

# Binomial sequence for selective quadrupolar $^{23}\text{Na}$ in vitro and in vivo NMR and MRI

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## Introduction

Sodium NMR and MRI is a non-invasive technique, in which elegant tailored experiments is capable of separating the intracellular and extracellular sodium ions. Intracellular sodium ions exhibit a quadrupolar interaction, while the extracellular do not. By monitoring exclusively the intracellular component of the total sodium concentration, valuable metabolic insight might be obtained. Binomial sequences are a simple but powerful water suppression technique in liquid state NMR. We want to explore the possibility for the use of binomial sequences for in vitro and in vivo sodium intra and extra cellular pool selective excitation. Recently [1, 2], have implemented a sequence denoted as quadrupolar jump and return (QJR) which in principle is a  $1\bar{1}$  binomial jump and return used for water suppression applied on spin  $3/2$  nuclei. This sequence, however, showed new and extremely interesting trends for in vivo sodium NMR and MRI, as the sequence suppresses both the signal from extracellular sodium and the satellite transitions of the intracellular sodium increasing the central transition of the later. In this study we investigate by simulations and experiments, the binomial series on a  $^{23}\text{Na}$  liquid crystal, for further in vivo and in vitro implementation.

## Method

Simulation where performed in the open source software Simpson [3], where the different binomial sequences, where simulated and their response where observed. The NMR experiment where performed on a 7 T horizontal bore magnet, bore diameter 11 cm. (Oxford Instruments, Oxford, UK) with a Unity Inova console (Varian, Paolo Alto, CA, USA). The experimental results where performed on a Sodium Linoleate sample, showing quadrupolar coupling CQ of 4000 Hz.

## Results

Both experiments (fig. 1) and simulations (fig. 2) suggest that the normal ( $S=1/2$ ) properties of the binomial sequences hold as long as the flip angle is approximately  $1/4$  of the optimal 90 degree flip angle. It also shows that the higher order has narrower excitation bands as one move up through the binomial order. The  $1\bar{1}$ ,  $1\bar{2}\bar{1}$ ,  $1\bar{3}\bar{3}\bar{1}$ ,  $1\bar{4}\bar{6}\bar{4}\bar{1}$ ,  $1\bar{5}\bar{1}\bar{0}\bar{1}\bar{0}\bar{5}\bar{1}$  type binomial sequences show good suppression, exclusively in the satellite transition. The signal gain achieved by QJR  $1\bar{1}$  experiment, is reproducible within the higher order QJR experiments  $1\bar{2}\bar{1}$ ,  $1\bar{3}\bar{3}\bar{1}$ ,  $1\bar{4}\bar{6}\bar{4}\bar{1}$ ,  $1\bar{5}\bar{1}\bar{0}\bar{1}\bar{0}\bar{5}\bar{1}$ .

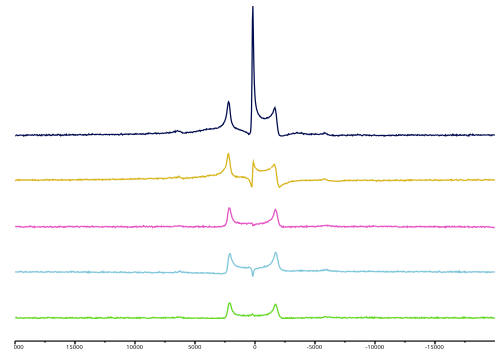


Figure 1 Experimental results of the low flip angle regime  $1\bar{1}$ ,  $1\bar{2}\bar{1}$ ,  $1\bar{3}\bar{3}\bar{1}$ ,  $1\bar{4}\bar{6}\bar{4}\bar{1}$ ,  $1\bar{5}\bar{1}\bar{0}\bar{1}\bar{0}\bar{5}\bar{1}$  from top to bottom. Sodium Linoleate 24 w% liquid crystal sample showing a CQ = 4000 Hz, with broad satellites. Shows increasing suppression of the central transition, for the higher order binomial sequences.

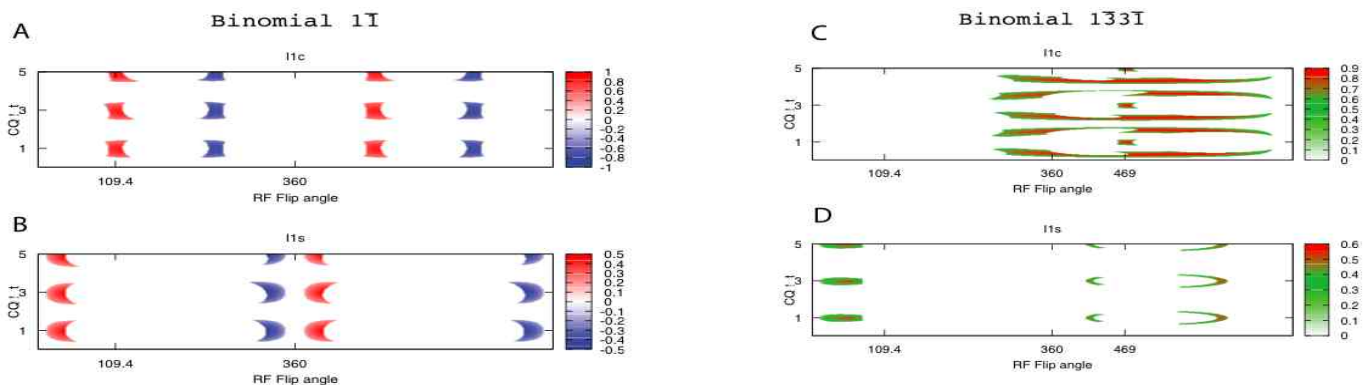


Figure 2 The effect of quadrupolar coupling CQ and the inter pulse delay versus the total flip angle. Plot A and C shows the central transition Ic and plot B and D shows the satellite transition Is components of the signal. The plot shows intensity if the counterpart intensities are in the range  $[-0.1:0.1]$  and the projection onto the given operator is larger than 0.5 in the  $1\bar{1}$  case and 0.2 in the  $1\bar{3}\bar{3}\bar{1}$  case. The plot shows the cyclic and the power domain responses, showing the narrow band selectivity for higher order binomial sequences and the double experiment trends of the jump and return type experiments ( $1\bar{1}$ ) 54.7 degrees for each of the two pulses, while ( $1\bar{3}\bar{3}\bar{1}$ ) is 469 degrees, divided on the 8 subpulses. The low flip angle regime is around 22.2 degrees, shown in both Is cases.

## Conclusion

We have demonstrated  $^{23}\text{Na}$  binomial sequences as a general tool for sodium NMR and MRI, where the higher order binomial experiments can be used if narrow band excitation/suppression is needed, for in vivo or in vitro systems.

## References

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