

# Novel 4-Azapregnene Derivatives as Potential Anticancer Agents: Synthesis, Antiproliferative Activity and Molecular Docking Studies

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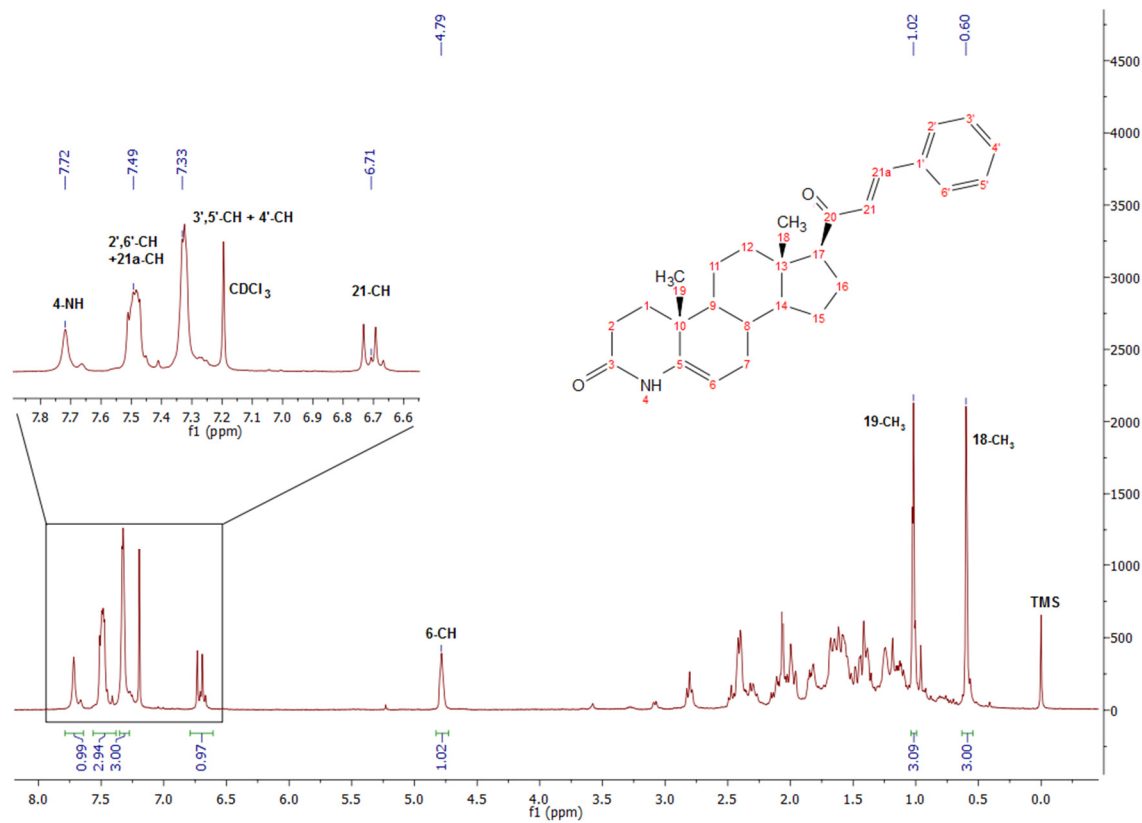
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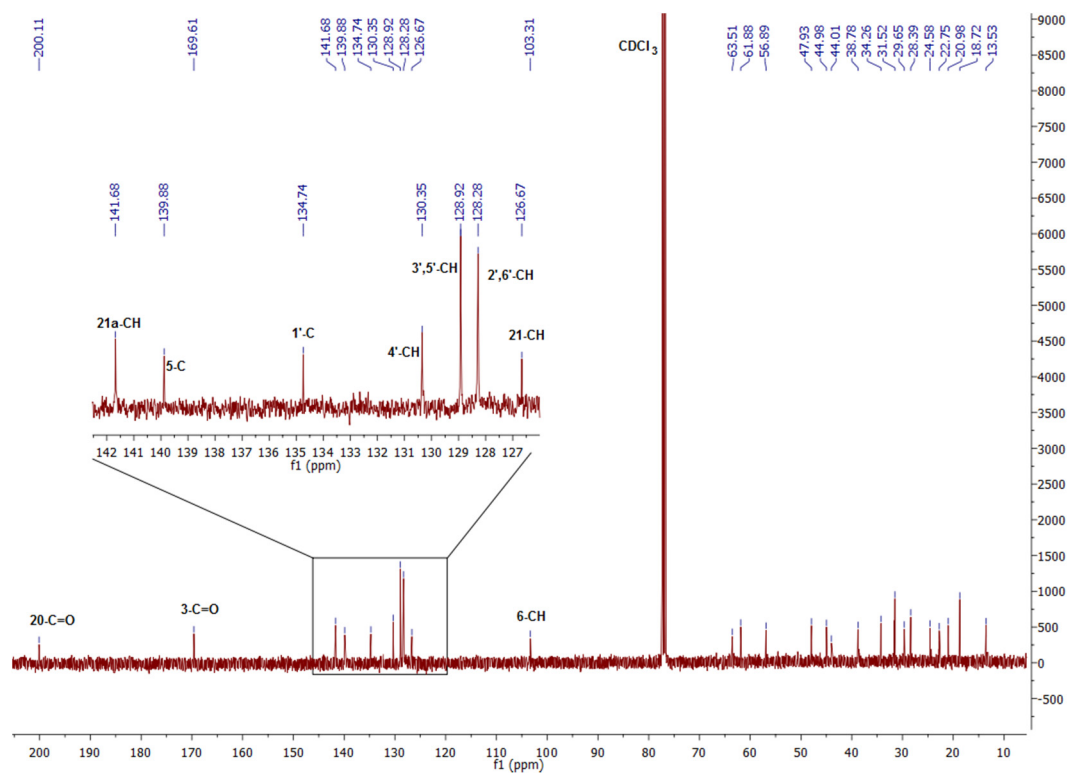
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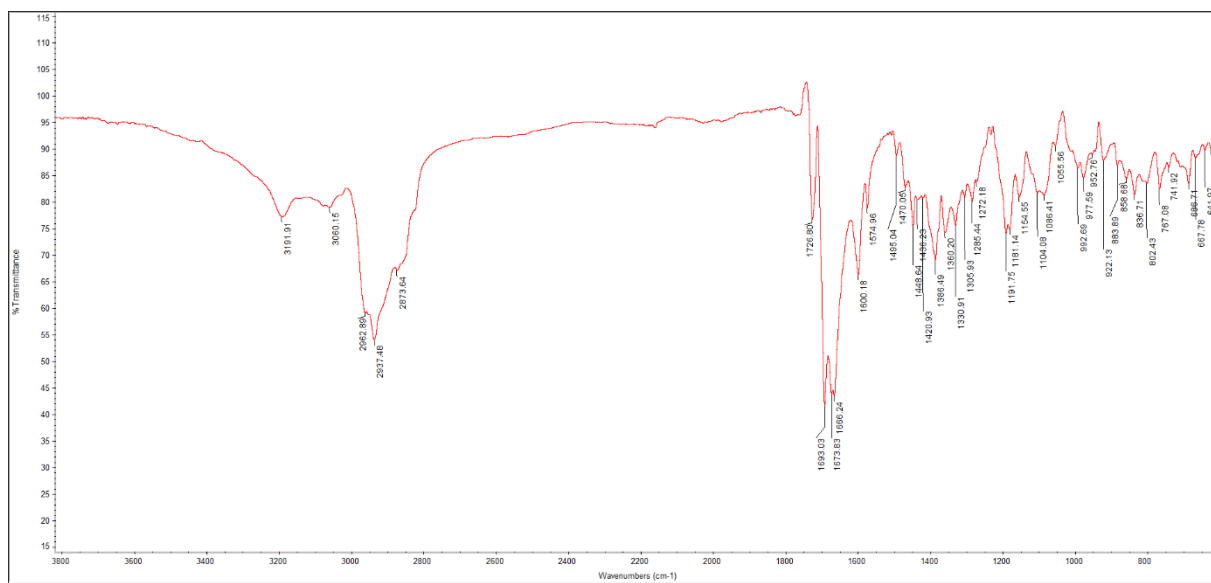
# <sup>1</sup>H NMR spectrum of compound 3a



