

Article

Synthesis of New Brassinosteroid 24-Norcholane Type Analogs Conjugated in C-3 with Benzoate Groups

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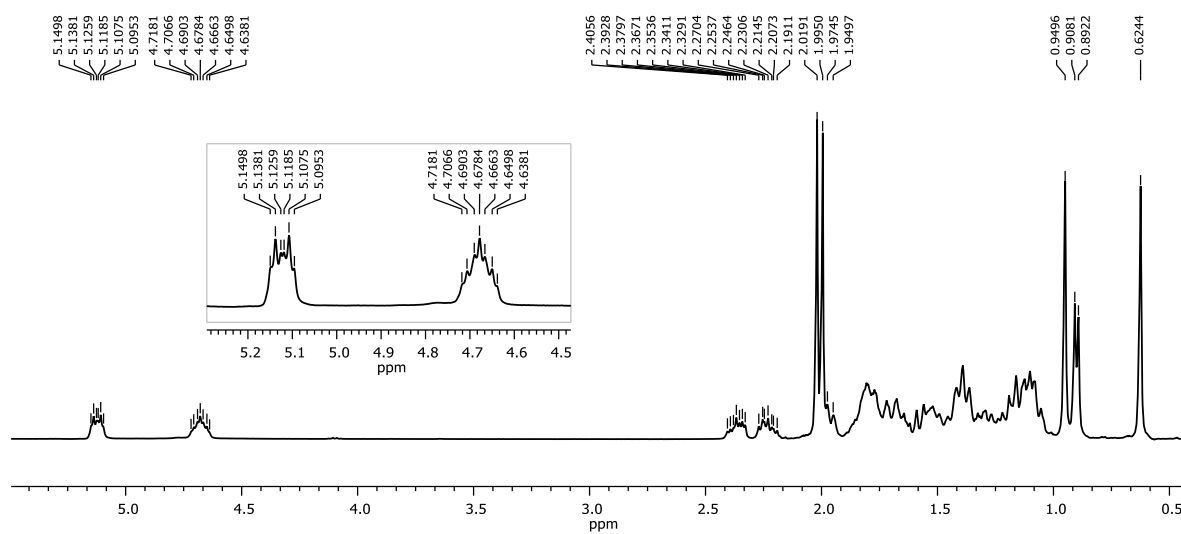
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Supplementary Materials: The following are available online at www.mdpi.com/xxx/s1, **Figure S1**: NMR spectra of 3 α ,6 α -diacetox-5 β -cholan-24-oic acid (**22**), **Figure S2**: NMR spectra of 24-nor-5 β -cholan-22-ene-3 α ,6 α -diyl diacetate (**23**), **Figure S3**: NMR spectra of 24-nor-5 β -chol-22-ene-3 α ,6 α -diol (**24**), **Figure S4**: NMR spectra of 6 α -hydroxy-24-nor-5 β -chol-22-en-3-one (**25**), **Figure S5**: NMR spectra of 24-nor-5 β -chol-22-ene-3,6-dione (**26**), **Figure S6**: NMR spectra of 3 α -hydroxy-24-nor-5 β -chol-22-en-6-one (**27**), **Figure S7**: NMR spectra of 3 α -hydroxy-24-nor-5 α -chol-22-en-6-one (**28**), **Figure S8**: NMR spectra of 6-oxo-24-nor-5 α -chol-22-en-3 α -yl 4-methylbenzoate (**29**), **Figure S9**: NMR spectra of 6-oxo-24-nor-5 α -chol-22-en-3 α -yl 2-fluorobenzoate (**30**), **Figure S10**: NMR spectra of (22*R*)-22,23-dihydroxy-6-oxo-24-nor-5 α -cholan-3 α -yl 4-methylbenzoate (**18a**), **Figure S11**: NMR spectra of (22*S*)-22,23-dihydroxy-6-oxo-24-nor-5 α -cholan-3 α -yl 4-methylbenzoate (**18b**), **Figure S12**: NMR spectra of (22*R*)-22,23-dihydroxy-6-oxo-24-nor-5 α -cholan-3 α -yl 2-fluorobenzoate (**19a**), **Figure S13**: NMR spectra of (22*S*)-22,23-dihydroxy-6-oxo-24-nor-5 α -cholan-3 α -yl 2-fluorobenzoate (**19b**), **Figure S14**: HRMS (API⁺) spectrum of 3 α -hydroxy-24-nor-5 α -chol-22-en-6-one (**28**), **Figure S15**: HRMS (API⁺) spectrum of 6-oxo-24-nor-5 α -chol-22-en-3 α -yl 4-methylbenzoate (**29**), **Figure S16**: HRMS (API⁺) spectrum of 6-oxo-24-nor-5 α -chol-22-en-3 α -yl 2-fluorobenzoate (**30**), **Figure S17**: HRMS (API⁺) spectrum of (22*R*)-22,23-dihydroxy-6-oxo-24-nor-5 α -cholan-3 α -yl 4-methylbenzoate (**18a**), **Figure S18**: HRMS (API⁺) spectrum of (22*S*)-22,23-dihydroxy-6-oxo-24-nor-5 α -cholan-3 α -yl 4-methylbenzoate (**18b**), **Figure S19**: HRMS (API⁺) spectrum of (22*R*)-22,23-dihydroxy-6-oxo-24-nor-5 α -cholan-3 α -yl 2-fluorobenzoate (**19a**), **Figure S20**: HRMS (API⁺) spectrum of (22*S*)-22,23-dihydroxy-6-oxo-24-nor-5 α -cholan-3 α -yl 2-fluorobenzoate (**19b**).

¹H-NMR



¹³C-NMR

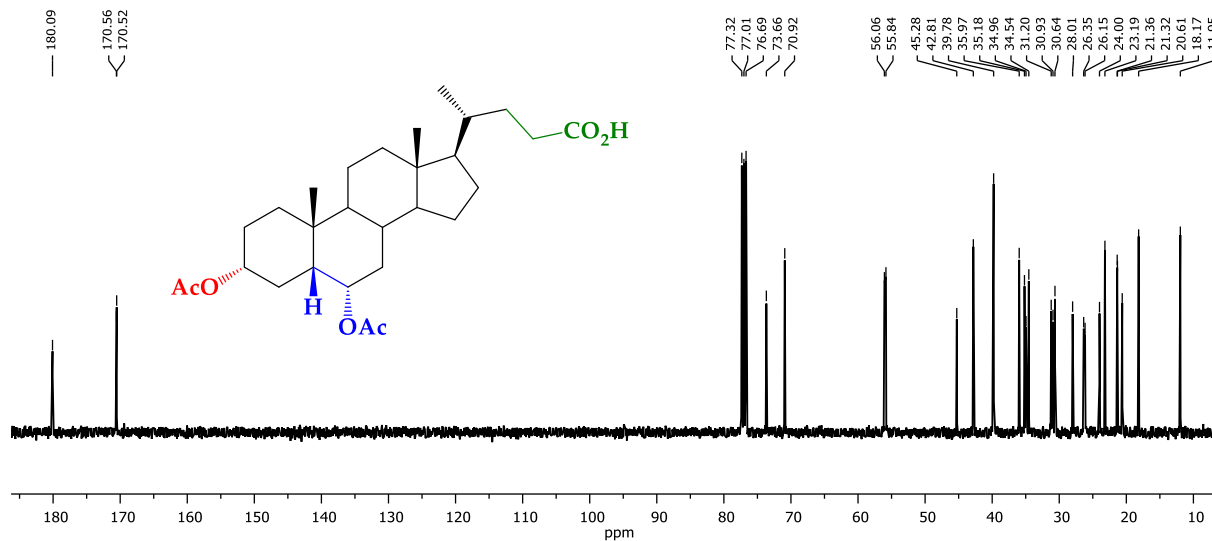
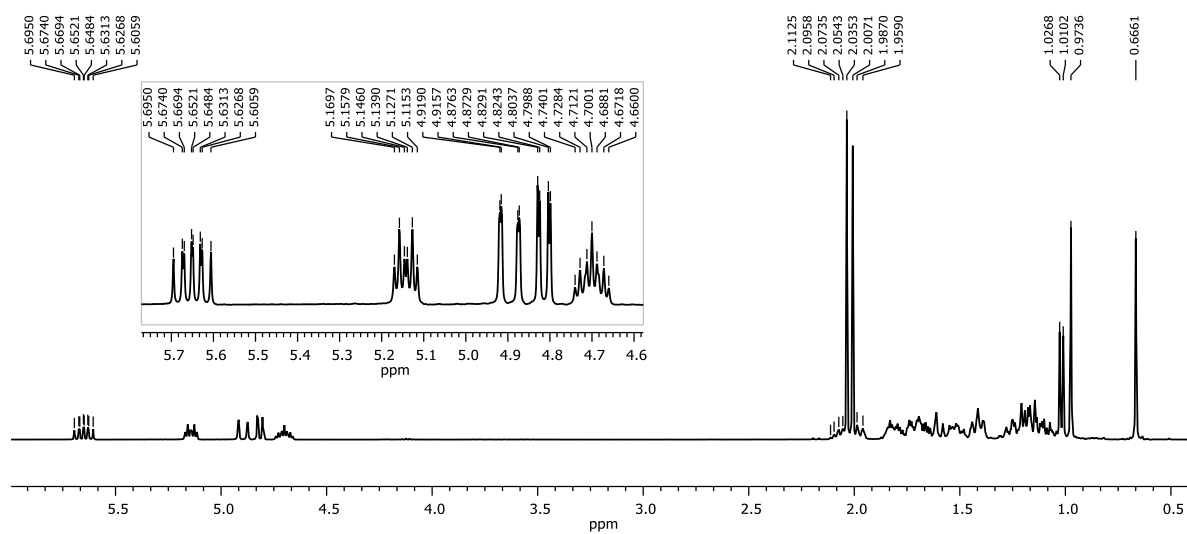


