



*John*

**Phytochemical and Antimicrobial  
Compounds from *Barbeya  
oleoides* Schweinf and *Solanum  
schimperianum* Hochst**

By mai Mohammed Al-oqail

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*Solanum schimperianum* Hochst



*Barbeya oleoides*



*Solanum schimperianum*

# OUTLINES

Introduction

Specific research objective

Preliminary phytochemical screening

Phytochemical study

Biological study

Conclusion

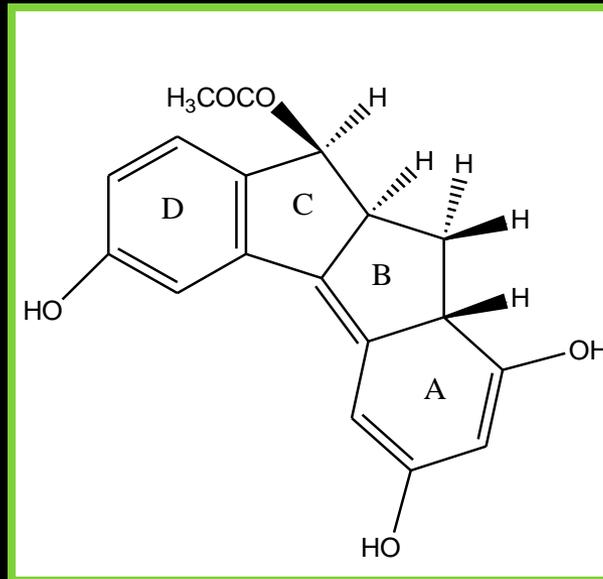
# Introduction

# 1-*Barbeya oleoides*

- ▶ Family Barbeyaceae
- ▶ One plant species
- ▶ Bushy shrub or small tree up to 5 m high
- ▶ Northeast Africa, Arabian peninsula



# Barbyol



•B. Ahmed *et al*, *Zeitschrift für Naturforschung*, **57c** (2002).

## 2- *Solanum schimperianum*

- ▶ Family Solanaceae
- ▶ 90 genera and some 2600 species.
- ▶ Annual, perennial trees or shrubs
- ▶ The nightshade or potato family

•W. C. Evans. *Trease and Evans Pharmacognosy*. 15th edition, (2002).

★ Source of common cultivated crops



*Solanum tuberosum*



*Solanum melongena*

★ Source of a medicine or narcotic



*Atropa belladonna*



*Datura stramonium*

# Ornamentals



**Browallia White**



**Cestrum parqui**



**Salpiglossis sinuata**

# Active Constituents

- ▶ Alkaloids
- ▶ Steroidal saponins
- ▶ Withanolides
- ▶ Flavones
- ▶ Carotenoids
- ▶ Anthraquinones
- ▶ Pungent principle
- ▶ Coumarins

# *Genus Solanum*

1700 species



# Folk Use of Different *Solanum* species

Brazil

*S. paniculatum*



Gastric and liver disorders

Germany

*S. tuberosum*



Antispasmodic and antacid

Kenya

*S. incanum*



In injuries and against snake bite

India

*S. xanthocarpum*



Diabetes mellitus

South Africa

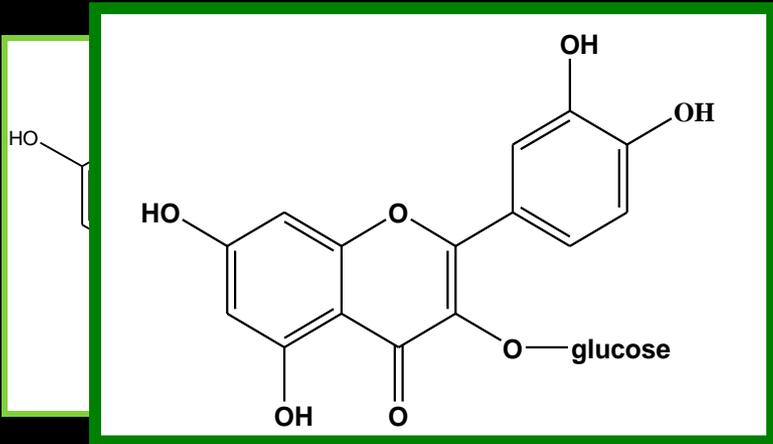
*S. aculeastrum*



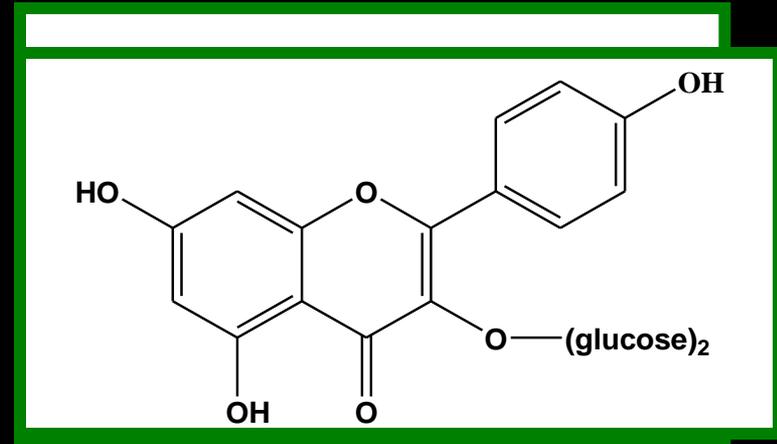
Treatment of cancer and gonorrhoea

# *Solanum schimperianum* Hochst

- ★ Southern region of Saudi Arabia
- ★ Four glycoalkaloids,  $\alpha$  and  $\beta$ -solamargine,  $\beta$  and  $\gamma$ -solamarine
- ★ One coumarin
- ★ **Four flavonol**
- ★ *Solanum schimperianum* Hochst has antiplasmodial activity



Isoquercetin  
Rutin



3-Kämpferol-3-glucoside

## Research objectives

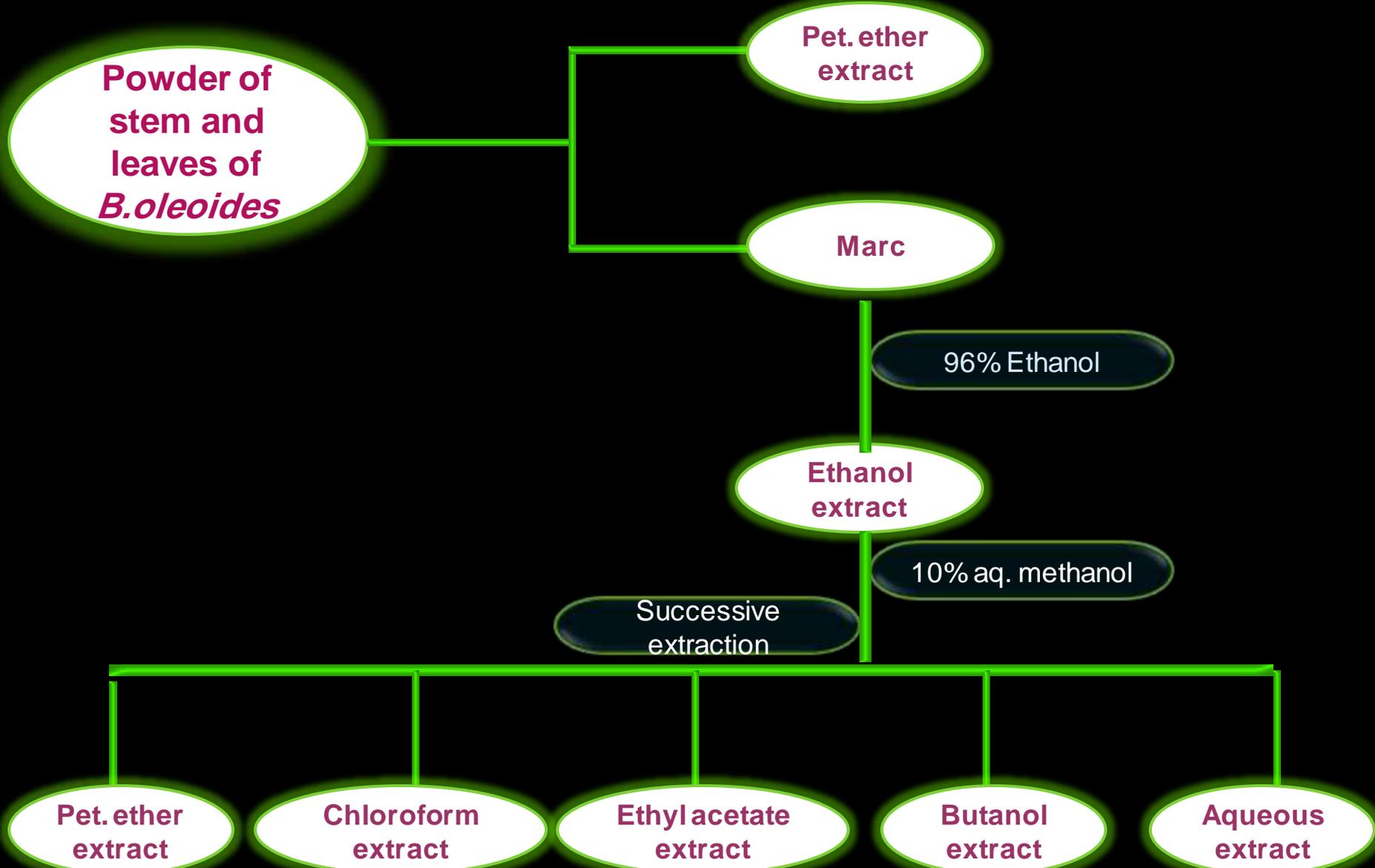
- 1- Preliminary phytochemical screening.
- 2- Investigation of the lipid content of *B. oleoides* .
- 3- Isolation and structure elucidation of different compounds present in *B. oleoides* and *S. schimperianum*.
- 4- Chemical derivatization on small scale of selected compounds.
- 5- The biological activity was concerned on antimicrobial activities of different extracts and isolated compounds of both plants.
- 6- Evaluation of other biological activities of different extracts and or isolated compounds including antioxidant, smooth muscle relaxant and antihypertensive activities.
- 7- Comparison of the obtained results with literature data for the some isolated compound.

**Preliminary Phytochemical  
Screening of *Barbeya  
oleoides* Schweinf and  
*Solanum shimperianum*  
Hochst**

G.E. Trease and W.C. Evans, Pharmacognosy, 15<sup>th</sup> ed (2002)

# 1- Whole powdered plant

# 2- Successive extracts



**Results of phytochemical screening of the powder of stem and leaves of *B. oleoides* Schweinf**

<b>Active constituents</b>	<b>Result</b>
<b>Alkaloids</b>	—
<b>Carbohydrates and/or glycosides</b>	+ ✓
<b>Anthraquinones</b>	—
<b>Flavonoids</b>	+ ✓
<b>Saponins</b>	+ ✓
<b>Triterpenoids and/or sterols</b>	+ ✓
<b>Tannins</b>	+
<b>Volatile constituents</b>	— ✓

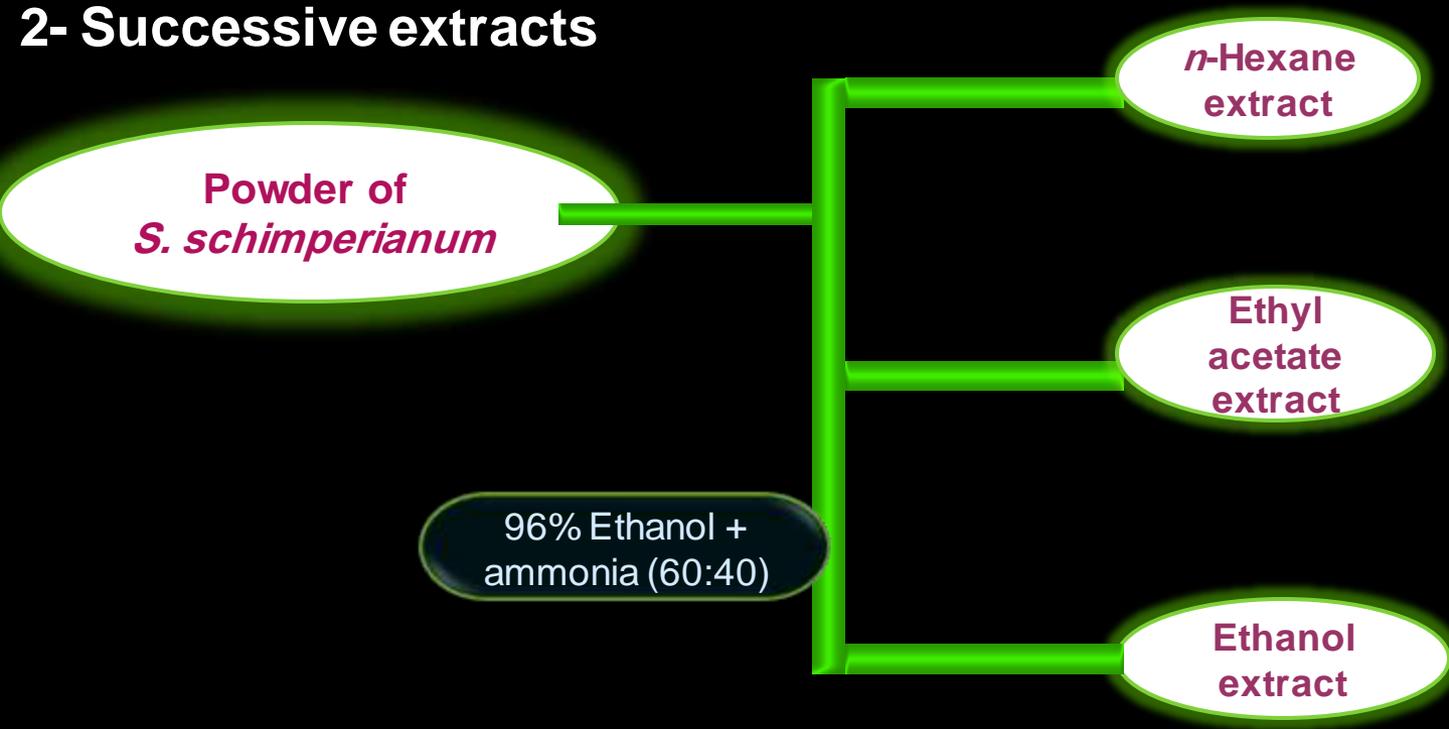
- negative; + positive



*Solanum schimperianum*

1- Whole powdered plant

2- Successive extracts



## Results of phytochemical screening of the powder of *S. schimperianum* Hochst

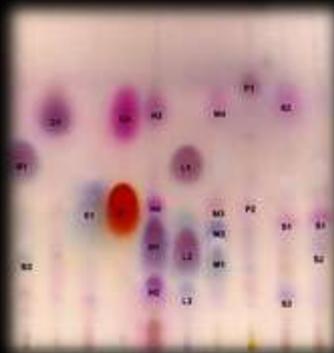
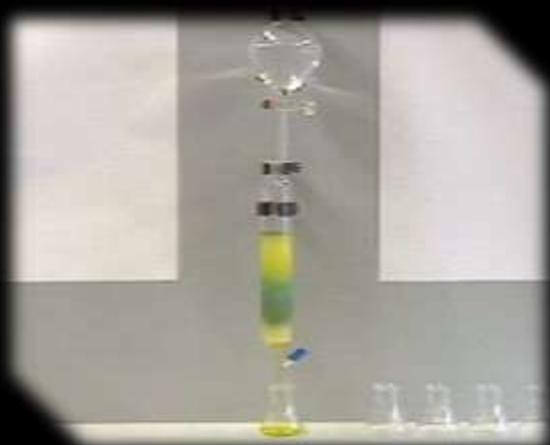
Active constituents	Result
<b>Alkaloids</b>	+ ✓
<b>Carbohydrates and/or glycosides</b>	+ ✓
<b>Anthraquinones</b>	-
<b>Flavonoids</b>	+ ✓
<b>Saponins</b>	+ ✓
<b>Triterpenoids and/or sterols</b>	+ ✓
<b>Tannins</b>	-
<b>Volatile constituents</b>	-

- negative; + positive

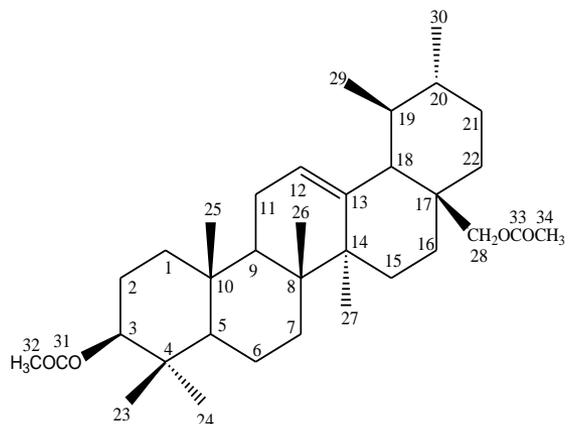
Results of phytochemical screening of the successive extracts of the whole plant of *S. schimperianum* Hochst.

