

**A New Steroidal 5,7-Diene Derivative, 3 $\beta$ -Hydroxyandrosta-5, 7-Diene-17 $\beta$ -Carboxylic Acid, Shows Potent Anti-proliferative Activity**

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<sup>3</sup>Department of Pharmacognosy and Research Institute of Pharmaceutical Sciences, School of Pharmacy, University of Mississippi, University, MS 38677, USA

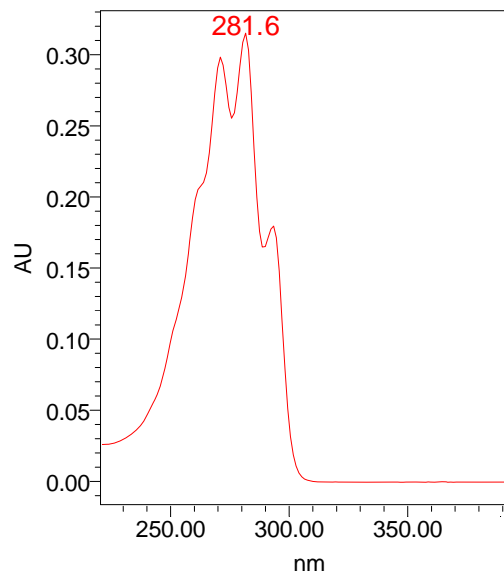
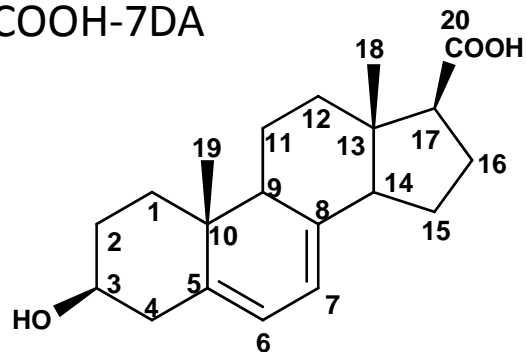
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Kim and Chen are the first authors

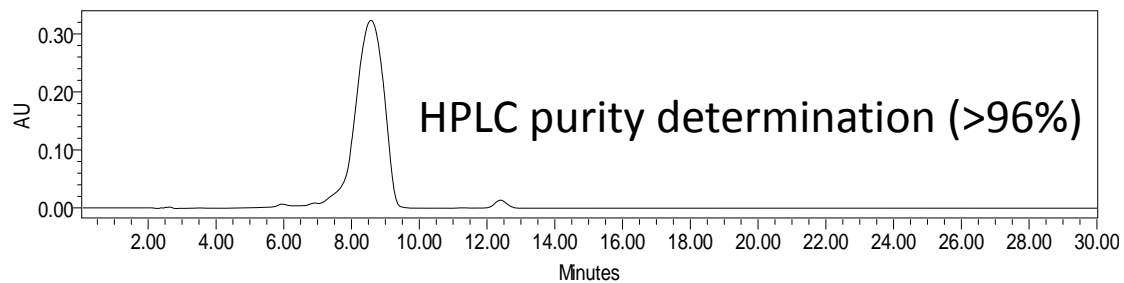
**Supplementary Materials**

Compound purity determination by HPLC, UV spectra of these compounds, and complete 1D and 2D NMR spectra used for full structural assignments are included in these supplementary materials.