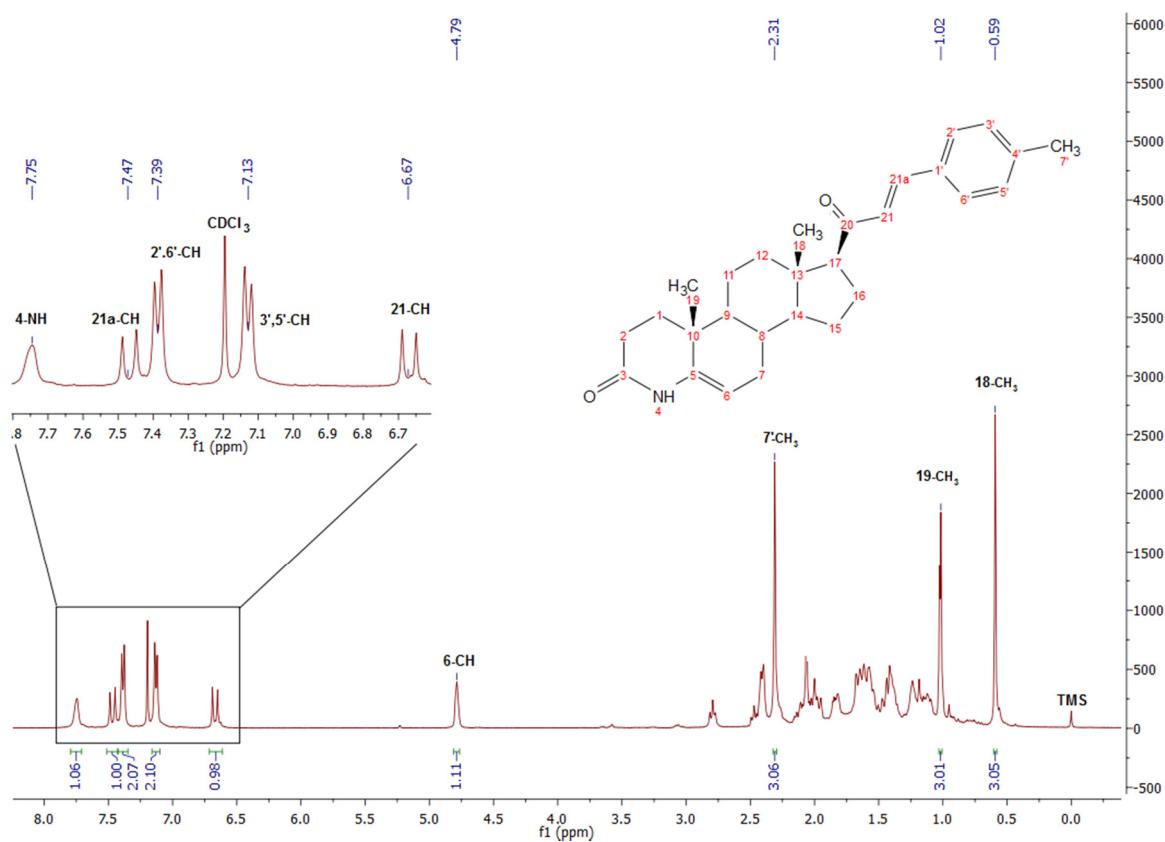
# <sup>13</sup>C NMR spectrum of compound 3a