Constituents tested	n-hexane fraction	Ethyl acetate fraction	Ethanol fraction
<b>Alkaloids</b>	—	—	+ ✓
<b>Carbohydrates And/or glycoside</b>	—	+ ✓	+ ✓
<b>Anthraquinones</b>	—	—	—
<b>Cardiac glycosides</b>	—	—	—
<b>Flavonoids: -Aglycone -Glycosides</b>	— —	+ ✓ +	+ ✓ —
<b>Saponins</b>	—	—	+ ✓
<b>Triterpens and/or sterols</b>	+ ✓	+ ✓	+ ✓
<b>Tannins</b>	—	—	—
<b>Volatile constituents</b>	—	—	—

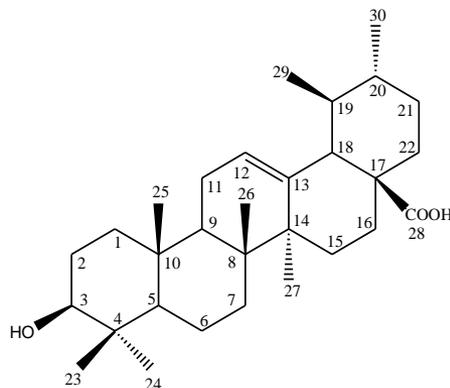
**Phytochemical study of  
*Barbeya oleoides* and  
*Solanum shimperianum***



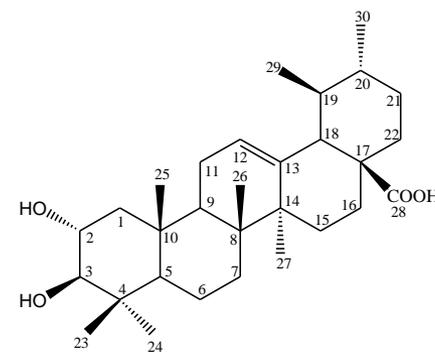
## Structures of isolated compounds from *Barbeya oleoides*



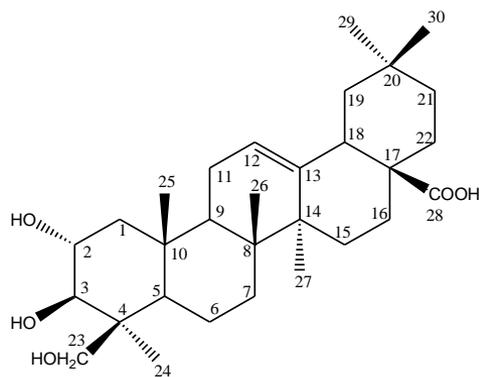
B-1 (Uvaol diacetate)



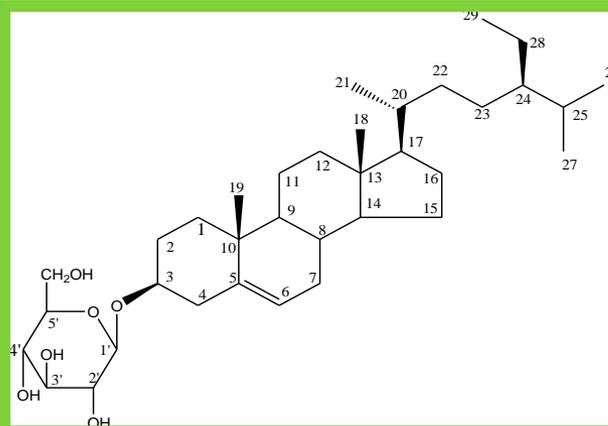
B-2 (Ursolic acid)



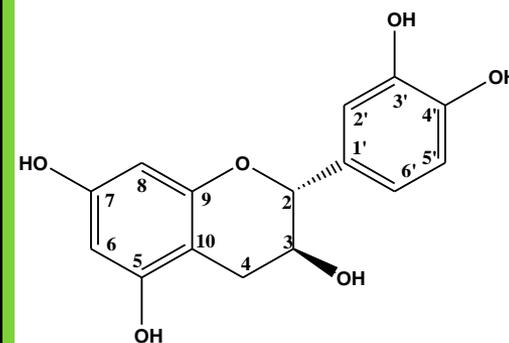
B-3 (Corsolic acid)



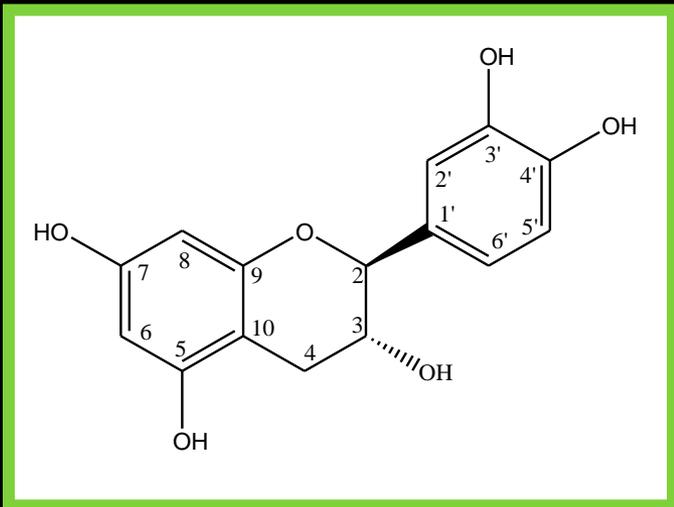
B-4 (Arjunolic acid)



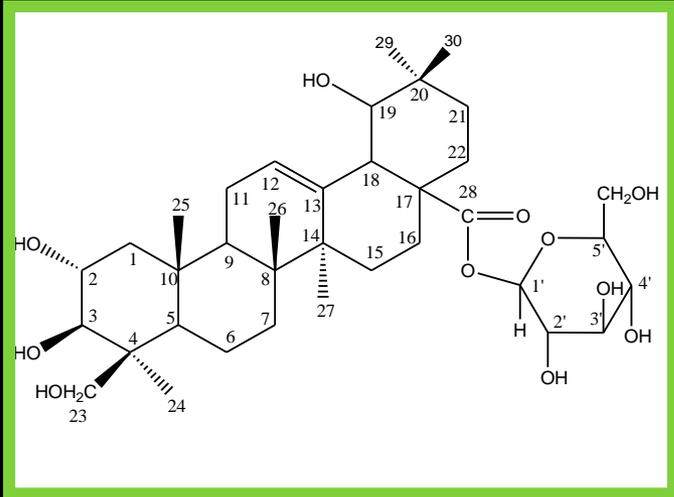
B-5 ( $\beta$ -sitosterol-3-O- $\beta$ -D-glucoside)



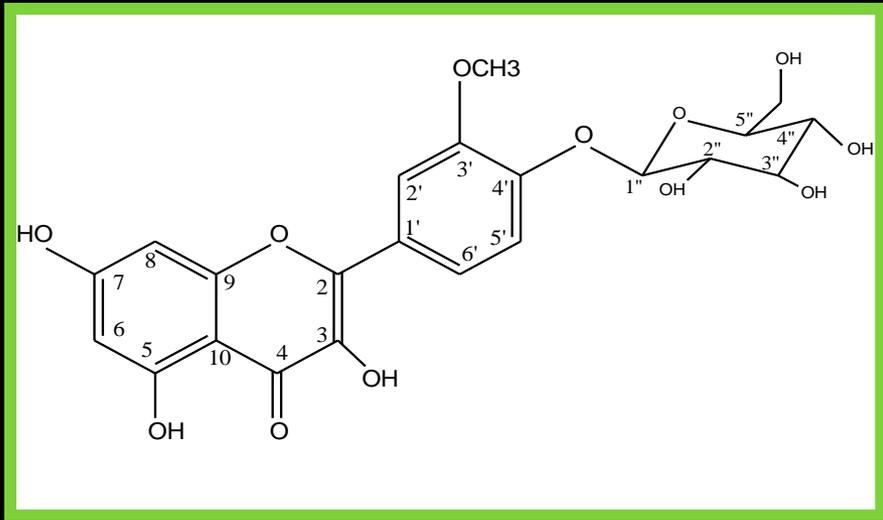
B-6 (Catechin)



