

Supporting information

Synthesis of novel heterocyclic oleanolic acid derivatives with improved antiproliferative activity in solid tumor cells

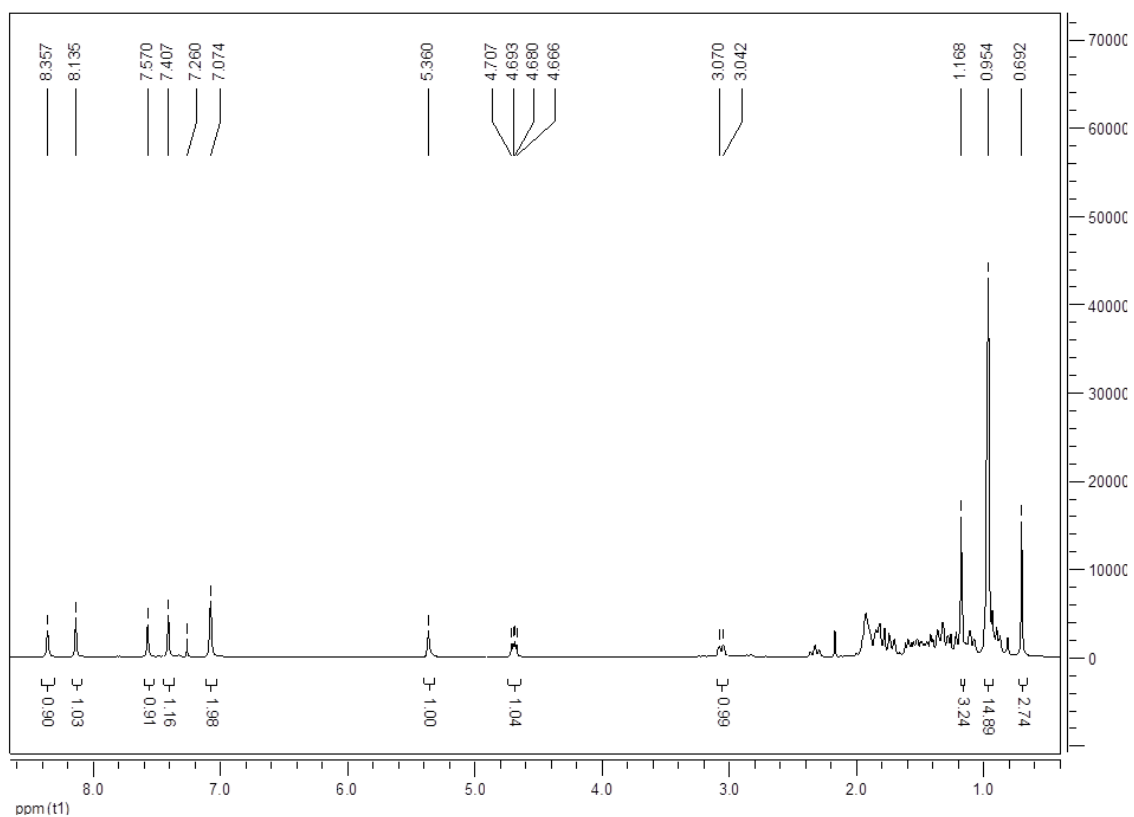
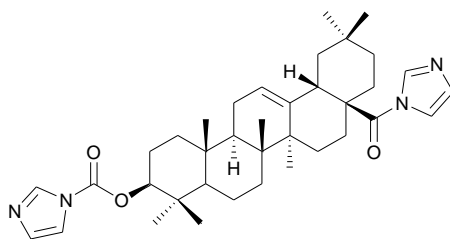
Ana S. Leal, Jorge A.R. Salvador and Yongkui Jing

Table of contents

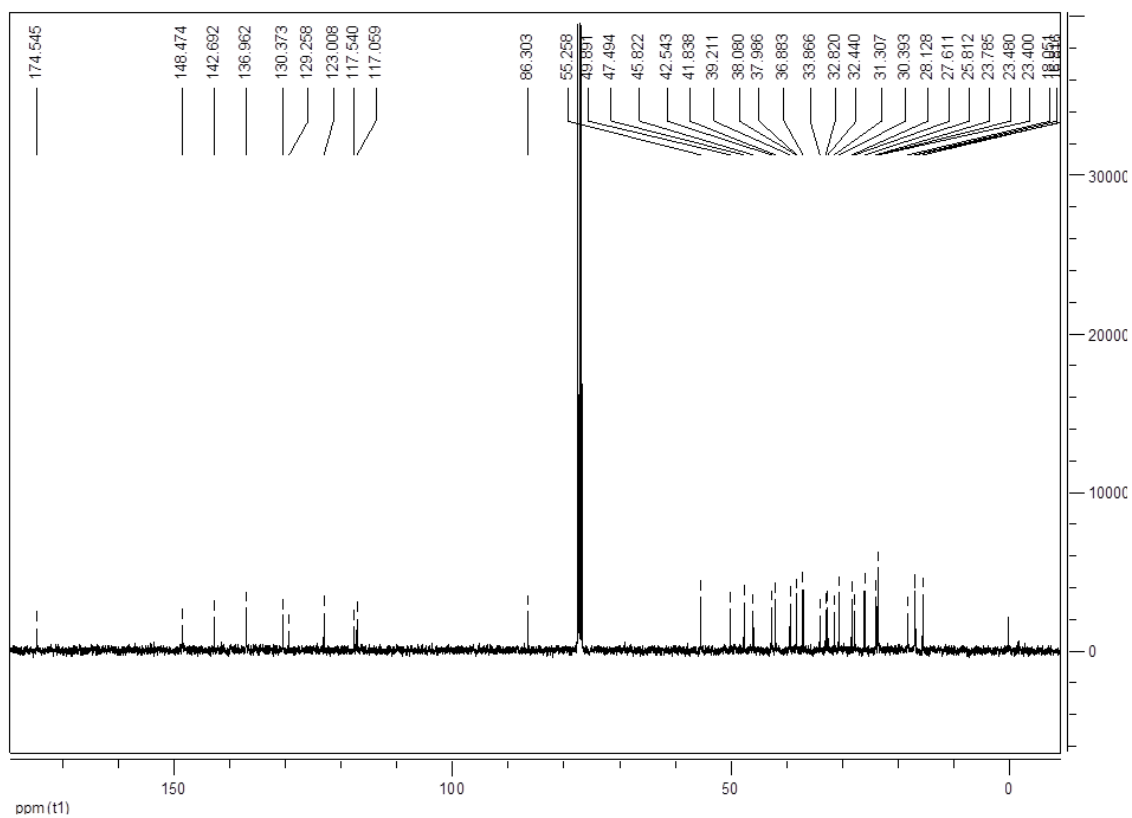
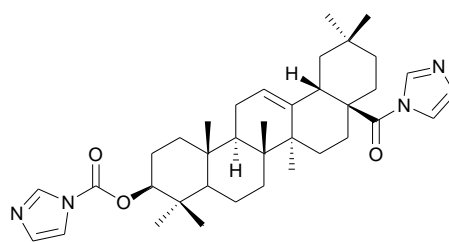
1. Spectral data for compound 15	S2
2. Spectral data for compound 16	S6
3. Spectral data for compound 17	S12
4. Spectral data for compound 18	S18
5. Spectral data for compound 19	S24
6. Spectral data for compound 20	S28
7. Spectral data for compound 21	S34
8. Spectral data for compound 22	S40
9. Spectral data for compound 23	S44
10. Spectral data for compound 24	S48
11. Spectral data for compound 25	S52
11. Spectral data for compound 26	S56
13. Spectral data for compound 27	S62
14. Spectral data for compound 28	S68

1. Spectral data for compound **15**

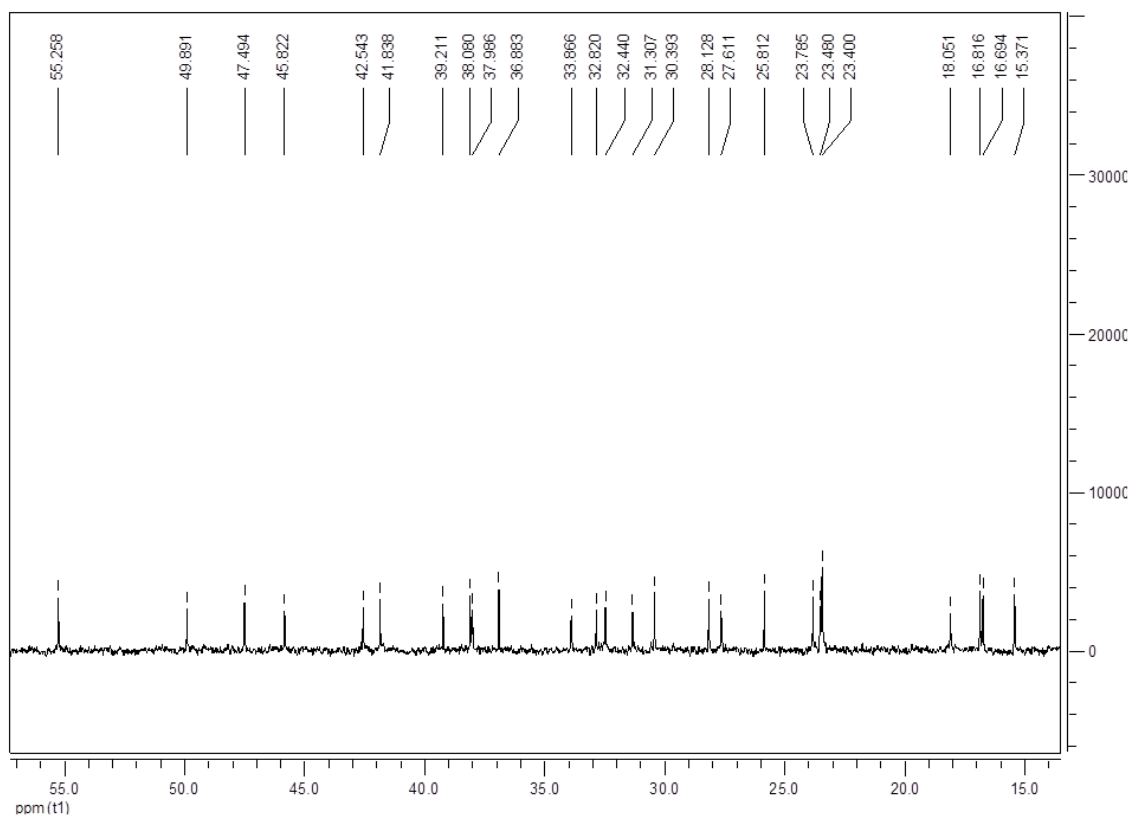
^1H NMR spectrum for compound **15** recorded in CDCl_3 .



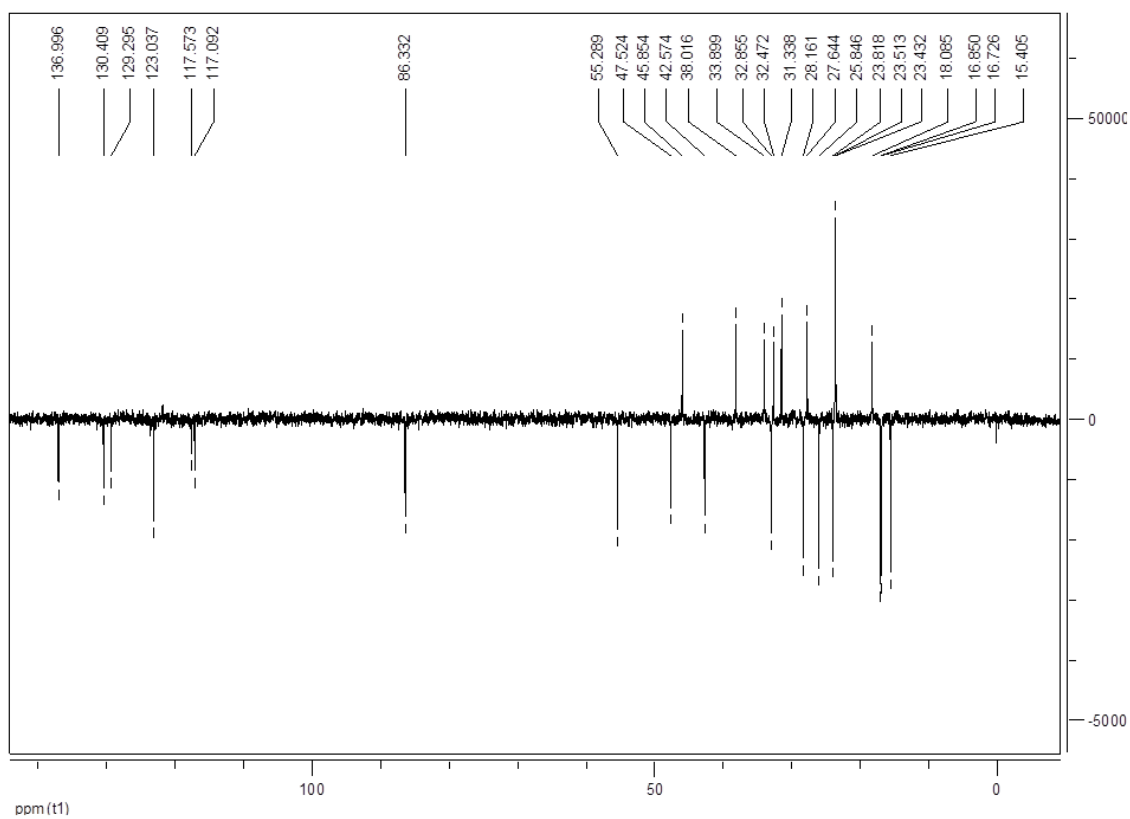
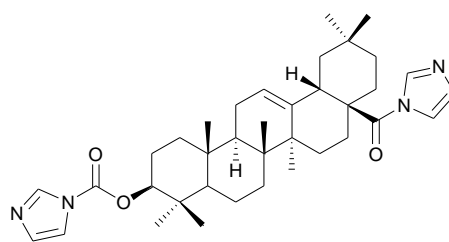
^{13}C NMR spectrum for compound **15** recorded in CDCl_3 .



^{13}C NMR spectrum detail of compound **15**.

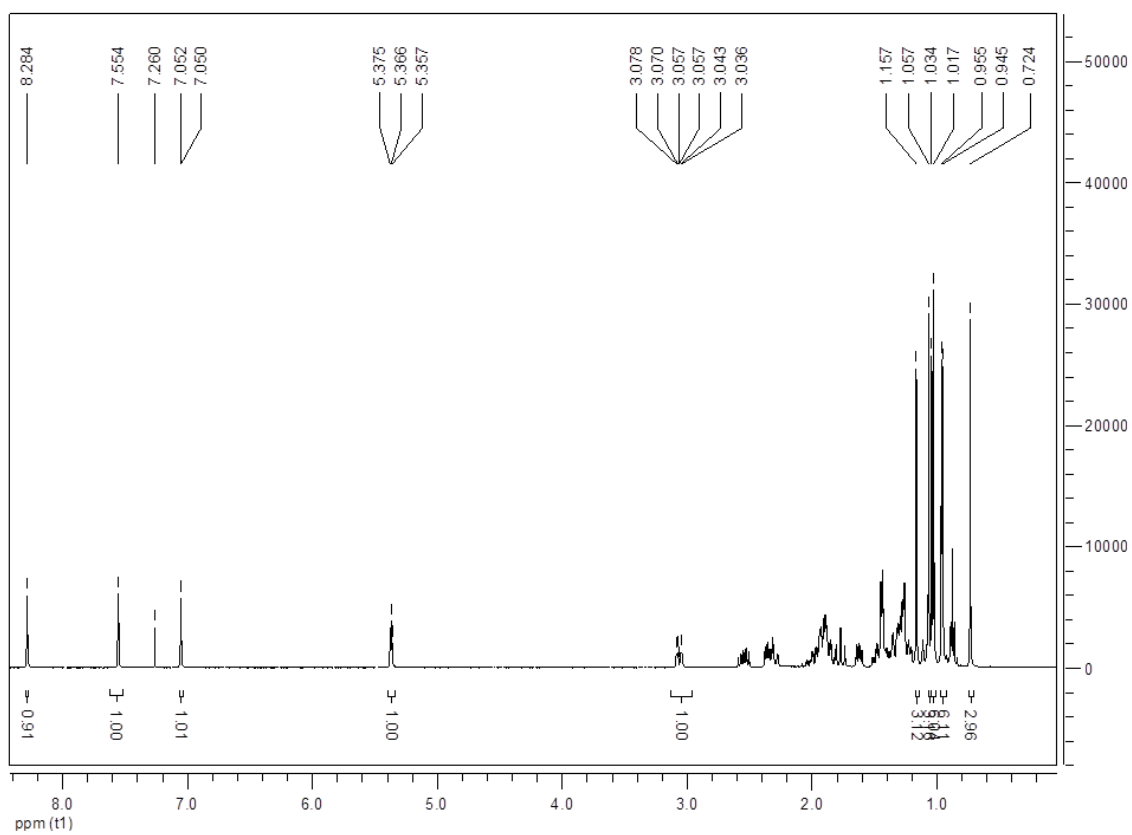
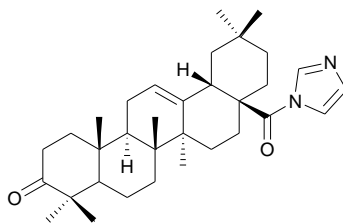


DEPT-135 NMR spectrum for compound **15** recorded in CDCl₃

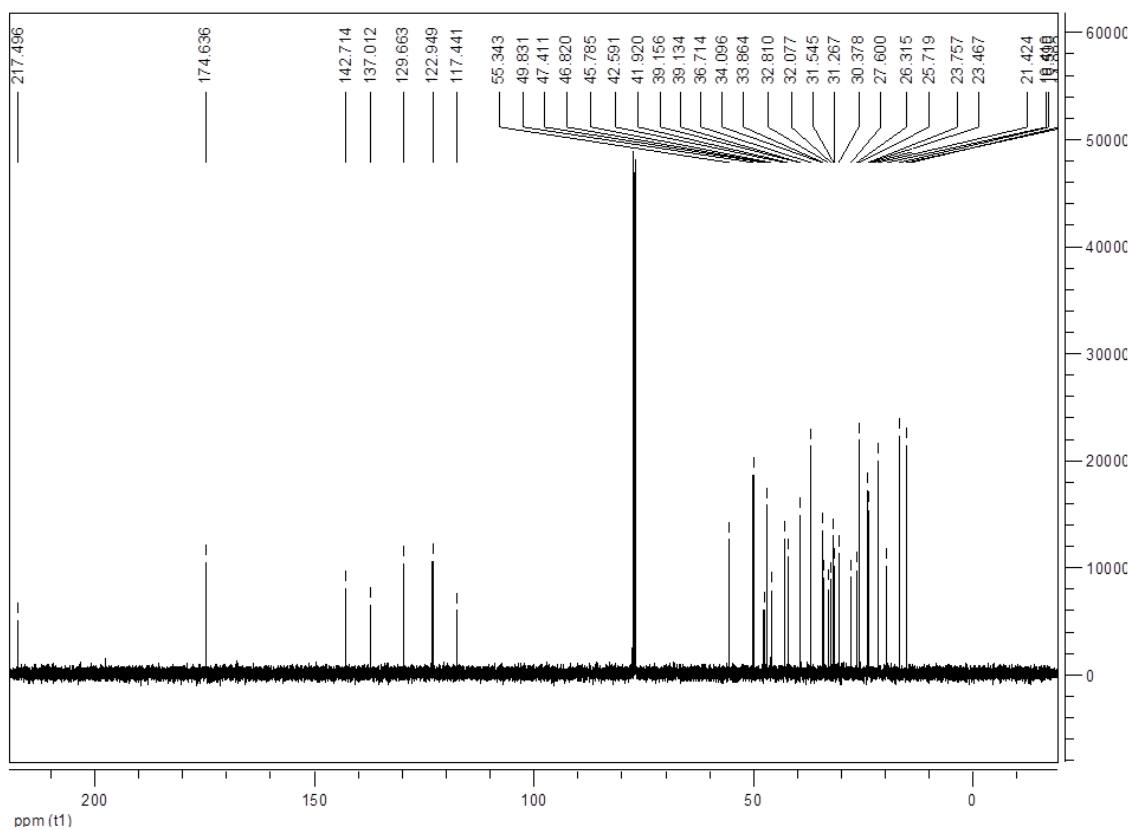
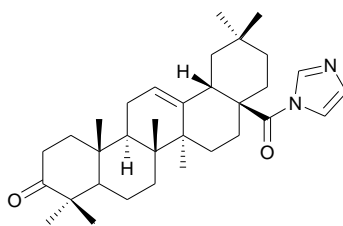


2. Spectral data for compound 16

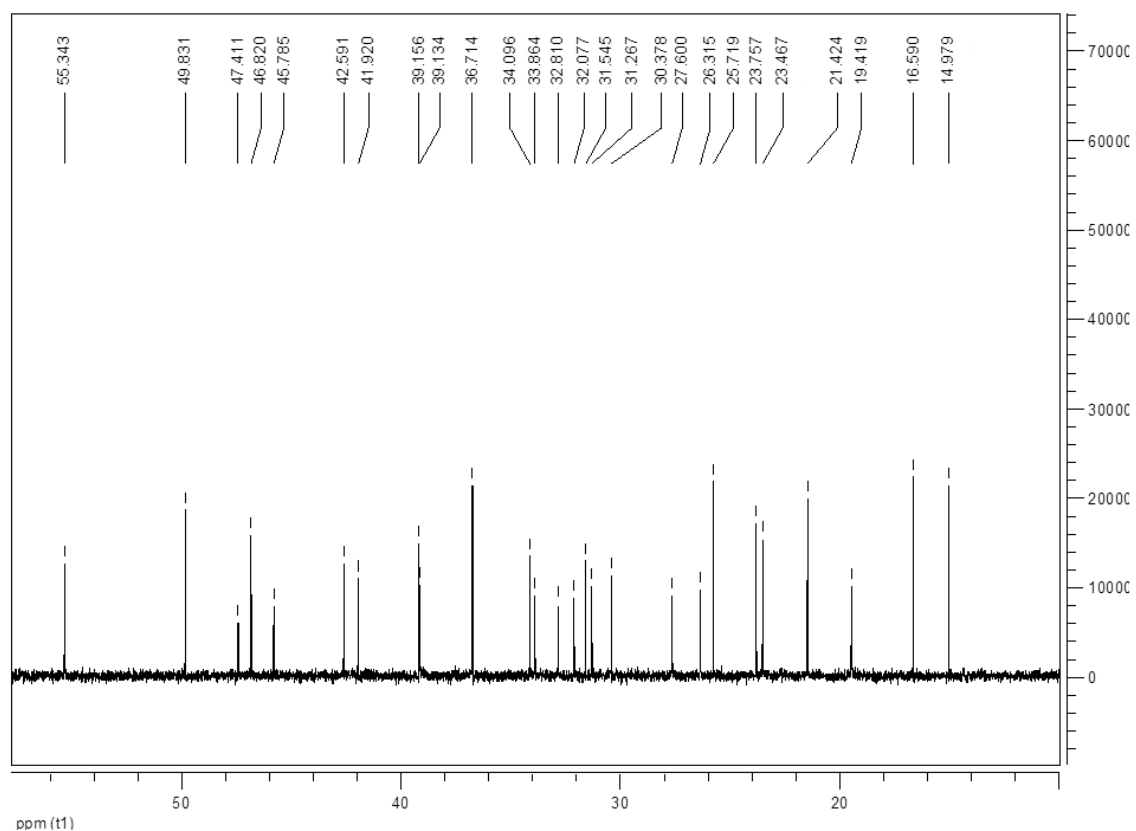
^1H NMR spectrum for compound **16** recorded in CDCl_3 .



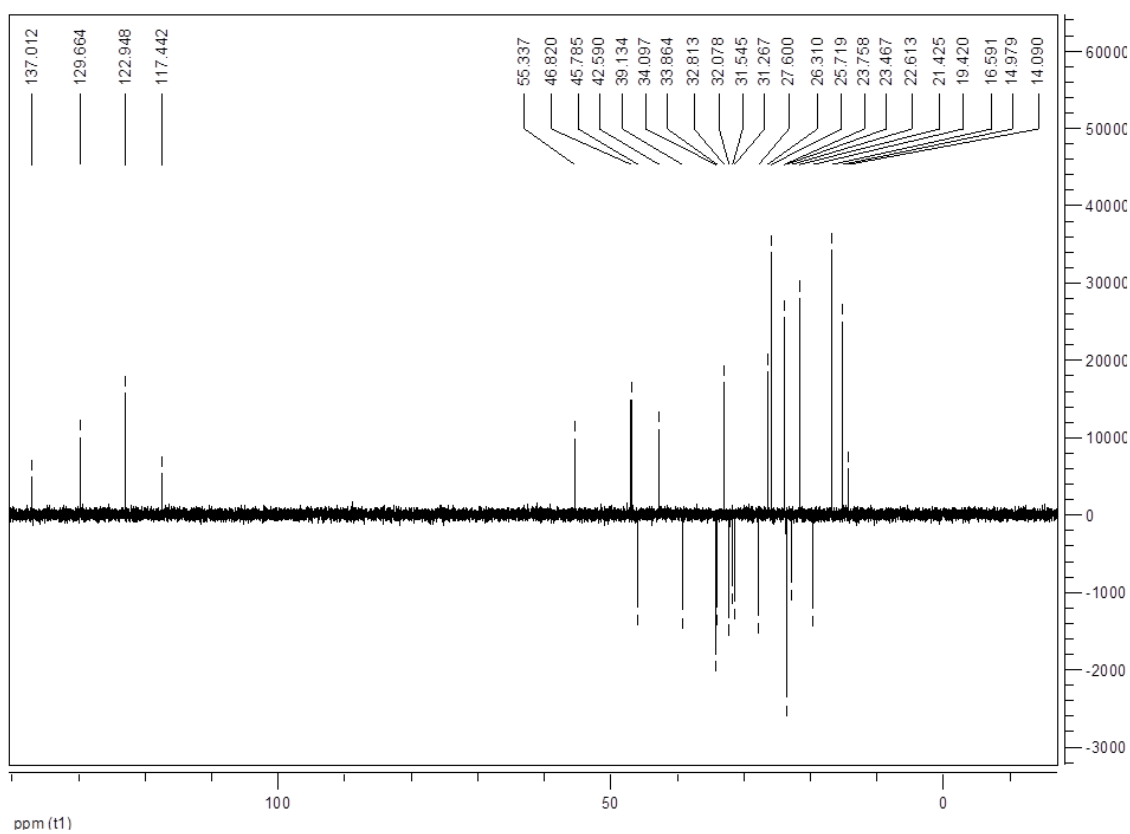
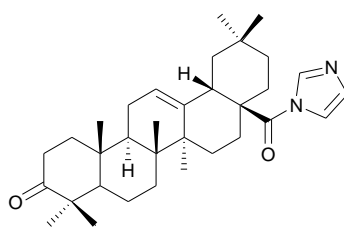
^{13}C NMR spectrum for compound **16** recorded in CDCl_3 .



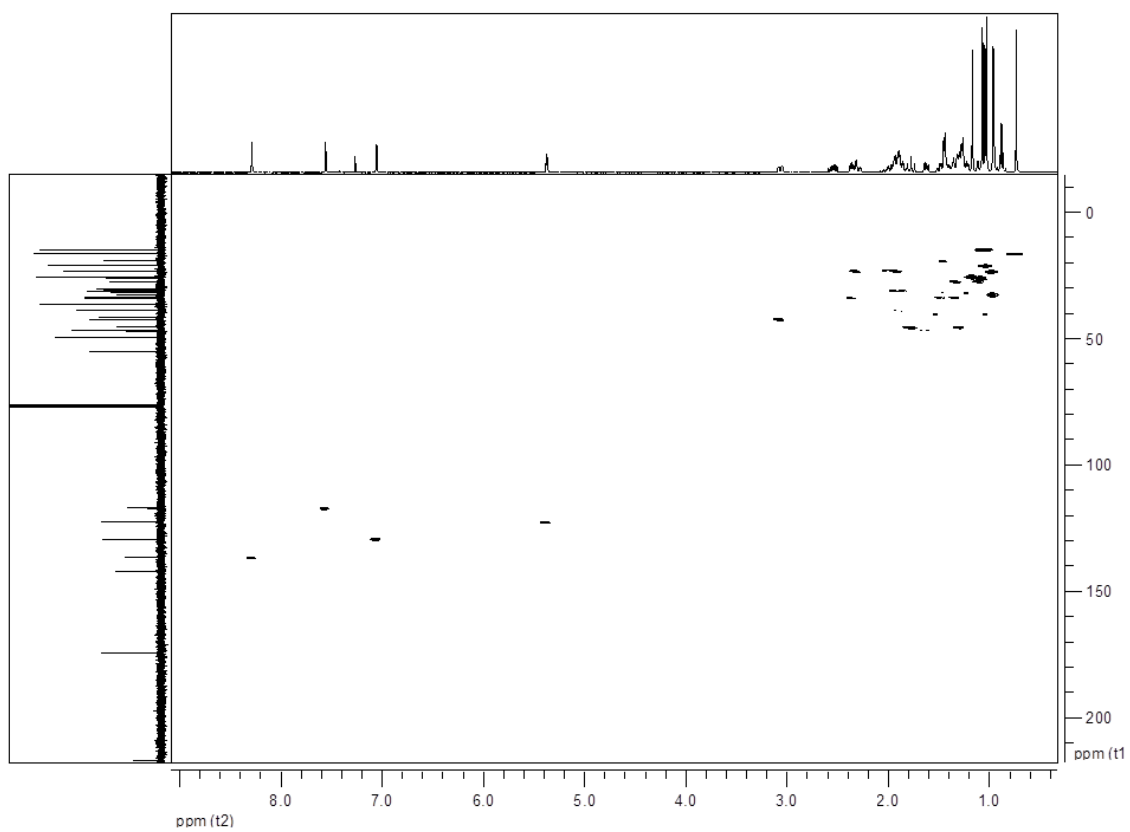
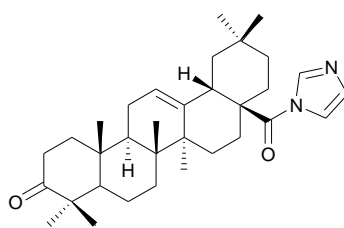
^{13}C NMR spectrum detail of compound **16**.



