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(71) Applicant *(for all designated States except US)*: **AGENCY FOR SCIENCE, TECHNOLOGY AND RESEARCH** [SG/SG]; 1 Fusionopolis Way #20-10, Connexis, Singapore 138632 (SG).

(72) Inventors; and

(75) Inventors/Applicants *(for US only)*: **LEE, Dong-Yup** [KR/SG]; c/o Bioprocessing Technology Institute, 20 Biopolis Way #06-01, Centros, Singapore 138668 (SG). **LEE, Terk Shuen** [SG/SG]; c/o Bioprocessing Technology Institute, 20 Biopolis Way #06-01, Centros, Singapore 138668 (SG). **HO, Ying Swan** [SG/SG]; c/o Bioprocessing Technology Institute, 20 Biopolis Way #06-01, Centros, Singapore 138668 (SG).

(74) Agent: **VIERING, JENTSCHURA & PARTNER LLP**; P.O. Box 1088, Rochor Post Office, Rochor Road, Singapore 911833 (SG).

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(54) Title: A METHOD, AN APPARATUS, AND A COMPUTER PROGRAM PRODUCT FOR IDENTIFYING METABOLITES FROM LIQUID CHROMATOGRAPHY-MASS SPECTROMETRY MEASUREMENTS

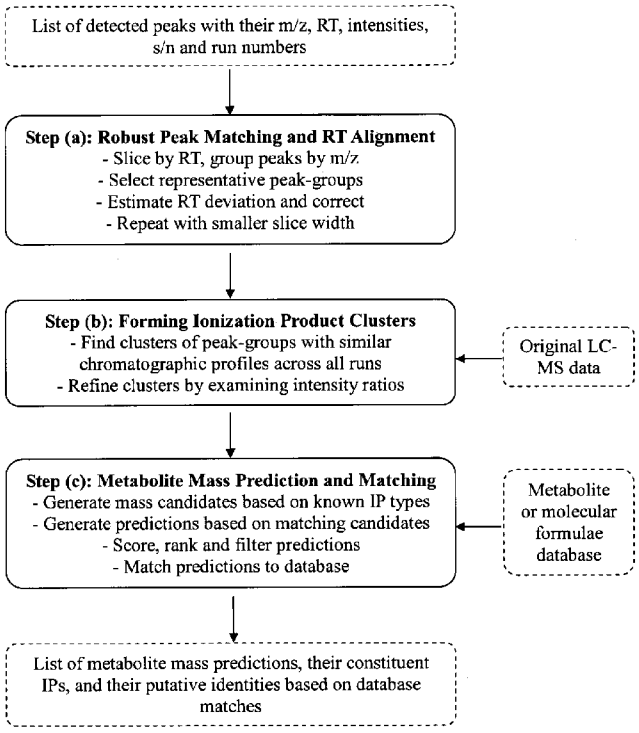


FIGURE 1

(57) Abstract: The present invention relates to a method for identifying metabolites present in a set of samples. The method may include: (a) forming a plurality of peak-groups, wherein each peak-group comprises mass peaks representative of a specific ion in each chromatographic run; (b) forming a plurality of clusters, wherein each cluster comprises at least one peak-group of (a) each having similar chromatographic profiles; and (c) generating a list of metabolite predictions, wherein each metabolite prediction is selected from the plurality of clusters of (b).

WO 2012/125121 A1

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