



***PULSE PROGRAM
CATALOGUE:
II. BIOMOLECULAR
NMR EXPERIMENTS***

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***TOPSPIN v2.0
NMRGuide***



UAB

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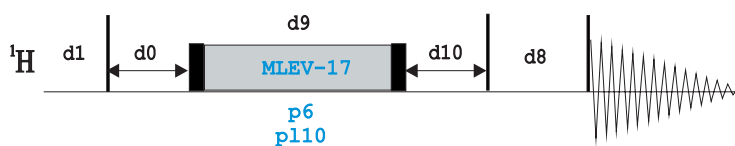
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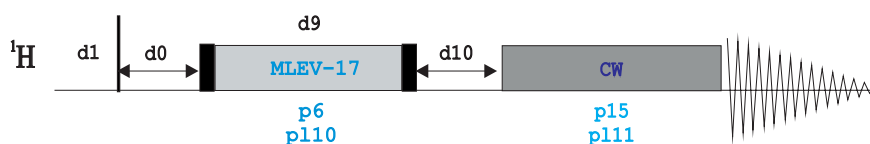
3D HOMONUCLEAR
EXPERIMENTS

3D TOCSY-NOESY experiment (**mlevnoesy3d**)
3D TOCSY-ROESY experiment (**mlevroesy3d**)
3D NOESY-TOCSY experiment (**noesymlev3d**)
3D NOESY-TOCSY experiment using presaturation (**noesymlevpr3d**)
3D NOESY-NOESY experiment using presaturation (**noesyoesypr3d**)

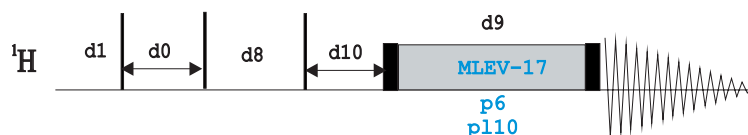
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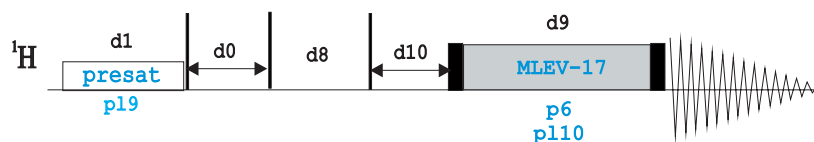
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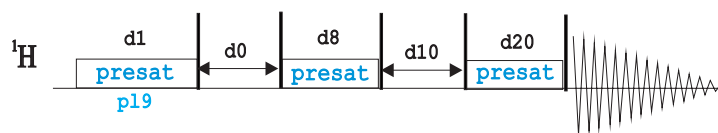
noesymlev3d



noesymlevpr3d



noesyoesypr3d



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3D PHASE-CYCLED
DOUBLE-RESONANCE
EXPERIMENTS

3D ^1H - ^{13}C TOCSY-HMQC experiment using presaturation (**mlevhmqcpr3d**)
 3D ^1H - ^{13}C NOESY-HMQC experiment using presaturation (**noesyhmqcpr3d**)
 3D ^1H - ^{13}C HMQC-TOCSY experiment using BIRD (**hmqcmlevbi3d**)
 3D ^1H - ^{13}C HMQC-NOESY experiment using BIRD (**hmqcnoesybi3d**)

Timing diagram for the 1H and X channels. The 1H channel shows a sequence of delays (d1, d2, d2, d7, d2, d2) followed by a block labeled 'MLEV-17_y' with delays d9 and d10. The X channel shows a sequence of delays (d0, d0) followed by a block labeled 'GARP'. The diagram is labeled 'p6 p110' and 'p112'.

^1H

d1
presat
p19

Δ

d0

d0

d9
MLEV-17
p6
p110

d2

X

d10

d10

GARP
p112

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3D HCCH-COSY
3D HCCH-TOCSY

- **HCCH-COSY**

ge-3D HC(C)H-COSY experiment (**hcchcogp3d** | HCCHCOGP3D)

- **HCCH-TOCSY**

ge-3D HC(C)H-TOCSY experiment (**hcchdigp3d** | HCCHDIGP3D)

ge-3D (H)CCH-TOCSY experiment (**hcchdigp3d2** | HCCHDIGP3D2)

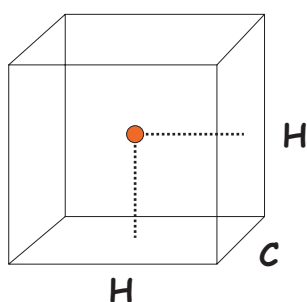
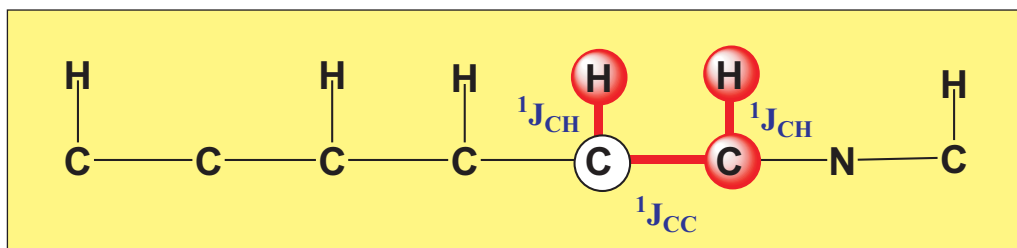
ge-3D HC(C)H-TOCSY using adiabatic TOCSY experiment (**hcchatgp3d** | HCCHATGP3D)

- **ge-2D Long-range HCCH correlation**

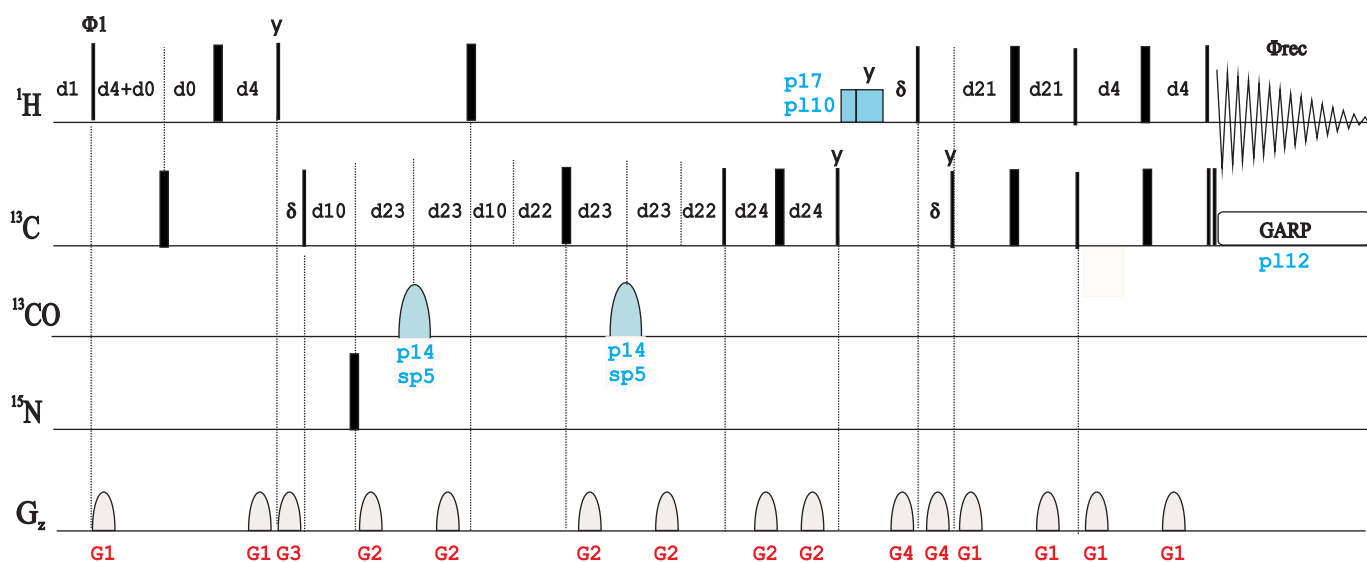
Phase-sensitive ge-2D Long-range HCCH using echo-antiecho (**hcchetgplr**)

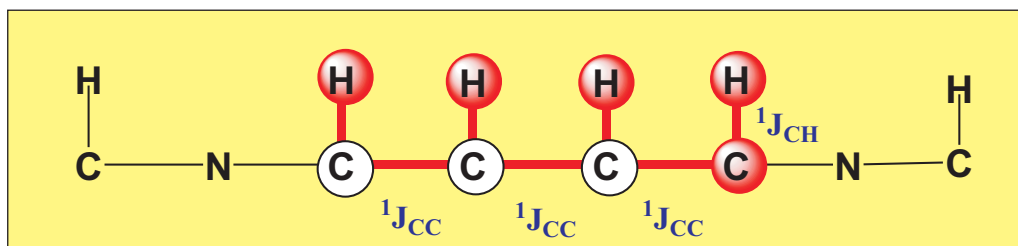
Also see:

- 2D ADEQUATE
- HCCH-type experiments in Nucleic Acids

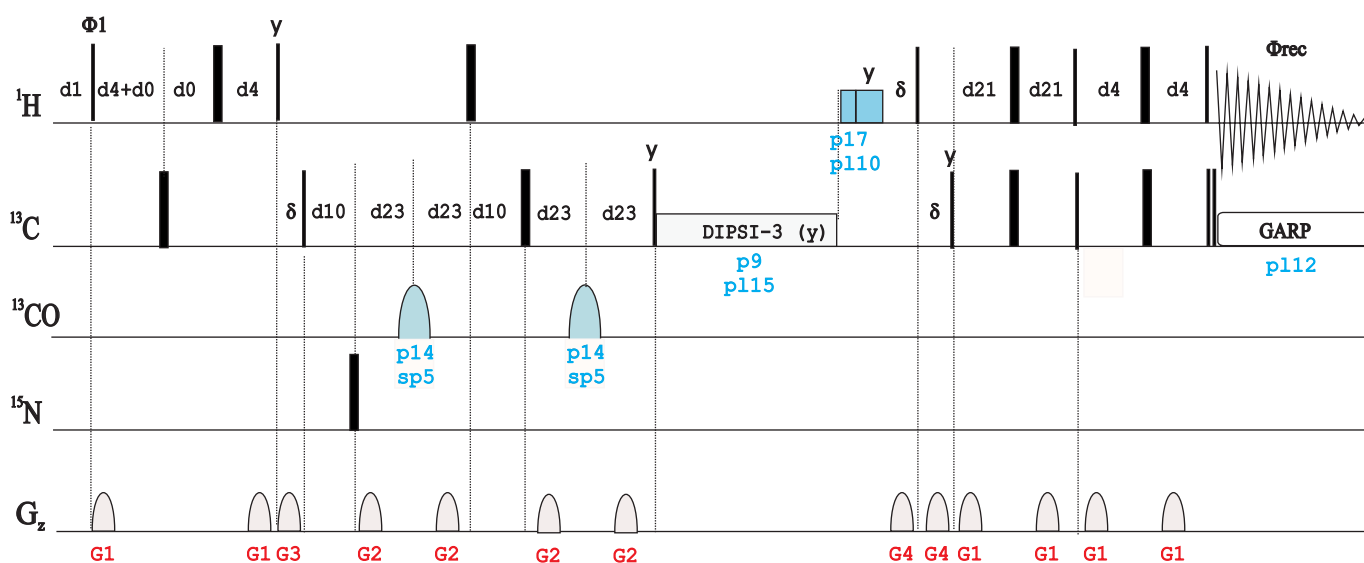


hcchcogp3d

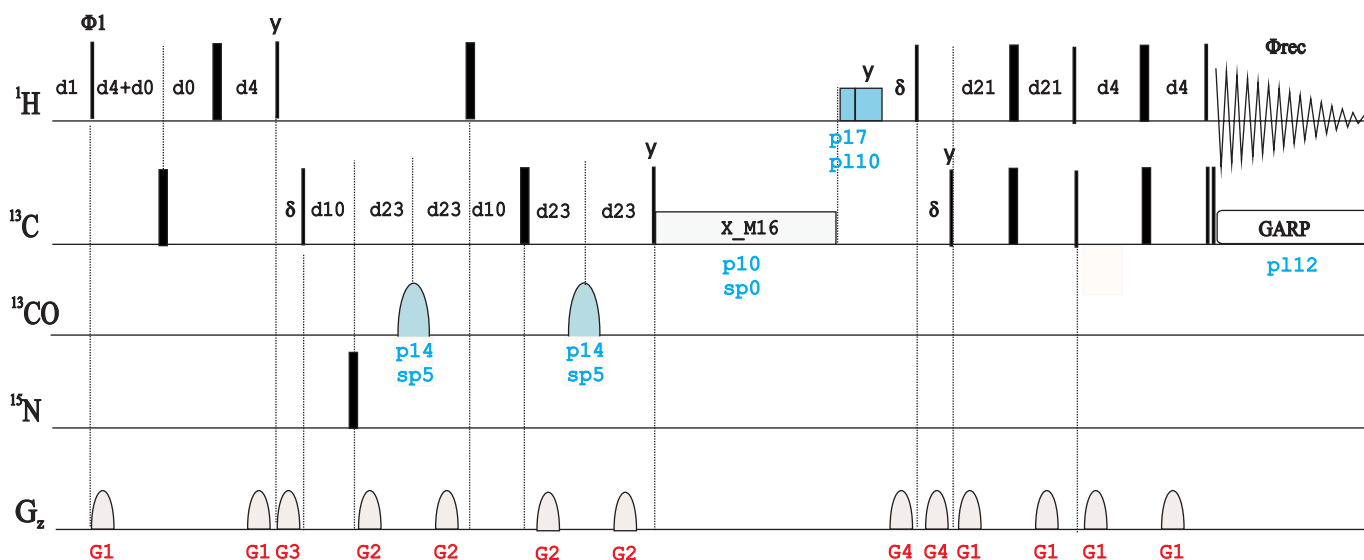


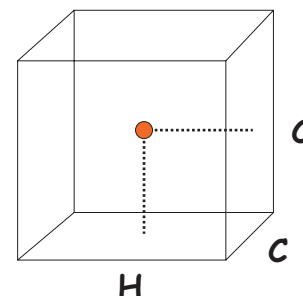
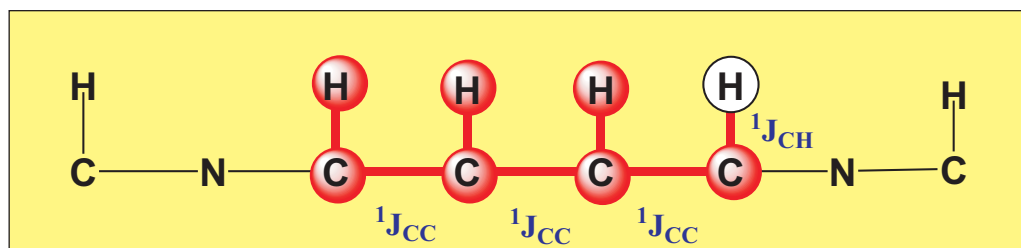


hcchdlgp3d

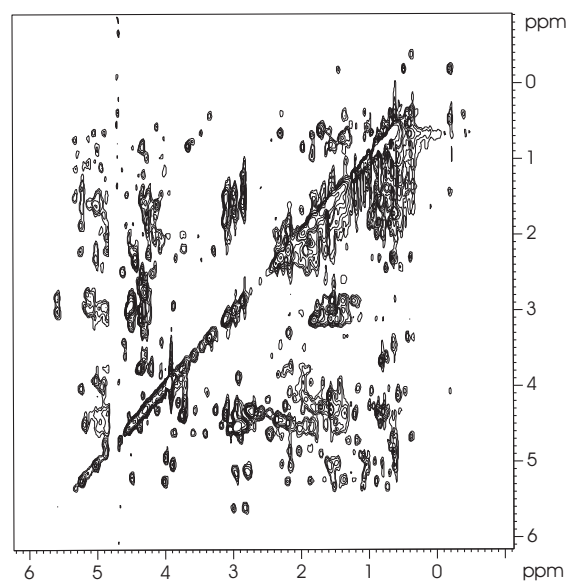
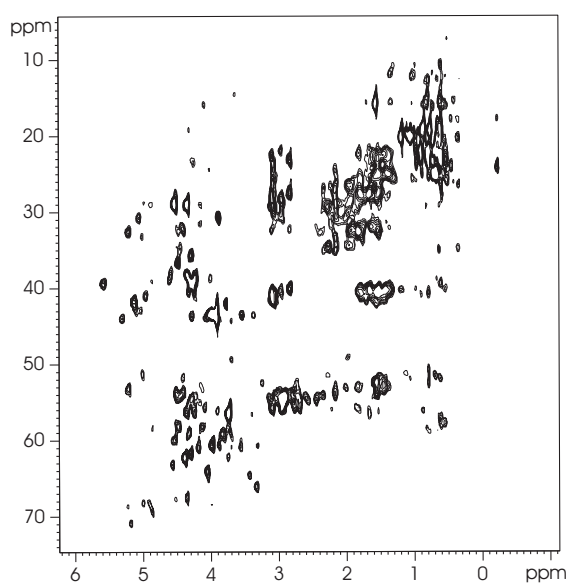
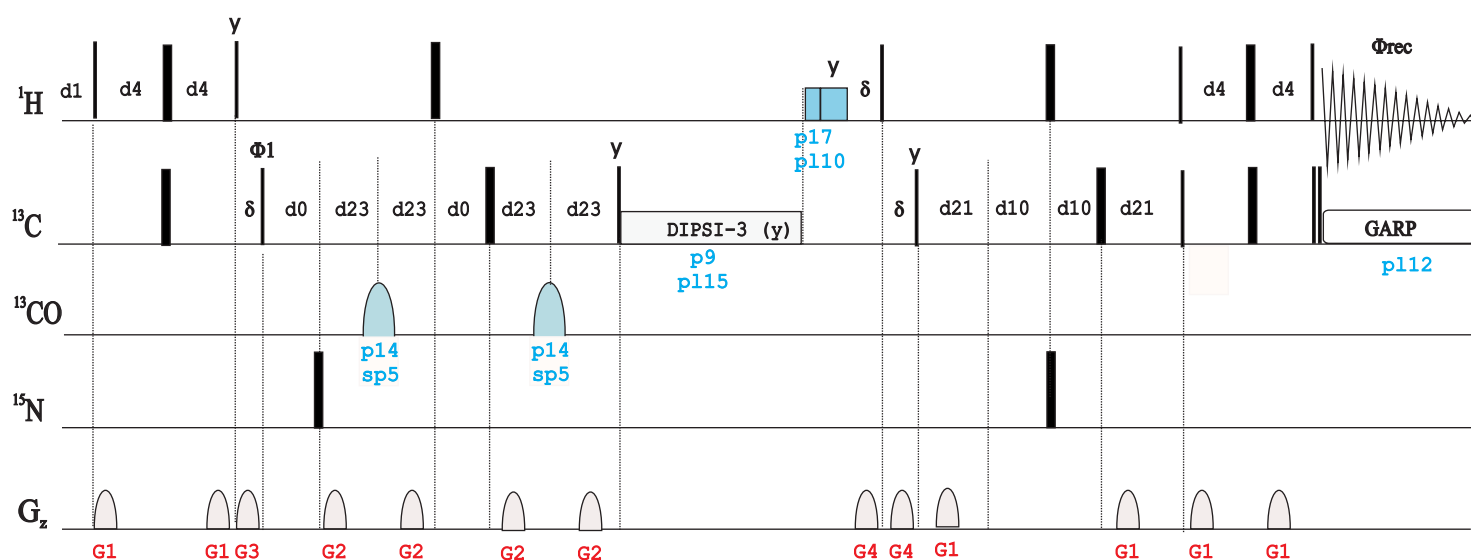


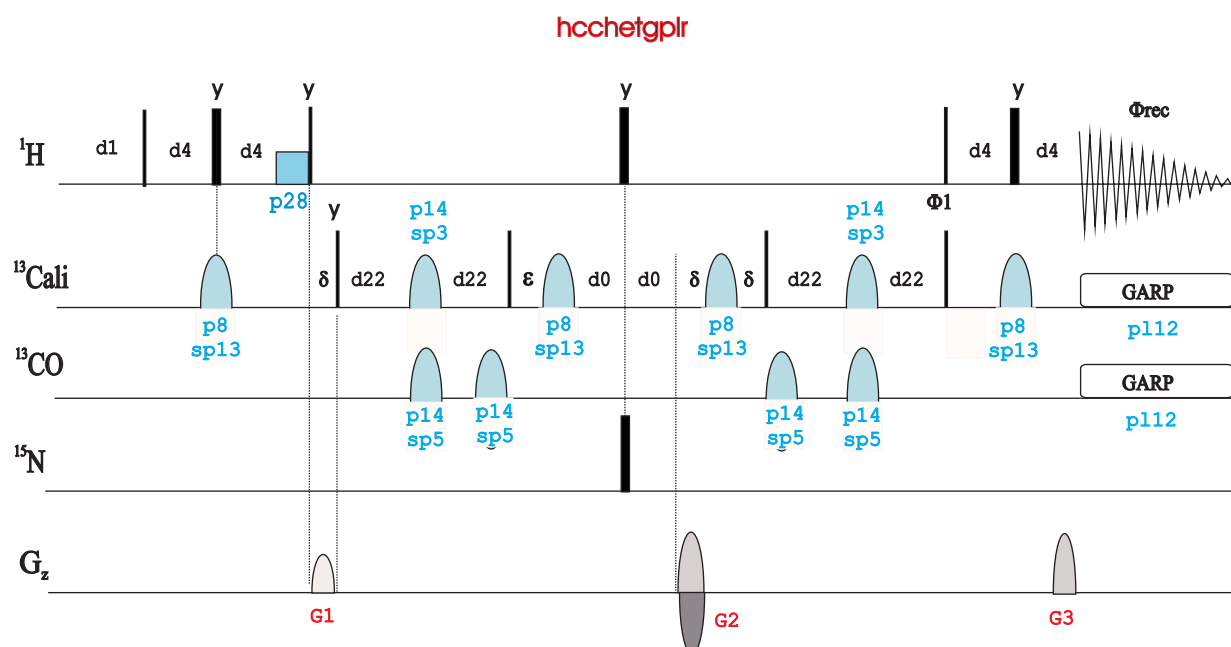
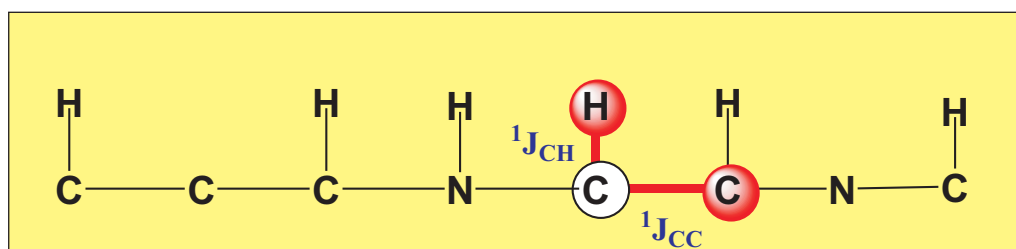
hcchatgp3d





hcchdipg3d2





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3D TOCSY-HSQC
EXPERIMENT

- **Gradient-enhanced from f2 channel:**

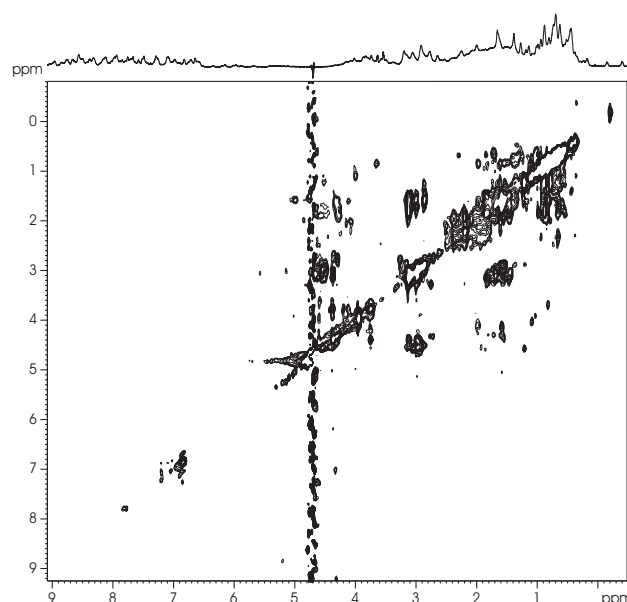
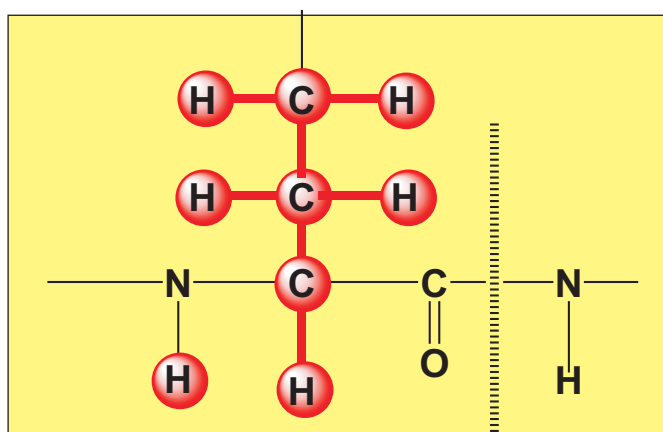
ge-3D ^1H - ^{13}C TOCSY-HSQC experiment using echo-antiecho (**mlevhsqcetgp3d** | MLEVHSQCETGP3D)

- **Gradient-enhanced from f3 channel:**

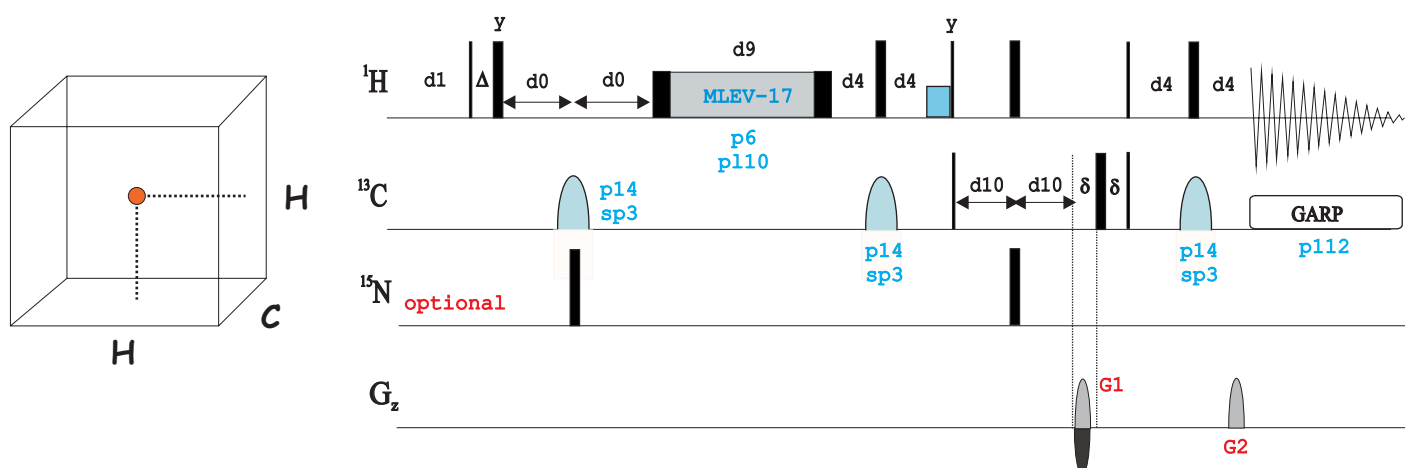
ge-3D ^1H - ^{15}N TOCSY-HSQC with MLEV using echo-antiecho (**mlevhsqcetf3gp3d** | MLEVHSQCETf3GP3D)

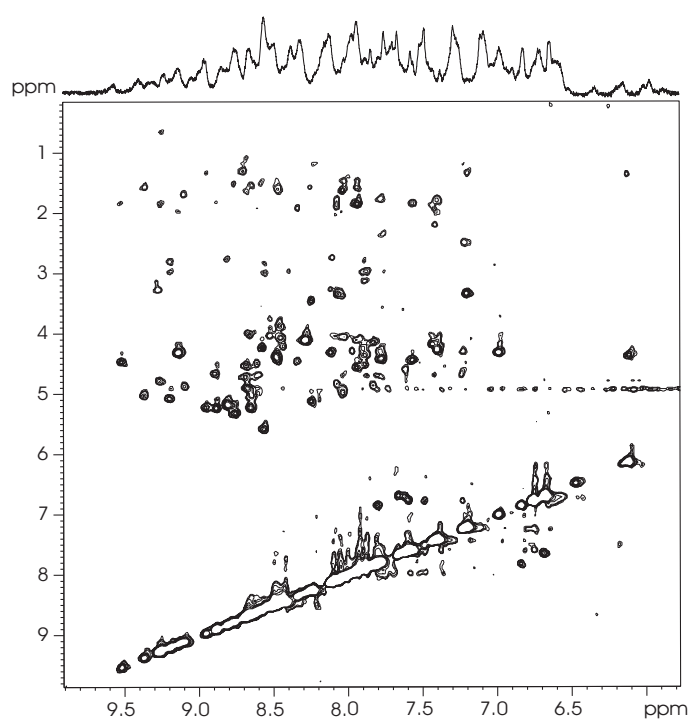
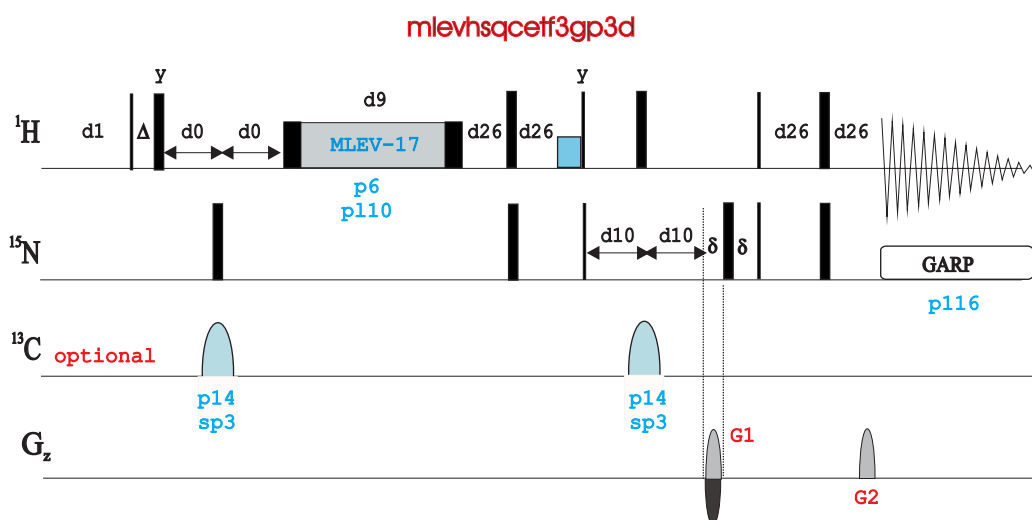
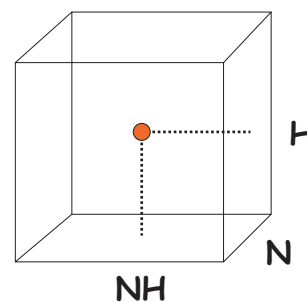
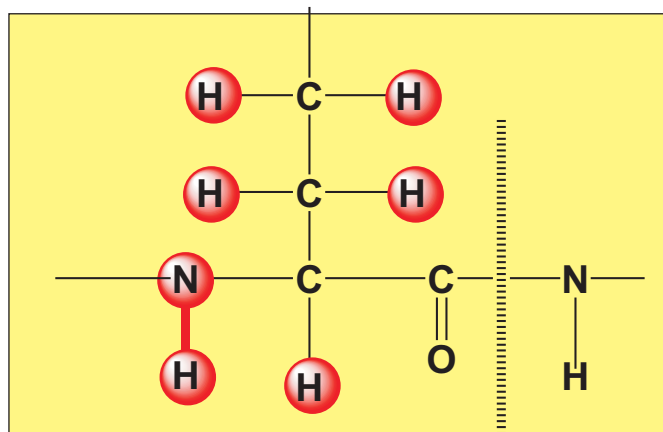
ge-3D ^1H - ^{15}N TOCSY-HSQC with DIPSI-2 and PEP (**dipsihsqcf3gpsi3d** | DIPSIHSQCF3GPSI3D)

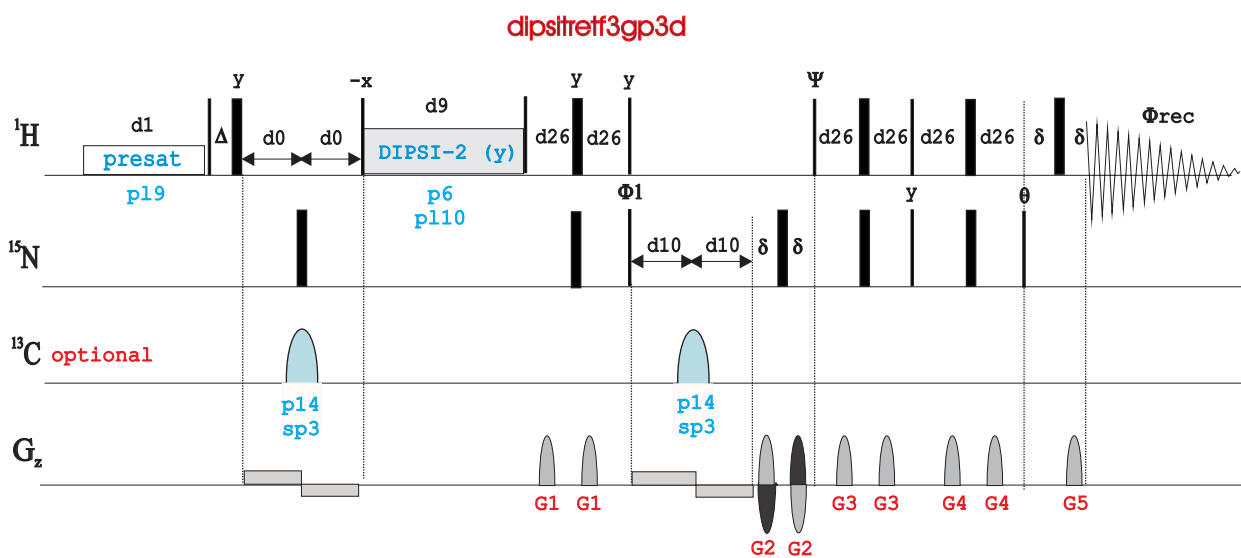
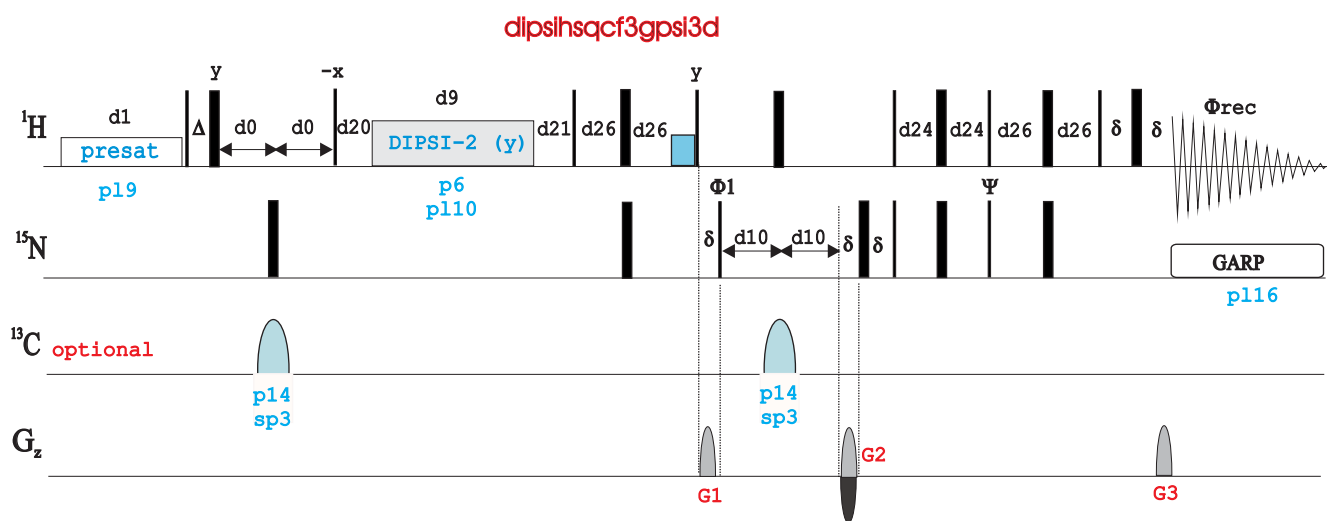
ge-3D ^1H - ^{15}N TOCSY-HSQC with DIPSI-2 using TROSY (**dipsitretf3gp3d** | DIPSIRETf3GP3D)



mlevhsqcetgp3d







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2D $^{13}\text{C}/^{15}\text{N}$ -FILTERED/EDITED
TOCSY EXPERIMENTS