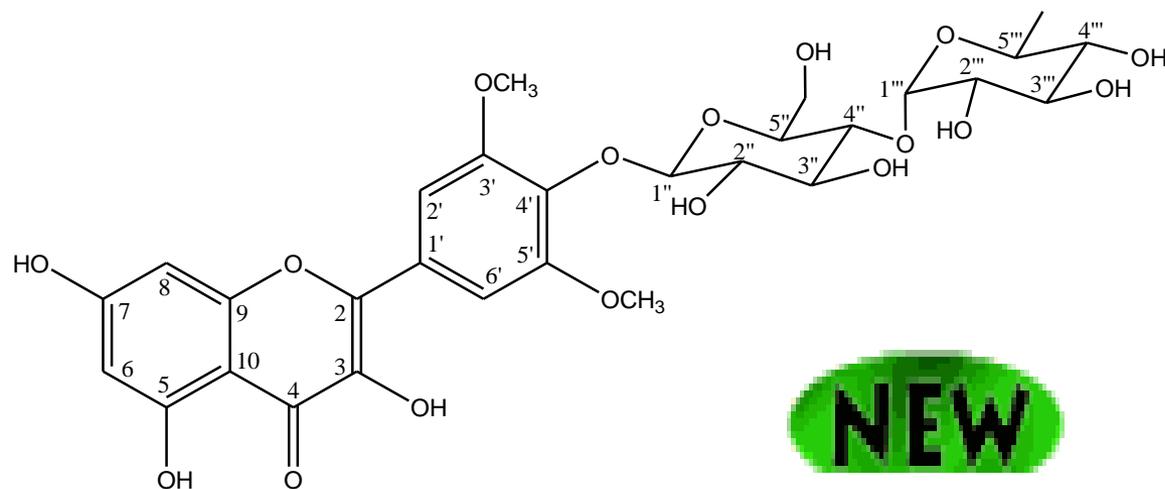
**B-7 (Epicatechin )**



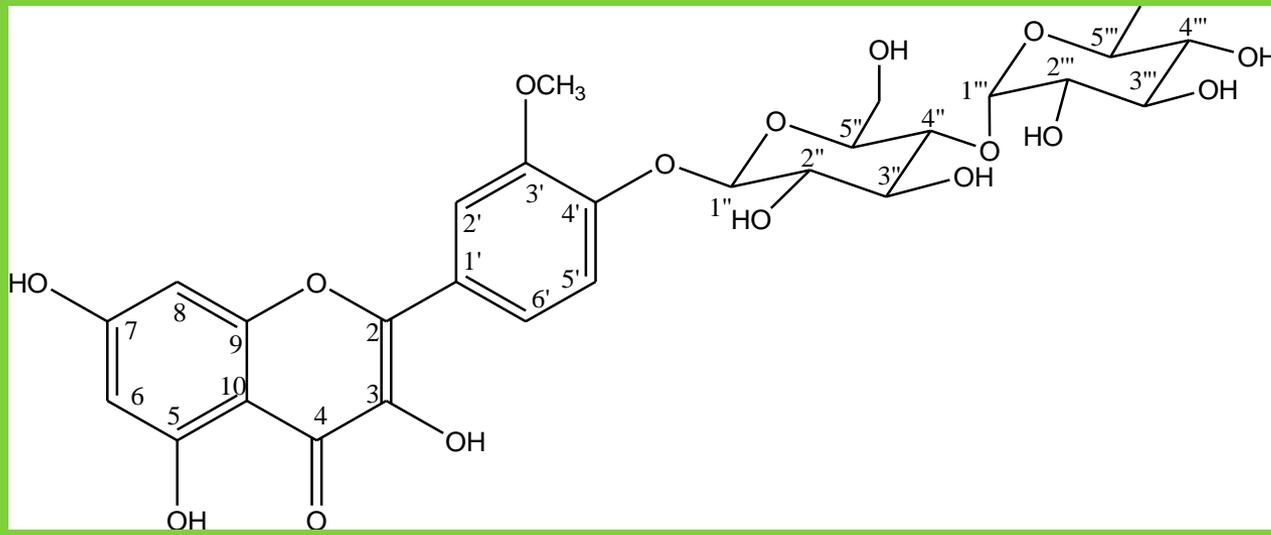
**B-8 (Arjunoglucoside I )**



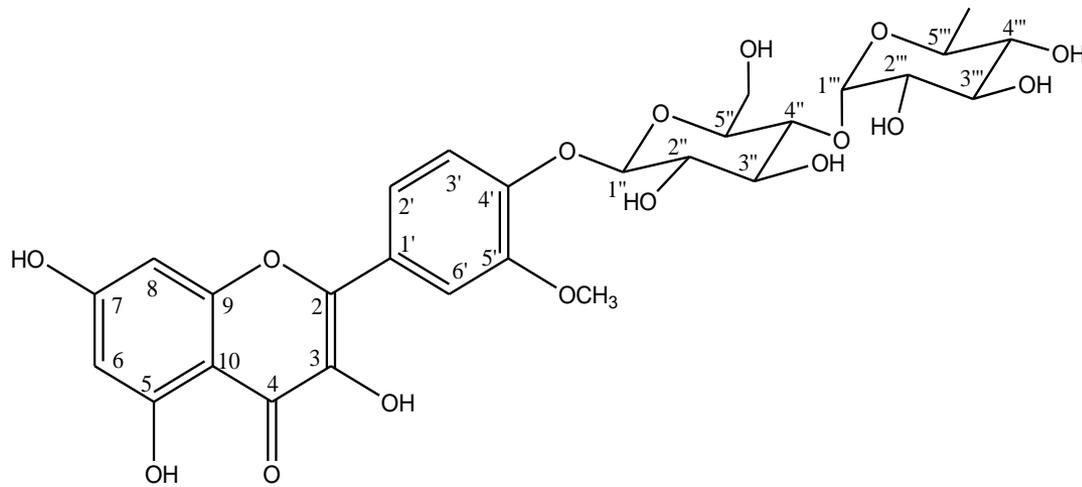
**B-9( Isorhamnetin-4'-O-glucoside)**



**B-10-(4'-O-(1''-4''-O-L-rhamnopyranosyl)-β-D-(glucopyranosyl-3',5' dimethoxymyricetin)**

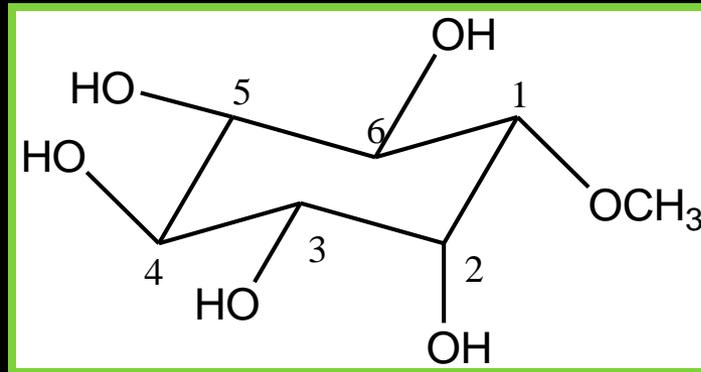


**B-11a (4'- O-(1'''-4''-O-L-rhamnopyranosyl)-β-D-(glucopyranosyl-3'-methoxyquercetin)**

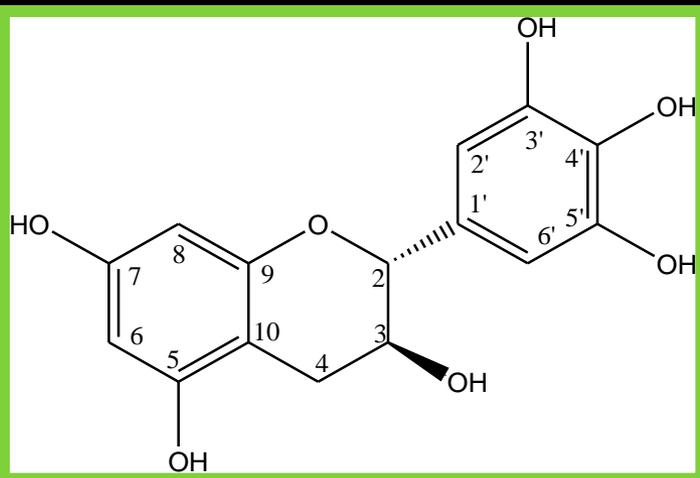


**B-11b (4'- O-(1'''-4''-O-L-rhamnopyranosyl)-β-D-(glucopyranosyl-5'-methoxyquercetin)**

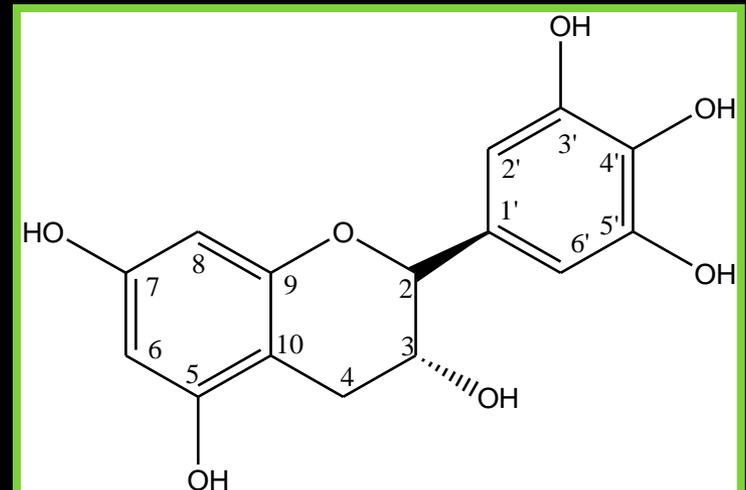
**NEW**



B-12 ( D (-) bornesitol)



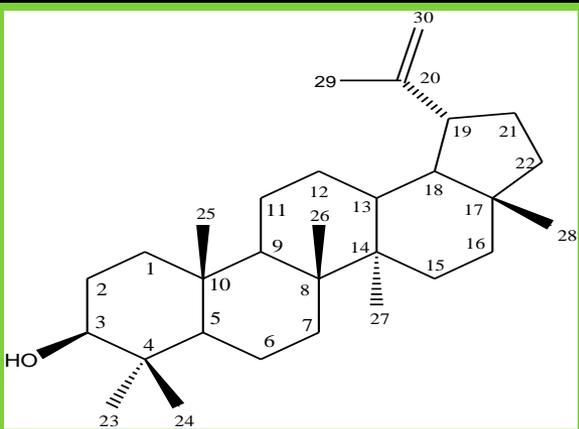
B-13 (Gallocatechin)



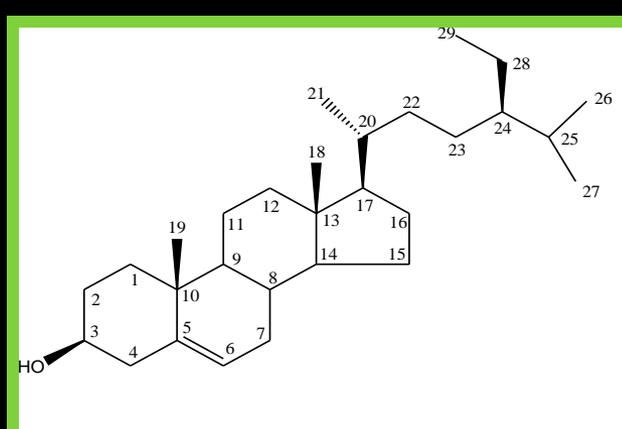
B-14 (Epigallocatechin)

*Solanum schimperianum* Hochst

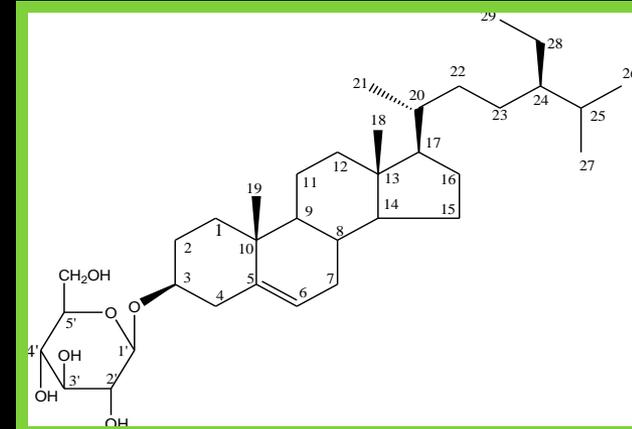
# Structures of isolated compounds from *Solanum schimperianum*



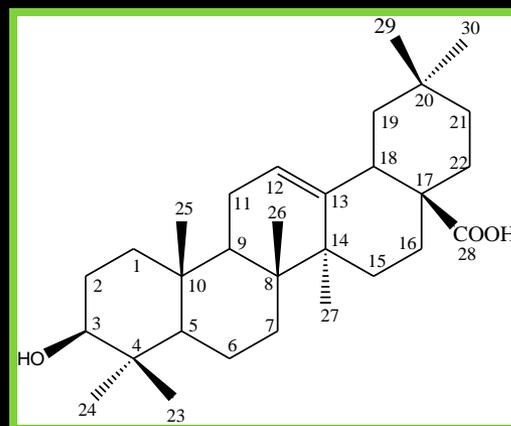
S-1 (Lupeol)



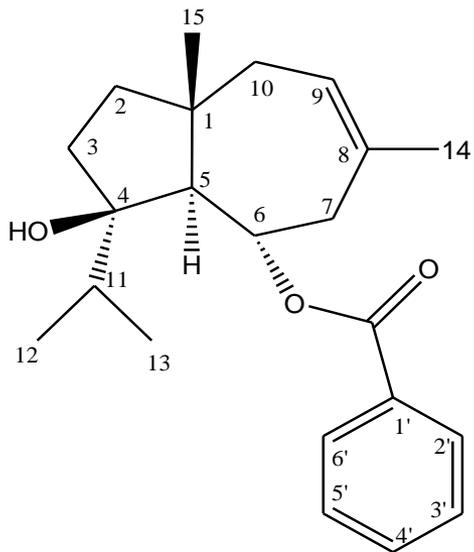
S-2 ( $\beta$ -Sitosterol)



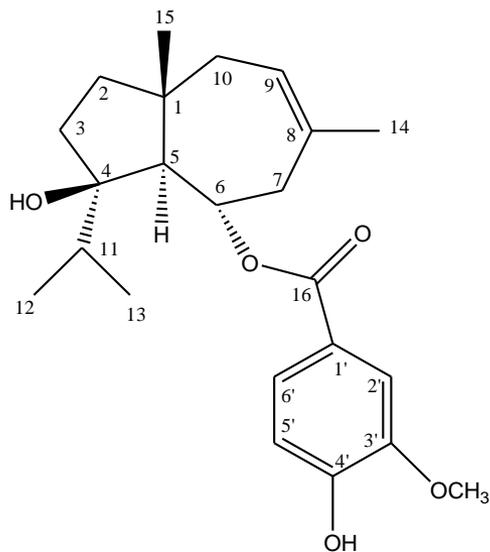
S-3 ( $\beta$ -Sitosterol-3- $\beta$ -D-glucoside)



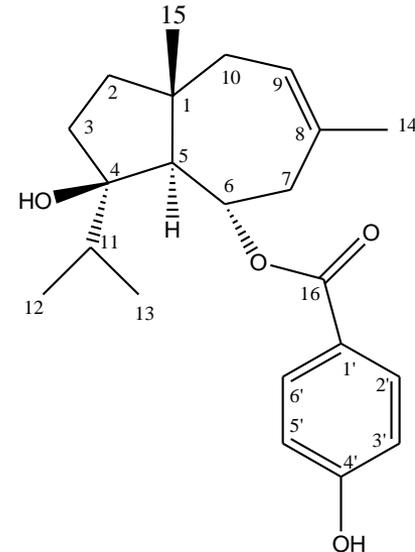
S-4 (Oleanolic acid)



S-5 (Teferidin)



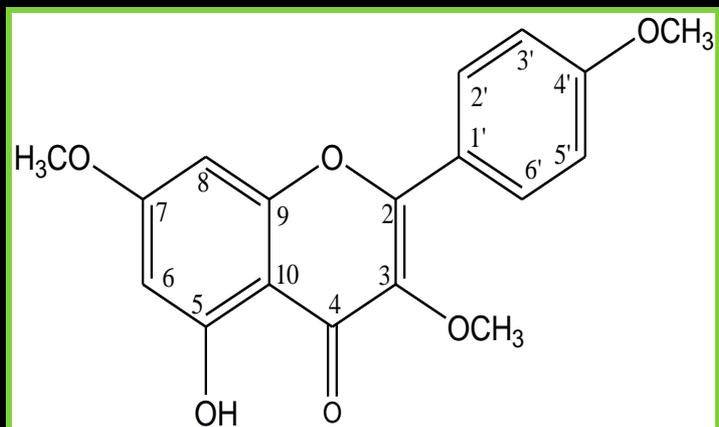
S-6 (Teferin)



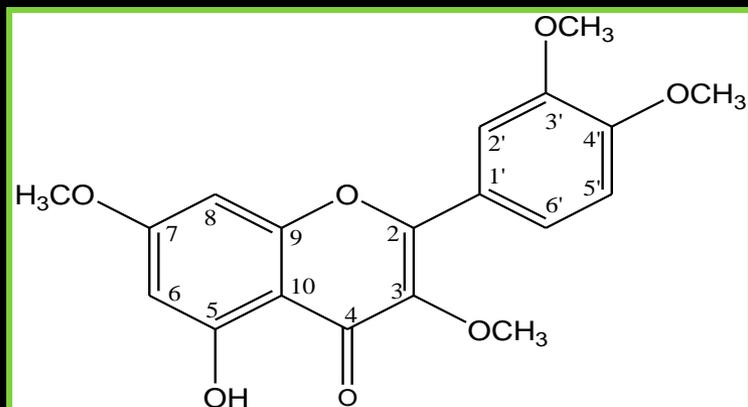
S-7 (Ferutinin)

FIRST TIME

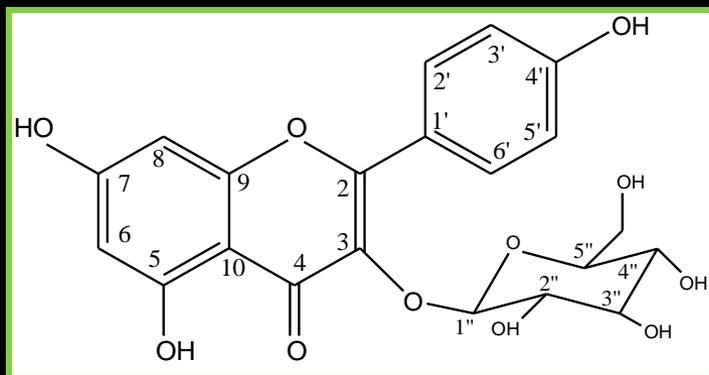
Solanaceae



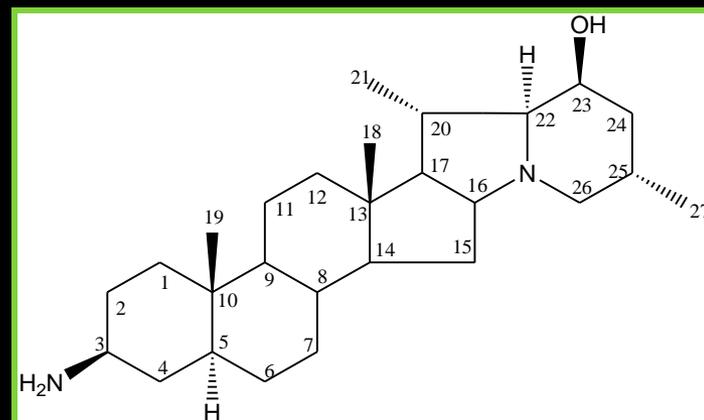
**S-8 (5-Hydroxy-3,7,4'- trimethoxyflavone)**



