



*Supplement of*

**Exclusively heteronuclear NMR experiments for the investigation of intrinsically disordered proteins: focusing on proline residues**

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1 **Supplementary information**

2 The pulse sequences used to acquire the 3D experiments to focus on proline residues are reported  
3 hereafter:

4 Pulse sequence 1 – **3D (H)CBCACON\_pro**

5 Pulse sequence 2 – **3D (H)CCCON\_pro**

6 Pulse sequence 3 – **3D (H)CBCANCO\_pro**

7 Pulse sequence 4 – **3D (H)CACOCON\_pro**

```

8 Pulse sequence 1 – 3D (H)CBCACON_pro
9
10 ;c_hcbcacon_ia3d_pro
11 ;avance-version (20/07/28)
12 ;(H)CbCaCON
13 ;3D sequence with
14 ; 13C detected correlation for triple resonance using
15 ; multiple inept transfer steps
16 ;
17 ; F2(Ha/b) -> F1(Ca/b,t1) -> F1(Ca) -> F1(C=O)
18 ; -> F3(N,t2) -> F1(C=O,t3)
19 ;
20 ;on/off resonance 13C pulses using shaped pulses
21 ;phase sensitive (t1)
22 ;phase sensitive (t2)
23 ;using constant time in t1
24 ;using IPAP scheme for virtual decoupling
25 ;using selective N pulse for Pro
26 ;(use parameterset )
27 ;
28 ;M.G. Murralli, A. Piaj, W. Bermel, I.C. Felli & R. Pierattelli,
29 ; ChemBioChem 19, 1625-1629 (2018)
30 ;W. Bermel, I. Bertini, V. Csizmok, I. C. Felli, R. Pierattelli &
31 ; P. Tompa, J. Magn. Reson. 198, 275-281 (2009)
32 ;(W. Bermel, I. Bertini, I.C. Felli, R. Kuemmerle
33 ; & R. Pierattelli, J. Magn. Reson. 178, 56-64 (2006) )
34 ;(W. Bermel, I. Bertini, L. Duma, I.C. Felli, L. Emsley, R. Pierattelli,
35 ; P.R. Vasos, Angew. Chem. Int. Ed. 44, 3089-3092 (2005) )
36 ;(L. Duma, S. Hediger, A. Lesage & L. Emsley,
37 ; J. Magn. Reson. 164, 187-195 (2003) )
38 ;
39 ;$CLASS=HighRes
40 ;$DIM=3D
41 ;$TYPE=
42 ;$SUBTYPE=
43 ;$COMMENT=
44
45
46 prosol relations=<triple_c>
47
48
49 #include <Avance.incl>
50 #include <Grad.incl>
51 #include <Delay.incl>
52
53
54 "p4=p3*2"

```

```

55 "p22=p21*2"
56 "d11=30m"
57 "d12=20u"
58
59 "d3=1.1m"
60 "d4=1.8m"
61 "d22=4.5m"
62 "d23=16.6m"
63 "d25=4.0m"
64
65
66 "d0=3u"
67 "d10=3u"
68 "d20=d25-p12-4u"
69
70 "in0=inf1/2"
71 "in10=inf2/2"
72
73 "in20=in0"
74
75 "td1=tdmax(td1,d20*2,in20)"
76
77
78 "DELTA=d10*2+larger(p4,p8)"
79 "DELTA1=d25-d0-larger(p12,p22)-d3-p4"
80 "DELTA2=d23-d22-p12"
81 "DELTA3=d23-p12-larger(p12,p59)/2-4u"
82 "DELTA4=d23/2-p12/2"
83 "DELTA5=d25-p12-4u"
84 "DELTA6=d23-d22-p12-larger(p12,p59)/2"
85
86
87 "l0=1"
88
89
90 "spoff13=bf1*((cnst22/2-cnst21/2)/1000000)"
91 "spoff23=0"
92 "spoff24=0"
93 "spoff25=0"
94 "spoff26=bf1*((cnst21-cnst23)/1000000)"
95 "spoff27=bf1*((cnst22-cnst21)/1000000)"
96
97 "o1_F1=bf1*cnst23/1000000"
98
99 aqseq 321
100
101
102 1 ze

```

103 d11 pl12:f2 pl16:f3  
104 2 d11 do:f2 do:f3  
105 3 d1 fq=cnst23(bf ppm):f1  
106 d12 pl2:f2 pl3:f3  
107 50u UNBLKGRAD  
108  
109 (p3 ph1):f2  
110 d4  
111 (center (p12:sp24 ph1) (p4 ph1):f2 )  
112 d4  
113 (p3 ph2):f2  
114  
115 p16:gp1  
116 d16  
117  
118 (p11:sp23 ph3)  
119 d0  
120 (center (p12:sp26 ph6) (p22 ph1):f3 )  
121 d3  
122 (p4 ph6):f2  
123 DELTA1  
124 (p12:sp24 ph1)  
125 d20  
126 (p12:sp26 ph1)  
127 4u  
128 (p11:sp25 ph1)  
129  
130 4u  
131 (p12:sp26 ph1)  
132 DELTA5  
133 (p12:sp24 ph1)  
134 4u  
135 (p12:sp26 ph1)  
136 DELTA5  
137 (p11:sp23 ph1)  
138  
139 p16:gp2  
140 d16 fq=cnst21(bf ppm):f1  
141  
142 (p11:sp23 ph5)  
143 d22  
144 (p12:sp27 ph1)  
145 DELTA6  
146 (center (p12:sp24 ph1) (p59:sp46 ph1):f3 )  
147 DELTA3  
148 (p12:sp27 ph1)  
149 4u  
150 (p11:sp25 ph1)

```

151
152   p16:gp3
153   d16 pl3:f3
154
155   (p21 ph4):f3
156   d10
157   (center (p8:sp13 ph6) (p4 ph6):f2 )
158   d10
159   (p22 ph1):f3
160   DELTA
161   (p21 ph1):f3
162
163   p16:gp4
164   d16 pl12:f2
165
166   if "lO %2 == 1"
167     {
168     (p11:sp23 ph1)
169     DELTA4
170     (p12:sp27 ph1)
171     DELTA4
172     (center (p12:sp24 ph1) (p22 ph1):f3 )
173     DELTA4
174     (p12:sp27 ph1)
175     DELTA4 pl16:f3
176     }
177   else
178     {
179     (p11:sp23 ph7)
180     d22
181     (p12:sp27 ph1)
182     DELTA2
183     (center (p12:sp24 ph1) (p22 ph1):f3 )
184     DELTA4
185     DELTA4 pl16:f3
186     (p12:sp27 ph1)
187     }
188
189   4u BLKGRAD
190   go=2 ph31 cpd2:f2 cpd3:f3
191   d11 do:f2 do:f3 mc #0 to 2
192
193   # ifdef LABEL_F1
194     F1(iu0, 2)
195   # else
196     F2(iu0, 2)
197   # endif /*LABEL_F1*/
198

