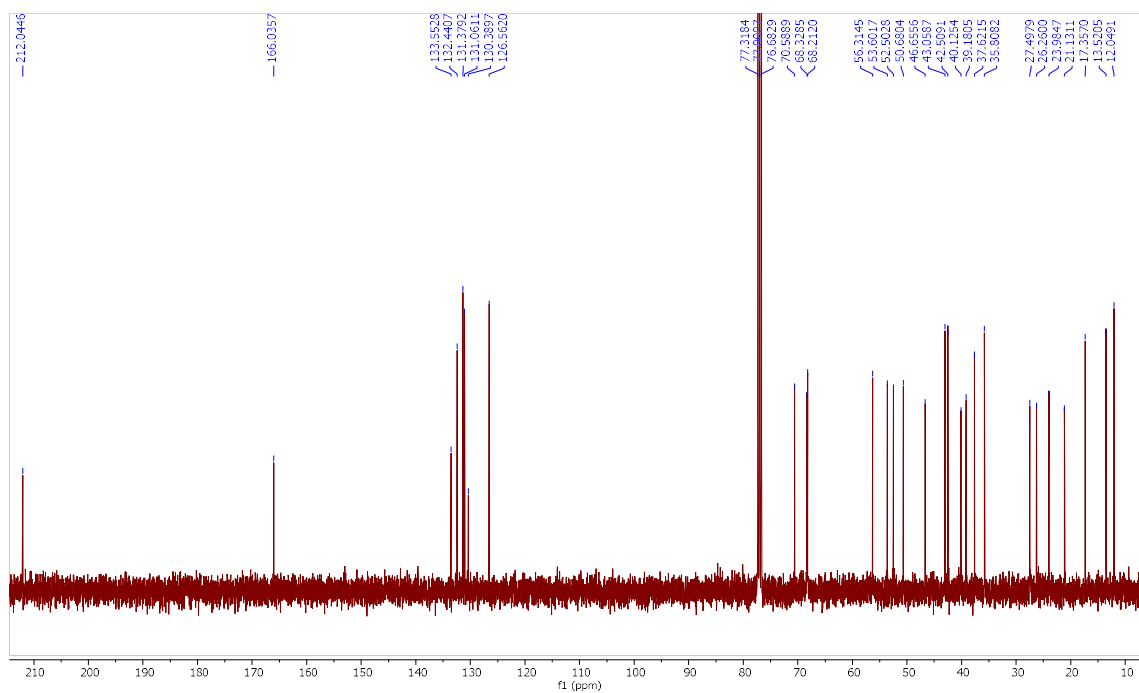


Fig. S23. ^{13}C NMR Spectrum of $2\alpha,3\alpha$ -Dihydroxy-6-oxo-23,24-dinor- 5α -cholan-22-yl-(2-chloro)-benzoate (**19**).