# 17-COOH-7DA

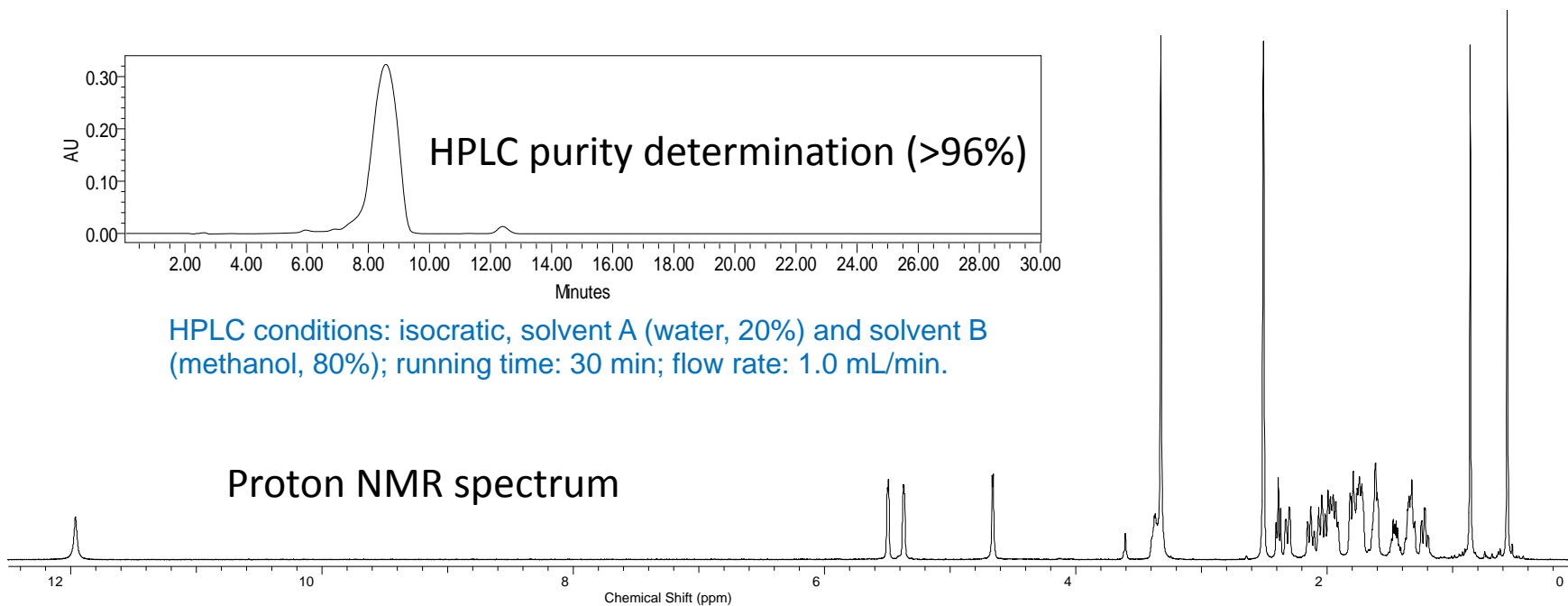


UV spectrum

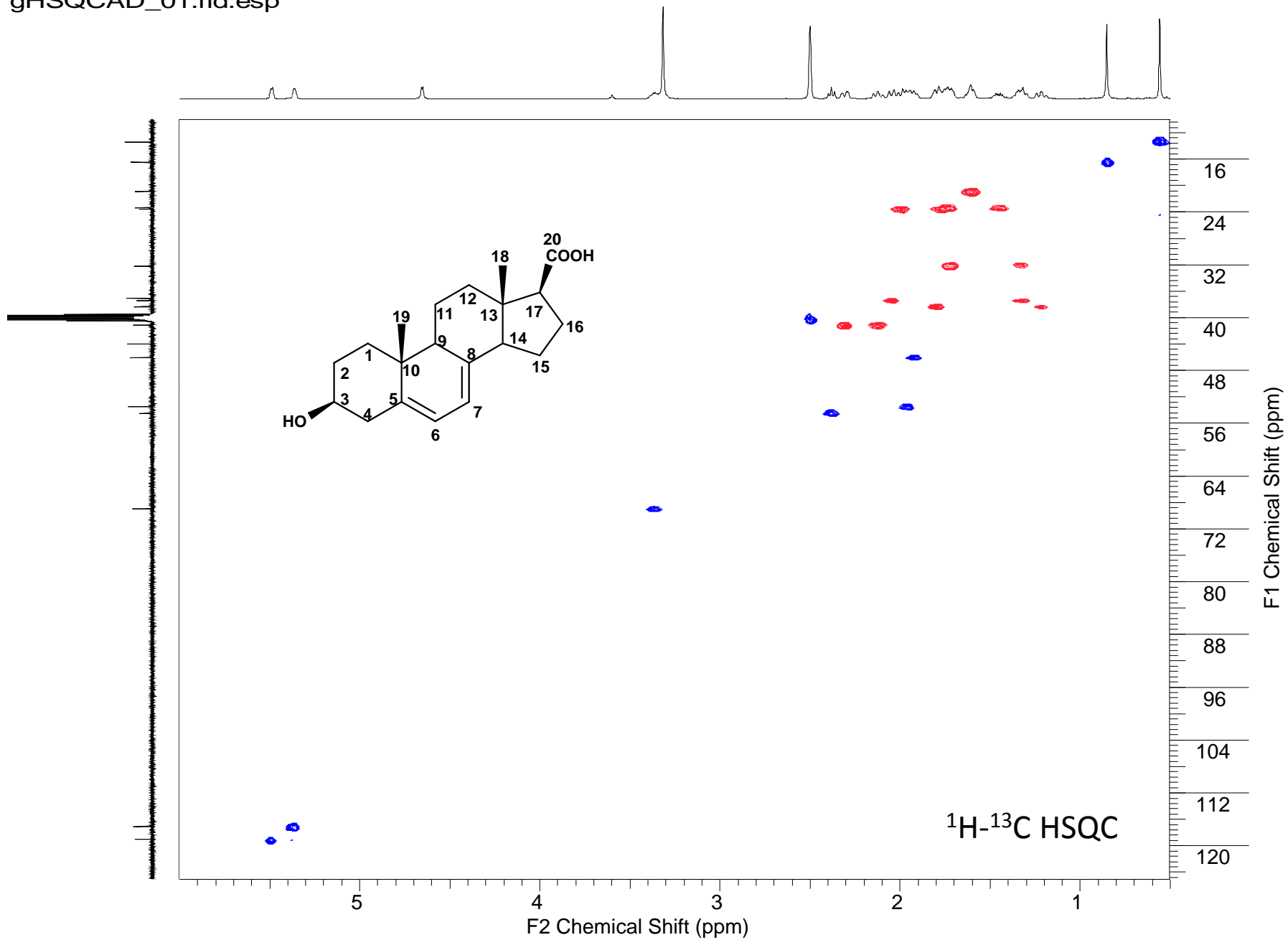


HPLC conditions: isocratic, solvent A (water, 20%) and solvent B (methanol, 80%); running time: 30 min; flow rate: 1.0 mL/min.

