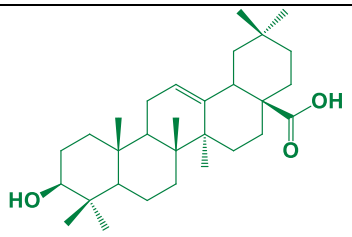
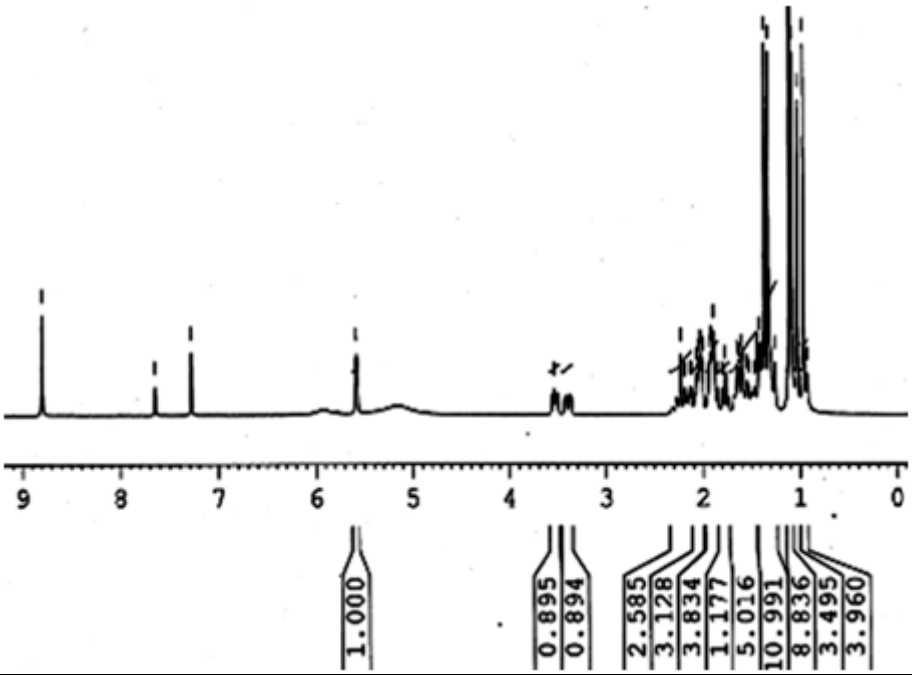
Supplementary Data

