

## Supplementary materials

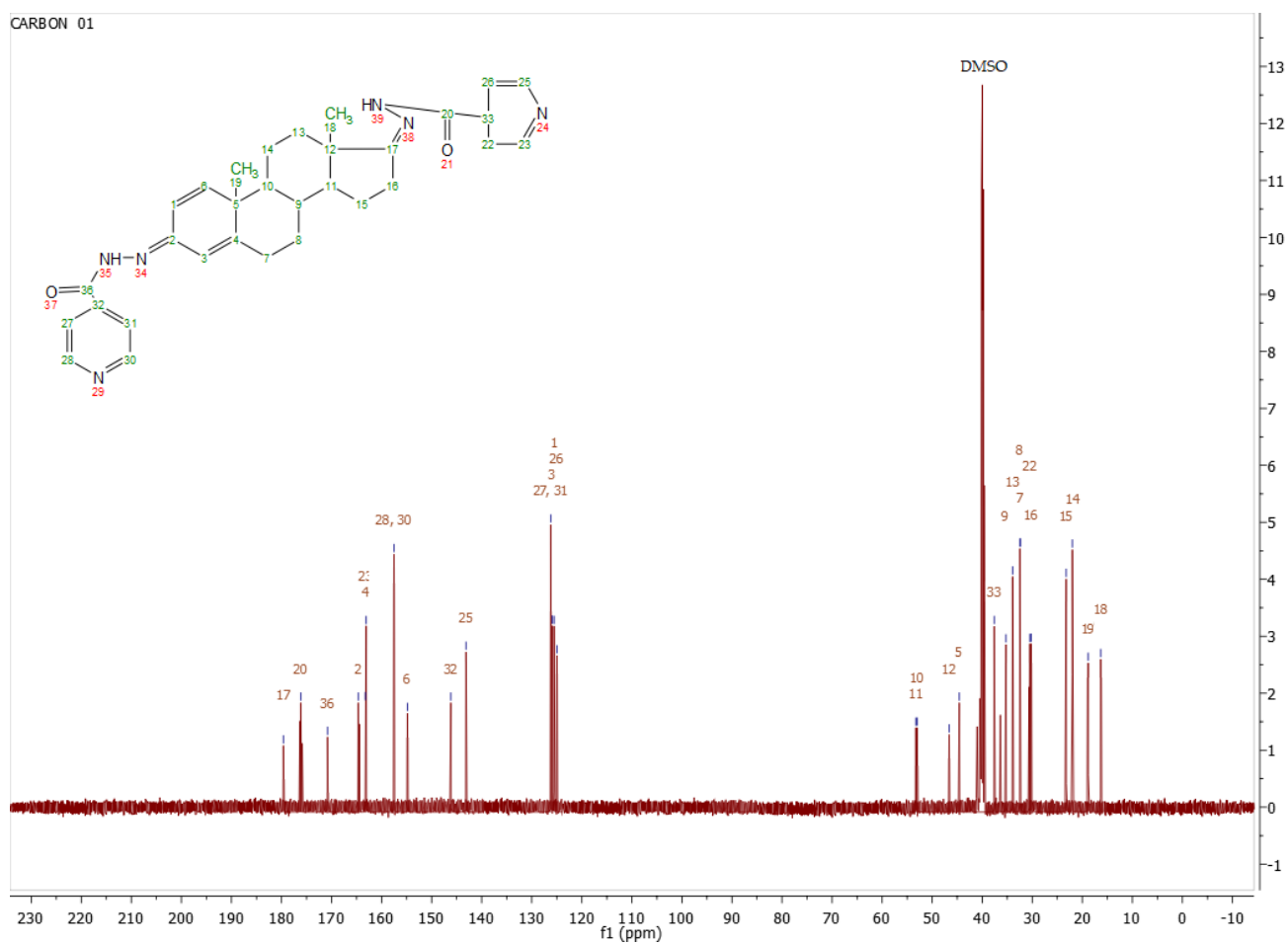


Figure S1:  $^{13}\text{C}$  NMR spectrum of compound 1 in DMSO- $d_6$

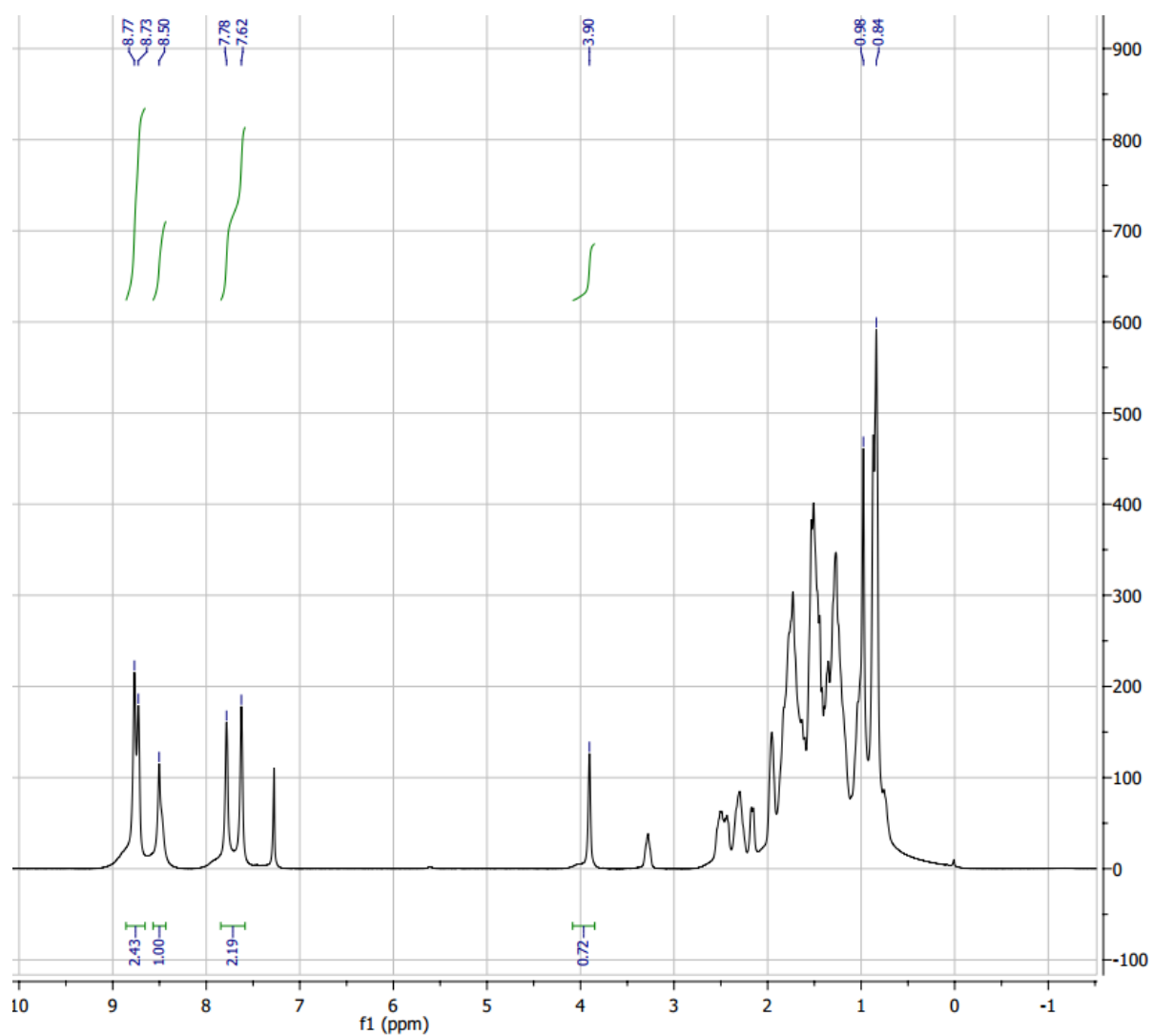


Figure S2:  $^1\text{H}$  NMR spectrum of 3 $\beta$ -azido-5 $\alpha$ -androstan-17-one isonicotinoylhydrazone (compound **2**) in  $\text{CDCl}_3$

