

## Supplementary Materials

# In Silico and Experimental Investigation of the Biological Potential of Some Recently Developed Carprofen Derivatives

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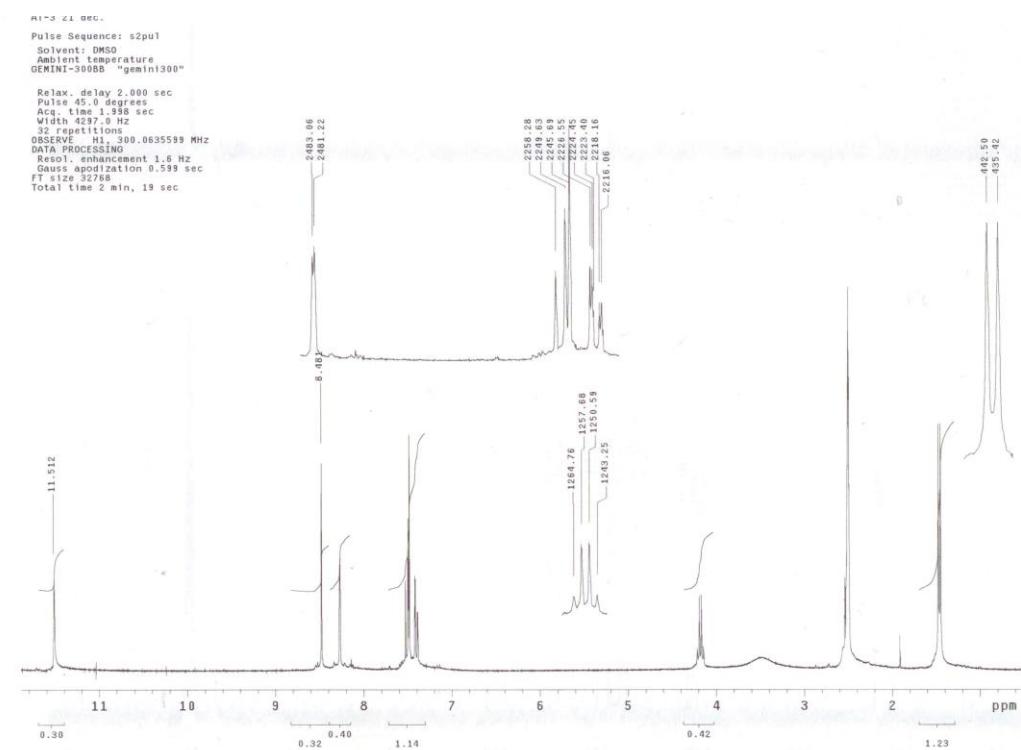
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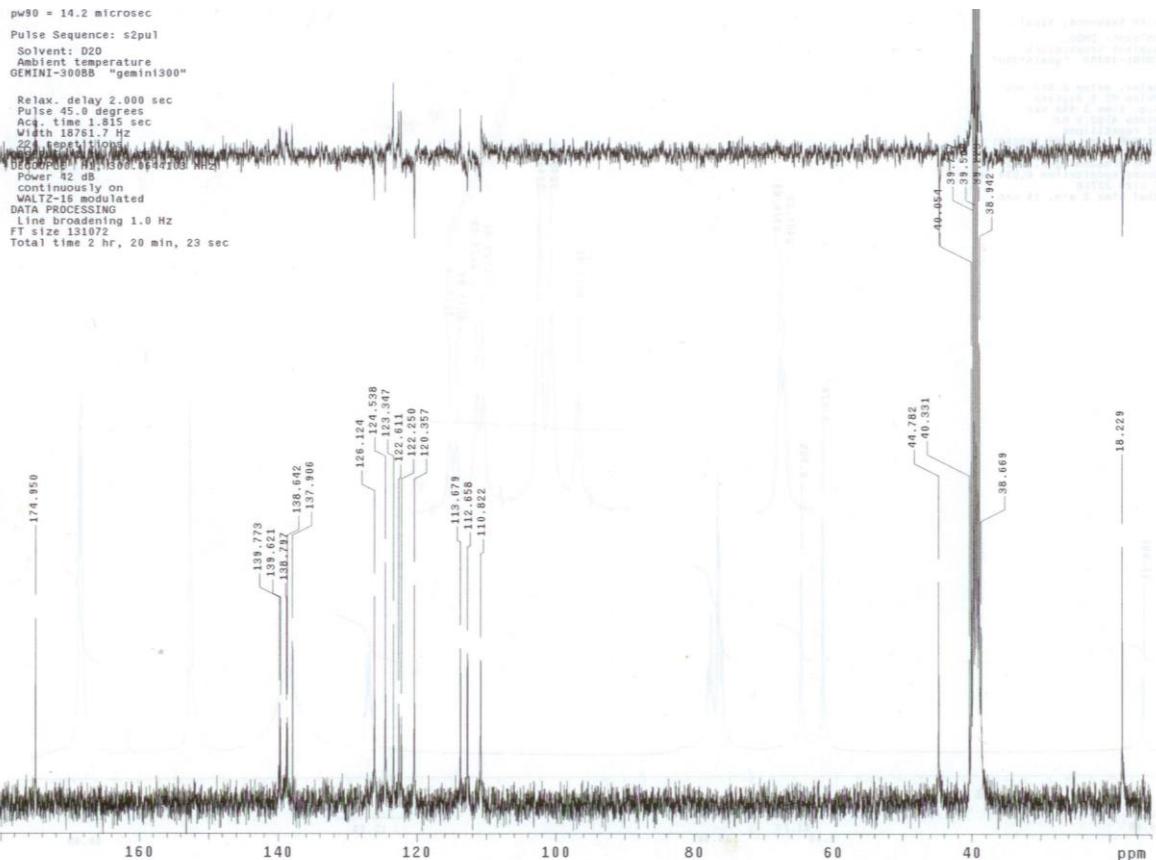
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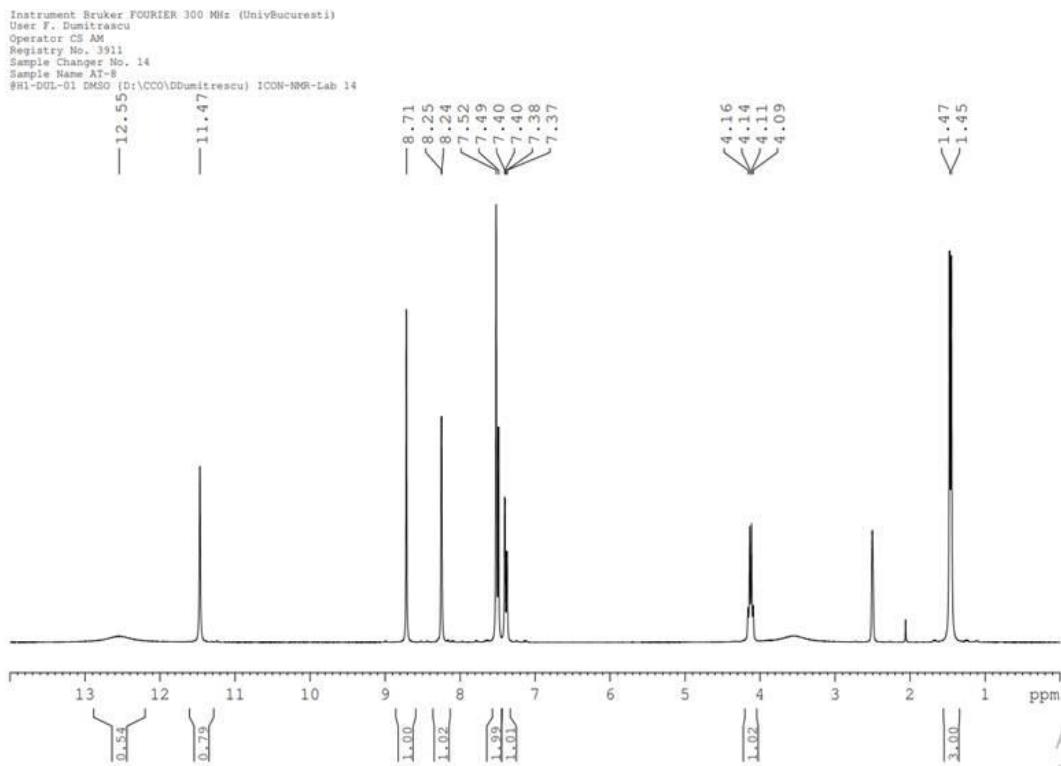
† These authors equally contribute to this work.