Figure S1: NMR spectra of 3α,6α-diacetoxy-5β-cholan-24-oic acid (**22**)

¹H-NMR



¹³C-NMR

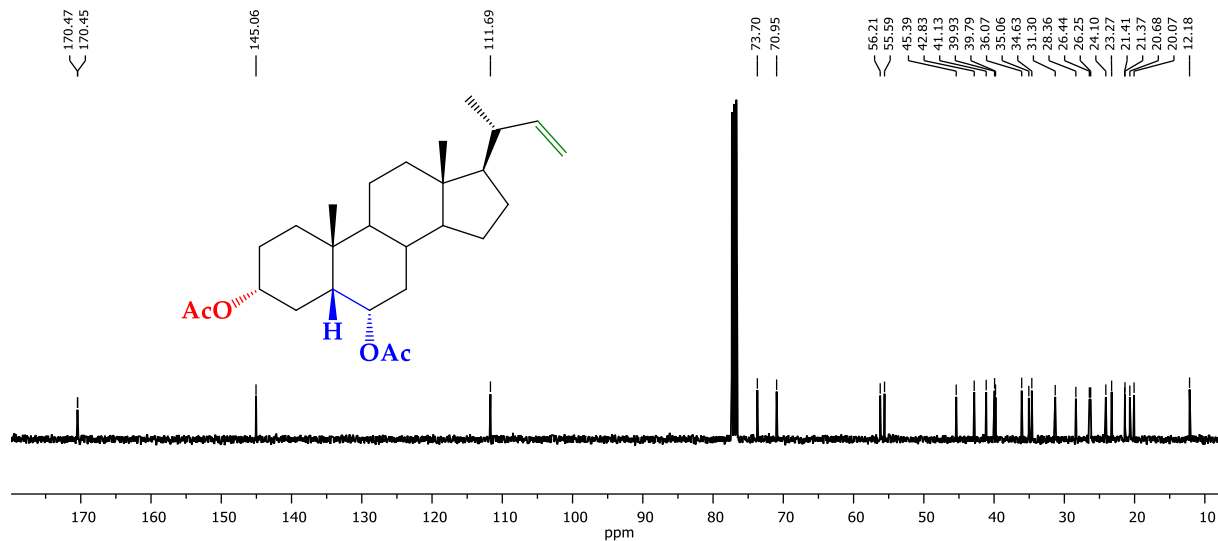
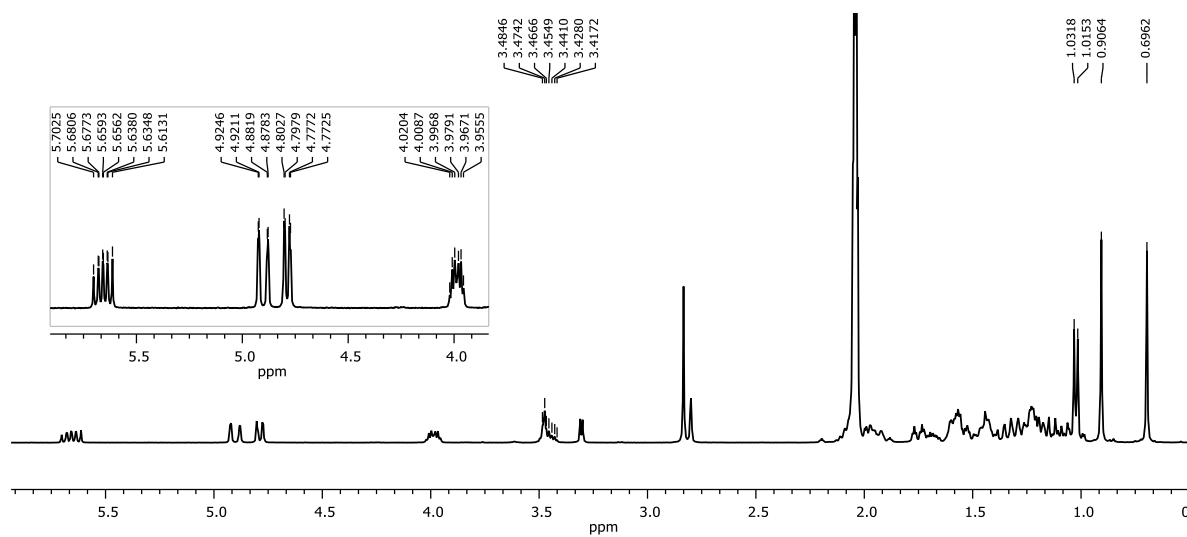


Figure S2: NMR spectra of 24-nor-5 β -cholan-22-ene-3 α ,6 α -diyl diacetate (23)

^1H -NMR



^{13}C -NMR

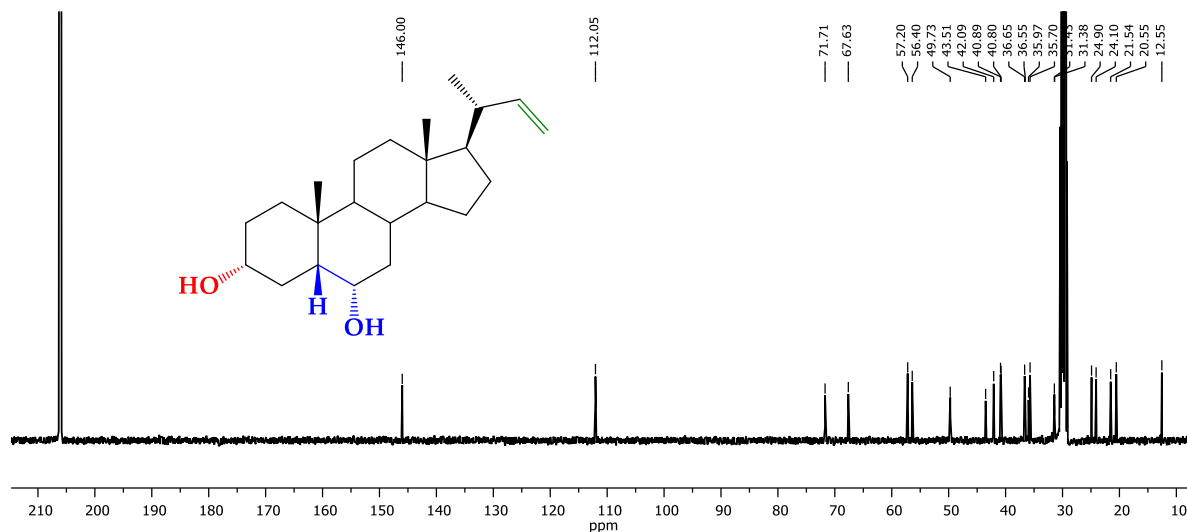


Figure S3: NMR spectra of 24-nor-5 β -chol-22-ene-3 α ,6 α -diol (**24**)

