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Abstracts and Posters

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TI

Bilateral acute retinal necrosis following Shingrix vaccine in a locally immunosuppressed host

Wang, Yao. **2020 COS Annual Meeting and Exhibition** (Jun 22, 2020)

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AU,AUFN,AULN
PUB

AB

Abstract (summary) [Translate](#)

Purpose: To the best of our knowledge, we report the first case of acute retinal necrosis (ARN) following H_z/S_u (Shingrix) shingles vaccine in a locally immunosuppressed 83-year-old host. Study Design: Observational case report in the setting of a tertiary care ophthalmology referral centre. Methods: The patient's clinical records were reviewed including history, clinical examinations, imaging and investigations. A thorough review of the literature was conducted. Results: An 83-year-old man with an ocular history significant for herpes zoster keratouveitis

Indexing (details) Cite

IF

Identifier (keyword) acute retinal necrosis, shingles, vaccine, immunocompromise

TI

Title Bilateral acute retinal necrosis following Shingrix vaccine in a locally immunosuppressed host

AU,AUFN,AULN

Author Wang, Yao ¹

¹ Queen's University

CFTI

Conference title 2020 COS Annual Meeting and Exhibition

ESDT

Conference start date 2020-06-26

EVDT

Conference end date 2020-06-28

CG, CCNT

Conference location Online

LA

Language English

DTYPE

Document type Conference Poster, Conference Abstract

PUB

Publication title 2020 COS Annual Meeting and Exhibition

PSTYPE

Publication type Conference Papers & Proceedings

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Publication date Jun 22, 2020

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AN

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First available 2020-08-19


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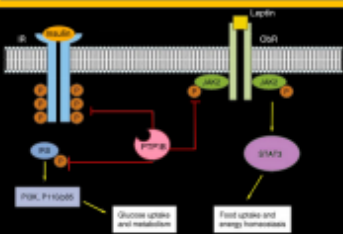
Pharmacophore-docking virtual screening of protein tyrosine phosphatase 1b identifies natural products with potential activity against diabetes mellitus type-2 and obesity

Ho Yueng Hsing¹, Selestin Rathnasamy^{1,2}, Roza Dianita¹ and **Habibah A. Wahab^{1,2}**

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INTRODUCTION

Growing incidence of Type-2 Diabetes Mellitus (T2DM) together with obesity, shows the complexity and progressive nature of these metabolic disorders and alarms the necessity to explore new and alternative therapeutic pathways and drugs. Insulin and leptin resistance are the most common pathophysiological link between T2DM and obesity. Protein tyrosine phosphatase 1B (PTP1B) is thought to interfere with glucose homeostasis and satiety through downregulation of insulin and leptin signaling pathways. Thus, drugs that are potent to impede this enzyme should be effective in treating T2DM and obesity.

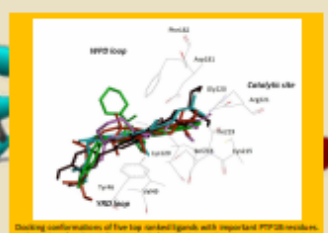


*PDB structure with ID 1C83 in complex with the ligand 6-(oxalyl-amino)-1h-indole-5-carboxylic acid (OAI) was used for this study.

RESULTS



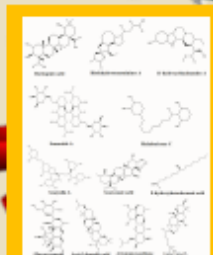
Compounds that showed best docking interactions with PTP1B structure



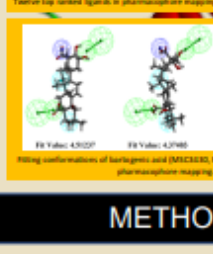
Docking conformation of the top ranked ligand with important PTP1B residues. The order of ranking of compounds from highest to lowest: MDC238 (green) > MDC238 (red) > MDC265 (purple) > S1 (blue) > MDC237 (dark green)

Sample	IC ₅₀ (µg/ml)	Sample	IC ₅₀ (µg/ml)
Standard	81.54 ± 1.22	Mandarin orange (L)	33.26 ± 18.88
<i>P. amaryllifolius</i> (L)	94.28 ± 2.43	Platanus guineensis (L)	36.73 ± 8.22
<i>Vitex negundo</i> (L)	89.83 ± 2.68	<i>Oslea indica</i> (SP)	38.24 ± 6.79
<i>Piper nigrum</i> (F)	81.29 ± 19.28	<i>Cordia alliodora</i> (L)	25.54 ± 19.78
<i>Cynchophagen nardus</i> (L)	79.78 ± 6.12	<i>Antiaropsis heterophylla</i> (R)	9.82 ± 12.12
<i>Cynchophagen nardus</i> (F)	66.90 ± 6.42	<i>Myrsine javanica</i> (F)	2.81 ± 6.97
<i>Cynchophagen nardus</i> (L)	66.82 ± 13.28	<i>Acrostichum volatile</i> (F)	2.28 ± 12.82
<i>Mandarin orange</i> (F)	62.86 ± 23.87	<i>Morone bonensis</i> (L)	< 200
<i>Calophyllum inophyllum</i> (L)	48.58 ± 21.89	<i>Antiaropsis heterophylla</i> (L)	< 200
<i>Mimodora charantifolia</i> (L)	42.38 ± 16.62	<i>Amorfrutia molleoides</i> (L)	< 200
<i>Mimodora charantifolia</i> (L)	42.18 ± 7.71	-	-

IC₅₀ cannot be determined, (L) leaves, (F) fruit, (R) root, (S) bark, (SP) whole plant

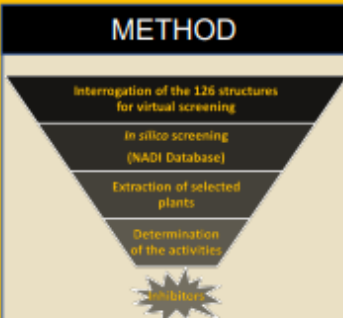


Top five best ranked ligands in pharmacophore mapping



Fitting conformations of barbigens acid (MDC238, Ranked 1st, 2nd and 3rd) in pharmacophore mapping

METHOD



*ChemDraw Ultra 8.0 and AutoDock 4.2 were used to illustrate ligand structure and run molecular docking simulation and virtual screening, respectively.
 *Discovery Studio 2.5 and 4.0 Client were used for pharmacophore mapping and protein-ligand interactions visualization.
 *4000 natural compounds from NADI database were screened for activity.
 *Methanol crude extracts of selected plants were prepared using maceration technique.
 *PTP1B calorimetric assay kit (cat. no: 539736) was used for in vitro assay

CONCLUSION

Our virtual screening study and enzymatic assays indicated the promising PTP1B inhibitory activity of *Pandanus amaryllifolius* leaves, *Vitex negundo* leaves and *Piper nigrum* fruit. Further fractionation or isolation of active principles from these plants can provide a good platform to develop promising anti-diabetic or -obesity drugs through PTP1B-targeted approach. However, taken into account the limitations targeting only the catalytic region of PTP1B, future experiments should include all possible binding pockets.

REFERENCES

- WHO. Global report on diabetes [Internet]. World Health Organization; 2016 [cited 2023 Feb 20]; 88 p.
- Sharma, S and Singh, R. (2018). Protein tyrosine phosphatase-98 (PTP-98): a novel and challenging therapeutic target for type-2 diabetes and obesity. *International Journal of Advanced Research and Development*. 9(4) p 53-62.

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