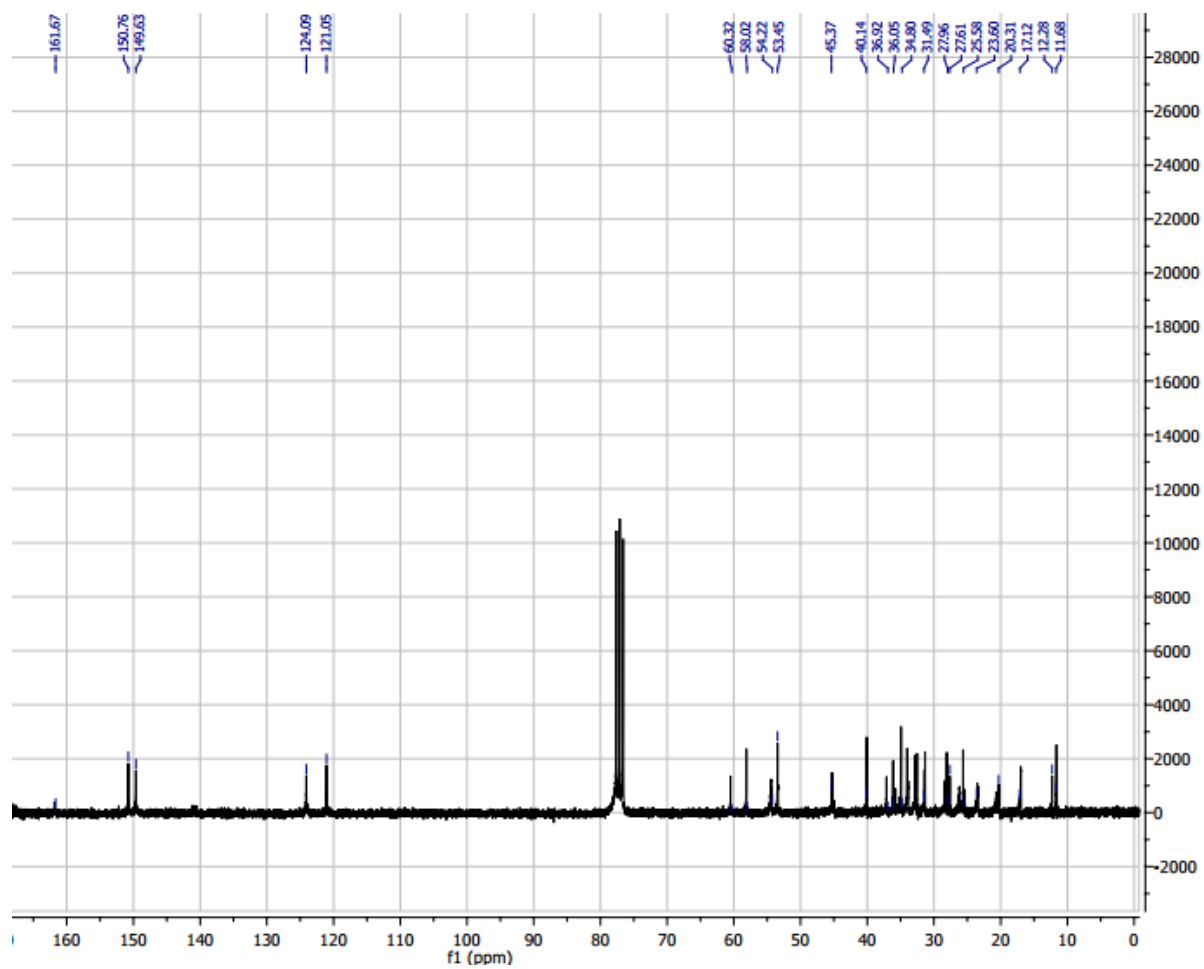


Figure S3: <sup>13</sup>C NMR spectrum of 3β-azido-5α-androstan-17-one isonicotinoylhydrazone (compound **2**) in CDCl<sub>3</sub>

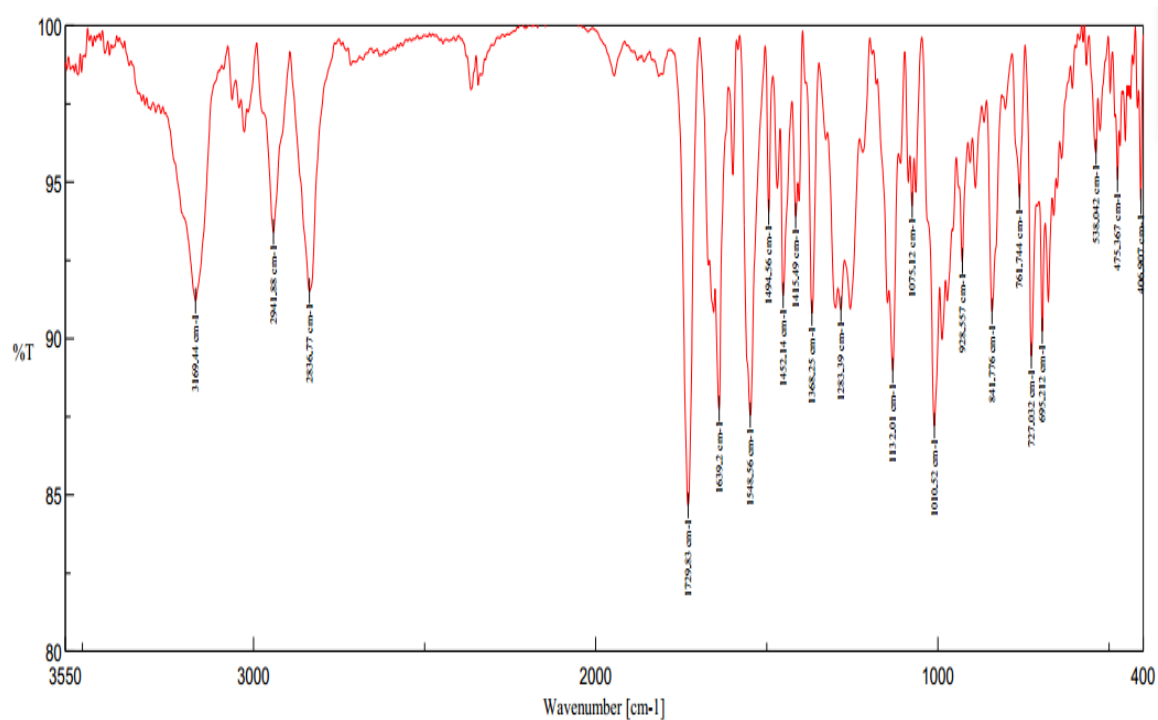


Figure S4: IR spectrum of 3β-phenylacetoxy-5α-androstan-17-one isonicotinoylhydrazone (compound 3) in KBr

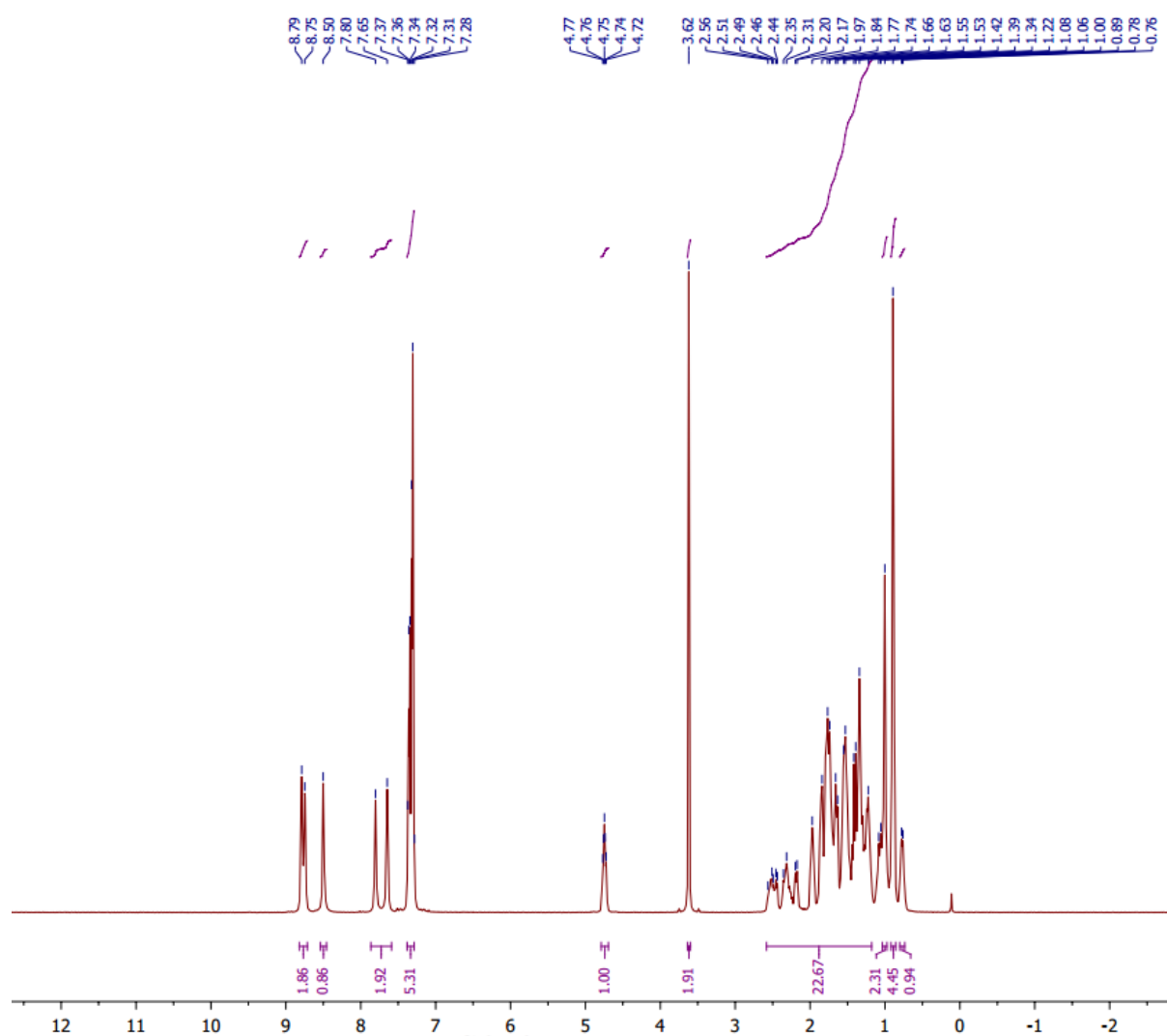


Figure S5:  $^1\text{H}$  NMR spectrum of 3 $\beta$ -phenylacetoxy-5 $\alpha$ -androstan-17-one isonicotinoylhydrazone (compound **3**) in  $\text{CDCl}_3$

