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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)

Highlighting: Off | Single | Multi

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 Hz/Su (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 <sup>1</sup>

<sup>1</sup> 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

DT, YR

**Publication date** Jun 22, 2020

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AN

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FAV

**First available** 2020-08-19


UD

**Updates** 2020-08-19

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UNIVERSITI SAINS MALAYSIA



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

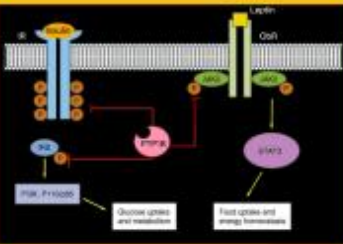
Ho Yueng Hsing<sup>1</sup>, Selestin Rathnasamy<sup>1,2</sup>, Roza Dianita<sup>1</sup> and **Habibah A. Wahab<sup>1,2\*</sup>**

<sup>1</sup>School of Pharmaceutical Sciences, Universiti Sains Malaysia, 11800 Minden, Penang, Malaysia  
<sup>2</sup>USM-RIKEN Centre for Aging Science (URICAS), Universiti Sains Malaysia, 11800 Minden, Penang, Malaysia

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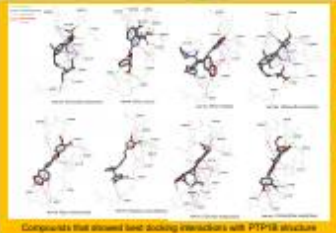
### INTRODUCTION

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.

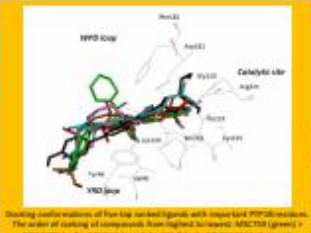


\*PDB structure with ID 1C83 in complex with the ligand 6-(oxalylamino)-1h-indole-5-carboxylic acid (OAI) was used for this study.

### RESULTS



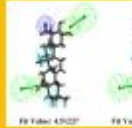
Compounds that showed best docking interactions with PTP1B structure



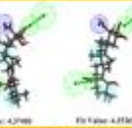
Docking conformation of the top ligand (green) with impacted PTP1B structure. The order of docking of residues from right to left are: SH2C18 (green) + SH2C20 (red) + SH2C19 (orange) + SH2 (black) + SH2C17 (blue) (left)

Sample	IC <sub>50</sub> (Inhibition)	Sample	IC <sub>50</sub> (Inhibition)
Sorrelis	81.54 ± 1.82	Mandarin orange (L)	15.56 ± 0.28
<i>P. amaryllifolius</i> (L)	54.28 ± 2.41	Platium gramine (L)	18.73 ± 8.22
<i>Vitex negundo</i> (L)	81.83 ± 3.85	<i>Opur sativa</i> (MF)	28.24 ± 6.75
<i>Piper nigrum</i> (F)	81.28 ± 18.18	<i>Cordia alliodora</i> (L)	25.56 ± 0.98
<i>Cyrtopogon nardus</i> (L)	79.78 ± 6.12	<i>Antiarum arborescens</i> (B)	9.82 ± 22.53
<i>Cyrtopogon nardus</i> (F)	66.98 ± 6.81	<i>Mysticium fragrans</i> (F)	2.81 ± 6.97
<i>Cyrtopogon nardus</i> (L)	66.02 ± 13.28	<i>Boerhaavia diffusa</i> (F)	2.38 ± 12.82
<i>Mandarin orange</i> (F)	62.06 ± 20.87	<i>Maranta arundinacea</i> (L)	< 90
<i>Calophyllum inophyllum</i> (L)	68.98 ± 21.85	<i>Antiarum arborescens</i> (L)	< 90
<i>Morinda charitadiif</i>	62.88 ± 18.82	<i>Antiarum arborescens</i> (L)	< 90
<i>Morinda charitadiif</i> (L)	62.08 ± 1.71		


IC<sub>50</sub> cannot be determined. (L) leaves, (F) fruit, (B) bark, (MF) whole plant



Fit Value: 4.5107



Fit Value: 4.2788

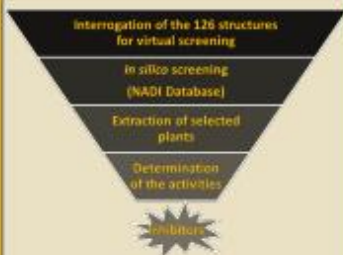


Fit Value: 4.3748

Fit Value: 4.5107    Fit Value: 4.2788    Fit Value: 4.3748

Binding conformations of ligands (red) and SH2C18, SH2C19, SH2 and SH2C20 in pharmacophore mapping

### METHOD



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

### 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

1. WHO. Global report on diabetes (Geneva): World Health Organization; 2016 [Cited 2019 Feb 20]; 68 p.
2. Sharma, D and Singh, R. (2018). Protein tyrosine phosphatase-1B (PTP-1B): a novel and challenging therapeutic target for type-2 diabetes and obesity. International Journal of Advanced Research and Development. 8(4) p 53-62.

### ACKNOWLEDGEMENT

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Accession number	AN	an(5e73657dcde2b641284aae7a)	A unique document identification number assigned by the information provider
All fields except poster	ALL	all(tdm2 OR "type 2 diabetes")	Searches all fields except the text of the poster. Use proximity and/or Boolean operators to narrow search results
All fields + text of poster	--	vildagliptin AND (tdm2 OR "type 2 diabetes")	Search all fields including the text of the poster with no field code
Author <sup>1</sup> Author First Name Author Last Name	AU AUFN AULN	au("rathnasamy, selestin") aufn(selestin) auln(rathnasamy)	Sometimes only the first author is included in the AU field, but the other authors may be included on the poster, so a search without any field qualification may return more results
Author affiliation	AF	af(novartis) au(novartis) novartis	Sometimes the author's affiliation is not included in the AF or AU field, but it is included on the poster so a search without any qualification may return more results.
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Conference title	CFTI	cfti(cos 2020)	Also searchable with CF
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Document type <sup>1</sup>	DTYPE	dtype(conference poster) dtype(conference abstract)	All items in Morressier are posters submitted to life science conferences. Most of them (but not all) also have an abstract. Occasionally posters are subject to embargo and withdrawn.
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