spinflex Technical Report: Comparison between Bruker X-band pulsed spectrometer and the spinflex spinUP-X and Q systems

The capabilities of the spinflex spinUP-X system were compared to those available form a commercial system by Bruker (Elexsys E-580). Two main important parameters are compared: spin sensitivity and signal stability. The systems are compared under the same conditions as much as possible: In both system we use the same sample – standard Double electron electron resonance (DEER) sample of stable bi-radical, supplied by Bruker, containing nitroxide bi-radical (DEER-Q, Bruker P.N E3005327) placed in a quartz tube with i.d. of 2 mm and o.d of 3 mm (for X-band measurements) or i.d of 1.4 mm and o.d of 1.6 mm (for Q-band measurements). At X-band, for both systems the sample is measured in a Bruker MD4 X-band resonator at room temperature and both spectrometers make use of a similar 1 kW TWT power amplifier. At Q-band, the Bruker system uses EN 5107D2 resonator with 2 mm sample access while the spinUP-Q system uses our own 1.6 sample access dielectric resonator.

- **Sensitivity:** Figure 1 shows a comparison between the Bruker system measurement and the SpinUP system, for field-swept echo data, measured with the parameters given in Table 1. It is clear that the spinUP system is comparable in its performance to the Bruker system. The signal-to-noise-ratio is slightly lower for the spinUP compared to the Bruker system, but since spinUP measured the sample with a longer interpulse delay, there is some significant signal decay (~25%-30%) at room temperature that has to be accounted for. Thus, overall, sensitivity is very much the same. It should be noted that the noise DC bias level of the Bruker system is significantly larger than the one in the spinUP system. Spectral shape is a bit different due to the way the field-swept echo data is processed.

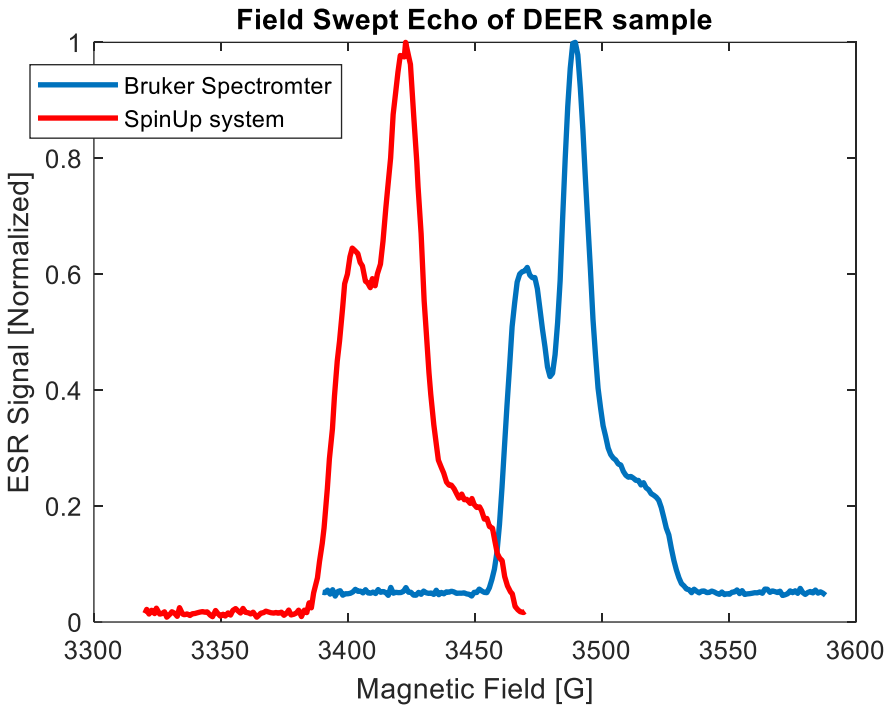

Figure 4: Field Swept Echo data acquired for a standard DEER sample with both systems (Bruker, and SpinUp)

