Poster program

Posters will be presented as follows:

Odd number - Monday evening 17:25 – 18:30

Even number - Wednesday evening 17:25 – 18:30

A - Monday lunch

B - Tuesday lunch

C - Wednesday lunch

A. P450 mechanisms

1A **Ms Julie Ducharme,** McGill University, Canada
Probing the P450 3A4 allosteric site via bioconjugation of ligand analogues

2B **Prof Laura Furge,** Kalamazoo College, USA
Tryptophan-75 is a potential gating residue of cytochrome P450 2D6

3C **Dr Anna Haduch,** Institute of Pharmacology Polish Academy of Sciences, Poland
The effect of ageing and tryptophan hydroxylase 2 (TPH2) deficit on the CYP2D activity in rat brain and liver

4A **Mr Joshua Harbort,** The University of Queensland, Australia
Determination of the distal ligand coordination to resting state cytochrome P450 CYP199A4 and its correlation to activity

5B **Ms Gabriela Schröder,** North Carolina State University; Oak Ridge National Laboratory, USA
Investigating the catalytic cycle and redox partner protein dependent dynamics of cytochrome P450 (CYP450) by neutron scattering

6C **Dr Grazyna Szklarz,** West Virginia University, USA
Molecular basis for caffeine oxidation by human cytochromes P450 1A1 and 1A2

B. P450 structural biology

7A **Dr Thomas Lautier,** Université de Toulouse, INSA, France
Ordered chimerogenesis applied to CYP2B P450 enzymes

8B **Ms Lorela Paco,** University of Washington, USA
Ligand-dependent dynamics of cytochrome P450 3A4 in nanodiscs

9C **Mr Irwin R Selvam,** University of Manchester, UK
Ongoing characterisation of the promising targets CYP121 and CYP141 from Mycobacterium tuberculosis H37Rv

10A **Mr Matthew Snee,** University of Manchester, UK
Structural characterisation of CYP142A1 from Mycobacterium tuberculosis in complex with novel inhibitory compounds

C. Biophysical approaches

11B **Mr Matthew Podgorski,** The University of Adelaide, Australia
Investigation of different cytochrome P450 substrate binding modes using CYP199A4

D. Redox partner or other protein-protein interactions

12C **Mr Simon Jensen,** University of Copenhagen, Denmark
Regulation of cytochrome P450 oxidoreductase by small-molecules: Single molecule insights linking conformational sampling to function

E. Molecular modelling

13A **Dr Pramod Nair,** Flinders University, Australia
Comparison of computational methods for site(s) of metabolism (SOM) prediction of protein kinase inhibitors metabolised by CYP3A4

14B **Prof Laura Furge,** Kalamazoo College, USA
Pathways and energetics of ligand unbinding in CYP2D6

F. Novel P450 support systems

15C **Ms Thien Kim Le,** Chonnam National University, South Korea
Light-driven biocatalytic C-hydroxylation by CYP102A1 through direct transfer of photoinduced electrons

16A **Dr Silas Mellor,** Copenhagen University, Denmark
Electron carrier engineering towards increased partitioning of photosynthetic reducing power to cytochrome P450 catalysis

17B **Ms Chan Mi Park,** Chonnam National University, South Korea
Characterization of NADP+-specific glucose-6-phosphate dehydrogenase from Solanum lycopersicum and application to NADPH-generating system for P450-catalyzed reactions

H. Protein engineering of P450s

18C **Miss Wenyu Chen,** University of Oxford, UK
Site-directed mutagenesis of P450BM3 to improve steroid hydroxylation

19A **Miss Stephlina D'Cunha,** The University of Queensland, Australia
Ancestral reconstruction of human cytochrome P450 enzyme 2D6, an important drug metabolising enzyme

20B **Miss Raine Thomson,** The University of Queensland, Australia
Thermostability correlates with evolutionary age in ancestors of promiscuous xenobiotic-metabolizing enzymes, suggesting a robust ancestor facilitated evolutionary diversification

21C **Mr Matthew Fisher,** University of Oxford, UK
A toolbox for selective beta-caryophyllene oxidation by engineered CYP102A1