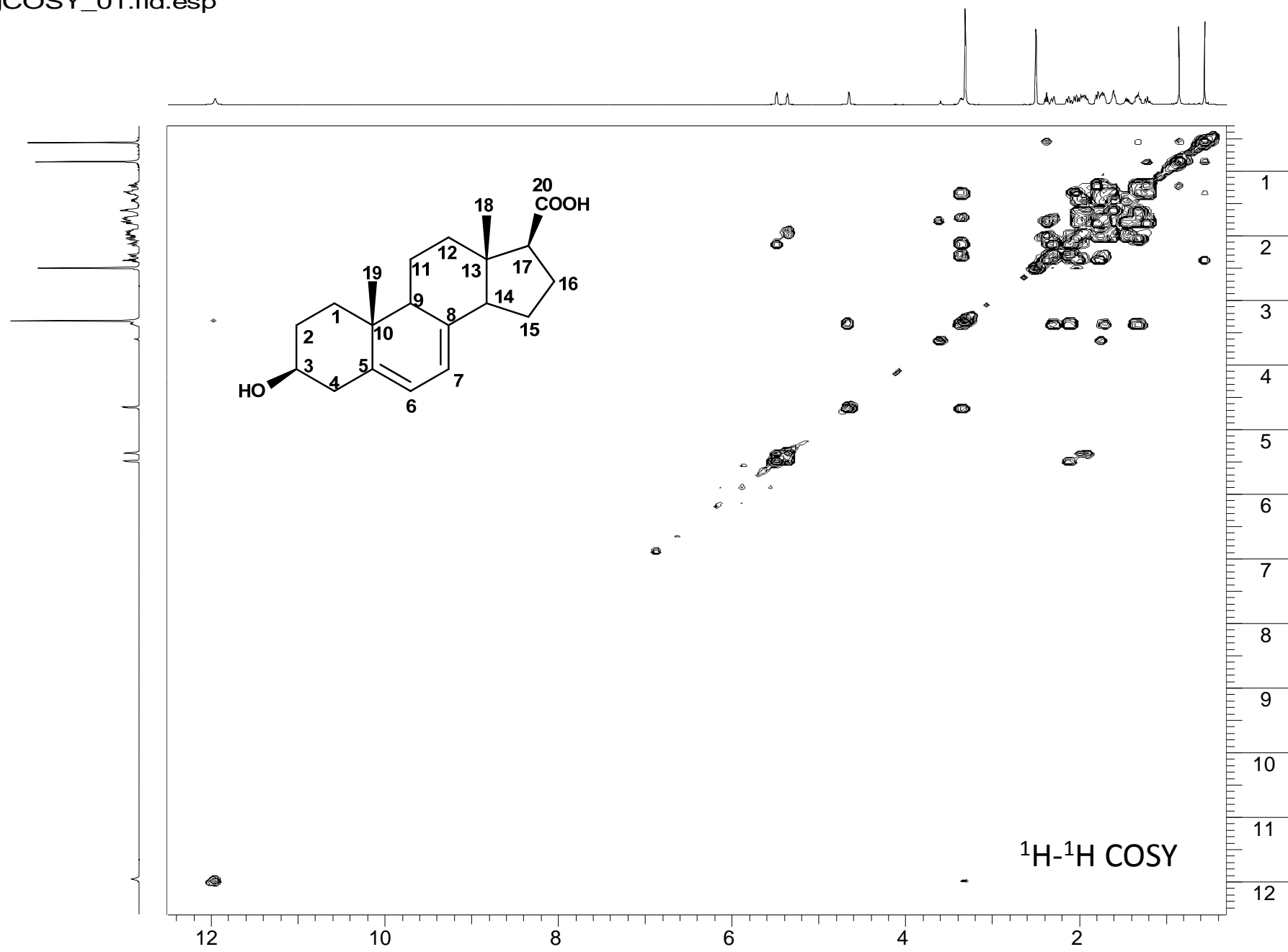
## Proton NMR spectrum

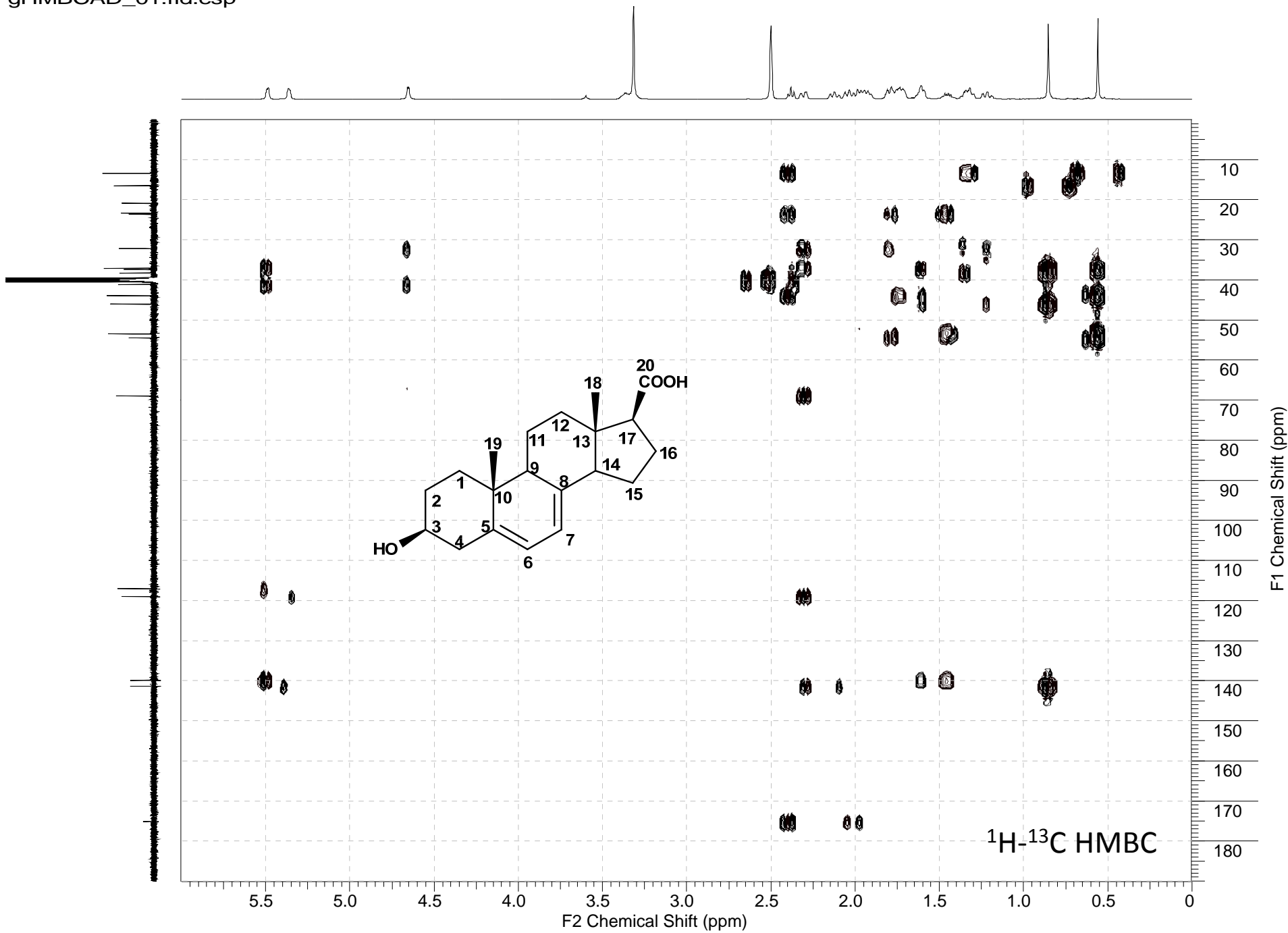


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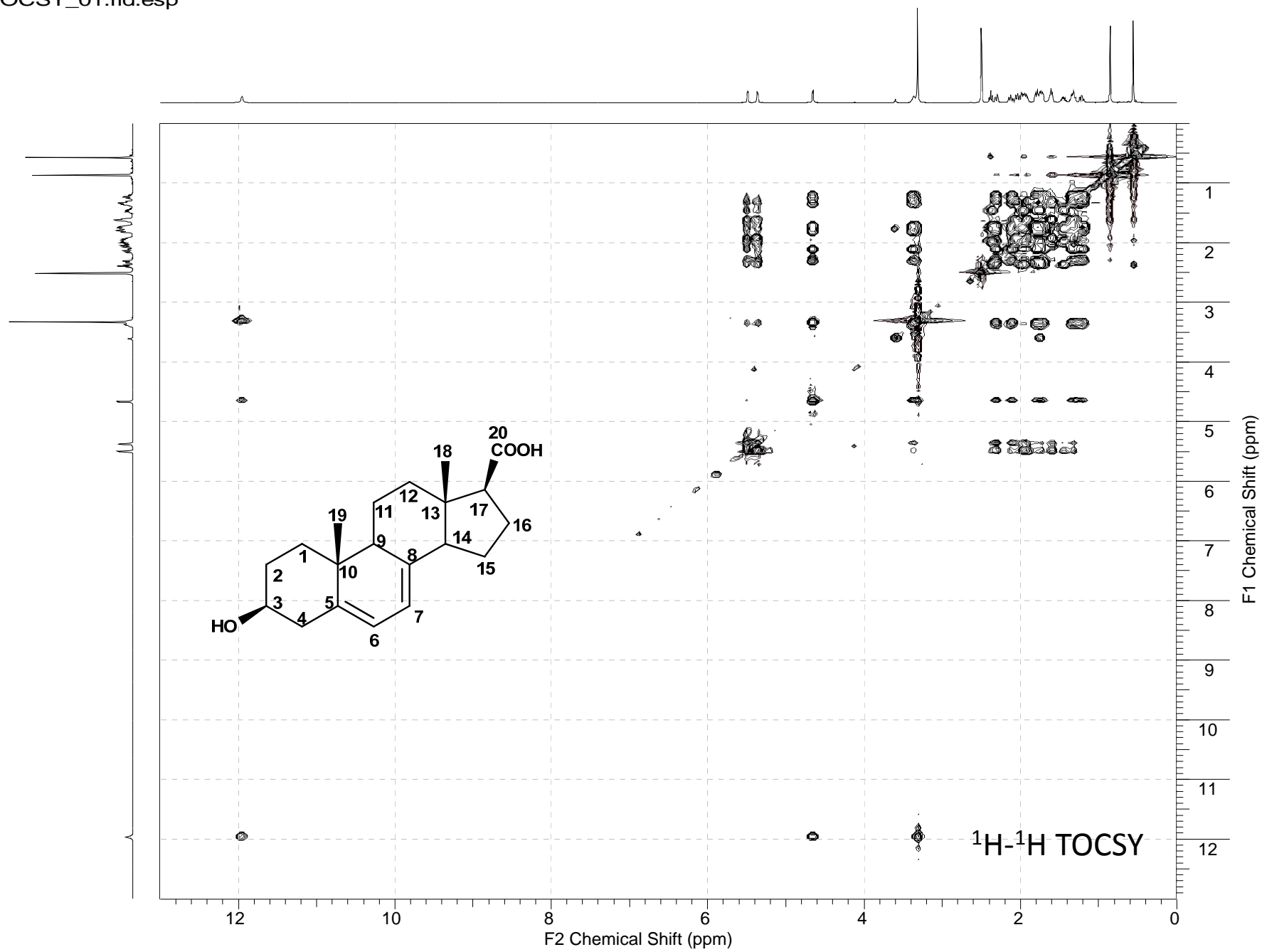


