

Supplementary Material

Solid-State NMR Characterization of Mefloquine Resinate Complexes Designed for Taste- Masking Pediatric Formulations

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- Figure S1** ¹³C CPMAS NMR spectra of mefloquine hydrochloride obtained at 9800 and 10000 Hz spinning frequencies. (*) denotes spinning sidebands.
- Figure S2** ¹³C CPMAS NMR spectra of mefloquine hydrochloride (sample MQ), with contact time 1100 μ s and a variation of recycle time (s).
- Figure S3** ¹³C CPMAS NMR spectra of mefloquine hydrochloride (sample MQ), with a variation in contact time (in μ s).
- Figure S4** ¹³C CPMAS NMR spectra of potassium polacrilin resin (sample R), obtained with a variation in contact time (in μ s).
- Figure S5** ¹³C CPMAS NMR spectrum of the mefloquine-resinate (sample MQ-R), with a variation in contact time (in μ s).
- Figure S6** ¹³C solution NMR spectrum (DMSO-*d*₆) of sample MQ.
- Figure S7** Distribution of T_{CH} for the carbons of mefloquine, MQ (blue); MQ-R complex (orange); and resin R (green).
- Figure S8** Dependence of C2 signal intensity (vertical scale, arbitrary unities) on the contact time t_c (horizontal scale, in s unities) for the samples mefloquine hydrochloride (MQ) and mefloquine-polacrilin complex (MQ-R).
- Figure S9** Dependence of C7 signal intensity (vertical scale, arbitrary unities) on the contact time t_c (horizontal scale, in s unities) for the samples mefloquine hydrochloride (MQ) and mefloquine-polacrilin complex (MQ-R).
- Figure S10** Dependence of C5 signal intensity (vertical scale, arbitrary unities) on the contact time t_c (horizontal scale, in s unities) for the samples mefloquine hydrochloride (MQ) and mefloquine-polacrilin complex (MQ-R).
- Figure S11** Dependence of C6 signal intensity (vertical scale, arbitrary unities) on the contact time t_c (horizontal scale, in s unities) for the samples mefloquine hydrochloride (MQ) and mefloquine-polacrilin complex (MQ-R).
- Figure S12** Dependence of C12 signal intensity (vertical scale, arbitrary unities) on the contact time t_c (horizontal scale, in s unities) for the samples mefloquine hydrochloride (MQ) and mefloquine-polacrilin complex (MQ-R).
- Figure S13** Dependence of C signal intensity (vertical scale, arbitrary unities) on the contact time t_c (horizontal scale, in s unities) for carbons in the sample of polacrilin resin (R).

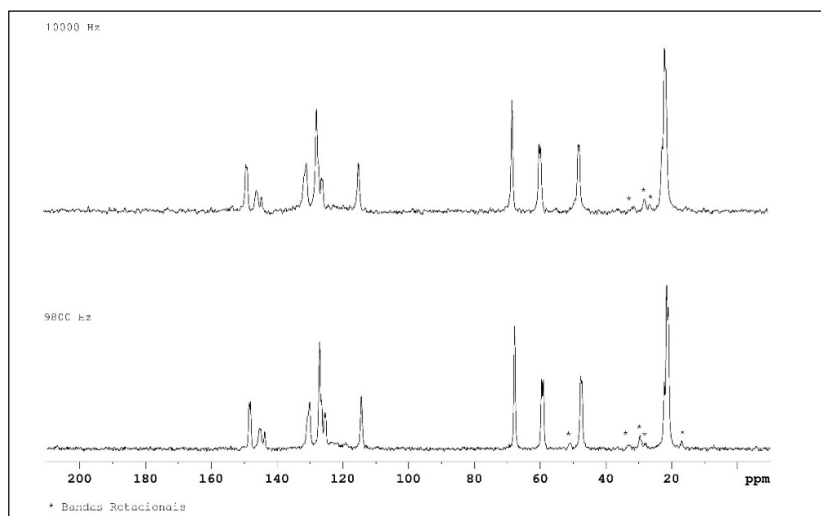


Figure S1 - ^{13}C CPMAS NMR spectra of mefloquine hydrochloride (sample MQ) obtained at 9800 and 10000 Hz spinning frequencies. (*) denotes spinning sidebands.

