Supplementary Materials

Phytochemical Analysis of *Anastatica hierochuntica* and *Aerva javanica* Grown in Qatar: Their Biological Activities and Identification of Active Ingredients.

Vandana Thotathil, Naheed Sidiq, Ameena Fakroo and Lakshmaiah Sreerama*

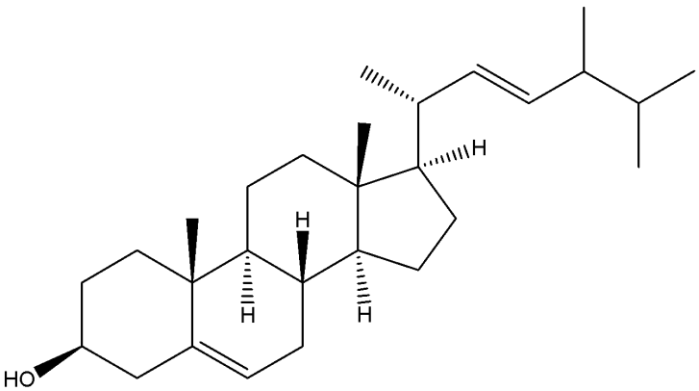
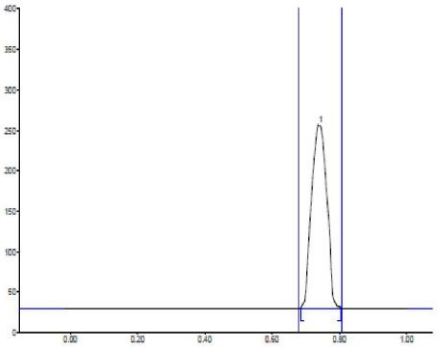
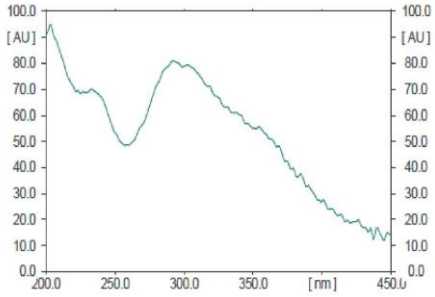
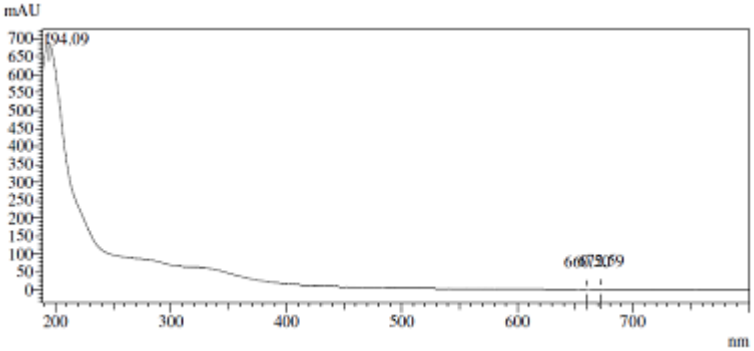
Department of Chemistry and Earth Sciences, Chemistry Program, College of Arts and Sciences, Qatar University, P.O. Box 2713, Doha, Qatar
* Correspondence: author: lsreerama@qu.edu.qa

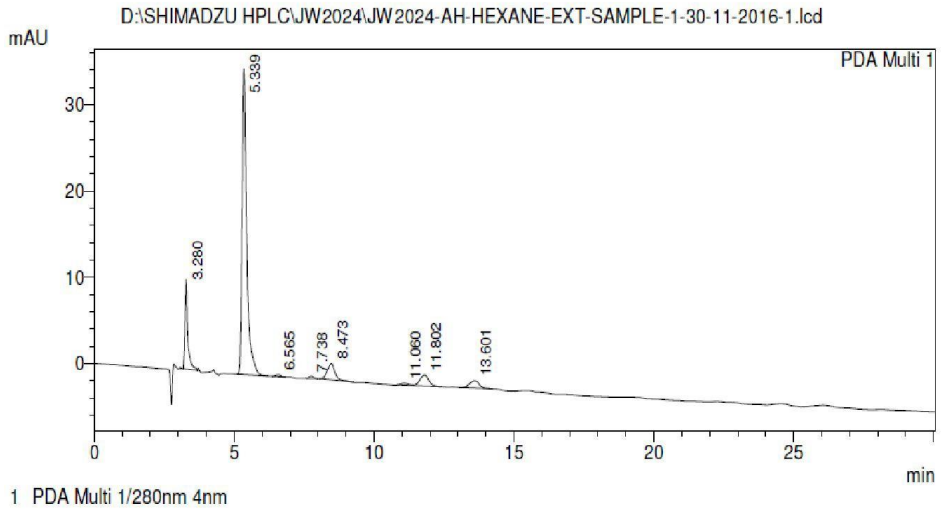
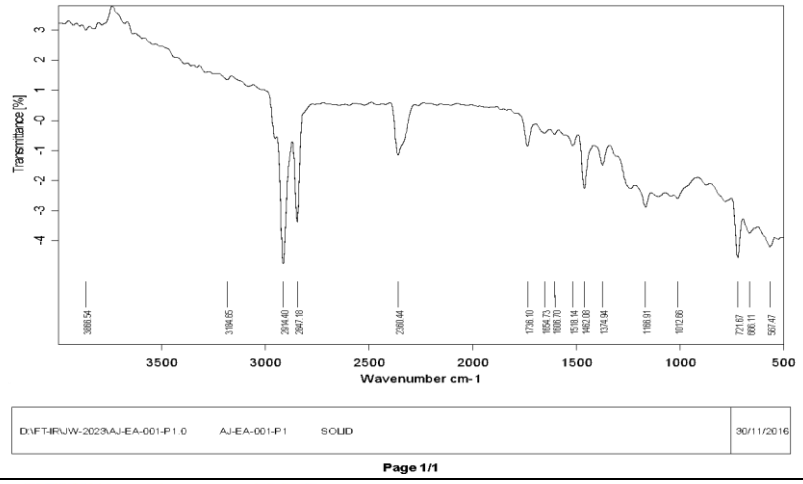
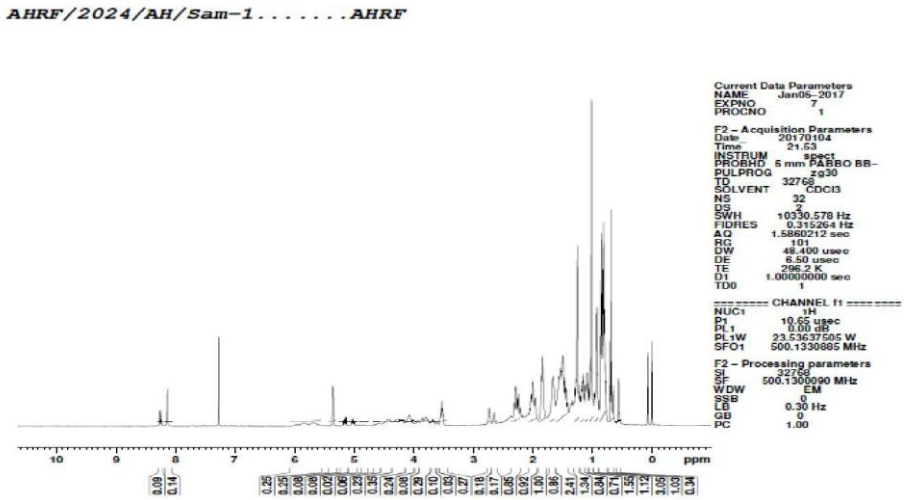
Anastatica Hierochuntica

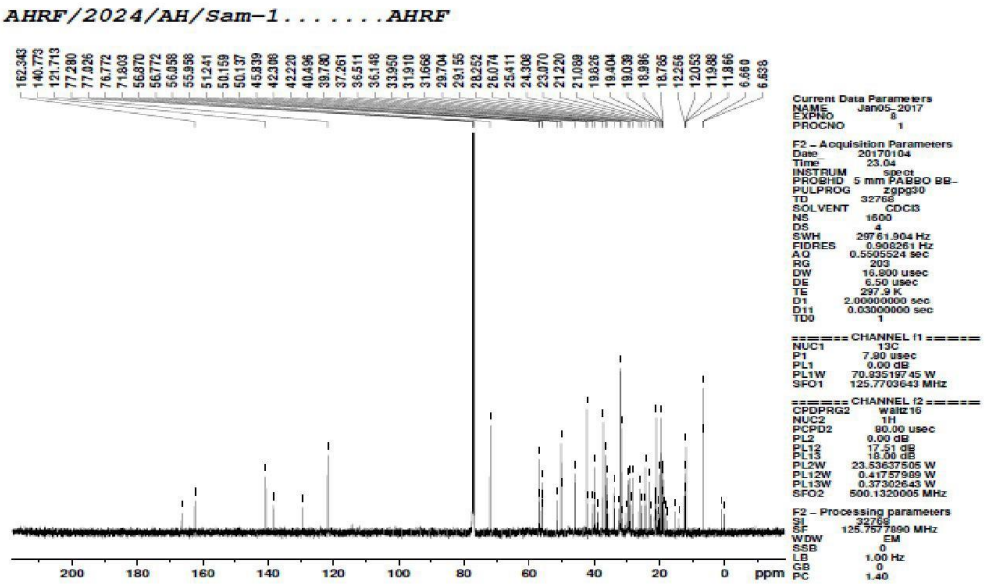
Phytochemical analysis of the Isolated Compounds

The hexane fraction was subjected to HPTLC and HPLC analysis. Three pure compounds were isolated and subjected to IR and NMR analysis for further identification.