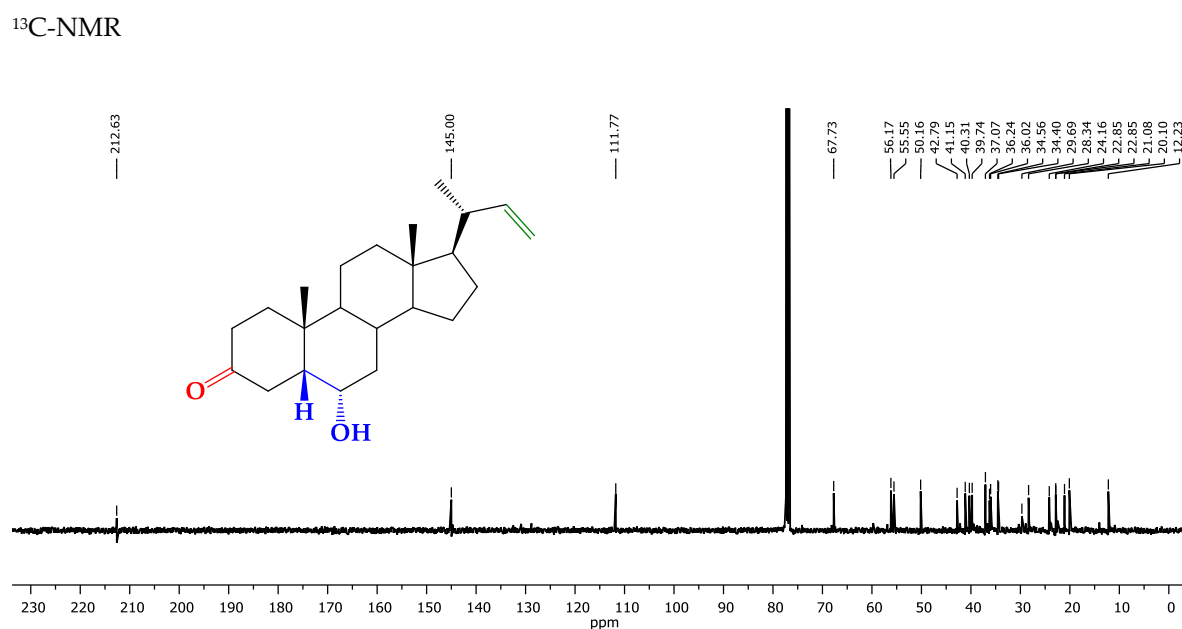
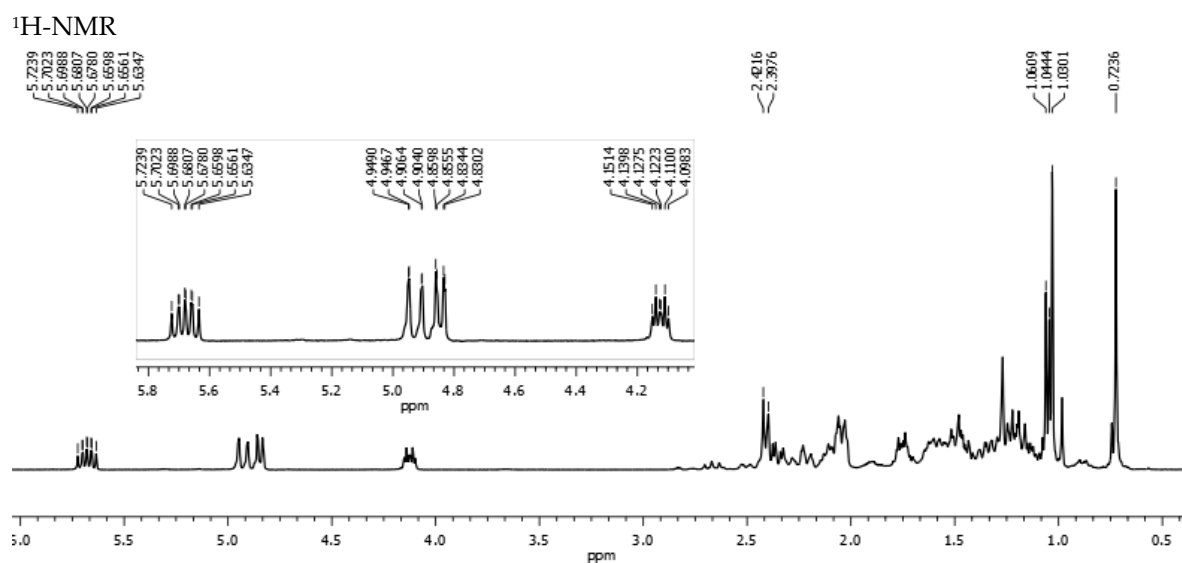
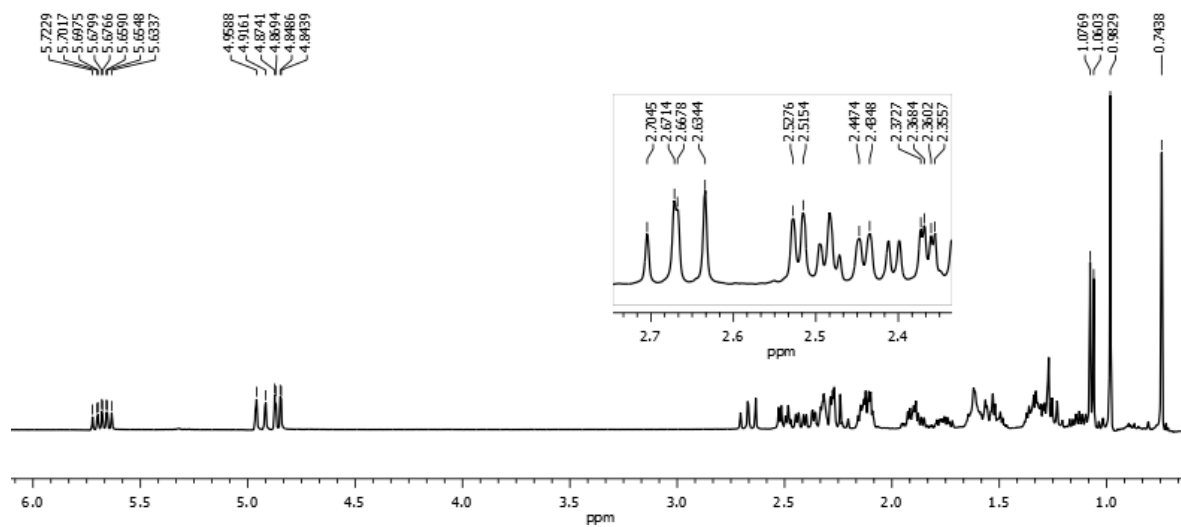


Figure S4: NMR spectra of 6α-hydroxy-24-nor-5β-chole-22-en-3-one (25)

¹H-NMR



¹³C-NMR

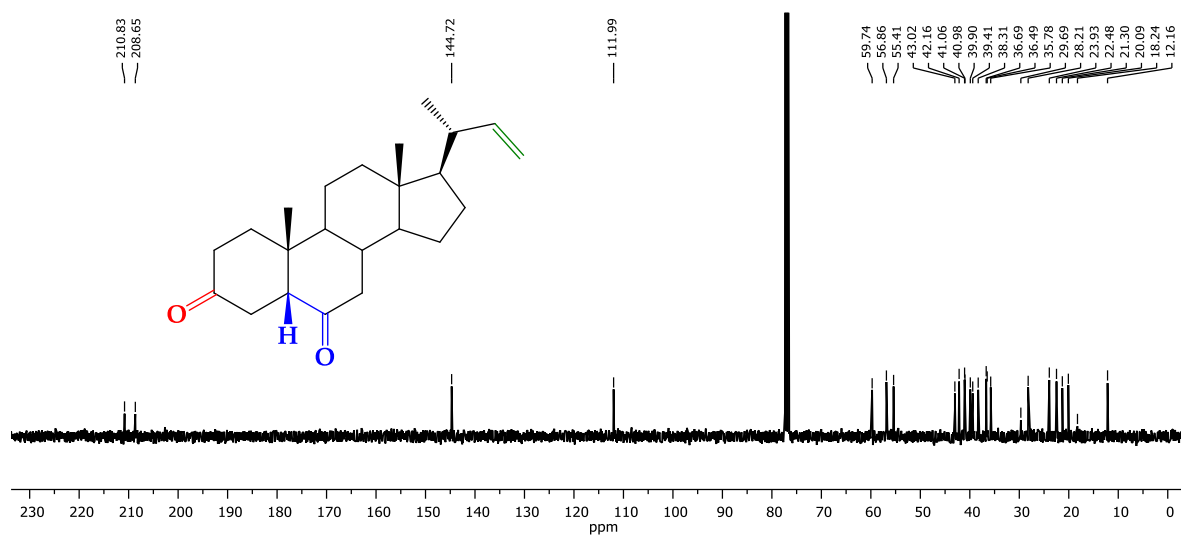
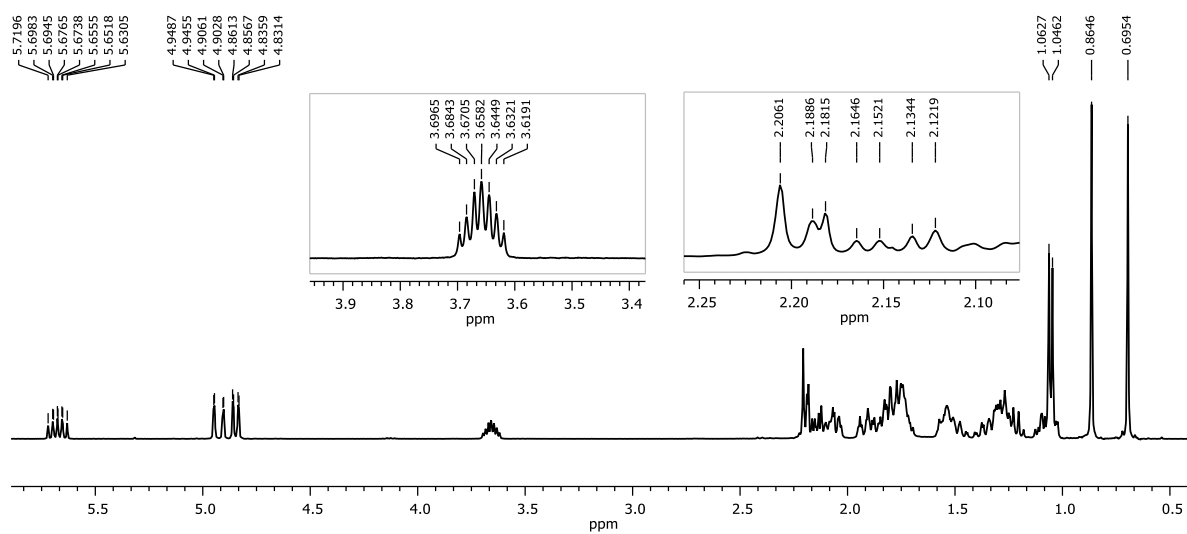


Figure S5: NMR spectra of 24-nor-5 β -chol-22-ene-3,6-dione (**26**)