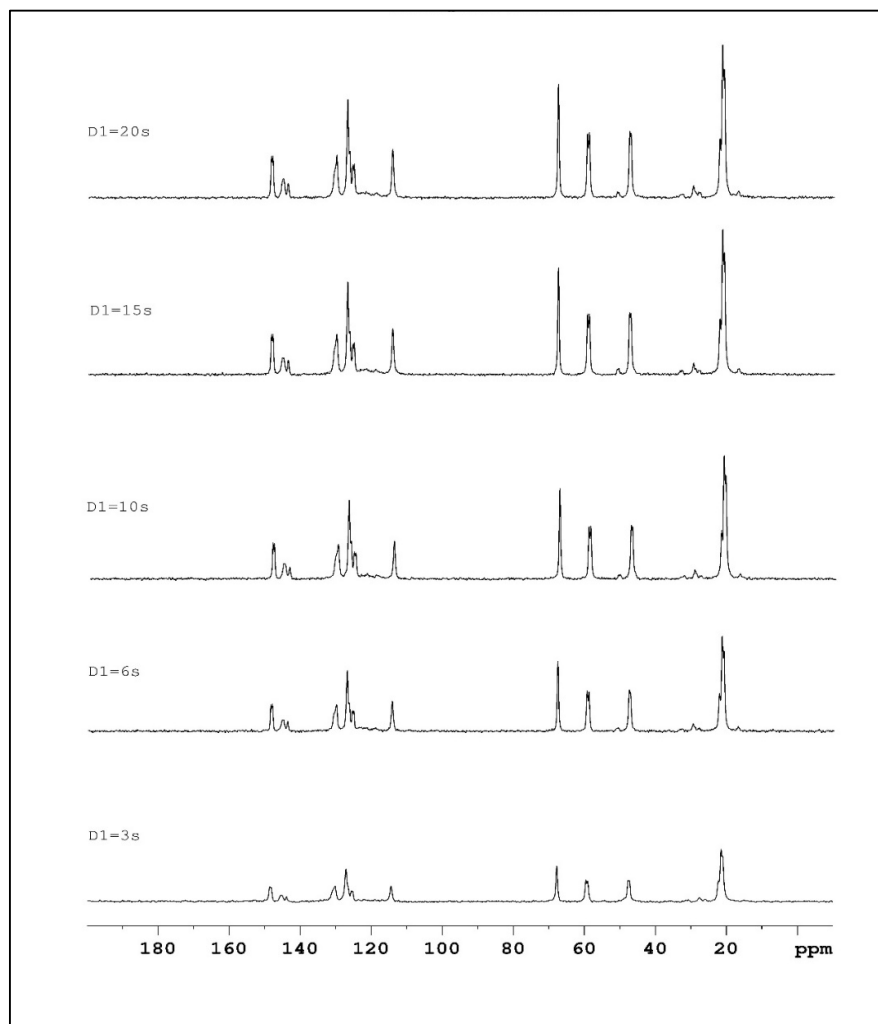


Figure S2 – ^{13}C CPMAS NMR spectra of mefloquine hydrochloride (sample MQ), with contact time $1100\mu\text{s}$ and a variation of recycle time (s).