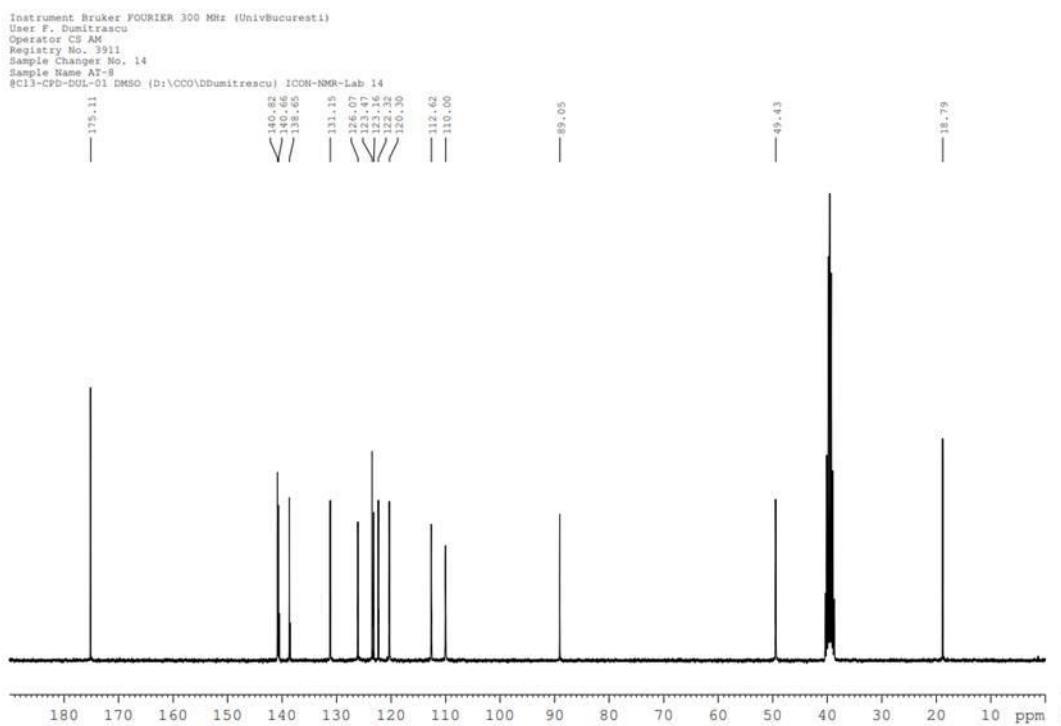
**Figure S1a.** The  $^1\text{H}$ -NMR spectrum of 2-(3-Bromo-6-chloro-9H-carbazol-2-yl)propanoic acid (**2**).



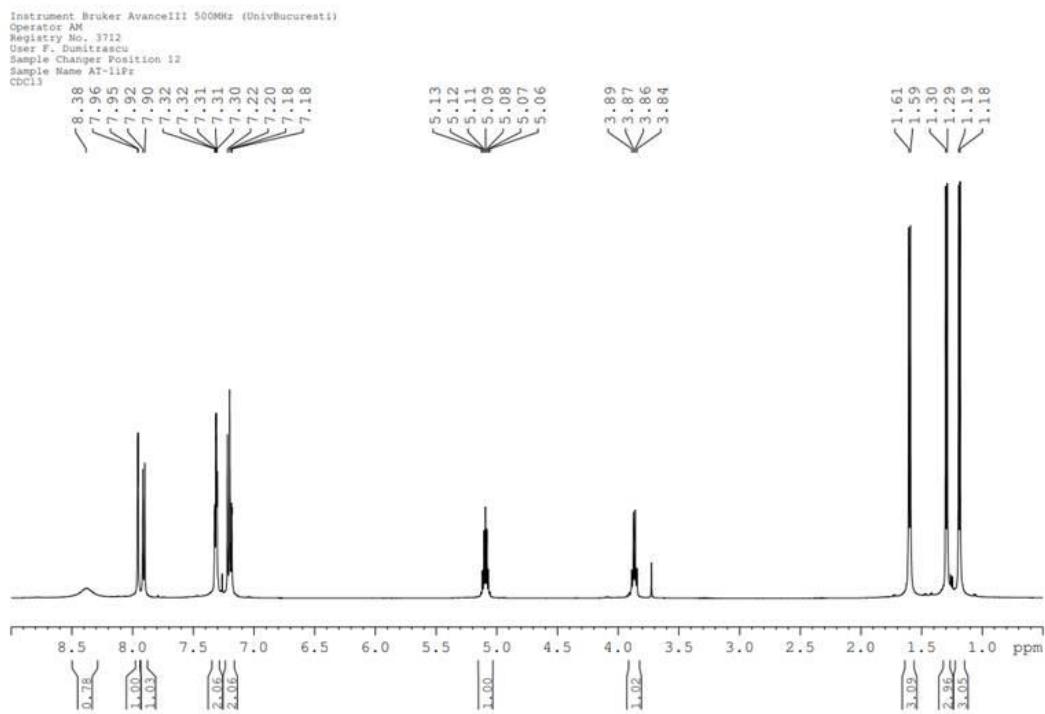
**Figure S1b.** The  $^{13}\text{C}$ -NMR spectrum of 2-(3-Bromo-6-chloro-9H-carbazol-2-yl)propanoic acid (**2**).