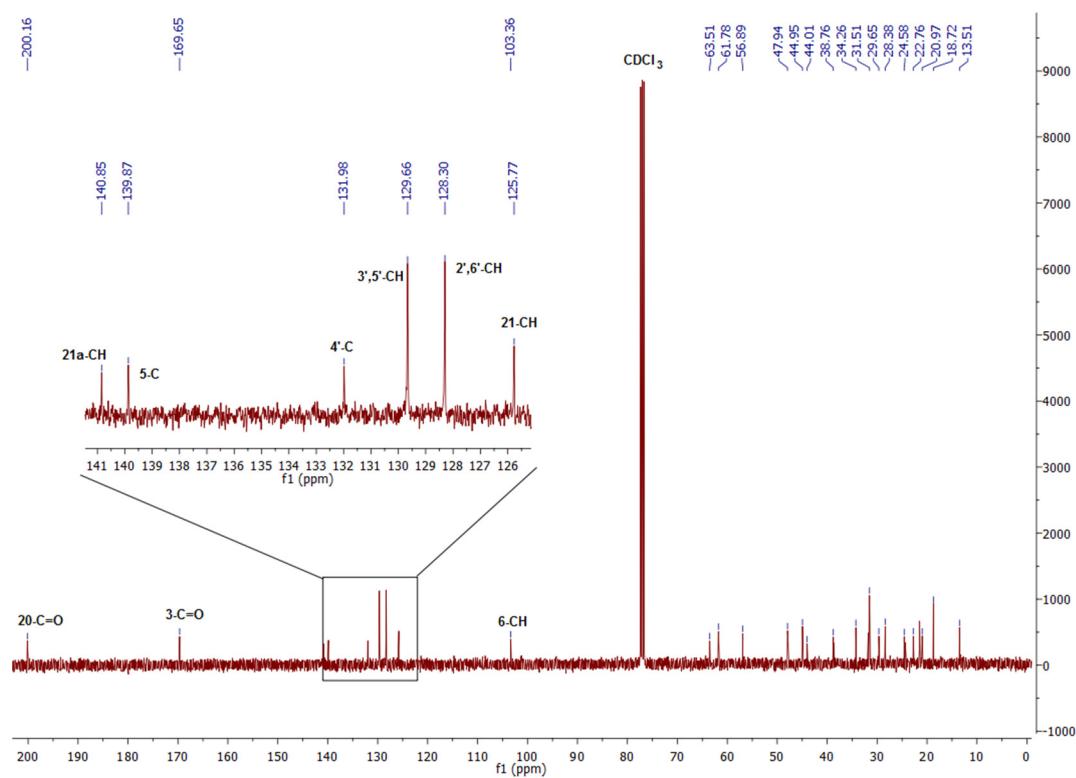
## IR spectrum of compound 3a



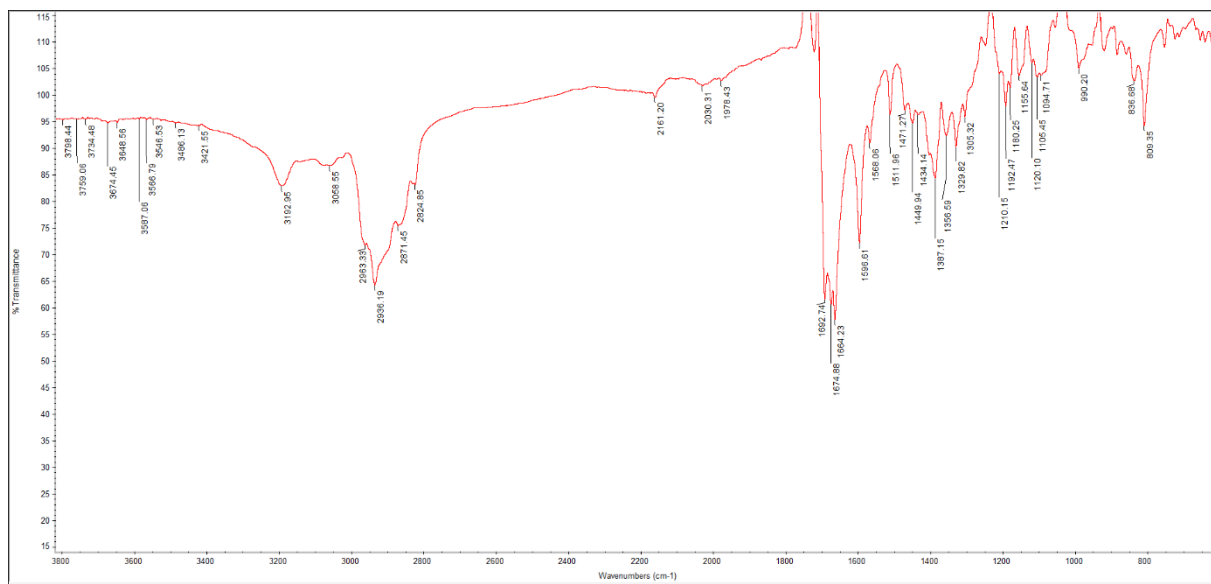
# <sup>1</sup>H NMR spectrum of compound 3b



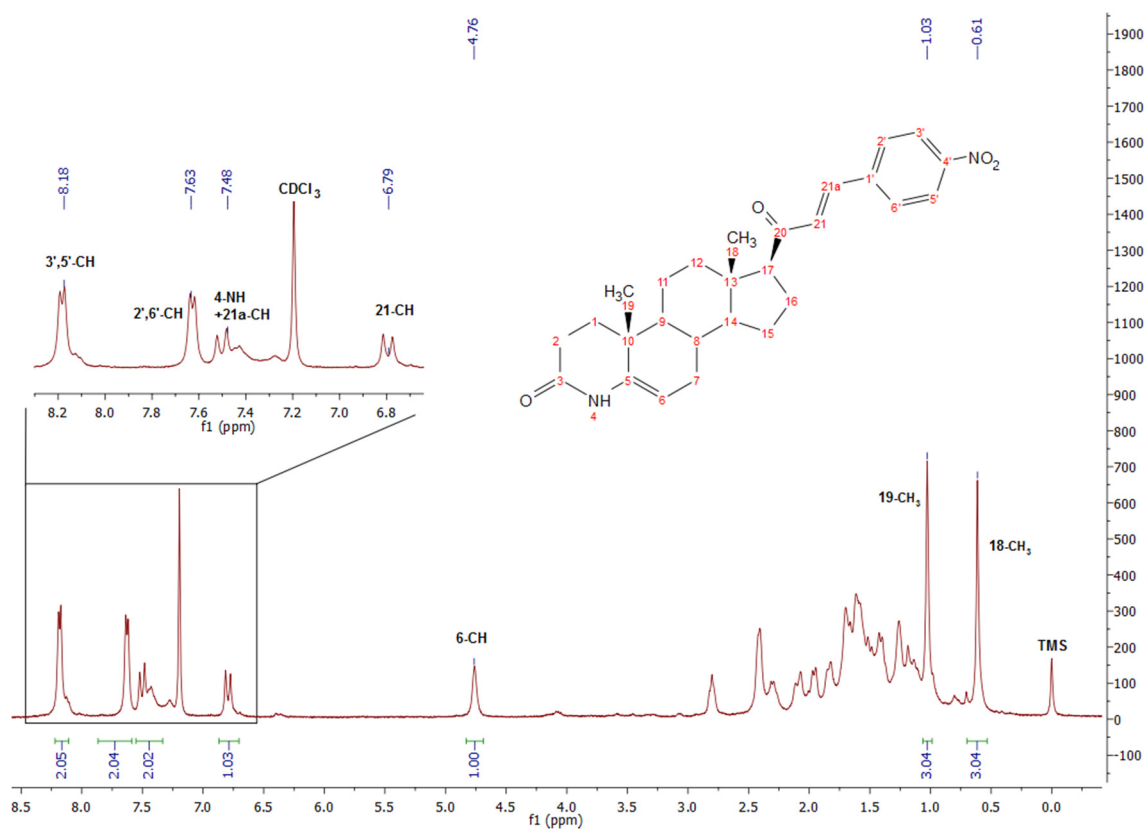
# <sup>13</sup>C NMR spectrum of compound 3b