22A **Ms Xiao Juie Wong,** University of Oxford, UK
Wood aroma synthesis by P450-catalysed sesquiterpene oxidation

23B **Dr Konrad Viehrig,** Technical University of Denmark, Denmark
Engineering of geraniol oxidase for heterologous production of plant terpenoids in baker's yeast Saccharomyces cerevisae

24C **Mr Yuan Zhang,** University of Oxford, UK
Selective remote functionalisation of azepane by engineered CYP102A1

I. Biotechnological applications of P450s

25A **Mr Saurabh Kumar Ahirwar,** The University of Adelaide, Australia
Exploring the activity and selectivity of the CYP101B1 and CYP101C1 enzymes from Novosphingobium aromaticivorans

26B **Mr Jong-Min (Joseph) Baek,** The University of Queensland, Australia
The vertebrate ancestor of cytochrome P450 family 3: Optimization of expression and reaction conditions for industrial application

27C **Ms Alessia Andrews,** The University of Manchester, UK
Biochemical studies of peroxygenase enzymes for applications in the fuel industry

28A **Mr Ngoc Tan Cao,** Chonnam National University, South Korea
Regioselective hydroxylation of monacolin J by CYP102A1 to produce 6'-hydroxymethyl metabolite, an inhibitor of HMG-CoA reductase

29B **Mr Heon Jeong,** Chonnam National University, South Korea
Generation of metabolites of neohesperidin dihydrochalcone by bacterial CYP102A1

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30C **Miss Bethan Jones,** University of Manchester, UK
Regio- and enantio-selective chemo-enzymatic C-H-lactonization of decanoic acid to (S)-δ-decalactone

31A **Dr Nico Kress,** University of Manchester, UK
Identification and characterization of new thermostable self-sufficient cytochrome P450 monooxygenases

32B **Ms Ngoc Anh Nguyen,** Chonnam National University, South Korea
Biocatalytic production of a potent inhibitor of adipocyte differentiation from apple-derived phloretin

33C **Ms Thi Huong Ha Nguyen,** Chonnam National University, South Korea
Regioselective hydroxylation of naringin dihydrochalcone, an artificial sweetener, to catechol product, neoeriocitrin dihydrochalcone, by Bacillus megaterium CYP102A1

34A **Ms Silja Strohmaier,** The University of Queensland, Australia
The ability of P450s to be supported by oxygen surrogates is substrate-dependent

35B **Ms Silja Strohmaier,** The University of Queensland, Australia
NADPH - and redox partner-free catalysis by ancestral cytochrome P450 enzymes

36C **Mr Dominic Whittall,** University of Manchester, UK
Profound alteration of P450 BM3 regioselectivity via a single point mutation

37A **Dr Julien Tailhades,** Monash University, Australia
P450-mediated oxidation cascade applied to vancomycin substrates: A serendipity story

38B **Mr Yongwei Zhao,** Monash University, Australia
P450 enzyme cascade to generate tetracyclic teicoplanin

J. Bioinformatics

39C **Ms Courtney Lewis,** University of The Sunshine Coast, Australia
Defining the CYP450 repertoire across metamorphosis in spiny lobsters

40A **Dr Tomer Ventura,** University of The Sunshine Coast, Australia
Closing gaps in invertebrate development using crustacean CYP450 omics, 3D modelling and rapid in vitro assays

K. Novel P450s from microbes

41B **Miss Ava Ho,** The University of Queensland, Australia
Potential steroid metabolising Cytochrome P450s from Rhodococcus rhodochrous

42C **Assoc Prof Brian Monk,** University of Otago, New Zealand
Exploring the impact of amino acid changes on fungal sterol 14α-demethylase structure and function using a yeast model

43A **Ms Yasmeen Ruma,** University of Otago, New Zealand
Development of Cryptococcus neoformans and Candida parapsilosis lanosterol 14α-demethylase as drug targets

44B **Mr Hayama Tsutsumi,** The University of Tokyo, Japan
Two novel cytochrome P450s involved in the biosynthesis of benzastatins