```

```

199     F1PH(calph(ph3, +90), caldel(d0, +in0) & caldel(d20, -in20))
200     F2PH(calph(ph4, +90), caldel(d10, +in10))
201 exit
202
203
204 ph1=0
205 ph2=1
206 ph3=0 2
207 ph4=0 0 2 2
208 ph5=0 0 0 0 2 2 2 2
209 ph6=0 0 0 0 0 0 0 2 2 2 2 2 2 2 2
210 ph7=3
211 ph31=0 2 2 0 2 0 0 2
212
213
214 ;p1 : f1 channel - power level for pulse (default)
215 ;p2 : f2 channel - power level for pulse (default)
216 ;p3 : f3 channel - power level for pulse (default)
217 ;p12: f2 channel - power level for CPD/BB decoupling
218 ;p16: f3 channel - power level for CPD/BB decoupling
219 ;sp13: f1 channel - shaped pulse 180 degree (adiabatic)
220 ;sp23: f1 channel - shaped pulse 90 degree (on resonance)
221 ;sp24: f1 channel - shaped pulse 180 degree (on resonance)
222 ;sp25: f1 channel - shaped pulse 90 degree (on resonance)
223 ;           for time reversed pulse
224 ;sp26: f1 channel - shaped pulse 180 degree (C=O off resonance)
225 ;sp27: f1 channel - shaped pulse 180 degree (Ca off resonance)
226 ;sp46: f3 channel - shaped pulse 180 degree (N, selective for Pro)
227 ;p3 : f2 channel - 90 degree high power pulse
228 ;p4 : f2 channel - 180 degree high power pulse
229 ;p8 : f1 channel - 180 degree shaped pulse for inversion (adiabatic)
230 ;p11: f1 channel - 90 degree shaped pulse
231 ;p12: f1 channel - 180 degree shaped pulse
232 ;p16: homospoil/gradient pulse           [1 msec]
233 ;p21: f3 channel - 90 degree high power pulse
234 ;p22: f3 channel - 180 degree high power pulse
235 ;p59: f3 channel - 180 degree shaped pulse (N, selective for Pro)
236 ;d0 : incremented delay (F1 in 3D)       [3 usec]
237 ;d1 : relaxation delay; 1-5 * T1
238 ;d3 : 1/(6J(HCa))                        [1.1 msec]
239 ;d4 : 1/(4J(HCa))                        [1.8 msec]
240 ;d10: incremented delay (F2 in 3D)       [3 usec]
241 ;d11: delay for disk I/O                 [30 msec]
242 ;d12: delay for power switching          [20 usec]
243 ;d16: delay for homospoil/gradient recovery
244 ;d20: decremented delay (F1 in 3D) = d25+d0-p12-4u
245 ;d22: 1/(4J(COCa))                      [4.5 msec]
246 ;d23: 1/(4J(NCO))                      [16.6 msec]

```

```

247 ;d25: 1/(8J'(CaCb)) [4.0 msec]
248 ;cnst21: CO chemical shift (offset, in ppm)
249 ;cnst22: Calpha chemical shift (offset, in ppm)
250 ;cnst23: Caliphatic chemical shift (offset, in ppm)
251 ;o1p: CO chemical shift (cnst21)
252 ;l0: flag to switch between inphase and antiphase
253 ;in0: 1/(2 * SW(Ca/b)) = DW(Ca/b)
254 ;nd0: 2
255 ;in10: 1/(2 * SW(N)) = DW(N)
256 ;nd10: 2
257 ;in20: = in0
258 ;ns: 16 * n
259 ;ds: >= 32
260 ;td1: number of experiments in F1
261 ;td2: number of experiments in F2
262 ;FnMODE: States-TPPI (or TPPI) in F1 td1 max = n * d20 / in20 (n = 4 or = 2 with LABEL_F2)
263 ;FnMODE: States-TPPI (or TPPI) in F2
264 ;cpd2: decoupling according to sequence defined by cpdprg2
265 ;cpd3: decoupling according to sequence defined by cpdprg3
266 ;pcpd2: f2 channel - 90 degree pulse for decoupling sequence
267 ;pcpd3: f3 channel - 90 degree pulse for decoupling sequence
268
269
270 ;for z-only gradients:
271 ;gpz1: 50%
272 ;gpz2: 30%
273 ;gpz3: 19%
274 ;gpz4: 13%
275
276 ;use gradient files:
277 ;gpnam1: SMSQ10.100
278 ;gpnam2: SMSQ10.100
279 ;gpnam3: SMSQ10.100
280 ;gpnam4: SMSQ10.100
281
282
283 ;preprocessor-flags-start
284 ;LABEL_F2: to do ipap in F2 start experiment with
285 ; option -DLABEL_F2 (eda: ZGOPTNS)
286 ;preprocessor-flags-end
287
288
289 ;use AU-program splitcomb [ipap 2] (F1 or F2 with LABEL_F2) to process data
290
291
292
293 ;$ld: $
294

```



```

295 Pulse sequence 2 – 3D (H)CCCON_pro
296
297 ;c_hcccon_ia3d_pro
298 ;avance-version (20/07/28)
299 ;(H)CC(CO)N
300 ;3D sequence with
301 ; 13C detected correlation for triple resonance using
302 ; multiple inept transfer steps and
303 ; C-C FLOPSY16 spinlock
304 ;
305 ; F1(Cali,t1) -> F1(Ca) -> F1(C=O)
306 ; -> F3(N,t2) -> F1(C=O,t3)
307 ;
308 ;on/off resonance 13C pulses using shaped pulses
309 ;phase sensitive (t1)
310 ;phase sensitive (t2)
311 ;using IPAP scheme for virtual decoupling
312 ;using selective N pulse for Pro
313 ;(use parameterset )
314 ;
315 ;M.G. Murralli, A. Piaj, W. Bermel, I.C. Felli & R. Pierattelli,
316 ; ChemBioChem 19, 1625-1629 (2018)
317 ;W. Bermel, I. Bertini, I.C. Felli, R. Kuemmerle
318 ; & R. Pierattelli, J. Magn. Reson. 178, 56-64 (2006)
319 ;
320 ;$CLASS=HighRes
321 ;$DIM=3D
322 ;$TYPE=
323 ;$SUBTYPE=
324 ;$COMMENT=
325
326
327 prosol relations=<triple_c>
328
329
330 #include <Avance.incl>
331 #include <Delay.incl>
332 #include <Grad.incl>
333
334
335 "p4=p3*2"
336 "p22=p21*2"
337 "d11=30m"
338 "d12=20u"
339
340 "d3=0.95m"