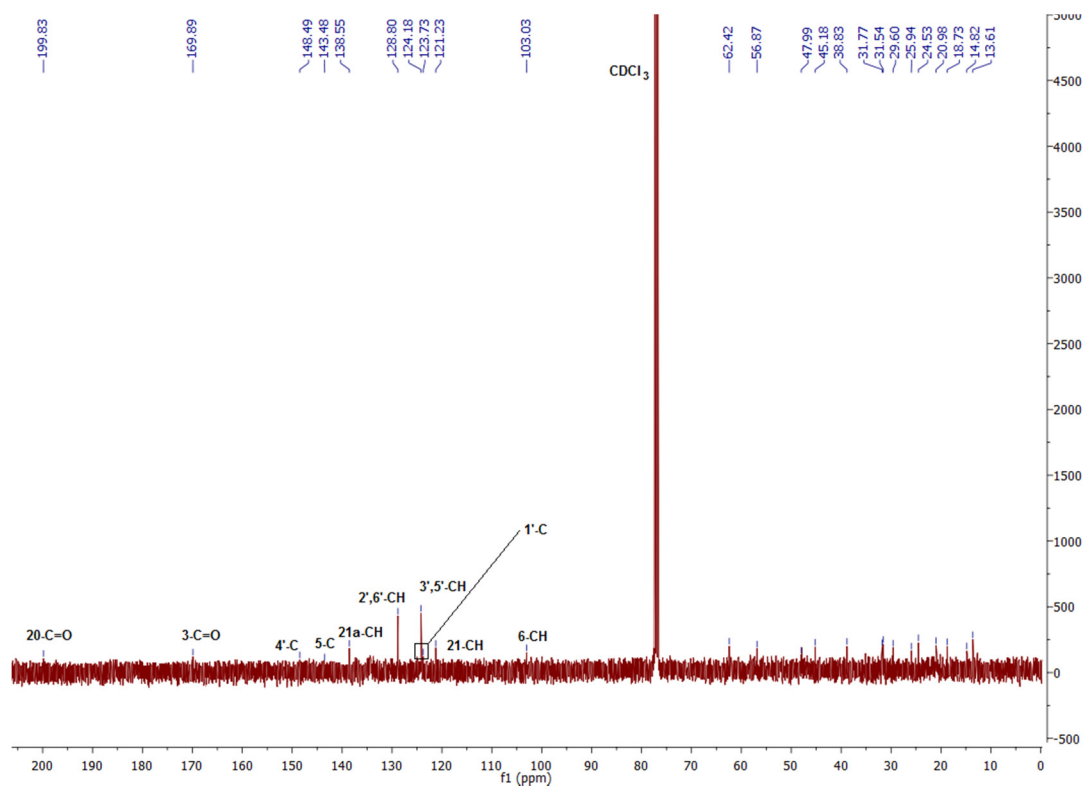
## IR spectrum of compound 3b



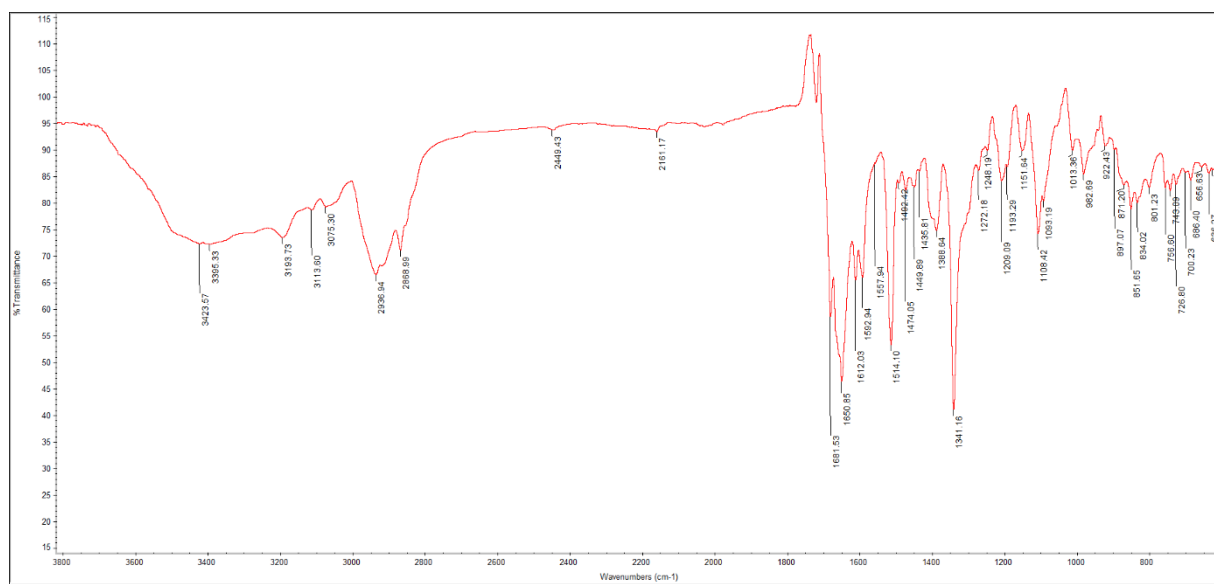
# <sup>1</sup>H NMR spectrum of compound 3c



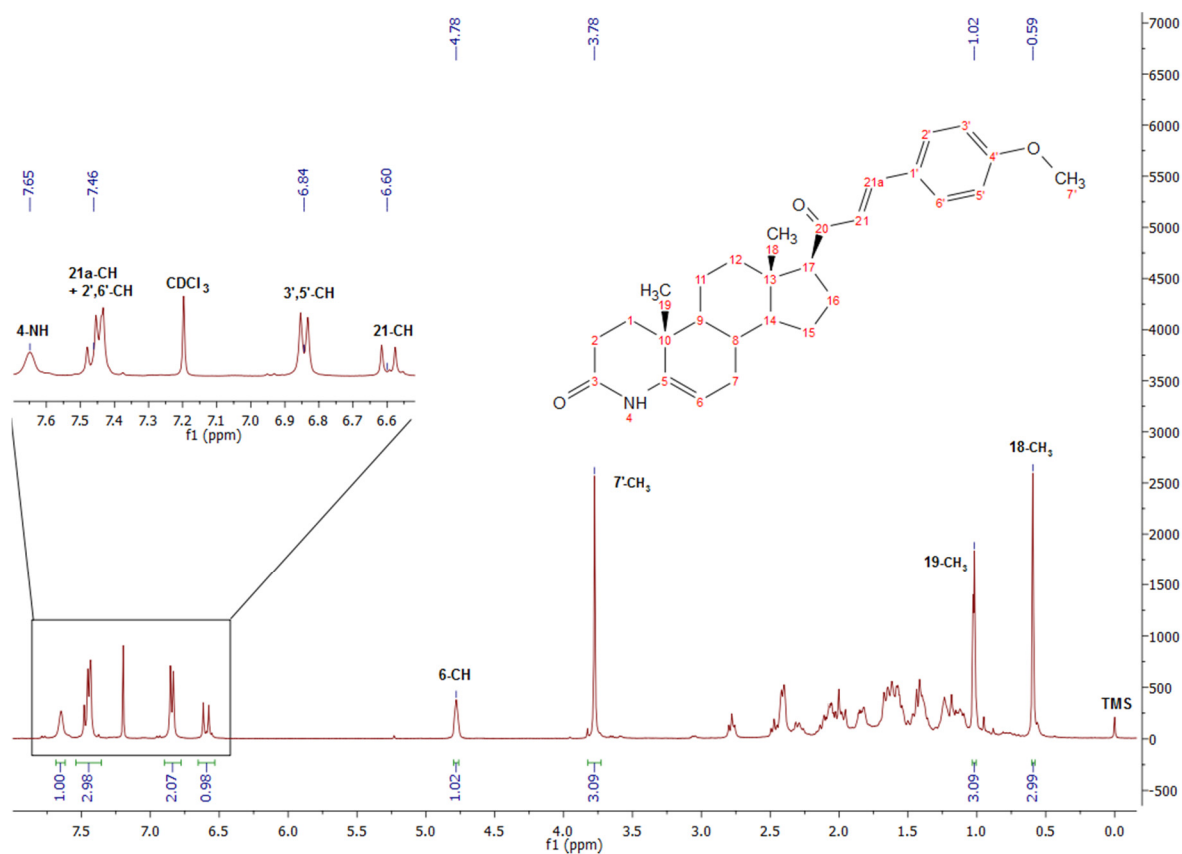
# <sup>13</sup>C NMR spectrum of compound 3c