2D X-filtered/edited TOCSY

ge-2D w_1 - ^{13}C , ^{15}N -filtered/edited TOCSY experiment

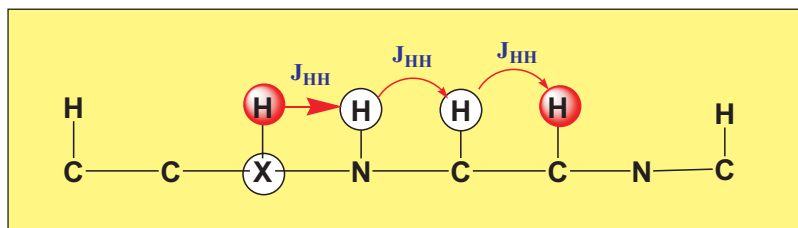
ge-2D w_1 - ^{13}C , ^{15}N -filtered/edited TOCSY using DIPSI2 and WATERGATE
(**dipsi2gp phwgx1**)

ge-2D w_2 - ^{13}C , ^{15}N -filtered/edited NOESY experiment

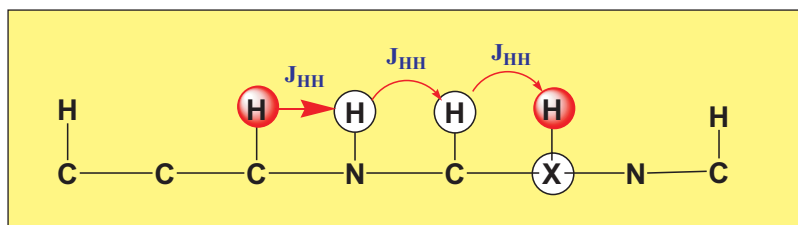
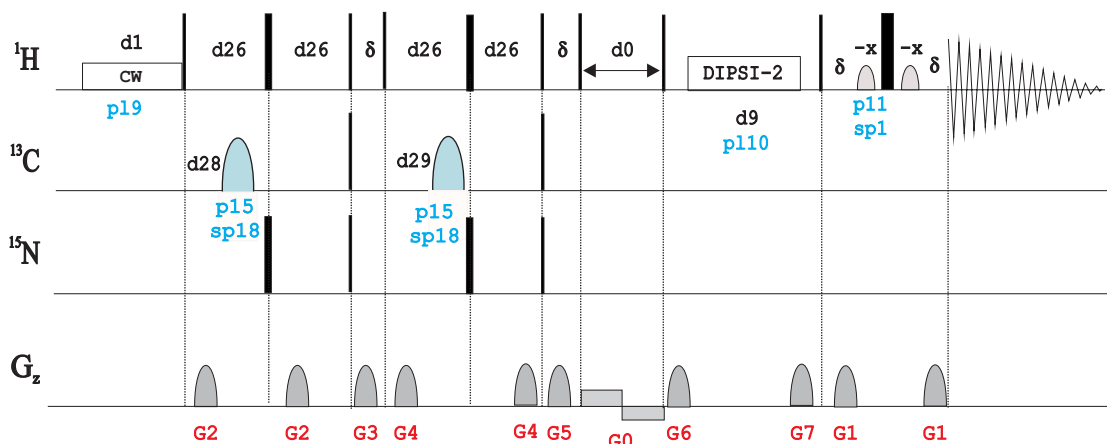
ge-2D w_2 - ^{13}C , ^{15}N -filtered/edited TOCSY using DIPSI2 and WATERGATE
(**dipsi2gp phwgx2**)

ge-2D w_1, w_2 - ^{13}C , ^{15}N -filtered/edited NOESY experiment

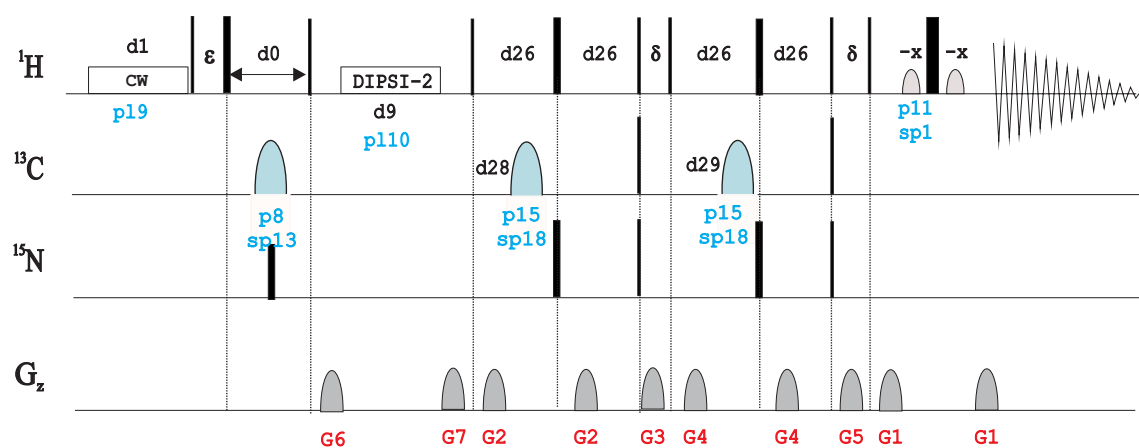
Phase-sensitive ge-2D w_1, w_2 ^{13}C , ^{15}N -filtered/edited TOCSY using DIPSI2 and
WATERGATE (selective pulses) (**dipsi2gp phwgxf**)

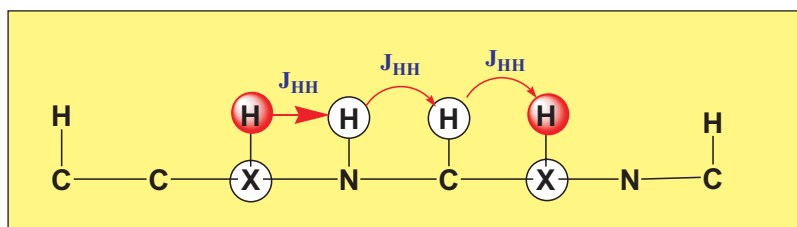


d1psi2gp phwgx1

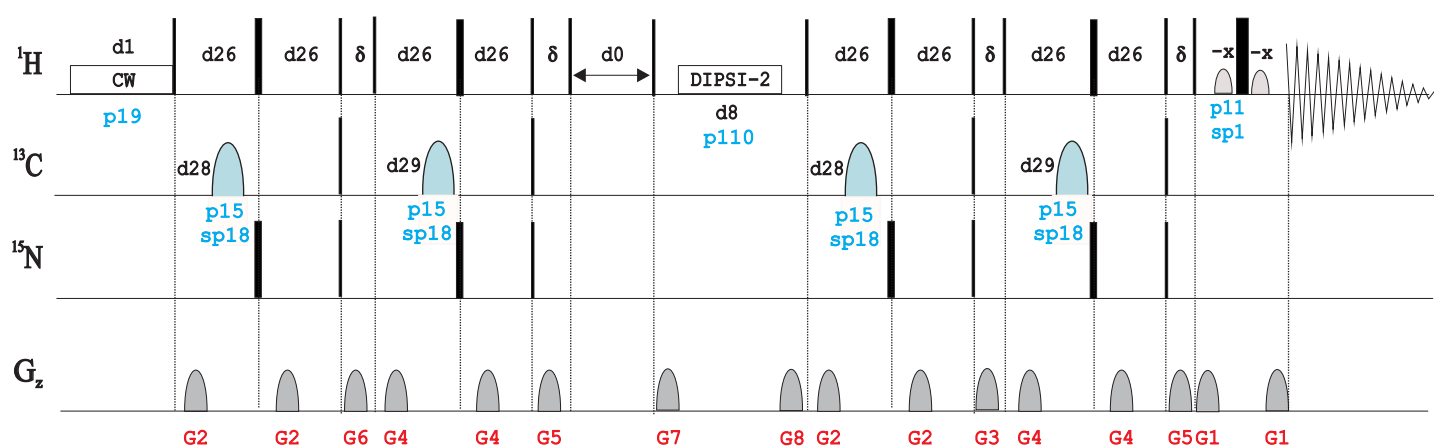


d1psi2gp phwgx2





dipsl2gpplhwgxf



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3D NOESY-HSQC
EXPERIMENTS

3D NOESY-HSQC

- **Gradient-enhanced from f2 channel:**

3D ^1H - ^{13}C NOESY-HSQC experiment

using echo-antiecho (**noesyhsqcetgp3d** | NOESYHSQCETGP3D)

using PEP (**noesyhsqcetgps3d** | NOESYHSQCETGPS3D)

- **Gradient-enhanced from f3 channel:**

- 3D ^1H - ^{15}N NOESY-HSQC experiment

- using echo-antiecho (**noesyhsqcetf3gp3d** | NOESYHSQCETF3GP3D)

- using PEP (**noesyhsqcf3gps3d** | NOESYHSQCF3GPS3D)

- using PEP and water flip-back (**noesyhsqcfpf3gps3d** | NOESYHSQCFF3GPS3D)

- using WATERGATE (**noesyhsqcf3gp193d** | NOESYHSQCF3GP193D)

- using TROSY (**noesytretf3gp3d** | NOESYTRETF3GP3D)

- using ZQ-TROSY (**noesytzgp3d** | NOESYTZGP3D)

- **Gradient-enhanced from f2 and f3 channel:**

3D NOESY- ^{13}C , ^{15}N -HSQC experiment

with simultaneous evolution (**noesyhsqcgpsm3d.2** | NOESYHSQCGPSM3D.2)

with simultaneous evolution, sensitivity improvement and adiabatic ^{13}C pulses

(**noesyhsqcgpsism3d** | NOESYHSQCGPSISM3D)

with simultaneous evolution and editing between labeled-unlabeled part

(**noesyhsqcedgpsm3d** | NOESYHSQCEDGPSM3D)

with simultaneous evolution, sensitivity improvement and editing between labeled-

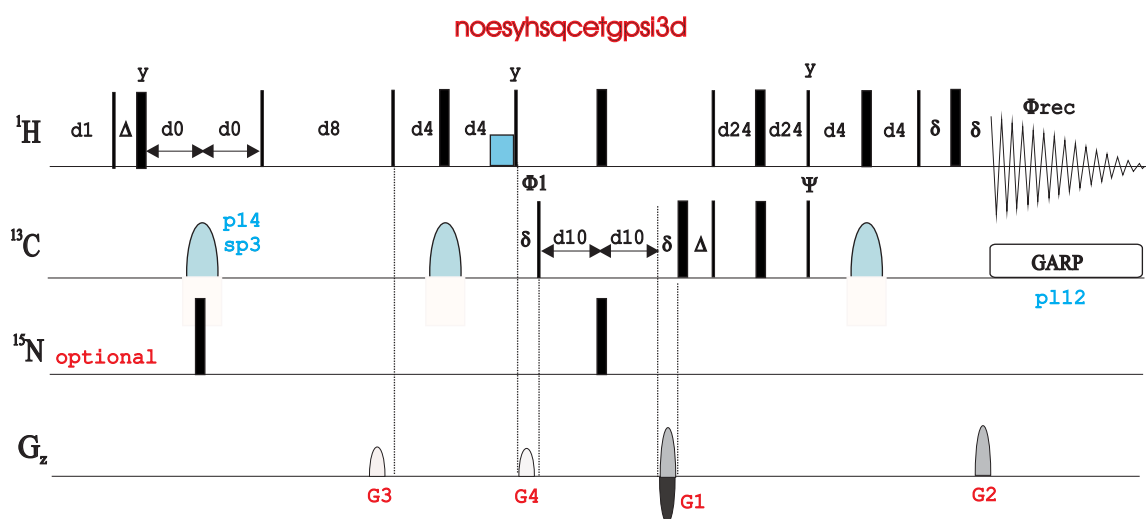
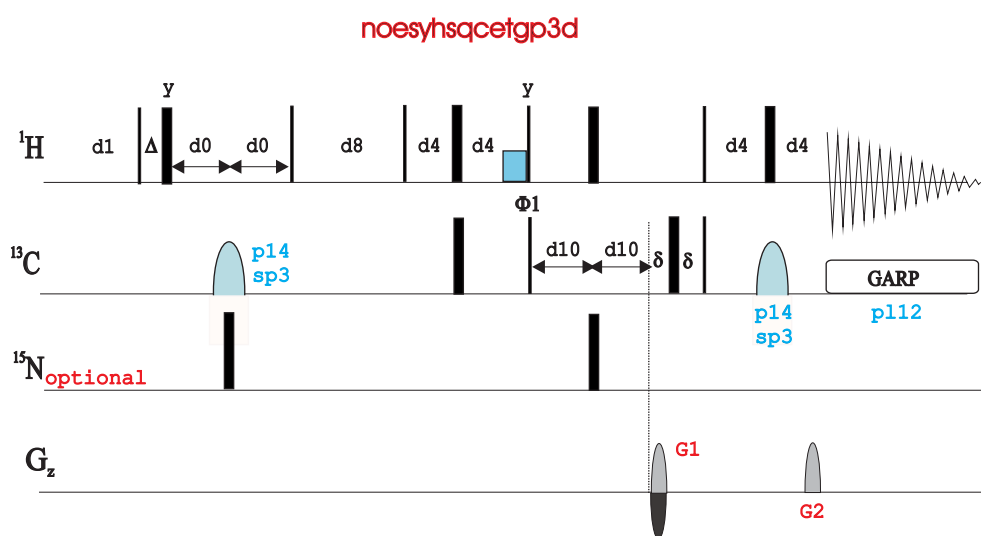
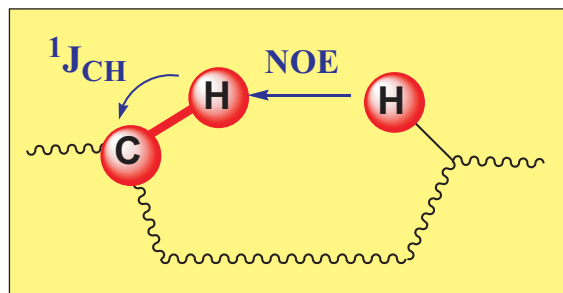
unlabeled part (**noesyhsqcedgpsism3d** | NOESYHSQCEDGPSISM3D)

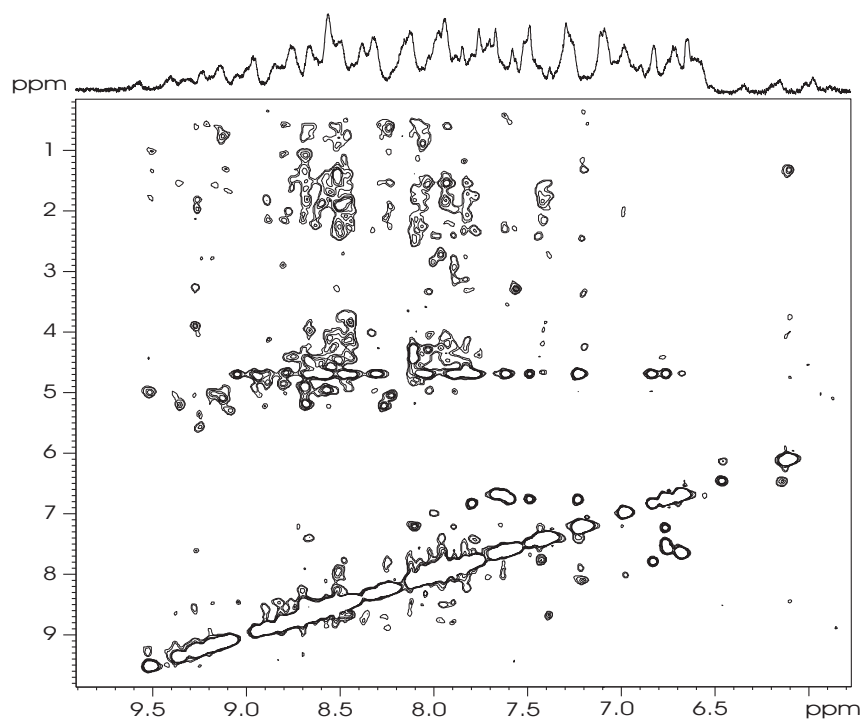
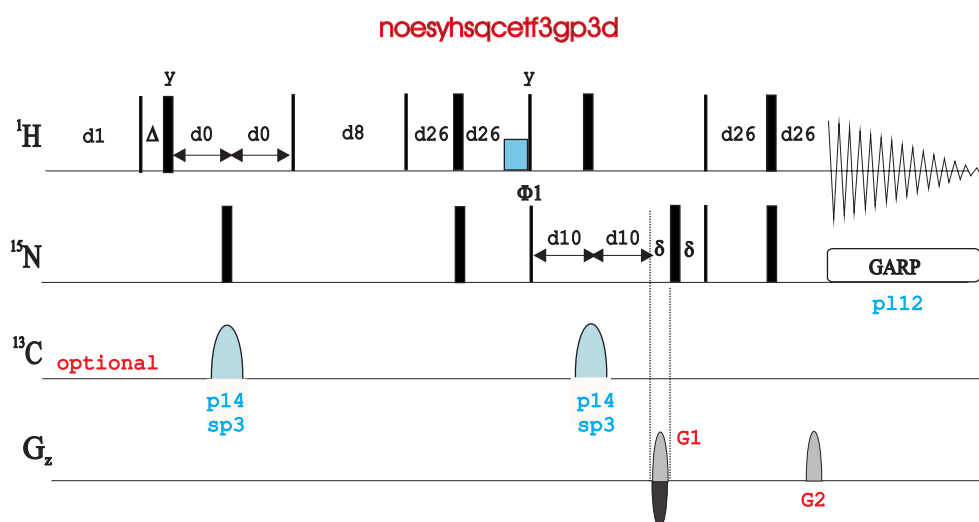
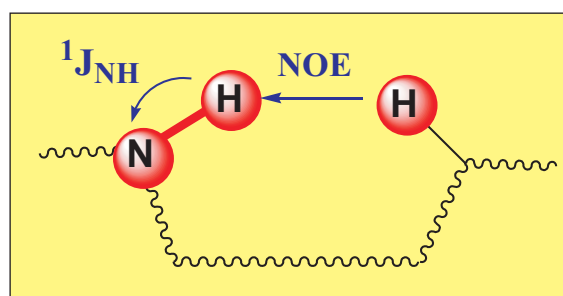
Related Experiments:

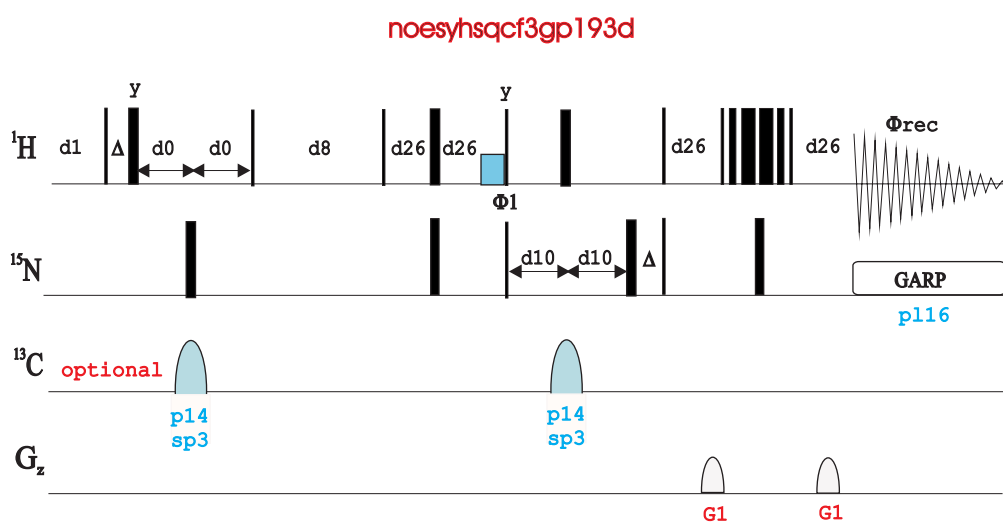
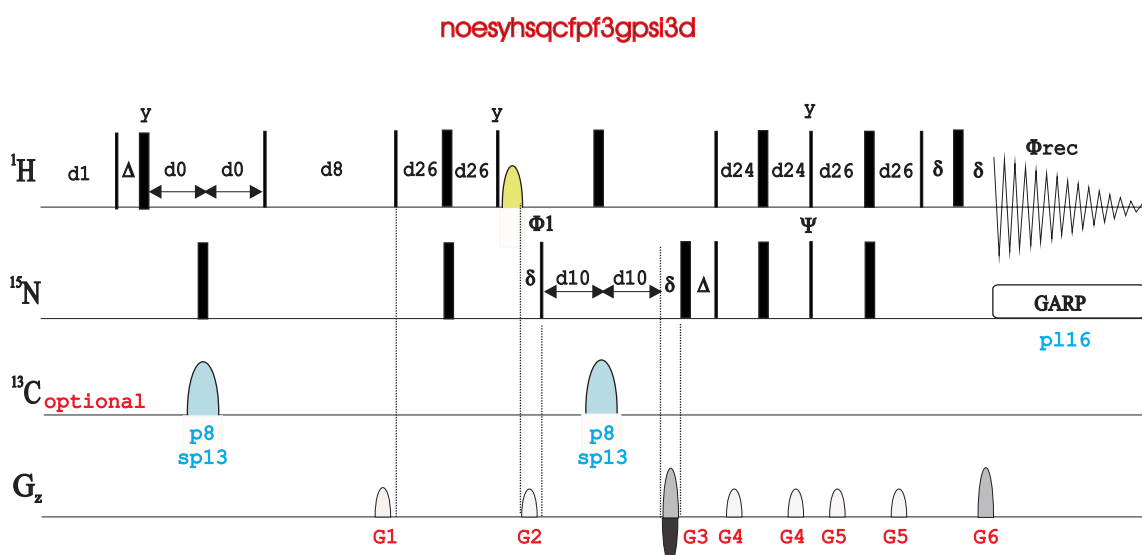
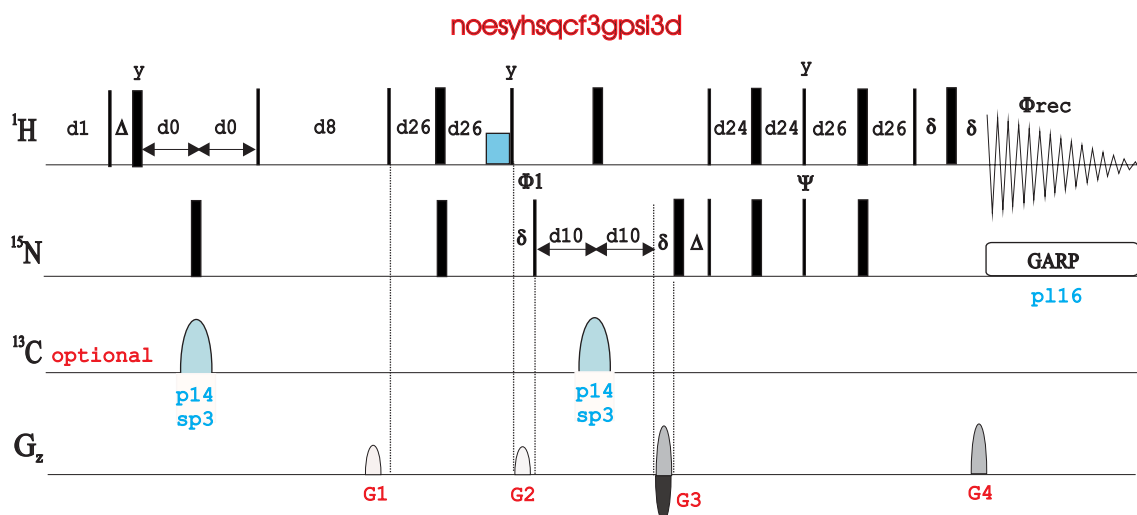
2D NOESY

3D HSQC-NOESY-HSQC

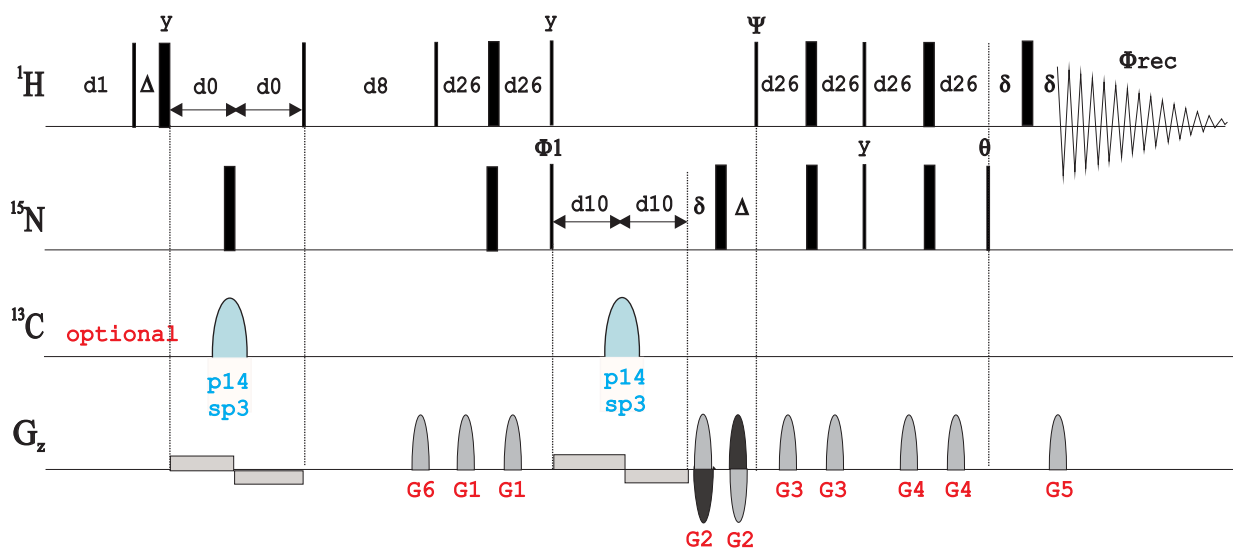
2D & 3D X-filtered/edited NOESY



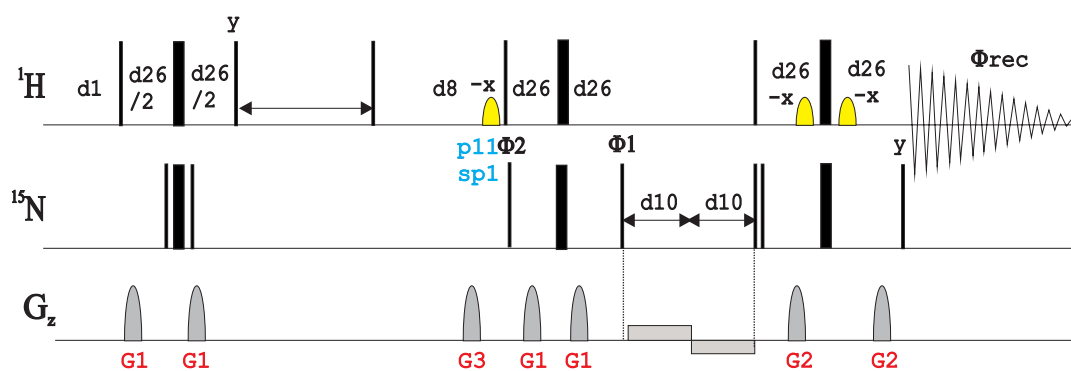


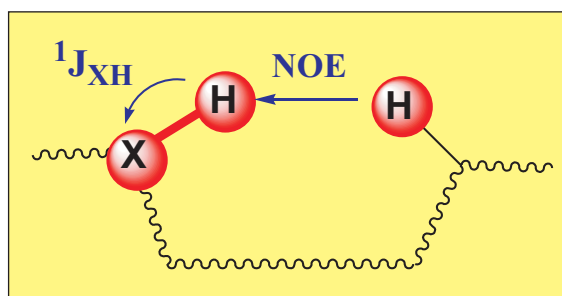


noesytreff3gp3d

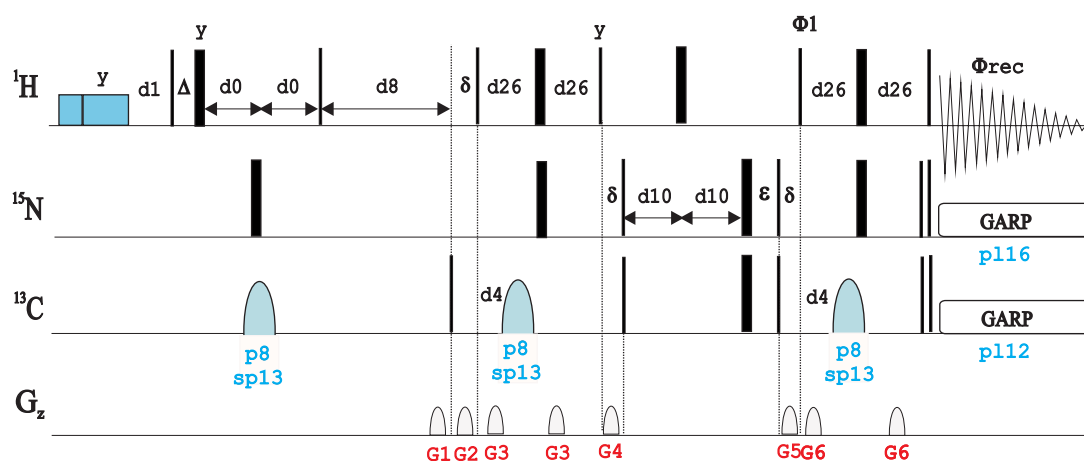


noesytzgp3d

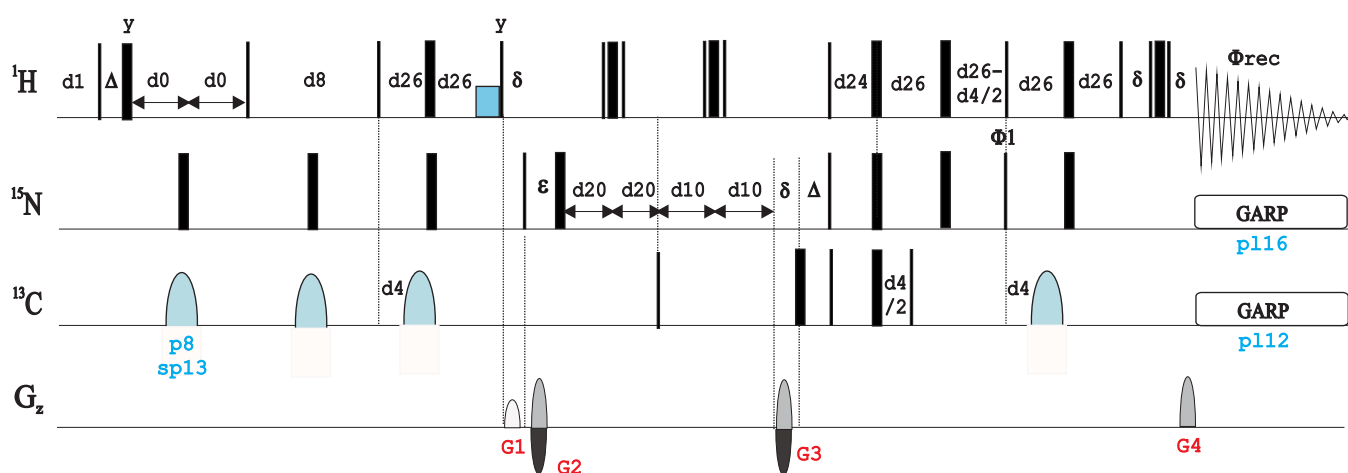




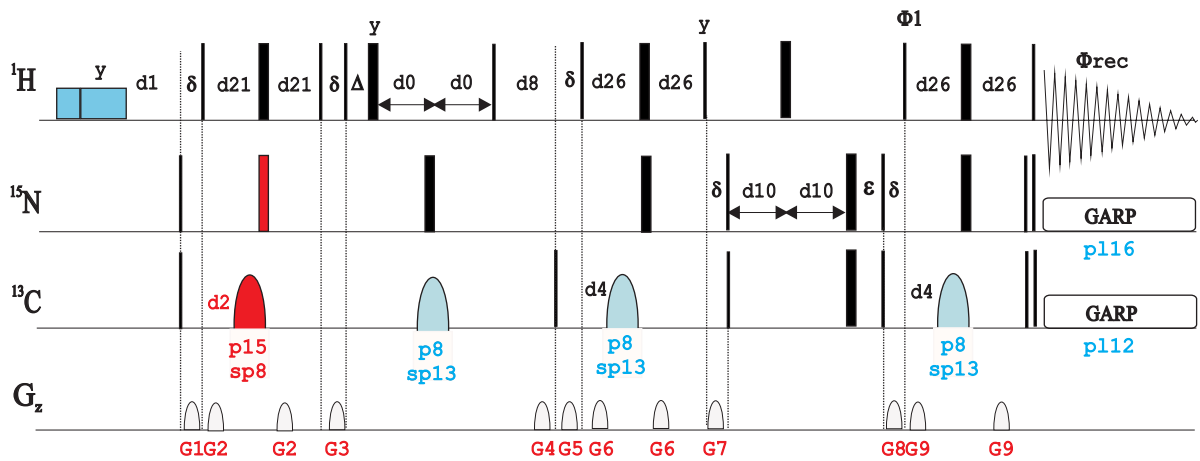
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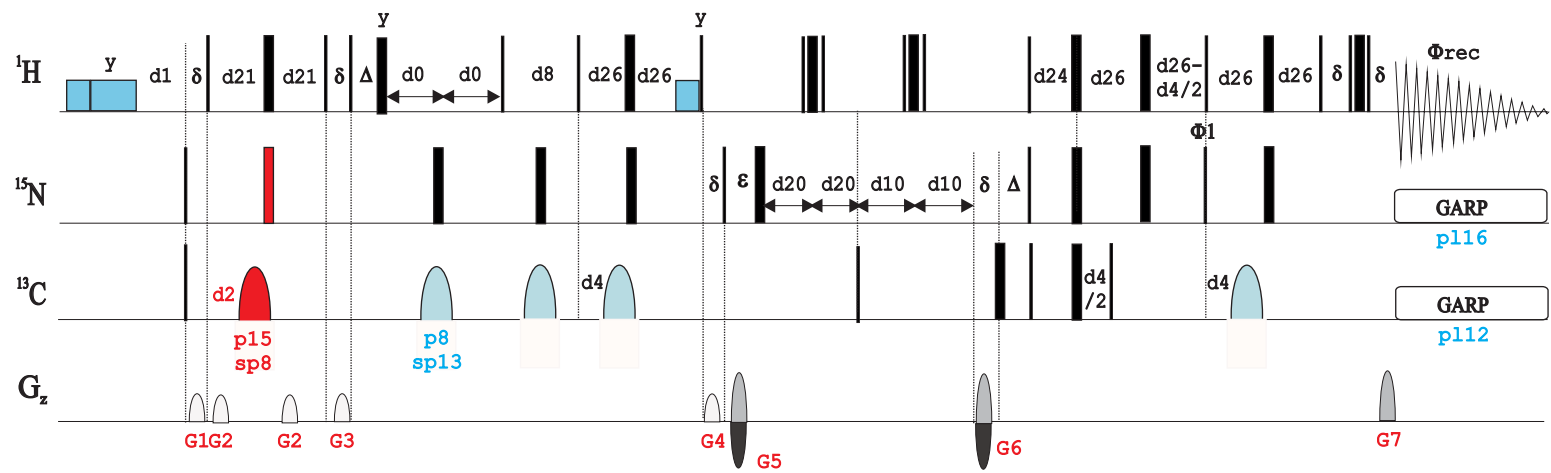
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noesyhsqcedgpsm3d



noesyhsqcedgpsism3d

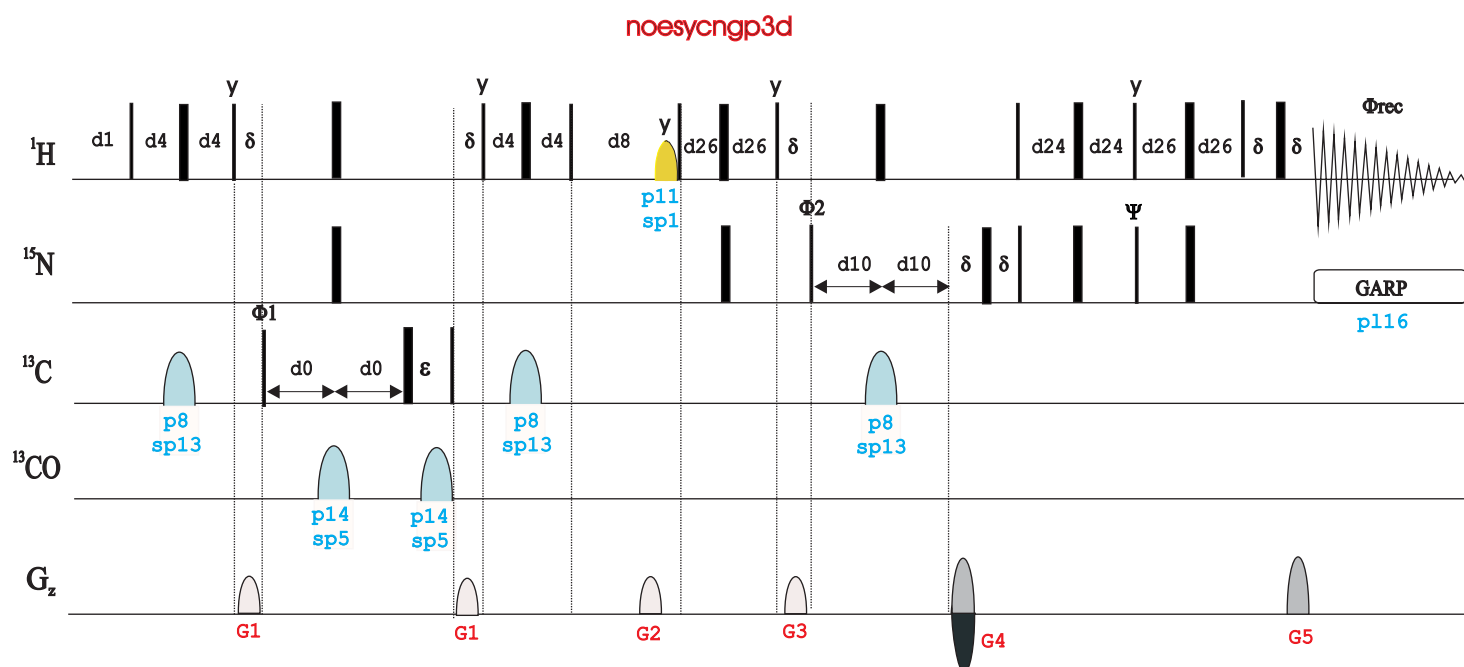
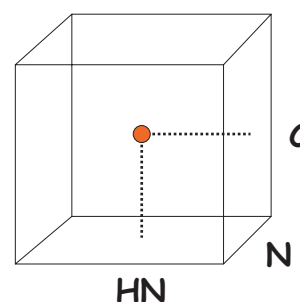
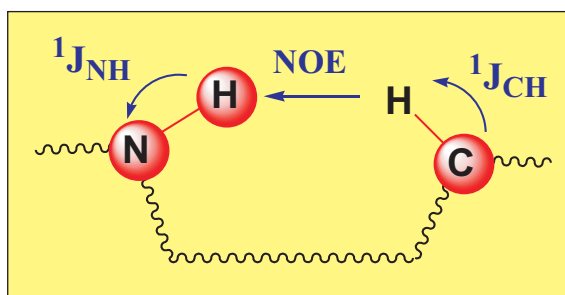


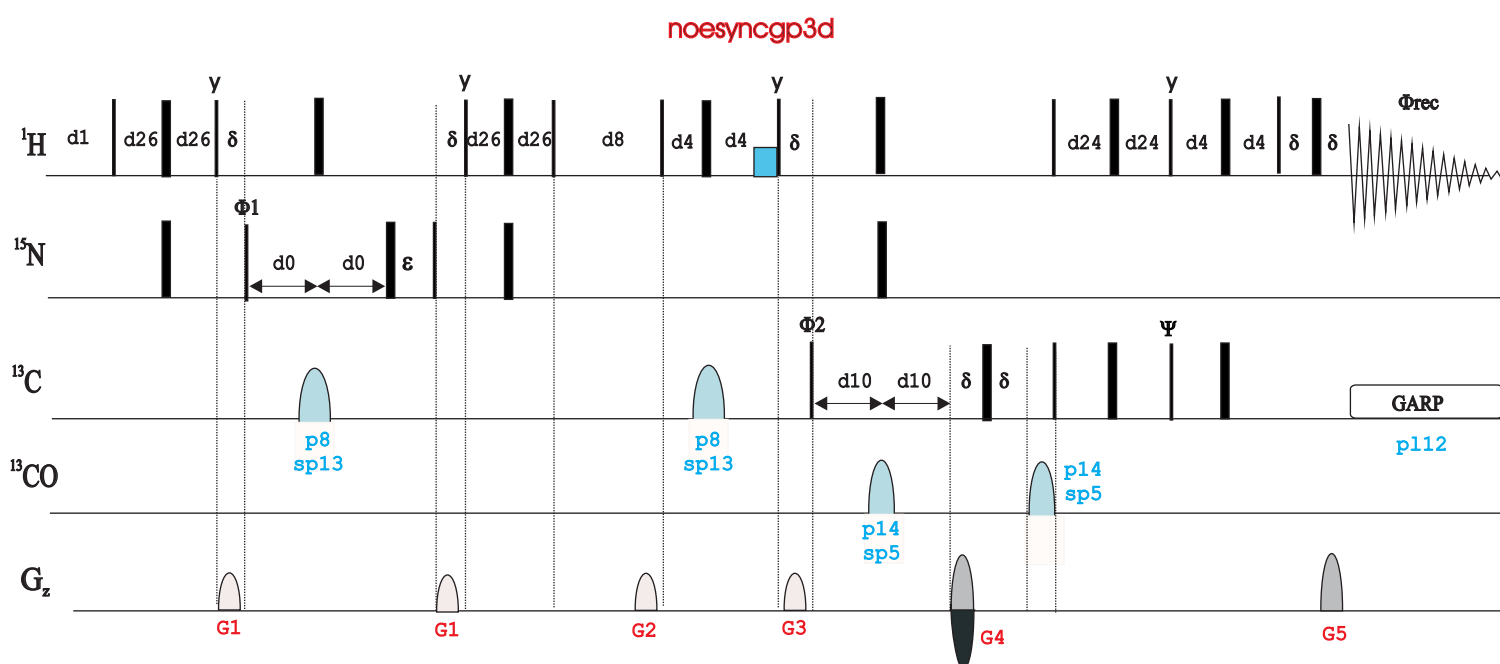
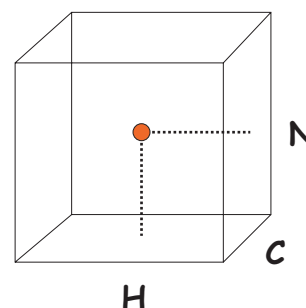
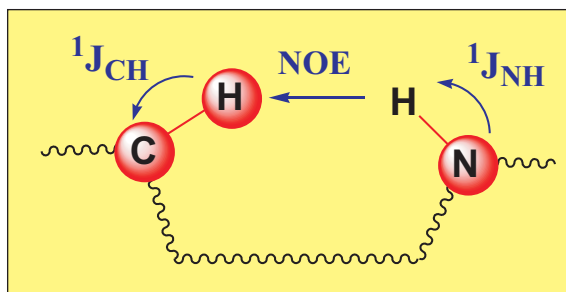
BRUKER PULSE PROGRAM CATALOGUE

