

Supporting Information

Compact NMR Spectroscopy for Low-Cost Identification and Quantification of PVC Plasticizers

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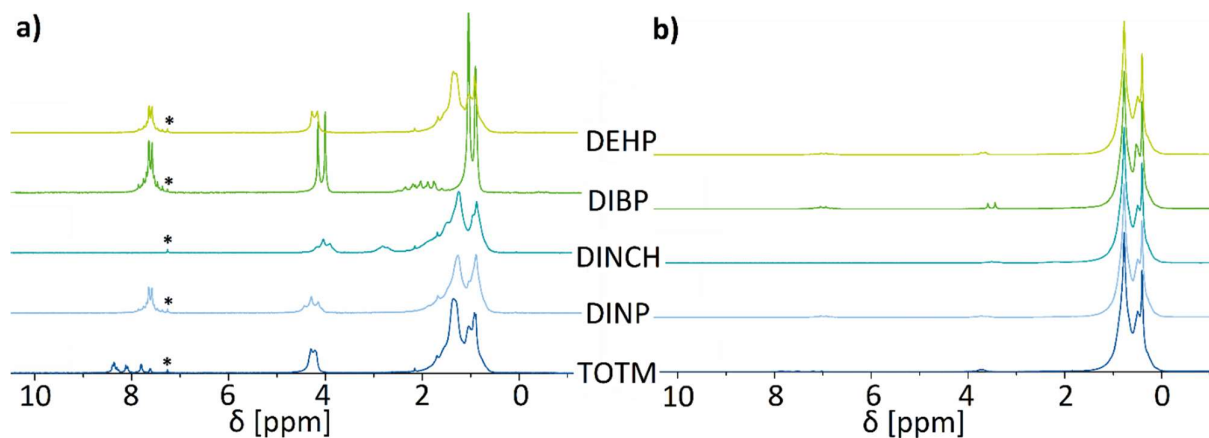


Fig. S1. 40 MHz ^1H NMR spectra of the investigated plasticizers at concentrations of 10 vol.% in a) deuterated chloroform and b) non-deuterated n-hexane without zoom. Spectra have been referenced to the residual deuterated chloroform (signal marked with asterisk at 7.26 ppm) and n-hexane (0.8 ppm) peaks, respectively.

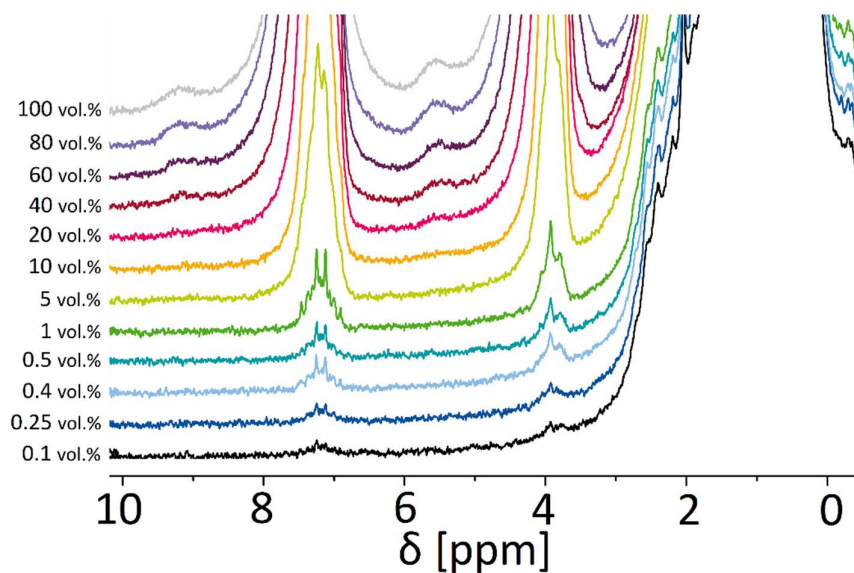


Fig S2. 40 MHz ^1H NMR spectra of DINP in non-deuterated hexane at varying concentrations. All spectra have been referenced to the signal of the n-hexane (0.8 ppm) peak. The specific resonances at around 7 ppm can be observed even at concentrations as low as 0.1 vol.% with only 4 scans.