L. Novel reactions/novel chemistry

45C **Mr Joel Lee,** The University of Adelaide, Australia
P450 catalysed citran-ring formation in Bruceol Biosynthesis

M. P450s in drug and other human xenobiotic metabolism (DMPK)

46A **Mr Przemysław Danek,** Institute of Pharmacology Polish Academy of Sciences, Poland
The effect of the novel atypical antipsychotic drug asenapine on human cytochrome P450 1A (CYP1A) expression and activity

47B **Dr Porntipa Korprasertthaworn,** Mahidol University, Thailand
The inhibitory effects of Thai herb extracts on CYP450-mediated anticancer metabolism

48C **Dr Ilia Denisov,** University of Illinois, USA
Allosteric interactions in CYP3A4 probed by site directed mutations

49A **Prof Yasuhiro Masubuchi,** Chiba Institute of Science, Japan
Time-dependent inhibition of CYP1A2 by stiripentol and its structurally related methylenedioxyphenyl compounds

50B **Dr Hideo Shiohira,** University of The Ryukyus Hospital, Japan
Increased plasma tacrolimus concentration after a single intravenous administration of voriconazole: A case of drug-drug interaction

51C **Prof Toshiro Niwa,** Shinshu University Hospital, Japan
Dopamine formation from p-tyramine mediated by human CYP2D6 in the brain

52A **Miss Sian Thistlethwaite,** University of Manchester, UK
Bacterial P450 engineering for production of valuable drug metabolites

53B **Mrs Susanne Steinbrecht,** Institute of Biotechnology, Germany
Metabolic activity testing can underestimate acute drug cytotoxicity as revealed by HepG2 cell clones overexpressing cytochrome P450 2C19 and 3A4

54C **Prof Qing-Yu Zhang,** University of Arizona, USA
Effects of arsenic exposure on CYP expression and drug metabolism

55A **Dr Satoshi Yamaori,** Shinshu University Hospital, Japan
Characterization of epalrestat as a highly selective CYP4A11 inhibitor

N. Pharmacogenetics

56B **Mr Masaki Kumondai,** Tohoku University, Japan
Functional characterization of 11 allelic variants of CYP2C9 identified in 3554 Japanese individuals

57C **Assoc Prof Amit Pandey,** University of Bern, Switzerland
Variability in drug metabolizing cytochrome P450 CYP2C9, CYP2C19 and CYP3A5 activities caused by Genetic Variations in Cytochrome P450 Oxidoreductase (POR)

58A **Assoc Prof Pavel Soucek,** Charles University, Czech Republic
Pharmacogenomics of cytochromes P450 in breast cancer patients

59B **Dr Yune-Fang Ueng,** National Research Institute of Chinese Medicine, Taiwan
The association of CYP2D6(C100T) allele and blood lipid levels with plasma endoxifen level in breast cancer patients in Taiwan

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O. P450 regulation

60C **Dr Ewa Bromek,** Institute of Pharmacology Polish Academy of Sciences, Poland
The expression of cytochrome P450 in the liver is regulated by the GluN2B subunit NMDA receptor antagonist CP-101,606

61A **Prof Władysława Daniel,** Institute of Pharmacology Polish Academy of Sciences, Poland
The positive allosteric modulator of mGlu5 receptor (VU 0360172), but not the mGlu2/3 receptor agonist (LY354740) affects liver cytochrome P450

62B **Dr Gábor Mátis,** University of Veterinary Medicine Budapest, Hungary
Nutritional modulation of intestinal cytochrome P450 enzymes in broiler chicken

63C **Dr Gábor Mátis,** University of Veterinary Medicine Budapest, Hungary
Investigations on hepatic and intestinal cytochrome P450 enzymes in wild boar and domestic pig

64A **Prof Petr Pavek, Charles University,** Czech Republic
Stilbene compound trans-3,4,5,4´-tetramethoxystilbene regulates constitutive androstane receptor (Car) target genes, but does not possess proliferative activity in mouse liver

