



Research Article

**Phytochemical Investigation and
Molecular Modelling of Steroidal Glycoalkaloid
from *Solanum Xanthocarpum***

Patel V.B.^{1*}, Rathod I.S.², Patel J.M.¹, Brahmbhatt M.R.¹

¹K.J College of Pharmacy, At & Po., Vadasma, Dist., Mehsana, Gujarat, India

²L.M.College of Pharmacy, Dept. of Pharmaceutical Chemistry, Ahmedabad

Abstract

The kantakari having a botanical name is *Solanum xanthocarpum*, synonym *Solanum surattense* and it belongs to family solanaceae. A dried ripe berries containing more amount of glycoalkaloid compare to all parts of the plant. Glycoalkaloids consist of perhydro 1, 2-cyclopentanophenanthrene nucleus, the solanum alkaloid having N- analog of steroidal saponins. The isolated compounds were evaluated by physical and chemical methods and further elucidated by analytical specification using UV, Infrared and Mass spectroscopic methods. Molecular Modelling and comparison study used as a potassium sparing diuretic and the isolated, the 3D compound, structure of the spironolactone and solasodine were generated, energy minimized and superimposed using software, finally determine RMSD for both spironolactone and isolated compound having a low value that shown spironolactone and solasodine had a structural similarity so solasodine gave pharmacological action similar to spironolactone.

Key words: RMSD, spironolactone, 3D structure, glycoalkaloids, canrenone

INTRODUCTION

The botanical name of kantakari is *Solanum xanthocarpum*, synonym *Solanum surattense* and it belongs to family Solanaceae. The plant occurs throughout India, often in waste places, on

*Corresponding author

Email : viba135patel@yahoo.co.in

roadsides and in open scrublands. It is a prickly, usually spreading or diffused perennial, woody at base. The young branches are densely covered with minute star-shaped hairs. The branches zigzag, spread close to the ground are covered with yellow, sharp, shining prickles, about 1.5 cm long. The leaves are up to 10 cm in length, their midribs and other nerves with sharp yellow prickles. The flowers are purple, about 2 cm long, few together in small bunch opposite the leaves. The fruits are glabrous, globular drooping berries, 1.5-2 cm, yellow or pale with green veins. A glucoalkaloid termed solasonine is found in the fruits. A sterol known as carpesterol and solasodine are also present. Potassium nitrate, a fatty acid, a resinous and phenolic substance, diosgenin and sitosterol are present. Dry fruits contain traces of isochlorogenic, neochlorogenic, chlorogenic and caffeic acids. Solasodine, solasonine, solamargine are present in fruits of Nepalese plant. Quercetin isolated together with apigenin and sitosterol. ^[1, 2] Solasodine content was 0.75 and 1.7% on dry weight basis in unripe and ripe berries respectively. The basic moiety of solasodine and solasonine consist of perhydro 1, 2- cyclopentanophenanthrene nucleus. The solanum alkaloid having N- analog of steroidal saponins. The center of chirality 22 and 25 permit the existence of 4 side chain diastereomer for the spirosolane. Spirolactone also having a steroid nucleus. ^[4]

EXPERIMENTAL

Plant material

The ripe berries of *Solanum xanthocarpum* were collected during month of March-May from the region of North Gujarat. The plant had id 821562-1 in Index Kewensis. The Plant materials were dried in Hot air oven at a constant temperature at 60°C.

Table 1 Physical and Chemical evaluation of isolated compounds

	Solasodine	Solasonine
Physical evaluation		
Molecular Formula	C ₂₇ H ₄₃ NO ₂	C ₄₅ H ₇₃ NO ₁₆
Molecular Weight	413.6	884.4
Melting Point	208-210(200-202)	291-295(284-286)
Chemical Evaluation		
Mobile phase: Ethyl acetate: Hexane (20:80)	Orange spot	Orange spot
Spraying reagent: Dragendroff reagent	R _f : 0.27	R _f : 0.6

Phytochemical screening

The dried berries powder was passed through sieve 40 #. The two compounds solasodine and solasonine was isolated by extraction and hydrolysis method. [3,5]

Methods

The isolated compounds were evaluated by physical and chemical methods. [6]