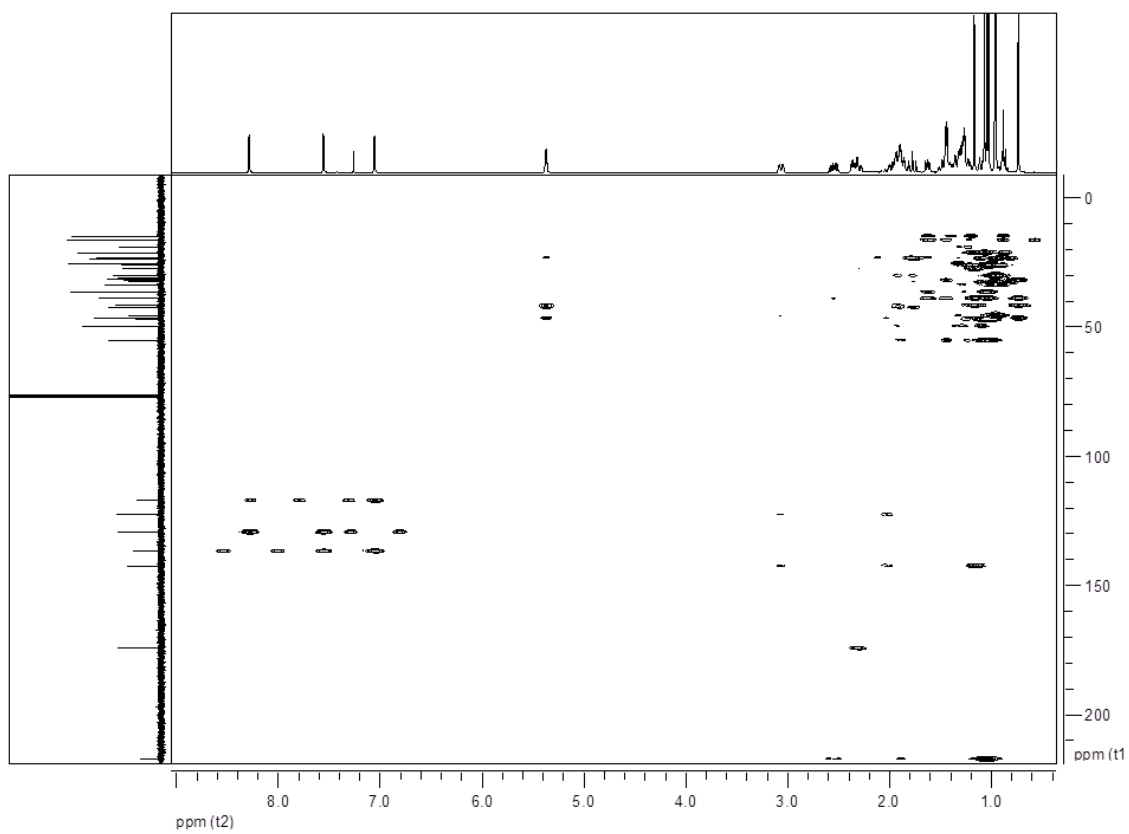
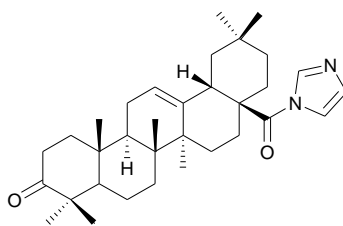
DEPT-135 NMR spectrum for compound **16** recorded in CDCl₃.



HMQC NMR spectrum for compound **16** recorded in CDCl₃.

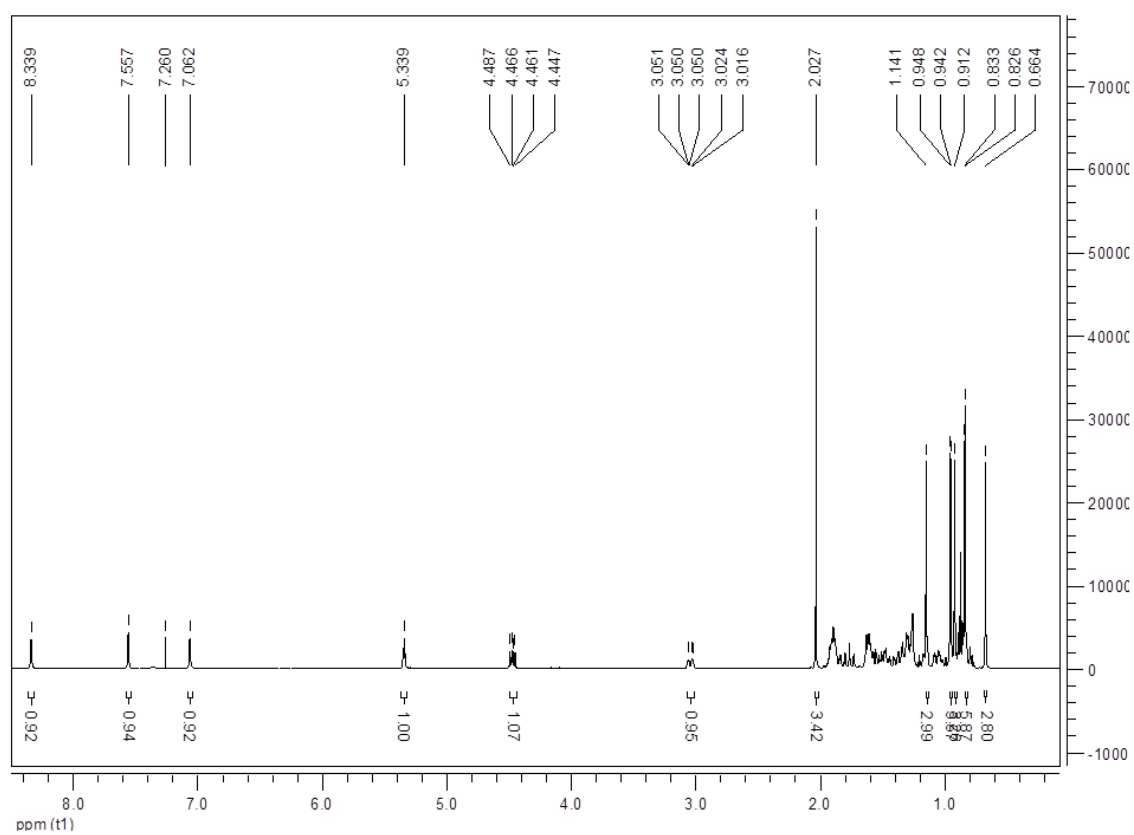
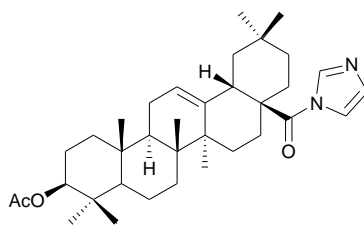


HMBC NMR spectrum for compound **16** recorded in CDCl₃.

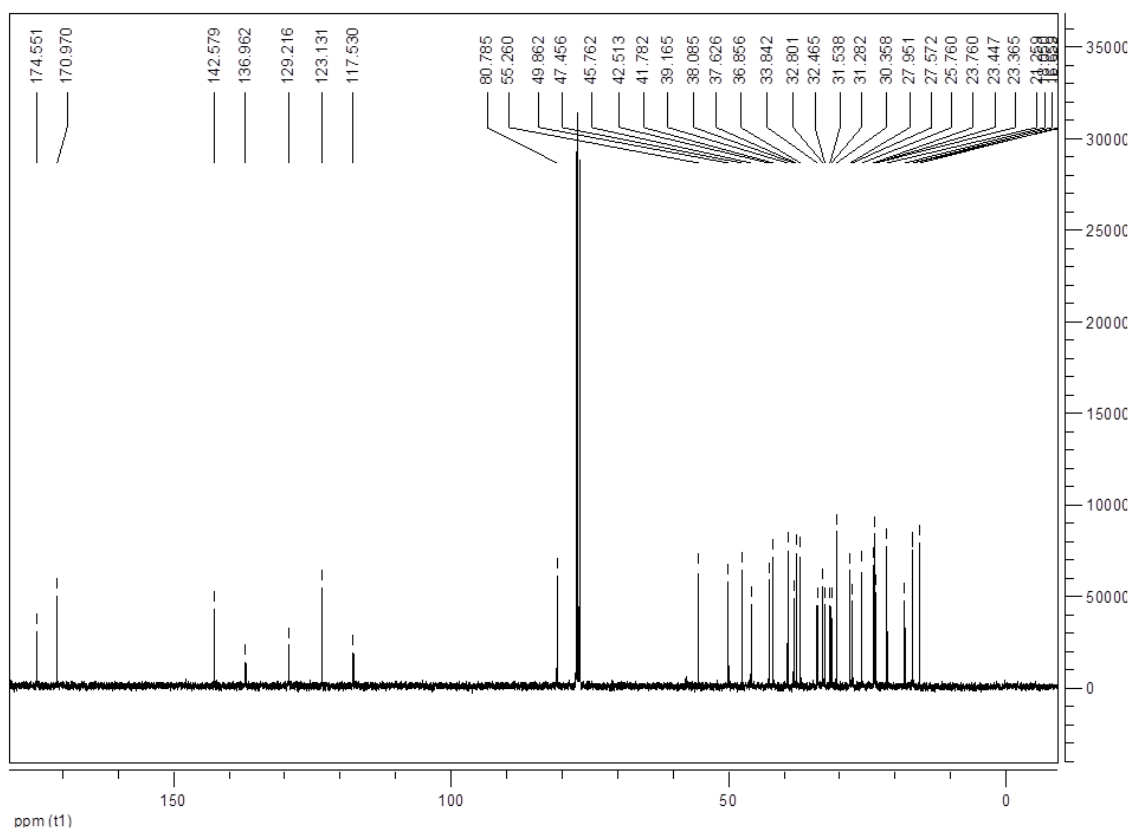
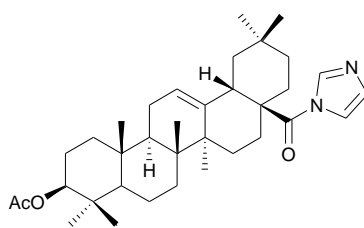


3. Spectral data for compound 17

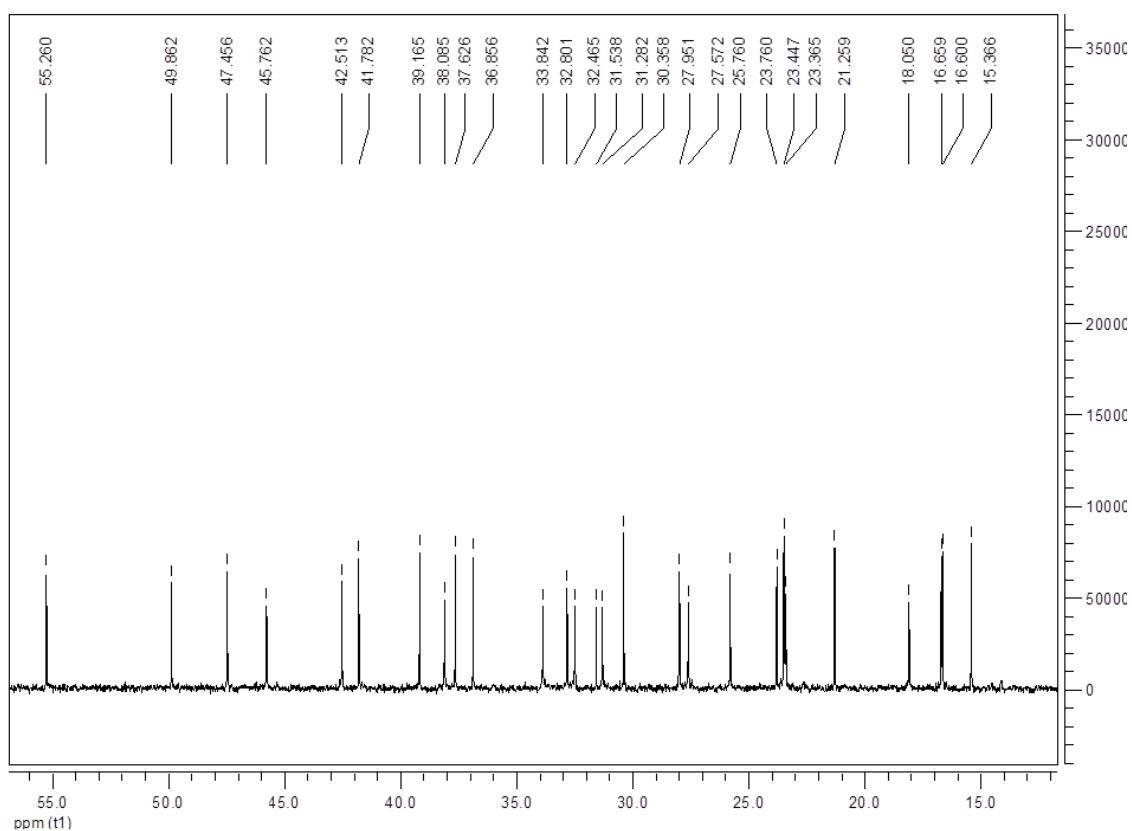
^1H NMR spectrum for compound 17 recorded in CDCl_3 .



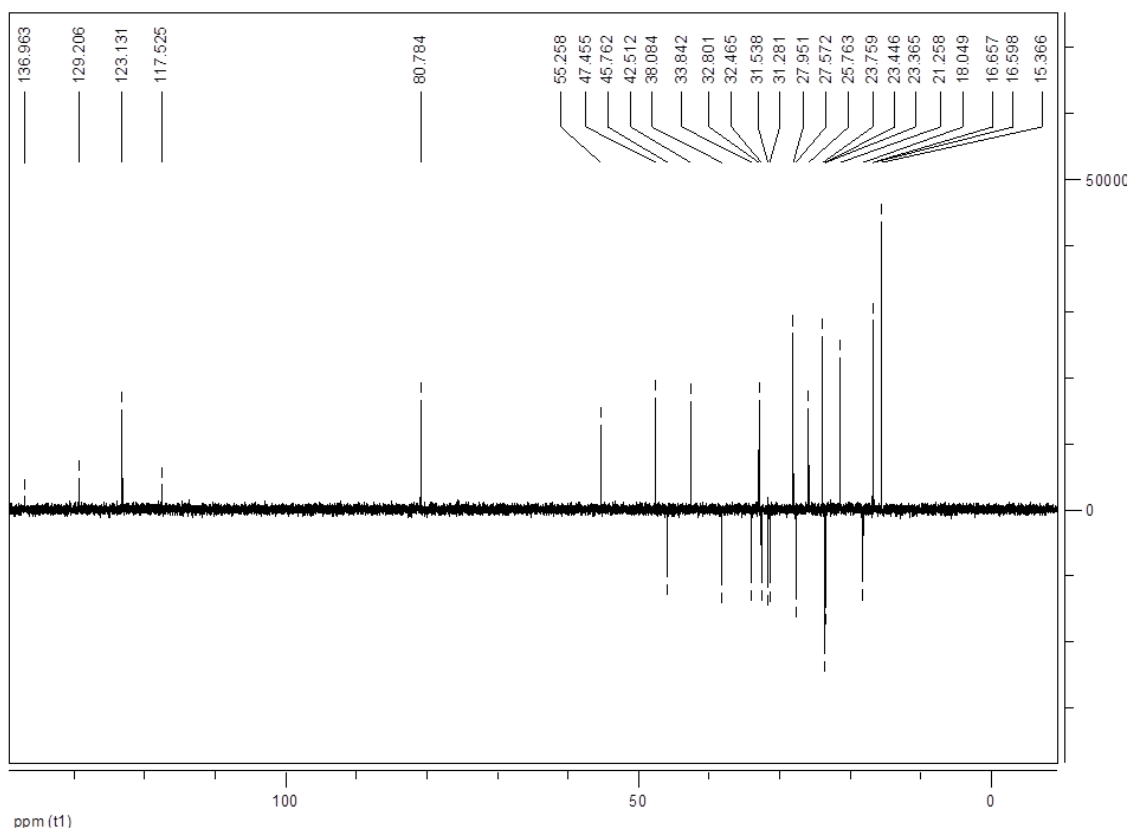
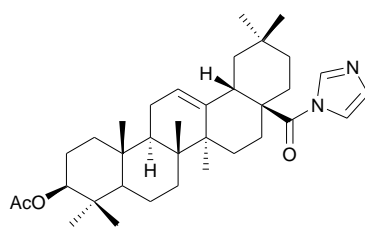
^{13}C NMR spectrum for compound **17** recorded in CDCl_3 .



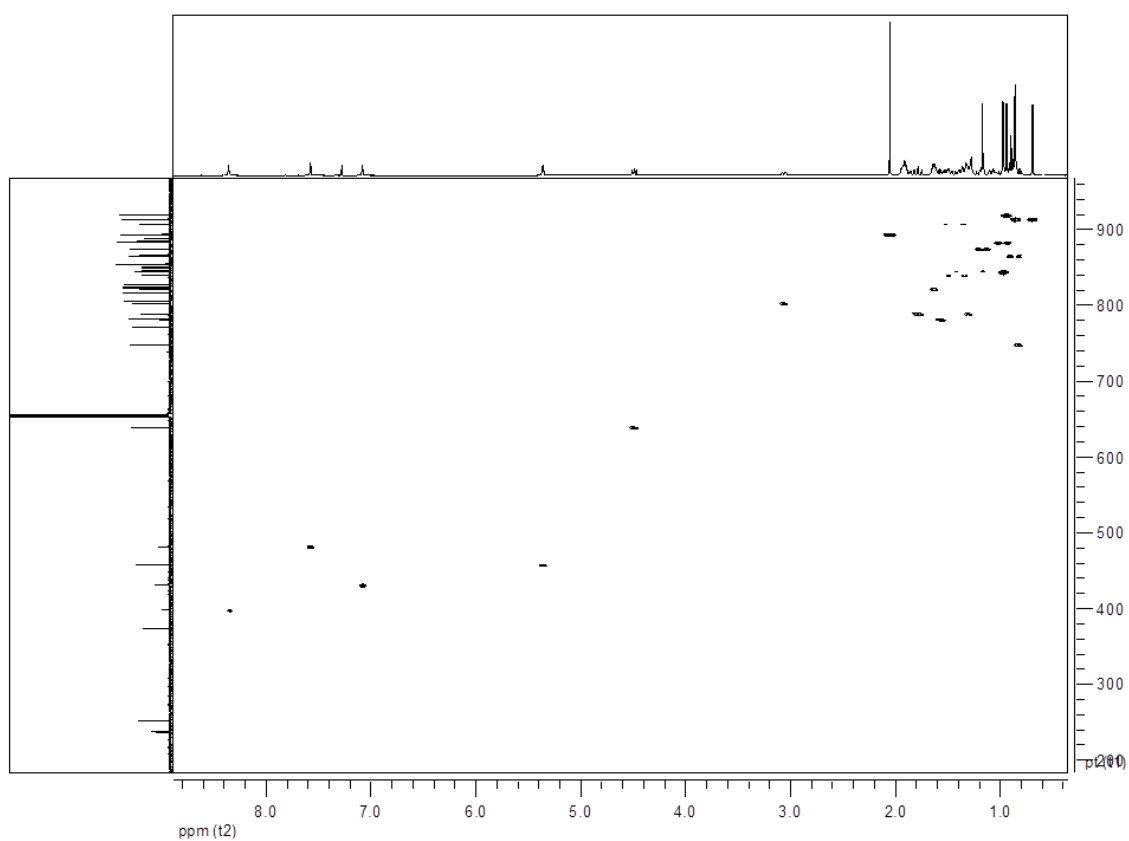
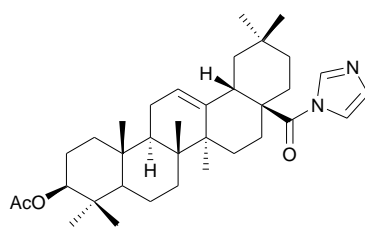
^{13}C NMR spectrum detail of compound **17**.



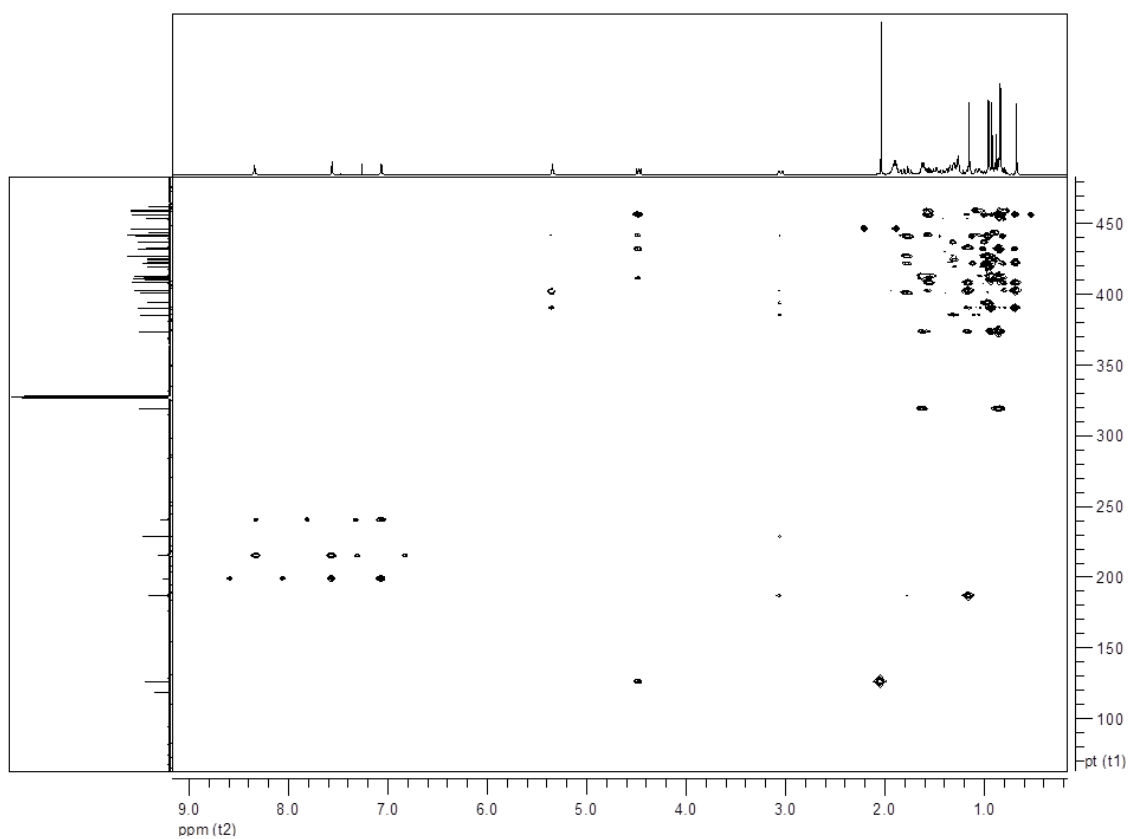
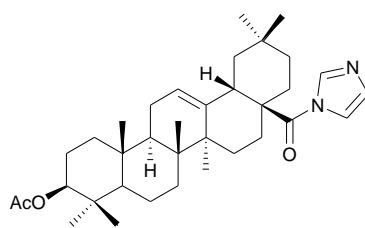
DEPT-135 NMR spectrum for compound **17** recorded in CDCl₃.



HMQC NMR spectrum for compound **17** recorded in CDCl₃.

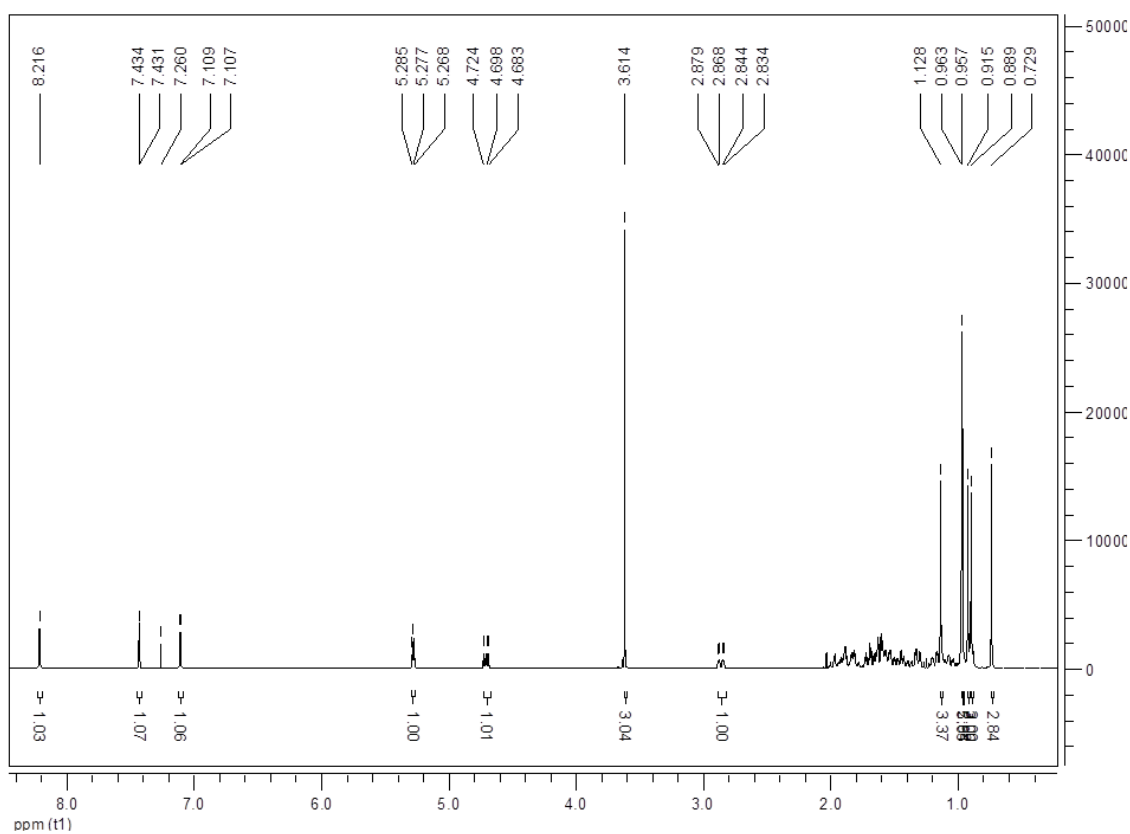
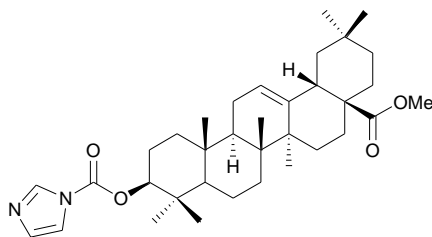


HMBC NMR spectrum for compound **17** recorded in CDCl₃.