A) NMR Spectra of isolated and synthesized compounds

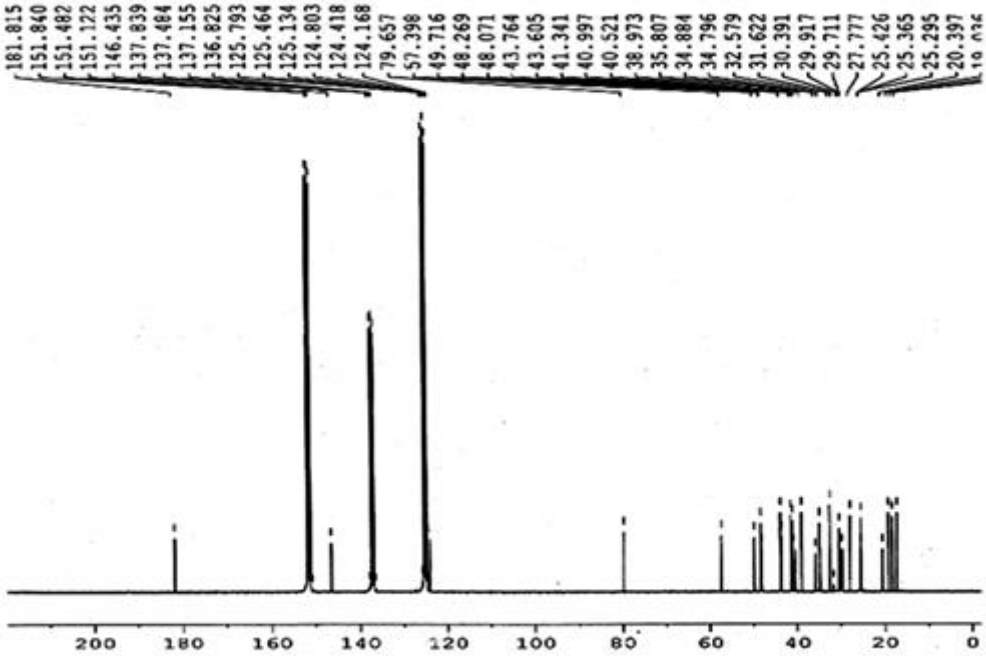


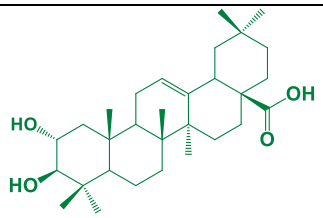
Compound **1**

^{1}H NMR



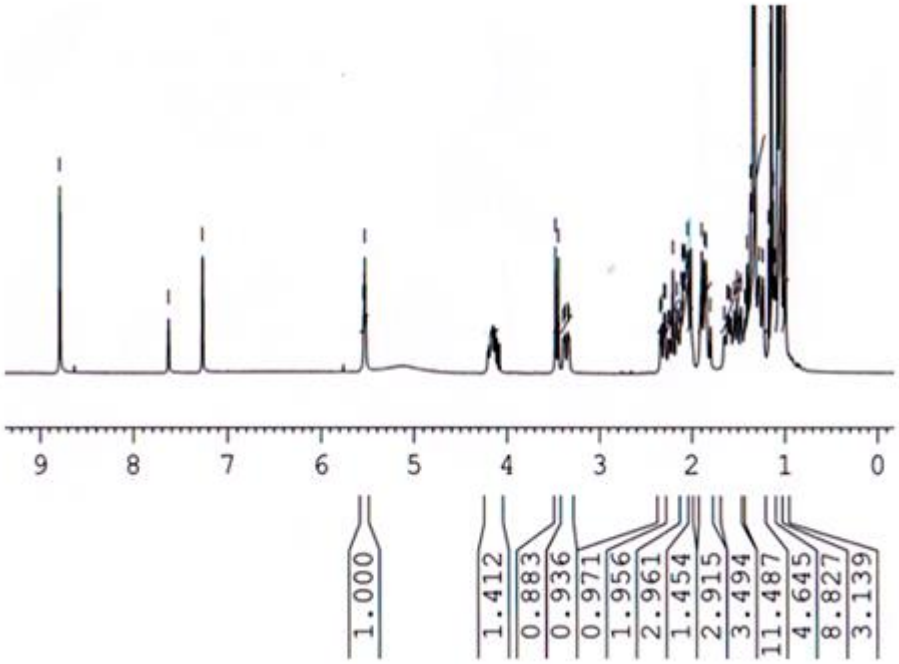
^{13}C NMR



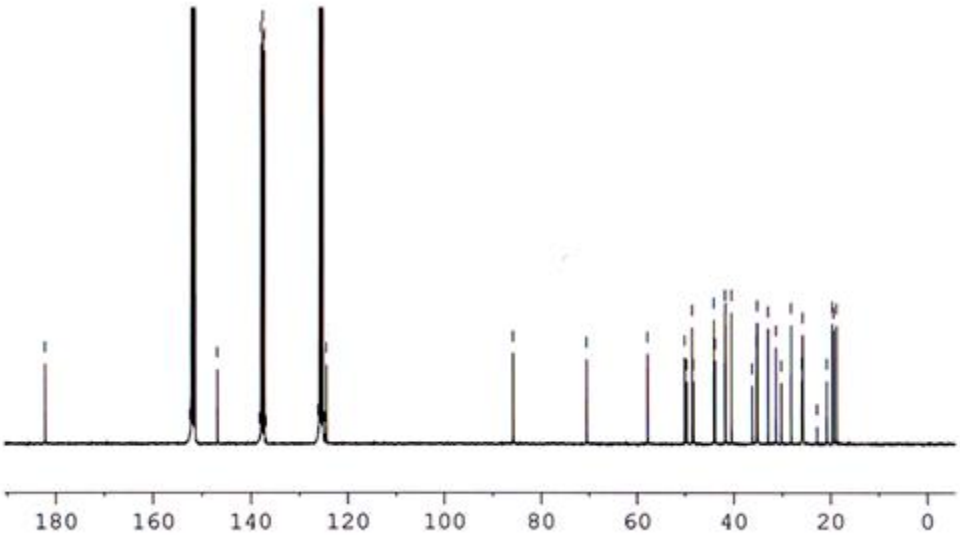


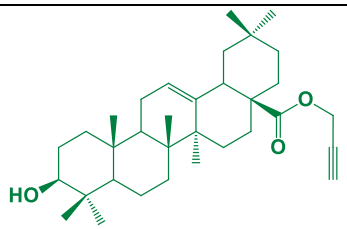
Compound **2**

^{1}H NMR



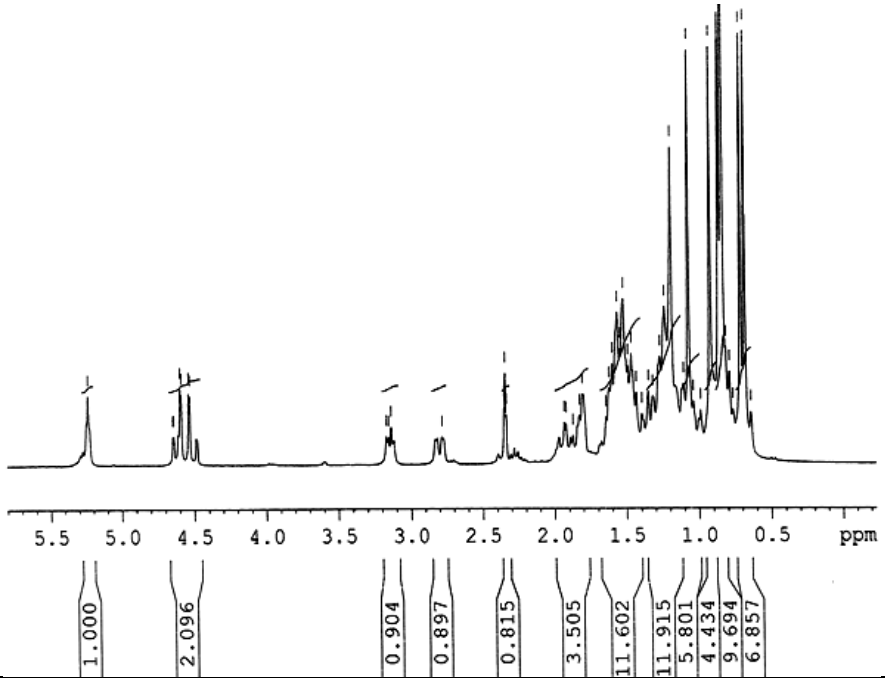
^{13}C NMR



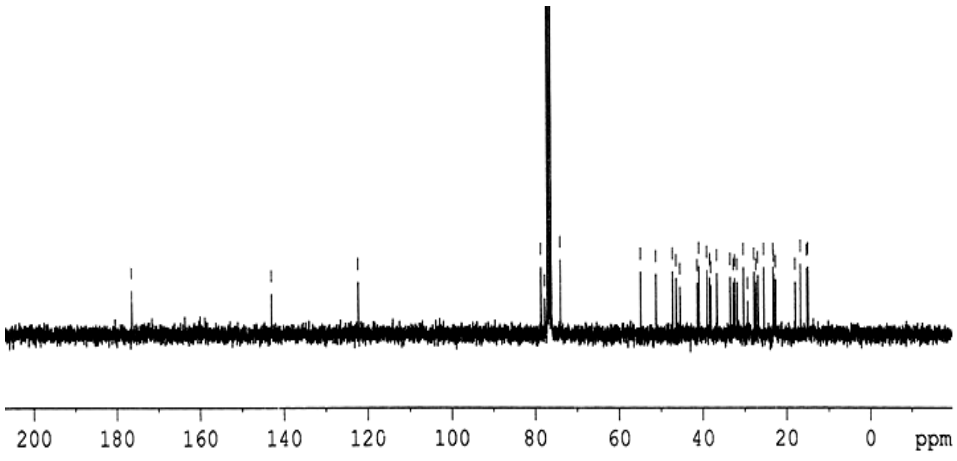


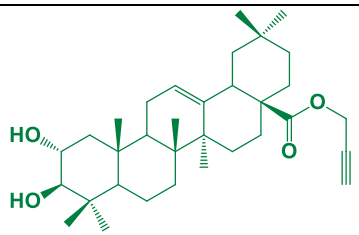
Compound **3**

^{1}H NMR



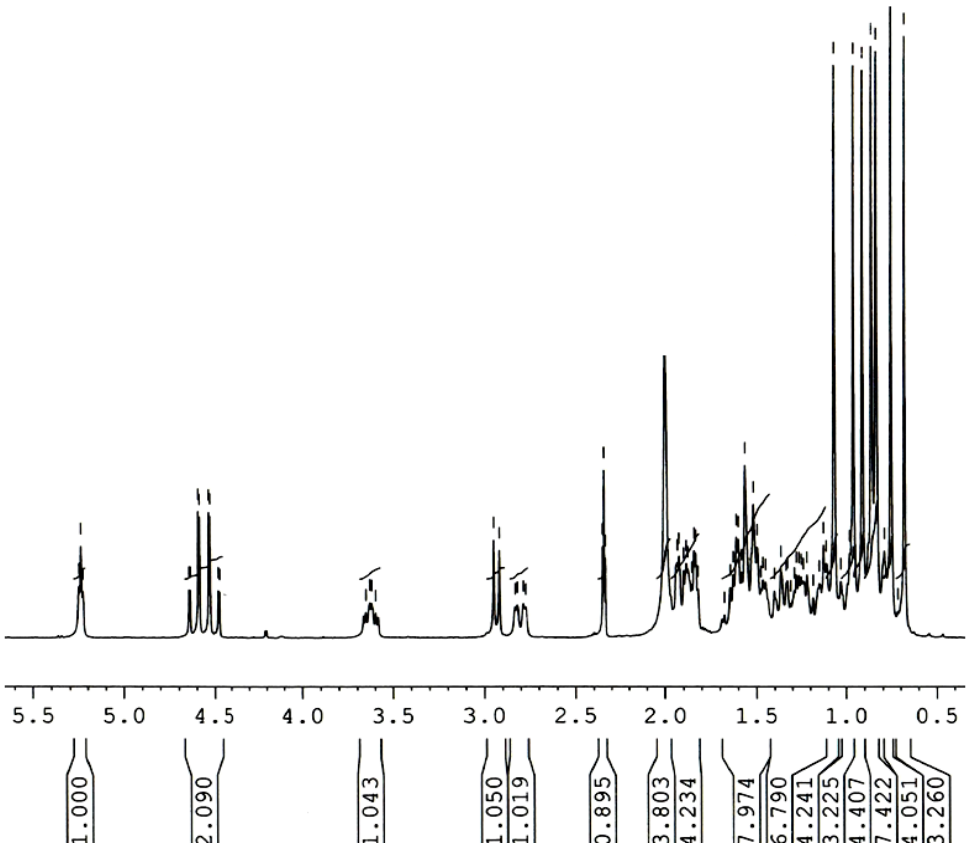
^{13}C NMR