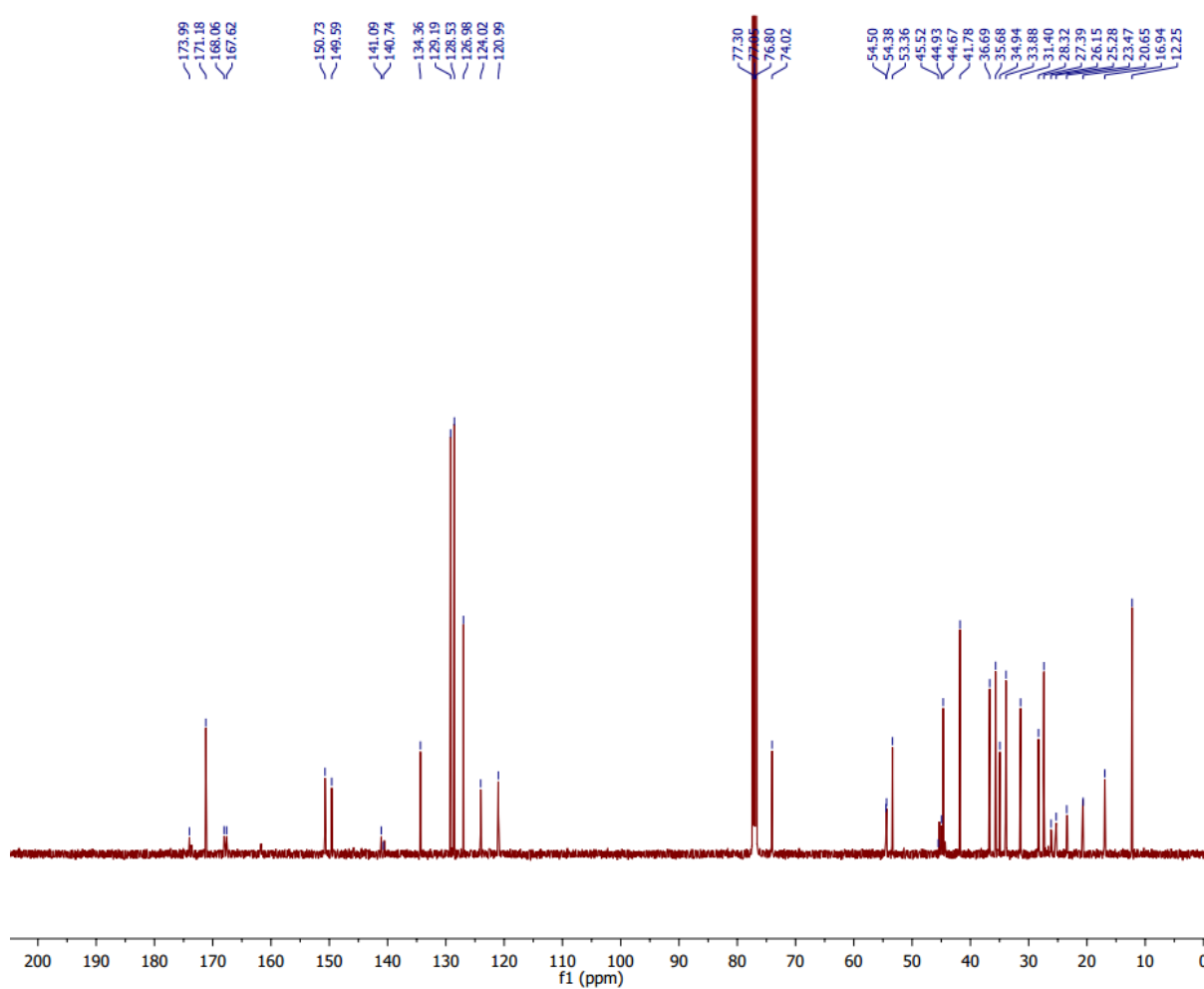


Figure S6:  $^{13}\text{C}$  NMR spectrum of 3 $\beta$ -phenylacetoxy-5 $\alpha$ -androstan-17-one isonicotinoylhydrazone (compound **3**) in  $\text{CDCl}_3$

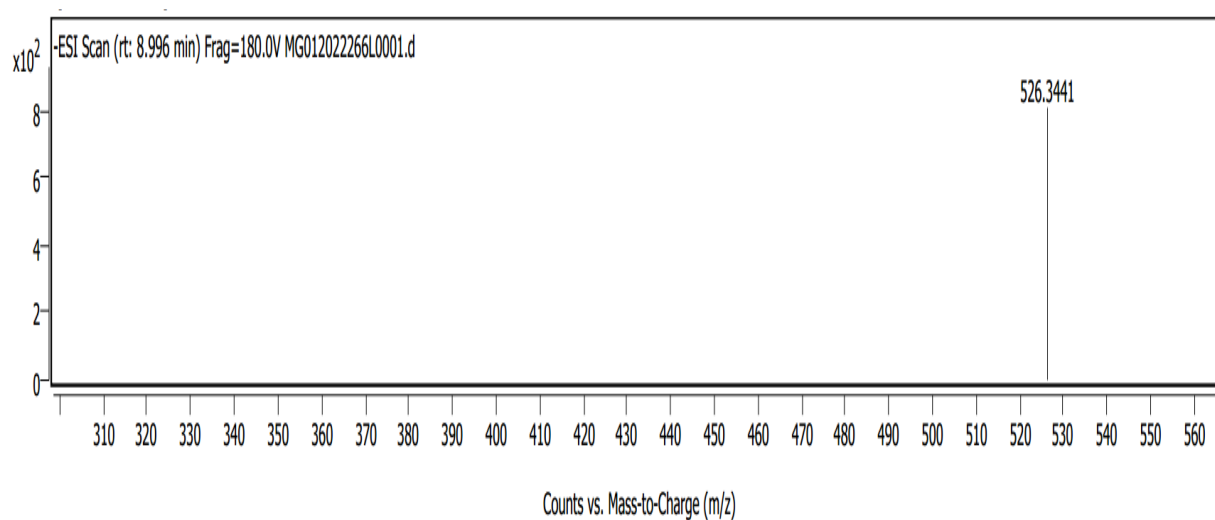


Figure S7: MS spectrum of 3 $\beta$ -phenylacetoxy-5 $\alpha$ -androstan-17-one isonicotinoylhydrazone (compound **3**)

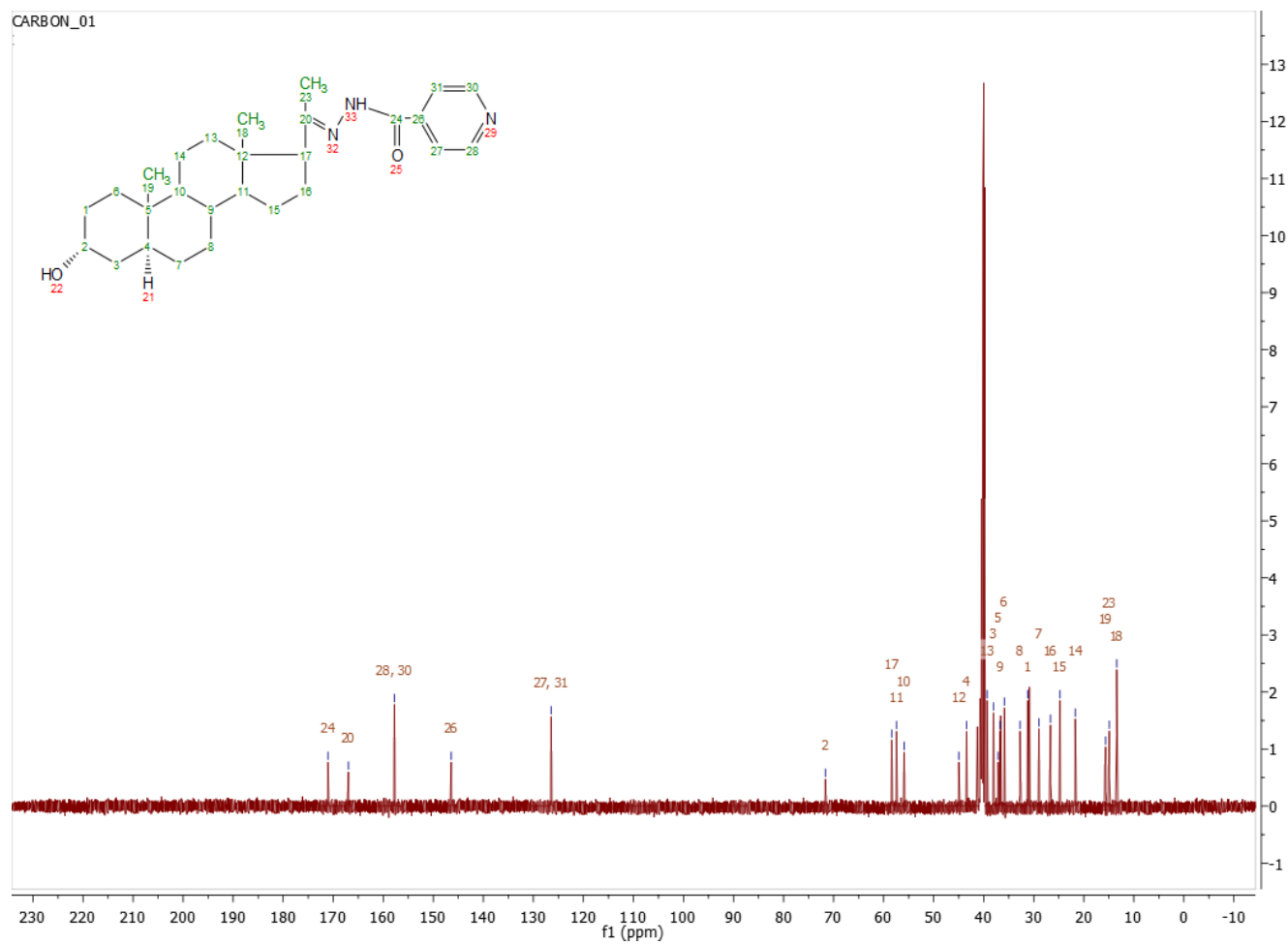


Figure S8:  $^{13}\text{C}$  NMR spectrum of compound **4** in  $\text{d}_6\text{-DMSO}$