```

341 "d4=1.8m"  
342 "d22=4.5m"  
343 "d23=16.6m"  
344  
345  
346 "d0=3u"  
347 "d10=3u"  
348  
349 "in0=inf1/2"  
350 "in10=inf2/2"  
351  
352  
353 "DELTA=d10\*2+p8"  
354 "DELTA1=d3/2"  
355 "DELTA2=d3/2+p22+p4+d0\*2"  
356 "DELTA3=d23-d22-p12"  
357 "DELTA4=d23-p12-larger(p12,p59)/2-4u"  
358 "DELTA5=d23/2-p12/2"  
359 "DELTA6=d23-d22-p12-larger(p12,p59)/2"  
360  
361  
362 "FACTOR2=(d9/(p6\*188.448))"  
363 "l1=FACTOR2"  
364  
365  
366 "l0=1"  
367  
368  
369 "spoff13=bf1\*((cnst22/2-cnst21/2)/1000000)"  
370 "spoff22=bf1\*((cnst21-cnst22)/1000000)"  
371 "spoff23=0"  
372 "spoff24=0"  
373 "spoff25=0"  
374 "spoff26=bf1\*((cnst21-cnst23)/1000000)"  
375 "spoff27=bf1\*((cnst22-cnst21)/1000000)"  
376 "spoff28=0"  
377  
378  
379 "o1\_F1=bf1\*cnst23/1000000"  
380  
381  
382 aqseq 321  
383  
384  
385 1 ze  
386 d11 pl12:f2 pl16:f3  
387 2 d11 do:f2 do:f3  
388 3 d1 fq=cnst23(bf ppm):f1

389 d12 pl2:f2 pl3:f3  
390 50u UNBLKGRAD  
391  
392 (p3 ph1):f2  
393 d4  
394 (center (p12:sp24 ph1) (p4 ph1):f2 )  
395 d4  
396 (p3 ph8):f2  
397  
398 (p11:sp23 ph3)  
399 d0  
400 (p22 ph1):f3  
401 DELTA1  
402 (p12:sp26 ph1)  
403 DELTA1  
404 (p4 ph1):f2  
405 d0  
406 (p12:sp24 ph1)  
407 DELTA2  
408 (p12:sp26 ph1)  
409 DELTA1  
410 (p11:sp25 ph1)  
411  
412 p19:gp1  
413 d16 pl10:f1  
414 ;begin FLOPSY16  
415 4 p6\*0.511 ph11  
416 p6\*1.067 ph12  
417 p6\*1.822 ph13  
418 p6\*1.767 ph14  
419 p6\*1.444 ph15  
420 p6\*1.767 ph14  
421 p6\*1.822 ph13  
422 p6\*1.067 ph12  
423 p6\*0.511 ph11  
424  
425 p6\*0.511 ph21  
426 p6\*1.067 ph22  
427 p6\*1.822 ph23  
428 p6\*1.767 ph24  
429 p6\*1.444 ph25  
430 p6\*1.767 ph24  
431 p6\*1.822 ph23  
432 p6\*1.067 ph22  
433 p6\*0.511 ph21  
434  
435 p6\*0.511 ph21  
436 p6\*1.067 ph22

437 p6\*1.822 ph23  
438 p6\*1.767 ph24  
439 p6\*1.444 ph25  
440 p6\*1.767 ph24  
441 p6\*1.822 ph23  
442 p6\*1.067 ph22  
443 p6\*0.511 ph21  
444  
445 p6\*0.511 ph11  
446 p6\*1.067 ph12  
447 p6\*1.822 ph13  
448 p6\*1.767 ph14  
449 p6\*1.444 ph15  
450 p6\*1.767 ph14  
451 p6\*1.822 ph13  
452 p6\*1.067 ph12  
453 p6\*0.511 ph11  
454  
455 p6\*0.511 ph11  
456 p6\*1.067 ph12  
457 p6\*1.822 ph13  
458 p6\*1.767 ph14  
459 p6\*1.444 ph15  
460 p6\*1.767 ph14  
461 p6\*1.822 ph13  
462 p6\*1.067 ph12  
463 p6\*0.511 ph11  
464  
465 p6\*0.511 ph11  
466 p6\*1.067 ph12  
467 p6\*1.822 ph13  
468 p6\*1.767 ph14  
469 p6\*1.444 ph15  
470 p6\*1.767 ph14  
471 p6\*1.822 ph13  
472 p6\*1.067 ph12  
473 p6\*0.511 ph11  
474  
475 p6\*0.511 ph21  
476 p6\*1.067 ph22  
477 p6\*1.822 ph23  
478 p6\*1.767 ph24  
479 p6\*1.444 ph25  
480 p6\*1.767 ph24  
481 p6\*1.822 ph23  
482 p6\*1.067 ph22  
483 p6\*0.511 ph21  
484

485 p6\*0.511 ph21  
486 p6\*1.067 ph22  
487 p6\*1.822 ph23  
488 p6\*1.767 ph24  
489 p6\*1.444 ph25  
490 p6\*1.767 ph24  
491 p6\*1.822 ph23  
492 p6\*1.067 ph22  
493 p6\*0.511 ph21  
494  
495 p6\*0.511 ph21  
496 p6\*1.067 ph22  
497 p6\*1.822 ph23  
498 p6\*1.767 ph24  
499 p6\*1.444 ph25  
500 p6\*1.767 ph24  
501 p6\*1.822 ph23  
502 p6\*1.067 ph22  
503 p6\*0.511 ph21  
504  
505 p6\*0.511 ph11  
506 p6\*1.067 ph12  
507 p6\*1.822 ph13  
508 p6\*1.767 ph14  
509 p6\*1.444 ph15  
510 p6\*1.767 ph14  
511 p6\*1.822 ph13  
512 p6\*1.067 ph12  
513 p6\*0.511 ph11  
514  
515 p6\*0.511 ph11  
516 p6\*1.067 ph12  
517 p6\*1.822 ph13  
518 p6\*1.767 ph14  
519 p6\*1.444 ph15  
520 p6\*1.767 ph14  
521 p6\*1.822 ph13  
522 p6\*1.067 ph12  
523 p6\*0.511 ph11  
524  
525 p6\*0.511 ph21  
526 p6\*1.067 ph22  
527 p6\*1.822 ph23  
528 p6\*1.767 ph24  
529 p6\*1.444 ph25  
530 p6\*1.767 ph24  
531 p6\*1.822 ph23  
532 p6\*1.067 ph22