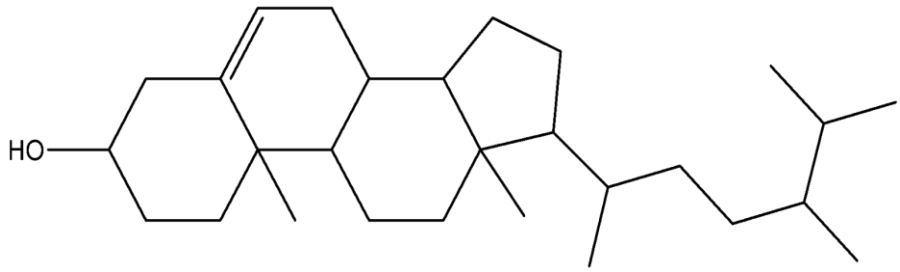
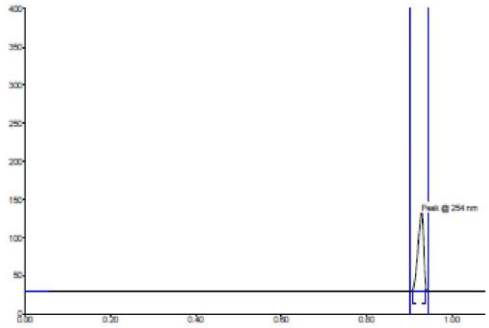
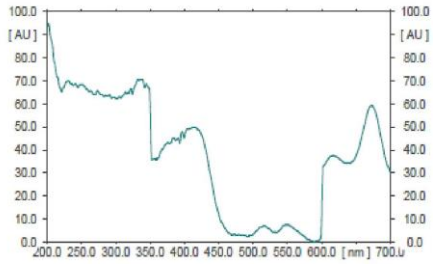
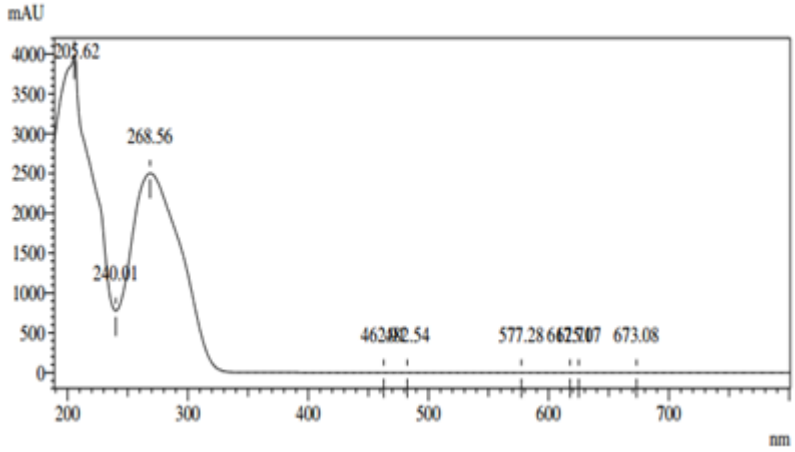
COMPOUND 1 (AH-HX-001-P1)

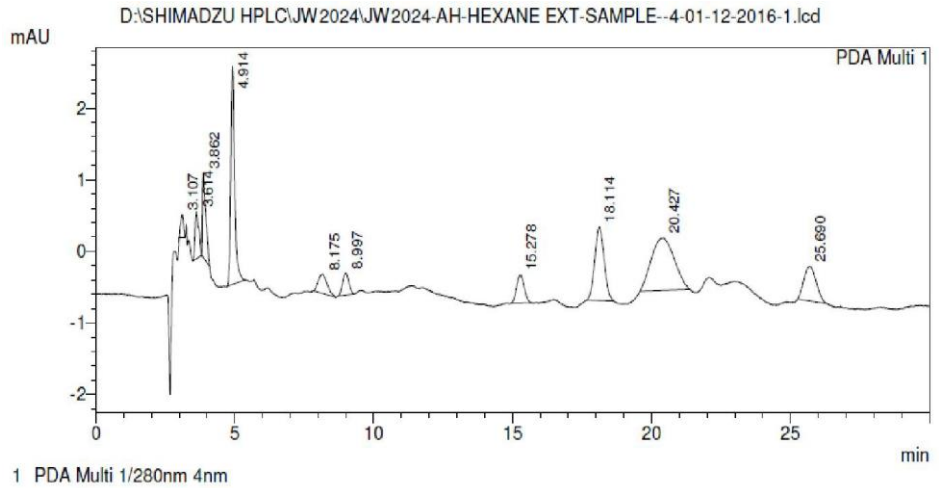
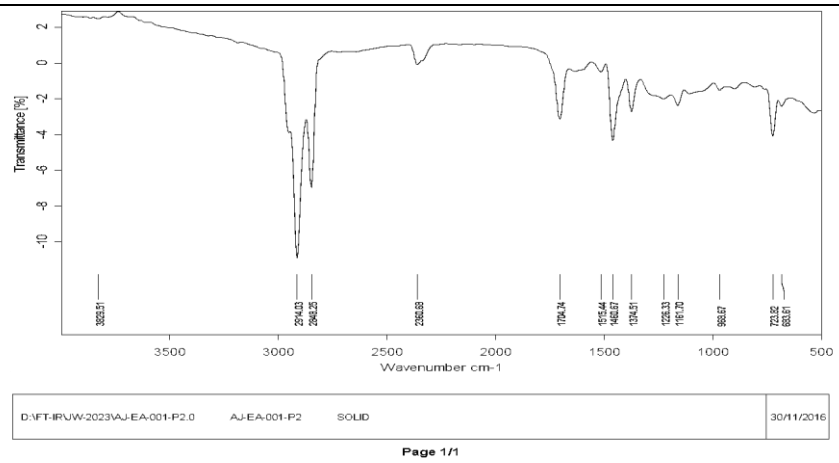
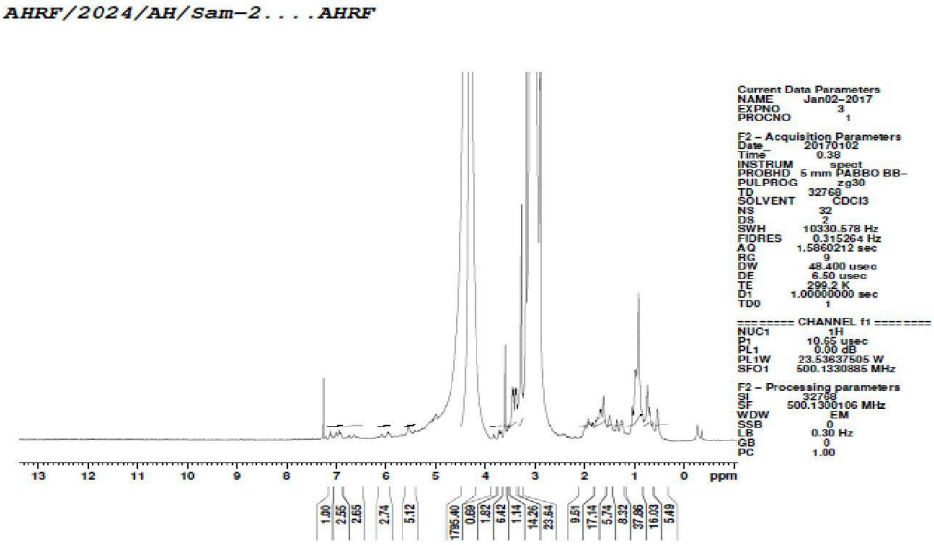
SPECIFICATON	**SPECTRUM**
Probable structure	β-Sitosterol 
CAMAG HPTLC Scanner III Mobile Phase: Hex: EtoAc (7:3) Rf: 0.74 λ max: 203nm	 
UV spectrum PDA detector: 200-800nm λ max: 194 nm	

SHIMADZU SPD-20A HPLC Column: Enable C_{18}, 4.6x250mm (5micron) Mobile Phase: ACN:H_2O (15:85) with 0.1% H_3PO_4 λ max: 280nm Inj. Vol: 20µl Flow rate: 1.0ml/min Rt: 5.339 min	
Bruker FT-IR Wavelength scan: 500-4000cm^{-1}	
BRUKER NMR 400MHz ^{1}HNMR($CDCl_3$):	