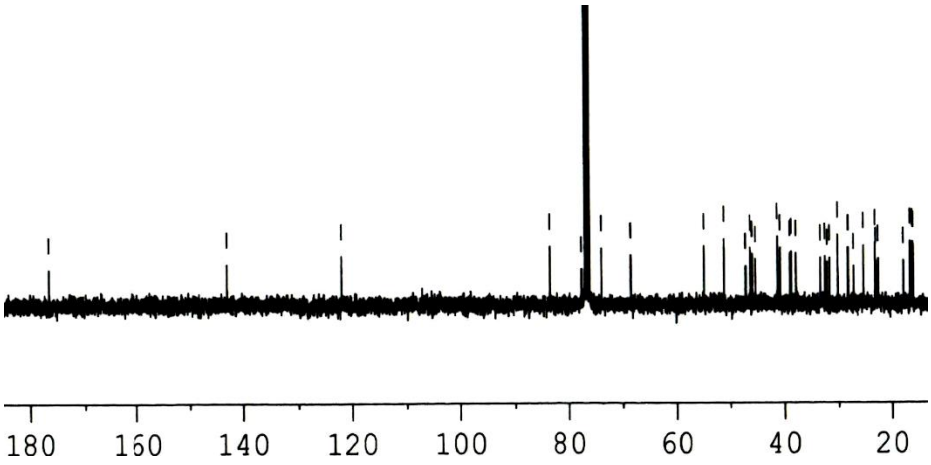


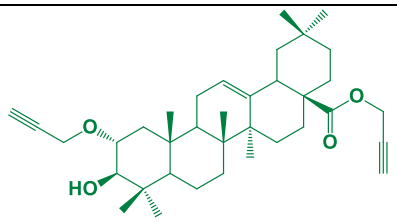
Compound **4**

^{1}H NMR



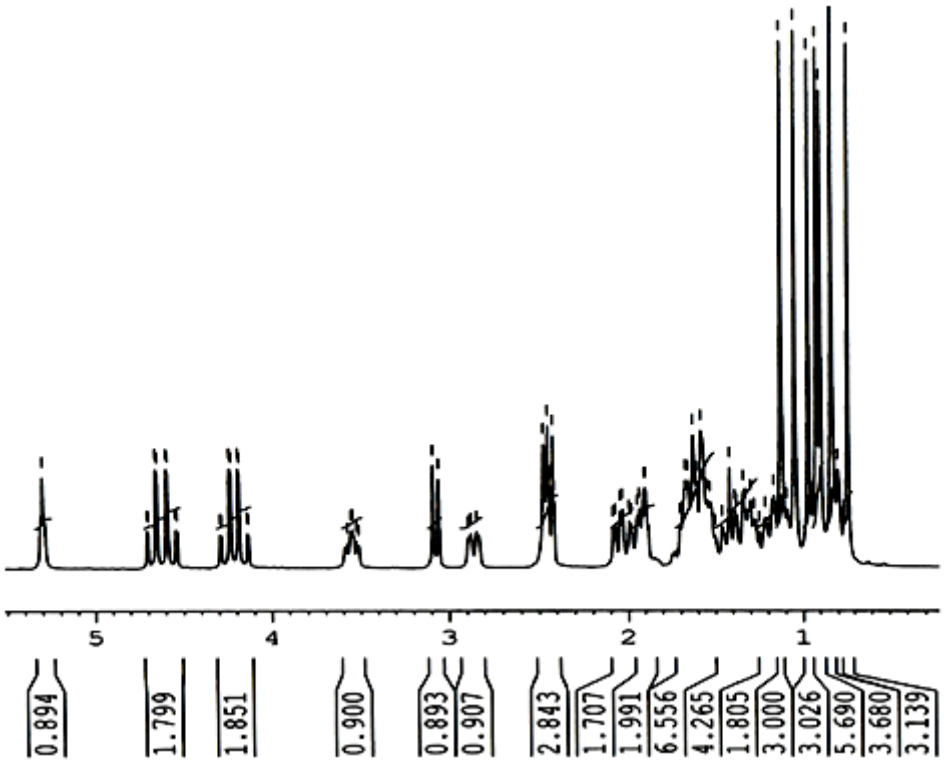
^{13}C NMR



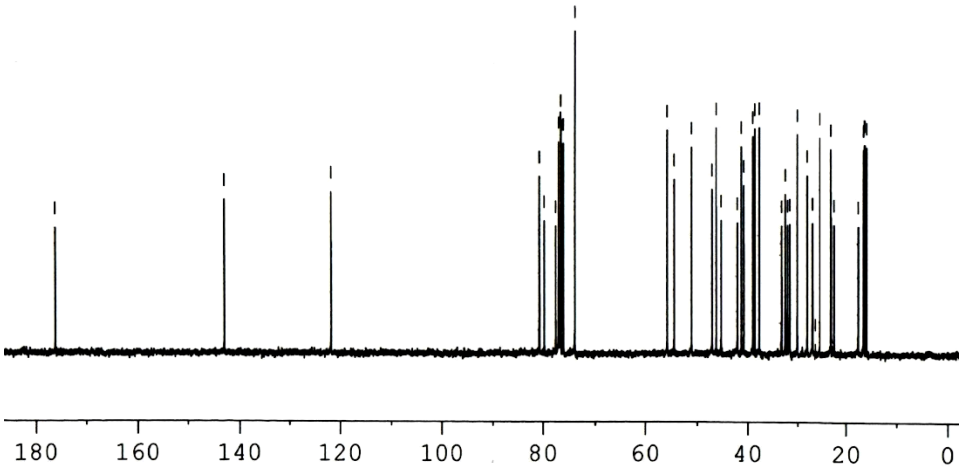


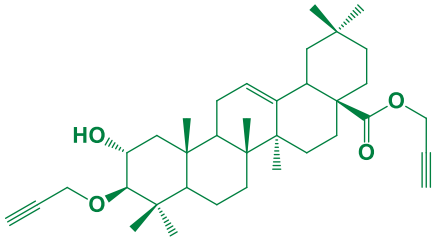
Compound **5**

^{1}H NMR



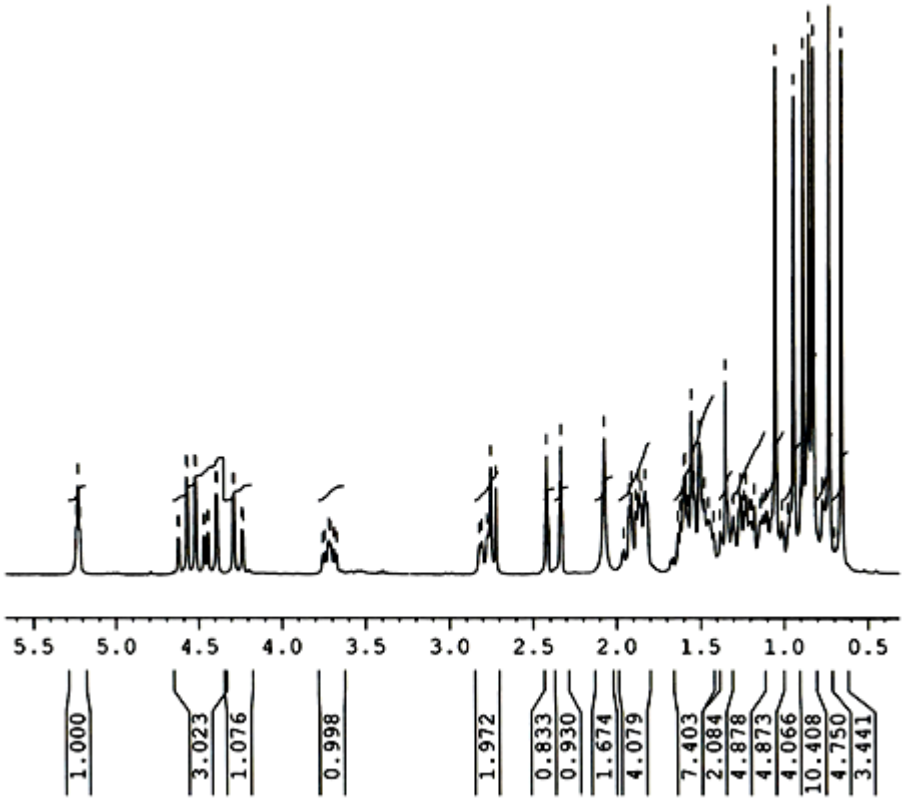
^{13}C NMR



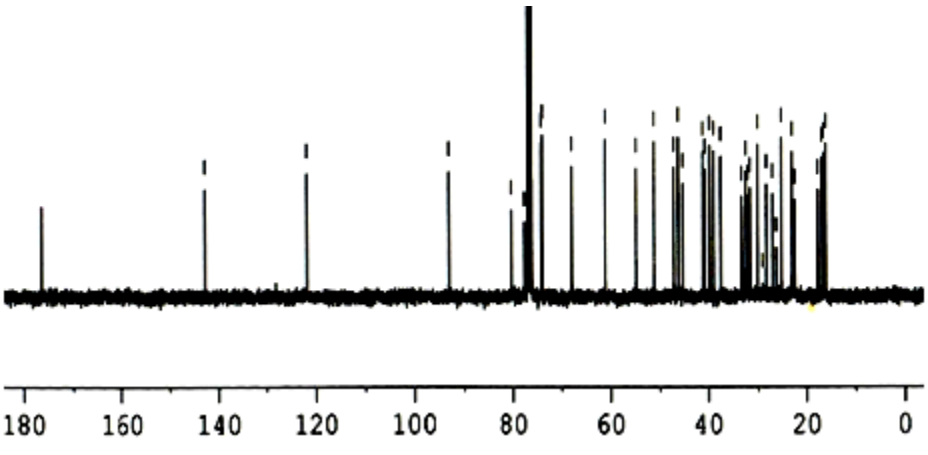


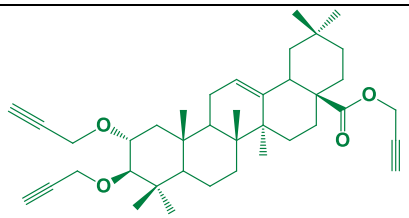
Compound **6**

^{1}H NMR



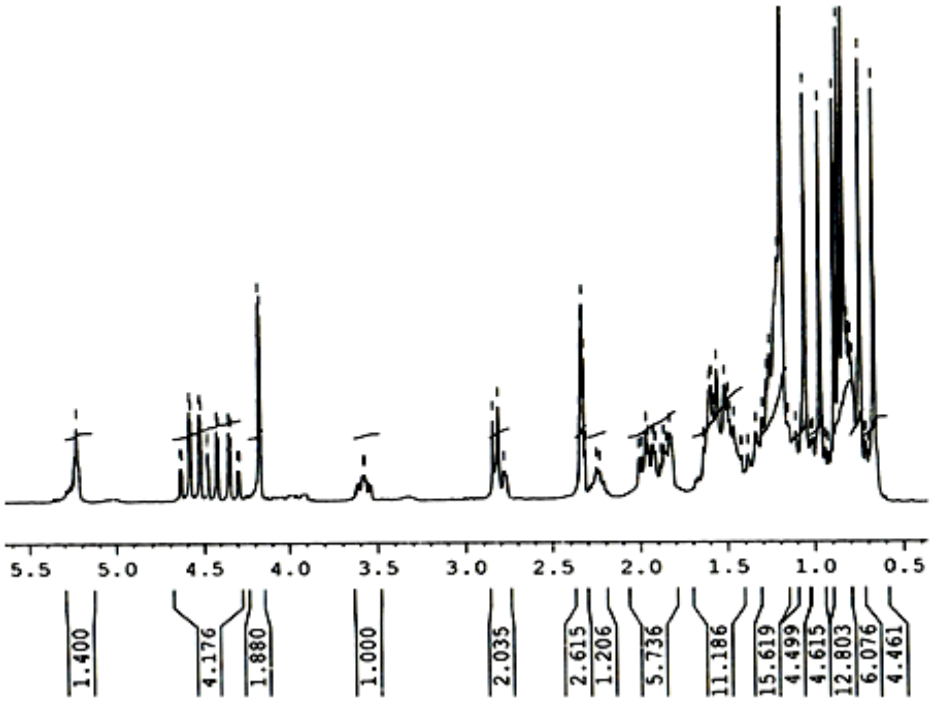
^{13}C NMR



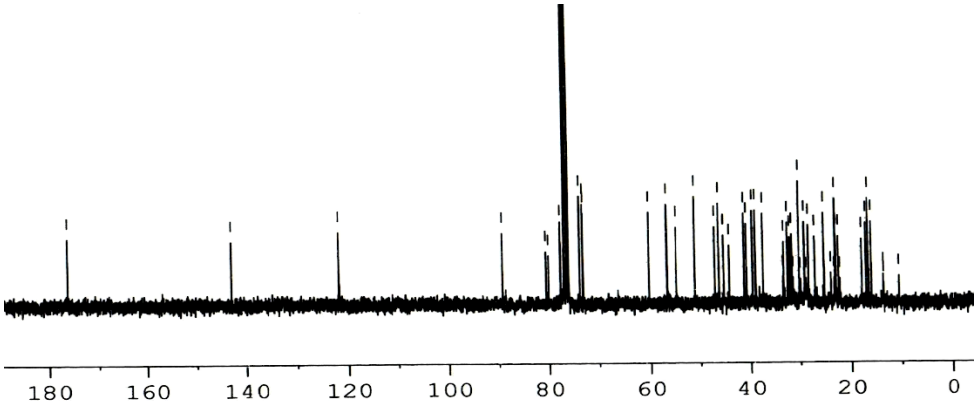


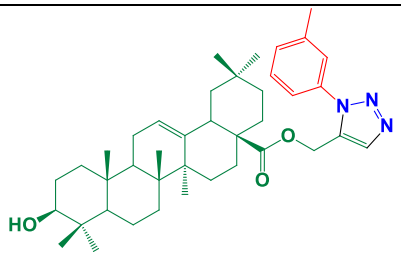