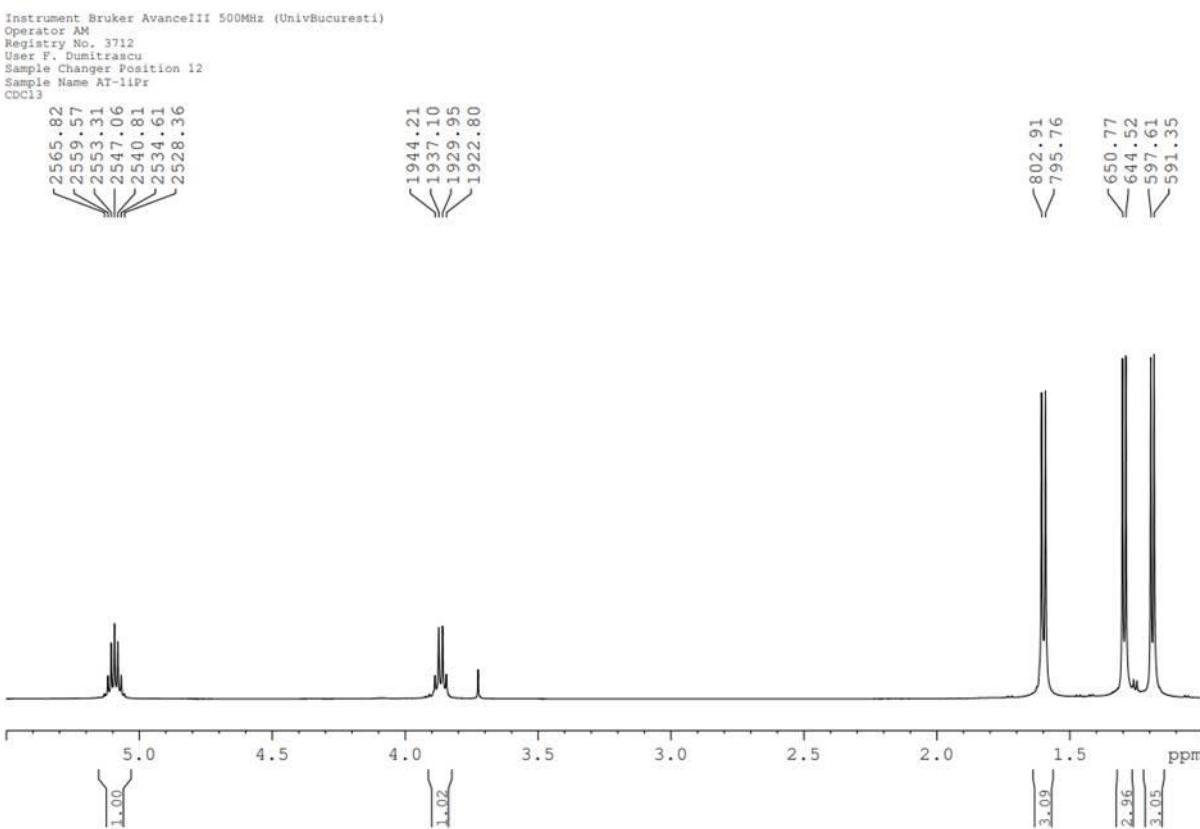
**Figure S2a.** The  $^1\text{H}$ -NMR spectrum of 2-(3-Iodo-6-chloro-9H-carbazol-2-yl)propanoic acid (**3**).



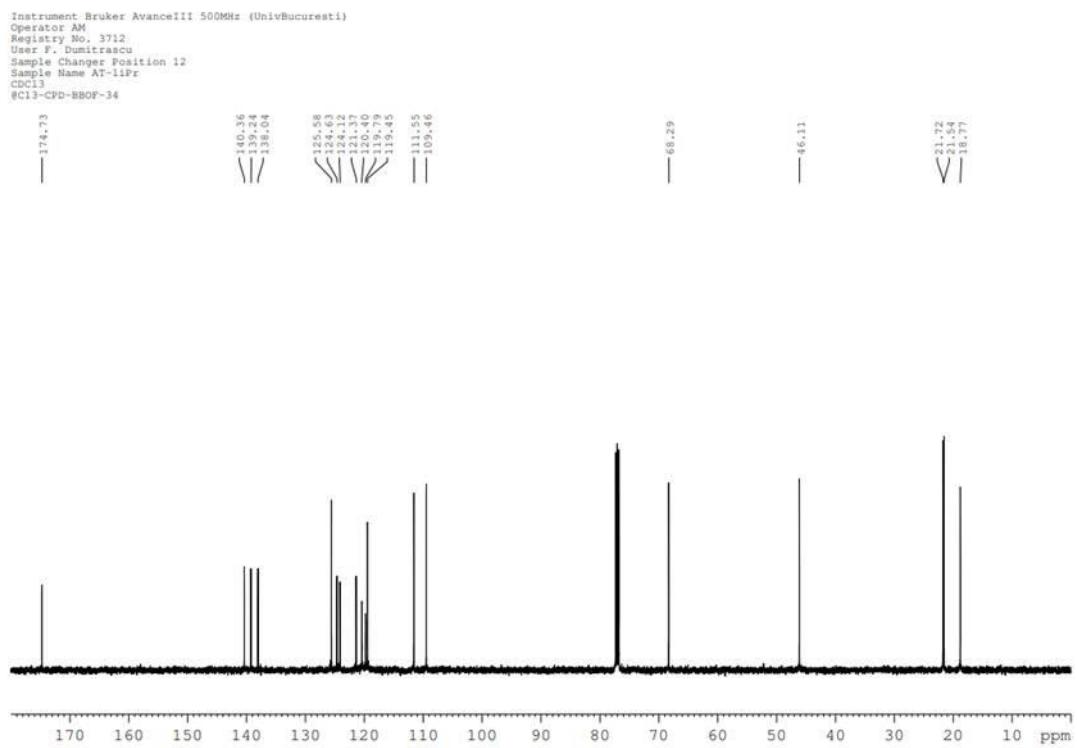
**Figure S2b.** The  $^{13}\text{C}$ -NMR spectrum of 2-(3-Iodo-6-chloro-9H-carbazol-2-yl)propanoic acid (**3**).