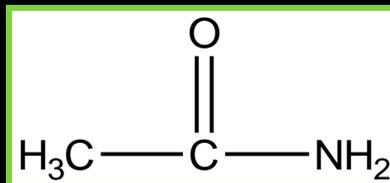
**S-9 (Retusin)**



**S-10 (Kaempferol-3-O-glucopyranoside)**

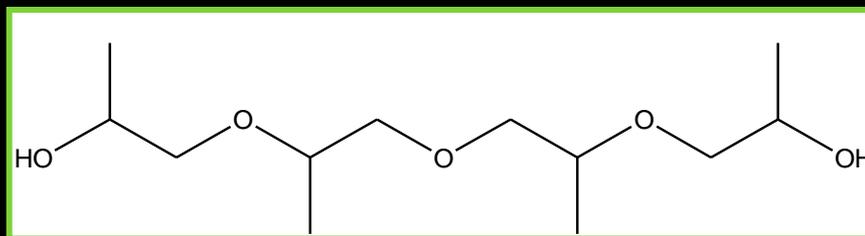


**S-11 (Solanopubamine)**



S-12 (Acetamide)

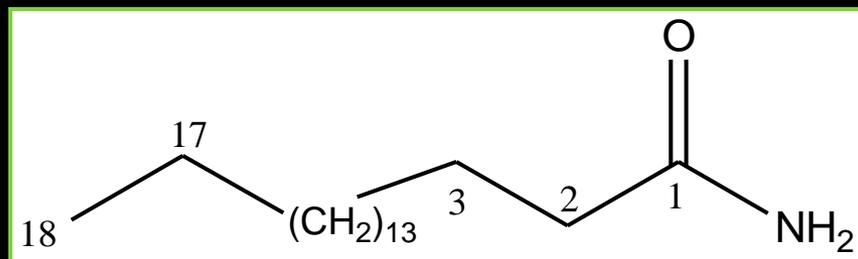
SECOND  
TIME



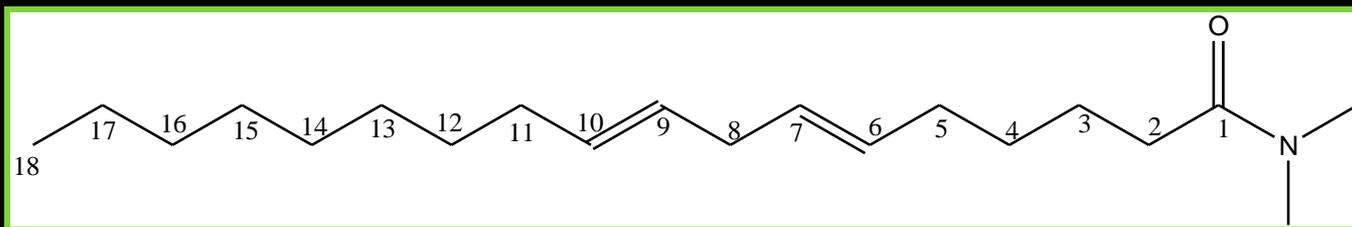
S-13 (1-{1-[2-(2 Hydroxypropoxy) propoxy] propan-2-yloxy} propan-2-ol)

FIRST  
TIME

NATURE



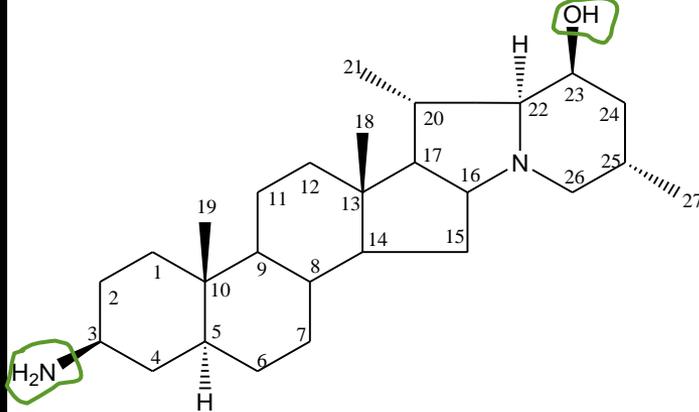
S-14 (Stearamide)



S-15 ( 6E,9E)-N,N-dimethyloctadeca-6,9-dieneamide

FIRST  
TIME

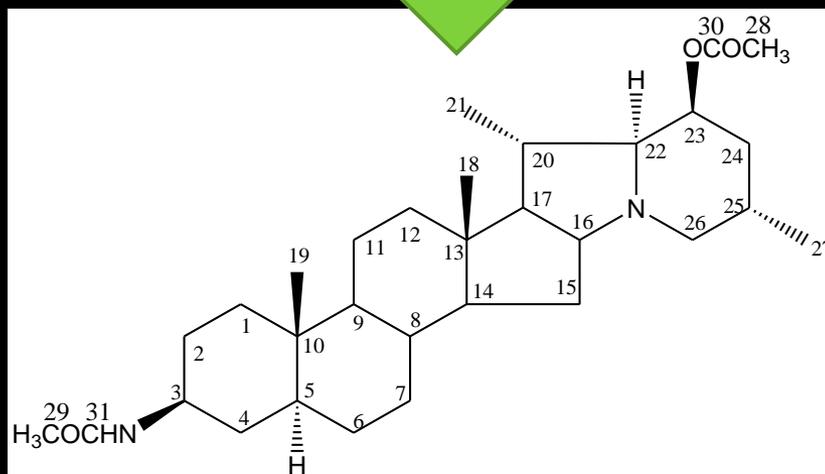
Solanaceae



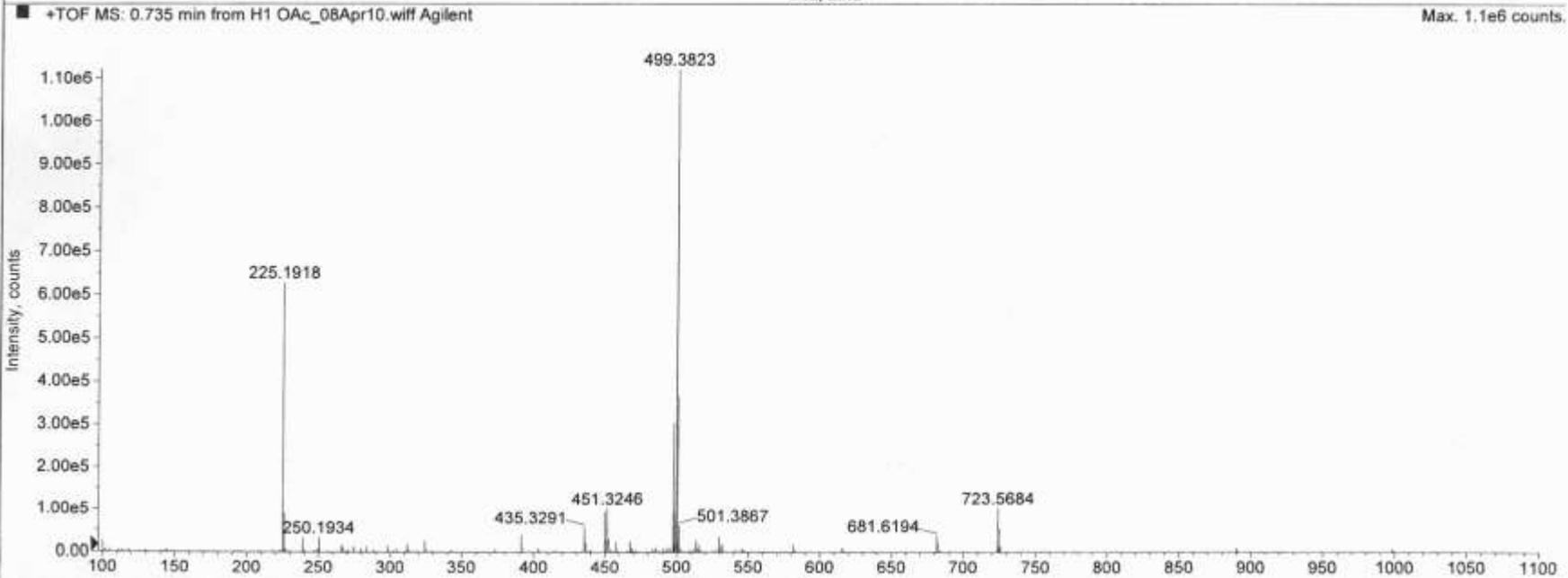
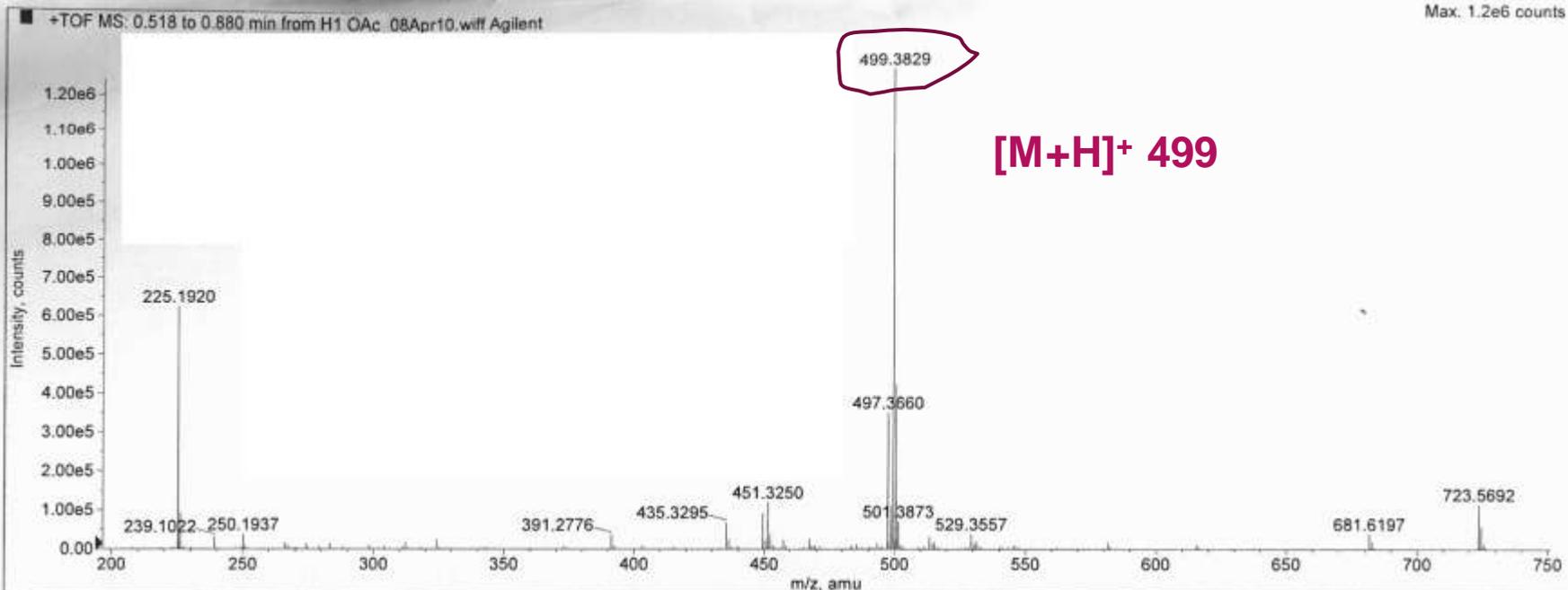
S-11 (Solanopubamine)

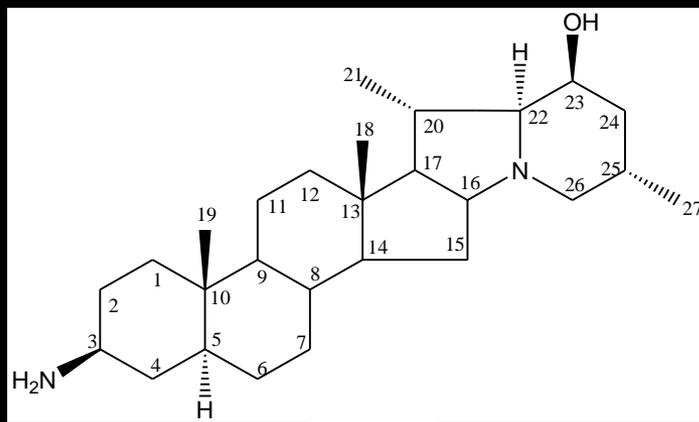
Acetylation

Pyridine  
Acetic anhydride



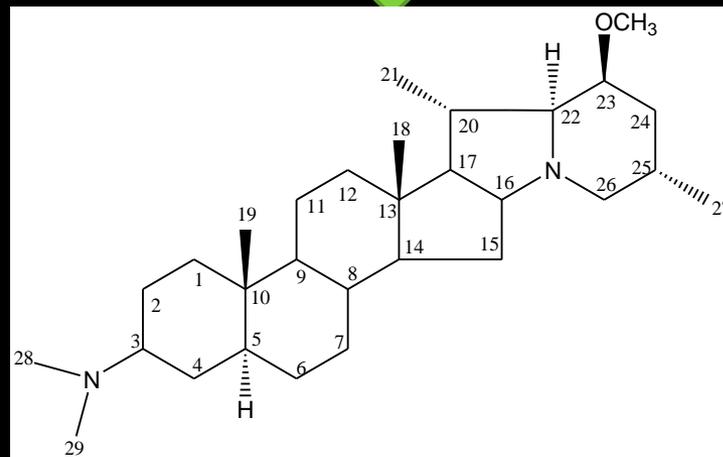
S-11a (3-N, 23-O-diacetyl-solanopubamine)