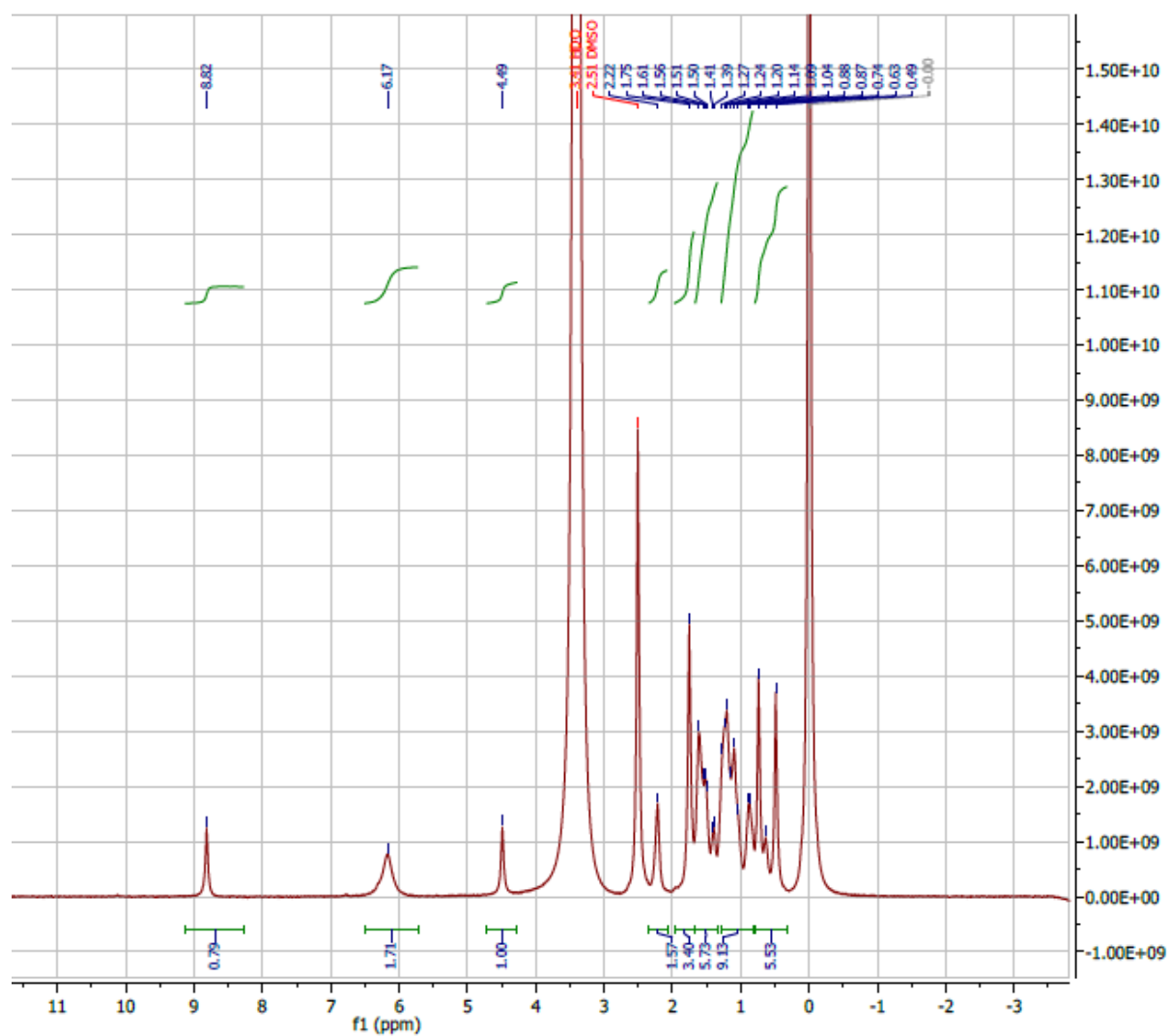


Figure S9:  $^1\text{H}$  NMR spectrum of 3 $\alpha$ -hydroxy-5 $\alpha$ -pregnan-20-one thiosemicarbazone (compound 5) in  $\text{d}_6$ -DMSO



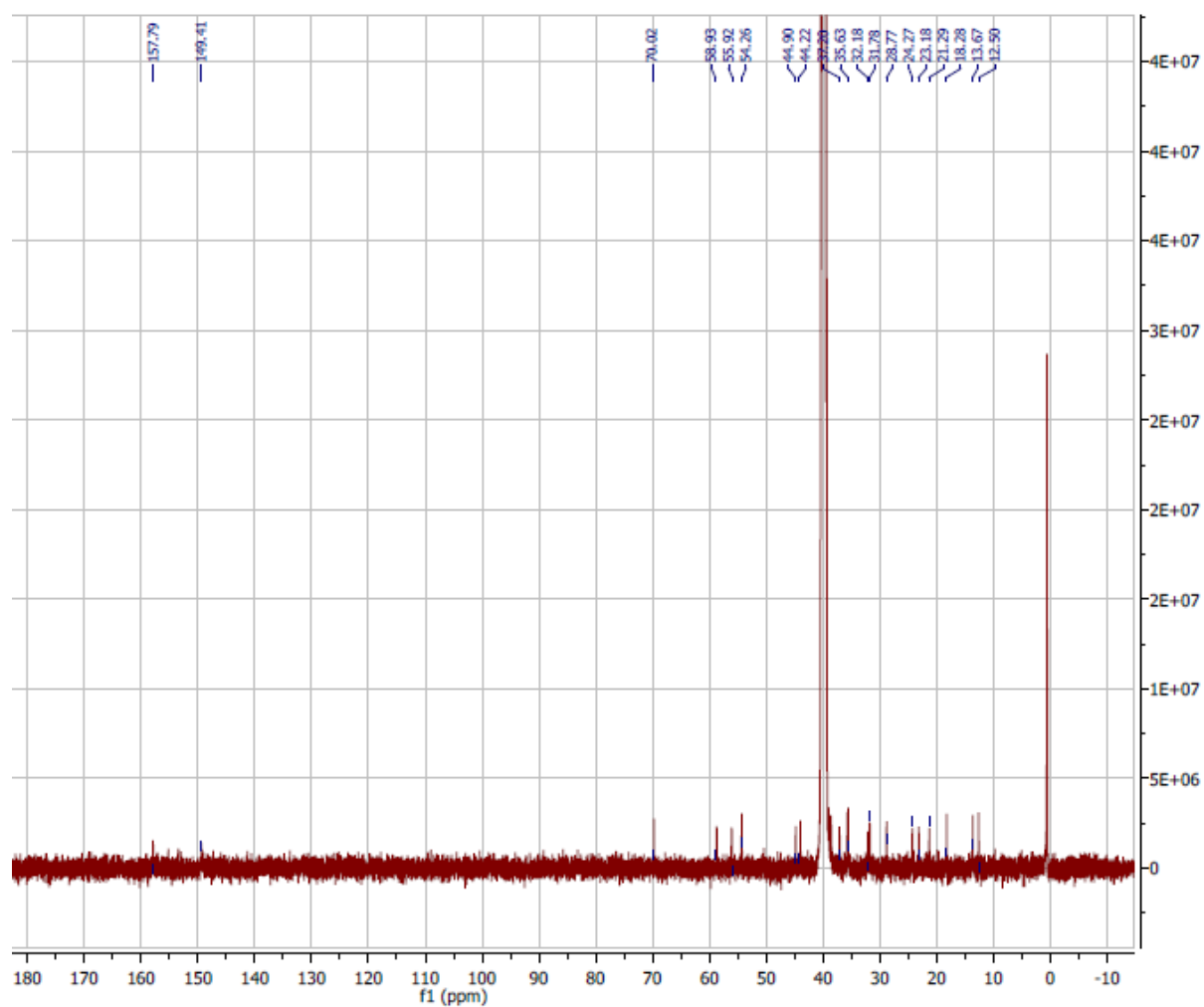


Figure 10:  $^{13}\text{C}$  NMR spectrum of 3 $\alpha$ -hydroxy-5 $\alpha$ -pregnan-20-one thiosemicarbazone (compound **5**) in  $\text{d}_6\text{-DMSO}$