**Figure S3a.** The <sup>1</sup>H-NMR spectrum of Isopropyl 2-(6-chloro-9H-carbazol-2-yl)propanoate (**4**).



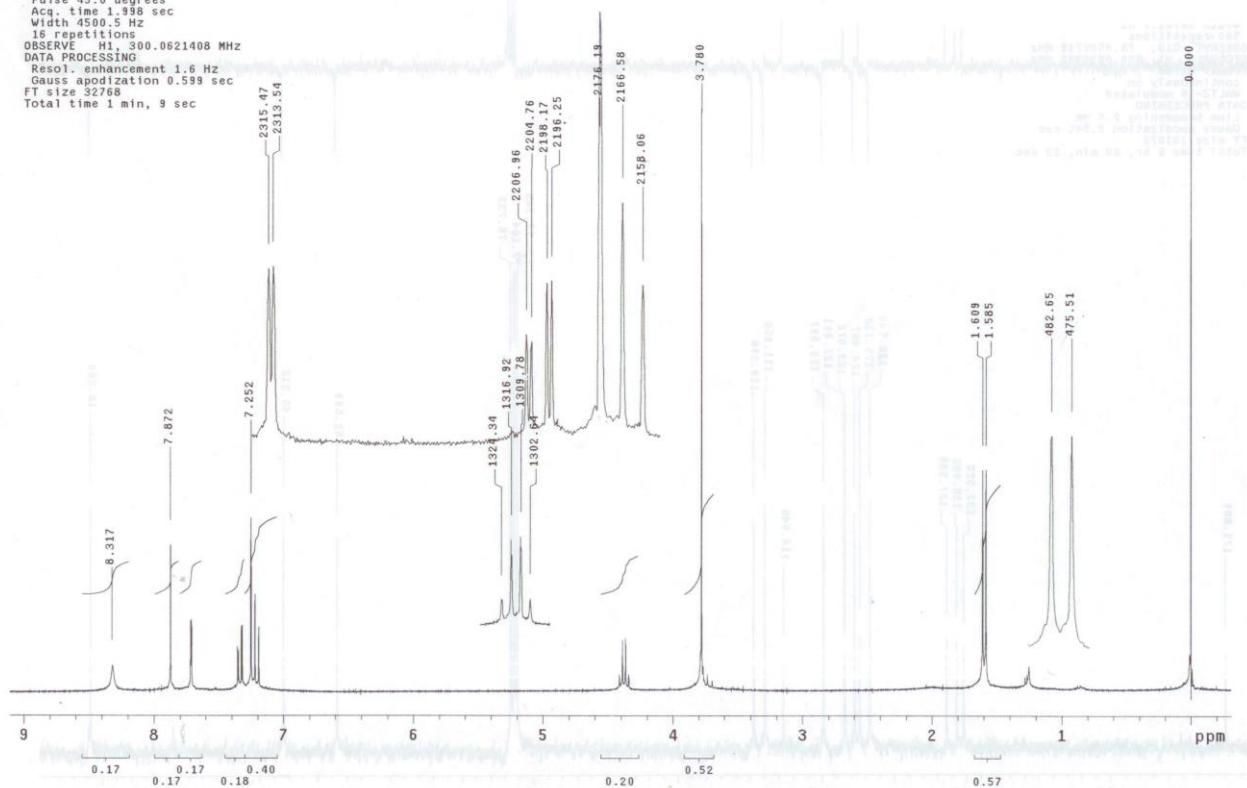
**Figure S3b.** The <sup>1</sup>H-NMR spectrum (details) of Isopropyl 2-(6-chloro-9H-carbazol-2-yl)propanoate (**4**).



**Figure S3c.** The <sup>13</sup>C-NMR spectrum of Isopropyl 2-(6-chloro-9H-carbazol-2-yl)propanoate (**4**).

Pulse Sequence: s2pul  
 Solvent: CDCl<sub>3</sub>  
 Ambient temperature  
 GEMINI-300BB "gemini300"

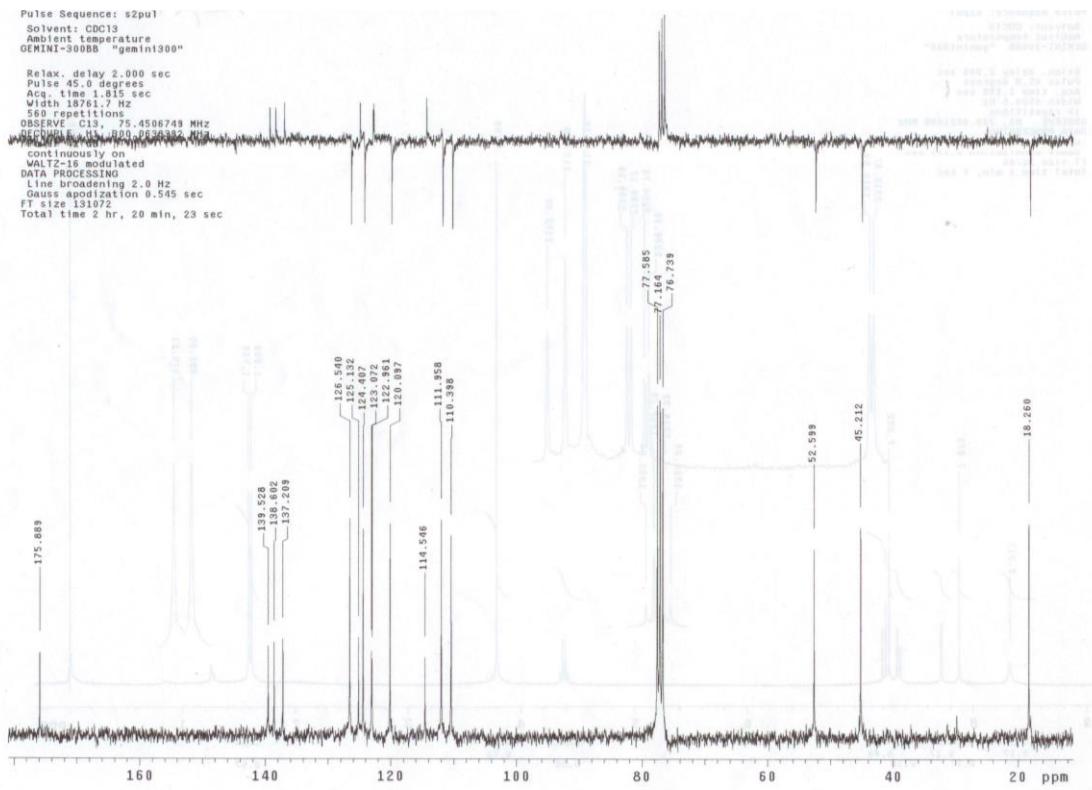
Relax. delay 2.000 sec  
 Pulse 45.0 degrees  
 Acq. time 1.998 sec  
 Width 1.600 Hz  
 16 repetitions  
 OBSERVE H1, 300.0621408 MHz  
 DATA PROCESSING  
 Resol. enhancement 1.6 Hz  
 Gauss apodization 0.599 sec  
 FT size 32768  
 Total time 1 min, 9 sec



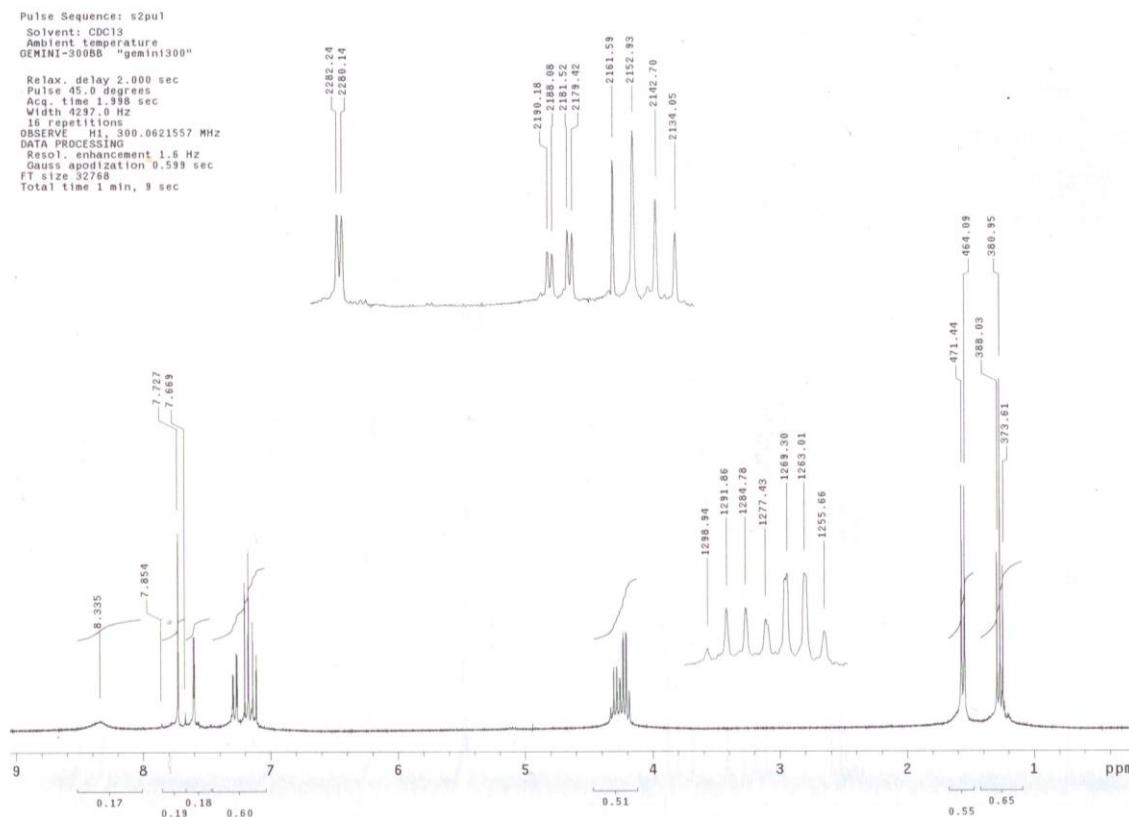
**Figure S4a.** The <sup>1</sup>H-NMR spectrum of Methyl 2-(3-Bromo-6-chloro-9H-carbazol-2-yl)propanoate (**5**).

