OIL PALM METABOLOME DATABASE

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provides

defining

and

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omics

the

in

powerful tools

signalling networks in plants. Metabolome data

refers to the collection of metabolites within a

biological system under a specific set of conditions

(Jorge et al., 2016). It complements the information

derived from genomics, transcriptomics and

proteomics to assist in providing a system

approach for holistic biological interpretation. From hydrophilic to hydrophobic chemicals,

metabolites function as immediate signatures of biochemical activity and thus represent the

molecular phenotype. This makes metabolites

the excellent candidates for biomarkers and

particularly useful for understanding disease

states and other important industrial traits such as

Oil palm R&D via metabolomics has been

intensified since the last 10 years to complement

genomic discoveries, driven by instrumentation and informatics advances such as mass spectrometry

and chemometrics (Masura *et al.,* 2017; Ramli *et al.,* 2016). The resulting large metabolome data

sets require suitable tools and resources for data interpretation. The unambiguous identification

of metabolites in highly complex oil palm

biological samples have generated a vast amount

of data, which comprise data ID, mass spectra,

chemical nomenclature and structure, molecular

formula and metabolite profile information. In

view of this, the Oil Palm Metabolome Database (OPMDB) was established to aid in cataloguing

and assigning metabolome data observed in

metabolomics experiments. Here, we report on the utility of currently available OPMDB for natural

product discoveries and recommendations on

yield and quality.

etabolomics, the newest of the

for

status and perturbations

approaches

metabolic pathways

how the research community can contribute its metabolome data to OPMDB.

NOVELTY

OPMDB provides the oil palm industry and academia with the primary and updated comprehensive registry of oil palm metabolite description, analysis spectra and structural information from multi-analysis metabolomics platforms.

BENEFITS

- Access to searchable oil palm metabolome database based on metabolomics experiment by MPOB and other researchers;
- Provision of an oil palm metabolome database as reference for metabolomists and other scientists; and
- Availability of a comprehensive resource centre that integrates spectroscopic and chemical data for growing number of identified oil palm metabolites.

DATABASE DESCRIPTION

Database Content

OPMDB was designed and developed based on extensive set of associated information for oil palm (including other species related to oil palm *e.g. Ganoderma*) to facilitate metabolomics research. It was designed to suit different types of data inputs, such as texts, numbers, chromatogram or spectra images (.png, .jpg/.jpeg and .gif format) and chemical structure images (.mol format) (Ishak *et al.*, 2015). *Figure 1* shows the OPMDB search result of a metabolite and its experimental related information based on published studies conducted by MPOB and its collaborators.







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		Browse 🕈 Metabolite 🕈 Study L	istings					
LIST OF STUDIES								
common Name	Citric acid		(i) Matabalita Information					
JPAC Name	3-carboxy-3-hydroxypen	tane-1,5-dioic acid	(i) Metabolite Information					
)ther Name(s)	3-carboxy-3-hydroxypen	tanedioic acid						
letabolite Class	Organic acids							
lolecular Formula	C ₆ H ₈ O ₇							
Nolecular Weight (g/mol)	192.1235							
SMILES	OC(=0)CC(0)(C(=0)0)	O(O=)))						
CAS No.	77-92-9							
PubChem No.	22230							
ChEBI No.	30769							
			(ii) Experimental Detaile					
RECORD 1			(ii) Experimental Details					
Date Created	14/03/2016	Date Updated	11/04/2016					
Author(s)	Nurul Liyana Rozali, Ahmad Ku	shairi Din, Umi Salamah Ramli, Idris Abu Se	man					
Research/Study Title	Discriminative analysis of partia approach using GCxGC-MS (T	ally tolerant and susceptible parental palms (oF)	Elaeis guineensis) towards understanding basal stem rot via metabolomic					
		Under Review						
Publication Status	Under Review							
Publication Status Keywords		asal stem rot, 2-dimensional gas chromatogr	aphy mass spectrometer time-of-flight (GCxGC-MS (ToF)), Metabolomics					
		asal stem rot, 2-dimensional gas chromatogr	aphy mass spectrometer time-of-flight (GCxGC-MS (ToF)), Metabolomics View Details					
Keywords		asal stem rot, 2-dimensional gas chromatogr						
Keywords RECORD 2	Oil palm (Elaeis guineensis), B		View Details					
Keywords RECORD 2	Oil palm (Elaeis guineensis), B 29/03/2016	Date Updated						
Keywords RECORD 2 Date Created Author(s)	Oil paim (Elaeis guineensis), B 29/03/2016 Noor Idayu Tahir, Nurul Liyana	Date Updated Rozali, Umi Salamah Ramli	View Details					
Keywords RECORD 2 Date Created Author(s)	Oil paim (Elaeis guineensis), B 29/03/2016 Noor Idayu Tahir, Nurul Liyana Organic acids of oil paim leave	Date Updated Rozali, Umi Salamah Ramli	View Details					
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Figure 1. Study record example that includes (i) metabolite information – common name, IUPAC name, chemical structure, molecular formula, molecular weight, mass-to-charge ratios, fragments/spectra images and so forth, and (ii) experimental details - researcher information, related references, tissue sources (materials), methodology and instrument information.

