Supporting Information for:

perfectBASH: Band-selective homonuclear decoupling in peptides and peptidomimetics

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1 Experiments on the Elastin fragment GVG(VPGVG)$_3$

1.1 Elastin sample and experimental setups

The sample contains the elastin fragment GVG(VPGVG)$_3$ (10% w/w) dissolved in a 50mM sodium phosphate buffer pH 7 in H$_2$O/D$_2$O 80:20[1]. Experiments were done on a Bruker Avance III system with 600.3 MHz proton base frequency, equipped with a 5 mm triple-resonance broadband inverse probe ($^1$H, $^2$H, $^{31}$P, BB) with z-gradient. The maximum z-gradient strength was experimentally determined to be (0.494 ± 0.007) T m$^{-1}$ using a stimulated echo experiment on a doped water sample[2].

A 90° proton pulse with duration of 11.1 μs was used. Gradients used for coherence selection had durations of 1 ms and smoothed square shape (SMSQ) digitized using 100 points. All gradients strengths are given as a fraction of the maximum amplitude and were followed by a recovery delay of 200 μs.

All bandwidths given for the pulse shapes used for frequency selective refocusing were calculated with the Bruker Shape Tool of TopSpin 3.2 using the “Calculate Bandwidth for Refocusing –My” option. The numbers given are calculated by default for 70% of the maximum refocusing profile. Note, however, that at least 95% of the maximum refocusing profile is recommended to obtain clean homonuclear decoupled spectra using the perfectBASH scheme. The pulses used herein were adjusted to fulfill this criterion.

1.2 Conventional $^1$H spectra

The $^1$H spectrum in Figure 1-1a) was acquired using the zgesgp pulse programs from the Bruker pulse sequence library. Excitation sculpting was executed with 2.5 ms long soft rectangular pulses (Squa100.1000) with 4.68 ppm offset and flanked in each case by gradients with 31% and 11% strength, respectively.

1.3 $^1$H-experiments with perfectBASH band selective decoupling

1D $^1$H-perfectBASH experiments were acquired with the pulse sequence in the SI chapter 5.1 including an option for solvent presaturation during the relaxation delay. In all experiments this option was checked to attenuate the strong water signal. Water was presaturated for 1 s, the offset was set on 4.697 ppm and the RF-power was 4.5*10$^{-5}$ W. All spectra were measured at 300 K. The spectra were collected with 10 kHz spectral width and the interferogram based acquisition mode using 32 data-chunks of 20 ms duration.
Several $^1$H-perfect BASH spectra of the elastin sample were acquired applying different selective refocusing pulses. For the spectra in Figure 1-1 c), Figure 1-2 b), Figure 1-3 b) and Figure 1-4 a) a 2.6 ms long twofold phase-modulated RSnob pulse with two offsets was used. The phase-modulated pulse, digitized in 10000 points with two offset frequencies at 0 Hz (=SPOFFS) and 2500 Hz (=SPOFFS + 2500 Hz) was created using Bruker ShapeTool of TopSpin 3.2 with the “Multiple Phase Modulation” option. The quality of the frequency selective refocusing was checked with a gradient selected selective spin echo (selgpse) and is shown in Figure 1-1 b). The offset of the selective pulse was set to 3.99 ppm.

The spectra in Figure 1-2 a) and Figure 1-4 b) were acquired using a 1.6 ms long ReBurp pulse (3600 Hz bandwidth, 5.98 ppm offset) and a 4.5 ms long ReBurp pulse (1290 Hz bandwidth, 3.92 ppm offset), respectively. Coherence selection was enforced in all experiments with gradients of $G_1=33\%$ strength in the first echo block and $G_2=82\%$ in the second echo block respectively. 8 transients per data-chunk were accumulated and a relaxation delay of 2 s was used.

For FID reconstruction the $pshift$ AU from the Manchester NMR Methodology Group web pages (http://nmr.chemistry.manchester.ac.uk) was used yielding a 646.8 ms FID, which was zero filled to 32768 complex points and multiplied with an exponential apodization function (1 Hz line broadening) before Fourier transformation.
1.4 *perfectBASH* spectra of the elastin fragment GVG(VPGVG)$_3$

Figure 1-1: Proton spectra of the elastin fragment GVG(VPGVG)$_3$ obtained with (a) conventional $^1$H (600.3 MHz proton base frequency), (b) a gradient selected selective spin echo using a 2.6 ms two-fold phase-modulated RSnob refocusing pulse and (c) 1D $^1$H-*perfectBASH* using a 2.6 ms two-fold phase-modulated RSnob refocusing pulse.
Figure 1-2: 1D $^1$H-$\text{perfectBASH}$ spectra of the elastin fragment GVG(VPGVG)$_3$ obtained with (a) a 1.6 ms ReBurp refocusing pulse and (b) a 2.6 ms two-fold phase-modulated RSnob refocusing pulse. All spectra were obtained with 600.3 MHz proton base frequency.

Figure 1-3: Expansions of the amide- and $\alpha$-proton region of (a) the conventional $^1$H-spectrum (600.3 MHz proton base frequency) and (b) the 1D $^1$H-$\text{perfectBASH}$ spectrum, illustrating the incomplete homonuclear decoupling of the amide- and $\alpha$-protons of glycine.
Figure 1-4: 1D $^1$H-\textit{perfectBASH} spectra obtained with (a) a 2.6 ms twofold phase-modulated RSnob refocusing pulse and (b) a 4.5 ms ReBurp refocusing pulse (1290 Hz bandwidth, 3.92 ppm offset). All spectra were obtained with 600.3 MHz proton base frequency. In the spectrum (a) the amide- as well as the $\alpha$-proton region is band selectively homonuclear decoupled, hence the diastereotopic and mutually coupled $\alpha$-protons of the glycine amino acids are not fully decoupled. In spectrum (b) only the $\alpha$-proton region is band selectively homonuclear decoupled using the \textit{perfectBASH} sequence. The mutually coupled $\alpha$-protons of glycine should be decoupled in this case and should appear as singlets. However the quality of the spectrum is only marginally improved due to the clustered and strongly coupled nature of the glycine $\alpha$-protons.
2 Cyclosporine A

2.1 NOESY vs. EASY-ROESY

Under the chosen measurement conditions (700.17 MHz and 300 K) the longitudinal nuclear overhauser effect of the cyclosporine A sample seems to be near the zero crossing. This is illustrated with a zero-quantum filtered NOESY \((\text{noesygpphzs})\) spectrum (Figure 2-1), which shows only little cross peaks with comparably low intensity. In contrast, the EASY-ROESY \((\text{roesyadjsphpr})\) spectrum (Figure 2-2) shows significantly more cross peaks.

![Figure 2-1: Zero-Quantum filtered NOESY of cyclosporine A in benzene-\(d_6\), obtained at 700.17 MHz and 300 ms mixing time.](image-url)
2.2 Cyclosporine A spin system used for simulations

The reduced spin system used for the simulations of cyclosporine A only contains the amide-, α-, N-methyl- and some side chain protons with chemical shifts close to the α-proton region. Chemical shifts were extracted from a 1D $^1$H-PSYCHE[3] spectrum and a $^1$H,$^{13}$C-HSQC (hsqcetgpsp.2). J-coupling constants were determined from the conventional proton spectrum. To treat the effects of relaxation during the experiment at least phenomenologically, $T_2$-rates were estimated for the sites considered, and also fed into the simulation program. For a rough estimate of $T_2$, we assumed that $T_2 \approx T_1$ to be valid. We are well aware, that this is by no means a rigorous treatment of the effects of relaxation during the pulse sequence. The $T_2$-relaxation times were determined with a series of inversion recovery experiments ($t_{1ir}$), using seven delays (5 ms, 10 ms, 50 ms, 500 ms, 1.25 s, 4 s and 30 s) and subsequent fitting of the integrals. The spectral parameters for the spin system input file are listed in the table below. A simulated proton spectrum of the reduced spin system is shown in Figure 2-3.
<table>
<thead>
<tr>
<th>Proton assignment</th>
<th>Chemical Shift δ / ppm</th>
<th>J-coupling constant *J_{ij} / Hz</th>
<th>Relaxation times T1 ≈ T2 / ms</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 MeBmt</td>
<td>α 5.7216</td>
<td>3J_{α,β} = 7.61</td>
<td>587.4</td>
</tr>
<tr>
<td></td>
<td>β 4.1917</td>
<td></td>
<td>584.7</td>
</tr>
<tr>
<td></td>
<td>γ 3.7166</td>
<td></td>
<td>690.0</td>
</tr>
<tr>
<td></td>
<td>ε 5.6394</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>ζ 5.5211</td>
<td>3J_{ε,ζ} = 14.9</td>
<td>1154.0</td>
</tr>
<tr>
<td>2 Abu</td>
<td>α 5.1125</td>
<td>3J_{α,β} = 9.76</td>
<td>880.6</td>
</tr>
<tr>
<td></td>
<td>NH 8.2483</td>
<td></td>
<td>479.0</td>
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<td>3 Sar</td>
<td>α 4.0027</td>
<td></td>
<td>415.3</td>
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<tr>
<td></td>
<td>NMe 3.0664</td>
<td></td>
<td>851.7</td>
</tr>
<tr>
<td>4 MelLeu</td>
<td>α 5.5827</td>
<td></td>
<td>842.0</td>
</tr>
<tr>
<td></td>
<td>NMe 2.9671</td>
<td></td>
<td>743.3</td>
</tr>
<tr>
<td>5 Val</td>
<td>α 4.8763</td>
<td>3J_{α,β} = 9.92, 3J_{ε,ζ} = 8.66</td>
<td>827.0</td>
</tr>
<tr>
<td></td>
<td>β 2.6128</td>
<td></td>
<td>504.7</td>
</tr>
<tr>
<td></td>
<td>NH 7.4459</td>
<td></td>
<td>599.6</td>
</tr>
<tr>
<td>6 MelLeu</td>
<td>α 5.3782</td>
<td></td>
<td>549.0</td>
</tr>
<tr>
<td></td>
<td>NMe 3.2182</td>
<td></td>
<td>728.5</td>
</tr>
<tr>
<td>7 Ala</td>
<td>α 4.8011</td>
<td></td>
<td>1063.0</td>
</tr>
<tr>
<td></td>
<td>NH 7.9611</td>
<td>3J_{α,β} = 7.30</td>
<td>471.0</td>
</tr>
<tr>
<td>8 Ala</td>
<td>α 4.8251</td>
<td>3J_{α,β} = 7.31</td>
<td>1063.0</td>
</tr>
<tr>
<td></td>
<td>NH 7.6066</td>
<td></td>
<td>687.0</td>
</tr>
<tr>
<td>9 MelLeu</td>
<td>α 5.8634</td>
<td></td>
<td>421.9</td>
</tr>
<tr>
<td></td>
<td>NMe 2.9212</td>
<td></td>
<td>790.2</td>
</tr>
<tr>
<td>10 MelLeu</td>
<td>α 5.3298</td>
<td></td>
<td>416.9</td>
</tr>
<tr>
<td></td>
<td>NMe 2.8419</td>
<td></td>
<td>907.8</td>
</tr>
<tr>
<td>11 MeVal</td>
<td>α 5.2528</td>
<td></td>
<td>794.5</td>
</tr>
<tr>
<td></td>
<td>NMe 2.5853</td>
<td></td>
<td>685.0</td>
</tr>
</tbody>
</table>