Pulse Sequence: s2pul  
 Solvent: CDCl<sub>3</sub>  
 Ambient temperature  
 GEMINI-300BB "gemini300"

Relax. delay 2.000 sec  
 Pulse 45.0 degrees  
 Acq. time 1.815 sec  
 Width 18761.7 Hz  
 160 repetitions  
 OBSERVE C13, 75.4506749 MHz  
 DECODED H1, 300.0621408 MHz  
 continuously on  
 WALTZ-16 modulated  
 DATA PROCESSING  
 Line broadening 2.0 Hz  
 Gauss apodization 0.545 sec  
 FT size 131072  
 Total time 2 hr, 20 min, 23 sec



**Figure S4b.** The <sup>13</sup>C-NMR spectrum of Methyl 2-(3-Bromo-6-chloro-9H-carbazol-2-yl)propanoate (**5**).



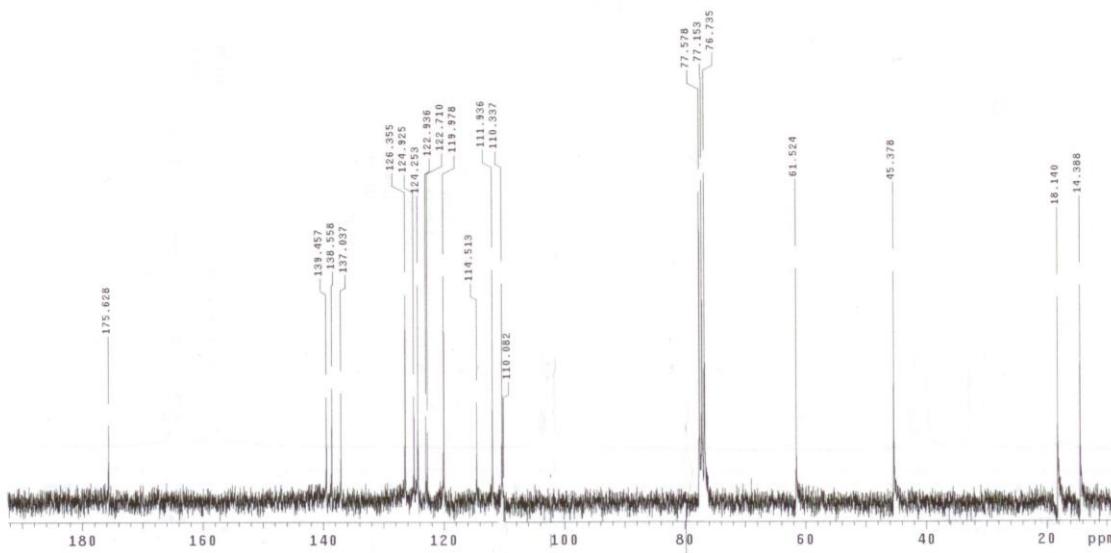
**Figure S5a.** The  $^1\text{H}$ -NMR spectrum of Ethyl 2-(3-Bromo-6-chloro-9H-carbazol-2-yl)propanoate (**6**).

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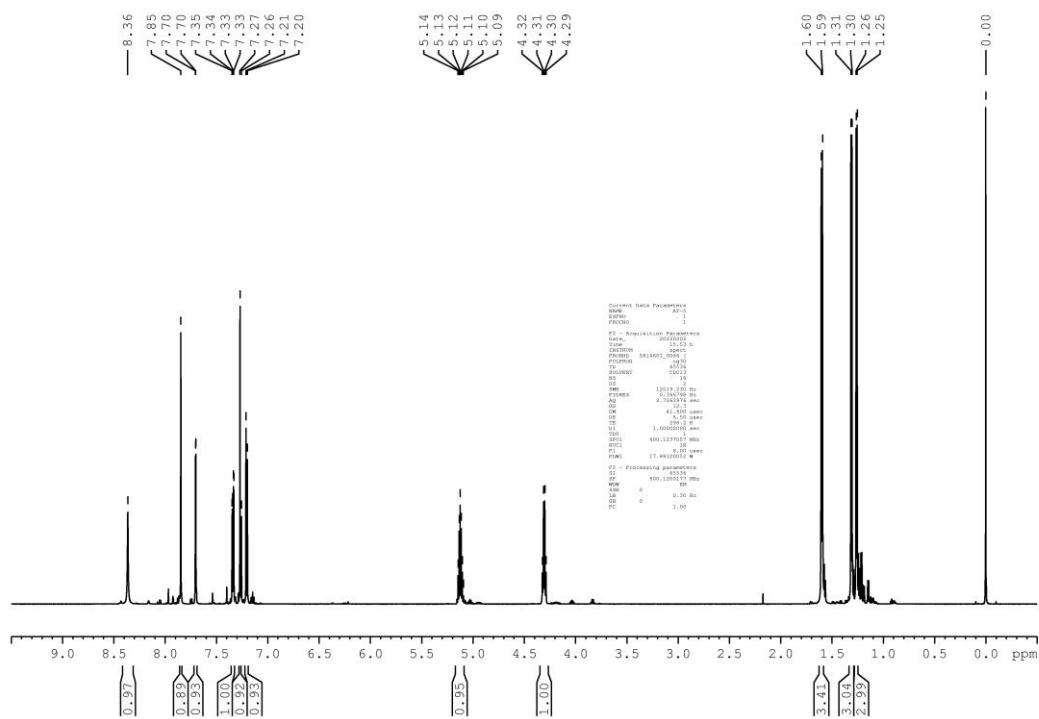
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
GEMINI-300B8 "gemini1300"

Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 1.000 sec
Width 17.0000 Hz
228 repetitions
OBSERVE C13, 75.4506775 MHz
SWEEP F1, 1.300.0636392 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA 1024 points
Line broadening 1.0 Hz
FT size 85536
Total time 2 hr, 11 min, 30 sec