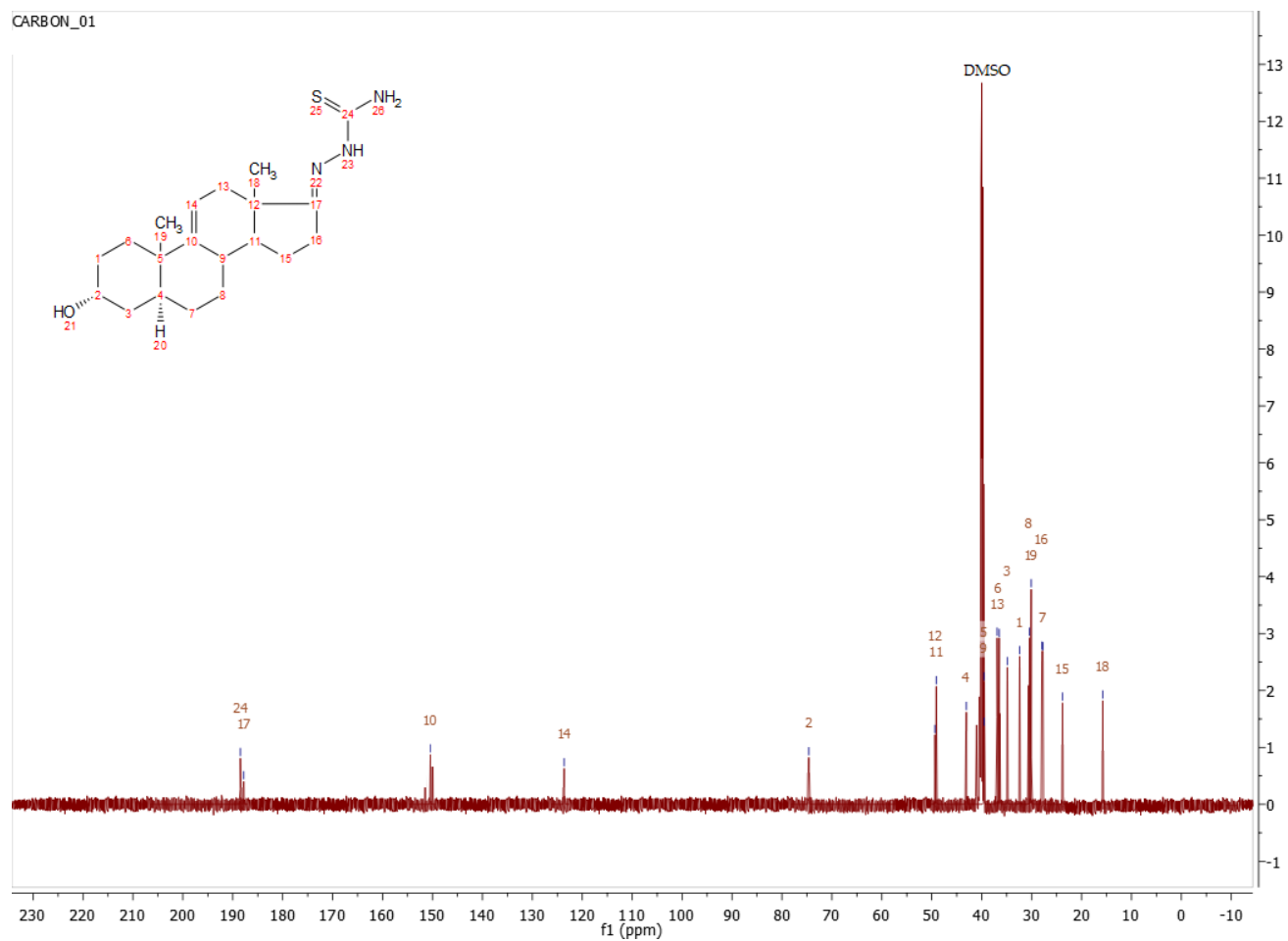


Figure S11:  $^{13}\text{C}$  NMR spectrum of compound 6 in  $\text{d}_6$ -DMSO

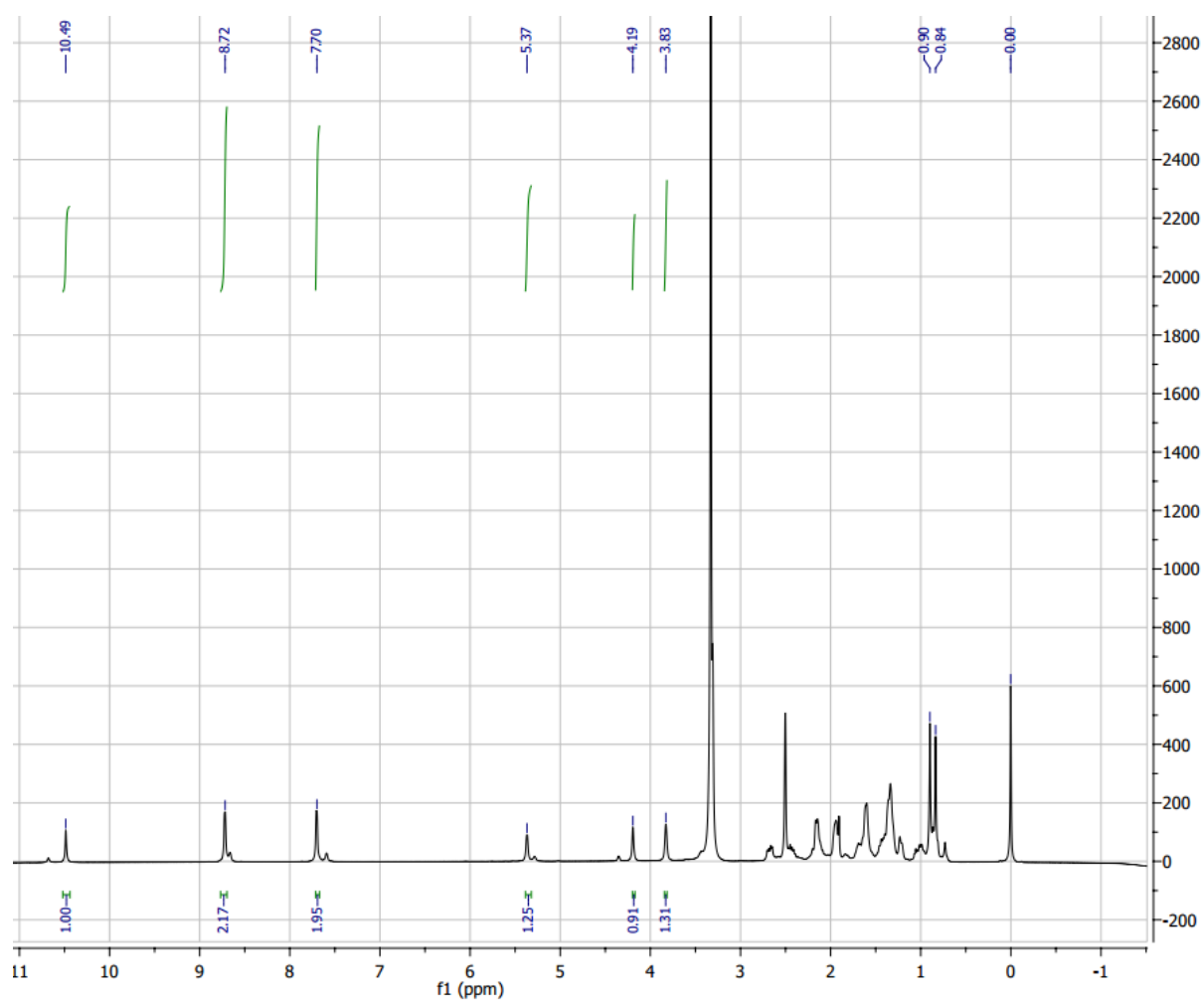


Figure S12:  $^1\text{H}$  NMR spectrum of 3 $\alpha$ -hydroxy-5 $\alpha$ -androst-9(11)-en-17-one isonicotinoylhydrazone (compound 7) in  $\text{d}_6\text{-DMSO}$

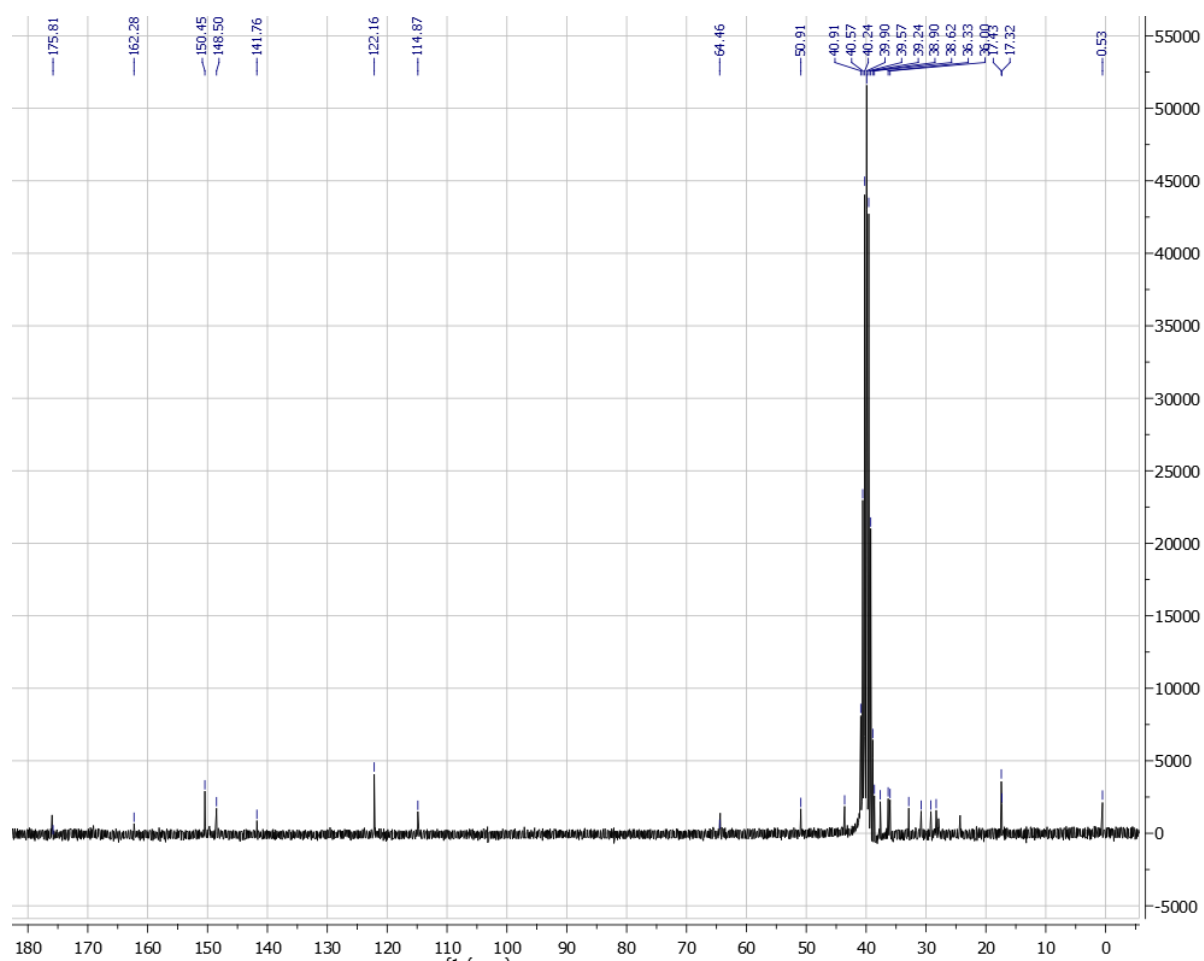


Figure S13:  $^{13}\text{C}$  NMR spectrum of 3 $\alpha$ -hydroxy-5 $\alpha$ -androst-9(11)-en-17-one isonicotinoylhydrazone (compound 7) in  $\text{d}_6\text{-DMSO}$

