Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information for: Rapid survey of nuclear quadrupole resonance by broadband excitation with comb modulation and dual-mode acquisition

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1 Derivation of Eqs. (2)-(4)

In general, an excitation pulse $f(t)$ with amplitude $\omega_1(t)$ and phase $\phi(t)$ is expressed as

$$f(t) = Ae^{i\phi(t)}. \tag{S1}$$

Now, let us recall Eq. (1):

$$\begin{aligned} g_1(t) &= \omega_{\max}[\mathrm{sech}(\beta t)]^{1-i\mu} \\ &= \omega_{\max}\mathrm{sech}(\beta t)[\mathrm{sech}(\beta t)]^{-i\mu}. \end{aligned} \tag{S2}$$

Comparing Eq. (S2) with Eq. (S1), we obtain

$$\omega_1(t) = \omega_{\max}\mathrm{sech}(\beta t), \tag{S3}$$

$$e^{i\phi(t)} = [\mathrm{sech}(\beta t)]^{-i\mu}. \tag{S4}$$

By taking natural logarithm of both sides of Eq. (S4), we obtain

$$\ln{[\mathrm{sech}(\beta t)]^{-i\mu}} = \ln e^{i\phi(t)}, \tag{S5}$$

$$-i\mu \ln{[\mathrm{sech}(\beta t)]} = i\phi(t), \tag{S6}$$

so that

$$\phi(t) = -\mu \ln[\mathrm{sech}(\beta t)]. \tag{S7}$$

The frequency in Eq. (3) is obtained by taking time derivative on Eq. (S4). Noting that

$$\mathrm{sech}(x) = \frac{1}{\cosh x}, \tag{S8}$$

and

$$(\mathrm{sech}(x))' = \left(\frac{1}{\cosh x}\right)' = \frac{-\sinh c}{\cosh^2 x} = -\frac{\tanh x}{\cosh x} = -\tanh x \mathrm{sech} x, \tag{S9}$$

we obtain

$$\begin{aligned} \frac{d\phi(t)}{dt} &= -\mu \frac{(\mathrm{sech}(\beta t))'}{\mathrm{sech}(\beta t)} \\ &= -\mu \frac{-\tanh(\beta t)\mathrm{sech}(\beta t)\cdot\beta}{\mathrm{sech}(\beta t)} \\ &= \mu\beta\tanh(\beta t) = \Delta\omega. \end{aligned} \tag{S10}$$

2 ^{35}Cl NQR rapid scan and FID signals of $KClO_3$ with various frequency offsets

All the following figures show the rapid scan signal (upper) and FID signal (lower) in ^{35}Cl NQR experiments of $KClO_3$ when the frequency offset of sweep center from resonance $\Delta\omega_c$ was $\pm 2\pi\cdot 10$, $-2\pi\cdot 50$, $\pm 2\pi\cdot 100$, $\pm 2\pi\cdot 150$ and $\pm 2\pi\cdot 200$ kHz. Red and green lines describe the in-phase and quadrature components of the magnetization, respectively. The comb-modulated HS pulse was aborted at time t indicated in the captions and in the figures by the broken lines.

