

Spectroscopic Data
of Steroid Glycosides:
Cardenolides and Pregnanes

Volume 4

Volume 1
SPECTROSCOPIC DATA OF STEROID GLYCOSIDES:
CHOLESTANES, ERGOSTANES, WITHANOLIDES,
STIGMASTANE

Edited by Viqar Uddin Ahmad and Anwer Basha

Volume 2
SPECTROSCOPIC DATA OF STEROID GLYCOSIDES:
STIGMASTANES, FUROSTANES, SPIRTOSTANES

Edited by Viqar Uddin Ahmad and Anwer Basha

Volume 3
SPECTROSCOPIC DATA OF STEROID GLYCOSIDES:
SPIROSTANES, BUFANOLIDES, CARDENOLIDES

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Volume 5
SPECTROSCOPIC DATA OF STEROID GLYCOSIDES:
PREGNANES, ANDROSTANES, AND MISCELLANEOUS

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Volume 6
SPECTROSCOPIC DATA OF STEROID GLYCOSIDES:
MISCELLANEOUS STEROIDS AND INDEXES

Edited by Viqar Uddin Ahmad and Anwer Basha

Spectroscopic Data of Steroid Glycosides: Cardenolides and Pregnanes

Volume 4

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PREFACE

The present volumes reproduce the spectroscopic data of naturally occurring steroidal glycosides as far as they are available in the chemical literature published until the end of 2004. Steroids have the basic skeleton of cyclopentanoperhydrophenanthrene. Generally they do not have methyl groups attached to C-4 and thus differ from triterpenes. Many of the steroidal glycosides, or saponins, have interesting biological activities and constitute the active principles of the natural drugs. The cardiac glycosides (cardenolides) included in the present work act as life-saving medicines in certain ailments.

Not included in this work are the glycosides of steroidal alkaloids. However, the compounds which contain a nitrogen atom in the sugar or in the ester moiety (e.g. nicotinoyl moiety) are included.

The steroidal glycosides are arranged according to the class of their aglycones (steroidal parts). Within each class increasing molecular weight is taken as the basis for this arrangement. If the compounds of the same class have the same molecular weight, then the glycosides with lesser number of carbon atoms come earlier than those with more carbon atoms. Finally, if all these factors are the same, then the compounds are arranged in alphabetical order.

The chemical shifts in the proton nuclear magnetic resonance (PMR) spectral data are arranged according to the increasing δ (ppm) values. Each signal represents one proton unless indicated otherwise. The small alphabets used as superscript in PMR and ^{13}C -NMR (CMR)-spectral data mean that the assignments are ambiguous and may be reversed with signals having the same superscripts. The signals masked by solvent peaks or by other signals of the compound are marked by an asterisk.

Compounds can be easily located in this book with the help of the four indexes at the end of the last volume. The trivial names of the compounds given by the original authors are used as the heading of the compound. If no trivial name has been given, then the name of the plant from which the glycoside has been isolated followed by the word "saponin" or "glycoside" and then the numerical order are used as the main heading. For the subheading, the name of the aglycone (trivial names if available) followed by names of the sugars are used with clear indication of glycosidic linkages and branching of the sugar chain if present.

I am very grateful to Ms. Judy Watson of Chemical Abstract Service who has helped me greatly in finding the registry numbers of several compounds. This work would not have been possible without the help of literature surveyors Dr. Akbar Ali, Dr. Hidayat M. Khan, Dr. M. Athar Abbasi, Mr. Touseef Ali Khan, Mr. Umair Quyyum Khan, Miss. Humera Zaheer, Miss. Rukhsana Kausor, Miss Husna Qamar, Miss. Fouzia Shamim,

Ms. Zeenat Siddiqui, Muhammad Zubair, Afsar Khan, and Shazia Yasmeen to whom my sincere thanks are due. The whole book has been typed, composed, and structures drawn by Mr. Rafat Ali, Mr. Shabbir Ahmed, and Tariq Ilyas and I wish to express my sincere thanks to them.

ABBREVIATIONS

Aco	Acofrose
Afr	Acrofriose
Agl	Aglycone
All	Allose
Alt	Altrose
Ang	Angeloyl
Ant	Antirose
Ara	Arabinose
Boi	Boivinosé
Ben	Benzoyl
Can	Canarose
Cin	Cinnamoyl
CMR	¹³ C-Nuclear Magnetic Resonance
Cym	Cymarose
DAC	4-Deoxy-4-aminocymarose
DMC	4-Deoxy-4-methylaminocymarose
Dal	6-Deoxyallose
Ddg	Dideoxygulopyranoside
Def	2-Deoxyfucose
Dex	6-Deoxy-D-glycero-L-threo-4-hexosulose
DHMP	2,3-Dihydroxy-3-methylpentanoyl
DMB	Dimethoxybenzoyl
DMC	4-Deoxy-4-methylaminocymarose
Dil	Digitalose
Din	Diginose
Dix	Digitoxose
Dma	Deoxymethylallose
DMP	3,4-Dimethyl-2(<i>E</i>)-pentenoyl
DMX	Dimethylxylose
EI	Electron ionization
ESI	Electro-spray ionization
F	Furanosyl
FAB	Fast Atom Bombardment
FD	Field desorption
Fuc	Fucose
Gal	Galactose

Glc	Glucose
Glum	6-Deoxy- α -L-glucopyranoside
Gum	Gulomethylose
HMB	Hydroxymethoxybenzoyl
HMG	Hydroxymethylglutaroyl
HR	High resolution
Ike	Ikemoyl (3,4-dimethyl-2-pentenoyl)
LD	Laser Desorption
Meb	2-Methylbutanoyl
MeXyl	Methylxylose
MGI	Methylglucose
Neg	Negative
Nic	Nicotinoyl
Ole	Oleandrose
Oli	Olivose
PMB	<i>Para</i> -methoxybenzoyl
Pos	Positive
PMR	Proton Magnetic Resonance
Qui	Quinovose
Rha	Rhamnose
Sar	Sarmentose
Tam	Talomethylose
Tar	Triacetylalabinose
The	Thevetose
TMB	Trimethoxybenzoyl
TOF	Time of flight
Xyl	Xylose

CONTENTS

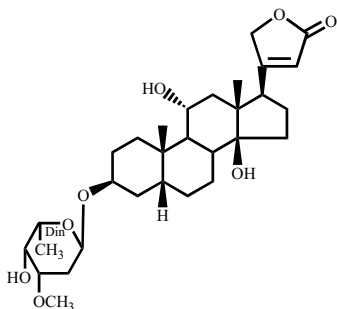
Cholestane	1-394
Ergostane	395-522
Withanolides	523-565
Stigmastane	566-725
Furostane	726-1158
Spirostane	1159-1916
Bufanolide	1917-2027
Cardenolide	2028-2759
Pregnane	2760-3737
Androstane	3738-3742
Misc.	3743

Indexes

Compound Index	3744-3829
Plant Source Index	3830-3864
Registry Number Index	3865-3976
Molecular Formula Index	3977-4176

DIVOSTROSIDE

Sarmentogenin 3-O- α -L-diginopyranoside



Source : *Strophanthus divaricatus* (Lour.) Hook. et Arn.^{1,2}
(Apocynaceae), *S. divaricatus* calli³

Mol. Formula : C₃₀H₄₆O₈

Mol. Wt. : 534

M.P. : 195-199°C²

[α]_D²² : -54.5° (c=0.56, MeOH)²

Registry No. : [76704-78-4]

PMR (CDCl₃, 400 MHz)² : δ 0.88 (s, 3xH-18)^a, 1.05 (s, 3xH-19)^a, 1.24 (d, $J=6.0$ Hz, 3xH-6 of Din), 3.39 (s, OCH₃ of Din), 4.74 (dd, $J=18.0, 1.0$ Hz, H-21A), 4.97 (s, H-1 of Din), 5.00 (dd, $J=18.0, 1.0$ Hz, H-21B), 5.84 (t, $J=1.0$ Hz, H-22).