NMRGuide

3D HSQC-NOESY-HSQC
EXPERIMENTS

- ge-3D ^1H - ^{13}C HSQC-NOESY- ^1H - ^{15}N HSQC (**noesyngp3d** | NOESYNGP3D)
- ge-3D ^1H - ^{15}N HSQC-NOESY- ^1H - ^{13}C HSQC (**noesyngp3d** | NOESYNGP3D)





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NMRGuide

2D X-FILTERED/EDITED
NOESY EXPERIMENTS

2D w_1 - ^{13}C -filtered/edited NOESY experiment

Phase-sensitive w_1 -filtered/edited NOESY without decoupling (**noesyphx1**)
 Phase-sensitive w_1 -filtered/edited NOESY with decoupling (**noesydcphx1**)
 Phase-sensitive w_1 -filtered/edited NOESY with presaturation and without decoupling (**noesyphprx1**)
 Phase-sensitive w_1 -filtered/edited NOESY with presaturation and with decoupling (**noesydcphprx1**)

2D w_2 - ^{13}C -filtered/edited NOESY experiment

Phase-sensitive w_2 -filtered/edited NOESY without decoupling (**noesyphx2**)
 Phase-sensitive w_2 -filtered/edited NOESY with decoupling (**noesydcphx2**)
 Phase-sensitive w_2 -filtered/edited NOESY with presaturation and without decoupling (**noesyphprx2**)
 Phase-sensitive w_2 -filtered/edited NOESY with presaturation and with decoupling (**noesydcphprx2**)

ge-2D w_1, w_2 ^{13}C -filtered/edited NOESY experiment

Phase-sensitive ge-2D w_1, w_2 ^{13}C -filtered/edited NOESY with presaturation (**noesygpphprxf** | **NA_NOESYGPPHPRXF**)
 Phase-sensitive ge-2D w_1, w_2 ^{13}C -filtered/edited NOESY with WATERGATE (3-9-19) (**noesygpphxf19** | **NA_NOESYGPPHXF19**)

ge-2D w_1, w_2 ^{15}N -filtered/edited NOESY experiment

Phase-sensitive ge-2D w_1, w_2 ^{15}N -filtered/edited NOESY using WATERGATE (3-9-19) (**noesyf3gpphxf19** | **NOESYF3GPPHXF19**)

ge-2D w_1 - $^{13}\text{C}, ^{15}\text{N}$ -filtered/edited NOESY experiment

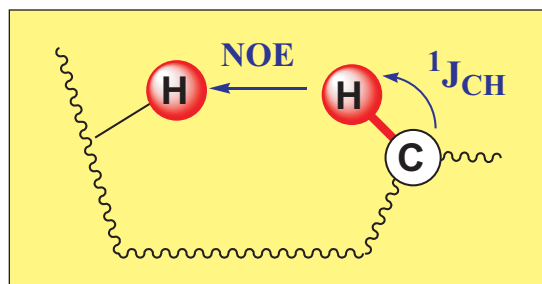
ge-2D w_1 - $^{13}\text{C}, ^{15}\text{N}$ -filtered/edited NOESY using WATERGATE (**noesygpphwgx1** | **NOESYGPPHWGX1**)

ge-2D w_2 - $^{13}\text{C}, ^{15}\text{N}$ -filtered/edited NOESY experiment

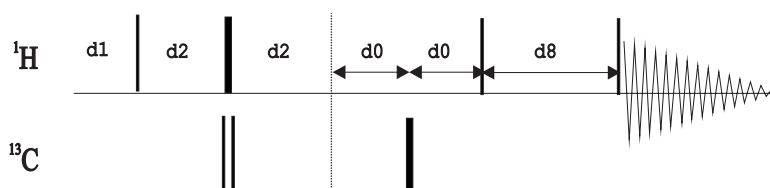
ge-2D w_2 - $^{13}\text{C}, ^{15}\text{N}$ -filtered/edited NOESY using WATERGATE (**noesygpphwgx2** | **NOESYGPPHWGX2**)

ge-2D w_1, w_2 $^{13}\text{C}, ^{15}\text{N}$ -filtered/edited NOESY experiment

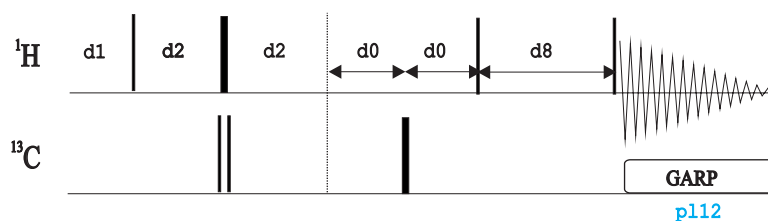
Phase-sensitive ge-2D w_1, w_2 $^{13}\text{C}, ^{15}\text{N}$ -filtered/edited NOESY with WATERGATE (selective pulses) (**noesygpphwgxf** | **NOESYGPPHWGXf**)
 Phase-sensitive ge-2D w_1, w_2 $^{13}\text{C}, ^{15}\text{N}$ -filtered/edited NOESY with WATERGATE (selective pulses) (**noesygpphwgxf.2** | **NOESYGPPHWGXf.2**)



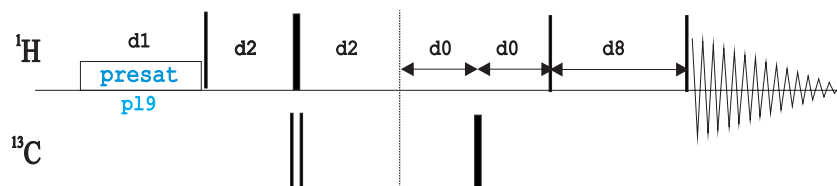
noesyphx1



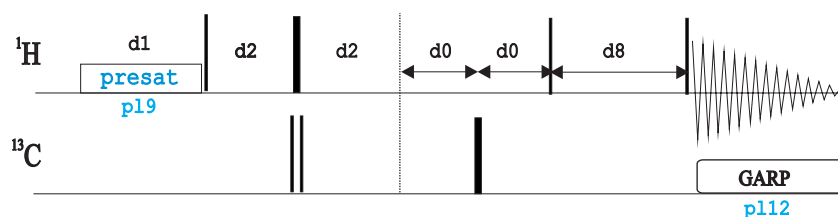
noesydcphx1

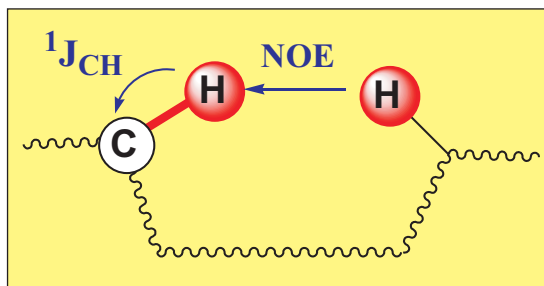


noesyphprx1

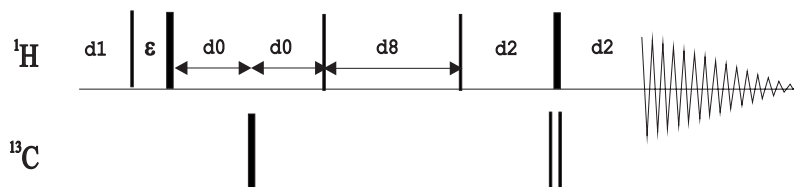


noesydcphprx1

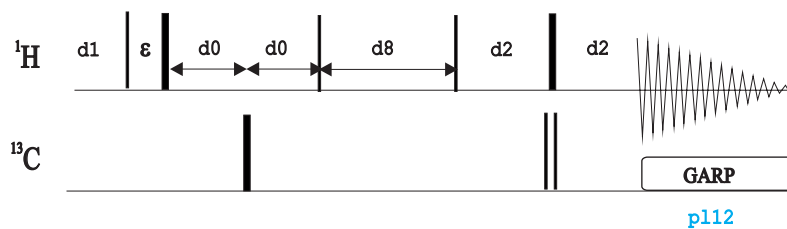




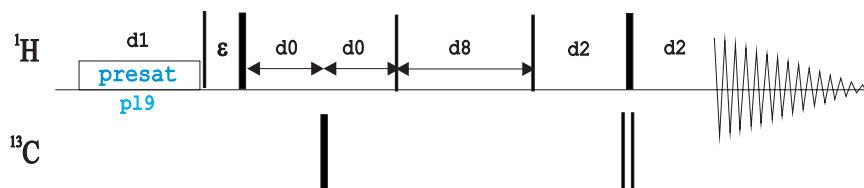
noesyphx2



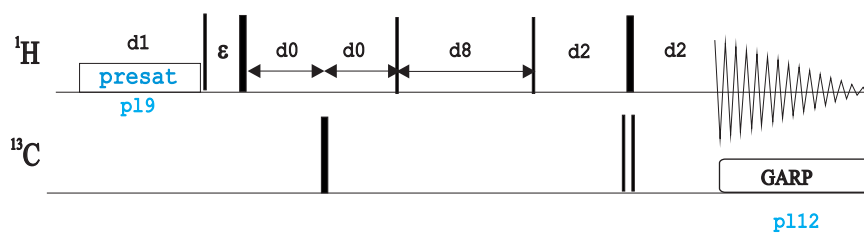
noesydcphx2

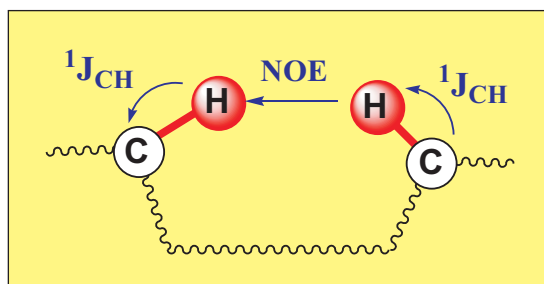


noesyphprx2

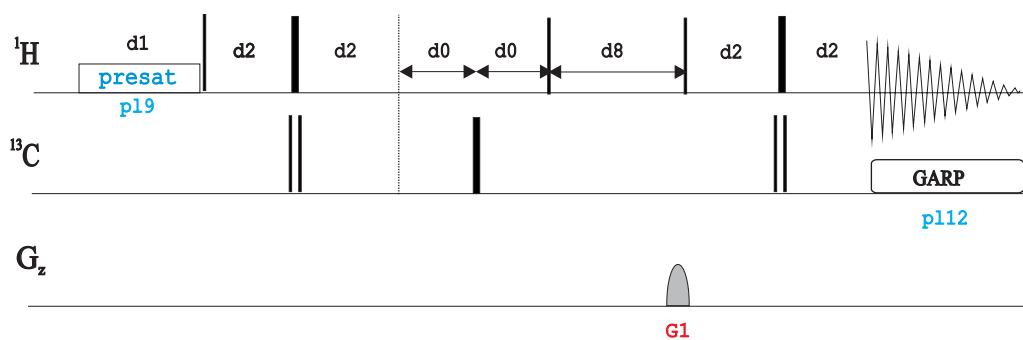


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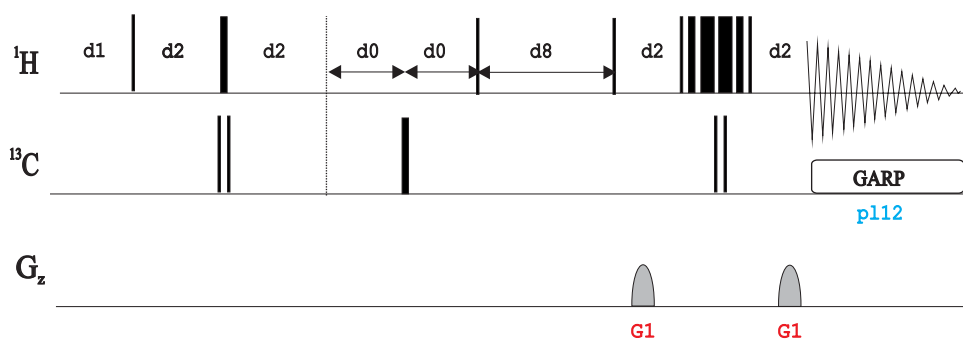


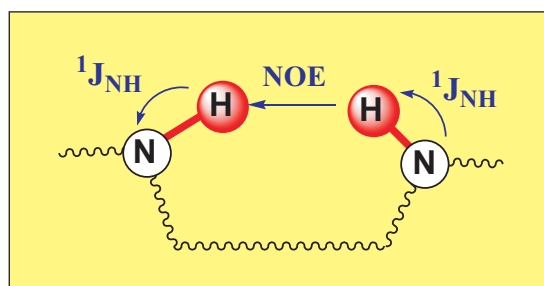


noesygp-phprxf

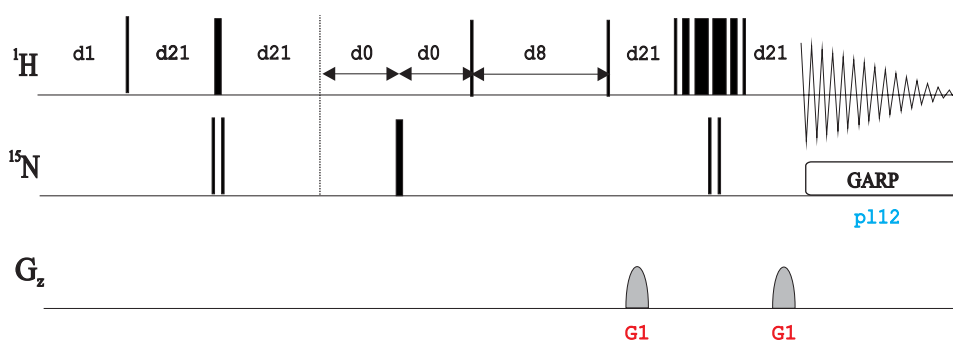


noesygp-phxf19



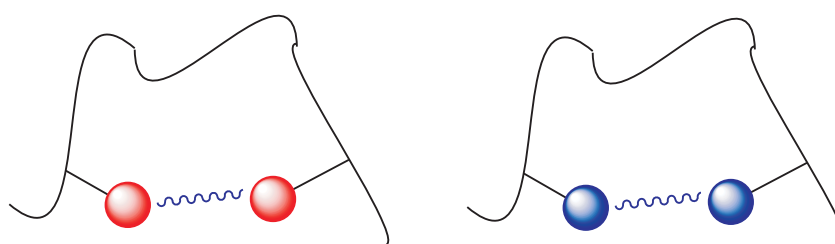


noesyf3gpphxf19

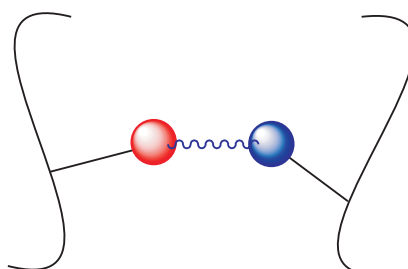


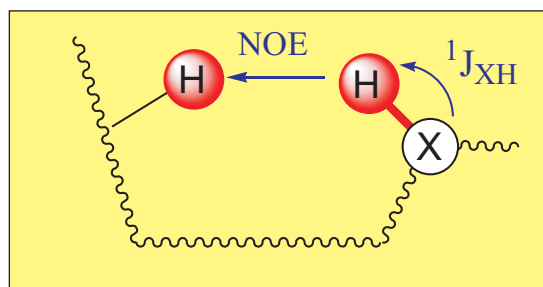
Unlabeled
 Labeled

Intramolecular NOEs

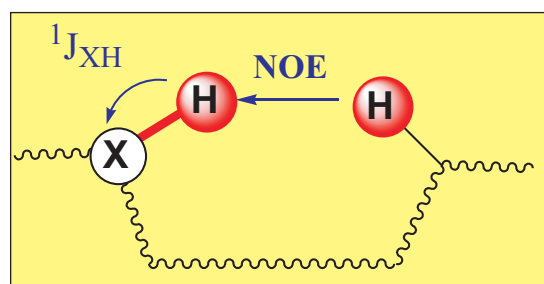
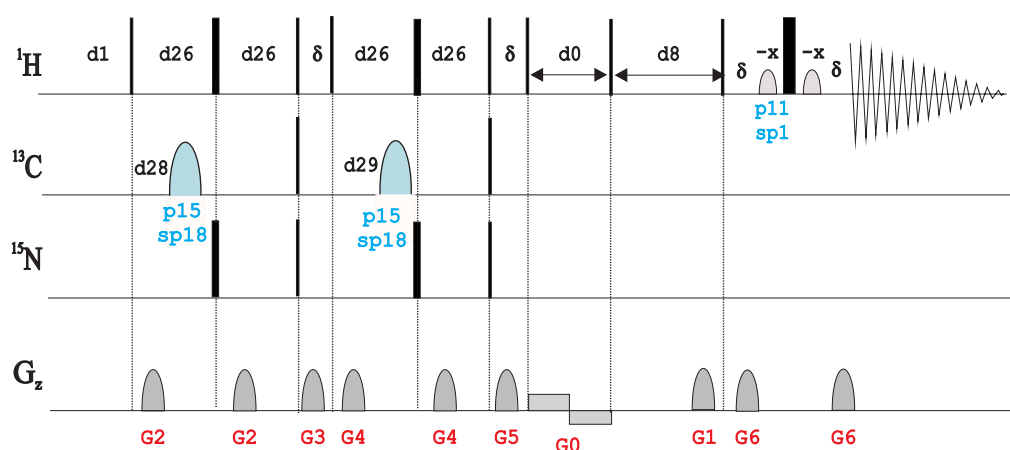


Intermolecular NOEs

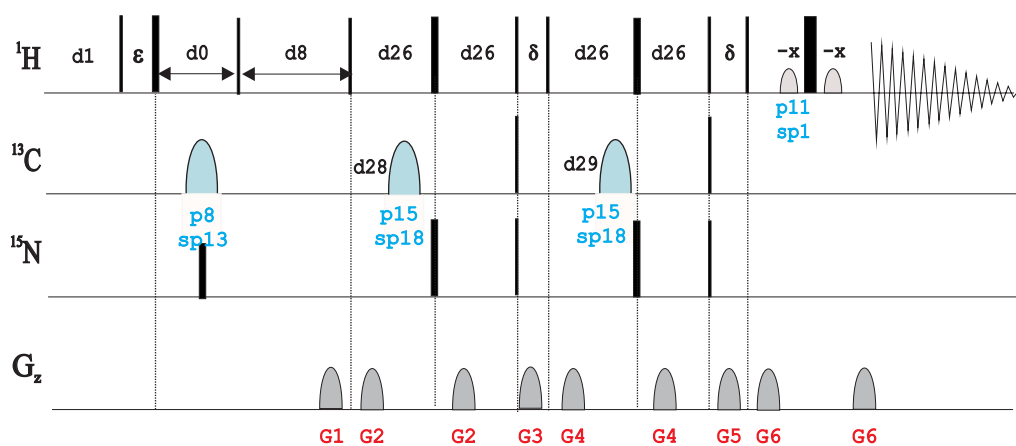


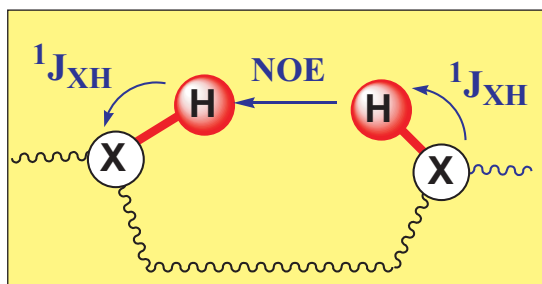


noesygp phw gx1

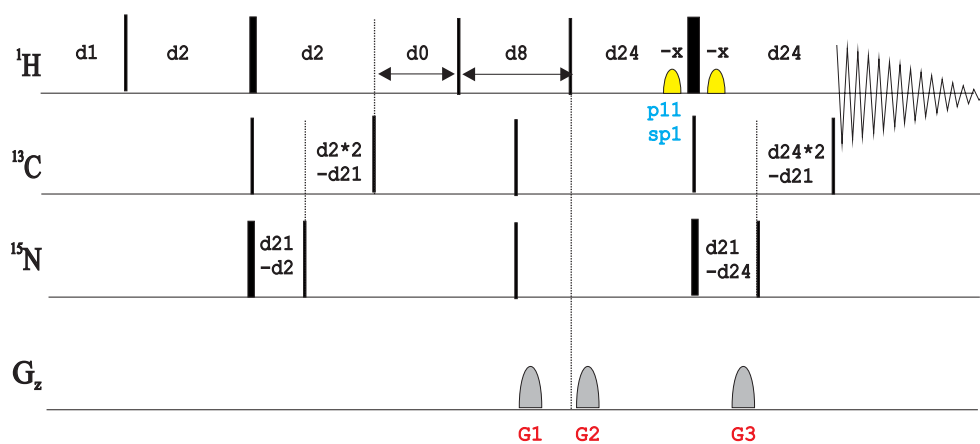


noesygp phw gx2

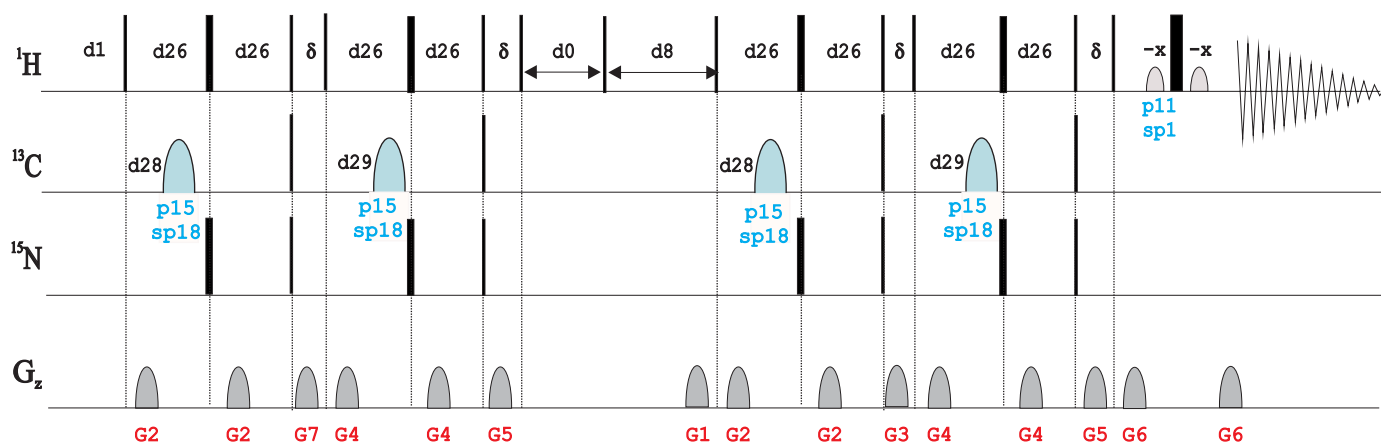




noesygp phw gxf



noesygp phw gxf.2



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3D X-FILTERED/EDITED
NOESY-HSQC & HSQC-NOESY
EXPERIMENTS

ge-3D ^{13}C , ^{15}N -filtered/edited NOESY-HSQC experiment

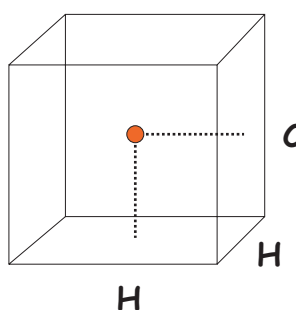
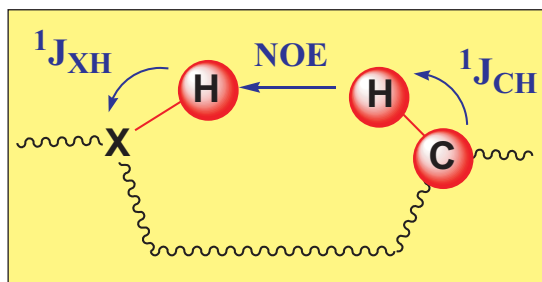
w_1 - ^{13}C , ^{15}N -filtered/edited 3D NOESY- ^1H - ^{13}C -HSQC using WATERGATE
(**noesyhsqcgpwgx13d**| NOESYHSQCGPWGX13D)
 w_1 - ^{13}C , ^{15}N -filtered/edited 3D NOESY- ^1H - ^{15}N -HSQC using WATERGATE
(**noesyhsqcf3gpwgx13d**| NOESYHSQCF3GPWG13D)
 w_1 - ^{13}C , ^{15}N -filtered/edited 3D NOESY- ^1H - ^{15}N -HSQC using PEP and echo-antiecho
(**noesyhsqcfpf3gpsix13d**)

ge-3D ^{13}C , ^{15}N -filtered/edited HSQC-NOESY experiment

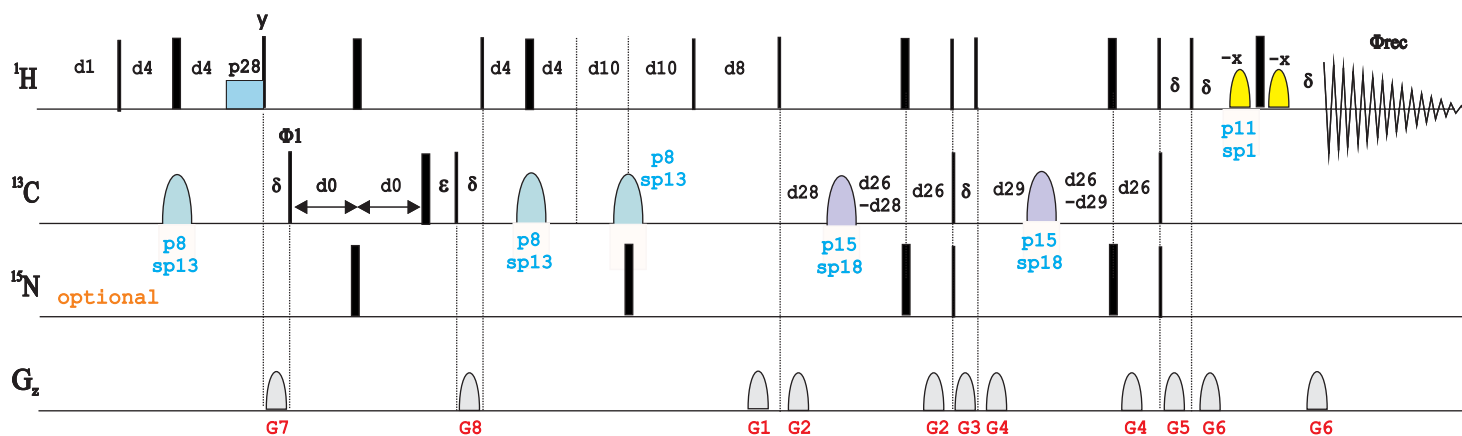
w_2 - ^{13}C , ^{15}N -filtered/edited 3D ^1H - ^{13}C -HSQC-NOESY using WATERGATE
(**hsqcgpnogx33d**| HSQCGPNOWGX33D)
 w_2 - ^{13}C , ^{15}N -filtered/edited 3D ^1H - ^{15}N -HSQC-NOESY using WATERGATE
(**hsqcf3gpnogx33d**| HSQCF3GPNOWGX33D)

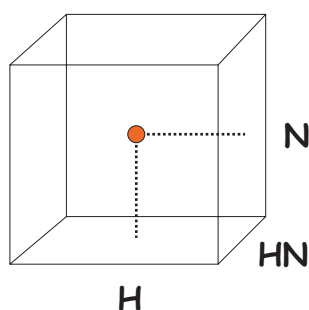
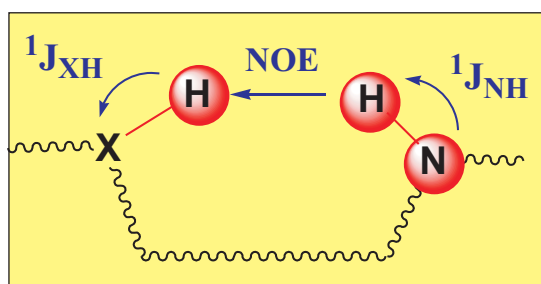
Also see:

NOESY-HSQC, HSQC-NOESY, and HSQC-NOESY-HSQC

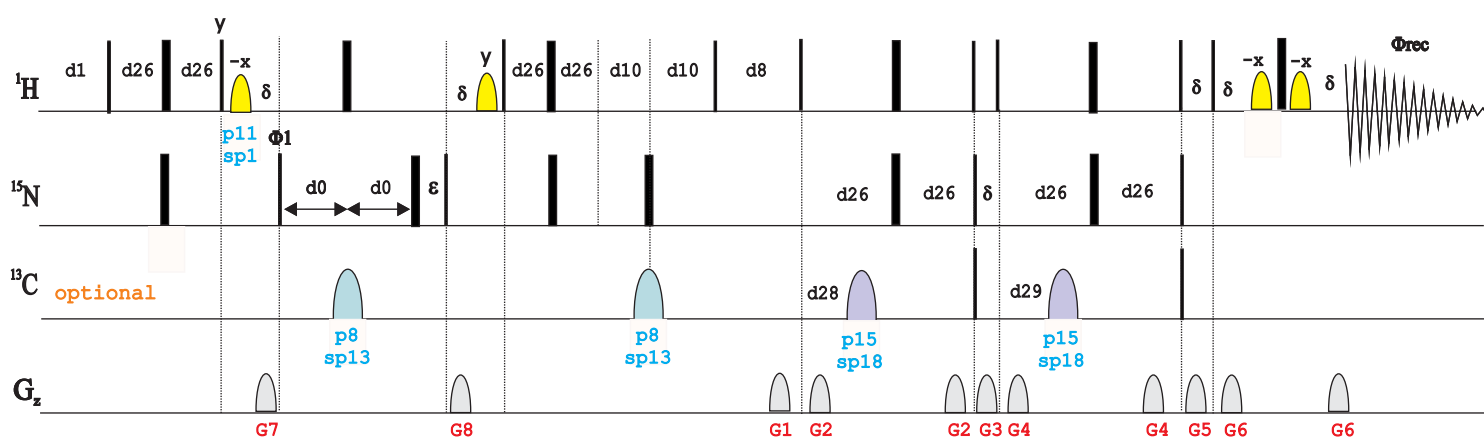


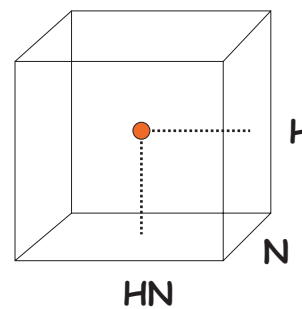
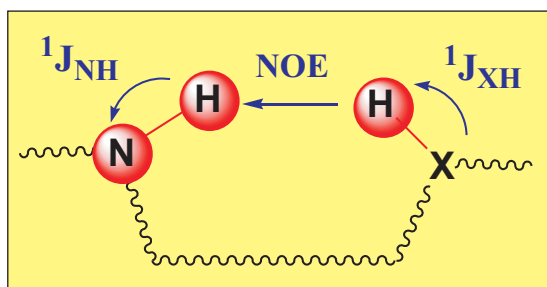
hsqcgpnwngx33d



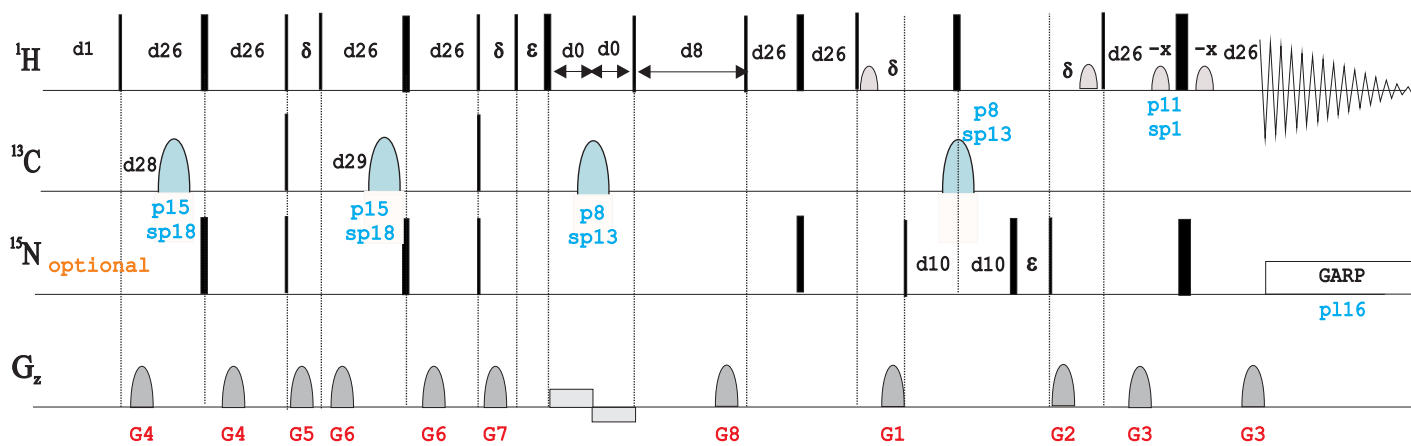


hsqcf3gpnowgx33d

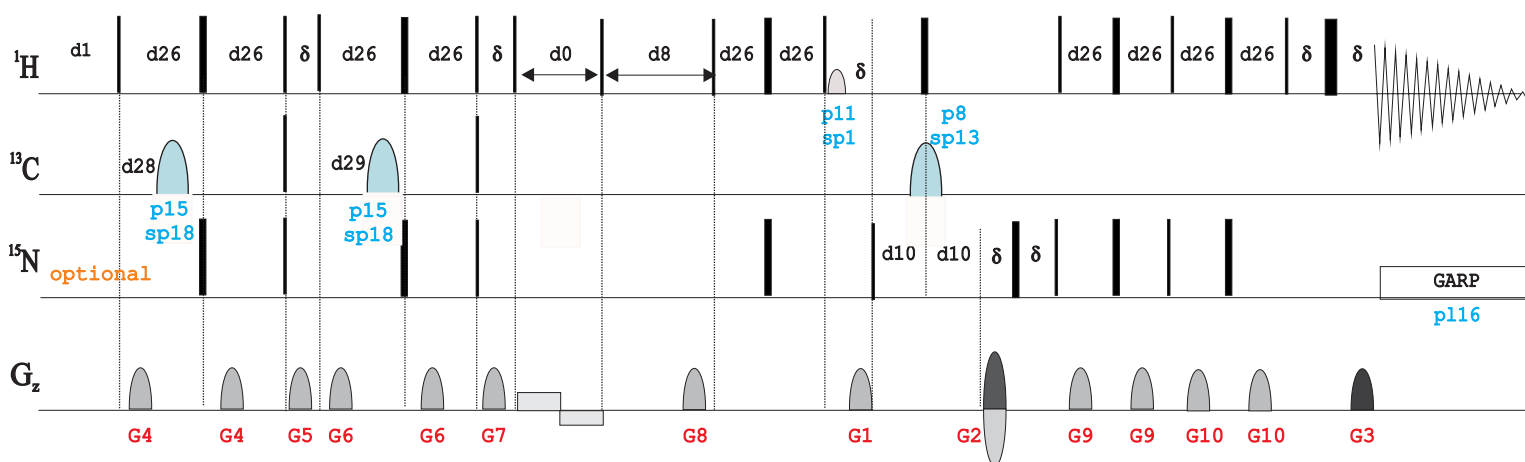


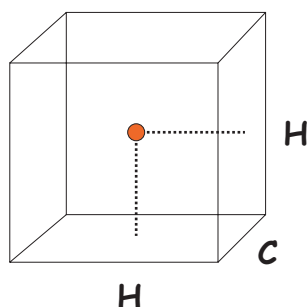
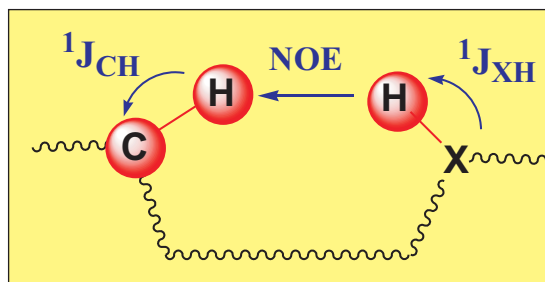