¹H-NMR



¹³C-NMR

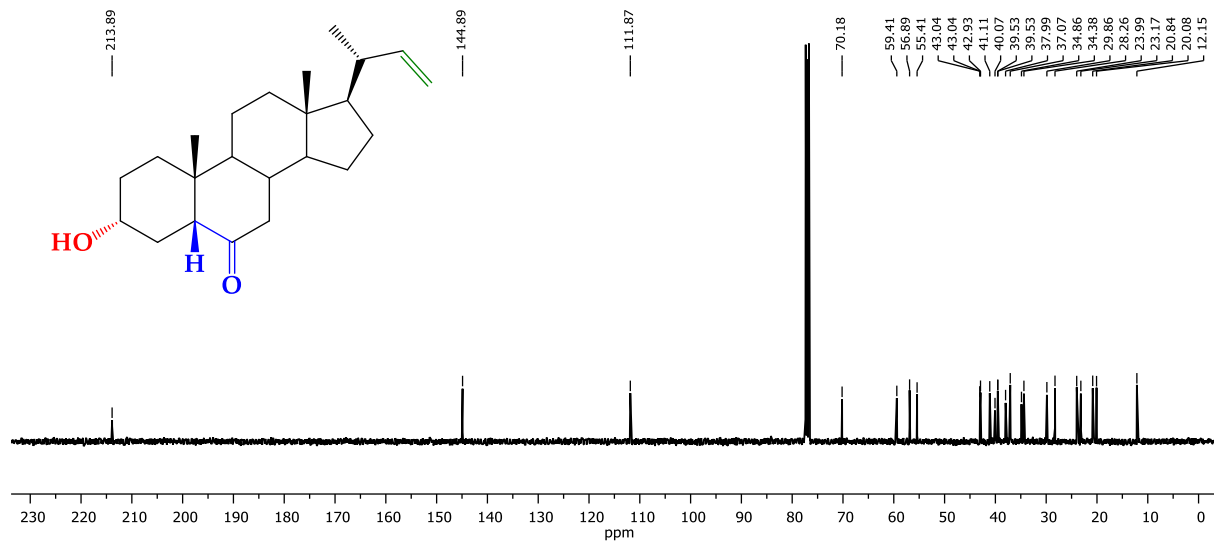
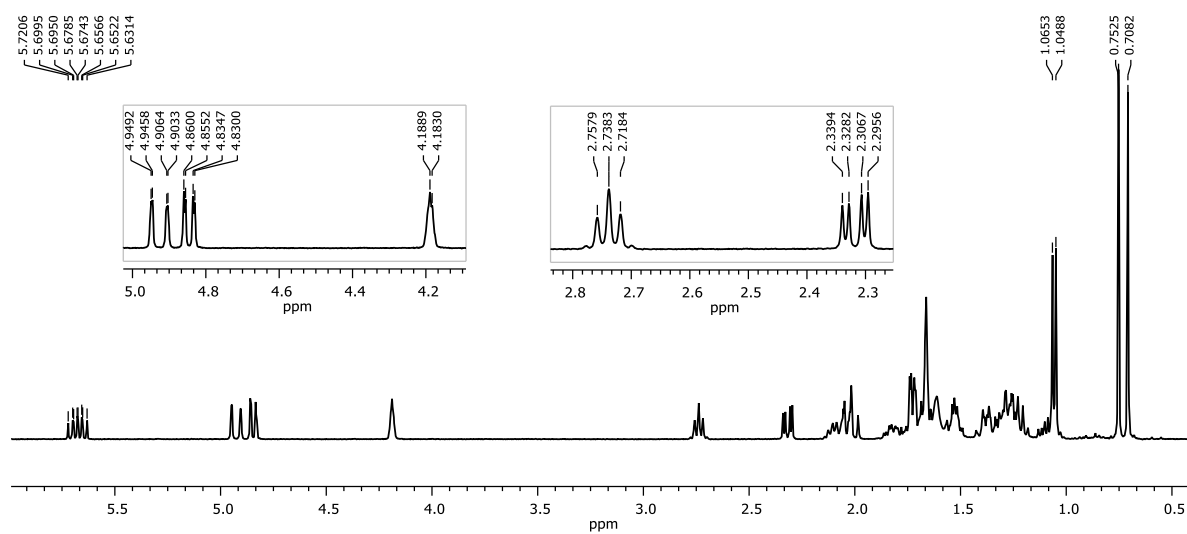


Figure S6: NMR spectra of 3α-hydroxy-24-nor-5β-chole-22-en-6-one (27)

¹H-NMR



¹³C-NMR

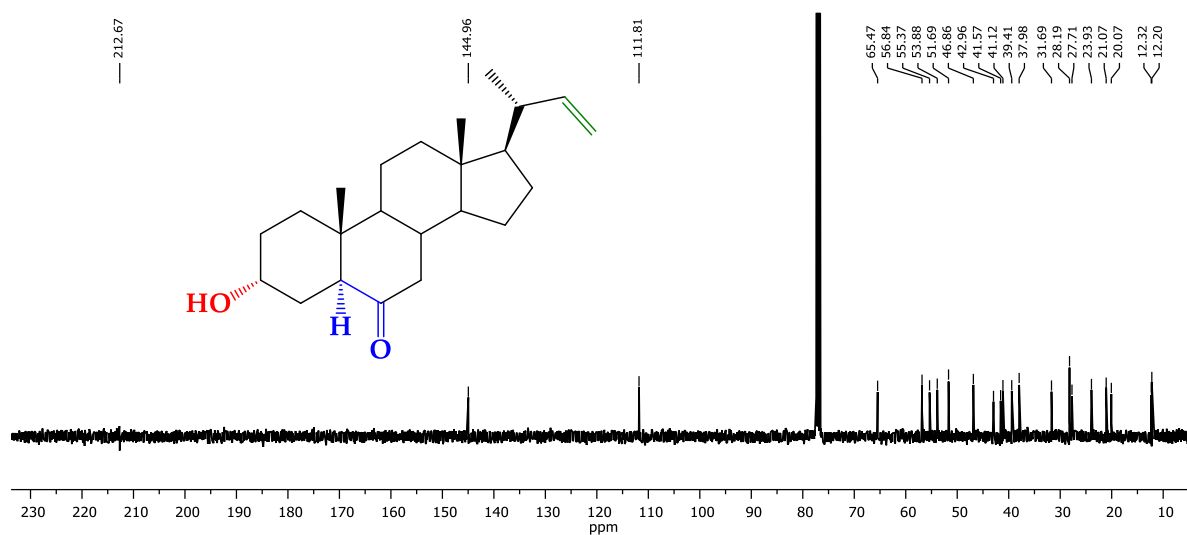
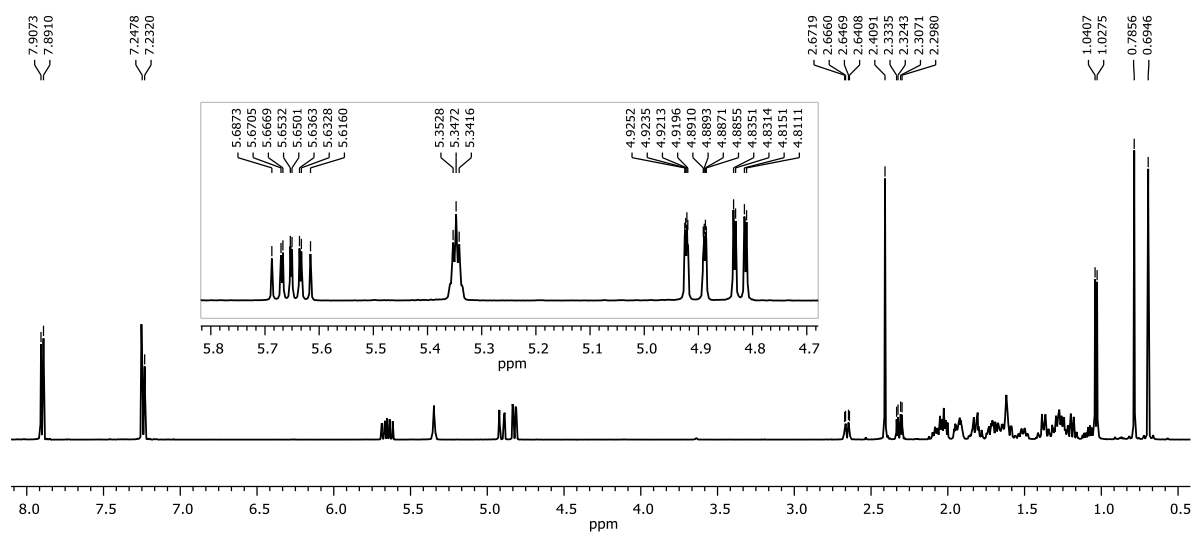


Figure S7: NMR spectra of 3α-hydroxy-24-nor-5α-chole-22-en-6-one (28)

¹H-NMR



¹³C-NMR

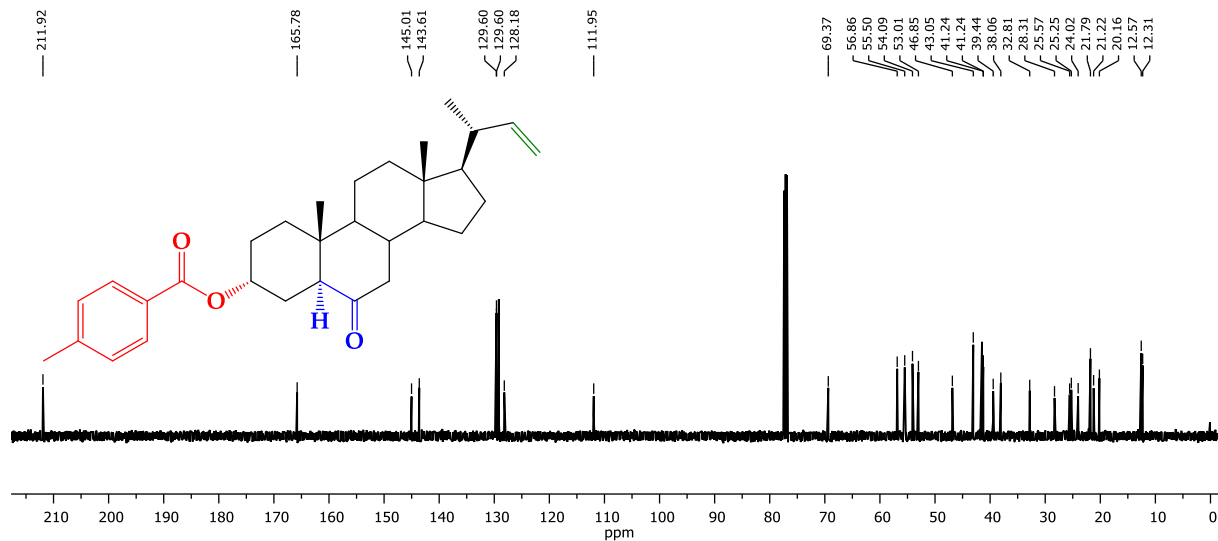
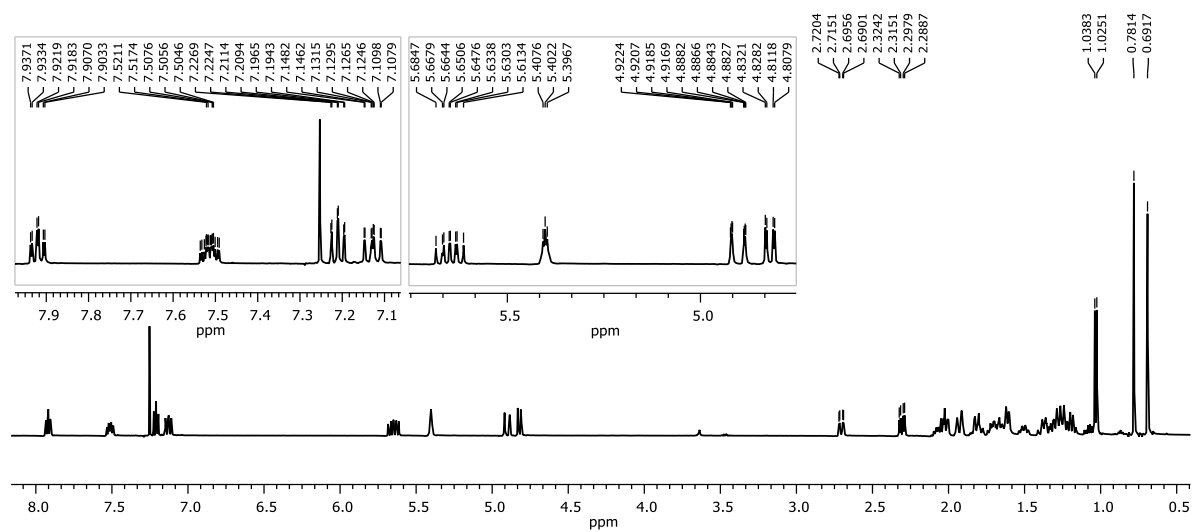