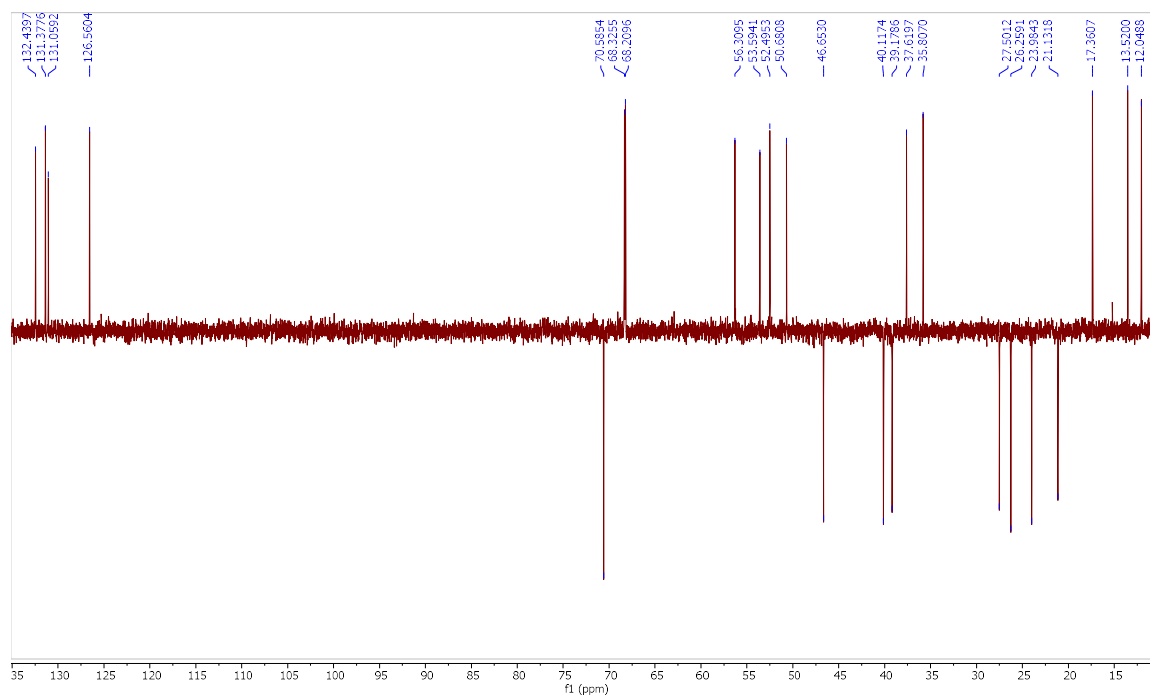


Fig. S24. ^{13}C DEPT-135 NMR Spectrum of $2\alpha,3\alpha$ -Dihydroxy-6-oxo-23,24-dinor- 5α -cholan-22-yl-(2-chloro)-benzoate (**19**).

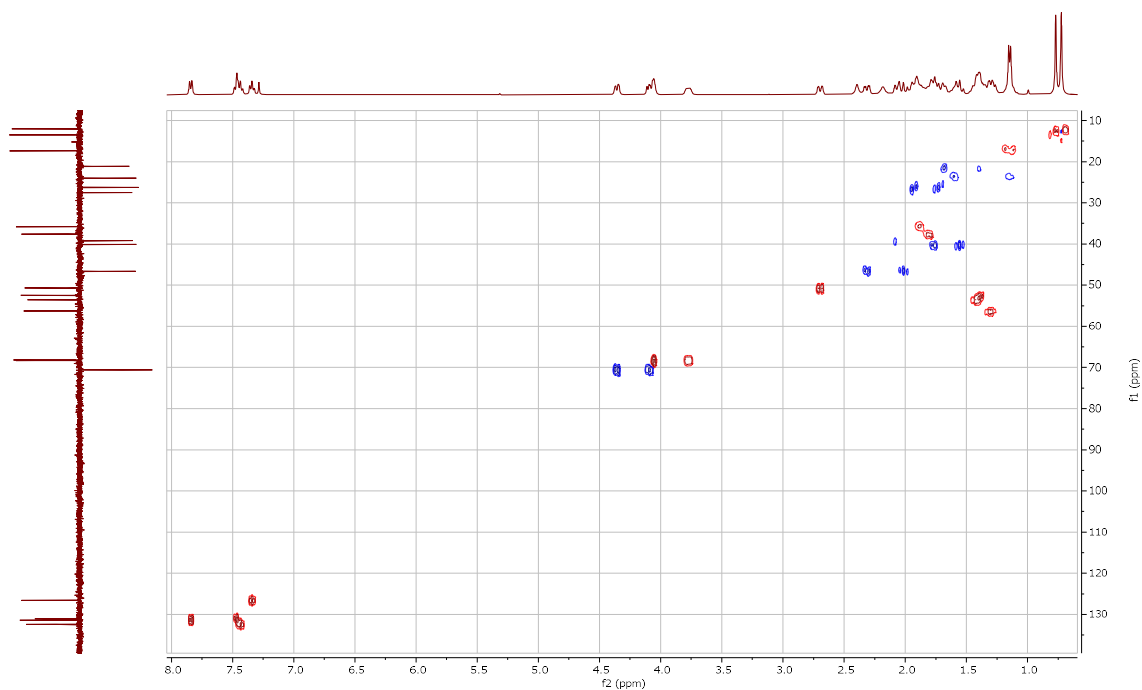


Fig. S25. 2D ^1H - ^{13}C HSQC NMR Spectrum of $2\alpha,3\alpha$ -Dihydroxy-6-oxo-23,24-dinor- 5α -cholan-22-yl-(2-chloro)-benzoate (**19**).