533 p6\*0.511 ph21  
534  
535 p6\*0.511 ph21  
536 p6\*1.067 ph22  
537 p6\*1.822 ph23  
538 p6\*1.767 ph24  
539 p6\*1.444 ph25  
540 p6\*1.767 ph24  
541 p6\*1.822 ph23  
542 p6\*1.067 ph22  
543 p6\*0.511 ph21  
544  
545 p6\*0.511 ph21  
546 p6\*1.067 ph22  
547 p6\*1.822 ph23  
548 p6\*1.767 ph24  
549 p6\*1.444 ph25  
550 p6\*1.767 ph24  
551 p6\*1.822 ph23  
552 p6\*1.067 ph22  
553 p6\*0.511 ph21  
554  
555 p6\*0.511 ph11  
556 p6\*1.067 ph12  
557 p6\*1.822 ph13  
558 p6\*1.767 ph14  
559 p6\*1.444 ph15  
560 p6\*1.767 ph14  
561 p6\*1.822 ph13  
562 p6\*1.067 ph12  
563 p6\*0.511 ph11  
564  
565 p6\*0.511 ph11  
566 p6\*1.067 ph12  
567 p6\*1.822 ph13  
568 p6\*1.767 ph14  
569 p6\*1.444 ph15  
570 p6\*1.767 ph14  
571 p6\*1.822 ph13  
572 p6\*1.067 ph12  
573 p6\*0.511 ph11  
574 lo to 4 times l1  
575 ;end FLOPSY16  
576  
577 4u  
578 p19:gp2  
579 d16 fq=cnst22(bf ppm):f1  
580 20u pl12:f2

```

581 20u cpd2:f2
582
583 (p11:sp23 ph1)
584 d22
585 (p12:sp22 ph1)
586 4u
587 (p25:sp28 ph1)
588 d22
589 (p12:sp22 ph1)
590 4u
591 (p11:sp25 ph2)
592
593 4u do:f2
594 p16:gp3
595 d16 fq=cnst21(bf ppm):f1
596 20u cpd2:f2
597
598 (p11:sp23 ph1)
599 d22
600 (p12:sp27 ph1)
601 DELTA6
602 (center (p12:sp24 ph1) (p59:sp46 ph1):f3 )
603 DELTA4
604 (p12:sp27 ph1)
605 4u
606 (p11:sp25 ph1)
607
608 4u do:f2
609 p16:gp4
610 d16 pl3:f3
611 20u cpd2:f2
612
613 (p21 ph4):f3
614 d10
615 (p8:sp13 ph6)
616 d10
617 (p22 ph1):f3
618 DELTA
619 (p21 ph5):f3
620
621 if "l0 %2 == 1"
622 {
623 (p11:sp23 ph1)
624 DELTA5
625 (p12:sp27 ph1)
626 DELTA5
627 (center (p12:sp24 ph1) (p22 ph1):f3 )
628 DELTA5

```

```

629     (p12:sp27 ph1)
630     DELTA5 pl16:f3
631     }
632 else
633     {
634     (p11:sp23 ph7)
635     d22
636     (p12:sp27 ph1)
637     DELTA3
638     (center (p12:sp24 ph1) (p22 ph1):f3 )
639     DELTA5
640     DELTA5 pl16:f3
641     (p12:sp27 ph1)
642     }
643
644 4u BLKGRAD
645 go=2 ph31 cpd3:f3
646 d11 do:f2 do:f3 mc #0 to 2
647
648 # ifdef LABEL_F1
649     F1(iu0, 2)
650 # else
651     F2(iu0, 2)
652 # endif /*LABEL_F1*/
653
654     F1PH(calph(ph3, +90), caldel(d0, +in0))
655     F2PH(calph(ph4, +90), caldel(d10, +in10))
656 exit
657
658
659 ph1=0
660 ph2=1
661 ph3=1 3
662 ph4=0 0 0 0 2 2 2 2
663 ph5=0 0 0 0 0 0 0 2 2 2 2 2 2 2 2
664 ph6=0
665 ph7=3
666 ph8=1 1 3 3
667
668 ph11=(720) 0
669 ph12=(720) 90
670 ph13=(720) 135
671 ph14=(720) 630
672 ph15=(720) 45
673
674 ph21=(720) 360
675 ph22=(720) 450
676 ph23=(720) 495

```



```

677 ph24=(720) 270
678 ph25=(720) 405
679
680 ph31=0 2 2 0 2 0 2 0 2 2 0 0 2 0 2 2 0
681
682
683 ;p1 : f1 channel - power level for pulse (default)
684 ;p2 : f2 channel - power level for pulse (default)
685 ;p3 : f3 channel - power level for pulse (default)
686 ;p10: f1 channel - power level for TOCSY-spinlock
687 ;p12: f2 channel - power level for CPD/BB decoupling
688 ;p16: f3 channel - power level for CPD/BB decoupling
689 ;sp13: f1 channel - shaped pulse 180 degree (adiabatic)
690 ;sp22: f1 channel - shaped pulse 180 degree (C=O off resonance)
691 ;sp23: f1 channel - shaped pulse 90 degree (on resonance)
692 ;sp24: f1 channel - shaped pulse 180 degree (on resonance)
693 ;sp25: f1 channel - shaped pulse 90 degree (on resonance)
694 ;           for time reversed pulse
695 ;sp26: f1 channel - shaped pulse 180 degree (C=O off resonance)
696 ;sp27: f1 channel - shaped pulse 180 degree (Ca off resonance)
697 ;sp28: f1 channel - shaped pulse 180 degree (Ca on resonance)
698 ;           sp28 requires higher selectivity than sp24
699 ;sp46: f3 channel - shaped pulse 180 degree (N, selective for Pro)
700 ;p3 : f2 channel - 90 degree high power pulse
701 ;p4 : f2 channel - 180 degree high power pulse
702 ;p6 : f1 channel - 90 degree low power pulse
703 ;p8 : f1 channel - 180 degree shaped pulse for inversion (adiabatic)
704 ;p11: f1 channel - 90 degree shaped pulse
705 ;p12: f1 channel - 180 degree shaped pulse
706 ;p16: homospoil/gradient pulse           [1 msec]
707 ;p19: gradient pulse 2                   [500 usec]
708 ;p21: f3 channel - 90 degree high power pulse
709 ;p22: f3 channel - 180 degree high power pulse
710 ;p25: f1 channel - 180 degree shaped pulse (Ca, sp28)
711 ;p59: f3 channel - 180 degree shaped pulse (N, selective for Pro)
712 ;d0 : incremented delay (F1 in 3D)       [3 usec]
713 ;d1 : relaxation delay; 1-5 * T1
714 ;d3 : 1/(6J(HCa))                       [950 usec]
715 ;d4 : 1/(4J(HCa))                       [1.8 msec]
716 ;d9 : TOCSY mixing time                  [12 msec]
717 ;d10: incremented delay (F2 in 3D)       [3 usec]
718 ;d11: delay for disk I/O                 [30 msec]
719 ;d12: delay for power switching          [20 usec]
720 ;d16: delay for homospoil/gradient recovery [150 usec]
721 ;d22: 1/(4J(COCa))                      [4.5 msec]
722 ;d23: 1/(4J(NCO))                      [16.6 msec]
723 ;cnst21: CO chemical shift (offset, in ppm)
724 ;cnst22: Calpha chemical shift (offset, in ppm)