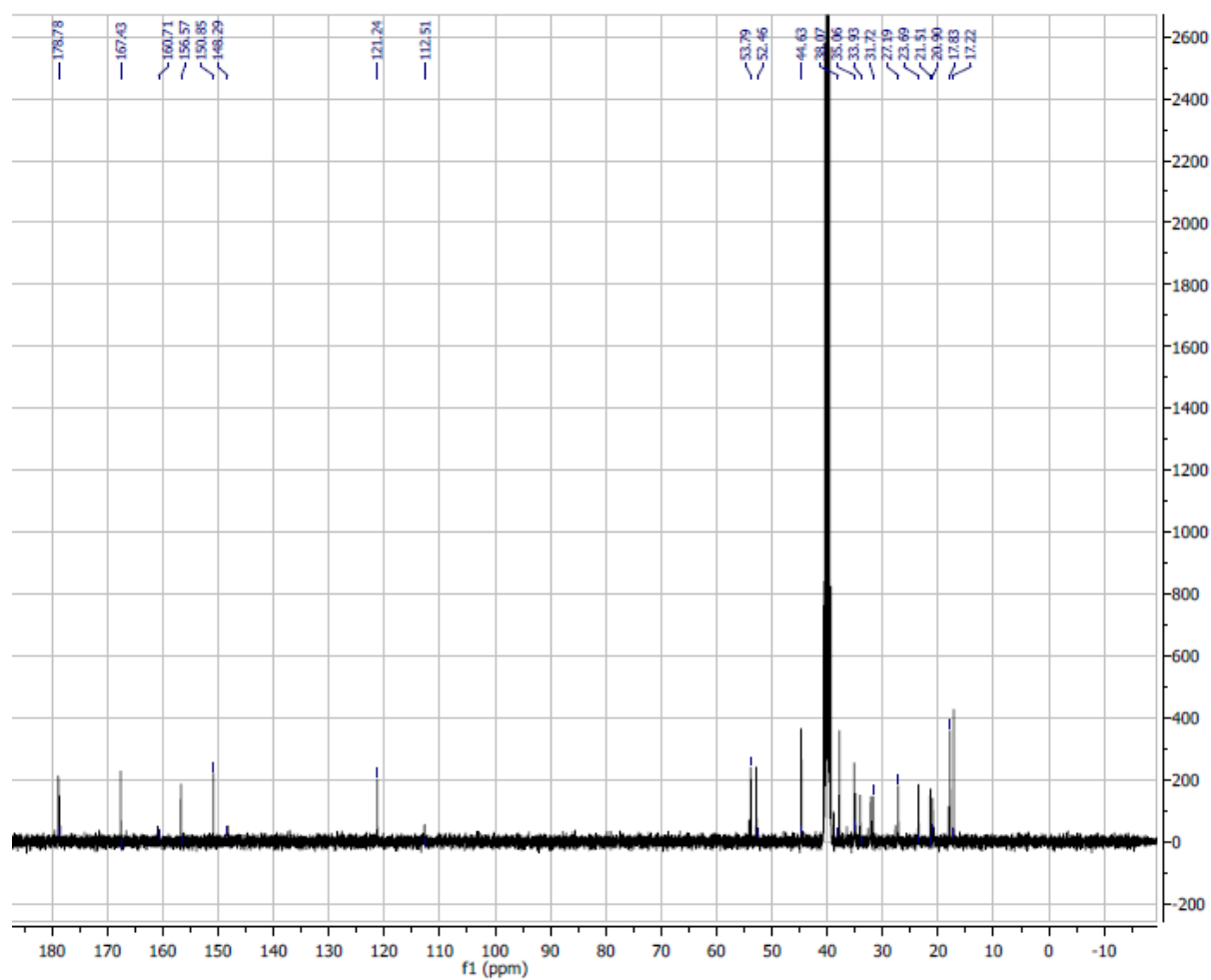


Figure S14:  $^{13}\text{C}$  NMR spectrum of androsta-1,4-diene-3,17-dione dithiosemicarbazone (compound 8) in  $\text{d}_6$ -DMSO

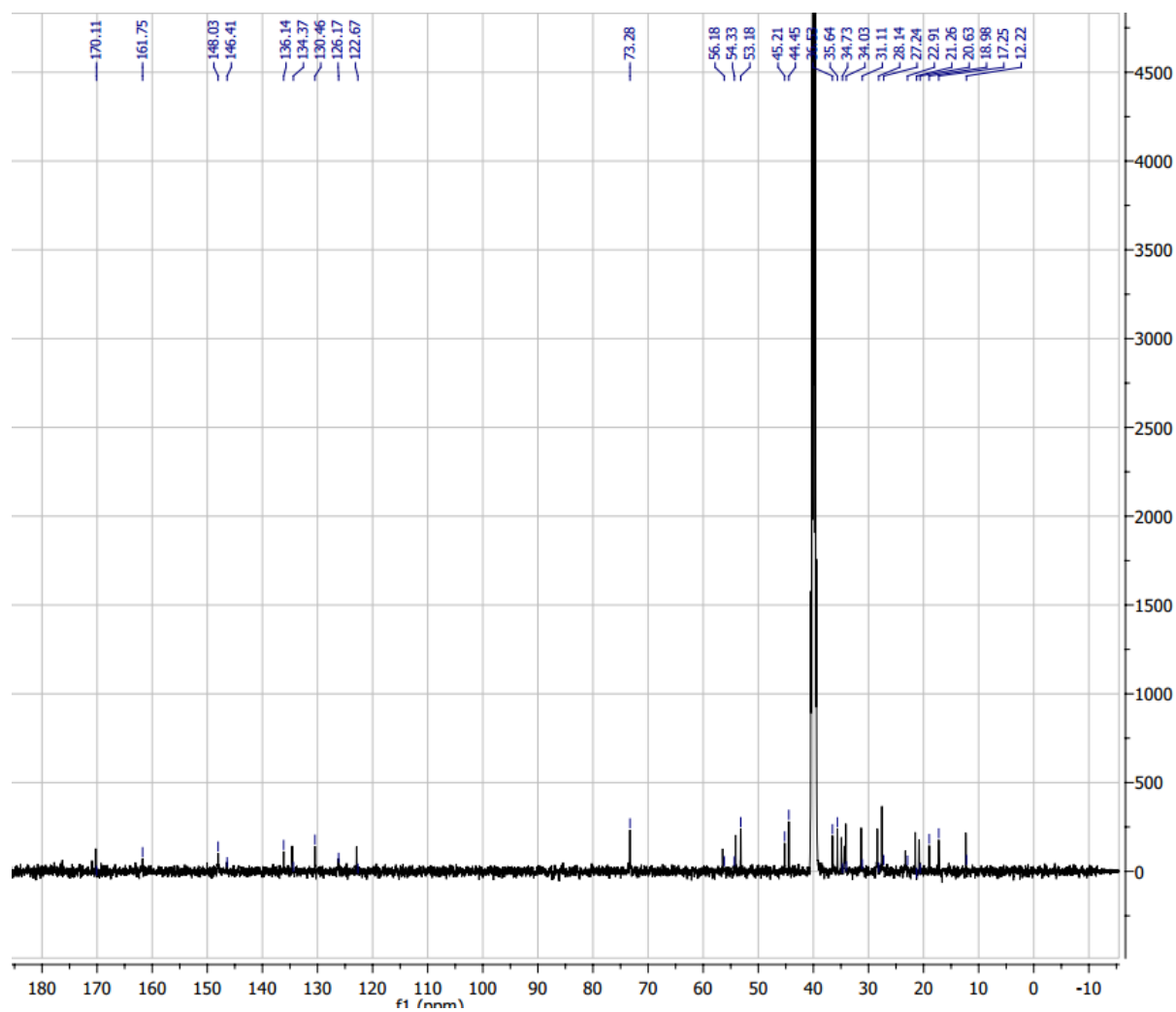


Figure S15: <sup>13</sup>C NMR spectrum of 3β-acetoxy-5α-androstan-17-one *m*-nitrobenzoylhydrazone (compound **9**) in d<sub>6</sub>-DMSO