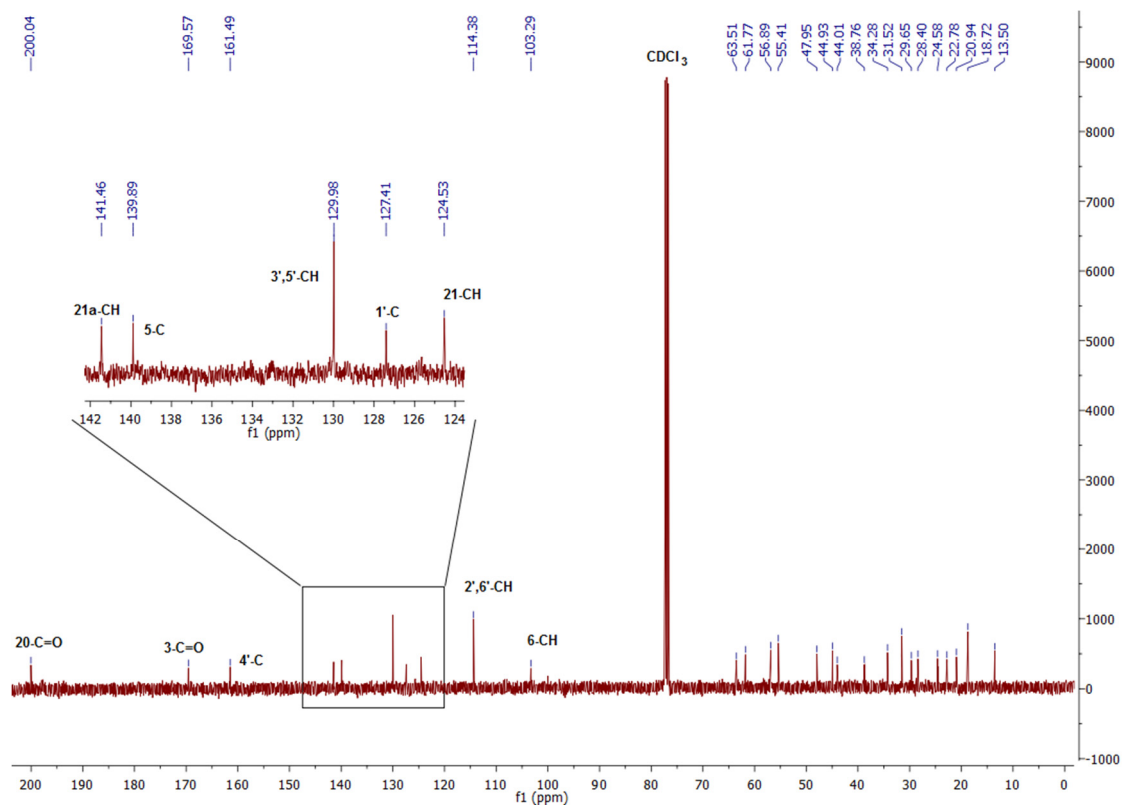
## IR spectrum of compound 3c



# <sup>1</sup>H NMR spectrum of compound 3d

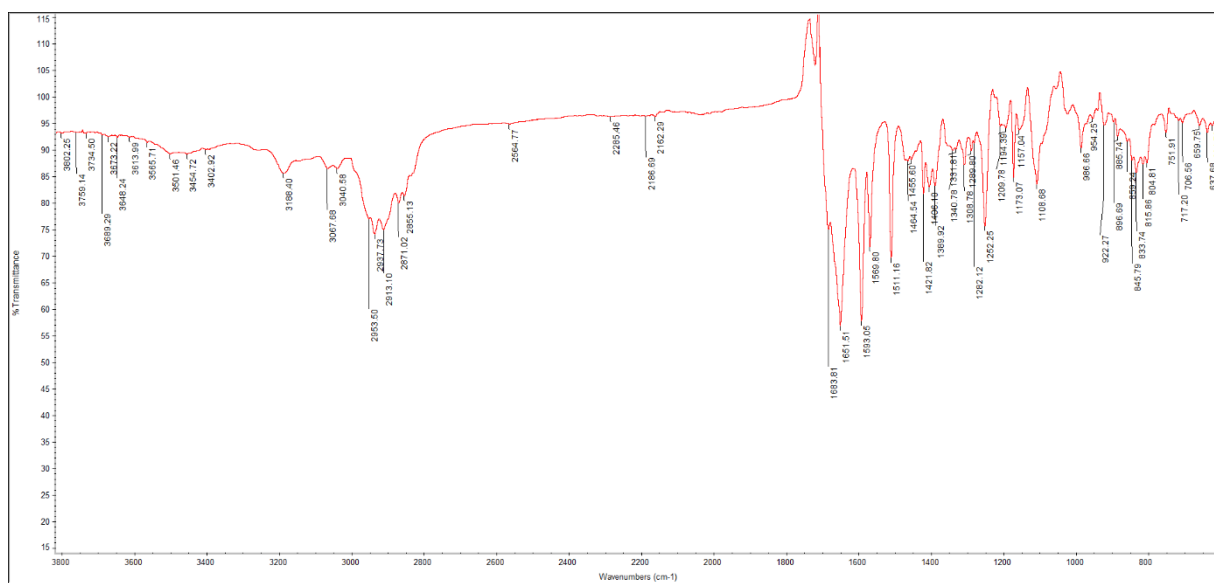


# <sup>13</sup>C NMR spectrum of compound 3d

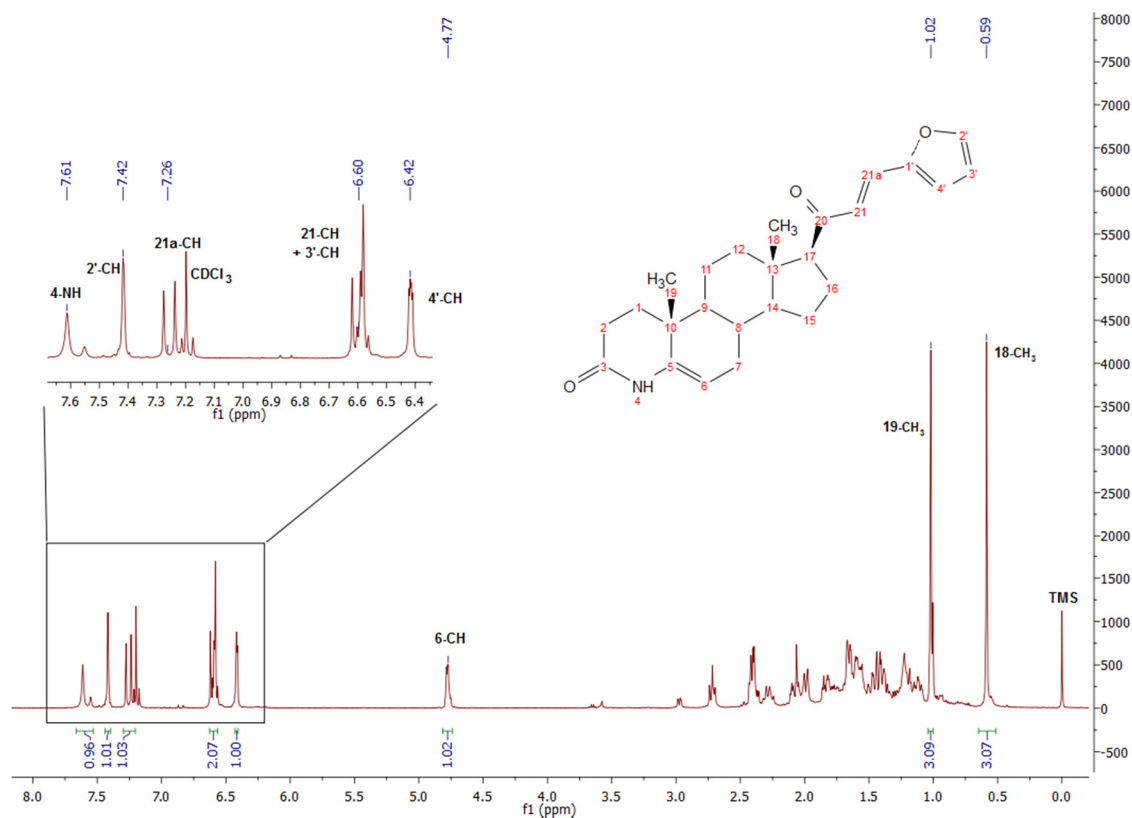