Figure 2-3: Proton spectra of cyclosporine A in benzene-d_6 obtained (a) experimentally (600.3 MHz proton base frequency, 300 K) and (b) via simulation using the Bruker NMRSim package and the reduced cyclosporine A system described above.
2.3 Pulse design

Figure 2-4: Simulated refocusing profiles of tested selective refocusing pulses potentially usable for perfectBASH band selective homonuclear decoupling of the amide- and $\alpha$-protons in cyclosporine A. In (a) profiles for a 400 $\mu$s Gaussian refocusing pulse (blue), a 800 $\mu$s RSnob refocusing pulse (red) and 1.49 ms ReBurp (green). In (b) simulated refocusing profile for a two-fold phase modulated RSnob-refocusing pulse (purple) or ReBurp-refocusing pulse (orange) with two different offsets at 5.32 ppm in the $\alpha$-H-region and 7.79 ppm in the amide-region of cyclosporine A. For better clarity, the profiles were calculated for inversion, but do not differ substantially from the case of refocusing. The profiles were simulated for 600.3 MHz proton base frequency.
2.4 Simulated and experimental spectra

Figure 2-5: Comparison between experimental (b and d) and simulated (a and c) 1D $^1$H-perfectBASH spectra of the $\alpha$-proton region of cyclosporine A. In (a) and (b) a 800 $\mu$s RSnob refocusing pulse (2920 Hz bandwidth, 6.52 ppm offset) was used for selective refocusing, whereas in (c) and (d) a 1.49 ms ReBurp refocusing pulse (3900 Hz bandwidth, 6.52 ppm offset) was applied. All spectra were obtained with 600.3 MHz proton base frequency.
Figure 2-6: Comparison between experimental (b and d) and simulated (a and c) 1D $^1$H-$\text{perfectBASH}$ spectra of the amide-proton region of cyclosporine A. In (a) and (b) a 800 $\mu$s RSnob refocusing pulse (2920 Hz bandwidth, 6.52 ppm offset) was used for selective refocusing, whereas in (c) and (d) a 1.49 ms ReBurp refocusing pulse (3900 Hz bandwidth, 6.52 ppm offset) was applied. All spectra were obtained with 600.3 MHz proton base frequency.
2.5 Simulated spectra with further tested pulse shapes

Figure 2-7: 1D $^1$H-spectrum (a) and simulated (b – f) 1D $^1$H-perfectBASH spectra of the $\alpha$-proton region of cyclosporine A. The spectra were obtained using (b) a 2.6 ms ReBurp refocusing pulse (2236 Hz bandwidth), (c) a 1.1 ms RSnob refocusing pulse (2120 Hz bandwidth), (d) a 400 $\mu$s Gaussian refocusing pulse (2205 Hz bandwidth), (e) a 1.5 ms twofold phase-modulated RSnob pulse with two offsets at 5.32 ppm ($\alpha$-proton region) and 7.79 ppm (amide-proton region) and (e) a 5 ms twofold phase-modulated ReBurp pulse with two offsets at 5.32 ppm ($\alpha$-proton region) and 7.79 ppm (amide-proton region). The refocusing profiles of the last two pulses are shown in Figure 2-4b. All spectra were obtained with 600.3 MHz proton base frequency.
Figure 2-8: 1D $^1$H-spectrum (a) and simulated (b – f) 1D $^1$H-perfectBASH spectra of the amide-proton region of cyclosporine A. The spectra were obtained using (b) a 2.6 ms ReBurp refocusing pulse (2236 Hz bandwidth), (c) a 1.1 ms RSnob refocusing pulse (2120 Hz bandwidth), (d) a 400 μs Gaussian refocusing pulse (2205 Hz bandwidth), (e) a 1.5 ms twofold phase-modulated RSnob pulse with two offsets at 5.32 ppm ($\alpha$-proton region) and 7.79 ppm (amide-proton region) and (e) a 5 ms twofold phase-modulated ReBurp pulse with two offsets at 5.32 ppm ($\alpha$-proton region) and 7.79 ppm (amide-proton region). The refocusing profiles of the last two pulses are shown in Figure 2-4b. All spectra were obtained with 600.3 MHz proton base frequency.
3 Experiments on the hexameric oligourea sample

3.1 Experimental section

Experiments were done on a Bruker Avance III with 700.17 MHz proton base frequency, equipped with a QCI probe ($^1$H, $^{13}$C, $^{19}$F, $^{15}$N) with z-gradient (0.53 T m$^{-1}$ maximum gradient strength). Sample temperature was regulated at 320 K using a BCU-Xtreme unit. Temperature calibration was performed using an ethyleneglycol-$d_6$ sample. The 90° proton pulse duration was 6.99 μs.

Gradients used for coherence selection had durations of 1 ms and smoothed square shape (SMSQ) digitized using 100 points. All gradients strengths are given as a fraction of the maximum amplitude and were followed by a recovery delay of 200 μs.

The band selective homonuclear decoupled spectra of the β-proton and α$_1$-proton region independently were acquired with the 1D $^1$H-HOBS scheme and with a band selective Zangger-Sterk type interferogram-based acquisition[4].

3.1.1 1D $^1$H-HOBS

1D $^1$H-HOBS spectra were acquired using the 1D $^1$H-HOBS sequence in chapter 5.3. The strong water signal was presaturated with continuous low power irradiation lasting for 1 s, the offset was set on 4.61 ppm.

Both spectra were collected with 5 kHz spectral width and 12798 complex points (640 ms acquisition time). For HOBS decoupling during acquisition the FID was cut into 32 blocks of 20 ms duration separated by the decoupling pulses. The band selective decoupling of the β-proton region (Figure 3-2b) was performed with a ReBurp refocusing pulse with a duration of 17 ms (345 Hz bandwidth) and 4.67 ppm offset. The α$_1$-proton region (Figure 3-3b) was decoupled using a 15 ms ReBurp refocusing pulse (390 Hz bandwidth) with 4.12 ppm offset.

Gradients for coherence selection in the selective refocusing element (G$_1$) before acquisition had durations of 1 ms and 17% gradient strength, the gradients during real-time decoupling had durations of 500 μs and strengths of $G_2$=7 % and $G_3$=5 %, respectively.

32 transients were accumulated and a relaxation delay of 2 s was used. The acquired FIDs were zero filled to 65536 complex points and multiplied with an exponential apodization function (1 Hz line broadening) before Fourier transformation.

3.1.2 Interferogram-based acquisition

The Zangger-Sterk type interferogram-based acquisition was performed with the Zangger-Sterk pulse sequence used in the PEPSIE paper[5]. The FID was acquired in 32 data-chunks with duration of 20 ms each. Band selective decoupling of the β-proton region (Figure 3-2c) was performed with a ReBurp refocusing pulse with a duration of 17 ms (345 Hz bandwidth) and 4.67 ppm offset. The α$_1$-proton region (Figure 3-3c) was decoupled using a 15 ms ReBurp refocusing pulse (390 Hz bandwidth) with
4.12 ppm offset. The gradient for coherence selection had gradient strength of 83%, the slice-selection gradient was switched off. 32 transients were accumulated and a relaxation delay of 2 s was used. For FID reconstruction the \textit{pshift} AU from the Manchester NMR Methodology Group web pages (http://nmr.chemistry.manchester.ac.uk) was used yielding a 646.8 ms FID, which was zero filled to 65536 complex points and multiplied with an exponential apodization function (0.3 Hz line broadening) before Fourier transformation.

\subsection*{3.2 Resulting spectra}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig3-1.png}
\caption{Simulated refocusing profiles of a 17 ms ReBurp refocusing pulse (345 Hz bandwidth) with 4.67 ppm offset for band selective decoupling of the $\beta$-proton region (blue profile) and of a 15 ms ReBurp refocusing pulse (390 Hz bandwidth) with 4.12 ppm offset for band selective decoupling of the $\alpha_1$-proton region (red profile). Probably there is partial co-refocusing of the other proton group ($\beta$- and $\alpha_r$-protons, respectively) at the edges of the refocusing profile. For better clarity, the profiles were calculated for inversion, but do not differ substantially from the case of refocusing. The profiles were simulated for 700.17 MHz proton base frequency.}
\end{figure}
Figure 3-2: Spectra of the hexameric oligoureza with homonuclear decoupling of the β-proton region, obtained using (a) conventional $^1$H (700.17 MHz proton base frequency), (b) HOBS, (c) band selective homonuclear decoupling using the Zangger-Sterk type interferogram-based acquisition and (d) perfectBASH. For selective refocusing a 17 ms ReBurp refocusing pulse (345 Hz bandwidth) with 4.67 ppm offset was used in (b) and (c), in spectrum (d) a 4.5 ms Reburp refocusing pulse (1290 Hz bandwidth) with 4.37 ppm offset was applied. Spectrum (b) shows broadened lines and significant distortions, which result from the long interruptions of the FID ($\approx$ 17 ms) in the real-time acquisition scheme. Using the band selective variant of the Zangger-Sterk type interferogram-based acquisition the homonuclear decoupling quality is improved significantly. Nevertheless, the distortions in spectrum (c) result from two mutually coupled protons of the benzylic protecting group.
Figure 3-3: Spectra of the hexameric oligourea with homonuclear decoupling of the $\alpha_1$-proton region, obtained using (a) conventional $^1$H (700.17 MHz proton base frequency), (b) HOBS, (c) band selective homonuclear decoupling using the Zangger-Sterk type interferogram-based acquisition and (d) perfectBASH. For selective refocusing a 15 ms ReBurp refocusing pulse (390 Hz bandwidth) with 4.12 ppm offset was used in (b) and (c), in spectrum (d) a 4.5 ms Reburp refocusing pulse (1290 Hz bandwidth) with 4.37 ppm offset was applied. Spectrum (b) shows similar distortions like spectrum (b) in Figure 3-2. This can be solved using the band selective variant of the Zangger-Sterk type interferogram-based acquisition. However, in the present case partial co-refocusing of $\beta$-protons happens.
**Figure 4-1:** $F1$-perfectBASH CLIP-COSY (a) and $F1$-perfectBASH relayed-CLIP-COSY (b; with two transfer steps) of the backbone proton region of cyclosporine A. The dotted lines indicate the positions, at which the $F2$-traces shown in Figure 4-2 have been extracted. The red trace belongs to the $\alpha$-proton of amino acid 5-valine, as indicated in the structure above. The blue trace belongs to the amide-proton of the same amino acid. Both positive and negative contours are shown in black, to avoid confusion stemming from the signal sign changes expected in the case of the relayed experiment. The spectra were obtained with 600.3 MHz proton base frequency.
Figure 4-2: Comparison of extracted F2-traces of the (a, red) 5α- and (b, blue) 5NH-proton from the $F_1$-perfectBASH CLIP-COSY, the $F_1$-perfectBASH relayed-CLIP-COSY (two transfer steps) and the $F_1$-perfectBASH TOCSY (Figure 5 in the main text). In (a) the CLIP-COSY delivers only two correlations from the 5α-proton to the 5β- and 5NH-proton, respectively. The relayed-CLIP-COSY shows two extra correlation stemming from a two-step transfer originating from the 5α-proton to the two methyl groups 5γ₁ and 5γ₂, whereas the TOCSY exhibit all correlations from the whole spin system of amino acid 5-valine. The traces were extracted from spectra, which were obtained with 600.3 MHz proton base frequency.
5  Bruker pulse sequence codes

