

Supplementary Data

Synthesis of novel androstane-N-cyclohexyl-17-carboxamides, and their effect on th

e 5 α -reductase isoform 2, the androgen receptor, and androgen-dependent glands

Juan C. Lopez-Lezama^{1,2}, Marisa Cabeza³, Yvonne Heuze⁴, Araceli Sánchez³, José L. Rojas⁵ and Norma A. Valencia-Islas^{1*}.

¹Universidad Nacional de Colombia, Sede Bogotá, Facultad de Ciencias, Departamento de Farmacia. Cra. 30 No. 45-03, Bogotá, Colombia.

²*Current address*: Universidad El Bosque, Facultad de Medicina, Bogotá, Colombia.

³Departamento de Sistemas Biológicos, Universidad Autónoma Metropolitana-Xochimilco, Calzada del Hueso #1100. Colonia Villa Quietud, CP 04960, Ciudad de México, México.

⁴Departamento de Producción Agrícola y Animal. Universidad Autónoma Metropolitana-Xochimilco, Calzada del Hueso 1100. Col. Villa Quietud, 04960 Ciudad de México.

⁵Universidad Nacional de Colombia, Sede Bogotá, Facultad de Ciencias, Departamento de Química. Cra. 30 No. 45-03, Bogotá, Colombia.

Corresponding author:

Norma A. Valencia-Islas. Universidad Nacional de Colombia, Sede Bogotá, Facultad de Ciencias, Departamento de Farmacia. Cra. 30 No. 45-03, Bogotá, Colombia.

E-mail: navalenciai@unal.edu.co

[Phone: \(571\) + 3165000 Ext. 14629](tel:+5713165000). [Fax: \(571\) + 3165000 Ext. 14639](tel:+5713165000).

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Figure S28. ESI-MS spectrum of N-cyclohexyl-3-oxoandrosta-4,16-diene-17-carboxamide (**8**).

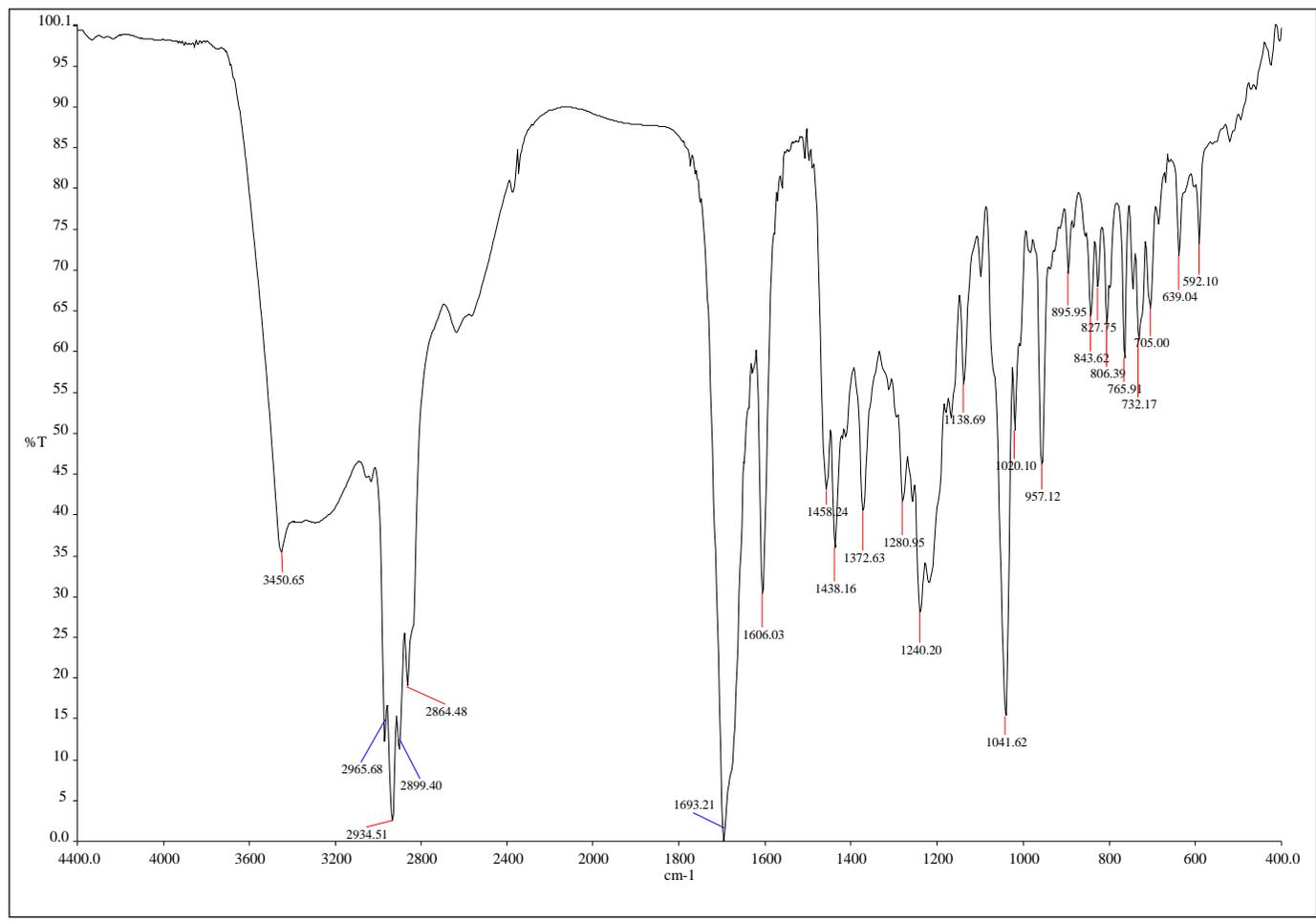


Figure S1. IR (KBr, cm⁻¹) spectrum of 3β-hydroxyandrosta-5,16-diene-17-carboxylic acid (**2**).

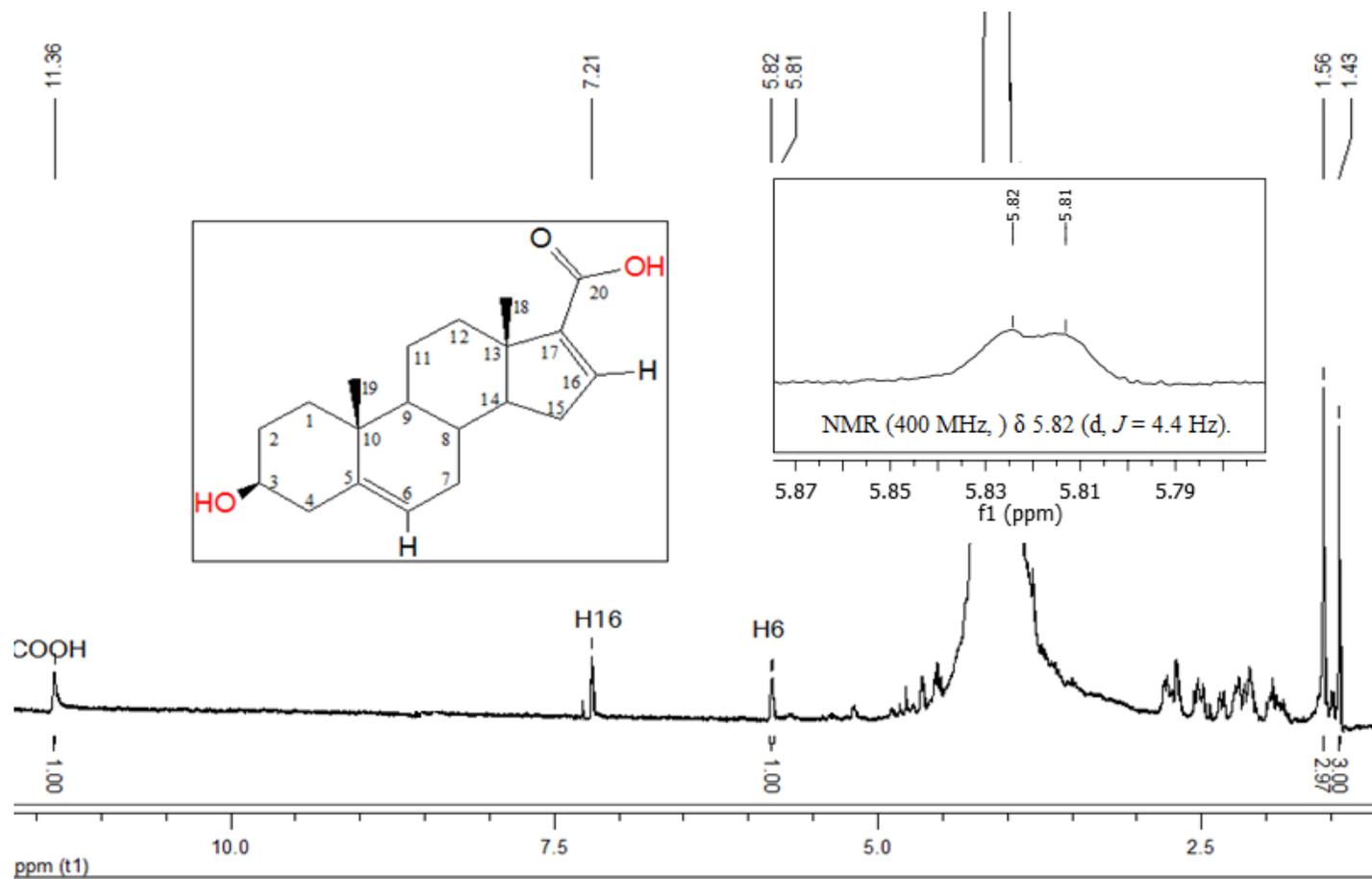


Figure S2. ¹H NMR spectrum of 3β-hydroxyandrosta-5,16-diene-17-carboxylic acid (**2**) (1,4-dioxane-d₈, 400 MHz).

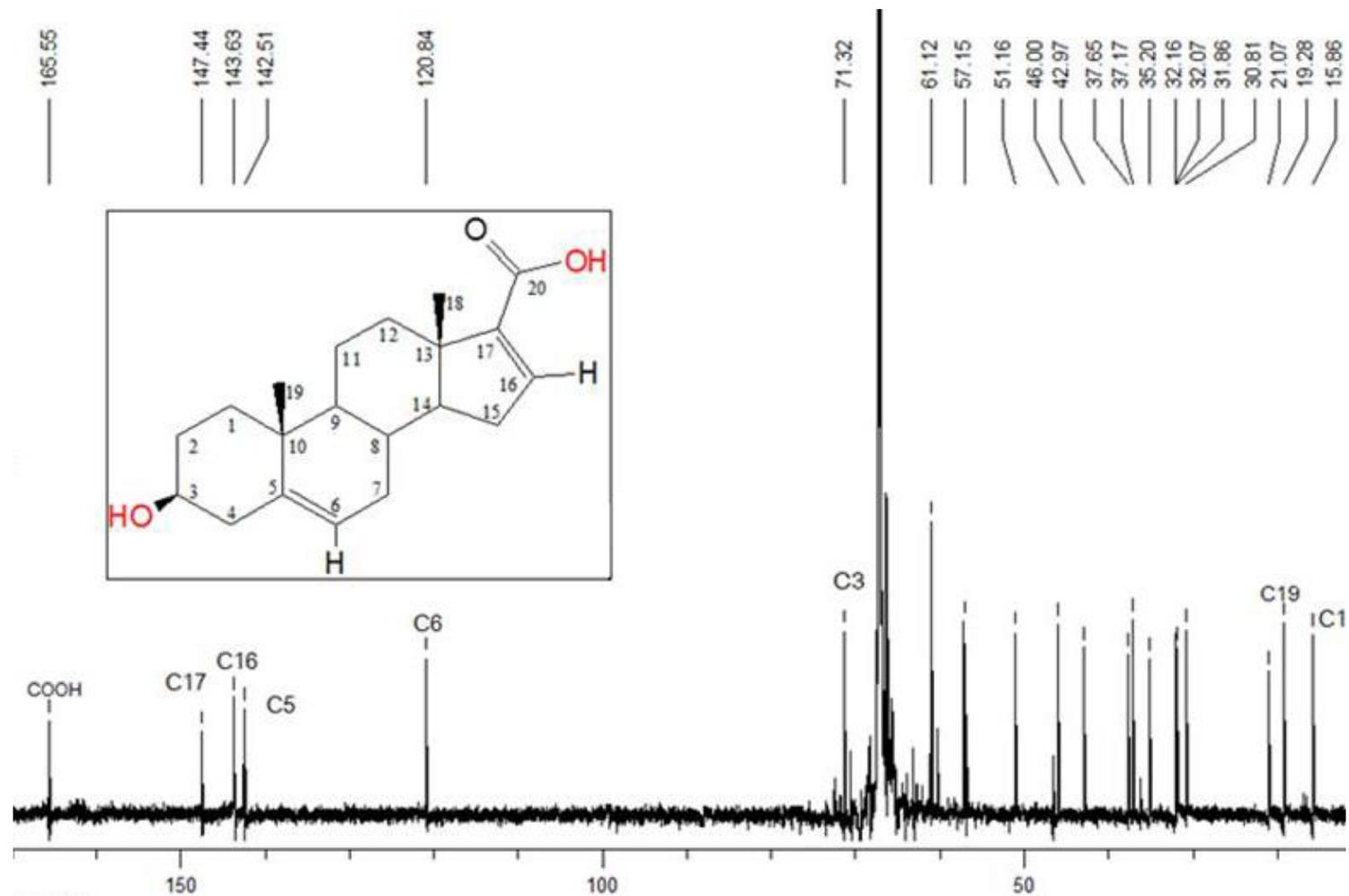


Figure S3. ^{13}C NMR spectrum of 3 β -hydroxyandrosta-5,16-diene-17-carboxylic acid (**2**) (1,4-dioxane- d_8 , 100 MHz).