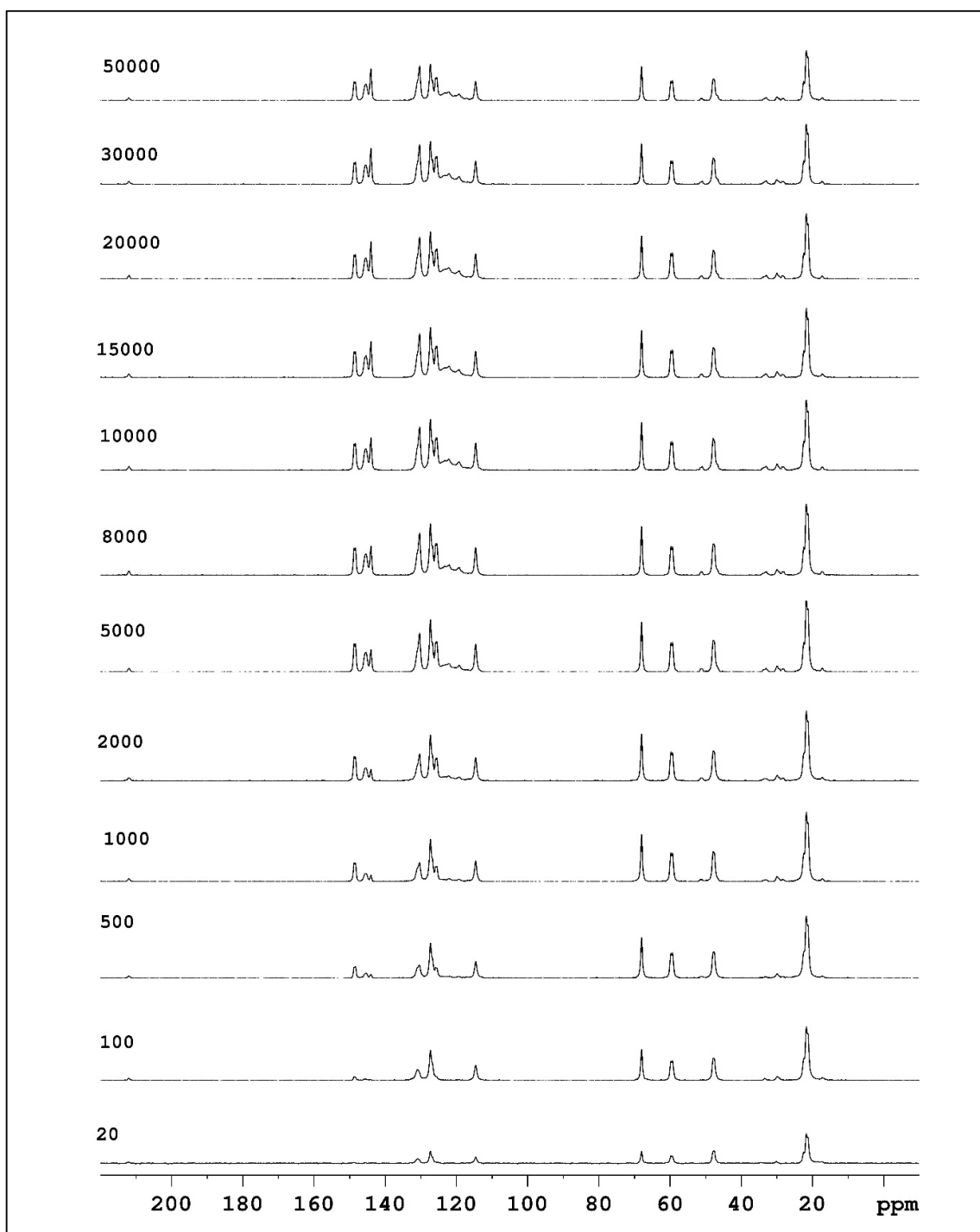


Figure S3 – ^{13}C CPMAS NMR spectra of mefloquine hydrochloride (sample MQ), with a variation in contact time (in μs).