5.1 1D $^1$H-experiment with perfectBASH decoupling

; 1D 1H-PERFECT-BASH
;
; This pulse sequence is part of the paper:
; perfectBASH: Band selective homonuclear decoupling in peptides and peptidomimetics
; Authors: Julian Ilgen, Lukas Kaltschnee, Christina M. Thiele
;
; Julian Ilgen and Lukas Kaltschnee
; Technical University Darmstadt
; Avance II+/III Version
; Topspin 3.6
;
; Description and Comments:
; The pulse sequence has been coded for test purposes only and may contain errors.
; It does contain arguments that can lead to hardware damages if acquisition parameters
; are set unfavorably. The functionality of the pulse sequence itself may differ
; depending on the hardware as well as the software used to execute it. Functionality
; on differing systems cannot be granted.
; Any use of this pulse sequence on a spectrometer is at your own risk!
; By using this pulse sequence or any modification of it in any published material
; you agree to acknowledge the above-mentioned publication.
;
; band selective homonuclear decoupling using frequency selective pulses incorporated in Perfect-Echo
; pulse sequence is based on 1D 1H-PEPSIE
; interferogramm based acquisition mode in pseudo direct dimension
; J is refocussed at centre of chunk
; option for solvent presaturation during relaxation delay
; presaturation offset defined via cnst40 [ppm]
; data can be reconstructed using the "pshift" macro available at http://nmr.chemistry.manchester.ac.uk
; avance-version (12/01/11)
;
; Relevant papers:
; (4) L. Kaltschnee, A. Kolmer, I. Timari, V. Schmidts, R. W. Adams, M. Nilsson, K. E. Köver, G. A. Morris and C. M. Thiele,
; Chem. Commun., 2014, 50, 15702 - 15705
;
; $CLASS=HighRes
; $DIM=2D
; $TYPE=
; $SUBTYPE=
; $COMMENT=

#include <Avance.incl>
#include <Grad.incl>

define delay tauA
define delay tauB
define delay tauC

"d11=30m"
"d12=20u"
"in0=inf1/2"
"tauA=in0+\{de\"2\*cnst4\}+de" 
"p2=p1\^2.0"
tauB = in0 / 2 - p16 - d16 - 10u

tauC = in0 / 2 + 10u + (dw * 2 * cnst4) + de

cnst21 = cnst20 * bf1 ; offset calculation for frequency selective refocusing

cnst22 = cnst21 - o1

spoffs2 = cnst22

#ifdef CWPR ; solvent presaturation

d18 = d1 - d17

cnst41 = cnst40 * bf1

cnst42 = cnst41 - o1
#endif /*CWPR*/

; start pulsesquence;
1 ze
2 d11
3 d12

#ifdef CWPR ; begin of solvent presaturation

d12 fq = 0 : f1

d12 fq = cnst42 : f1 ; set frequency on f1-channel to solvent shift for presaturation [fq = SFO1 + cnst42]

d12 pl9 : f1 ; set power level on f1-channel for presaturation

d18 ; residual relaxation delay

d17 cw : f1 ph29

4u do : f1

d12 fq = 0 : f1 ; reset frequency on f1-channel [fq = SFO1]

d12 pl1 : f1 ; reset power level on f1-channel
#endif /*CWPR*/

#else ; no solvent presaturation

d1

d12 pl1 : f1
#endif /*CWPR*/

50u UNBLERGRAD

4 (p1 ph1) : f1 ; 90 degree pulse excitation

10u
d0 ; Incremented delay

tauA pl0 : f1 ; power switching f1-channel

p16 : gp1
d16

(p12 : mp2 ph2 : r) : f1 ; first frequency selective refocusing pulse

p16 : gp1
d16
tauA pl1 : f1 ; power switching f1-channel
d0 ; Incremented delay

10u
5 (p1 ph3) : f1 ; 90 degree pulse for perfect echo J-removal
d0       ; Incremented delay

tauB

10u

p16:gp2*0.5     ; CTP, +0.5
d16

[p2 ph4]:f1     ; hard 180 degree pulse
tauc p10:f1     ; power switching f1-channel

p16:gp2*-0.5    ; CTP, -0.5
d16

[p12:sp2 ph5:r]:f1     ; second frequency selective refocusing pulse

p16:gp2*-1.0    ; CTP, -1
d16 pl1:f1     ; power switching f1-channel

10u BLKGRAD

; incremented delay

6 go=2 ph31
30u
d11 mc #0 to 2 PiQEF(caldel(d0, +in0))

exit

;Phase Cycling

rph1       ; Hard 90
rph2       ; First selective 180
rph3       ; Hard 90
rph4       ; Hard 180
rph5       ; Second selective 180
rph29      ; CW solvent presaturation
rph31      ; Receiver

ph1= 0 2
ph2= 1 1 2 2 3 3 0 0
ph3= 1 3
ph4= 0
ph5= 0
ph29=0
ph31=2 0 0 2 2 0 0 2

rph31= rph1+p h2*2 + ph3*0 + ph4*2 + ph5*2  ; Receiver

zp1 : f1 channel = 90 degree high power pulse
zp2: f1 channel = high power 180 pulse width
zp12: duration of selective 180 pulse
zp16: CTP gradient pulse width

zp1 : f1 channel = power level for pulse (default)
zp9 : f1 channel = power level for continuous wave for solvent presaturation

zp: selective pulse power level
zpoffs2: selective pulse offset
zpnam2: file name for selective pulse [ReBurp.1000]

zp: CTP gradient 20-50% first echo
zp: CTP gradient 50-90% second echo
zpnam1: SMSQ10.100
zpnam2: SMSQ10.100

z00: incremented delay, set initial value to 0 s
zd1 : relaxation delay: 1=5 * T1
zd11: delay for disk I/O [30 msec]
; S25: delay for power switching [20 usec]
; d16: gradient recovery delay
; d17: delay for solvent presaturation
; d18: reduced relaxation delay
; td1: number of chunks to acquire

; NS: number of scans
; DS: number of dummy scans
; cnst4: number of points to drop at the beginning of each FID
; cnst20: offset for selective refocusing [ppm]
; cnst40: solvent offset [ppm]
; cnst42: difference for frequency switching on f1-channel

; FnMODE: QF

; preprocessor-flags-start
; CWPR: presaturation of solvent at beginning of pulse sequence
; option =DCWPR (eda: ZGOPTNS)
; preprocessor-flags-end
5.2 RESET-compatible 1D-perfectBASH sequence

; 1D 1H-PERFECT-BASH FOR RESET-PROCESSING
;
; This pulse sequence is part of the paper:
; perfectBASH: Band selective homonuclear decoupling in peptides and peptidomimetics
; Authors: Julian Ilgen, Lukas Kaltschnee, Christina M. Thiele
;
; Julian Ilgen and Lukas Kaltschnee
; Technical University Darmstadt
; Avance II+/III Version
; Topspin 3.x
;
; Description and Comments:
; The pulse sequence has been coded for test purposes only and may contain errors.
; It does contain arguments that can lead to hardware damages if acquisition parameters
; are set unfavorably. The functionality of the pulse sequence itself may differ
; depending on the hardware as well as the software used to execute it. Functionality
; on differing systems cannot be granted.
; Any use of this pulse sequence on a spectrometer is at your own risk!
; By using this pulse sequence or any modification of it in any published material
; you agree to acknowledge the above-mentioned publication.
;
; Band selective homonuclear decoupling using frequency selective pulses incorporated in Perfect-Echo
; Pulse sequence based on 1D 1H-PEPSIE
; interferogram acquisition mode in pseudo indirect dimension
; J is refocused at centre of chunk
; option for solvent presaturation during relaxation delay
; presaturation offset defined via cnst40 [ppm]
; Data can be reconstructed using the Bruker "proc_reset" AU-program, details see Ref. (5)
; avance-version (12/01/11)
;
; Relevant papers:
; Chem. Commun.; 2014, 50, 15702 – 15705
;
; @CLASS=HighRes
; @DIM=2D
; @STYPE=
; @SUBTYPE=
; @COMMENT=
;
#include <Avance.incl>
#include <Grad.incl>

define delay tauA

define delay tauB

define delay tauC

"in0=de*l31"
"tauA=in0+(dw*2*l30)+de"
"p2=p2+2.0"
"tauB=in0/2-p16-d16-10u"
"tauC=in0/2+p16+d16-10u"
"cnst21=cnst20+bw1" ; offset calculation for frequency selective refocusing
**cnst22=cnst21-o1**