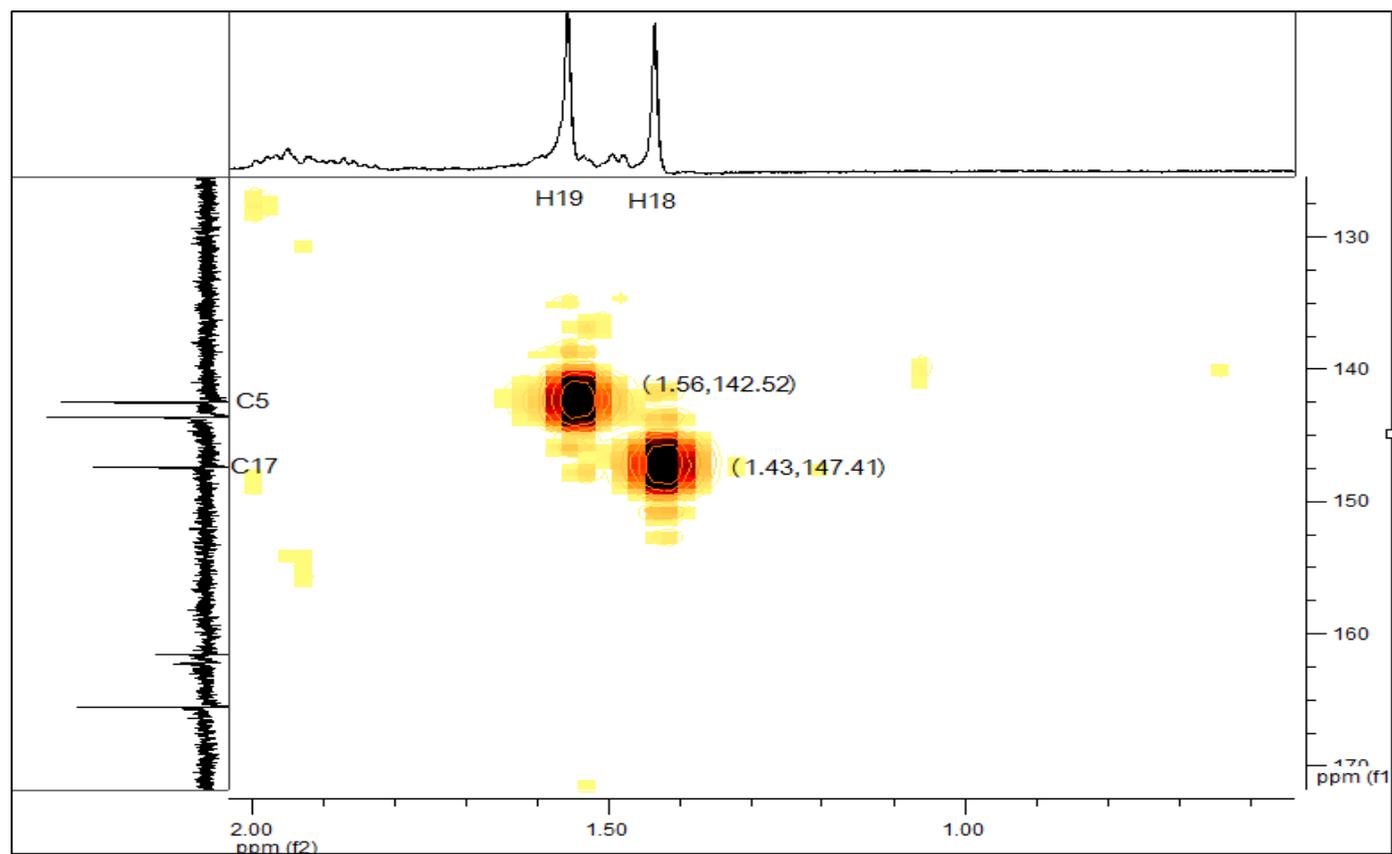


Figure S4. HMBC spectrum of 3 β -hydroxyandrosta-5,16-diene-17-carboxylic acid (**2**) (1,4-dioxane-d₈).

Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [MF-Linear]
RT : 1.16 min Scan# : (22,32)
BP : m/z 18.0000 Int. : 211.87
Output m/z range : 14.2433 to 351.3353 Cut Level : 0.00 %

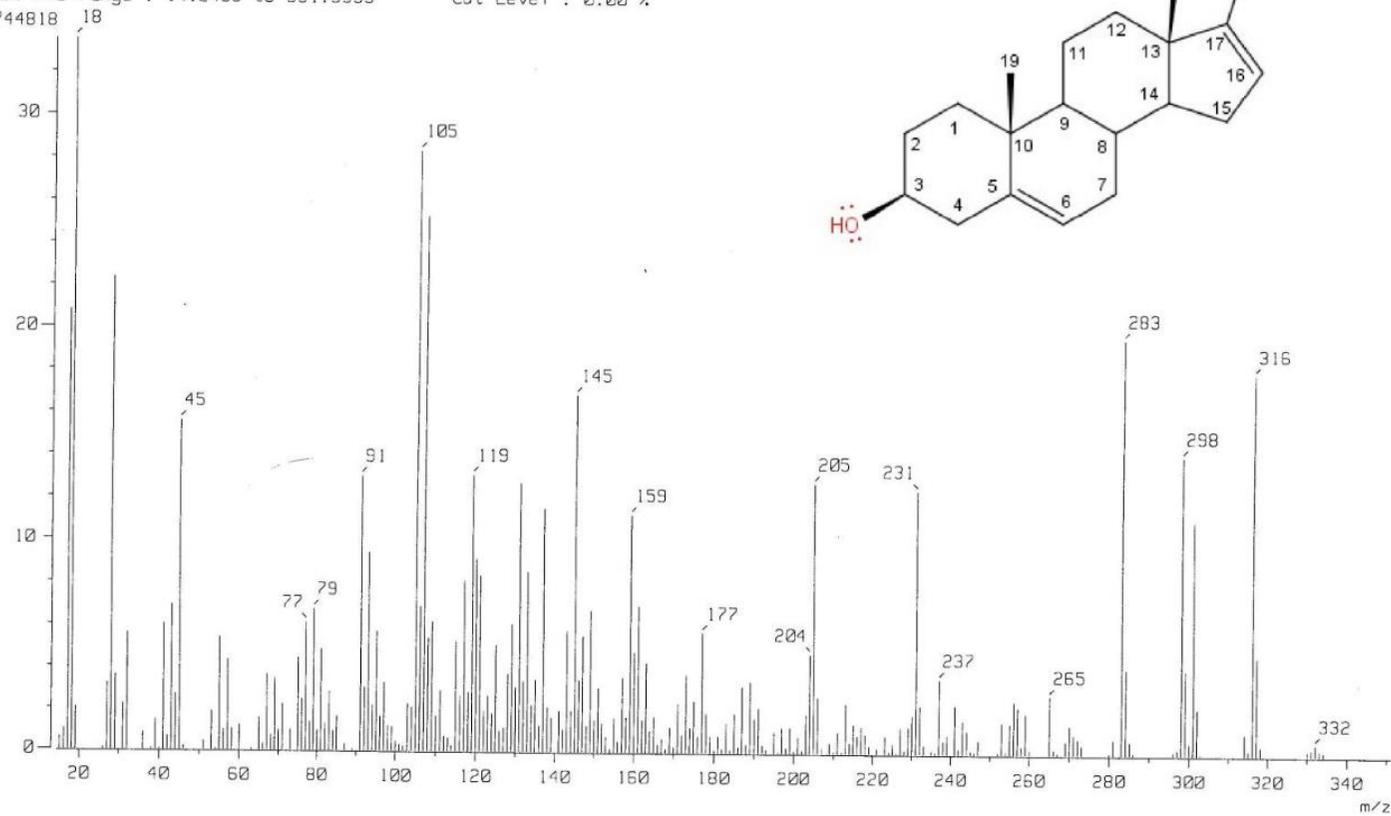


Figure S5. EIMS spectrum of 3β-hydroxyandrosta-5,16-diene-17-carboxylic acid (2).

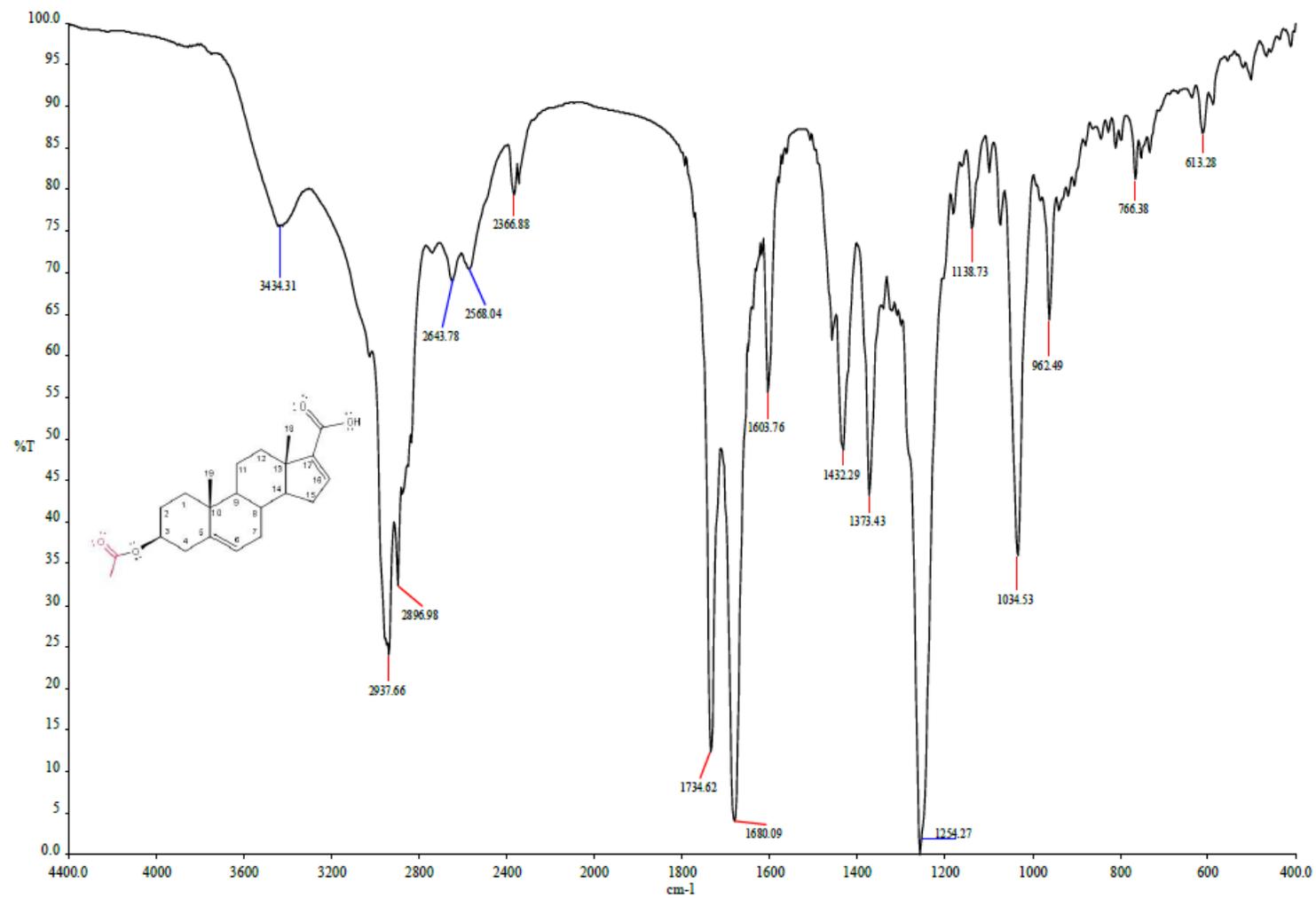


Figure S6. IR (KBr, cm⁻¹) spectrum of 3β-acetoxyandrosta-5,16-diene-17-carboxylic acid (**3**).