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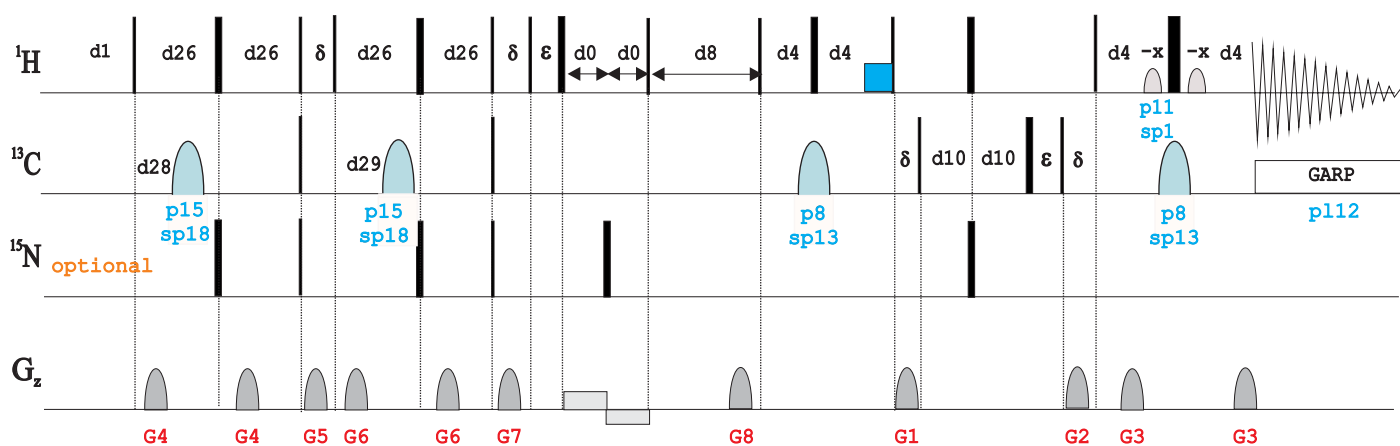


noesyhsqcfpf3gpsk13d





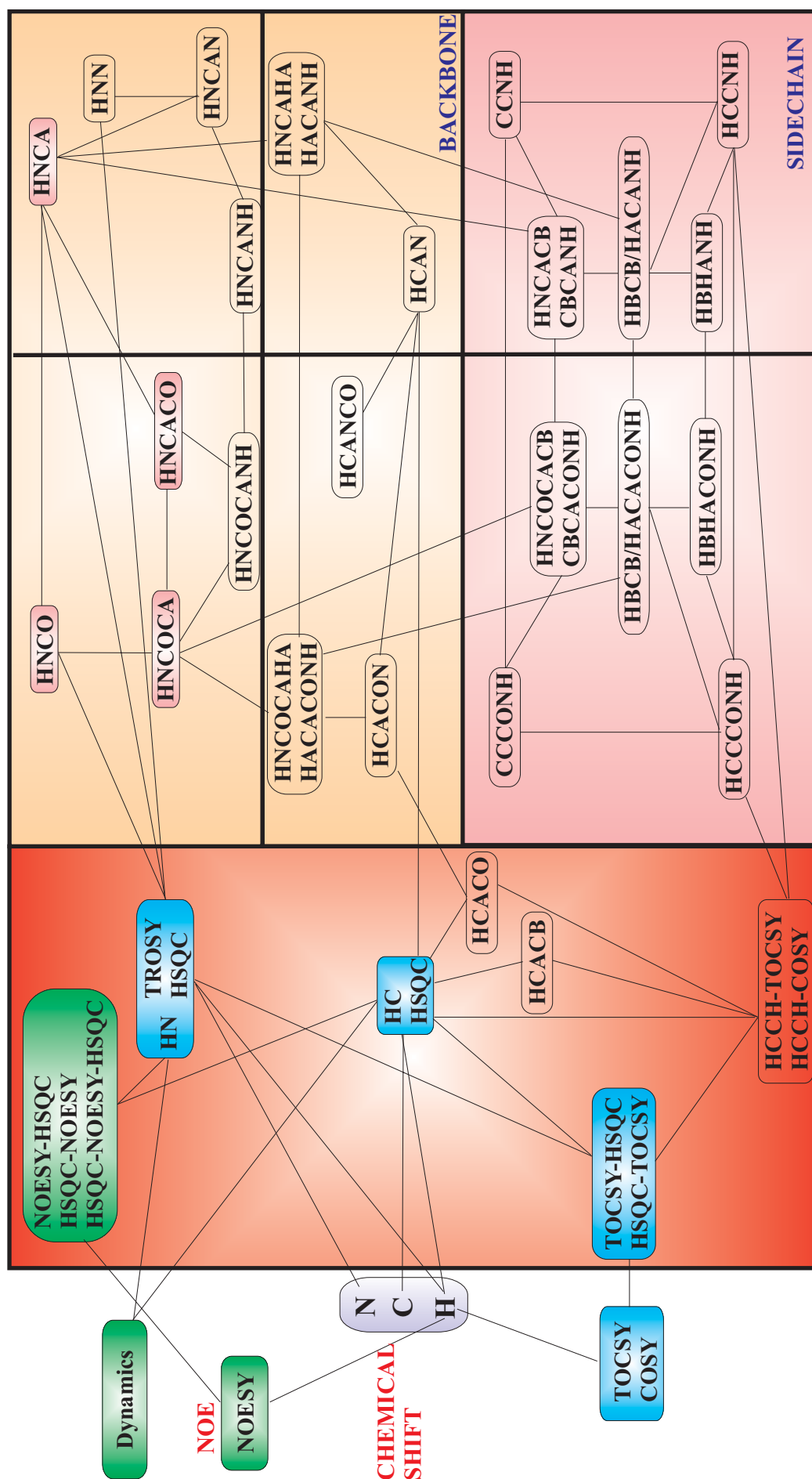
noesyhsqcgpwgx13d



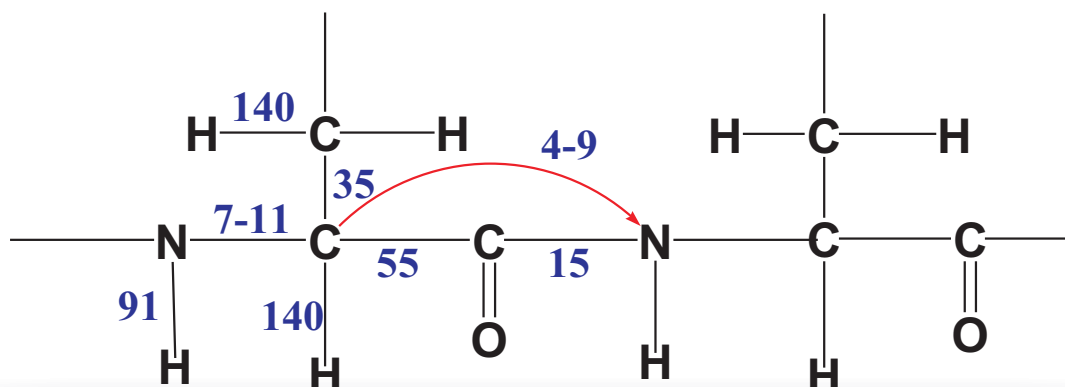
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PROTEIN NMR
BACKBONE EXPERIMENTS



Interpulse delays are optimized as a function of the following heteronuclear coupling constants:



Identifier	Power	Duration	spsam	cpdprg	Description	Remarks
PROTON PULSES & POWER LEVELS						
p1,p2	pl1				High Power Pulse	
p6	pl10	25u			TOCSY	
p15	pl11				ROESY	Power as 125u pulse
p26,pcpd1	pl19	55-65u		dipsi2	Decoupling pulse	
p11	sp1	1.5-2m	SINC1.1000		Water flipback pulse	
CARBON PULSES & POWER LEVELS						
p3,p4	pl2				High Power Pulse	
p9	pl15	25u		dipsi3	CC-TOCSY or HC-Cross polarization	
p13	sp2	410u	G4.256		on-resonance 90° (Cali or CO)	
p13	sp8	410u	G4tr.256		on-resonance time-reversed 90° (Cali or CO)	
p14	sp3	256u	G3.256		on-resonance 180° (Cali or CO)	
p14	sp5/sp7	256u	G3.256		off-resonance 180° (Cali or CO)	
p24	sp9	768u	G3.256		on-resonance 180° (CA)	
p24	sp7	2m	Crp60comp.4		Adiabatic 180° refocusing	Power as 25u pulse
p8	sp13	500u	Crp60,0.5,20.1		Adiabatic 180° inversion	Power as 25u pulse
pcpd2	pl12	60u-80u		garp	Low Power Pulse for broadband decoupling	
pcpd2, p31	sp15,pl13	1.5m	CHIRP95	p5m4sp180.p31	Adiabatic Decoupling	Power as GARP + 2dB
pcpd2, p31	sp15,pl28	768u	G3.256	mlevsp180.p31	CA or CO selective decoupling	
pcpd2, p31	sp15,pl28	100u	Gauss5.256	mlevsp180.p31	Selective CO Decoupling	Power as 25u pulse
NITROGEN PULSES & POWER LEVELS						
p21,p22	pl3				High Power Pulse	
pcpd3	pl16	200-300u		garp	Low Power Pulse for broadband decoupling	
DEUTERIUM PULSES & POWER LEVELS						
pcpd4	pl17	250u		garp	Low Power Pulse for broadband decoupling	

Delay	Coupling Constant	length (ms)	Remarks	Experiment
d3	1/(3JCH)	2.2		
d4	1/(4JCH)	1.6-1.8		
d21	1/(6JCH)	1.1		
d21	1/(2JNH)	5.5		
d22	1/(4JCOCA)	4.0		
d22	1/(2JCOCA)	3.6	Two-bond	
d22	1/(2JCOCA)	4.4	One-bond	
d23	1/(2JNCO)	12.0		
d24	1/(4JCC)	3.6		
d26	1/(4JNH)	2.3		
d21	T(N)	12.4		
d23	T(C)	12.0	2T=24ms<1/4JCH	

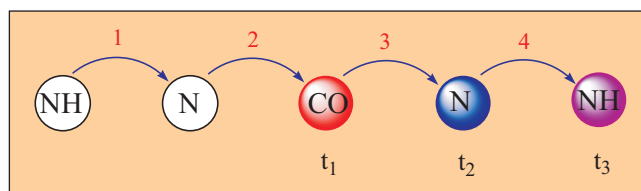
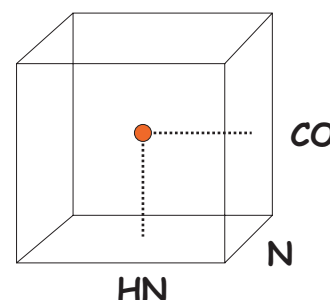
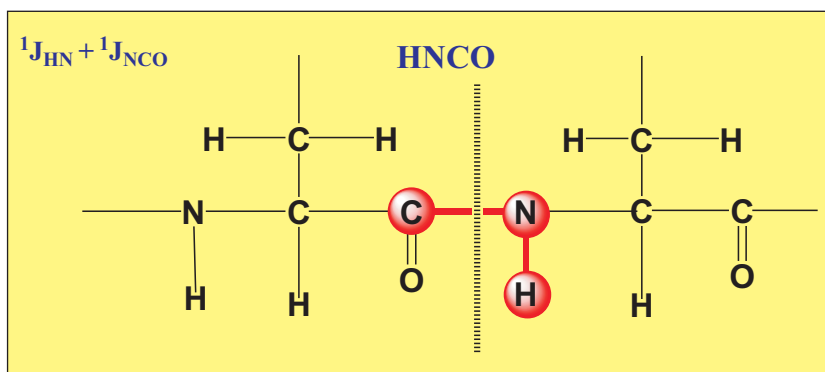
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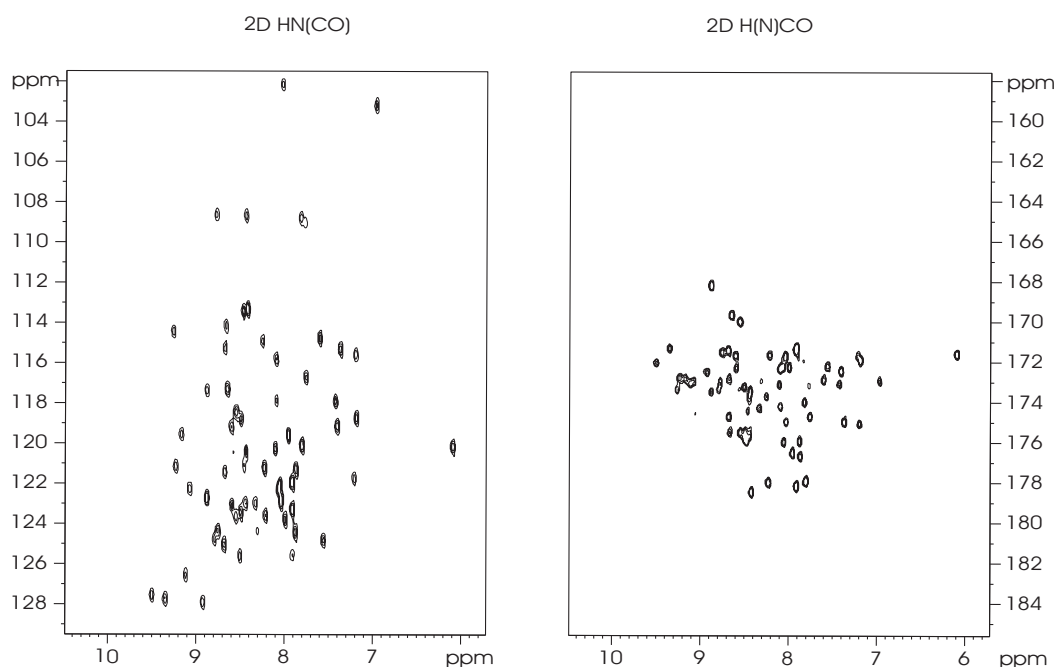
3D HNCO

- 3D HNCO using PEP (**hncogp3d** | **HNCOGP3D**)
- 3D HNCO using WATERGATE (**hncogpwg3d** | **HNCOGPWG3D**)
- 3D HNCO using TROSY (**trhncogp3d** | **TRHNCOGP3D**):
 - using echo-antiecho gradient (**trhncoetgp3d** | **TRHNCOETGP3D**)
 - with ^2H -decoupling (**trhncogp2h3d** | **TRHNCOGP2H3D**)

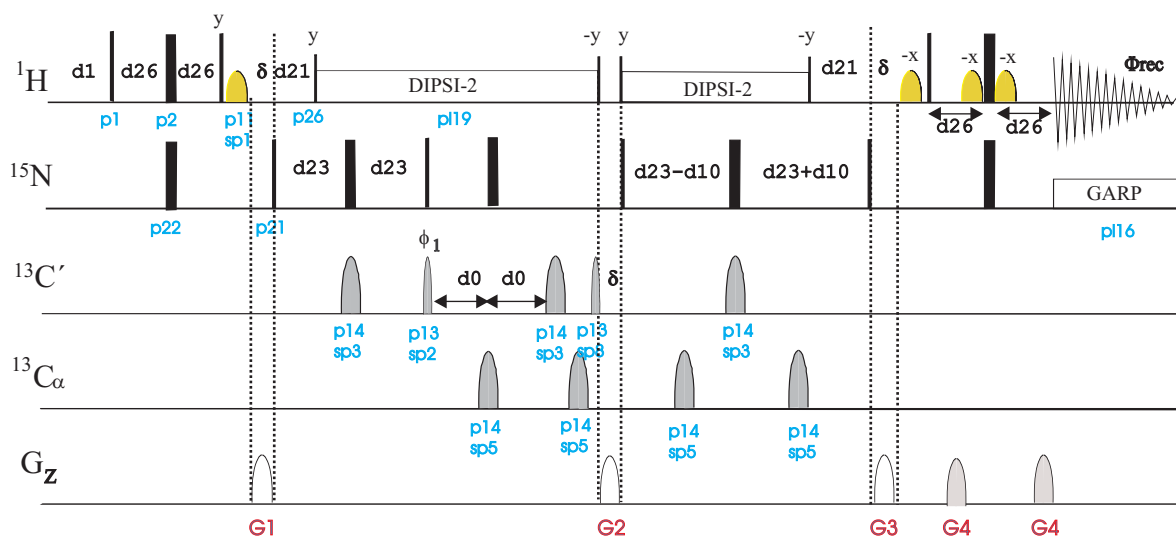
Also see: Coupling constants in proteins



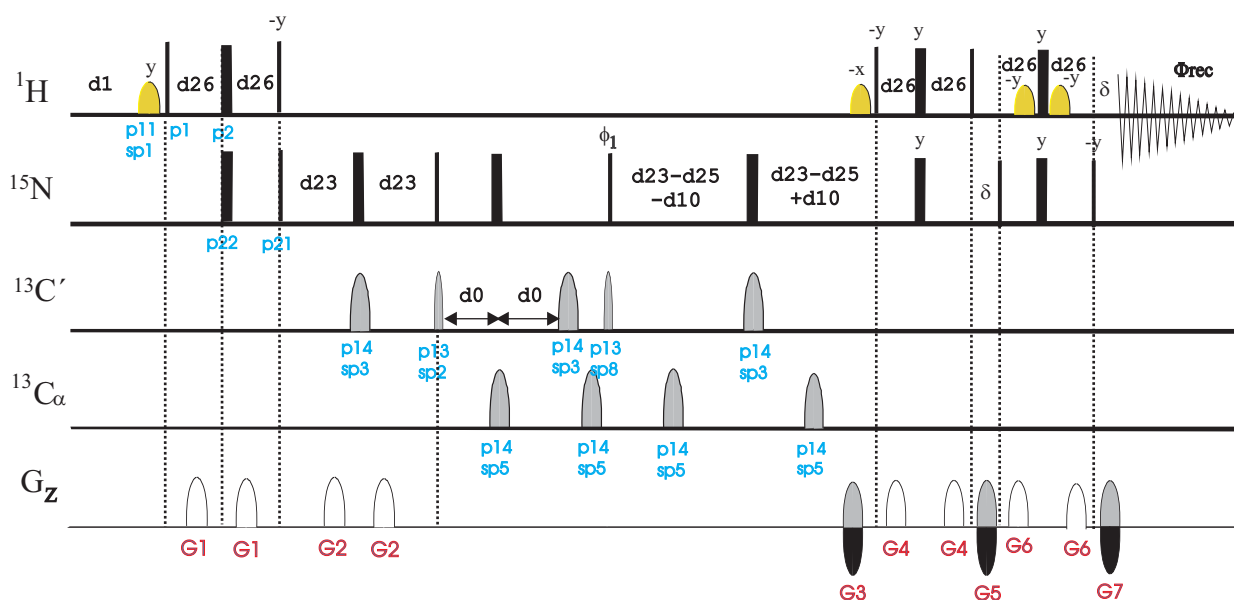
$$\begin{aligned} d26 &= 1/4J(\text{NH}) = 2.5\text{m} \\ d21 &= 1/2J(\text{NH}) = 5.5\text{m} \\ d23 &= 1/4J(\text{NCO}) = 12\text{m} \end{aligned}$$



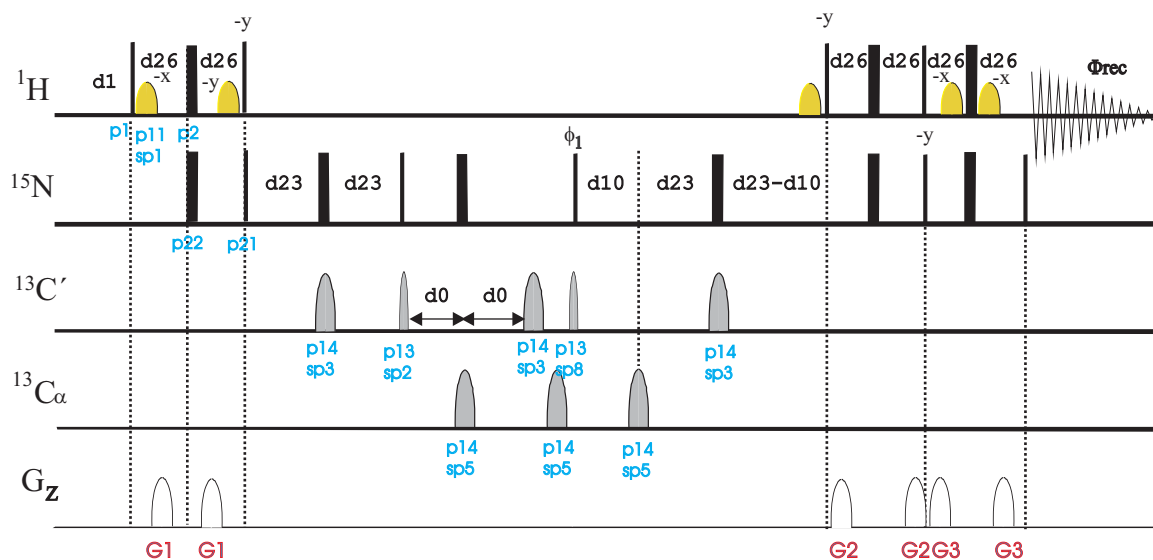
hncogpwg3d



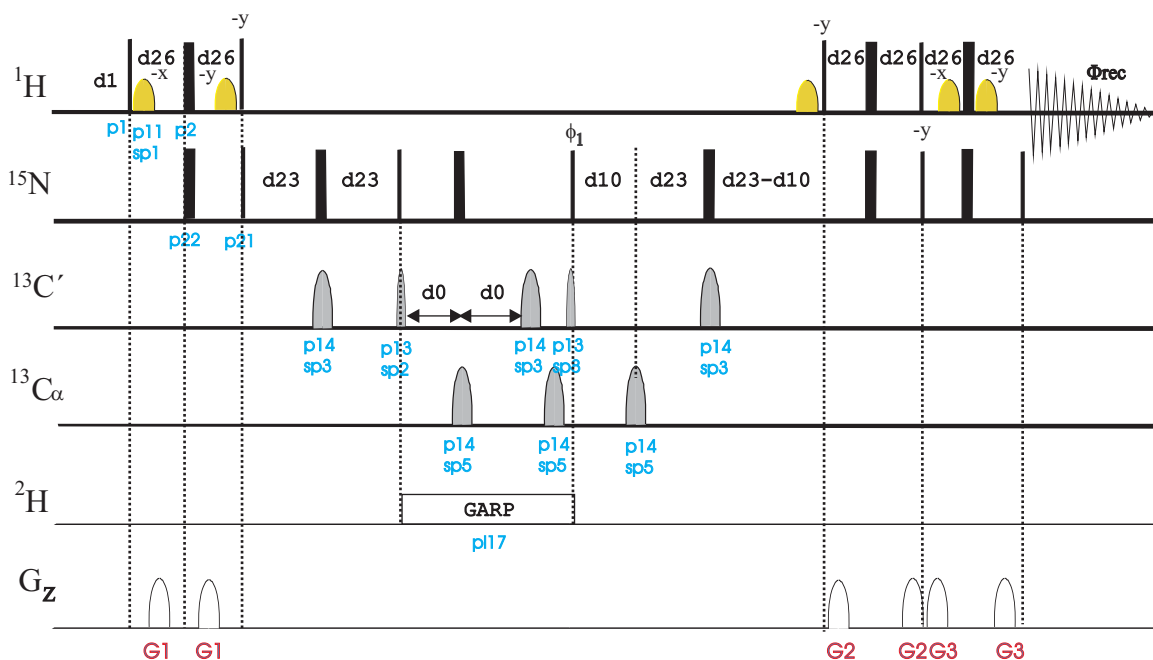
trhncogtgp3d



trhncogp3d



trhncogp2h3d



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3D HNCA

3D HNCA experiment

3D HNCA using PEP (**hncagp3d** | HNCAGP3D)

- with ^2H -decoupling (**hncagp2h3d** | HNCAGP2H3D)

3D HNCA using WATERGATE (**hncagpwg3d** | HNCAGPWG3D)

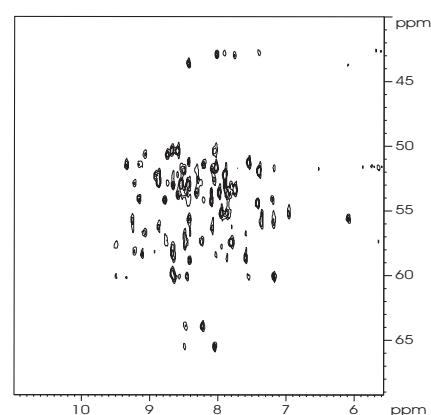
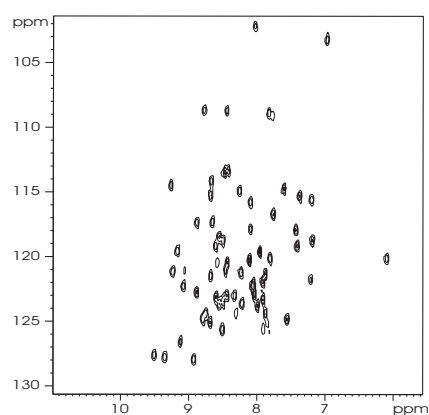
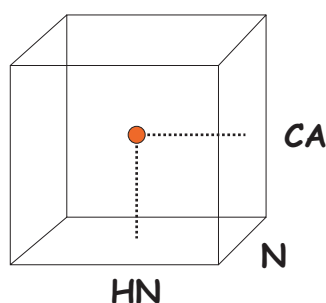
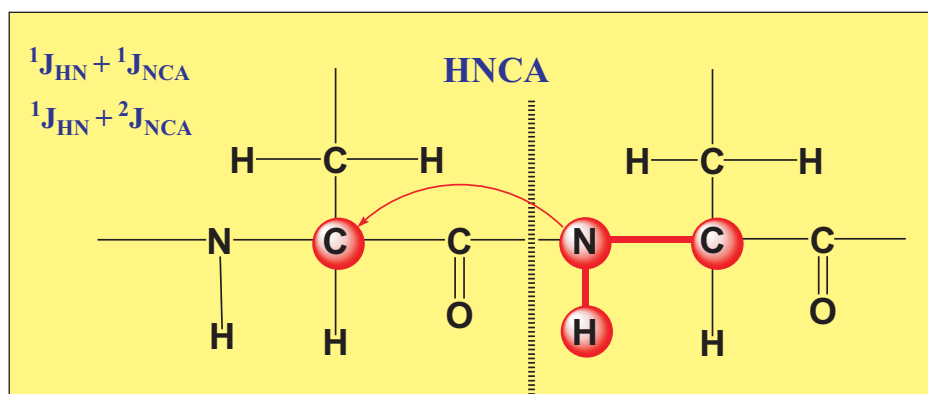
- with ^2H -decoupling (**hncagpwg2h3d** | HNCAGPWG2H3D)

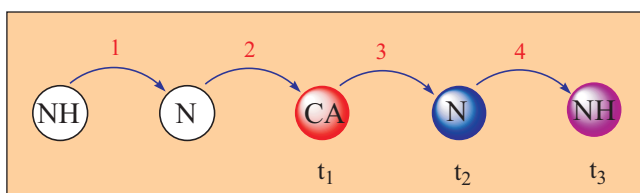
3D HNCA with selective Cb/C=O decoupling (**hncadhgp3d**)

3D HNCA using TROSY(**trhncagp3d2.2** | TRHNCAGP3D2.2) :

- using echo-antiecho gradient (**trhncagetp3d** | TRHNCAGTGP3D)
- using echo-antiecho gradient and with ^2H -decoupling (**trhncagetp2h3d** | TRHNCAGTGP2H3D)
- with HMQC steps (**trhncagp3d.2** | TRHNCAGP3D.2)
- with $^1\text{H}\alpha$ -decoupling (**trhncagp3d2** | TRHNCAGP3D2)
- with $^1\text{H}\alpha$ -decoupling and HMQC steps (**trhncagp3d** | TRHNCAGP3D)
- with ^2H -decoupling and HMQC steps (**trhncagp2h3d** | TRHNCAGP2H3D)
- with ^2H -decoupling (**trhncagp2h3d2** | TRHNCAGP2H3D2)

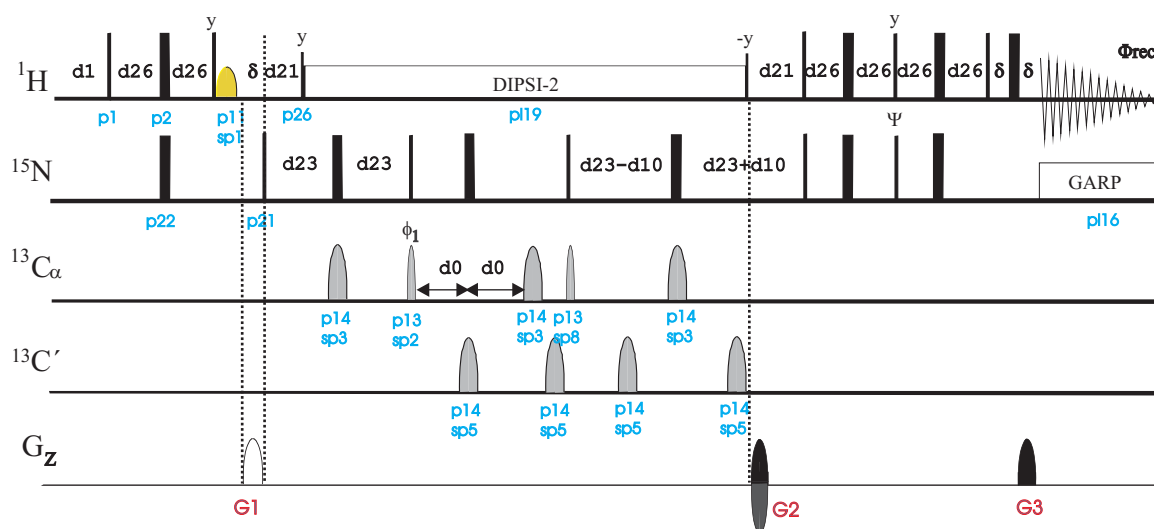
Also see: intra-HNCA, sequential-HNCA, HN(CO)CA



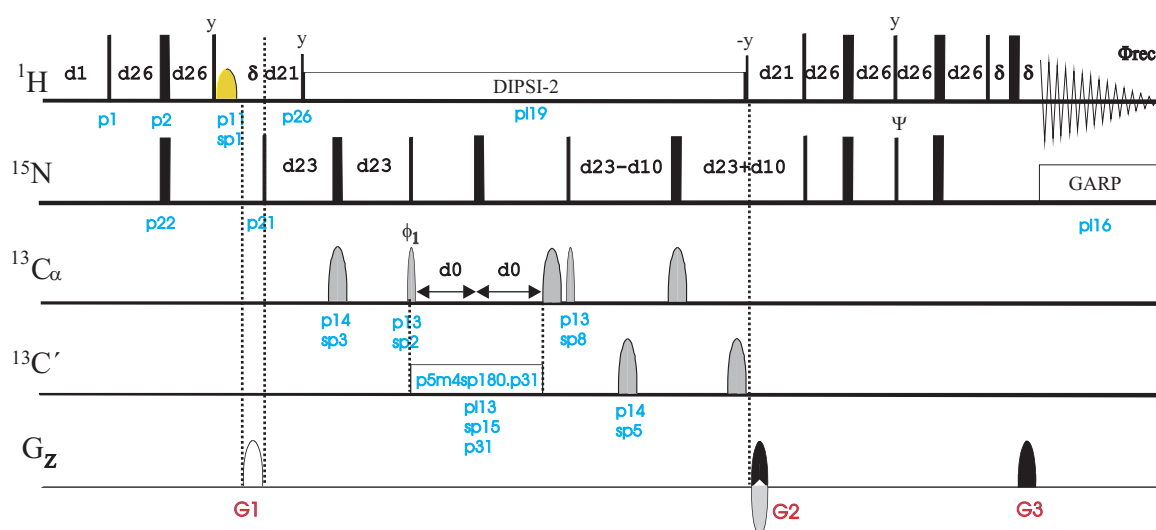


$d26=1/4J(\text{NH})=2.5\text{m}$
 $d21=1/2J(\text{NH})=5.5\text{m}$
 $d23=1/4J(\text{NCA})=12\text{m}$

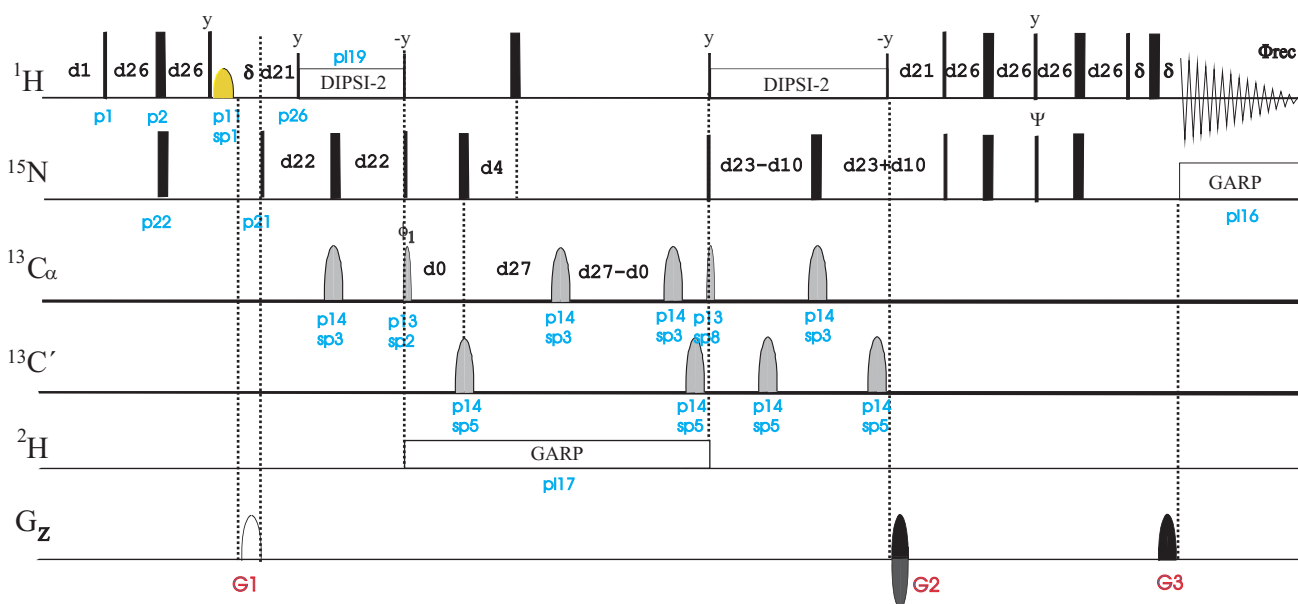
hncagp3d



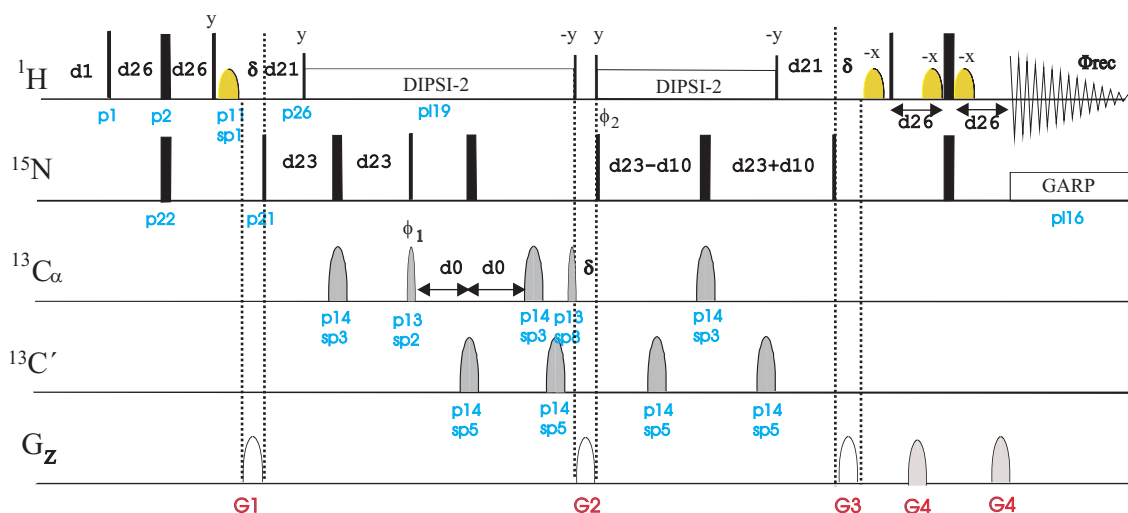
hncadhgp3d



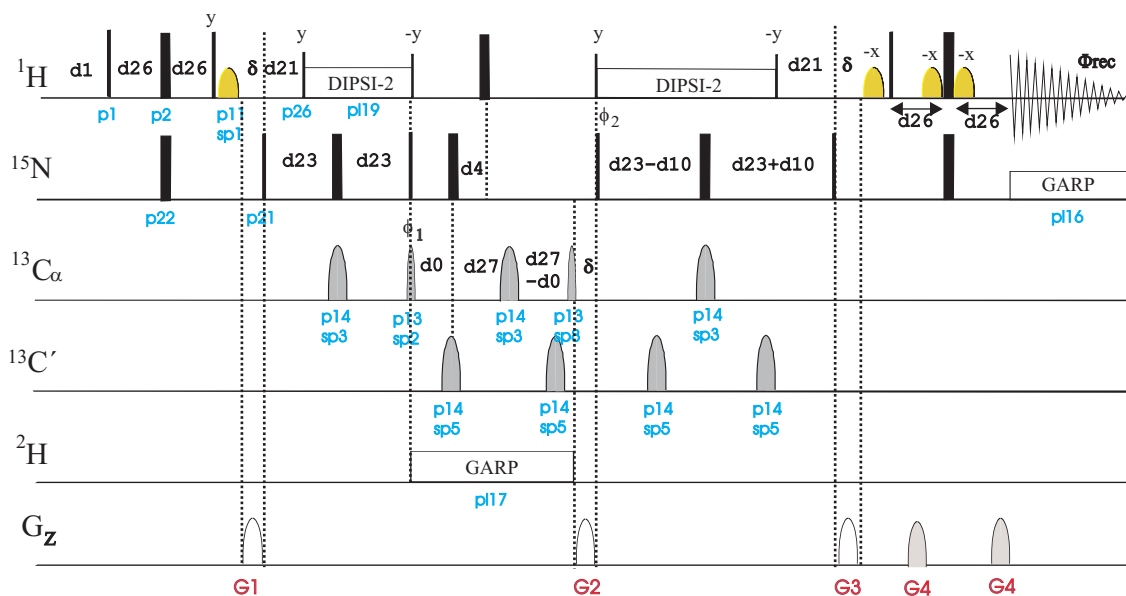
hncagp2h3d

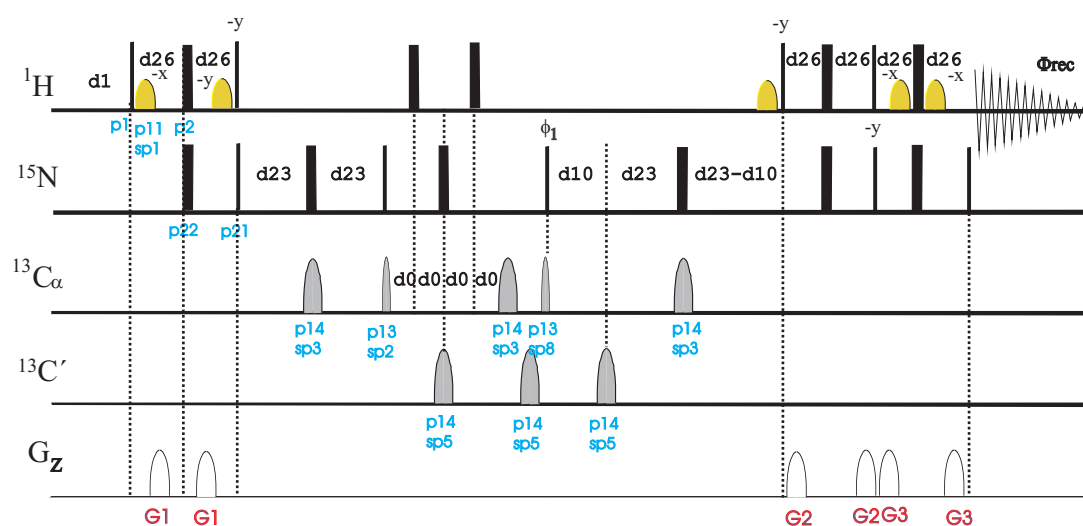
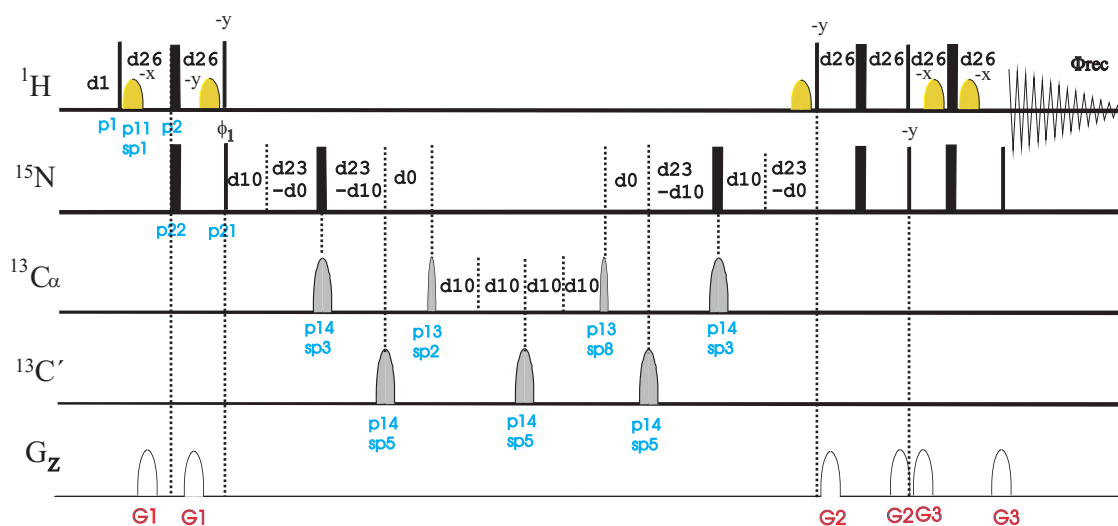