**spoffs2=cnst22**

```c
#ifdef CWPR  ; solvent presaturation
  "d18=d1-d17"
  "cnst41=cnst40*bf1"
  "cnst42=cnst41-o1"
#else
#endif /*CWPR*/

; start pulse sequence;
1 ze
2 d11
3 d12

#ifdef CWPR  ; begin of solvent presaturation
  d12 fq=0:f1
  d12 fq=cnst42 :f1 ; set frequency on f1-channel to solvent shift for presaturation [fq=SFO1+cnst42]
  d12 pl9:f1 ; set power level on f1-channel for presaturation
  d18 ; residual relaxation delay
  d17 cw:f1 ph29 ; solvent presaturation
  4u do:f1
  d12 fq=0:f1 ; reset frequency on f1-channel [fq=SFO1]
  d12 pl1:f1 ; reset power level on f1-channel
#else ; no solvent presaturation
  d1
#endif /*CWPR*/

50u UNBLKGRAD
4 (p1 ph1):f1 ; 90 degree pulse excitation
10u
d0 ; incremented delay
tauA p10:f1 ; power switching f1-channel
pl6:gp1
d16
(p12:sp2 ph2:r):f1 ; first frequency selective refocusing pulse
pl6:gp1
d16
tauA p11:f1 ; power switching f1-channel
d0 ; incremented delay
10u
5 (p1 ph3):f1 ; 90 degree pulse for perfect echo J-removal
d0 ; incremented delay
tauB
10u
pl16:gp2*0.5 ; CTP, +0.5
d16
{p2 ph4):f1 ; hard 180 degree pulse
tauC pl10:f1 ; power switching f1-channel
pl16:gp2*0.5 ; CTP, -0.5
d16
{p12:sp2 ph5:r):f1 ; second frequency selective refocusing pulse
pl16:gp2*-1.0 ; CTP, -1
d16 pl11:f1 ; power switching f1-channel
10u BLKGRAD
d0 ; incremented delay
6 go=2 ph31
30u
d11 mc #0 to 2 P1QF(naldel(d0, +in0))
exit
rPhase Cycling
rph1 ; Hard 90
rph2 ; First selective 180
rph3 ; Hard 90
rph4 ; Hard 180
rph5 ; Second selective 180
rph29 ; CW solvent presaturation
rph31 ; Receiver
ph1= 0 2
ph2= 1 1 2 3 3 0 0
ph3= 1 3
ph4= 0
ph5= 0
ph29=0
ph31=2 0 0 2 0 0 2
rph31= rph1 + ph2*2 + ph3*0 + ph4*2 + ph5*2 ; Receiver
rp1 : f1 channel - 90 degree high power pulse
rp2 : f1 channel - high power 180 pulse width
rp12: duration of selective 180 pulse
rp16: CTP gradient pulse width
rp11 : f1 channel - power level for pulse (default)
rp19 : f1 channel - power level for continuous wave for solvent presaturation
rzp2: selective pulse power level
rzpoffs2: selective pulse offset
rzpnam2: file name for selective pulse [ReBurp.1000]
rgps1: CTP gradient 20-50% first echo
rgps2: CTP gradient 50-90% second echo
rgpnam1: SMSQ10.100
rgpnam2: SMSQ10.100
z00: incremented delay, set initial value to 0 s
zd1 : relaxation delay: 1=5 * T1
zd11: delay for disk I/O [30 msec]
zd12: delay for power switching [20 usec]
zd16: gradient recovery delay
zd17: delay for solvent presaturation
;d18: reduced relaxation delay

;cnst4: number of points to drop at the beginning of each FID
;cnst20: offset for selective refocusing [ppm]
;cnst40: solvent offset [ppm]
;cnst42: difference for frequency switching on f1-channel
;l29: total number of points in reconstructed FID
;l30: number of complex points at the beginning not to be included in reconstruction
;l31: number of complex points along the acquisition dimension per block block length about 8 to 10ms
;in0: increment for d0 ; dw*l31
;td1: number of chunks to acquire

;NS: number of scans
;DS: number of dummy scans
;
;PARAM: QF

;preprocessor-flags-start
; CWPR: presaturation of solvent at beginning of pulsesequence
; option -DCWPR (eda: ZGOPTNS)
;preprocessor-flags-end
5.3 1D $^1$H-HOBS sequence

; 1D 1H-HOBS
;
; advance-version (14/07/25)
; 1D sequence
; bandselective homodecoupling during acquisition
; based on HOBS sequence from Ref. (1)
; including presaturation during relaxation delay
; presaturation offset defined with cnst40
; calculation of offsets for selective refocusing pulses
;
; Literature;
;
; (2) J. Ying, J. Roche & A. Bax, J. Magn. Reson. 241, 97-102 (2014)
;
; $CLASS=HighRes
; $DIM=1D
; $TYPE=
; $SUBTYPE=
; $COMMENT=

#include <Avance.incl>
#include <Grad.incl>
#include <Delay.incl>
#include <De.incl>

"p2=p1*2"
"d11=30m"
"d12=20u"

"p29=300u"
"d3=d12/2u"

"d62=d1/10*2m" ; duration of one "real-time" chunk
"d63=d62/2" ; half duration for first chunk

; Calculations solvent presaturation;
ifdef CWPR
"d18=d1-d17"
"cnst41=cnst40*bf1"
"cnst42=cnst41-o1"
else
endif /*CWPR*/

"COUNTER=trunc((cnst31/100)*l0)+1"
"131=10*COUNTER"

"spoff35=bf1*(cnst21/1000000)-o1" ; offset for selective refocusing pulse

"acq=pi*2/V1"

dwellmode explicit

1 se
2 d11
3 d12

ifdef CWPR ; begin of solvent presaturation

d12 fq=0:f1
d12 fq=cnst42 :f1 ; set frequency on f1-channel to solvent shift for presaturation [fq=DF01+cnst42]

endif /*CWPR*/
"COUNTER=trunc((cnst31/100)*l0)+1"
"131=10*COUNTER"

"spoff35=bf1*(cnst21/1000000)-o1" ; offset for selective refocusing pulse

"acq=pi*2/V1"

dwellmode explicit

1 se
2 d11
3 d12

ifdef CWPR ; begin of solvent presaturation

d12 fq=0:f1
d12 fq=cnst42 :f1 ; set frequency on f1-channel to solvent shift for presaturation [fq=DF01+cnst42]

endif /*CWPR*/
S31

; set power level on f1-channel for presaturation

; residual relaxation delay

d17 cw:f1 ph29
4u do:f1

d12 fq=0:f1 ; reset frequency on f1-channel [fq=SFO1]
d12 pl1:f1 ; reset power level on f1-channel

#else ; no solvent presaturation
d1
d12 pl1:f1
#endif /*CWPR*/

50u UNBLKGRAD
(p1 ph1):f1
d3

p28:gp1
d16 pl0:f1

[p46:sp35 ph1]:f1
12u

p28:gp1
d16 pl0:f1

ACQ_START(ph30,ph31) ; total delay here=de

0.1u REC_UNBLK
0.05u DWL_CLK_ON
d63:r
0.05u DWL_CLK_OFF
0.1u REC_BLK

4 p29:gp2
d16 pl1:f1
(p2 ph2):f1
p29:gp2
d16

p29:gp3
d16 pl0:f1
5u
[p46:sp35 ph3]:f1
5u
p29:gp3
d16
0.1u REC_UNBLK
0.05u DWL_CLK_ON
d62:r
0.05u DWL_CLK_OFF
0.1u REC_BLK

p29:gp2
d16 pl1:f1
(p2 ph2):f1
p29:gp2
d16 pl0:f1

p29:gp3
d16
5u
[p46:sp35 ph3]:f1
p29:gp3

d16

0.1u REC_UNBLK
0.05u DWL_CLK_ON
d62:r
0.05u DWL_CLK_OFF
0.1u REC_BLK

10 to 4 times 131

d62

rcyc=2
30m mc 0 to 2 PO(xd)
exit

ph1=0 2 2 0 1 3 3 1
ph2=0 2
ph3=0 2
ph29=0 0 0 0 0 0 0 0 ; Continuous_wave_water_presaturation
ph30=0
ph31=0 2 2 0 1 3 3 1

; p1 : f1 channel - high power pulse
; p2 : f1 channel - 180 degree high power pulse
; p28: duration of CTP gradient pulse 1
; p29: duration of CTP gradient pulse 2
; p46: f1 channel - duration of 180 degree shaped pulse
; p11 : f1 channel - power level for pulse (default)
; p19 : f1 channel - power level for continuous wave for water presaturation

; sp35: f1 channel - region selective refocusing pulse [RSnob, ReBurp]
;r41 : relaxation delay; 1-5 * T1
;r411: delay for disk I/O [30 msec]
r412: delay for power switching [20 usec]
r416: delay for homospoil/gradient recovery
;r417: delay for solvent presaturation
;r418: reduced relaxation delay
;r412: length of block between decoupling pulses : = aq/l0 [< 20-25 msec]
r413: = d62/2

; cnst21: chemical shift for selective pulse [offset, in ppm]
; cnst31: = v9, random variation of +/- v9 %
; cnst40: solvent offset [ppm]
; cnst42: difference for frequency switching on f1-channel

; l0 : number of blocks during acquisition time adjust to get d62 as required
; nsa: 1 * n, total number of scans: NS * TDO
; rns: 4

; use gradient files:
; gppnam1: SMSQ10.100
; gppnam2: SMSQ10.100
; gppnam3: SMSQ10.100
; gppz1: 17%
; gppz2: 7%
; gppz3: 5%

; preprocessor-flags-start
; LABEL_CWPR: presaturation of solvent at beginning of pulse sequence
; option -DCWPR (eda: ZGOPTNS)
; preprocessor-flags-end
5.4 2D TOCSY with F1-perfectBASH homonuclear decoupling

; 2D TOCSY WITH HOMODECOPLING IN F1 USING PERFECT-BASH
;
; This pulse sequence is part of the paper:
; perfectBASH: Band selective homonuclear decoupling in peptides and peptidomimetics
; Authors: Julian Ilgen, Lukas Kaltschnee, Christina M. Thiele
;
; Julian Ilgen and Lukas Kaltschnee
; Technical University Darmstadt
; Avance II+/III Version
; Topspin 3.x
;
; Description and Comments:
; The pulse sequence has been coded for test purposes only and may contain errors.
; It does contain arguments that can lead to hardware damages if acquisition parameters
; are set unfavorably. The functionality of the pulse sequence itself may differ
; depending on the hardware as well as the software used to execute it. Functionality
; on differing systems cannot be granted.
; Any use of this pulse sequence on a spectrometer is at your own risk!
; By using this pulse sequence or any modification of it in any published material
; you agree to acknowledge the above-mentioned publication.
;
; with DIPSI-2 for isotropic mixing
; zero-quantum filtration before and after isotropic mixing
; phase sensitive
; band selective homonuclear decoupling using frequency selective pulses incorporated in Perfect-Echo
; homodecoupling scheme based on PEPSIE and F1-PSYCHE-TOCSY from Ref. (5)