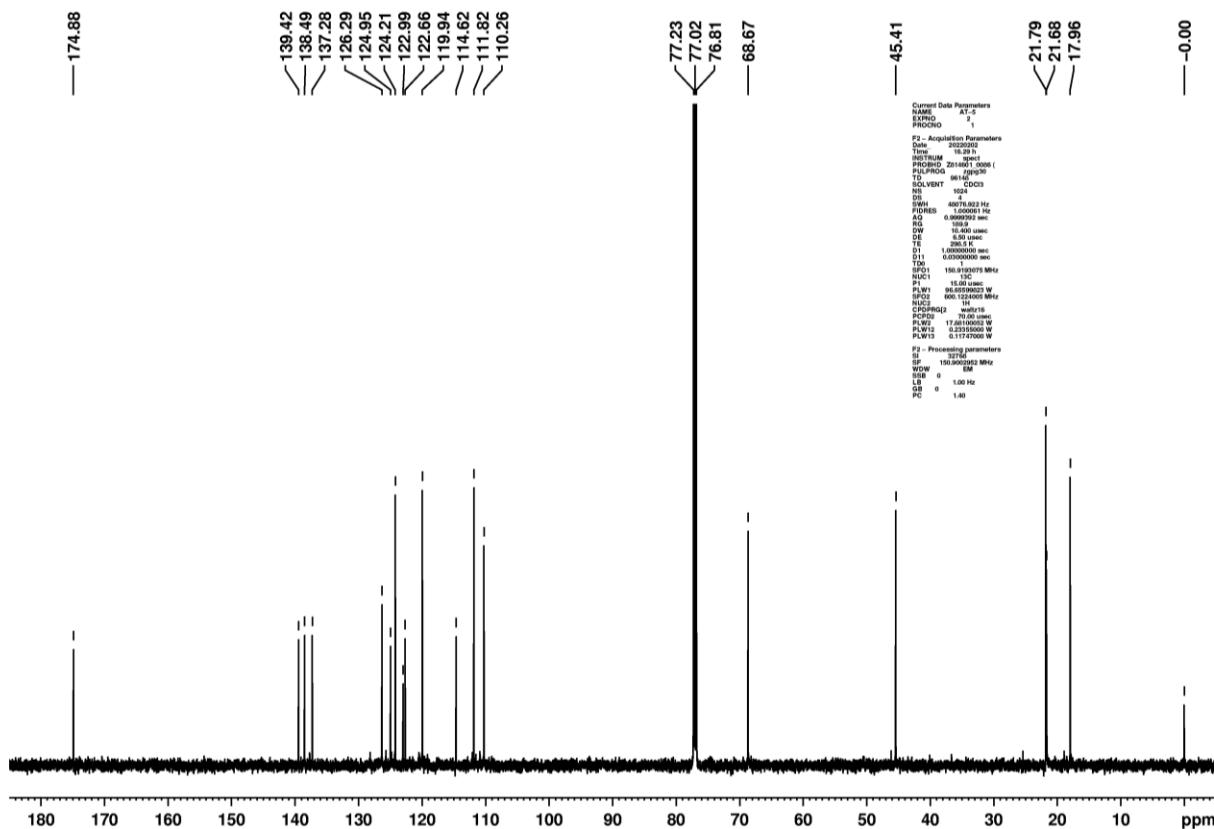
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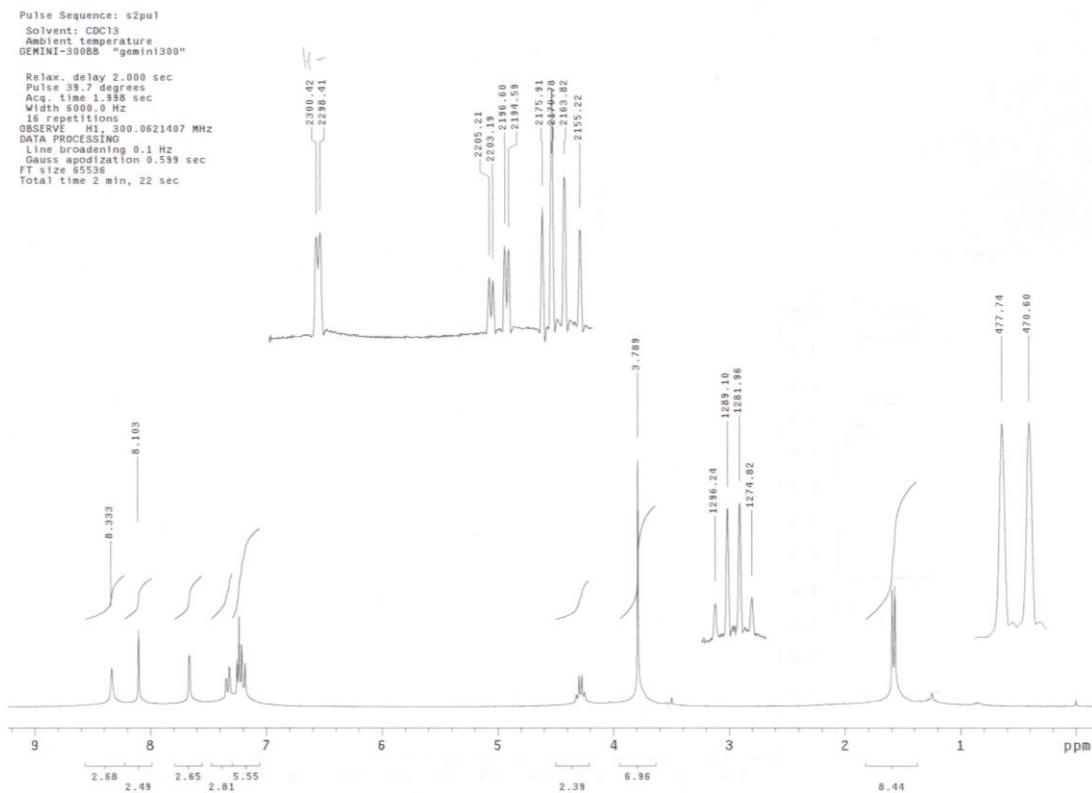
**Figure S5b.** The  $^{13}\text{C}$ -NMR spectrum of Ethyl 2-(3-Bromo-6-chloro-9H-carbazol-2-yl)propanoate (**6**).