```

```

725 ;cnst23: Caliphatic chemical shift (offset, in ppm)
726 ;o1p: CO chemical shift (cnst21)
727 ;l0: flag to switch between inphase and antiphase
728 ;l1: loop for FLOPSY16 cycle: ((p6*188.448) * l1) = mixing time
729 ;inf1: 1/SW(Cali) = 2 * DW(Cali)
730 ;inf2: 1/SW(N) = 2 * DW(N)
731 ;in0: 1/(2 * SW(Cali)) = DW(Cali)
732 ;nd0: 2
733 ;in10: 1/(2 * SW(N)) = DW(N)
734 ;nd10: 2
735 ;ns: 16 * n
736 ;ds: >= 32
737 ;td1: number of experiments in F1
738 ;td2: number of experiments in F2
739 ;FnMODE: States-TPPI (or TPPI) in F1
740 ;FnMODE: States-TPPI (or TPPI) in F2
741 ;cpd2: decoupling according to sequence defined by cpdprg2
742 ;cpd3: decoupling according to sequence defined by cpdprg3
743 ;pcpd2: f2 channel - 90 degree pulse for decoupling sequence
744 ;pcpd3: f3 channel - 90 degree pulse for decoupling sequence
745
746
747 ;for z-only gradients:
748 ;gpz1: 60%
749 ;gpz2: 50%
750 ;gpz3: 19%
751 ;gpz4: 11%
752
753 ;use gradient files:
754 ;gpnam1: SMSQ10.100
755 ;gpnam2: SMSQ10.100
756 ;gpnam3: SMSQ10.100
757 ;gpnam4: SMSQ10.100
758
759
760 ;preprocessor-flags-start
761 ;LABEL_F2: to do ipap in F2 start experiment with
762 ; option -DLABEL_F2 (eda: ZGOPTNS)
763 ;preprocessor-flags-end
764
765
766
767 ;use AU-program splitcomb [ipap 2] (F1 or F2 with LABEL_F2) to process data
768
769
770
771 ;$Id: $

```

```

772 Pulse sequence 3 – 3D (H)CBCANCO_pro
773
774 ;c_hcbcanco_ia3d_pro
775 ;avance-version (20/07/28)
776 ;(H)CbCaNCO
777 ;3D sequence with
778 ; 13C detected correlation for triple resonance using
779 ; multiple inept transfer steps
780 ;
781 ; F2(Ha/b) -> F1(Ca/b,t1) -> F1(Ca)
782 ; -> F3(N,t2) -> F1(C=O,t3)
783 ;
784 ;on/off resonance 13C pulses using shaped pulses
785 ;phase sensitive (t1)
786 ;phase sensitive (t2)
787 ;using constant time in t1
788 ;using constant time in t2
789 ;using IPAP scheme for virtual decoupling
790 ;using selective N pulse for Pro
791 ;(use parameterset )
792 ;
793 ;M.G. Murralli, A. Piai, W. Bermel, I.C. Felli & R. Pierattelli,
794 ; ChemBioChem 19, 1625-1629 (2018)
795 ;W. Bermel, I. Bertini, V. Csizmok, I. C. Felli, R. Pierattelli &
796 ; P. Tompa, J. Magn. Reson. 198, 275-281 (2009)
797 ;(W. Bermel, I. Bertini, I.C. Felli, R. Kuemmerle
798 ; & R. Pierattelli, J. Magn. Reson. 178, 56-64 (2006) )
799 ;
800 ;$CLASS=HighRes
801 ;$DIM=3D
802 ;$TYPE=
803 ;$SUBTYPE=
804 ;$COMMENT=
805
806
807 prosol relations=<triple_c>
808
809
810 #include <Avance.incl>
811 #include <Grad.incl>
812 #include <Delay.incl>
813
814
815 "p4=p3*2"
816 "p22=p21*2"
817 "d11=30m"

```

818 "d12=20u"  
819  
820 "d3=1.1m"  
821 "d4=1.8m"  
822 "d22=4.5m"  
823 "d23=11.0m"  
824 "d25=4.0m"  
825 "d27=16.0m"  
826  
827  
828 "d0=3u"  
829 "d10=d23"  
830 "d20=d25-p12-4u"  
831 "d30=d27-larger(p12,p59)/2"  
832  
833 "in0=inf1/2"  
834 "in10=inf2/2"  
835  
836 "in20=in0"  
837 "in30=in10"  
838  
839 "td1=tdmax(td1,d20\*2,in20)"  
840 "td2=tdmax(td2,d30\*2,in30)"  
841  
842  
843 "DELTA1=d25-d0-larger(p12,p22)-d3-p4"  
844 "DELTA2=d27-d10-p12-larger(p12,p59)/2"  
845 "DELTA3=d27/2-p12/2"  
846 "DELTA4=d27-d22-p12"  
847  
848  
849 "l0=1"  
850  
851  
852 "spoff23=0"  
853 "spoff24=0"  
854 "spoff25=0"  
855 "spoff26=bf1\*((cnst21-cnst23)/1000000)"  
856 "spoff27=bf1\*((cnst22-cnst21)/1000000)"  
857  
858  
859 "o1\_F1=bf1\*cnst23/1000000"  
860  
861  
862 aqseq 321  
863  
864  
865 1 ze