; J is refocussed at the beginning of mixing
; option for solvent presaturation during relaxation delay possible in zg-options
; presaturation offset defined via const40 [ppm]
; advance-version (12/01/11)
;
; Relevant Papers:
; (4) L. Kaltschnee, A. Kolmer, I. Timari, V. Schmidts, R. W. Adams, M. Nilsson, K. E. Köver, G. A. Morris and C. M. Thiele,
; Chem. Commun.; 2014, 50, 15702 - 15705
;
#define delay tauA
;Calculations isotropic mixing and zero-quantum filtration;
"FACTOR1=(d9/(p6*115.112))/2+0.5"
"l1=FACTOR1*2"
"d12=20u"
"p21=p11"
"p22=p12"
"d11=30m"
;Calculations PerfectBASH;
"p2=p1*2.0"    ; 180 high power pulse
"in0=inf1/2"
"d0=0u" ; incremented delay for chemical shift evolution during homodecoupling-block
"tauA=p16+d16"
"const21=const20*bf1" ; offset calculation for frequency selective refocusing
"const22=const21-o1"
"spoffs40=const22"

;; Calculations solvent presaturation;;
#ifdef CWPR
"d18=d1-d19"
"const41=const40*bf1"
"const42=const41-o1"
#else
#endif /*CWPR*/

;; start pulsesequence;;
1 se
2 d11
3 d12
#ifdef CWPR ; begin of solvent presaturation
d12 fq=0:f1

d12 fq=const42 :f1 ; set frequency on f1-channel to solvent shift for presaturation [fq=SFO1+const42]
d12 pl9:f1 ; set power level on f1-channel for presaturation
d18 ; residual relaxation delay

d19 cw:f1 ph29 ; solvent presaturation
4u do:f1

d12 fq=0:f1 ; reset frequency on f1-channel [fq=SFO1]
d12 pl1:f1 ; reset power level on f1-channel
#else ; no solvent presaturation
d1
d12 pl1:f1
#endif /*CWPR*/

50u UNBLKGRAD

4 p1 ph1 ; 90 degree excitation pulse
5u ; beginning of decoupling using PerfectBASH
5u p10:f1 ; power switching f1-channel
d0 ; Incremented delay
tauA
p16:gp1 ; CTP 1
d16 ; gradient recovery delay
(p40:sp40 ph5:r):f1 ; first selective refocusing pulse
p16:gp1 ; CTP 1
d16 ; gradient recovery delay
tauA p11:f1 ; power switching f1-channel
d0 ; Incremented delay
10u
5 (p1 ph6):f1 ; 90 high power pulse for perfect echo J-removal
d0 ; Incremented delay
p16:gp2 ; CTP 2
d16 ; gradient recovery delay
(p2 ph7):f1 ; 180 high power pulse

10u
p16:gp2 ; CTP 2
d16 ; gradient recovery delay
p16:gp3 ; CTP 3
d16 ; gradient recovery delay
(p40:sp40 ph8:r):f1 ; second selective refocusing pulse
d16 ; gradient recovery delay
p16:gp3 ; CTP 3
d16

10u p11:f1 ; power switching f1-channel
d0 ; incremented delay F1-dimension
6 p1 ph2 ; 90 degree pulse at begin of isotropic mixing step
5u p10:f1

(center (p21:gp11) (p11:sp1 ph4):f1 ) ; first z-filter element
d17 ; gradient recovery delay

5u p110:f1

7 p6*3.556 ph23 ; begin isotropic mixing using dipsi-2
p6*4.556 ph25
p6*3.222 ph23
p6*3.167 ph25
p6*0.333 ph23
p6*2.722 ph25
p6*4.167 ph23
p6*2.944 ph25
p6*4.111 ph23
p6*3.556 ph25
p6*4.556 ph23
p6*3.222 ph25
p6*3.167 ph23
p6*0.333 ph25
p6*2.722 ph23
p6*4.167 ph25
p6*2.944 ph23
p6*4.111 ph23
p6*3.556 ph25
p6*4.556 ph23
p6*3.222 ph25
p6*3.167 ph23
p6*0.333 ph25
p6*2.722 ph23
p6*4.167 ph25
p6*2.944 ph23
p6*4.111 ph23
p6*3.556 ph25
p6*4.556 ph23
p6*3.222 ph25
p6*3.167 ph23
p6*0.333 ph25
p6*2.722 ph23
p6*4.167 ph25
p6*2.944 ph23
p6*4.111 ph23
p6*3.556 ph25
p6*4.556 ph23
p6*3.222 ph25
p6*3.167 ph23
p6*0.333 ph25
p6*2.722 ph23
p6*4.167 ph25
p6*2.944 ph25
p6*4.111 ph23
p6*3.556 ph25
p6*4.556 ph23
p6*3.222 ph25
p6*3.167 ph25
p6*0.333 ph25
p6*2.722 ph25
p6*4.167 ph25
p6*2.944 ph25
p6*4.111 ph23

10 to 7 times l1
5u pl10:f1

pl7:gp4 ; purge gradient
d17 ; gradient recovery delay

| center (p22:gp12) (p12:sp2 ph4:f1) | ; second z-filter element
d17 ; gradient recovery delay

50u BLKGRAD
5u pl11:f1

8 pl ph3 ; 90 degree pulse at end of isotropic mixing step
gp=2 ph31
d11 mc #0 to 2 F1PH(calph(ph1, +90) & calph(ph5, +90) & calph(ph6, +90) & calph(ph7, +90) & calph(ph8, +90), caldel(d0, +in0))
exit

ph1= 0 2 ; Hard 90 excitation
ph2= 0 0 0 0 2 2 2 2 ; Hard 90 before mixing
ph3= 0 0 2 2 ; Hard 90 after mixing
ph4= 0 ; adiabatic 180 (z-filter element)
ph5= 1 1 3 3 ; First selective refocusing pulse
ph6= 1 3 ; Hard 90 Perfect-Echo J-removal
ph7= 0 ; Hard 180
ph8= 0 ; Second selective refocusing pulse
ph23=3 ; dispsi-2
ph25=1 ; dispsi-2
ph29=0 ; CW-presaturation
ph31=0 2 2 0 0 2 ; receiver

zp1: high power 90 pulse width
zp2: high power 180 pulse width
zp6: 90 degree low power pulse
zp11: duration of first ZQC dephasing element
zp12: duration of second ZQC dephasing element
zp16: duration of CTP gradient
zp17: duration of CTP gradient
zp21: duration ZQC dephasing gradient
zp22: duration ZQC dephasing gradient
zp40: duration of selective 180 pulse
zp11: f1 channel - power level for pulse (default)
zp19 : f1 channel - power level for presaturation
zp110: DIPSI-2 power

rzp1: first adiabatic 180 pulse power level
rzpoffs1: first adiabatic 180 pulse offset (0 Hz)
ruzpoffs2: second adiabatic 180 pulse power level
rzpoffs2z: second adiabatic 180 pulse offset (0 Hz)
rz偏好 selective refocusing pulse
rzp40 : RF power of selective 180 pulse
zspnam40: file name for selective 180 pulse

zd0 : incremented delay
zd1 : relaxation delay
zd9 : TOCSY mixing time
zd16: gradient recovery delay, homodecoupling
zd17: gradient recovery delay, mixing step
zd18: residual relaxation delay
zd19: delay for solvent presaturation

rgpz1: CTP gradient
rgpz2: CTP gradient
rgpz3: CTP gradient
rgps4: Purge gradient
rgps11: ZQC gradient 1-3%
rgps12: ZQC gradient 1-3% 
rgnam1: SMSQ10.100
rgnam2: SMSQ10.100
rgnam3: SMSQ10.100
rgnam4: SMSQ10.100
rgnam11: RECT.1
rgnam12: RECT.1

cnst20: offset for selective refocusing [ppm]
cnst40: solvent offset [ppm]
cnst42: difference for frequency switching on f1-channel

r11 : loop for DIPI cycle
rin0 : 1/(2 * SW) = DW
NS : number of scans 8*n
DS : number of dummy scans 16
tdl1 : number of t1 increments
MC2 : TPPI or States-TPPI

;preprocessor-flags-start
;LABEL_CWPR: presaturation of solvent at beginning of pulse sequence
; option -DCWPR (eda: ZGOPTNS)
;preprocessor-flags-end
5.5 2D NOESY with F1-perfectBASH homonuclear decoupling

; 2D NOESY WITH HOMODECOUPLING IN F1 USING PERFECT-BASH
;
; This pulse sequence is part of the paper:
; perfectBASH: Band selective homonuclear decoupling in peptides and peptidomimetics*
; Authors: Julian Ilgen, Lukas Kaltschnee, Christina M. Thiele
;
; Julian Ilgen and Lukas Kaltschnee
; Technical University Darmstadt
; Avance II+/III Version
; Topspin 3.x
;
; Description and Comments:
; The pulse sequence has been coded for test purposes only and may contain errors.
; It does contain arguments that can lead to hardware damages if acquisition parameters
; are set unfavorably. The functionality of the pulse sequence itself may differ
; depending on the hardware as well as the software used to execute it. Functionality
; on differing systems cannot be granted.
; Any use of this pulse sequence on a spectrometer is at your own risk!
; By using this pulse sequence or any modification of it in any published material
; you agree to acknowledge the above-mentioned publication.
;
; 2D homonuclear correlation via dipolar coupling
; dipolar coupling may be due to noe or chemical exchange
; zero-quantum filtration during mixing
; phase sensitive
; band selective homonuclear decoupling using frequency selective pulses incorporated in Perfect-Echo
; homodecoupling scheme based on PEPSIE and F1-PSYCHE-TOCSY from Ref. (7)
; J is refocussed at the beginning of mixing
; option for solvent presaturation during relaxation delay possible in zg-options
; presaturation offset defined via cnst40 [ppm]
; advance-version {12/01/11}
;
; Relevant Papers:
; Chem. Commun.; 2014, 50, 15702 – 15705
;
; $CLASS=HighRes
; $DIM=2D
; $TYPE=
; $SUBTYPE=
; $COMMENT=

#define delay tauA
#define delay TAU

d11=30m
"d11=30m"
d12=20u
"d12=20u"

; ; Definition NOESY mixing:
"TAU=d8-(p32+16+20+20u)"
"p11=p32" ; adiabatic pulse as long as ZQC dephasing gradient
;Calculations PerfectBASH;
"p2=p1*2.0" ; 180 high power pulse
"in0=inf1/2" ; incremented delay for chemical shift evolution during homodecoupling-block
"d0=0u" ; incremented delay for chemical shift evolution during homodecoupling-block
"ttau=p16+d16"
"cnst21=cnst20*bf1" ; offset calculation for frequency selective refocusing
"cnst22=cnst21-o1"
"spoffs40=cnst22"

;Calculations solvent presaturation;
#ifdef CWPR
"d18=d1-d19"
"cnst41=cnst40*bf1"
"cnst42=cnst41-o1"
#else
#endif /*CWPR*/

;begin pulsesquence;

1 ze
2 d11
3 d12
4u
#ifdef CWPR ; begin of solvent presaturation

d12 fq=0:f1

d12 fq=cnst42:f1 ; set frequency on f1-channel to solvent shift for presaturation [fq=SFO1+cnst42]

d12