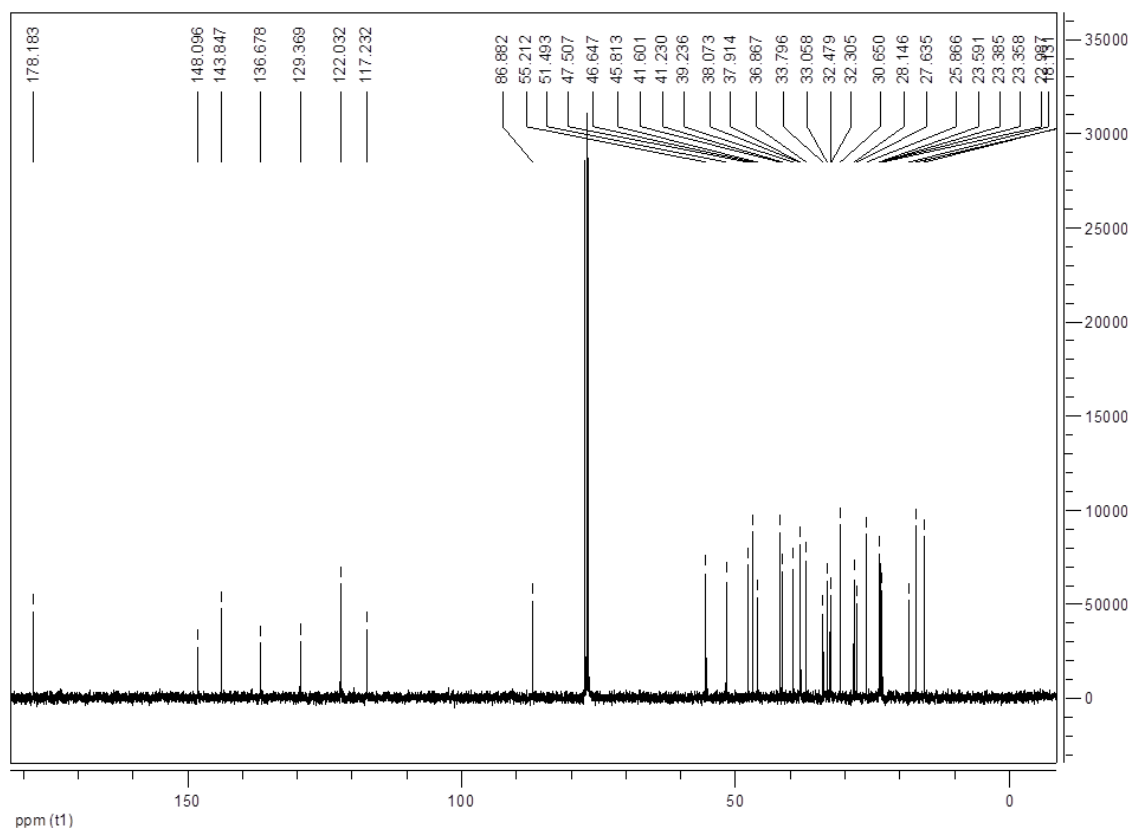
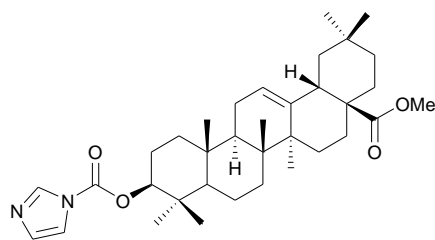


4. Spectral data for compound **18**

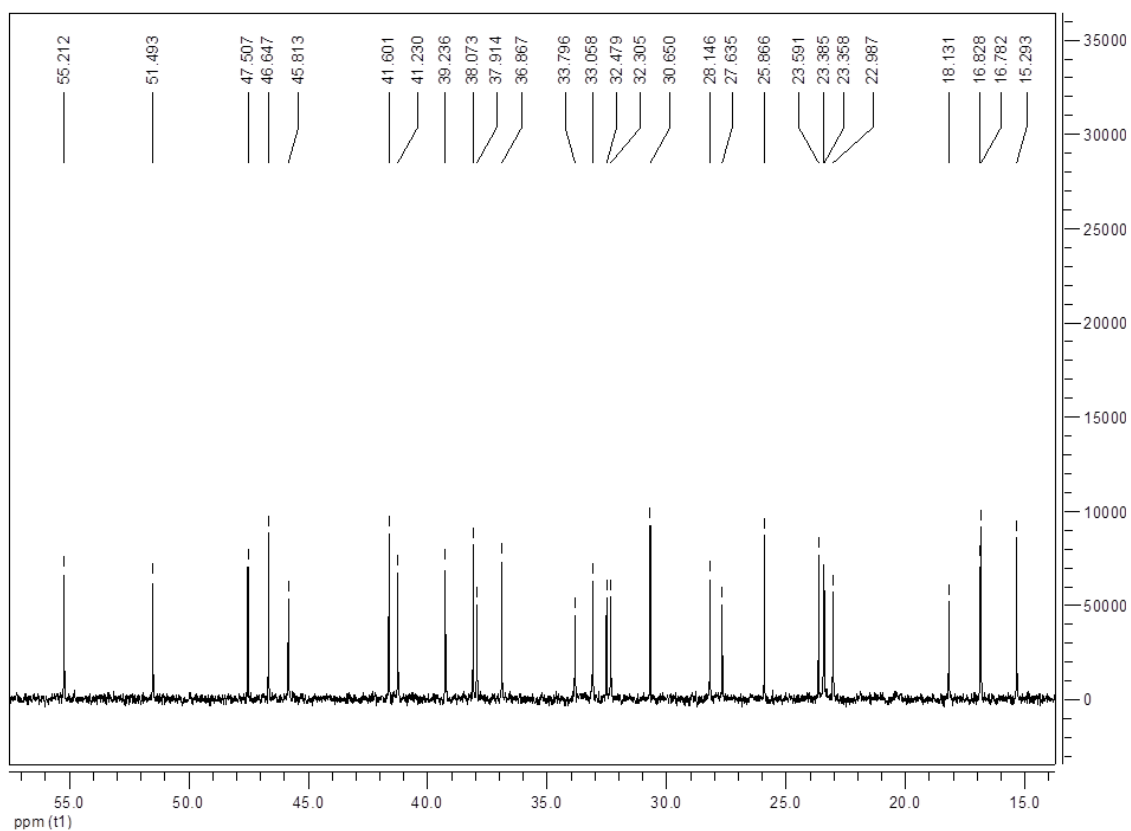
^1H NMR spectrum for compound **18** recorded in CDCl_3 .



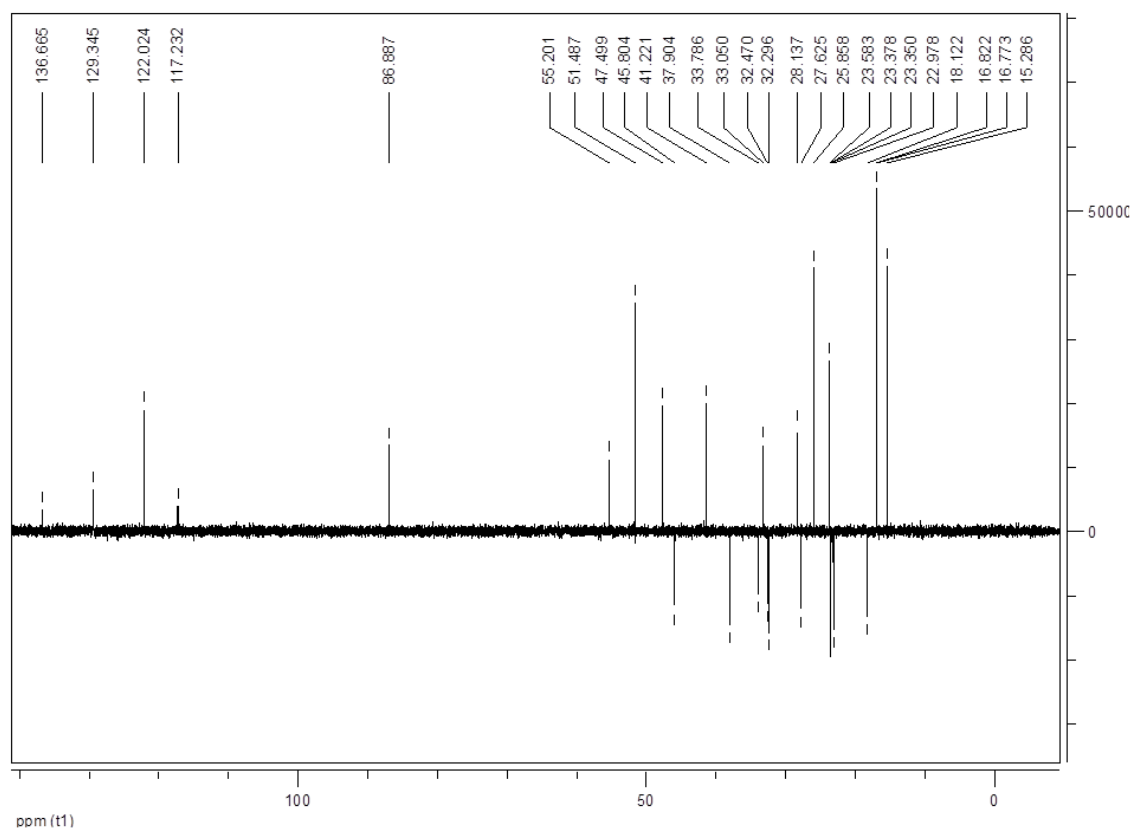
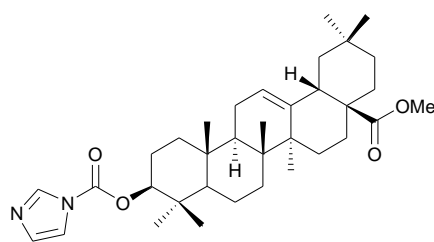
^{13}C NMR spectrum for compound **18** recorded in CDCl_3 .



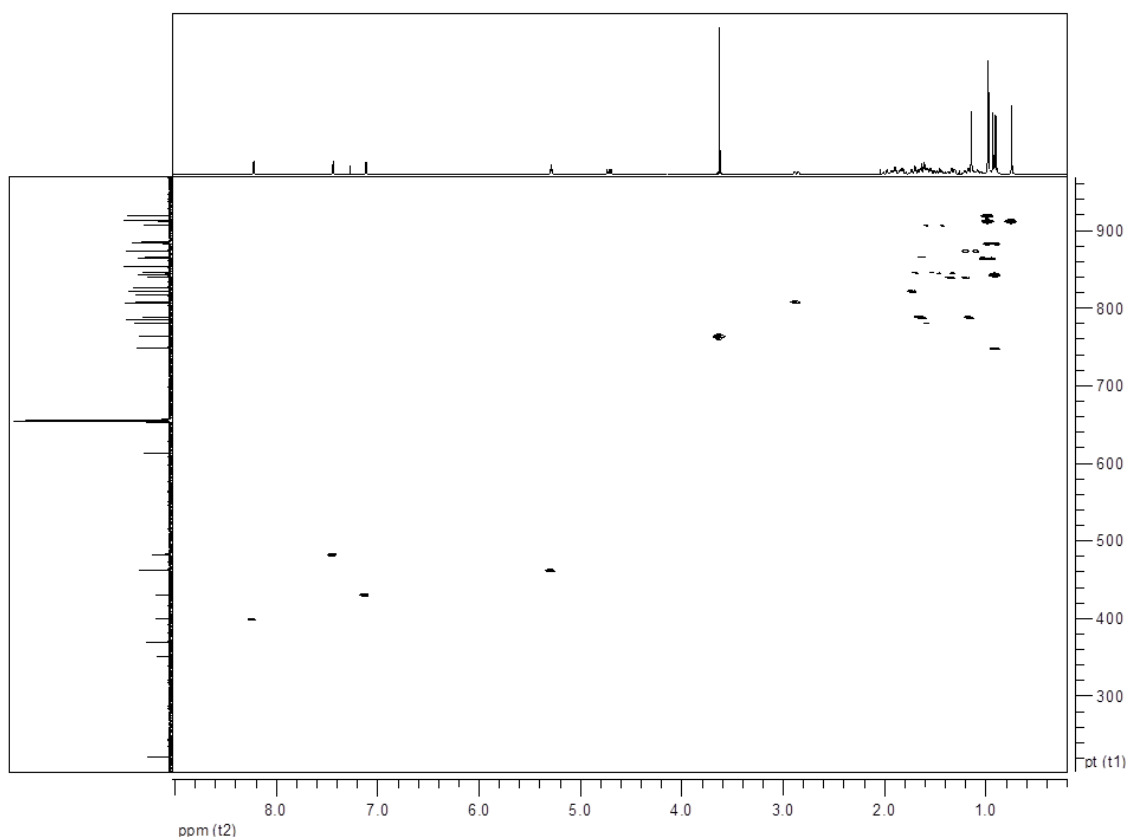
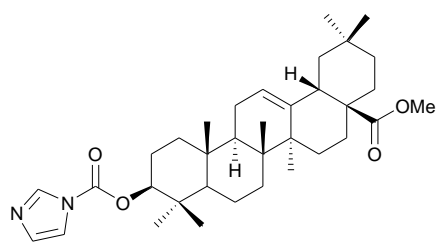
^{13}C NMR spectrum detail of compound **18**.



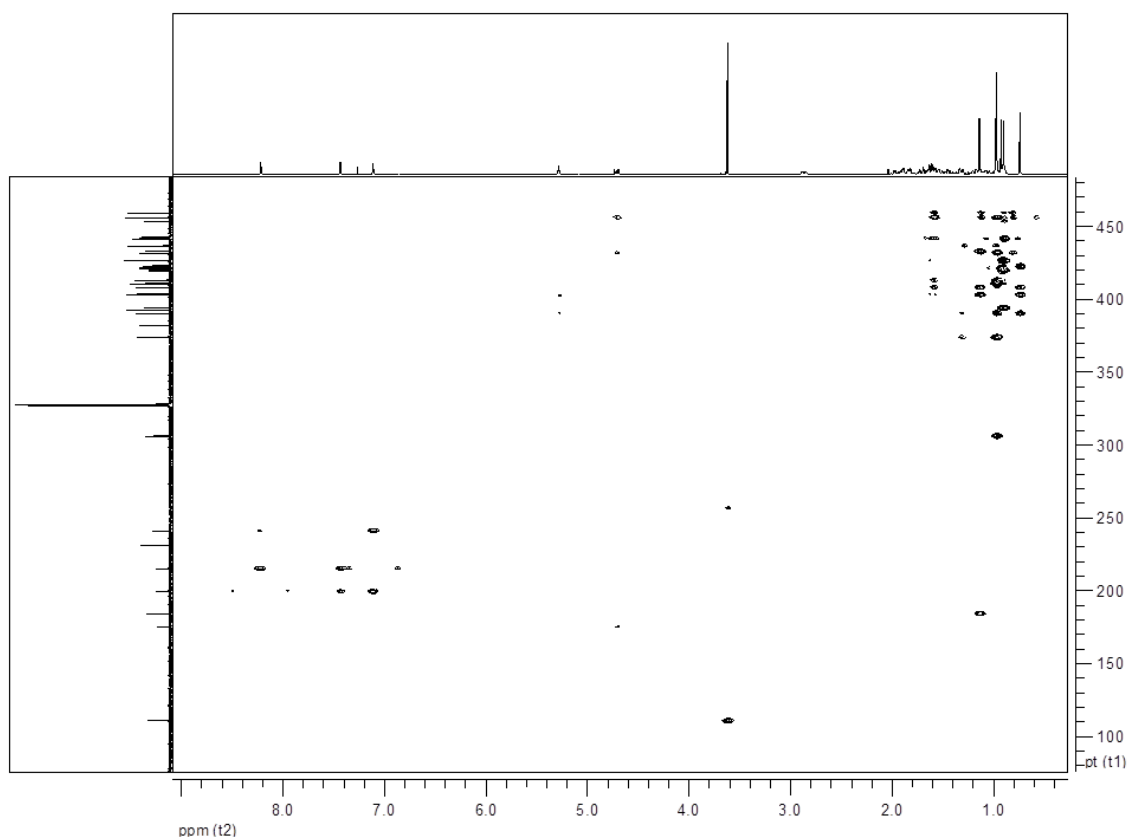
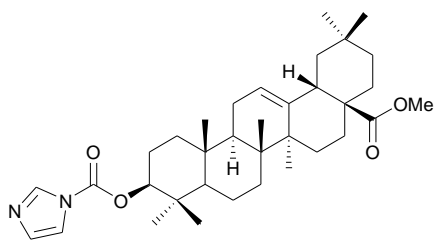
DEPT-135 NMR spectrum for compound **18** recorded in CDCl₃.



HMQC NMR spectrum for compound **18** recorded in CDCl₃.

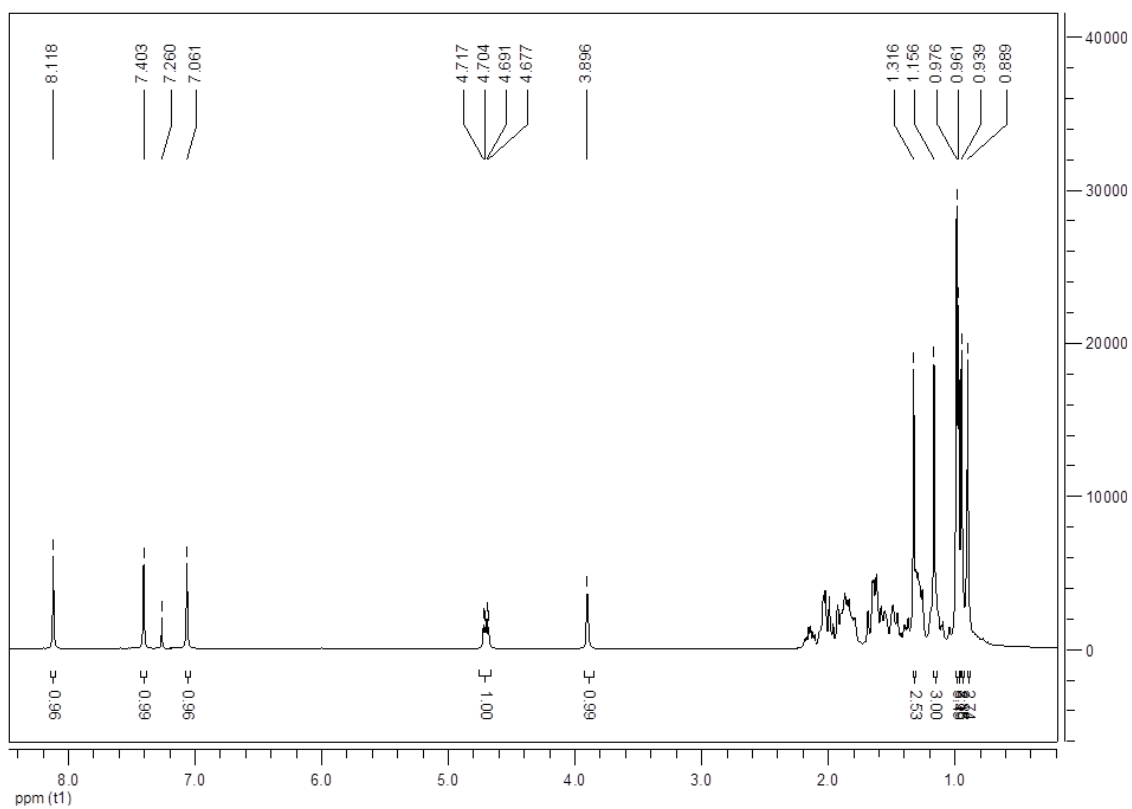
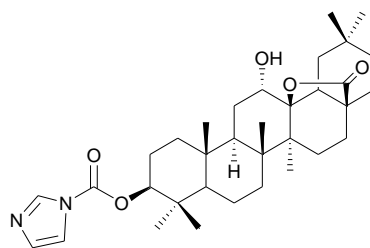


HMBC NMR spectrum for compound **18** recorded in CDCl₃.

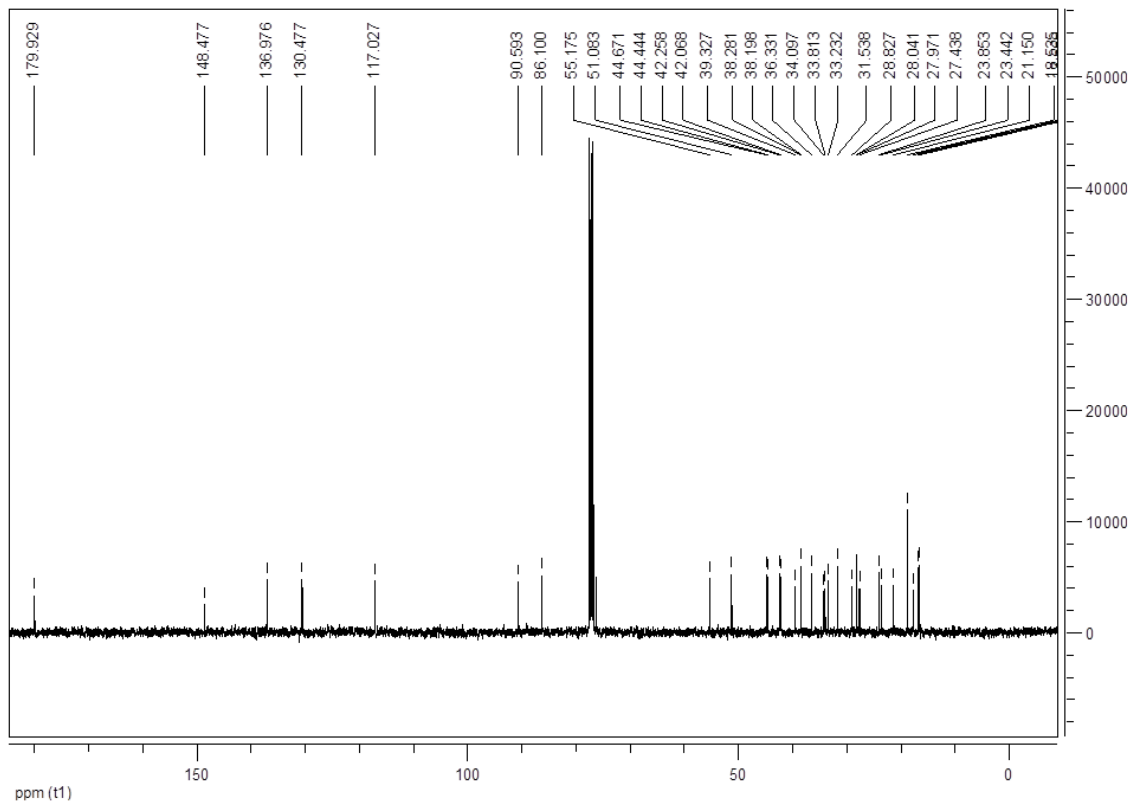
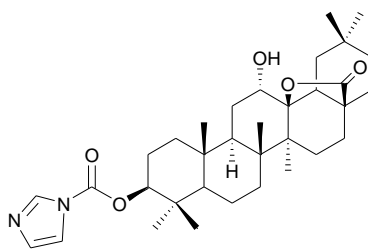


5. Spectral data for compound **19**

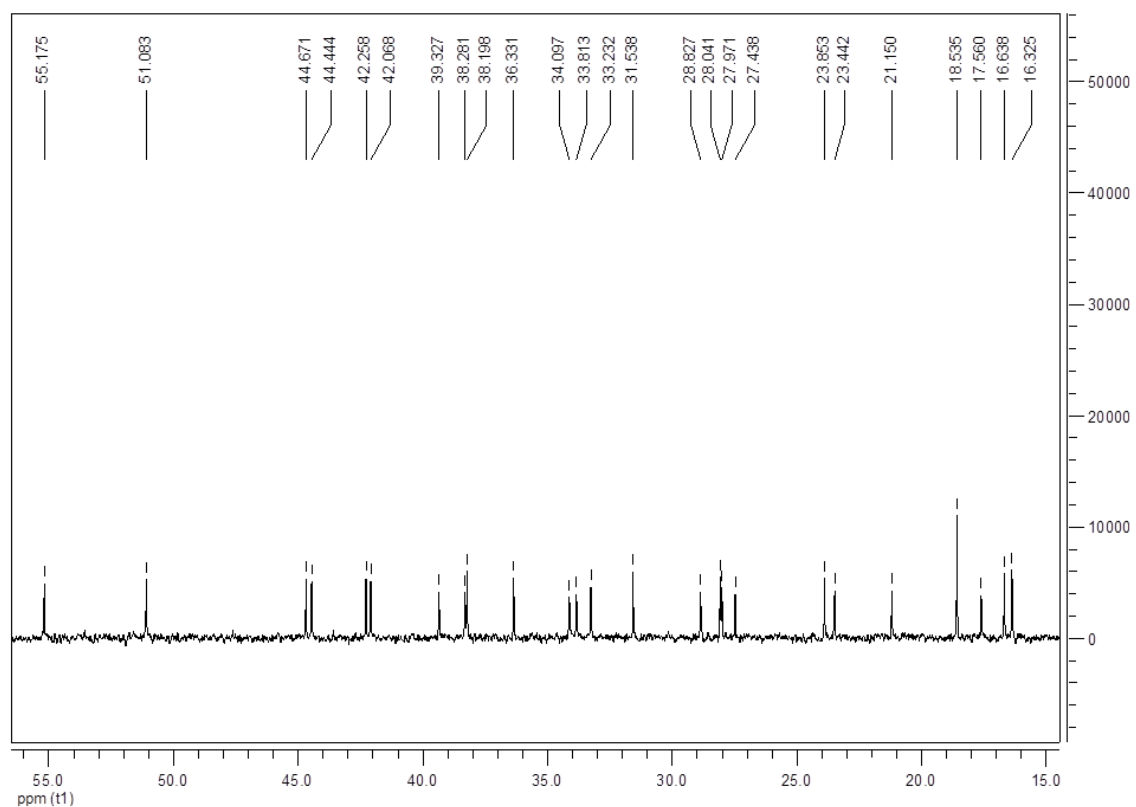
^1H NMR spectrum for compound **19** recorded in CDCl_3 .



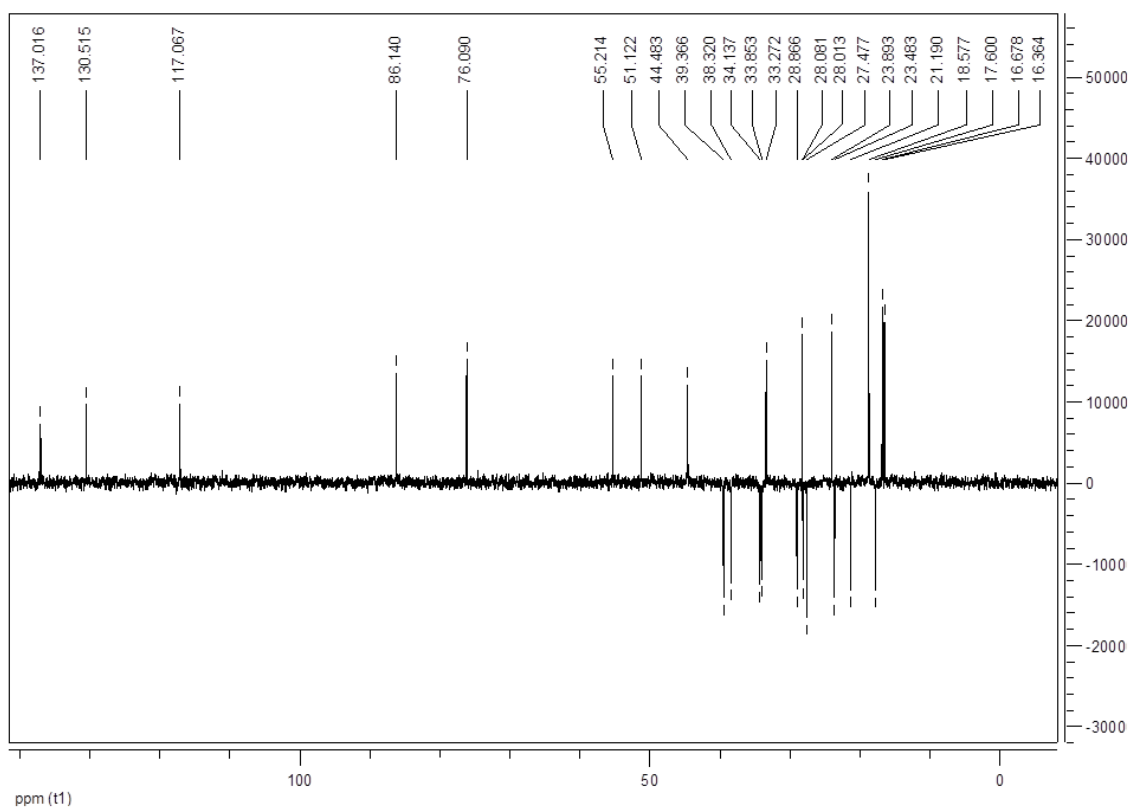
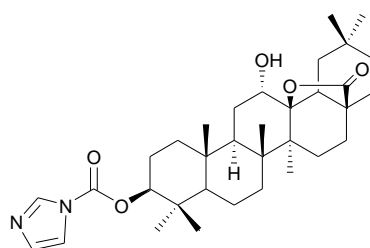
^{13}C NMR spectrum for compound **19** recorded in CDCl_3 .



^{13}C NMR spectrum detail of compound **19**.