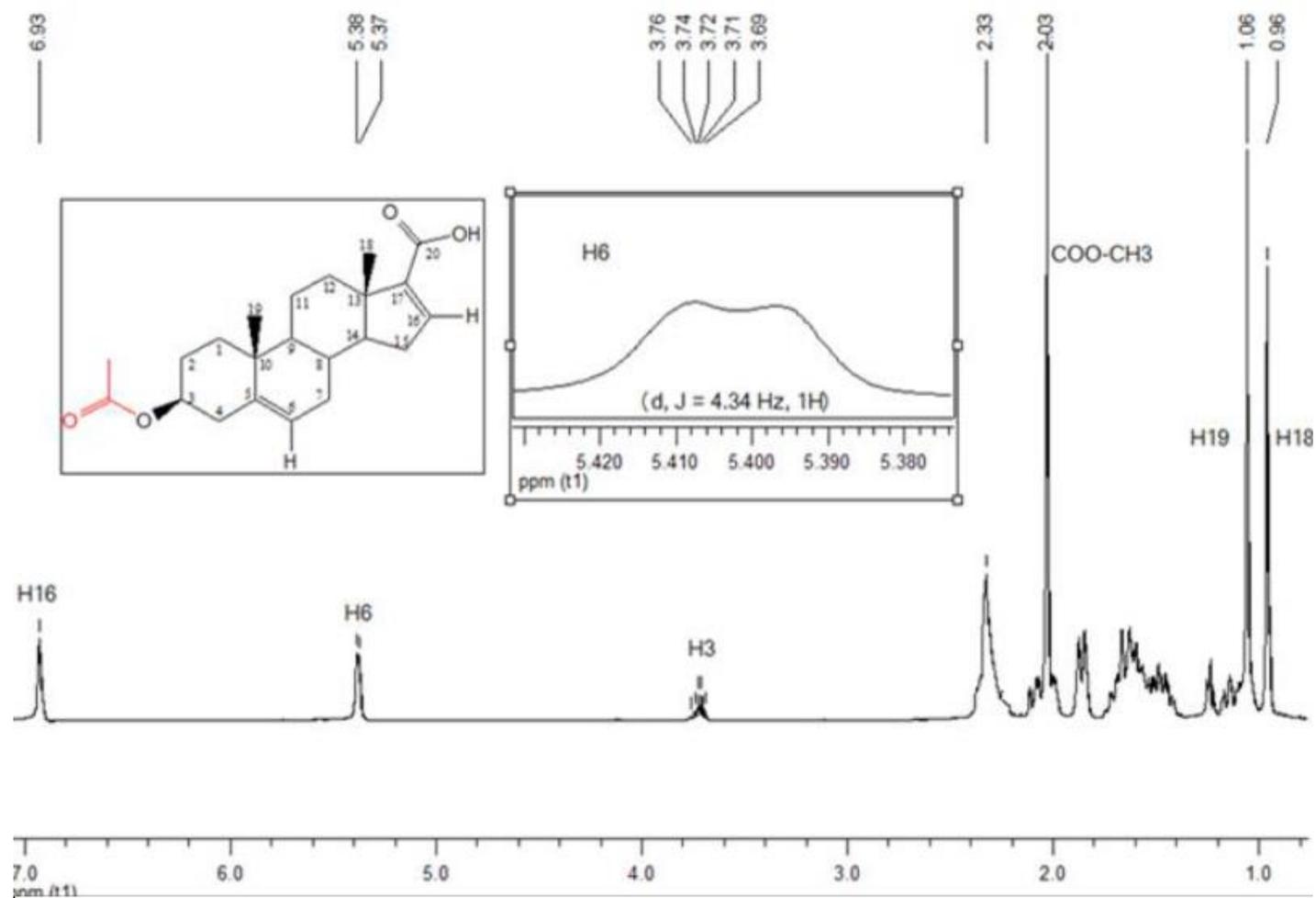


Figure S7. ^1H NMR spectrum of 3 β -acetoxyandrosta-5,16-diene-17-carboxylic acid (**3**). (CDCl_3 , 400 MHz).

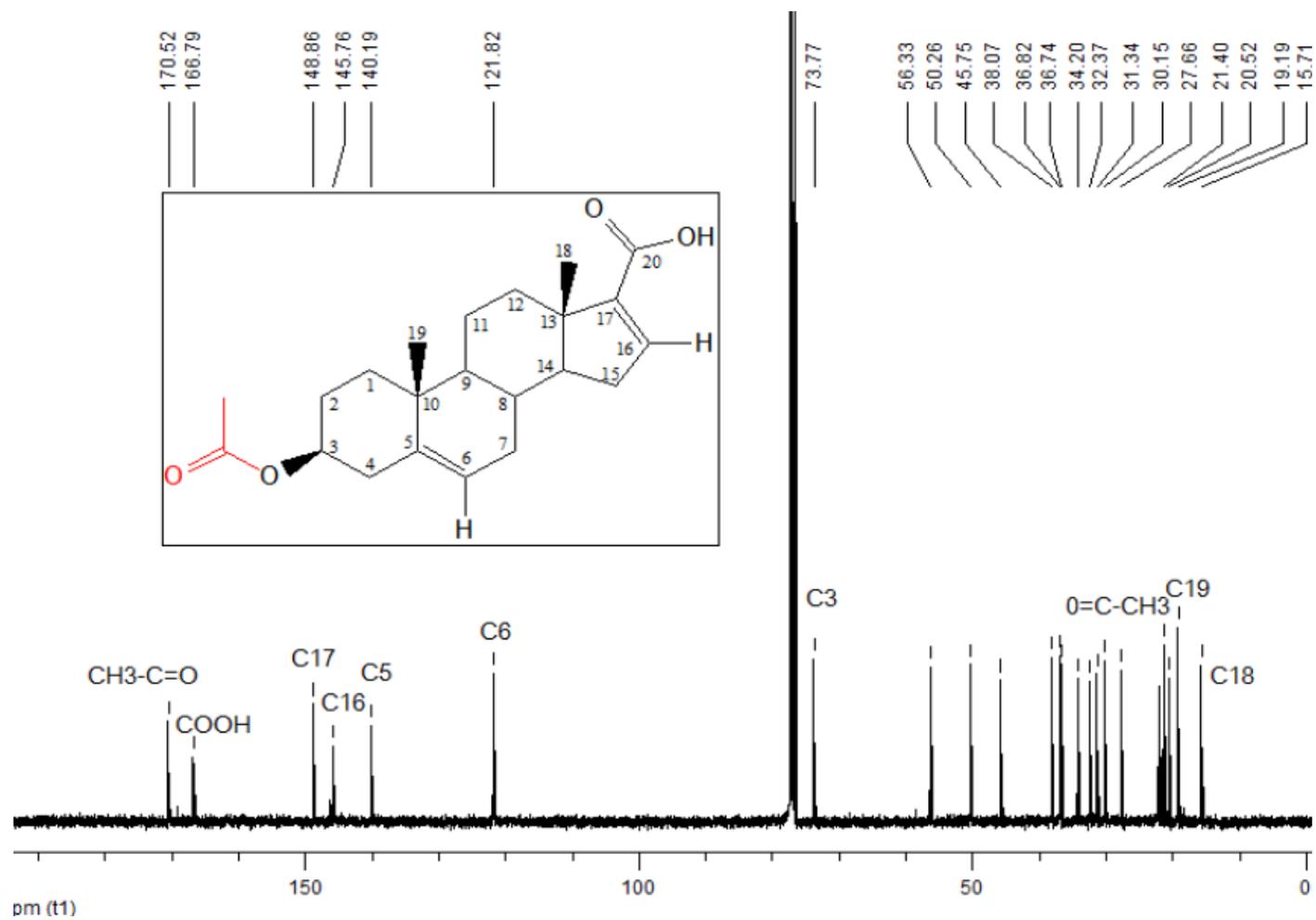


Figure S8. ¹³C NMR spectrum of 3β-acetoxyandrosta-5,16-diene-17-carboxylic acid (**3**) (CDCl₃, 100 MHz).

Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [MF-Linear]
RT : 1.03 min Scan# : (20,29)
BP : m/z 298.0000 Int. : 488.89
Output m/z range : 13.0564 to 447.4777 Cut Level : 0.00 %

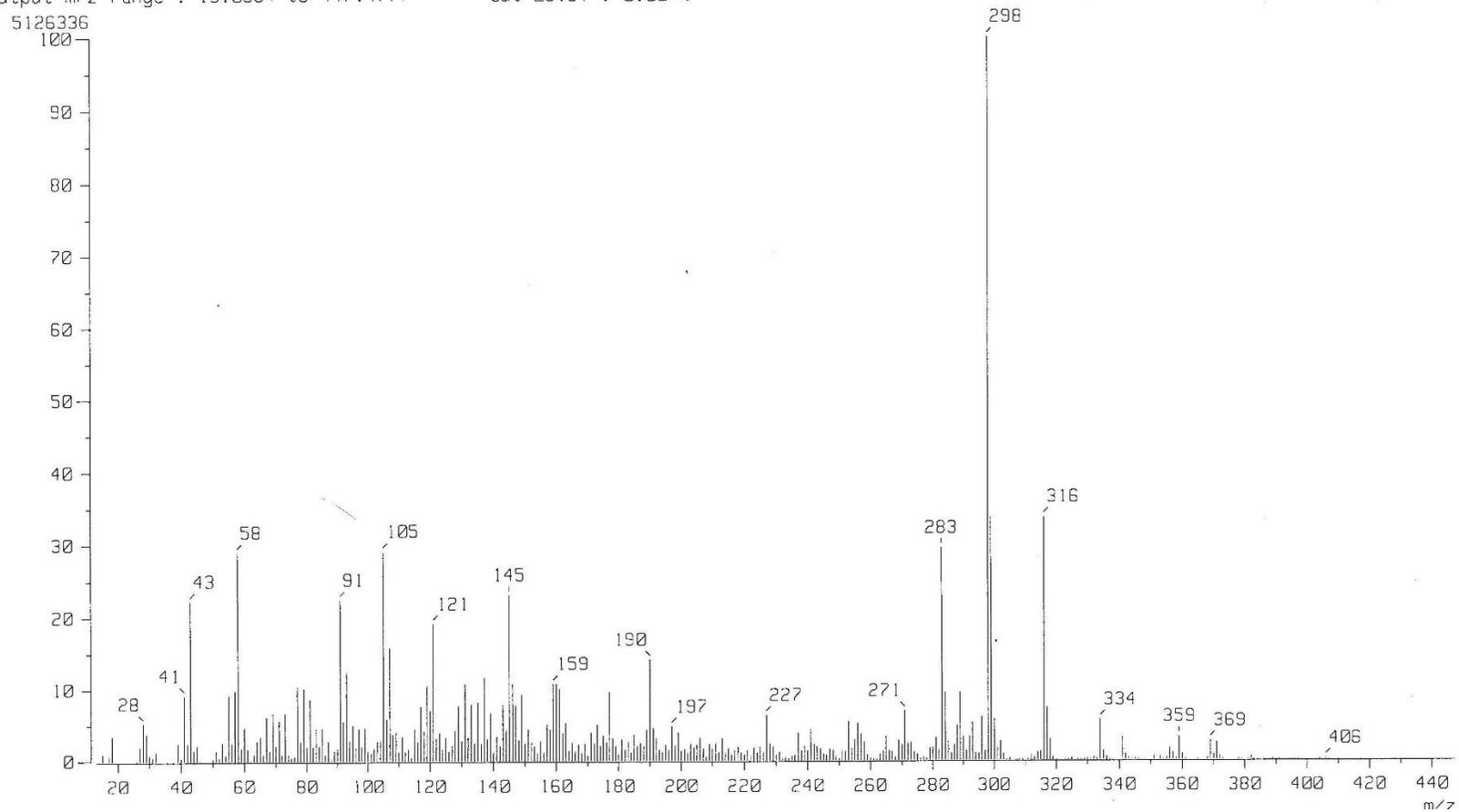


Figure S9. EIMS spectrum of 3 β -acetoxyandrosta-5,16-diene-17-carboxylic acid (**3**).

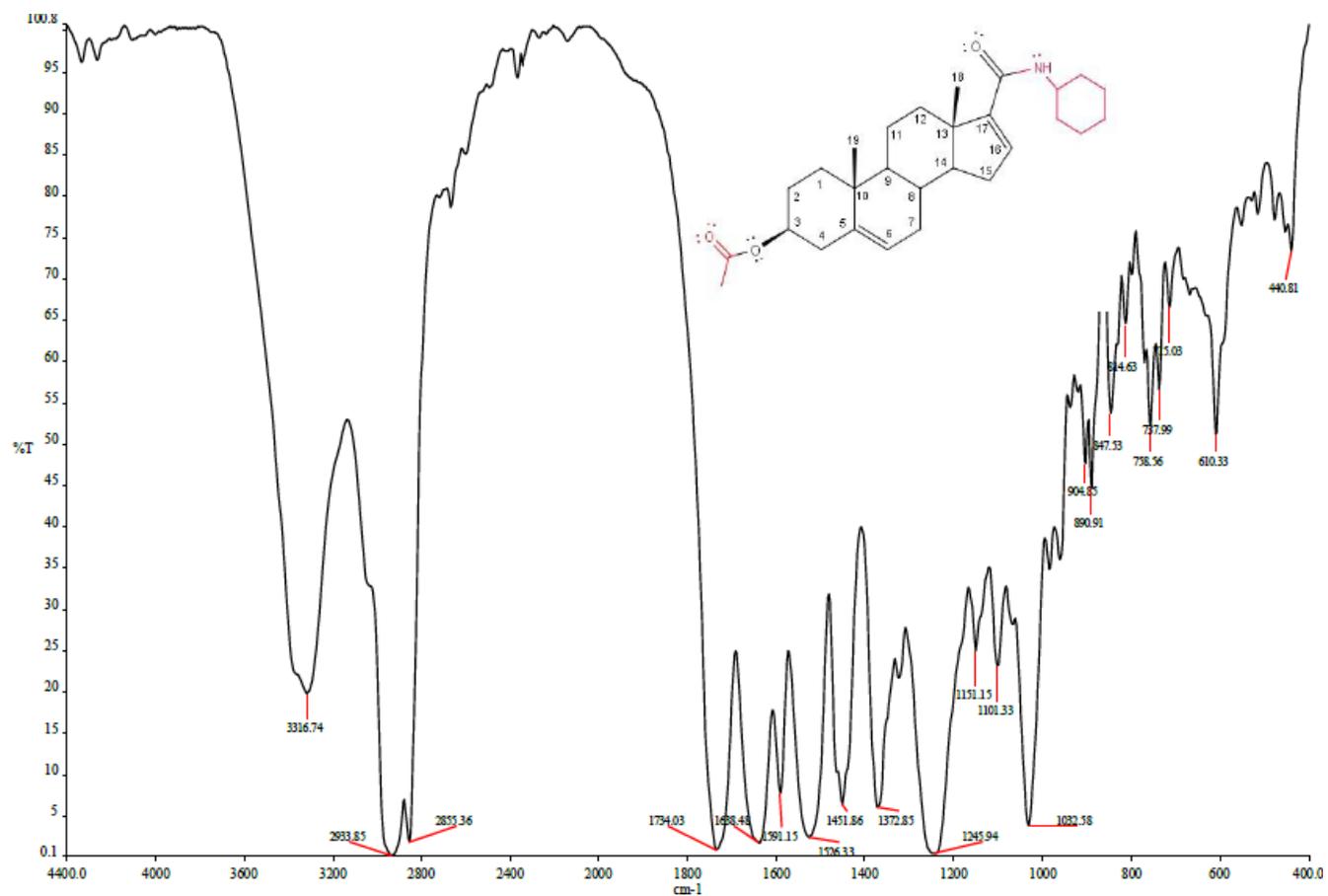


Figure S10. IR (KBr, cm^{-1}) spectrum of N-cyclohexyl-3 β -acetoxyandrosta-5,16-diene-17-carboxamide (5).