d18 p19:f1 ; residual relaxation delay + set power level on f1-channel for presaturation
d19 cw:f1 ph29 ; solvent presaturation
4u d0:f1
d12 fq=0:f1 ; reset frequency on f1-channel [fq=SFO1]
d12 p11:f1 ; reset power level on f1-channel
#else ; no solvent presaturation
d1
d12 p11:f1
#endif /*CWPR*/

50u UNBLKGRAD
4 p1 ph1 ; 90 high power excitation pulse
5u
5u p10:f1 ; power switching f1-channel
d0 ; incremented delay
tauA
p17:gp1 ; CTP 1
d17 ; gradient recovery delay
(p-01ap40 ph5:r):f1 ; first selective refocusing pulse
p17:gp1 ; CTP 1
d17 ; gradient recovery delay
tauA p11:f1 ; power switching f1-channel
S40

10u

5 (p1 ph6):f1 ; 90 high power pulse for perfect echo J-removal
d0 ; Incremented delay
p17:gp2 ; CTP 2
d17 ; gradient recovery delay

[p2 ph4]:f1 ; 180 high power pulse
10u

pl7:gp2 ; CTP 2
d17 ; gradient recovery delay
p17:gp3 ; CTP 3
d17 pl0:f1 ; gradient recovery delay + power switching f1-channel

[p40:sp40 ph4:r]:f1 ; second selective refocusing pulse
d17 ; gradient recovery delay
p17:gp3 ; CTP 3
d17

10u pl1:f1 ; power switching f1-channel
d0 ; incremented delay
(p1 ph2) ; 90 high power pulse at beginning of NOESY mixing time
10u pl0:f1 ; power switching f1-channel

center(p32:sp29 ph4:r):f1 (pl1:gp1)) ; Thrippleton-Keeler z-filter element
d16 ; gradient recovery delay
p16:gp4 ; purge gradient
d16 pl1:f1 ; gradient recovery delay and power switching f1-channel

10u BLKGRAD
TAU ; mixing time

(p1 ph3) ; 90 high power pulse at end of NOESY mixing time
go=2 ph31
d11 mc #0 to 2 F1PH(calph(ph1, +90) & calph(ph5, +90) & calph(ph6, +90) & calph(ph4, +90), caldel(d0, +in0))
exit

rphase cycling
ph1=0 2 ; Hard 90 Excitation
ph2=0 0 0 0 0 0 0 0 2 2 2 2 2 2 2 2 2 ; Hard 90 Begin NOESY mixing
ph3=0 0 0 2 2 2 2 ; Hard 90 End NOESY mixing
ph4=0 ; adiabatic 180 zfilter & Hard 180 & 2nd sel. 180
ph5=1 3 3 ; 1st sel. 180
ph6=1 3 1 3 ; Hard 90 Perfect Echo
ph29=0 ; CW_Presaturation
ph31=2 0 0 0 2 0 2 2 0 2 2 0 2 2 0 2 0 0 ; Receiver

zp1 : f1 channel = 90 degree high power pulse
zp2: f1 channel = 180 degree pulse width
zp11: duration of 3QC dephasing gradient
zp16: purge gradient pulse during NOESY mixing time [5m]
zp17: homospoil/gradient pulse during F1-homodecoupling [1m]
zp32: f1 channel = 180 degree shaped pulse (adiabatic)
zp40: duration of selective 180 pulse

zp11 : f1 channel = power level for pulse (default)
zp19 : f1 channel = power level for presaturation
5.6 2D EASY-ROESY with F1-perfectBASH homonuclear decoupling

; 2D EASY-ROESY with homodecoupling in F1 using Perfect-BASH
;
; This pulse sequence is part of the paper:
; perfectBASH: Band selective homonuclear decoupling in peptides and peptidomimetics
; Authors: Julian Ilgen, Lukas Kaltschnee, Christina M. Thiele
;
; Julian Ilgen and Lukas Kaltschnee
; Technical University Darmstadt
; Avance II+/III Version
; Topspin 3.x
;
; Description and Comments:
; The pulse sequence has been coded for test purposes only and may contain errors.
; It does contain arguments that can lead to hardware damages if acquisition parameters
; are set unfavorably. The functionality of the pulse sequence itself may differ
; depending on the hardware as well as the software used to execute it. Functionality
; on differing systems cannot be granted.
; Any use of this pulse sequence on a spectrometer is at your own risk!
; By using this pulse sequence or any modification of it in any published material
; you agree to acknowledge the above-mentioned publication.
;
; jump-symmetrized with adiabatic spinlocks for mixing
; correction to ensure symmetrically shifted offsets for spin-locking
; midpoint of symmetric offset shifting of spin-lock defined via cnst32 [ppm] and should be set center of 1H spectrum
; phase sensitive
; band selective homonuclear decoupling using frequency selective pulses incorporated in Perfect-Echo
; homodecoupling scheme based on PEPSIE and F1-PSYCHE-ROESY from Ref. (5)
; J is refocussed at the beginning of mixing
; option for solvent presaturation during relaxation delay possible in zg-options
; presaturation offset defined via cnst40 [ppm]
; advance-version (12/01/11)
;
; Relevant Papers:
; Chem. Commun. 2014, 50, 15702 – 15705
;(7) Procházková, E., Kolmer, A., Ilgen, J., Schwab, M., Kaltschnee, L., Federer, M., Schmidt, V., Wende, R. C.,
; Schreiner, P. R., Thiele, C. M., Angew. Chem. Int. Ed. 2016, 55, 15754-15759
;
;
#define pulse P_SL
#define delay tauA
"d11=30m"
"d12=20u"
;;calculations for ROESY-Spinlock;
"cnst24=1000000.0*tan((cnst28*2*PI)/360.0)/(dw*4)"
"if ( cnst24 > 6500 ) {cnst25 = 6400.0;} else {cnst25 = cnst24;}

#include <Avance.incl>
#include <Grad.incl>

include <Avance.incl>
#include <Grad.incl>

define pulse P_SL
#define delay tauA
"d11=30m"
"d12=20u"
;;calculations for ROESY-Spinlock;
"cnst24=1000000.0*tan((cnst28*2*PI)/360.0)/(dw*4)"
"if ( cnst24 > 6500 ) {cnst25 = 6400.0;} else {cnst25 = cnst24;}

S42
"if ( cnst24 > 6500 ) \{ cnst29 = atan(cnst25*4*dw/1000000.0)*360.0/(2*PI); \} else \{ cnst29=cnst28; \}"

"if (cnst26<cnst25) \{ cnst27=cnst25; \} else \{ if (cnst26>6500) \{ cnst27=6400; \} else \{ cnst27=cnst26; \} \}"

"cnst30=abs(cnst27/tan((cnst29*2*PI)/360.0))" ; requested offset shifting for low- and high-field SL, if offset o1 is 1H-spectrum center

"cnst33=o1-(cnst32*bf1)" ; difference between PerfectBASH offset and 1H-spectrum center, to allow symmetrical spin-locking, cnst32 defines the midpoint of symmetrical offset shifting!!

"cnst34=cnst30*cnst33" ; correction for lowfield SL offset
"cnst35=cnst30+cnst33" ; correction for highfield SL offset

define list<frequency> roesylist={"f1", 0.0, -cnst34, cnst35, 0} ;

"p30=1000000.0/(cnst27*4)"
"p273=(p30/plw1) + (p30/plw1)"
"spw10=plw1/cnst31"
"spw12=plw1/cnst31"
"spw13=plw1/cnst31"
"spw16=plw1/cnst31"
"spw17=plw1/cnst31"
"cnst23=cnst30+cnst31+p30"
"p1=1m"
"P_30=plw1/2"
"spoff10=0"
"spoff12=0"
"spoff13=0"
"spoff16=0"
"spoff17=0"
"p2=1.0"
"in0=inf1/2"
"d0=0u" ; incremented delay for chemical shift evolution during homodecoupling-block
"tauA=p16+d16" ; offset calculation for frequency selective refocusing
"cnst21=cnst20*bf1" ; offset calculation for frequency selective refocusing
"spoffs40=cnst22"

;;Calculations PerfectBASH;;
"p2=p1*2.0" ; 180 high power pulse
"in0=inf1/2" ;
"d0=0f" ; incremented delay for chemical shift evolution during homodecoupling-block
"tauA=p16+d16" ; offset calculation for frequency selective refocusing
"cnst21=cnst20*bf1" ; offset calculation for frequency selective refocusing
"spoffs40=cnst22"

;;Calculations solvent presaturation;;
#ifdef CWPR
"d18=d1-d19" ; changed according to use ppm values for solvent offset
"cnst41=cnst40*bf1" ; changed according to use ppm values for solvent offset
"cnst42=cnst41-o1"
#else
#endif /*CWPR*/

;; start pulsedsequence ;;
1 ze
2 d11
3 d12 roesylist:f1
 4u roesylist:inc
#ifdef CWPR ; begin of solvent presaturation
"d12 fq=0:f1"
"d12 fq=cnst42:f1" ; set frequency on f1-channel to solvent shift for presaturation [fq=fP01+cnst42]
"d12 d18 p19:f1" ; residual relaxation delay + set power level on f1-channel for presaturation
"d19 cw:f1 ph29" ; solvent presaturation
 4u do:f1
d12 fq=0:f1 ; reset frequency on f1-channel [fq=fP01]
d12 pll:f1 ; reset power level on f1-channel

#else ; no solvent presaturation
d1
d12 pll:f1
#endif /*CWPR*/

50u UNBLEGRAD

4 p1 ph1 ; 90 high power excitation pulse
5u
5u p10:f1 ; power switching f1-channel
d0 ; Incremented delay

tauA

p17:gp3 ; CTP 3
d17 ; gradient recovery delay

(p40:sp40 ph2:r):f1 ; first selective refocusing pulse

p17:gp3 ; CTP 3
d17 ; gradient recovery delay
tauA pll:f1 ; power switching f1-channel
d0 ; Incremented delay

10u

5 (p1 ph3):f1 ; 90 high power pulse for perfect echo J-removal
d0 ; Incremented delay

p17:gp4 ; CTP 4
d17 ; gradient recovery delay

(p2 ph4):f1 ; 180 high power pulse

10u

p17:gp4 ; CTP 4
d17 ; gradient recovery delay

p17:gp5 ; CTP 5
d17 p10:f1 ; gradient recovery delay + power switching f1-channel

(p40:sp40 ph5:r):f1 ; second selective refocusing pulse

p17:gp5 ; CTP 5
d17

10u pll:f1 ; power switching f1-channel
d0 ; Incremented delay

6 (p1 ph6):f1 ; 90 high power pulse before ROESY mixing

4u

p16:gp1 ; purge gradient
d16 roesylist:f1 ; gradient recovery delay
4u roesylist,inc

#endif AV2

(p41:sp12 ph6):f1 ; adiabatic ramp up (lowfield, positive offset)
3u

(P_SL:sp10 ph6):f1 ; low field spinlock
3u
; adiabatic ramp down (lowfield, positive offset)
#  else
  [p41:sp12 ph6]:f1
  [P_SL:sp10 ph6]:f1
  [p41:sp13 ph6]:f1
#  endif /*AV2*/
4u
4u roesylist:f1
4u roesylist.inc

#  ifdef AV2
  [p41:sp16 ph6]:f1
  3u
  [P_SL:sp10 ph6]:f1
  3u
  [p41:sp17 ph6]:f1
#  else
  [p41:sp16 ph6]:f1
  [P_SL:sp10 ph6]:f1
  [p41:sp17 ph6]:f1
#  endif /*AV2*/
4u

p16:gp2
  ; purge gradient
d16 roesylist:f1
  ; gradient recovery delay
4u roesylist.inc
4u p11:f1
4u BLKGRAD

[p1 ph7]
  ; 90 high power pulse after ROESY mixing
go=2 ph31
d11 mc #0 to 2 F1PH(calph(ph1, +90) & calph(ph2, +90) & calph(ph3, +90) & calph(ph4, +90) & calph(ph5, +90), caldel(d0, +in0))
exit

ph1= 0 2
  ; Hard 90 excitation
2h3= 1 1 1 1 2 2 2 2
  ; First selective 180
ph4= 0
  ; Hard 180
ph5= 0
  ; Second selective 180
ph6= 0
  ; Hard 90 ROESY mixing begin
ph7= 2 2 0 0 3 3 1 1
  ; Hard 90 ROESY mixing end
ph29=0
  ; CW presaturation
ph31=0 2 2 0 3 1 1 3
  ; Receiver

zp1 : f1 channel - 90 degree high power pulse
zp2: high power 180 pulse width
zp5: f1 channel = pulse for ROESY spinlock
zp6: purge gradient pulse during ROESY mixing time
zp7: homospoil/gradient pulse during F1-homodecoupling
zp8: f1 channel - 90 degree pulse at sp10
zp35: f1 channel - 90 degree pulse at sp40
zp40: duration of selective 180 pulse
zp41: f1 channel = shaped pulse for adiabatic ramp
zp41: [lm]
zp11 : f1 channel = power level for pulse (default)
zp19 : f1 channel = power level for presaturation

zp12: f1 channel = shaped pulse for ROESY-spinlock (= p11 + cnst31)
zp13: Gaussrampdown.1
zp13: Gaussrampup.1
zp16: f1 channel = shaped pulse for adiabatic ramp down (highfield, negative offset) (= p11 + cnst31)
spnam16: Gaussramp-down.1
spnam17: Gaussramp-up.1
spw40: RF power of selective 180 pulse
spnam40: file name for selective 180 pulse

rgsz1: purge gradient 31% ROESY element
rgsz2: purge gradient 11% ROESY element
rgsz3: CTP gradient (20-50%) homodecoupling F1-dimension
rgsz4: CTP gradient (20-50%) homodecoupling F1-dimension
rgsz5: CTP gradient (20-50%) homodecoupling F1-dimension
rgpsm1: SMSQ10.100
rgpsm2: SMSQ10.100
rgpsm3: SMSQ10.100
rgpsm4: SMSQ10.100
rgpsm5: SMSQ10.100

rso : incremented delay (2D)
rd1 : relaxation delay; 1=5 * T1
rd11: delay for disk I/O [30 msec]
rd12: delay for power switching [20 usec]
rd16: delay for homospoil/gradient recovery
rd17: delay for homospoil/gradient recovery in F1-dimension
rd18: reduced relaxation delay
rd19: delay for solvent presaturation
rcnst20: offset for selective refocusing [ppm]
rcnst23: (for display purpose only)
rcnst24: min. RF field strength to make sure that the carrier is shifted to the edge of the spectrum
rcnst25: reduced min. RF field strength in case an upper limit of 6.5kHz is exceeded
rcnst26: requested RF field strength (gammaB1) for ROESY spinlock
rcnst27: used RF field strength (gammaB1) for ROESY spinlock
rcnst28: requested tilt angle for ROESY spinlock (between axis of spinlock and z-axis) [45 degree]
rcnst29: used tilt angle for ROESY spinlock (between axis of spinlock and z-axis)
rcnst30: low and highfield offset, calculated from gammaB1 (rcnst27) for tilt angle (rcnst29)
rcnst31: difference in power level (dB) for spinlock relative to pl1
rcnst40: solvent offset [ppm]
rcnst41: spectrum center [Hz]
rcnst42: difference for frequency switching on f1-channel

rin0: 1/(1 * SW) = 2 * DW
rn0: 1
nN1 : 8*n
nDE : 16
rtol1 : number of t1 increments
FnMODE: States-TPPI, TPPI, States or QSEQ

;preprocessor-flags-start
;CWPR: presaturation of solvent at beginning of pulse sequence
; option -DCWPR (eda: ZGOPTNS)
;preprocessor-flags-end
5.7 2D CLIP-COSY with F1-perfectBASH homonuclear decoupling

; 2D CLIP-COSY WITH HOMODECOUPLING IN F1 USING PERFECT-BASH
;
; This pulse sequence is part of the paper:
; perfectBASH: Band selective homonuclear decoupling in peptides and peptidomimetics
; Authors: Julian Ilgen, Lukas Kaltschnee, Christina M. Thiele
;
; Julian Ilgen and Lukas Kaltschnee
; Technical University Darmstadt
; Avance II+/III Version
; Topspin 3.x
;
; Description and Comments:
; The pulse sequence has been coded for test purposes only and may contain errors.
; It does contain arguments that can lead to hardware damages if acquisition parameters
; are set unfavorably. The functionality of the pulse sequence itself may differ
; depending on the hardware as well as the software used to execute it. Functionality
; on differing systems cannot be granted.
; Any use of this pulse sequence on a spectrometer is at your own risk!
; By using this pulse sequence or any modification of it in any published material
; you agree to acknowledge the above-mentioned publication.
;
; Clean In-phase COSY
; 2D H,H-correlation using in-phase transfer
; based on the CLIP-COSY pulse sequence from Ref. (1)
; phase sensitive
; band selective homonuclear decoupling in F1 using frequency selective pulses incorporated in Perfect-Echo
; J is refocussed at the beginning of mixing
; option for solvent presaturation during relaxation delay possible in zg-options
; presaturation offset defined via cnst40 [ppm]
; advance-version (12/01/11)
;
; Relevant Papers:
; Chem. Commun.; 2014, 50, 15702 – 15705
;
#define delay tauA
;;;;CLIP-COSY statements;;;;
*p2=p1+2*
"d6=1s/(cnst1*4)" ; coupling evolution delay in mixing step
"d11=30m"
"d12=20u"
*p35=p32*
*p36=p33*
;;;;Calculations PerfectBASH;;;;
*p2=p1+2.0* ; 180 high power pulse
"in0=inf1/2"
"\$d0=0u"    ; incremented delay for chemical shift evolution during homodecoupling-block  
"tauA=p16+\$d16"  
"cnst21=cnst20*bf1"    ; offset calculation for frequency selective refocusing  
"cnst22=cnst21-01"  
"spoffs40=cnst22"  

;;;Calculations solvent presaturation;;  
 ifdef CWPR  
    \$d18=\$d1-\$d19"  
    "cnst41=cnst40*bf1"  
    "cnst42=cnst41-01"  
 ifdef /*CWPR*/  

 ;begin pulseequence;;  
 1 se  
 2 d11  
 3 d12  
 4u  
     ifdef CWPR  
     d12 fq=0:f1  
     d12 fq=cnst42 :f1    ; set frequency on f1-channel to solvent shift for presaturation [fq=SFO1+cnst42]  
     d12 pl9:f1    ; set power level on f1-channel for presaturation  
     d18    ; residual relaxation delay  
     d19 cw:f1 ph29  
     4u do:f1  
     d12 fq=0:f1    ; reset frequency on f1-channel [fq=SFO1]  
     d12 pl1:f1    ; reset power level on f1-channel  
 else  
     d1  
     d12 pl1:f1  
 endif /*CWPR*/  

 50u UNBLKGRAD  

 4 p1 ph1    ; 90 high power excitation pulse  
 5u  
 5u p10:f1    ; power switching f1-channel  
 0d    ; Incremented delay  
 tauA  
 p16:gp1    ; CTP 1  
 d16    ; gradient recovery delay  
 (p40:sp40 ph10:rr):f1    ; first selective refocusing pulse  
 p16:gp1    ; CTP 1  
 d16    ; gradient recovery delay  
 tauA p11:f1    ; power switching f1-channel  
 0d    ; Incremented delay  
 10u  
 5(p1 ph11):f1    ; 90 high power pulse for perfect echo J-removal
d0 ; Incremented delay
p16:gp2 ; CTP 2
d16 ; gradient recovery delay
(p2 ph12):f1 ; 180 high power pulse
10u
p16:gp2 ; CTP 2
d16 ; gradient recovery delay
p16:gp3 ; CTP 3
d16 pl0:f1 ; gradient recovery delay + power switching f1-channel
(p40:sp40 ph12:z):f1 ; second selective refocusing pulse
p16:gp3 ; CTP 3
d16 ; gradient recovery delay
10u pl1:f1 ; power switching f1-channel
d0 ; Incremented delay
6 p1 ph7 ; first Thrippleton-Keeler-filter
5u pl0:f1
(center(p35:gp11) (p32:sp28 ph8):f1)
5u
d16 pl1:f1
7 p1 ph2 ; Begin in-phase COSY mixing
d6
p2 ph3
d6
p1 ph4
d6
p2 ph3
d6
8 p1 ph5 ; second Thrippleton-Keeler-filter
5u pl0:f1
(center(p36:gp12) (p33:sp29 ph9):f1)
5u
d16 pl1:f1
p16:gp13 ; Purge gradient
5u
d16 BLKGRAD
9 p1 ph6
go=2 ph31
d11 mc #0 to 2 PIPH(calph(ph1, +90) & calph(ph10, +90) & calph(ph11, +90) & calph(ph12, +90) & caldel(d0, +in0)) exit
rphase cycling
ph1=0 2 ; 90 excitation
ph2=2 2 2 0 0 0 0 ; 90 begin mixing
ph3=0 ; 90 mixing element
ph4=1 ; 90 mixing element
ph5=0 0 2 2 ; 90 end mixing and begin second z-filter
ph6=0 ; 90 begin acquisition
ph7=0 ; 90 begin first z-filter
ph8=0 ; 180 adiabatic first z-filter
ph9=2 ; 180 adiabatic second z-filter
ph10=1 1 1 2 2 2 ; 180 first selective refocusing
ph11=1 3 1 3 ; 90 Perfect-Echo
S50

ph12=0 ; 180 hard + second selective refocusing
ph29=0 ; CW presaturation
ph31=0 2 2 0 0 2 2 0 ; receiver

rp1: 90 degree high power pulse
rp2: 180 degree high power pulse
rp16: homospoil/gradient pulse
rp32: 180 degree adiabatic pulse for ZQC-dephasing
rp33: 180 degree adiabatic pulse for ZQC-dephasing
rp35: duration ZQC-dephasing gradient
rp36: duration ZQC-dephasing gradient
rp40: duration of selective refocusing pulse
rp50: zero power