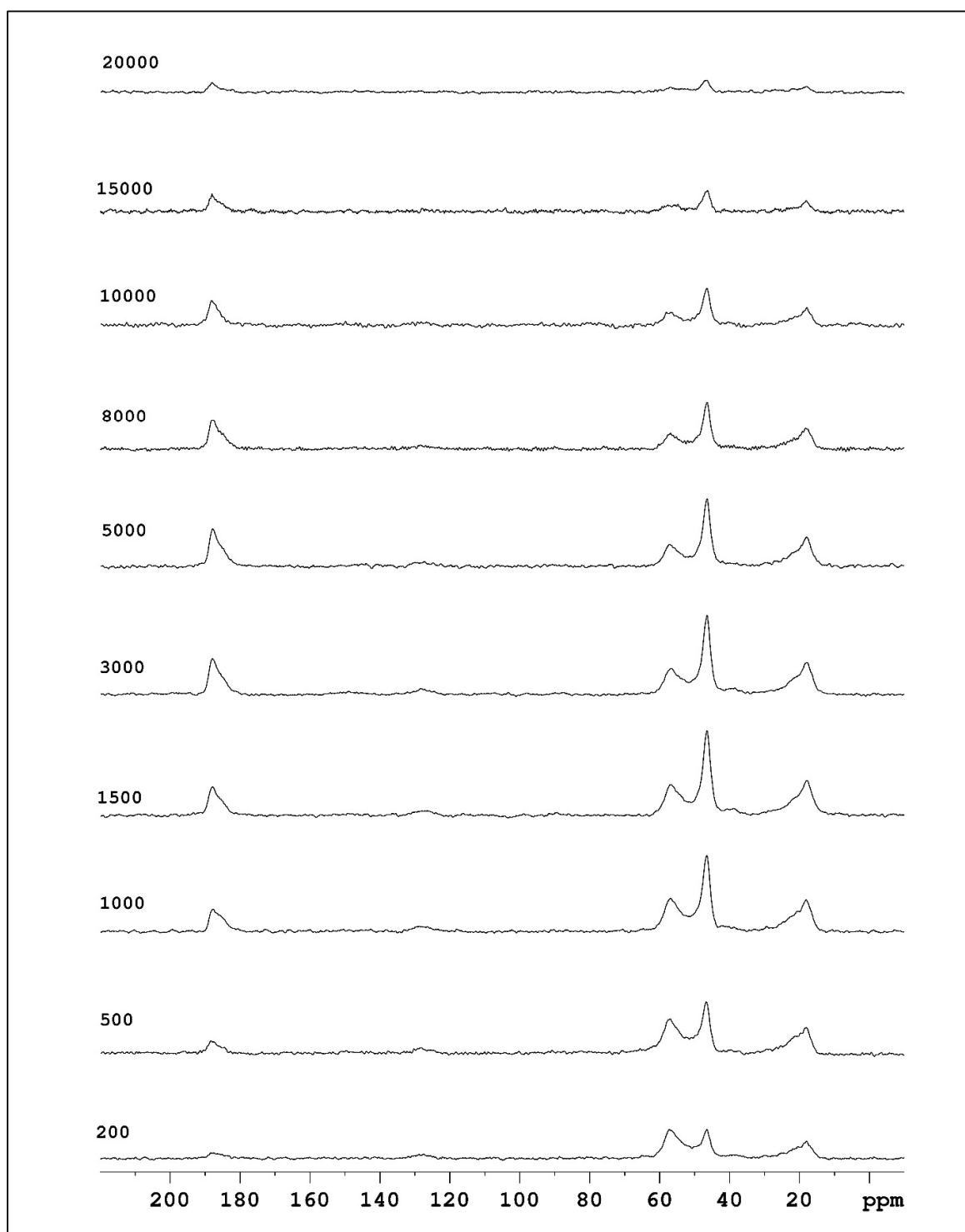


Figure S4 – ^{13}C CPMAS NMR spectra of potassium polacrilin resin (sample R), obtained with a variation in contact time (in μs).