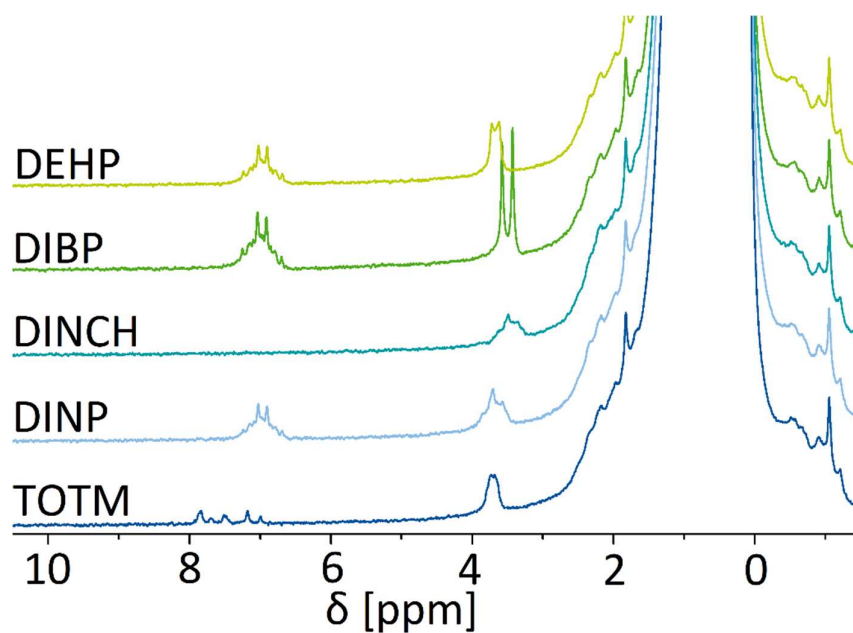


Fig S3. 40 MHz ^1H NMR spectra of all investigated plasticizers in non-deuterated n-hexane at a concentration of 1 vol. %. All spectra have been referenced to the signal of the n-hexane (0.8 ppm) peak.

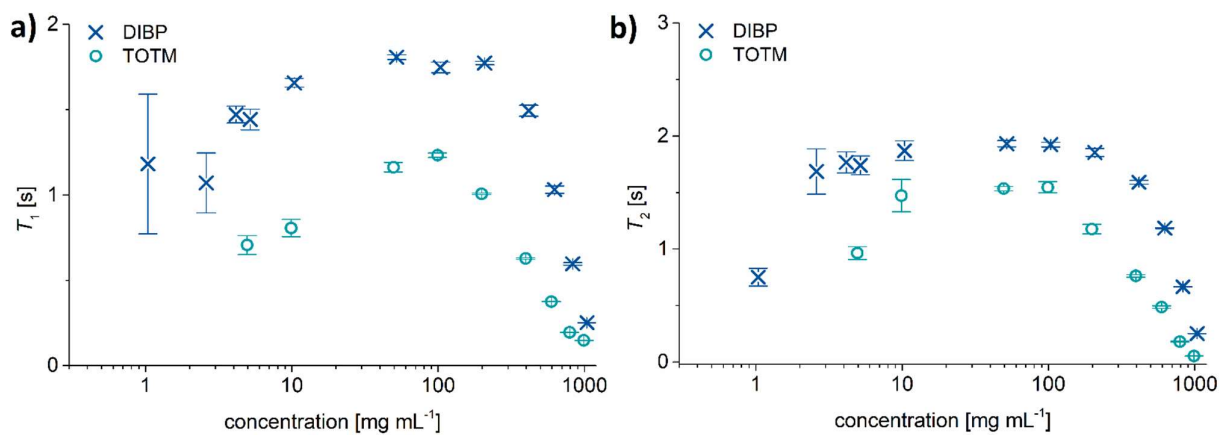


Fig S4. ^1H -NMR a) T_1 and b) T_2 relaxation times of TOTM and DIBP at all investigated concentrations measured at 40 MHz. For each concentration, the reported relaxation times are the average of three measurements.

