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

Targeted ^{13}C metabolic tracer fate association study and regression analysis reveal diverse cellular phenotypes

László G Boros
Harbor-UCLA Medical Center, USA

Regression statistics in this targeted tracer fate association study (TTFAS) is shown to reveal associations among diverse phenotypic metabolic products in fumarate hydratase-deficient UOK kidney tumor cells with defective glutaminolysis, reductive carboxylation for lipogenic citrate production, as well as the Warburg effect, using the [1,2-13C2]-D-glucose tracer. These co-existing profiles were revealed in previous ^{13}C-glutamine and ^{13}C-glucose tracer experiments. Herein UOK cells show a close Warburg-type correlation between consumption of glucose for 13C-lactic acid production (R2>0.98; glucose to lactate). On the other hand, proliferation-related macromolecule 13C labeling, such as that of RNA-derived ribose and lignoceric acid, correlates with the glucose-derived internally cross-labeled ^{13}C-glutamine fraction (R2>0.98; glutamate to lignocerate and RNA ribose). The TTFAS approach reliably re-produces results and conclusions obtained via multiple 13C-tracer metabolic flux analyses using a single metabolic tracer to trim down versatilities, cost and time, involved in multiple metabolic tracer studies using ^{13}C and deuterium as labeling atoms for diverse products.

Boros@LABIOMED.org

Solid state analytical techniques to characterize cocrystals: Ciprofloxacin–hippuric acid co-crystal

Pawanpreet Singh and **Renu Chadha**
University Institute of Pharmaceutical Sciences, India

Co-crystals are crystalline single phase materials composed of two or more different molecular and/or ionic compounds generally in a stoichiometric ratio which are neither solvates nor simple salts. They are of interest to both academic research as well as industry as they represent the opportunity to access new solid forms with modified physical properties including dissolution rate, physical stability and altered pharmacokinetic profile of the API subjected for co-crystallization. The present work represents Ciprofloxacin-Hippuric acid cocrystal which was prepared by solvent assisted grinding method. It was primarily characterized by FTIR showing shift in –COOH stretch at 3264.1 cm-1 in cocrystal as compared to 3405.2 and 3343.9 cm-1 in drug and coformer respectively. The C-N stretch also shifted from 1380 cm-1 to 1385.2 cm-1. The cocrystal was then confirmed by Differential scanning calorimetry showing single melting endothermic transition at 218.9oC irrespective of both components showing formation of new stable phase. XRPD pattern of cocrystal shows disappearance of two major peaks at 14.7 and 24.9o 2θ while another major peak shows drastic shift from 25.5 to 19.5o 2θ. Fortunately, the development of XRPD equipment and structure solving algorithms makes it possible to extract the crystal structure from the XRPD pattern. Recently, peers introduced a protocol to confirm the refined result using combination of XRPD and solid state NMR data. The NMR chemical shift values (1H, 13C, 15N) were also computed to validate the refined cocrystal structure.

p.s.chadha87@gmail.com