The isolated compounds were elucidated by analytical specification using UV, Infrared and Mass spectroscopic methods. [7]

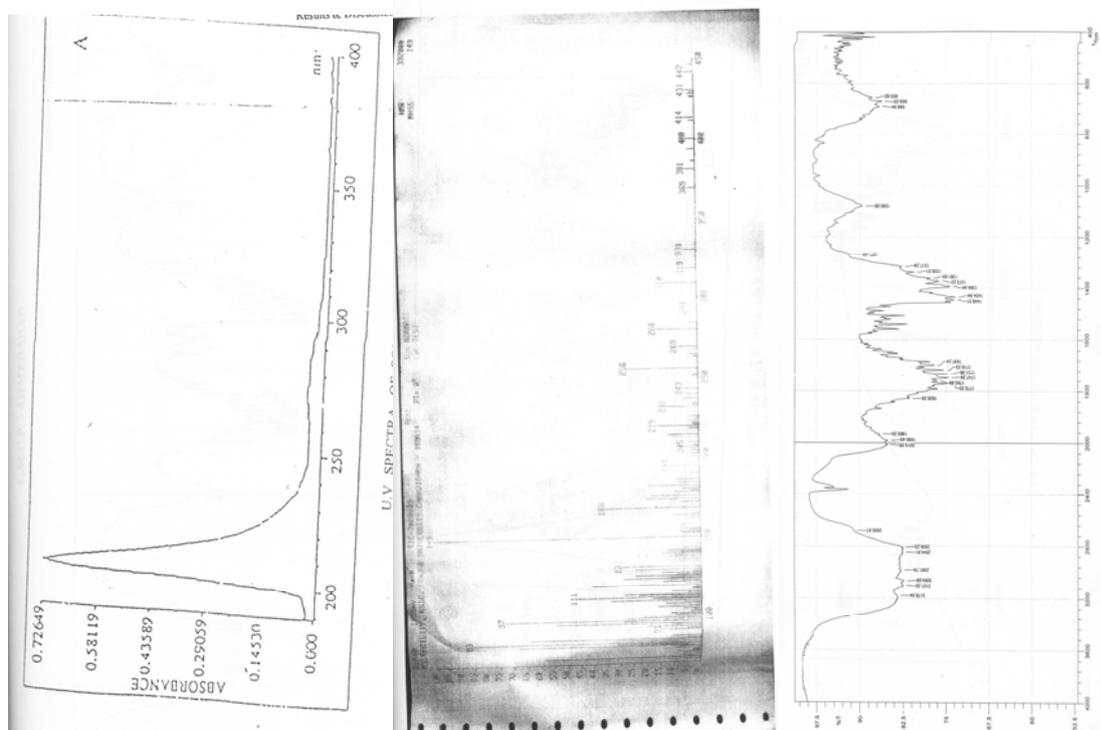
Molecular Modelling and comparison study

The structure of the spironolactone and solasodine were generated, energy minimized and superimposed using PC based CS Chem 3D Pro software (Cambridge soft corporation). The RMSD (Root Mean Square Distance) was determined for both isolated compounds. Also the Triangular Pharmacophore of solasodine and canrenone, the active metabolite of spironolactone was compared.

RESULTS AND DISCUSSION

The evaluation parameter of isolated compounds showed in Table 1 and it was concluded that the isolated compounds were solasodine and solasonine.

Figure 1 UV, GC-MS and IR spectra of solasodine



It was further validated by spectral analysis (Figure 1&2). The isolated compound solasodine in Methanol showed absorbance peak at 210 nm. Both compounds showed identical pattern of UV spectra which was confirmed that the entire compound was belong to same series.

The presence of broad/sharp peak at 3450 cm^{-1} showed the primary alcohol. The broad peak of 3362 cm^{-1} showed the presence of secondary amine. The sharp peak at 1060, 1239 cm^{-1} indicated presence of C-O-C (ether). Solasodine was characterized by Mass spectrum analysis. Solasodine gave M+1 peak at the molecular weight 414. Other prominent peaks were obtained at 398, 385, 271, 138 and 114. The fragment of m/z 138 and 114 were characteristic for spirosolane ring of solasodine.