hncagpwg3d



hncagpwg2h3d





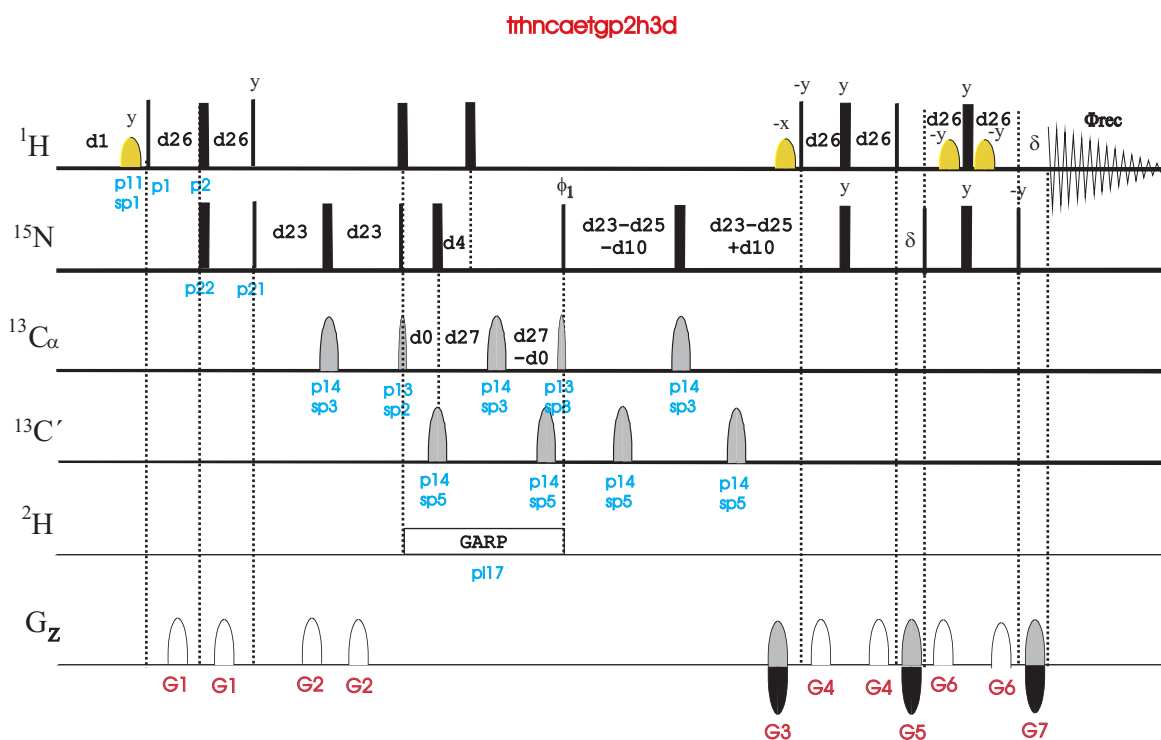
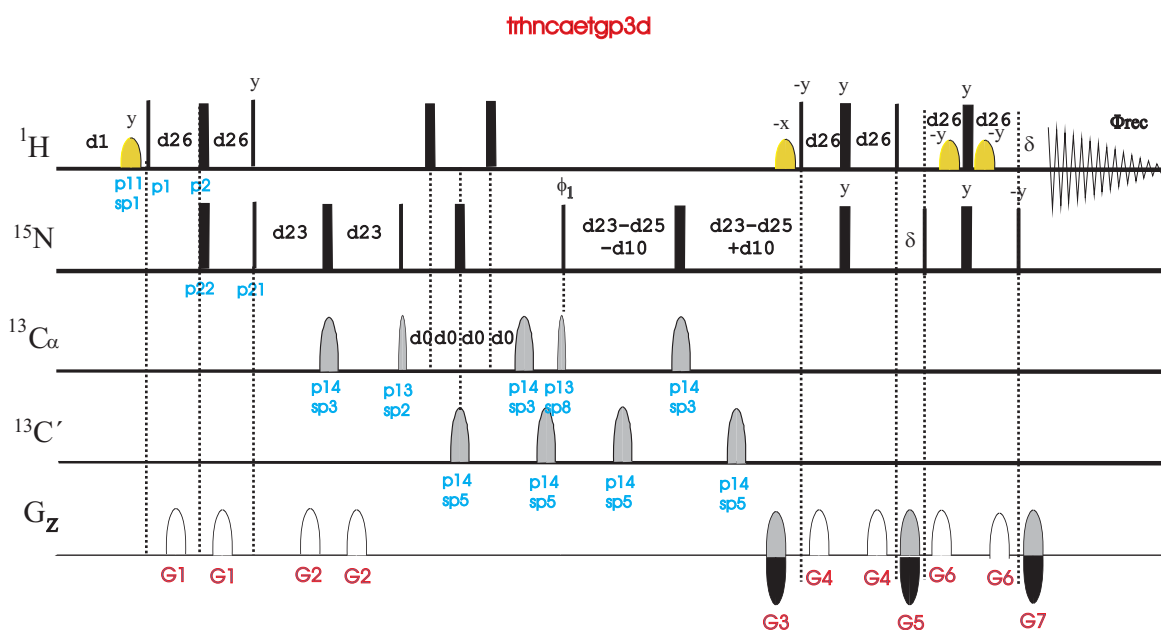
[illegible]

The diagram illustrates the timing of the DIPSI-2 experiment across five channels: ^1H , ^{15}N , $^{13}\text{C}_\alpha$, $^{13}\text{C}'$, and G_z . The experiment is divided into two main sections: **G1** and **G2**, separated by a dashed vertical line. The **DIPSI-2** block is located in the ^{15}N channel.

- ^1H Channel:** Shows pulses labeled d1, -x, d26, -y, y, d1, -y, d26, d26, d26, -x, d26, -x, and a free induction decay (FID) signal labeled Φ_{rec} .
- ^{15}N Channel:** Shows pulses labeled p1, p11, p2, sp1, d23, d23, d10, d23, d23-d10, and -y.
- $^{13}\text{C}_\alpha$ Channel:** Shows pulses labeled d0, d0, p14, p13, p14, p13, and p14.
- $^{13}\text{C}'$ Channel:** Shows pulses labeled p14, p14, p14, and p14.
- G_z Channel:** Shows pulses labeled G1, G1, G2, G2G3, and G3.

Vertical dotted lines indicate the timing of the pulses across all channels. The **DIPSI-2** block is a rectangular pulse in the ^{15}N channel, occurring between the first and second y-pulses.





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3D HN(CO)CA

3D HN(CO)CA experiment

3D HN(CO)CA using PEP (**hncocagp3d** | HNCOCAGP3D)

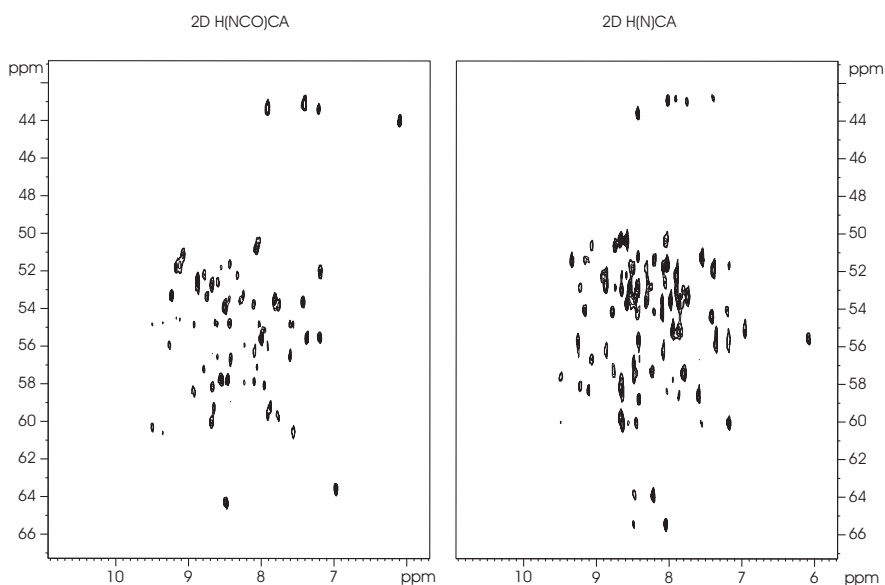
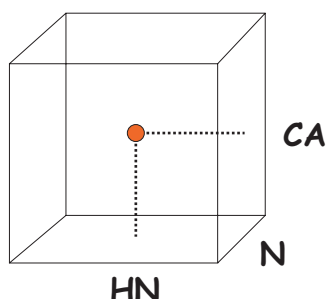
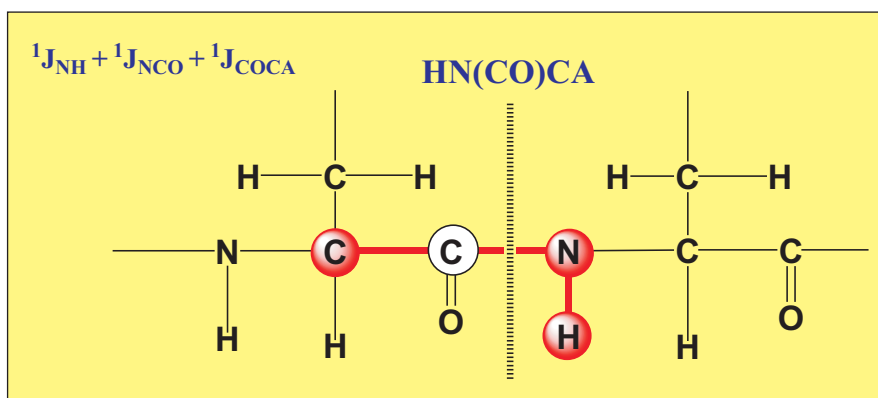
- with ^2H -decoupling (**hncocagp2h3d** | HNCOCAGP2H3D)

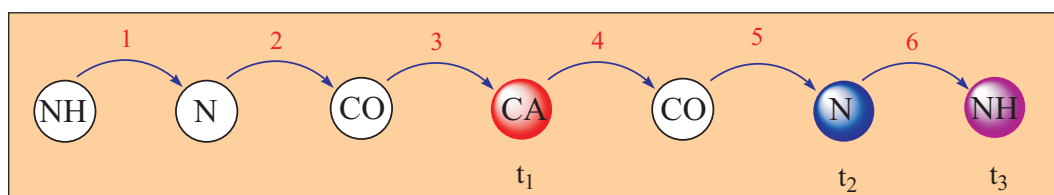
3D HN(CO)CA using WATERGATE (**hncocagpwg3d** | HNCOCAGPWG3D)

- with ^2H -decoupling (**hncocagpwg2h3d** | HNCOCAGPWG2H3D)

3D HN(CO)CA using TROSY (**trhncocagp3d** | TRHNCOCAGP3D):

- with ^2H -decoupling (**trhncocagp2h3d** | TRHNCOCAGP2H3D)
- using echo-antiecho gradient (**trhncocaetgp3d** | TRHNCOCAETGP3D)
- using echo-antiecho gradient and with ^2H -decoupling (**trhncocaetgp2h3d** | TRHNCOCAETGP2H3D)

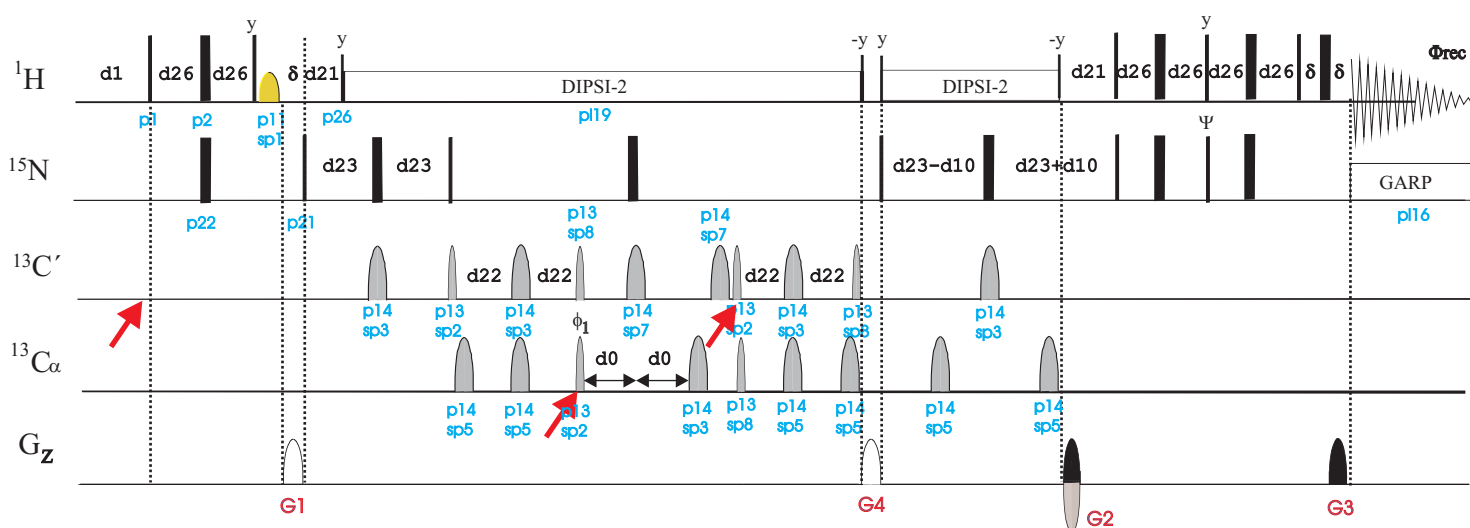




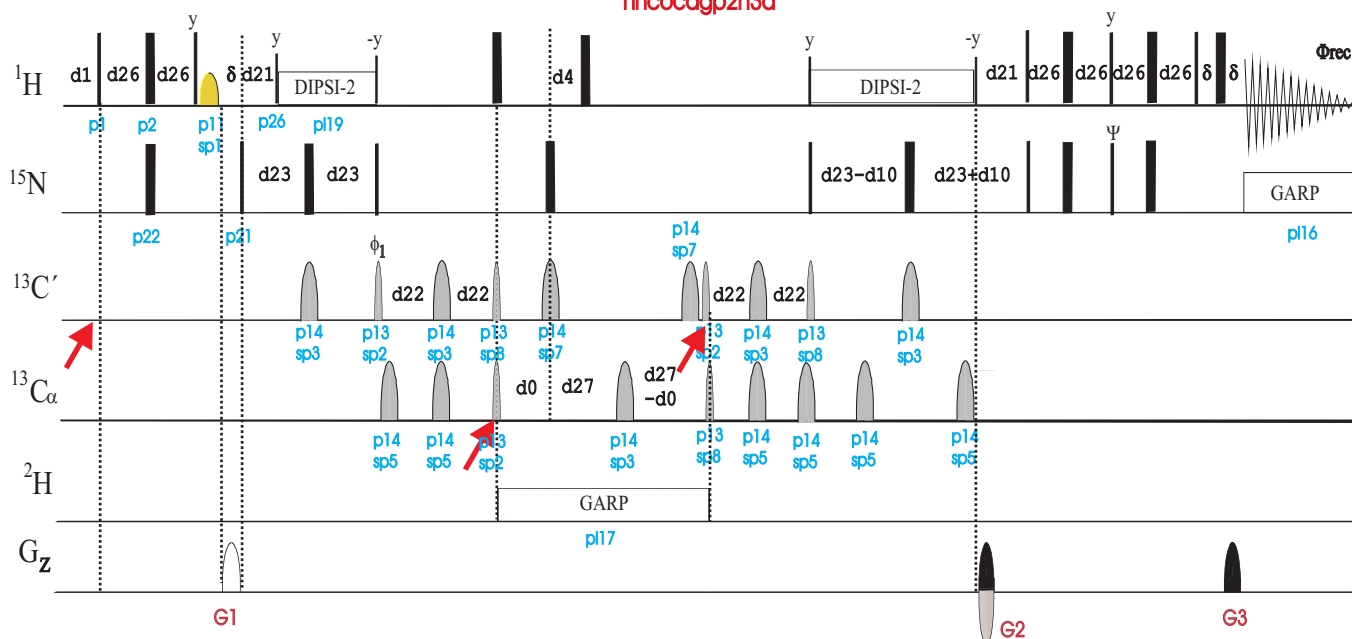
$d26=1/4J(\text{NH})=2.3\text{m}$
 $d21=1/2J(\text{NH})=5.5\text{m}$
 $d23=1/4J(\text{NCO})=12\text{m}$
 $d22=1/4J(\text{COCA})=4\text{m}$

$d27=\text{CT}(\text{CA})=13.8\text{m}$
 $d4=1/4J(\text{CH})=1.7\text{m}$

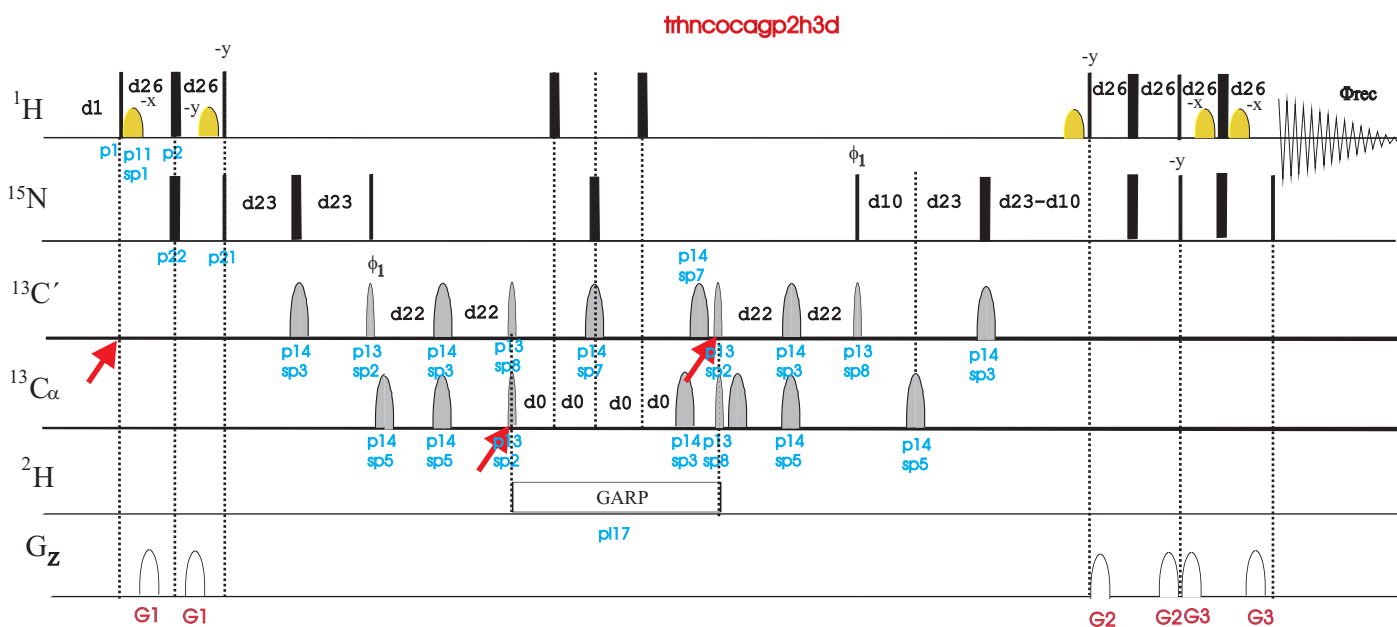
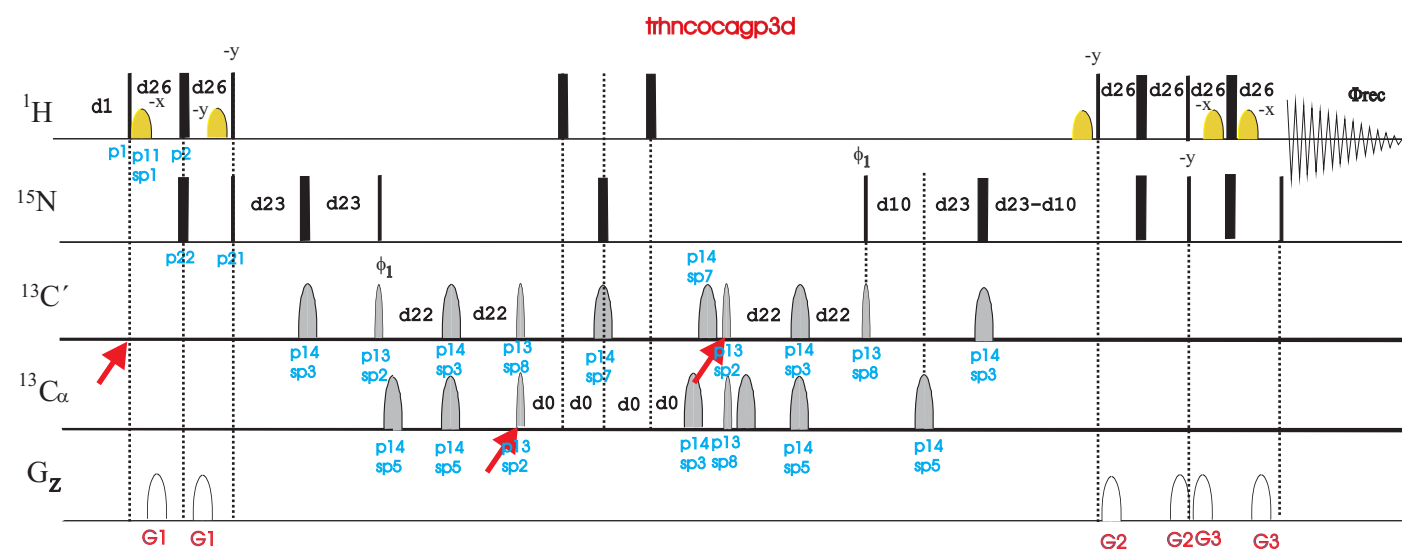
hncocagp3d



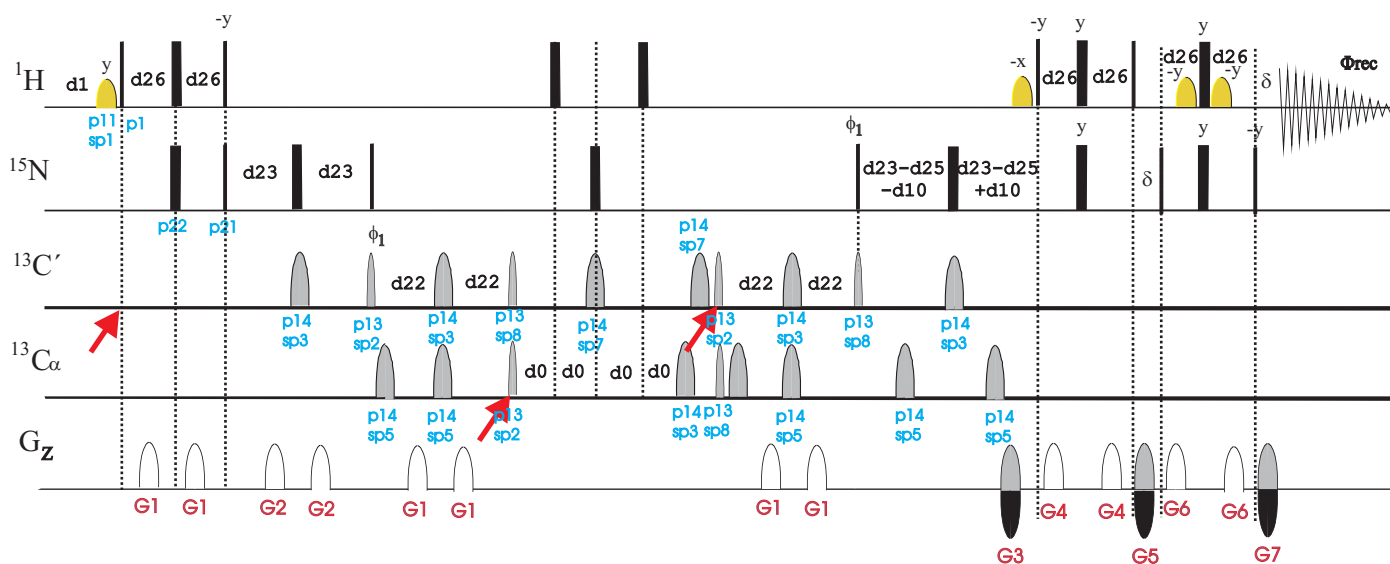
hncocagp2h3d



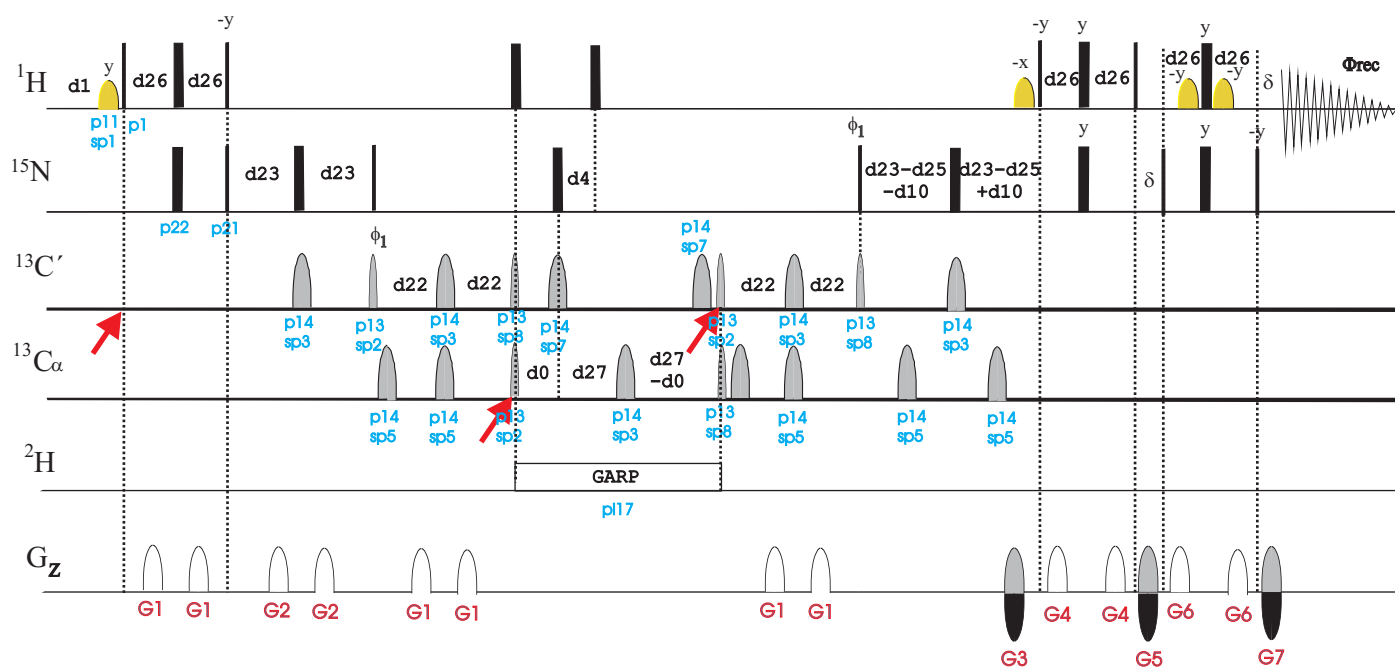
[illegible]



trhncocaetgp3d



trhncocetgp2h3d



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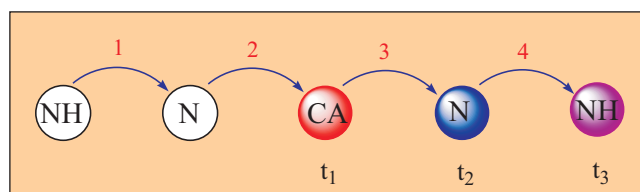
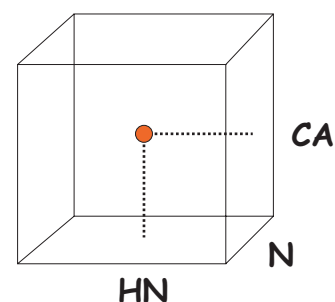
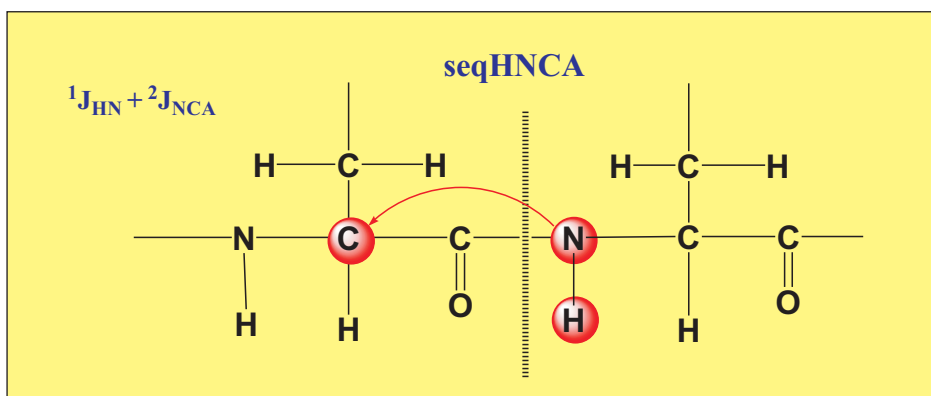
3D SEQUENTIAL HNCA

3D sequential-HNCA experiment

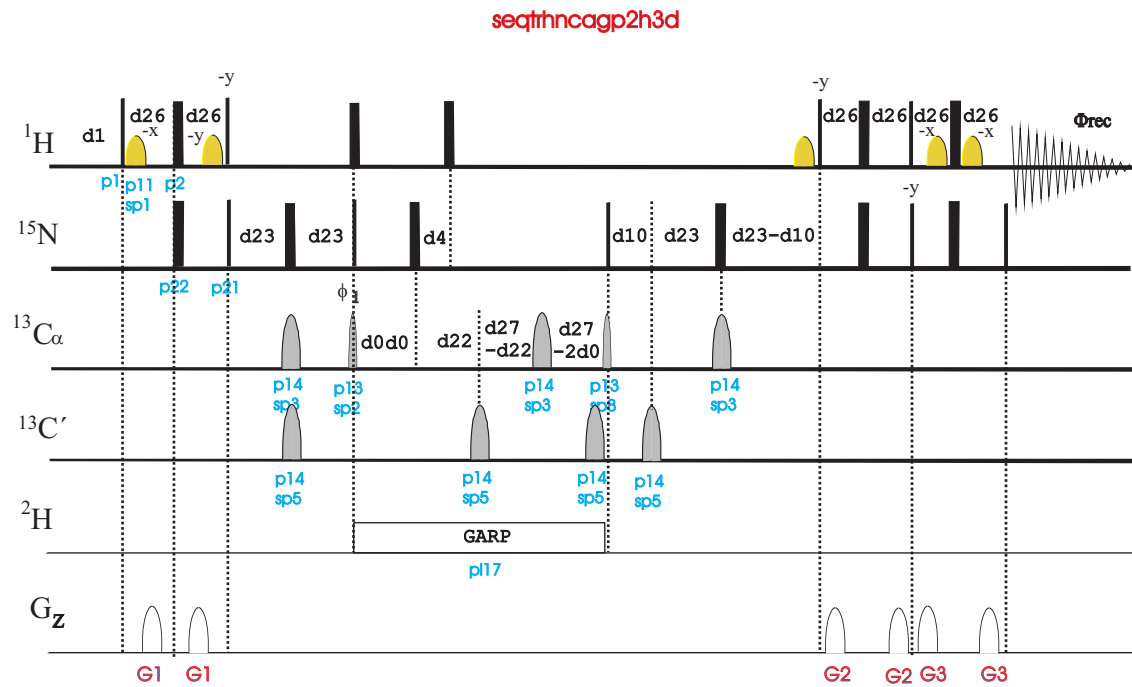
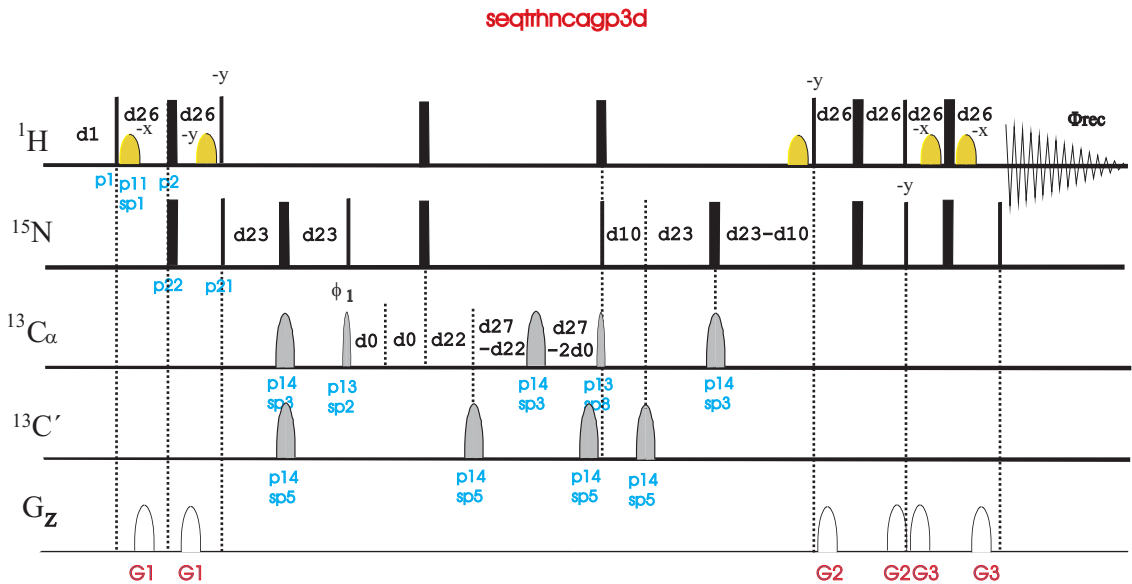
3D Sequential HNCA using TROSY (**seqtrhncagp3d** | **SEQTRHNCAGP3D**)

- with ^2H -decoupling (**seqtrhncagp2h3d** | **SEQTRHNCAGP2H3D**)
- with gradient echo-antiecho (**seqtrhncagp3d** | **SEQTRHNCAGP3D**)
- with gradient echo-antiecho and with ^2H -decoupling (**seqtrhncagp2h3d** | **SEQTRHNCAGP2H3D**)