866 d11 pl12:f2 pl16:f3  
867 2 d11 do:f2 do:f3  
868 3 d12 fq=cnst23(bf ppm):f1  
869 d1  
870 d12 pl2:f2 pl3:f3  
871 50u UNBLKGRAD  
872  
873 (p3 ph1):f2  
874 d4  
875 (center (p12:sp24 ph1) (p4 ph1):f2 )  
876 d4  
877 (p3 ph2):f2  
878  
879 p16:gp1  
880 d16  
881  
882 (p11:sp23 ph3)  
883 d0  
884 (center (p12:sp26 ph6) (p22 ph1):f3 )  
885 d3  
886 (p4 ph1):f2  
887 DELTA1  
888 (p12:sp24 ph1)  
889 d20  
890 (p12:sp26 ph1)  
891 4u  
892 (p11:sp25 ph1)  
893  
894 d23  
895 (center (p12:sp24 ph1) (p22 ph1):f3 )  
896 d23 pl12:f2  
897 (p11:sp23 ph1)  
898  
899 p16:gp2  
900 d16 fq=cnst21(bf ppm):f1  
901 20u cpd2:f2  
902  
903 (p21 ph4):f3  
904 d10  
905 (p12:sp27 ph6)  
906 DELTA2  
907 (center (p12:sp24 ph6) (p59:sp46 ph1):f3 )  
908 d30 pl3:f3  
909 (p21 ph1):f3  
910  
911 4u do:f2  
912 p16:gp3  
913 d16

```

914 20u cpd2:f2
915
916 if "l0 %2 == 1"
917 {
918 (p11:sp23 ph5)
919 DELTA3
920 (p12:sp27 ph1)
921 DELTA3
922 (center (p12:sp24 ph1) (p22 ph1):f3 )
923 DELTA3
924 (p12:sp27 ph1)
925 DELTA3 pl16:f3
926 }
927 else
928 {
929 (p11:sp23 ph7)
930 d22
931 (p12:sp27 ph1)
932 DELTA4
933 (center (p12:sp24 ph1) (p22 ph1):f3 )
934 DELTA3
935 DELTA3 pl16:f3
936 (p12:sp27 ph1)
937 }
938
939 4u BLKGRAD
940
941 go=2 ph31 cpd3:f3
942 d11 do:f2 do:f3 mc #0 to 2
943
944 # ifdef LABEL_F1
945 F1(iu0, 2)
946 # else
947 F2(iu0, 2)
948 # endif /*LABEL_F1*/
949
950 F1PH(calph(ph3, +90), caldel(d0, +in0) & caldel(d20, -in20))
951 F2PH(calph(ph4, +90), caldel(d10, +in10) & caldel(d30, -in30))
952 exit
953
954
955 ph1=0
956 ph2=1
957 ph3=0 2
958 ph4=0 0 2 2
959 ph5=0 0 0 0 2 2 2 2
960 ph6=0 0 0 0 0 0 0 2 2 2 2 2 2 2 2
961 ph7=3 3 3 3 1 1 1 1

```

```

962 ph31=0 2 2 0 2 0 0 2
963
964
965 ;p1 : f1 channel - power level for pulse (default)
966 ;p2 : f2 channel - power level for pulse (default)
967 ;p3 : f3 channel - power level for pulse (default)
968 ;p12: f2 channel - power level for CPD/BB decoupling
969 ;p16: f3 channel - power level for CPD/BB decoupling
970 ;sp23: f1 channel - shaped pulse 90 degree (on resonance)
971 ;sp24: f1 channel - shaped pulse 180 degree (on resonance)
972 ;sp25: f1 channel - shaped pulse 90 degree (on resonance)
973 ;           for time reversed pulse
974 ;sp26: f1 channel - shaped pulse 180 degree (C=O off resonance)
975 ;sp27: f1 channel - shaped pulse 180 degree (Ca off resonance)
976 ;sp46: f3 channel - shaped pulse 180 degree (N, selective for Pro)
977 ;p3 : f2 channel - 90 degree high power pulse
978 ;p4 : f2 channel - 180 degree high power pulse
979 ;p11: f1 channel - 90 degree shaped pulse
980 ;p12: f1 channel - 180 degree shaped pulse
981 ;p16: homospoil/gradient pulse           [1 msec]
982 ;p21: f3 channel - 90 degree high power pulse
983 ;p22: f3 channel - 180 degree high power pulse
984 ;p59: f3 channel - 180 degree shaped pulse (N, selective for Pro)
985 ;d0 : incremented delay (F1 in 3D)           [3 usec]
986 ;d1 : relaxation delay; 1-5 * T1
987 ;d3 : 1/(6J(HCa))                           [1.1 msec]
988 ;d4 : 1/(4J(HCa))                           [1.8 msec]
989 ;d10: incremented delay (F2 in 3D) = d23
990 ;d11: delay for disk I/O                       [30 msec]
991 ;d12: delay for power switching               [20 usec]
992 ;d16: delay for homospoil/gradient recovery
993 ;d20: decremented delay (F1 in 3D) = d25-p12-4u
994 ;d22: 1/(4J(COCa))                           [4.5 msec]
995 ;d23: 1/(4J(NCa))                           [11.0 msec]
996 ;d25: 1/(8J'(CaCb))                         [4.0 msec]
997 ;d27: 1/(4J(NCO))                           [16.0 msec]
998 ;d30: decremented delay (F2 in 3D) = d27-larger(p12,p59)/2
999 ;cnst21: CO chemical shift (offset, in ppm)
1000 ;cnst22: Calpha chemical shift (offset, in ppm)
1001 ;cnst23: Caliphatic chemical shift (offset, in ppm)
1002 ;o1p: CO chemical shift (cnst21)
1003 ;l0: flag to switch between inphase and antiphase
1004 ;inf1: 1/SW(Ca) = 2 * DW(Ca)
1005 ;inf2: 1/SW(N) = 2 * DW(N)
1006 ;in0: 1/(2 * SW(Ca)) = DW(Ca)
1007 ;nd0: 2
1008 ;in10: 1/(2 * SW(N)) = DW(N)
1009 ;nd10: 2

```

```

1010 ;in20: = in0
1011 ;in30: = in10
1012 ;ns: 16 * n
1013 ;ds: >= 32
1014 ;td1: number of experiments in F1
1015 ;td2: number of experiments in F2
1016 ;FnMODE: States-TPPI (or TPPI) in F1
1017 ;FnMODE: States-TPPI (or TPPI) in F2
1018 ;cpd2: decoupling according to sequence defined by cpdprg2
1019 ;cpd3: decoupling according to sequence defined by cpdprg3
1020 ;pcpd2: f2 channel - 90 degree pulse for decoupling sequence
1021 ;pcpd3: f3 channel - 90 degree pulse for decoupling sequence
1022
1023
1024 ;for z-only gradients:
1025 ;gpz1: 50%
1026 ;gpz2: 30%
1027 ;gpz3: 19%
1028
1029 ;use gradient files:
1030 ;gpnam1: SMSQ10.100
1031 ;gpnam2: SMSQ10.100
1032 ;gpnam3: SMSQ10.100
1033
1034
1035
1036 ;preprocessor-flags-start
1037 ;LABEL_F2: to do ipap in F2 start experiment with
1038 ; option -DLABEL_F2 (eda: ZGOPTNS)
1039 ;preprocessor-flags-end
1040
1041
1042
1043 ;use AU-program splitcomb [ipap 2] (F1 or F2 with LABEL_F2) to process data
1044
1045
1046
1047 ;$Id: $
1048