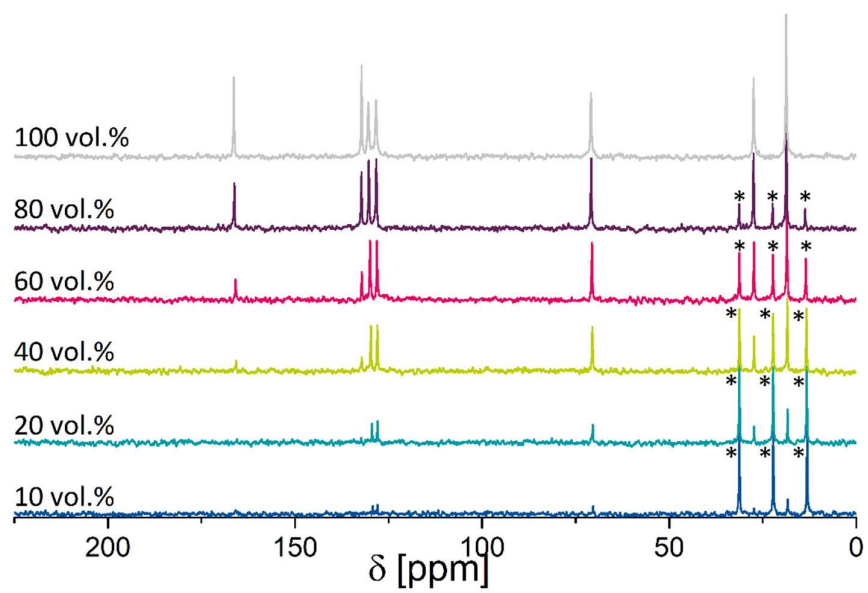


Fig S5. ¹³C spectra of DIBP at various concentrations recorded at 40 MHz. The asterisks correspond to the signals from n-hexane.

Table S1. Results of gravimetric analyses of unknown PVC samples used for solvent extraction discussed in section 2.3.

| sample | initial sample mass [g] | sample mass after | | mass difference [g] | mass difference [wt.%] |
|----------------------|-------------------------|---------------------------|--|---------------------|------------------------|
| | | extraction and drying [g] | | | |
| 1a CDCl ₃ | 130.7 | 82.9 | | 47.8 | 36.57% |
| 1a C ₆ | 130.1 | 82.6 | | 47.5 | 36.51% |
| 1b CDCl ₃ | 131.2 | 81.9 | | 49.3 | 37.58% |
| 1b C ₆ | 131.7 | 82.4 | | 49.3 | 37.43% |
| 1c CDCl ₃ | 130.2 | 82.4 | | 47.8 | 36.71% |
| 1c C ₆ | 120.2 | 74.1 | | 46.1 | 38.35% |
| 2a CDCl ₃ | 144.5 | 107.4 | | 37.1 | 25.67% |
| 2a C ₆ | 143.9 | 107.7 | | 36.2 | 25.16% |
| 2b CDCl ₃ | 144.3 | 105.6 | | 38.7 | 26.82% |
| 2b C ₆ | 142.5 | 107 | | 35.5 | 24.91% |
| 2c CDCl ₃ | 137.1 | 102.7 | | 34.4 | 25.09% |
| 2c C ₆ | 116.7 | 88.2 | | 28.5 | 24.42% |
| 3a CDCl ₃ | 198.6 | 187.3 | | 11.3 | 5.69% |
| 3a C ₆ | 192.4 | 177.6 | | 14.8 | 7.69% |
| 3b CDCl ₃ | 194.9 | 181.5 | | 13.4 | 6.88% |
| 3b C ₆ | 195.3 | 180.6 | | 14.7 | 7.53% |
| 3c CDCl ₃ | 163.4 | 156.3 | | 7.1 | 4.35% |
| 3c C ₆ | 183.5 | 170.7 | | 12.8 | 6.98% |
| 4a CDCl ₃ | 154.5 | 102.5 | | 52 | 33.66% |
| 4a C ₆ | 154.7 | 104.5 | | 50.2 | 32.45% |
| 4b CDCl ₃ | 150.8 | 99.9 | | 50.9 | 33.75% |
| 4b C ₆ | 152.6 | 103.4 | | 49.2 | 32.24% |
| 4c CDCl ₃ | 146.9 | 98.7 | | 48.2 | 32.81% |
| 4c C ₆ | 145.4 | 98.5 | | 46.9 | 32.26% |
| 5a CDCl ₃ | 304.9 | 265.7 | | 39.2 | 12.86% |
| 5a C ₆ | 305.3 | 266.9 | | 38.4 | 12.58% |
| 5b CDCl ₃ | 303.8 | 268.4 | | 35.4 | 11.65% |
| 5b C ₆ | 301.7 | 264.7 | | 37 | 12.26% |
| 5c CDCl ₃ | 300.4 | 265.8 | | 34.6 | 11.52% |
| 5c C ₆ | 283.3 | 250.2 | | 33.1 | 11.68% |