PMR (C₅D₅N, 300 MHz)³ : δ 1.00 (s, 3xH-18), 1.10 (s, 3xH-19), 1.39 (d, $J=6.0$ Hz, 3xH-6 of Din), 2.29 (dd, $J=12.0, 3.5$ Hz, H-2A of Din), 2.85 (dd, $J=9.0, 5.0$ Hz, H-17 α), 3.22 (s, OCH₃ of Din), 3.80 (ddd, $J=12.0, 5.0, 3.0$ Hz, H-3 of Din), 4.04 (br s, H-3), 4.92 (dd, $J=18.0, 1.5$ Hz, H-21A), 5.13 (br d, $J=3.0$ Hz, H-1 of Din), 5.19 (dd, $J=18.0, 1.5$ Hz, H-21B), 6.00 (br s, H-22).

CMR (C₅D₅N, 100 MHz)² : δ C-1) 33.9^a (2) 28.2 (3) 72.5 (4) 31.1 (5) 38.9 (6) 27.3^b (7) 22.3 (8) 42.3 (9) 41.4 (10) 37.1 (11) 67.7^c (12) 50.6 (13) 50.3 (14) 84.3 (15) 33.7^a (16) 27.8^b (17) 51.3 (18) 17.7 (19) 24.5 (20) 175.4 (21) 73.8 (22) 117.7 (23) 174.5 **Din** (1) 96.4 (2) 31.4 (3) 76.0 (4) 67.1 (5) 67.8^c (6) 17.7 (OCH₃) 55.0.

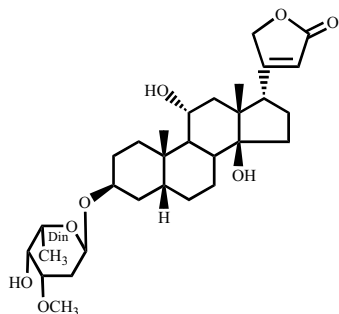
Mass (FAB, Positive ion)³ : m/z 557 [M+Na]⁺.

Mass (F.D.)² : m/z 535 [M+H]⁺, 490, 389, 145.

References

1. O. Renkonen, O. Schindler and T. Reichstein, *Helv. Chim. Acta*, **42**, 160, 182 (1959).
2. R.F. Chen, F. Abe, T. Yamauchi and M. Taki, *Phytochemistry*, **26**, 2351 (1987).
3. K. Kawaguchi, I. Asaka, M. Hirotoni, T. Furuya and S. Katsuki, *Phytochemistry*, **34**, 1317 (1993).

17 β H-DIVOSTROSIDE
17 β H-Sarmentogenin-3-O- α -L-diginopyranoside



Source : Tissue cultures plants from *Strophanthus divaricatus* calli (Lour.) Hook. et Arn. (Apocynaceae)

Mol. Formula : C₃₀H₄₆O₈

Mol. Wt. : 534

[α]_D²³ : -50.9° (c=0.53, MeOH)

Registry No. : [152323-38-1]

PMR (C₅D₅N, 300 MHz) : δ 1.15 (s, 3xH-18 and 3xH-19), 1.40 (d, J =6.0 Hz, 3xH-6 of Din), 2.30 (dd, J =12.0, 3.5 Hz, H-2A of Din), 3.22 (OCH₃ of Din), 3.27 (dd, J =9.5, 9.5 Hz, H-17 β), 3.80 (ddd, J =12.0, 5.0, 3.0 Hz, H-3 of Din), 3.98 (m, H-11 β), 4.07 (br s, H-3 α), 4.66 (dd, J =17.5, 1.5 Hz, H-21A), 4.81 (dd, J =17.5, 1.5 Hz, H-21B), 5.15 (br d, J =3.0 Hz, H-1 of Dig), 5.96 (br d, J =1.5 Hz, H-22).

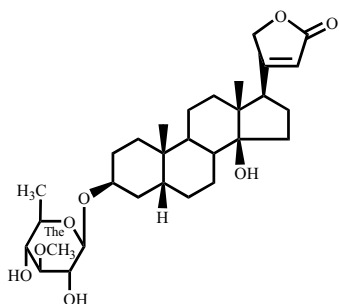
CMR (C₅D₅N, 75 MHz) : δ 34.3 (2) 28.4 (3) 72.7 (4) 31.3 (5) 39.2 (6) 27.8 (7) 22.0 (8) 42.8 (9) 41.3 (10) 37.2 (11) 67.8 (12) 42.6 (13) 50.0 (14) 84.9 (15) 32.0 (16) 25.1 (17) 49.3 (18) 19.8 (19) 24.6 (20) 172.7 (21) 74.2 (22) 116.8 (23) 174.7 **Din** (1) 96.7 (2) 31.5 (3) 76.2 (4) 67.3 (5) 67.9 (6) 17.8 (OCH₃) 55.0.

Mass (FAB-MS) : m/z 557 [M+Na]⁺.

Reference

1. K. Kawaguchi, I. Asaka, M. Hirotsani, T. Furuya and S. Katsuki, *Phytochemistry*, **34**, 1317 (1993).

HONGKELIN, HONGHELIN
Digitoxigenin 3-O- β -D-thevetopyranoside



Source : *Adenium honghel* A. DC.¹ (Apocynaceae),

Adenium obesum Fosk.² (Apocynaceae)

Mol. Formula : C₃₀H₄₆O₈

Mol. Wt. : 534

M.P. : 130-135°C¹

[α]_D²⁶ : -10.3° (MeOH)¹

Registry No. : [560-67-8]

UV² : 220 (log ϵ , 4.25) nm.

IR² : 1780, 1740, 1620 cm⁻¹.

PMR (CDCl₃, 60 MHz)² : δ 0.87 (s, CH₃), 0.93 (s, CH₃), 3.60 (s, OCH₃), 4.00 (1H), 4.90 (2H), 5.83 (1H).

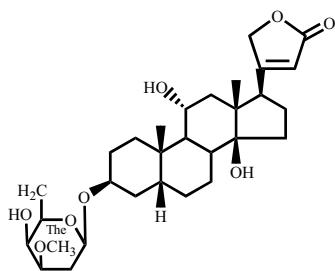
Mass (E.I.)² : m/z 534 [M]⁺, 357, 339, 203.

References

1. K. Reyle and T. Reichstein, *Helv. Chim. Acta*, **35**, 195 (1952).
2. J.J. Hoffmann, J.R. Cole, *J. Pharm. Sci.*, **66**, 1336 (1977).

KWANGOSIDE

Sarmentogenin 3-O- β -D-diginopyranoside



Source : *Strophanthus amboensis* (Schinz) Engl. et Pax.¹,

S. vanderijstii Staner.² (Apocynaceae)

Mol. Formula : C₃₀H₄₆O₈

Mol. Wt. : 534

M.P. : 212-217°C²

[α]_D¹⁹ : -9.4° ± 1.5° (c=0.163, CHCl₃)²

UV (EtOH)² : λ_{max} 217 (log ϵ , 4.23) nm..

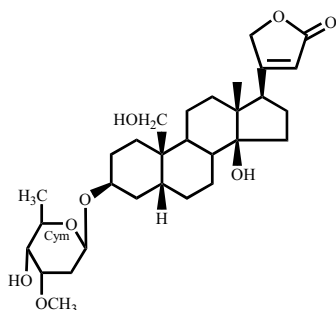
Biological Activity : Lethal dose 0.3276 ± 0.0249 mg/kg in cats.¹

References

1. O. Schindler, *Helv. Chim. Acta*, **39**, 64 (1956).
2. H. Lichti, C. Tamm and T. Reichstein, *Helv. Chim. Acta*, **39**, 1933 (1956).