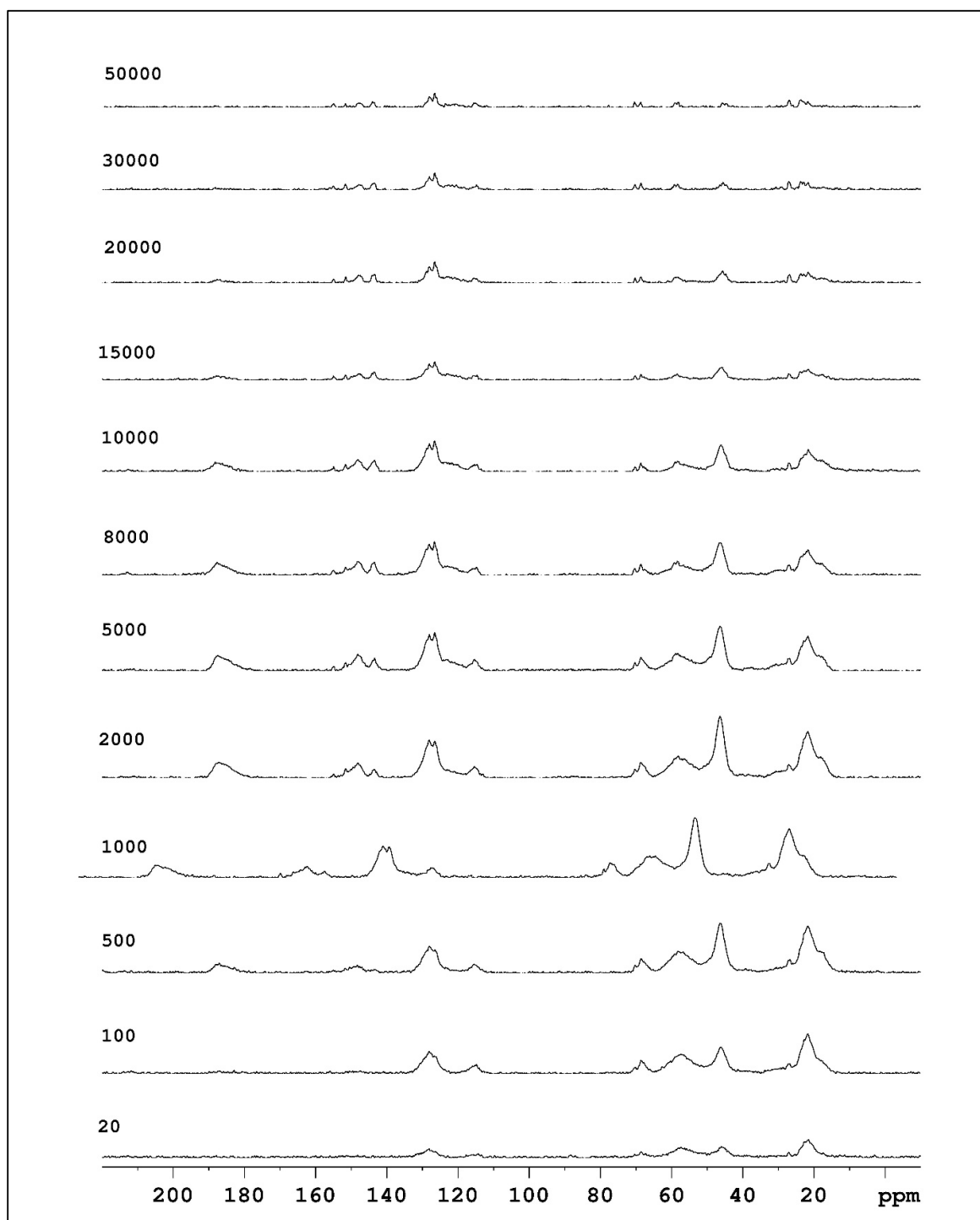


Figure S5 – ^{13}C CPMAS NMR spectrum of the mefloquine-resinate (sample MQ-R), with a variation in contact time (in μs).

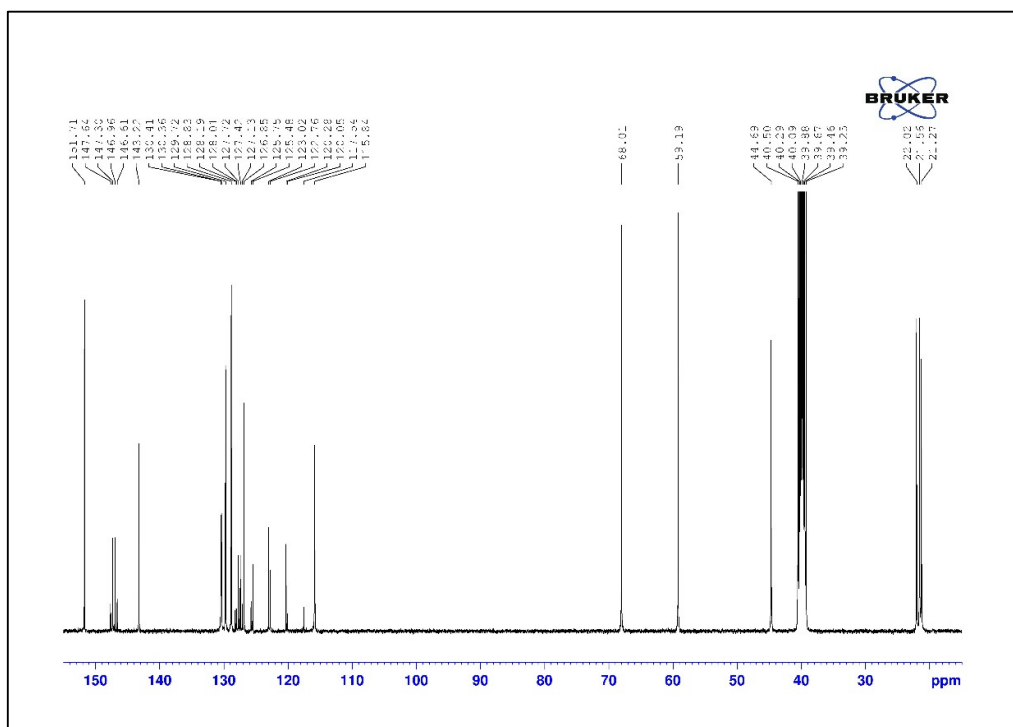


Figure S6 – ^{13}C NMR (500 MHz, $\text{DMSO}-d_6$) spectrum of the MQ sample.