Figure S8: NMR spectra of 6-oxo-24-nor-5 α -chol-22-en-3 α -yl 4-methylbenzoate (29)

^1H -NMR



^{13}C -NMR

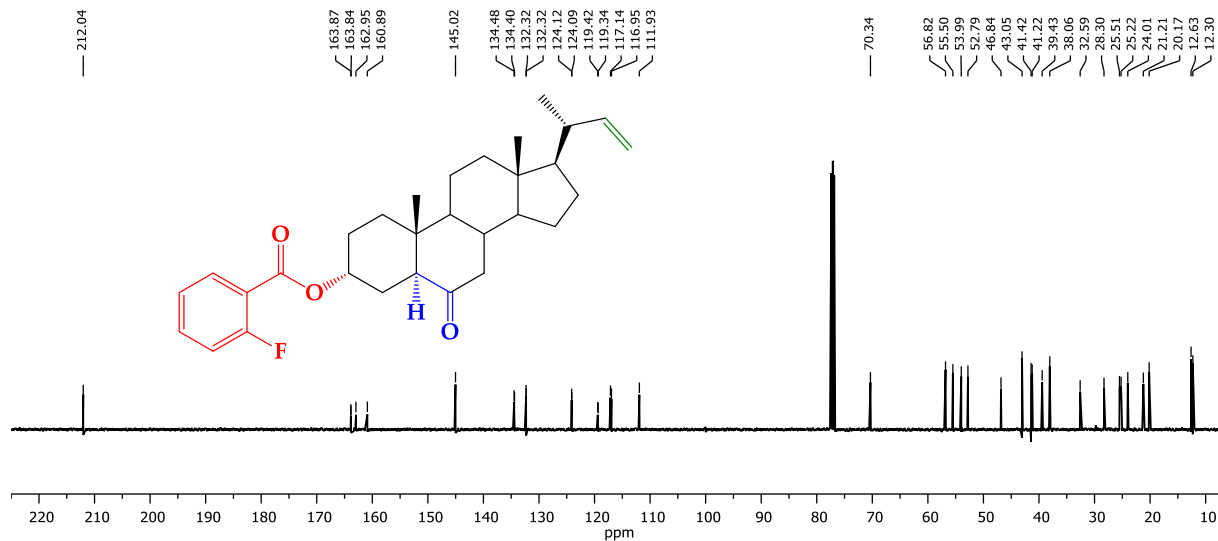
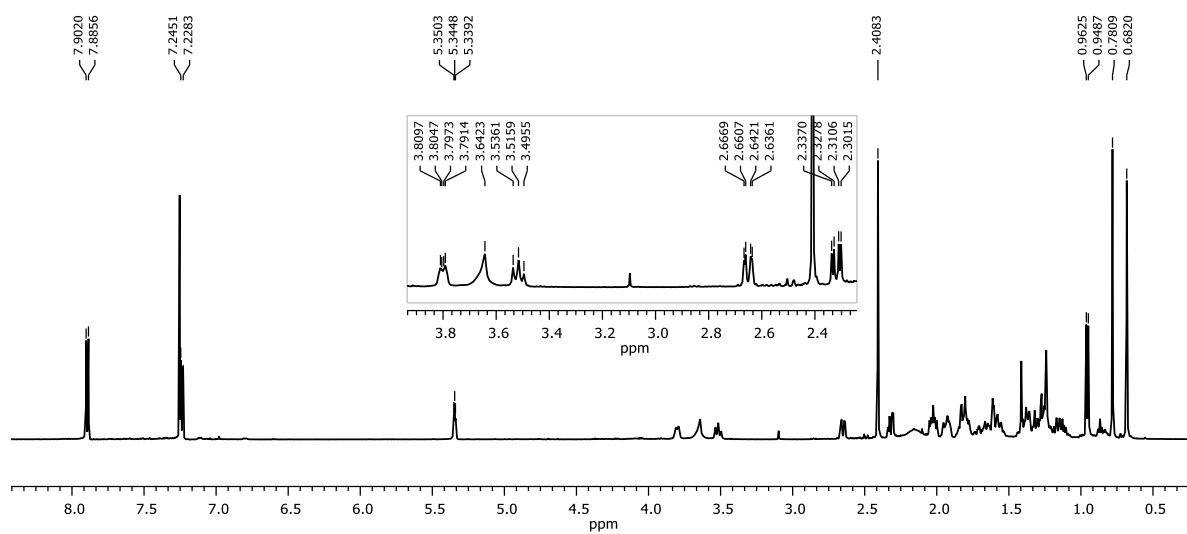


Figure S9: NMR spectra of 6-oxo-24-nor-5 α -chol-22-en-3 α -yl 2-fluorobenzoate (**30**)

¹H-NMR



¹³C-NMR

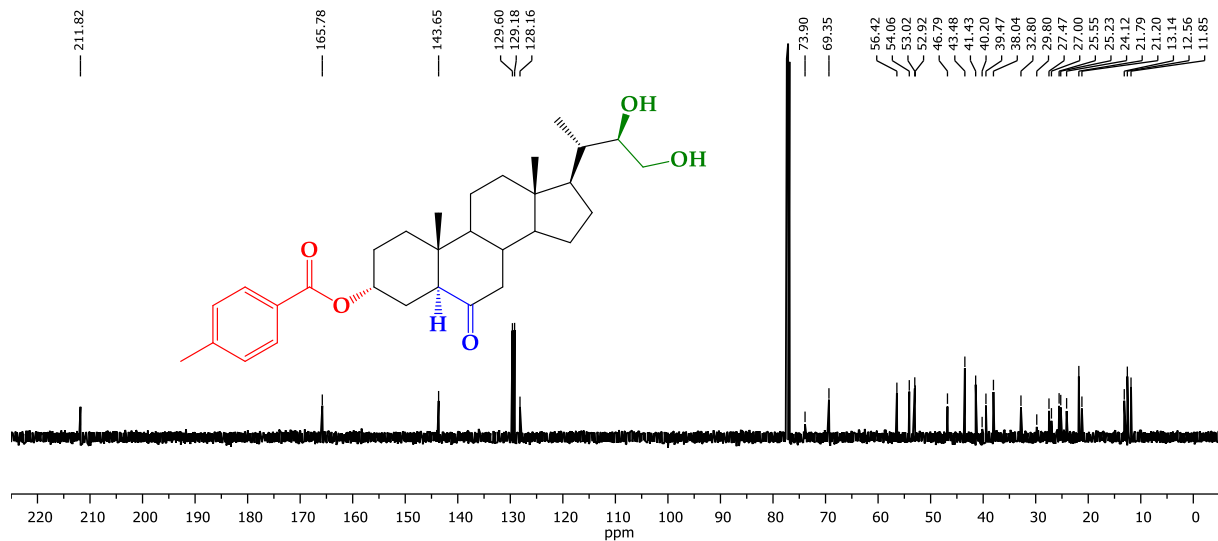
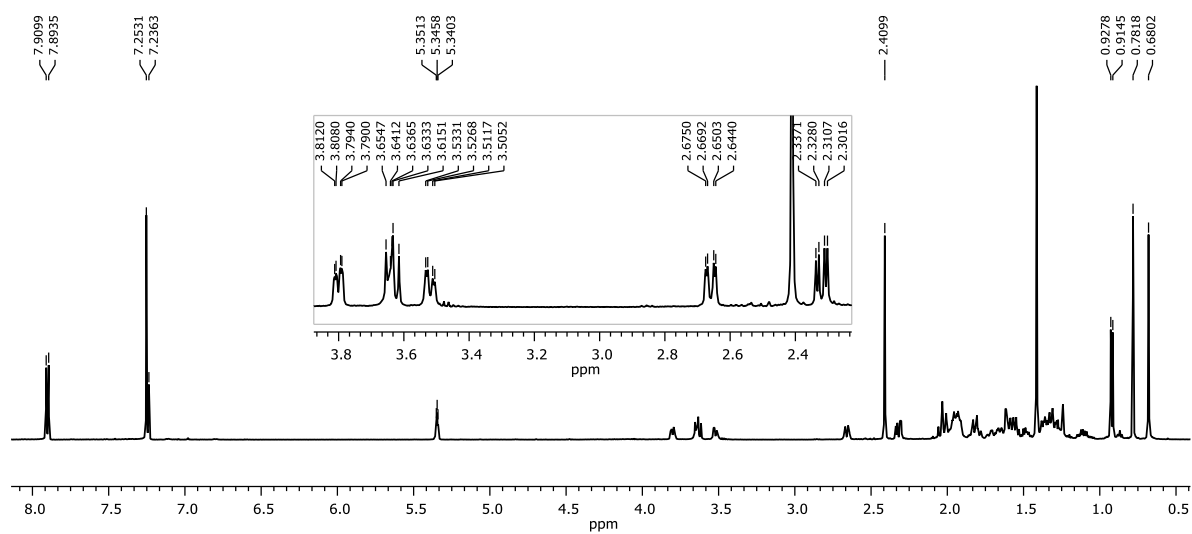