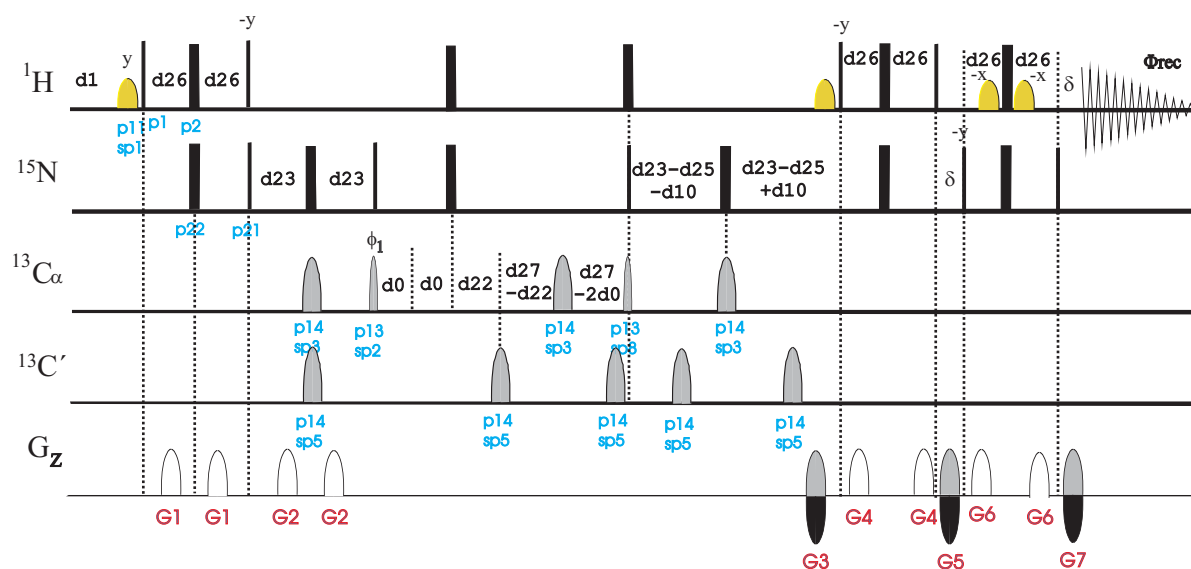
Also see: HNCA, intra-HNCA, , HN(CO)CA



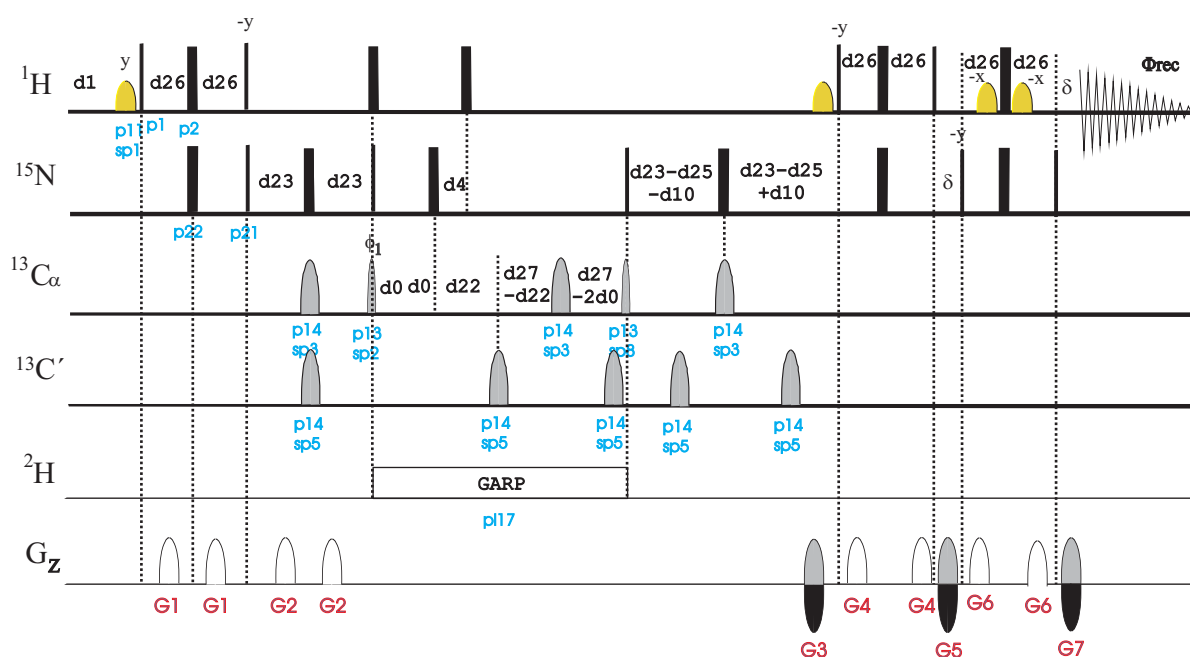
$d26 = 1/4J(\text{NH}) = 2.3\text{m}$
 $d23 = 1/4J(\text{NCA}) = 12\text{m}$
 $d22 = 1/4J(\text{CACO}) = 4.5\text{m}$
 $d27 = 1/4J(\text{CACB}) = 13.3\text{m}$
 $d25 = 1/4J(\text{NH}) = 2.3\text{m}$



seqtrhncatgp3d



seqtrhncatgp2h3d



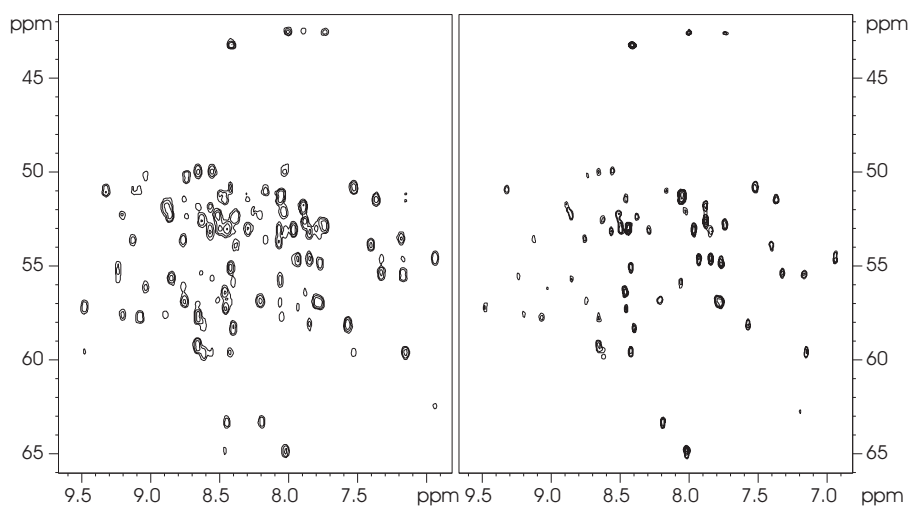
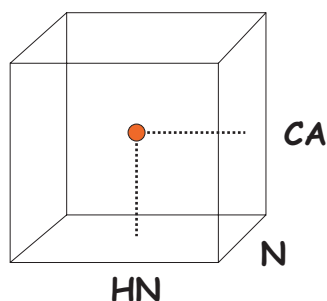
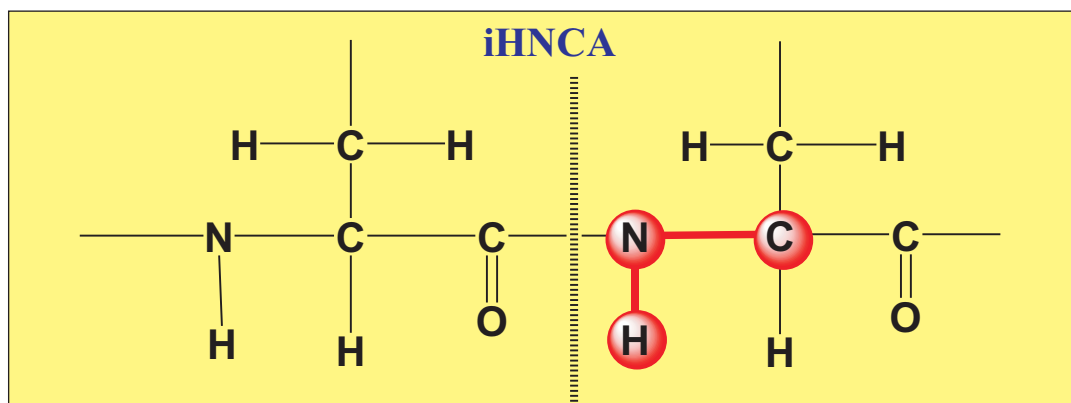
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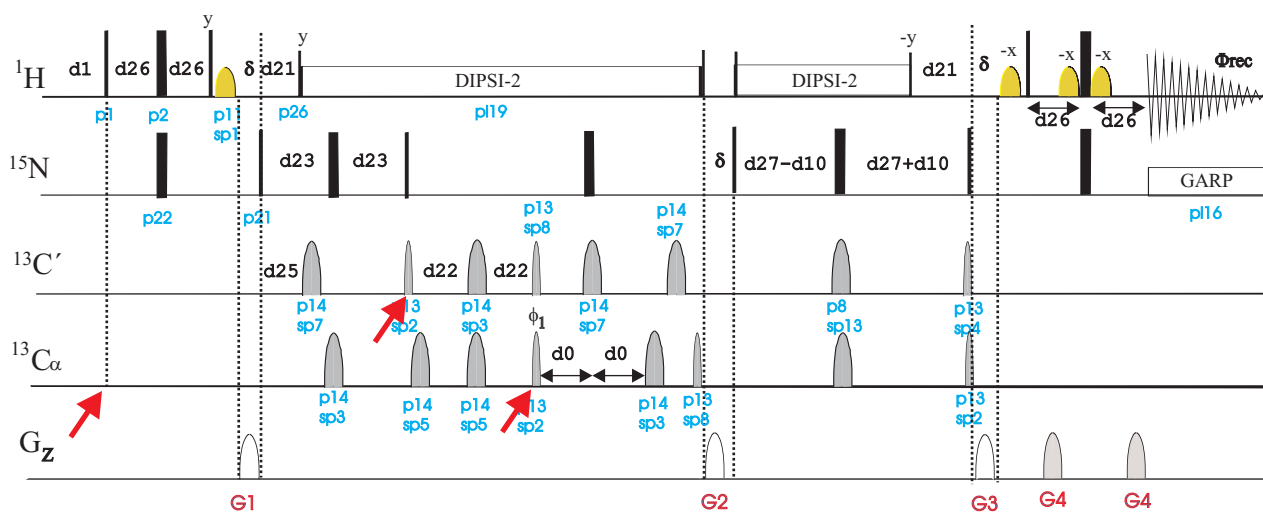
3D INTRA-HNCA

3D intra-HNCA experiment

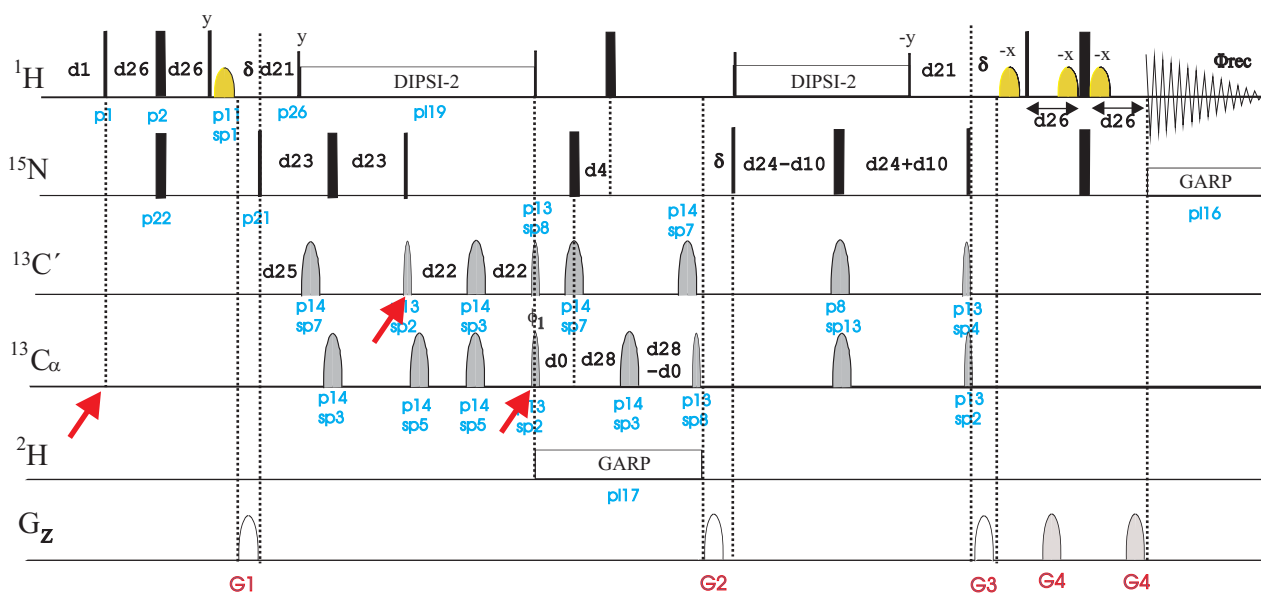
- 3D Intra-HNCA using PEP (**hncaigp3d** | HNCAIGP3D)
 - with ^2H -decoupling (**hncaigp2h3d** | HNCAIGP2H3D)
- 3D Intra-HNCA using WATERGATE (**hncaigpwg3d** | HNCAIGPWG3D)
 - with ^2H -decoupling (**hncaigpwg2h3d** | HNCAIGPWG2H3D)
- 3D Intra-HNCA using TROSY (**trhncaigp3d** | TRHNCAIGP3D)
 - with ^2H -decoupling (**trhncaigp2h3d** | TRHNCAIGP2H3D)
 - with gradient echo-antiecho (**trhncaietgp3d** | TRHNCAIETGP3D)
 - with gradient echo-antiecho and with ^2H -decoupling (**trhncaietgp2h3d** | TRHNCAIETGP2H3D)



hncalgpwg3d



hncalgpwg2h3d





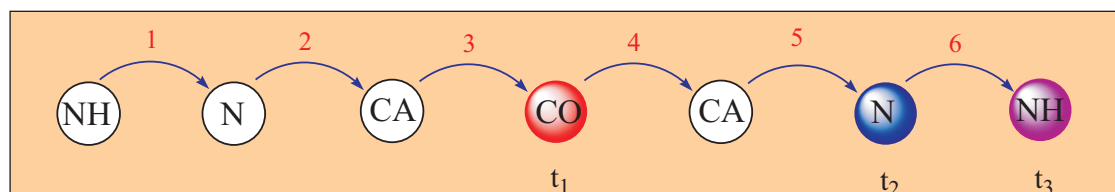
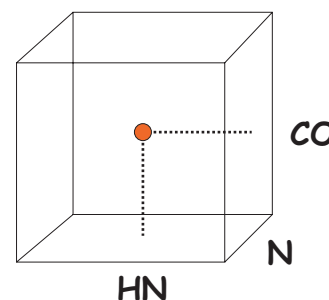
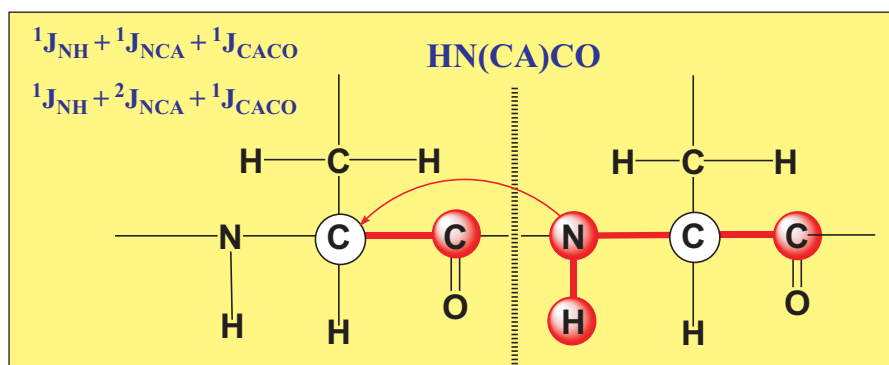
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3D HN(CA)CO

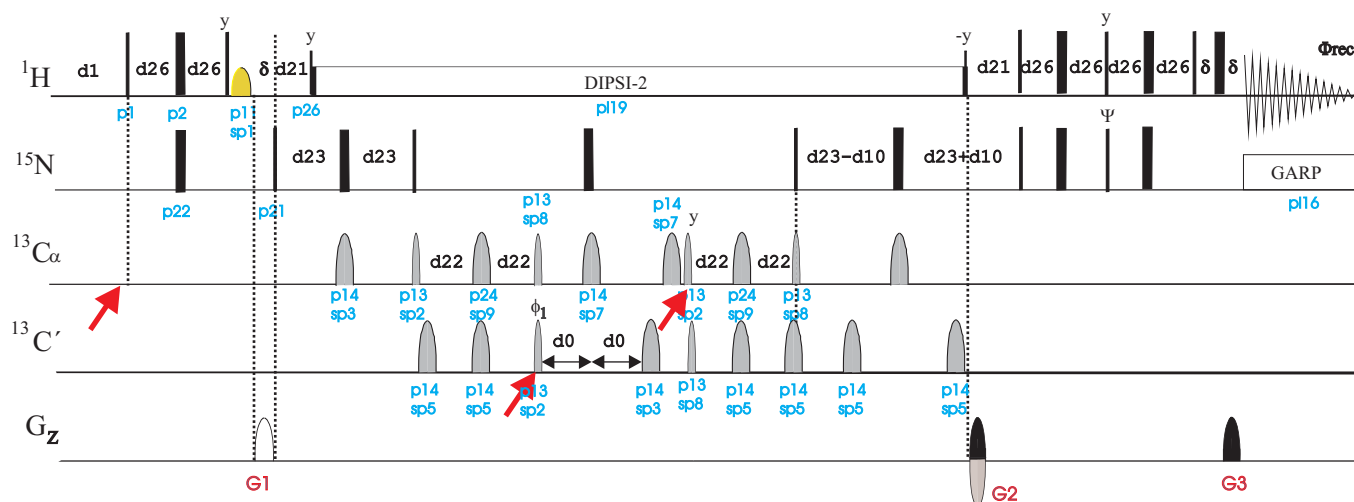
3D HN(CA)CO experiment

- 3D HN(CA)CO using PEP (**hncacogp3d** | HNCACOGP3D)
- with ^2H -decoupling and suppression of protonated carbons (**hncacogp2h3d** | HNCACOGP2H3D)
 - with ^2H -decoupling (**hncacogp2h3d.2** | HNCACOGP2H3D.2)
- 3D HN(CA)CO using WATERGATE (**hncacogpwg3d** | HNCACOGPWG3D)
- with ^2H -decoupling and suppression of protonated carbons (**hncacogpwg2h3d** | HNCACOGPWG2H3D)
- 3D HN(CA)CO using TROSY (**trhncacogp3d** | TRHNCACOGP3D)
- with ^2H -decoupling (**trhncacogp2h3d** | TRHNCACOGP2H3D)
 - using echo-antiecho gradient (**trhncacoetgp3d** | TRHNCACOETGP3D)
 - using echo-antiecho gradient and with ^2H -decoupling (**trhncacoetgp2h3d** | TRHNCACOETGP2H3D)

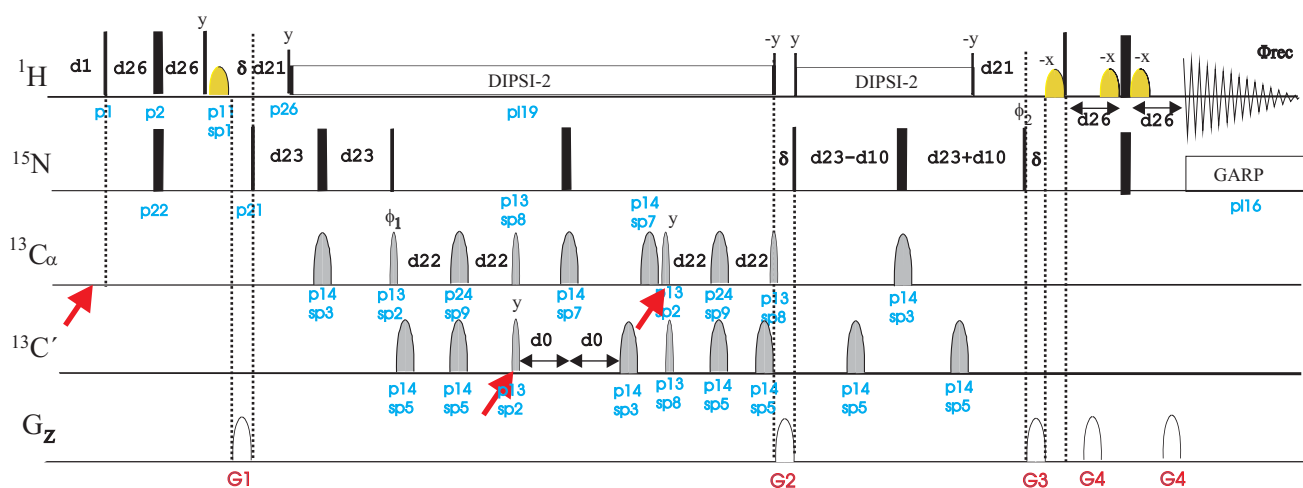


$$\begin{aligned} d26 &= 1/4J(\text{NH}) = 2.3\text{m} \\ d21 &= 1/2J(\text{NH}) = 5.5\text{m} \\ d23 &= 1/4J(\text{NCO}) = 12\text{m} \\ d22 &= 1/4J(\text{COCA}) = 4\text{m} \\ d4 &= 1/4J(\text{CH}) = 1.7\text{m} \end{aligned}$$

hncacogp3d

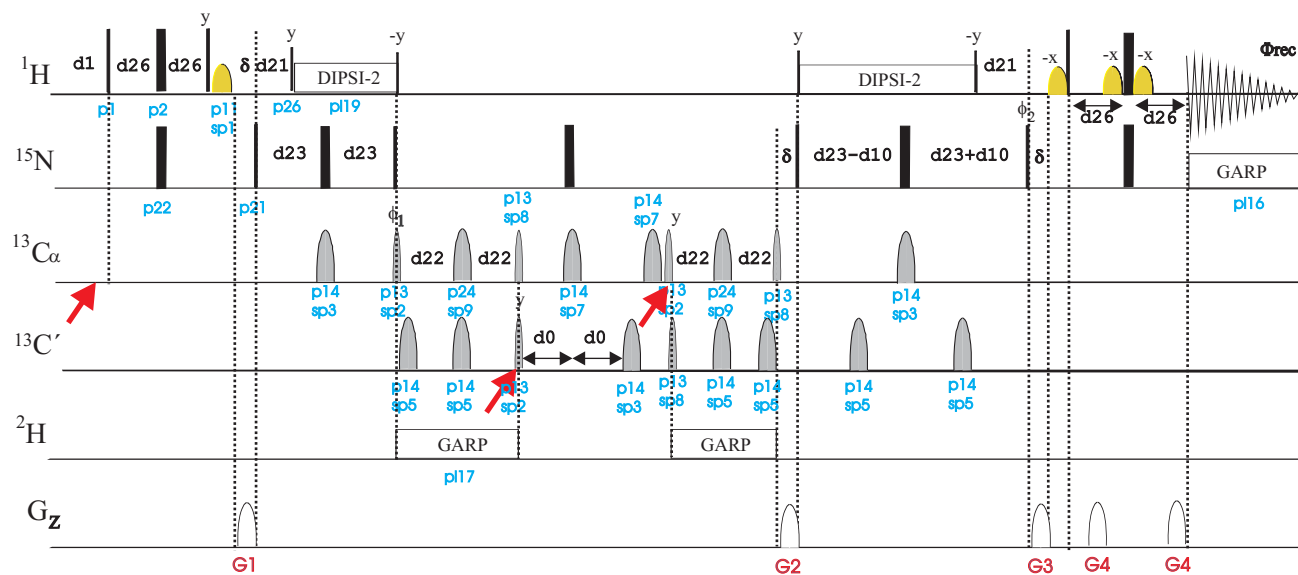


hncacogpwg3d

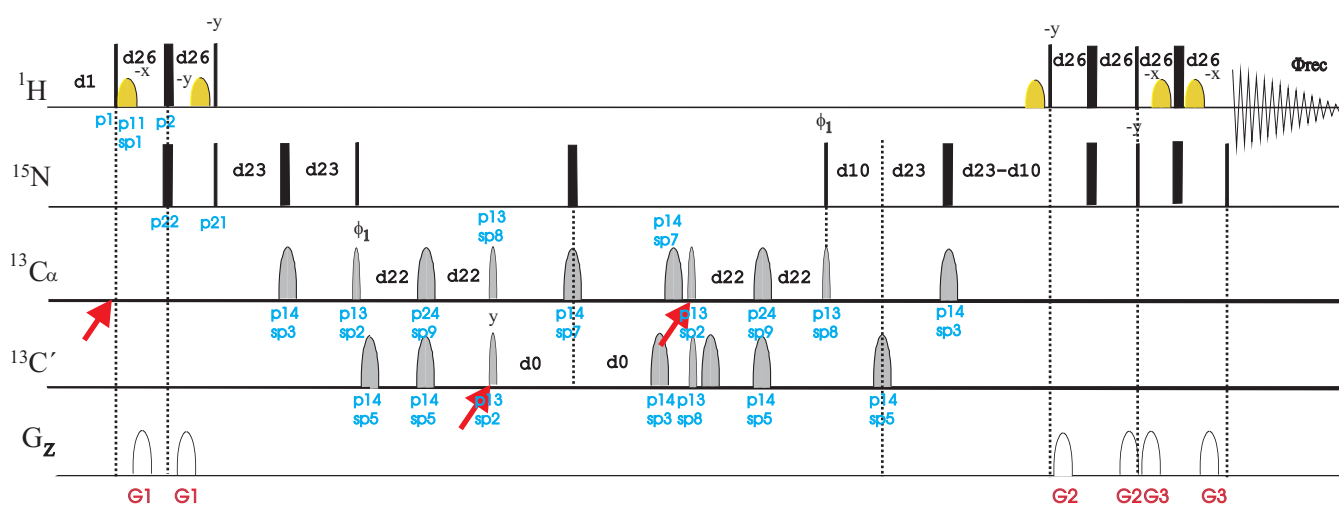




hncacogpwg2h3d



trhncacogp3d

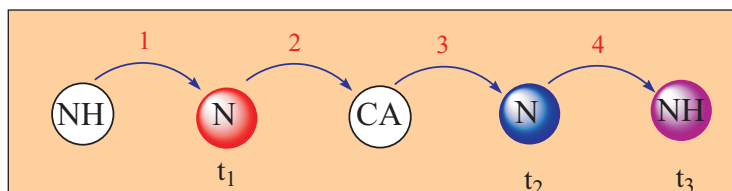
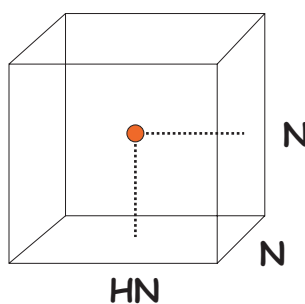
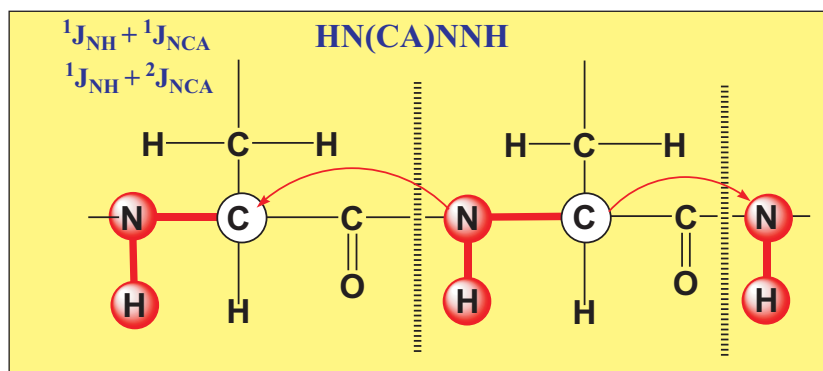


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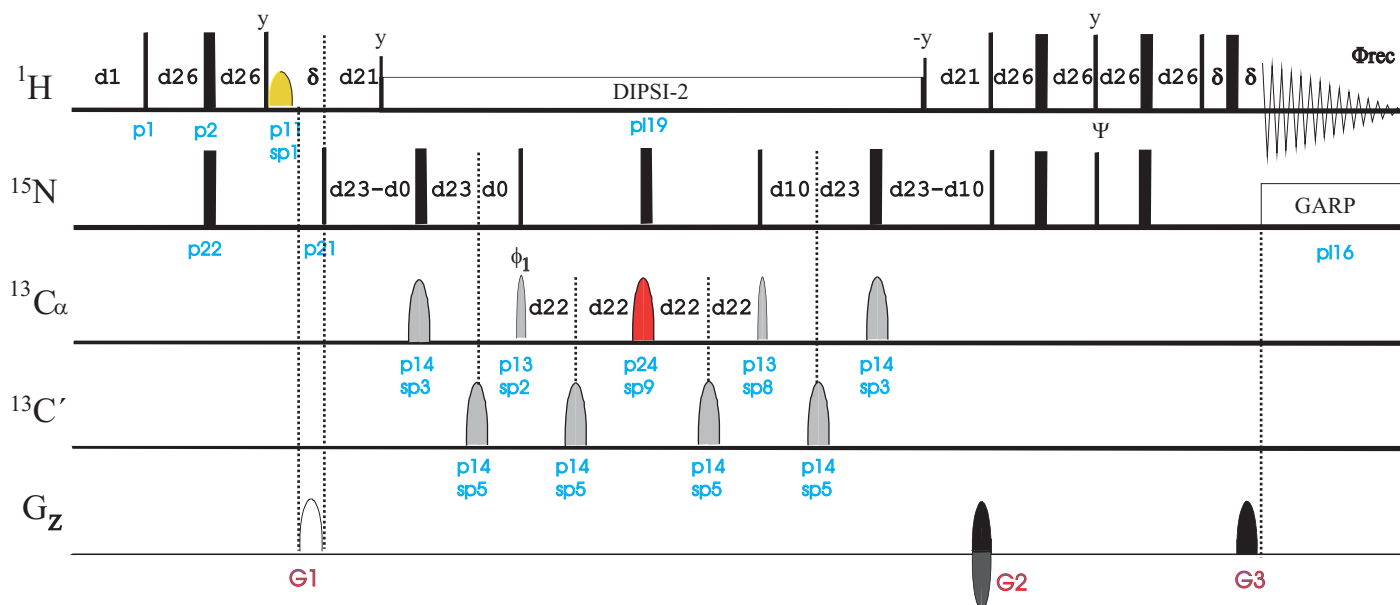
3D HN(CA)NNH

- 3D HN(CA)NNH using PEP (**hncannhgp3d** | HNCANNHGP3D)
- 3D HN(CA)NNH with ^2H -decoupling and PEP (**hncannhgp2h3d** | HNCANNHGP2H3D)

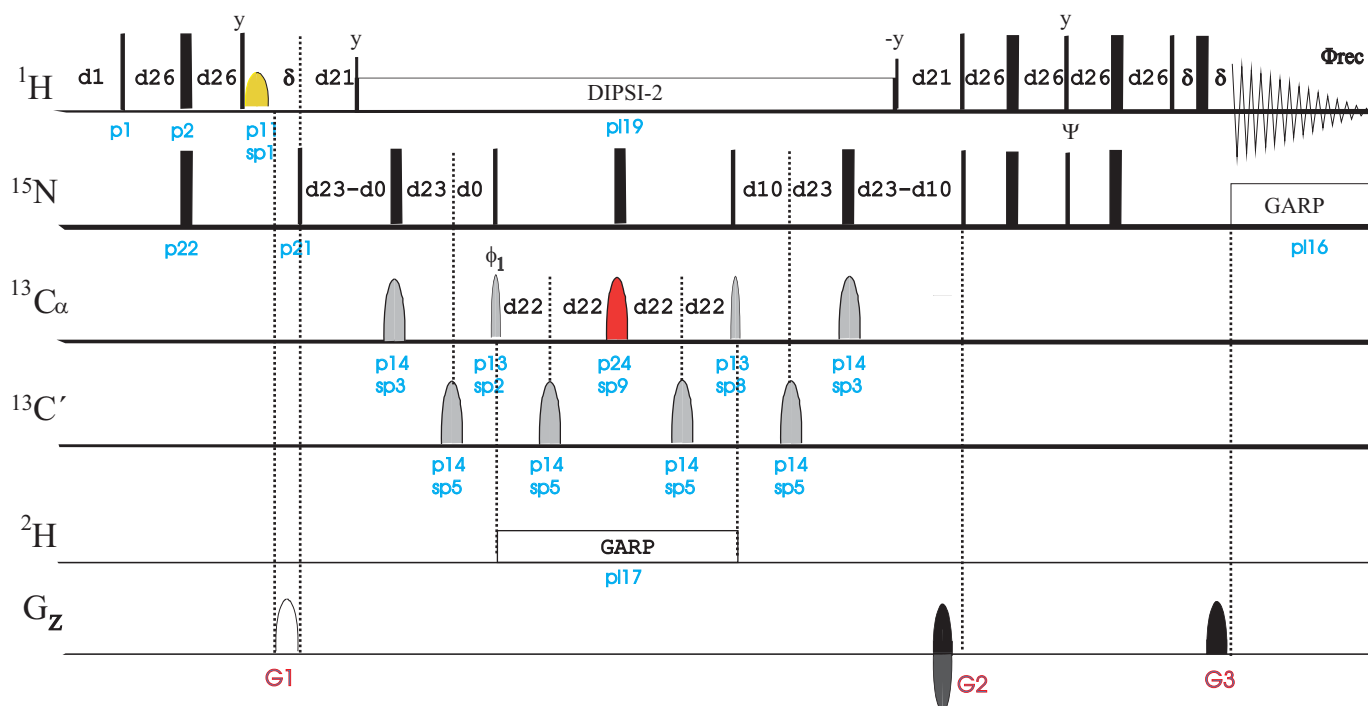


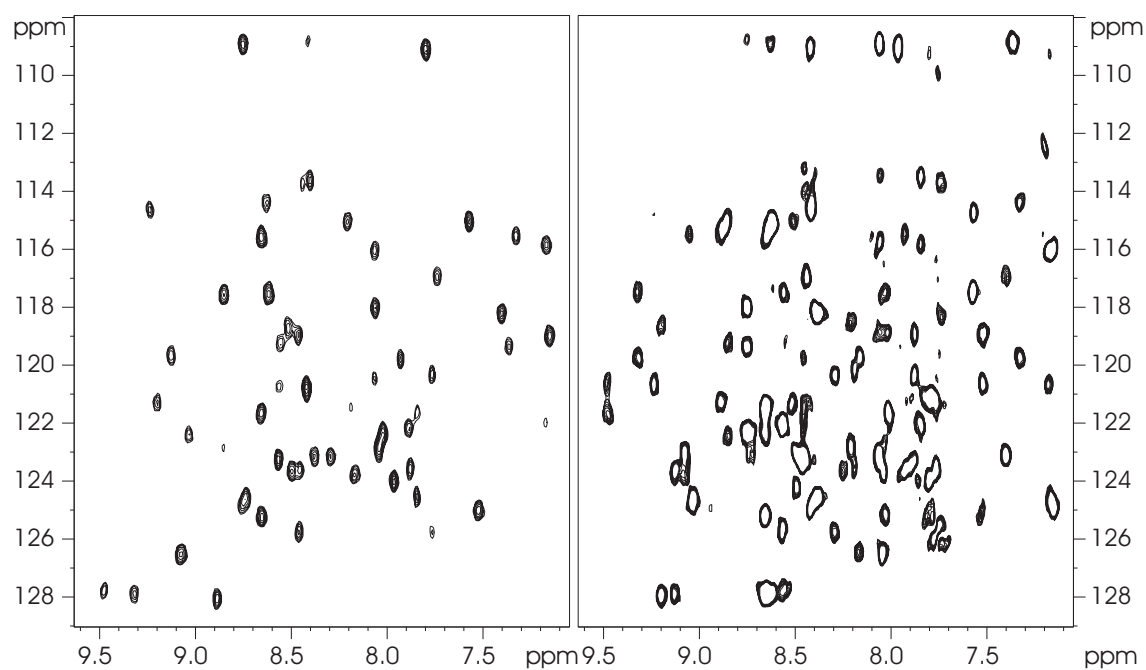
$d26 = 1/4J(\text{NH}) = 2.3\text{m}$
 $d21 = 1/2J(\text{NH}) = 5.5\text{m}$
 $d23 = 1/4J(\text{NCA}) = 12\text{m}$
 $d22 = 1/4J(\text{NCA}) = 12.5\text{m}$

hncannhgp3d



hncannhgp2h3d



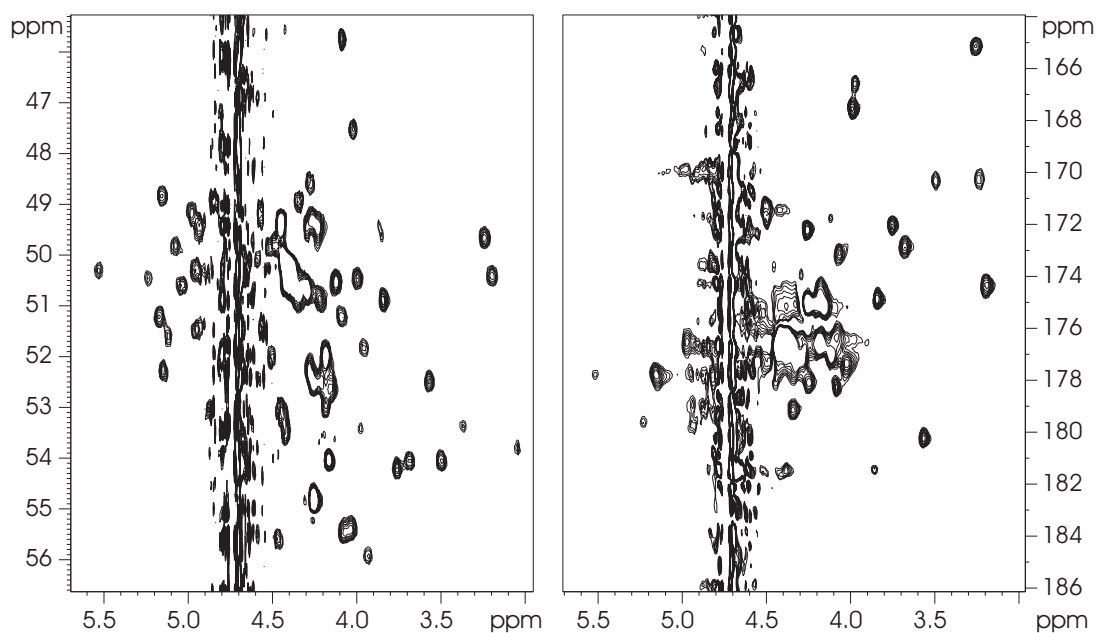
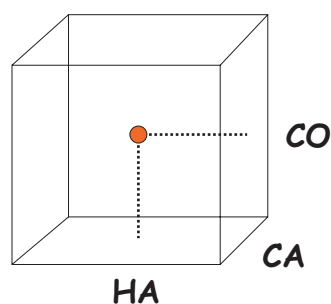
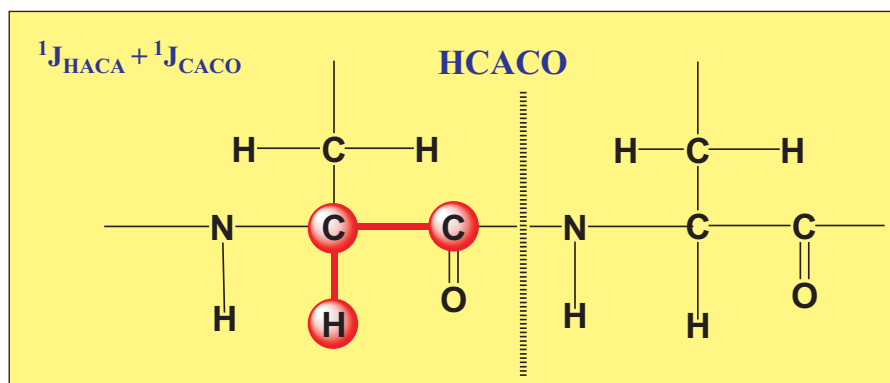


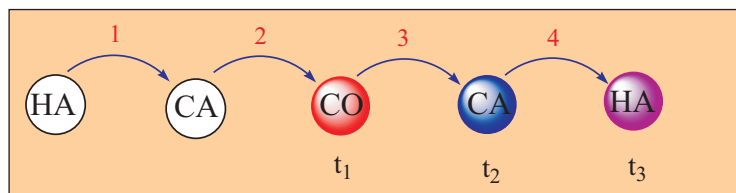
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3D HCACO

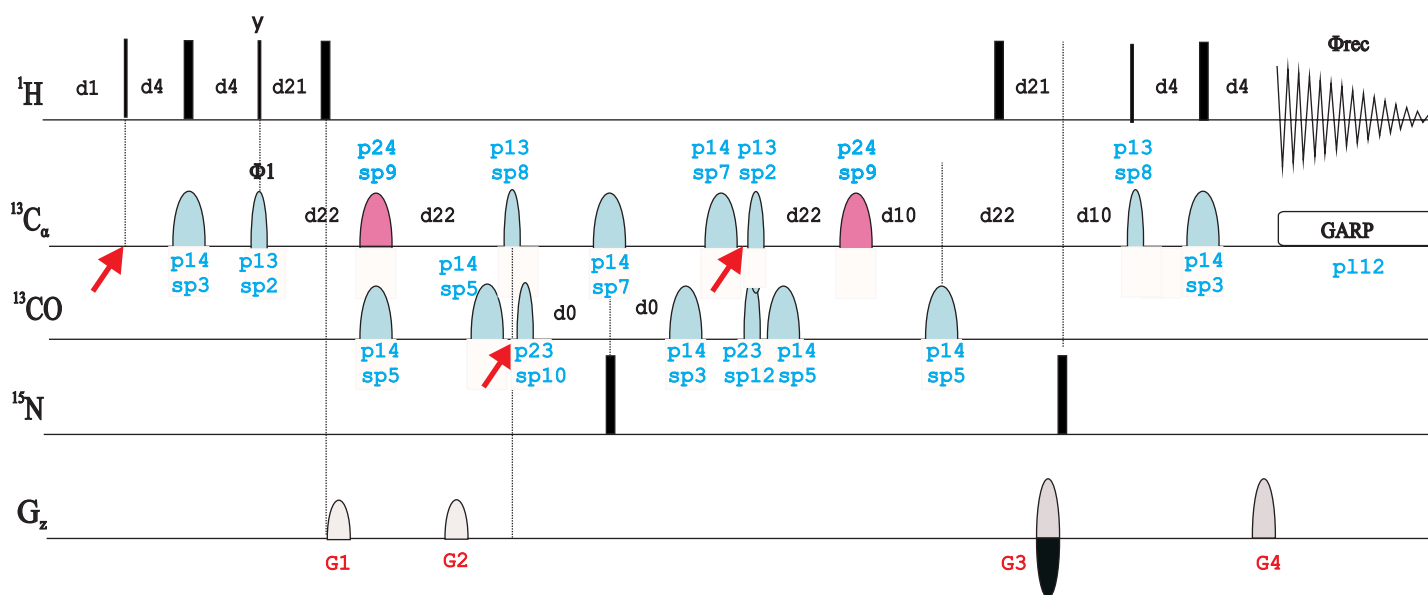
3D HCACO experiment (**hcacogp3d** | HCACOGP3D)