Compound **7**

^{1}H NMR



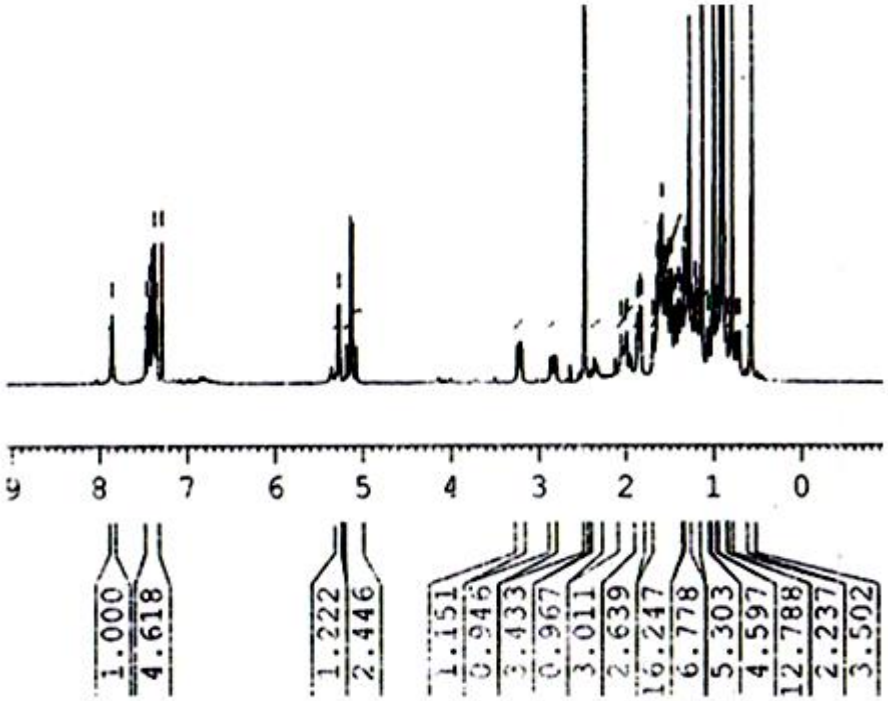
^{13}C NMR



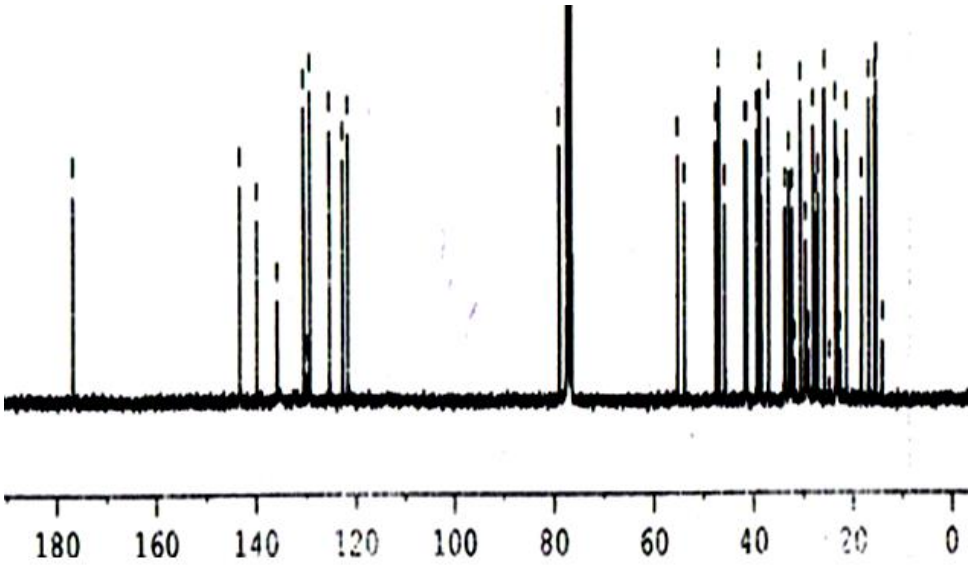


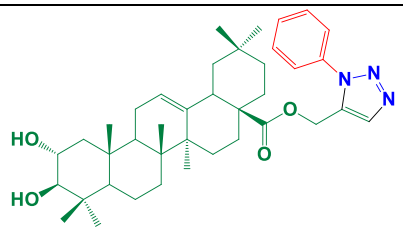
Compound **8**

^{1}H NMR



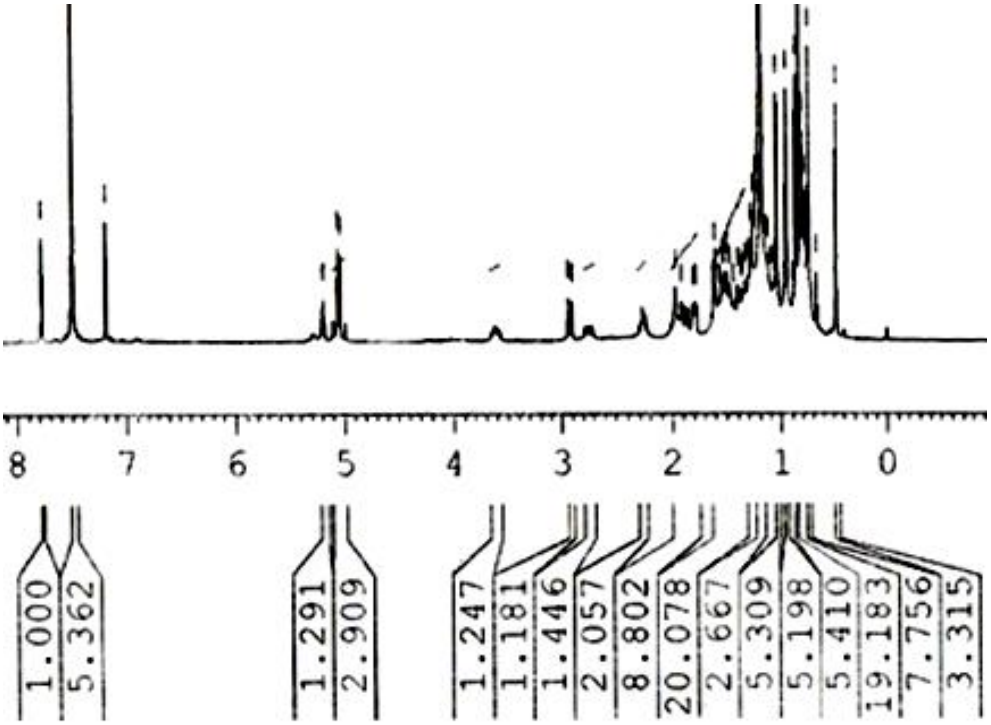
^{13}C NMR



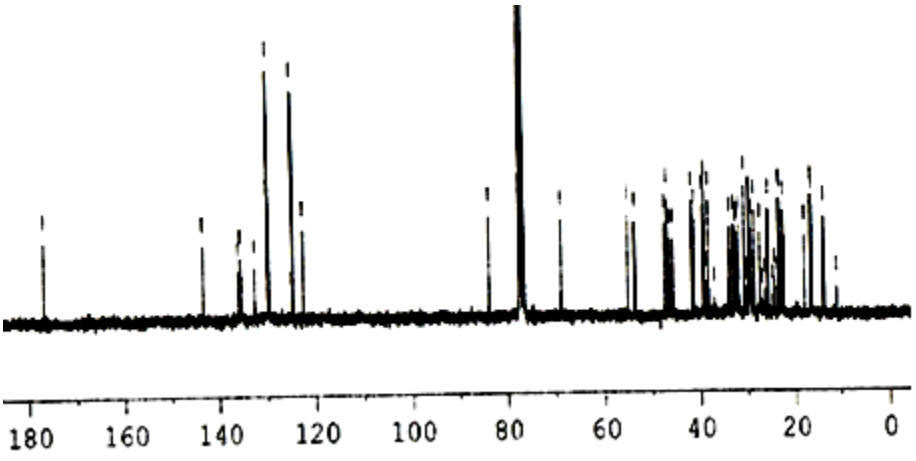


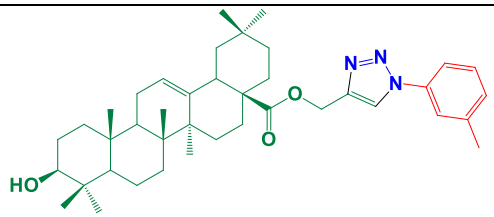
Compound **9**

^{1}H NMR



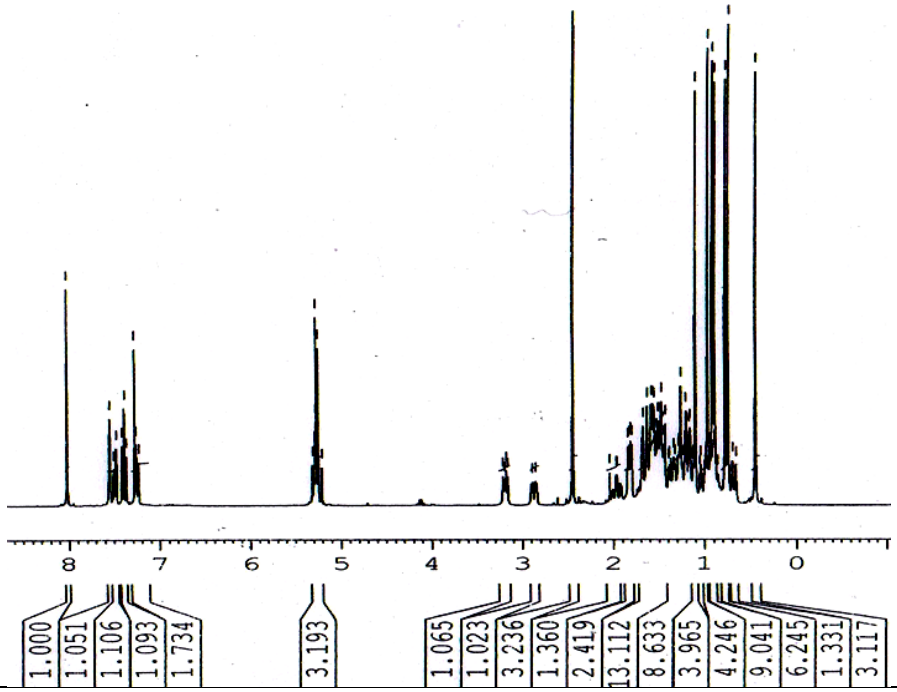
^{13}C NMR



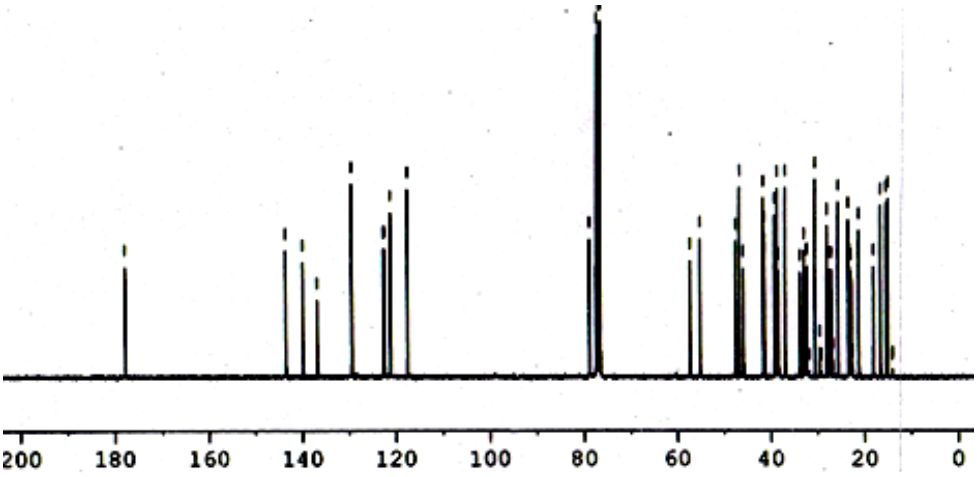


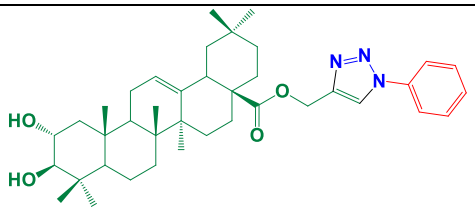
Compound **10**

^{1}H NMR



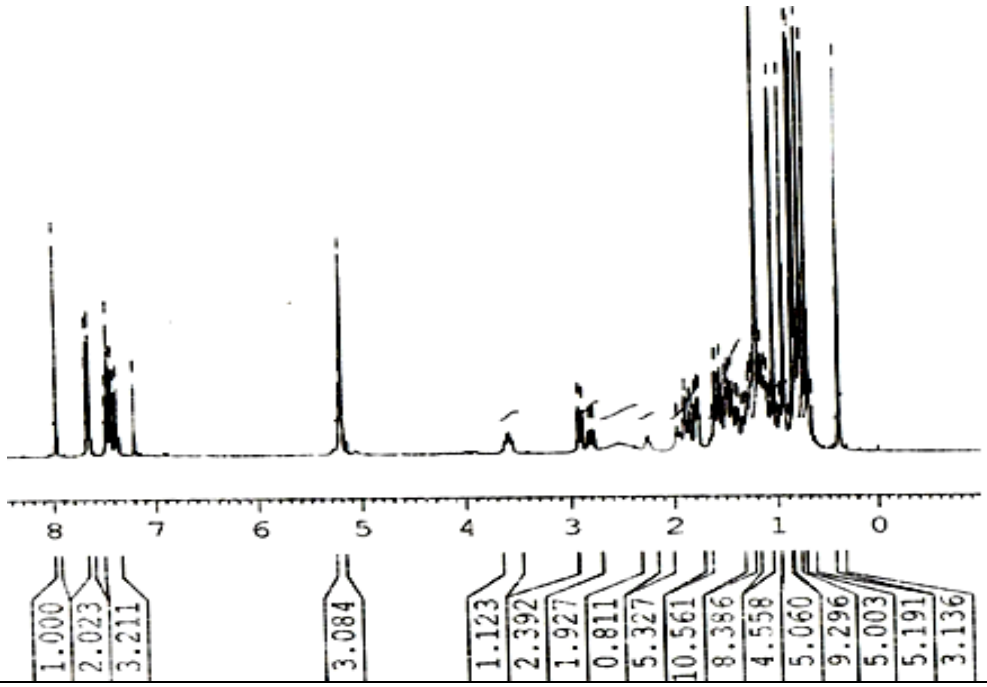