MAQUIROSIDE A

Cannogenol 3-O- β -D-cymaroside



Source : *Maquira calophylla* (P&E) C.C. Berg.
(Moraceae)

Mol. Formula : C₃₀H₄₆O₈

Mol. Wt. : 534

M.P. : 123-125°C

[α]_D²⁵ : +17.9° (c=0.07, CHCl₃)

Registry No. : [110187-24-1]

UV (EtOH) : λ_{\max} 218 (ϵ , 5628), 290 (ϵ , 239) nm.

IR (CHCl₃) : 3568, 3322, 2933, 2870, 1740, 1615, 1448, 1085 cm⁻¹.

PMR (CDCl₃, 360 MHz) : δ 0.87 (s, 3xH-18), 1.23 (d, $J=6.0$ Hz, 3xH-6 of Cym), 1.30-2.00 (m, ~25H), 2.07 (m, H-2 of Cym), 2.76 (m, H-17), 3.22 (dd, $J=3.4, 9.0$ Hz, H-4 of Cym), 3.43 (s, OCH₃), 3.50 (m, H-5 of Cym), 3.64 (m, H-3 of Cym), 3.54 and 3.80 (ABq, $J=11.0$ Hz, 2xH-19), 4.02 (br s, H-3), 4.72 (dd, $J=1.5, 9.0$ Hz, H-1 of Cym), 4.89 (ABq, $J_{AB}=6.0$ Hz, $J_{21,22}=1.5$ Hz, 2xH-21), 5.88 (s, H-22).

CMR (C₅D₅N, 22.5 MHz) : δ C-1) 30.8 (2) 27.2 (3) 71.0 (4) 30.8 (5) 35.9 (6) 27.2 (7) 24.8 (8) 42.0 (9) 30.0 (10) 39.9 (11) 21.9 (12) 40.5 (13) 50.2 (14) 84.9 (15) 33.0 (16) 27.4 (17) 51.6 (18) 16.3 (19) 65.5 (20) 175.9 (21) 73.7 (22) 117.7 (23) 174.5 Cym (1) 96.6 (2) 36.2 (3) 79.0 (4) 74.3 (5) 73.2 (6) 19.1 (OCH₃) 58.0.

Mass (C.I., Isobutane, H.R.) : m/z 535.3353 [(M+Na), calcd. for 535.3271].

Mass (C.I.) : m/z (rel.intens.) 535 [M⁺ + H, 2.3%], 391 (21.6), 389 (2.6), 373 (24.2), 355 (44.95), 219 (12.3), 179 (3.9), 165 (1.7), 162 (1.1), 147 (14.7), 145 (100), 144 (6.0), 117 (10), 111 (20.2), 100 (2.9), 87 (87.2), 86 (3.2), 74 (37.9).

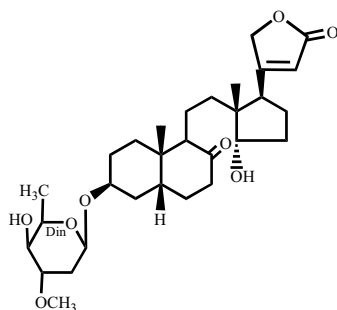
Biological Activity : Maquiroside exhibited activity against the KB cell culture system with an ED₅₀=0.013 μ g/ml.

Reference

1. J.M. Rovinski, G.L. Tewalt and A.T. Sneden, *J. Nat. Prod.*, **50**, 211 (1987).

NERIASIDE

Neriagenin 3-O- β -D-diginopyranoside



Source : *Nerium odorum* Soland.(Apocynaceae)

Mol. Formula : C₃₀H₄₆O₈

Mol. Wt. : 534

[α]_D²⁵ : -17.6°

Registry No. : [68165-55-9]

UV (MeOH) : λ_{\max} 217 nm.

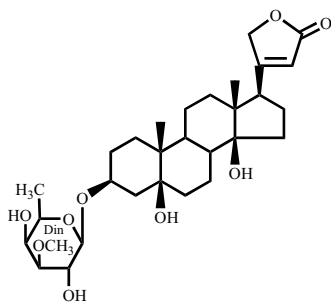
PMR : δ 0.76 (s, 3xH-18), 0.80 (s, 3xH-19), 1.34 (d, $J=6.0$ Hz, 3xH-6 of Din), 2.91 (dd, $J=9.0, 9.0$ Hz, H-17), 3.44 (s, OCH₃ of Din), 3.76 (d, $J=3.0$ Hz, H-4 of Din), 4.15-4.35 (2H), 4.58 (dd, $J=4.0, 9.0$ Hz, H-1 of Din), 4.82 (s, 2xH-21), 5.98 (s, H-22).

Reference

1. T. Yamauchi and F. Abe, *Tetrahedron Lett.*, 1825 (1978).

NERIDIGINOSIDE

3 β ,5 β ,14 β -Trihydroxy-card-20(22)-enolide 3-O- β -D-diginyopyranoside



Source : *Nerium oleander* Linn. (Apocynaceae)

Mol. Formula : C₃₀H₄₆O₈

Mol. Wt. : 534

M.P. : 195.8-196.5°C

[α]_D²⁶ : +38.31° (c=0.522, CHCl₃)

Registry No. : [221380-14-9]

UV (MeOH) : λ_{\max} 219 nm.

IR (CHCl₃) : 3450, 1780 and 1740 cm⁻¹.

PMR (CDCl₃, 500 MHz) : δ 1.00 (s, 3xH-18), 1.05 (s, 3xH-19), 1.10 (dddd, $J=14.0, 3.0, 3.0, 3.0$ Hz, H-11A), 1.32 (d, $J=6.5$ Hz, 3xH-6 of Din), 1.38 (m, H-7A), 1.38 (ddd, $J=11.5, 11.0, 4.5$ Hz, H-12A), 1.42 (m, H-1A), 1.48 (m, H-15A), 1.51 (m, H-2A), 1.51 (m, H-7B), 1.57 (ddd, $J=11.5, 4.5, 3.0$ Hz, H-12B), 1.60 (dd, $J=10.0, 5.0$ Hz, H-4A), 1.61 (m, H-2B), 1.62 (ddd, $J=14.5, 6.5, 3.0$ Hz, H-15B), 1.68 (ddd, $J=12.5, 12.0, 9.5$ Hz, H-2A of Din), 1.70 (m, H-6A), 1.74 (m, H-16A), 1.76 (m, H-9), 1.79 (m, H-8), 1.82 (m, H-1B), 1.94 (ddd, $J=12.5, 5.0, 2.0$ Hz, H-2B of Din), 1.95 (m, H-6B), 2.10 (m, H-11B), 2.15 (dd, $J=10.0, 4.5$ Hz, H-4B), 2.15 (m, H-16B), 2.74 (dd, $J=9.5, 6.0$ Hz, H-17), 3.33 (ddd, $J=12.0, 5.0, 3.5$ Hz, H-3 of Din), 3.38 (s, OCH₃ of Din), 3.40 (dq, $J=6.5, 3.5$ Hz, H-5 of Din), 3.67 (br t, $J=3.5$ Hz, H-4 of Din), 4.05 (br s, $W_{1/2}=7.0$ Hz, H-3), 4.44 (dd, $J=9.5, 2.0$ Hz, H-1 of Din), 4.80 (dd, $J=18.0, 1.5$ Hz, H-21A), 4.98 (dd, $J=18.0, 1.5$ Hz, H-21B), 5.85 (t, $J=1.5$ Hz, H-22).