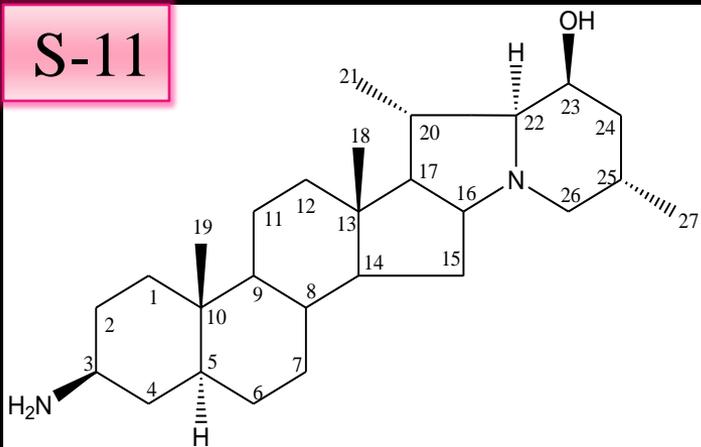
Methylation

CH<sub>3</sub>I/MgCO<sub>3</sub>

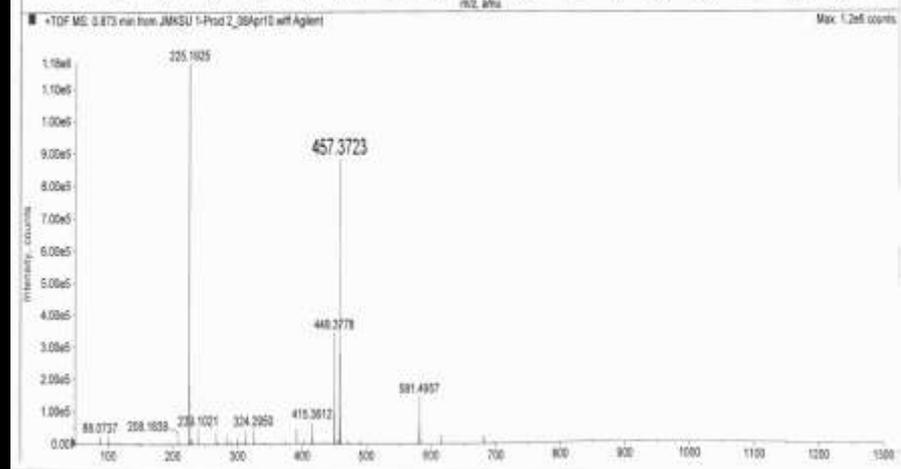
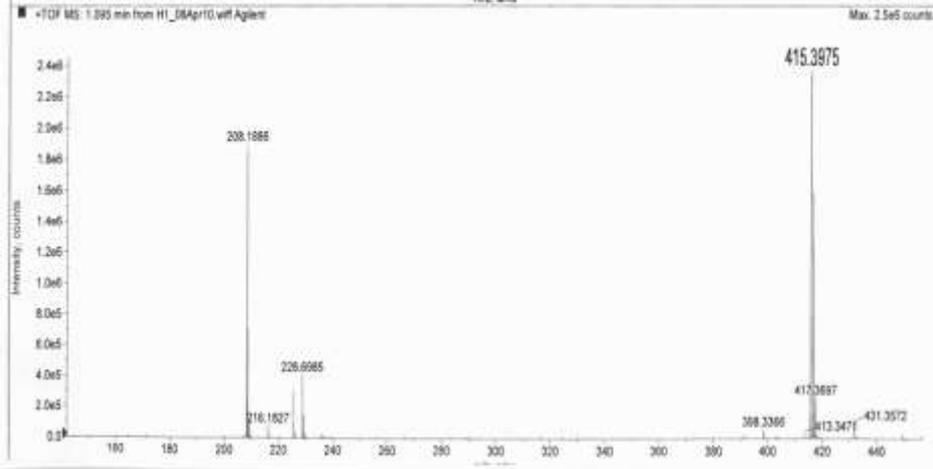
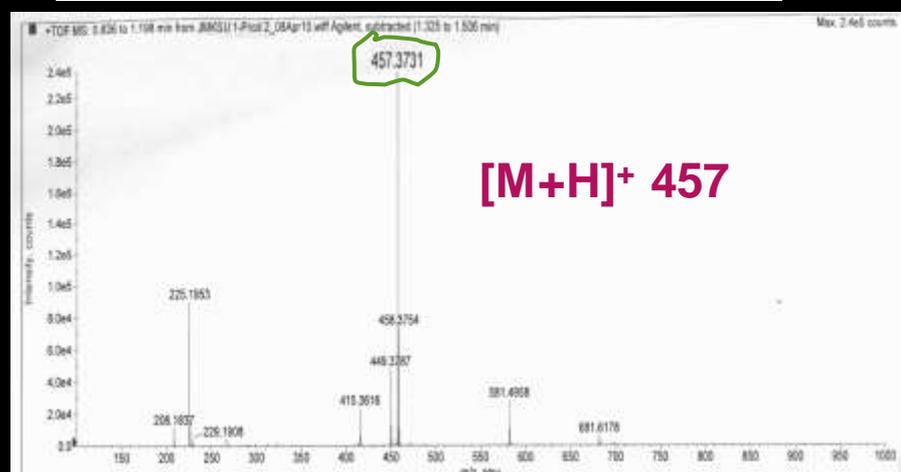
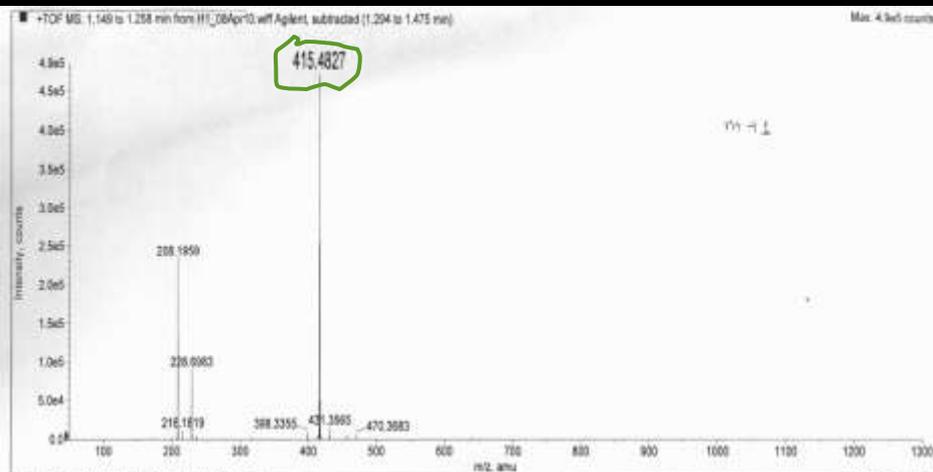
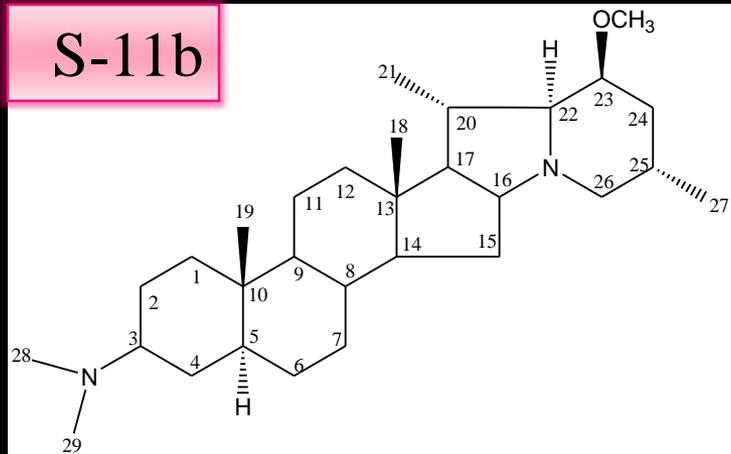


S-11b (3,3-N,N-Dimethyl-23-O-methylsolanopubamine)

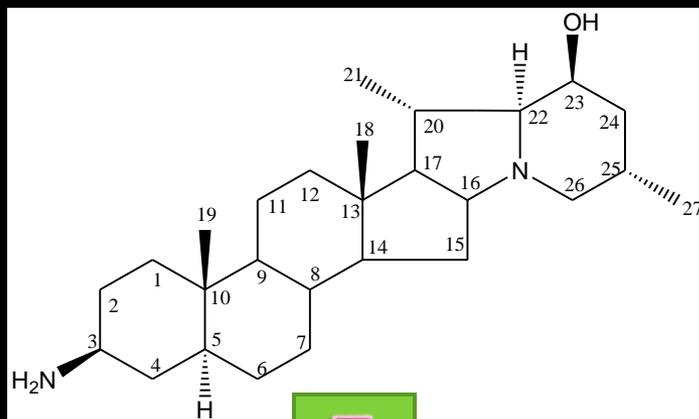
S-11



S-11b

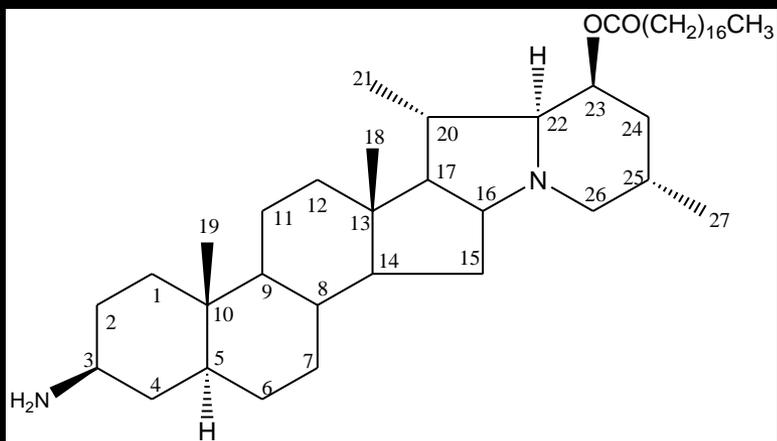


**FIRST  
TIME**

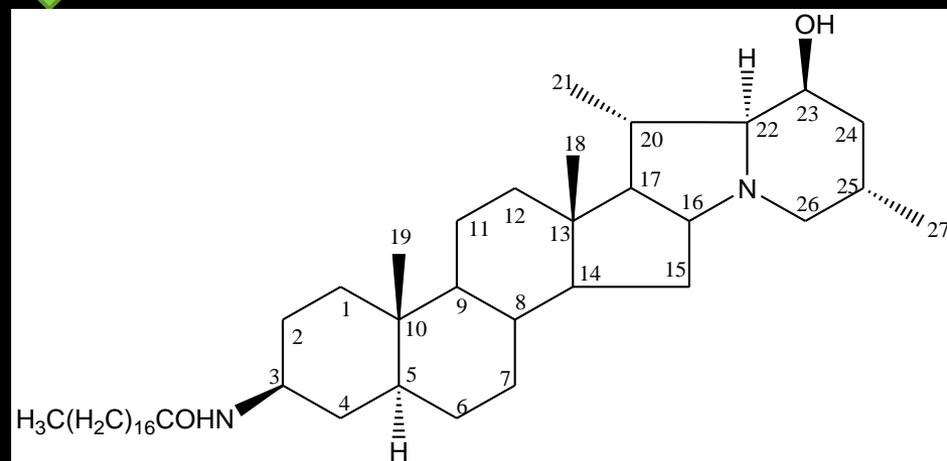


**Esterification**

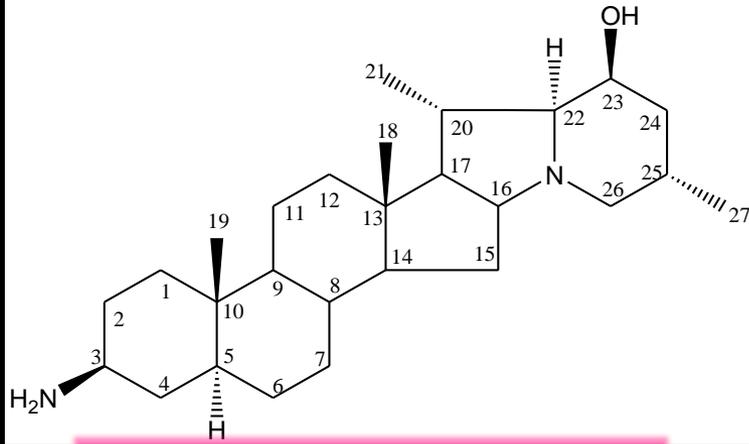
**Octadecanoic acid**



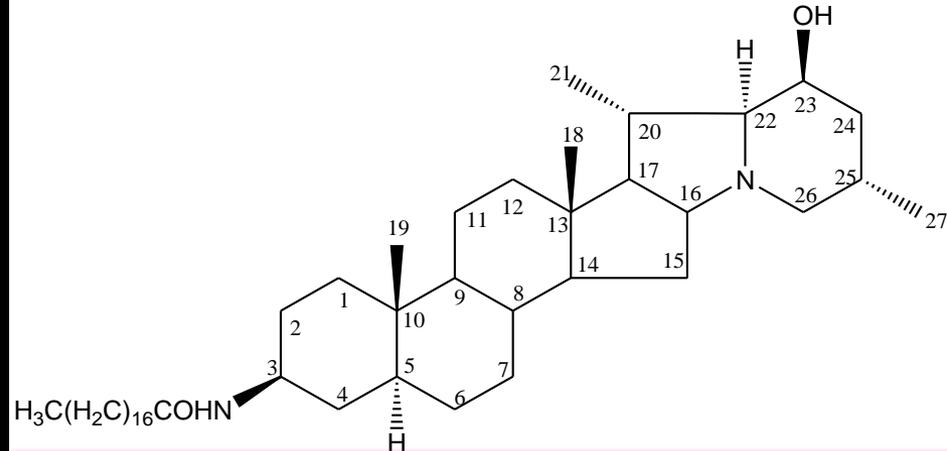
**S-11d (23-*O*-octadecanoate-solanopubamine)**