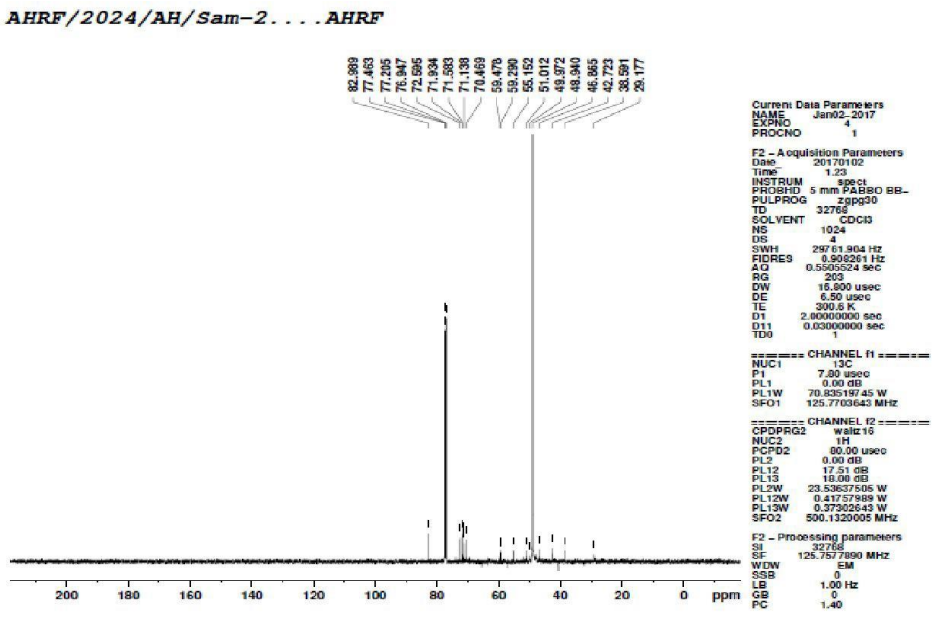
BRUKER NMR 400MHz ^{13}CNMR($CDCl_3$):	

COMPOUND 2 (AH-HX-001-P4)

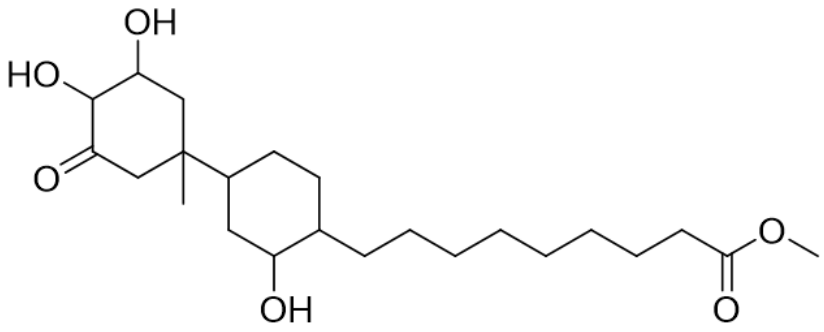
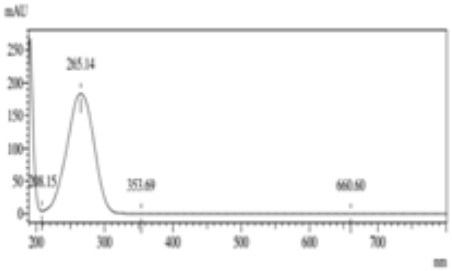
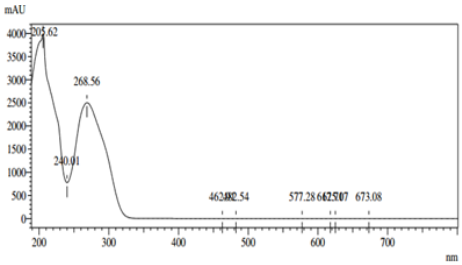
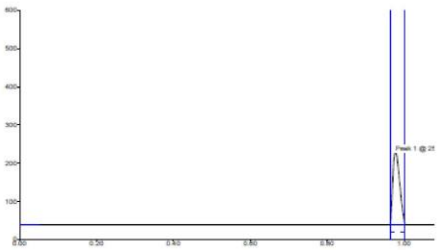
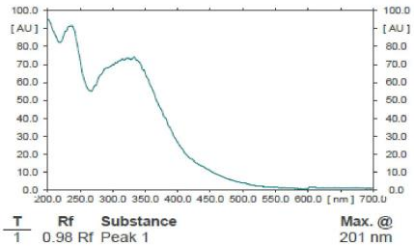
SPECIFICATON	SPECTRUM
Probable structure	Campesterol 
CAMAG HPTLC Scanner III Mobile Phase: Hex: EtoAc (7:3) Rf: 0.93 λ max: 202 nm	  T Rf Substance Max. @ 1 0.93 Rf Peak 202 nm
UV spectrum PDA detector: 200-800nm λ max: 205, 268nm	

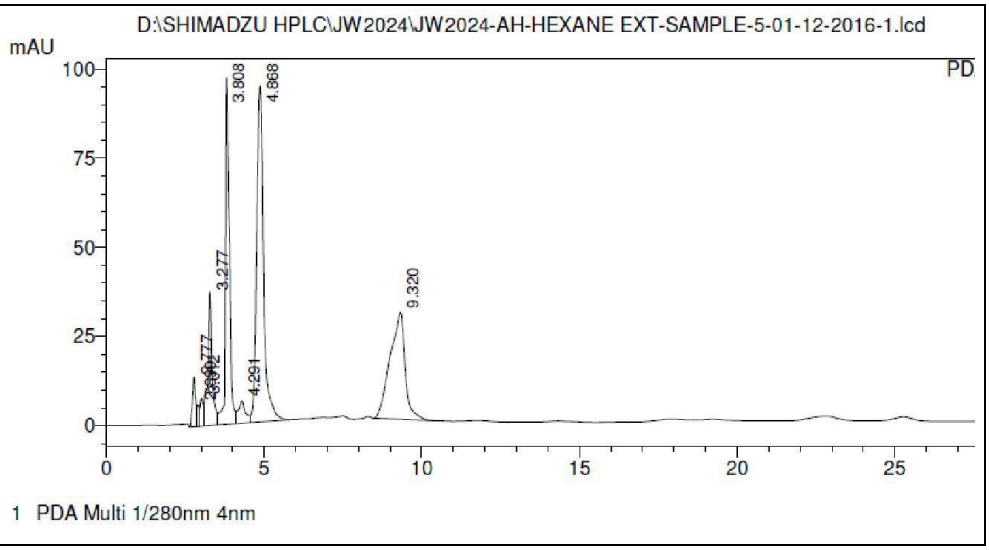
SHIMADZU SPD-20A HPLC Column: Enable C_{18}, 4.6x250mm (5micron) Mobile Phase: ACN:H_2O (15:85) with 0.1% H_3PO_4 λ max: 280nm Inj. Vol: 20µl Flow rate: 1.0ml/min Rt: 4.914 min	
Bruker FT-IR Wavelength scan: 500-4000cm^{-1}	
BRUKER NMR 400MHz ^{1}HNMR($CDCl_3$):	