^{13}C NMR



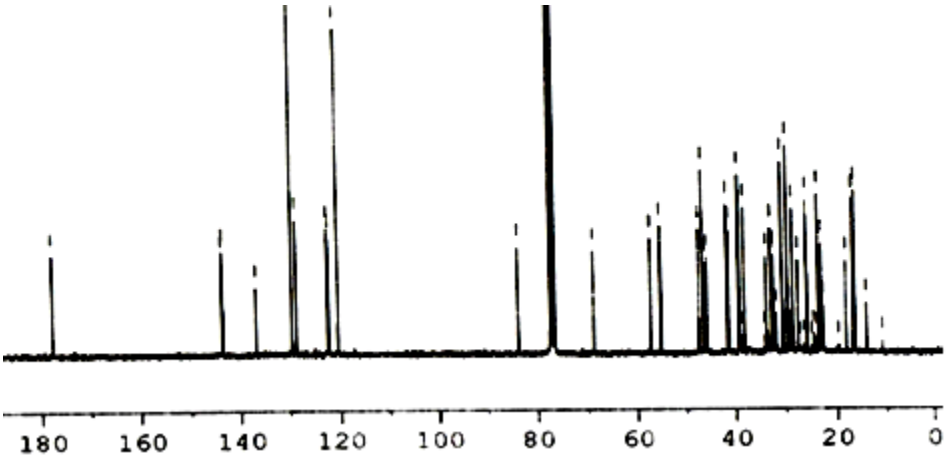


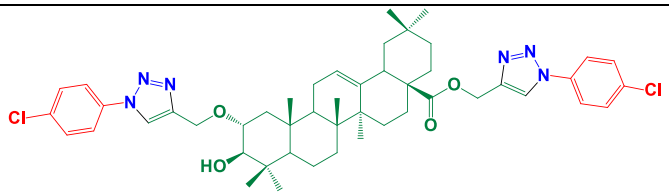
Compound **11**

^{1}H NMR



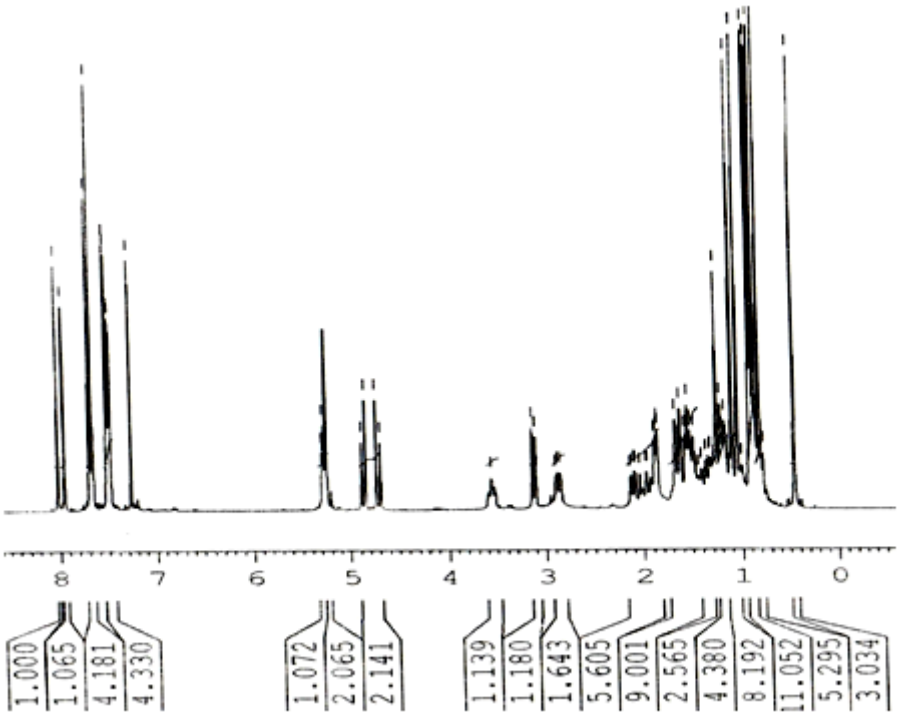
^{13}C NMR



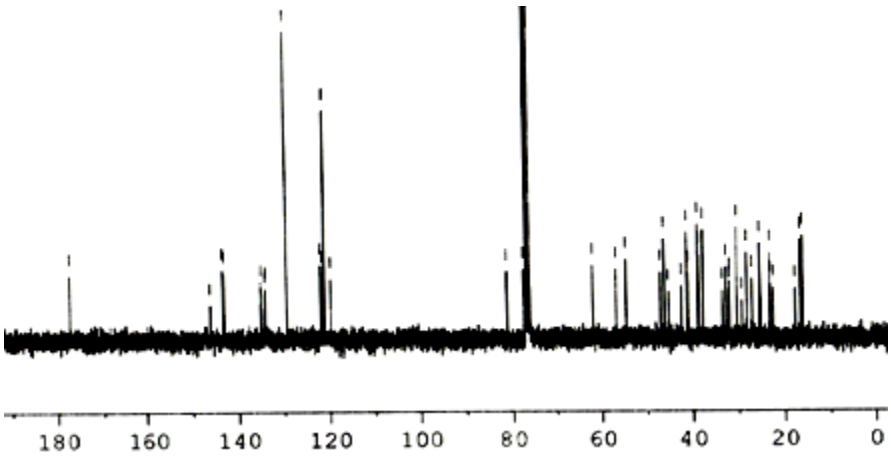


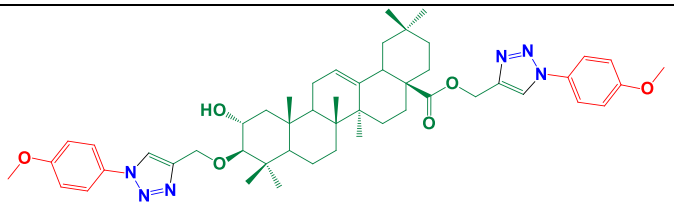
Compound **12**

^{1}H NMR



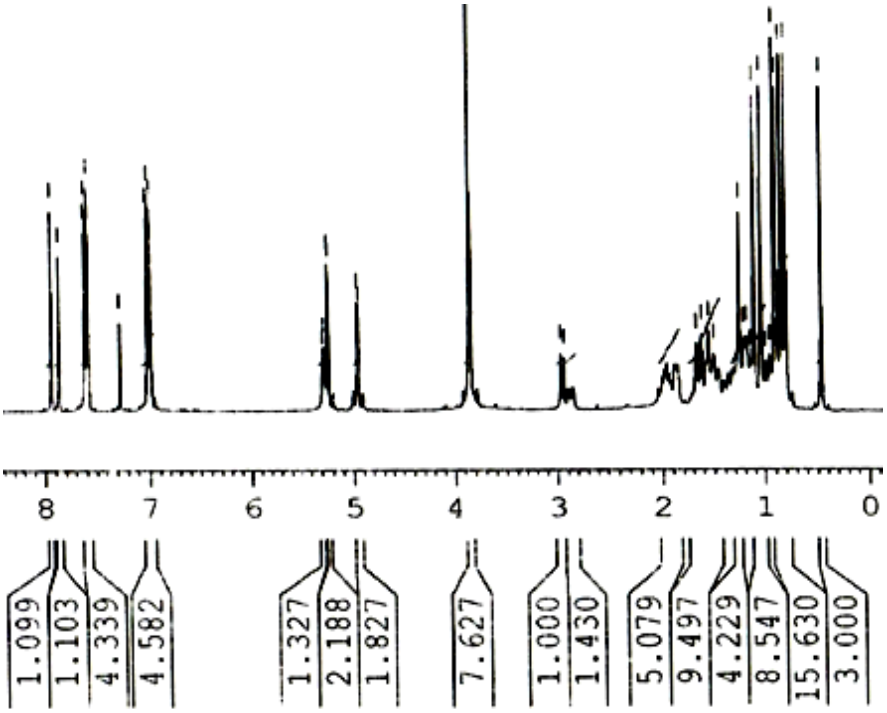
^{13}C NMR



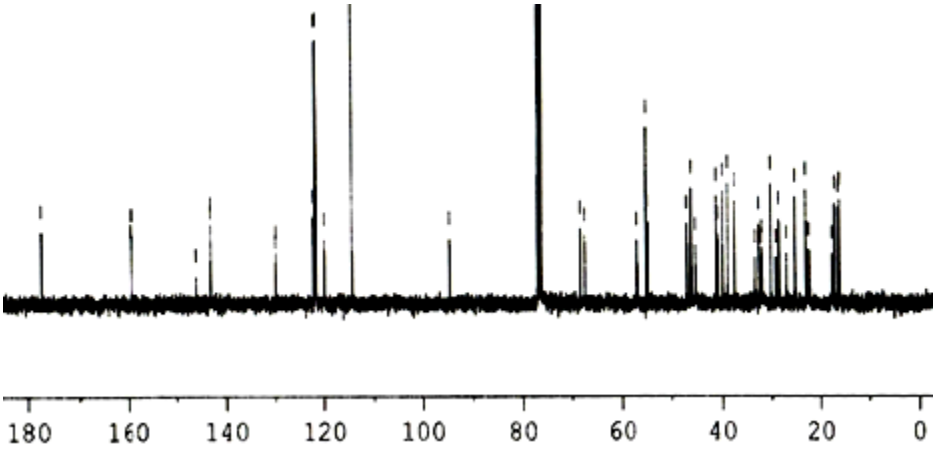


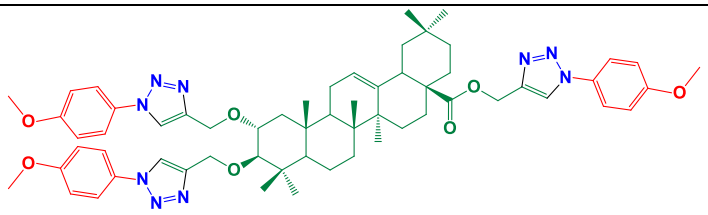
Compound **13**

^{1}H NMR



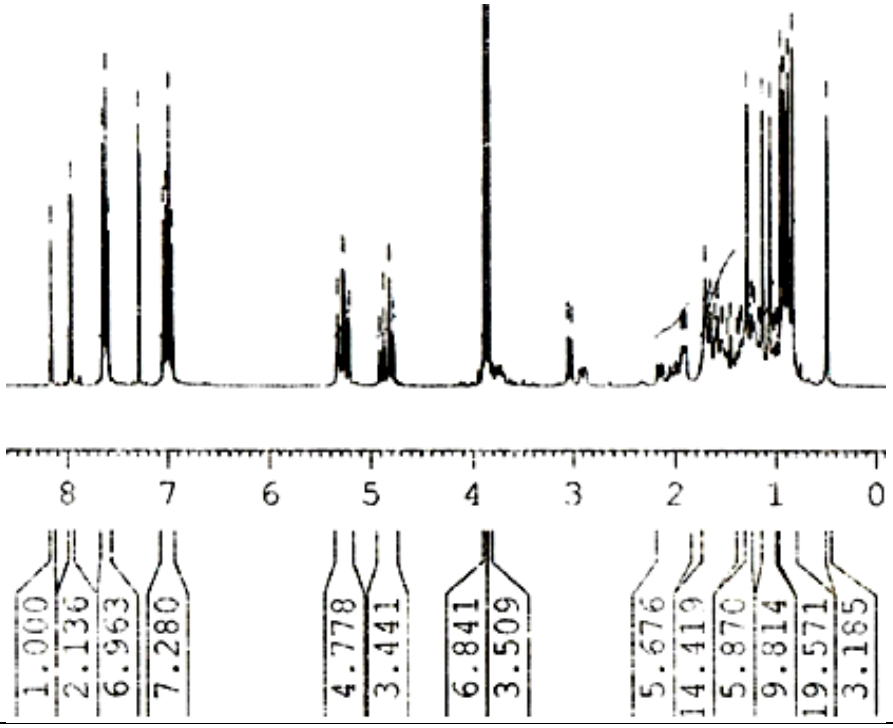
^{13}C NMR



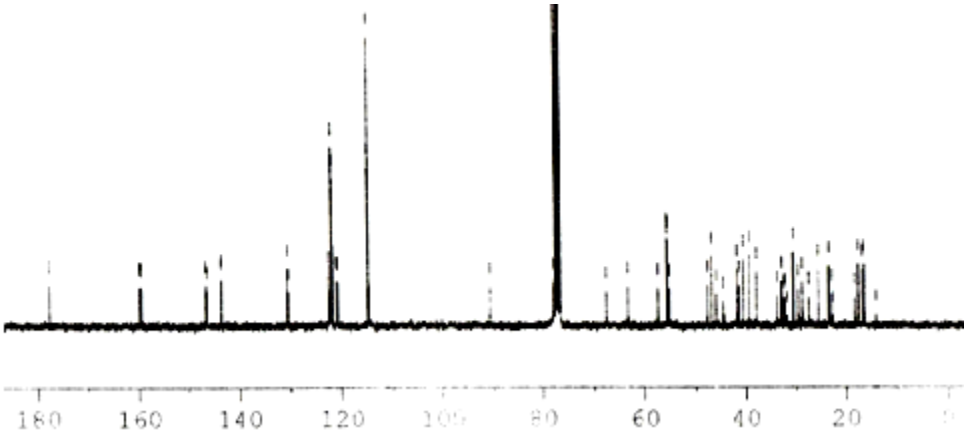