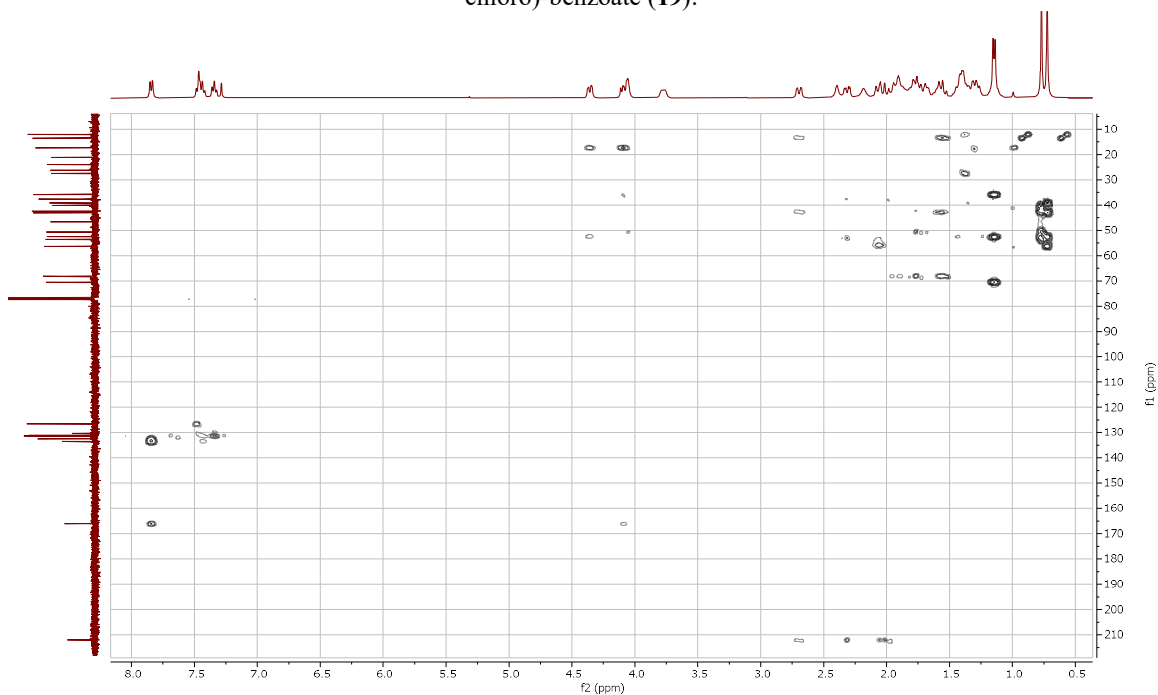


Fig. S26. 2D ^1H - ^{13}C HMBC NMR Spectrum of $2\alpha,3\alpha$ -Dihydroxy-6-oxo-23,24-dinor- 5α -cholan-22-yl-(2-chloro)-benzoate (**19**).

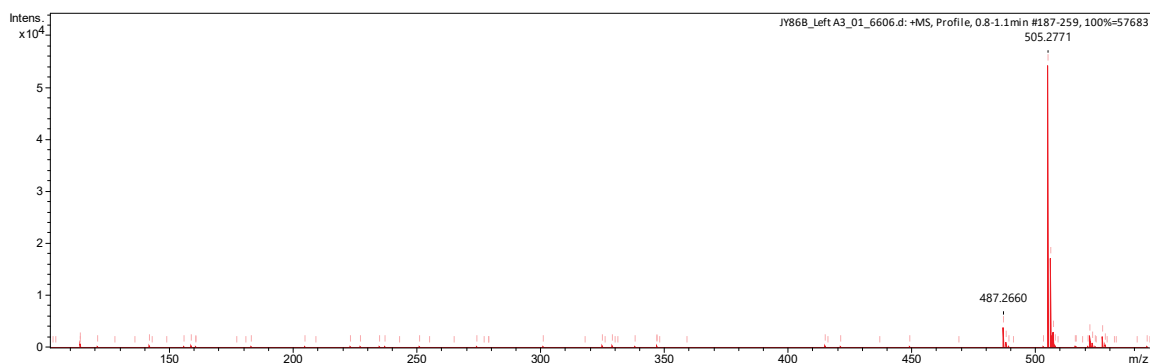


Fig. S27. HRMS spectrum of 2 α ,3 α -Dihydroxy-6-oxo-23,24-dinor-5 α -cholan-22-yl-(2-chloro)-benzoate (**19**).