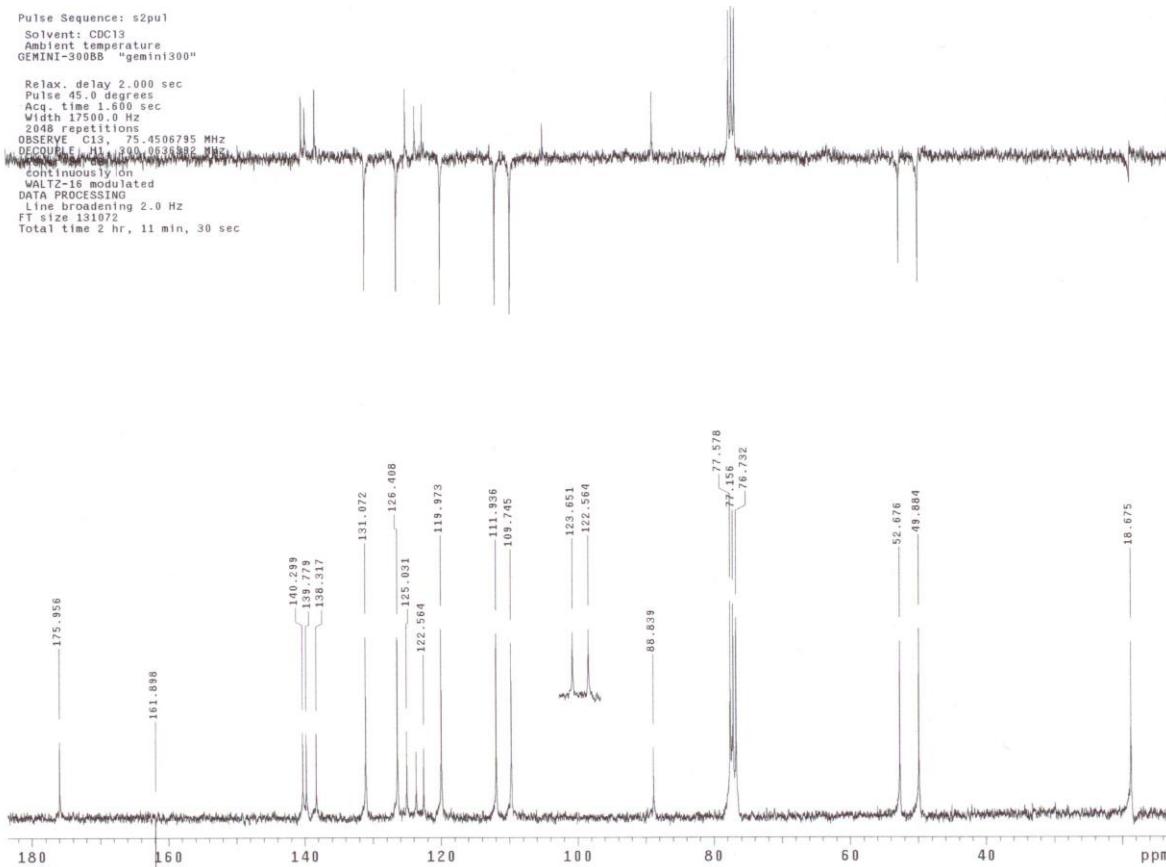
**Figure S6a.** The <sup>1</sup>H-NMR spectrum of Isopropyl 2-(3-Bromo-6-chloro-9H-carbazol-2-yl)propanoate (**7**).



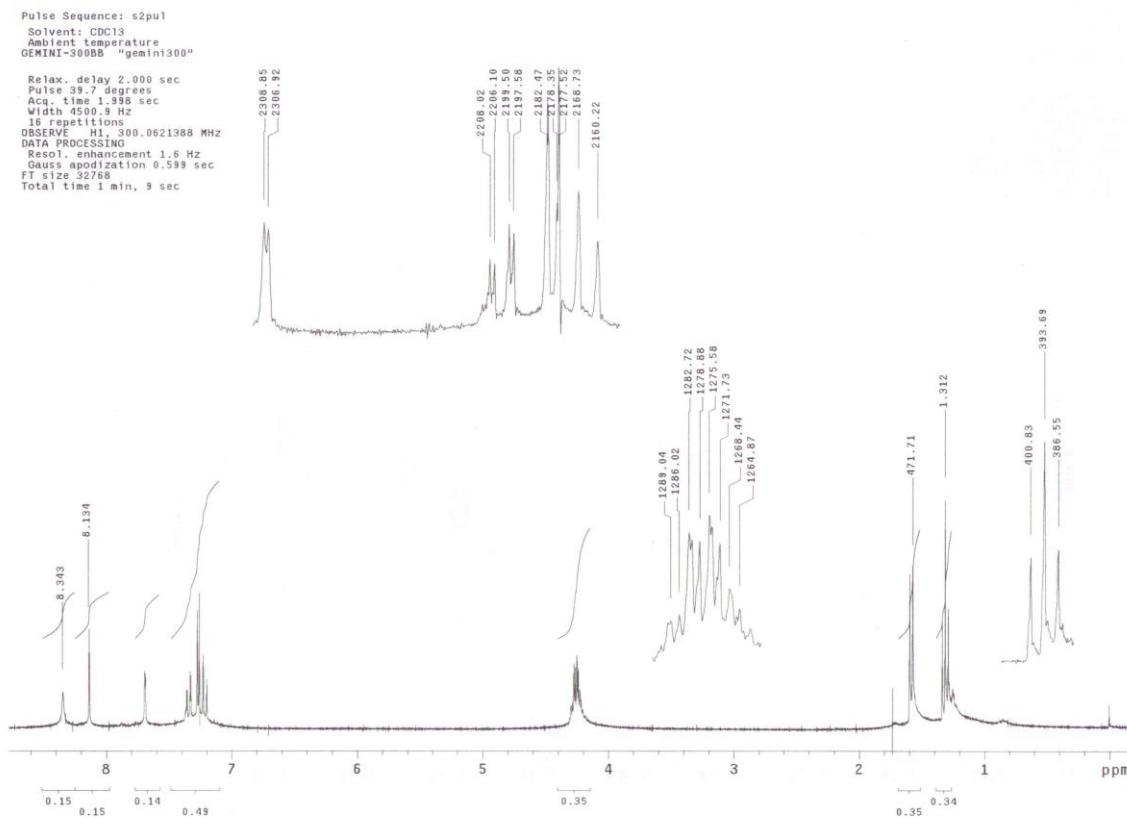
**Figure S6b.** The <sup>13</sup>C-NMR spectrum of Isopropyl 2-(3-Bromo-6-chloro-9H-carbazol-2-yl)propanoate (**7**).



**Figure S7a.** The  $^1\text{H}$ -NMR spectrum of Methyl 2-(3-iodo-6-chloro-9H-carbazol-2-yl)propanoate (**8**).



**Figure S7b.** The  $^{13}\text{C}$ -NMR spectrum of Methyl 2-(3-iodo-6-chloro-9H-carbazol-2-yl)propanoate (**8**).



**Figure S8a.** The  $^1\text{H}$ -NMR spectrum of Ethyl 2-(3-iodo-6-chloro-9H-carbazol-2-yl)propanoate (**9**).

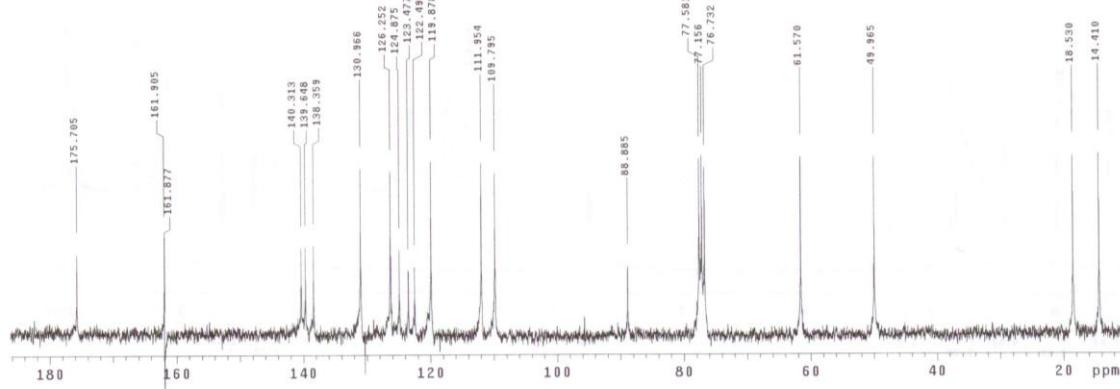
Pulse Sequence: s2pu1  
Solvent: CDCl<sub>3</sub>  
Ambient temperature  
GEMINI-300BB "gemini300"