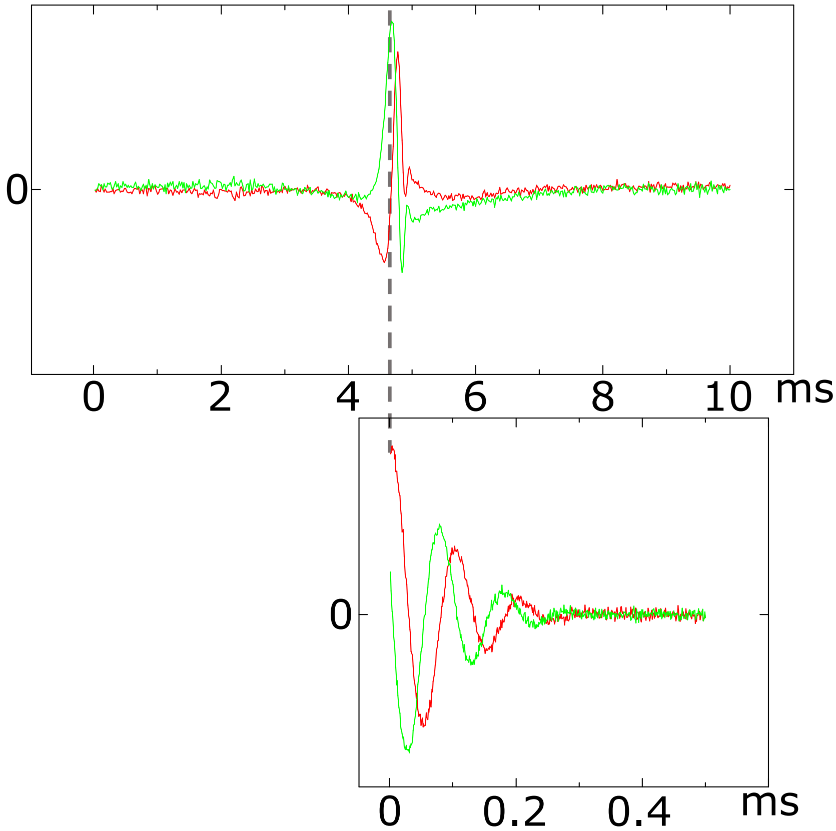

Figure S1: $\Delta\omega_c = 2\pi \cdot 10$ kHz, $t = 4.68$ ms.

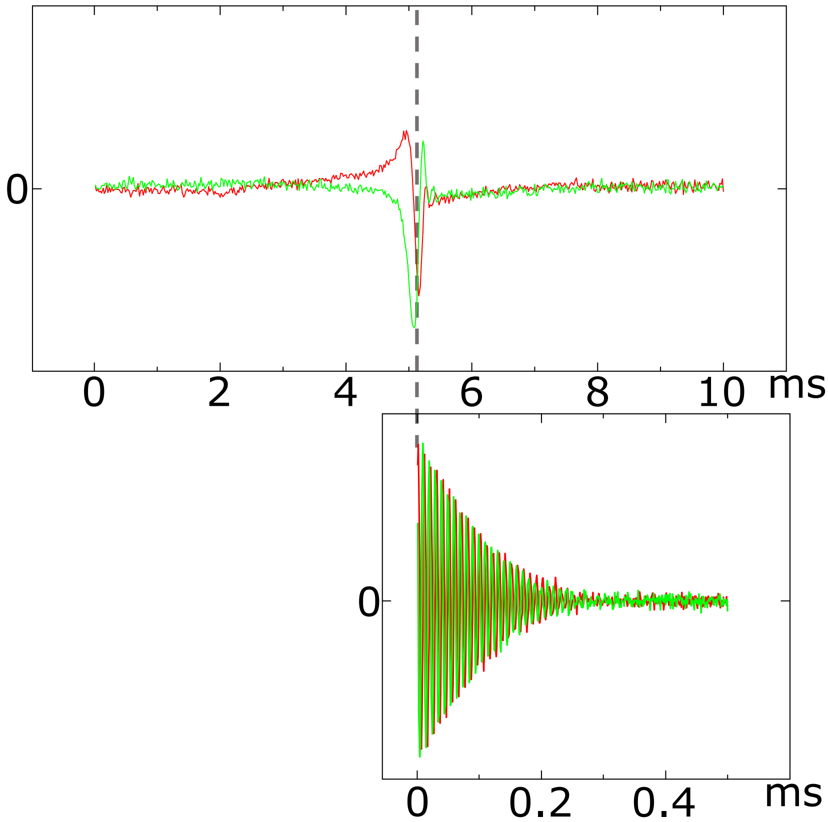

Figure S2: $\mathit{\Delta}\omega_{\mathrm{c}} = 2\pi \cdot 100$ kHz, $t = 5.10$ ms.