CMR (CDCl₃, 125 MHz) : δ C-1) 26.89 (2) 27.01 (3) 72.20 (4) 35.03 (5) 74.50 (6) 32.04 (7) 17.60 (8) 36.94 (9) 35.54 (10) 35.19 (11) 22.47 (12) 40.38 (13) 50.42 (14) 85.90 (15) 29.86 (16) 27.38 (17) 51.84 (18) 18.42 (19) 25.36 (20) 174.30 (21) 73.37 (22) 117.90 (23) 174.20 **Din** (1) 97.80 (2) 31.71 (3) 78.03 (4) 67.19 (5) 70.40 (6) 16.80 (OCH₃) 55.73.

Mass (H.R.) : m/z 390.2410 [C₂₃H₃₄O₅], 373.2318 [C₂₃H₃₃O₄], [C₂₃H₃₁O₃], 337.2108 [C₂₃H₂₉O₂], 208.1161 [C₁₂H₁₆O₃], 181.0882 [C₁₀H₁₃O₃], 161.0850 [C₇H₁₃O₄], 145.0901 [C₇H₁₃O₃].

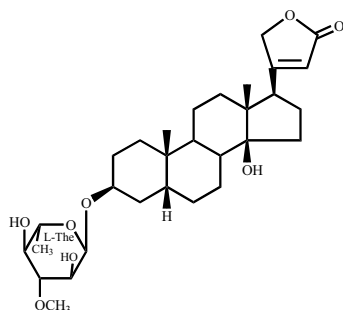
Biological Activity : The compound showed sedation in mice at 25 mg/kg dose.

Reference

1. S. Begum, B.S. Siddiqui, R. Sultana, A. Zia and A. Suria, *Phytochemistry*, **50**, 435 (1999).

NERIIFOLIN

Digitoxigenin 3-O- α -L-thevetopyranoside



Source : *Thevetia neriifolia* Juss. ex Steud.¹, *T. peruviana* Pers. Schum.² (Apocynaceae), *T. thevetodes*³, *T. ahouai* (L.) A. DC.⁴, *Cerbera odollam* Gaertn.⁵ (Apocynaceae), *C. manghas* L.⁶

Mol. Formula : C₃₀H₄₆O₈

Mol. Wt. : 534

M.P. : 218-225°C¹

[α]_D : -50.2° (MeOH)¹

Registry No. : [466-07-9]

PMR (CDCl₃, 60/250 MHz)⁷ : δ 0.88 (s, 3xH-18), 0.97 (s, 3xH-19), 1.26 (d, $J=6.3$ Hz, 3xH-6 of The), 2.0-2.25 (m, 2xH-16), 2.78 (dd, $J=8.8, 5.0$ Hz, H-17), 3.15 (t, $J=9.0$ Hz, H-4 of The), 3.25 (t, $J=8.9$ Hz, H-3 of The), 3.58 (dd, $J=8.9, 4.4$ Hz, H-2 of The), 3.69 (s, OCH₃), 3.74 (dq, $J=9.0, 6.3$ Hz, H-5 of The), 3.97 (m, H-3), 4.82 (dd, $J=18.0, 1.5$ Hz, H-21A), 4.86 (d, $J=4.4$ Hz, H-1 of The), 4.98 (dd, $J=18.0, 1.5$ Hz, H-21B), 5.88 (t, $J=1.5$ Hz, H-22).

CMR (CDCl₃, 22.63 MHz)⁷ : δ C-1) 30.6^a (2) 26.5^a (3) 73.3 (4) 30.0^a (5) 36.9 (6) 26.5^a (7) 21.2^b (8) 41.8 (9) 35.9 (10) 35.3 (11) 21.4^b (12) 40.0 (13) 50.3 (14) 85.5 (15) 33.2 (16) 26.9 (17) 50.9 (18) 15.8 (19) 23.9 (20) 174.6 (21) 73.4 (22) 117.8 (23) 174.6 **The** (1) 97.2 (2) 73.0 (3) 84.7 (4) 74.7 (5) 67.5 (6) 17.5 (OCH₃) 60.6.

Mass (E.I.)⁹ : m/z 534 [M]⁺, 516 [M-H₂O]⁺, 502, 484, 459, 440, 430, 417, 403, 385, 375 [Agl+H], 353, 339, 323, 257, 246, 231, 229, 217, 213, 203, 165, 177, 163, 147, 145, 128, 121, 105, 87, 85, 74.

Mass (F.I.) : m/z 534 [M]⁺, 516 [M-H₂O]⁺, 375 [Agl+H], 373 [Agl-H]⁺, 357, 339, 317, 299, 179, 169, 161, (sugar), 143.

2'-O-Acetate :

PMR (C_5D_5N , 400 MHz)⁸ : δ 0.83 (s, 3xH-18)^a, 1.02 (s, H-19)^a, 1.61 (d, $J=6.0$ Hz, H-6 of The), 2.80 (dd, $J=9.0$, 6.0 Hz, H-17), 3.66 (t, $J=9.0$ Hz, H-4 of The), 3.84 (OCH₃ of The), 4.00 (t, $J=9.0$ Hz, H-3 of The), 4.08 (dd, $J=4.0$, 9.0 Hz, H-2 of The), 4.18 (br s, H-3 α), 4.31 (m, H-5 of The), 5.03 (H-21A), 5.24 (d, $J=4.0$ Hz, H-5 of The), 5.31 (dd, $J=18.0$, 1.0 Hz, H-21B), 6.13 (br s, H-22).

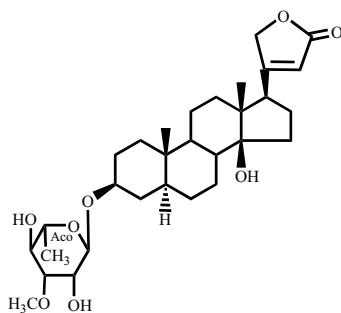
CMR (C_5D_5N , 100 MHz)⁸ : δ C-1) 30.3 (2) 26.9^a (3) 73.7 (4) 31.0 (5) 36.8 (6) 27.1^a (7) 21.5^b (8) 41.9 (9) 35.8 (10) 35.5 (11) 21.9^b (12) 39.8 (13) 50.1 (14) 84.6 (15) 33.2 (16) 27.1^a (17) 51.5 (18) 16.2 (19) 23.8 (20) 175.9 (21) 73.6 (22) 117.6 (23) 174.4 **The** (1) 98.9 (2) 73.4 (3) 85.4 (4) 76.6 (5) 68.9 (6) 18.5 (OCH₃) 60.5.

Biological Activity : Increase muscle tone and abolishes peristaltic motion of guinea pig ileum,¹⁰ cardiotoxic,¹¹ insecticidal,³ cytotoxic,³ strong inotropic activity.¹²

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NERIIFOSIDE

3 β ,14 β -Dihydroxy-5 α -carda-20:22-enolide 3-O- α -L-acofrioside**Source :** *Thevetia neriiifolia* Juss. (Apocynaceae)**Mol. Formula :** C₃₀H₄₆O₈**Mol. Wt. :** 534**M.P. :** 210-212°C**Registry No. :** [145921-45-5]**UV** (MeOH) : λ_{\max} 217 nm.**IR** (CHCl₃) : 3400, 2900-2850, 1780, 1740, 1600, 1120, 1020 cm⁻¹.