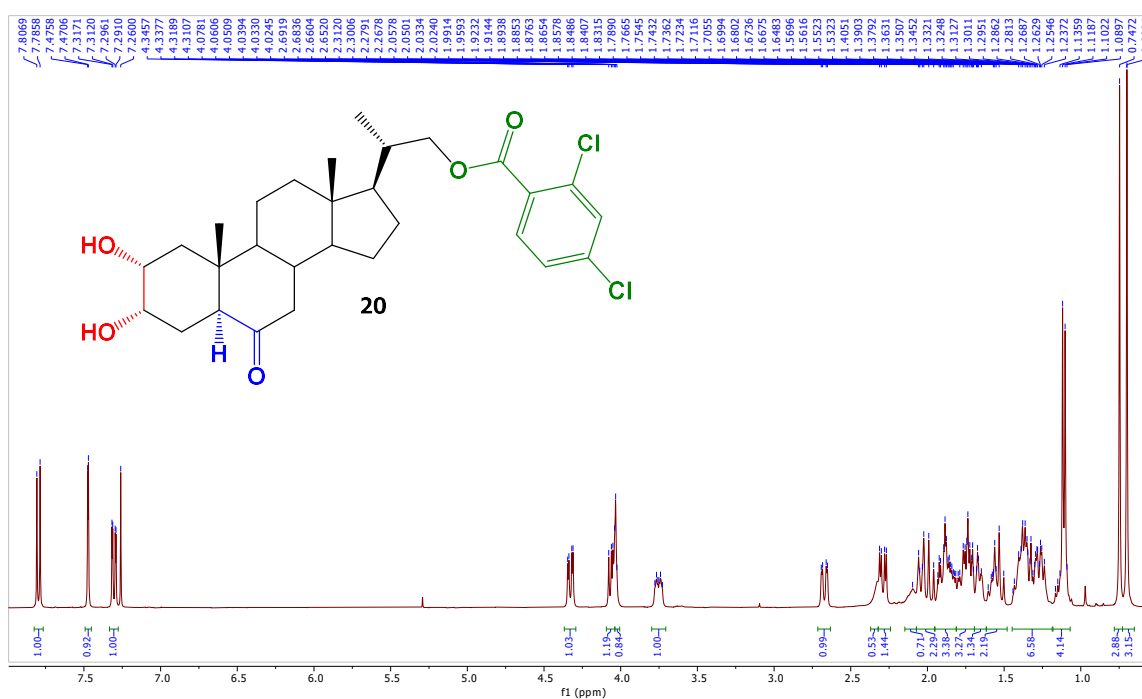


Fig. S28. ^1H NMR Spectrum of 2 α ,3 α -Dihydroxy-6-oxo-23,24-dinor-5 α -cholan-22-yl-(2,4-dichloro)-benzoate (**20**).