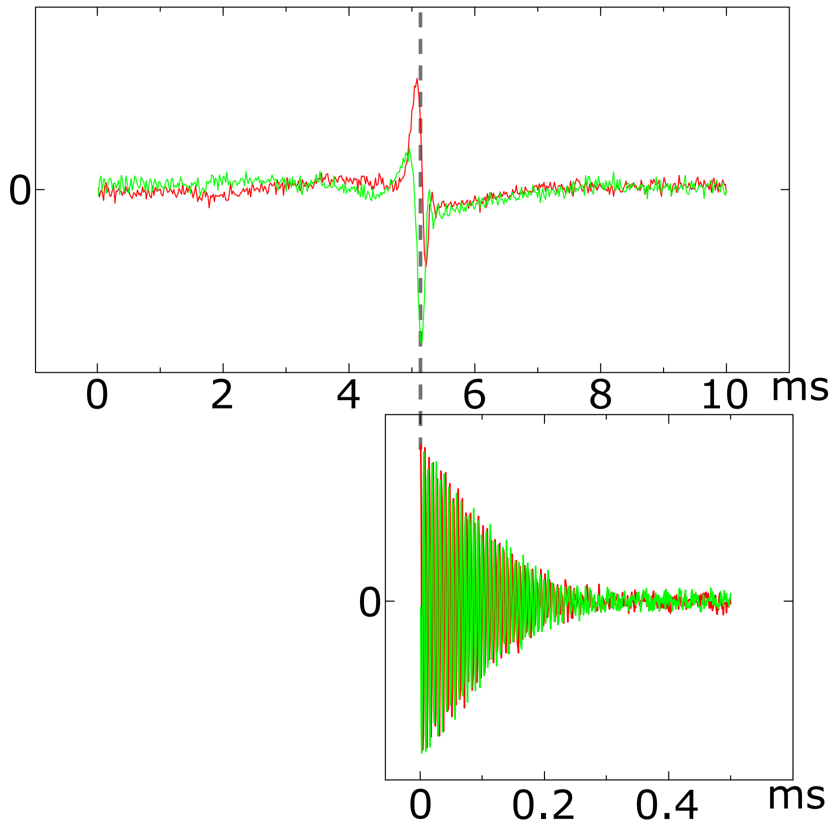

Figure S3: $\Delta\omega_c = 2\pi \cdot 150$ kHz, $t = 5.10$ ms.

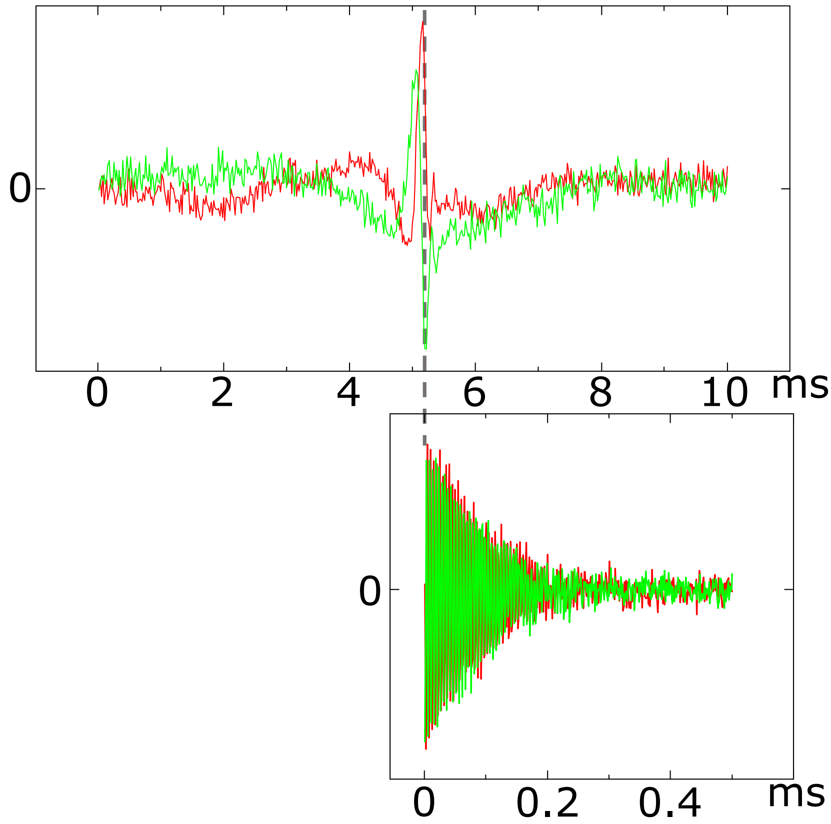

Figure S4: $\Delta\omega_c = 2\pi \cdot 200$ kHz, $t = 5.10$ ms.