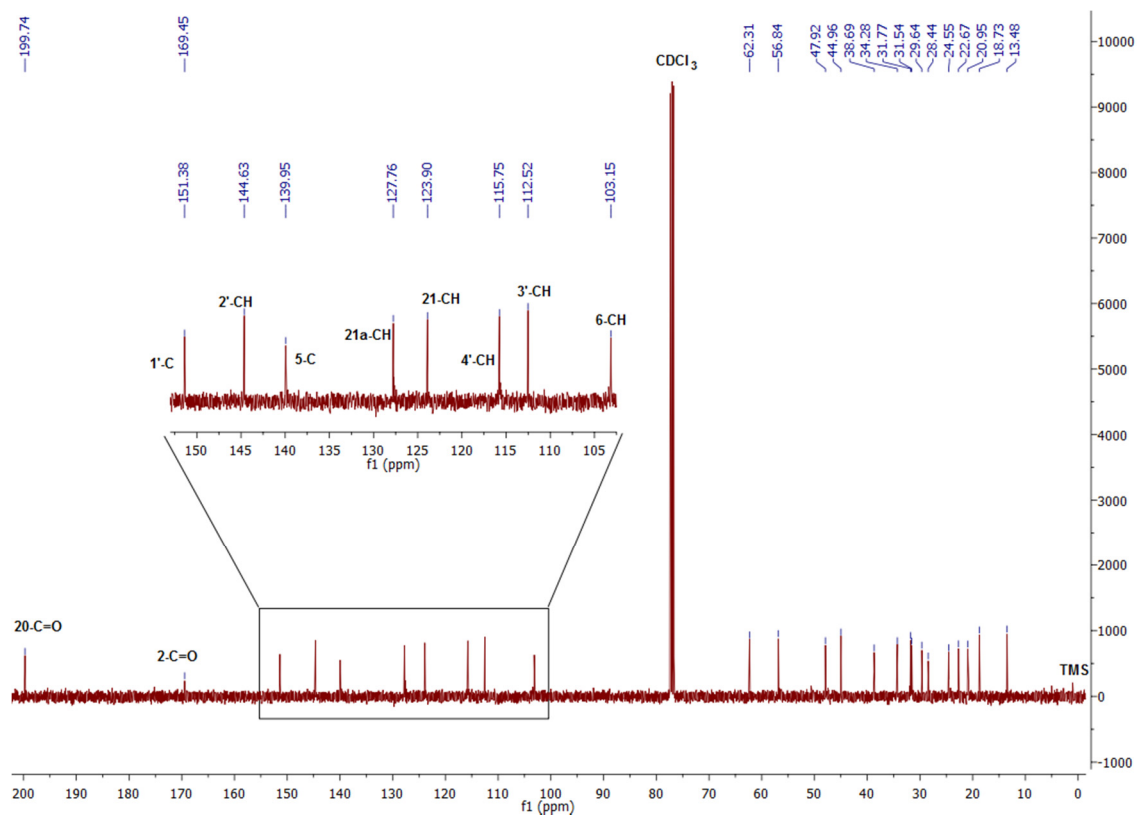
## IR spectrum of compound 3d



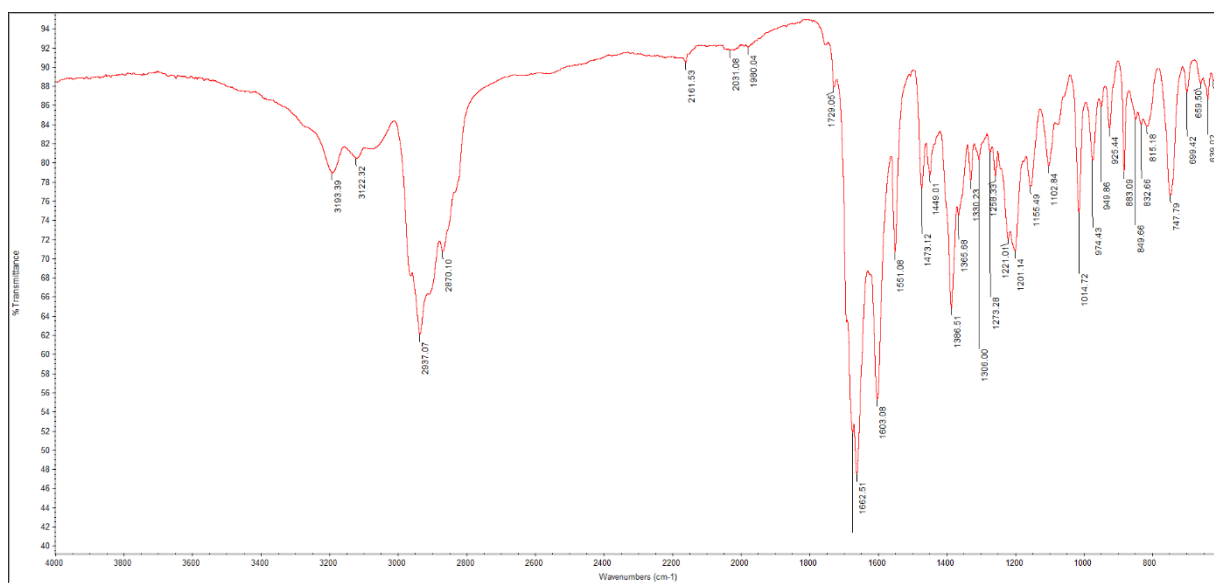
# <sup>1</sup>H NMR spectrum of compound 3e



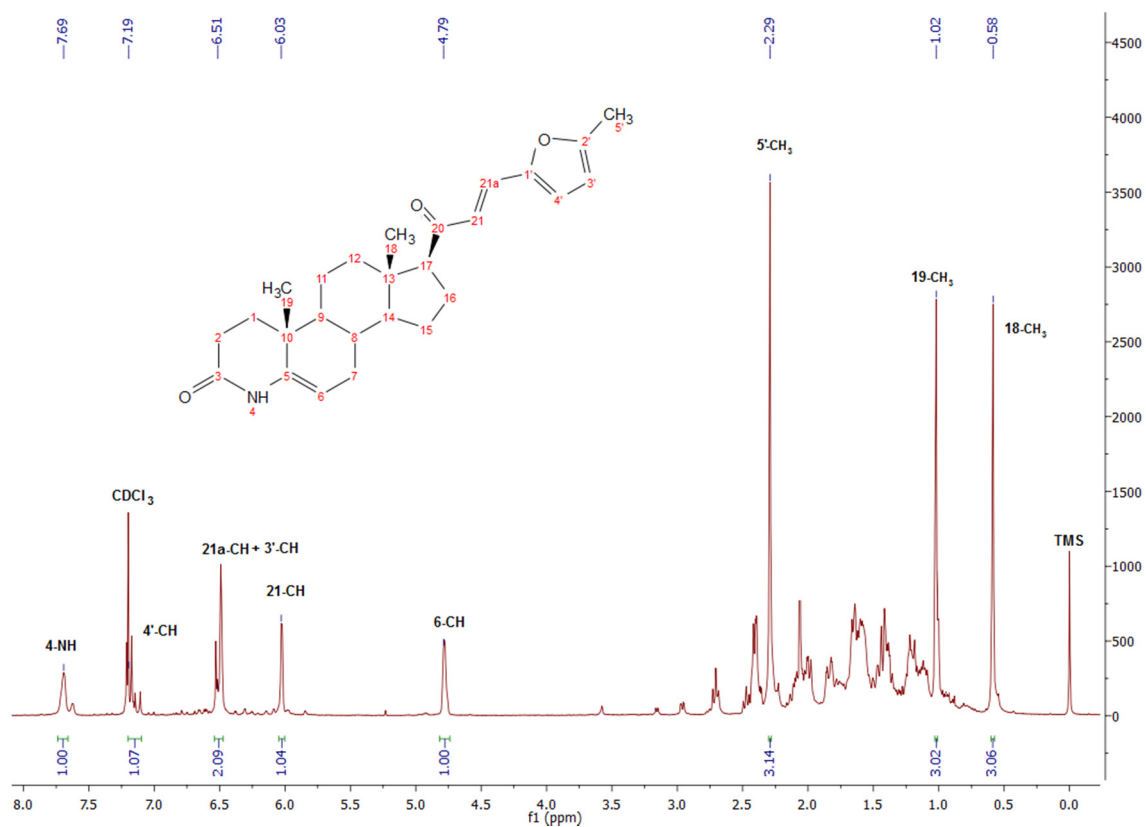
# <sup>13</sup>C NMR spectrum of compound 3e



