OIL PALM METABOLOME DATABASE

NUR 'AIN ISHAK; NOOR IDAYU TAHIR; NURAZAH ZAIN; NURUL LIYANA ROZALI; MOHD AMIN AB HALIM; ABRIZAH OTHMAN and UMI SALAMAH RAMLI

840

MPOB INFORMATION SERIES • ISSN 1511-7871 • JULY 2020 MPOB TS No. 191

Metabolomics, the newest of the omics approaches provides powerful tools for defining the status and perturbations in metabolic pathways and 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 yield and quality.

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 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.

ISSN 1511-7871
9 771511 787001

Head of Corporate Implementation and Consultancy Unit, Malaysian Palm Oil Board. 6, Persiaran Institusi, Bandar Baru Bangi, 43000 Kajang, Selangor, Malaysia.
Tel: 03-8769 4574 Fax: 03-8926 1337 E-mail: tot@mpob.gov.my Website: www.mpob.gov.my

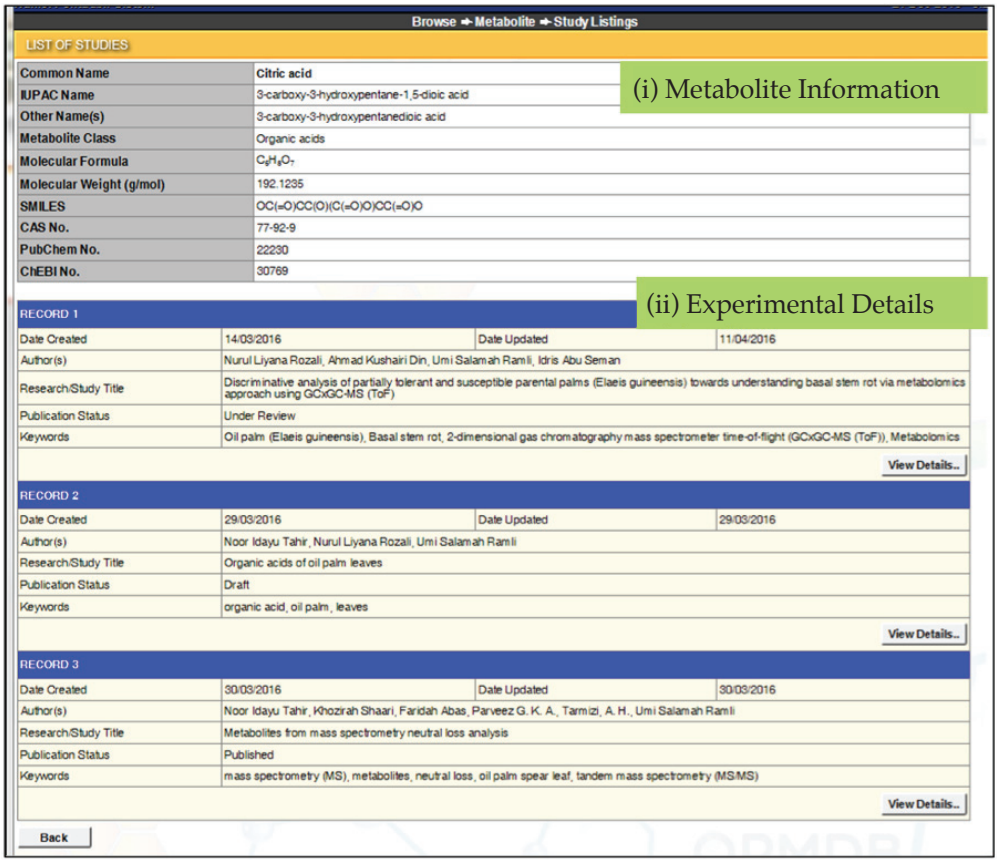

Figure 1. Study record example that includes (i) metabolite information – common name, IUPAC name, chemical structure, molecular formula, molecular weight, mass-to-charge ratios, fragments/spectra images and so forth, and (ii) experimental details - researcher information, related references, tissue 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 (ii) experiment information (iii) instrument 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.

Figure 2. OPMDB search modules.

Figure 3. OPMDB browse menu.

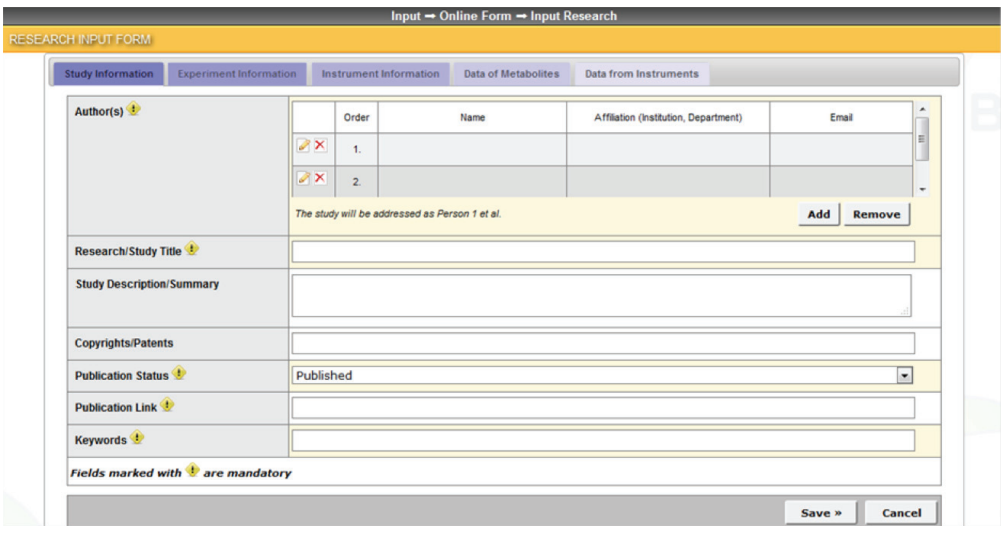

Figure 4. Data submission online form.

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/.

REFERENCES

Ishak, N A; Nurazah, Z; Rozali N L; Halim, M A; Rosli, R; Othman, A; Ramli, U S and Tahir, N I (2015). Construction of integrated oil palm metabolome chemical resources library. *Proc. of the 2015 PIPOC International Palm Oil Conference*. MPOB, Bangi. p. 381-385.

Jorge, T F; Rodrigues, J A; Caldana, C; Schmidt, R; Van Dongen, J T; Thomas-Oates, J and António, C (2016). Mass spectrometry-based plant metabolomics: Metabolite responses to abiotic stress. *Mass Spectrom. Rev., 35(5)*: 620-649.

Masura, S S; Tahir, N I; Rasid, O A; Ramli, U S; Othman, A; Masani, M Y A; Parveez, G K A and Kushairi, A (2017). Post-genomic technologies for the advancement of oil palm research. *J. Oil Palm Res., 29(4)*: 469-486.

Ramli, U S; Lau, B Y C; Tahir, N; Syahanim, S; Hassan, H; Nurazah, Z; Rozali, N L; Dzulkafli, S; Ishak, N A and Othman, A (2016). Proteomics and metabolomics: Spearheading oil palm improvement and sustainability. *The Planter, 92(1087)*: 727-737.

For more information, kindly contact:

Head of Corporate Implementation
and Consultancy Unit, MPOB
6, Persiaran Institusi,
Bandar Baru Bangi,
43000 Kajang, Selangor, Malaysia
Tel: 03-8769 4574
Fax: 03-8926 1337
E-mail: tot@mpob.gov.my
www.mpob.gov.my