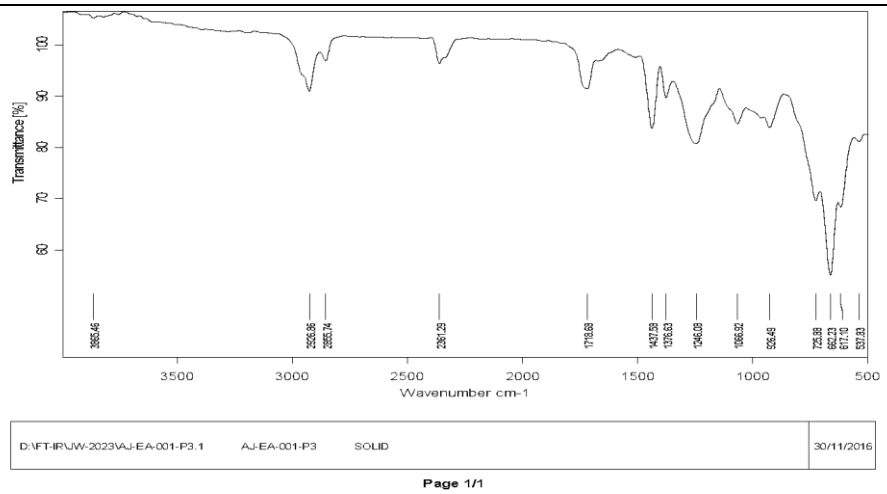
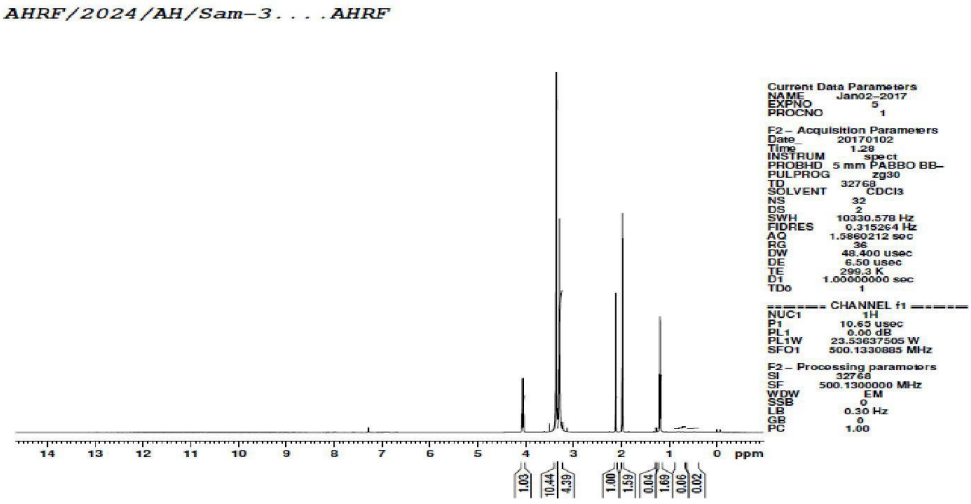
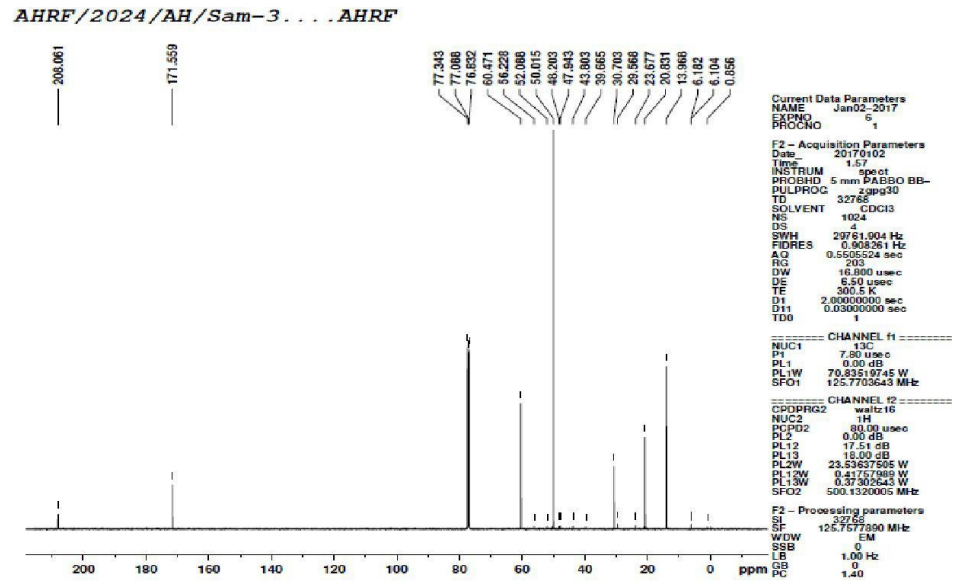
BRUKER NMR 400MHz
^{13}CNMR($CDCl_3$):



COMPOUND 3 (AH-HX-001-P5)

SPECIFICATON	SPECTRUM
Probable structure	Methyl- 9-(4-(3,4-dihydroxy-1'-methyl-5'-oxocyclohexyl)-2-hydroxycyclohexyl)nonanoate 
UV spectrum PDA detector: 200-800nm λ max: 205, 265nm	 
CAMAG HPTLC Scanner III Mobile Phase: Hex: EtoAc (7:3) Rf: 0.09 λ max: 201 nm	 

SHIMADZU SPD-20A HPLC Column: Enable C_{18}, 4.6x250mm (5micron) Mobile Phase: ACN:H_2O (15:85) with 0.1% H_3PO_4 λ max: 280nm Inj. Vol: 20µl Flow rate: 1.0ml/min Rt: 3.808min and 4.868min	

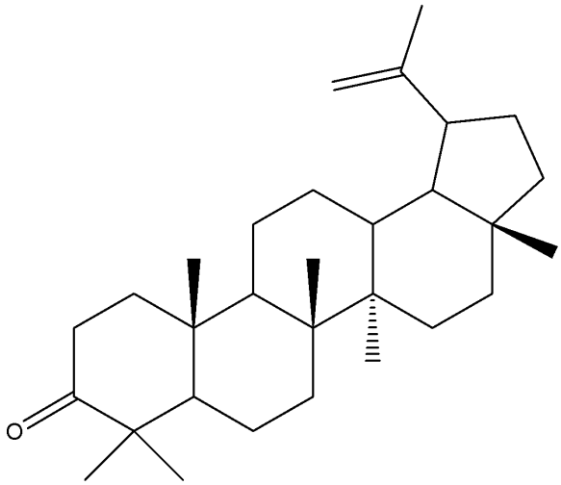
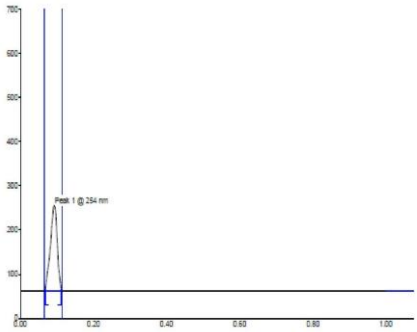
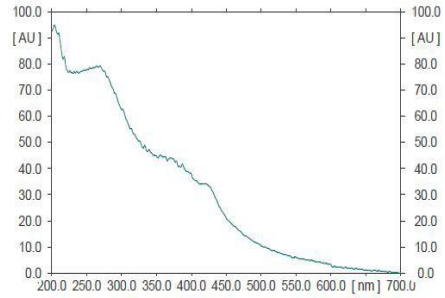
Bruker FT-IR Wavelength scan: 500-4000cm^{-1}	
BRUKER NMR 400MHz ^{1}HNMR($CDCl_3$):	
BRUKER NMR 400MHz ^{13}CNMR($CDCl_3$):	

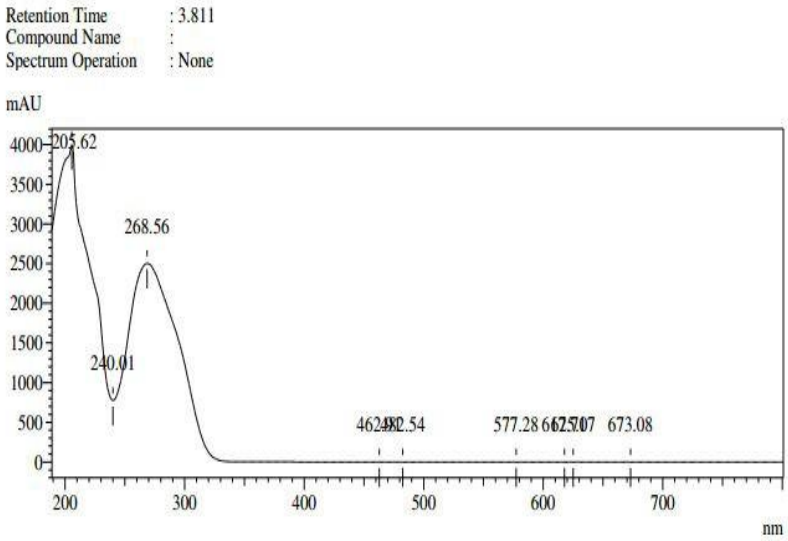
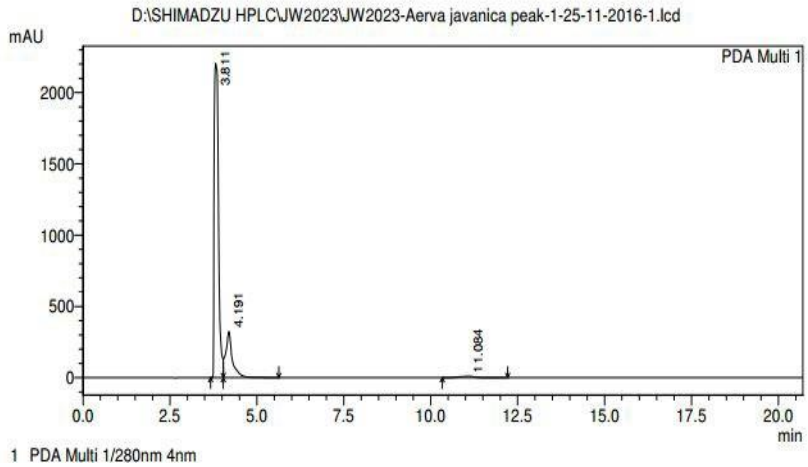
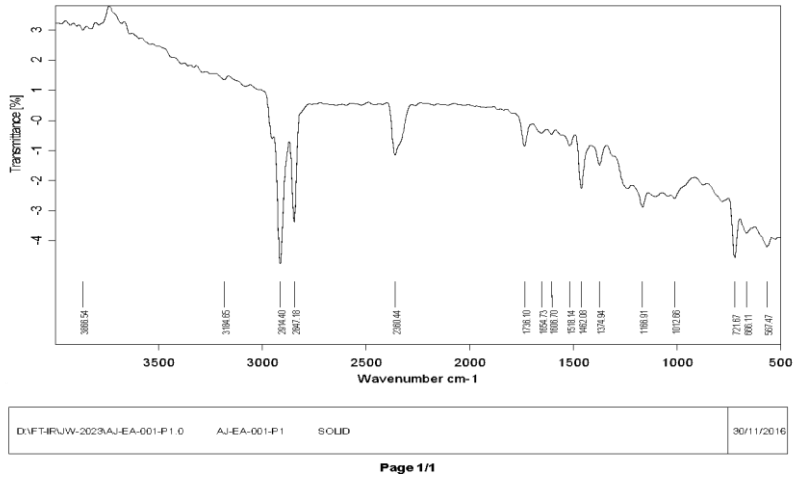
Aerva Javanica