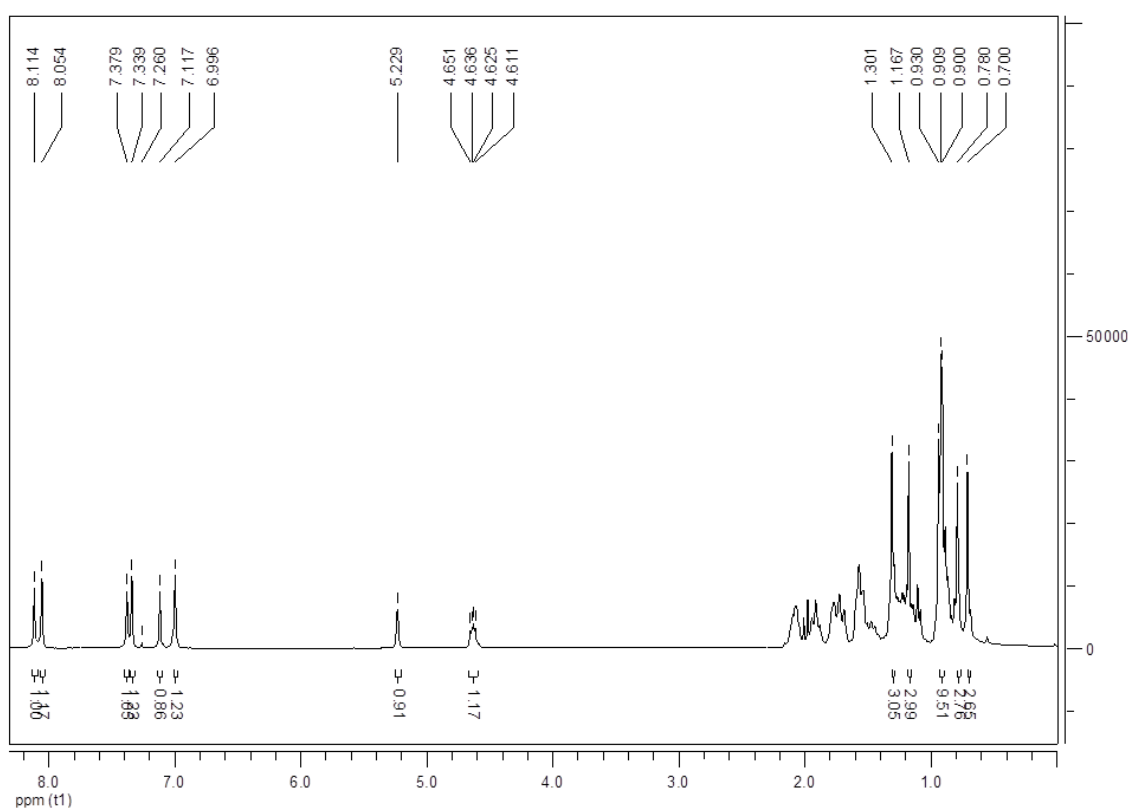
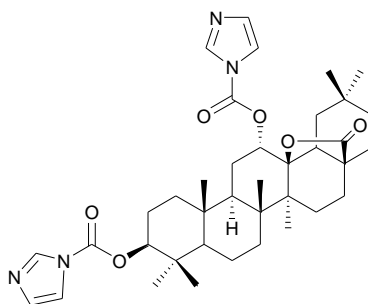


DEPT-135 NMR spectrum for compound **19** recorded in CDCl₃.

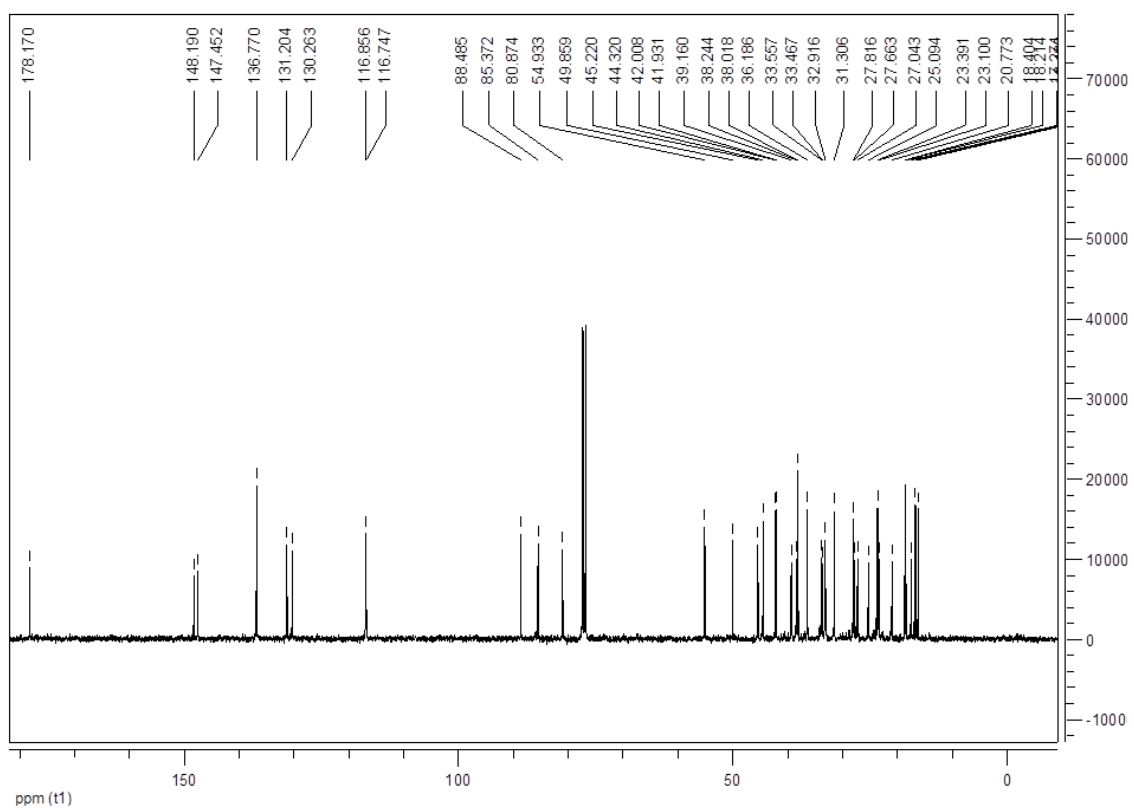
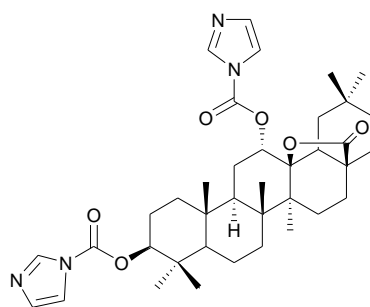


6. Spectral data for compound 20

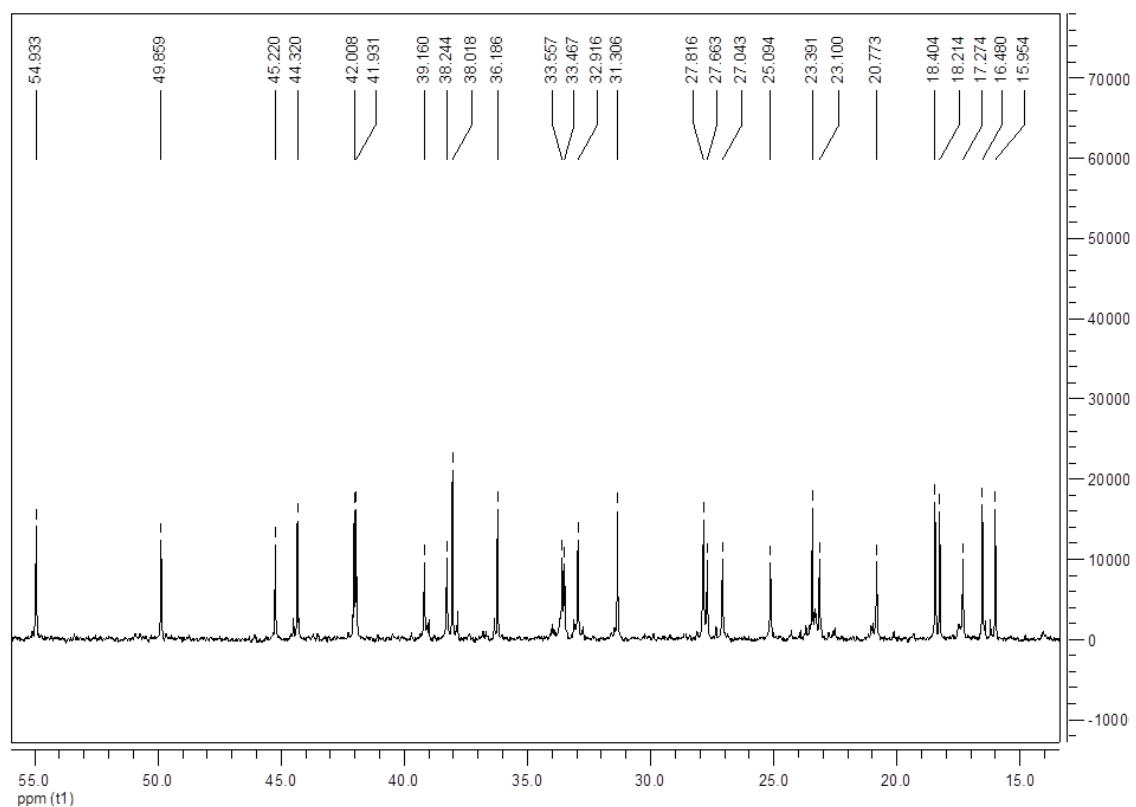
^1H NMR spectrum for compound **20** recorded in CDCl_3 .



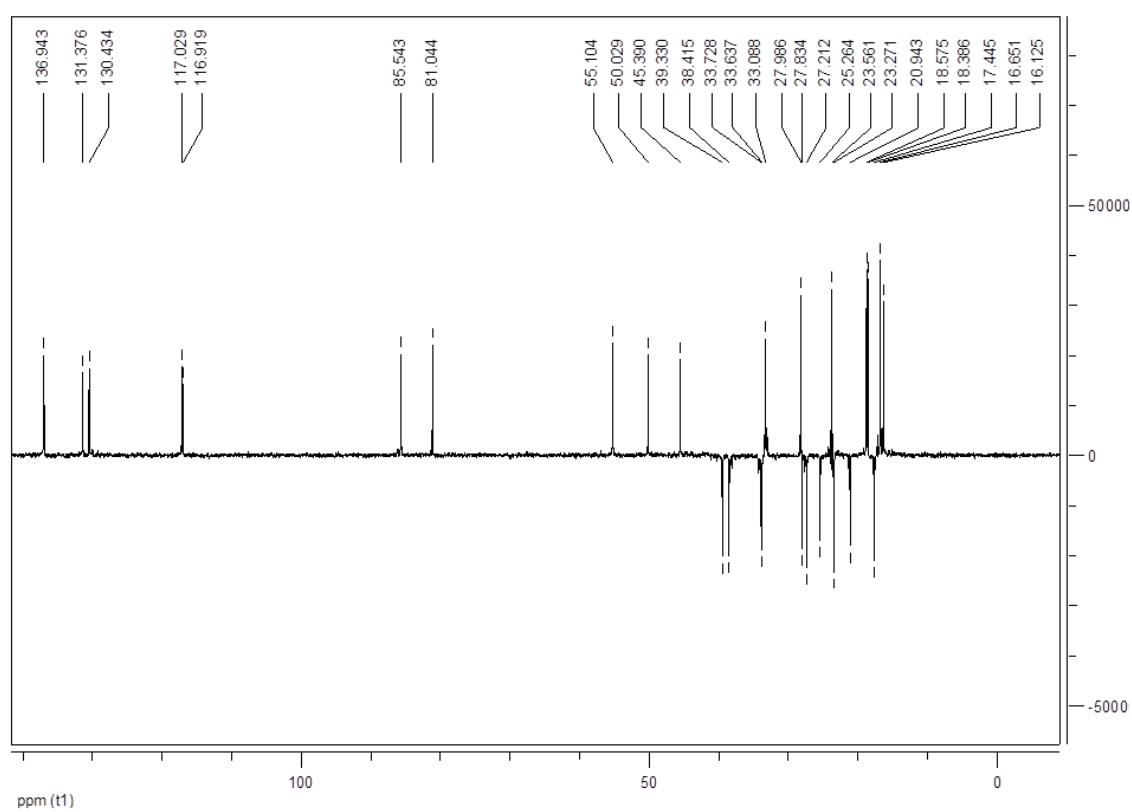
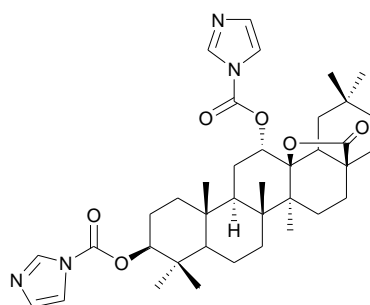
^{13}C NMR spectrum for compound **20** recorded in CDCl_3 .



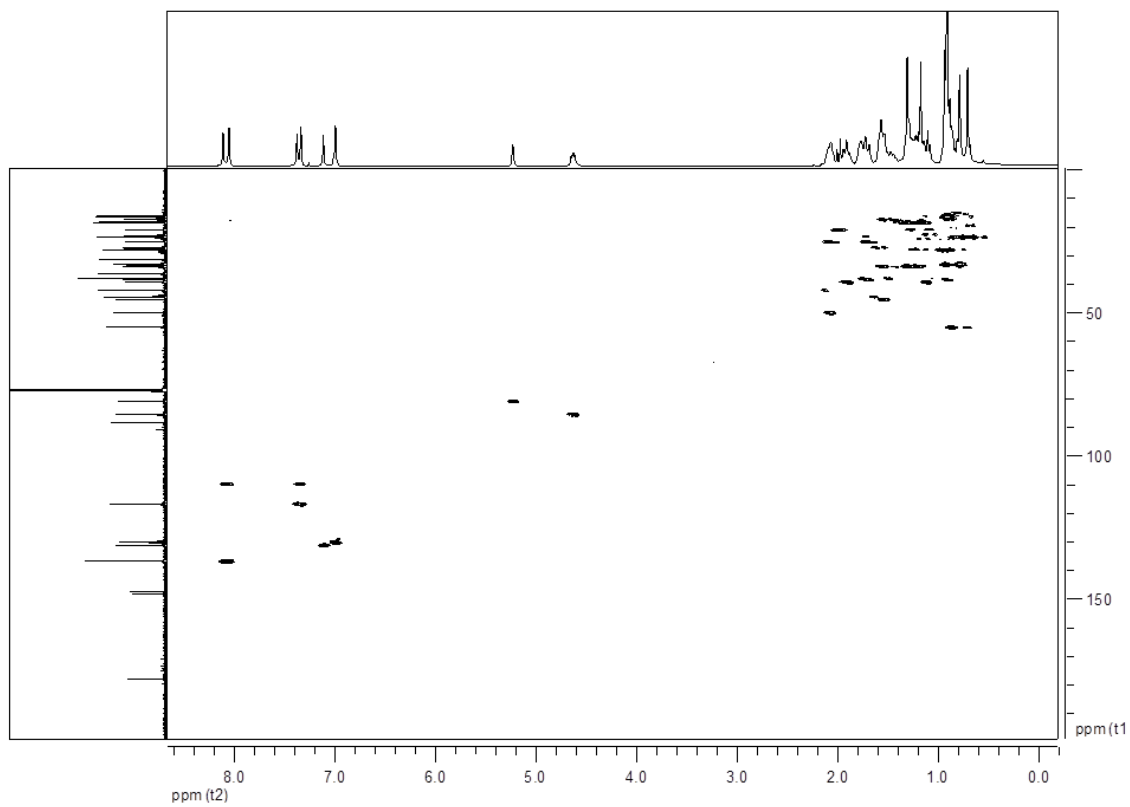
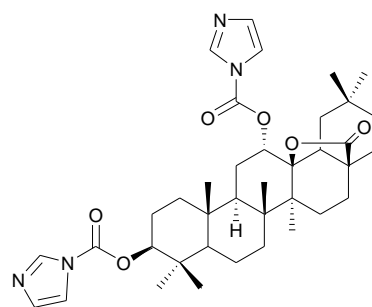
^{13}C NMR spectrum detail of compound **20**.



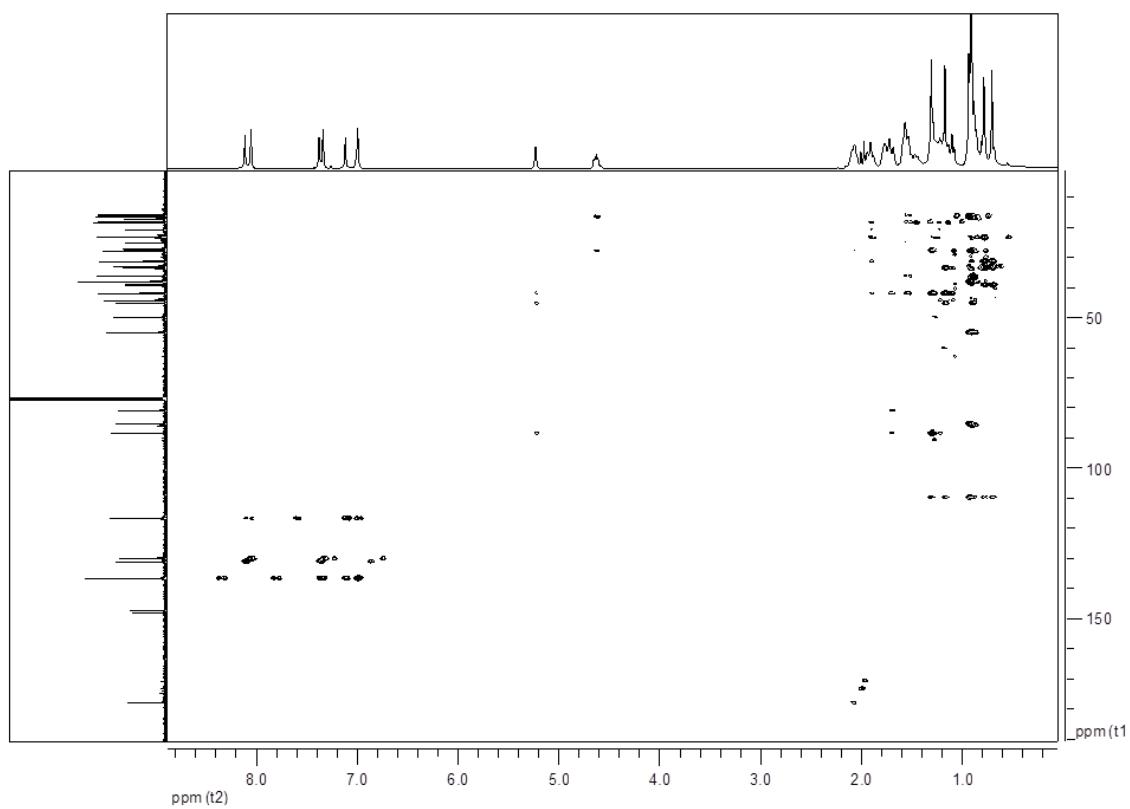
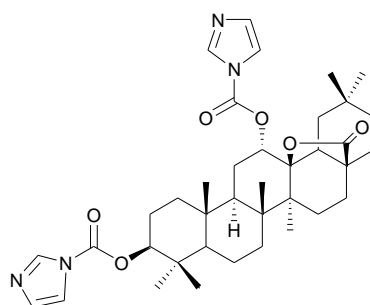
DEPT-135 NMR spectrum for compound **20** recorded in CDCl₃.



HMQC NMR spectrum for compound **20** recorded in CDCl₃.

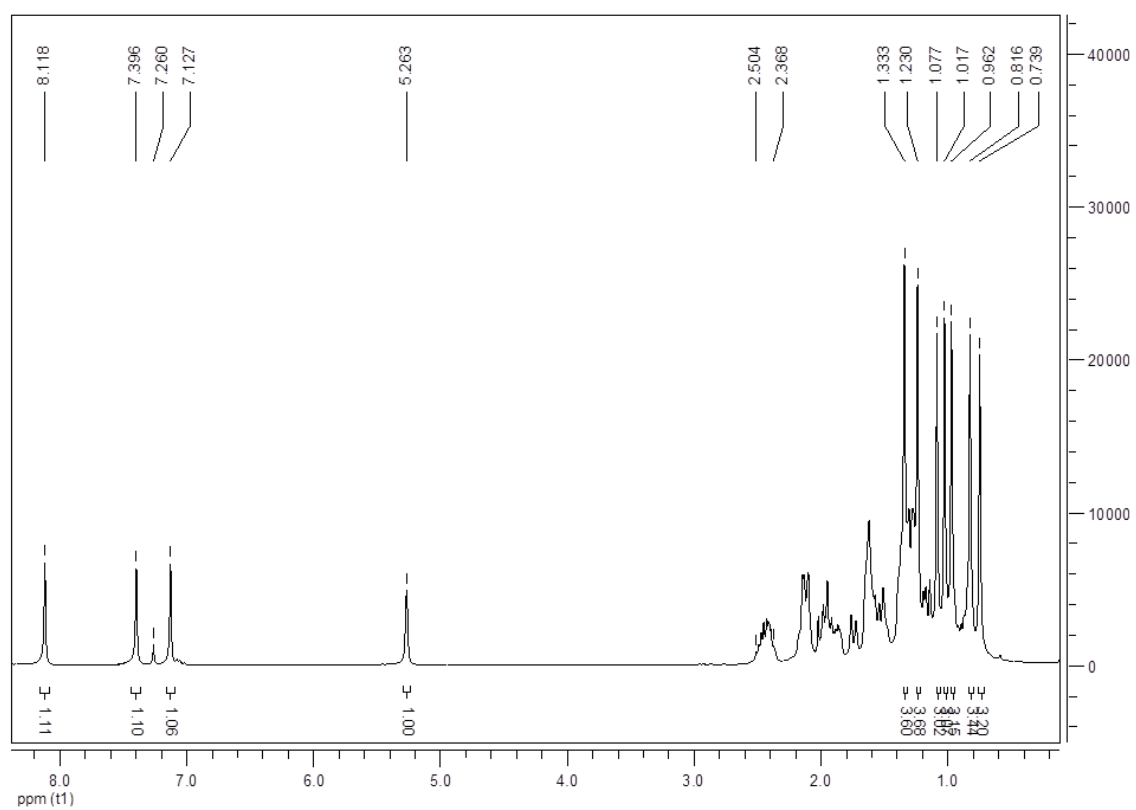
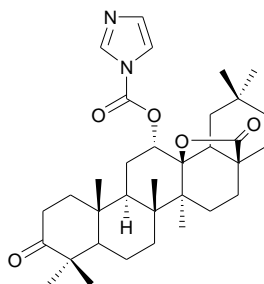


HMBC NMR spectrum for compound **20** recorded in CDCl₃.

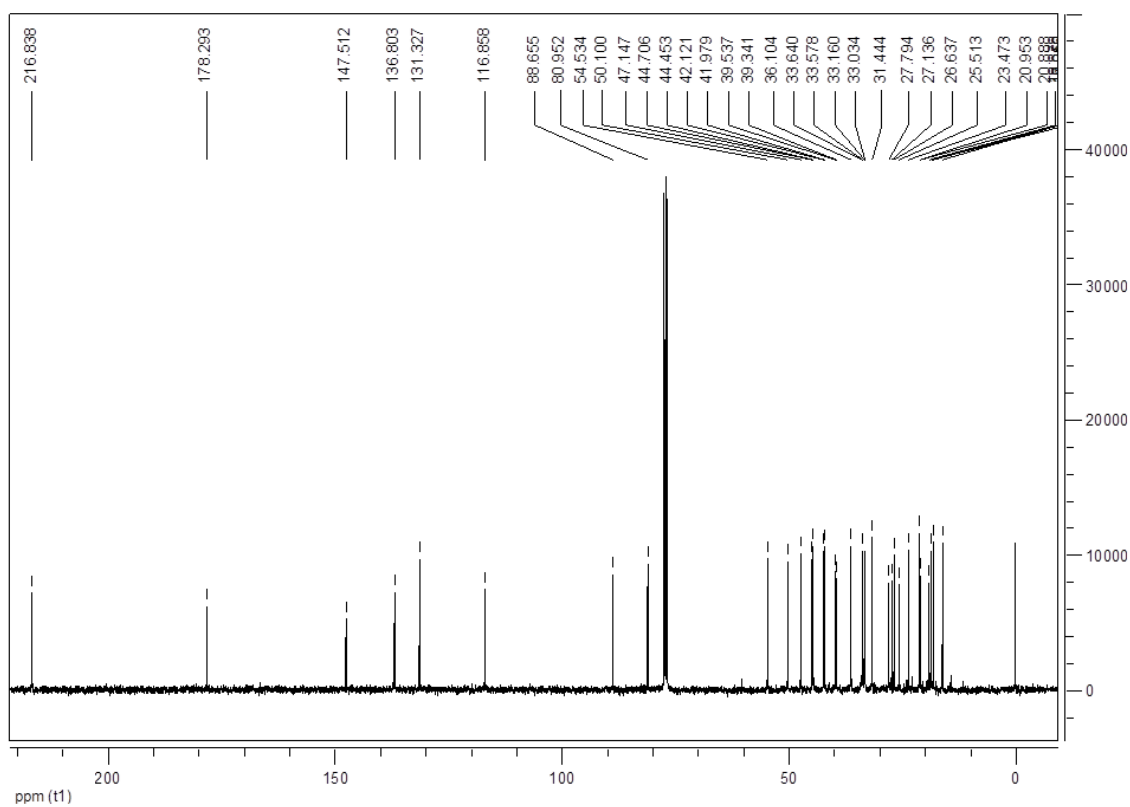
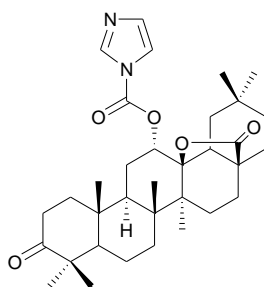


7. Spectral data for compound **21**

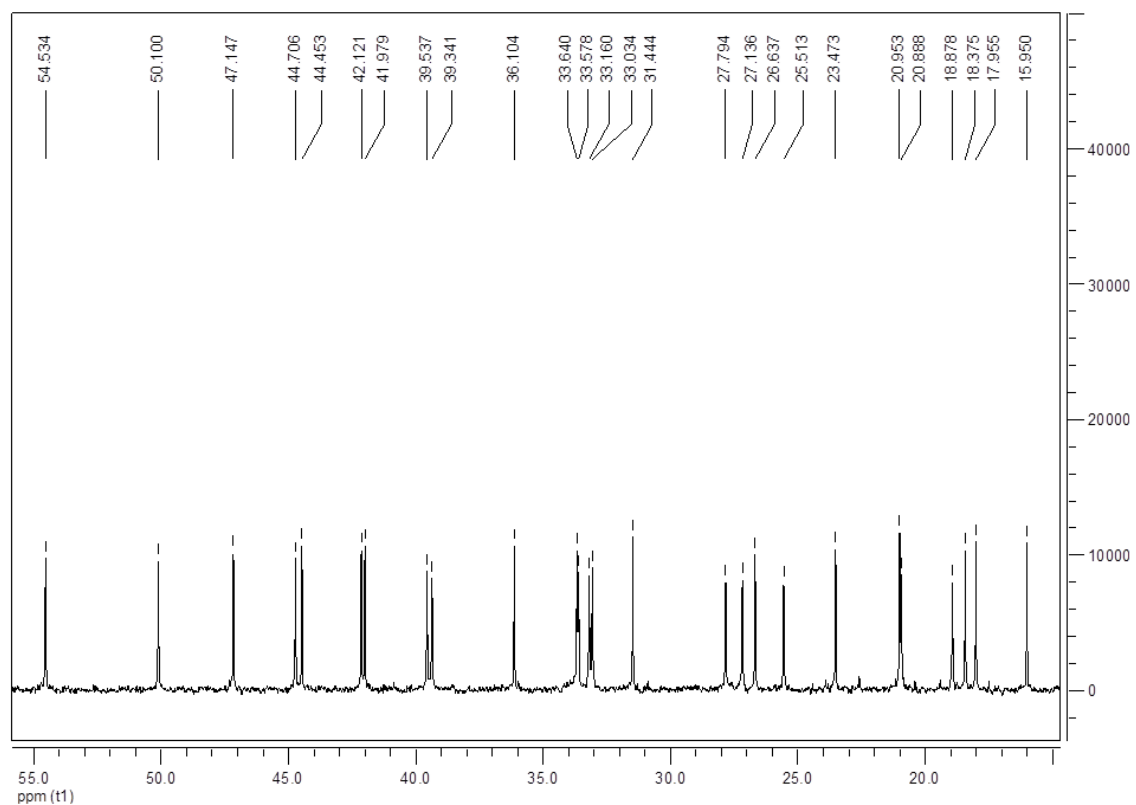
^1H NMR spectrum for compound **21** recorded in CDCl_3 .