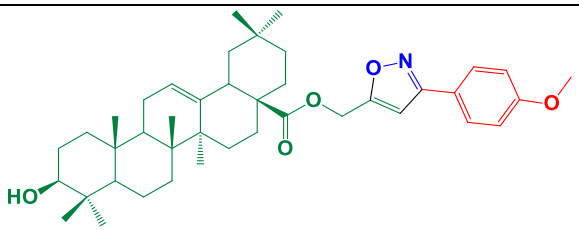
Compound **14**

^{1}H NMR



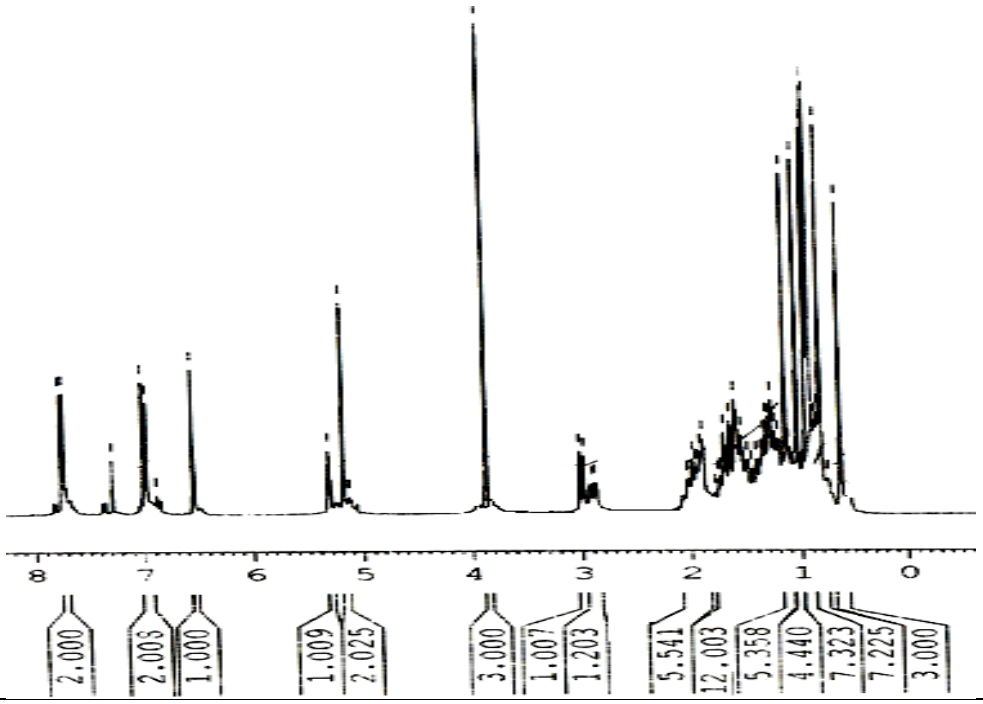
^{13}C NMR



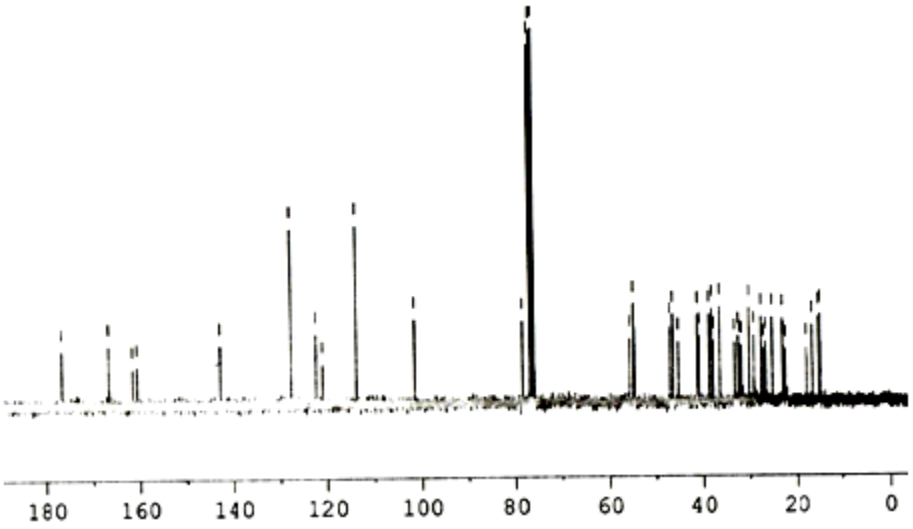


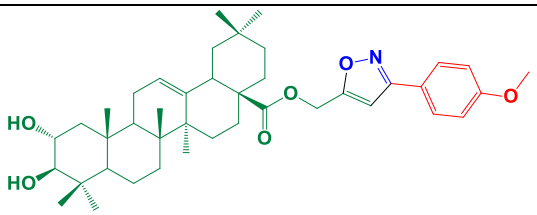
Compound **15**

^{1}H NMR



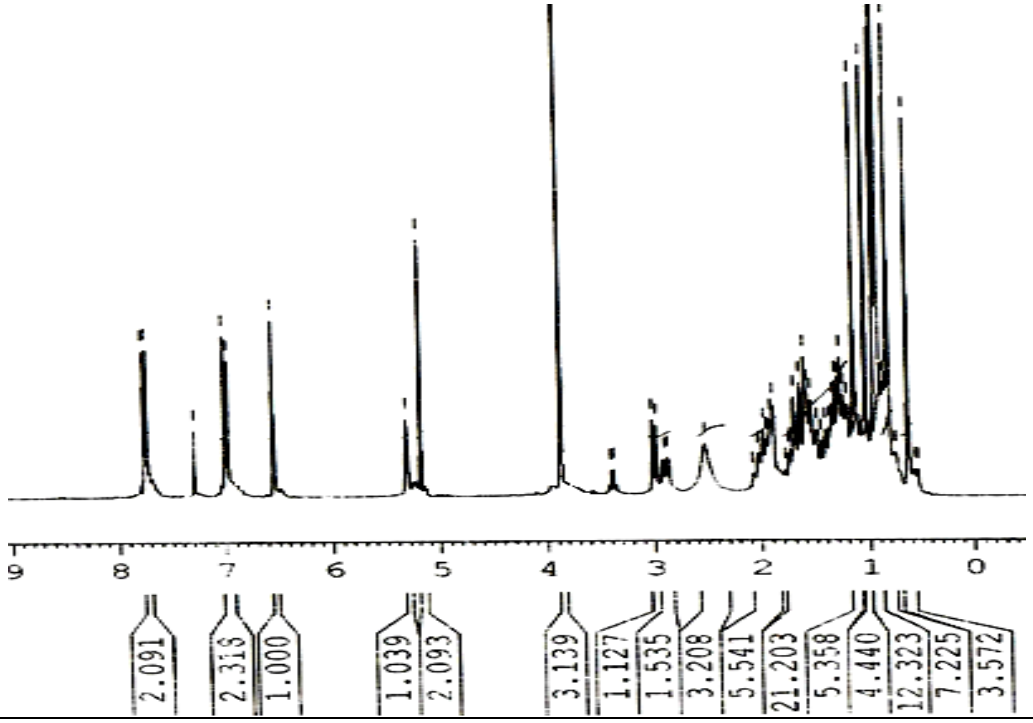
^{13}C NMR



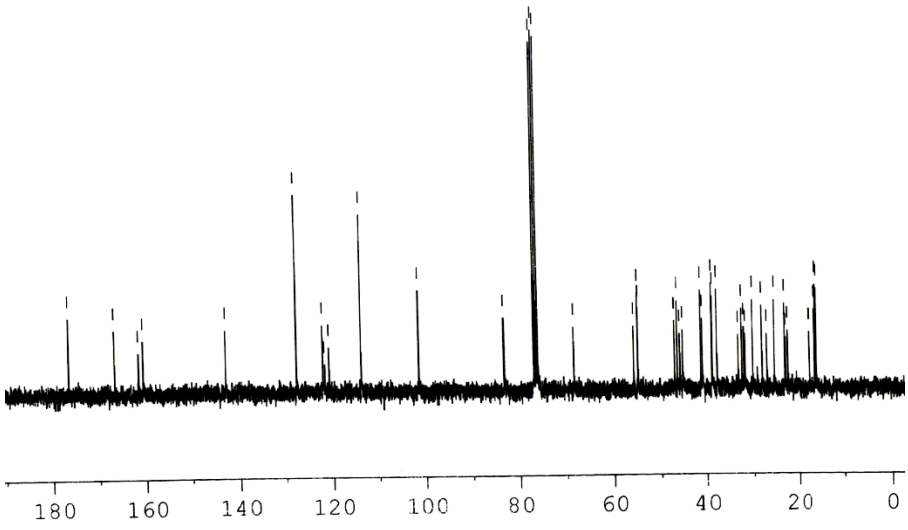


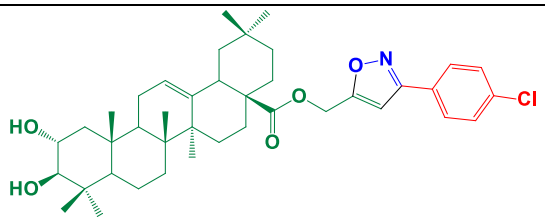
Compound **16**

^{1}H NMR



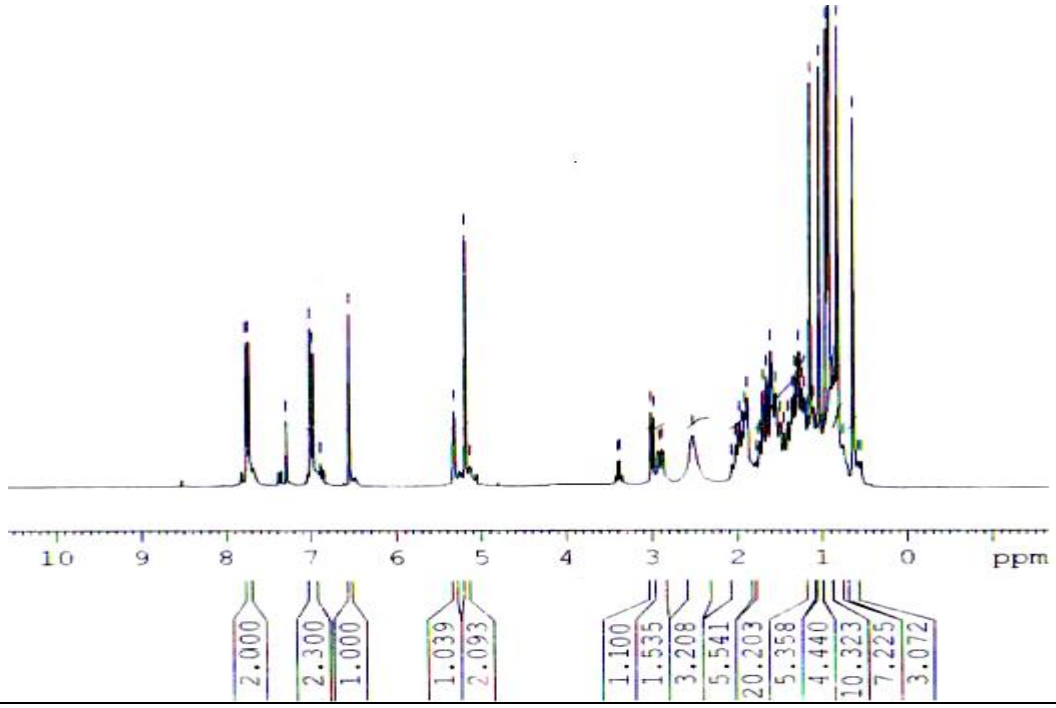
^{13}C NMR



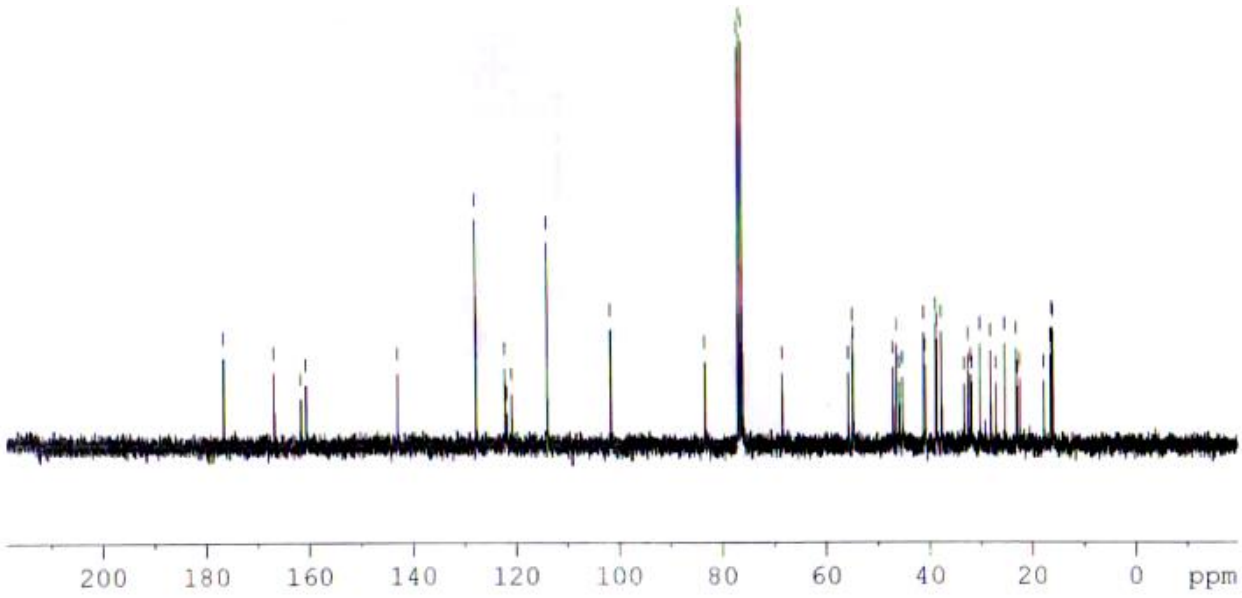


Compound **17**

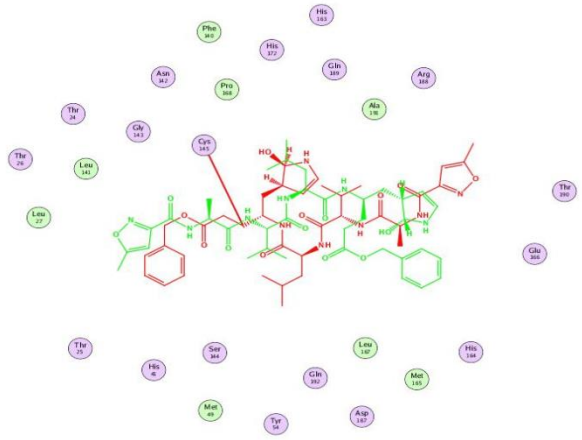