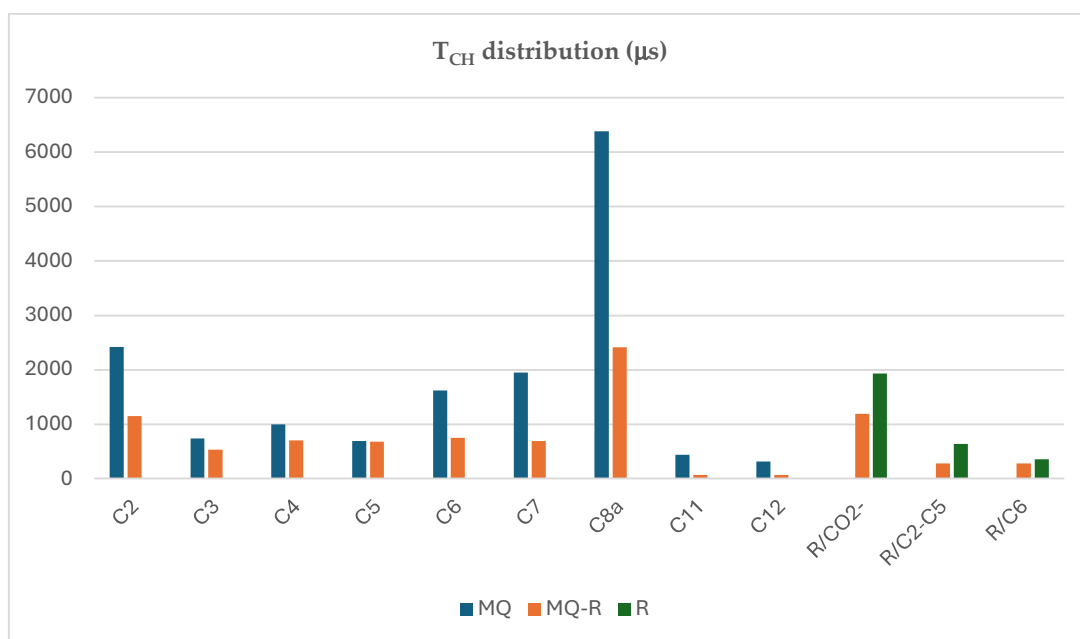
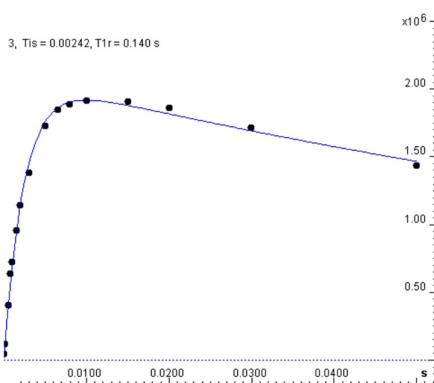


Figure S7. Distribution of T_{CH} for the carbons of mefloquine, MQ (blue); MQ-R complex (orange); and resin R (green).

C2 carbon

Mefloquine

$\delta = 145.2$ ppm



Mefloquine-polacrillin

$\delta = 148.0$ ppm

$\delta = 147.3$ ppm

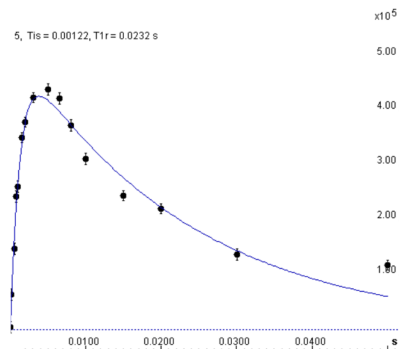
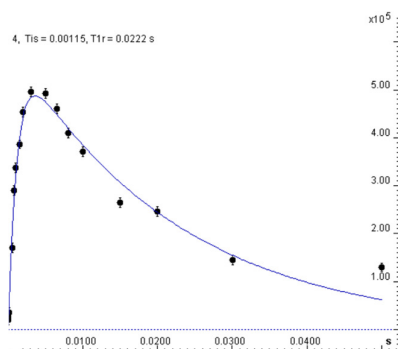
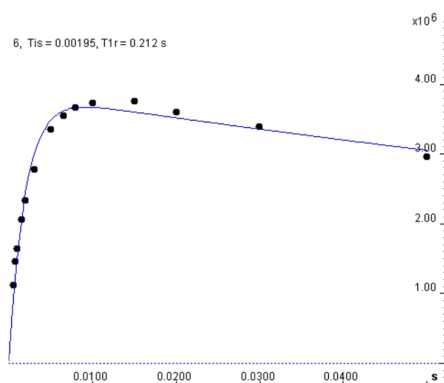


Figure S8. Dependence of C2 signal intensity (vertical scale, arbitrary unities) on the contact time t_c (horizontal scale, in s unities) for the samples mefloquine hydrochloride (MQ) and mefloquine-polacrillin complex (MQ-R).