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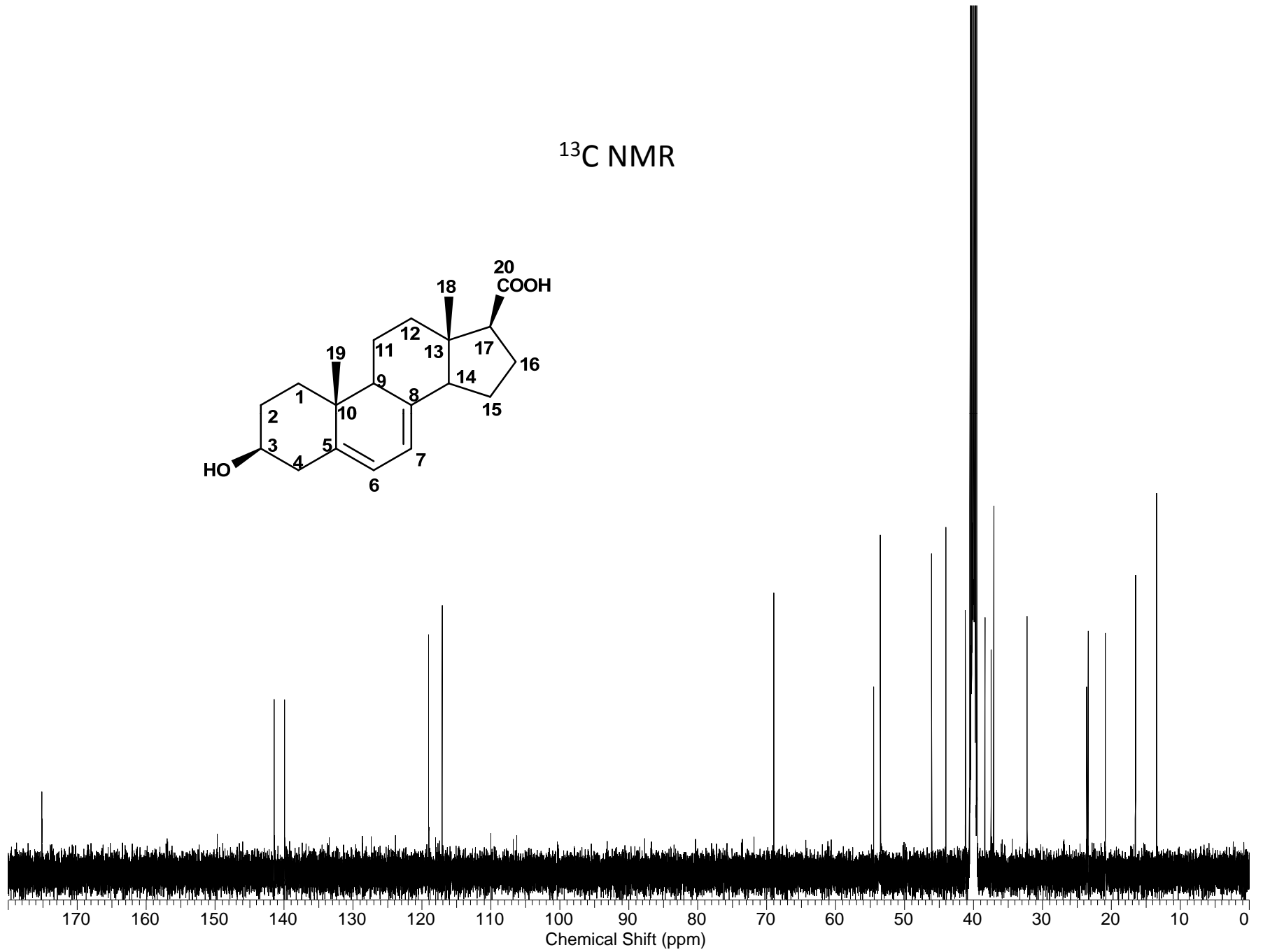
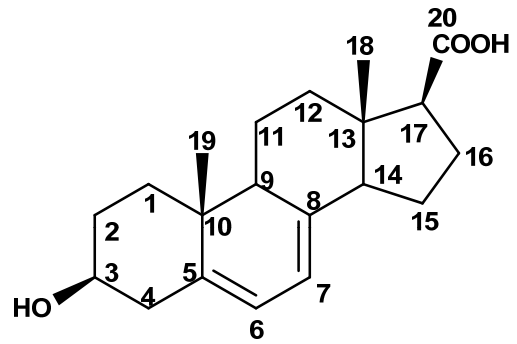




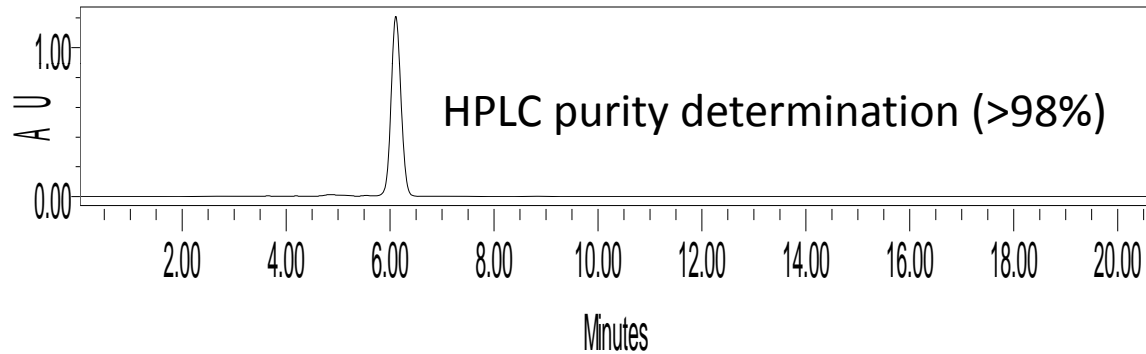
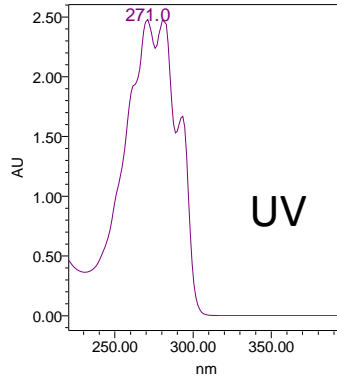
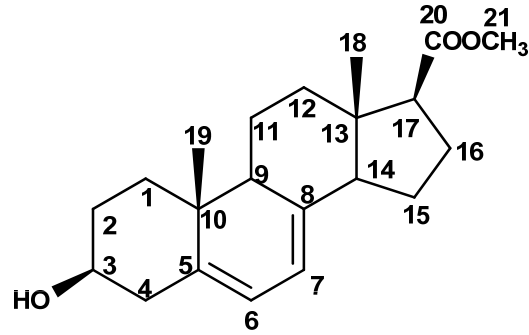
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$^{13}\text{C}$  NMR



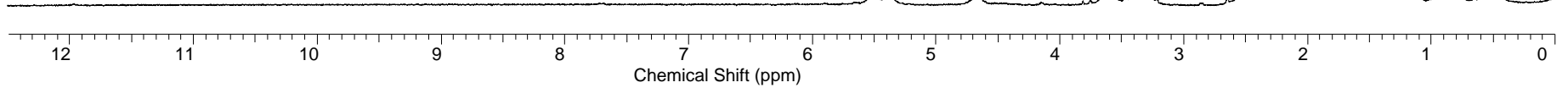
# 17-COOCH<sub>3</sub>-7DA



HPLC purity determination (>98%)

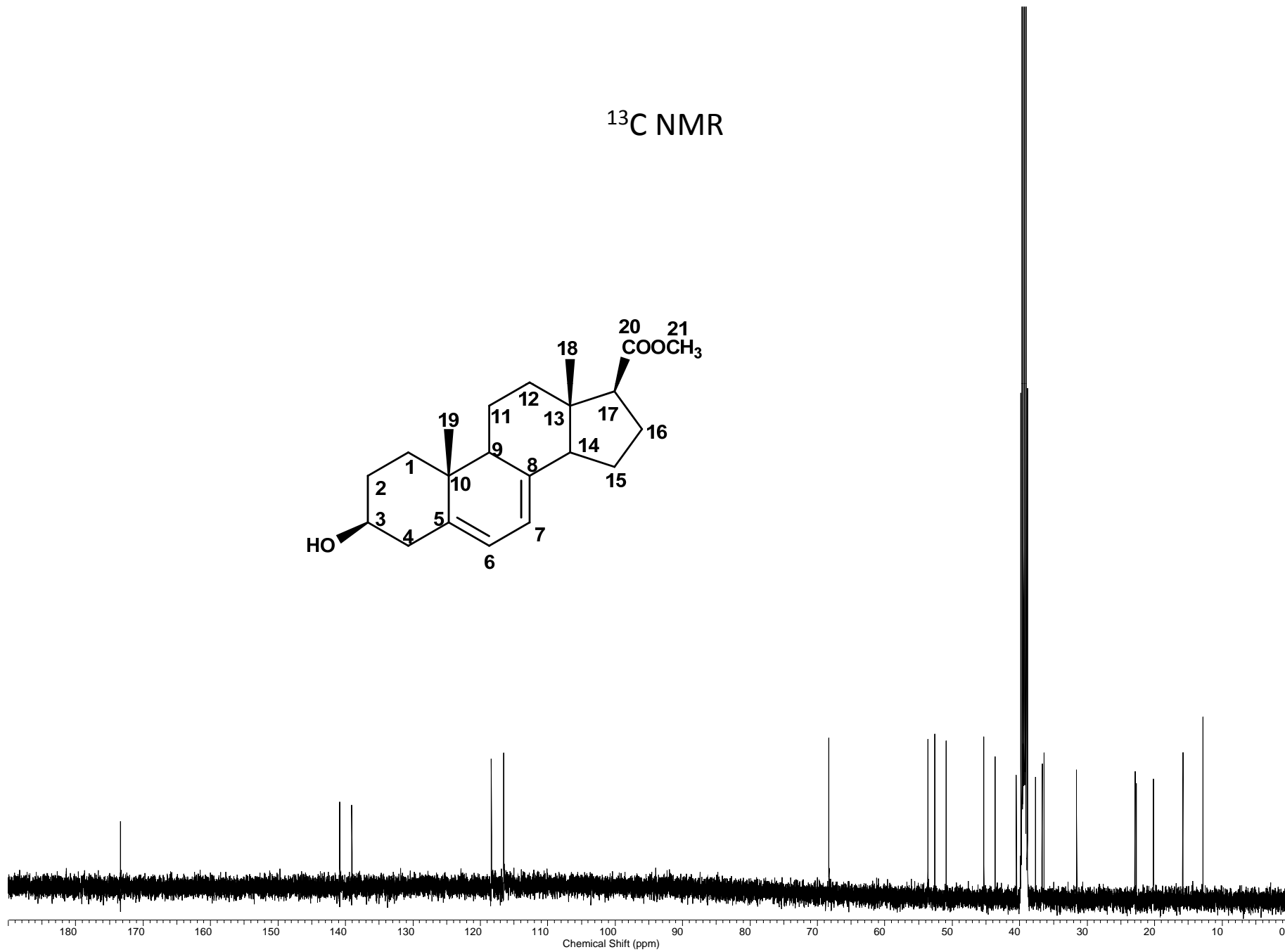
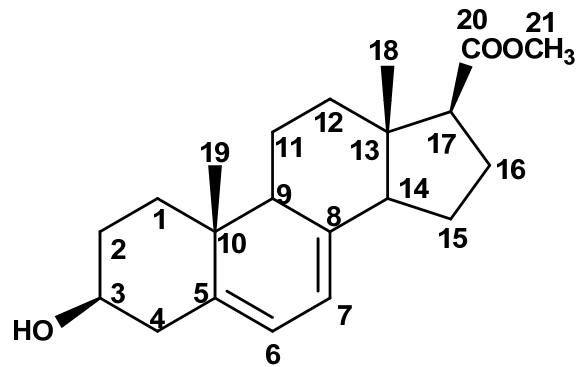
HPLC conditions: isocratic, solvent A (water, 10%) and solvent B (methanol, 90%); running time: 20 min; flow rate: 1.0 mL/min.

