OMICS International
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J Anal Bioanal Tech 2015, 6:4
http://dx.doi.org/10.4172/2155-9872.S1.022

Use of "Omics" technologies for mechanistic understandings of toxicological events

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Drug toxicity observed in pre-/non-clinical animal studies sometimes leads to discontinuation of drug candidates. Understanding the phenomena or backgrounds surrounding toxicological events occurred must be a key element for attrition improvement in research and development (R&D) of new chemical entities (NCEs), often requiring mechanistic investigations to understand toxicological mechanism of actions and then to make "Go" or "No go" decisions. In the post-genomic era, a battery of "Omics" technologies was introduced and has been rapidly increasing utilization, among which is the prefix of "toxico-" added to each omics technology in toxicology field. Especially, metabolomics in toxicology, which is so-called "toxicometabolomics", has been widely implemented in this area. The objectives are to identify and characterize the metabolites, both endogenous and exogenous, which are the end products of cellular metabolism and drug metabolism, respectively. Moreover, toxicometabolomics enables to capture the phenotypic changes in the events, which are generated by enzymatic proteins as resultants of gene expression, at the molecular level; therefore, smooth translation of the findings can be made into the clinic. The presentation in this session will review the usefulness of toxicometabolomics technologies which are generally nuclear magnetic resonance (NMR)-based and mass spectrometry (MS)-based, and other toxic-Omics technologies. Furthermore, today, newly introduced technology, MS imaging (MSI) is considered applicable in the toxicology field, hence its toxicological usability will be also reviewed.

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LC-MS based rapid secondary metabolite profiling and inhibitory effects of melanin synthesis from marine *Pseudoalteromonas* sp. M2

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The ocean has been large resource such as a marine flora, fauna and food resources. A marine bacterial strain that showed confluent growth on the marine broth and antibacterial activity, was isolated and identified based on the 16S rDNA sequence analysis as a strain of *Pseudoalteromonas* sp., thus named as *Pseudoalteromonas* sp. M2. This strain was produced various secondary metabolites as quinolone alkaloids, we identified nine 4-hydroxy-2-alkylquinoline secondary metabolites (pseudane-III, IV, V, VI, VII, VIII, IX, X, and XI) and closely related two unknown compounds by high-resolution and tandem mass spectrometry. The two unknown compounds were determined to be novel metabolites (2-isopentylquinolin-4-one and 2-(2,3-dimethylbutyl)quinolin-4-one) by NMR analysis. Among the isolated compounds, 2-(2, 3-dimethylbutyl) quinolin-4-one, pseudane-VI, and pseudane-VII showed the inhibition of melanin synthesis in the melan-a cells as 23.0, 28.2, and 42.7%, respectively. Especially, pseudane-VII showed the highest inhibitory effect at 8 μg/ml compared with other compounds. The production of 2-isopentylqunoline-4-one and 2-(2,3-dimetylbutyl) qunoline-4-(1H)-one from marine bacteria has not been reported before. The results of this study suggest that LC-MS/MS based metabolite screening was effective dereplication methods to improve the efficiency of the discovery process of novel metabolite and these compounds may be promising candidates for the development of effective bioactivity.

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