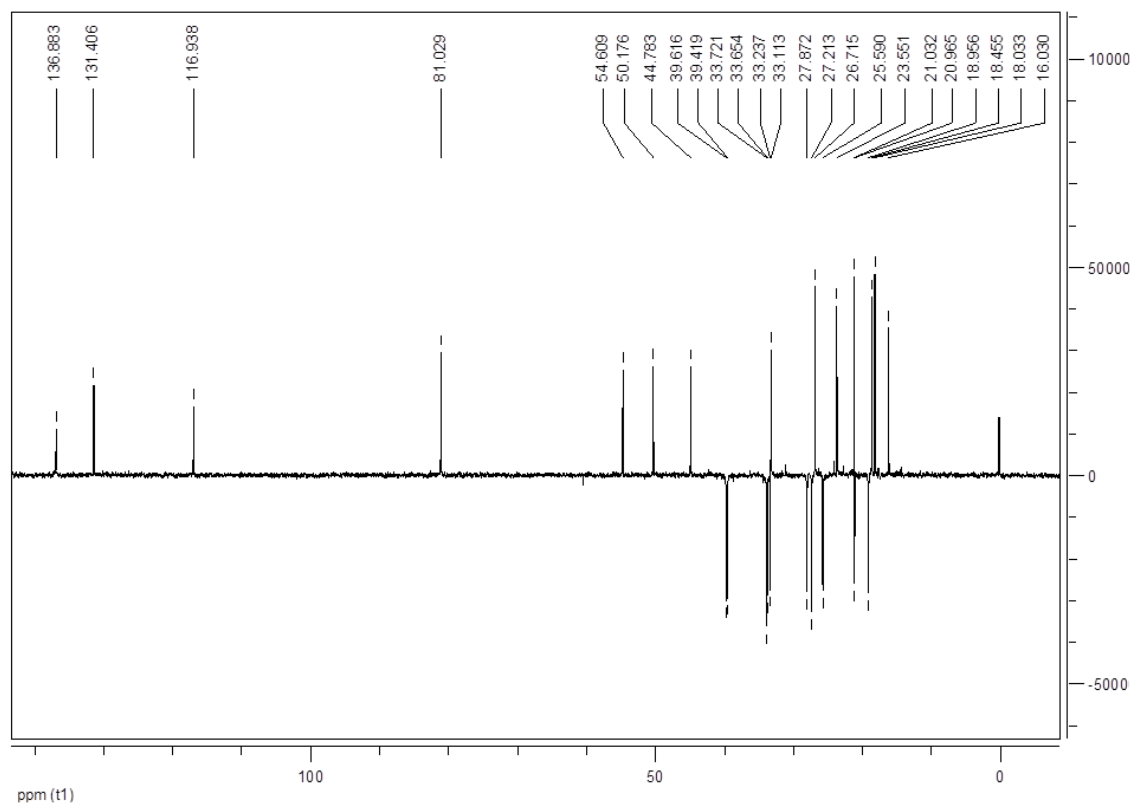
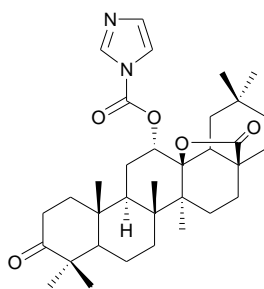
^{13}C NMR spectrum for compound **21** recorded in CDCl_3 .



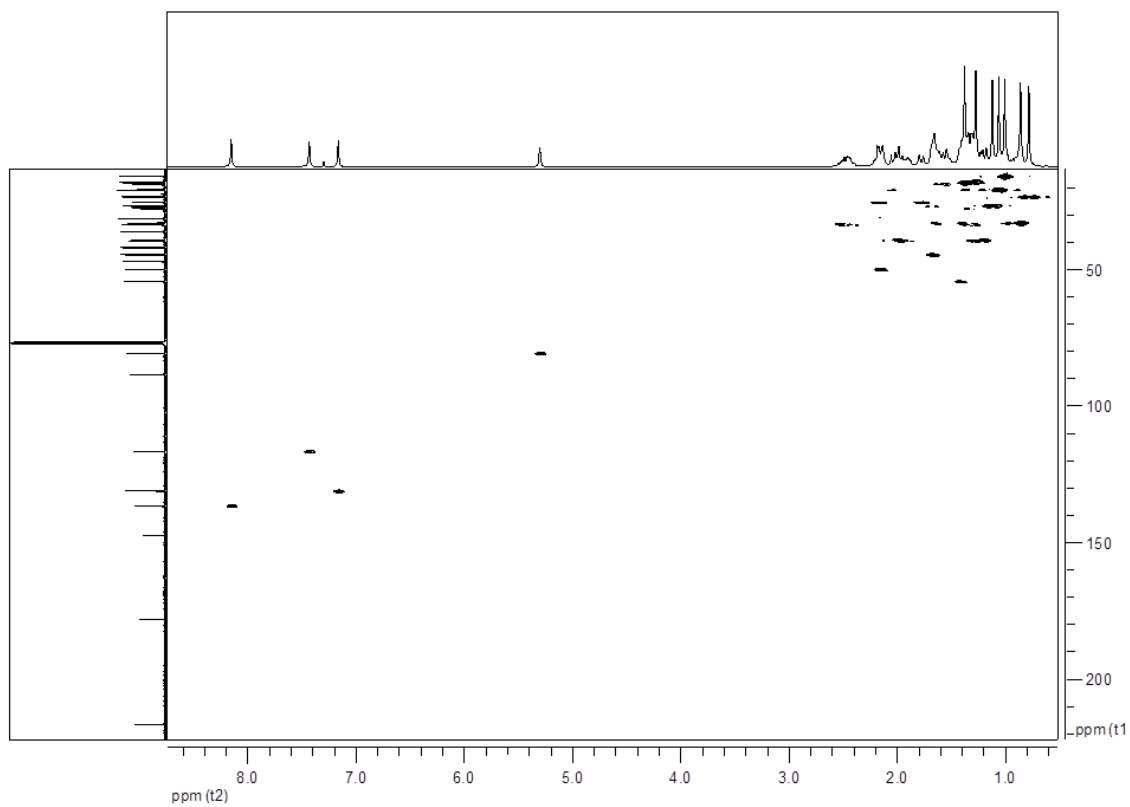
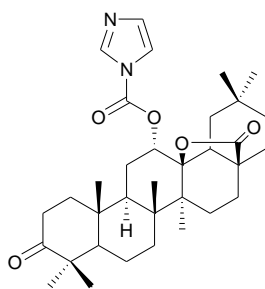
^{13}C NMR spectrum detail of compound **21**.



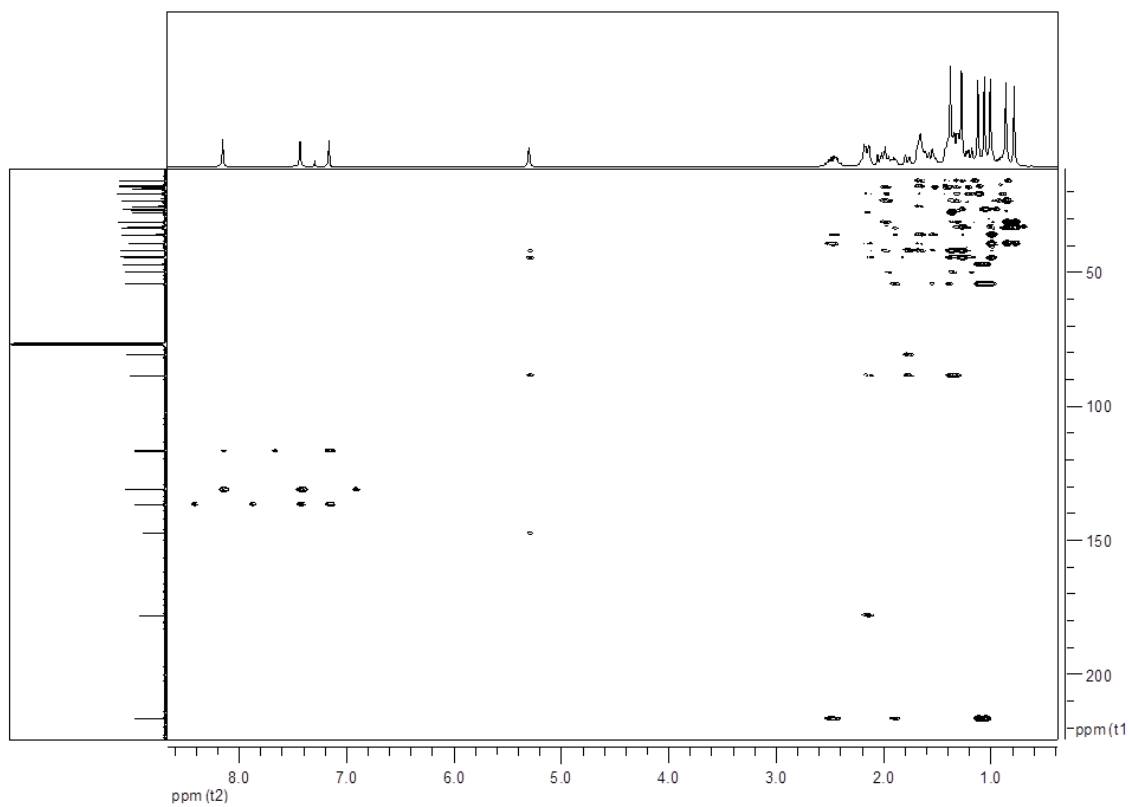
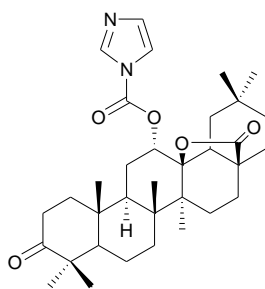
DEPT-135 NMR spectrum for compound **21** recorded in CDCl₃.



HMQC NMR spectrum for compound **21** recorded in CDCl₃.

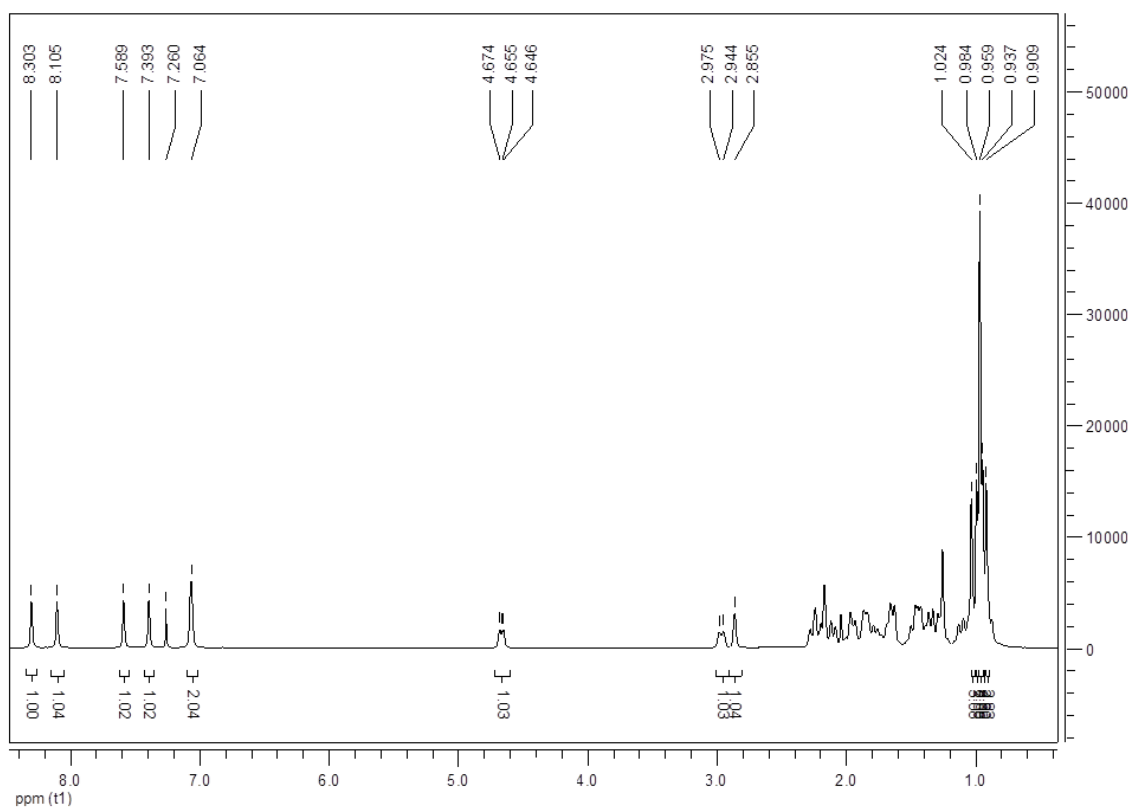
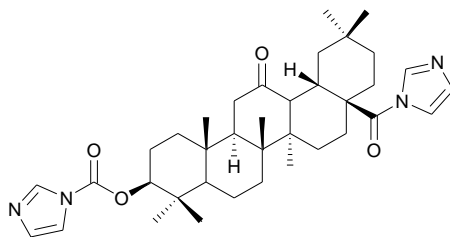


HMBC NMR spectrum for compound **21** recorded in CDCl₃.

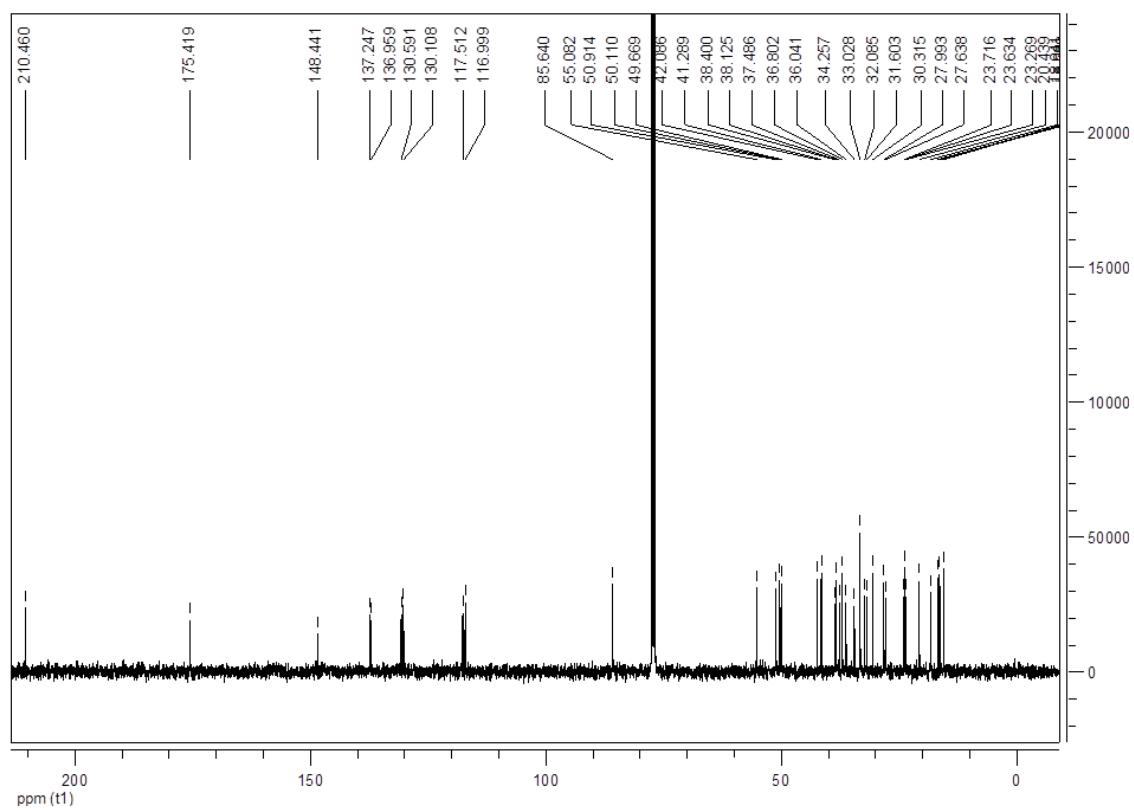
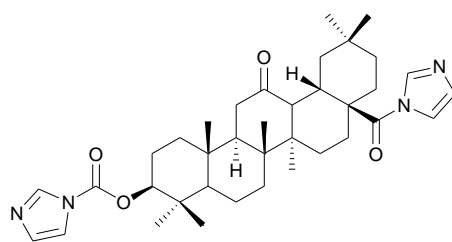


8. Spectral data for compound **22**

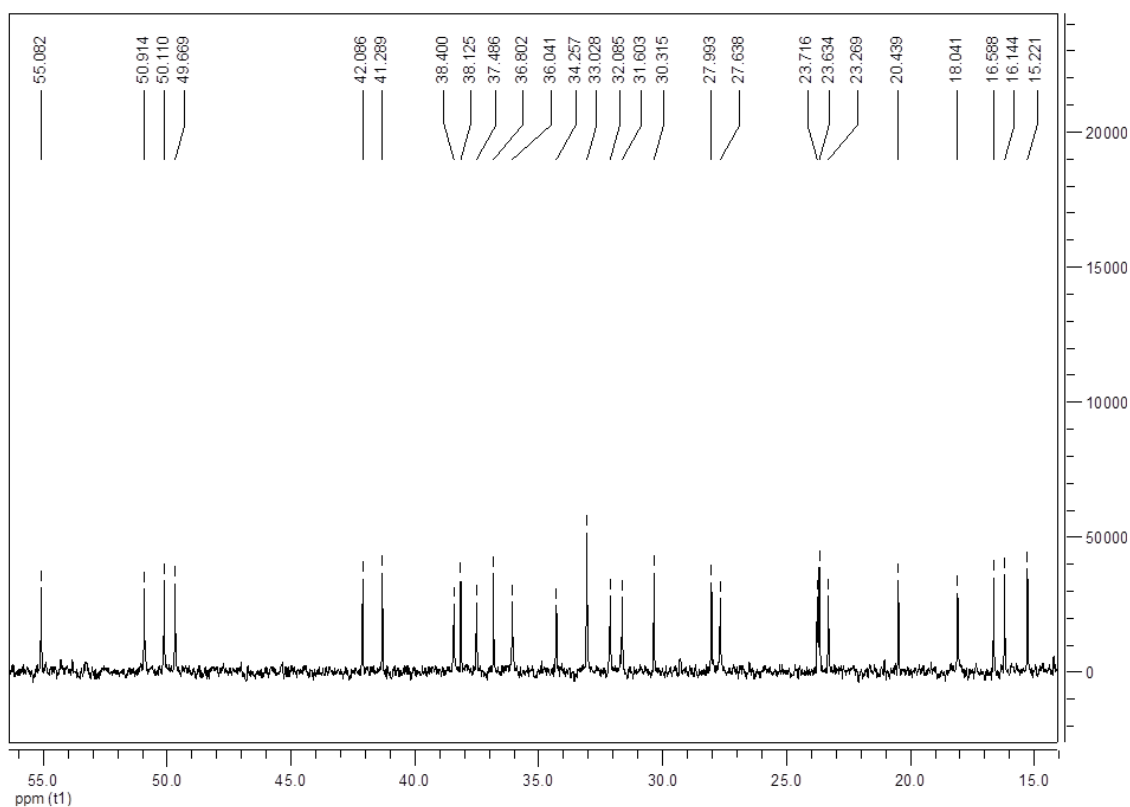
^1H NMR spectrum for compound **22** recorded in CDCl_3 .



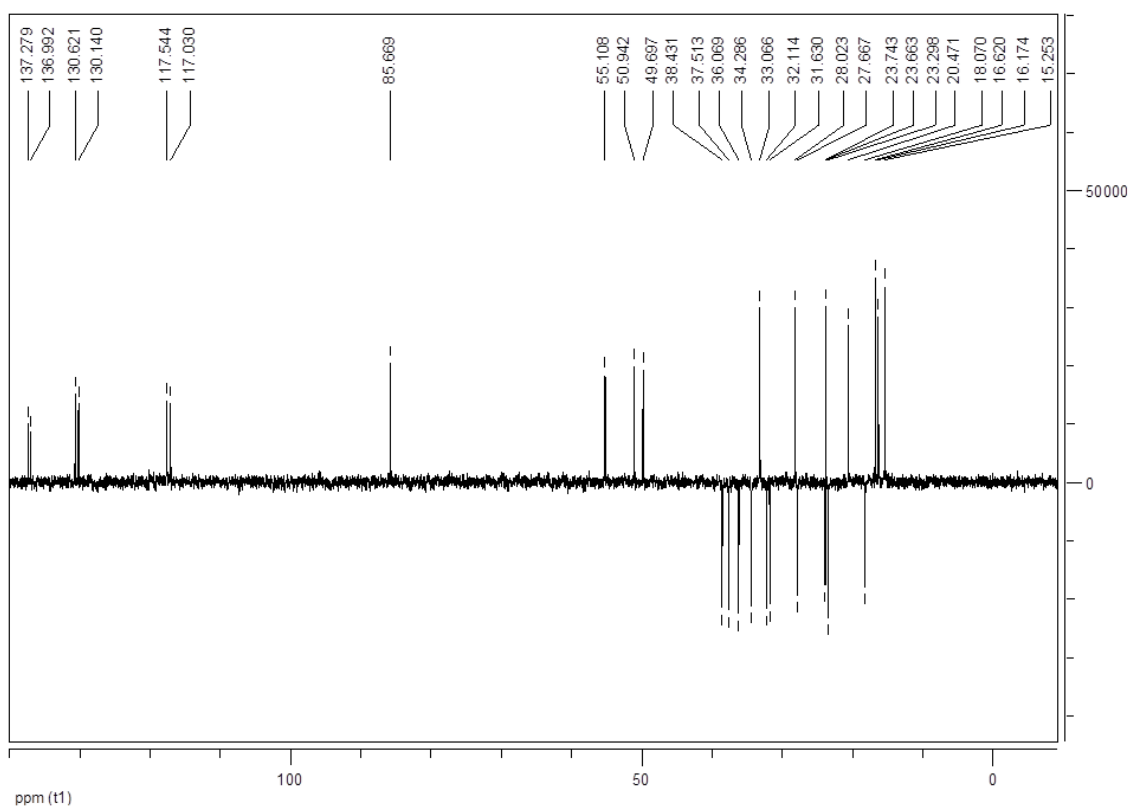
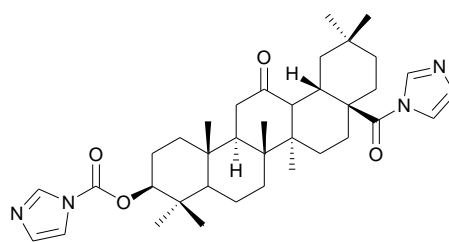
^{13}C NMR spectrum for compound **22** recorded in CDCl_3 .



^{13}C NMR spectrum detail of compound **22**.

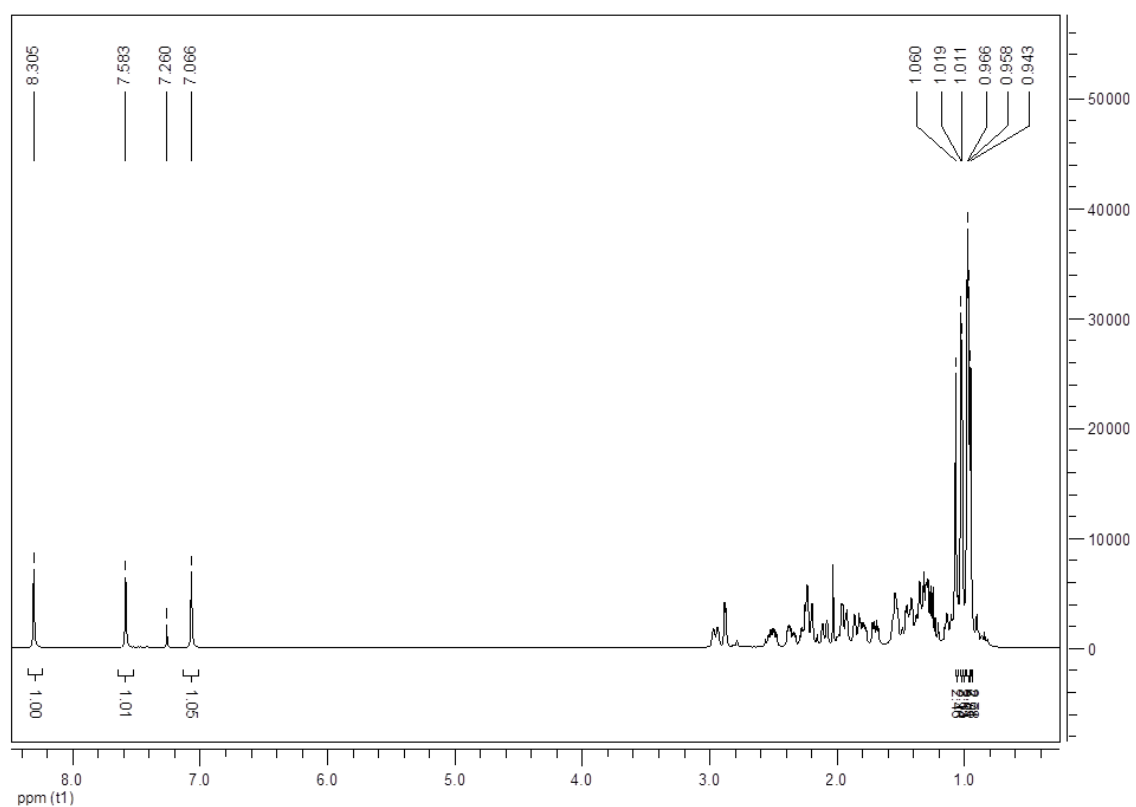
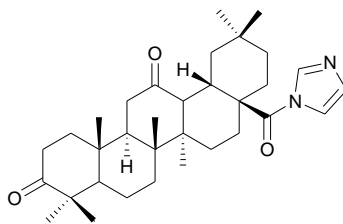


DEPT-135 NMR spectrum for compound **22** recorded in CDCl₃.

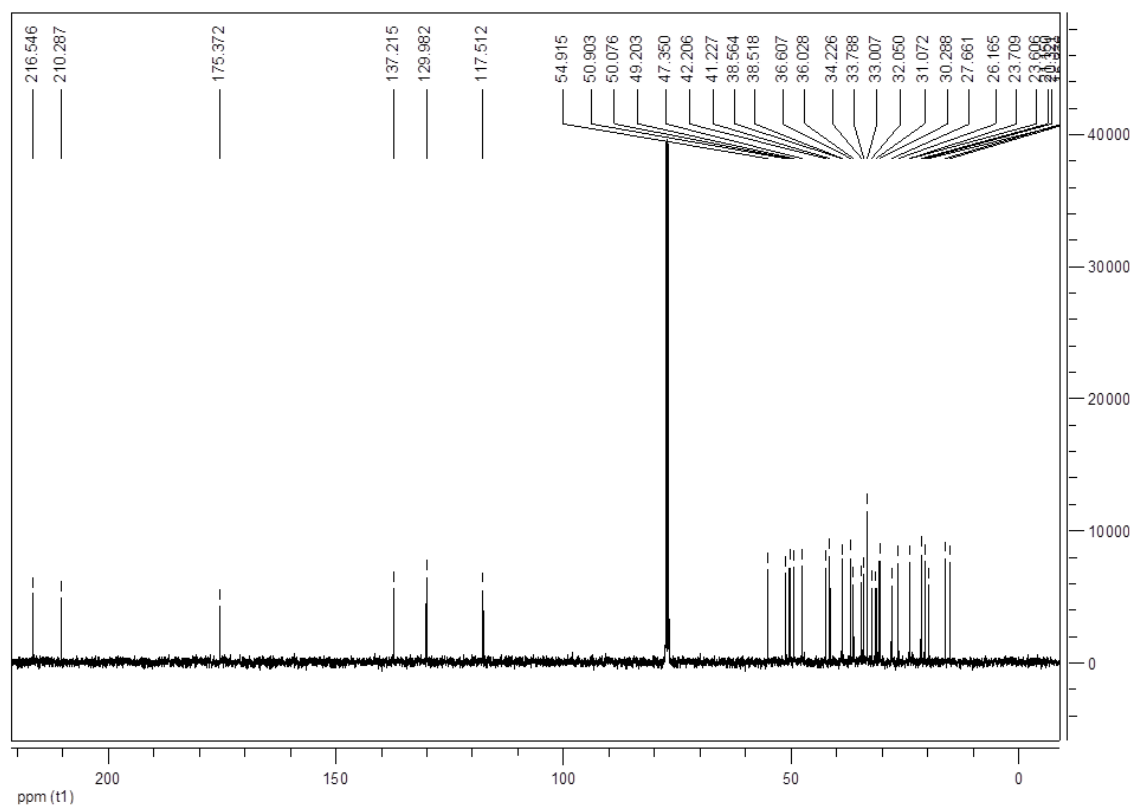
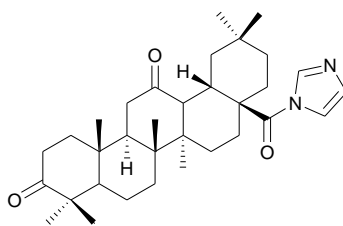


9. Spectral data for compound **23**

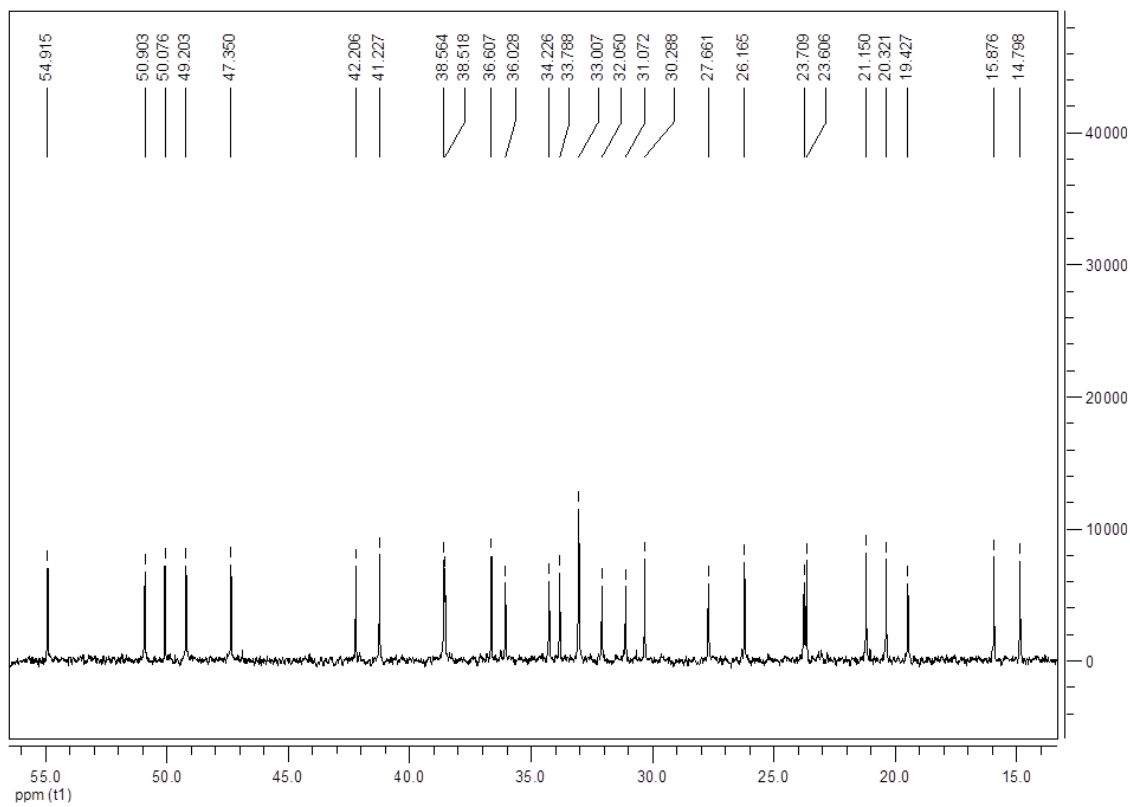
^1H NMR spectrum for compound **23** recorded in CDCl_3 .