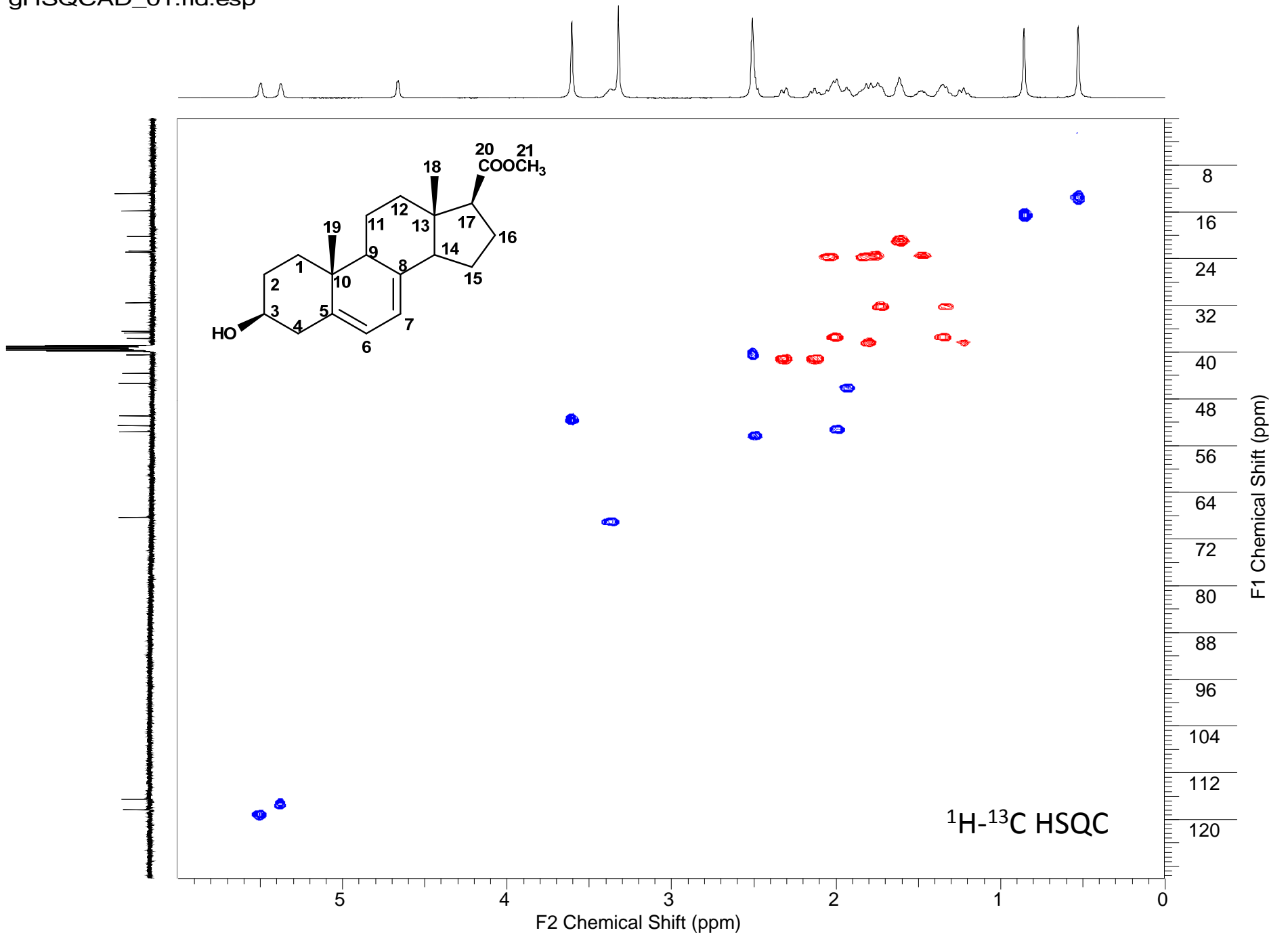
## Proton NMR spectrum

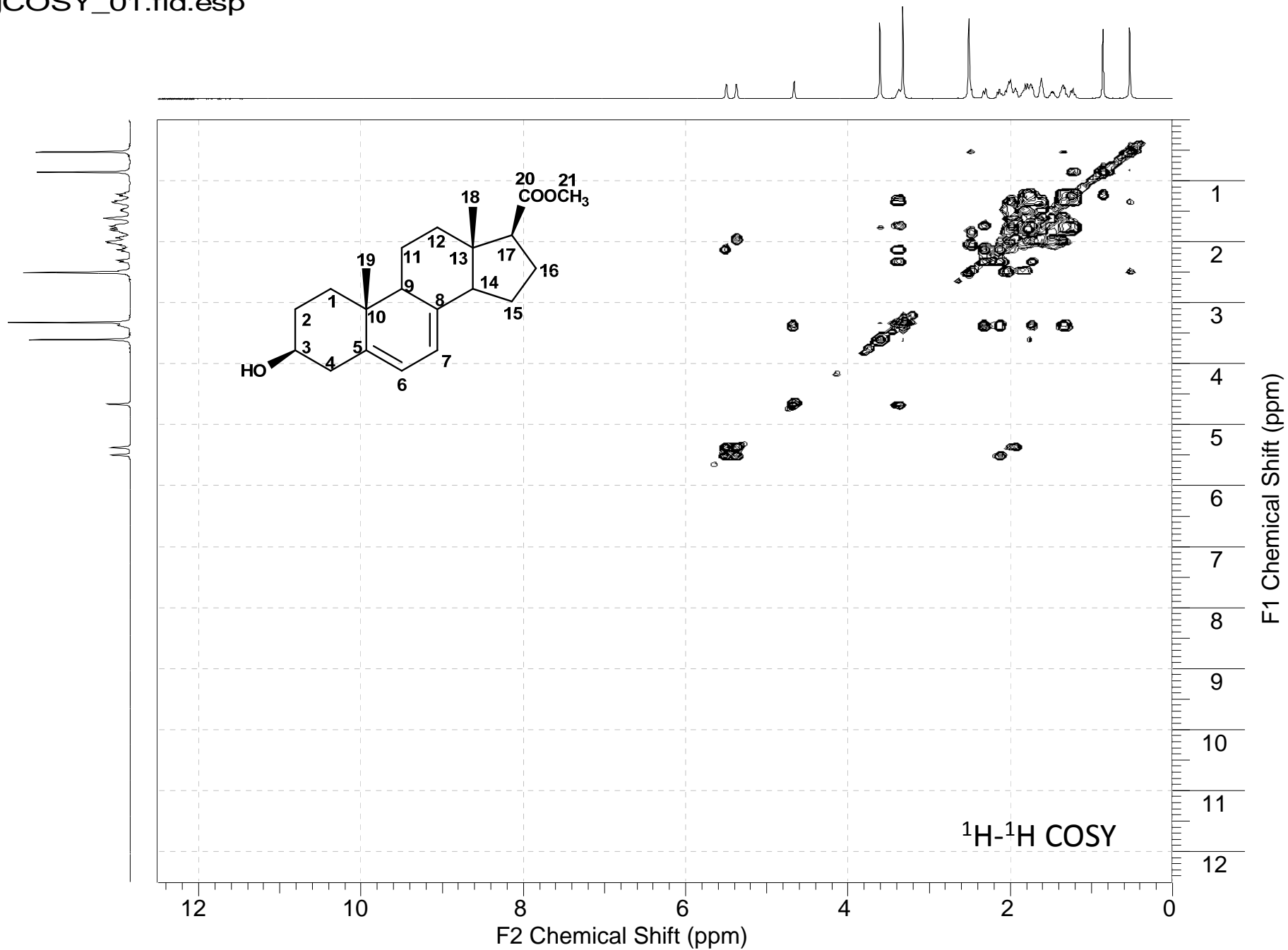


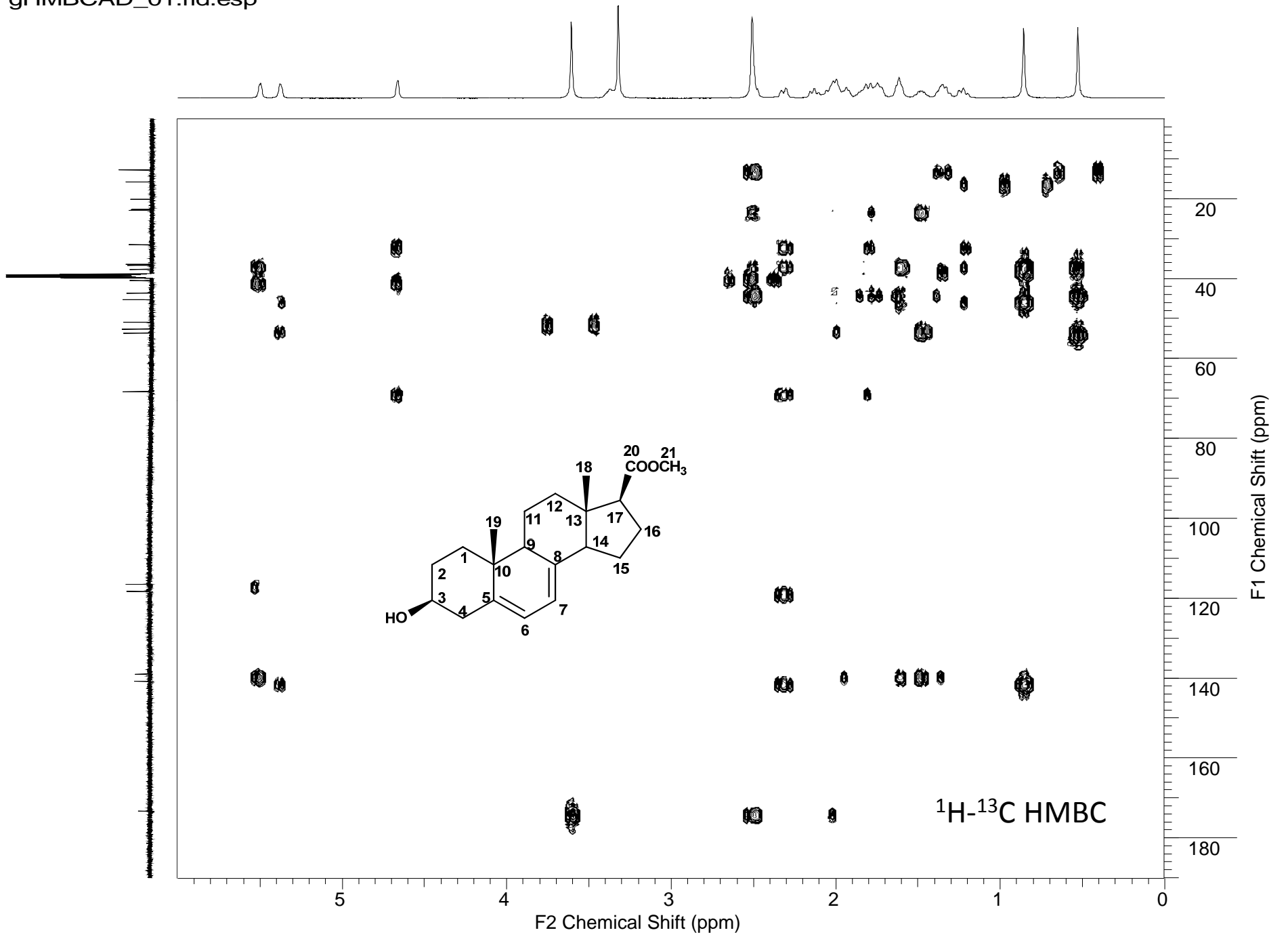