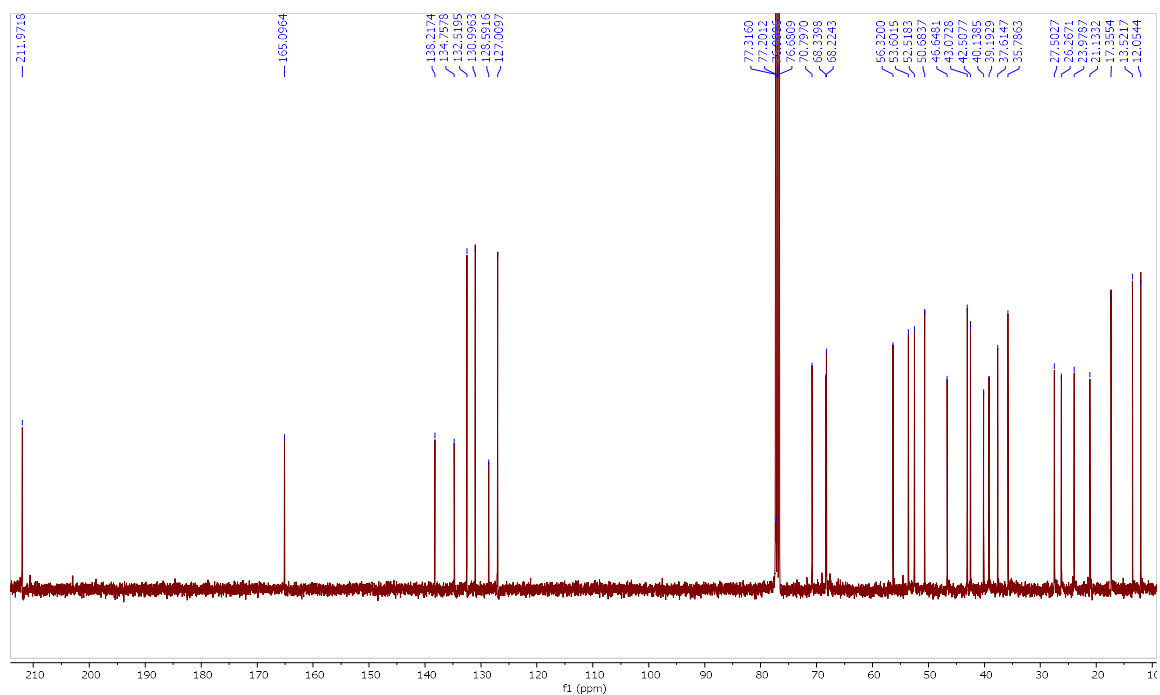


Fig. S29. ^{13}C NMR Spectrum of $2\alpha,3\alpha$ -Dihydroxy-6-oxo-23,24-dinor- 5α -cholan-22-yl-(2,4-dichloro)-benzoate (**20**).