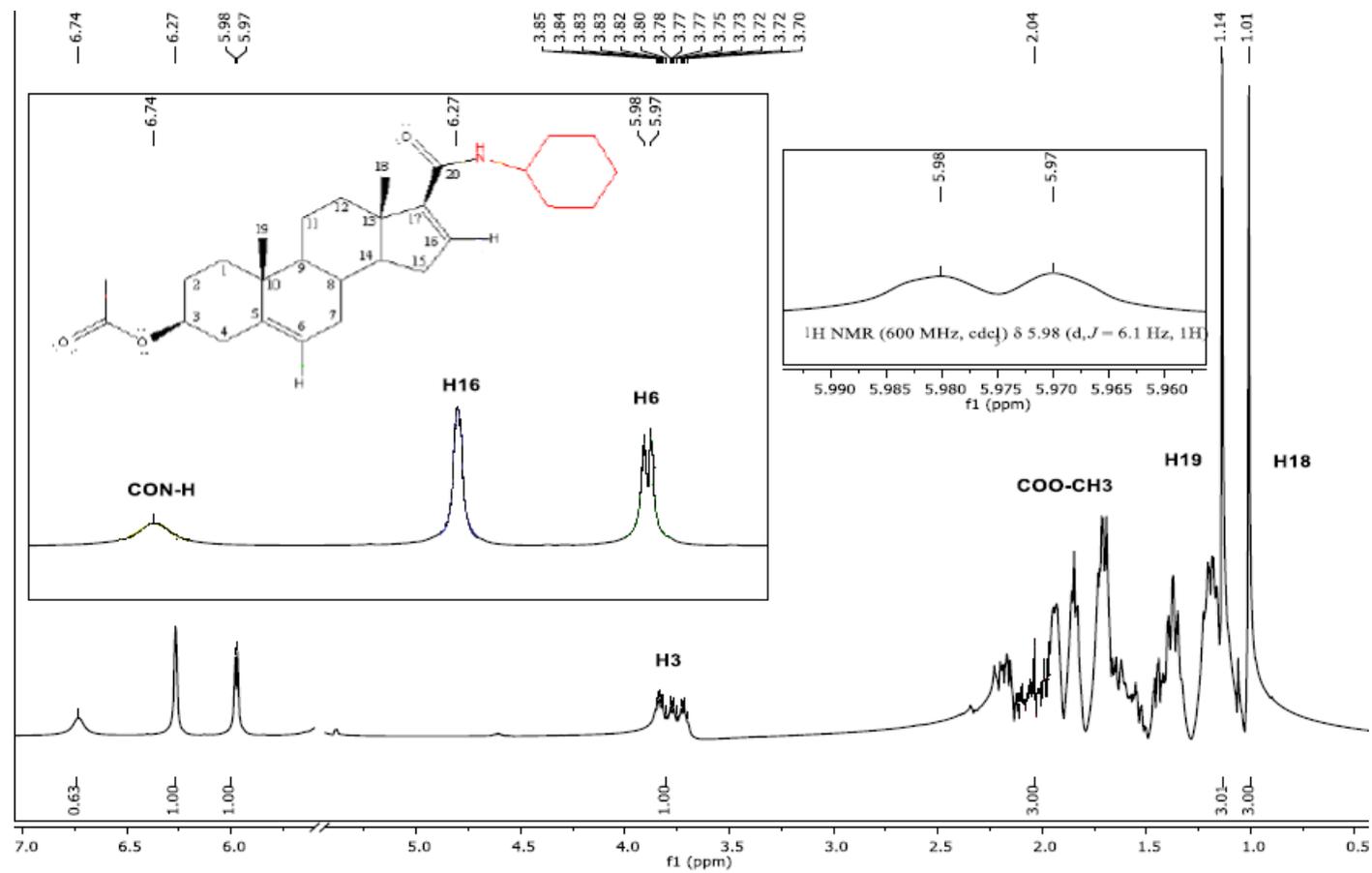


Figure S11. ¹H NMR spectrum of N-cyclohexyl-3β-acetoxyandrosta-5,16-diene-17-carboxamide (5) (CDCl₃, 600 MHz).

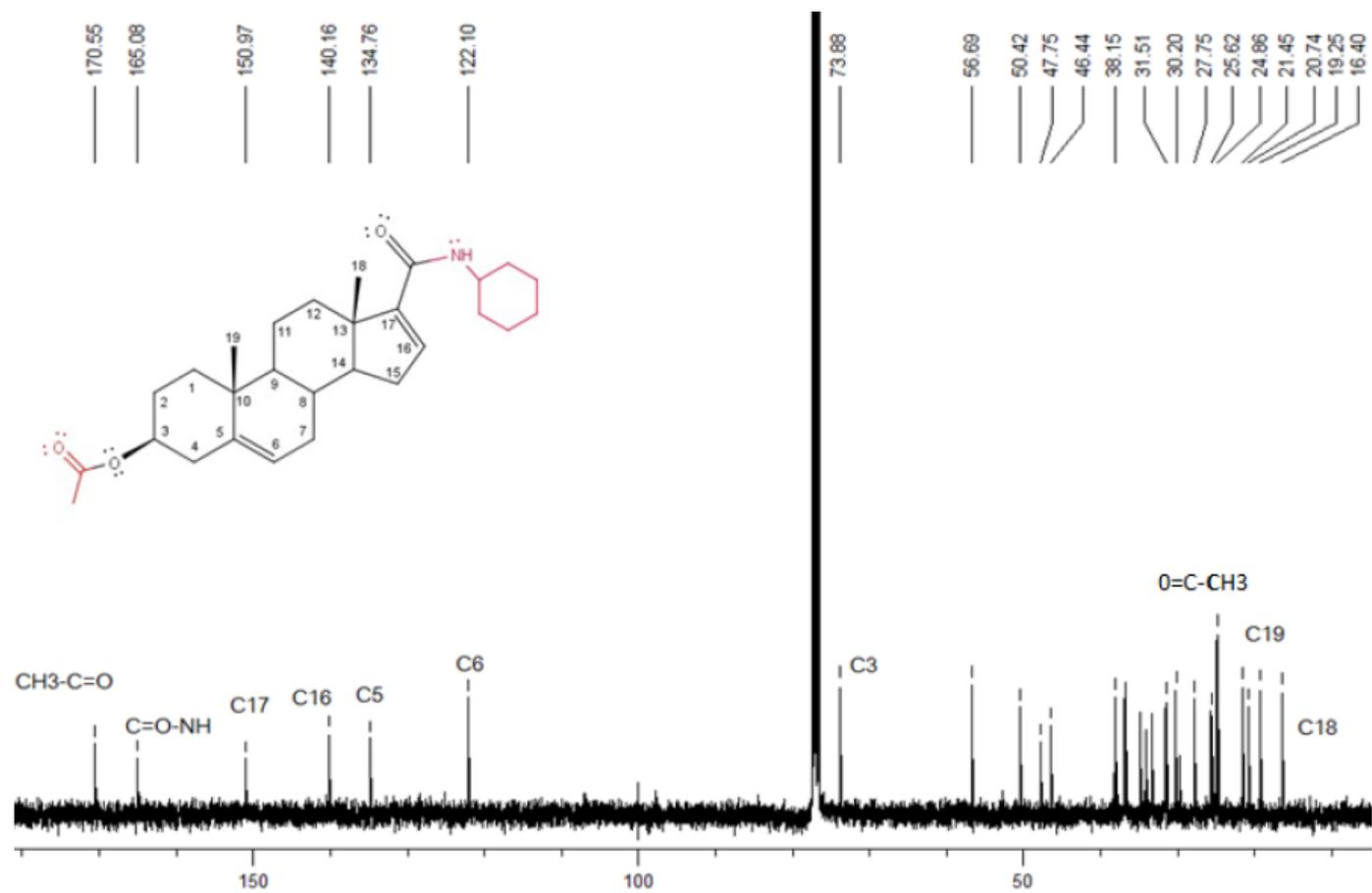


Figure S12. ¹³C NMR spectrum of N-cyclohexyl-3β-acetoxyandrosta-5,16-diene-17-carboxamide (5) (CDCl₃, 125 MHz).

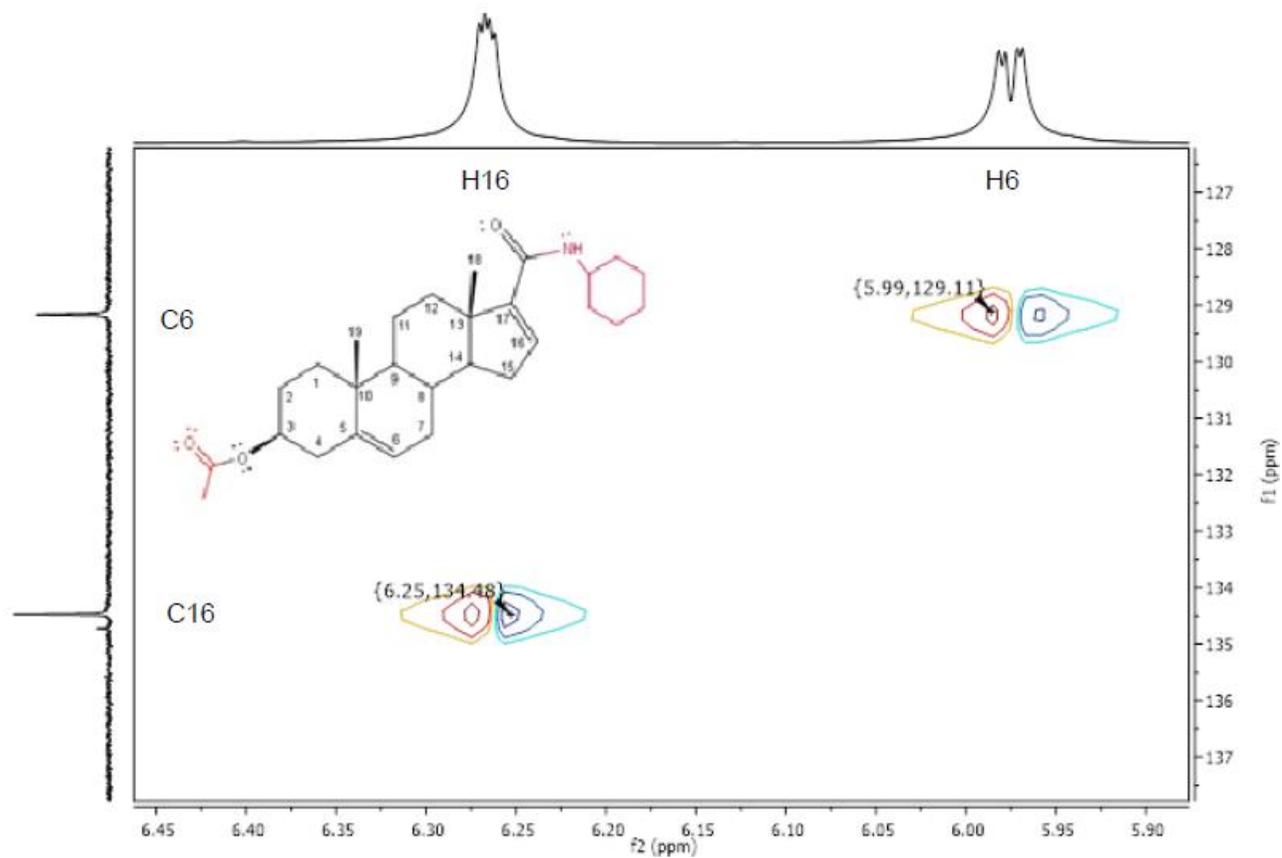


Figure S13. Expansion of HSQC spectrum of N-cyclohexyl-3 β -acetoxyandrosta-5,16-diene-17-carboxamide (**5**) (CDCl_3).