# $^{13}\text{C}$ NMR

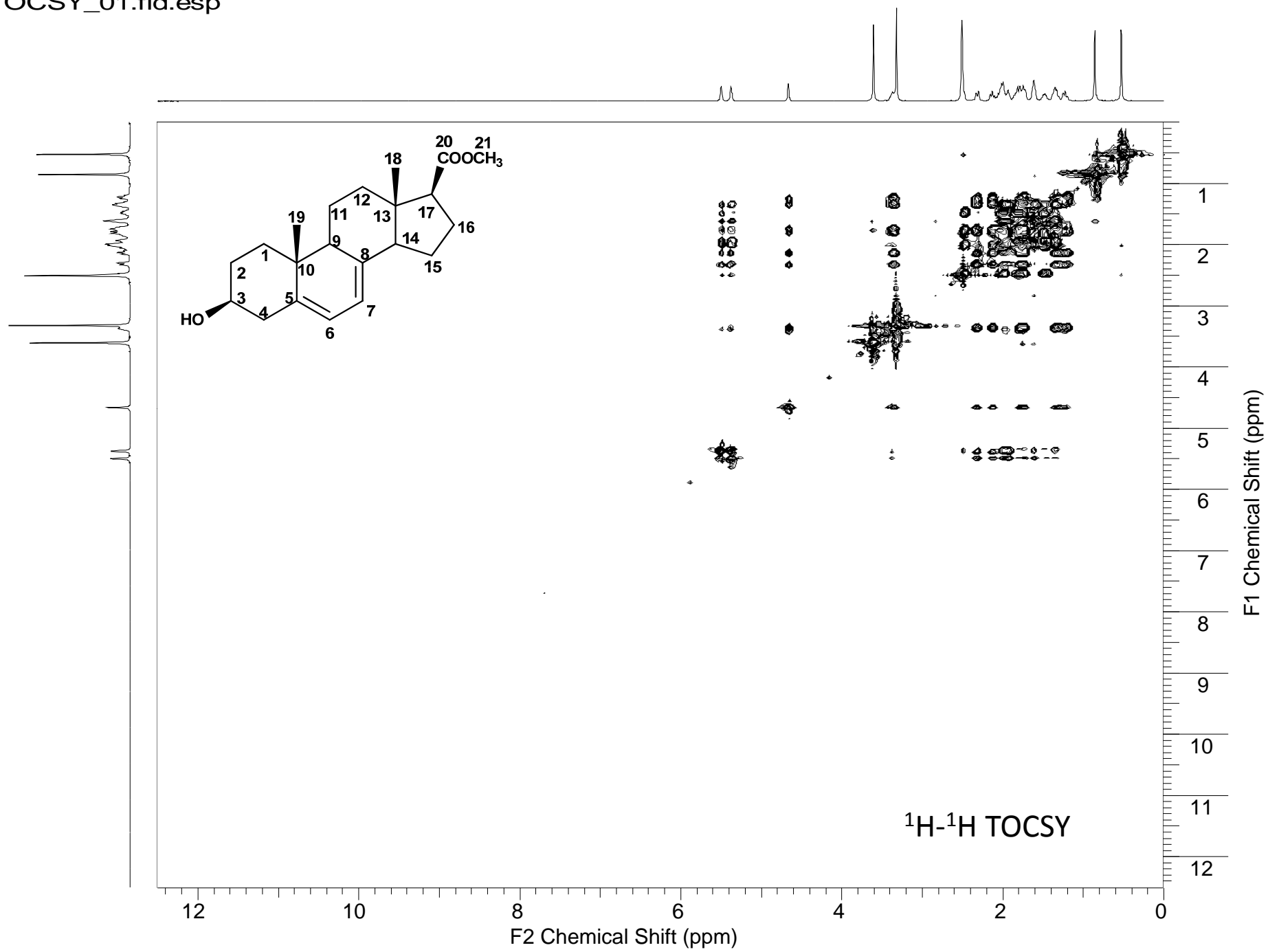




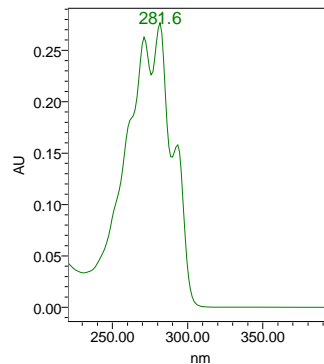
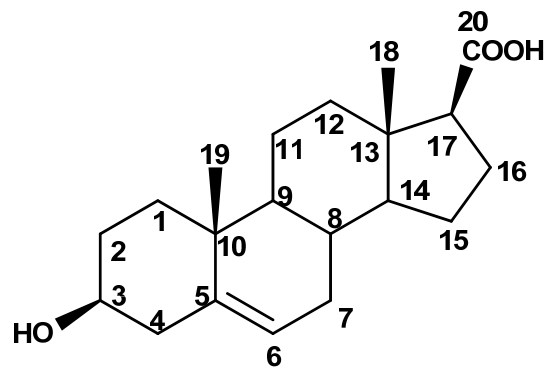