PMR (CDCl₃, 400 MHz) : δ 0.80 (s, 3xH-19), 0.87 (s, 3xH-18), 1.16 (m, H-5), 1.29 (d, $J=6.21$ Hz, H-6 of Aco), 1.36 (m, 3xH-12), 1.38 (m, H-2A), 1.39 (m, H-12B), 1.51 (m, H-11A), 1.52 (m, H-8), 1.55 (m, H-11B), 1.64 (m, 2xH-4), 1.70 (m, H-1A), 1.75 (m, H-1B), 1.77 (m, H-2B), 1.82 (m, 2xH-6), 2.05 (m, H-15A), 2.07 (m, H-15B), 2.12 (m, H-16A), 2.16 (m, H-16B), 2.16 (m, 2xH-7), 2.75 (dd, $J=9.26, 5.58$ Hz, H-17), 3.38 (dd, $J=9.20, 3.19$ Hz, H-3 of Aco), 3.46 (s, OCH₃), 3.46 (t, $J=9.20$ Hz, H-4 of Aco), 3.76 (dq, $J=9.20, 6.21$ Hz, H-5 of Aco), 3.96 (m, H-3), 3.98 (dd, $J=3.19, 1.69$ Hz, H-2 of Aco), 4.76 (dd, $J=17.99, 1.17$ Hz, H-21A), 4.96 (d, $J=1.69$ Hz, H-1 of Aco), 4.97 (dd, $J=17.99, 1.82$ Hz, H-21B), 5.85 (dd, $J=1.82, 1.17$ Hz, H-22).

CMR (CDCl₃, 75 MHz) : δ C-1) 37.3 (2) 29.1 (3) 71.9 (4) 33.9 (5) 44.3 (6) 28.6 (7) 26.9 (8) 41.8 (9) 49.9 (10) 36.0 (11) 21.2 (12) 40.0 (13) 49.5 (14) 85.5 (15) 33.2 (16) 27.4 (17) 51.0 (18) 15.8 (19) 12.2 (20) 174.2 (21) 73.4 (22) 117.8 (23) 174.2 **Aco** (1) 97.5 (2) 67.6 (3) 81.4 (4) 72.0 (5) 67.7 (6) 17.6 (OCH₃) 57.0.

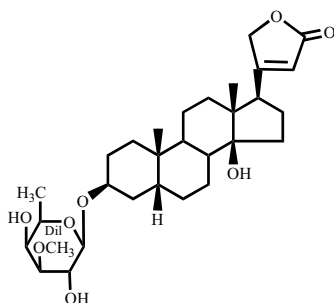
Mass (HRMS) : m/z 374.2429 (C₂₃H₃₄O₄, AgI), 356.2366 (C₂₃H₃₂O₃), 338.2291 (C₂₃H₃₀O₂), 257.1950 (C₁₈H₂₅O), 181.0917 (C₁₀H₁₃O₃), 109.0943 (C₈H₁₃), 84.9795 (C₄H₄O₂), 57.0507 (C₃H₅O), 55.0396 (C₃H₃O).

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ODOROSIDE H

3-O- β -D-digitalopyranoside



Source : *Strophanthus gracilis* K. Sch. et Pax.¹, *S. vanderijstii* Staner.² (Apocynaceae), *Nerium odorum* Soland.³ (Apocynaceae), *Nerium oleander* L.⁴ (Apocynaceae), *Carissa ovata* R.Br. var. *stolonifera* F.M. Bailey⁵, *C. lanceolata* R.Br.⁵ (Apocynaceae), *Digitalis purpurea* L.⁶ (Scrophulariaceae) *Mandevilla pentlandiana* (A.DC.)⁷ (Apocynaceae)

Mol. Formula : C₃₀H₄₆O₈
Mol. Wt. : 534
M.P. : 236-239°C⁴
[α]_D¹⁷ : +8 ± 2° (c=0.9972, MeOH)⁵
Registry No. : [18810-25-8]

UV (MeOH)⁴ : λ_{\max} 217 nm.

IR (KBr)⁴ : 3400 (OH), 2885 (C-H, aliphatic), 1778, 1735 (α,β -unsaturated γ -lactone) and 1670 cm⁻¹.

CMR (CDCl₃, 25 MHz)⁷ : δ C-1) 30.5 (2) 26.8^a (3) 75.0 (4) 30.5 (5) 36.8 (6) 27.1^a (7) 21.7^b (8) 42.0 (9) 36.2 (10) 35.6 (11) 21.9^b (12) 40.4 (13) 50.4 (14) 85.8 (15) 32.7 (16) 27.4 (17) 51.5 (18) 15.8 (19) 23.5 (20) 176.4^c (21) 74.6 (22) 117.0 (23) 177.6^c **Dil** (1) 102.5 (2) 70.8 (3) 84.0 (4) 68.1 (5) 70.6 (6) 16.3 (CH₃) 56.6.

CMR (C₅D₅N, 22.63 MHz)⁸ : δ **Dil** C-1) 103.6 (2) 70.9 (3) 85.1 (4) 68.7 (5) 71.0 (6) 17.4 (OCH₃) 57.2.

Mass (FD)⁹ : m/z (rel.intens.) 535 [(M+H)⁺, 100], 517 [(M+H-H₂O)⁺, 41.7], 375 (Agl, 46.7), 357 (53.0), 161 (Dil, 50.0).

Mass (FAB, Positive ion)⁹ : m/z (rel.intens.) 535 [(M+H)⁺, 20], 517 [(M+H-H₂O)⁺, 9.7], 375 (Agl, 34.0), 357 (39.6), 161 (Dil, 62.3), 129 (100).

Mass (FAB, Negative ion)⁹ : m/z (rel.intens.) 533 [(M-H)⁻, 77.6], 373 [(Agl)⁻, 21.5], 355 [(Agl-H₂O)⁻, 13.1].

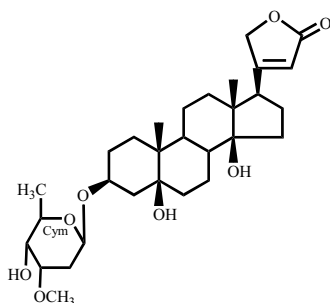
Biological Activity : Causes sedation in mice at a dose of 25 mg/kg.⁴

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PERIPLOCYMARIN
Periplogenin 3-O-[β -D-cymaropyranoside]



Source : *Periploca graeca* L.¹ (Asclepiadaceae), *Strophanthus nicholsonii* Holm² (Apocynaceae), *S. hypoleucus* Stapf.³, *S. eminii* Asch. et Pax.⁴, *S. mirabilis* Gilg.⁵, *S. preussi* Engl. et Pax.⁶, *S. ledienii* Stein.⁷, *S. hispidus* P. DC.⁸, *S. kombe* Oliv.⁹, *Pentopetia androsaemifolia* Decne¹⁰ (Periplocaceae), *Castilla elastica* Cerv.¹¹ (Moraceae), *Periploca sepium* Bge.¹² (Asclepiadaceae)

Mol. Formula : C₃₀H₄₆O₈

Mol. Wt. : 534

M.P. : 138-145°C (methanol-ether)²;
210-212°C (acetone)

[α]_D¹⁶ : 28.8 \pm 2° (MeOH)³

Registry No. : [32476-67-8]

CMR (C₅D₅N, 100.6 MHz)¹² : δ C-1) 25.44 (2) 26.22 (3) 75.34 (4) 34.23 (5) 73.53 (6) 33.91 (7) 23.67 (8) 40.96 (9) 40.16 (10) 40.78 (11) 21.62 (12) 39.25 (13) 49.48 (14) 85.60 (15) 33.10 (16) 26.88 (17) 50.74 (18) 15.72 (19) 16.78 (20) 174.25 (21) 73.41 (22) 117.85 (23) 174.20 **Cym** (1) 96.49 (2) 34.69 (3) 77.30 (4) 72.36 (5) 71.00 (6) 18.23 (OCH₃) 57.38.

Mass (S.I.)¹² : m/z 535 [M+H]⁺.

Biological Activity : Highly toxic, LD₅₀ 0.154 mg/kg in cats.