Figure S10: NMR spectra of (22R)-22,23-dihydroxy-6-oxo-24-nor-5α-cholan-3α-yl 4-methylbenzoate (18a)

¹H-NMR



¹³C-NMR

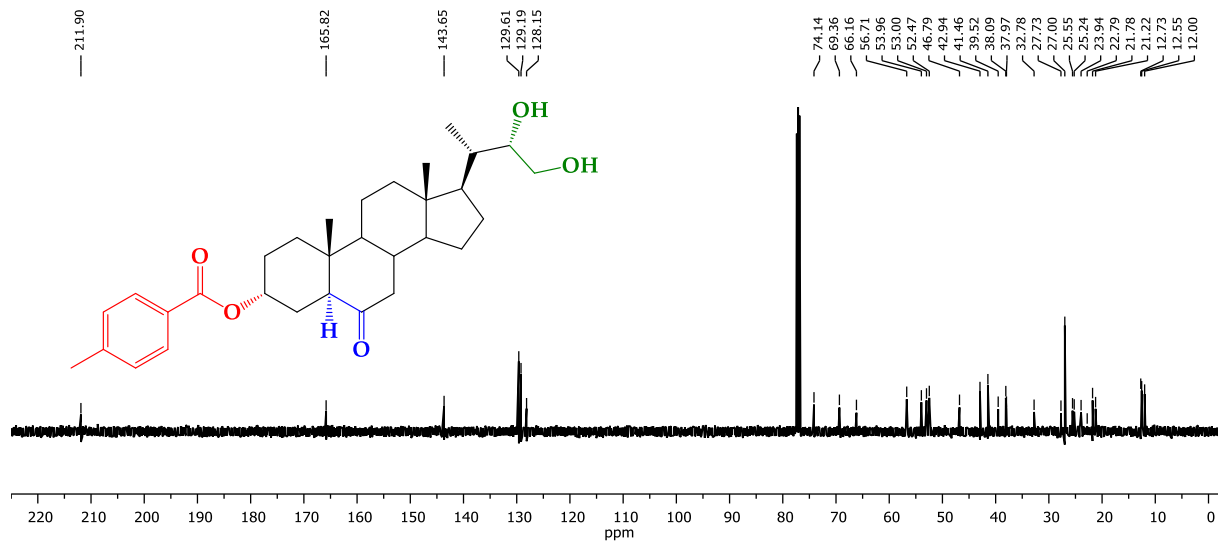
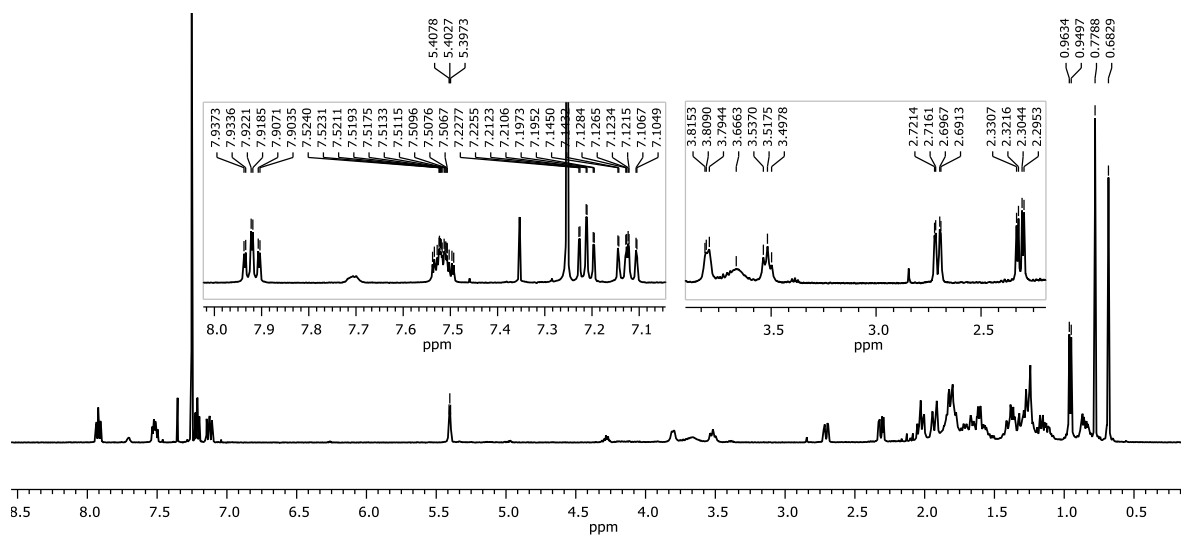


Figure S11: NMR spectra of (22S)-22,23-dihydroxy-6-oxo-24-nor-5 α -cholan-3 α -yl 4-methylbenzoate (18b)

¹H-NMR



¹³C-NMR

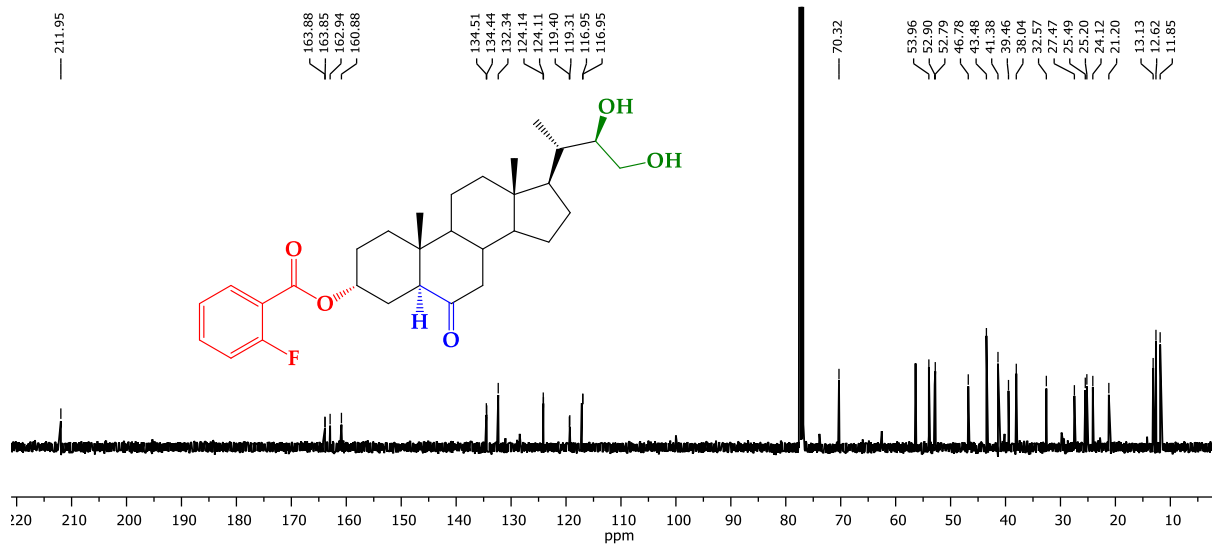
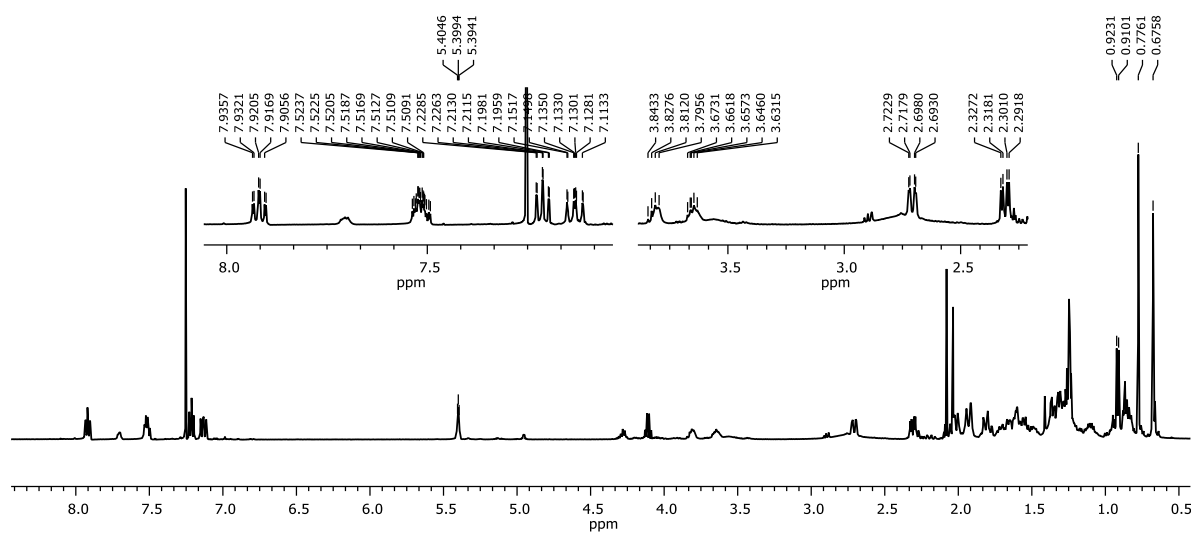


Figure S12: NMR spectra of (22*R*)-22,23-dihydroxy-6-oxo-24-nor-5α-cholan-3α-yl 2-fluorobenzoate (**19a**)