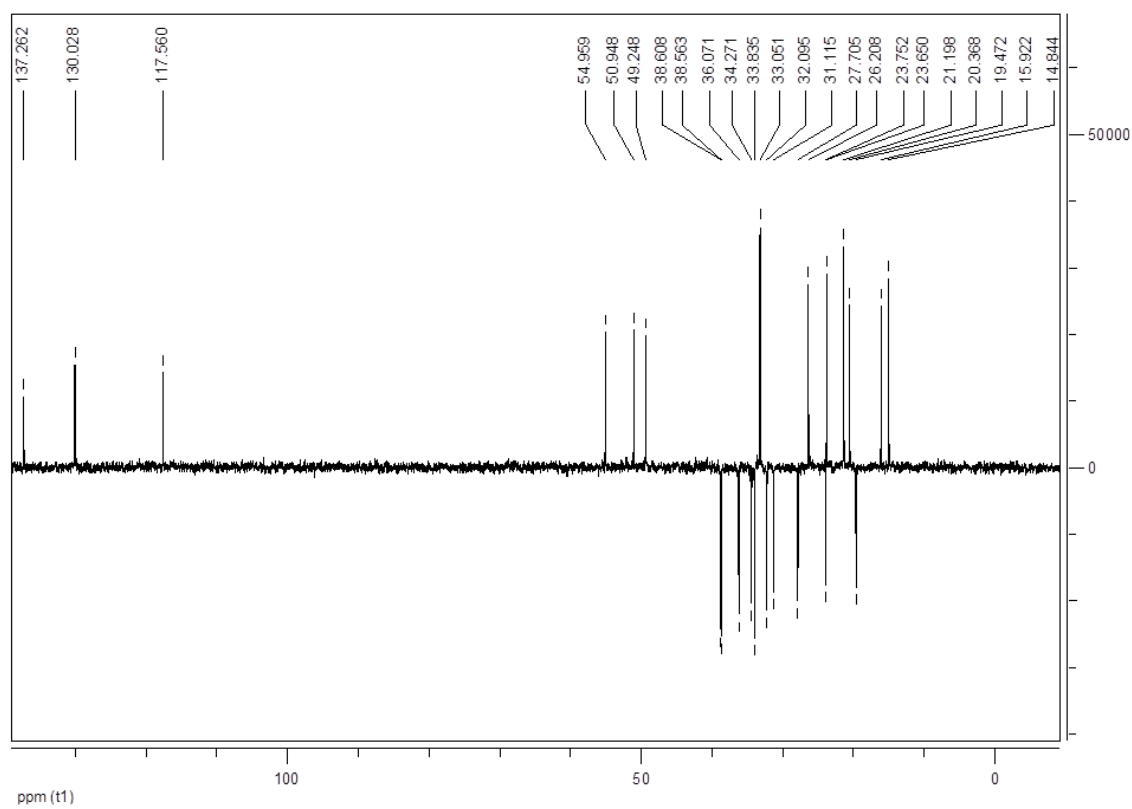
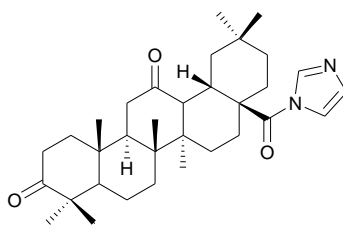
^{13}C NMR spectrum for compound **23** recorded in CDCl_3 .



^{13}C NMR spectrum detail of compound **23**.

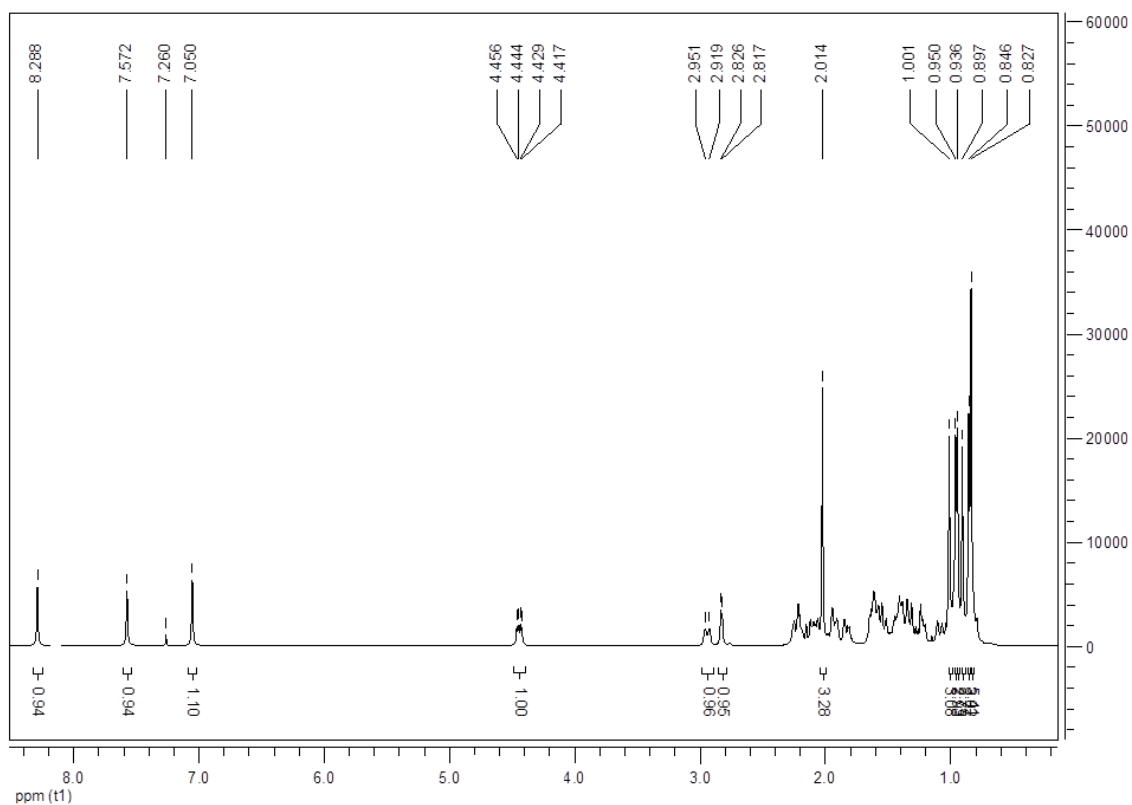
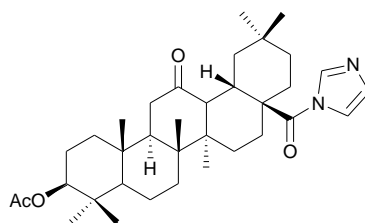


DEPT-135 NMR spectrum for compound **23** recorded in CDCl₃.

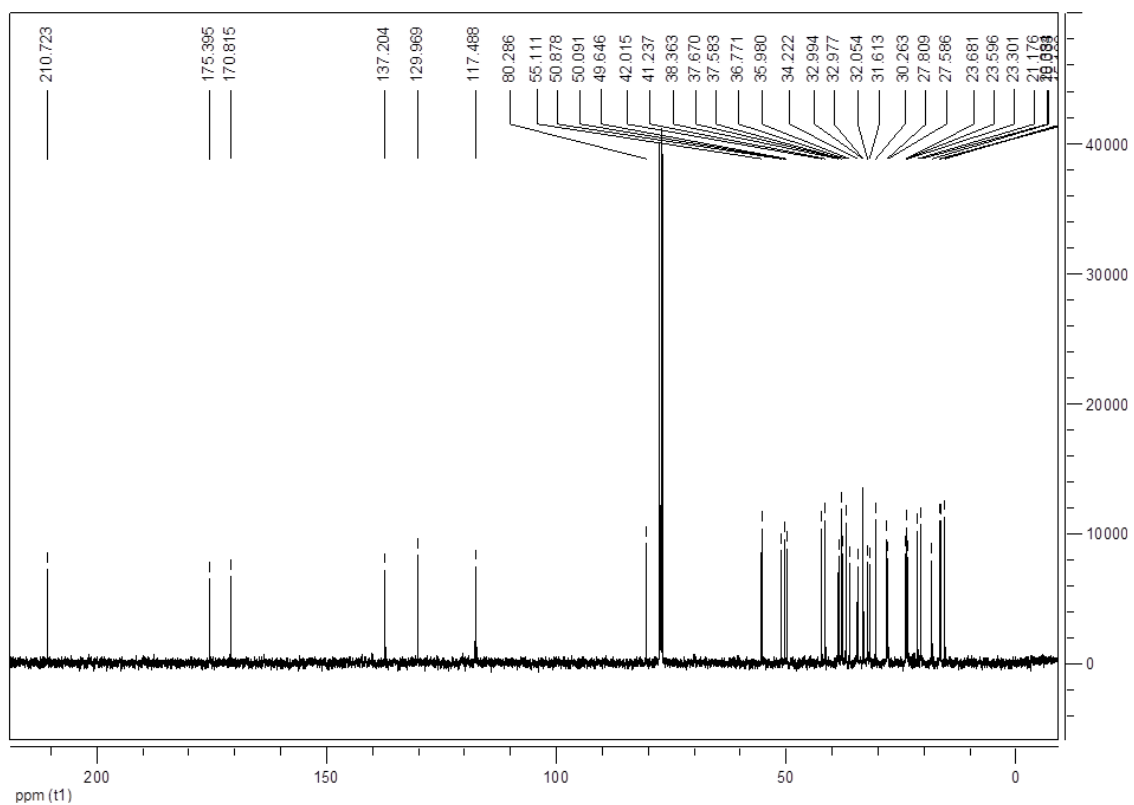
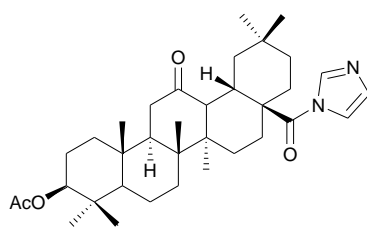


10. Spectral data for compound **24**

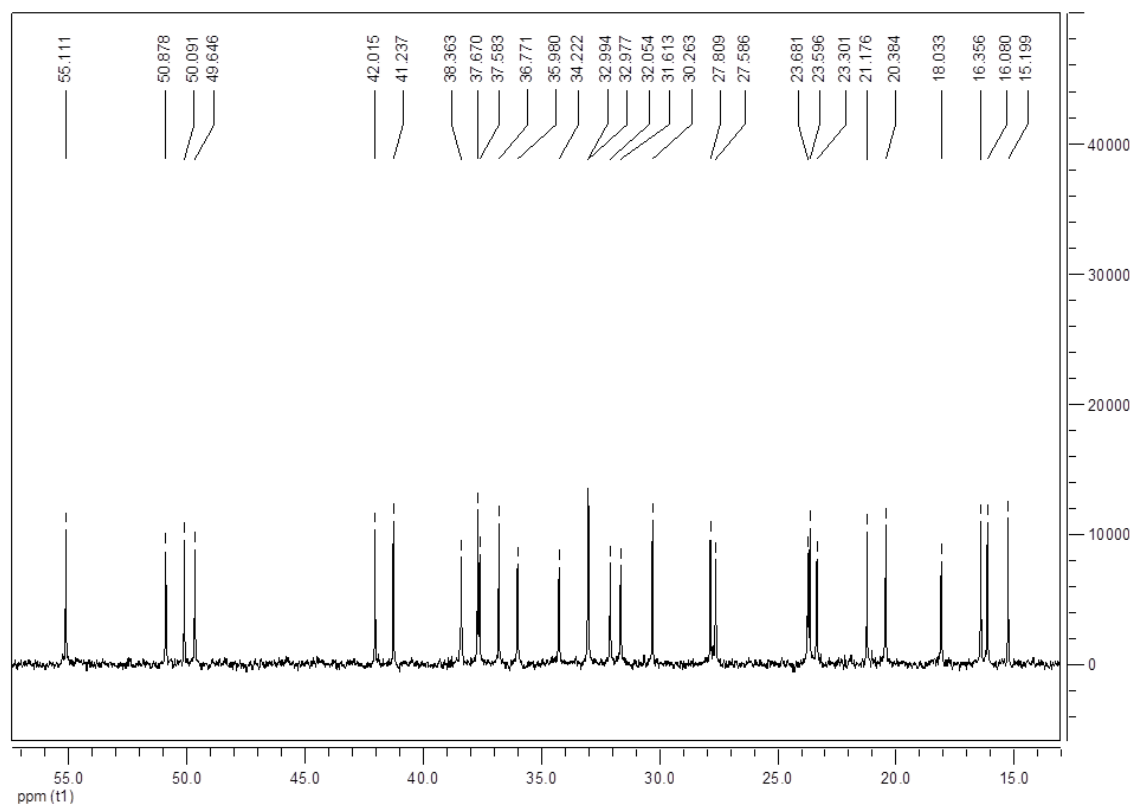
^1H NMR spectrum for compound **24** recorded in CDCl_3 .



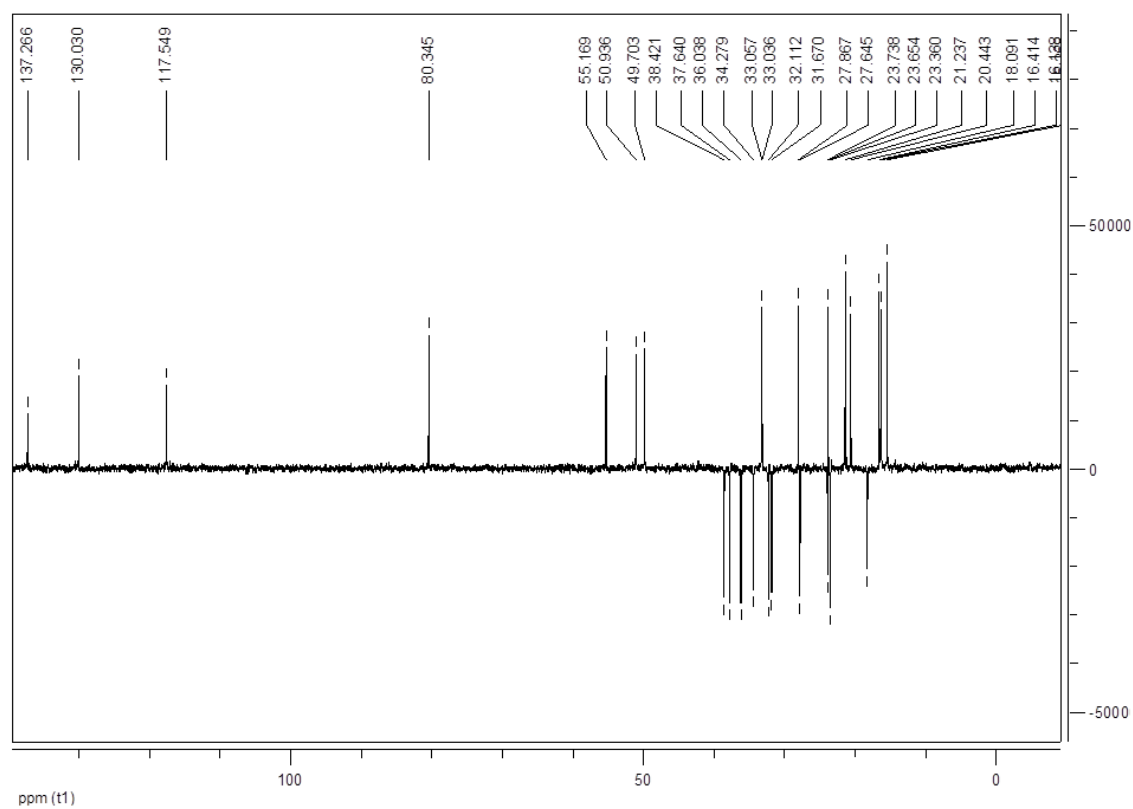
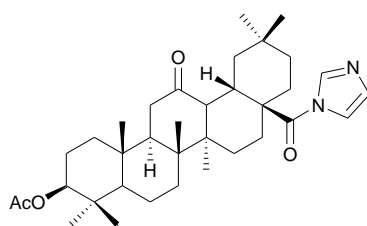
^{13}C NMR spectrum for compound **24** recorded in CDCl_3 .



^{13}C NMR spectrum detail of compound **24**.

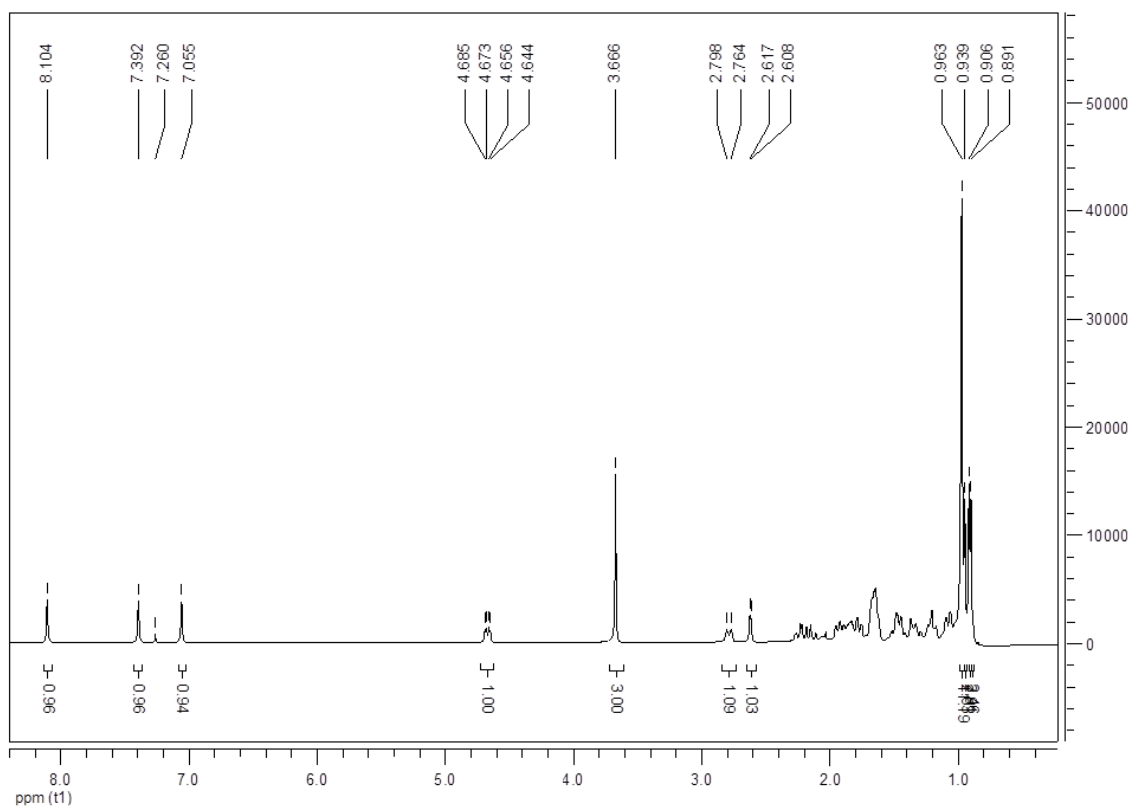
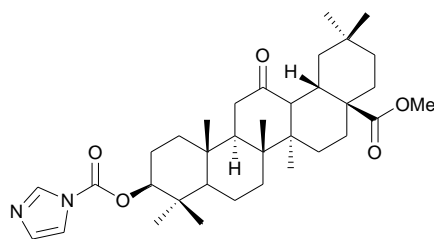


DEPT-135 NMR spectrum for compound **24** recorded in CDCl₃.

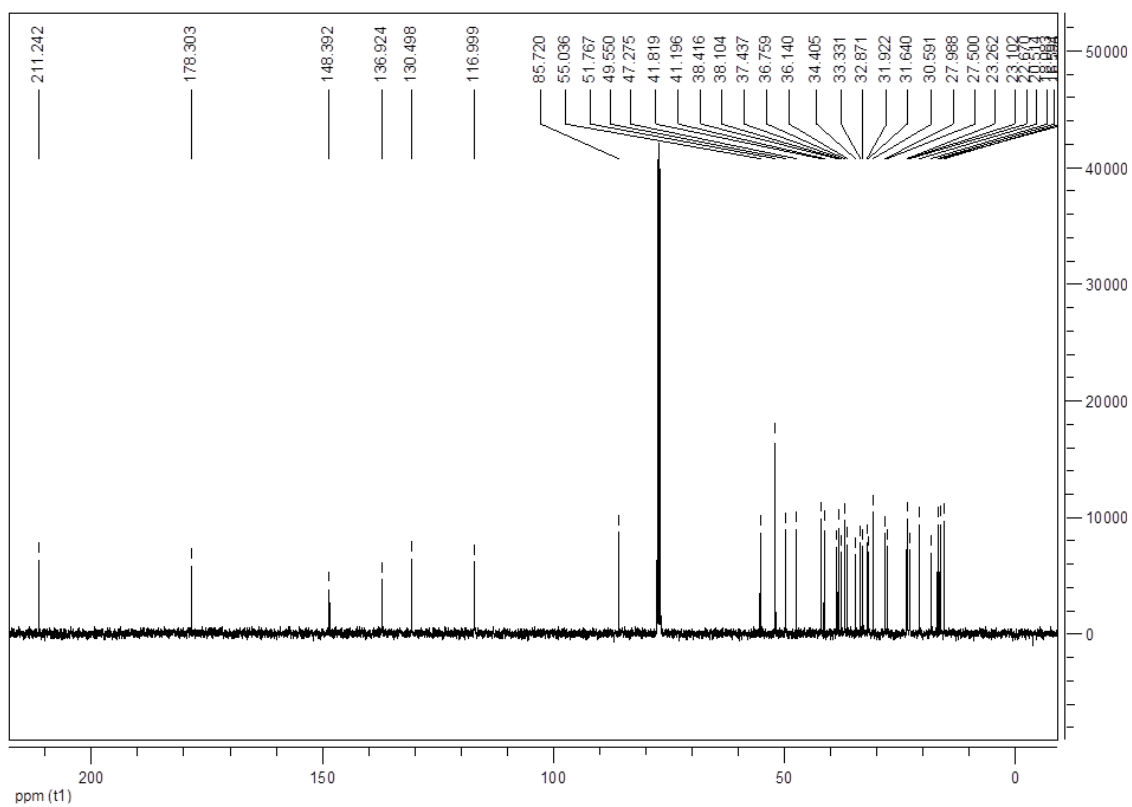
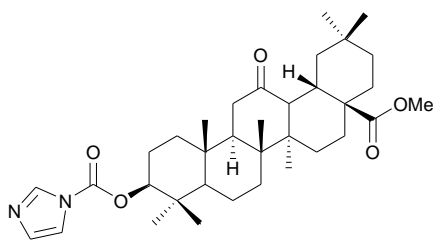


11. Spectral data for compound **25**

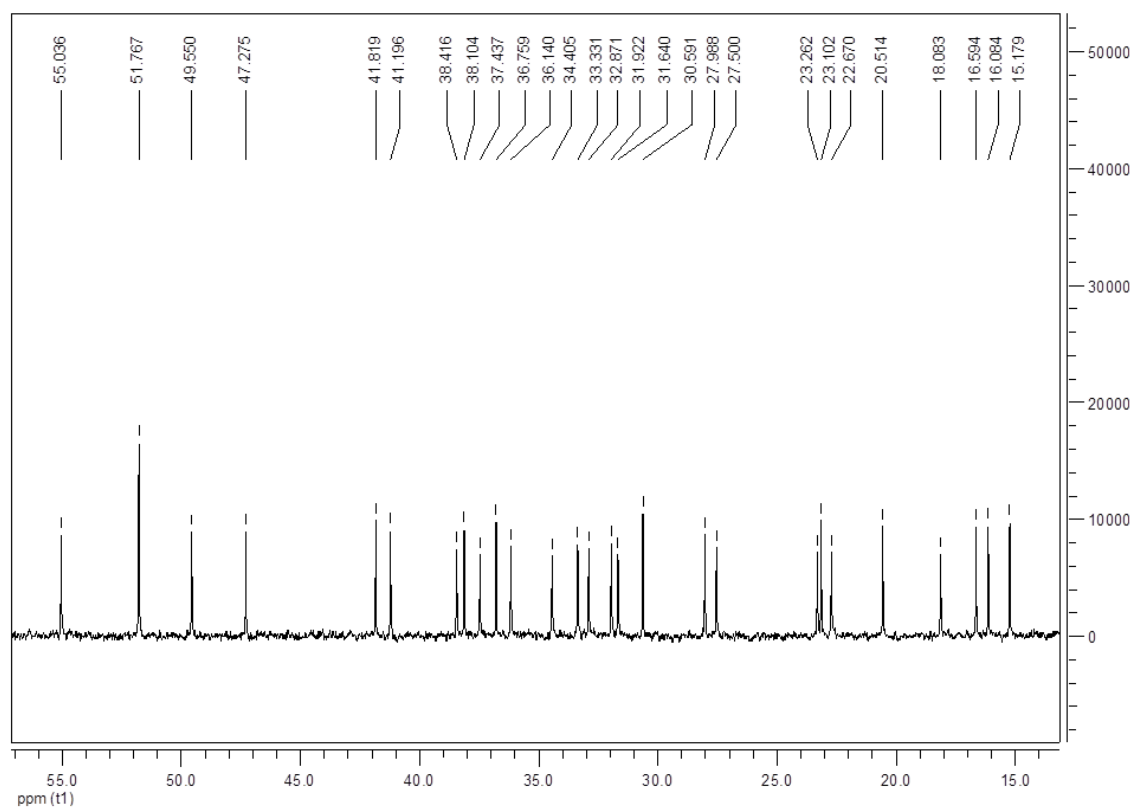
¹H NMR spectrum for compound **25** recorded in CDCl₃.