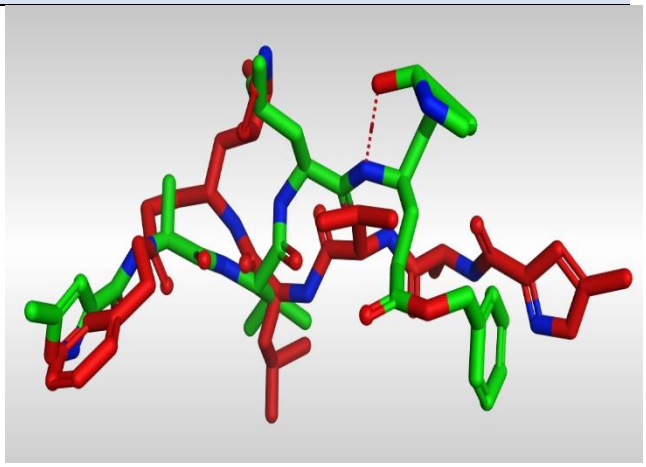
^{1}H NMR



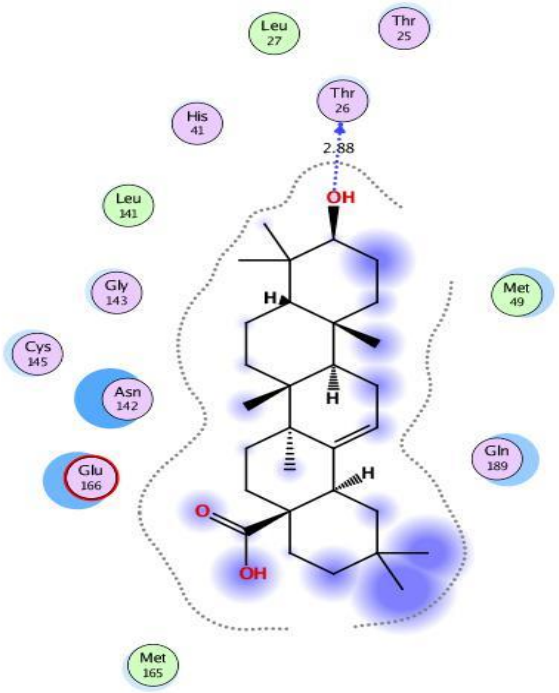
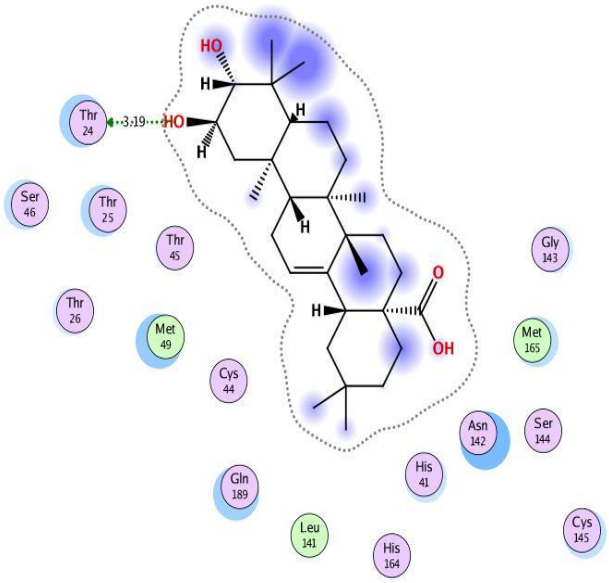
^{13}C NMR

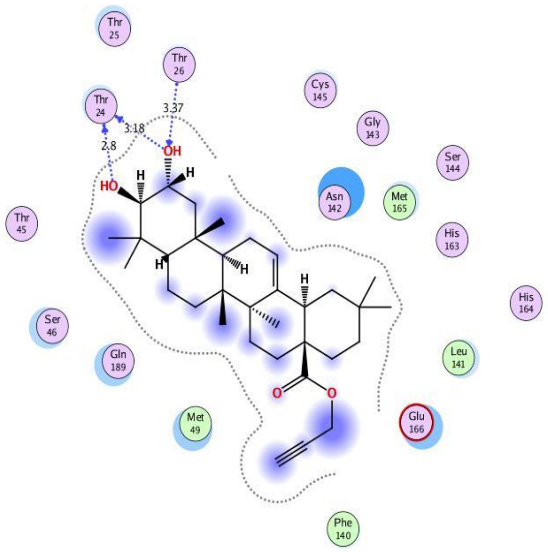
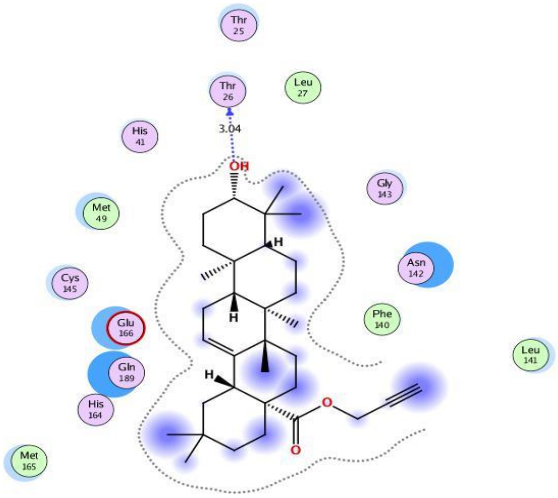
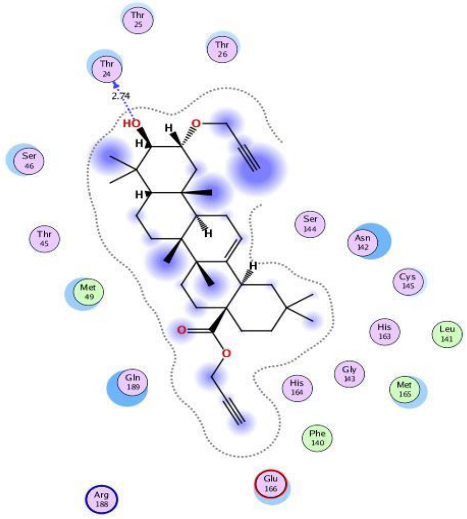


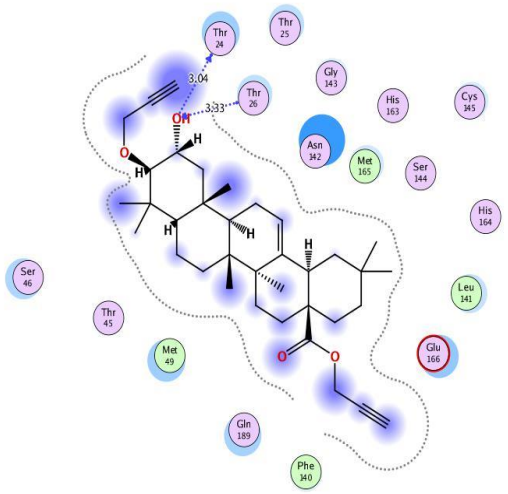
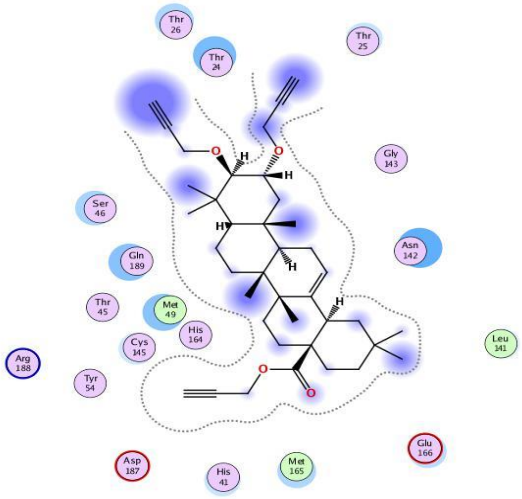
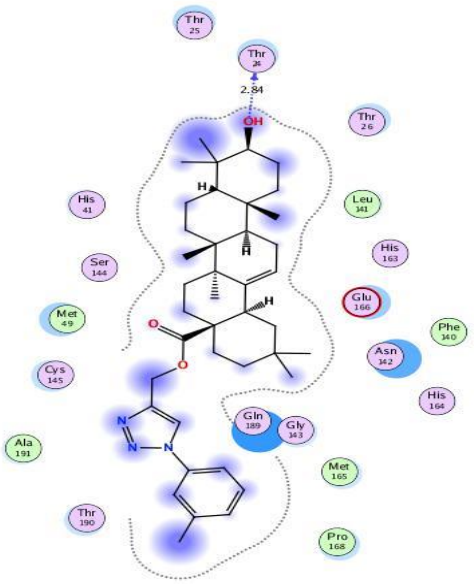
Supplementary Table (S1). 2 D and 3 D representations of the redocking process between the native co-crystallized N3 inhibitor (red) and the docked one (green).

