# Acquisition of quantitative $^{13}C$ NMR spectra in a short time with EXACT (EXtended ACquisition Time) acquisition Method (SI)

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# 1 Experimental

Camphor, Strychnine, and DEET (Diethyl meta toluamide) samples were prepared as follows: 30 mg of Camphor and 30 mg of Strychnine were dissolved separately in 800µl $CDCl_3$ each and used for the analysis. DEET (100µl) sample was mixed with 900µl of deuterated chloroform to make a 10% sample.

All sequences were programmed using C and MAGICAL languages compatible with the VNMRJ4 software. Spectra were acquired without the need for any window function processing after acquisition and FT. Windowed acquisition with the default constant sampling is used.

The EXACT and the SRT NMR experiments were carried out on Varian VNMRS 500 MHz spectrometers equipped with either a OneNMR probe or an Auto_X_DB_9070 probe. The duration of the 90° pulse on the $^{13}C$ observed channel was calibrated to 9µs and the 180° refocusing pulse on the proton decoupler channel was calibrated to 25µs using the auto_X_DB_9070 probe equipped spectrometer. Using the OneNMR probe equipped spectrometer, the 180° refocusing pulse was calibrated to 12µs and the 90 pulse was calibrated to 9µs.

All experiments were run at 25°C. All $^{13}C$ spectra were collected with 248.7 ppm spectral width (31250 Hz) and 32768 complex points and used Waltz-16 decoupling for the CPD (indicated by black rectangles in the pulse sequence in Figure 1). Acquisition times (including all chunks and gaps) were 1s for all the experiments. Relaxation delays and chunk lengths were varied as described in the main text,

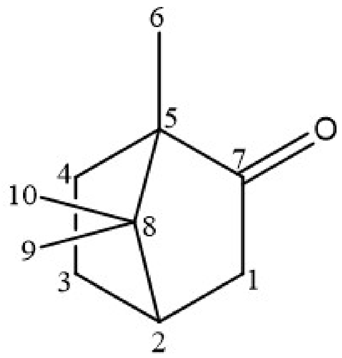
IST was used to reconstruct the unmeasured datapoints in the EXACT spectra. IT is an algorithm of the Compressed Sensing family, based on the assumption of spectral sparcity: the fact that an NMR spectrum has much more baseline points than “meaningful” ones, i.e. those contributing to peaks. It is an iterative algorithm in which we take the Fourier transform of the FID in each iteration; perform a thresholding operation, i.e. “cut” the peak tops which are above a pre-defined threshold; take the inverse Fourier transform of the thresholding result; and, finally, redefine non-measured points keeping the registered ones. When the output stops improving considerably from iteration to iteration, the algorithm is considered to be converged and yielding a reconstructed spectrum that is close enough to the one we would get if we had no gaps. More details on how to set the parameters of the algorithm can be found in reference, see also Fig.3 there for an illustration. Scripts for performing the reconstructions are available in the Supporting Information of references 9-11 of the main paper and were performed using Python wrappers of the MDDNMR software package (can be downloaded at http://mddnmr.spektrino.com/download).

Data processing and analysis were performed in Mestrenova 11.0. Processing of the SRT FIDs was performed by adding the two processed FIDs prior to the Fourier transform. The spectra were zero-filled to 256K datapoints prior to integration and baseline corrected with a 3$^{rd}$ oder polynomial fit.

# 2 Camphor experimental results

## 2.1 Table 1: Camphor $^{13}C$ numbers and assignment in ppm.

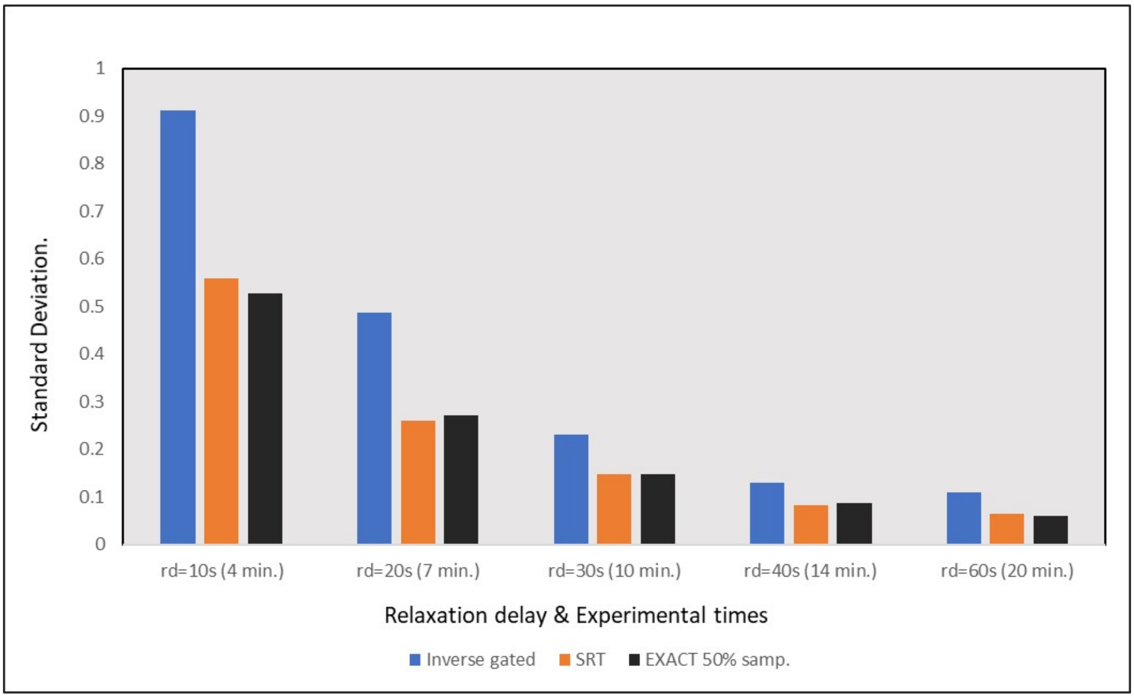
| Carbon | $^{13}C$ Assignment (ppm) |
|---|---|
| C1 | 43.04 |
| C2 | 43.29 |
| C3 | 27.03 |
| C4 | 29.9 |
| C5 | 57.68 |
| C6 | 9.22 |
| C7 | 219.65 |
| C8 | 46.77 |
| C9 | 19.12 |
| C10 | 19.76 |