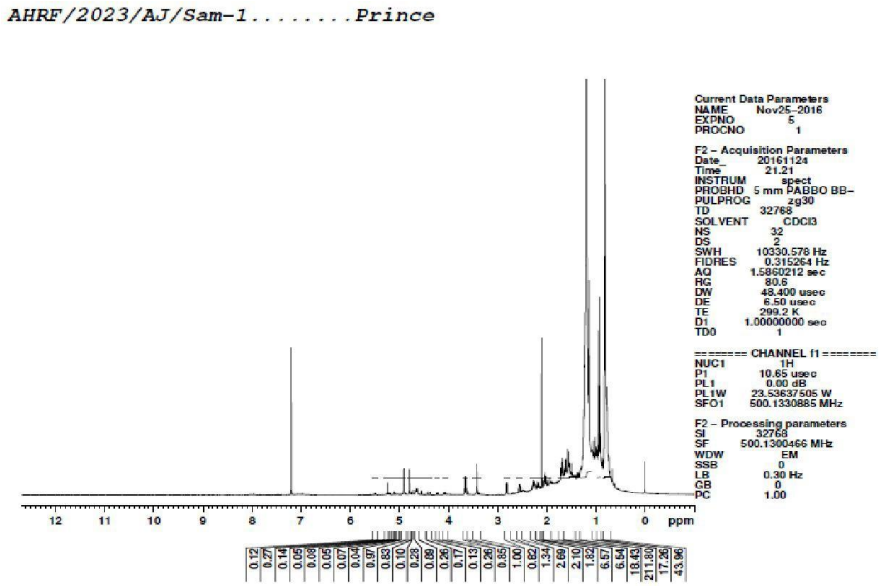
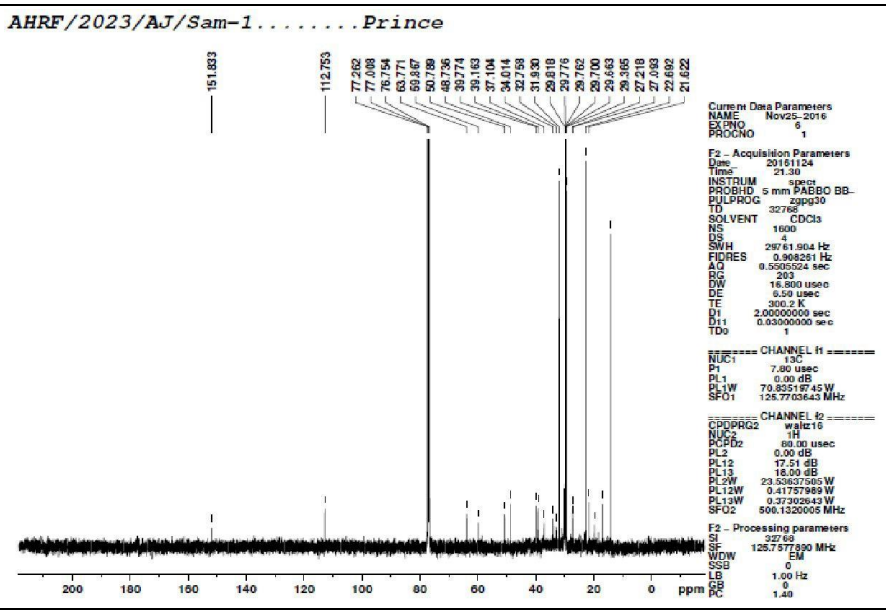
Phytochemical analysis of the Isolated Compounds

The ethyl acetate fraction was subjected to HPTLC and HPLC analysis. Three pure compounds were isolated and subjected to IR and NMR analysis for further identification.

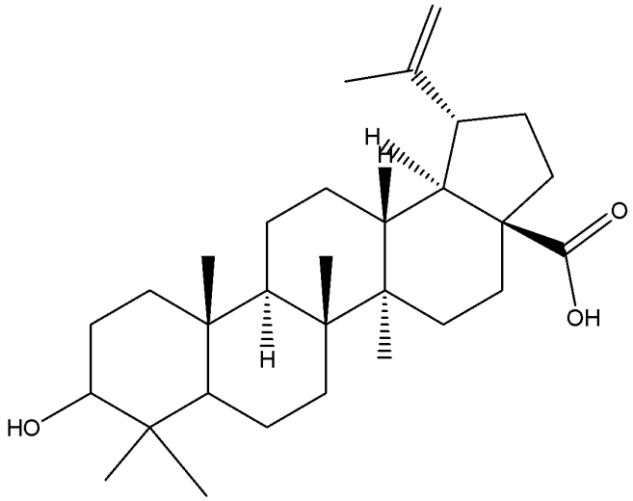
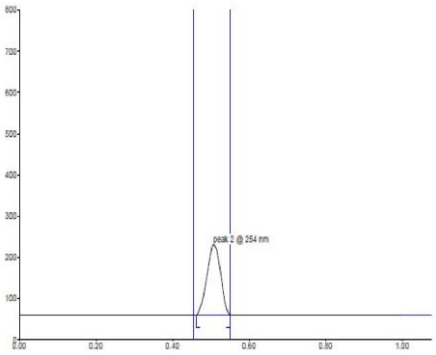
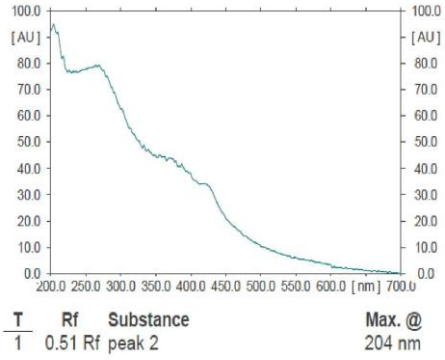
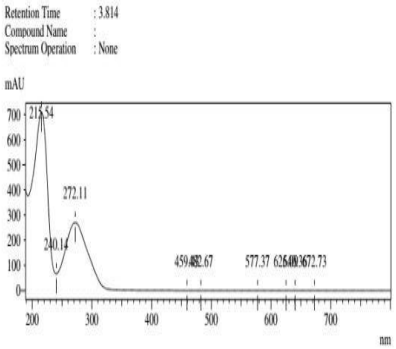
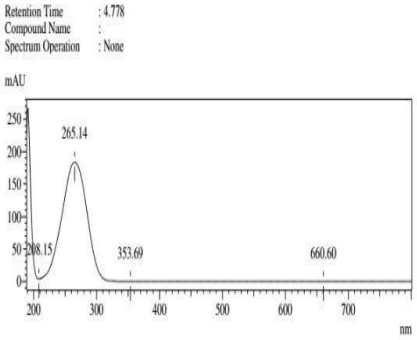
COMPOUND 1 (AJ-EA-001-P1)