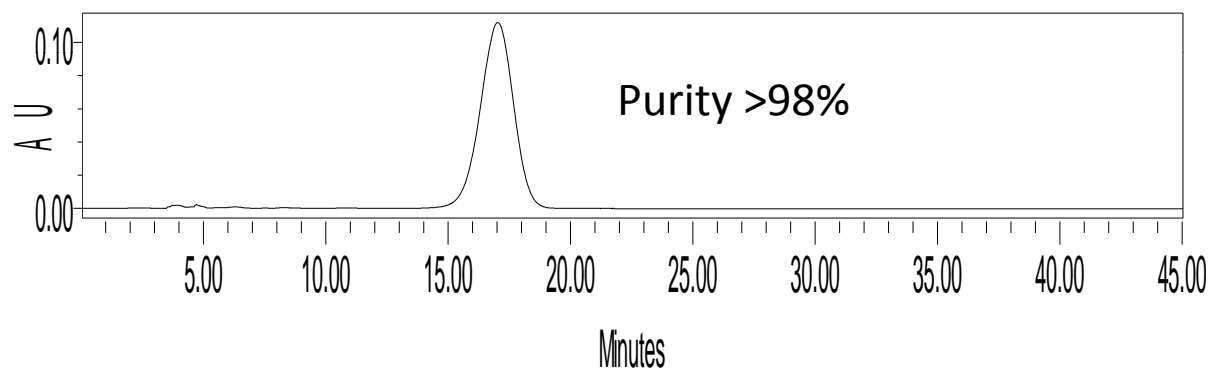
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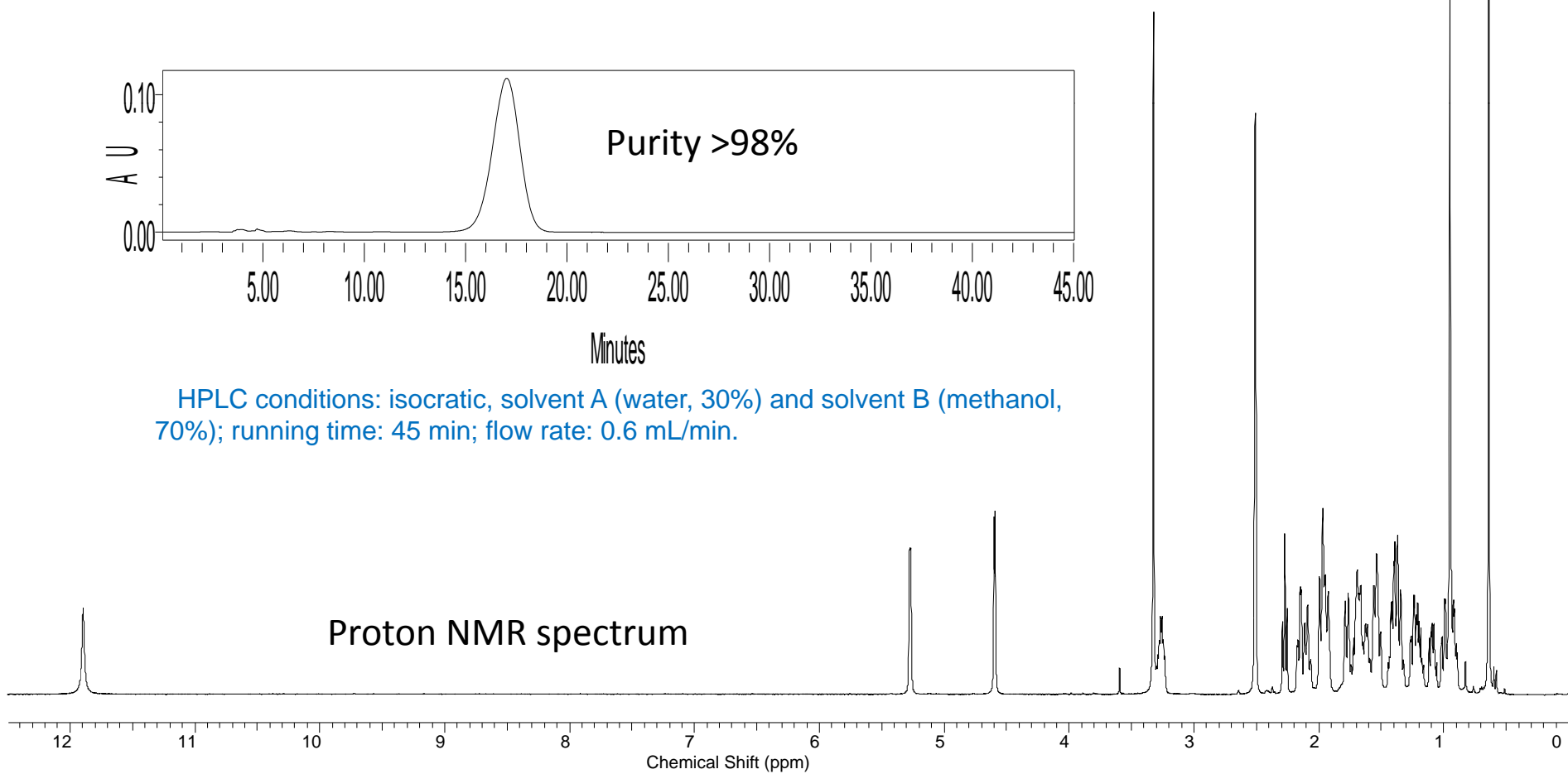
# 17-COOH-Pregnenolone (17-COOH-A)