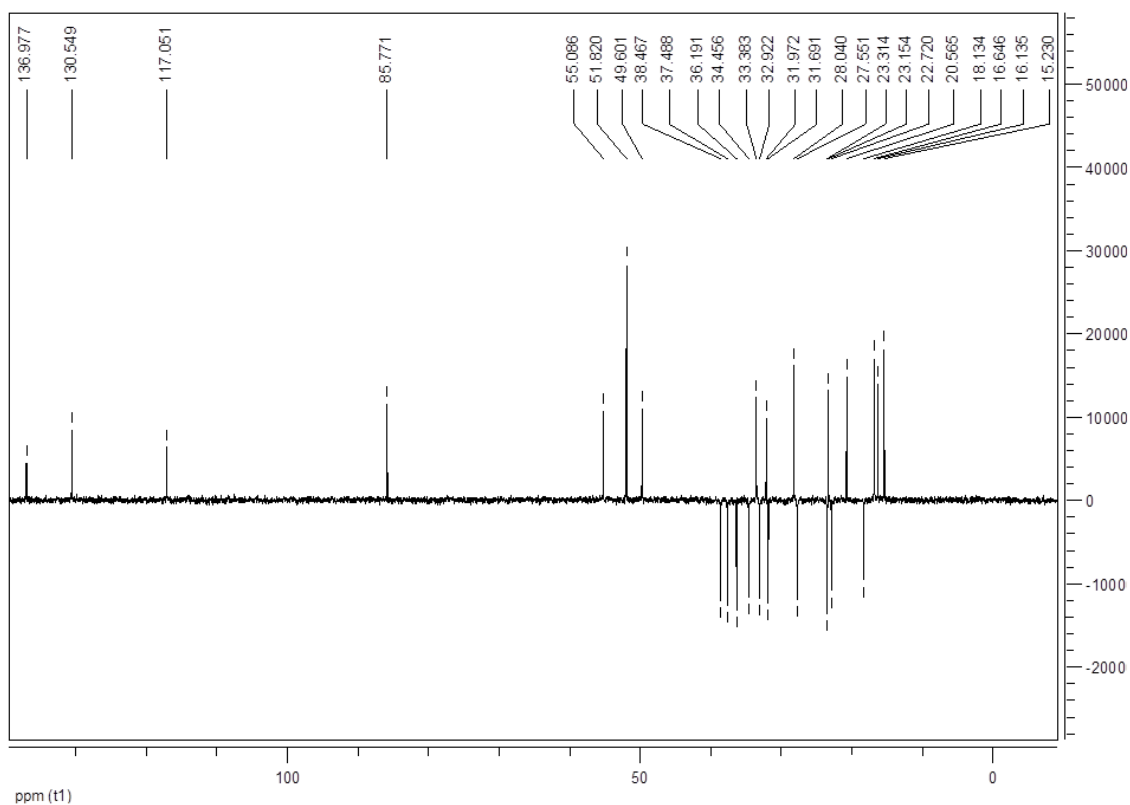
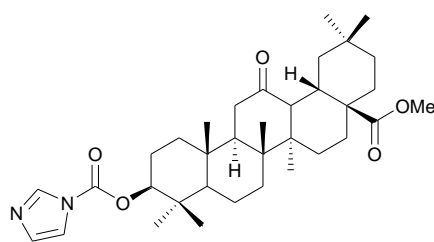
^{13}C NMR spectrum for compound **25** recorded in CDCl_3 .



^{13}C NMR spectrum detail of compound **25**.

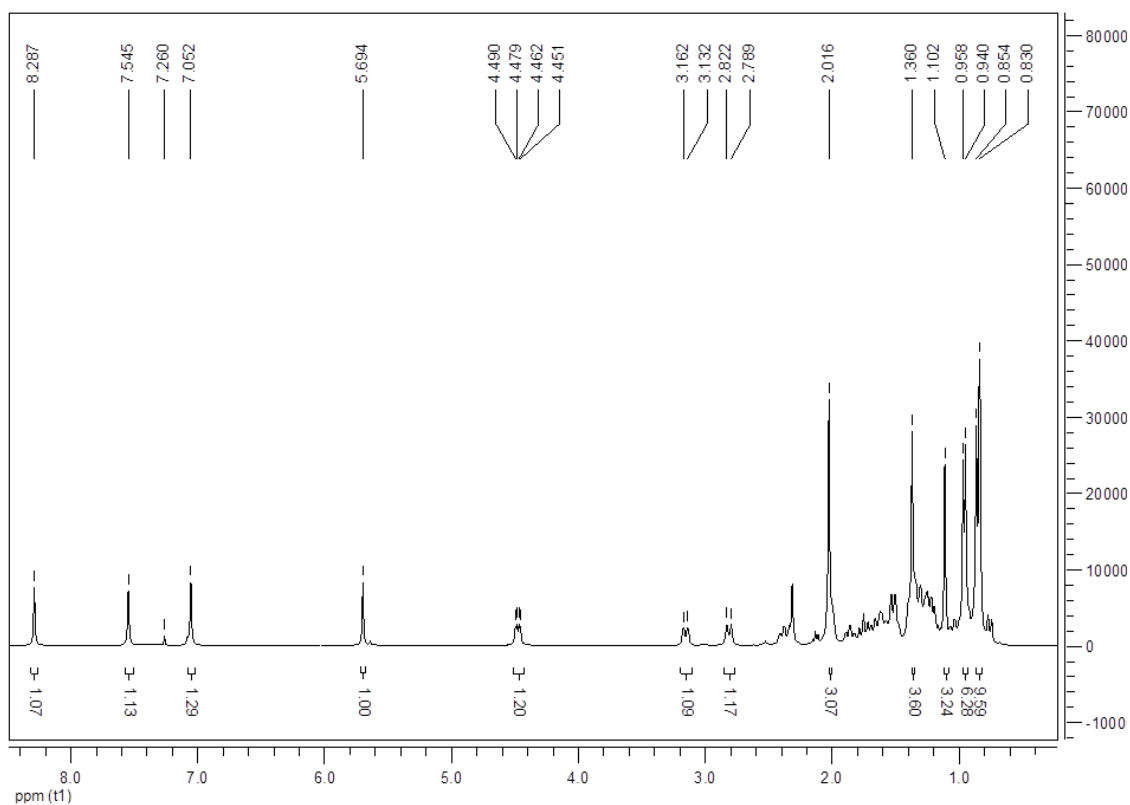
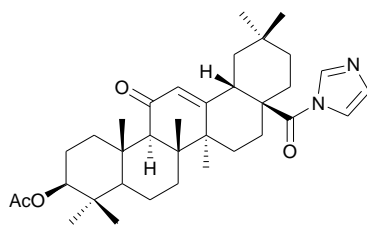


DEPT-135 NMR spectrum for compound **25** recorded in CDCl₃.

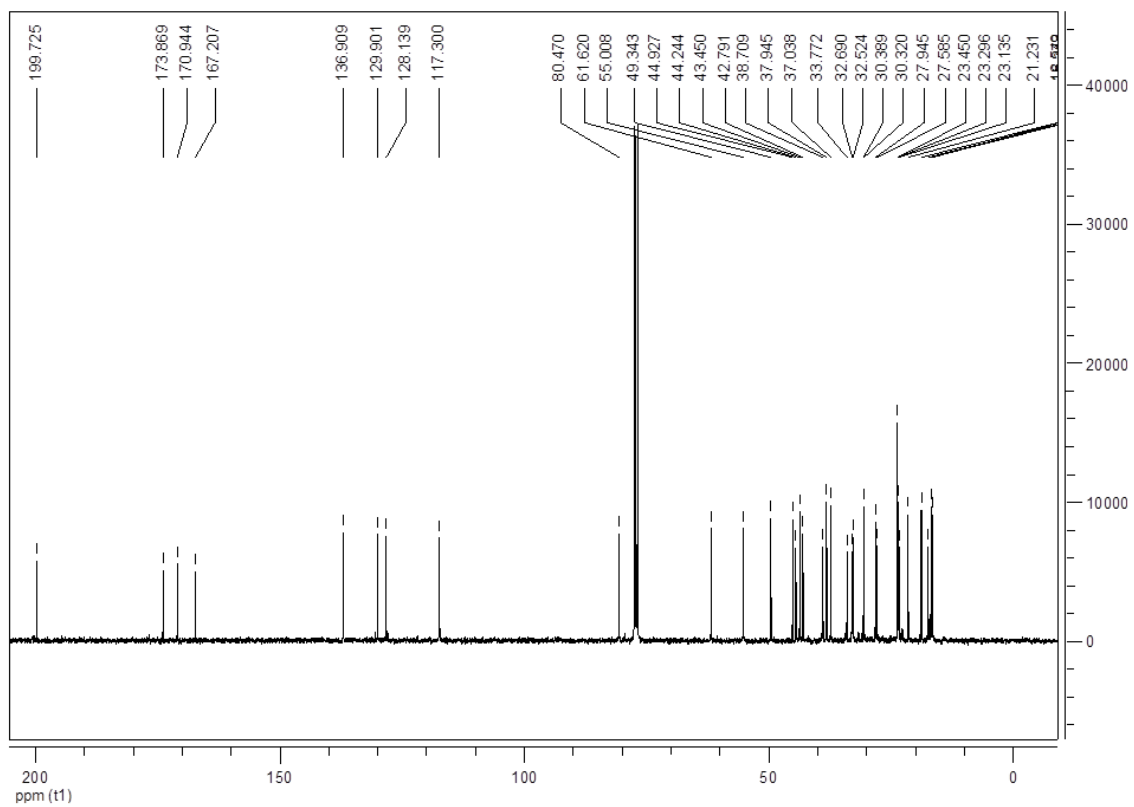
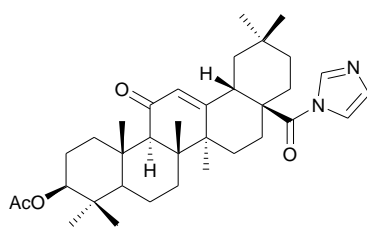


11. Spectral data for compound 26

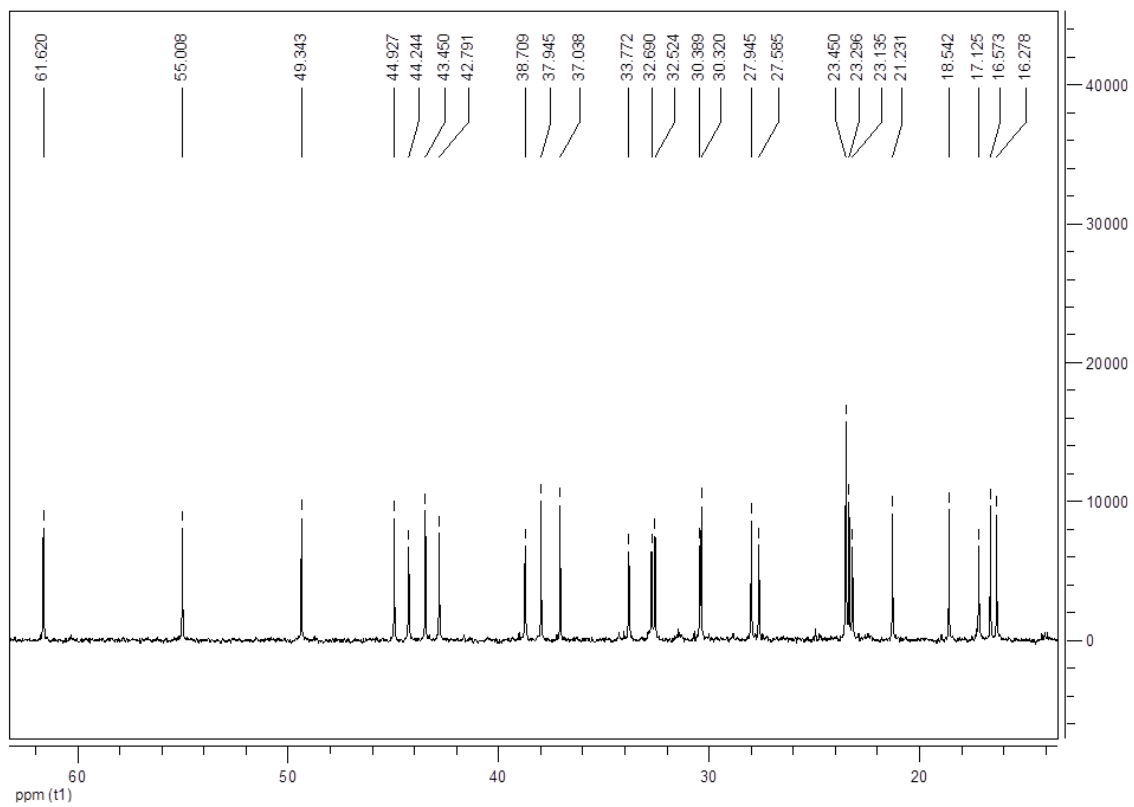
^1H NMR spectrum for compound 26 recorded in CDCl_3 .



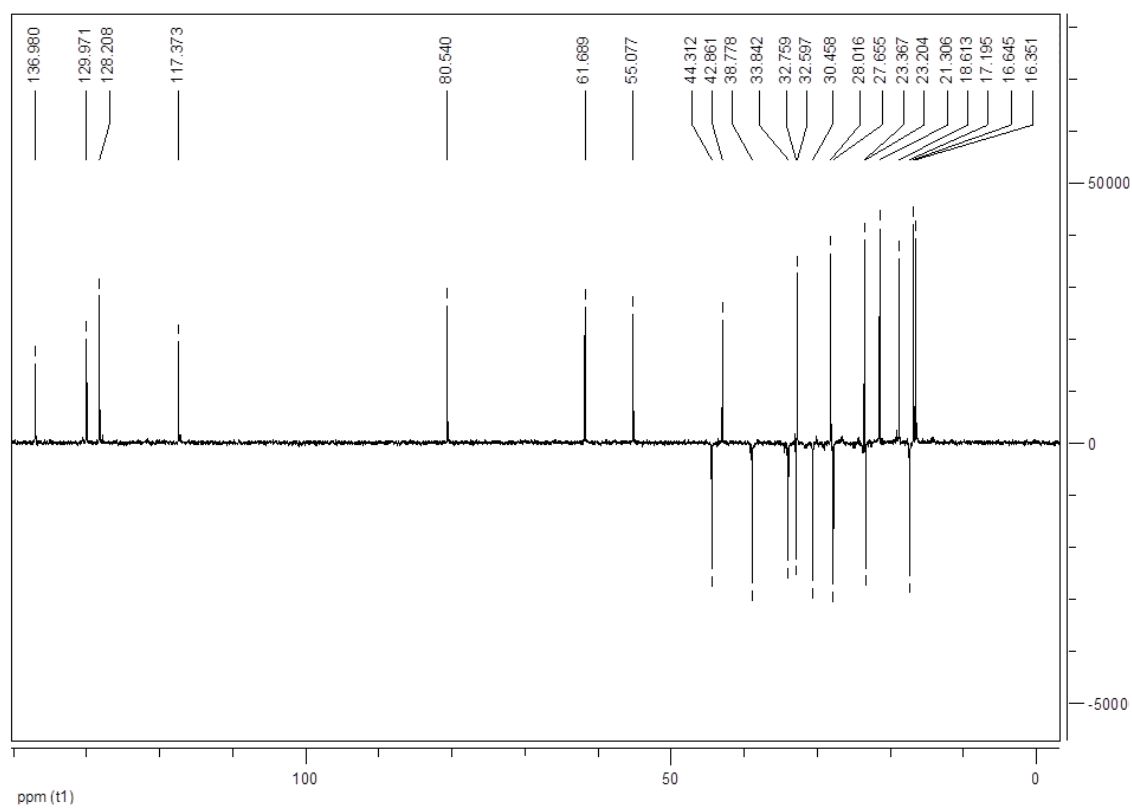
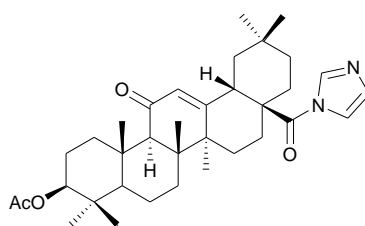
^{13}C NMR spectrum for compound **26** recorded in CDCl_3 .



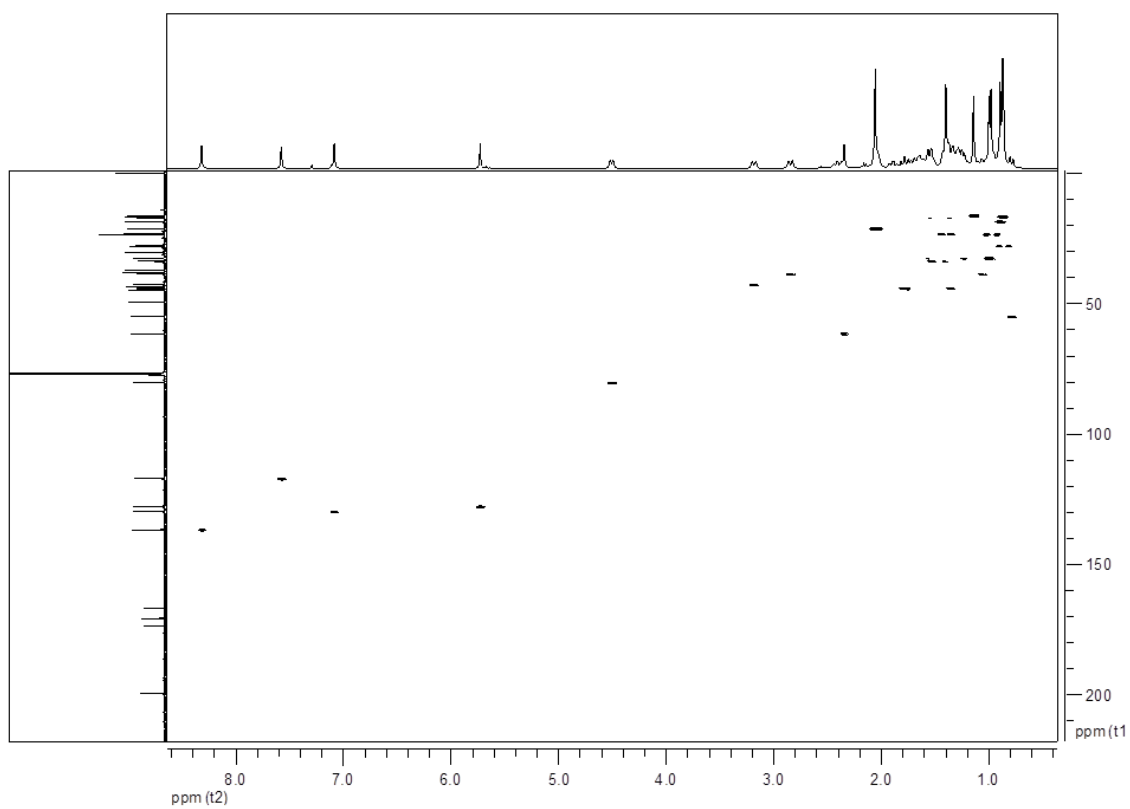
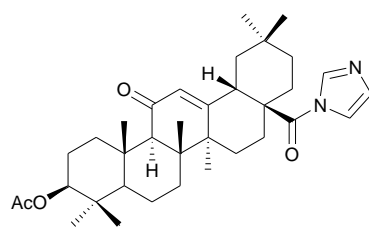
^{13}C NMR spectrum detail of compound **26**.



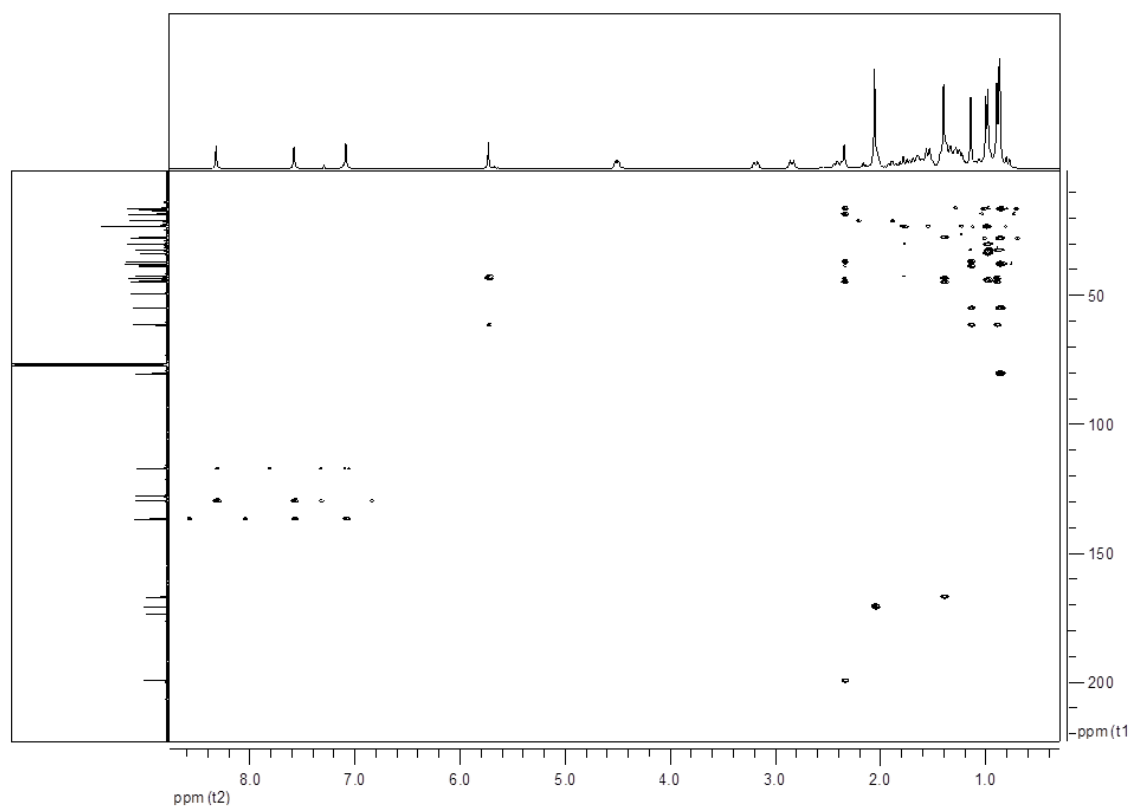
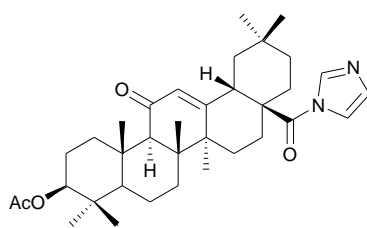
DEPT-135 NMR spectrum for compound **26** recorded in CDCl₃.



HMQC NMR spectrum for compound **26** recorded in CDCl₃.

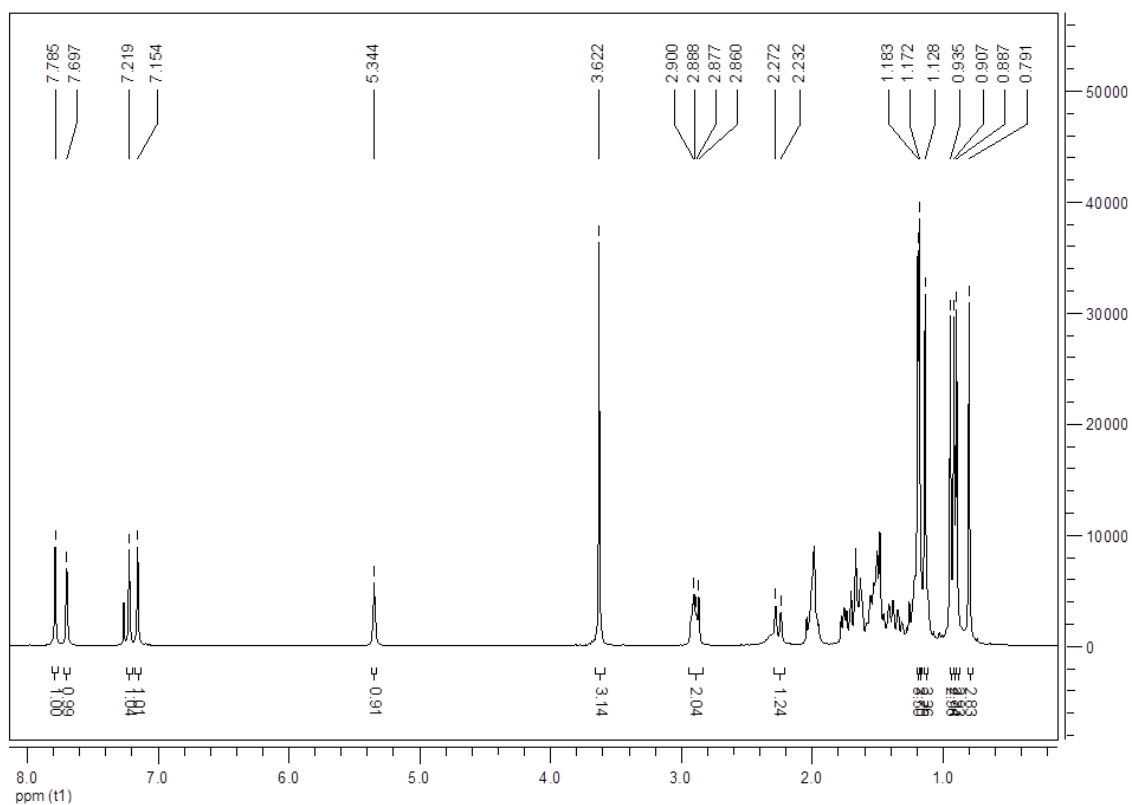
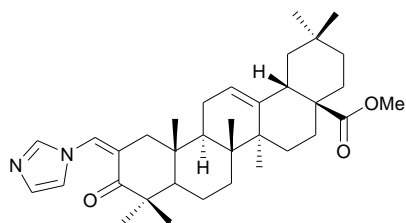


HMBC NMR spectrum for compound **26** recorded in CDCl₃.

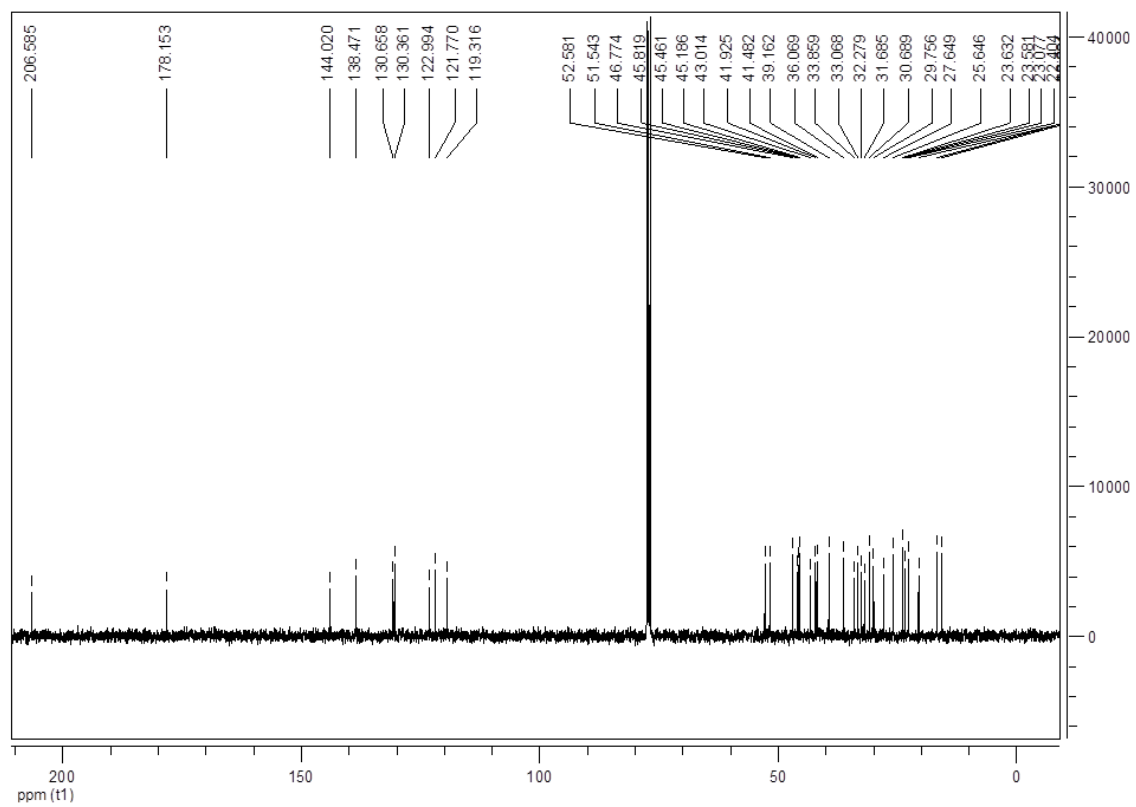
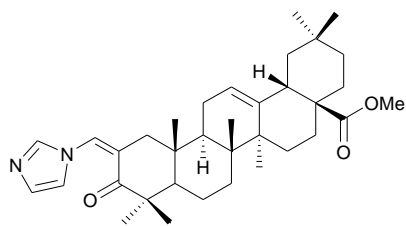


13. Spectral data for compound **27**

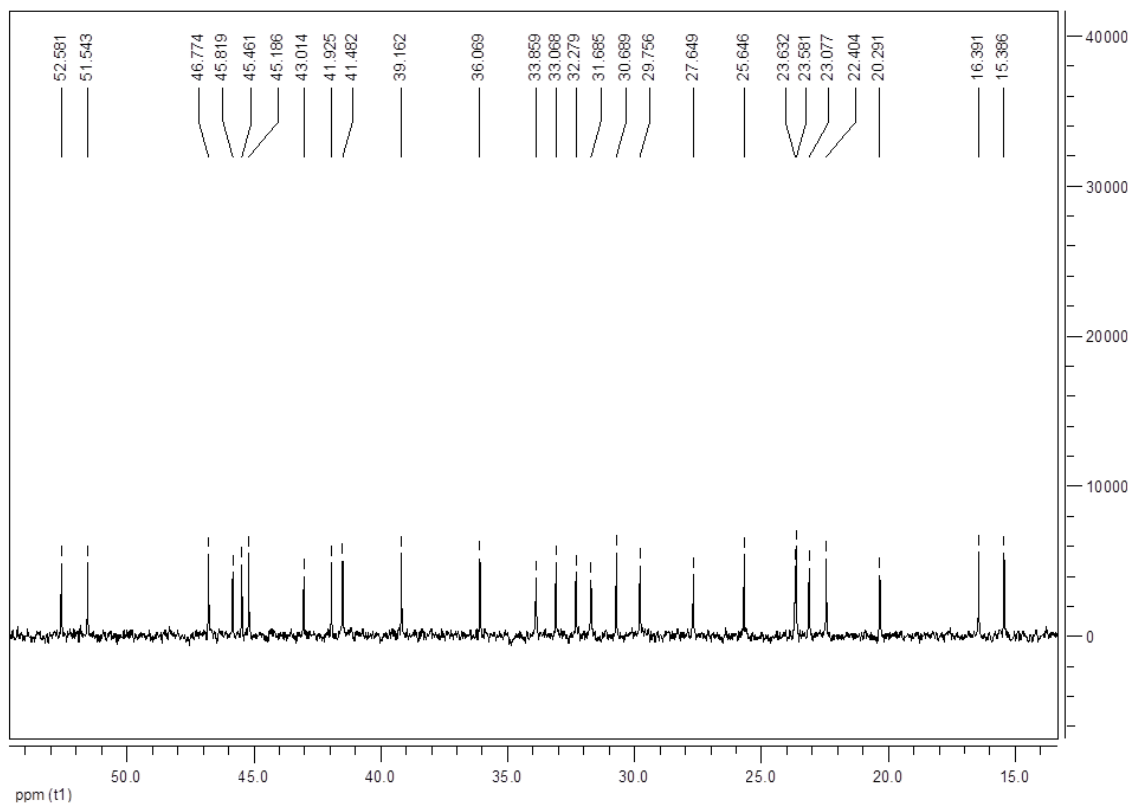
¹H NMR spectrum for compound **27** recorded in CDCl₃.