```



```

1049 Pulse sequence 4 – 3D (H)CACOCON_pro
1050
1051 ;c_hcacocon_ia3d_pro
1052 ;avance-version (20/07/28)
1053 ;(Hca)COCON-TOCSY
1054 ;3D sequence with
1055 ; homonuclear Hartman-Hahn transfer using MOCCA-XY16
1056 ; sequence for mixing
1057 ;
1058 ; F2(H) -> F1(Ca) -> F1(C=O,t1, MOCCA) -> F3(N,t2) -> F1(C=O,t3)
1059 ;
1060 ;on/off resonance 13C pulses using hard and shaped pulses
1061 ;phase sensitive (t1)
1062 ;phase sensitive (t2)
1063 ;using semi-constant time in t1
1064 ;using IPAP scheme for virtual decoupling
1065 ;using selective N pulse for Pro
1066 ;(use parameterset )
1067 ;
1068 ;M.G. Murralli, A. Piai, W. Bermel, I.C. Felli & R. Pierattelli,
1069 ; ChemBioChem 19, 1625-1629 (2018)
1070 ;I.C. Felli, R. Pierattelli, S.J. Glaser & B. Luy,
1071 ; J. Biomol. NMR 43, 187-196 (2009)
1072 ;W. Bermel, I. Bertini, I.C. Felli, Y.-M. Lee, C. Luchinat & R.
1073 Pierattelli,
1074 ; J. Am. Chem. Soc. 128, 3918-3919
1075 ;S. Balayssac, B. Jimenez & M. Piccioli,
1076 ; J. Magn. Reson. 182, 325-329 (2006)
1077 ;
1078 ;$CLASS=HighRes
1079 ;$DIM=3D
1080 ;$TYPE=
1081 ;$SUBTYPE=
1082 ;$COMMENT=
1083
1084 prosol relations=<triple_c>
1085
1086 #include <Avance.incl>
1087 #include <Delay.incl>
1088 #include <Grad.incl>
1089
1090
1091 "p22=p21*2"
1092 "d11=30m"
1093 "d12=20u"
1094
1095 "d3=1.1m"
1096 "d4=1.8m"
1097 "d22=4.5m"

```

```

1098 "d23=16.6m"
1099
1100 "d21=300u"
1101
1102
1103 "d10=3u"
1104 "d28=3u"
1105 "d0=d22"
1106 "d20=d22+d28-4u"
1107
1108 "in0=inf1/2"
1109 "in10=inf2/2"
1110
1111 "FACTOR1=d20*10000000*2/td1"
1112 "INCR1=FACTOR1/10000000"
1113
1114 "if ( INCR1 > in0 ) { in20 = in0; } else { in20 = INCR1; }"
1115 "if ( INCR1 > in0 ) { in28 = 0; } else { in28=in0-INCR1; }"
1116
1117 "TAU=d21/2"
1118
1119 "FACTOR2=(d9/((d21+p14))*16)"
1120 "l1=FACTOR2*16"
1121
1122 "d31=(d21+p14)*l1"
1123
1124 "DELTA=d10*2+p8"
1125 "DELTA1=d4-larger(p4,p25)/2"
1126 "DELTA2=d22-d3-p4"
1127 "DELTA3=d23/2-p12/2"
1128 "DELTA4=d23-d22-p12"
1129 "DELTA5=d23-larger(p12,p59)/2"
1130
1131 "l0=0"
1132
1133 "spoff13=bf1*((cnst21/2+cnst22/2)/1000000)-o1"
1134 "spoff23=0"
1135 "spoff24=0"
1136 "spoff25=0"
1137 "spoff26=bf1*((cnst22-cnst21)/1000000)"
1138 "spoff27=bf1*((cnst21-cnst22)/1000000)"
1139
1140
1141 "o1_F1=bf1*cnst21/1000000"
1142
1143
1144 aqseq 321
1145
1146
1147 1 ze
1148     d11 p112:f2 p116:f3
1149 2 d11 do:f2 do:f3

```

```

1150 4u BLKGRAD
1151 d1 p11:f1 p12:f2
1152 20u rpp11
1153 50u UNBLKGRAD
1154 d12 cpd3:f3
1155 20u fq=cnst22(bf ppm):f1
1156
1157 (p3 ph1):f2
1158 DELTA1
1159 (center (p25:sp28 ph1) (p4 ph1):f2 )
1160 DELTA1
1161 (p3 ph2):f2
1162
1163 (p11:sp23 ph1)
1164 d3
1165 (p4 ph1):f2
1166 DELTA2
1167 (p12:sp27 ph1)
1168 4u
1169 (p25:sp28 ph1)
1170 d22
1171 (p12:sp27 ph1)
1172 4u
1173 (p11:sp25 ph5)
1174
1175 p16:gp4
1176 d16 fq=cnst21(bf ppm):f1
1177
1178 (p11:sp23 ph3)
1179 d0
1180 (p12:sp26 ph1)
1181 d28
1182 (p12:sp24 ph1)
1183 d20
1184 (p12:sp26 ph1)
1185 4u
1186 (p11:sp25 ph4)
1187
1188 4u do:f3
1189 p16:gp1
1190 d16 p120:f1
1191
1192 ;begin MOCCA-XY16
1193 4 TAU
1194 (p14 ph11)
1195 TAU ipp11
1196 lo to 4 times l1
1197 ;end MOCCA-XY16
1198
1199 p16:gp2
1200 d16 p112:f2 p13:f3
1201 20u cpd2:f2