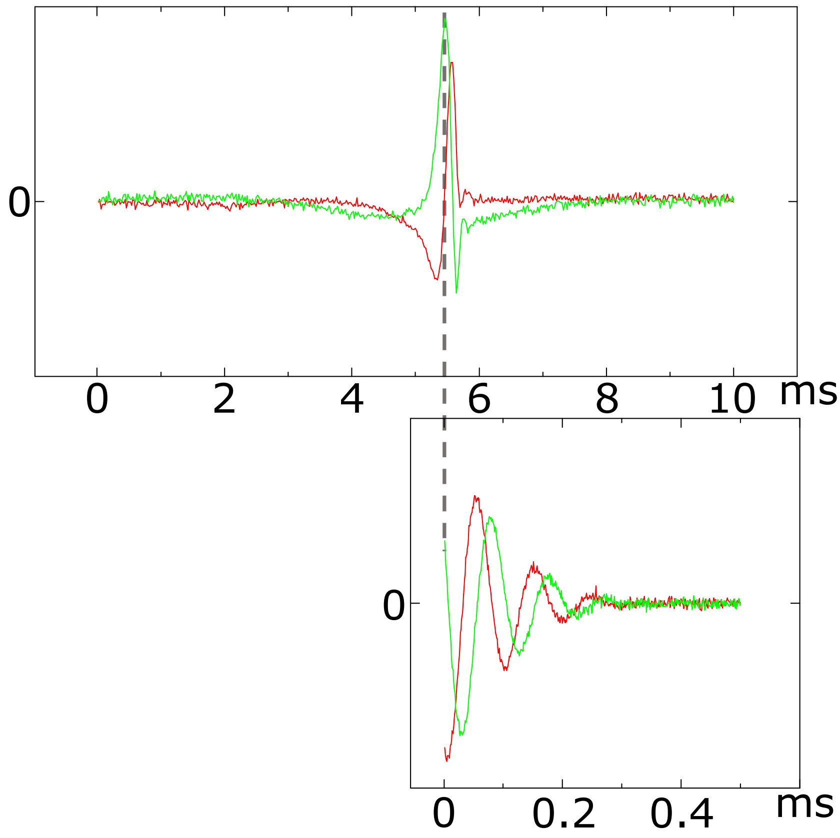

Figure S5: $\Delta\omega_c = -2\pi \cdot 10$ kHz, $t = 5.46$ ms.