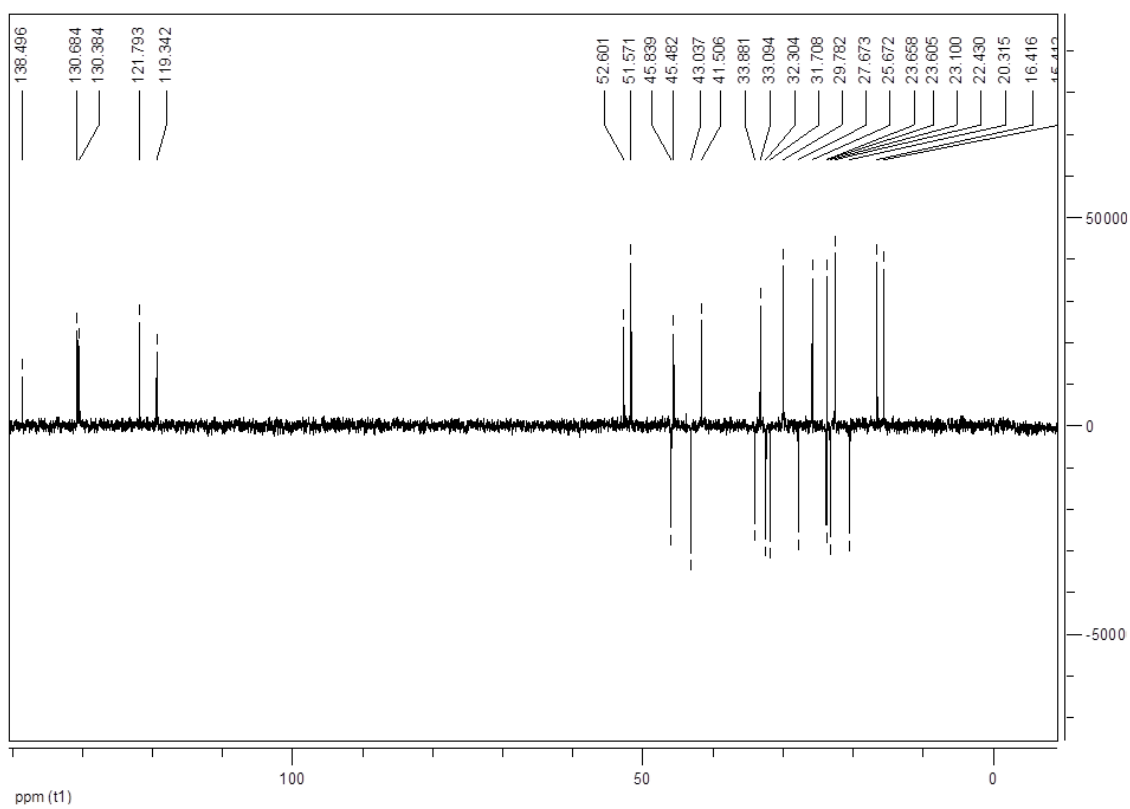
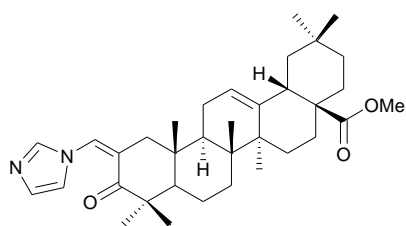
^{13}C NMR spectrum for compound **27** recorded in CDCl_3 .



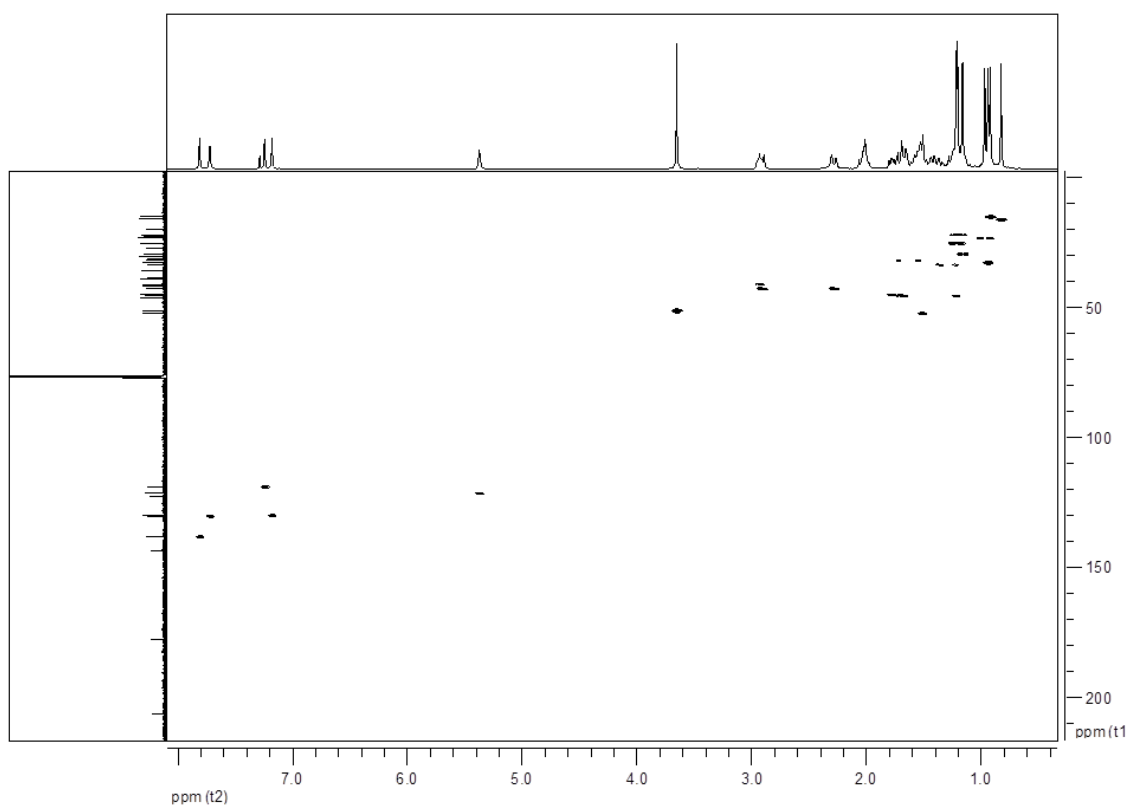
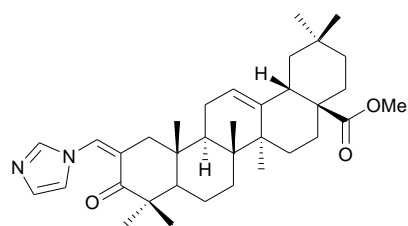
^{13}C NMR spectrum detail of compound **27**.



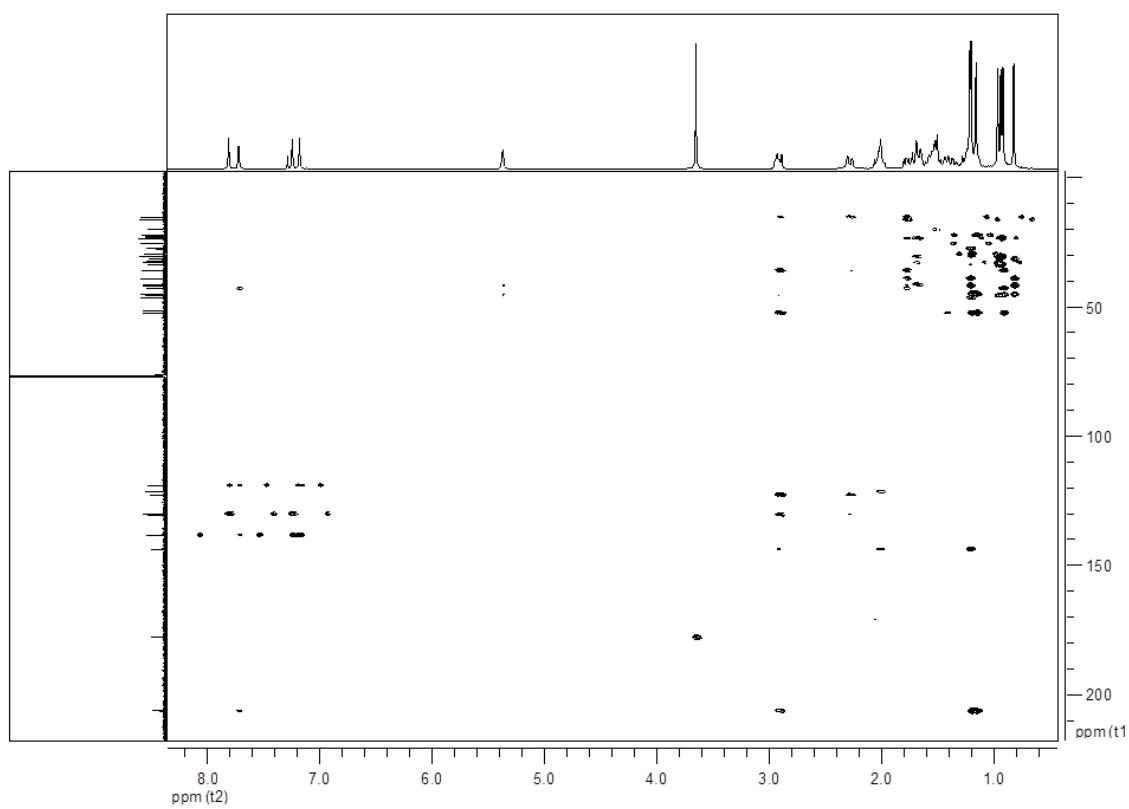
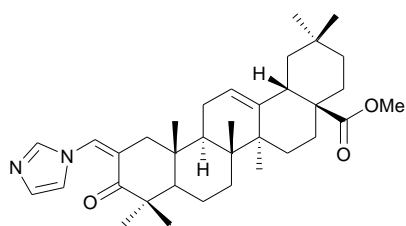
DEPT-135 NMR spectrum for compound **27** recorded in CDCl₃.



HMQC NMR spectrum for compound **27** recorded in CDCl₃.

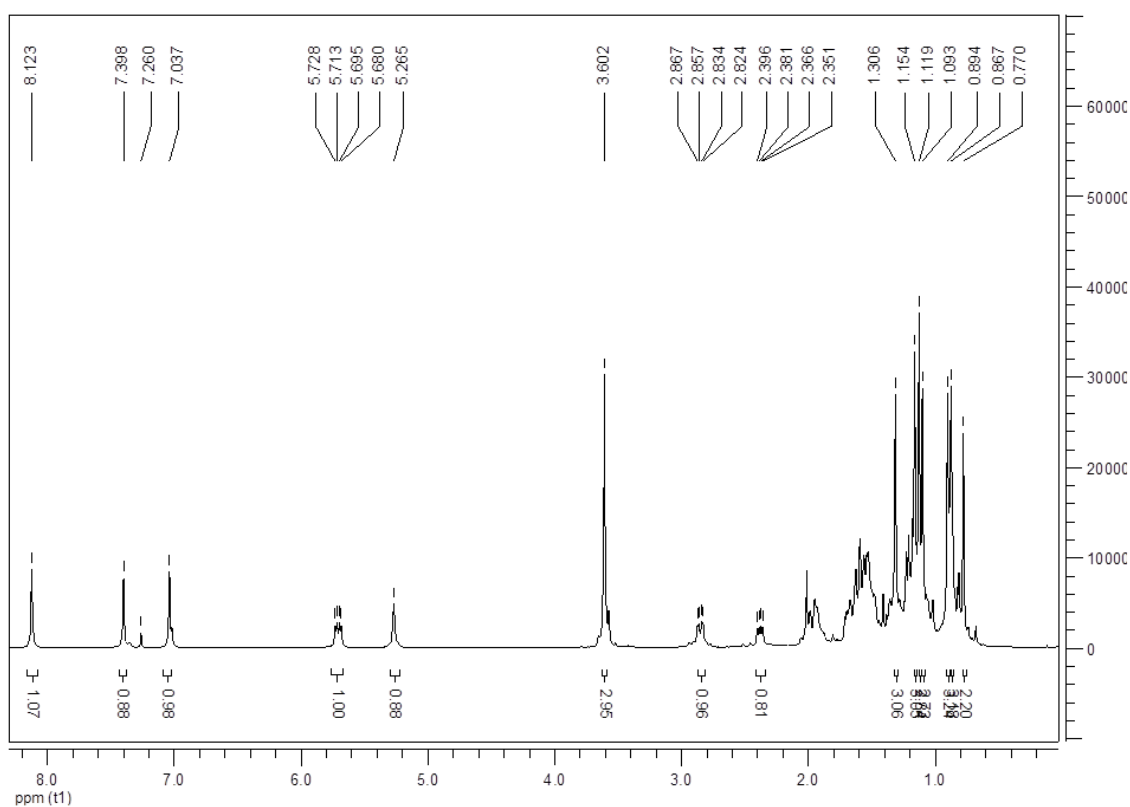
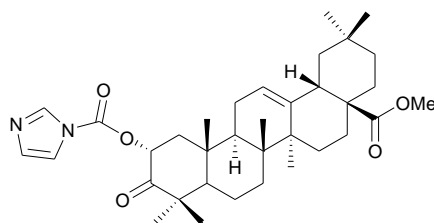


HMBC NMR spectrum for compound **27** recorded in CDCl₃.

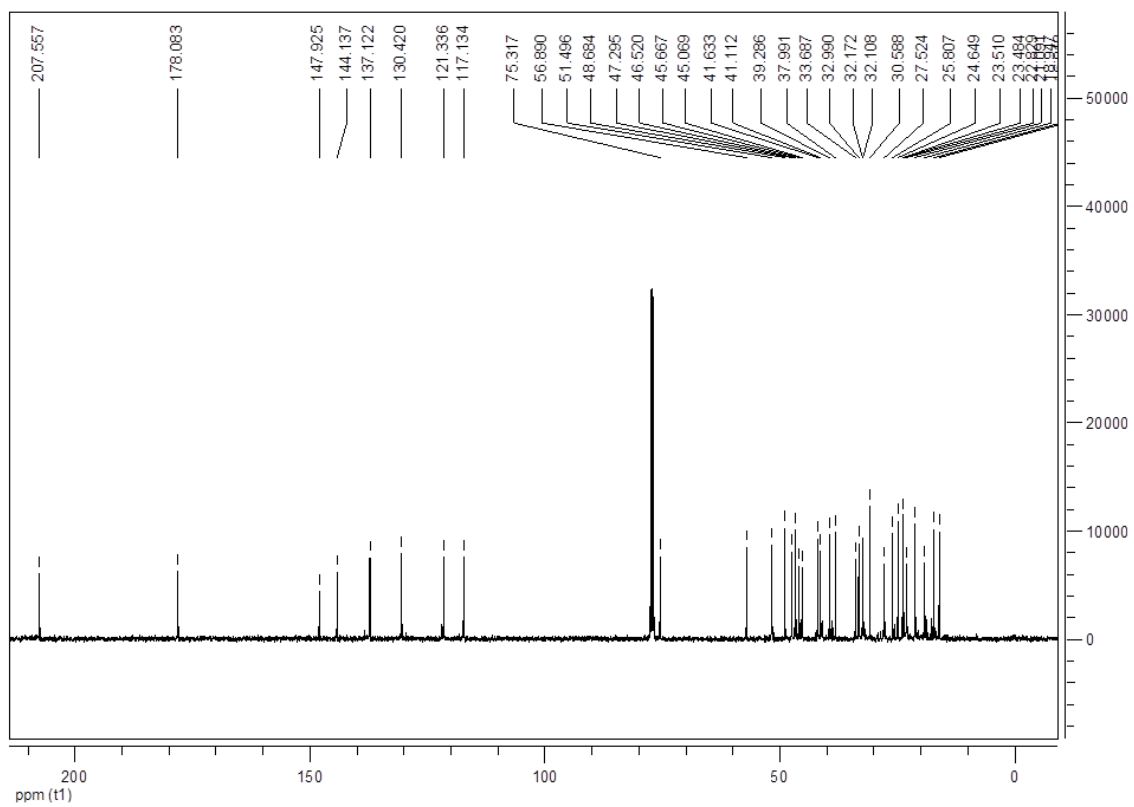
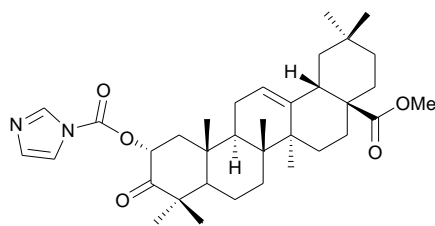


14. Spectral data for compound **28**

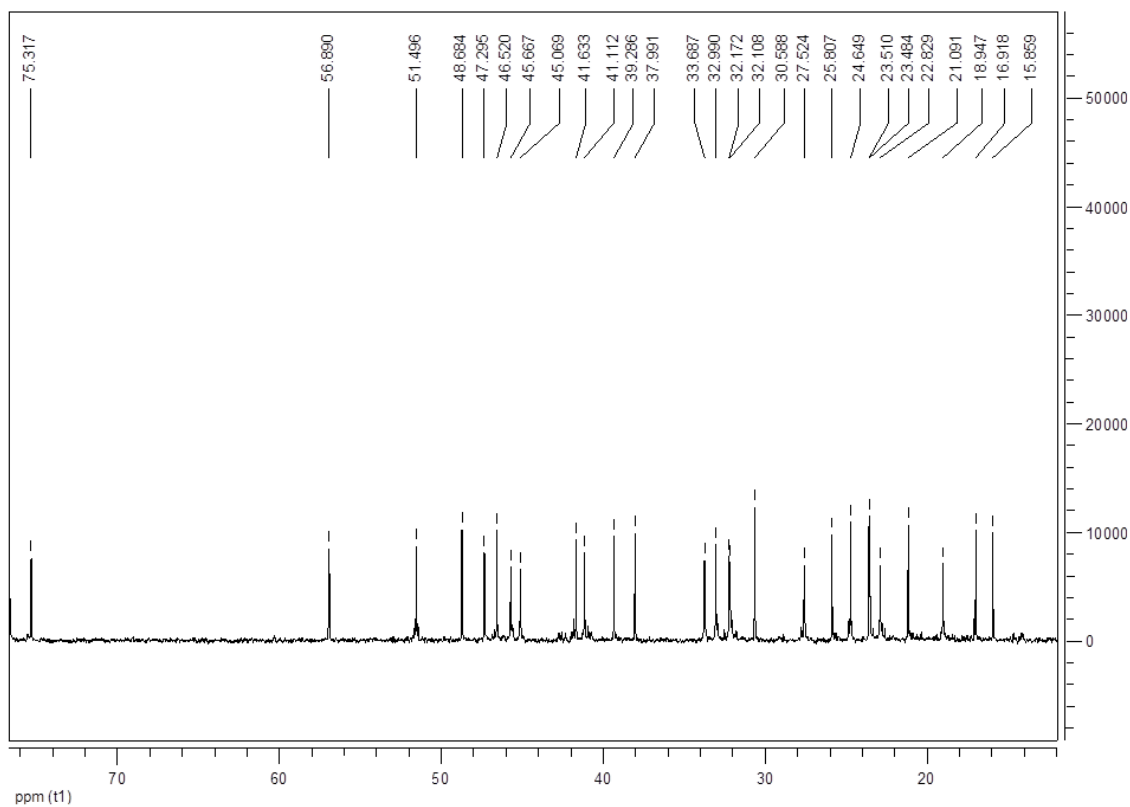
^1H NMR spectrum for compound **28** recorded in CDCl_3 .



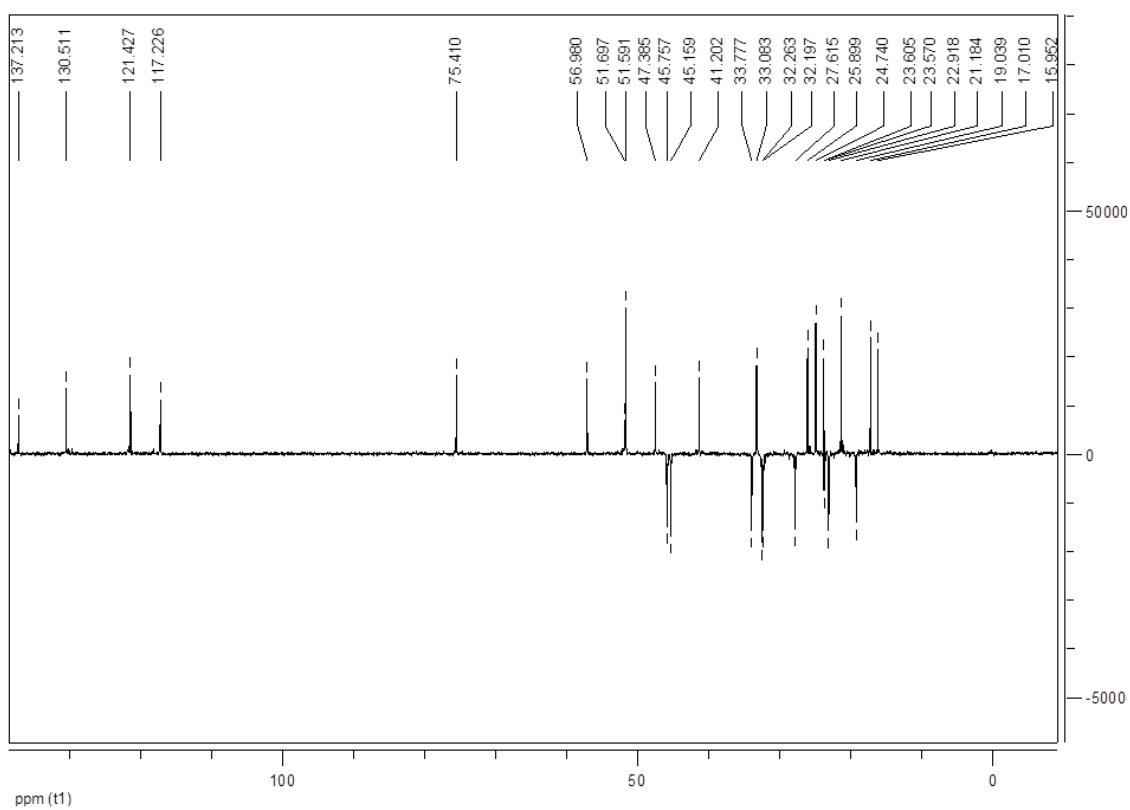
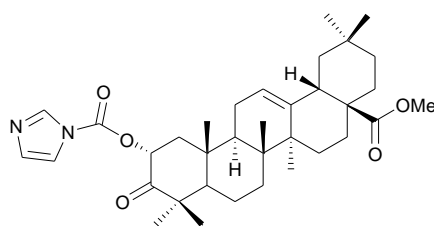
^{13}C NMR spectrum for compound **28** recorded in CDCl_3 .



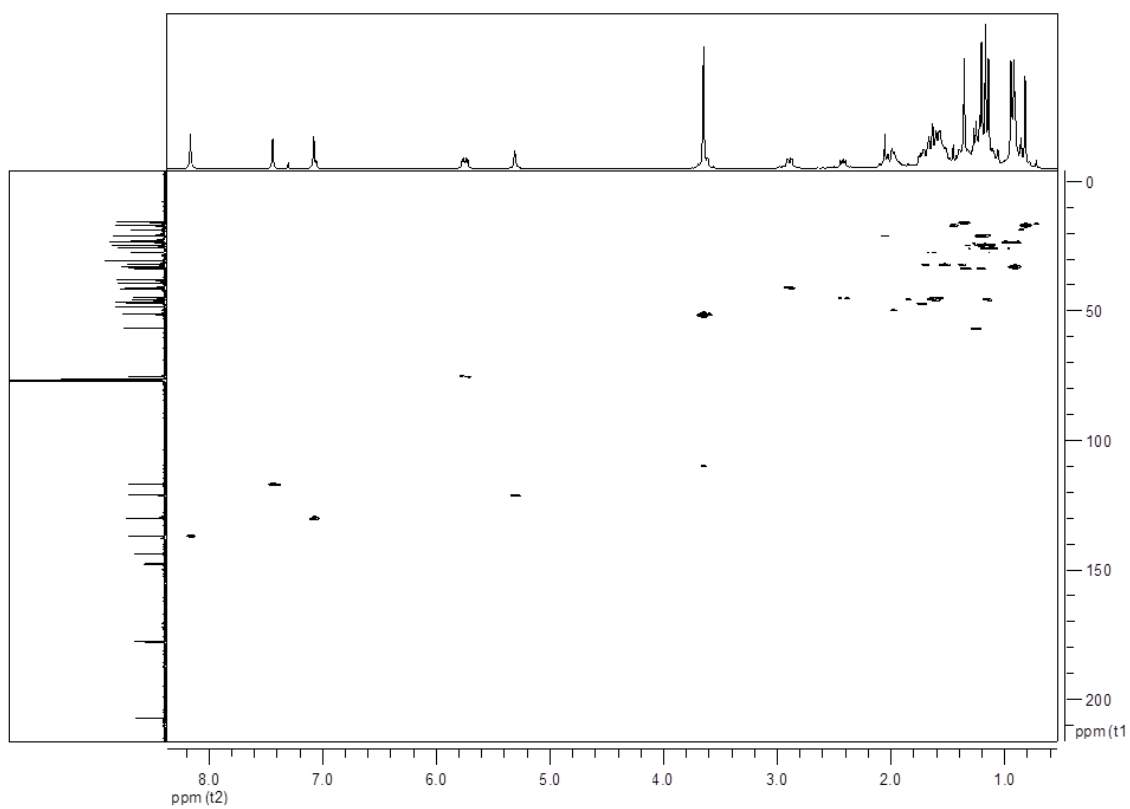
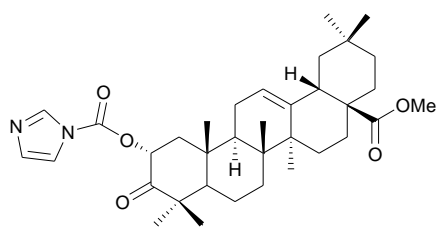
^{13}C NMR spectrum detail of compound **28**.



DEPT-135 NMR spectrum for compound **28** recorded in CDCl₃.



HMQC NMR spectrum for compound **28** recorded in CDCl₃.



HMBC NMR spectrum for compound **28** recorded in CDCl₃.