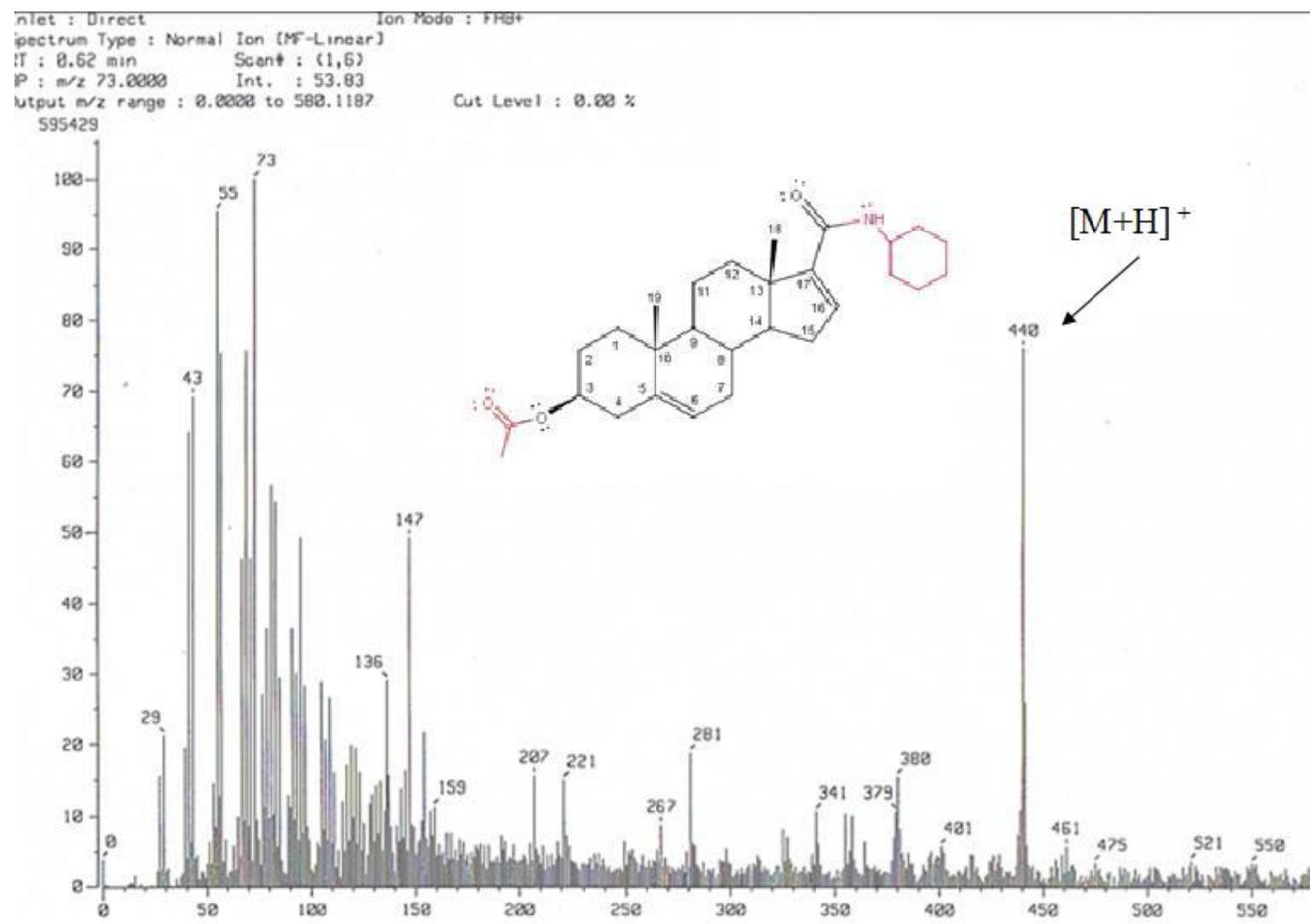


Figure S14. FAB-MS spectrum of N-cyclohexyl-3β-acetoxyandrosta-5,16-diene-17-carboxamide (5).

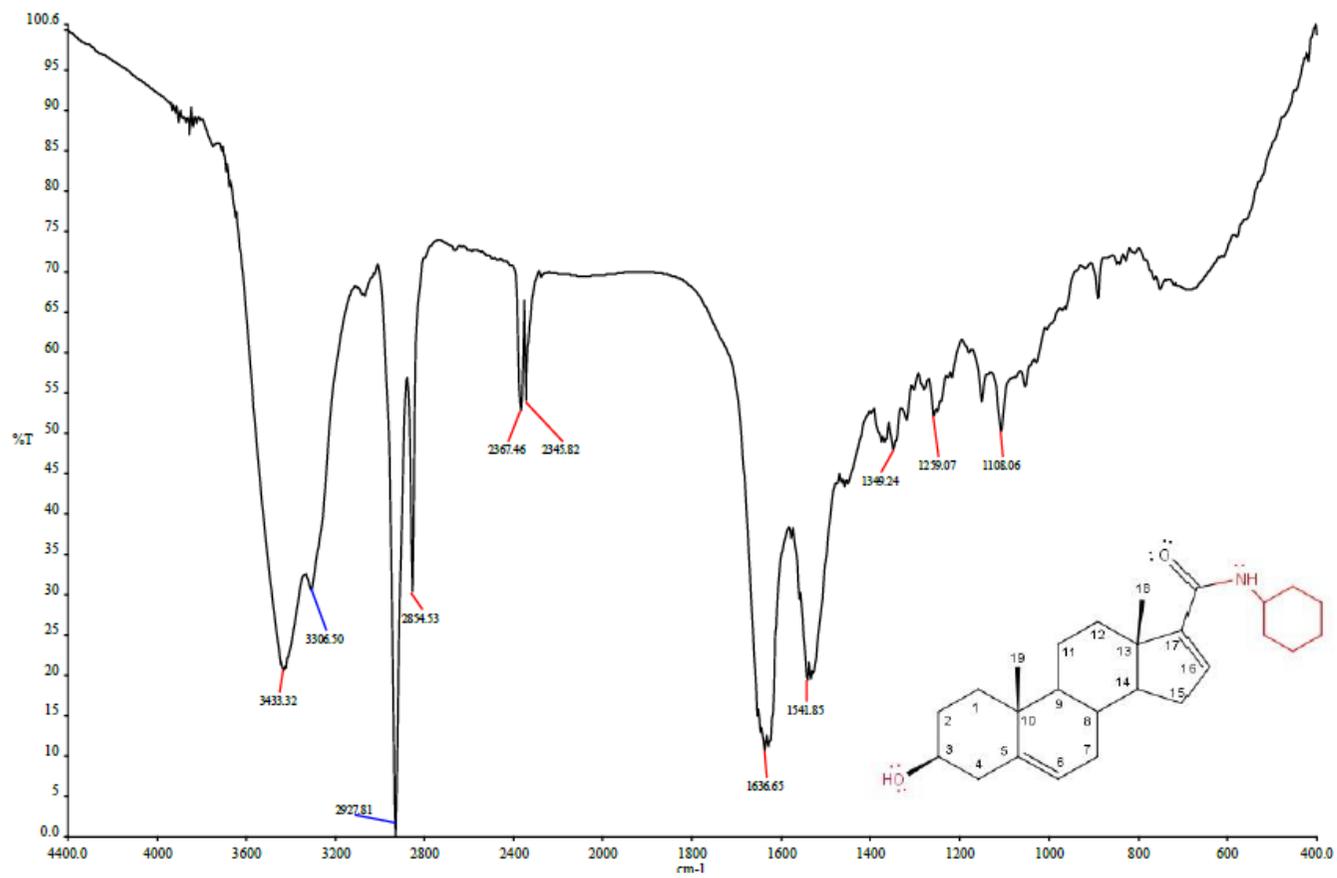


Figure S15. IR (KBr, cm⁻¹) spectrum of N-cyclohexyl-3β-hydroxyandrost-5,16-diene-17-carboxamide (**6**).

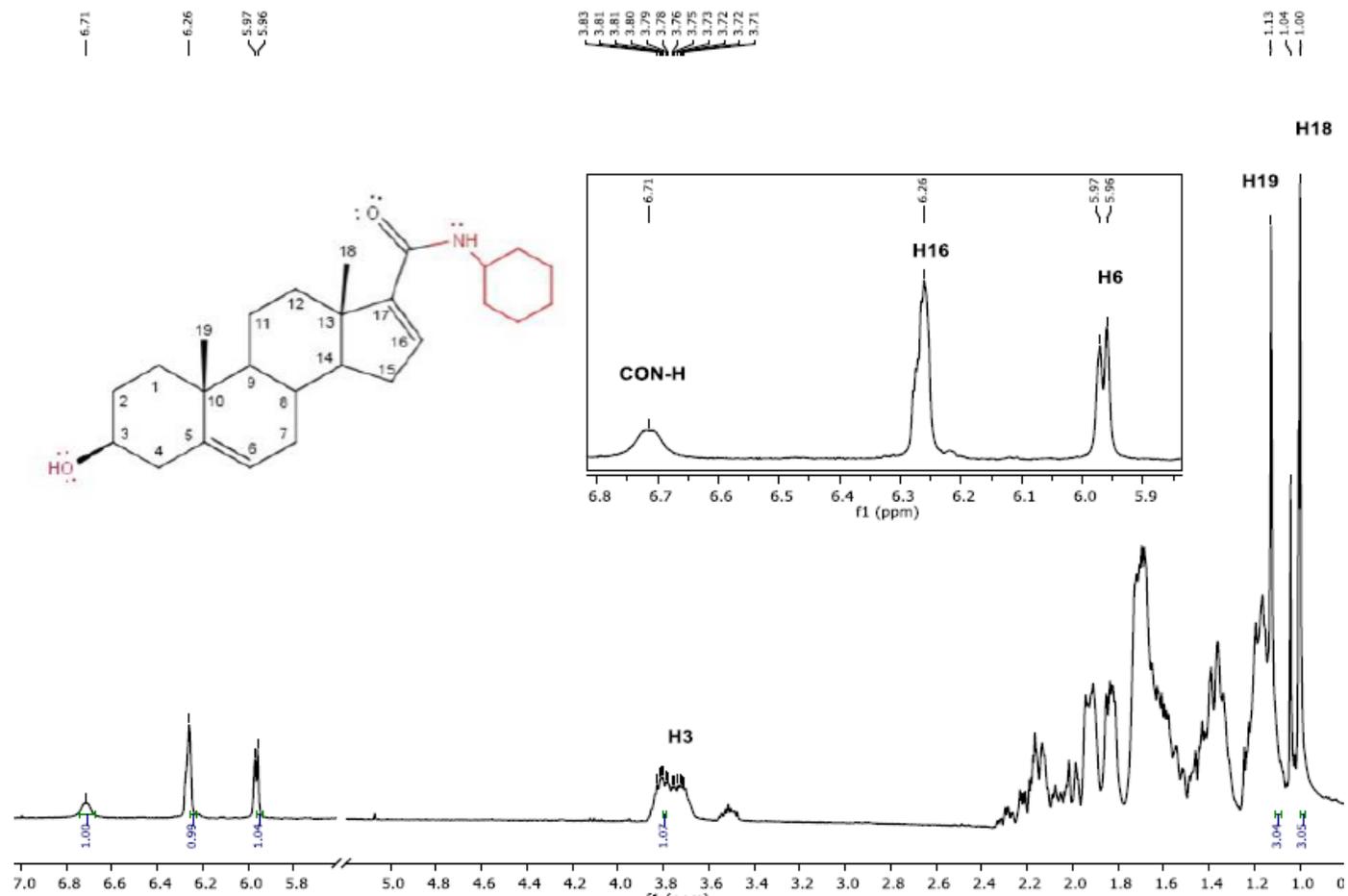


Figure S16. ¹H NMR spectrum of N-cyclohexyl-3β-hydroxyandrosta-5,16-diene-17-carboxamide (**6**) (CDCl₃, 400 MHz).

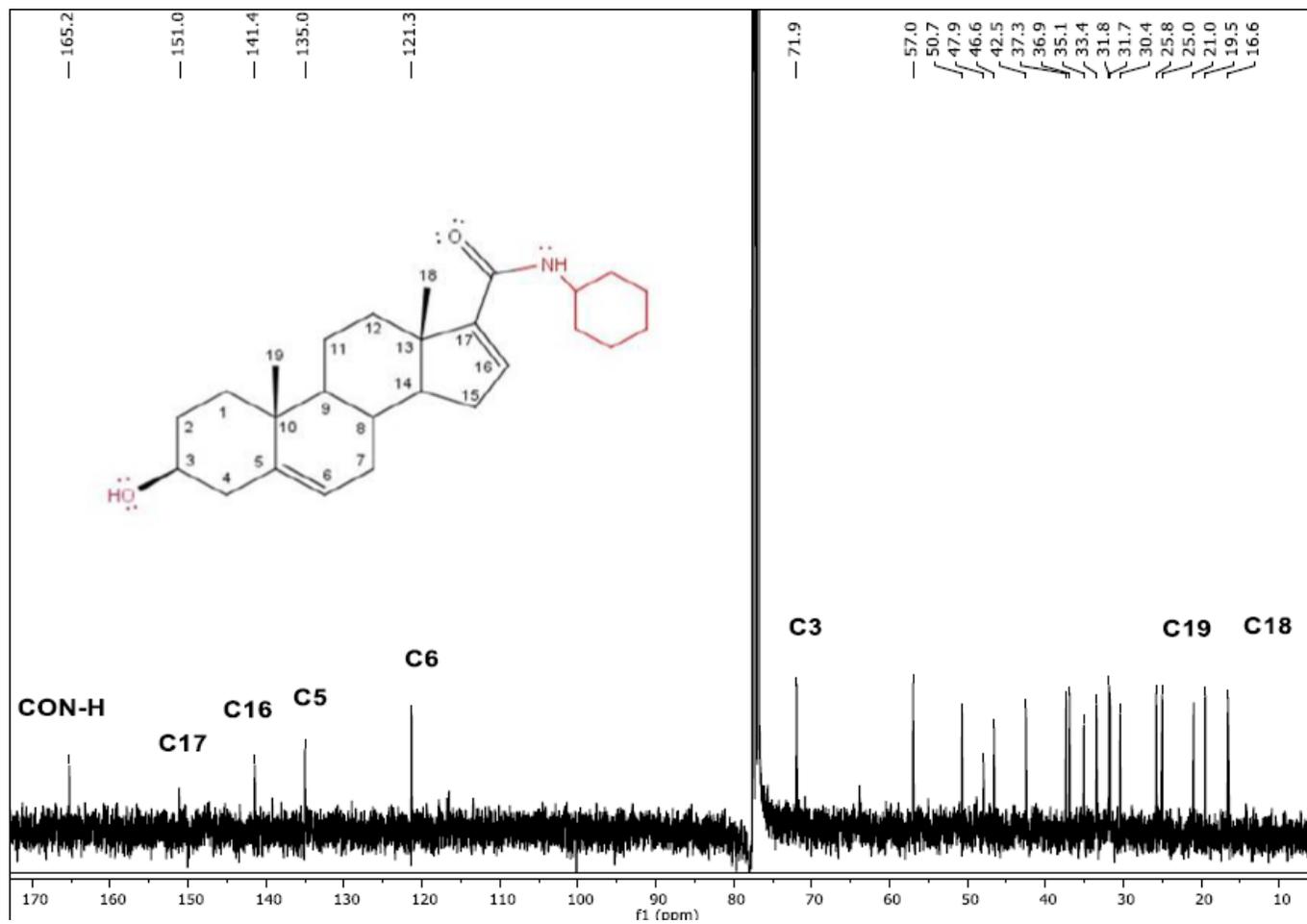


Figure S17. ¹³C NMR spectrum of N-cyclohexyl-3β-hydroxyandrosta-5,16-diene-17-carboxamide (**6**) (CDCl₃, 100 MHz).