$d4 = 1/4J(\text{CAHA}) = 1.7\text{m}$
 $d21 = 1/4J(\text{CH})$ or $1/6J(\text{CH}) = 1.7\text{m}$ or 1.2m
 $d22 = 1/4J(\text{CACO}) = 4.5\text{m}$

hcaacogp3d



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3D MISCELLANEOUS
PROTEIN NMR

3D HN(CA)HA (**hncah3d**)

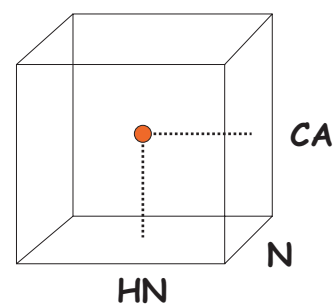
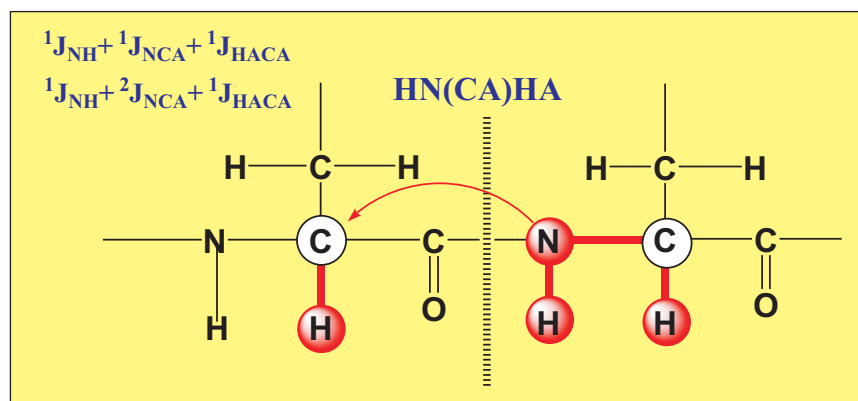
2D H(CA)N with ^2H -decoupling (**hcangp2h**)

2D H[CACO]N with ^2H -decoupling (**hcacong2h**)

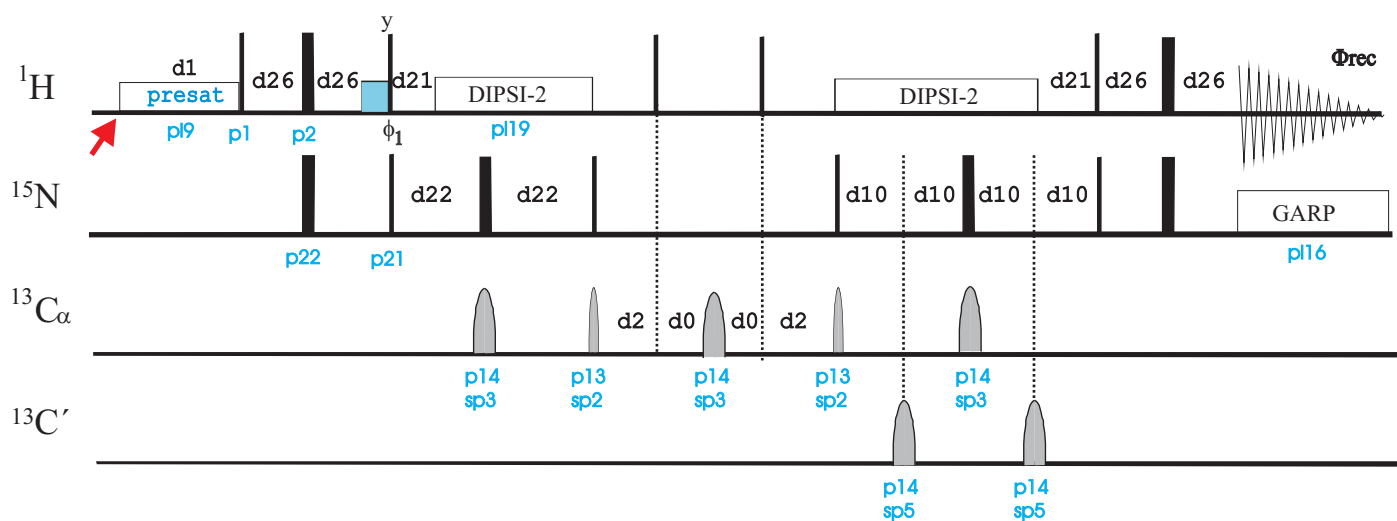
3D HCAN using PEP (**hcangp3d**)

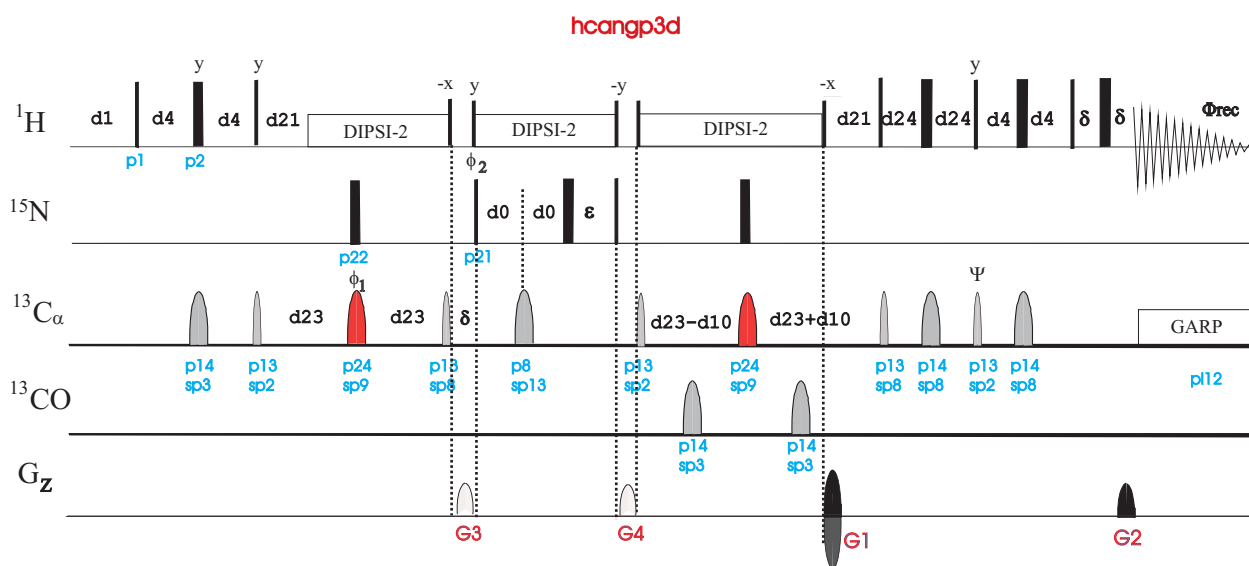
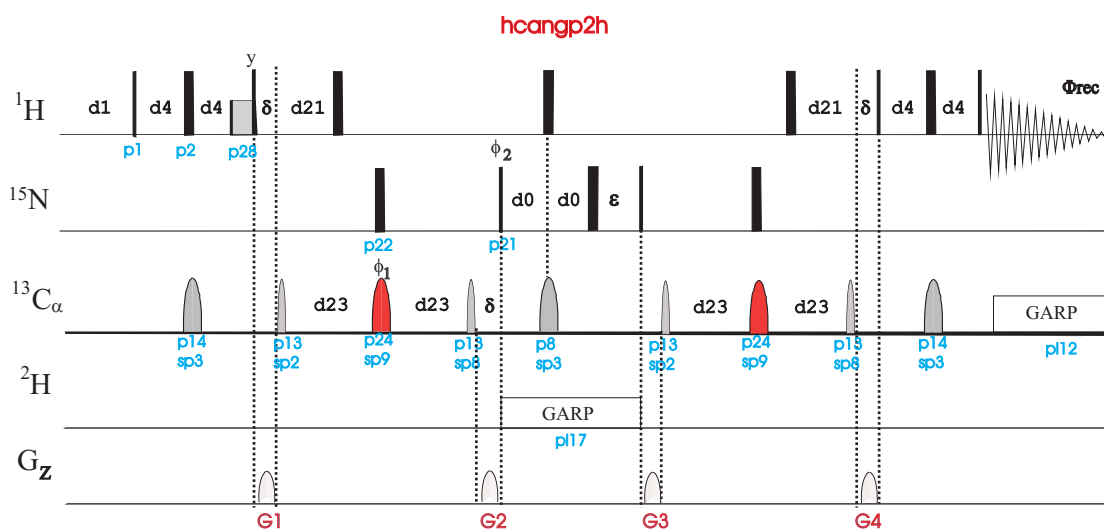
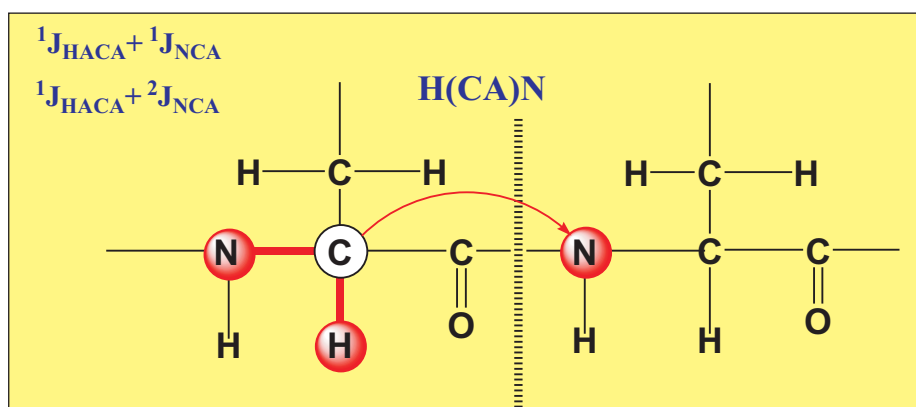
3D HCACON using PEP (**hcacong3d**)

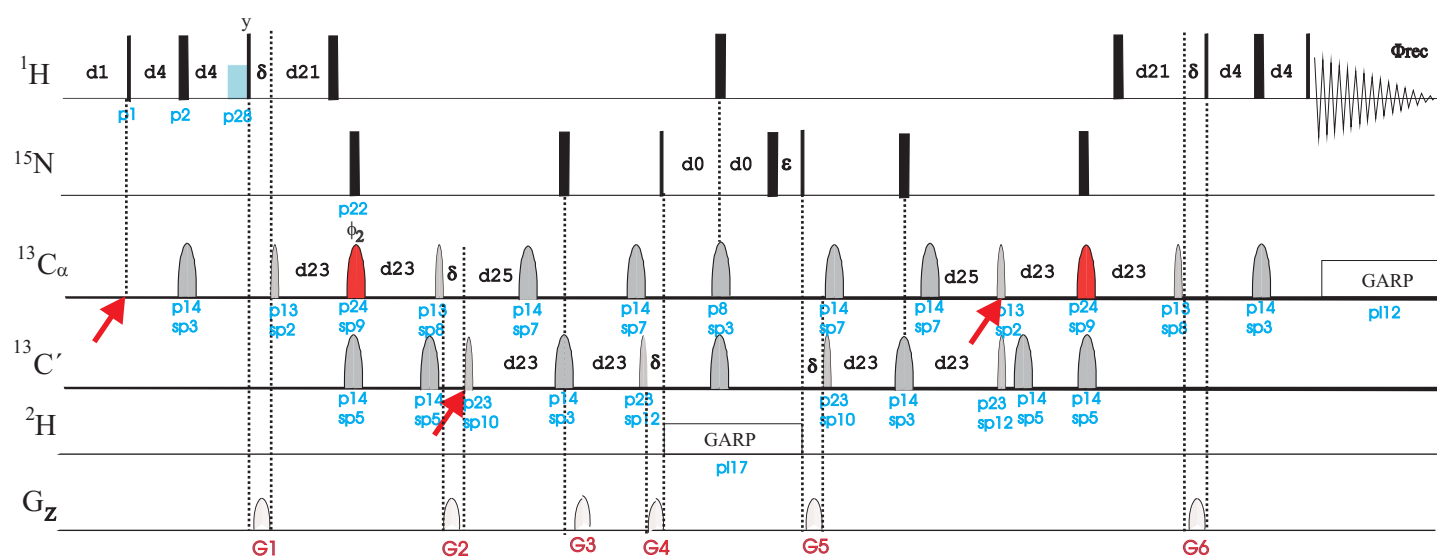
3D HCBCACON (**hcbcacong3d**)

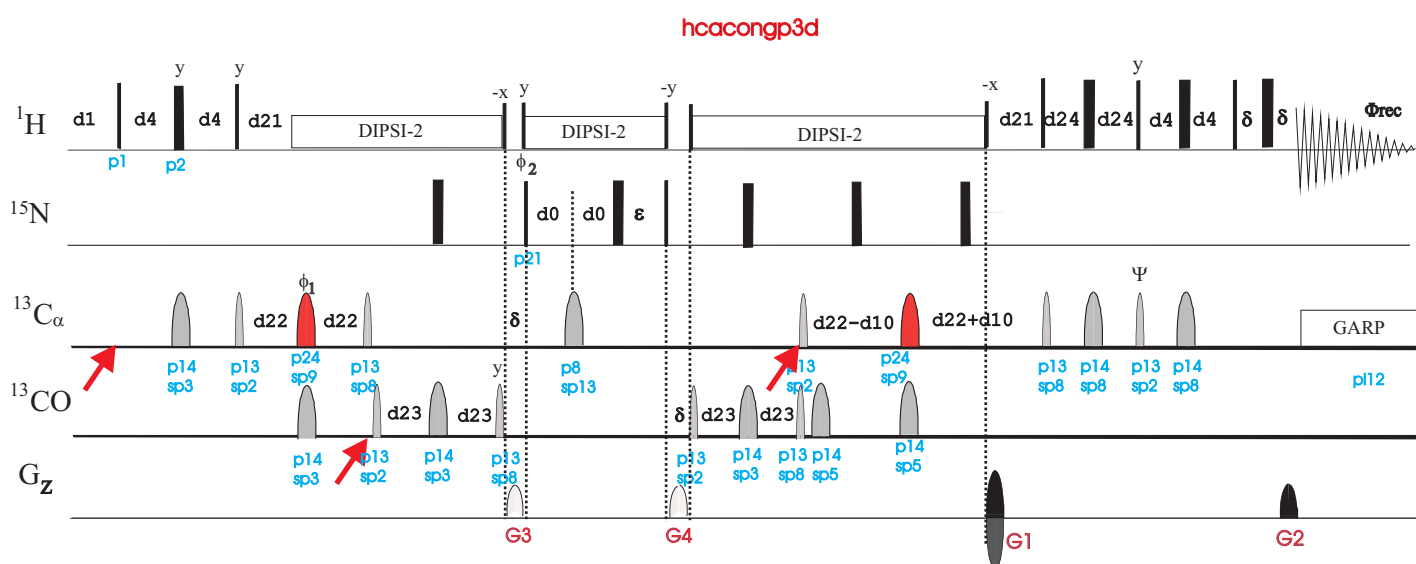
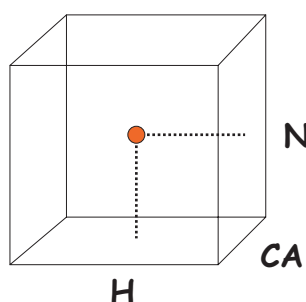


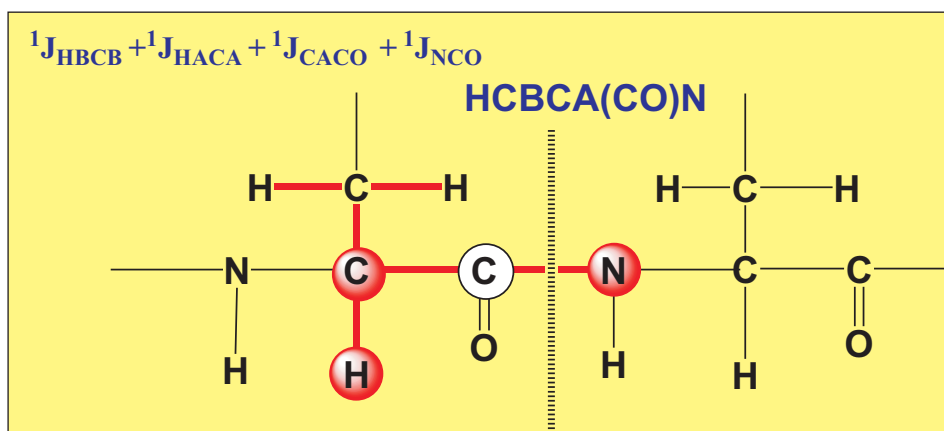
hncah3d



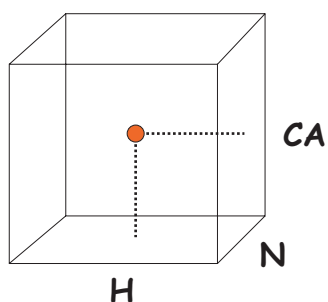
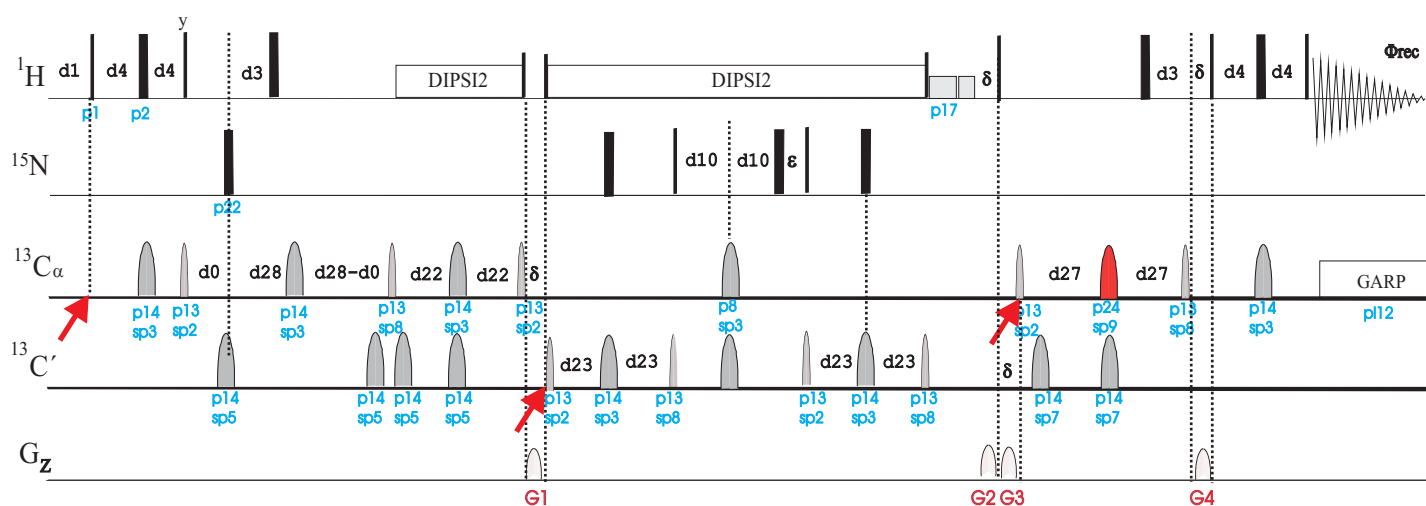








hcbcacong3d

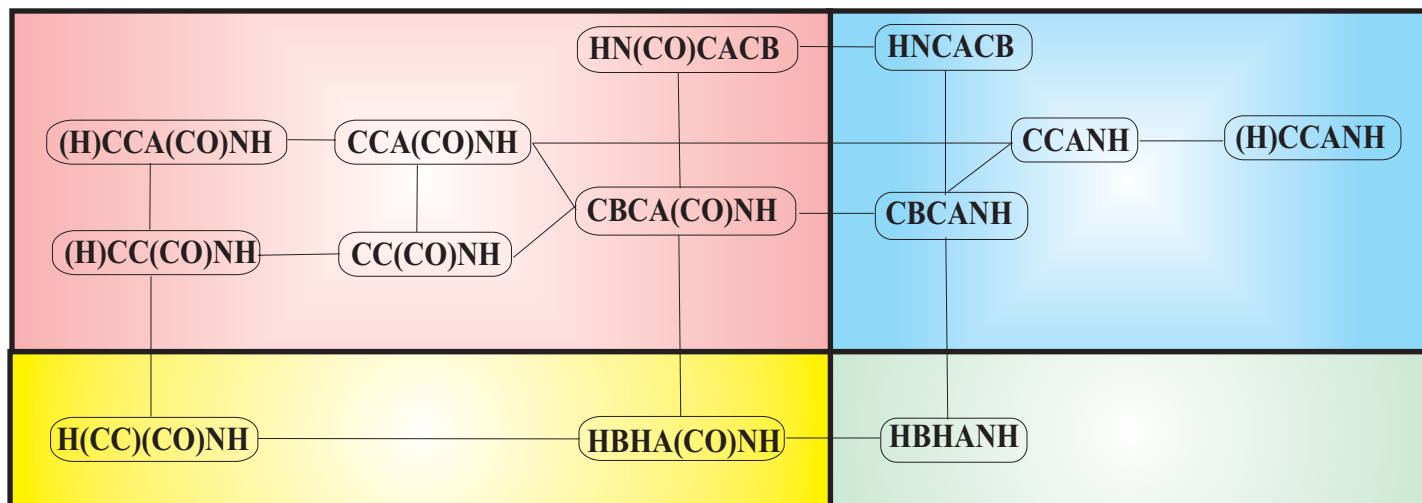


BRUKER PULSE PROGRAM CATALOGUE

NMRGuide

PROTEIN NMR.
BACKBONE-SIDECHAIN
3D EXPERIMENTS

BACKBONE-SIDECHAIN

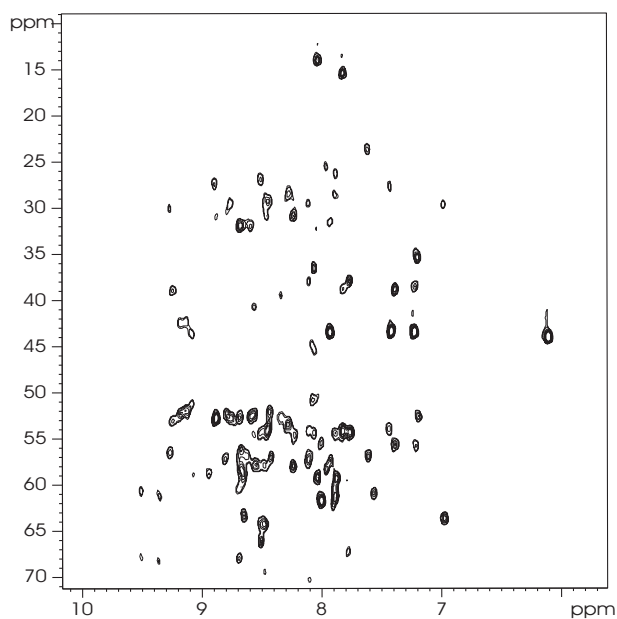
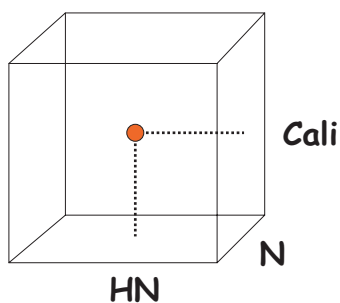
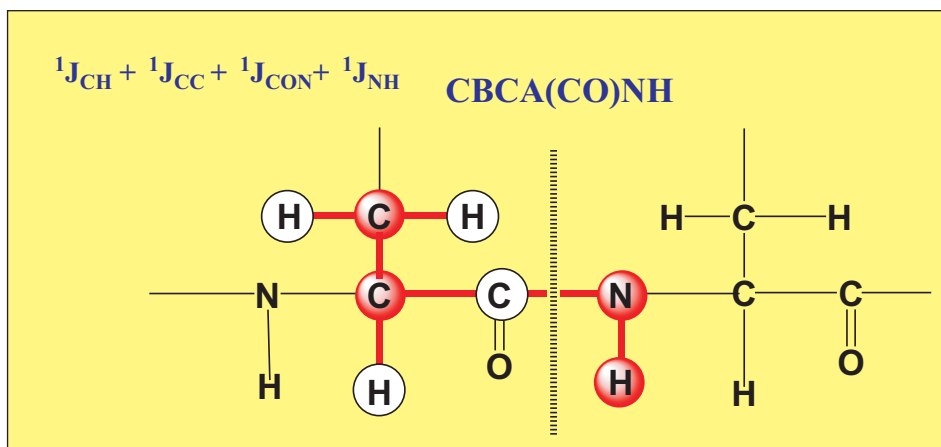


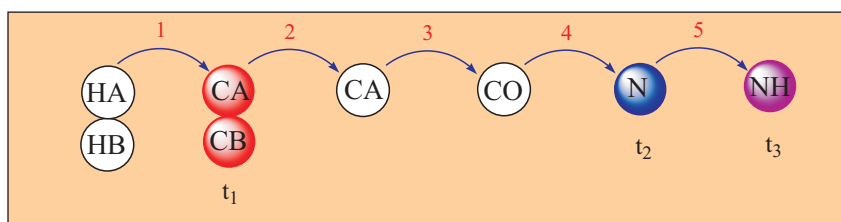
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NMRGuide

3D CBCA(CO)NH

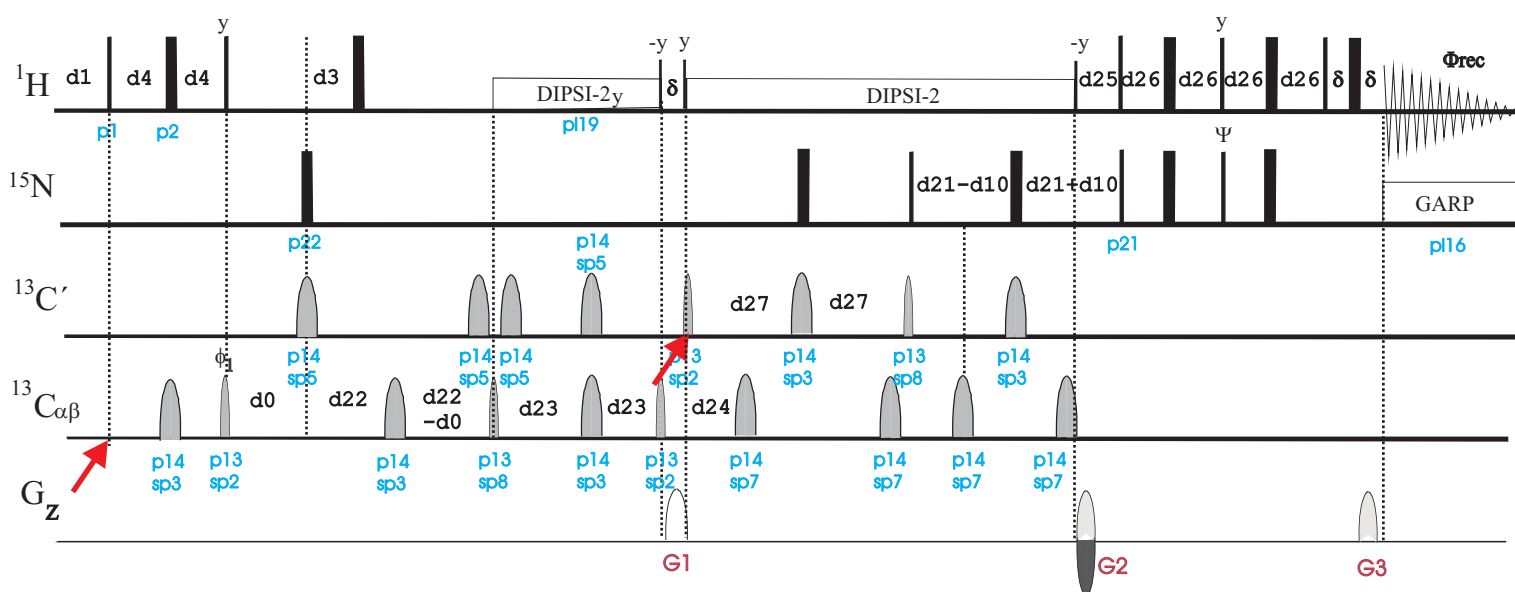
- 3D CBCA(CO)NH using PEP (**cbcaconhgp3d** | CBCACONHGP3D)
- 3D CBCA(CO)NH using WATERGATE (**cbcaconhgpwg3d** | CBCACONHGPWG3D)
- 3D CBCA(CO)NH using TROSY (**trcbcaconhgp3d** | TRCBCACONHGP3D)
- 3D CBCA(CO)NH using TROSY and gradient echo-antiecho (**trcbcaconhetgp3d** | TRCBCACONHETGP3D)



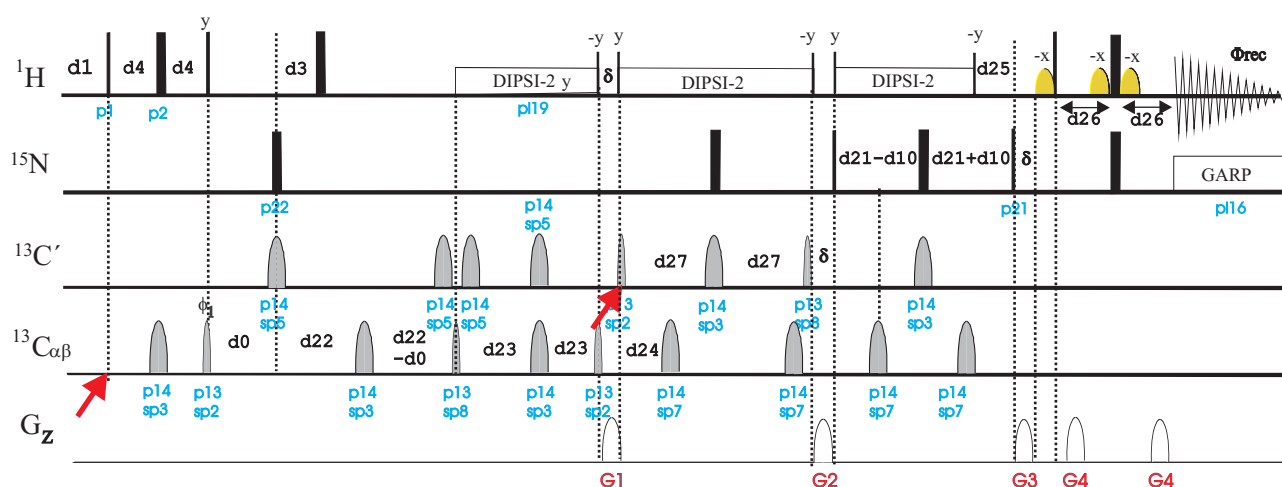


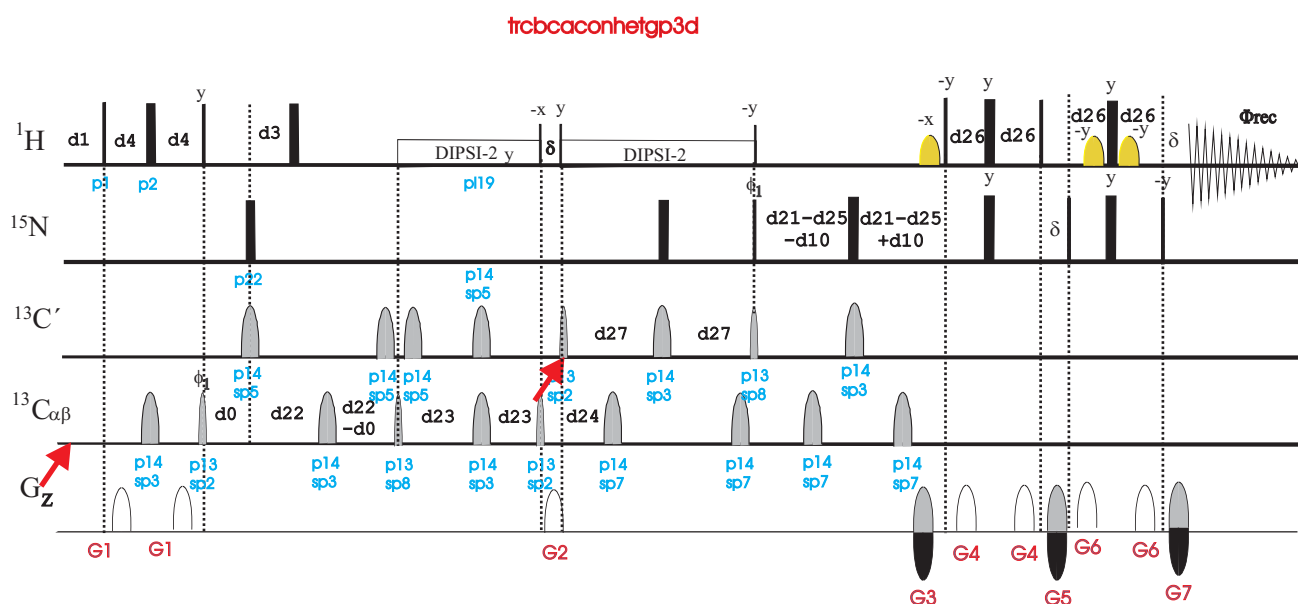
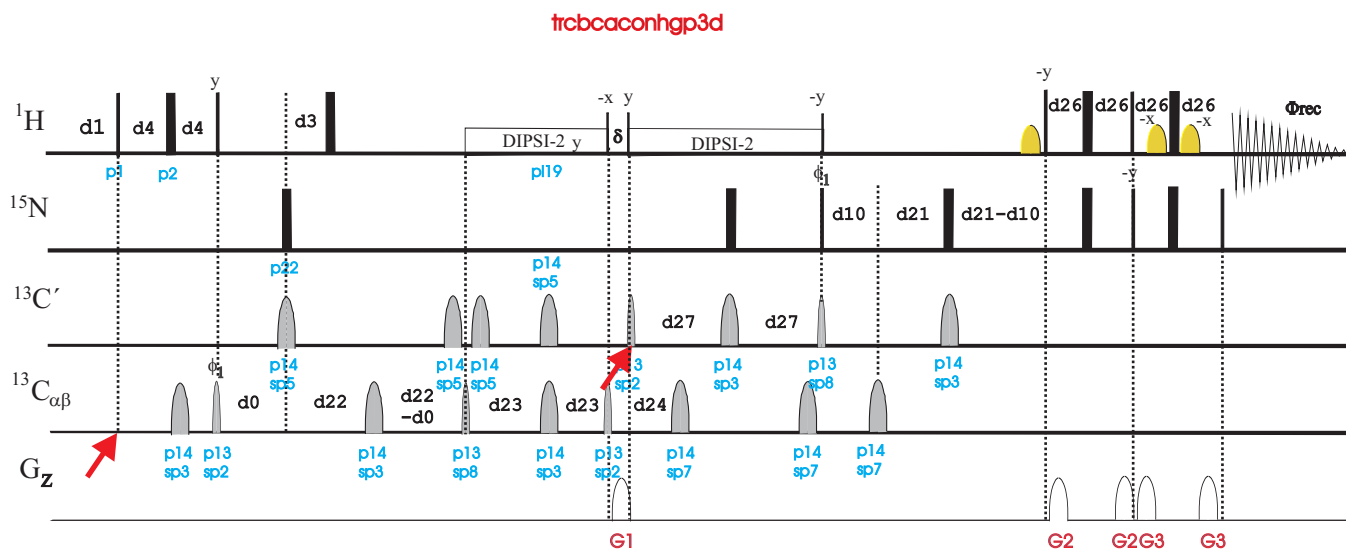
$d4=1/4J(\text{CH})=1.7\text{m}$
 $d3=1/6J(\text{CH})=1.1\text{m}$
 $d22=1/4J(\text{CBCA})=3.6\text{m}$
 $d23=1/4J(\text{CBCA})=3.6\text{m}$
 $d24=1/4J(\text{CACO})=4.4\text{m}$
 $d27=1/4J(\text{NCO})=12.4\text{m}$
 $d21=1/4J(\text{NCO})=12.4\text{m}$
 $d25=1/2J(\text{NH})=5.5\text{m}$
 $d26=1/4J(\text{NH})=2.3\text{m}$

cbcacaonhgp3d



cbcacaonhgpwg3d





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NMRGuide

3D HN(CO)CACB

3D HN(CO)CACB experiment

3D HN(CO)CACB using PEP (**hncocacbgp3d** | HNCOCACBGP3D):

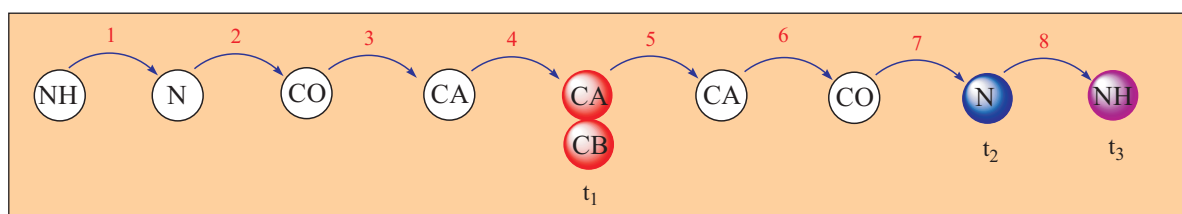
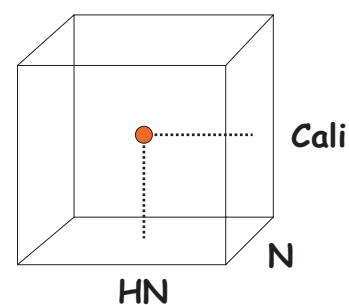
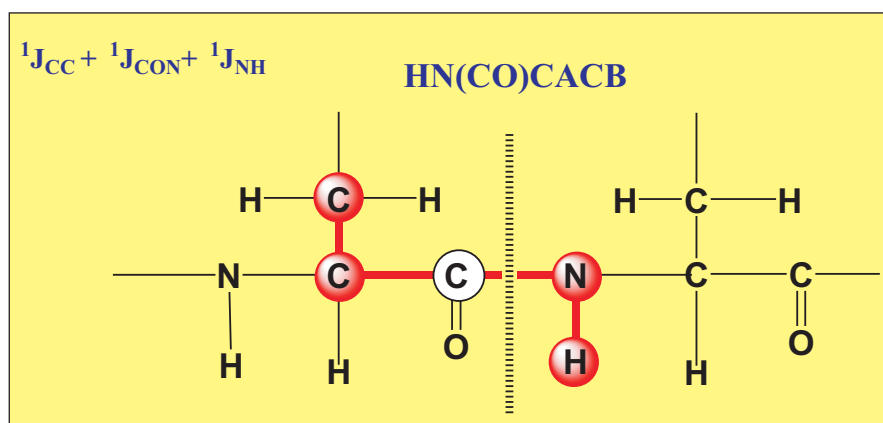
- with ^2H -decoupling (**hncocacbgp2h3d** | HNCOCACBGP2H3D)

3D HN(CO)CACB using WATERGATE (**hncocacbgpwg3d** | HNCOCACBGPWG3D)

- with ^2H -decoupling (**hncocacbgpwg2h3d** | HNCOCACBGPWG2H3D)