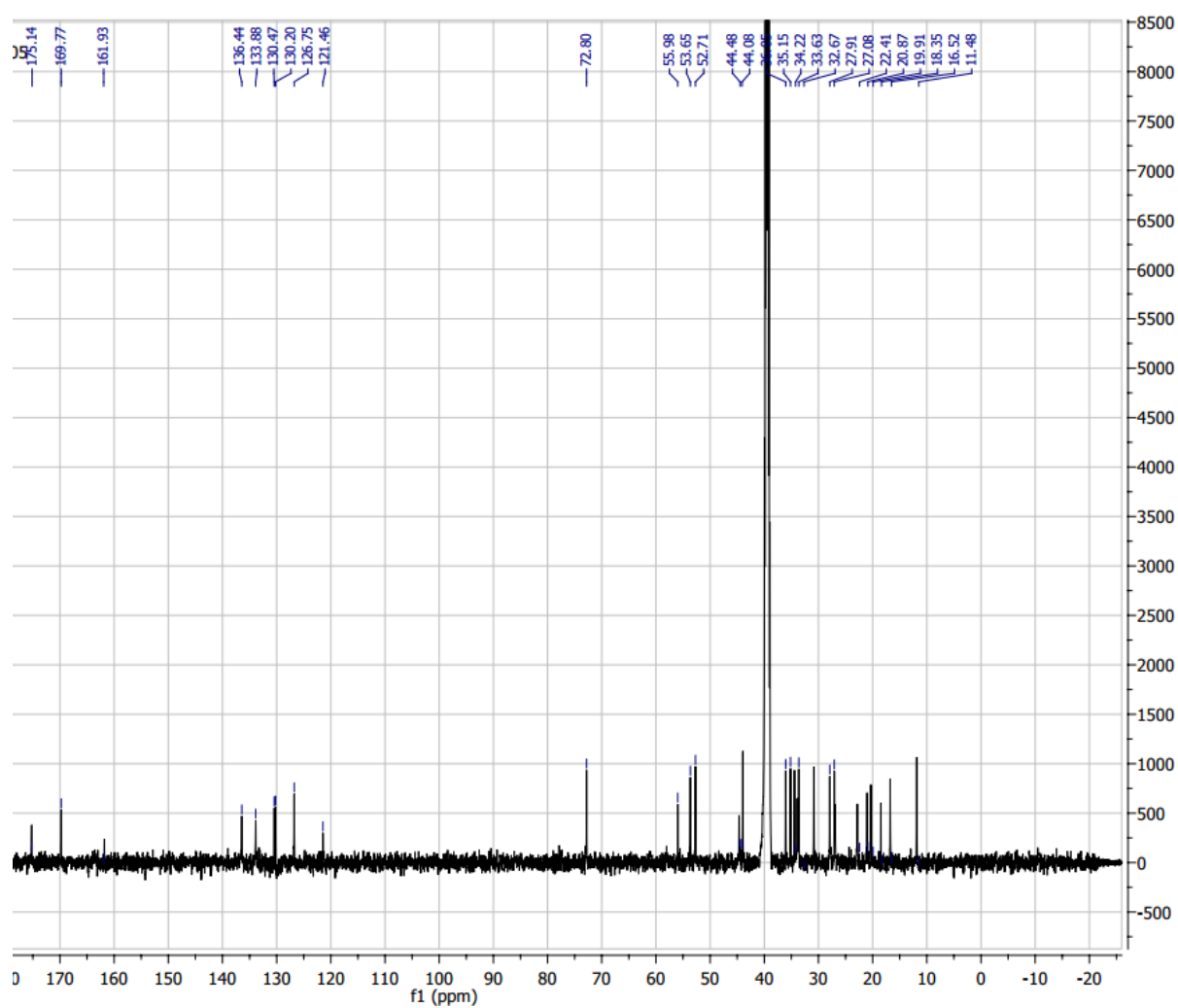


Figure S16: <sup>13</sup>C NMR spectrum of 3 $\beta$  -acetoxy-5 $\alpha$ -androstan-17-one *m*-bromobenzoylhydrazone (compound **10**) in d<sub>6</sub>-DMSO

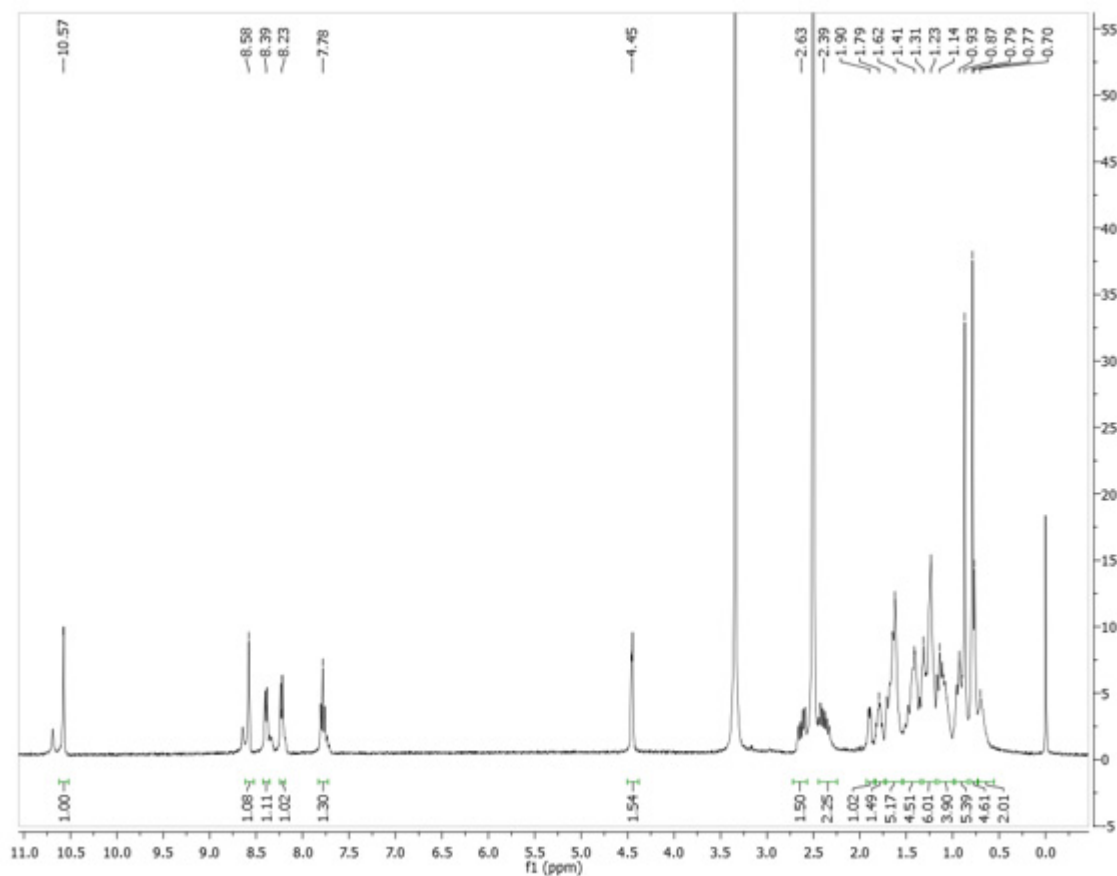


Figure S17:  $^1\text{H}$  NMR spectrum of 3 $\alpha$  -hydroxy-5 $\alpha$ -androstan-17-one *m*-nitrobenzoylhydrazone (compound **11**) in  $\text{d}_6$ -DMSO

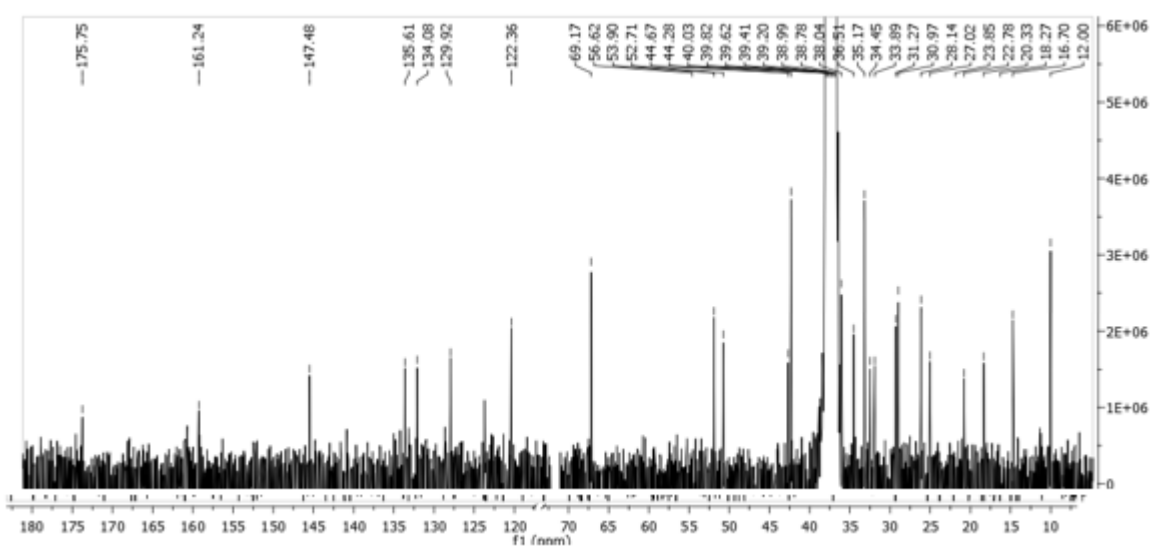


Figure S18:  $^{13}\text{C}$  NMR spectrum of 3 $\alpha$  -hydroxy-5 $\alpha$ -androstan-17-one *m*-nitrobenzoylhydrazone (compound **11**) in  $\text{d}_6$ -DMSO



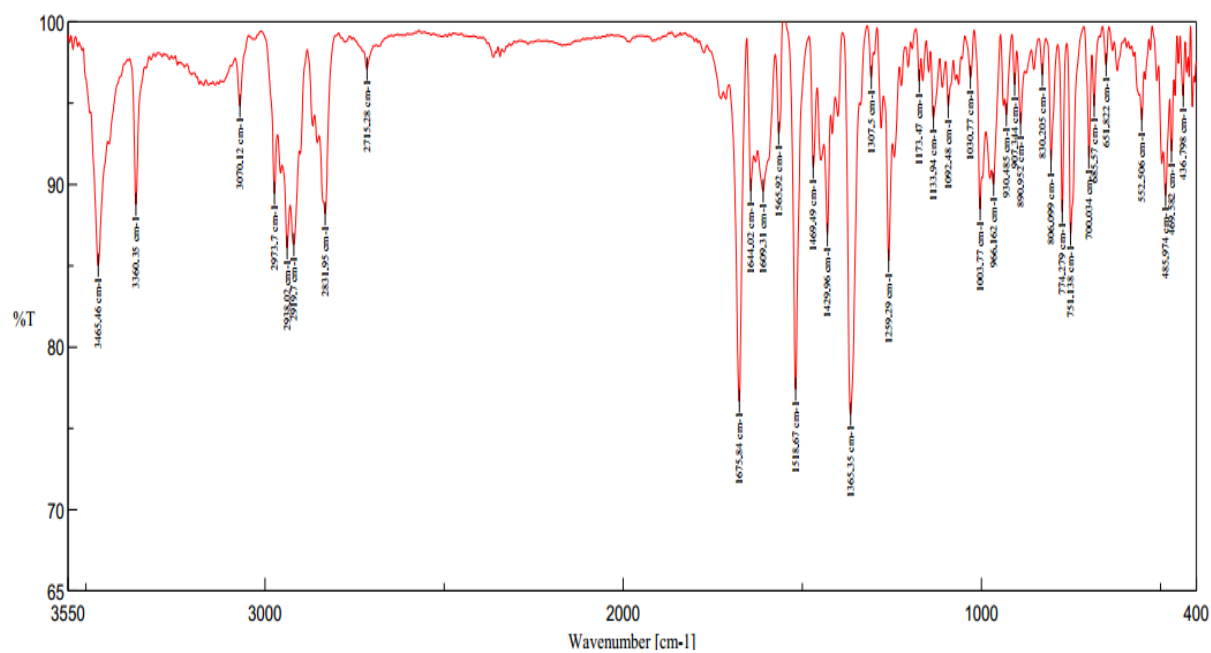


Figure S19: IR spectrum of 3α-hydroxy-5α-androstan-17-one *m*-bromobenzoylhydrazone (compound 12) in KBr