Acetate : Constituent of *Strophanthus kombe* Oliv.¹³ (Apocynaceae)

Mol. Formula : C₃₂H₄₈O₉; **Mol. Wt. :** 576; **M.P. :** 129-137°C¹³; **[α]_D¹³ :** 46.1 \pm 5° (c=0.477, CHCl₃)¹³

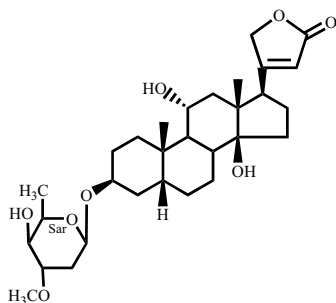
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SARMENTOCYMARIN

Sarmentogenin 3-O- β -D-sarmentopyranoside



Source : Seeds of *Strophanthus sarmentosus* P.DC.¹, *S. hispidus* P.DC.², *S. gerrardi* Stapf.³, *S. courmontii* Sacl.⁴, *S. petersianus* Klotzch, *S. grandiflorus* N.E.Br. Gilg., *Strophanthus* sp. var. *sarmentogenifera*⁵, *S. vanderijstii* Staner.⁷ (Apocynaceae), *Cryptolepis buchanani* Roem. et Schult.⁸ (Asclepiadaceae)

Mol. Formula : C₃₀H₄₆O₈
Mol. Wt. : 534
M.P. : 129-132°C (dehydrate)⁵, 206-208°C⁵
[α]_D²⁵ : -13.2° \pm 1° (c=2.0387, MeOH)⁵
Registry No. : [98633-61-5]

UV (EtOH)⁷ : λ_{\max} 218 (log ϵ , 4.22) nm.

CMR (C₅D₅N, 22.63 MHz)⁹ : δ Sar C-1) 97.3 (2) 33.6 (3) 80.3 (4) 67.9 (5) 69.9 (6) 17.5 (OCH₃) 56.7.

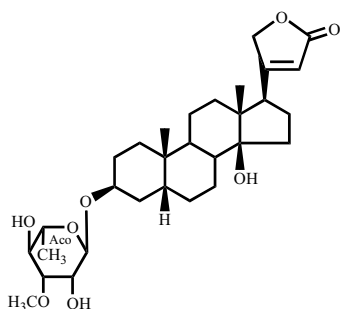
Biological Activity : Toxic, LD₅₀ 0.202 mg/kg in cats.⁹

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SOLANOSIDE, 3'-O-METHYLEVOMONOSIDE
Digitoxigenin 3-O- α -L-acofrioside



Source : *Vallisneria spiralis* (L.) O.K. (Apocynaceae)^{1,2}, *Cerbera odollam* Gaertn.³, *C. manghas* L.³, *Thevetia ahouai* (L.) A. DC. (Apocynaceae)⁴, *Thevetia nerifolia* Juss (Apocynaceae)⁵
Mol. Formula : C₃₀H₄₆O₈
Mol. Wt. : 534
M.P. : 203-204°C^d
[α]_D²⁵ : -20.6° (MeOH)^d
Registry No. : [4356-33-6]

IR (KBr)^d : 3600, 3460, 3005, 1788, 1742, 1620, 1442, 1376, 1096, 1040, 975, 915, 890, and 780 cm⁻¹.

PMR (CDCl₃, 60/250 MHz)^d : δ 0.88 (s, 3xH-18), 0.94 (s, 3xH-19), 1.29 (d, $J=6.3$ Hz, 3xH-6 of Aco), 2.0-2.25 (m, 2xH-16), 2.28 (dd, $J=9.0, 5.3$ Hz, H-17), 3.42 (dd, $J=9.2, 3.1$ Hz, H-3 of Aco), 3.50 (s, OCH₃), 3.50 (t, $J=9.1$ Hz, H-4), 3.73 (dq, $J=9.0, 6.3$ Hz, H-5 of Aco), 3.97 (m, H-3), 4.02 (dd, $J=3.1, 1.7$ Hz, H-2 of Aco), 4.82 (dd, $J=18.0, 1.5$ Hz, H-21A), 4.92 (d, $J=1.7$ Hz, H-1 of Aco), 4.99 (dd, $J=18.0, 1.5$ Hz, H-21B), 5.88 (t, $J=1.5$ Hz, H-22).

CMR (CDCl₃, 22.63 MHz)^d : δ C-1) 30.4^a (2) 26.5^a (3) 71.7 (4) 29.4^a (5) 36.5 (6) 26.6 (7) 21.2^b (8) 41.8 (9) 35.7 (10) 35.2 (11) 21.4^b (12) 40.0 (13) 50.3 (14) 85.5 (15) 33.1 (16) 26.9 (17) 50.9 (18) 15.8 (19) 23.8 (20) 174.6 (21) 73.5 (22) 117.7 (23) 174.6 Aco (1) 97.3 (2) 67.4 (3) 81.4 (4) 71.7 (5) 67.7 (6) 17.6 (OCH₃) 57.0

Mass (E.I.)^d : m/z (rel. intens.) 534 (M⁺, 0.2), 403 (9.8) 385 (2), 375 (10.5), 357 [(m-sugar-H)⁺, 89.4], 356 (48.4), 339 [(357-H)⁺, 96.4], 246 [(357-C₆H₇O₂)⁺, 56.8], 231 (11.3), 203 [(246-CH₃-CO)⁺, 96], 181 (22.9), 177 (22.8), 161 [(M-H-

Aglycone) (30.5)], 149 (16.3), 147 (22.8), 135 (18), 129 (24), 121 (25.8) 111 (25.3), 109 (30.4), 107 (32.5), 105 (25.4), 95 (48), 85 (52.9), 74 [(100) CH₃OCH=CHOH].

Biological Activity : Toxic, lethal dose cats 0.175 ± 0.009 mg/kg.¹ Cytotoxic against human epidermoid carcinoma of nasopharynx (KB) test system.⁴

Mono-O-Acetate : Position of acetyl group not certain.

Source : *Vallisneria spiralis* Roth. O.K. (Apocynaceae)¹; **Mol. Formula** : C₃₂H₄₈O₉; **Mol. Wt.** : 576; **M.P.** : 135-141°C; **[α]_D²⁴** : -15.1±2° (c=1.03, MeOH)

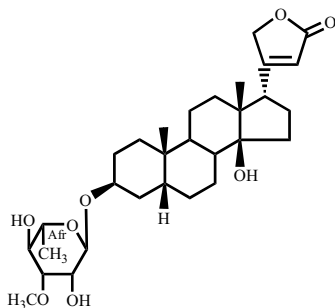
IR (KBr) : 3460 (br), 2932, 2881, 1779, 1754, 1736, 1623, 1443, 1373, 1237 cm⁻¹.

Biological Activity : Toxic, lethal dose for cats 0.317 ± 0.012 mg/kg.¹

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17α-SOLANOSIDE 17α-Digitoxigenin 3-O-α-L-acofriose



Source : *Cerbera odollam* Gaertn., *C. manghas* L. (Apocynaceae)

Mol. Formula : C₃₀H₄₆O₈

Mol. Wt. : 534

M.P. : 247-248°C

[α]_D²⁷ : -30.4° (c=0.14, MeOH)

Registry No. : [111613-31-1]

PMR (C₅D₅N, 400 MHz) : δ 0.93 (s, 3xH-18)^a, 1.20 (s, 3xH-19)^a, 1.66 (d, *J*=6.0 Hz, 3xH-6 of Afr), 3.43 (t, *J*=9.0 Hz, H-17), 3.55 (OCH₃ of Afr), 3.95 (dd, *J*=3.0, 9.0 Hz, H-3 of Afr), 4.21 (br s, H-3α), 4.29 (m, H-5 of Afr), 4.30 (t, *J*=9.0

Hz, H-4 of Afr), 4.57 (dd, $J=2.0, 3.0$ Hz, H-2 of Afr), 4.82 (H-21A), 4.95 (dd, $J=18.0, 2.0$ Hz, H-21B), 5.42 (d, $J=2.0$ Hz, H-1 of Afr), 6.13 (br s, H-22).