From Molecular modeling it was shown that spironolactone and solasodine had a structural similarity. Solasodine may be give pharmacological action similar to spironolactone. It was summarized in Table 2 that the distance between triangular pharmacophore of spironolactone and solasodine were 0.462. The low RMSD value suggests that close structure similarity.

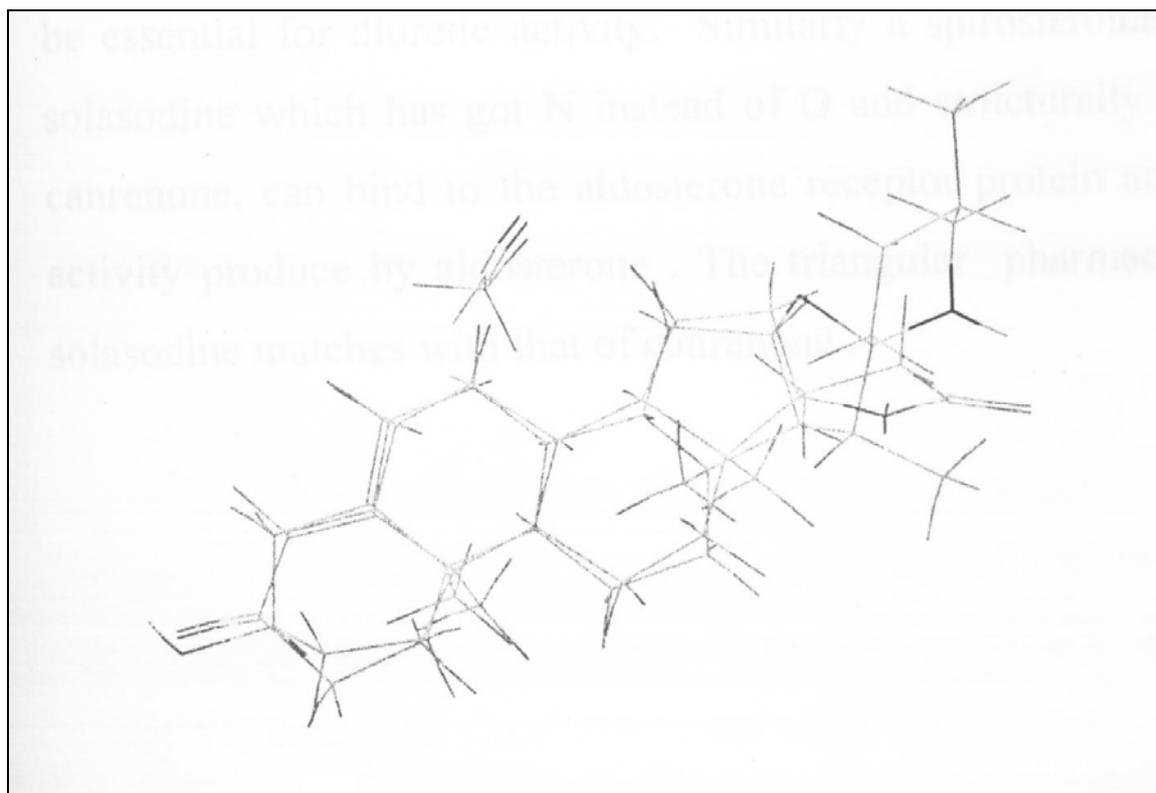
Table 2 Comparison of Triangular pharmacophore

Compound	A	B	C
Spironolactone	10.894 A	2.277	12.732
Solasodine	11.029	2.281	13.145
Difference	0.135	0.004	0.413

The measurement of RMSD between the two energy minima structure of solasodine and spironolactone considering 8 fix reference point was found to be 0.462. The low RMSD value suggest good 3D similarity between spironolactone and solasodine which was shown by super impositioning of 3D structures. (Figure 2)

Spironolactone was significantly metabolized in liver to its active metabolite canrenone which had a lactone ring at C17 position. [3] It was assumed that two oxygen of lactone and one oxygen at C3 position of canrenone may be responsible for pharmacological activity. Similarly a spiro steroidal alkaloid solasodine which had got N instead of O and structurally similar to canrenone. Then find out triangular pharmacophore of solasodine match with the canrenone.

Figure 2



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