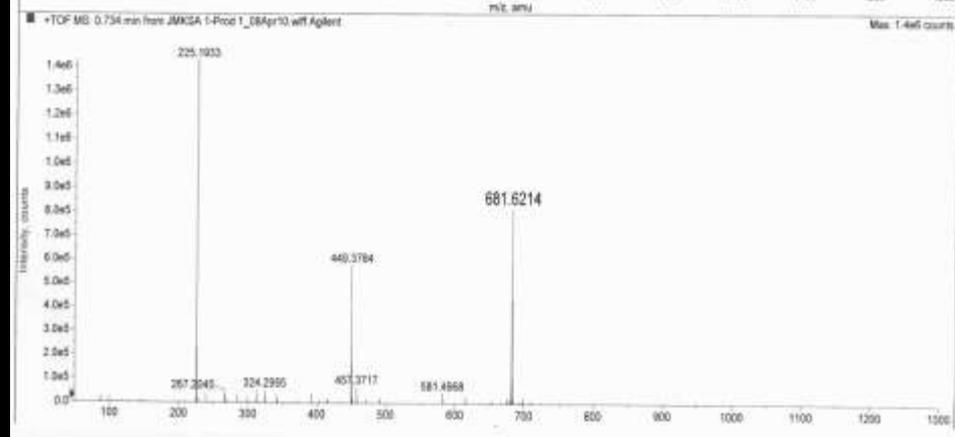
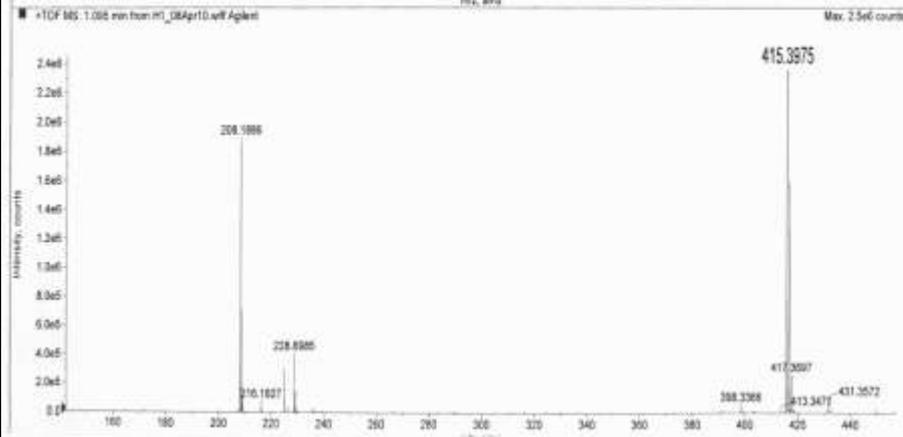
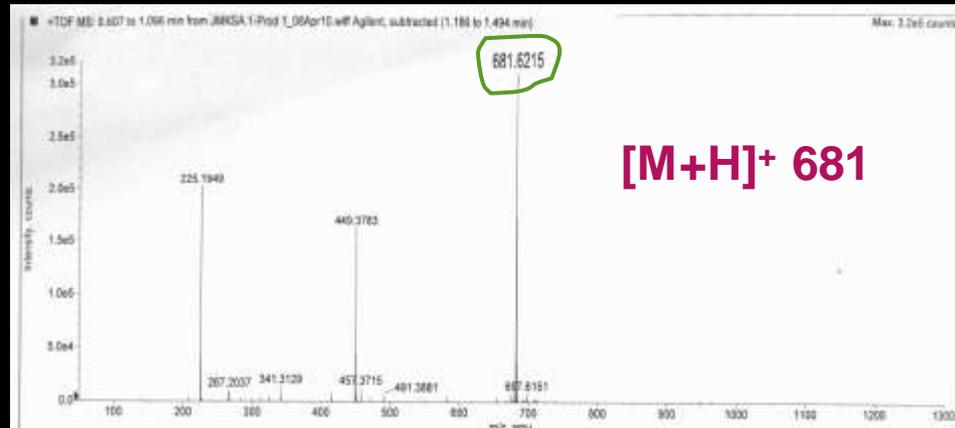
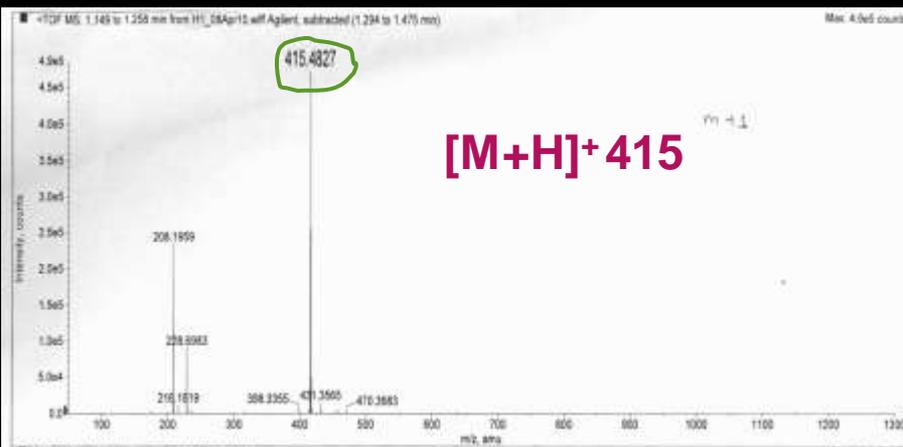
**S-11c (3-*N*-octadecanoate-solanopubamine)**

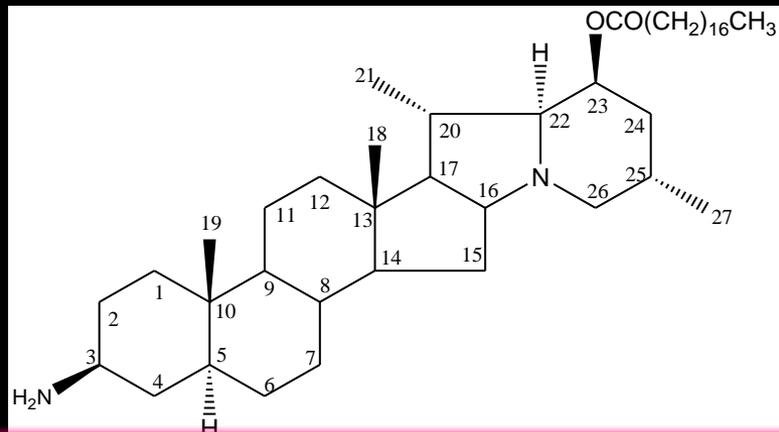


**S-11 (Solanopubamine)**

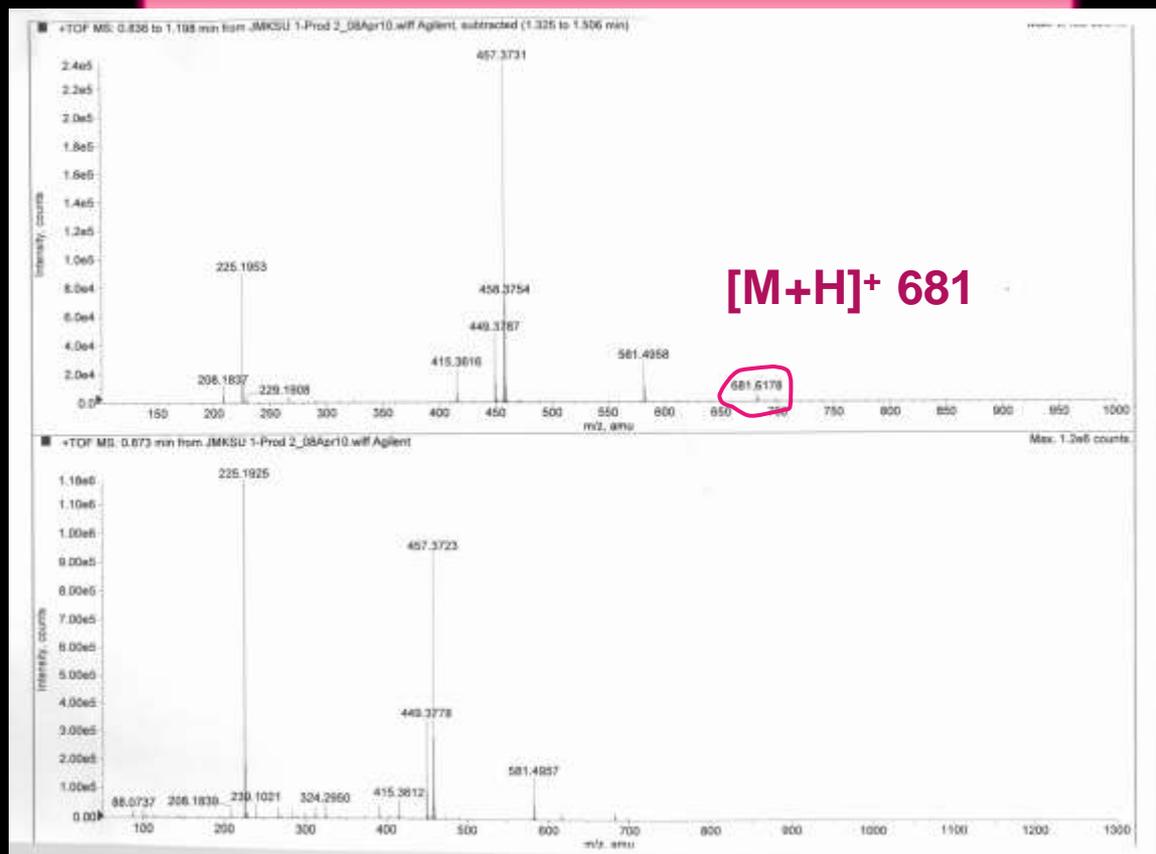


**S-11c (3-N-octadecanoate-solanopubamine)**



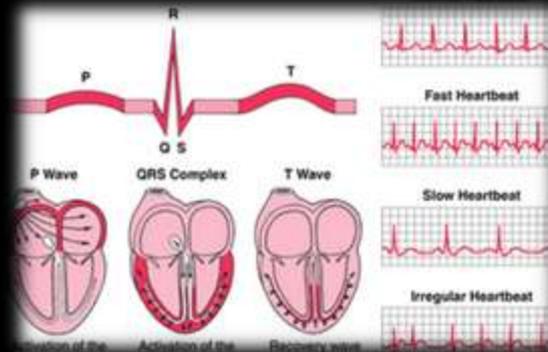


**S-11d (23-O-octadecanoate-solanopubamine)**





# Biological Study of *Barbeya oleoides* Schweinf and *Solanum* *schimperianum* Hostch



# Antimicrobial activity

## a. Antimicrobial screening by determination of zone of inhibition

Sample:

## b. Determination of minimum inhibitory concentration (MIC)

Method : Mitscher *et al.*

## Results of antimicrobial screening of extracts (1 mg/ml) *B. oleoides* Schweinf

Micro-organism	Inhibition zone									
	Leave					Stem				
	Petroleum ether extract	Chloroform extract	Ethyl acetate Extract	Butanol extract	Aqueous Extract	Petroleum ether extract	Chloroform Extract	Ethyl acetate extract	Butanol extract	Aqueous extract
<i>Bacillus subtilis</i>	+	+	+	-	-	+	-	+	+	-
<i>Staphylococcus aureus</i>	+	-	+	+	+	+	-	+	+	-
<i>Escherichia coli</i>	-	-	-	-	-	-	-	+	-	-
<i>Pseudomonas aeruginosa</i>	-	-	+	+	-	-	-	+	+	-
<i>Mycobacterium smegmatis</i>	-	-	+	+	+	-	-	+	+	-
<i>Candida albicans</i>	-	-	+	+	+	+	-	+	+	-

## MIC values of isolates B-2, B-3 and B-14 & B-15

Micro-organism	MIC in µg/ ml		
	B-2	B-3	B-14&B-15
<i>Bacillus subtilis</i>	50	25	25
<i>Staphylococcus aureus</i>	50	25	25

B-2 ( Ursolic acid)

B-3 ( Corsolic acid)

B-14&15 ( Gallocatechin and epigallocatechin)

## Results of antimicrobial screening of isolates B-2, B-3 and B-14& B-15 (100µg/ ml).

Micro-organism	Zone inhibition		
	B-2	B-3	B-14& B-15
<i>Bacillus subtilis</i>	+ ✓	+ ✓	+ ✓
<i>Staphylococcus aureus</i>	+ ✓	+ ✓	+ ✓
<i>Escherichia coli</i>	-	-	-
<i>Pseudomonas aeruginosa</i>	-	-	-
<i>Mycobacterium smegmatis</i>	-	-	-
<i>Candida albicans</i>	-	-	-

Results of antimicrobial screening of extracts (1 mg/ml) *S. schimperianum* Hochst

Micro-organism	Inhibition zone		
	<i>n</i> -hexane	Ethyl acetate Extract	Ethanol extract
<i>Bacillus subtilis</i>	+ ✓	–	+ ✓
<i>Staphylococcus aureus</i>	+ ✓	–	+ ✓
<i>Escherichia coli</i>		–	+ ✓
<i>Pseudomonas aeruginosa</i>	–	–	–
<i>Mycobacterium smegmatis</i>	–	–	+ ✓
<i>Candida albicans</i>	–	–	+ ✓



Results of MIC values of isolates compound S-11 from *S. schimperianum* Hostch

Micro-organism	MIC in µg/ ml of S-8
<i>Klepsiella pneumonia</i>	> 125.00 µg/ml
<i>Acinetobacter baumannii</i>	✓ > 31.25 µg/ml
<i>Escherichia coli</i>	> 62.50 µg/ml
<i>Pseudomonas aeruginosa</i>	✓ > 31,25 µg/ml
<i>Enterobacter</i>	> 62.50 µg/ml
<i>Methacilin resistant</i>	> 62.50 µg/ml
<i>Staphylococcous aureus</i>	
<i>Streptococcus pneumonia</i>	> 62.50 µg/ml
<i>Enterococcus faecalis</i>	> 62.50 µg/ml
<i>Enterococcus cloace</i>	> 62.50 µg/ml
<i>Staphylococcus epidermidis</i>	> 62.50 µg/ml
<i>Candida krusei</i>	> 125.00 µg/ml
<i>Aspergillus fumigatus</i>	> 126.00 µg/ml

S-11 (Solanobupamine)

Results of antimicrobial screening of isolates S-13, S-14 , and S-15 (100µg / ml). *S. schimperianum* Hostch

Micro-organism	Zone inhibition		
	S-13	S-14	S-15
<i>Bacillus subtilis</i>	–	–	–
<i>Staphylococcus aureus</i>	–	–	–
<i>Escherichia coli</i>	+ ✓	+ ✓	+ ✓
<i>Pseudomonas aeruginosa</i>	–	–	–
<i>Mycobacterium smegmatis</i>	–	–	–
<i>Candida albicans</i>	+ ✓	+ ✓	+ ✓

S-13 (1-{1-[2-(2 hydroxypropoxy) propoxy] propan-2-yloxy} propan-2-ol

S-14 (stearamide)

S-15 (6*E*, 9*E*-*N,N*-dimethyloctadeca-6,9-dienamide )

Results of antimicrobial screening of the synthetic compounds S-11a, S-11c and S-11d (100 µg / ml) from *S. schimperianum* Hostch

Micro-organism	Zone inhibition		
	S-11a	S-11c	S-11d
<i>Bacillus subtilis</i>	–	–	–
<i>Staphylococcus aureus</i>	–	–	–
<i>Escherichia coli</i>	+ ✓	+ ✓	+ ✓
<i>Pseudomonas aeruginosa</i>	–	–	–
<i>Mycobacterium smegmatis</i>	–	–	–
<i>Candida albicans</i>	+ ✓	+ ✓	+ ✓

S-11a (3-*N*,23-*O*-diacetyl-solanopubamine)

S-11c (3-*N*-octadecanoate-solanopubamine)

S-11d (23-*O*-octadecanoate-solanopubamine)

## Antihypertensive activity

**Animal:** Male Wistar rats

**Method:** K. E. H. El Tahir

Changes in blood pressure were quantified in mm Hg using the calibration system built-in the physiograph

Changes in the heart rate were calculated as percentage change compared with the pre-drug level.

