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1: ;hnngp3d
2: ;avance-version
3: ;3D HNN (800 MHz)
4: ;o2p = 56.0 ppm
5: ;Panchal et al J Biomol NMR 20, 135, 2001
6: ;Chugh J et al J Biomol NMR 40(2), 145-52, 2008
7: ;1) exclude Rance-Kay trick
8: ;2) use maximum resolution for t2 including also period k
9: ;3) water flip back and final watergate for water suppression
10:
11: ;sequence checkd and corrected by DMO
12:
13: ;edited by jc and dkg at 800 MHz
14:
15: ;$OWNER=guest
16: prosol relations =<triple>
17:
18: #include <Avance.incl>
19: #include <Grad.incl>
20:
21:
22:
23: ;##### constant values #####
24: "d2=2.25m"
25: ;"d4=2.7m-p2-3u-4u-p16-d16"
26: "d5=2.7m-p11-3u-4u-p16-d16" ;added DMO
27: "d6=5.4m" ;k
28: ;"d7=14m" ;Tn
29: "d11=30m"
30: "d14=p14"
31: ;"d15=12.5m" ;Tcn=12-17m
32: "d16=100u"
33:
34: ;##### center pulses #####
35: "d3=p21-p1"
36: "d8=(p14-p21*2)*0.5"
37:
38: ;##### incremented time t1 #####
39: "d0=3u" ;t1/2
40: "d9=d0+d14+d7+d8" ;t1/2 NOTE that d9<=d8+3u
41:
42: ;##### incremented time t2 #####
43: "d20=d9-d8" ;t2/2 decreased d20
44: ;d7=d9= 15ms = Tn
45: "d10=3u" ;t2/2 increased
46: "d21=d10+d9+d8+d7-d6-p1-p21*2-24u"
47:
48: "in9=in0"
49: "in20=in10"
50:
51: "spoff2=0"
52: "spoff3=0"
53: "spoff4=0"
54: "spoff5=bf2*(cnst21/1000000)-o2"
55: ;"spoff20=bf2*(cnst24/1000000)-o2" ;cnst24=64
56: aqseq 312
57:
58:
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59: 1 ze
60: d11 pl13:f3
61: 2 d11 pl13:f3
62: d1 pl1:f1
63: 20u pl2:f2
64: 50u UNBLKGRAD
65: (p1 ph0)
66: d2 pl3:f3
67: (d3 p1*2 ph0) (p21*2 ph0):f3
68: d2
69: (p1 ph9):f1
70: 3u
71: 20u pl11:f1
72: (p11:sp1 ph7:r):f1
73: 3u
74: p16:gp1
75: d16 pl1:f1
76: (p21 ph1):f3
77:
78: ;##### Start t1 d0=A ; d7=15m=B ; d9=C=15m-3u ; d6=5.4m=k #####
79:
80: (d6 p1 ph9 20u pl19 4u cpds1):f1 (d0 p14:sp5 ph0 d7 p14:sp3 ph0):f2 (d0 d14 d7 d8
p21*2 ph0 d9):f3
81:
82: ;##### end t1 #####
83:
84: (p21 ph2):f3
85: 4u do:f1
86: 20u pl1:f1
87: (p1 ph10):f1
88: 4u
89: p16:gp2
90: d16
91: (p1 ph9):f1
92: 3u
93: 20u pl19:f1
94: 4u cpds1:f1
95: (p13:sp2 ph2):f2
96: d15 ;Tcn = 12-16 ms
97: (d8 p21*2 ph0):f3 (p34:sp20 ph0):f2
98: d15 ;Tcn = 12-16 ms
99: (p13:sp4 ph0):f2
100: 4u do:f1
101: 20u pl1:f1
102: (p1 ph10):f1
103: 4u
104: p16:gp3
105: d16
106: (p1 ph9):f1
107: 3u
108: 20u pl19:f1
109: 4u cpds1:f1
110: (p21 ph8):f3
111: 5u
112:
113: ;##### Start t2 d10=F ; d20=D=15m-3u ; d7=E=15m ; d6=5.4m=k #####
114:
115: (d21 4u do 20u pl1 p1 ph10):f1 (d20 p14:sp3 ph0 d7 p14:sp5 ph0):f2 (d20 d8 p21*2
ph0 d7 d14 d8 d10):f3
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116:
117: ;##### end t2 #####
118:
119: (p21 ph0):f3
120: 4u
121: p16:gp5
122: d16
123: (p11:sp1 ph3:r):f1
124: 10u
125: 20u p11:f1
126: (p1 ph0):f1
127: 3u
128: p16:gp4
129: d16
130: 4u
131: d5 p111:f1 ;d4 substituted by d5 DMO
132: ;p11 ph4:r ;p2 substituted by p11 DMO
133: (p11:sp1 ph4:r):f1
134: 3u
135: 20u p11:f1
136: (d3 p1*2 ph5) (p21*2 ph0):f3
137: 3u
138: 20u p111:f1
139: ; p11 ph4:r
140: (p11:sp1 ph4:r):f1
141: 3u