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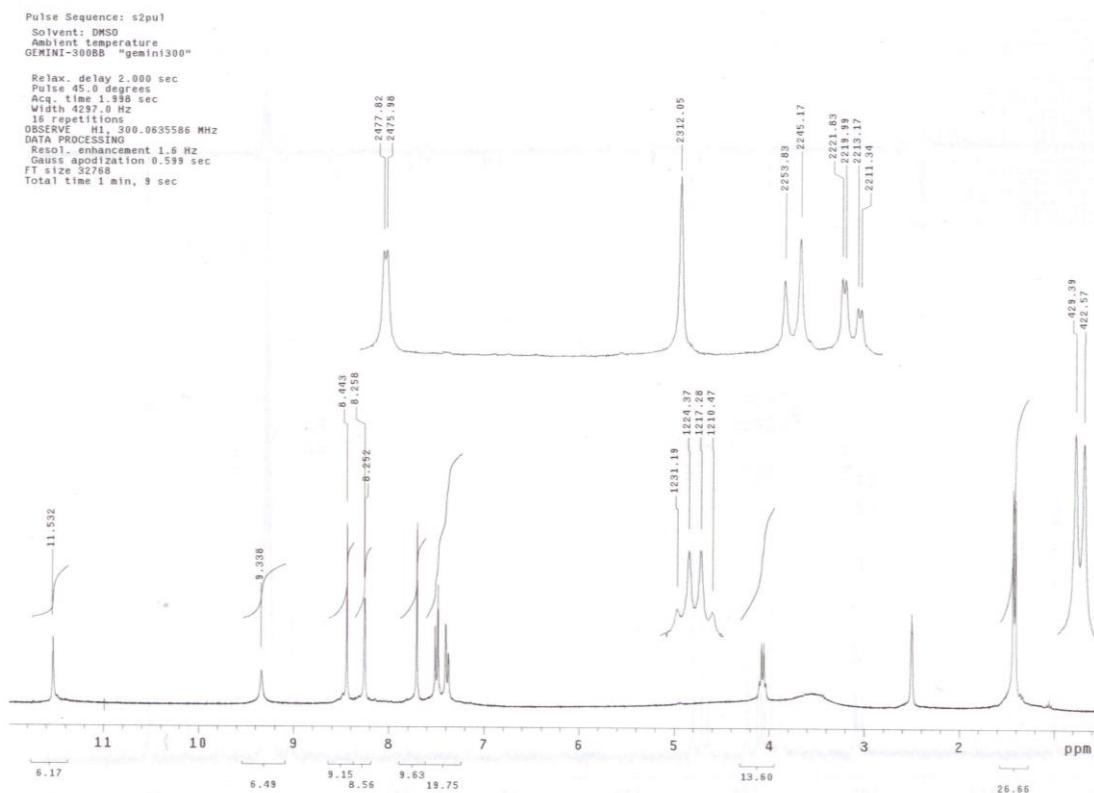
Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 1.560 sec
Width 17500.0 Hz
928 repetitions
OBSERVE C13, 75.4556801 MHz
DECOPULE H1, 300.6636392 MHz
SWP 57.0
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072

Total time 2 hr, 11 min, 30 sec

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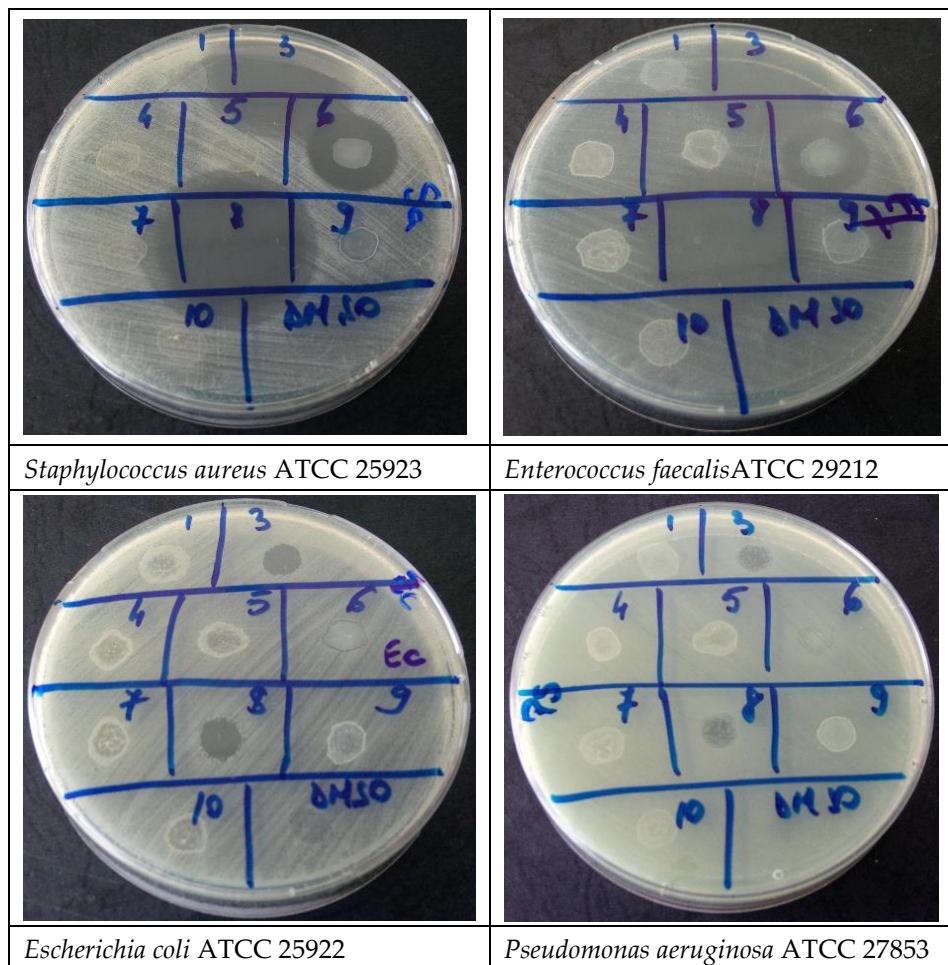
**Figure S8b.** The  $^{13}\text{C}$ -NMR spectrum of Ethyl 2-(3-iodo-6-chloro-9H-carbazol-2-yl)propanoate (**9**).



**Figure S9a.** The  $^1\text{H}$ -NMR spectrum of Hydrazide of 2-(3-Bromo-6-chloro-9H-carbazol-2-yl)propanoic acid (**10**).



**Figure S9b.** The  $^1\text{H}$ -NMR spectrum of Hydrazide of 2-(3-Bromo-6-chloro-9H-carbazol-2-yl)propanoic acid (**10**).



**Figure S10.** The Qualitative screening of the antimicrobial activity of the tested compounds (1- compound 4; 3- compound 2; 4- compound 5; 5- compound 7; 6- compound 10; 7- compound 6; 8- compound 3; 9- compound 8; 10- compound 9).