Inlet : Direct Ion Mode : FFB+
Spectrum Type : Normal Ion [MF-Linear]
RT : 1.24 min Scan# : (2,8)
BP : m/z 55.0000 Int. : 43.05
Output m/z range : 0.0000 to 436.7953 Cut Level : 0.00 %
537751

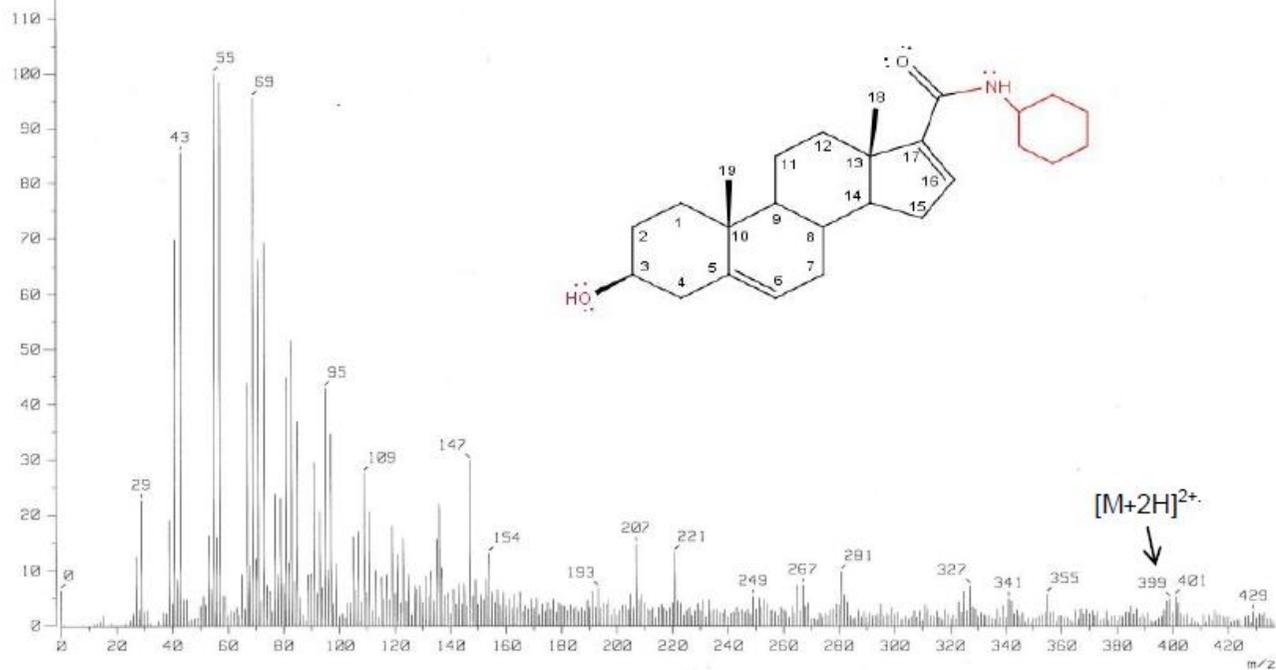


Figure S18. FAB-MS spectrum of N-cyclohexyl-3β-hydroxyandrost-5,16-diene-17-carboxamide (6).

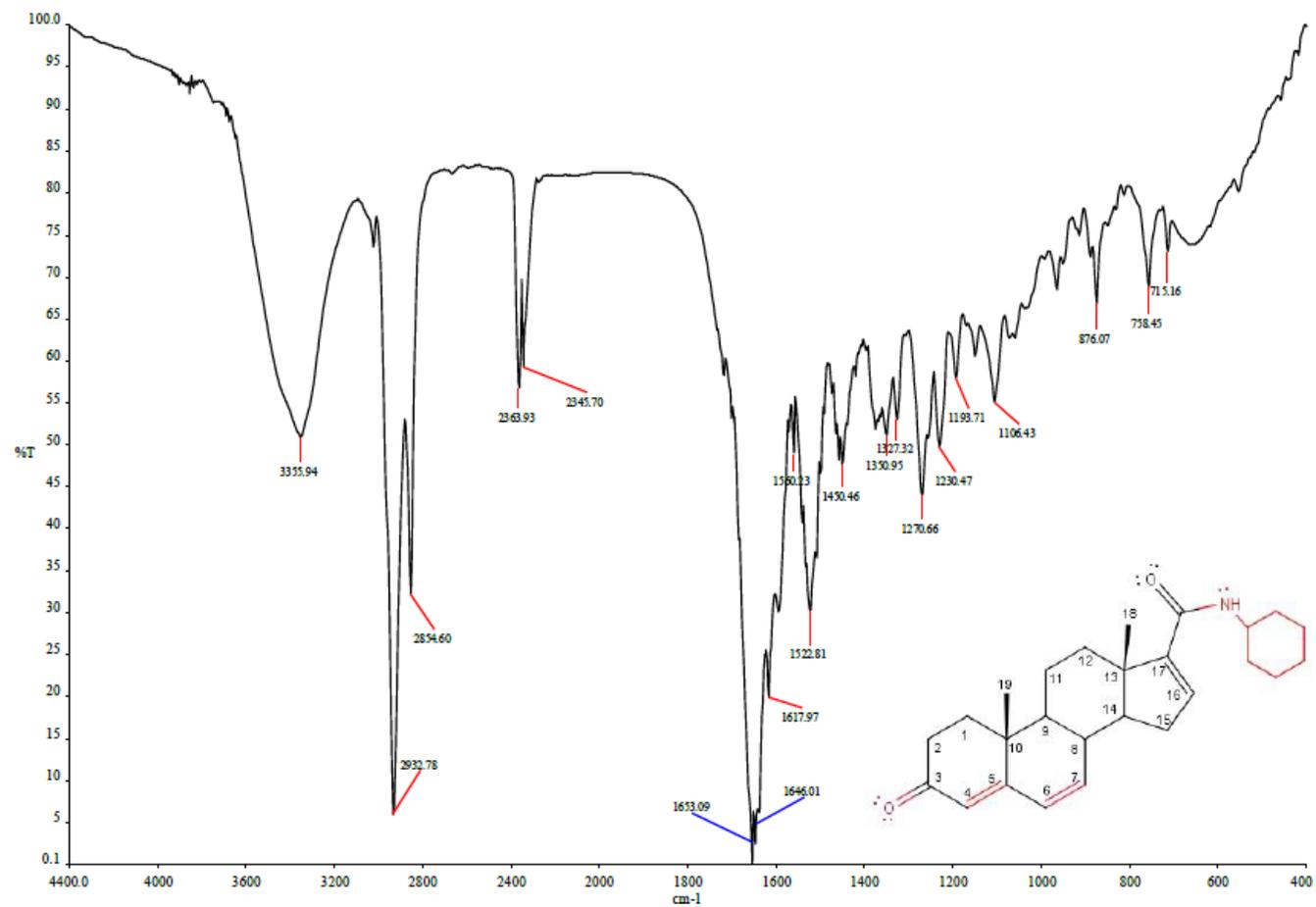


Figure S19. IR (KBr, cm⁻¹) spectrum of N-cyclohexyl-3-oxoandrosta-4,6,16-triene-17-carboxamide (7).

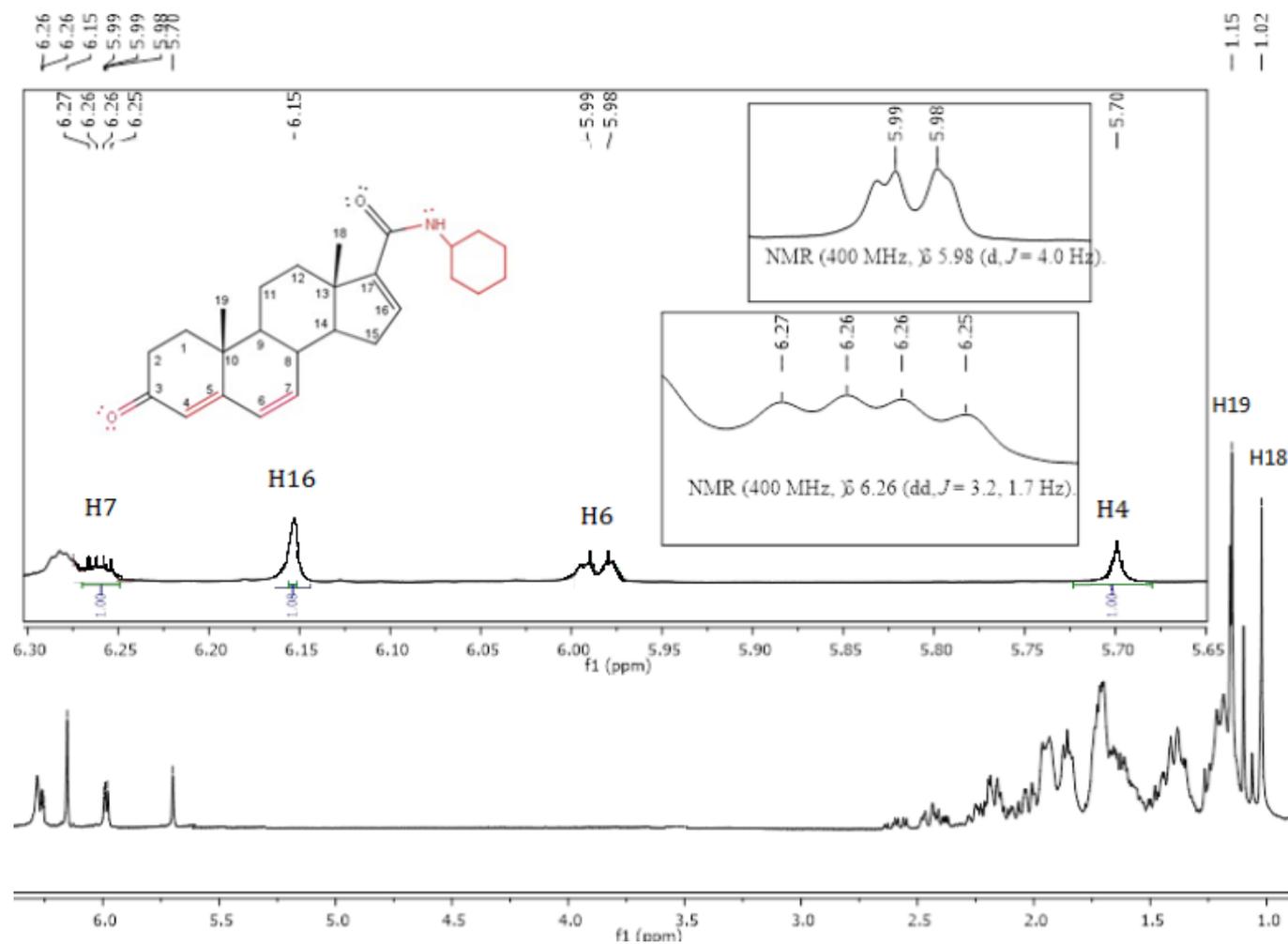


Figure S20. ^1H NMR spectrum of N-cyclohexyl-3-oxoandrosta-4,6,16-triene-17-carboxamide (**7**) (CDCl_3 , 400 MHz).