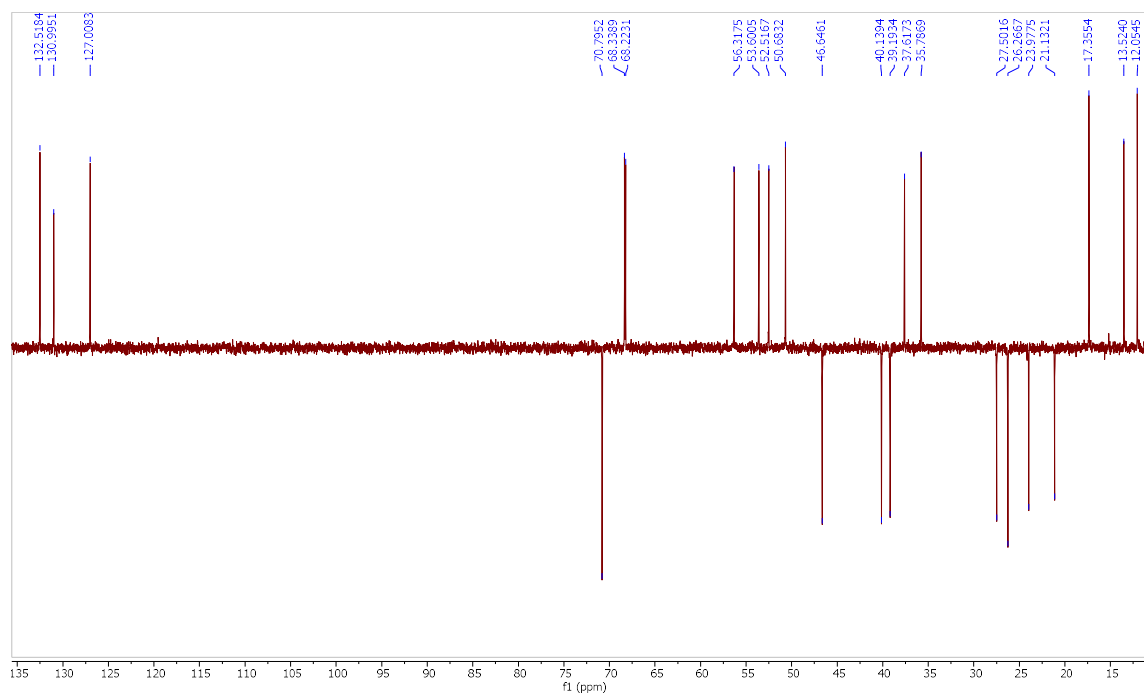


Fig. S30. ^{13}C DEPT-135 NMR Spectrum of $2\alpha,3\alpha$ -Dihydroxy-6-oxo-23,24-dinor- 5α -cholan-22-yl-(2,4-dichloro)-benzoate (**20**).

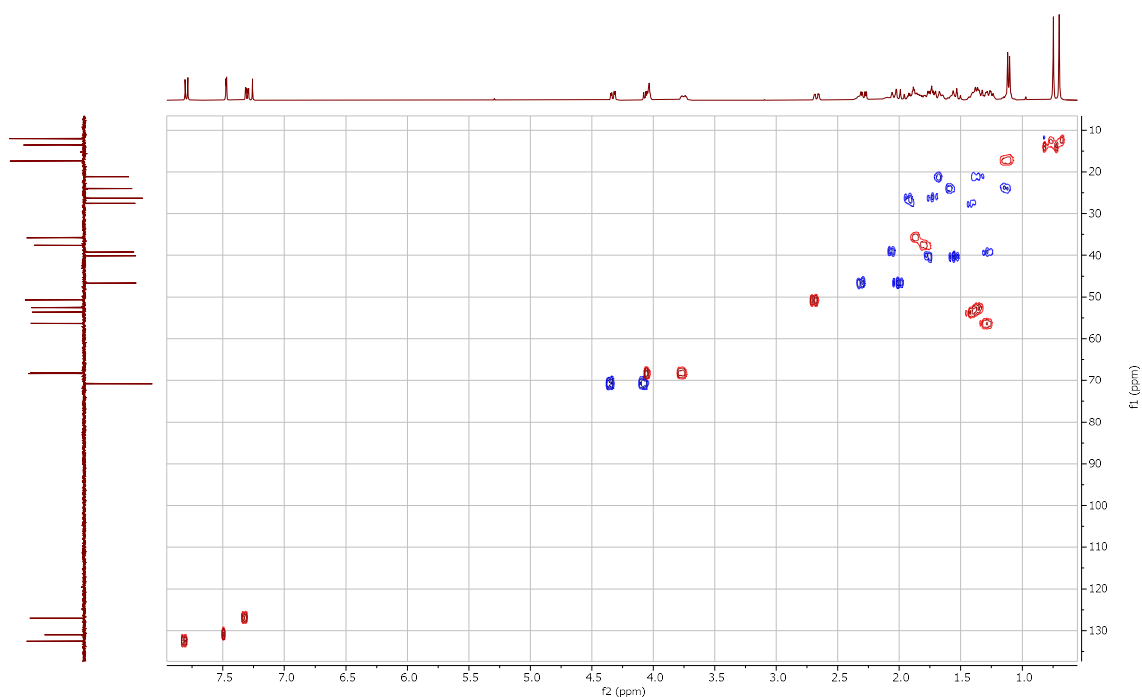


Fig. S31. 2D ^1H - ^{13}C HSQC NMR Spectrum of $2\alpha,3\alpha$ -Dihydroxy-6-oxo-23,24-dinor- 5α -cholan-22-yl-(2,4-dichloro)-benzoate (**20**).