**Effect of ethanol extracts of *B. oleoides* Schweinf on arterial blood pressure and heart rate.**

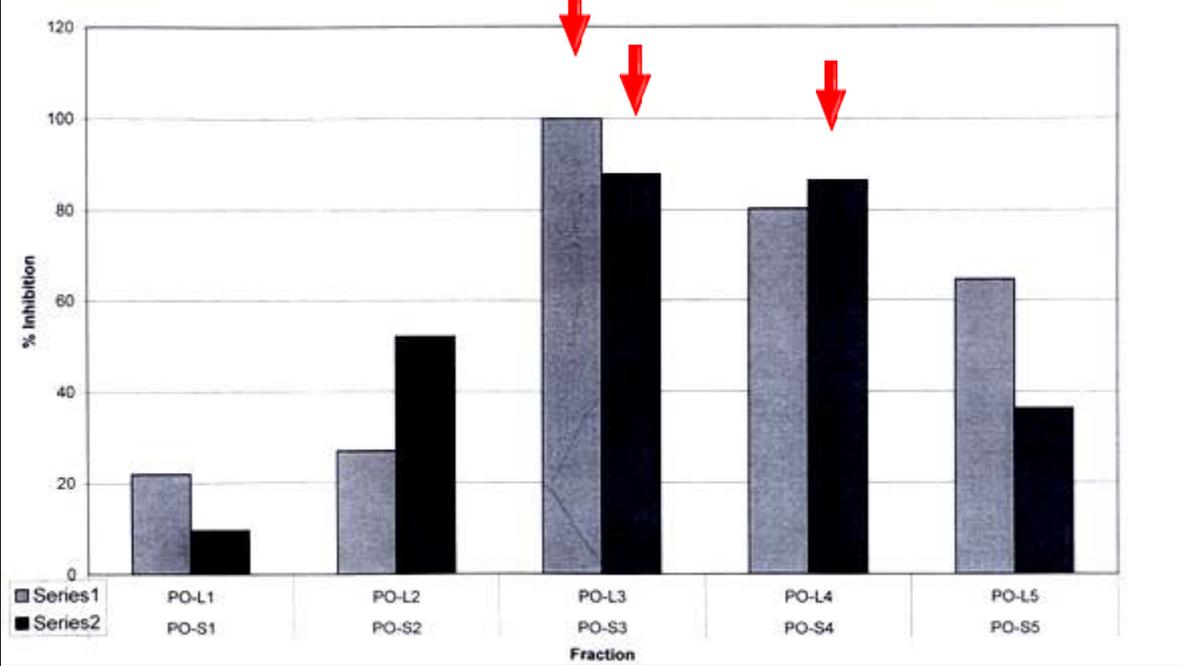
<b>Ethanol extract Dose</b>	<b>Decrease in arterial blood pressure (mm Hg)</b>	<b>Percentage decrease in heart rate</b>
<b>10 mg/Kg(I.P)</b>	<b>18 mm Hg</b>	<b>0</b>
<b>50 mg/ kg (I.P)</b>	<b>54 mm Hg</b>	<b>0</b>

## Antioxidant activity

**Sample:** different fractions of *B. oleoides*

**Method :** Thin –Layer Densitometry adopted to E. A. Abourashed, 2005 using DPPH.

Inhibition of DPPH by different fractions of *B.oleoides* Schweinf at 25ug/ml



PO-L3 Ethyl acetate extract of leave  
PO-L3 Ethyl acetate extract of stem  
PO-S4 Butanol extract of stem

## Spasmolytic activity

Effect of the different extracts on the spontaneously contracting rabbit jejunum.

Extract	% Inhibitor
BOB-S	65%
BOB-L	76%
Aqueous stem	55%
Ethyl acetate stem	80% ✓
Butanol stem	77%
Chloroform stem	92% ✓
Petroleum ether stem	68,2%

**Effect of tested compounds on the spasmogens-induced contractions on isolated guinea-pig ileum:**

<b>Compound</b> <b>dose(100</b> <b>µg/ml)</b>	<b>Inhibition %</b>		
	<b>Acetylcholine</b>	<b>Histamine</b>	<b>BaCl<sub>2</sub></b>
<b>B-13&amp;14</b>	<b>0</b>	<b>0</b>	<b>0</b>
<b>B-4</b>	<b>0</b>	<b>25</b>	<b>72</b>
<b>B-5</b>	<b>0</b>	<b>0</b>	<b>83</b>
<b>B-12</b>	<b>18</b>	<b>22</b>	<b>50</b>
<b>B-1</b>	<b>66</b> ✓	<b>35</b> ✓	<b>0</b> ✓

B-13&14 (Gallicocatechin & epigallocatechin

B-4 (arjulonic acid)

B-5 ( $\beta$ -Sitosterol -3- $\beta$ -O-glucoside)

B-12 (Borinisitol)

B-1 (Uvaol diacetate)

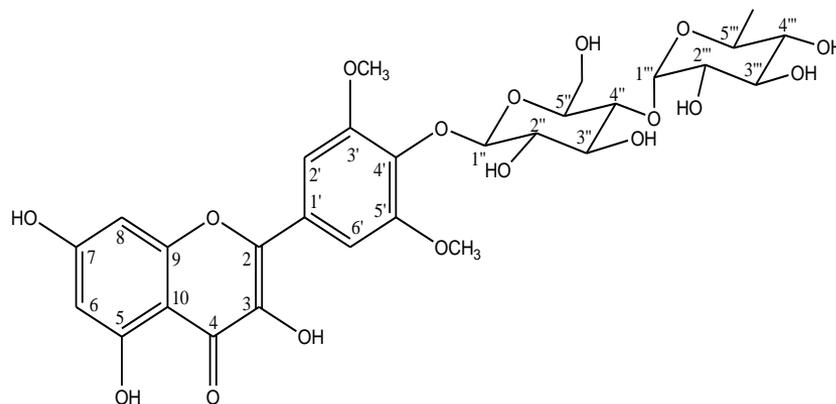
# Conclusion

This study is the first one that deals with phytochemical and antimicrobial activity of *B. oleoides* Schweinf and *S. schimperianum* Hochst growing in Saudi Arabia

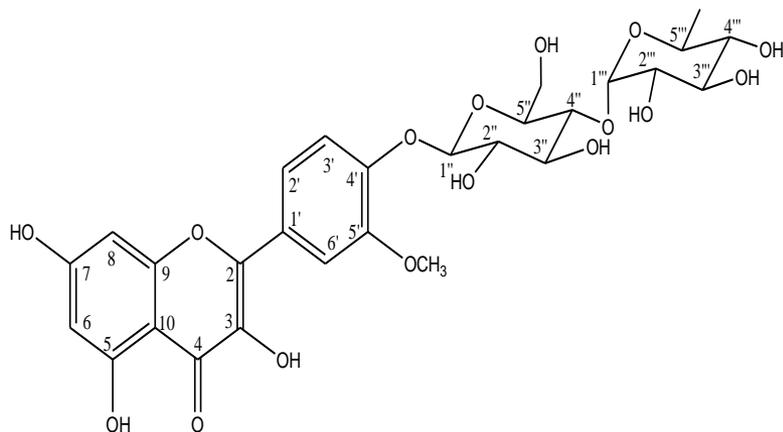
Phytochemical study of *B. oleoides* Schweinf resulted in isolation and characterization of 14 compounds

Phytochemical study of *S. schimperianum* Hochst resulted in isolation and characterization of 15 compounds

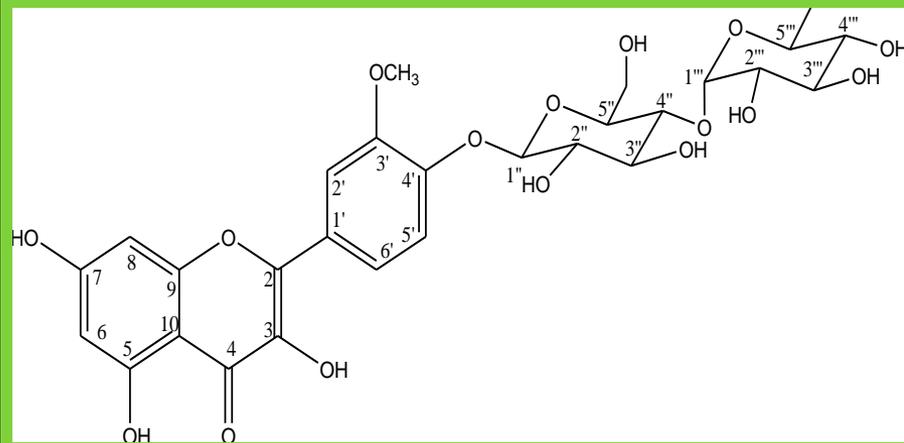
From *B. oleoides*, two compounds were isolated for first time from nature: B-10 and inseparable mixture of two isomeric compound B-11a & B-11b



**B-10-(4'-O-[1'''-4'']- rhamnopyranosyl) - $\beta$ -O-D glucopyranosyl, 3',5' dimethoxyquercetin)**

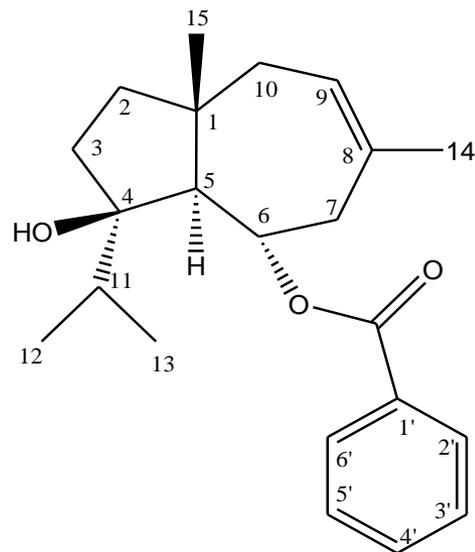


**B-11b (4'-O-[1'''-4'']-rhamnopyranosyl - $\beta$ -O-D-glucopyranosyl-5'-methoxyquercetin)**

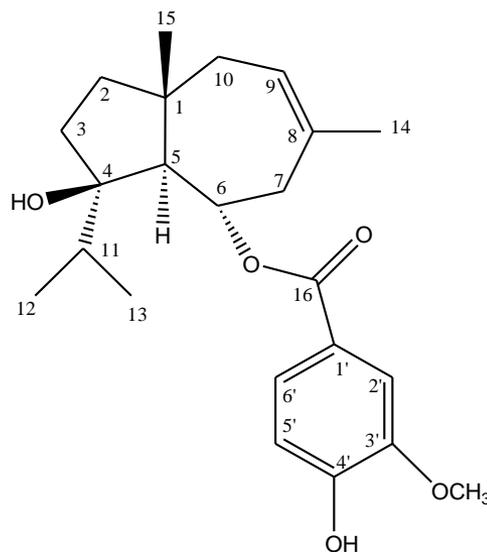


**B-11a (4'-O-[1'''-4'']-rhamnopyranosyl- $\beta$ -O-D-(glucopyranosyl-3'-methoxyquercetin)**

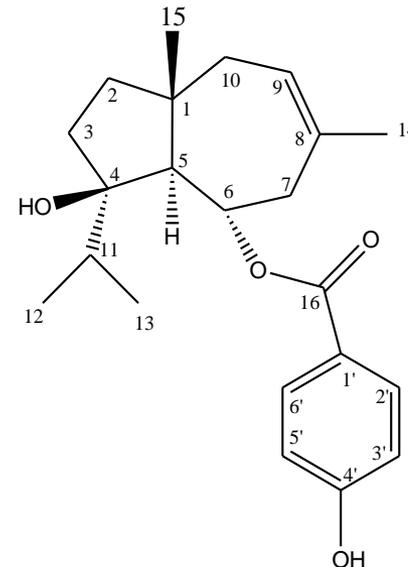
It was the first time to isolate Teferidin, teferin, ferutinin, stearamide and 6*E*,9*E*-*N,N*-dimethyloctadeca-6,9-dieneamide from family solanaceae



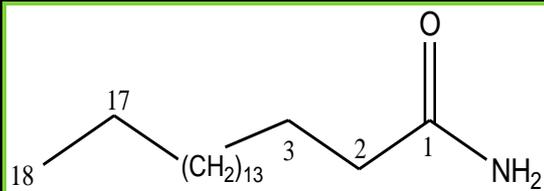
S-5 (Teferidin)



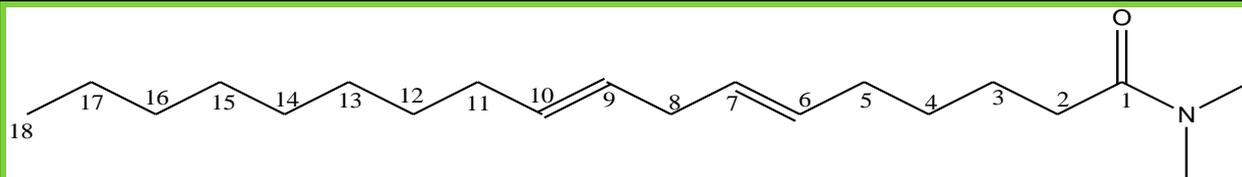
S-6 (Teferin)



S-7 (Ferutinin)

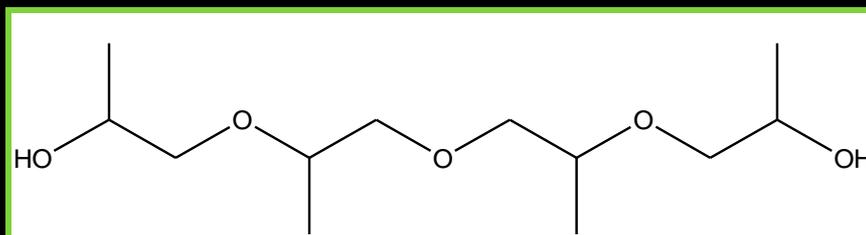


S-14 (Stearamide)

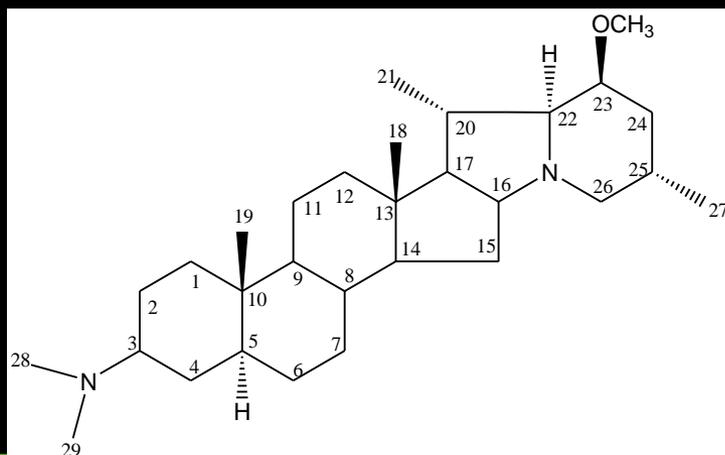


S-15 ( 6*E*,9*E*)-*N,N*-dimethyloctadeca-6,9-dieneamide

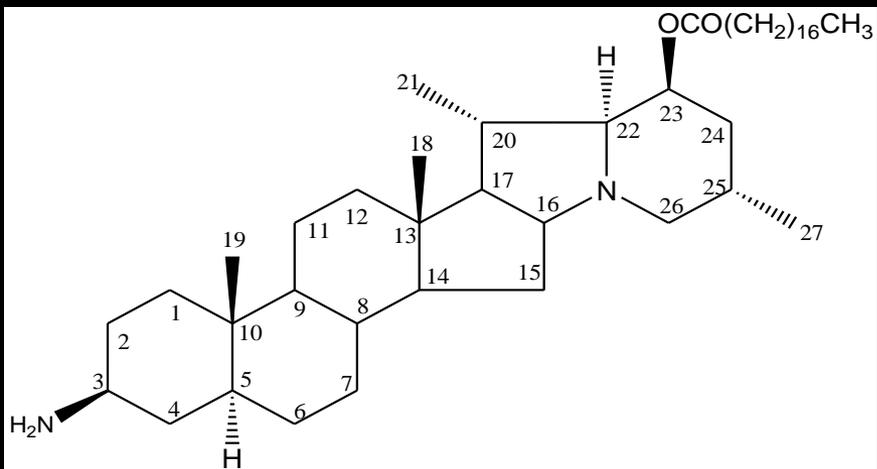
**It was the first time to isolate 1-{1-[2 (2hydroxypropoxy) propoxy] propan-2-yloxy} propan- 2-ol ] from nature**



