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In vitro cancer cell line classification using pattern recognition approach based on metabolite profiling (Article)

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Abstract

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This study aims to evaluate the feasibility of metabolite profiling for the characterisation and discrimination volatile compounds using the pattern recognition from in vitro cancer cell lines, which are lung, breast and colon cancer together with the blank medium as a control group. This study implemented the A549 (lung), MCF7 (breast) and HCT116 (colon). Cells were harvested and maintained until they grow as monolayer adherent and reach confluence 70-90% before sampling. The volatiles profile from the targeted cell line was established using headspace solid phase microextraction coupled to gas chromatography-mass spectrometry (HS-SPME/GCMS). Multivariate data analysis employed principal component analysis (PCA) to better visualise the subtle similarities and the differences among these data sets. A total of 116 volatile organic compounds were detected focused on a limited range of retention time from 3rd until 17th minutes, and 33 compounds were recognized as targeted compounds (peak area>1%). According to both results, the score and the loading plot explained 83% of the total variance. The volatiles compound has shown to be significantly distinguished among cancerous and control group based on metabolite profiling using pattern recognition approach.

Reaxys Database Information

View Compounds

Author keywords

GCMS | Headspace SPME | In Vitro Cell Line | Metabolite Profiling | Pattern Recognition

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