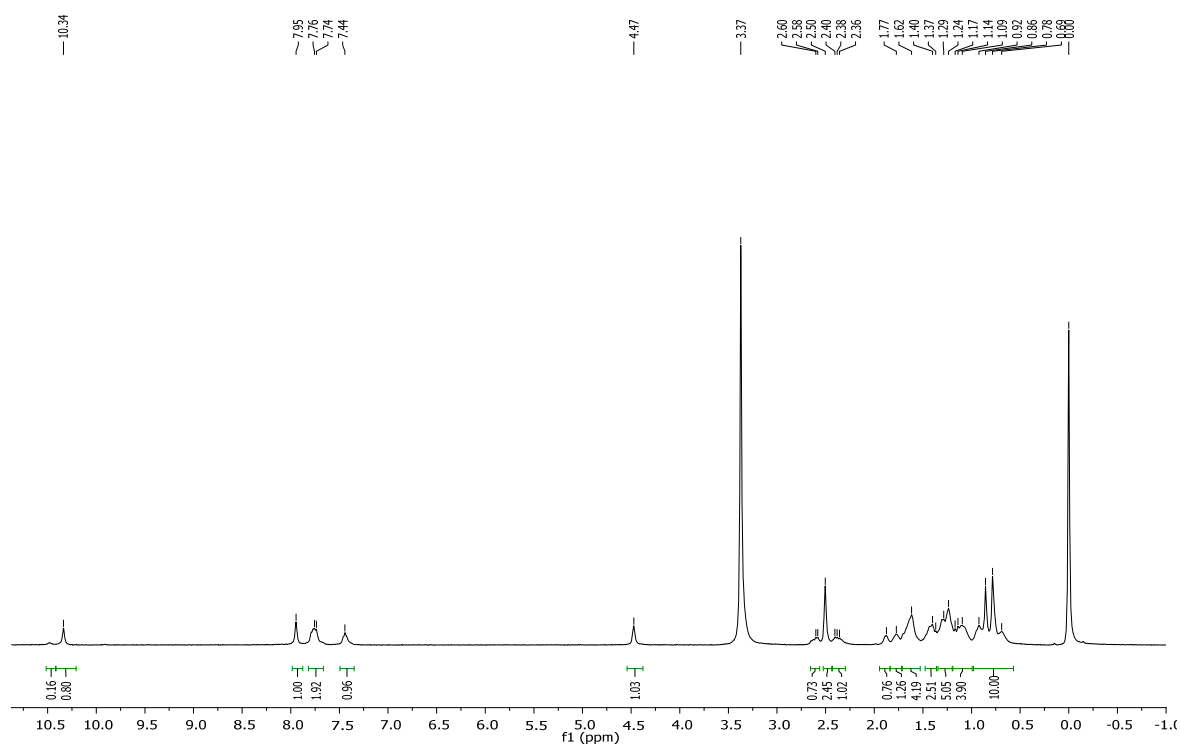


Figure S20: <sup>1</sup>H NMR spectrum of 3α-hydroxy-5α-androstan-17-one *m*-bromobenzoylhydrazone (compound 12) in d<sub>6</sub>-DMSO

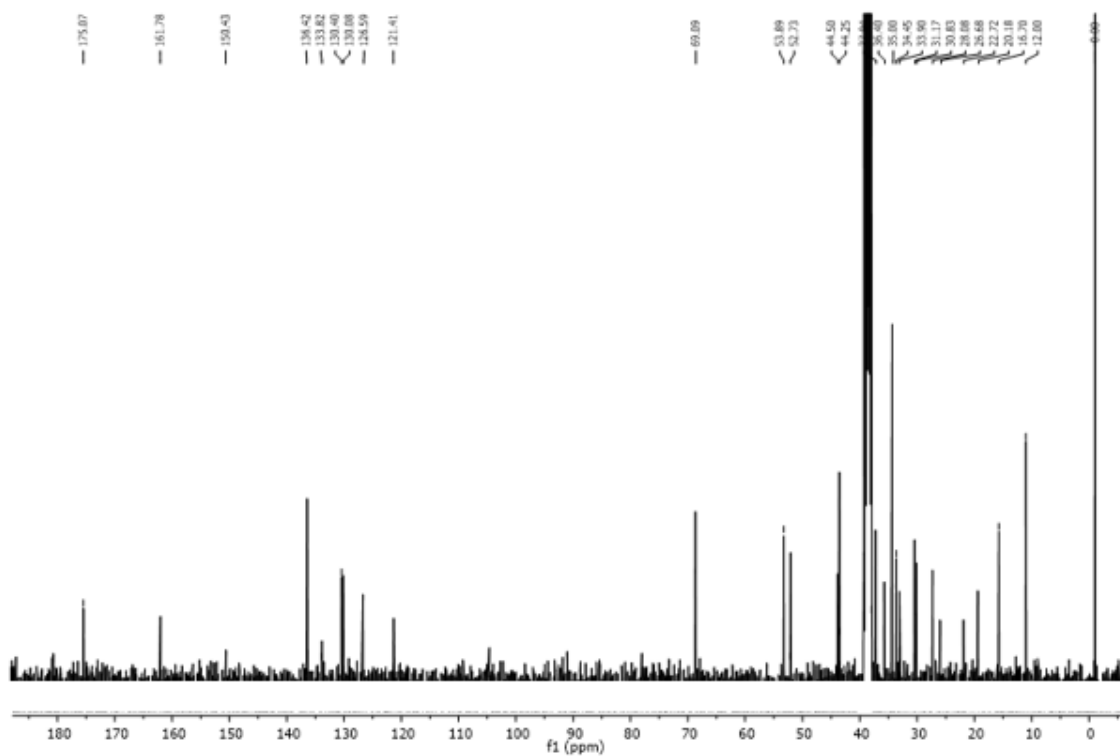


Figure S21: <sup>13</sup>C NMR spectrum of 3α-hydroxy-5α-androstan-17-one *m*-bromobenzoylhydrazone (compound **12**) in d<sub>6</sub>-DMSO

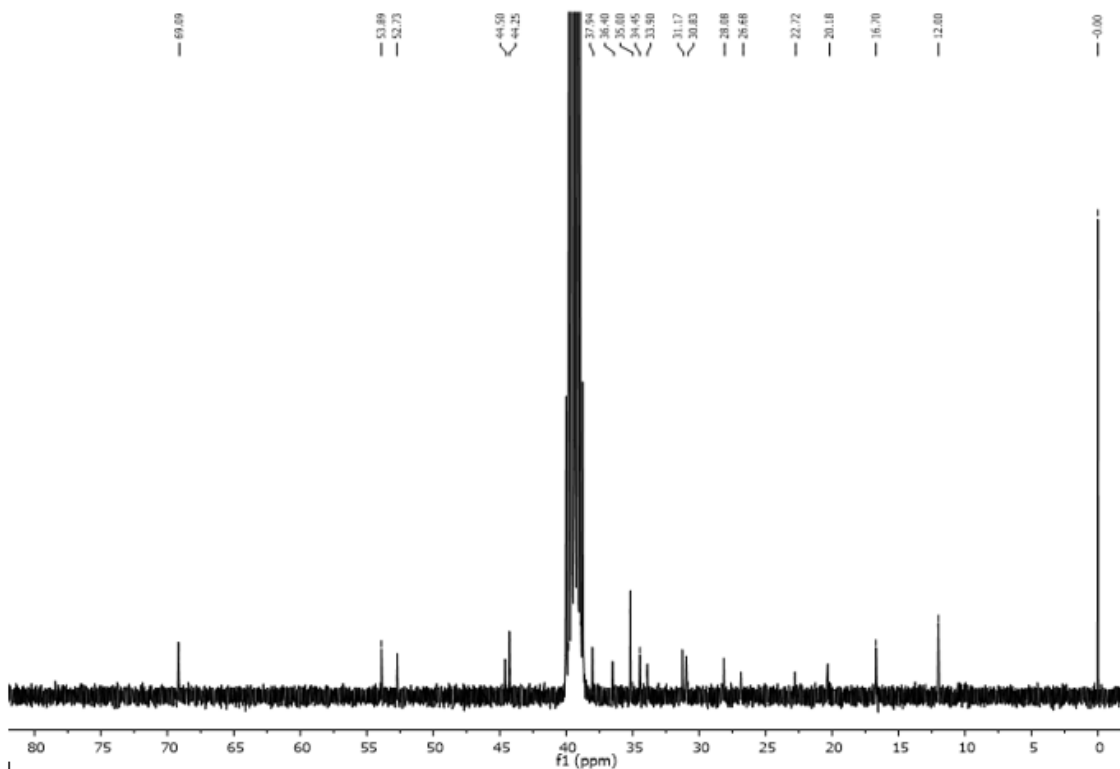


Figure S22: Fragment of <sup>13</sup>C NMR spectrum 3α-hydroxy-5α-androstan-17-one *m*-bromobenzoylhydrazone (compound **12**) in d<sub>6</sub>-DMSO