P. P450s in molecular toxicology

65B **Prof Young-Jin Chun,** Chung-ang University, South Korea
Human CYP1B1 protects cancer cell apoptosis through TRAIL-FOXO3-Skp2 pathway

66C **Miss Emily Fox,** University of Manchester, UK
The study of cytochrome P450s from environmentally sensitive species

Q. Human extrahepatic P450s

67A **Ms Sarah Glass,** Vanderbilt University School of Medicine, USA
Localization and quantification of cytochrome P450 27C1 in human skin

68B **Prof Tamihide Matsunaga,** Nagoya City University, Japan
Differentiation of human iPS cells into enterocyte-like cells using cAMP-activating compounds and these functions

R. P450s in human physiology and disease

69C **Dr Miyu Nishikawa,** Toyama Prefectural University, Japan
Comparative study of 25-hydroxyvitamin D3 treatment between Cyp27b1 knockout and Vdr (R270L) rats to evaluate clinical effects of 25(OH)D3

70A **Assoc Prof Amit Pandey,** University of Bern, Switzerland
Cytochrome P450 Aromatase (CYP19A1) deficiency caused by a Novel Mutation in the NADPH Cytochrome P450 Oxidoreductase

S. P450 evolution

71B **Mr Marcos Hamborg Vinde,** The University of Queensland, Australia
Exploring cytochromes P450-mediated diversification of the strigolactone structure via ancestral sequence reconstruction of the CYP711A family

72C **Mr Kurt Harris,** The University of Queensland, Australia
Ancestral reconstruction of cytochrome P450 family 1: Improved thermostability for biocatalysis and insights into CYP1 evolution

73A **Ms Connie Ross,** The University of Queensland, Australia
Ancestral sequence reconstruction of the CYP2U subfamily

U. P450s in plants and plant secondary metabolism

74B **Mr Justin Miller,** University of Illinois At Urbana-Champaign, USA
Investigation of structural residues required for metabolism of loganic acid by Camptotheca acuminata secologanic acid synthases (CYP72As)

75C **Dr Christian Molitor,** Technical University of Vienna, Austria
Heterologous expression of chalcone 3-hydroxylase from Dahlia variabilis in E. coli as a soluble enzyme

76A **Miss Lauren Salisbury,** The University of Queensland, Australia
Dioscorea transversa CYP90B57 catalyses the C22R-hydroxylation of cholesterol, an essential step in steroidal saponin biosynthesis

77B **Ms Julia Weissensteiner,** Technical University of Vienna, Austria
Characterization of a full-size CYP75A in Euphorbia pulcherrima

V. Terpenoid metabolism

78C **Mr Peter Giang,** The University of Queensland, Australia
Terpene-metabolising cytochromes P450 from Rhodococcus rhodochrous

W. P450s in steroid biosynthesis and metabolism

79A **Mr James Beckett,** The University of Queensland, Australia
Synthesis of hydroxycholesterols and derivatives for exploration of Cytochromes P450 in steroidal saponins biosynthesis and M. tuberculosis inhibition

80B **Dr Stella Child,** Vanderbilt University School of Medicine, USA
Arginine-124 is involved in electron transfer in a protozoan cytochrome P450 CYP51 enzyme

81C **Mr Luke Churchman,** The University of Queensland, Australia
Synthesis of intermediates in steroidal saponin biosynthesis

82A **Dr Michael Reddish,** Vanderbilt University School of Medicine, USA
Some reactions require commitment: Processivity of human P450 11B2 reactions

83B **Assoc Prof Amit Pandey,** University of Bern, Switzerland
Inhibitory effects of Curcuma longa extracts on the steroid metabolizing cytochrome P450 enzymes

X. P450s in insects / pesticides

84C **Mr Alex Giang,** The University of Melbourne, Australia
Evaluating the resistance potential of Drosophila melanogaster cytochrome P450 genes by transgenic overexpression

W. P450s in steroid biosynthesis and metabolism

85A **Assoc Prof Robert Tuckey,** The University of Western Australia, Australia
CYP27A1 but not CYP2R1 can metabolise vitamin D3-3-sulfate