Global Imaging Insights

Clinical Image

ISSN: 2399-7397

Modelling and simulation of ^{13}C, ^{15}N, ^{17}O NMR chemical shifts, ^{17}O and ^{14}N electric field gradients and measurement of ^{13}C and ^{15}N chemical shifts in DNA/RNA of human gum cancer cells, tissues and tumors using NMR biospectroscopic profiling for novel systems diagnostics

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Abstract

Differences in the cancers (treated and untreated) individuals and uninfected controls were identified with a NMR metabolomics approach. The current study was limited in sample size but provided original insights for modelling and simulation of ^{13}C, ^{15}N, ^{17}O NMR chemical shifts, ^{17}O and ^{14}N electric field gradients and measurement of ^{13}C and ^{15}N chemical shifts in DNA/RNA of human gum cancer cells, tissues and tumors using NMR biospectroscopic profiling of gum cancer cells, tissues and tumors for novel systems diagnostics. This work has demonstrated the reliability, simplicity, and predictive ability of NMR–based metabolomics in discriminating between the experimental groups studied in our sample.

Introduction

Modelling and simulation of ^{13}C, ^{15}N, ^{17}O NMR chemical shifts, ^{17}O and ^{14}N electric field gradients and measurement of ^{13}C and ^{15}N chemical shifts in DNA/RNA of human gum cancer cells, tissues and tumors using NMR biospectroscopic profiling of gum cancer cells, tissues and tumors for novel systems diagnostics was applied to determine the effect of human gum cancer infection on blood and plasma components. NMR biospectroscopic profile of the infected samples showed specific biomolecular information including reduction in body components especially DNA and RNA as compared to the healthy samples. Therefore, modelling and simulation of ^{13}C, ^{15}N, ^{17}O NMR chemical shifts, ^{17}O and ^{14}N electric field gradients and measurement of ^{13}C and ^{15}N chemical shifts in DNA/RNA of human gum cancer cells, tissues and tumors using NMR biospectroscopic profiling of gum cancer cells, tissues and tumors for novel systems diagnostics may be a suitable candidate for evaluating human gum cancer infection related changes in blood and plasma samples thus providing useful information that can really help in diagnosis especially at individual level and potentially early screening of the cancer [1-10].

Results and discussion

NMR biospectroscopy and its fingerprinting capabilities or rapid, high–throughput, and non–destructive analysis of a wide range of sample types producing a characteristic chemical "fingerprint" with a unique signature profile for modelling and simulation of ^{13}C, ^{15}N, ^{17}O NMR chemical shifts, ^{17}O and ^{14}N electric field gradients and measurement of ^{13}C and ^{15}N chemical shifts in DNA/RNA of human gum cancer cells, tissues and tumors using NMR biospectroscopic profiling of gum cancer cells, tissues and tumors for novel systems diagnostics. Nuclear magnetic resonance (NMR) biospectroscopy and an array of mass spectrometry (MS) techniques provide selectivity and specificity for modelling and simulation of ^{13}C, ^{15}N, ^{17}O NMR chemical shifts, ^{17}O and ^{14}N electric field gradients and measurement of ^{13}C and ^{15}N chemical shifts in DNA/RNA of human gum cancer cells, tissues and tumors using NMR biospectroscopic profiling of gum cancer cells, tissues and tumors for novel systems diagnostics, but demand costly instrumentation, complex sample pretreatment, are labor–intensive, require well–trained technicians to operate the instrumentation, and are less amenable for implementation in clinics. The potential for NMR biospectroscopy techniques to be brought to the bedside gives hope for

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Key words: *NMR biopectroscopy, gum cancer, cancer cells, cancer tissues, cancer tumors, modelling, simulation, chemical shifts, electric field gradients*

Received: March 11, 2021; **Accepted:** April 12, 2021; **Published:** April 16, 2021

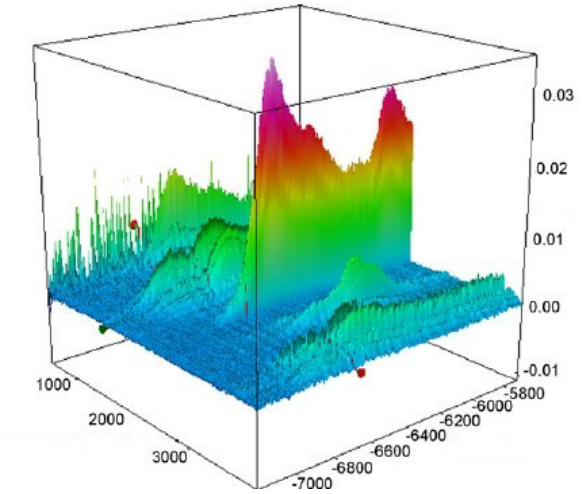

Figure 1. Simulation of ^{13}C, ^{15}N, ^{17}O NMR chemical shifts, ^{17}O and ^{14}N electric field gradients and measurement of ^{13}C and ^{15}N chemical shifts in DNA/RNA of human gum cancer cells, tissues and tumors using NMR biospectroscopic profiling of gum cancer cells, tissues and tumors for novel systems diagnostics

modelling and simulation of ^{13}C, ^{15}N, ^{17}O NMR chemical shifts, ^{17}O and ^{14}N electric field gradients and measurement of ^{13}C and ^{15}N chemical shifts in DNA/RNA of human gum cancer cells, tissues and tumors using NMR biospectroscopic profiling of gum cancer cells, tissues and tumors for novel systems diagnostics in the clinic. We discuss the utilization of current NMR biospectroscopy methodologies on biologic samples as an avenue towards rapid cost saving diagnostics for modelling and simulation of ^{13}C, ^{15}N, ^{17}O NMR chemical shifts, ^{17}O and ^{14}N electric field gradients and measurement of ^{13}C and ^{15}N chemical shifts in DNA/RNA of human gum cancer cells, tissues and tumors using NMR biospectroscopic profiling of gum cancer cells, tissues and tumors for novel systems diagnostics (Figure 1).

Conclusion

NMR biospectroscopic profile of the infected samples showed specific biomolecular information including reduction in body components especially DNA and RNA as compared to the healthy samples. Therefore, modelling and simulation of ^{13}C, ^{15}N, ^{17}O NMR chemical shifts, ^{17}O and ^{14}N electric field gradients and measurement of ^{13}C and ^{15}N chemical shifts in DNA/RNA of human gum cancer cells, tissues and tumors using NMR biospectroscopic profiling of gum cancer cells, tissues and tumors for novel systems diagnostics may be a suitable candidate for evaluating human gum cancer infection related changes in blood and plasma samples thus providing useful information that can really help in diagnosis especially at individual level and potentially early screening of the cancer. Future studies with larger subject numbers are warranted to expand upon the present findings.

Acknowledgement

This study was supported by the Cancer Research Institute (CRI) Project of Scientific Instrument and Equipment Development, the National Natural Science Foundation of the United Sates, the International Joint BioSpectroscopy Core Research Laboratory Program supported by the California South University (CSU), and the Key project supported by the American International Standards Institute (AISI), Irvine, California, USA.

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