C7 carbon

Mefloquine

$\delta = 130.1 \text{ ppm}$



Mefloquine-polacrillin

$\delta = 128.8 \text{ ppm}$

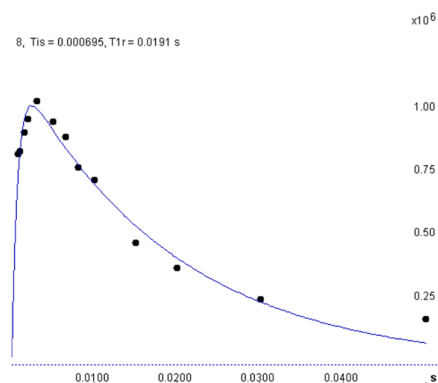


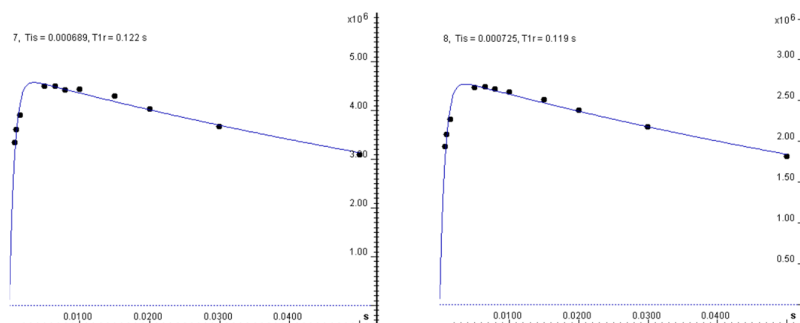
Figure S9. Dependence of C7 signal intensity (vertical scale, arbitrary unities) on the contact time t_c (horizontal scale, in s unities) for the samples mefloquine hydrochloride (MQ) and mefloquine-polacrillin complex (MQ-R).

C5 carbon

Mefloquine

$\delta = 127.1$ ppm

$\delta = 126.5$ ppm



Mefloquine-polacrillin

$\delta = 128.0$ ppm

$\delta = 127.5$ ppm

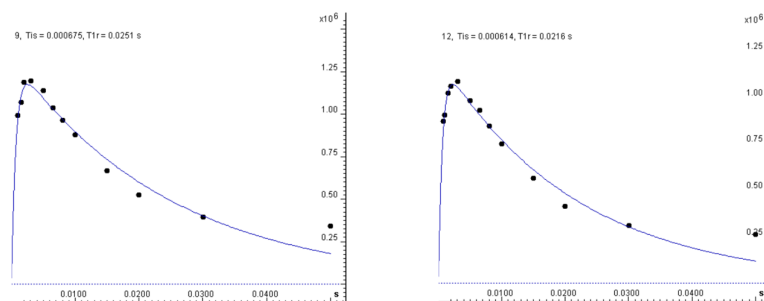
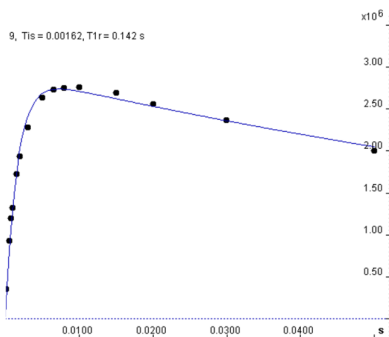


Figure S10. Dependence of C5 signal intensity (vertical scale, arbitrary unities) on the contact time t_c (horizontal scale, in s unities) for the samples mefloquine hydrochloride (MQ) and mefloquine-polacrillin complex (MQ-R).

C6 carbon

Mefloquine

$\delta = 125.6$ ppm



Mefloquine-polacrillin

$\delta = 126.6$ ppm

$\delta = 126.0$ ppm

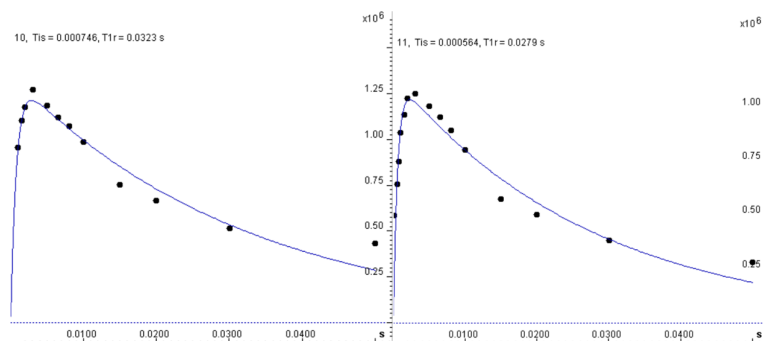


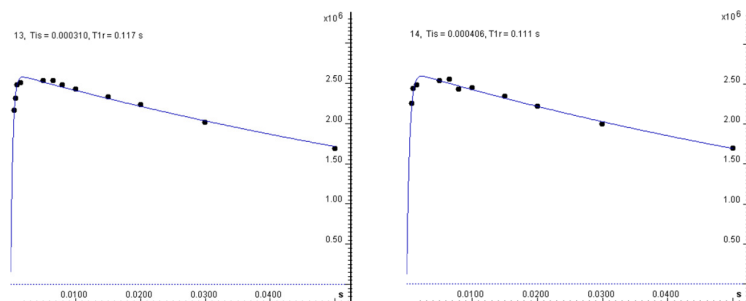
Figure S11. Dependence of C6 signal intensity (vertical scale, arbitrary unities) on the contact time t_c (horizontal scale, in s unities) for the samples mefloquine hydrochloride (MQ) and mefloquine-polacrillin complex (MQ-R).