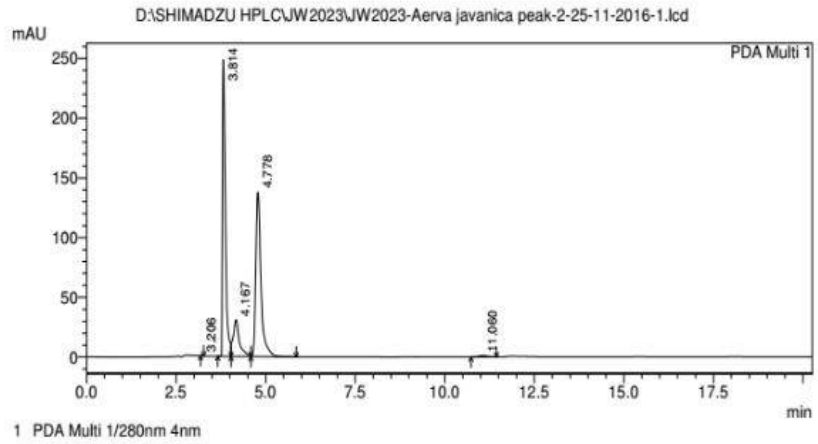
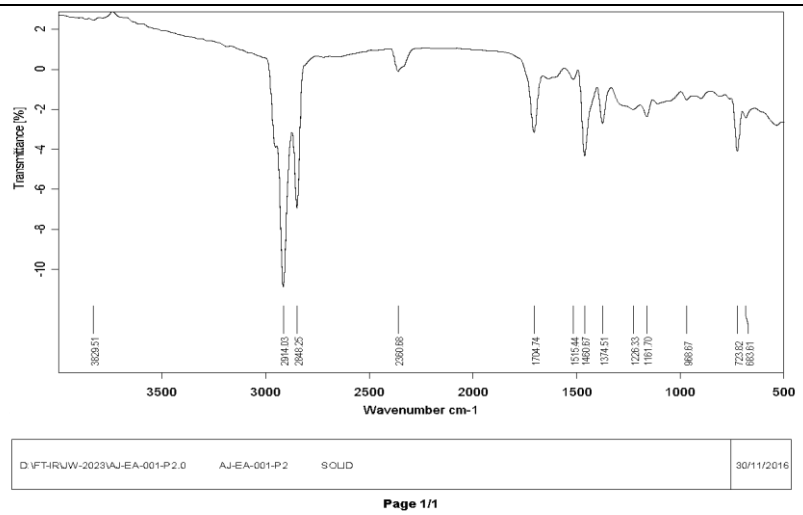
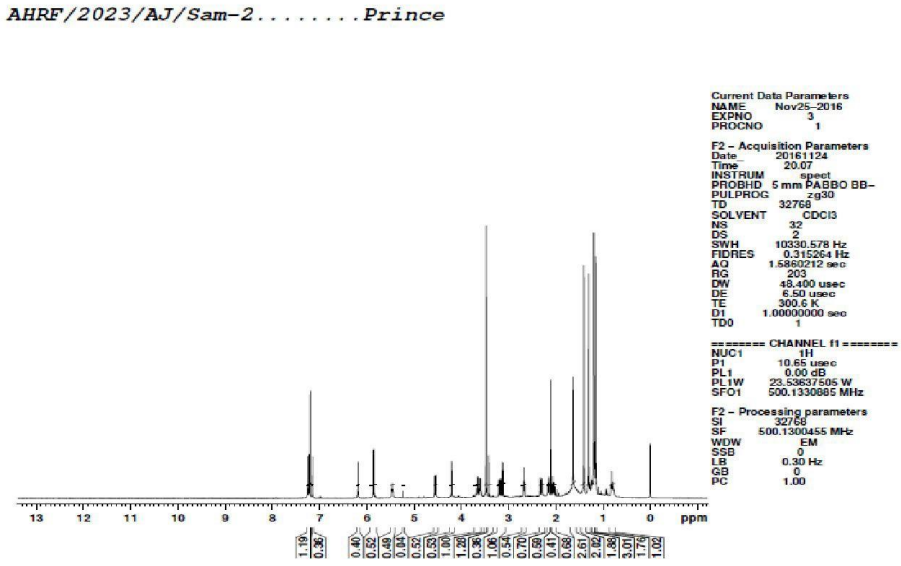
Probable structure	Lupenone 
CAMAG HPTLC Scanner III Mobile Phase: Hex: EtoAc (7:3) Rf: 0.09 λ max: 254nm	  T Rf Substance Max. @ 1 0.09 Rf peak 2 254 nm

UV spectrum PDA detector: 200-800nm λ max: 205, 268nm	
SHIMADZU SPD-20A HPLC Column: Enable C_{18}, 4.6x250mm (5micron) Mobile Phase: ACN:H_2O (15:85) with 0.1% H_3PO_4 λ max: 280nm Inj. Vol: 20µl Flow rate: 1.0ml/min Rt: 3.811min	
Bruker FT-IR Wavelength scan: 500-4000cm^{-1}	

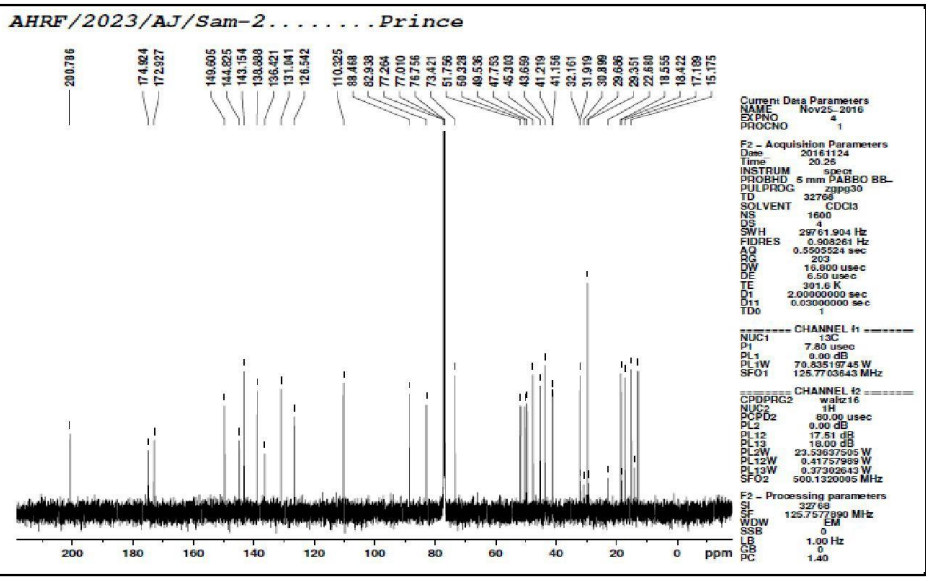
BRUKER NMR 400MHz ^{1}HNMR($CDCl_3$):	
BRUKER NMR 400MHz ^{13}CNMR($CDCl_3$):	

COMPOUND 2 (AJ-EA-001-P2)

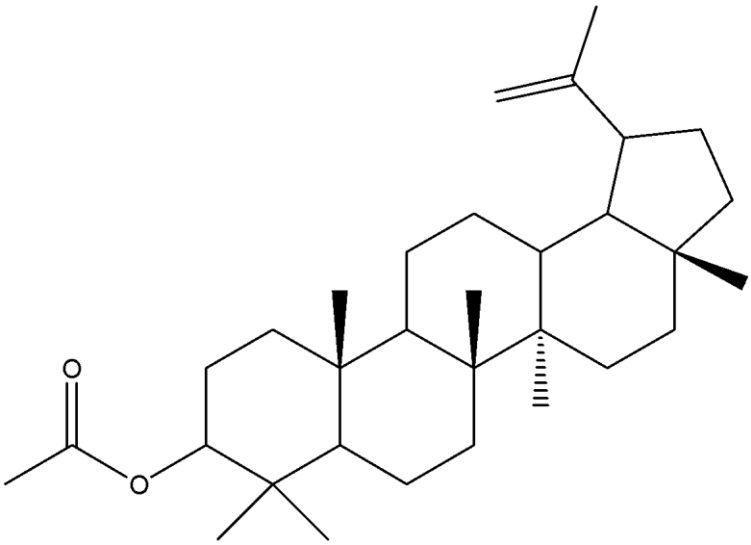
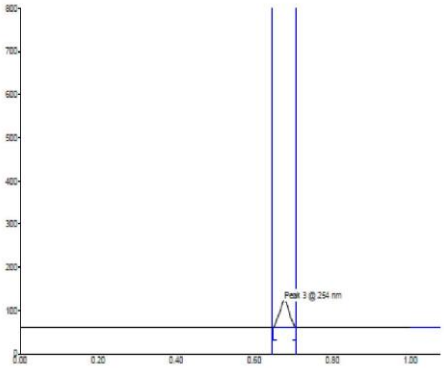
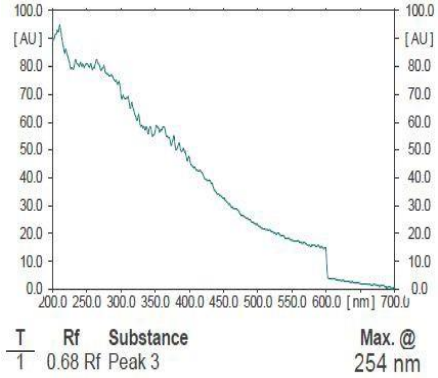
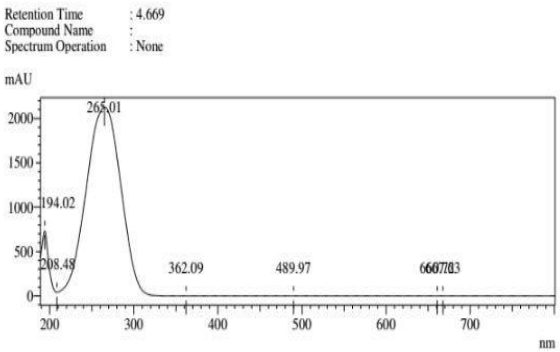
SPECIFICATON	SPECTRUM
Probable structure	Betulinic acid 
CAMAG HPTLC Scanner III Mobile Phase: Hex: EtoAc (7:3) Rf: 0.51 λ max: 204nm	  T Rf Substance Max. @ 1 0.51 Rf peak 2 204 nm
UV spectrum PDA detector λ max: Rt 3.814 – 215, 272nm Rt 4.778 – 265nm	 