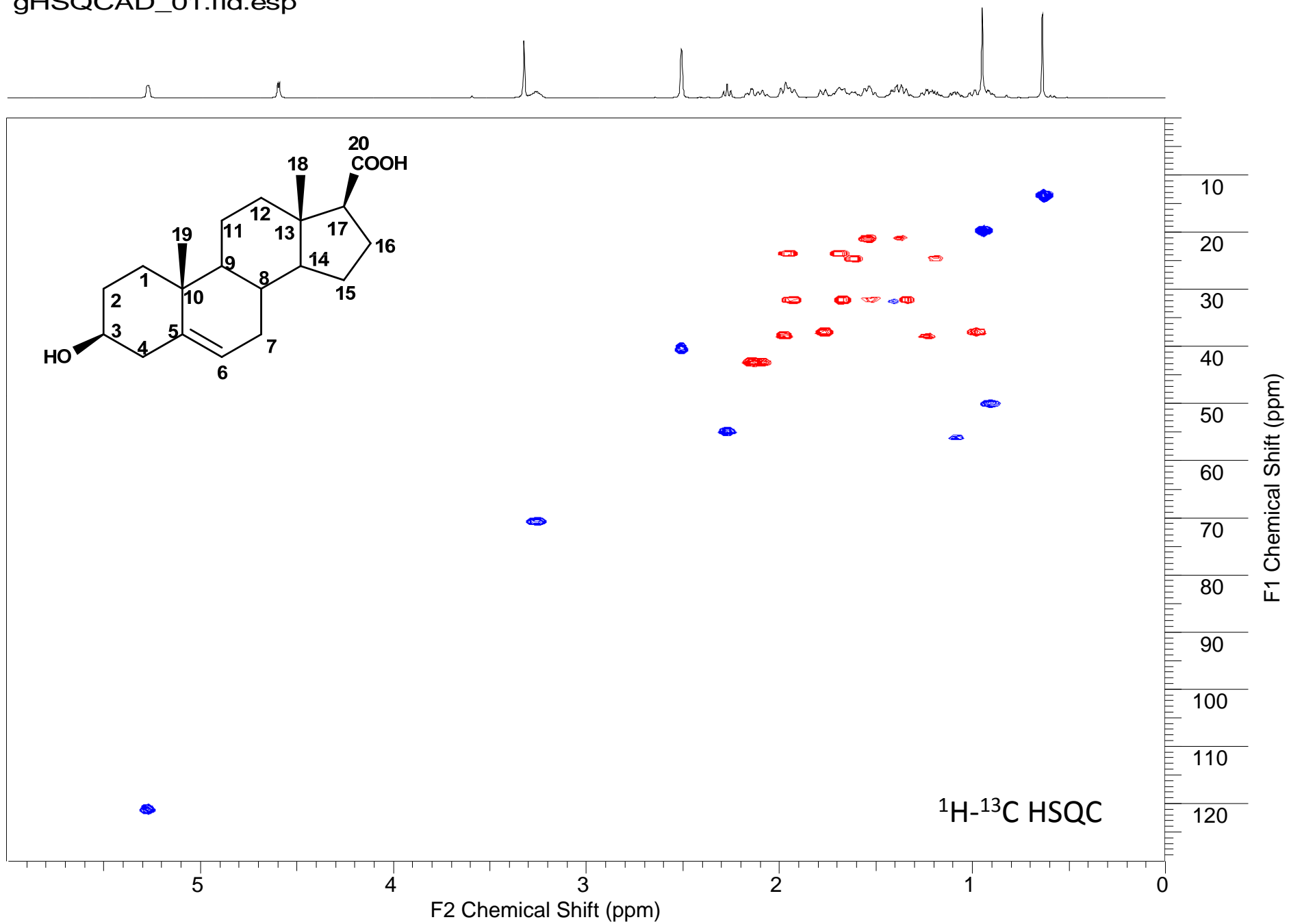
UV spectrum

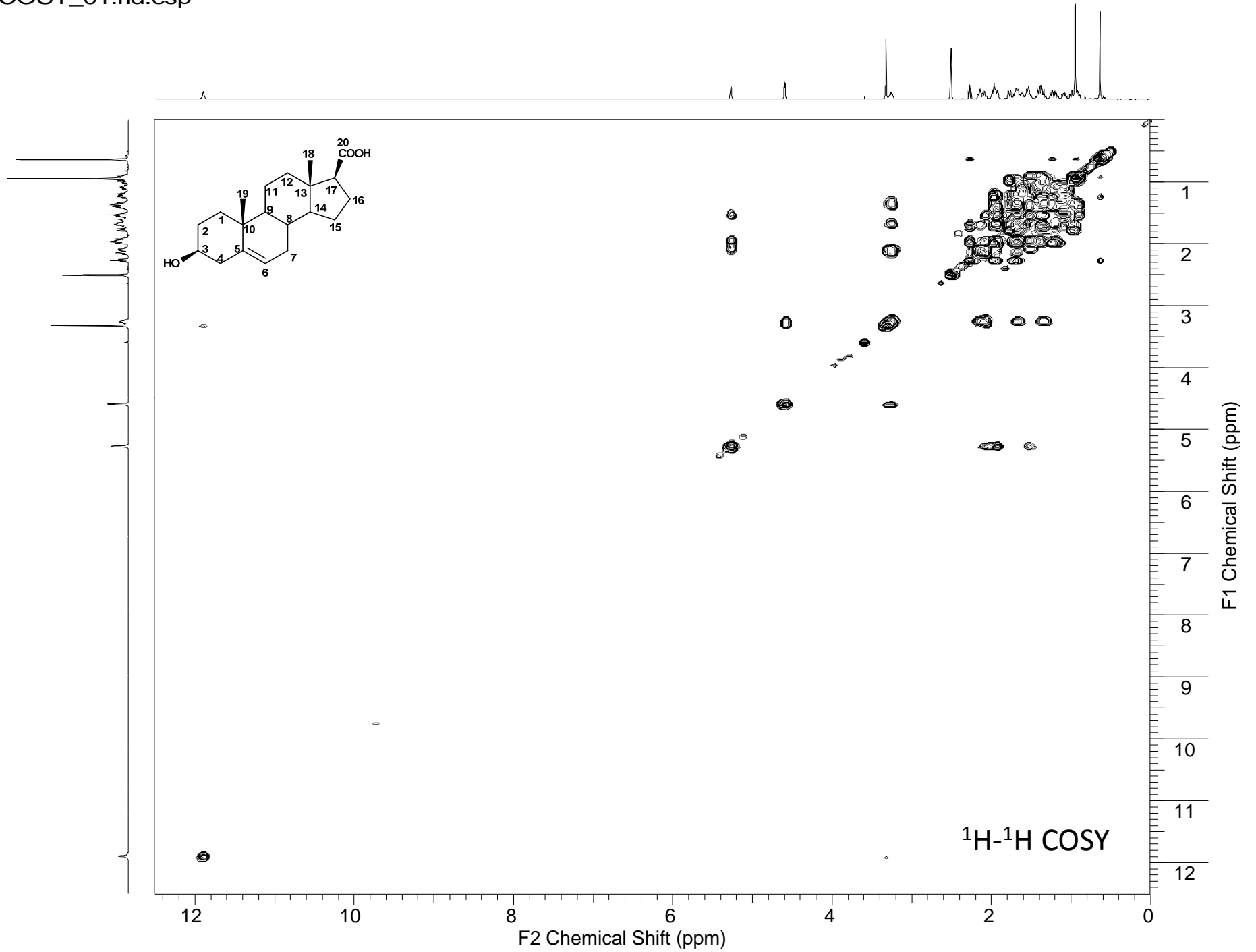


HPLC conditions: isocratic, solvent A (water, 30%) and solvent B (methanol, 70%); running time: 45 min; flow rate: 0.6 mL/min.



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