¹H-NMR



¹³C-NMR

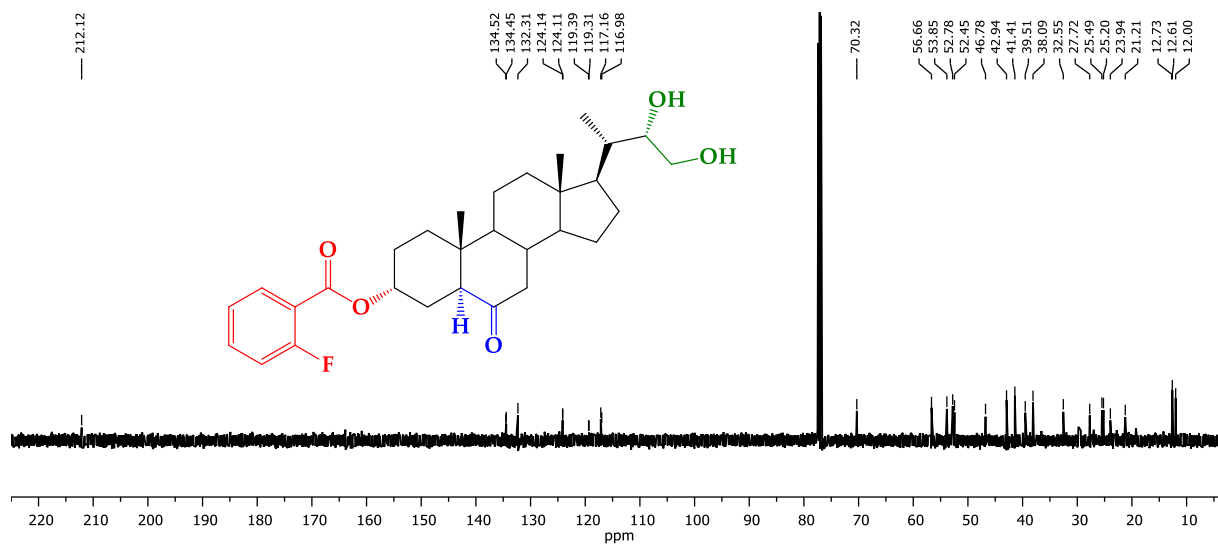


Figure S13: NMR spectra of (22S)-22,23-dihydroxy-6-oxo-24-nor-5 α -cholan-3 α -yl 2-fluorobenzoate (19b)

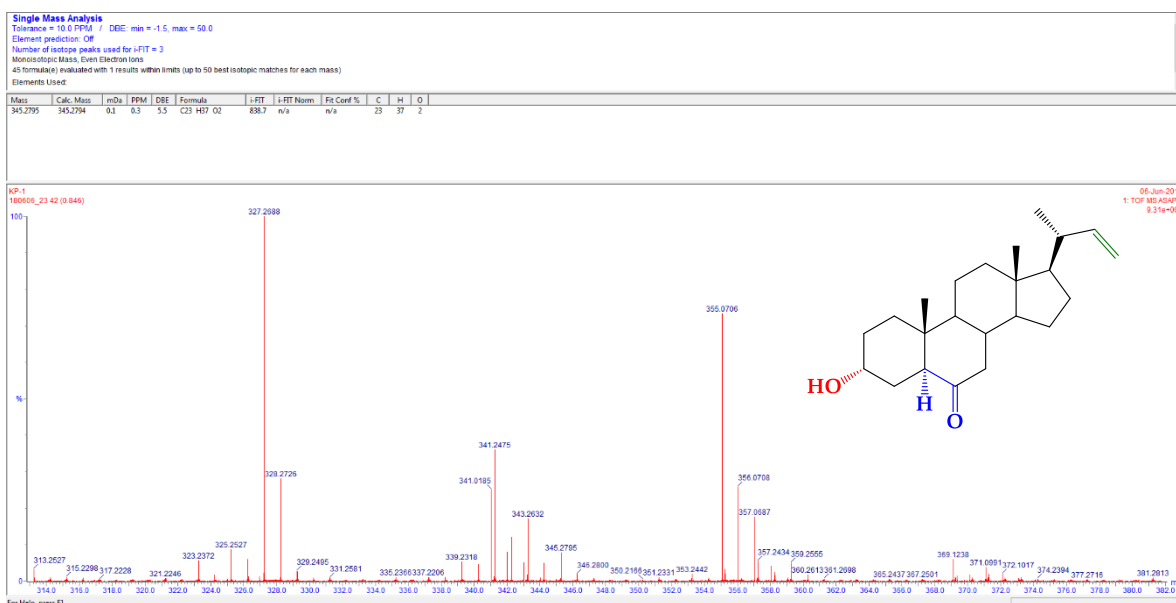


Figure S14: HRMS (API⁺) spectrum of 3α-hydroxy-24-nor-5α-chole-22-en-6-one (28)

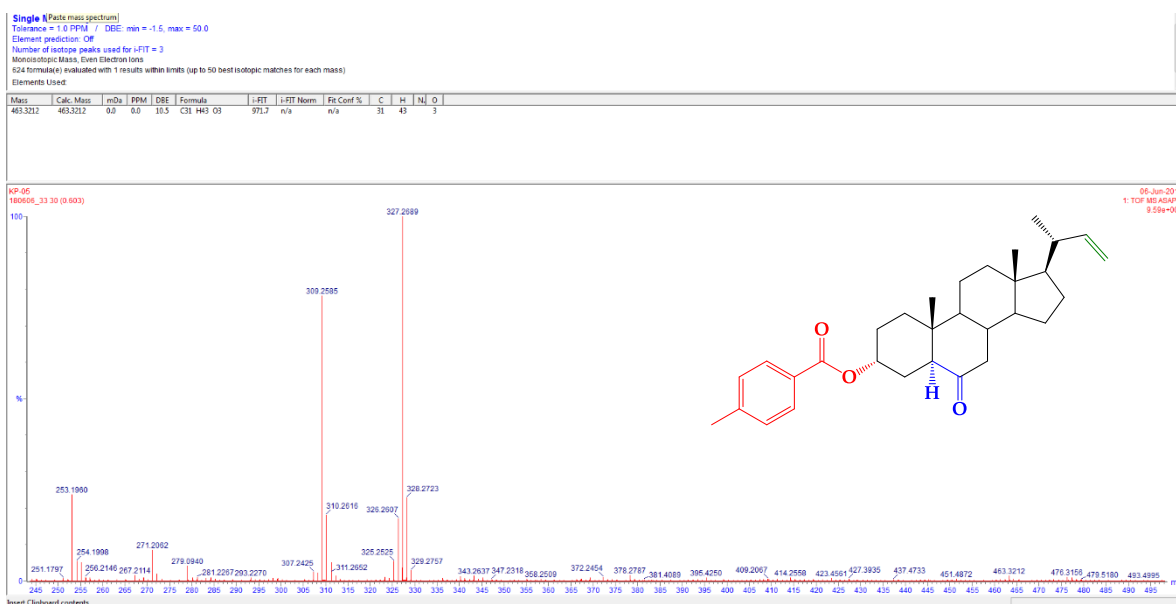


Figure S15: HRMS (API⁺) spectrum of 6-oxo-24-nor-5α-chole-22-en-3α-yl 4-methylbenzoate (29)

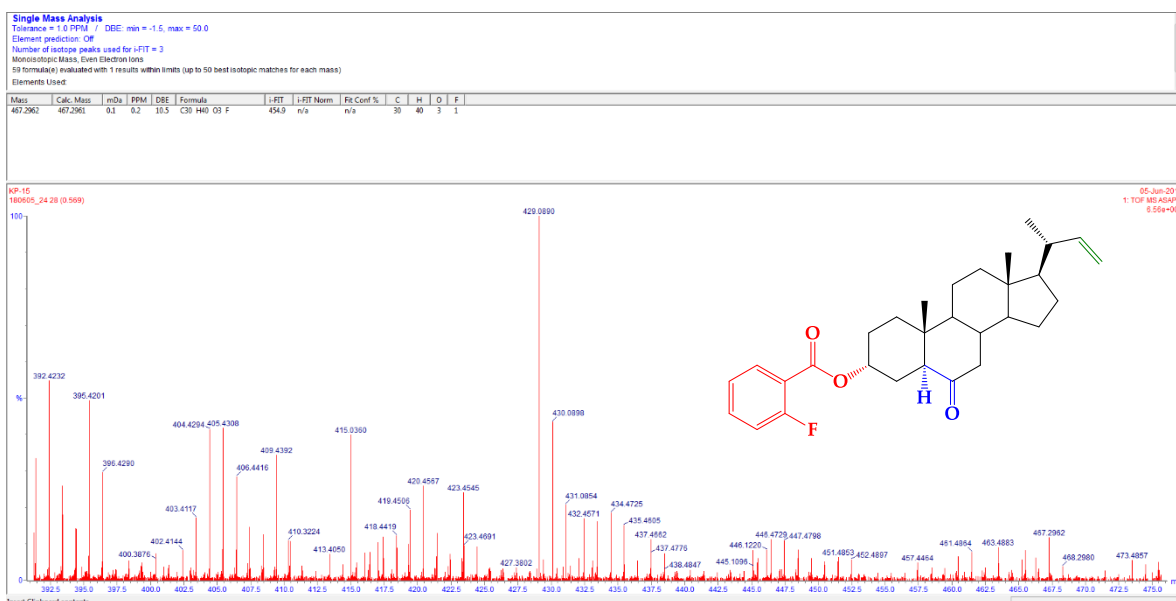


Figure S16: HRMS (API⁺) spectrum of 6-oxo-24-nor-5 α -chol-22-en-3 α -yl 2-fluorobenzoate (**30**)