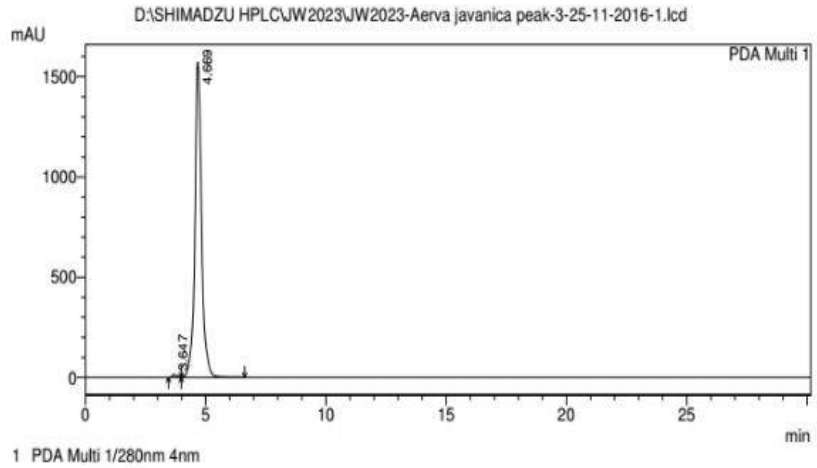
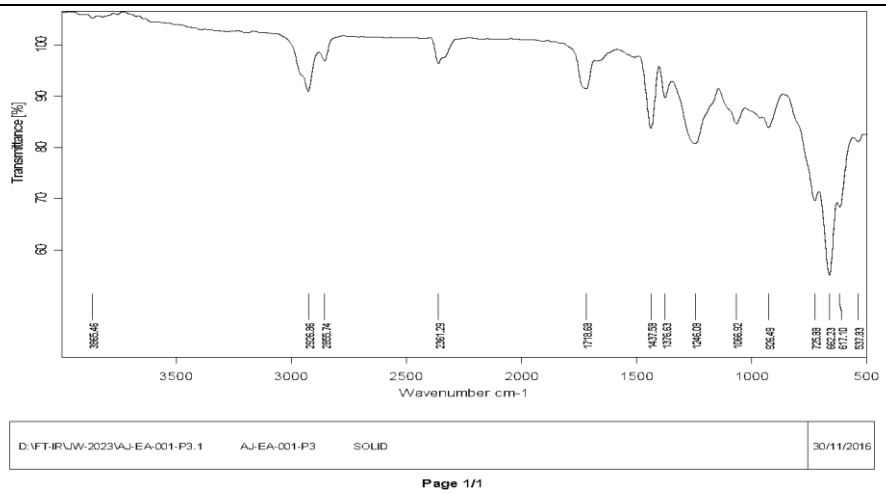
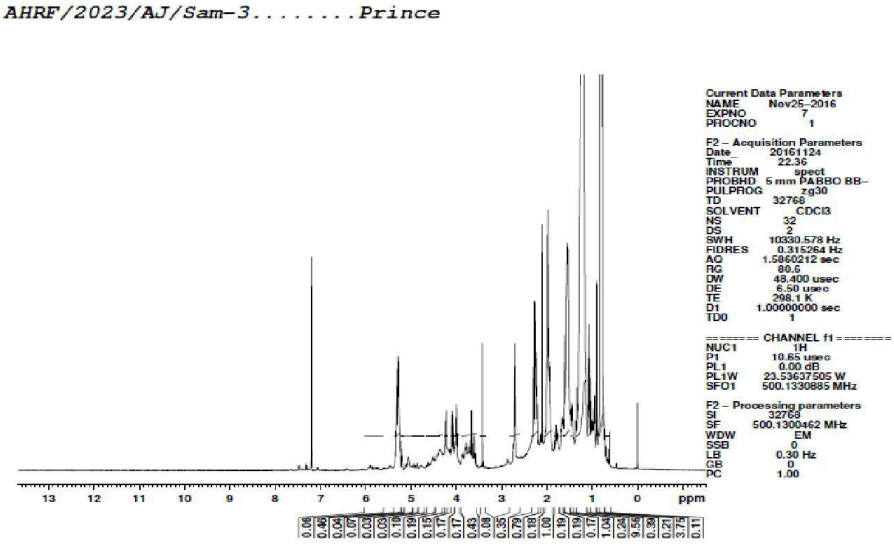
SHIMADZU SPD-20A HPLC Column: Enable C_{18}, 4.6x250mm (5micron) Mobile Phase: ACN:H_2O (15:85) with 0.1% H_3PO_4 λ max: 280nm Inj. Vol: 20µl Flow rate: 1.0ml/min Rt: 3.811min and 4.778min	
Bruker FT-IR Wavelength scan: 500-4000cm^{-1}	
BRUKER NMR 400MHz ^{1}HNMR($CDCl_3$):	

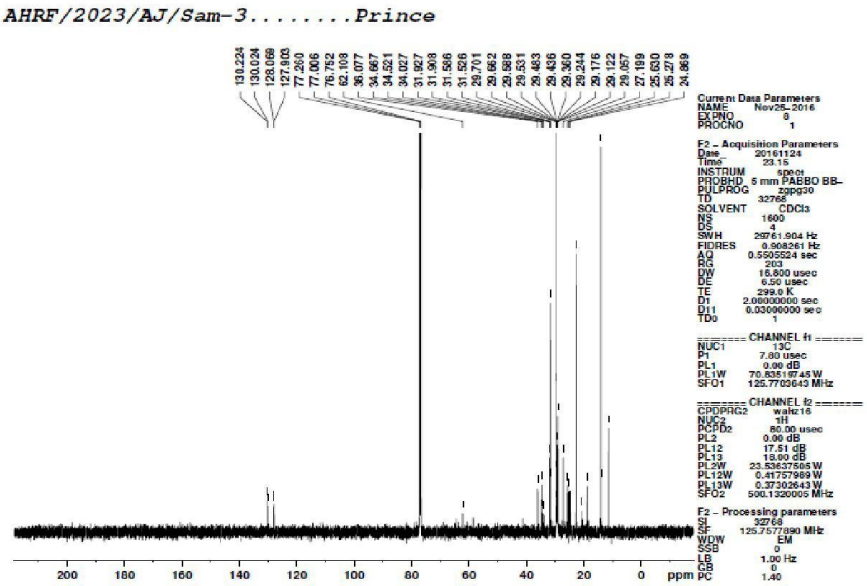
BRUKER NMR 400MHz
13CNMR($CDCl_3$):



COMPOUND 3 (AJ-EA-001-P6)

SPECIFICATON	SPECTRUM
Probable structure	Lupeol acetate 
CAMAG HPTLC Scanner III Mobile Phase: Hex: EtoAc (7:3) Rf: 0.68 λ max: 254nm	 
UV spectrum PDA detector λ max: 265nm	

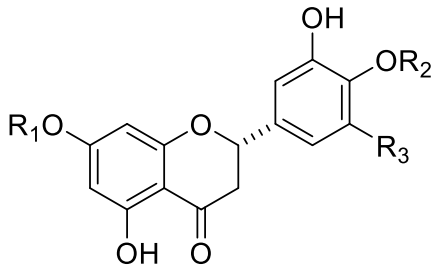
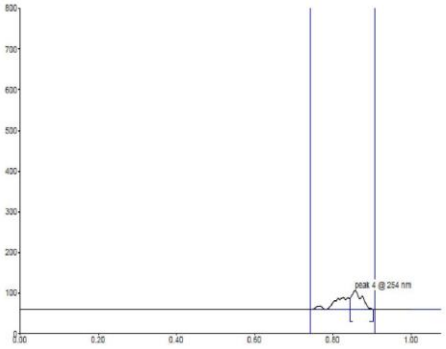
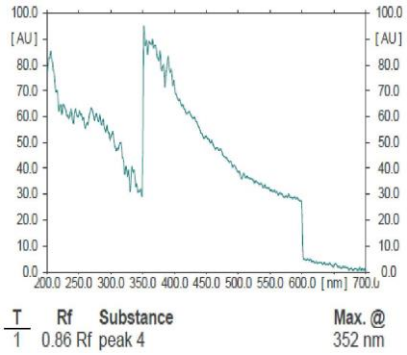
SHIMADZU SPD-20A HPLC Column: Enable C_{18}, 4.6x250mm (5micron) Mobile Phase: ACN:H_2O (15:85) with 0.1% H_3PO_4 λ max: 280nm Inj. Vol: 20µl Flow rate: 1.0ml/min Rt: 4.669min	
Bruker FT-IR Wavelength scan: 500-4000cm^{-1}	
BRUKER NMR 400MHz ^{1}HNMR($CDCl_3$):	