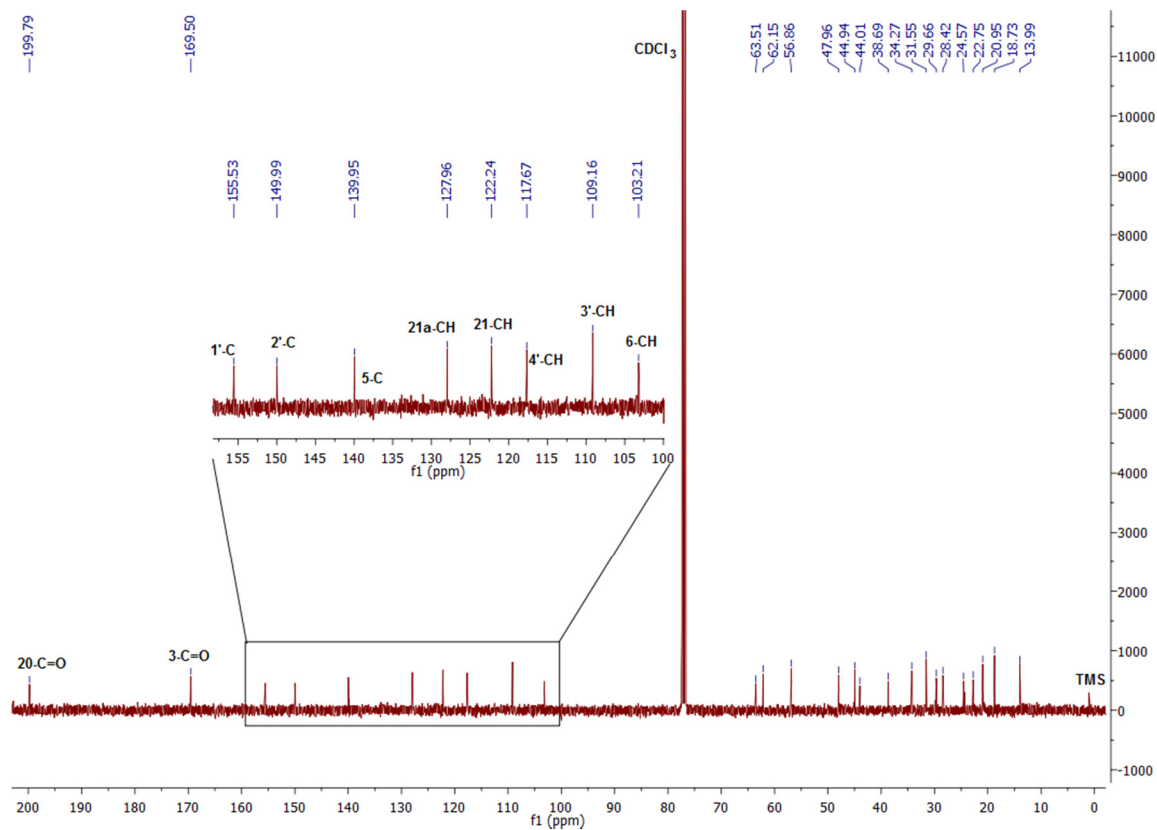
### IR spectrum of compound 3e



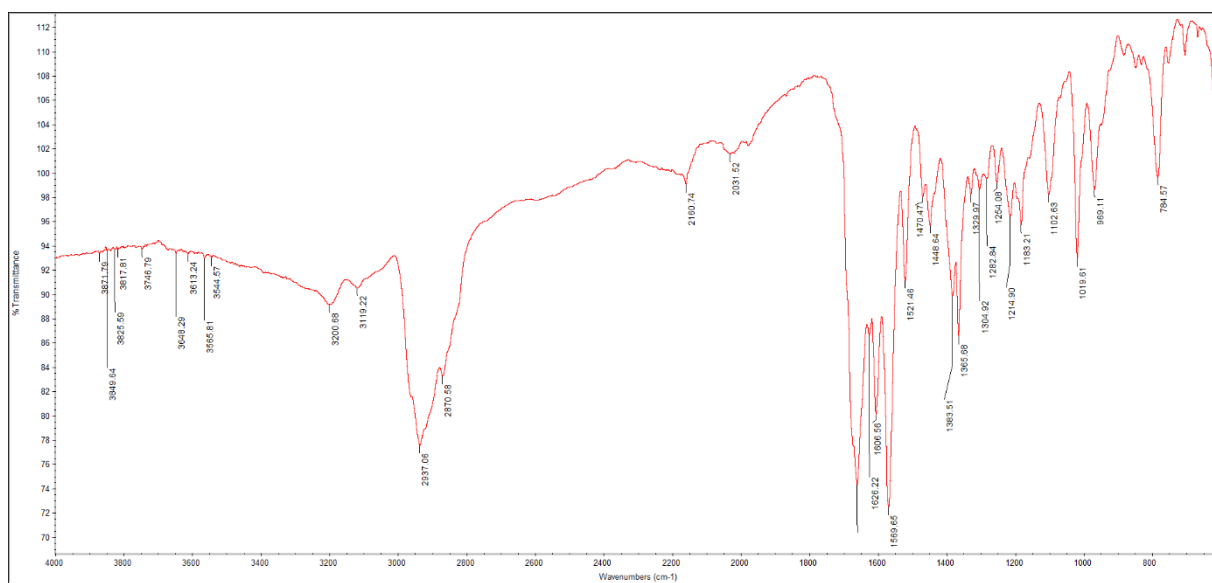
# <sup>1</sup>H NMR spectrum of compound 3f



