[P48] Global Mapping of Traditional Chinese Medicine (TCM) Into Bioactivity Space Improves Mechanistic Understanding and Discovers Relationships Between Medicinal Classes

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While Traditional Chinese Medicine (TCM) has been of great importance consistently throughout the years in the Far East, there is still lack of scientific rationale for the workings of TCM to be accepted into western scientific thinking. Given the tremendous increase in TCM data on the chemical ingredients, activities against protein targets, and biomarker readouts, we are now in the position to make a much stronger scientific case for this type of treatments. By using computational approaches, we could first establish the link between the top three enriched targets to the description of the respective medicinal subclass and we found that immunomodulatory targets, tyrosine-protein phosphatase non-receptor type 2 (PTPN2), steryl-sulfatase (STS), leukotriene B4 receptor 1 (LTB4-R1), protein kinase C beta type (PKC-β), and protein kinase C eta type (PKC-ε), are most frequently appeared as TCM views symptoms as the invasion of pathogenic factors, thus sensitise the immune system. In the second analysis, we are able for the first time to present a 'global TCM mapping' into bioactivity space. This study enabled us to discover connections between different subclasses that are not apparent by their compounds. Five major protein families were found to contribute the bioactivity profiles of the clusters in the dendrogram, which GPCR and protein kinase family are the two major protein families that contribute to the diversity of the bioactivity space due to various biological processes that the proteins are involved in. Hence, this study not only elucidates the mode-of-actions (MOAs) of the compounds per subclasses but also the patterns of bioactivity space acquire by the clusters.