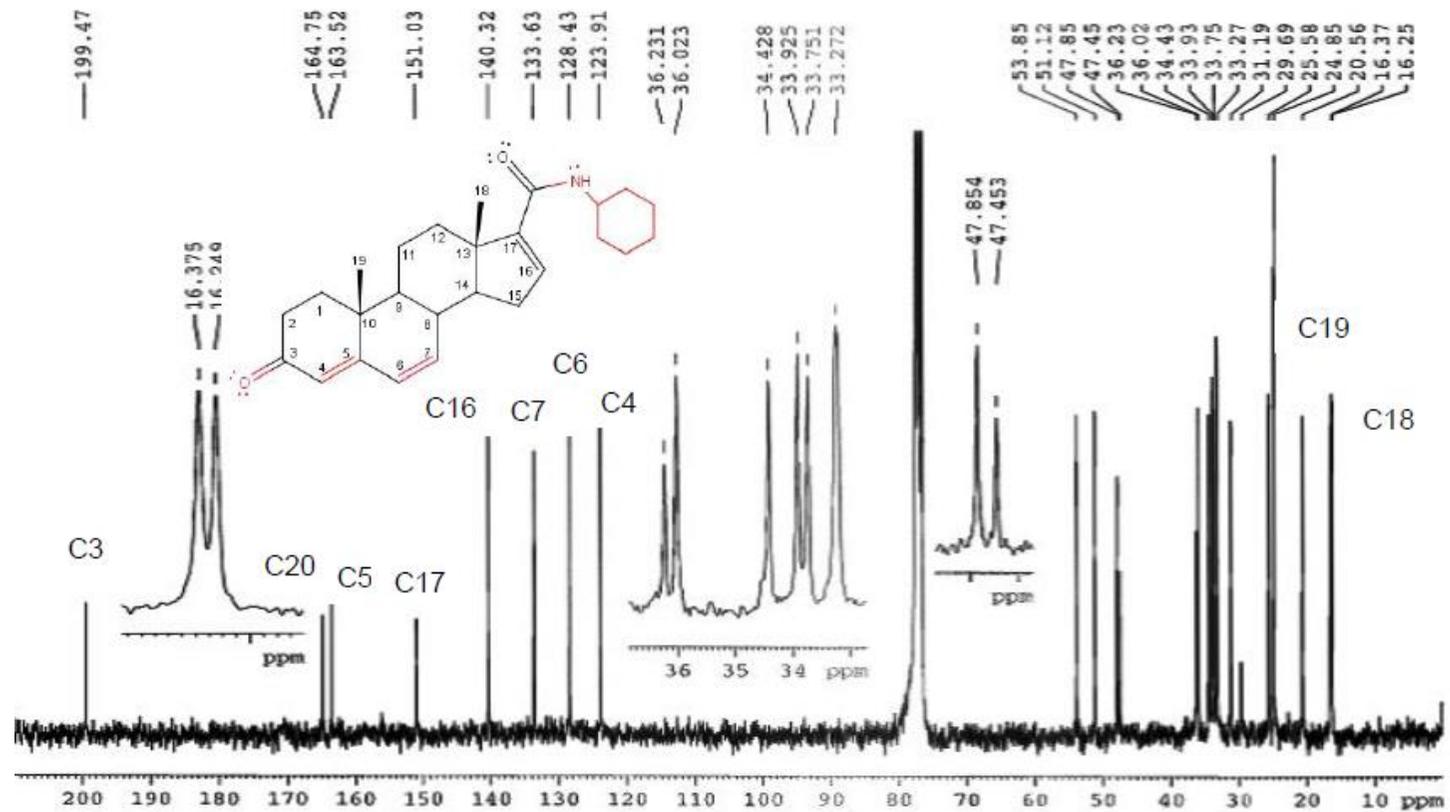


Figure S21. ¹³C NMR spectrum of N-cyclohexyl-3-oxoandrosta-4,6,16-triene-17-carboxamide (7) (CDCl₃, 75 MHz).

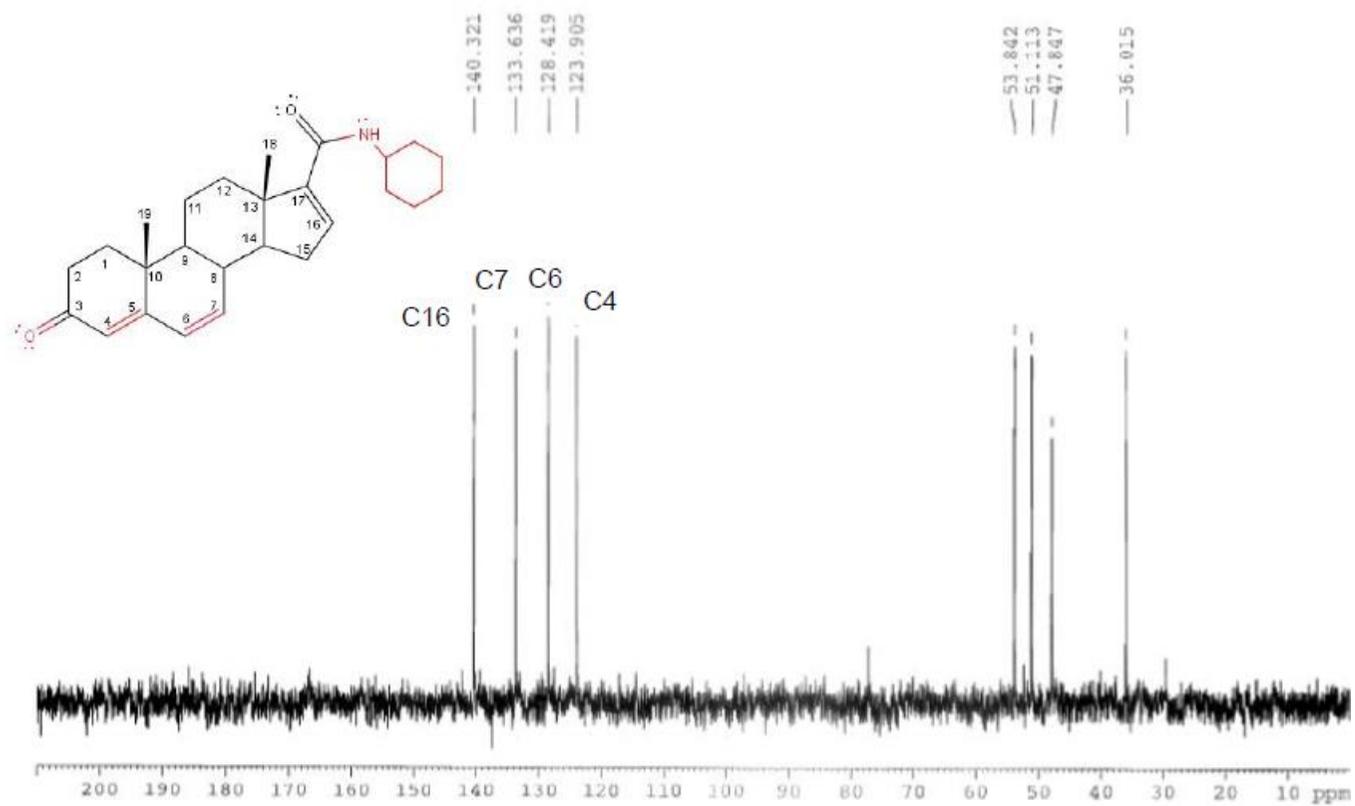


Figure S22. DEPT 90 spectrum of N-cyclohexyl-3-oxoandrosta-4,6,16-triene-17-carboxamide (7).

MS Spectrum

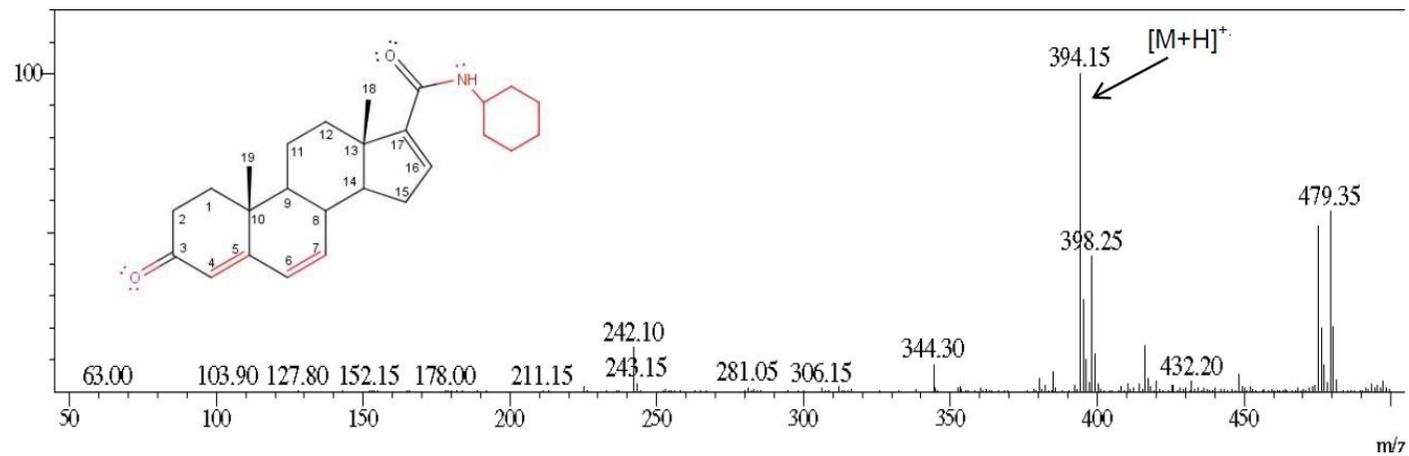


Figure S23. ESI-MS (+) spectrum of N-cyclohexyl-3-oxoandrosta-4,6,16-triene-17-carboxamide (7).

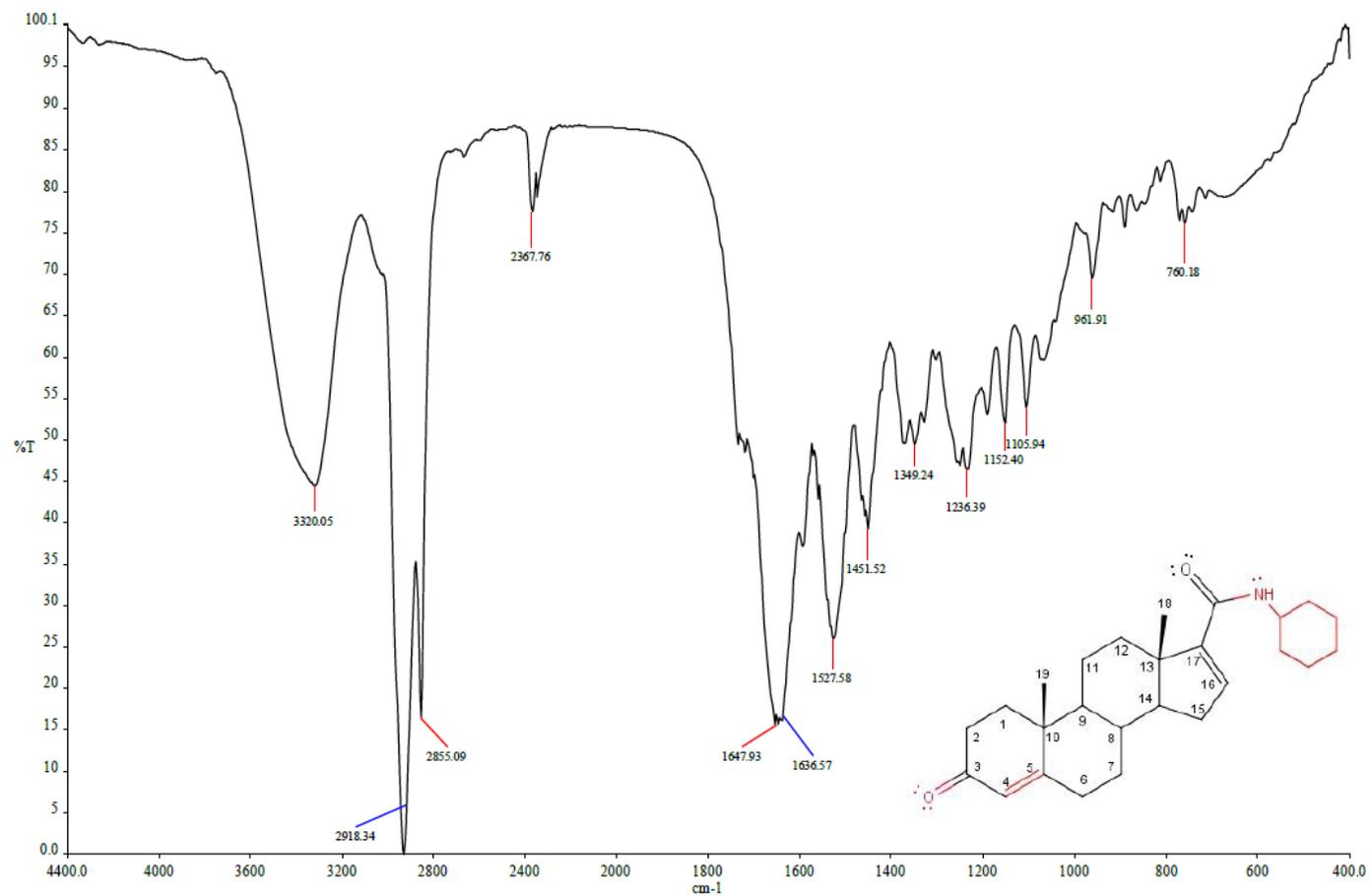


Figure S24. IR (KBr, cm⁻¹) spectrum of N-cyclohexyl-3-oxoandrosta-4,16-diene-17-carboxamide (**8**).