## 2.2 Table 2: Integrals and standard devotions of Camphor sample at different relaxation delays using inverse gated (IG), SRT, and EXACT acquisition methods.

| Inverse-gated Acquisition (Camphor) | | | | | |
|---|---|---|---|---|---|
| | **rd=10s** | **rd =20** | **rd =30s** | **rd =40s** | **rd =60s** |
| C1 | 3.13 | 2.00 | 1.41 | 1.19 | 1.13 |
| C2 | 2.83 | 1.95 | 1.30 | 1.06 | 1.16 |
| C3 | 2.90 | 1.80 | 1.50 | 1.16 | 0.97 |
| C4 | 2.50 | 1.71 | 1.44 | 1.28 | 1.01 |
| C5 | 0.81 | 0.74 | 0.88 | 0.88 | 0.77 |
| C6 | 2.57 | 1.92 | 1.26 | 1.14 | 1.07 |
| C7 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| C8 | 0.89 | 0.85 | 0.88 | 0.88 | 1.00 |
| C9 | 2.60 | 1.79 | 1.24 | 1.06 | 1.10 |
| C10 | 2.71 | 1.76 | 1.41 | 1.11 | 0.95 |
| **STDEV.** | **0.910** | **0.480** | **0.230** | **0.129** | **0.110** |
| **Semi-Real Time Acquisition (Camphor)** | | | | | |
| | **rd =10s** | **rd =20** | **rd =30s** | **rd =40s** | **rd =60s** |
| C1 | 2.27 | 1.54 | 1.22 | 1.20 | 1.0 |
| C2 | 2.03 | 1.42 | 1.25 | 1.06 | 1.08 |
| C3 | 1.99 | 1.35 | 1.06 | 1.01 | 1.02 |
| C4 | 2.09 | 1.29 | 1.08 | 1.06 | 1.05 |
| C5 | 0.85 | 0.76 | 0.76 | 0.92 | 0.87 |
| C6 | 1.88 | 1.42 | 1.11 | 0.95 | 1.05 |

| | | | | | |
|---|---|---|---|---|---|
| C7 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| C8 | 0.91 | 0.91 | 0.90 | 0.95 | 0.92 |
| C9 | 2.14 | 1.40 | 1.15 | 1.07 | 1.04 |
| C10 | 1.99 | 1.40 | 1.13 | 1.08 | 1.03 |
| **STDEV.** | **0.560** | **0.260** | **0.147** | **0.080** | **0.060** |
| **EXACT Acquisition 50% sampling density (Camphor)** | | | | | |
| | **rd =10s** | **rd =20s** | **rd =30s** | **rd =40s** | **rd =60s** |
| C1 | 2.15 | 1.55 | 1.17 | 1.19 | 0.99 |
| C2 | 1.95 | 1.45 | 1.24 | 1.07 | 1.04 |
| C3 | 2.01 | 1.36 | 1.07 | 1.02 | 1.00 |
| C4 | 1.92 | 1.32 | 1.06 | 1.06 | 1.04 |
| C5 | 0.80 | 0.74 | 0.76 | 0.90 | 0.86 |
| C6 | 1.86 | 1.42 | 1.11 | 0.95 | 1.03 |
| C7 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| C8 | 0.94 | 0.93 | 0.85 | 0.94 | 0.94 |
| C9 | 2.04 | 1.47 | 1.15 | 1.09 | 1.04 |
| C10 | 2.01 | 1.40 | 1.14 | 1.11 | 1.05 |
| **STDEV.** | **0.528** | **0.270** | **0.148** | **0.088** | **0.059** |
| **EXACT Acquisition 33% sampling density (Camphor)** | | | | | |
| | **rd =10s** | **rd =20s** | **rd =30s** | **rd =40s** | **rd =60s** |
| C1 | 2.1 | 1.42 | 1.05 | 1.07 | 0.97 |
| C2 | 1.83 | 1.13 | 1.10 | 1.014 | 1.12 |
| C3 | 1.72 | 1.28 | 1.16 | 1.01 | 0.97 |
| C4 | 1.61 | 1.11 | 1.29 | 1.14 | 1.17 |
| C5 | 0.89 | 0.8 | 0.73 | 0.9 | 0.9 |
| C6 | 1.82 | 1.38 | 1.27 | 1.21 | 0.94 |
| C7 | 1 | 1 | 1 | 1 | 1 |
| C8 | 1 | 0.96 | 0.83 | 0.91 | 0.92 |
| C9 | 1.84 | 1.32 | 1.06 | 1.14 | 0.97 |
| C10 | 1.85 | 1.42 | 1.16 | 1.12 | 0.94 |
| **STDEV.** | **0.434** | **0.215** | **0.178** | **0.102** | **0.087** |

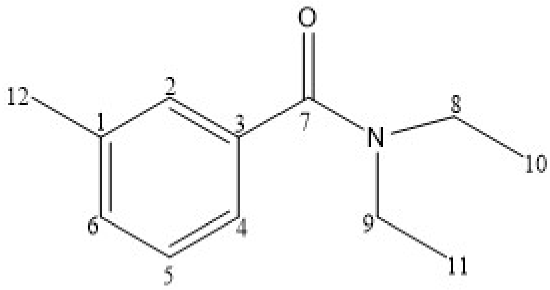


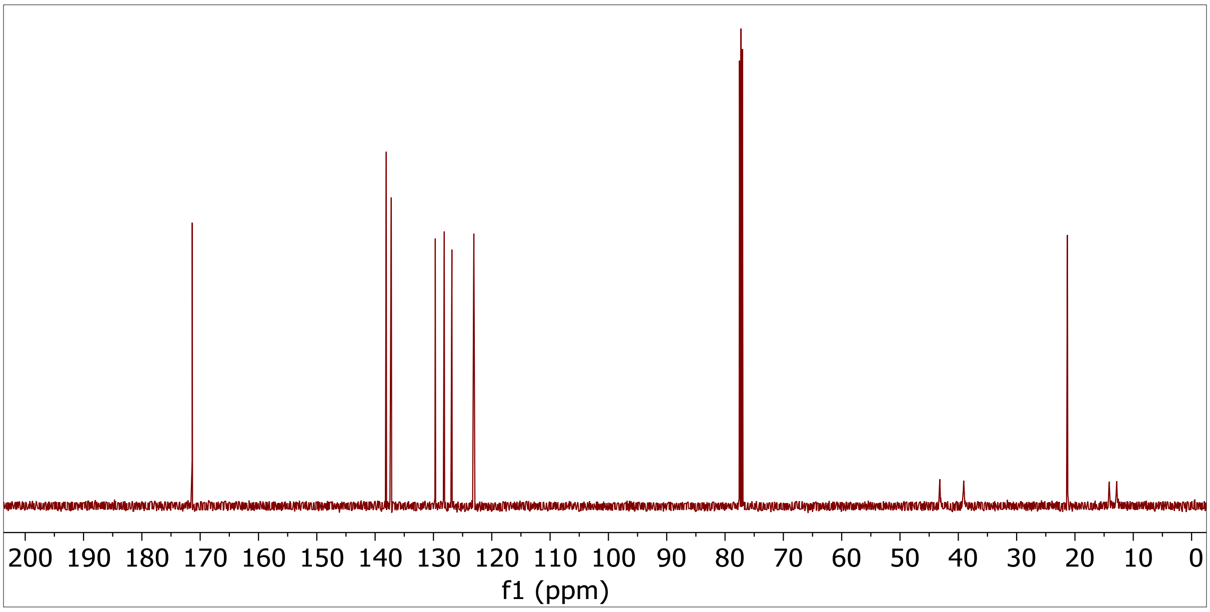

2.3 Figure S1: The standard deviations of the relative integrals of Camphor at different relaxation delays using inverse gated, SRT, and EXACT rec. Acquisition methods. The experimental time is the same using the inverse gated and the EXACT acquisition methods, however, it is double using the SRT acquisition method.

## 3 DEET experimental results

### 3.1 Table 3: DEET $^{13}C$ numbers and assignment in ppm

| Carbon | $^{13}C$ Assignment (ppm) |
|---|---|
| C1 | 138.16 |
| C2 | 126.87 |
| C3 | 137.23 |
| C4 | 123.10 |
| C5 | 128.17 |
| C6 | 129.72 |
| C7 | 171.43 |
| C8 | 39.12 |
| C9 | 43.23 |
| C10 | 12.89 |
| C11 | 14.18 |
| C12 | 21.34 |

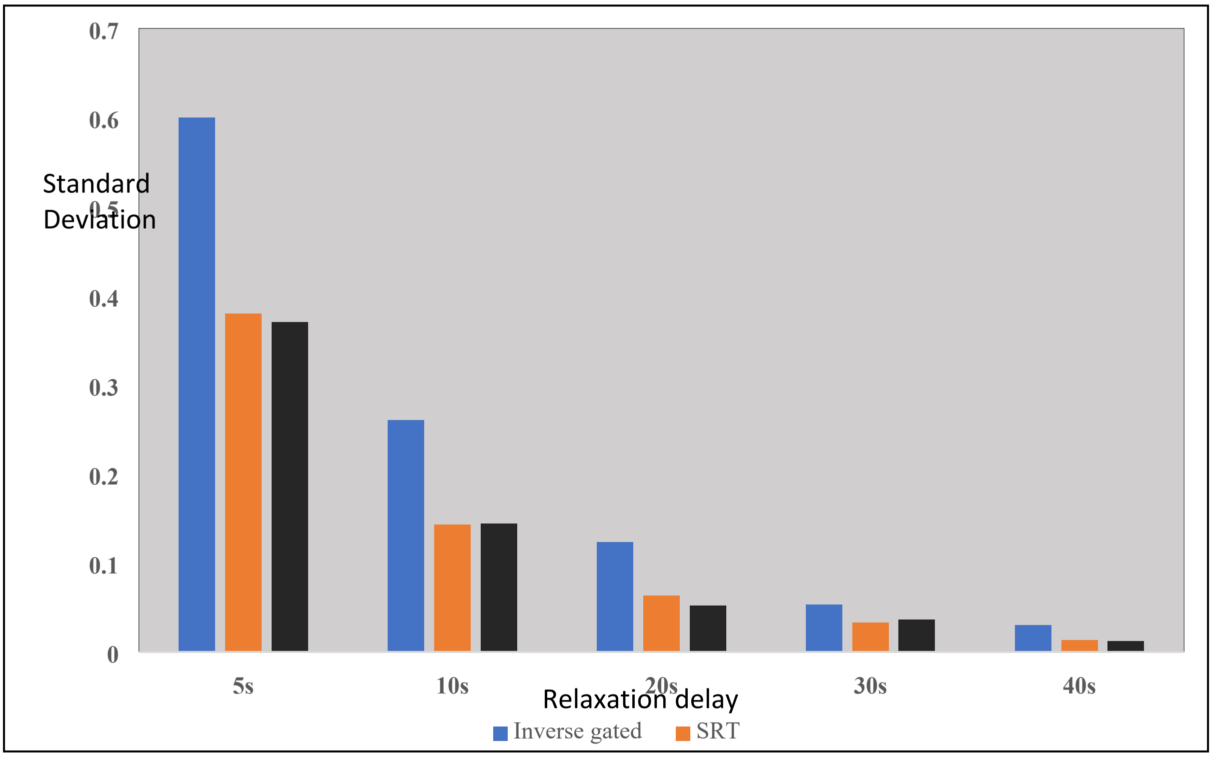





3.2 Figure S2: DEET $^{13}C$ NMR spectrum

3.3 Table 4: Integrals and standard devotions of DEET sample at different relaxation delays using inverse gated (IG), SRT, and EXACT acquisition methods.

| **Inverse Gated Acquisition (DEET)** | | | | | |
|---|---|---|---|---|---|
| | **rd =5s** | **rd =10s** | **rd =20s** | **rd =30s** | **rd =40s** |
| C1 | 1.40 | 1.46 | 1.29 | 1.15 | 1.04 |
| C2 | 2.40 | 1.73 | 1.25 | 1.03 | 1.01 |
| C3 | 1.36 | 1.33 | 1.20 | 1.06 | 1.03 |
| C4 | 2.32 | 1.73 | 1.25 | 1.06 | 0.95 |
| C5 | 2.64 | 1.72 | 1.28 | 1.00 | 1.01 |
| C6 | 2.43 | 1.64 | 1.17 | 0.98 | 0.97 |
| C7 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| C12 | 1.93 | 1.70 | 1.43 | 1.05 | 0.97 |
| | **0.610** | **0.262** | **0.122** | **0.053** | **0.031** |
| **Semi-Real Time Acquisition (DEET)** | | | | | |
| | **rd =5s** | **rd =10s** | **rd =20s** | **rd =30s** | **rd =40** |
| C1 | 1.28 | 1.16 | 1.05 | 1.06 | 1.02 |
| C2 | 1.91 | 1.21 | 1.05 | 1.09 | 0.98 |
| C3 | 1.25 | 1.04 | 0.99 | 1.06 | 1.00 |
| C4 | 1.97 | 1.15 | 0.89 | 1.02 | 1.00 |
| C5 | 1.96 | 1.33 | 0.99 | 1.07 | 1.02 |
| C6 | 1.81 | 1.17 | 0.97 | 1.08 | 1.01 |
| C7 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| C12 | 1.80 | 1.44 | 1.10 | 1.09 | 1.00 |
| | **0.383** | **0.143** | **0.063** | **0.0327** | **0.0130** |
| **EXACT Acquisition 50% sampling density (DEET)** | | | | | |
| | **rd =5s** | **rd =10s** | **rd =20s** | **rd =30s** | **rd=40** |
| C1 | 1.25 | 1.16 | 1.06 | 1.04 | 1.00 |
| C2 | 1.89 | 1.33 | 1.15 | 1.08 | 1.00 |
| C3 | 1.20 | 1.09 | 1.05 | 1.03 | 1.02 |
| C4 | 1.90 | 1.26 | 1.03 | 1.07 | 1.01 |
| C5 | 1.90 | 1.35 | 1.08 | 1.08 | 1.00 |
| C6 | 1.76 | 1.22 | 1.04 | 1.07 | 1.02 |
| C7 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| C12 | 1.86 | 1.44 | 1.14 | 1.12 | 1.03 |
| | **0.377** | **0.144** | **0.052** | **0.036** | **0.0119** |

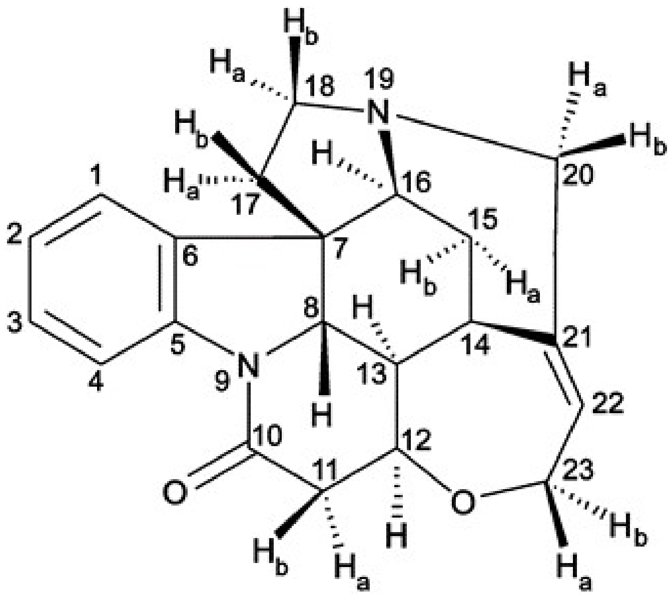


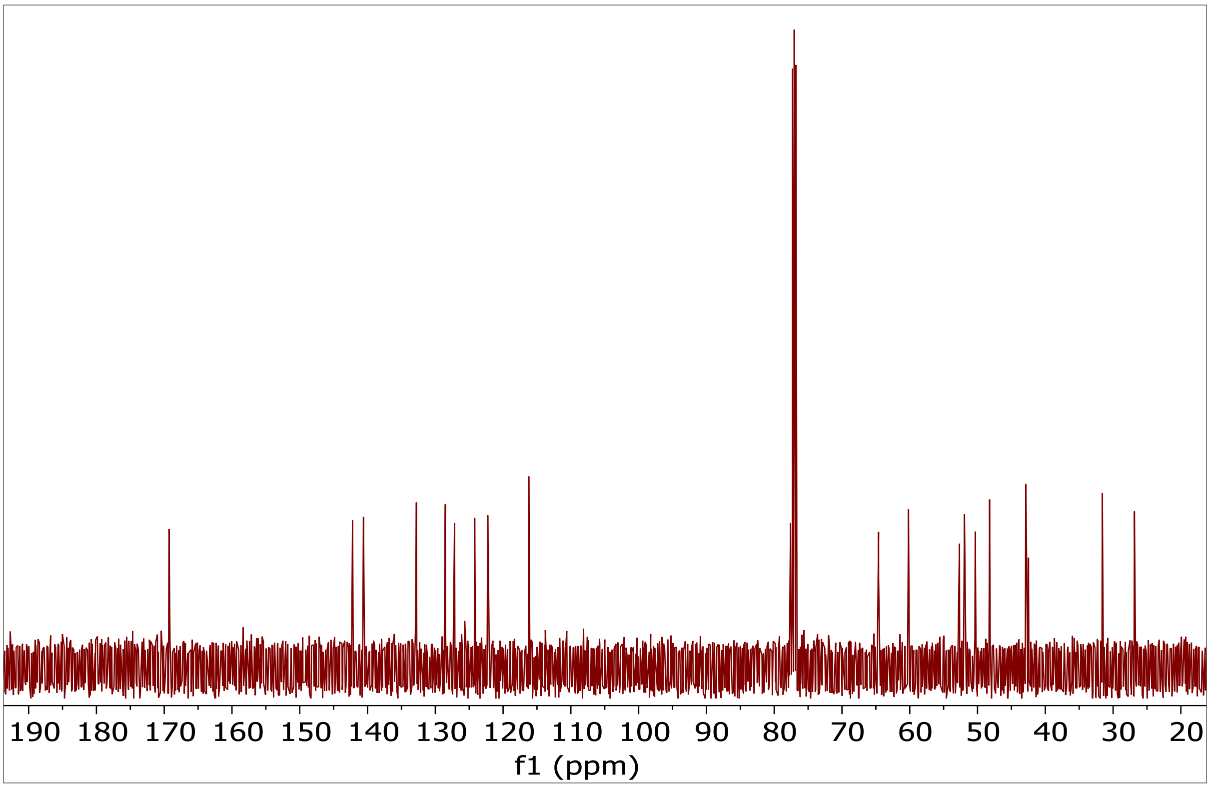

3.4 Figure S3: The standard deviations of the relative integrals of DEET at different relaxation delays using inverse gated, SRT, and EXACT rec. Acquisition methods. The experimental time is the same using the inverse gated and the EXACT acquisition methods, however, it is double using the SRT acquisition method.

# 4 Strychnine experimental results

## 4.1 Table 5: Strychnine $^{13}C$ numbers and assignment in ppm

| $^{13}C$ | $^{13}C$ Assignment |
|---|---|
| C1 | 122.19 |
| C2 | 124.12 |
| C3 | 128.48 |
| C4 | 116.22 |
| C5 | 142.27 |
| C6 | 132.8 |
| C7 | 51.99 |
| C8 | 60.15 |
| C10 | 169.27 |
| C11 | 42.47 |
| C12 | 77.64 |
| C13 | 48.28 |
| C14 | 31.68 |
| C15 | 26.9 |
| C16 | 60.22 |
| C17 | 42.9 |
| C18 | 50.34 |
| C20 | 52.71 |
| C21 | 140.63 |
| C22 | 127.08 |
| C23 | 64.61 |






4.2 Figure S4: Strychnine $^{13}C$ spectrum

4.3 Table 6: Integrals and standard devotions of strychnine sample at different relaxation delays using inverse gated (IG), SRT, and EXACT acquisition methods.

| Inverse Gated Acquisition (Strychnine) | | | | | | |
|---|---|---|---|---|---|---|
| | **rd=2.5s** | **rd=5s** | **rd=10s** | **rd=15s** | **rd=20 IG** | **rd=60 IG** |
| C1 | 1.85 | 1.78 | 1.05 | 0.88 | 0.63 | 0.82 |
| C2 | 2.01 | 1.74 | 1.08 | 0.84 | 0.75 | 0.64 |
| C3 | 2.06 | 1.72 | 1.42 | 1.03 | 0.71 | 0.66 |
| C4 | 2.29 | 2.04 | 1.02 | 0.87 | 0.76 | 0.75 |
| C5 | 1.20 | 1.17 | 0.8 | 1.08 | 1.04 | 0.93 |
| C6 | 0.93 | 1.14 | 0.73 | 0.89 | 0.75 | 0.93 |
| C7 | 1.03 | 1.77 | 0.63 | 0.66 | 0.76 | 0.77 |
| C8 | 2.67 | 1.42 | 0.94 | 1.32 | 1.19 | 0.92 |
| C10 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| C11 | 1.57 | 1.51 | 0.84 | 1.08 | 0.76 | 0.83 |
| C12 | 1.95 | 1.27 | 0.74 | 0.75 | 1.21 | 0.90 |
| C13 | 2.32 | 1.87 | 1.12 | 1.02 | 0.88 | 0.92 |
| C14 | 1.69 | 1.92 | 0.79 | 1.04 | 0.94 | 0.88 |

| | | | | | | |
|---|---|---|---|---|---|---|
| C15 | 1.11 | 2.04 | 0.96 | 0.95 | 0.77 | 0.80 |
| C16 | 2.18 | 2.13 | 0.93 | 1.08 | 1.03 | 0.98 |
| C17 | 1.92 | 1.57 | 1.01 | 0.71 | 0.87 | 0.79 |
| C18 | 1.62 | 1.66 | 0.93 | 0.87 | 0.72 | 0.64 |
| C20 | 1.16 | 1.3 | 0.82 | 0.69 | 0.94 | 0.74 |
| C21 | 1.60 | 2.06 | 0.93 | 1.23 | 0.93 | 0.90 |
| C22 | 1.88 | 1.91 | 0.89 | 0.85 | 1.06 | 0.77 |
| C23 | 1.76 | 1.82 | 0.78 | 1.21 | 0.71 | 0.75 |
| | **0.487** | **0.333** | **0.170** | **0.179** | **0.164** | **0.107** |

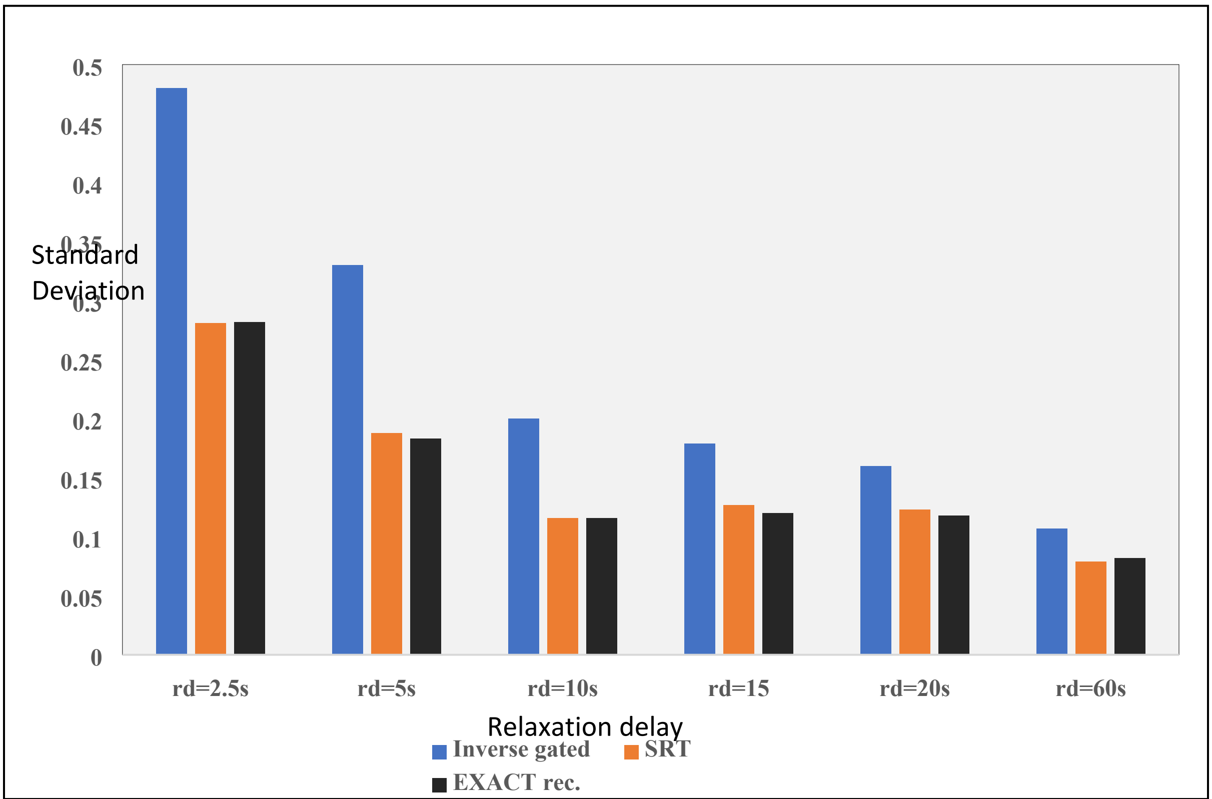
**Semi-Real Time Acquisition (Strychnine)**

| | **rd=2.5** | **rd=5s** | **rd=10s** | **rd=15s** | **rd=20s** | **rd=60** |
|---|---|---|---|---|---|---|
| C1 | 1.40 | 1.3 | 1.19 | 0.93 | 1.04 | 1.10 |
| C2 | 1.68 | 1.46 | 0.9 | 0.87 | 0.96 | 1.05 |
| C3 | 1.49 | 1.18 | 0.89 | 0.86 | 0.85 | 0.89 |
| C4 | 1.65 | 1.36 | 0.87 | 0.86 | 1.06 | 0.97 |
| C5 | 0.99 | 1.05 | 1.07 | 0.81 | 1.01 | 0.85 |
| C6 | 0.82 | 0.93 | 0.9 | 0.83 | 0.85 | 1.06 |
| C7 | 0.98 | 1.54 | 0.95 | 1.09 | 0.93 | 1.05 |
| C8 | 1.71 | 1.13 | 1.02 | 1.06 | 0.98 | 1.08 |
| C10 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| C11 | 1.48 | 1.05 | 0.99 | 0.83 | 0.86 | 0.91 |
| C12 | 1.51 | 1.36 | 0.99 | 1.23 | 1.04 | 1.04 |
| C13 | 1.49 | 1.17 | 1.12 | 0.96 | 1 | 1.01 |
| C14 | 1.36 | 1.37 | 0.72 | 0.85 | 0.81 | 1.06 |
| C15 | 1.05 | 1.68 | 0.84 | 0.85 | 0.69 | 0.97 |
| C16 | 1.55 | 1.10 | 1.00 | 1.18 | 1.17 | 1.11 |
| C17 | 1.05 | 1.26 | 0.96 | 0.94 | 1.09 | 1.07 |
| C18 | 1.02 | 1.05 | 0.97 | 0.78 | 0.91 | 0.99 |
| C20 | 1.09 | 1.14 | 0.74 | 1.05 | 1.11 | 0.92 |
| C21 | 0.9 | 1.16 | 0.83 | 0.8 | 1.07 | 1.08 |
| C22 | 1.28 | 1.11 | 0.96 | 1.04 | 1.05 | 0.85 |
| C23 | 1.18 | 1.29 | 0.81 | 0.94 | 0.76 | 1.01 |
| | **0.281** | **0.188** | **0.116** | **0.127** | **0.123** | **0.079** |

**EXACT Acquisition 50% sampling density (Strychnine)**

| | **rd=2.5** | **rd=5s** | **rd=10s** | **rd=15s** | **rd=20s** | **rd=60** |
|---|---|---|---|---|---|---|
| C1 | 1.41 | 1.36 | 1.32 | 1.12 | 1.17 | 1.08 |
| C2 | 1.57 | 1.60 | 1.11 | 1.00 | 1.15 | 0.90 |
| C3 | 1.48 | 1.43 | 1.06 | 0.97 | 1.26 | 0.91 |

| | | | | | | |
|---|---|---|---|---|---|---|
| C4 | 1.58 | 1.46 | 0.91 | 1.13 | 1.20 | 0.96 |
| C5 | 0.93 | 1.19 | 1.10 | 0.92 | 1.07 | 0.83 |
| C6 | 0.79 | 1.03 | 1.00 | 0.96 | 0.9 | 1.09 |
| C7 | 1.03 | 1.04 | 1.16 | 1.25 | 0.92 | 0.99 |
| C8 | 1.69 | 1.25 | 1.09 | 1.23 | 1.03 | 1.05 |
| C10 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| C11 | 1.46 | 1.34 | 1.13 | 0.96 | 0.86 | 0.91 |
| C12 | 1.64 | 1.63 | 1.14 | 1.22 | 1.11 | 1.11 |
| C13 | 1.54 | 1.64 | 1.35 | 1.06 | 1.09 | 0.97 |
| C14 | 1.43 | 1.3 | 1.08 | 1.03 | 0.84 | 1.09 |
| C15 | 1.07 | 1.12 | 1.09 | 0.96 | 0.94 | 1.02 |
| C16 | 1.62 | 1.35 | 1.27 | 1.23 | 0.99 | 1.03 |
| C17 | 1.10 | 1.17 | 1.06 | 1.19 | 0.87 | 1.06 |
| C18 | 1.03 | 1.24 | 1.14 | 1.06 | 1.02 | 0.96 |
| C20 | 1.05 | 1.22 | 1.01 | 1.20 | 0.97 | 0.92 |
| C21 | 0.92 | 1.35 | 0.89 | 0.82 | 1.13 | 1.05 |
| C22 | 1.25 | 1.27 | 1.14 | 1.10 | 0.94 | 0.85 |
| C23 | 1.19 | 1.33 | 1.00 | 1.13 | 1.09 | 0.91 |
| | **0.282** | **0.183** | **0.116** | **0.120** | **0.118** | **0.082** |




4.4 Figure S5: The standard deviations of the relative integrals of Strychnine at different relaxation delays using inverse gated, SRT, and EXACT rec. Acquisition methods. The experimental time is the same using the inverse gated and the EXACT acquisition methods, however, it is double using the SRT acquisition method.

# 5 Strychnine, Camphor, DEET mixture results

### 5.1 Table 7: Integrals average and standard deviation of Strychnine, Camphor, and DEET mixture using SRT acquisition method with 40s relaxation delay (rd).

| **SRT, rd=40s** | | | | | |
|---|---|---|---|---|---|
| **Strychnine** | | **Camphor** | | **DEET** | |
| C1 | 0.12 | C1 | 1.19 | C1 | 1.73 |
| C2 | 0.13 | C3 | 1.02 | C2 | 1.77 |
| C3 | 0.2 | C4 | 1.00 | C3 | 1.74 |
| C4 | 0.16 | C5 | 0.95 | C4 | 1.76 |
| C5 | 0.15 | C6 | 1.01 | C5 | 1.71 |
| C6 | 0.19 | C7 | 1.00 | C6 | 1.73 |
| C7 | 0.11 | C8 | 1.00 | C7 | 1.73 |
| C8 | 0.18 | C9 | 0.99 | C12 | 1.77 |
| C10 | 0.17 | C10 | 1.00 | | |
| C11 | 0.18 | | | | |
| C13 | 0.15 | | | | |
| C14 | 0.16 | | | | |
| C15 | 0.17 | | | | |
| C16 | 0.17 | | | | |
| C17 | 0.27 | | | | |
| C18 | 0.12 | | | | |
| C20 | 0.14 | | | | |
| C21 | 0.15 | | | | |
| C22 | 0.16 | | | | |
| C23 | 0.13 | | | | |
| **integrals average** | **0.160** | | **1.017** | | **1.742** |
| **std.** | **0.035** | | **0.067** | | **0.0218** |

### 5.2 Table 8: Integrals, Integrals average and standard deviation of Strychnine, Camphor, and DEET mixture using EXACT (with reconstruction) acquisition method with 40s relaxation delay (rd).

| **EXACT rd=40s** | | | | | |
|---|---|---|---|---|---|
| **Strychnine** | | **Camphor** | | **DEET** | |
| C1 | 0.12 | C1 | 1.26 | C1 | 1.69 |
| C2 | 0.15 | C3 | 1.00 | C2 | 1.72 |
| C3 | 0.22 | C4 | 0.96 | C3 | 1.69 |
| C4 | 0.14 | C5 | 0.87 | C4 | 1.73 |
| C5 | 0.14 | C6 | 0.99 | C5 | 1.71 |
| C6 | 0.18 | C7 | 1.00 | C6 | 1.69 |
| C7 | 0.13 | C8 | 0.94 | C7 | 1.72 |
| C8 | 0.16 | C9 | 0.95 | C12 | 1.75 |
| C10 | 0.16 | C10 | 0.96 | | |

| | | | | | |
|---|---|---|---|---|---|
| C11 | 0.14 | | | | |
| C13 | 0.15 | | | | |
| C14 | 0.14 | | | | |
| C15 | 0.17 | | | | |
| C16 | 0.18 | | | | |
| C17 | 0.26 | | | | |
| C18 | 0.12 | | | | |
| C20 | 0.15 | | | | |
| C21 | 0.14 | | | | |
| C22 | 0.19 | | | | |
| C23 | 0.13 | | | | |
| **integrals average** | **0.158** | | **0.992** | | **1.712** |
| **std.** | **0.034** | | **0.108** | | **0.021** |

5.3 Table 9: Integrals, Integrals average and standard deviation of Strychnine, Camphor, and DEET mixture using inverse gated (IG) acquisition method with 60s relaxation delay (rd)

| **IG, rd=60s** | | | | | |
|---|---|---|---|---|---|
| **Strychnine** | | **Camphor** | | **DEET** | |
| C1 | 0.12 | C1 | 1.16 | C1 | 1.81 |
| C2 | 0.15 | C3 | 1.01 | C2 | 1.65 |
| C3 | 0.28 | C4 | 0.95 | C3 | 1.80 |
| C4 | 0.14 | C5 | 0.83 | C4 | 1.77 |
| C5 | 0.17 | C6 | 1.00 | C5 | 1.61 |
| C6 | 0.17 | C7 | 1.00 | C6 | 1.67 |
| C7 | 0.17 | C8 | 0.87 | C7 | 1.78 |
| C8 | 0.13 | C9 | 1.02 | C12 | 1.70 |
| C10 | 0.16 | C10 | 1.01 | | |
| C11 | 0.16 | | | | |
| C13 | 0.13 | | | | |
| C14 | 0.16 | | | | |
| C15 | 0.15 | | | | |
| C16 | 0.15 | | | | |
| C17 | 0.25 | | | | |
| C18 | 0.12 | | | | |
| C20 | 0.12 | | | | |
| C21 | 0.13 | | | | |
| C22 | 0.22 | | | | |
| C23 | 0.11 | | | | |
| **integrals average** | **0.159** | | **0.983** | | **1.723** |
| **std.** | **0.044** | | **0.094** | | **0.071** |

Strychnine C12 and Camphor C2 could not be integrated due to signal overlap.

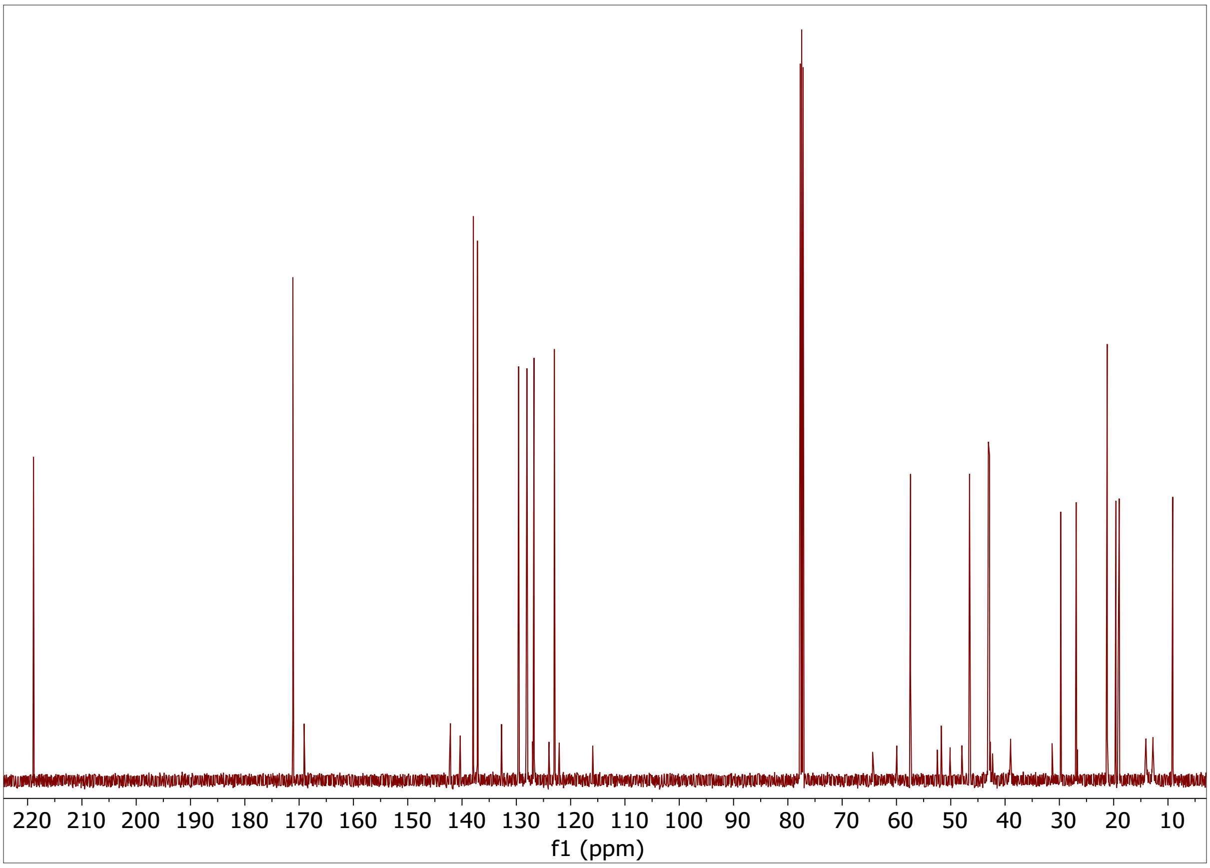



Figure 5.4 S6: Strychnine, Camphor, DEET mixture $^{13}C$ spectrum.

## 6 Varian-format pulse sequence for SRT and EXACT regular sampling

```
#include <standard.h>
void pulsesequence()
{

Double
chunkpoints = getval("chunkpoints"), /*number of datapoints collected*/
cycles = getval("cycles"), /*number of cycles*/
srt = getval("srt");/*for srt=0, FID starts with chunk, for srt=1, the FID strats with gap*/



initval(cycles,v20);
  /* equilibrium period */
  status(A);
  hsdelay(d1);

  /* --- tau delay --- */
  status(B);

  /* --- observe period --- */
  pulse(pw,oph);

/*--Acquisition start--*/

/*Preloop acquistion for srt = 0*/

if(srt==0)
{status(C);
decpower(42);                    /*Decpower statement for the WALTZ-16 status C*/
```

```
rcvron();
acquire (chunkpoints, 1/sw);
rcvroff();

status(B);
decpower(62);                    /*Decpower statement for the 180 pulse status B*/
 delay((0.5*chunkpoints/(2*sw))-pwx-rof1);
 decrgpulse(pwx*2, 1,rof1,rof2);
 delay((0.5*chunkpoints/(2*sw))-pwx-rof2-alfa);
}


/* Preloop acquistion for srt = 1 */

if(srt==1)
{
status(C);
decpower(42);
if (srt==1) {acquire (1,1/sw);
 rcvroff();

status(B);
decpower(62);
delay((0.5*chunkpoints/(2*sw))-pwx-0.5/sw-rof1);
decrgpulse(pwx*2,1,rof1,rof2);
 delay((0.5*chunkpoints/(2*sw))-pwx-rof2-alfa);}
```

```
starthardloop(v20);
  //decr(v20);
{

status(C);
decpower(42);
rcvron();
acquire(chunkpoints,1/sw);
rcvroff();

status(B);
decpower(62);
delay((0.5*chunkpoints/(2*sw))-pwx-rof1);          /*Delays by same length as chunk*/
decrgpulse(pwx*2,3,rof1,rof2);
delay((0.5*chunkpoints/(2*sw))-pwx-rof2-alfa);

status(C);
decpower(42);
rcvron();
acquire(chunkpoints,1/sw);
rcvroff();

status(B);
decpower(62);
delay((0.5*chunkpoints/(2*sw))-pwx-rof1);
decrgpulse(pwx*2,1,rof1,rof2);
delay((0.5*chunkpoints/(2*sw))-pwx-rof2-alfa);


endhardloop();
```

```
incr(v20);

}
```