142: d5 ;d4 substituted by d5 DMO
143: p16:gp4
144: d16 p116:f3
145: 4u BLKGRAD
146: go=2 ph31 cpd3:f3
147: d11 do:f3 mc #0 to 2
148: F1PH(ip1, id0 & dd9)
149: F2PH(rd0 & rd9 & ip8, id10 & dd20)
150: exit
151:
152: ph0=0
153: ph1=0 0 2 2
154: ph2=0 2
155: ph3=2
156: ph4=0
157: ph5=2
158: ph7=0
159: ph8=0 0 0 0 2 2 2 2
160: ph9=1
161: ph10=3
162: ph31=0 0 2 2 2 2 0 0
163:
164:
165: ;p34: 200-400-600us, f2 180 degree 13C shape
166: ;sp20: f2 power 180 (CA)
167: ;spnam20: Q3 gauss works fine
168: ;spoffs20: 56ppm for HNN and HNN-Ala and 64ppm for HNN-ST
169: ;d1: relaxation delay; 1-5*T1
170: ;d11: delay for disk I/O [30 msec]
171: ;p11: f1 power H high power pulse
172: ;p1: f1 90 degree high power p11 pulse
173: ;d2: 2.25-2.75m (Jhn=92Hz)
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174: ;d3: p21-p1 (center pulse)
175: ;pl2: f2 power C13 hard pulse (not used)
176: ;pl3: f3 power N15 hard pulse
177: ;p21: f3 90 degree high power N15 high power pl3 pulse
178: ;pl11: f1 power H2O soft rectangular pulse (1m)
179: ;pl1: f1 90 degree H2O low power pl11 rectangular pulse
180: ;pl3: 90 degree 13C shape
181: ;pl4: 180 degree 13C shape
182: ;gpz1: 30%
183: ;gpnam1: sine.100 shape of gradient pulse
184: ;sp5: f2 power 180 (CA) soft shaped
185: ;pl4: f2 soft shaped pulse 180 null at 18200 Hz
186: ;spnam5: use shape G3.256
187: ;spoff5: use offset 18200.0 Hz (600 MHz) on CO, null CA
188: ;spnam3: use shape G3.256
189: ;spoff3: use offset 0.0 Hz (600 MHz) on CA, null CO
190: ;d6: 5.4m (k in sequence)
191: ;pl19: f1 power for cpds1 decoupling
192: ;cpd1: dipsi2 (along x)
193: ;pcpd3: f1 cpds1 pulse length (60-70u) use 65u
194: ;d0: t1/2
195: ;d7: Tn [12-16m] use 15m
196: ;d9: d0+d14+d7+d8 (Tn-t1/2) SET ALWAYS d9<=d8+3u
197: ;gpz2: 30 % power level
198: ;gpnam2: sine.100 shape of gradient pulse
199: ;sp2: f2 power 90 (CA) soft shaped
200: ;spnam2: use shape G4.256
201: ;spoff2: use offset 0.0 on CA, null CO
202: ;sp4: f2 power 90 (CA) soft shaped
203: ;spnam4: use shape G4.256tr (time reverse shape)
204: ;spoff4: use offset 0.0 on CA, null CO
205: ;d15: [12-18m] Tcn, use 16m
206: ;gpz3: 30%
207: ;gpnam3: sine.100 shape of gradient pulse
208: ;d20: t2/2 (Tn-t2/2) [d9-d8]
209: ;d10: t2/2
210: ;spl: f1 power H2O soft shaped pulse
211: ;pl1: (2m) half-gaussian soft pulse with power spl
212: ;spnam1: hg.1000 half gaussian shape
213: ;pl6: gradient pulse 1 ms
214: ;gpz4: 80 %
215: ;gpnam4: sine.100 shape of gradient pulse
216: ;d4: 2.7m-p2-3u-4u-pl6-d16
217: ;pl16: f3 power level N15 cpd decoupling
218: ;cpd3: cpdprg3 decoupling sequence [garp]
219: ;pcpd3: f3 decoupling 90 degree pulse [>170 u]
220: ;l1: td1/2 STATES/TPPI
221: ;l2: td2/2 STATES/TPPI
222: ;in0: 1/(2* SW(N15)) = DW(N15)
223: ;in9: SET ALWAYS in9=in0
224: ;nd0: 2
225: ;in10: 1/(2* SW(N15)) = DW(N15)
226: ;in20: SET ALWAYS in20=in10
227: ;nd10: 2
228: ;NS: 8*n
229: ;DS: 16
230: ;td1: number of experiments N15
231: ;td2: number of experiments N15
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232: ;MC2: STATES-TPPI
233: