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# HW/SW Co-Design and test of a SoC-FPGA based NQR Compact Spectrometer

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## (1) NUCLEAR QUADRUPOLEAR RESONANCE

Nuclear Quadrupolar Resonance (NQR) is a spectroscopy technique that is used to study nuclei with spin superior to 1/2 like  $^{14}\text{N}$ ,  $^{35}\text{Cl}$ ,  $^{27}\text{Al}$  and  $^{127}\text{I}$  [1]. The NQR is well suited for a broad range of portable applications, nevertheless it suffers from a relatively weak sensitivity and susceptibility to external noise.

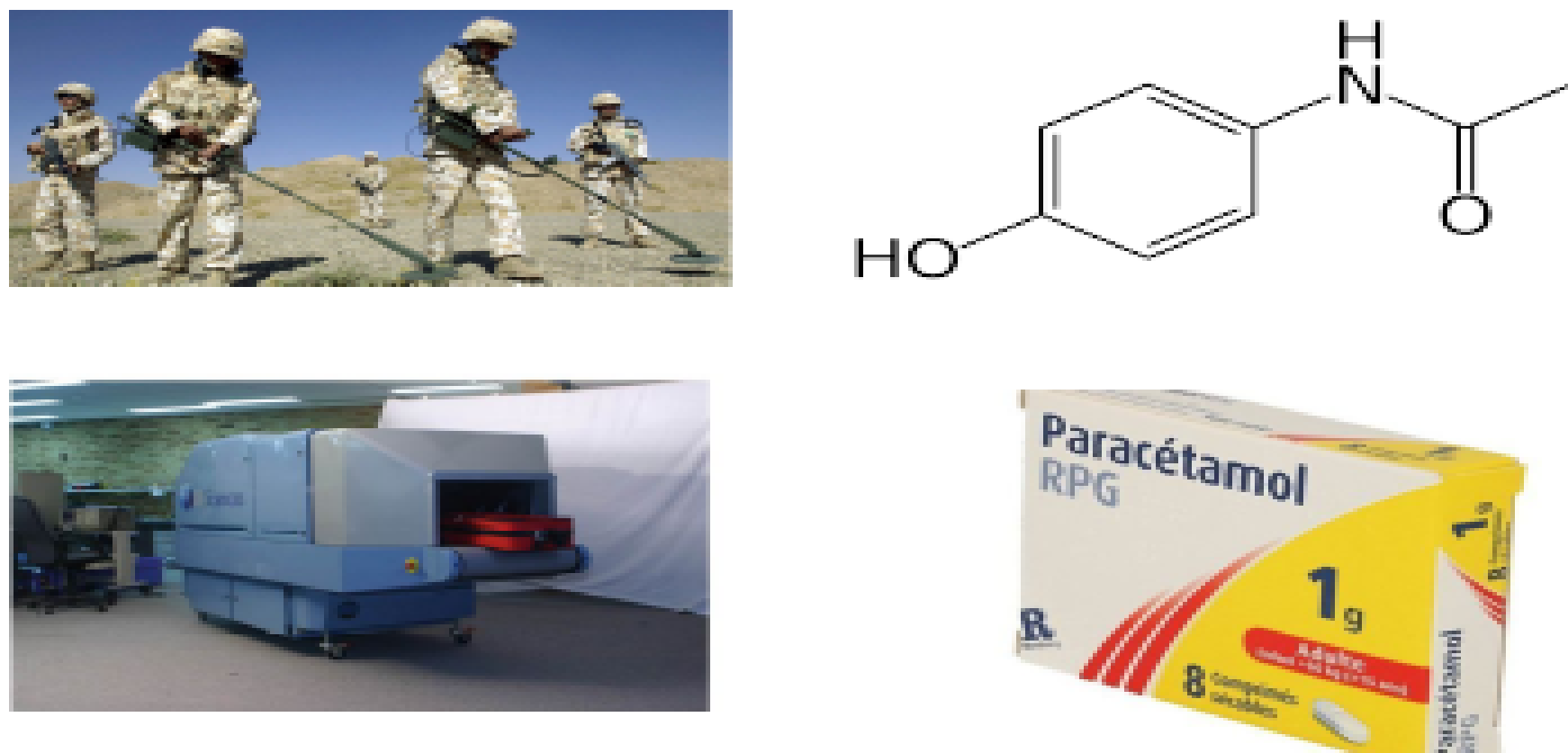


Fig. 1 NQR applications

Several portable spectrometers were presented in the literature, but those designed for NQR have critical components in the analog domain, inducing low sensitivity resulting from various types of noise. Moreover, they have limited performances [2].

## (2) PROPOSED SOLUTION

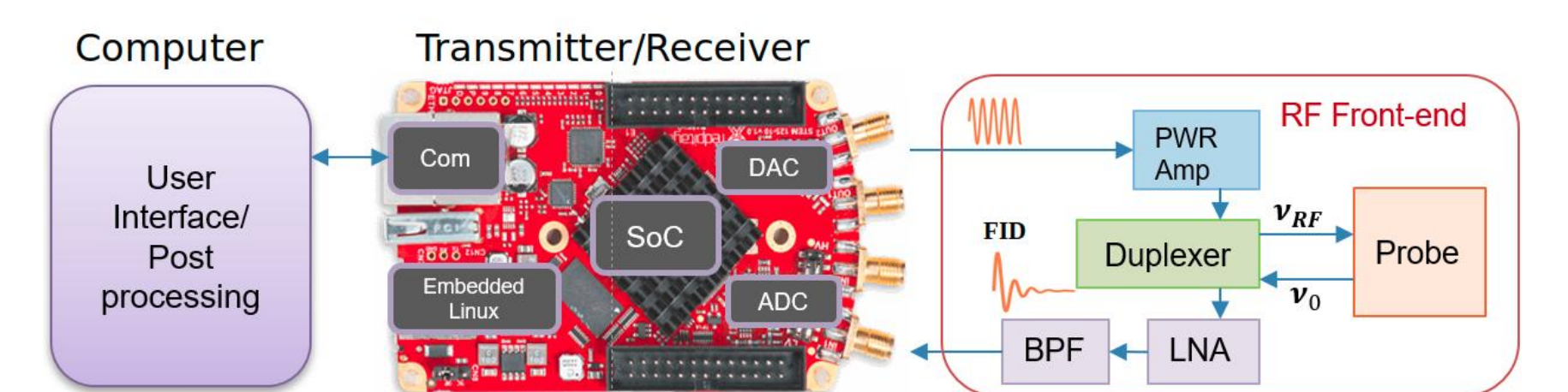


Fig. 2 New NQR spectrometer.

The work introduces a SoC-FPGA based [3] solution for spectrometer integration of key hardware and software parts including, a high resolution pulser, a fully controllable pulse transmitter, an acquisition module, in addition to embedded software applications. The objective is to increase portability, sensitivity and immunity to various noise sources.

## (3) SoC-FPGA HW/SW Co-DESIGN AND VERIFICATION

The proposed solution consists in digital hardware and software co-design of a SoC-FPGA. The used technology is a Zynq 7010 AP-SoC. Digital implementation and embedded software development were performed using Vivado, Xilinx IP catalog and SDK. The SoC-FPGA is located on the Redpitaya board.