rp11: f1 channel - power level for pulse (default)
rp19: f1 channel - power level for presaturation

zp28: adiabatic 180 pulse
zp29: adiabatic 180 pulse
zpnam28: file name for adiabatic 180 pulse
zpnam29: file name for adiabatic 180 pulse
zp40: selective 180 pulse
zpnam40: file name for selective 180 pulse

zd0: incremented delay
zd1: relaxation delay: 1-5*T1
zd6: 1/(4J(HH))
zd11: delay for disk I/O [30 msec]
zd12: delay for power switching [20 usec]
zd16: delay for homospoil/gradient recovery
zd18: reduced relaxation delay
zd19: delay for solvent presaturation

zf for z-only gradients:
 rgpz1: CTP gradient
 rgpz2: CTP gradient
 rgpz3: CTP gradient
 rgpz11: z-filter 7.2%
 rgpz12: z-filter -7.5%
 rgpz13: purge gradient -17.9%

rz use gradient files:
 rgpnam1: SMSQ10.100
 rgpnam2: SMSQ10.100
 rgpnam3: SMSQ10.100
 rgpnam11: RECT.1
 rgpnam12: RECT.1
 rgpnam13: SMSQ10.100

rconst1: > J(HH) [30Hz]
rconst20: offset for selective refocusing [ppm]
rconst40: solvent offset [ppm]

rin1: 1/SW = 2 * DW
rin0: 1/(1 * SW) = 2 * DW
ro0: 2
rNS: 8*n
rDS: 16
rd1: number of experiments
rFMODE: States-TPPI, TPPI, States or QSEQ

rpreprocessor-flags-start
rCNPR: presaturation of solvent at beginning of pulse sequence
; option -DCNPR (eda: ZGOPTNS)
rpreprocessor-flags-end
5.8 2D CLIP-COSY relayed (n=2) with F1-perfectBASH homonuclear decoupling

; RELAYED CLIP-COSY WITH F1-HOMODECOUPLING USING PERFECT-BASH
;
; This pulse sequence is part of the paper:
; perfectBASH: Band selective homonuclear decoupling in peptides and peptidomimetics
; Authors: Julian Ilgen, Lukas Kaltschnee, Christina M. Thiele
;
; Julian Ilgen and Lukas Kaltschnee
; Technical University Darmstadt
; Avance II+/III Version
; Topspin 3.0
;
; Description and Comments:
; The pulse sequence has been coded for test purposes only and may contain errors.
; It does contain arguments that can lead to hardware damages if acquisition parameters
; are set unfavourably. The functionality of the pulse sequence itself may differ
; depending on the hardware as well as the software used to execute it. Functionality
; on differing systems cannot be granted.
; Any use of this pulse sequence on a spectrometer is at your own risk!
; By using this pulse sequence or any modification of it in any published material
; you agree to acknowledge the above-mentioned publication.
;
; Clean In-phase COSY
; 2D H,H-correlation using in-phase transfer
; relayed CLIP-COSY with two steps
; pulse sequence is based on the CLIP-COSY relayed from Ref. (2)
; phase sensitive
; band selective homonuclear decoupling in F1 using frequency selective pulses incorporated in Perfect-Echo
; J is refocussed at the beginning of mixing
; option for solvent presaturation during relaxation delay possible in zg-options
; presaturation offset defined via cnst40 [ppm]
; advance-version (12/01/11)
;
; Relevant Papers:
;
$CLASS=HighRes
$DIM=2D
$TYPE=
$SUBTYPE=
$COMMENT=

#include <Avance.incl>
#include <Grad.incl>
#include <Delay.incl>
#include <De.incl>

define delay tauA

;CLIP-COSY statements;
"p2=p1/2"
"d0=1/(cnst1*4)" ; coupling evolution delay in mixing step
"d1=30m"
"d2=20u"
"p3=p32"
"p36=p33"

;Definitions for PerfectBASH;
"in0=inf1/2"
"\textit{d0}=0u" \quad \text{; incremented delay for chemical shift evolution during homodecoupling-block}
\texttt{tauA=p16+d16}
\texttt{cnst21=cnst20*bf1} \quad \text{; offset calculation for frequency selective refocusing}
\texttt{cnst22=cnst21-o1}
\texttt{spoffs40=cnst22}

\texttt{;;;;Calculations solvent presaturation;;}
\texttt{#ifdef CWPR}
\texttt{d18=d1-d19}
\texttt{cnst41=cnst40*bf1}
\texttt{cnst42=cnst41-o1}
\texttt{#else}
\texttt{#endif /*CWPR*/}

\texttt{;;;;begin pulsesequence;;}
1 \texttt{se}
2 \texttt{d11}
3 \texttt{d12}
4u

\texttt{#ifdef CWPR \quad \text{; begin of solvent presaturation}}
\texttt{d12 \texttt{fq}=0:f1}
\texttt{d12 \texttt{fq}=cnst42 :f1} \quad \text{; set frequency on f1-channel to solvent shift for presaturation \{\texttt{fq}=\texttt{SFO1}+\texttt{cnst42}\}}
\texttt{d12 \texttt{pl}9:f1} \quad \text{; set power level on f1-channel for presaturation}
\texttt{d18} \quad \text{; residual relaxation delay}
\texttt{d19 \texttt{cw}f1 \texttt{ph}20}
\texttt{4u \texttt{do}f1}
\texttt{d12 \texttt{fq}=0:f1} \quad \text{; reset frequency on f1-channel \{\texttt{fq}=\texttt{SFO1}\}}
\texttt{d12 \texttt{pl}1:f1} \quad \text{; reset power level on f1-channel}
\texttt{#else} \quad \text{; no solvent presaturation}
\texttt{d1}
\texttt{d12 \texttt{pl}1:f1}
\texttt{#endif /*CWPR*/}

50u \texttt{UNBLGRAD}

4 \texttt{pl \textit{ph}1} \quad \text{; 90 high power excitation pulse}
5u
5u \texttt{pl0:f1} \quad \text{; power switching f1-channel}
\texttt{d0} \quad \text{; Incremented delay}
\texttt{tauA}
\texttt{p16:gp1} \quad \text{; CTP 1}
\texttt{d16} \quad \text{; gradient recovery delay}
\texttt{(p40:sp40 \texttt{ph10:r}):f1} \quad \text{; first selective refocusing pulse}
\texttt{p16:gp1} \quad \text{; CTP 1}
\texttt{d16} \quad \text{; gradient recovery delay}
\texttt{tauA \texttt{pl}1:f1} \quad \text{; power switching f1-channel}
\texttt{d0} \quad \text{; incremented delay}
10u

5 \texttt{\{p1 \texttt{ph}11\}:f1} \quad \text{; 90 high power pulse for perfect echo J-removal}
\texttt{d0} \quad \text{; Incremented delay}
p16:gp2 ; CTP 2
d16 ; gradient recovery delay
(p2 ph12):f1 ; 180 high power pulse

d16 ; gradient recovery delay
p16:gp2 ; CTP 2
d16 ; gradient recovery delay
p16:gp3 ; CTP 3
d16 pl0:f1 ; gradient recovery delay + power switching f1-channel
(p40:sp40 ph12:z):f1 ; second selective refocusing pulse
p16:gp3 ; CTP 3
d16
10u pl1:f1 ; power switching f1-channel
d0 ; Incremented delay

6 p1 ph7 ; first Thrippleton-Keeler-filter
5u pl0:f1
(center(p35:gp11) (p32:sp28 ph8):f1)
5u
d16 pl1:f1

7 p1 ph2 ; begin in-phase COSY mixing
d6 ; 1st transfer
p2 ph3
d6
p1 ph3
d6
p2 ph4
d6
d6 ; 2nd transfer (relay)
p2 phi3
d6
p1 phi3
d6
p2 phi4
d6

8 p1 ph5 ; second Thrippleton-Keeler-filter
5u pl0:f1
(center(p36:gp12) (p33:sp29 ph9):f1)
5u
d16 pl1:f1
p16:gp13 ; purge gradient
5u
d16 BLKGRAD

9 p1 ph6
gs=2 ph3

d11 mc #0 to 2 P1PH(calph(ph1, +90) & calph(ph10, +90) & calph(ph11, +90) & calph(ph12, +90) & calph(ph1, +90) & calph(ph10, +90) & calph(ph11, +90) & calph(ph12, +90) , caldel(d0, +in0))
exit

; phase cycling
ph1=0 2 ; 90 excitation
ph2=2 2 2 0 0 0 0 ; 90 begin mixing
ph3= 1 3 ; 180 & 90 first mixing element
ph4= 3 2 ; 180 both mixing elements
ph13= 1 1 3 3 ; 180 & 90 second mixing element
ph5=0 0 2 2 ; 90 end mixing and begin second z-filter
ph6=0    ; 90 begin acquisition
ph7=0    ; 90 begin first z-filter
ph8=0    ; 180 adiabatic first z-filter
ph9=2    ; 180 adiabatic second z-filter
ph10=1 1 1 2 2 2     ; first selective refocusing pulse
ph12=0    ; 180 hard + second selective refocusing pulse
ph29=0    ; CW presaturation
ph31=0 2 2 0 0 2 2 0    ; receiver

zp1 : 90 degree high power pulse
zp2 : 180 degree high power pulse
zp16: homospoil/gradient pulse
zp12: 180 degree adiabatic pulse for ZQC-dephasing
zp35: 180 degree adiabatic pulse for ZQC-dephasing
zp36: duration x-filter dephasing gradient
zp40: duration of selective refocusing pulse
zp10: zero power
zp11 : f1 channel - power level for pulse (default)
zp19 : f1 channel - power level for presaturation
zp28: adiabatic dephasing pulse
zp38: adiabatic dephasing pulse
zpam28: file name for adiabatic 180 pulse
zpam29: file name for adiabatic 180 pulse
zp40: selective refocusing pulse
zpwe40: RF power of selective 180 pulse
zpam40: file name for selective 180 pulse (ReBurp.1000)
z0: incremented delay
zd1: relaxation delay: 1-5*T1
zd6: 1/4J(HH))
zd11: delay for disk I/O [30 msec]
zd12: delay for power switching [20 usec]
zd16: delay for homospoil/gradient recovery
zd18: reduced relaxation delay
zd19: delay for solvent presaturation
zf: for z-only gradients:
zp01: CTP gradient
zp02: CTP gradient
zp03: CTP gradient
zp011: z-filter 7.2%
zp012: z-filter -7.6%
zp013: purge gradient -17.9%
zpam01: SMSQ10.100
zpam02: SMSQ10.100
zpam03: SMSQ10.100
zpam11: RECT.1
zpam12: RECT.1
zpam13: SMSQ10.100
zconst1: > J(HH) [30Hz]
zconst20: offset for selective refocusing [ppm]
zconst40: solvent offset [ppm]
zi31: 1/SW = 2 * DW
zi30: 1/(1 * SW) = 2 * DW
zn0: 2
zn1: 8*n
zd1: 16
zd1: number of experiments
zFnMODE: States-TPPI, TPPI, States or QSEQ
zpreprocessor-flags-start
zCPWR: presaturation of solvent at beginning of pulsesequence
; option -ZCWPRA (eda: ZGOPTNS)
zpreprocessor-flags-end
6 References


