

# Obesity, Healthcare - Nutrition & Fitness

March 18 - 19, 2019 | New York, USA

SCIENTIFIC TRACKS | DAY 2

JOURNAL OF OBESITY & WEIGHT LOSS THERAPY 2019, VOLUME: 4 | DOI: 10.4172/2165-7904-C2-093

## GC-MS and molecular docking studies for identification of anti-diabetic compounds in methanolic extract of *hunteria umbellata* seeds

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The purpose of this study was to investigate the diabetic effect of phytocompounds synthesized from *Hunteria umbellata* using GC-MS analysis and molecular docking studies. Peroxisome proliferator-activated receptor gamma (PPAR- $\gamma$ ) agonists are beneficial in the treatment of diabetes by stimulating insulin sensitivity and antagonizing hepatic gluconeogenesis. The aim of the present study was to investigate PPAR- $\gamma$  agonist property of phytocompounds from *Hunteria umbellata* using in-silico approach. Molecular docking of *Hunteria*

*umbellata* on human PPAR- $\gamma$  protein was determined by Auto/Vina in Pymol 4.2 and compared with Gilbenclamide, a known agonist of PPAR- $\gamma$ . Our present study reports the phytochemical analysis of the extracts of the seeds and leaves of *Hunteria umbellata*. 21 compounds were revealed through GC-MS analysis and screened using Autodock/Vina against PPAR- $\gamma$ . Docking studies recommended that 2,2-Benzylidenebis (3-methylbenzofuran) an existing phytochemical from the seed of *Hunteria umbellata* had the highest fitness score of -11.3 Kcal/mol and hence could be a potent antidiabetic drug. *Hunteria umbellata* seed extract and its compound 2,2-Benzylidenebis (3-methylbenzofuran) have a significant antidiabetic activity against PPAR- $\gamma$ . Molecular binding interaction of an in-silico data demonstrated that 2,2-Benzylidenebis (3-methylbenzofuran) has

more specificity towards the PPAR- $\gamma$  binding site and could be a potent antidiabetic compound.

### Biography

Olusola Abiola Ladokun is a Professor of Nutritional Biochemistry in the Department of Biochemistry, Faculty of Sciences, Lead City University, Ibadan. She holds a PhD in Agricultural Biochemistry and Nutrition from the University of Ibadan, Ibadan, Nigeria. She is the current serving Dean of the Faculty of Basic Medical and Applied Sciences. She has to her credit several articles in both local and international journals, chapters in books and conference proceedings. Her areas of research include but not limited to Food Chemistry, Ethnopharmacology, and Functional Foods. She has attended and presented papers in conferences and workshops in Nigeria and Internationally.

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