Technical Architecture

The OPMDB construction is based on freely available open source software and tools. It is implemented on Linux server with Apache version 2.4.34, PHP version 7.2.8 and MariaDB server version 10.1.34. It is also equipped with ChemDoodle Web Components 7.0.2 visualisation tool (iChemLabs, LLC, US) and a chemical drawing function of PubChem Sketcher from National Center for Biotechnology Information (NCBI, USA).

Searching and Browsing for Data

The metabolome data collection can be retrieved via (i) basic search - by metabolite characteristics (name, weight, formula or m/z ratio) at the search box of OPMDB home page or (ii) advanced search - two methods of text/number search and molecular structure search by simplified molecular-input line-entry system (SMILES) (*Figure 2*).

OPMDB also provides a browsing function for a quick examination of relevant information required by the user. Browsing of the information in the OPMDB can be done by oil palm tree organs/parts, species (with relevance to oil palm), instruments, metabolite class or the latest entry of study (*Figure 3*). If the user registers and is currently logged into OPMDB, additional private studies will be displayed for viewing.

Submission of Metabolome Data to OPMDB

OPMDB is updated regularly and expands with new data. We also offer the OPMDB platform specifically for researchers to share metabolites identification information among laboratories engaged in metabolomics research by allowing registered users to submit their experimental data and descriptions via online form. The form is divided into 5 sections: (i) study information experiment information (iii) instrument (ii) information (iv) data of metabolites and (v) data from instrument (Figure 4). Submission will be reviewed by authorised personnel to verify the study. Users are recommended to submit studies that have been published. An approved study will then appear as the latest entry for the day and registered users will get to view the complete study record of the deposited metabolome record.



(ii) Advanced search

Text a	ind number		SMILE				
Nome About OFMD0 Emarce Extense Name: Anarymous User Advanced Search	Advanced Search Deserted	02 Jan 2019 7:06:36 PH	HODD OL PALM METABOLOME DATABASE (COMPA)				
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Author		Search					

Figure 2. OPMDB search modules.

		NPOB OIL PALM N	IETABOLOME DA	TABASE (O	PMDB)		
Home	About OPMDB	Browse Database	Advanced Search	Download	Log In		
Name: Anonyn	nous User	Oil Palm Diagram				15 Jan 2019 - 10:26:12	AM
		Group of Species					
		Species					
-		Tissue / Organ / Type			MPOB OIL PALM MI	ETABOLOME DATABASE (PMDB)
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Figure 3. OPMDB browse menu.

Study Information Experiment In	formation I	nstrument	Information	Data of Metabolites	Data from Instruments			
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	The sto	The study will be addressed as Person 1 et al.						
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Study Description/Summary								
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Publication Link 😟]
Keywords 🕩]
Keywords 😟]

Figure 4. Data submission online form.

CONCLUSION

OPMDB is the first and most comprehensive oil palm metabolomics database. It provides valuable information on oil palm natural chemicals and would serve as a reference for the scientific community as well as the palm oil industry. OPMDB can be accessed via http://opmdb.mpob. gov.my/.

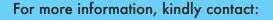
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