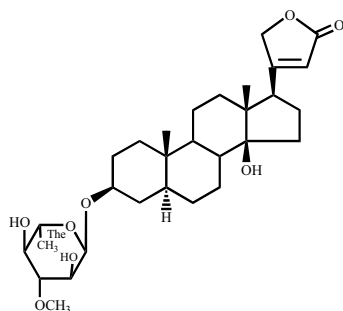
CMR (C_5D_5N , 100 MHz): δ C-1) 30.2 (2) 27.2^a (3) 72.4 (4) 31.0 (5) 37.2 (6) 26.9^a (7) 21.6 (8) 41.7 (9) 36.0 (10) 35.5 (11) 20.7 (12) 31.7 (13) 49.4 (14) 85.2 (15) 31.0 (16) 24.9 (17) 48.9 (18) 18.6 (19) 24.0 (20) 172.8 (21) 74.1 (22) 116.6 (23) 174.1 **Afr** (1) 99.7 (2) 70.0 (3) 82.8 (4) 72.3 (5) 68.8 (6) 18.6 (OCH₃) 57.0.

Mass (FAB): m/z 557.310 [(M+Na)⁺, calcd. 557.309].

Reference

1. T. Yamauchi, F. Abe and A.S.C. Wan, *Chem. Pharm. Bull.*, **35**, 2744 (1987).

THEVOFOLINE Uzarigenin3-O- α -L-thevatoside



Source : *Thevtia peruviana* (Pers.) K. Schum.
(Apocynaceae)

Mol. Formula : C₃₀H₄₆O₈

Mol. Wt. : 534

M.P. : 260°C

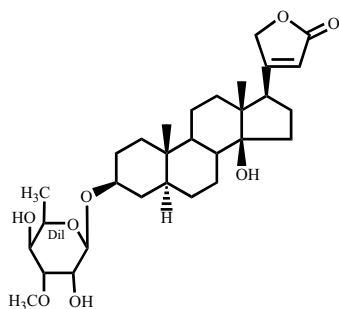
[α]_D²² : -66.0° (MeOH)

Registry No. : [34302-25-5]

Reference

1. M. Frerejacque and M. Durgeat, *Compte rend. Acad. Sci., Ser. D*, **272**, 2620 (1971).

UZARIGENIN 3-O- β -D-DIGITALOPYRANOSIDE



Source : *Nerium odorum* Sol. (Apocynaceae)

Mol. Formula : C₃₀H₄₆O₈

Mol. Wt. : 534

M.P. : 239-240°C¹

[α]_D : +4.2° (MeOH)¹

Registry No. : [61217-80-9]

UV (MeOH)¹ : λ_{\max} 218 (ϵ 15900) nm.

Mass (F.D.)² : m/z (rel.intens.) 535 [(M+H)⁺, 100], 517 [(M+H-H₂O)⁺, 17.5], 375 [(Agl+H)⁺, 40.4], 357 (57.9), 161 (63.2).

Mass (FAB, Positive ion)² : m/z (rel.intens.) 535 [(M+H)⁺, 59.5], 517 [(M+H-H₂O)⁺, 4.8], 375 (31.0), 357 (42.9), 161 (88.1), 129 (100).

Mass (FAB, Negative ion)² : m/z 355 [(M-H)⁻, 13.1].

Diacetate :

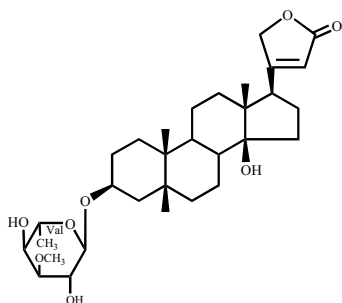
M.P. : 262-264°C¹; [α]_D : +66.7° (c=0.12)¹.

PMR (CDCl₃)¹ : δ 4.48 (d, $J=8.0$ Hz, H-1 of Dil), 5.01 (dd, $J=8.0, 10.0$ Hz, H-2 of Dil), 5.32 (dd, $J=1.4$ Hz, H-4 of Dil), 5.89 (H-22).

References

1. T. Yamauchi, M. Takahashi and F. Abe, *Phytochemistry*, **15**, 1275 (1976).
2. R. Isobe, T. Komori, F. Abe and T. Yamauchi, *Biomed. Environ. Mass Spectrom.*, **13**, 585 (1986).

VALLAROSIDE
Digitoxigenin 3-O- α -L-vallaropyranoside



Source : *Vallis solanacea* (Roth.) O.K.^{1,2}
 (Aspocynaceae)
Mol. Formula : C₃₀H₄₆O₈
Mol. Wt. : 534
M.P. : 122-124°C¹
[α]_D²⁴ : -46.5±2° (c=0.91, MeOH)¹
Registry No. : [4477-75-2]

IR (KBr)¹ : 3448 (br), 2932, 1779, 1742, 1628, 1628, 1449, 1377, 1344, 1287, 1256, 1190, 1158, 1051 cm⁻¹.

Biological Activity : Lethal dose for cats 0.1707±0.0068 mg/kg.¹

Acetate : Monoacetylvallaroside

Source : *Vallis solanacea* (Roth.) O.K (Apocynaceae), **Mol. Formula :** C₃₂H₄₈O₉, **Mol. Wt. :** 576,
M.P. : 196-199°C¹; [α]_D²⁷ : -38.2° (c=1.0, MeOH)¹

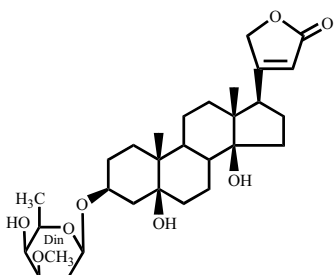
Position of acetyl group not certain.

IR (KBr)¹ : 3460 (br), 2924, 2881, 1776, 1739, 1618, 1445, 1368, 1230 cm⁻¹.

Biological Activity : Lethal dose for cats 0.3138±0.0230 mg/kg.¹

References

1. H. Kaufmann, W. Wehrli and T. Reichstein, *Helv. Chim. Acta*, **48**, 65 (1965).
2. H. Kaufmann, *Helv. Chim. Acta*, **48**, 83 (1965).
3. K.K. Chen, *J. Med. Chem.*, **13**, 1029 (1970).

VANDEROSIDE**Periplogenin 3-O- β -D-diginopyranoside**

Source : *Strophanthus vanderijstii* Staner. (Apocynaceae)

Mol. Formula : C₃₀H₄₆O₈

Mol. Wt. : 534

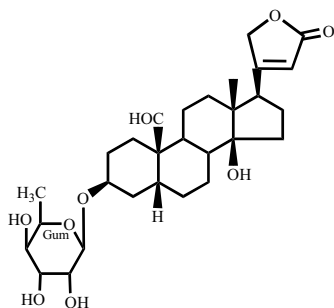
M.P. : 217-222°C

[α]_D²⁷ : +7.8 \pm 2.0° (c=1.32, CHCl₃)

UV (EtOH) : λ_{max} 218 (log ϵ , 4.25) nm.