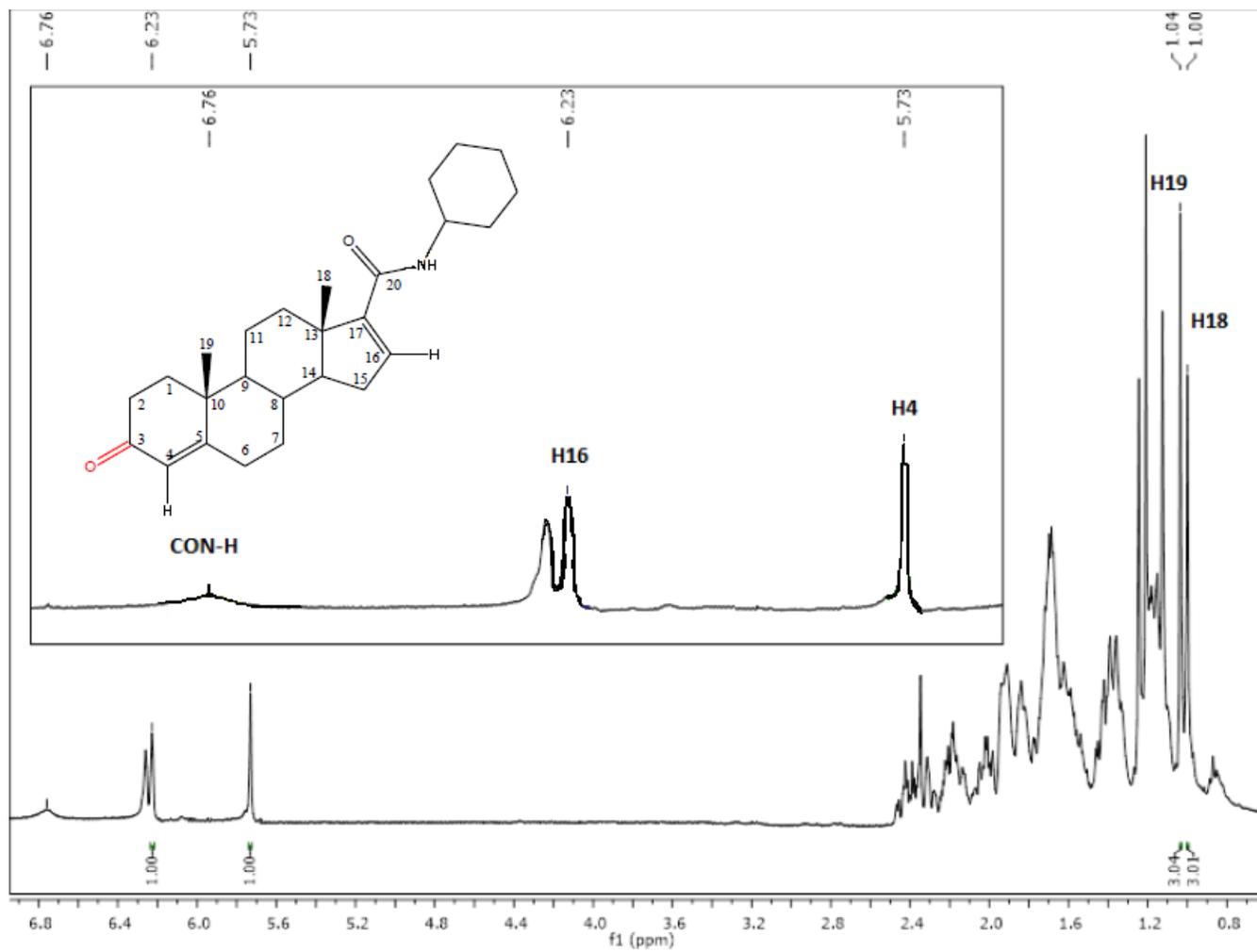


Figure S25. ¹H NMR spectrum of N-cyclohexyl-3-oxoandrosta-4,16-diene-17-carboxamide (**8**) (CDCl₃, 400 MHz).

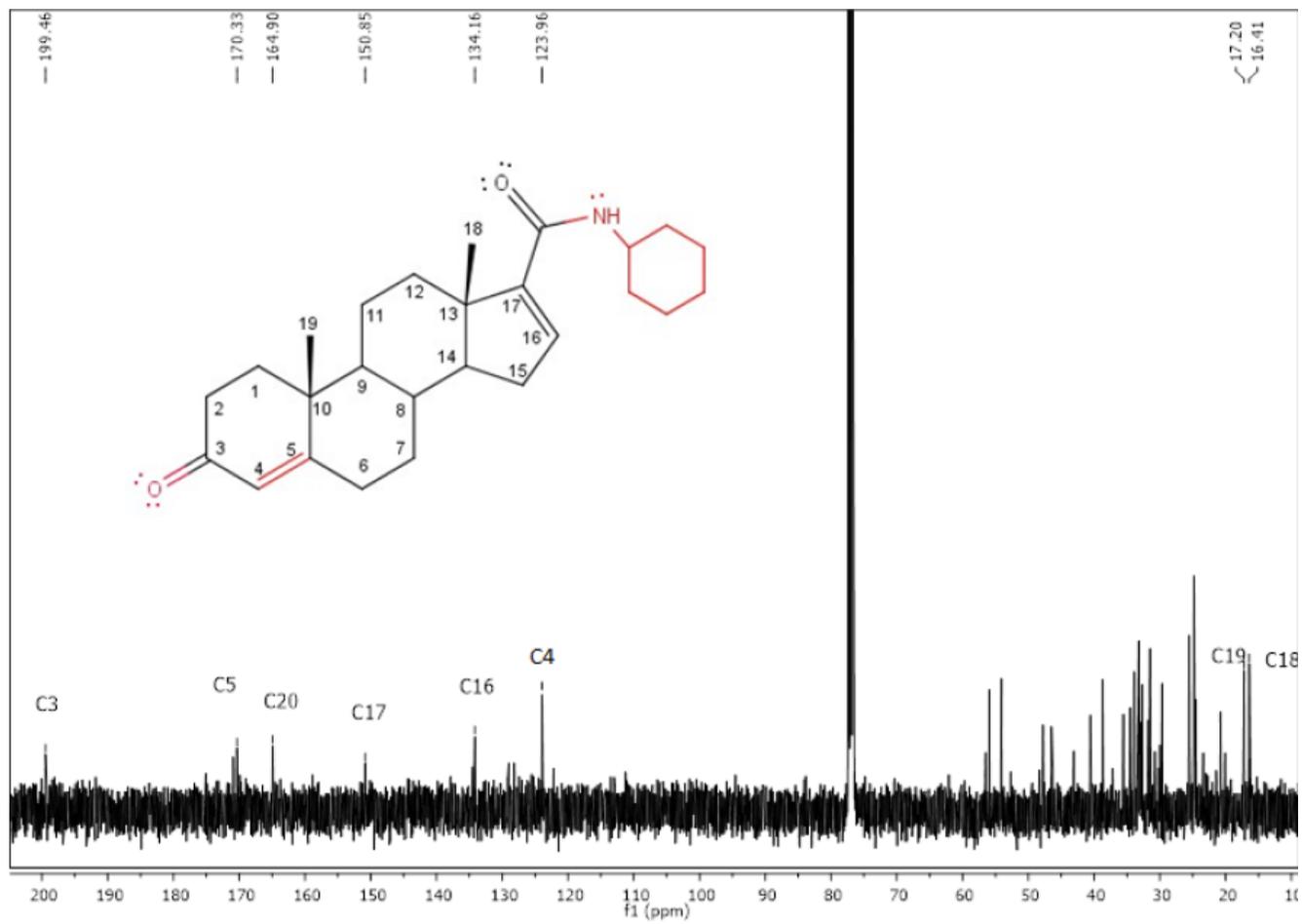


Figure S26. ^{13}C NMR spectrum of N-cyclohexyl-3-oxoandrosta-4,16-diene-17-carboxamide (**8**) (CDCl₃, 75 MHz).

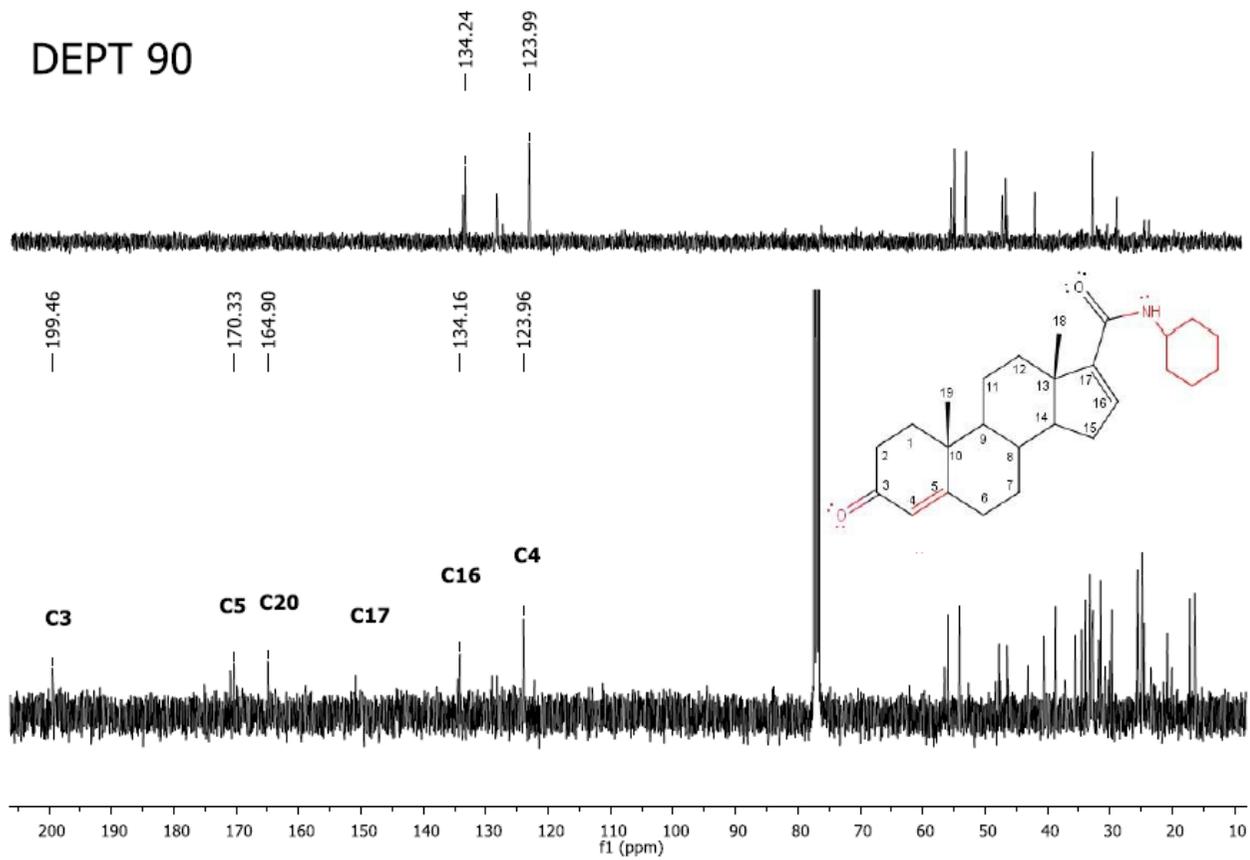


Figure S27. DEPT 90 spectrum of N-cyclohexyl-3-oxoandrosta-4,16-diene-17-carboxamide (**8**).

MS Spectrum

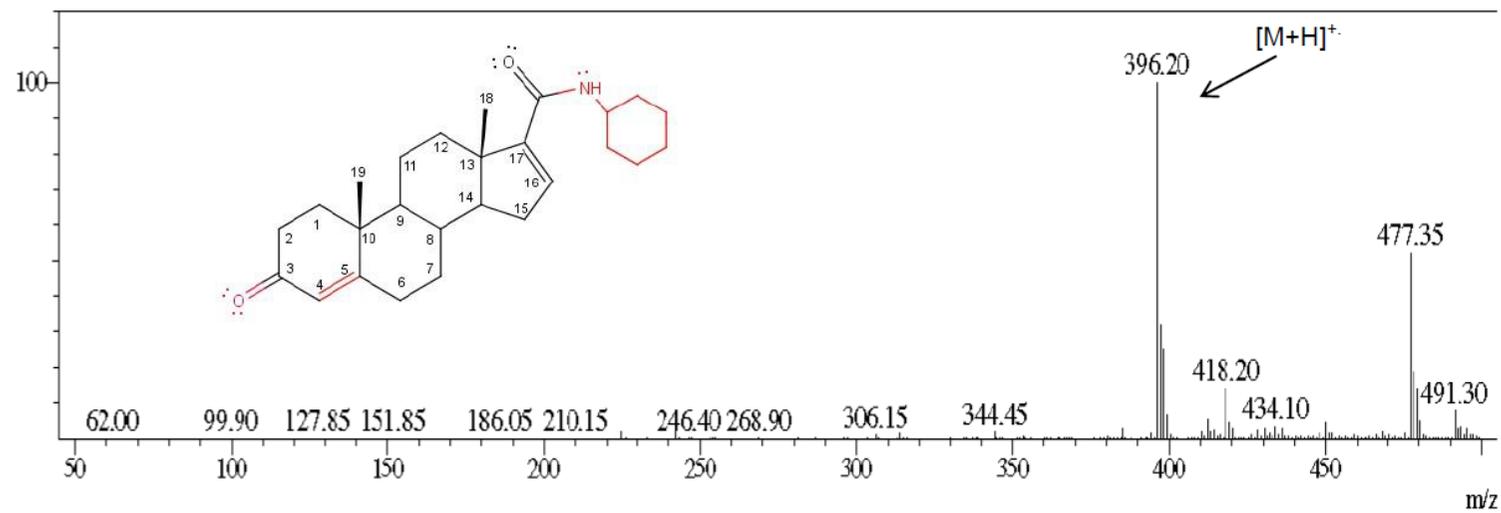


Figure S28. ESI-MS spectrum of N-cyclohexyl-3-oxoandrosta-4,16-diene-17-carboxamide (**8**).

