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Dynamic bioinformatics indices as the quantitative functional biomarkers for drug discovery and development

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Biomarkers usually consist of target markers, labeled markers and surrogate markers. Since they are parts of bioinformatics, it is proposed to add functional dynamic markers to promote functional relevance and practical usefulness. Unlike the conventional direct markers, the functional dynamic indices are intrinsic hidden properties that need to be revealed and quantitatively determined. The functional dynamics of a particle, molecule, drug or a defined system are all based on the median-effect equation as the general unified physico-chemical principle of the mass-action law as has been elaborated in Chou TC. Pharmacol. Rev. 58: 621-681, 2006 (free web access: http://pharmrev.aspetjournals.org/content/58/3/621). The dynamics is determined by the dose and effect algorithm of the mass-action law parameters such as the potency (the Dm value), the dynamic order (the m value) and the relevance index (the r value). The potency is defined as the median-effect dose; the dynamic order is represented by the shape of dose-effect curve (m=1, >1 and <1 indicates hyperbolic, sigmoidal and flat sigmoidal, respectively); and the relevance index is determined by the linear correlation coefficient of the median-effect plot (Chou TC. Integrative Biol. 3: 548-559, 2011; DOI: 10.1039/c0ib00130a). The functional dynamics can be quantified by the mass-action law algorithm, which is the basis for automated computer simulation (www.combosyn.com). The median-effect equation as the unified theory is for all dose-effect analysis (Dm, m, and r) and the combination index (CI) theorem is for all drug combinations where synergism (CI<1), additive effect (CI=1) and antagonism (CI>1), and to provide the dose-reduction index (DRI) for each drug where DRI>1, =1, and <1 indicate favorable dose reduction, no dose reduction, and unfavorable dose reduction, respectively; and also provide selectivity index [e.g., the therapeutic index (TD)x/(ED)x]. These indices are the most basic functional informatics that can be defined as biomarkers or bio-indices which are dimensionless quantities that make the mechanisms and units irrelevant. These new quantified index markers can be directly translated into therapeutic results.

Biography

Ting-Chao Chou received Ph.D. in Pharmacology from Yale University and postdoctoral training at the Johns Hopkins University School of Medicine. He joined Memorial Sloan-Kettering Cancer Center (MSKCC) and became a Member and a Professor of Pharmacology at Cornell University Graduate School of Medical Sciences in 1988. He is the Honorary Professor at Chinese Academy of Medical Sciences in Beijing and as the Visiting Professor at five other universities. Currently, he is the Director of Preclinical Pharmacology Core Laboratory at MSKCC.

Dr. Chou published 252 scientific articles, which have been cited over 13,210 times with H-index of 55. Dr. Chou derived median-effect equation of the mass-action law, and with Paul Talalay, introduced the combination index theorem (www.researcherid.com/rid/B-4111-2009). Chou is the co-inventor of 30 US patents and several of them are in clinical trials in U.S.

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