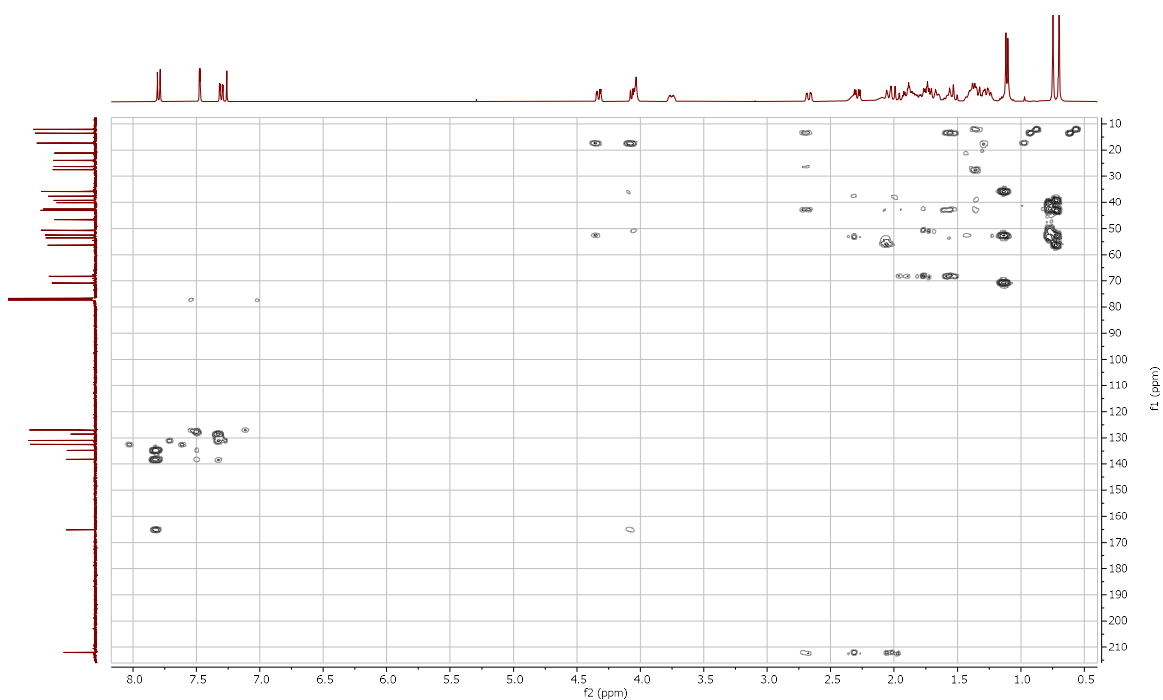


Fig. S32. 2D ^1H - ^{13}C HMBC NMR Spectrum of $2\alpha,3\alpha$ -Dihydroxy-6-oxo-23,24-dinor- 5α -cholan-22-yl-(2,4-dichloro)-benzoate (**20**).

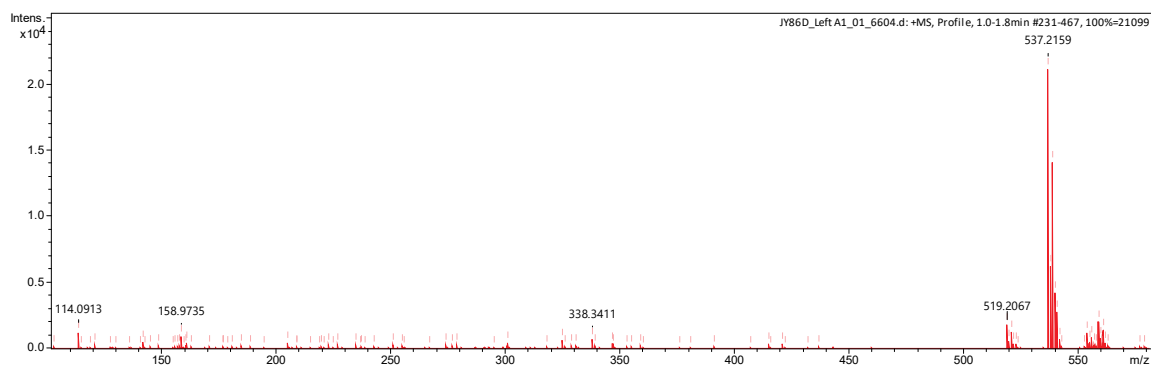


Fig. S33. HRMS spectrum of 2 α ,3 α -Dihydroxy-6-oxo-23,24-dinor-5 α -cholan-22-yl-(2,4-dichloro)-benzoate (**20**).