Reference

1. H. Lichti, C. Tamm and T. Reichstein, *Helv. Chim. Acta*, **39**, 1933 (1956).

CHEIRANT(H)OSIDE**Cannogenin 3-O-[6-deoxy- β -D-gulopyranoside]**

Source : *Cheiranthus allioni* Hort. (Syn. *Erysimum asperum*, Brassicaceae)

Mol. Formula : C₂₉H₄₂O₉

Mol. Wt. : 534

M.P. : 154-156°C

[α]_D²² : -41.3 \pm 3° (c=1.12, MeOH)

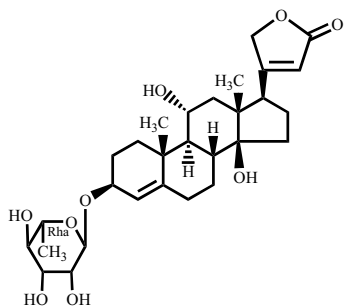
Registry No. : [29781-78-0]

UV (EtOH) : λ_{max} 217 (log ϵ , 4.19), 296 (log ϵ , 1.73) nm.

Reference

1. I.F. Makarevich, *Khim. Prir. Soedin.*, **6**, 331 (1970); *Chem. Nat. Comp.*, **6**, 331 (1970).

CHEIRANTHUS ALLIONI SAPONIN Ch-30
3 β ,11 α ,14-Trihydroxy-4,20(22)-dienolide 3-O-[α -L-rhamnopyranoside]



Source : *Cheiranthus allioni* Hort. (Brassicaceae)

Mol. Formula : C₂₉H₄₂O₉

Mol. Wt. : 534

M.P. : 268-275°C

[α]_D²⁰ : -38.2 \pm 3° (CHCl₃, MeOH)

Registry No. : [109138-53-6]

IR : 1630, 1620, 810 cm⁻¹.

Mass (FAB) : *m/z* 388, 370 [M-H₂O]⁺, 352 [M-2H₂O]⁺, 334 [M-3H₂O]⁺, 319 [M-3H₂O-CH₂]⁺, 217, 201, 199, 179, 173, 145, 91, 67, 55.

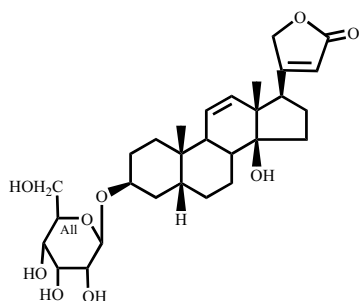
Biological Activity : Toxic, lethal dose 0.25 mg/kg in cats.

Reference

1. I.F. Makarevich, A.I. Pavlii and S.I. Makarevich, *Khim. Prir. Soedin.*, 119 (1987); *Chem. Nat. Comp.*, **23**, 101 (1987).

CHRYSOLINA POLITA SAPONIN 3

Δ^{11} -Digitoxigenin 3-O- β -allopyranoside



Source : *Chrysolina polita* (Chrysomelidae)

Mol. Formula : C₂₉H₄₂O₉

Mol. Wt. : 534

Registry No. : [115569-99-8]

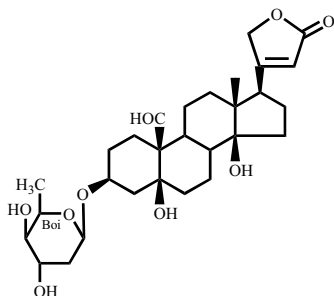
PMR (CD₃OD, 250 MHz) : δ 0.90 (s, 3xH-18), 0.90 (s, 3xH-19), 2.34 (br d, $J=11.0$ Hz, H-9), 2.91 (dd, $J=6.0, 6.0$ Hz, H-17), 3.49 (dd, $J=9.5, 3.0$ Hz, H-4 of All), 3.6-3.8 (H-5 and 2xH-6 of All), 4.05 (dd, $J=3.0, 3.0$ Hz, H-3 of All), 4.07 (br s, H-3), 4.70 (d, $J=8.0$ Hz, H-1 of All), 4.98 ($J=18.0, 2.0, 2.0$ Hz, 2xH-21), 5.48 (br s, H-11, H-12), 5.96 (br s, H-22).

Reference

1. S.V. Oycke, T. Randoux, J.C. Braekman, D. Daloze and J.M. Pasteels, *Bull. Soc. Chim. Belg.*, **97**, 297 (1988).

CORCHOROSIDE A

Strophanthidin 3-O- β -D-boivinopyranoside]



Source : *Corchorus capsularis* L.¹ (Tiliaceae), *C. olitorius* L.² (Tiliaceae), *Erysimum perofskianum* Fisch. et. Mey.³ (Cruciferae), *Castilla elastica* Cerv.⁴ (Moraceae) etc.

Mol. Formula : C₂₉H₄₂O₉

Mol. Wt. : 534

M.P. : 163-168°C⁵

[α]_D : 9.9°±2° (c=1.2, MeOH)¹

Registry No. : [508-76-9]

UV (EtOH)³ : λ_{\max} 216 (log ϵ , 4.18), 300 (log ϵ , 1.34) nm.

CD (MeOH, rel.intens.)² : 245.5 nm (+13.0), 306 (-1.4).

PMR (CD₃OD, 600 MHz)² : δ 0.84 (s, 3xH-18), 1.22 (d, $J=6.5$ Hz, 3xH-6 of Boi), 2.82 (m, H-17), 3.21 (m, H-4 of Boi), 3.94 (m, H-5 of Boi), 3.96 (m, H-3 of Boi), 4.17 (m, H-3), 4.87 (dd, $J=2.0, 10.0$ Hz, H-1 of Boi), 4.90, 5.02 (each 1H, dd, $J=2.0, 18.5$ Hz, 2xH-21), 5.89 (s, H-22), 10.04 (H-19).

CMR (CD₃OD, 150 MHz)² : δ C-1) 25.1 (2) 25.9 (3) 76.0 (4) 36.8 (5) 75.30^a (6) 37.1 (7) 23.2 (8) 42.5 (9) 40.4 (10) 56.1 (11) 18.9 (12) 40.5 (13) 50.7 (14) 85.9 (15) 32.4 (16) 27.9 (17) 51.7 (18) 16.1 (19) 210.1 (20) 178.1 (21) 75.27^a (22) 117.8 (23) 177.2 Boi (1) 99.0 (2) 34.7 (3) 70.29^b (4) 70.9 (5) 70.35^b (6) 16.9.

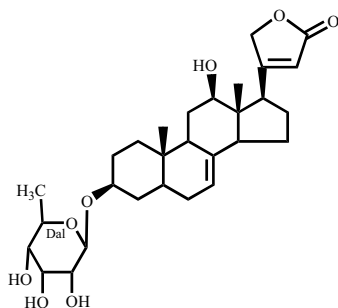
Mass (FAB, Negative ion)² : m/z 533 [M-H]⁻, 403 [Agl-H]⁻.

Biological Activity : Mean lethal dose in cats : 0.0768±0.053 mg/kg.³

References

1. M. Frerejacque and M. Durgeat, *Compt. Rend.*, **238**, 507 (1954).
2. T. Nakamura, Y. Goda, S. Sakai, K. Kondo, H. Akiyama and M. Toyoda, *Phytochemistry*, **49**, 2097 (1998).
3. Z. Kowalewski, H. Jäger, O. Schindler and T. Reichstein, *Helv. Chim. Acta*, **43**, 957 (1960).
4. P. Brauchli, O. Schindler and T. Reichstein, *Helv. Chim. Acta*, **44**, 904 (1961).
5. W. Kreis, C. Tamm and T. Reichstein, *Helv. Chim. Acta*, **40**, 593 (1957).

7,8-DIDEHYDROSYRIOGENIN 3-O-[6-DEOXY- β -D-ALLOPYRANOSIDE]



Source : *Asclepias syriaca* L. (Asclepiadaceae)

Mol. Formula : C₂₉H₄₂O₉

Mol. Wt. : 534

[α]_D²² : -54.6° (c=1.16, MeOH)

Registry No. : [676353-37-0]