Table S2. Mean results from each sample displayed in Table S1 and individual results from CDCl₃ and n-hexane extraction.

| sample | mean wt% | standard deviation | standard deviation [%] | mean wt% of CDCl ₃ extraction | standard deviation of CDCl ₃ extraction | standard deviation of CDCl ₃ extraction [%] | mean wt% of n-hexane extraction | standard deviation of n-hexane extraction | standard deviation of n-hexane extraction [%] |
|--------|----------|--------------------|------------------------|--|--|--|---------------------------------|---|---|
| 1 | 33.5% | 0.063 | 18.7% | 33.3% | 0.066 | 19.9% | 33.6% | 0.074 | 21.9% |
| 2 | 19.1% | 0.097 | 50.6% | 19.2% | 0.117 | 61.1% | 19.0% | 0.098 | 51.6% |
| 3 | 15.3% | 0.138 | 90.1% | 15.0% | 0.162 | 108.6% | 15.7% | 0.146 | 93.0% |
| 4 | 26.1% | 0.104 | 39.7% | 26.5% | 0.118 | 44.6% | 25.7% | 0.114 | 44.2% |
| 5 | 11.8% | 0.003 | 2.8% | 11.6% | 0.001 | 0.8% | 12.0% | 0.004 | 3.4% |

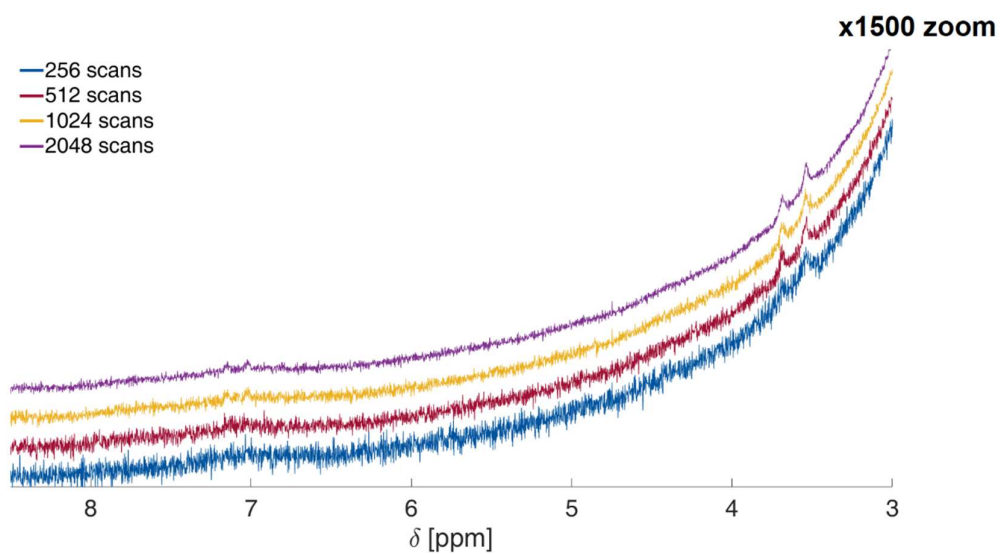


Fig S6. ¹H NMR spectra of a 0.05 mg mL⁻¹ DIBP solution in non-deuterated n-hexane in a stacked plot. SNRs at 3.5 ppm are 5.6, 8.5, and 8.7 for 512, 1024, and 2048 scans, respectively. SNRs at 7 ppm are 6.1, 7.0, and 7.5 for 512, 1024, and 2048 scans, respectively.