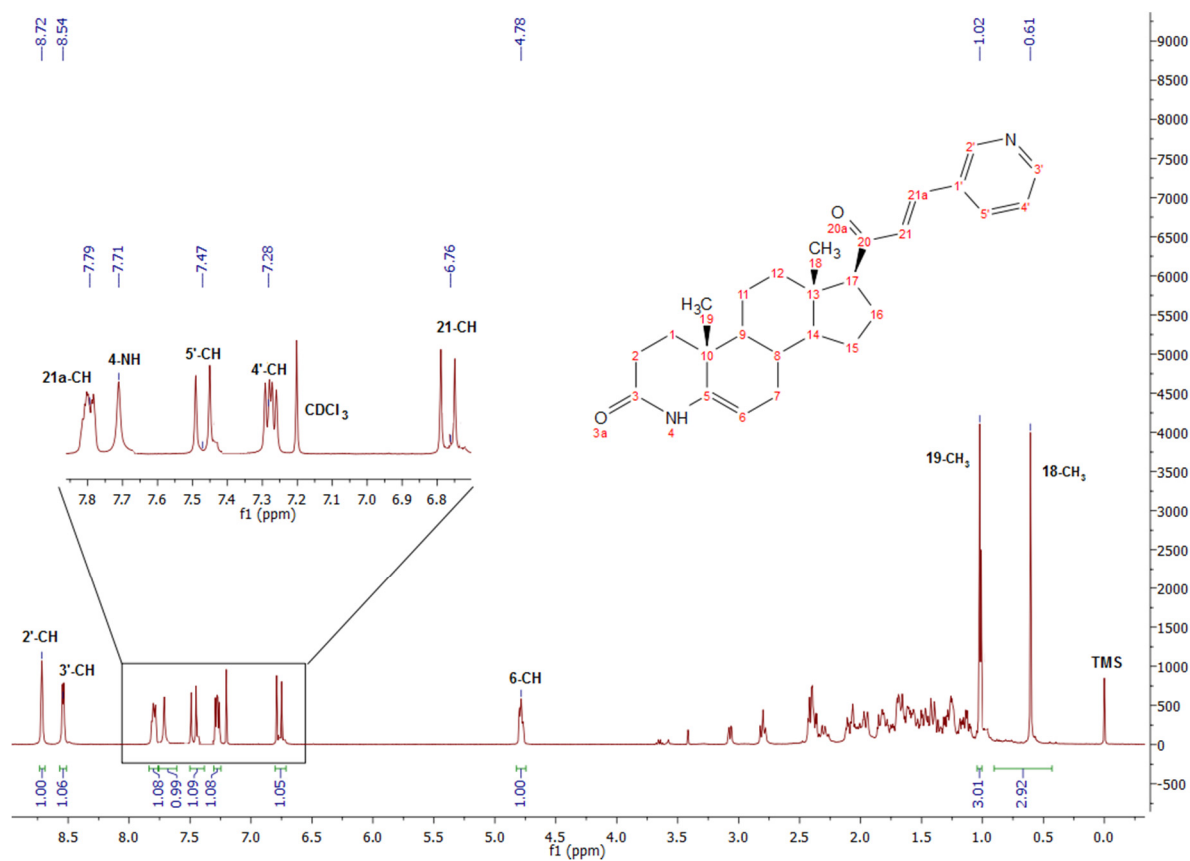
# <sup>13</sup>C NMR spectrum of compound 3f



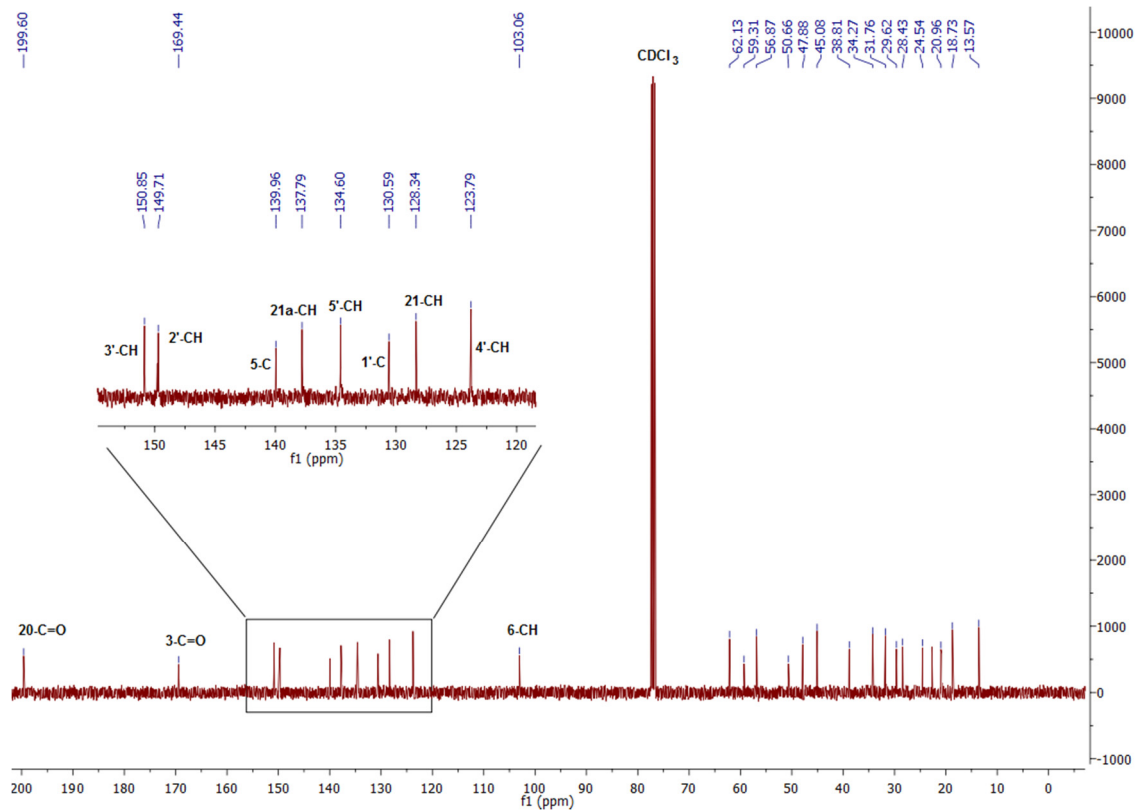
# IR spectrum of compound 3f



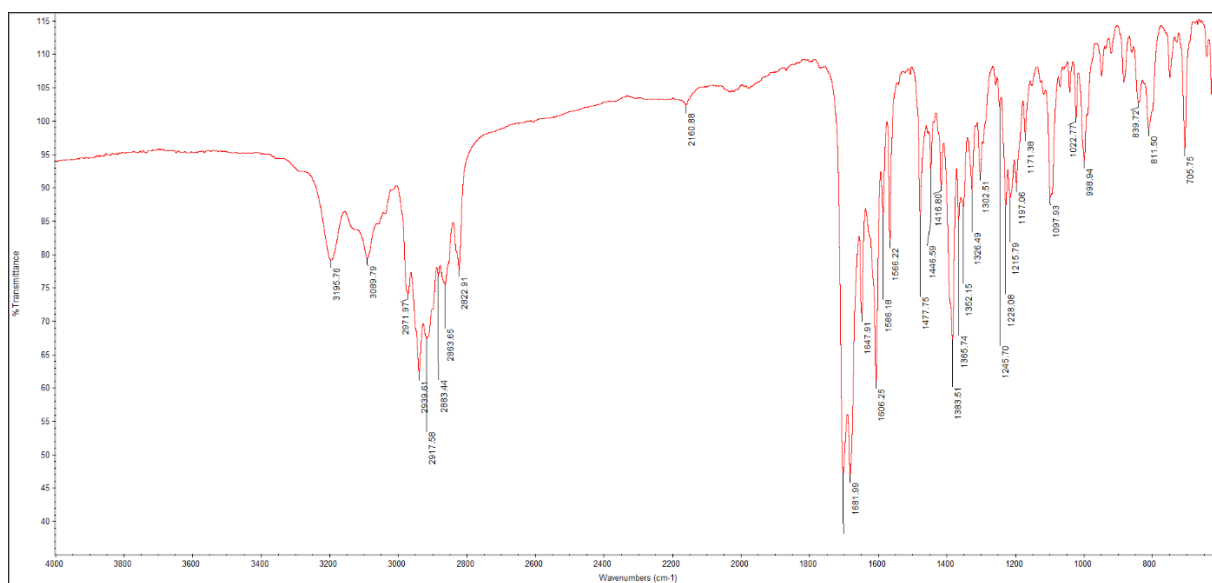
# <sup>1</sup>H NMR spectrum of compound 3g



# <sup>13</sup>C NMR spectrum of compound 3g



### IR spectrum of compound 3g



## S2. Flow cytometry additional data

Contour plots of flow cytometry assay with propidium iodide staining (for each FACS tube), in LNCaP cells after 24 and 72h of exposition to 50  $\mu$ M of steroid **3g** and finasteride (and respective controls).