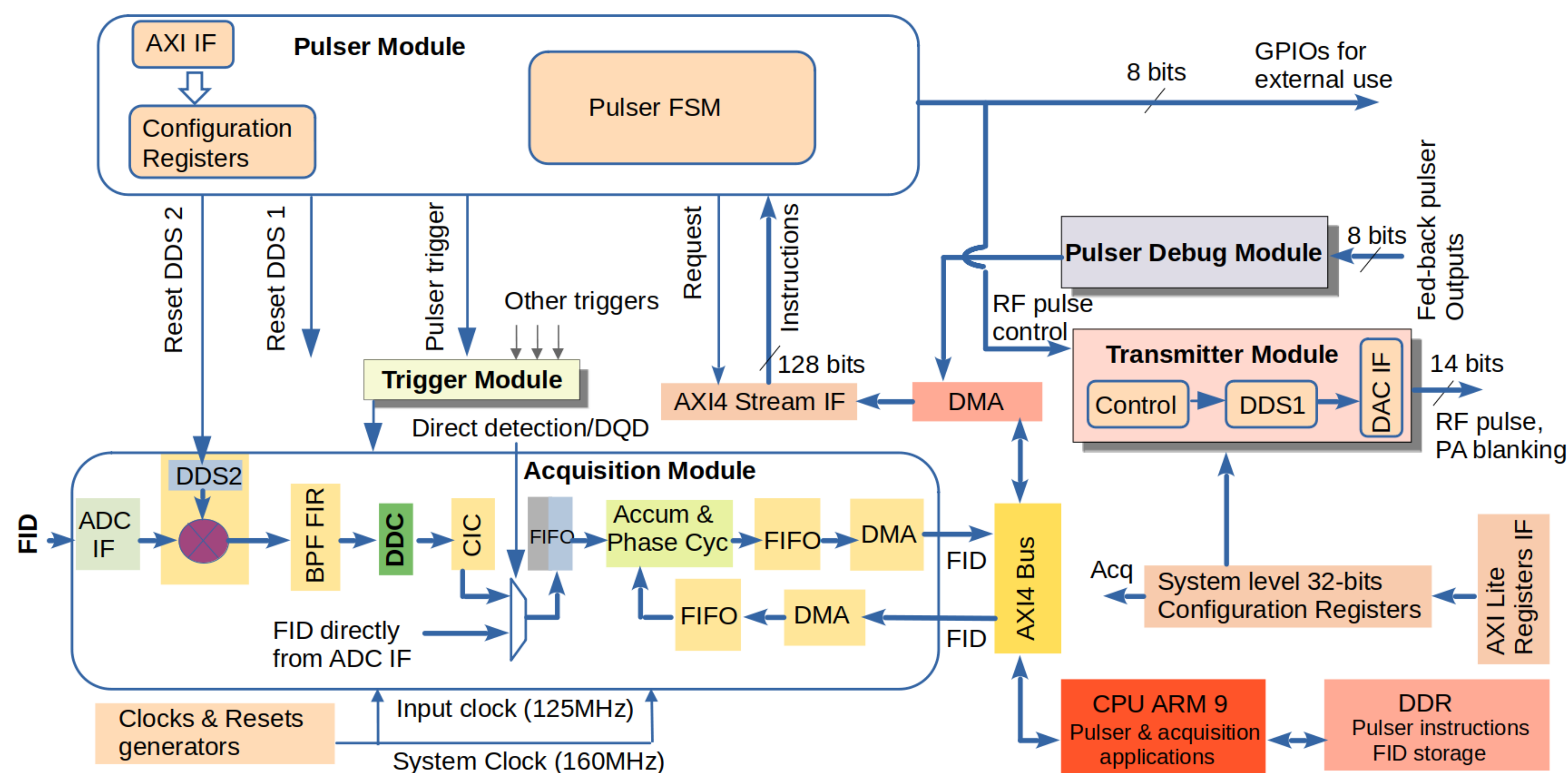


Fig. 3 Simplified diagram of the SoC-FPGA architecture

In the proposed solution, many of the traditional analog parts of the spectrometer are replaced by digital blocks that are integrated inside the SoC-FPGA.

The designed digital modules are:

- **An acquisition module:** processes the incoming signal FID and stores it inside the DDR via a Xilinx AXI DMA. Signal accumulation is done On-The-Fly on FPGA.
- **A pulser module:** generates the pulse sequence control signals (8 ns resolution).
- **A transmitter module:** based on a Xilinx DDS that is controlled in phase, and frequency. The RF pulse amplitude is also controlled digitally.
- **Auxiliary modules:** pulser debug module, trigger module, registers interface, etc.

SoC level integration and synchronization is performed by the usage and the configuration of the following Xilinx IPs: ARM 9 CPU, FIFOs, DMAs, DDR, AXI4 Bus, clocking wizard, etc.

Linux embedded applications were written in order to drive the pulser, the acquisition and the spectrometer. After rigorous bit-accurate RTL simulation and stand-alone on-target validation, the embedded system was interfaced with the analog front-end and the host post-processing software to validate its system level behavior.

## (4) VALIDATION RESULTS

The SoC-FPGA based NQR spectrometer was tested on reference samples (e.g., Sodium Nitrate, Hexamethylenetetramine, Sodium nitroprusside, Succinimide and 1,3,5-Trichlorobenzene) to check its functionality over the NQR frequency range. A sensitivity equivalent to Bruker spectrometer was obtained for  $^{35}\text{Cl}$  spectra (figure 4.d). The spectrometer was also tested on paracetamol to identify the synthesized polymorph (Monoclinic) and to analyze the impact of the tablet compression on the line width (figure 5).