	π/2 pulse length (rect)	π pulse length	Phase Cycle	Interpulse delay, τ	Number of scans	Average per scan	Shot repetition time	Noise bias (normalized)	Noise std (normalized)	Signal to noise std ratio
Bruker	12 ns	24 ns	+/- on first pulse	120 ns	16	10	2 ms	0.05	0.0034	294
SpinUp	12 ns	24 ns	+/- on first pulse	250 ns	1	160	2 ms	0.015	0.0042	238

Table 1: Parameters used for the sensitivity comparison measurements between the Bruker and the SpinUp system

- **Stability:** A second important comparison between Bruker and the spinUP system is related to the stability of the system. Such stability is important to carry out measurements, such as double electron electron resonance – DEER, where small changes in large signals are monitored as a function of pulse

sequence parameters. Figure 2 shows such comparison made for the same Bruker standard DEER sample. The measurements were carried out at room temperature with the same total measurement time of ~30 minutes. For both systems, the observe $\pi/2$ and π pulses were 20 and 40 ns, respectively, and the pump pulse was 30 ns. For the spinUP system we used Gaussian. It is clear that both systems give comparable results. The Bruker system gave slightly worse modulation depth, possibly due to the use of a slightly larger resonator, although power level for the spinUP-Q was lower (5 W vs. 10W for the Bruker). Keep in mind that for the spinUP-Q we measured the echo further away that enables to observe more modulation, but suffers more from T_2 decay.

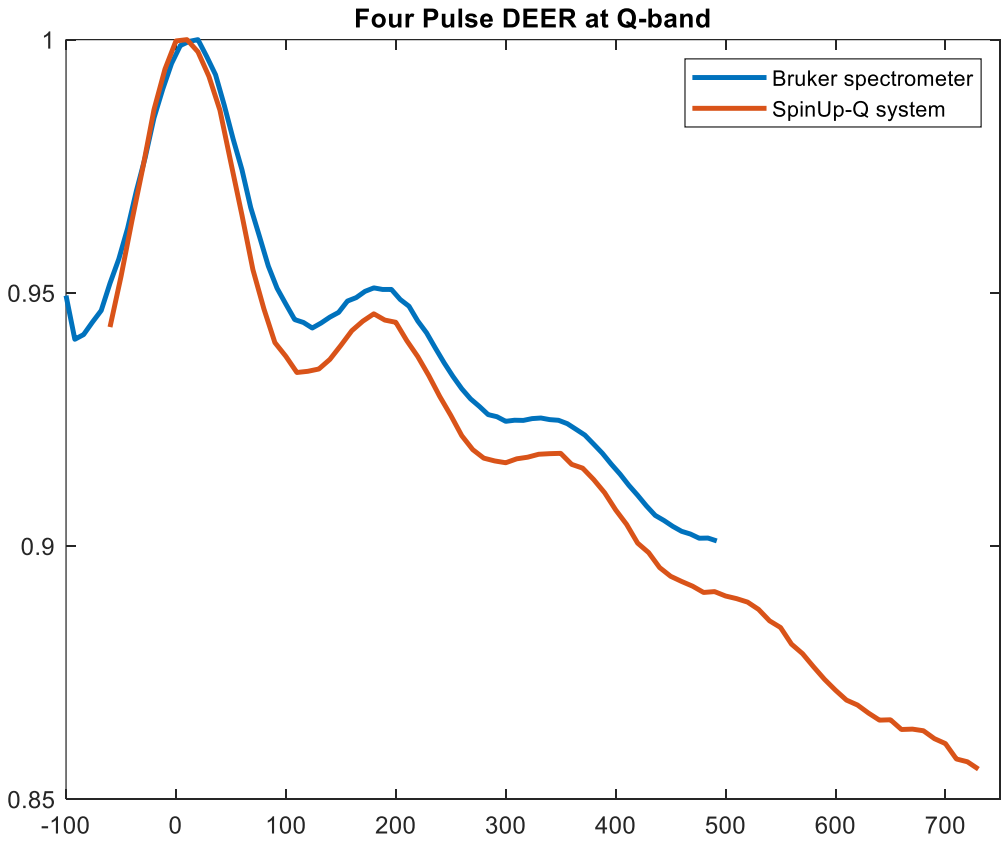

Figure 2: DEER data acquired for a standard DEER sample with both systems (Bruker, and SpinUP-Q).