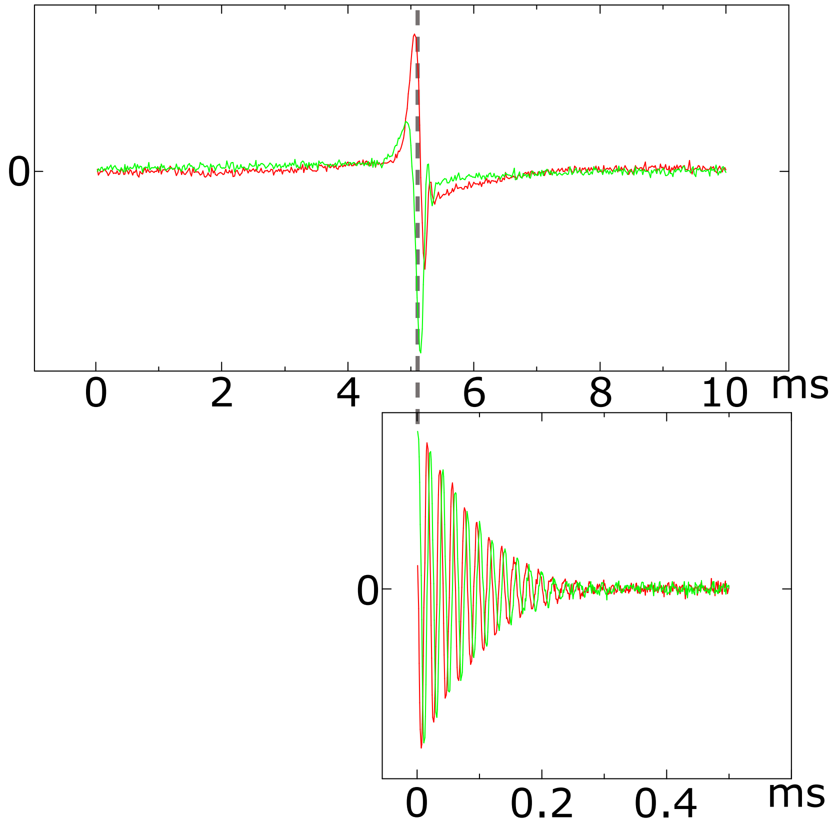

Figure S6: $\Delta\omega_c = -2\pi \cdot 50$ kHz, $t = 5.10$ ms.

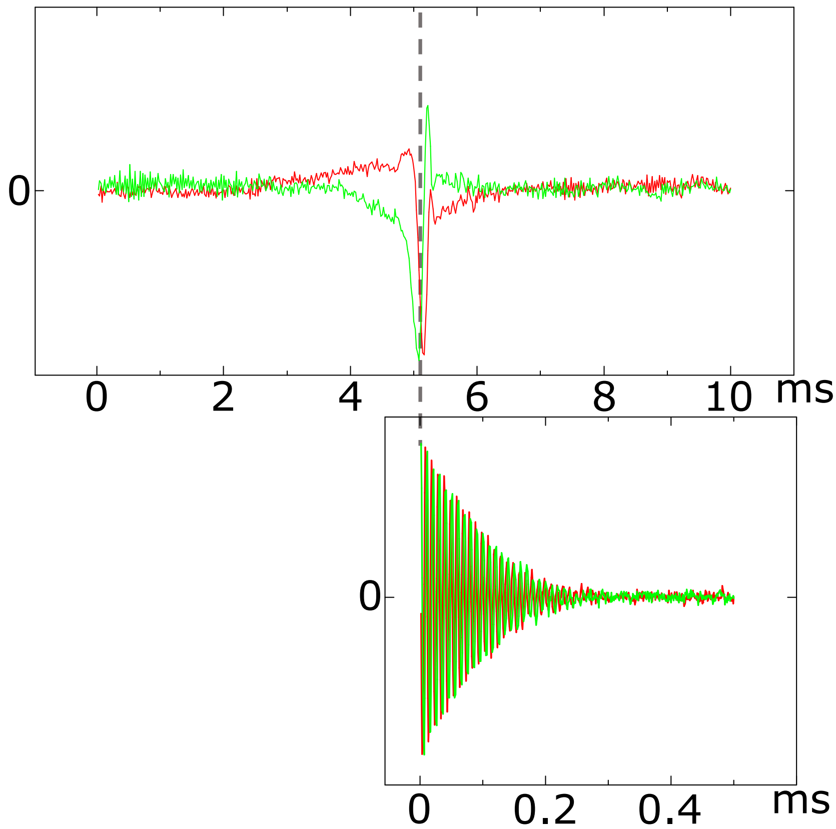

Figure S7: $\Delta\omega_c = -2\pi \cdot 100$ kHz, $t = 5.10$ ms.