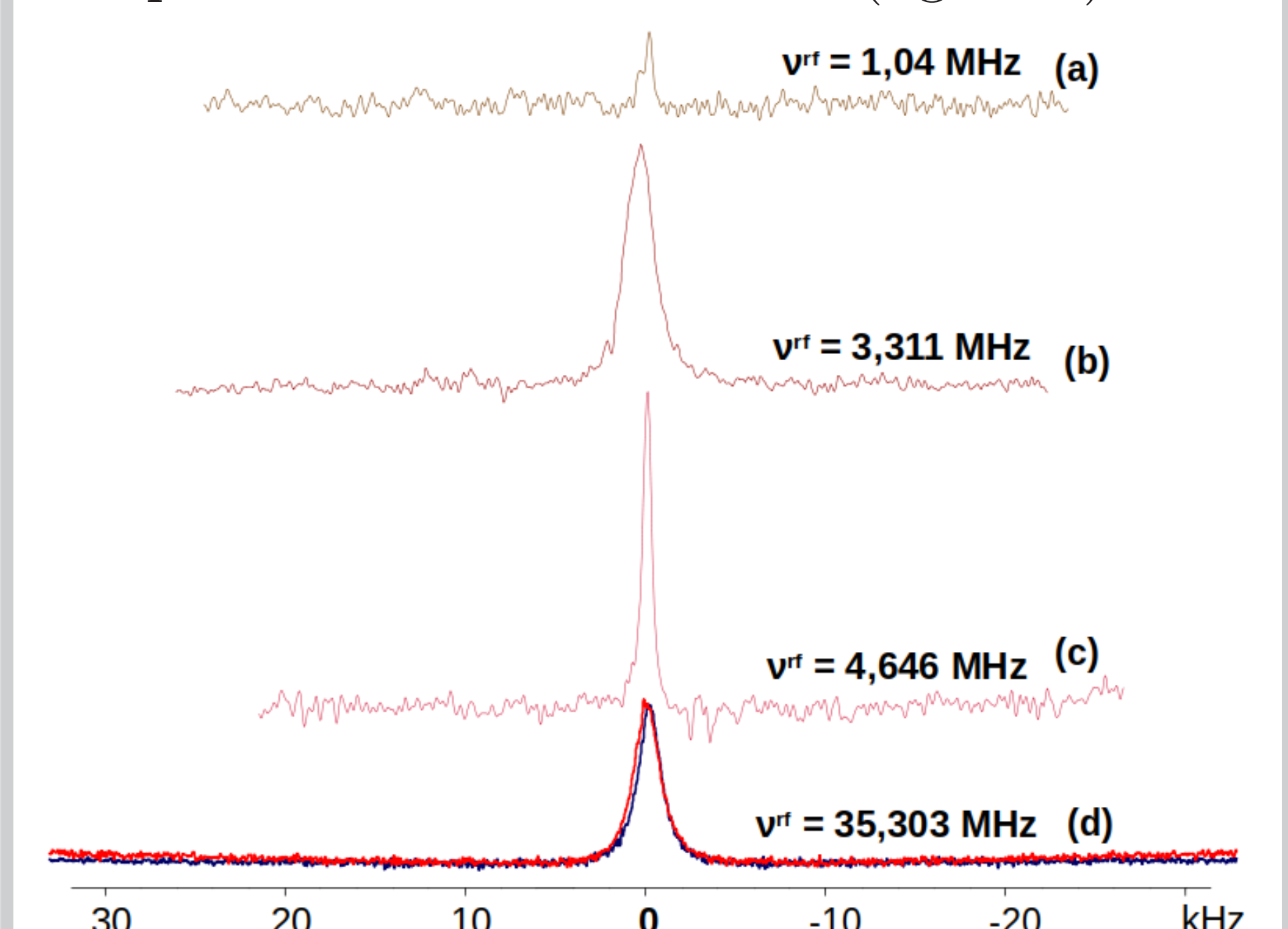


Fig. 4 Reference samples: lowest and highest frequencies of  $\text{NaNO}_2$  (a and c respectively), HMT frequency (b), 1,3,5-TCB sensitivity comparison between a Bruker commercial spectrometer and the SoC-FPGA spectrometer (d)

