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Cucurbitane derived terpenoidal moieties from under-utilised cucurbits as probable medicinal leads

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Objective: The present study was designed to phytochemically investigate and to screen the under-utilized cucurbit vegetables viz. Momordica balsamina, Coccinia indica and Trichosanthes dioica for their preventive effect against type-2 diabetes and to isolate the moderately polar cucurbitane type triterpenoids responsible for the biological effect.

Materials & Methods: The fruits of Momordica balsamina and Coccinia indica were extracted with chloroform and fractionated with hexane to create an extract rich in moderately polar components. These extracts rich in moderately polar components were used for evaluating the preventive effect of these cucurbit vegetables in nicotinamide/streptozotocin induced type-2 diabetes. Mildly diabetic animals were orally treated with chloroform extract of each fruits (250 mg/kg, BW) given daily for a week. Results and discussion: Both the extracts reduced fasting blood glucose significantly ($p<0.05$% vs. diabetic control) when estimated on seventh day of treatments. Pre-treatment with fruit extracts for seven days also blunted the OGTT curve and restricted the increment of blood glucose to 25 mg/dl after one hour of glucose challenge. Moreover, the treatment with fruit extracts resulted in significant improvement of lipid profile.

Conclusion: The phytochemical investigation focused on isolation and characterization of bioactive components revealed presence of β-Sitosterol 3-β-D-glucopyranoside, β-Sitosterol α-D-triglucoside, Cucurbit-5, 7-dien-ol, Cucurbiten- 3-D-glucoside, Cucurbiten-3β-ol-3-O-D-diglucosidic linolenate as main components. From the above results it was concluded that extract of fruits rich in cucurbitane type triterpenoidal moieties in M. balsamina and C. indica fruits possess preventive effects on diabetic hyperglycemia, hyperlipidemia and significant anti-diabetic potential.

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Current progress in structure-based rational drug design marks a new mindset in drug discovery

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As the paradigm of serendipity appears to have reached hard operational limitations in the field of drug discovery, there seems to be a renewed interest for investigating the detail of interactions between the ligands and their receptors. The past decade has witnessed a paradigm shift in preclinical drug discovery with structure-based drug design (SBDD) making a comeback while high-throughput screening (HTS) methods have continued to generate disappointing results. This is due to a deficit of information between identified hits and the many criteria that must be fulfilled in parallel to convert them into preclinical candidates that have a real chance to become a drug. Although accurate calculations of the free energy of binding are still elusive, receptor structure-based ligand interaction models may provide a wealth of information sufficient to allow feedback from experimental validation to be integrated in the model and generate workable information opening for rationally guided alternative proposals in chemical synthesis and testing plans during lead optimization. Unfortunately, in too many cases effective/operative structure-based models cannot be successfully elaborated. Although generally not overlooked, SBDD is hindered in practice mainly due to shortage of allocated time, insufficient expert manpower and dis-synchronization of the collaborative work between modelers and chemists. We propose to discuss some of the prerequisites and operational conditions when elaborating workable models throughout examples of prototypical situations covering the current possibilities and limitations of SBDD.

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