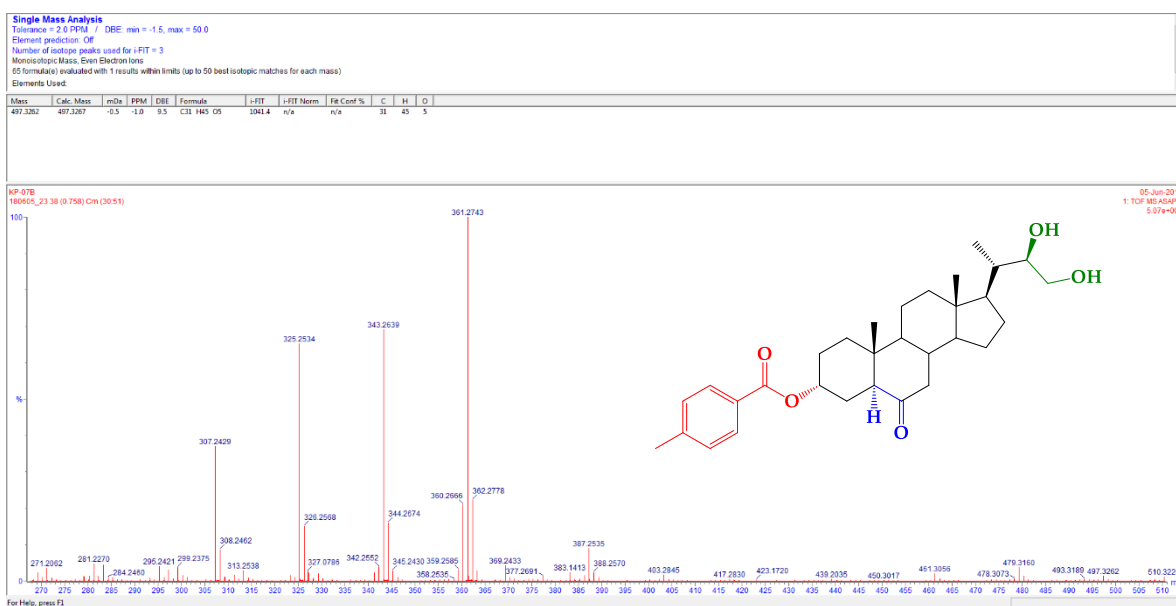


Figure S17: HRMS (API⁺) spectrum of (22*R*)-22,23-dihydroxy-6-oxo-24-nor-5 α -cholan-3 α -yl 4-methylbenzoate (**18a**)

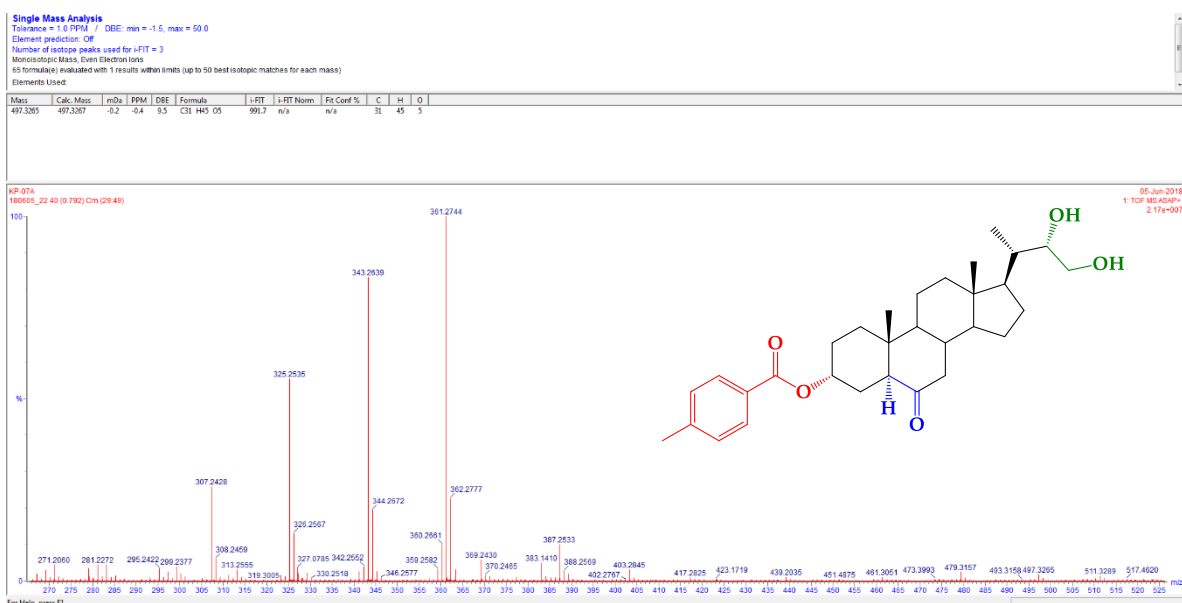


Figure S18: HRMS (API⁺) spectrum of (22S)-22,23-dihydroxy-6-oxo-24-nor-5α-cholan-3α-yl 4-methylbenzoate (18b)

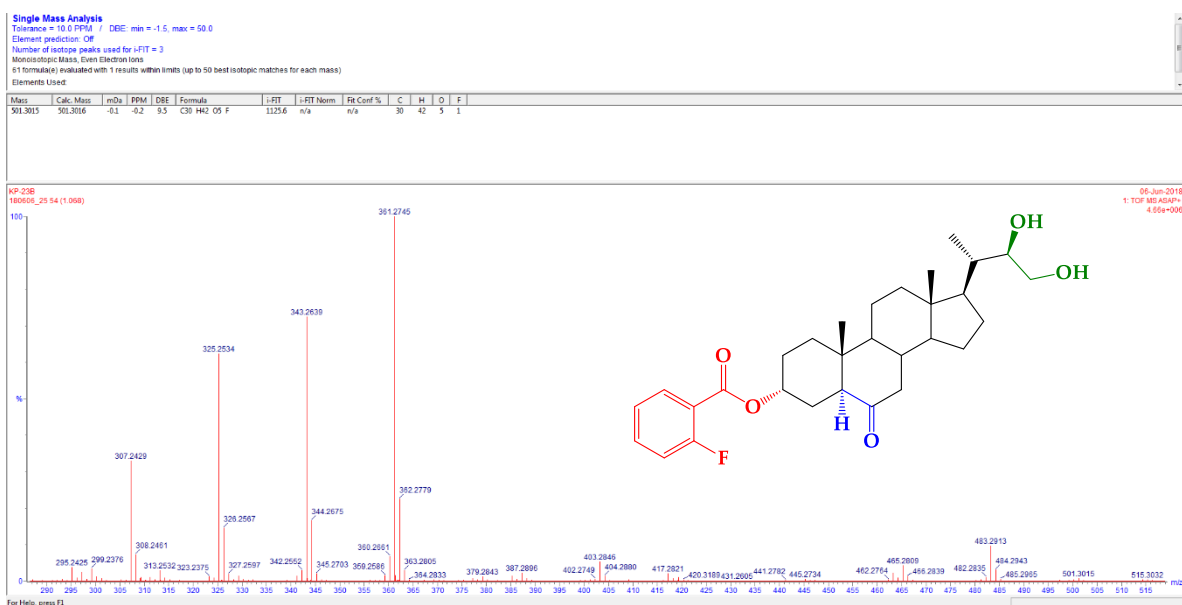


Figure S19: HRMS (API⁺) spectrum of (22R)-22,23-dihydroxy-6-oxo-24-nor-5α-cholan-3α-yl 2-fluorobenzoate (19a)

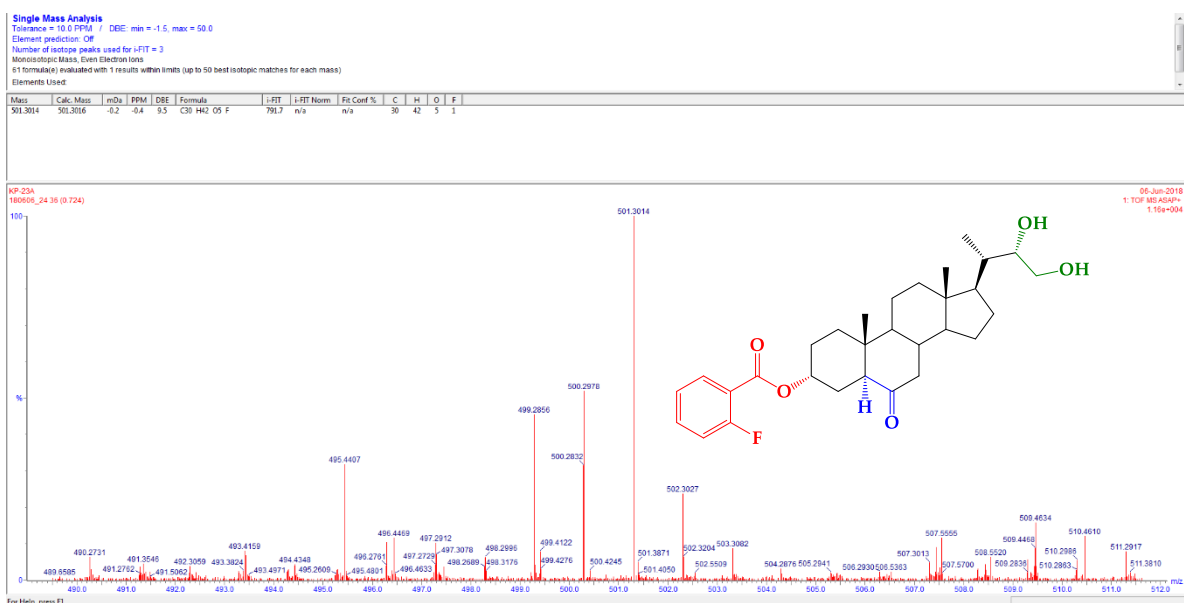


Figure S20: HRMS (API⁺) spectrum of (22*S*)-22,23-dihydroxy-6-oxo-24-nor-5α-cholan-3α-yl 2-fluorobenzoate (**19b**)