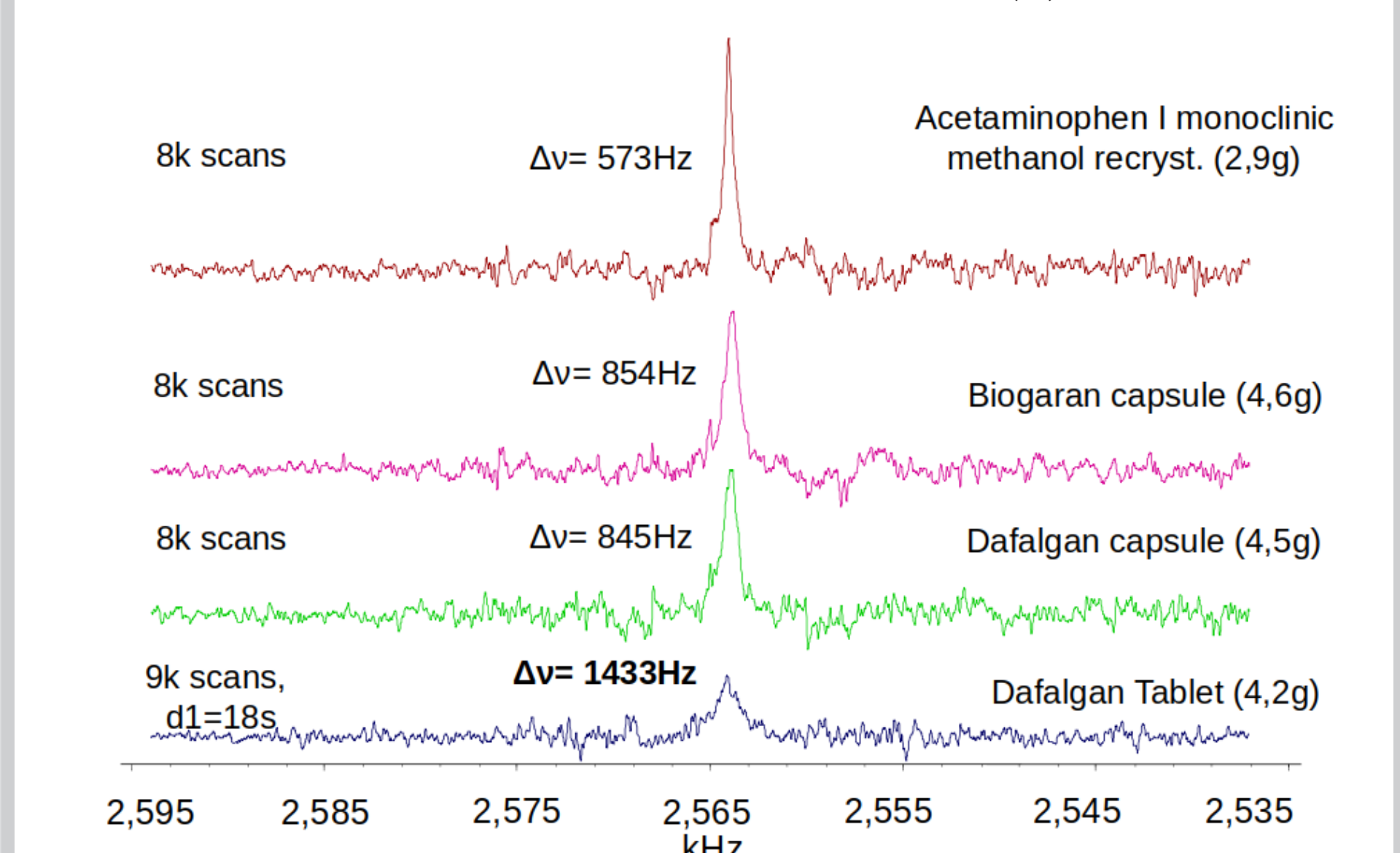


Fig. 5 Paracetamol analysis

## (5) CONCLUSION

The proposed SoC-FPGA architecture enabled significant instrument miniaturization and sensitivity improvement, resulting in a compact and performant NQR spectrometer. Experimental results, on reference and pharmaceutical samples, demonstrated the system's robust performance over the (0-62.5 MHz) frequency range needed for most NQR applications, highlighting its promising potential for pharmaceutical applications.

## (6) REFERENCES

- [1] B. H. Suits, "Nuclear Quadrupole Resonance Spectroscopy," in *Handbook of Applied Solid State Spectroscopy* (D. R. Vij, ed.), pp. 65–96, Boston, MA: Springer US, 2006.
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