```

```

1202
1203 (p11:sp23 ph1)
1204 DELTA5
1205 (center (p12:sp24 ph1) (p59:sp46 ph1):f3 )
1206 DELTA5
1207 (p11:sp25 ph2)
1208
1209 4u do:f2
1210 p16:gp3
1211 d16 p13:f3
1212 20u cpd2:f2
1213
1214 (p21 ph6):f3
1215 d10
1216 (p8:sp13 ph1)
1217 d10
1218 (p22 ph1):f3
1219 DELTA
1220 (p21 ph1):f3
1221
1222 if "l0 %2 == 0"
1223 {
1224 (p11:sp23 ph1)
1225 DELTA3
1226 (p12:sp26 ph1)
1227 DELTA3
1228 (center (p12:sp24 ph1) (p22 ph1):f3 )
1229 DELTA3
1230 (p12:sp26 ph1)
1231 DELTA3 p116:f3
1232 }
1233 else
1234 {
1235 (p11:sp23 ph7)
1236 d22
1237 (p12:sp26 ph1)
1238 DELTA4
1239 (center (p12:sp24 ph1) (p22 ph1):f3 )
1240 DELTA3
1241 DELTA3 p116:f3
1242 (p12:sp26 ph1)
1243 }
1244
1245 4u BLKGRAD
1246
1247 go=2 ph31 cpd3:f3
1248
1249 d11 do:f2 do:f3 mc #0 to 2
1250
1251 # ifdef LABEL_F1
1252 F1I(iu0, 2)
1253 # else

```

```

1254     F2I(iu0, 2)
1255 #   endif /*LABEL_F1*/
1256
1257     F1PH(calph(ph3, +90), caldel(d0, +in0) & caldel(d20, -in20) &
1258 caldel(d28, +in28))
1259     F2PH(calph(ph6, +90), caldel(d10, +in10))
1260
1261     d31
1262 exit
1263
1264
1265 ph1=0
1266 ph2=1
1267 ph3=0 2
1268 ph4=1 1 1 1 1 1 1 1 3 3 3 3 3 3 3 3
1269 ph5=0 0 0 0 2 2 2 2
1270 ph6=0 0 2 2
1271 ph7=3
1272 ph11=0 1 0 1 1 0 1 0 2 3 2 3 3 2 3 2
1273 ph31=0 2 2 0 2 0 0 2 2 0 0 2 0 2 2 0
1274
1275
1276 ;p11 : f1 channel - power level for pulse (default)
1277 ;p12 : f2 channel - power level for pulse (default)
1278 ;p13 : f3 channel - power level for pulse (default)
1279 ;p112: f2 channel - power level for CPD/BB decoupling
1280 ;p116: f3 channel - power level for CPD/BB decoupling
1281 ;p120: f1 channel - power level for TOCSY (high sel.)
1282 ;sp13: f1 channel - shaped pulse 180 degree (adiabatic)
1283 ;sp23: f1 channel - shaped pulse 90 degree (on resonance)
1284 ;sp24: f1 channel - shaped pulse 180 degree (on resonance)
1285 ;sp25: f1 channel - shaped pulse 90 degree (on resonance)
1286 ;
1287 ;sp26: f1 channel - shaped pulse 180 degree (Ca off resonance)
1288 ;sp27: f1 channel - shaped pulse 180 degree (C=O off resonance)
1289 ;sp28: f1 channel - shaped pulse 180 degree (Ca on resonance)
1290 ;
1291 ;sp46: f3 channel - shaped pulse 180 degree (N, selective for Pro)
1292 ;p3 : f2 channel - 90 degree high power pulse
1293 ;p4 : f2 channel - 180 degree high power pulse
1294 ;p8 : f2 channel - 180 degree shaped pulse for inversion (adiabatic)
1295 ;p11: f1 channel - 90 degree shaped pulse
1296 ;p12: f1 channel - 180 degree shaped pulse
1297 ;p14: f1 channel - 180 degree low power pulse at p120
1298 ;p16: homospoil/gradient pulse [1 msec]
1299 ;p21: f3 channel - 90 degree high power pulse
1300 ;p22: f3 channel - 180 degree high power pulse
1301 ;p25: f1 channel - 180 degree shaped pulse (Ca, sp28)
1302 ;p59: f3 channel - 180 degree shaped pulse (N, selective for Pro)
1303 ;d0 : incremented delay (F1 in 3D): = d22
1304 ;d1 : relaxation delay; 1-5 * T1
1305 ;d3 : 1/(6J(HCa)) [1.1 msec]

```

```

1306 ;d4 : 1/(4J(HCa)) [1.8 msec]
1307 ;d9 : TOCSY mixing time
1308 ;d10: incremented delay (F2 in 3D) [3 usec]
1309 ;d11: delay for disk I/O [30 msec]
1310 ;d12: delay for power switching [20 usec]
1311 ;d16: delay for homospoil/gradient recovery
1312 ;d20: decremented delay (F1 in 3D): = d22+d28-4u
1313 ;d21: delay for MOCCA sequence [300 usec]
1314 ;d22: 1/(4J(COCa)) [4.5 msec]
1315 ;d23: 1/(4J(NCO)) [15.0 msec]
1316 ;d28: incremented delay (F1 in 3D) [3 usec]
1317 ;d31: total mixing time as executed
1318 ;cnst21: CO chemical shift (offset, in ppm)
1319 ;cnst22: Calpha chemical shift (offset, in ppm)
1320 ;olp: CO chemical shift (cnst21)
1321 ;l0: flag to switch between inphase and antiphase
1322 ;l1: loop for MOCCA-XY16 cycle: ((TAU*2+p14)*16 * l1) = mixing time
1323 ;inf1: 1/SW(CO) = 2 * DW(CO)
1324 ;inf2: 1/SW(N) = 2 * DW(N)
1325 ;in0: 1/(2 * SW(CO)) = DW(CO)
1326 ;nd0: 2
1327 ;in10: 1/(2 * SW(N)) = DW(N)
1328 ;nd10: 2
1329 ;in20: = k * in0
1330 ;in28: = (1 - k) * in0
1331 ;ns: 8 * n
1332 ;ds: >= 32
1333 ;td1: number of experiments in F1
1334 ;td2: number of experiments in F2
1335 ;FnMODE: States-TPPI (or TPPI) in F1
1336 ;FnMODE: States-TPPI (or TPPI) in F2
1337 ;cpd2: decoupling according to sequence defined by cpdprg2
1338 ;cpd3: decoupling according to sequence defined by cpdprg3
1339 ;pcpd2: f2 channel - 90 degree pulse for decoupling sequence
1340 ;pcpd3: f3 channel - 90 degree pulse for decoupling sequence
1341
1342 ;for z-only gradients:
1343 ;gpz1: 80%
1344 ;gpz2: 70%
1345 ;gpz3: 30%
1346 ;gpz4: 50%
1347
1348 ;use gradient files:
1349 ;gpnam1: SMSQ10.100
1350 ;gpnam2: SMSQ10.100
1351 ;gpnam3: SMSQ10.100
1352 ;gpnam4: SMSQ10.100
1353
1354 ;use AU-program splitcomb [ipap 2] to process data
1355
1356 ;$Id: $

```