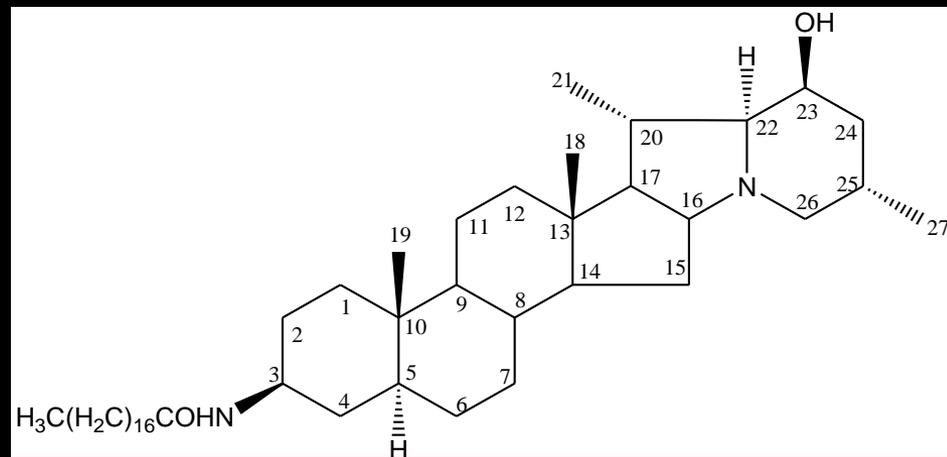
It was the first time to synthesis 3,3-*N,N*-Dimethyl-23-*O*-methylsolanopubamine , 3-*N*-octadecanoate-solanopubamine and 23-*O*-octadecanoate-solanopubamine



S-11b (3,3-*N,N*-Dimethyl-23-*O*-methylsolanopubamine)

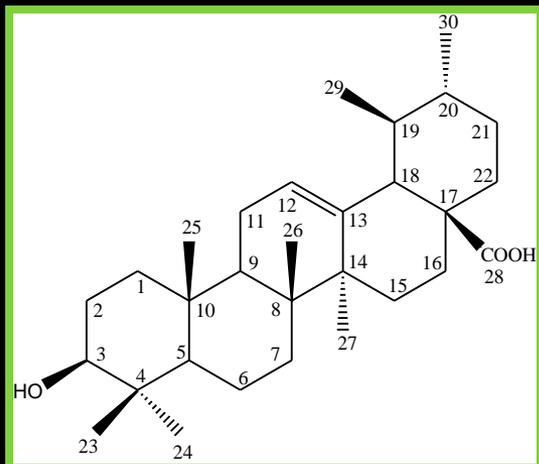


S-11d (23-*O*-octadecanoate-solanopubamine)

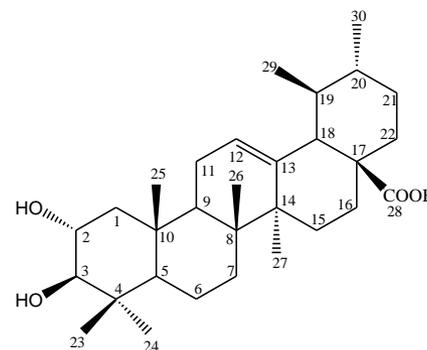


S-11c (3-*N*-octadecanoate-solanopubamine)

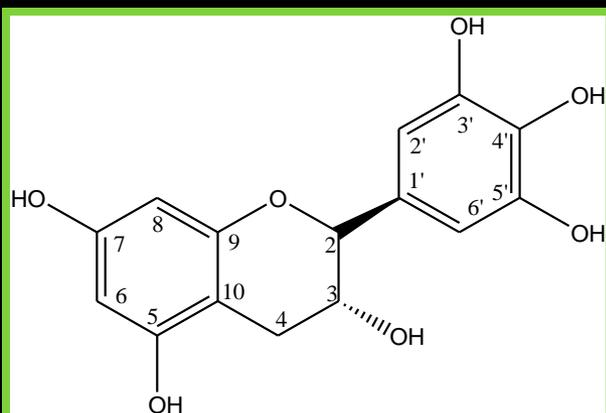
From *B. oleoides*: Ursolic acid (B-2), Corsolic acid (B-3) and galocatechin epimer (B-13 & B-14) showed good antimicrobial activity



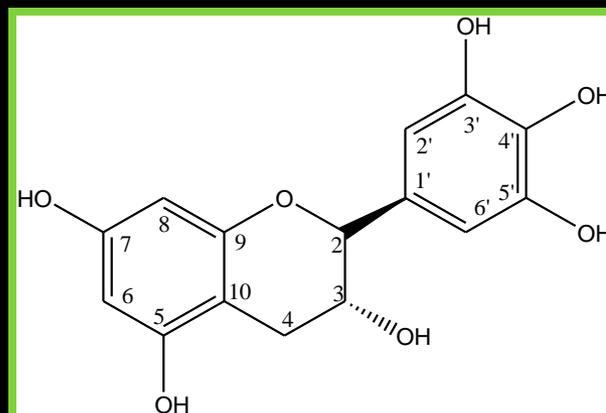
B-2 (Ursolic acid)



B-3 (Corsolic acid)

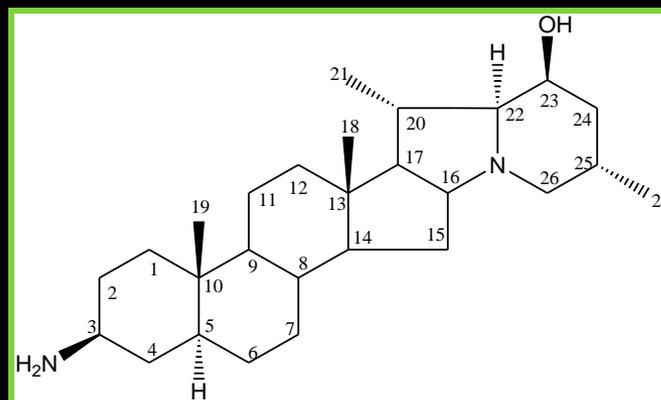


B-14 (Epigallocatechin)

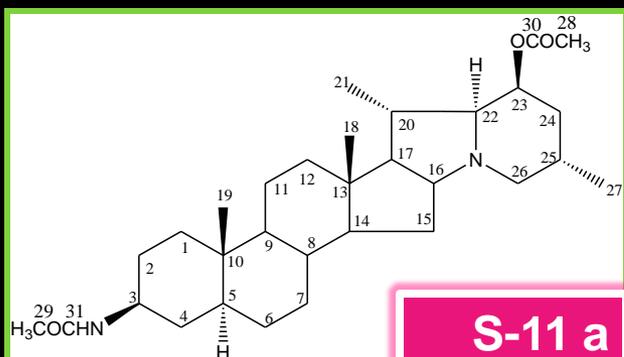


B-13 (Galocatechin)

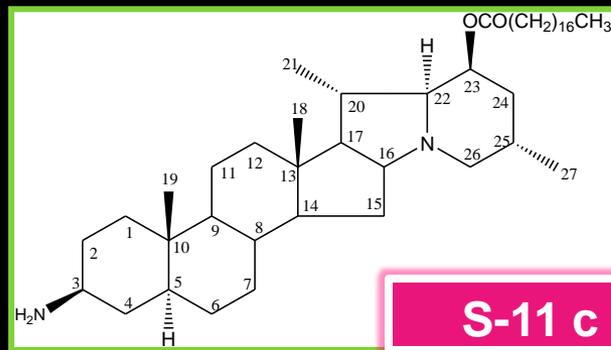
From *S. schimperianum* : S-11 and its synthetic compounds S-11a, S-11c and S-11d showed good antimicrobial activity



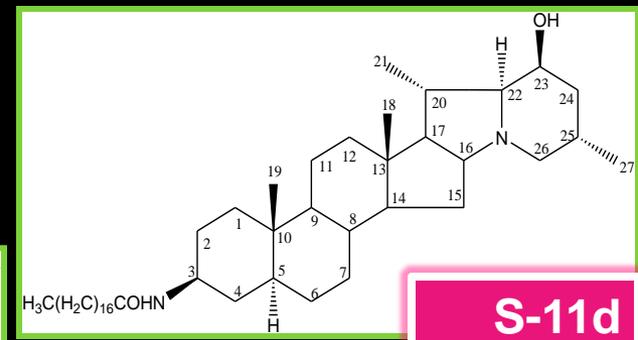
**S-11 (Solanopubamine)**



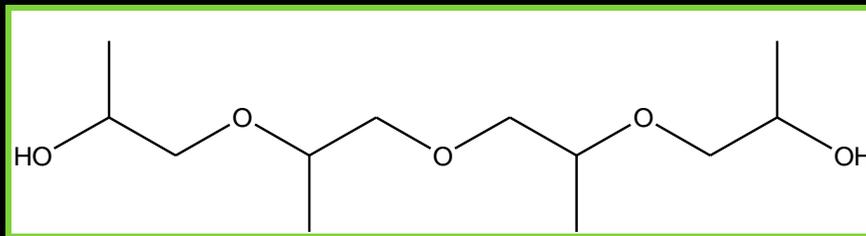
**S-11 a**



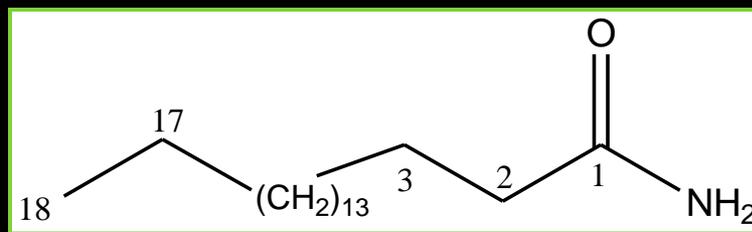
**S-11 c**



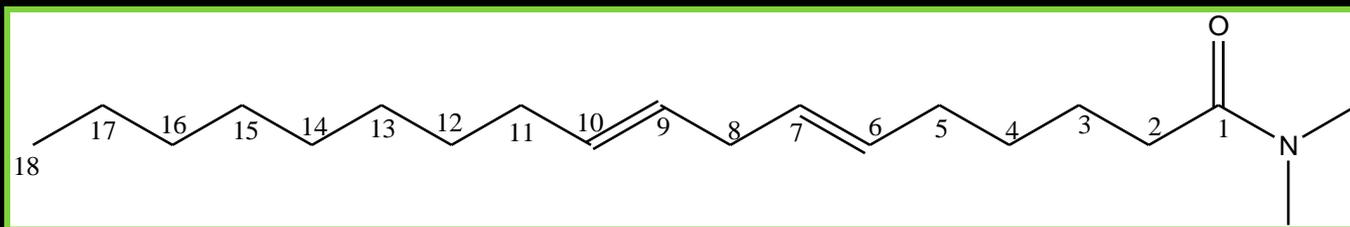
**S-11 d**



**S-13** (1-{1-[2-(2 Hydroxypropoxy) propoxy] propan-2-yloxy} propan-2-ol)

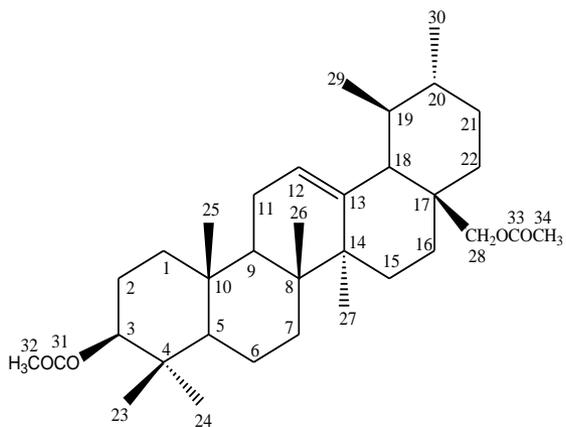


**S-14 (Stearamide)**

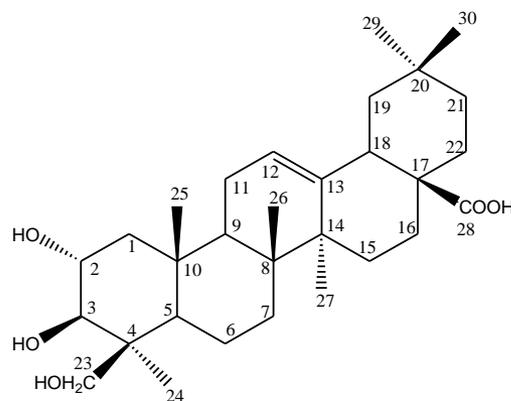


**S-15** ( 6*E*,9*E*)-*N,N*-dimethyloctadeca-6,9-dieneamide

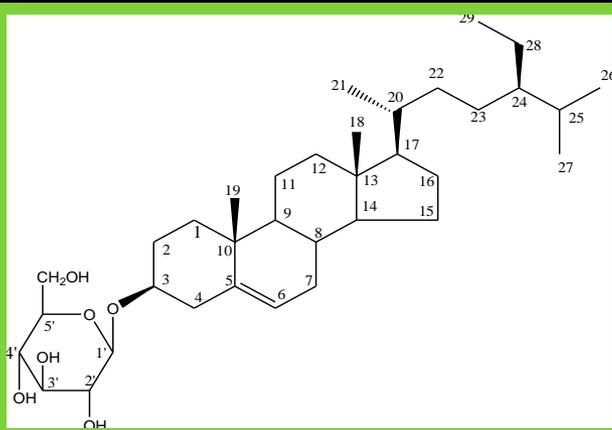
**Isolated compounds : B-1, B-4, B-5 and B-12 from *B. oleoides* showed spasmolytic activity**



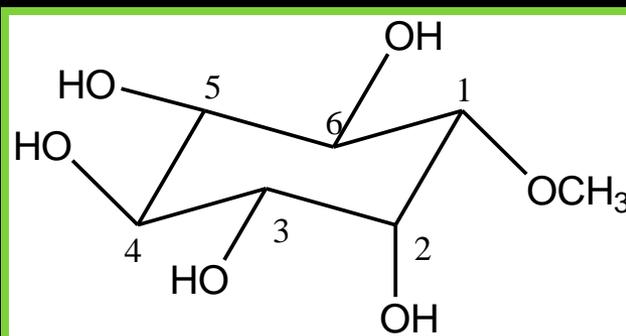
**B-1 (Uvaol diacetate)**



**B-4 (Arjunolic acid)**



**B-5 (β-sitosterol-3-O-β-D-glucoside)**



**B-12 ( D (-) bornesitol)**

**Ethanol extract from *B. oleoides* possess antihypertensive activity**

**Ethyl acetate and butanol extracts from *B. oleoides* showed marked antioxidant activity**



**Thank you**