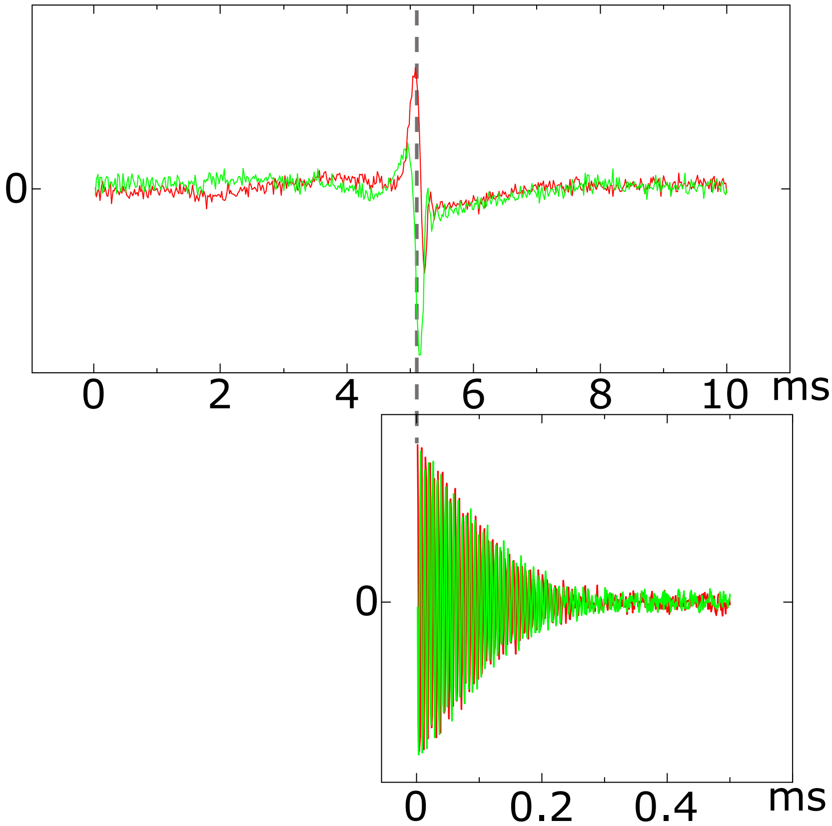

Figure S8: $\Delta\omega_c = -2\pi \cdot 150$ kHz, $t = 5.10$ ms.

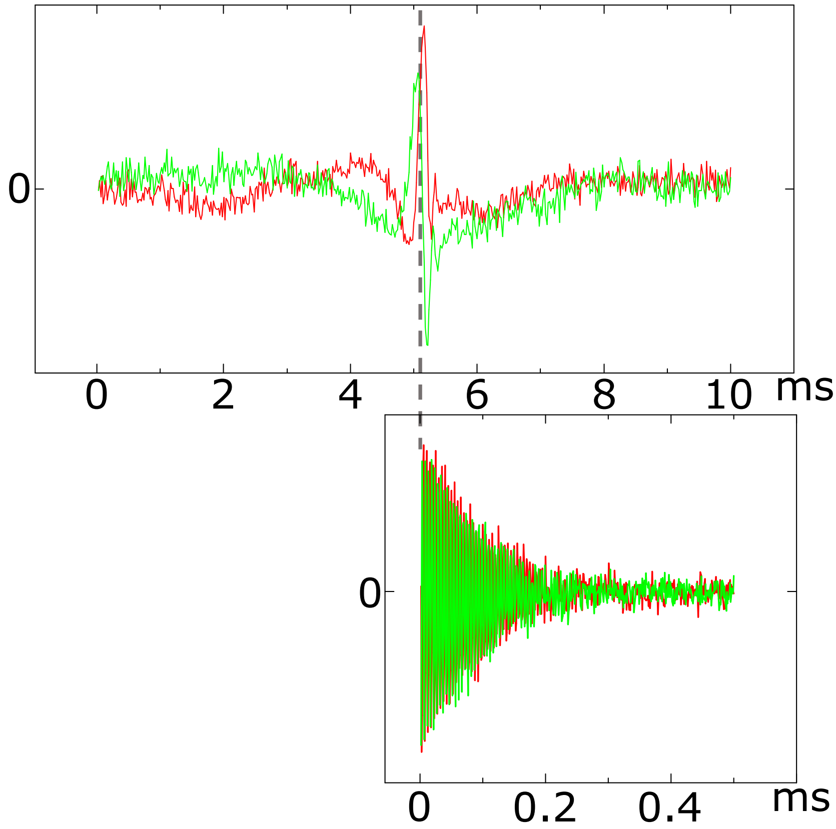

Figure S9: $\Delta\omega_c = -2\pi \cdot 200$ kHz, $t = 5.10$ ms.