C12 carbon

Mefloquine

$\delta = 59.5$ ppm

$\delta = 59.0$ ppm



Mefloquine-polacrillin

$\delta = 58.1$ ppm

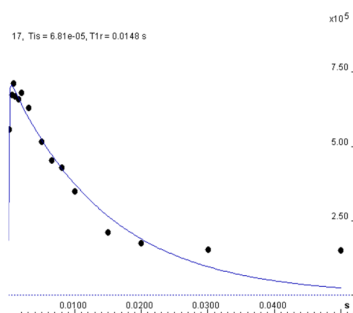
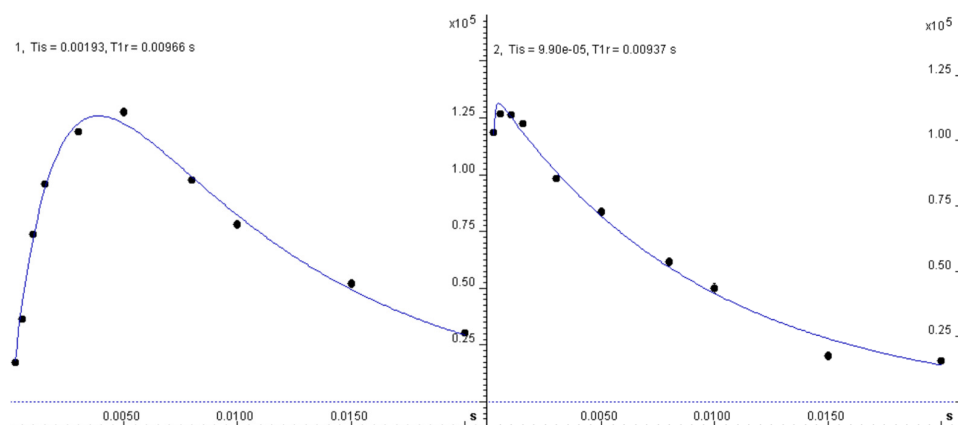


Figure S12. Dependence of C12 signal intensity (vertical scale, arbitrary unities) on the contact time t_c (horizontal scale, in s unities) for the samples mefloquine hydrochloride (MQ) and mefloquine-polacrillin complex (MQ-R).

Polacrilin Resin

C1 (COO⁻), $\delta = 186.5$ ppm

C2, C3, C4, C5, $\delta = 56.9$ ppm



C2, C3, C4, C5, $\delta = 46.4$ ppm

C6 (CH₃), $\delta = 18.1$ ppm

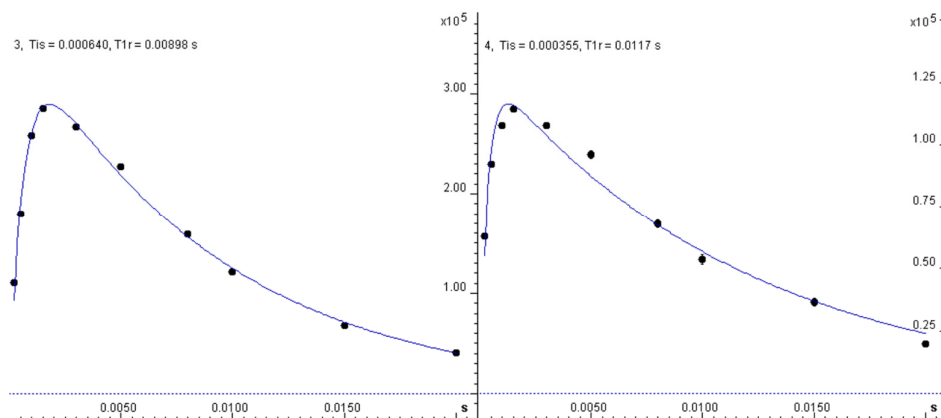


Figure S13. Dependence of C signal intensity (vertical scale, arbitrary unities) on the contact time t_c (horizontal scale, in s unities) for carbons in the sample of polacrilin resin (R).