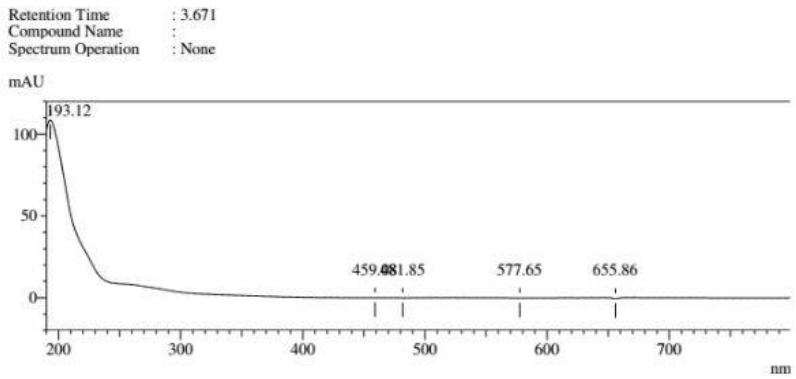
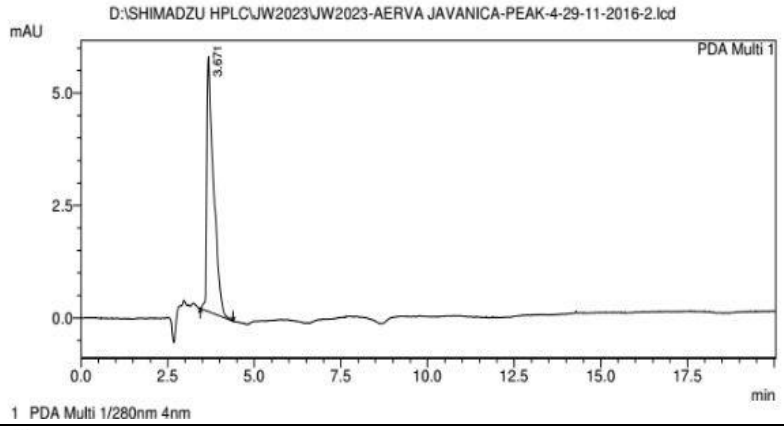
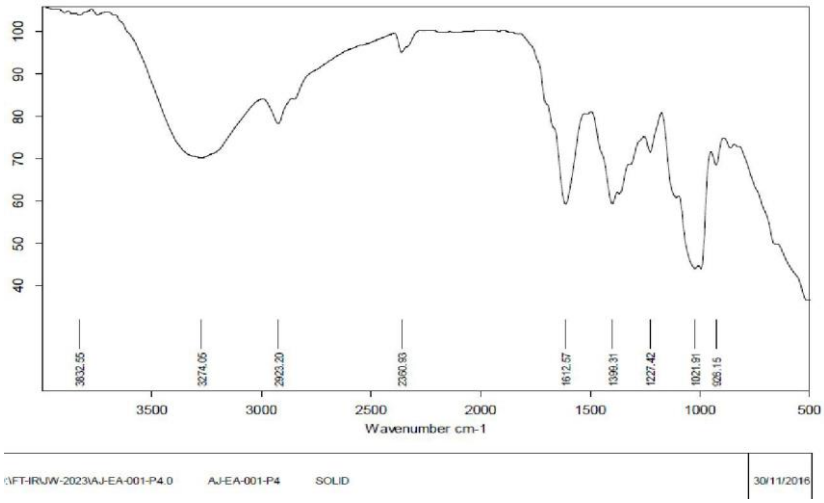
BRUKER NMR 400MHz 13CNMR($CDCl_3$):	

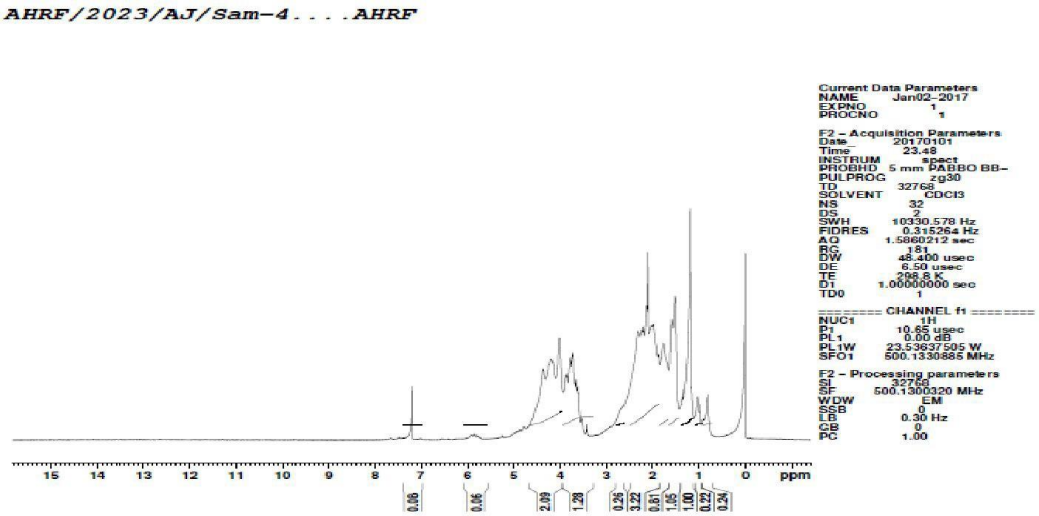
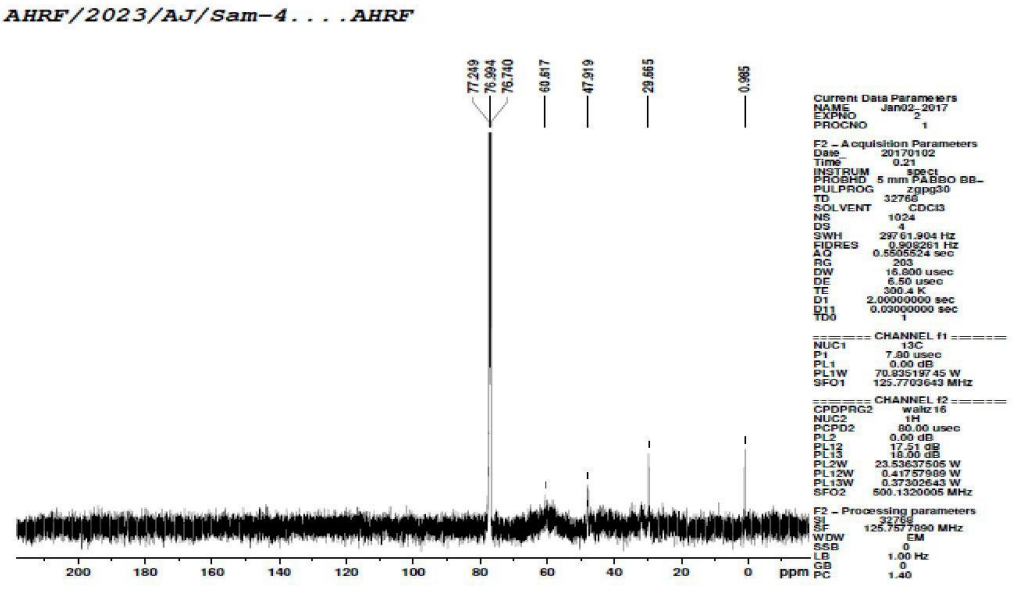
METHANOL EXTRACT

The methanol fraction were subjected to HPTLC and HPLC analysis. One pure compound was isolated and subjected to IR and NMR analysis for further identification.

COMPOUND 4 (AJ-ME-001-P3)

SPECIFICATON	SPECTRUM
Probable structure	Persinoside A and B  Persinoside A R_1=Me, R_2=Glc, R_3 = H Persinoside B R_1=Glc, R_2=H, R_3 = OH
CAMAG HPTLC Scanner III Mobile Phase: Hex: EtoAc (7:3) Rf: 0.81 λ max: 352nm	 

UV spectrum PDA detector: 200-800nm λ max: 195nm	
SHIMADZU SPD-20A HPLC Column: Enable C_{18}, 4.6x250mm (5micron) Mobile Phase: ACN:H2O (15:85) with 0.1% H3PO4 λ max: 280nm Inj. Vol: 20µl Flow rate: 1.0ml/min Rt: 3.671min	
Bruker FT-IR Wavelength scan: 500-4000cm^{-1}	

BRUKER NMR 400MHz ^{1}HNMR($CDCl_3$):	
BRUKER NMR 400MHz ^{13}CNMR($CDCl_3$):