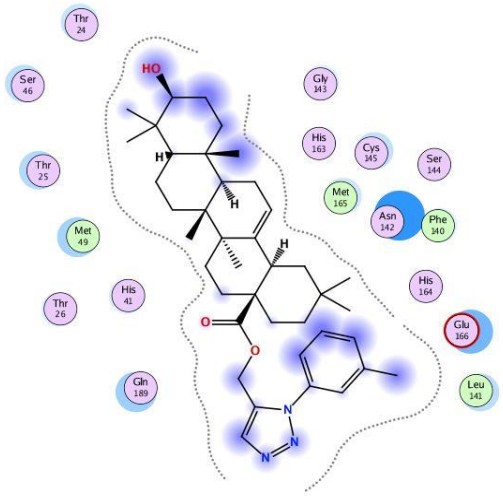
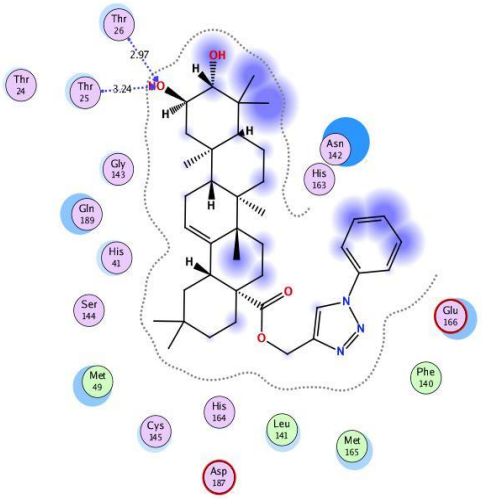
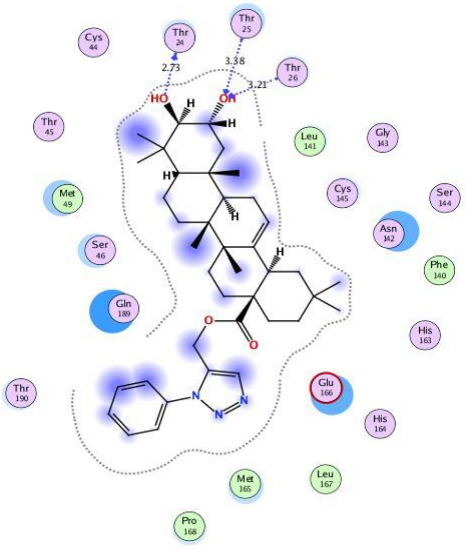
Redocked N3	
2D	**3D**
	

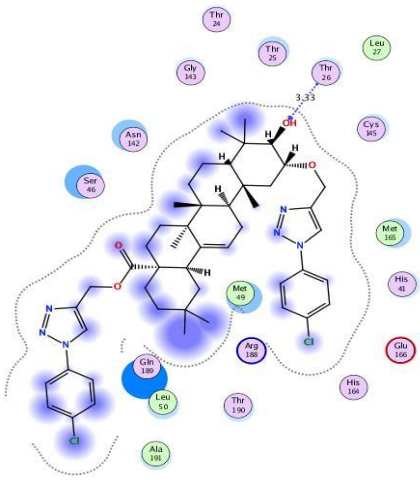
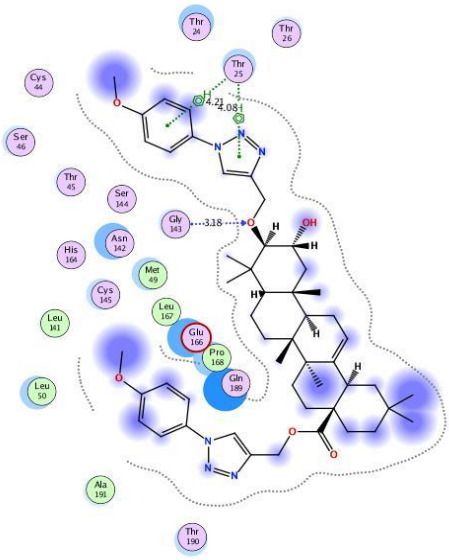
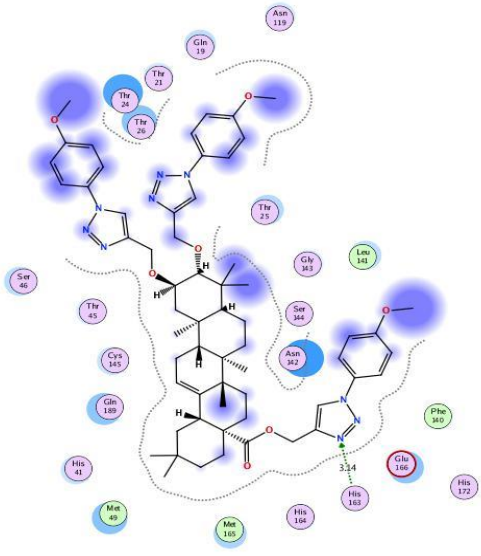
Supplementary Table (S2). 2 D pictures representing the binding interactions between the tested compounds (**1-17**) at the N3-binding pocket in comparison to the docked N3 inhibitor (**18**).

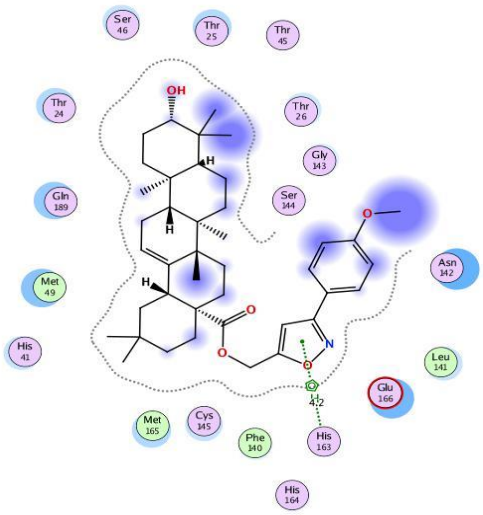
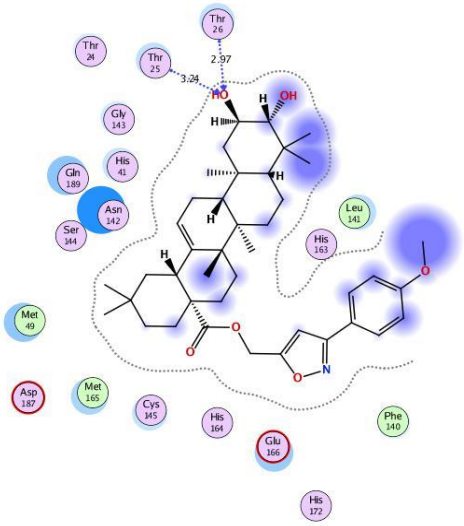
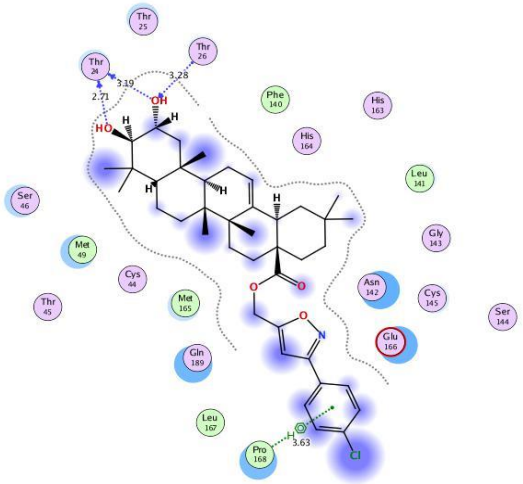
No.	2 D binding interactions
1	
2	

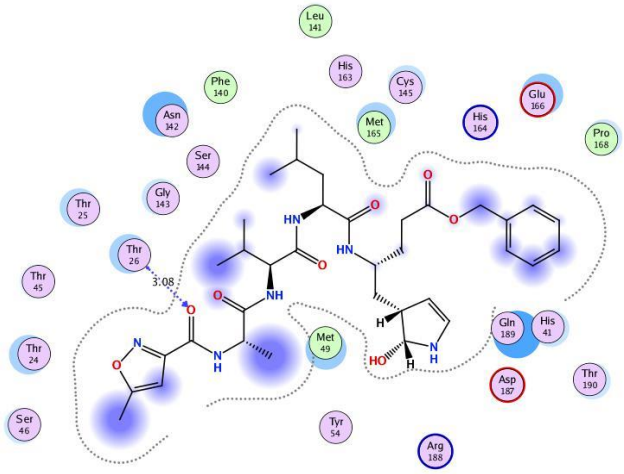
3	 Thr 25 Thr 26 Thr 24 3.37 3.18 2.8 OH HO Cys 145 Gly 143 Ser 144 Asn 142 Met 165 His 163 Thr 45 His 164 Ser 46 Gln 189 Leu 141 Met 49 Glu 166 Phe 140
4	 Thr 25 Thr 26 Leu 27 3.04 His 41 OH Gly 143 Met 49 Asn 142 Cys 145 Phe 140 Glu 166 Leu 141 Gln 189 His 164 Met 165
5	 Thr 25 Thr 26 Thr 24 2.74 HO Ser 46 Ser 144 Asn 142 Thr 45 Cys 145 Met 49 His 163 Leu 141 Gln 189 Gly 143 His 164 Met 165 Phe 140 Glu 166 Arg 188

6	 Thr 24 Thr 25 3.04 3.33 Gly 143 Thr 26 His 163 Cys 145 OH Asn 142 Met 165 Ser 144 His 164 Ser 46 Leu 141 Thr 45 Met 49 Glu 166 Gln 189 Phe 140
7	 Thr 26 Thr 24 Thr 25 Gly 143 Ser 46 Asn 142 Gln 189 Thr 45 Met 49 His 164 Cys 145 Leu 141 Arg 188 Tyr 54 Glu 166 Asp 187 His 41 Met 165
8	 Thr 25 Thr 26 2.84 OH Thr 26 His 41 Leu 141 His 163 Ser 144 Glu 166 Met 49 Phe 140 Asn 142 Cys 145 His 164 Gln 189 Gly 143 Ala 191 Met 165 Thr 190 Pro 168

9	 Thr 24 Ser 46 HO Gly 143 His 163 Cys 145 Ser 144 Thr 25 Met 165 Asn 142 Phe 140 Met 49 His 164 His 41 Thr 26 Glu 166 O O Gln 189 Leu 141 N N N
10	 Thr 26 2.97 OH Thr 24 Thr 25 3.24 HO Asn 142 Gly 143 His 163 Gln 189 His 41 Ser 144 Glu 166 O O N N Met 49 Phe 140 His 164 Cys 145 Leu 141 Met 165 Asp 187
11	 Cys 44 Thr 24 Thr 25 2.73 3.38 Thr 26 3.21 HO OH Thr 45 Leu 141 Gly 143 Met 49 Cys 145 Ser 144 Asn 142 Ser 46 Phe 140 Gln 189 O O His 163 Thr 190 Glu 166 N N N His 164 Met 165 Leu 167 Pro 168

12	
13	
14	

15	
16	
17	

18	 Leu 141 His 163 Cys 145 Phe 140 Glu 166 Asn 142 Met 165 His 164 Pro 168 Ser 344 Gly 143 Thr 25 Thr 26 3.08 Thr 45 Thr 24 Met 49 Gln 189 His 41 Asp 187 Thr 190 Ser 46 Tyr 54 Arg 188