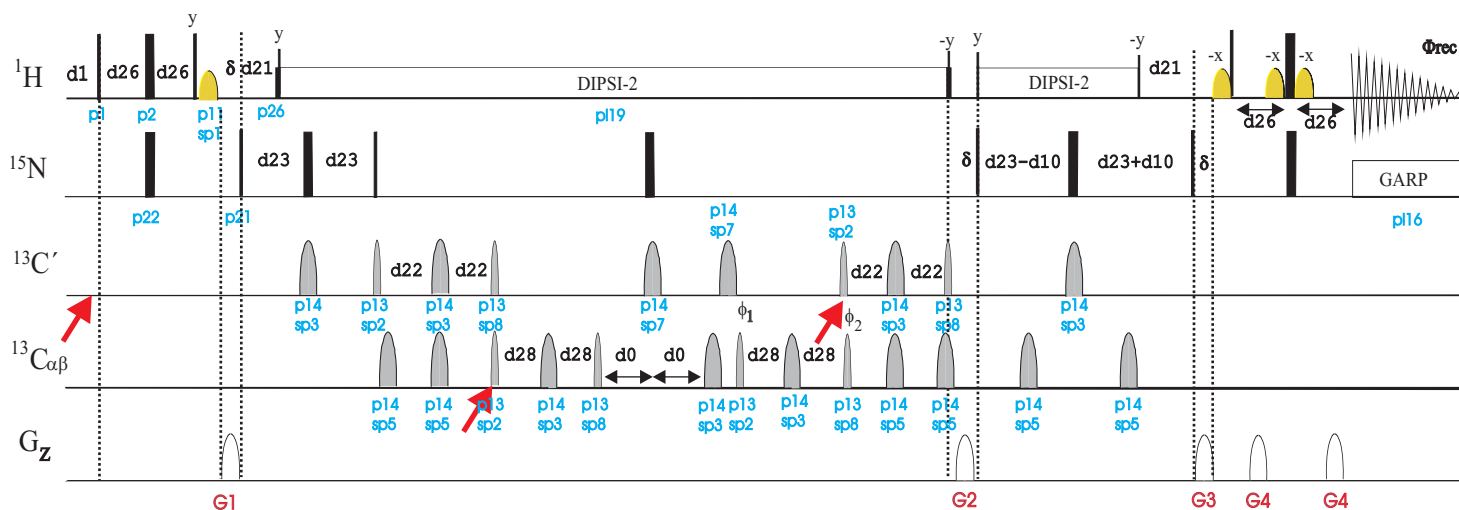
3D HN(CO)CACB using TROSY (**trhncocacbgp3d** | TRHNCOCACBGP3D):

- with ^2H -decoupling (**trhncocacbgp2h3d** | TRHNCOCACBGP2H3D)
- using gradient echo-antiecho (**trhncocacbetgp3d** | TRHNCOCACBETGP3D)
- using gradient echo-antiecho and with ^2H -decoupling (**trhncocacbetgp2h3d** | TRHNCOCACBETGP2H3D)

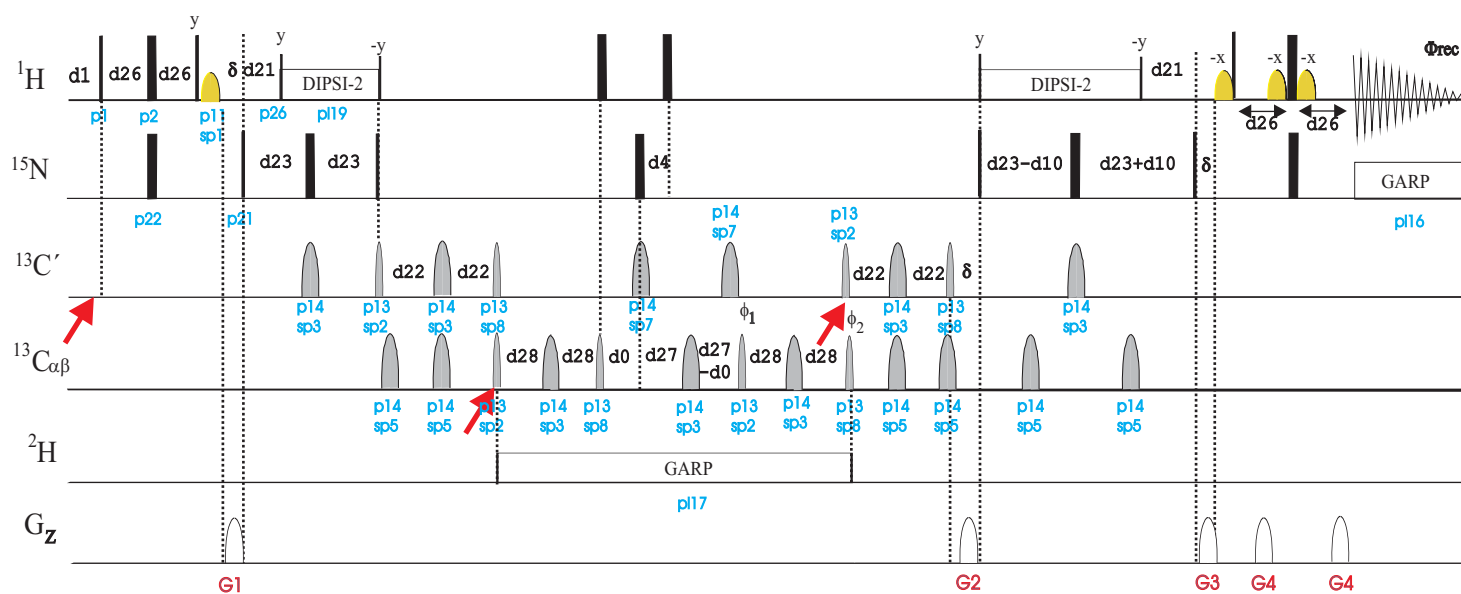


$d26 = 1/4J(\text{NH}) = 2.3\text{m}$
 $d21 = 1/2J(\text{NH}) = 5.5\text{m}$
 $d23 = 1/4J(\text{NCO}) = 12\text{m}$
 $d22 = 1/4J(\text{CACO}) = 4\text{m}$
 $d28 = 1/4J(\text{CACB}) = 3.6\text{m}$

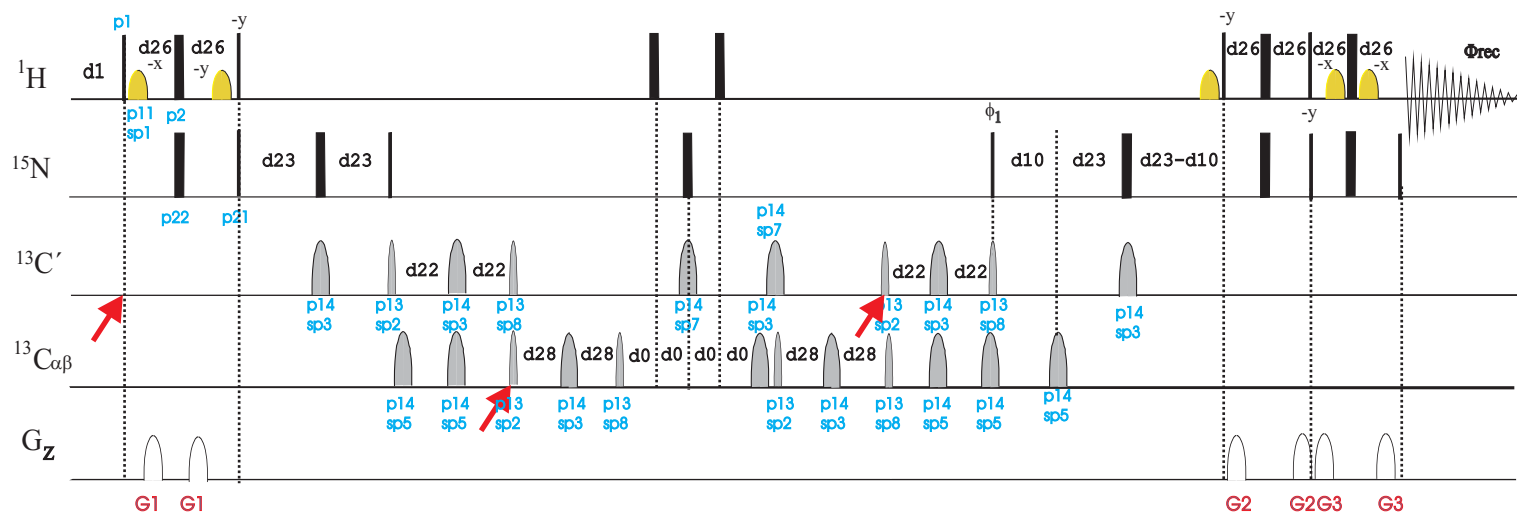
hncocacbgpwg3d



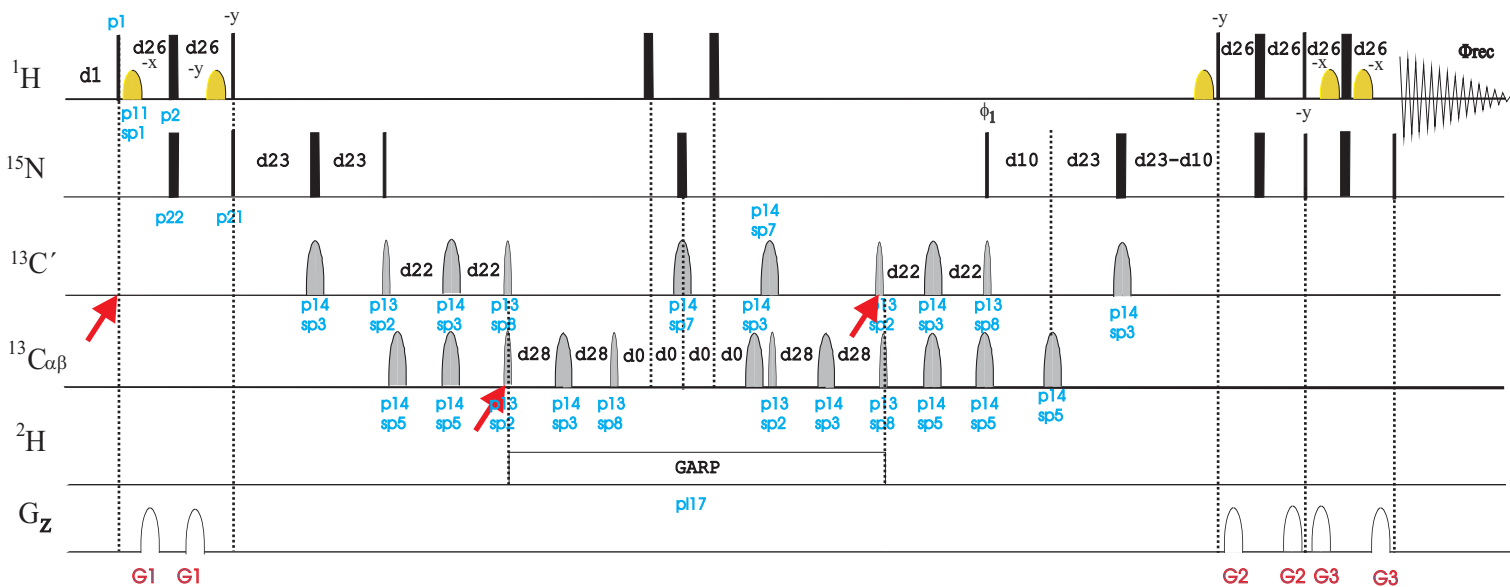
hncocacbgpwg2h3d



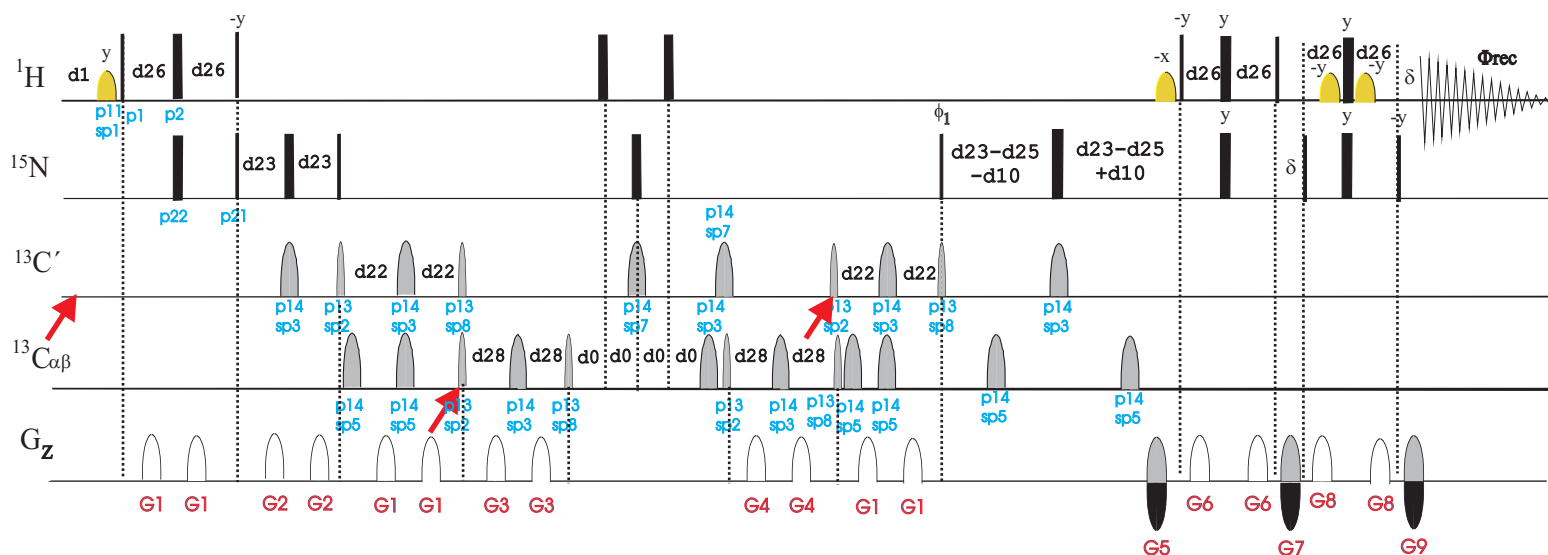
tfhncocacbgp3d



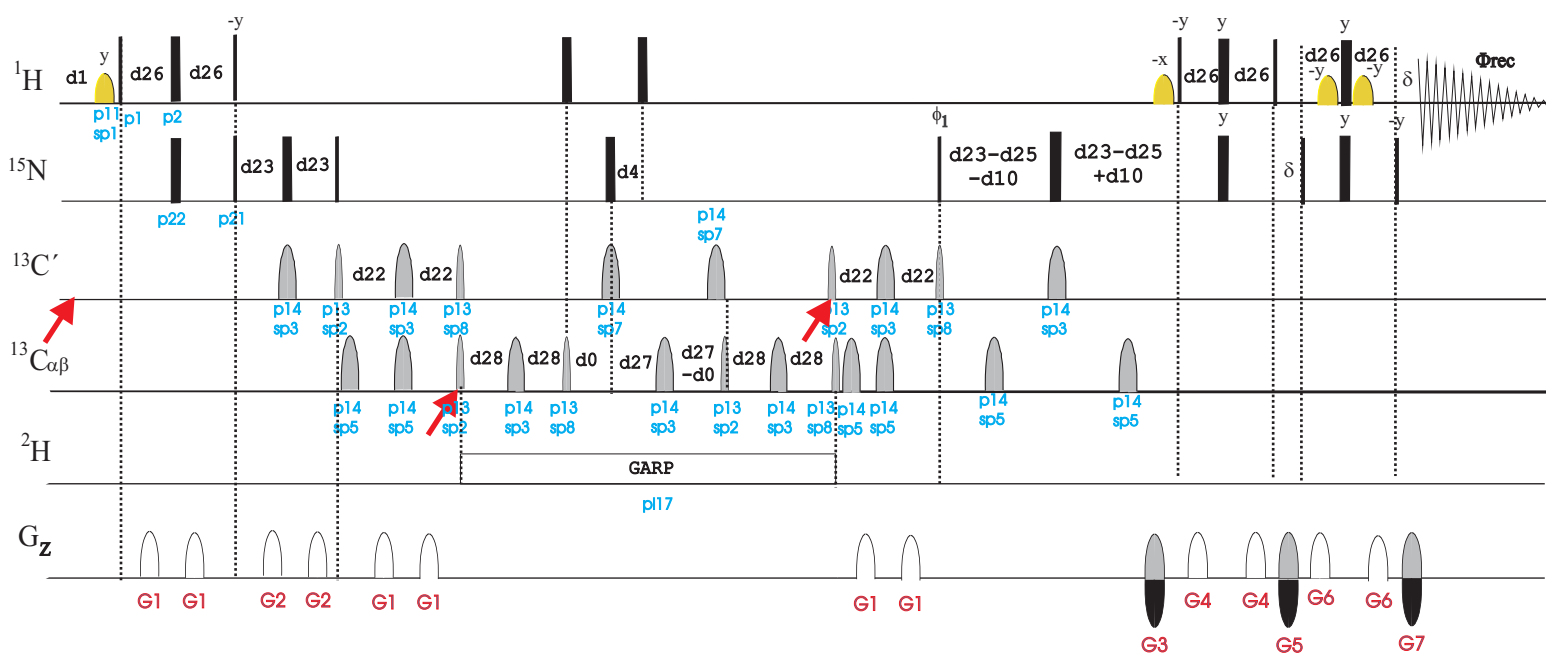
tfhncocacbgp2h3d



trhncocacbetgp3d



trhncocacbetgp2h3d

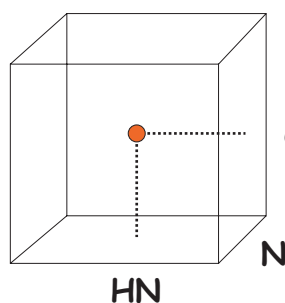
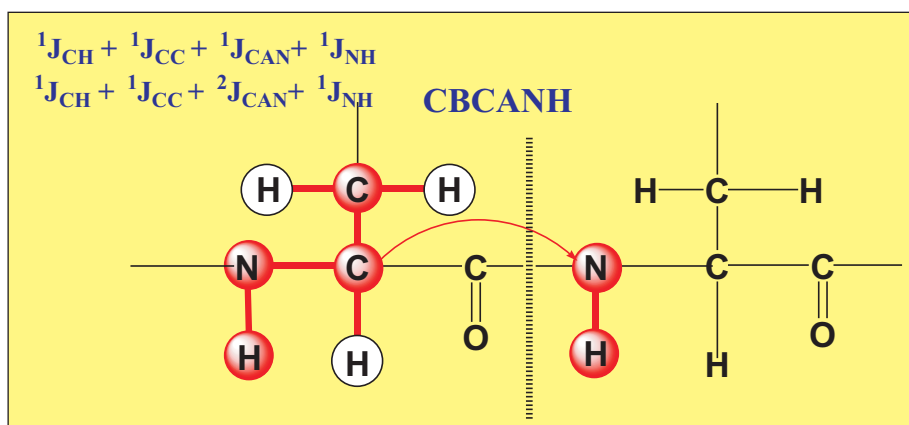


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3D CBCANH

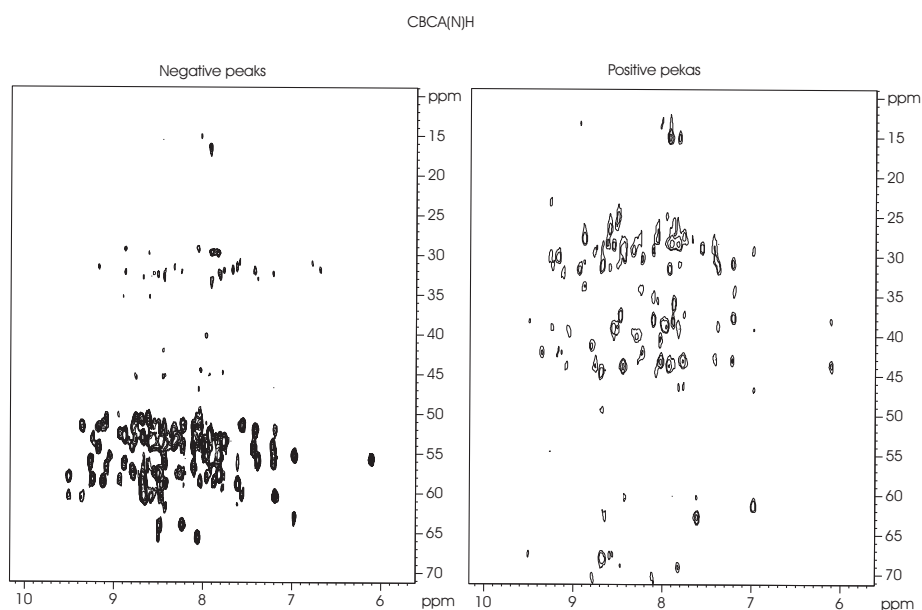
- 3D CBCANH using PEP (**cbcanhgp3d** | CBCANHGP3D)
- 3D CBCANH using WATERGATE (**cbcanhgpgwg3d** | CBCANHGPWG3D)
- 3D CBCANH using TROSY (**trcbcanhgp3d** | TRCBCANHGP3D)
- 3D CBCANH using TROSY and gradient echo-antiecho (**trcbcanhetgp3d** | TRCBCANHETGP3D)

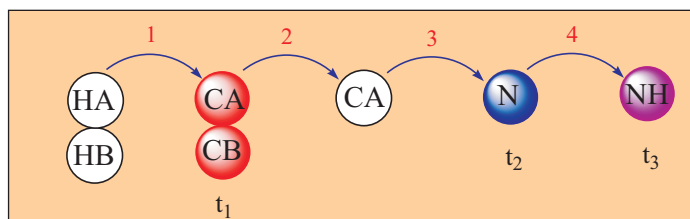


Cali

N

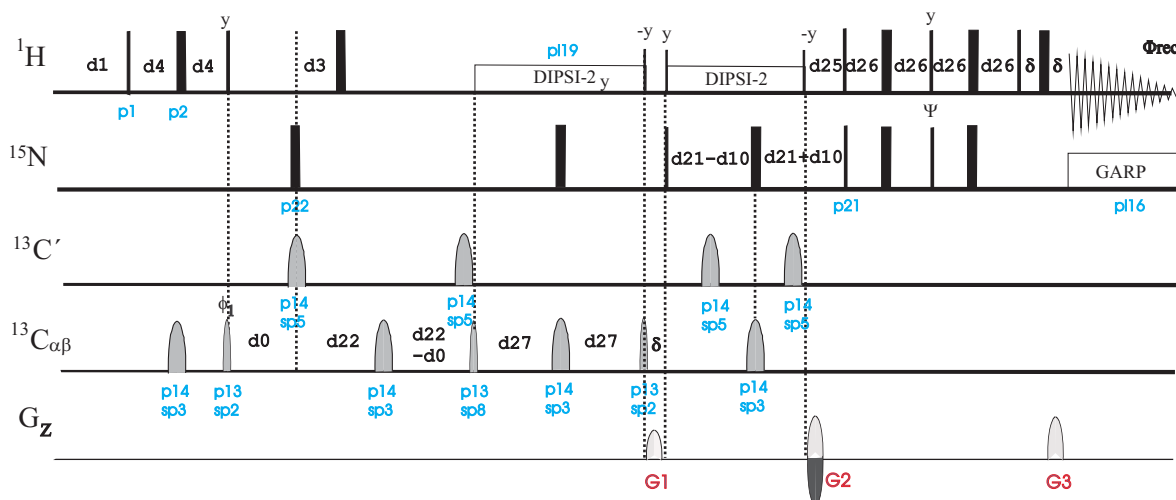
HN

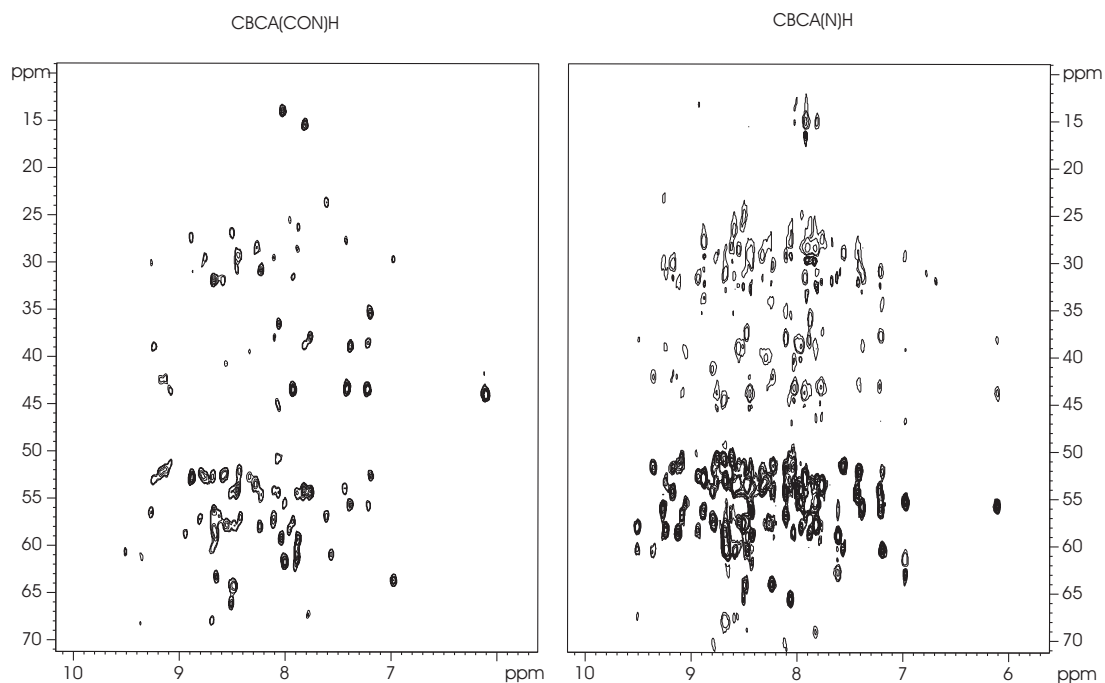
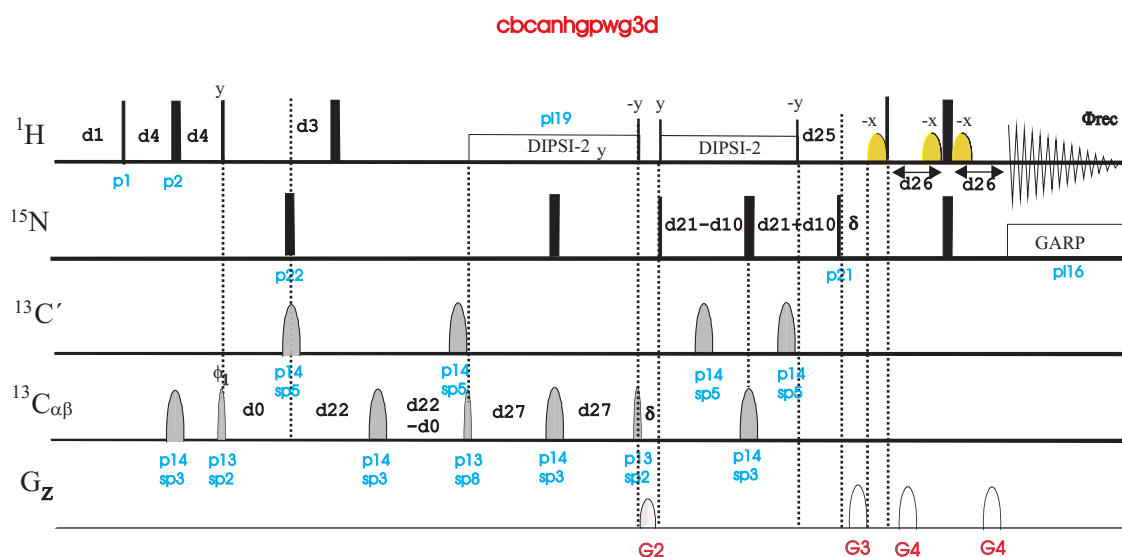




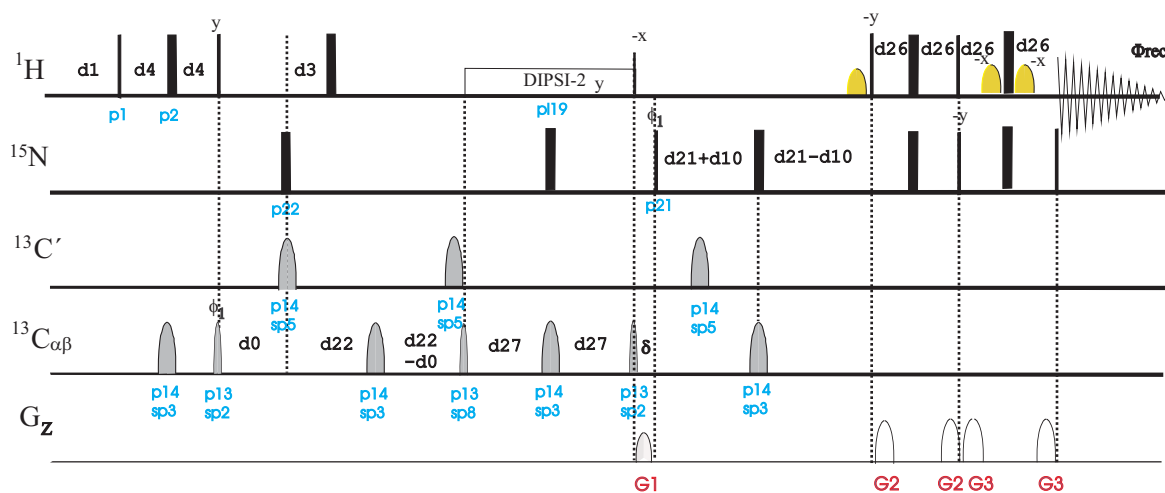
$d4=1/4J(\text{CH})=1.7\text{m}$
 $d3=1/6J(\text{CH})=1.1\text{m}$
 $d22=1/4J(\text{CBCA})=3.6\text{m}$
 $d27=1/4J(\text{NCO})=11\text{m}$
 $d21=1/4J(\text{NCO})=12.4\text{m}$
 $d25=1/2J(\text{NH})=5.5\text{m}$
 $d26=1/4J(\text{NH})=2.3\text{m}$

cbcanhg3d

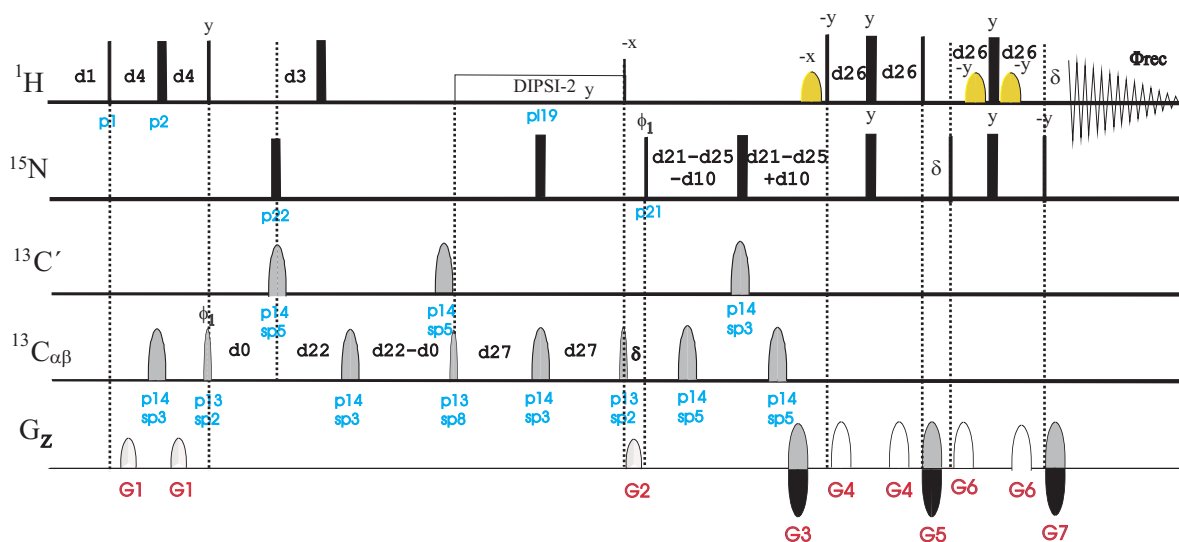




trcbcanhgp3d



trcbcanhetgp3d

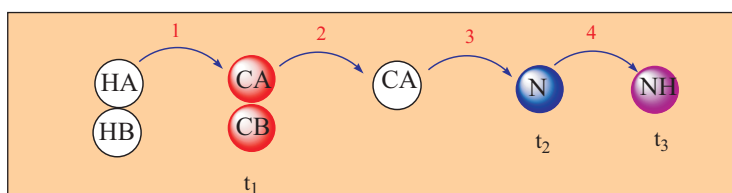
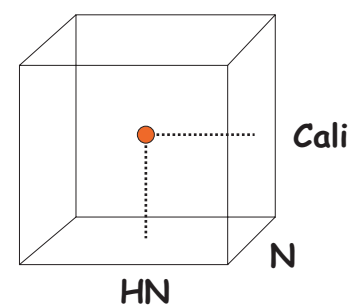
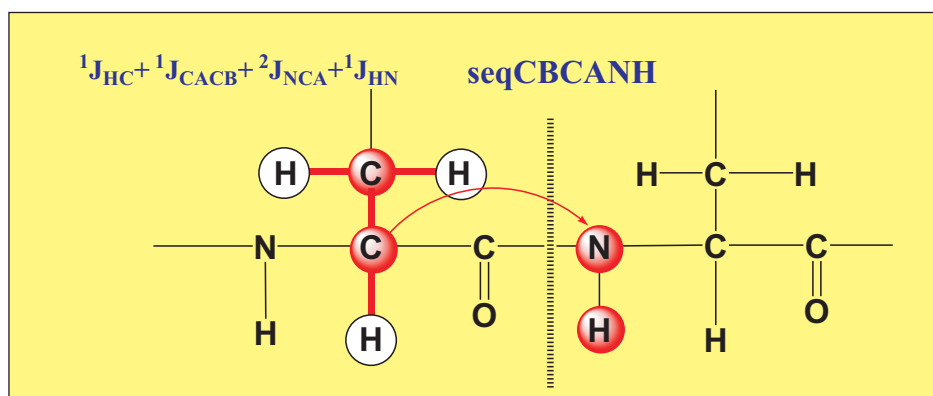


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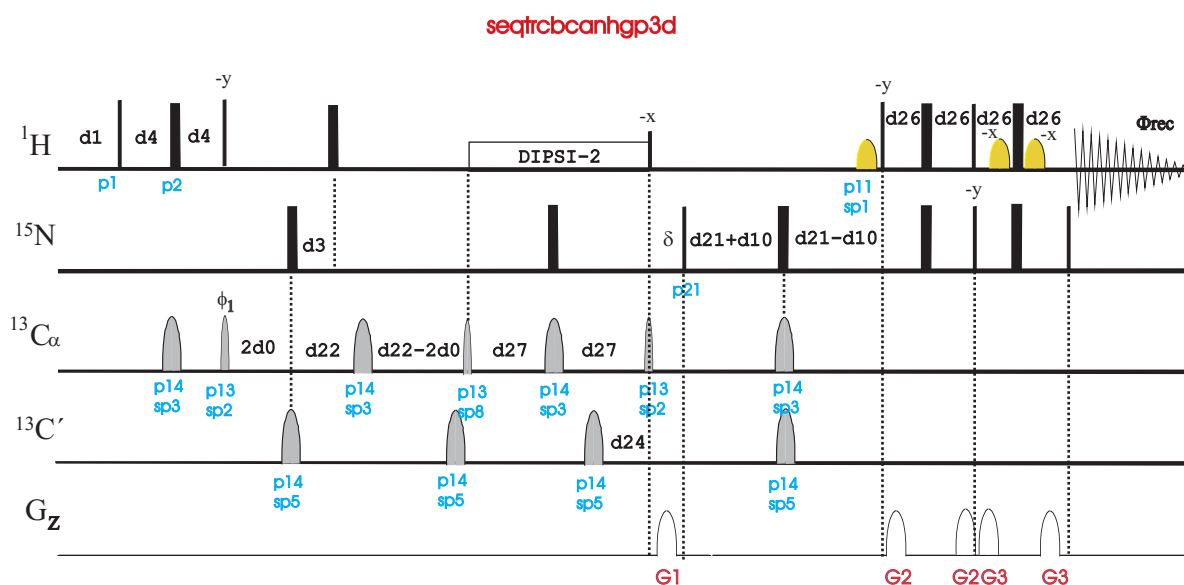
NMRGuide

3D SEQUENTIAL CBCANH

- 3D Sequential CBCANH using TROSY (**seqtrcbcanhgp3d** | SEQTRCBCANHGP3D)



$$\begin{aligned} d26 &= 1/4J(NH) = 2.3m \\ d21 &= 1/4J(NCA) = 12.4m \\ d22 &= 1/8J(CACB) = 3.6m \\ d27 &= 1/4J(NCA) = 11m \\ d24 &= 1/4J(CACO) = 4.5m \\ d4 &= 1/4J(CH) = 1.7m \\ d3 &= 1/6J(CH) = 1.1m \end{aligned}$$



BRUKER PULSE PROGRAM CATALOGUE

NMRGuide

3D HNCACB

3D HNCACB experiment

3D HNCACB using PEP (**hncacbgp3d** | HNCACBGP3D):

- with ^2H -decoupling (**hncacbgp2h3d** | HNCACBGP2H3D)

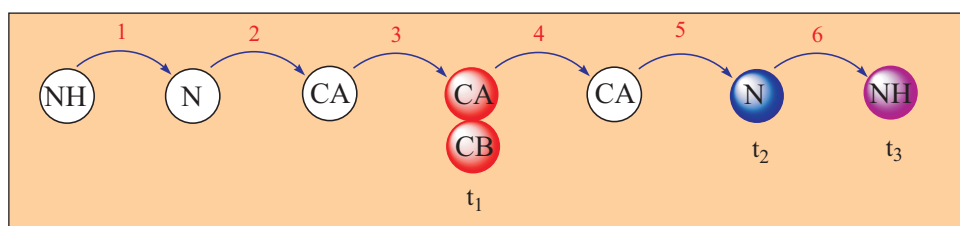
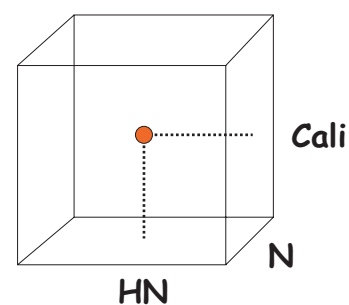
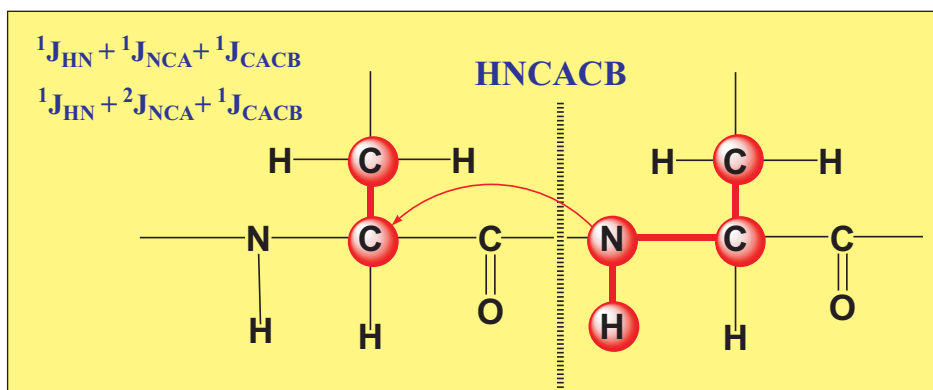
3D HNCACB using WATERGATE (**hncacbgpwg3d** | HNCACBGP2H3D)

- with ^2H -decoupling (**hncacbgpwg2h3d** | HNCACBGPWG2H3D)

3D HNCACB using TROSY (**trhncacbgp3d** | TRHNCACBGP3D) :

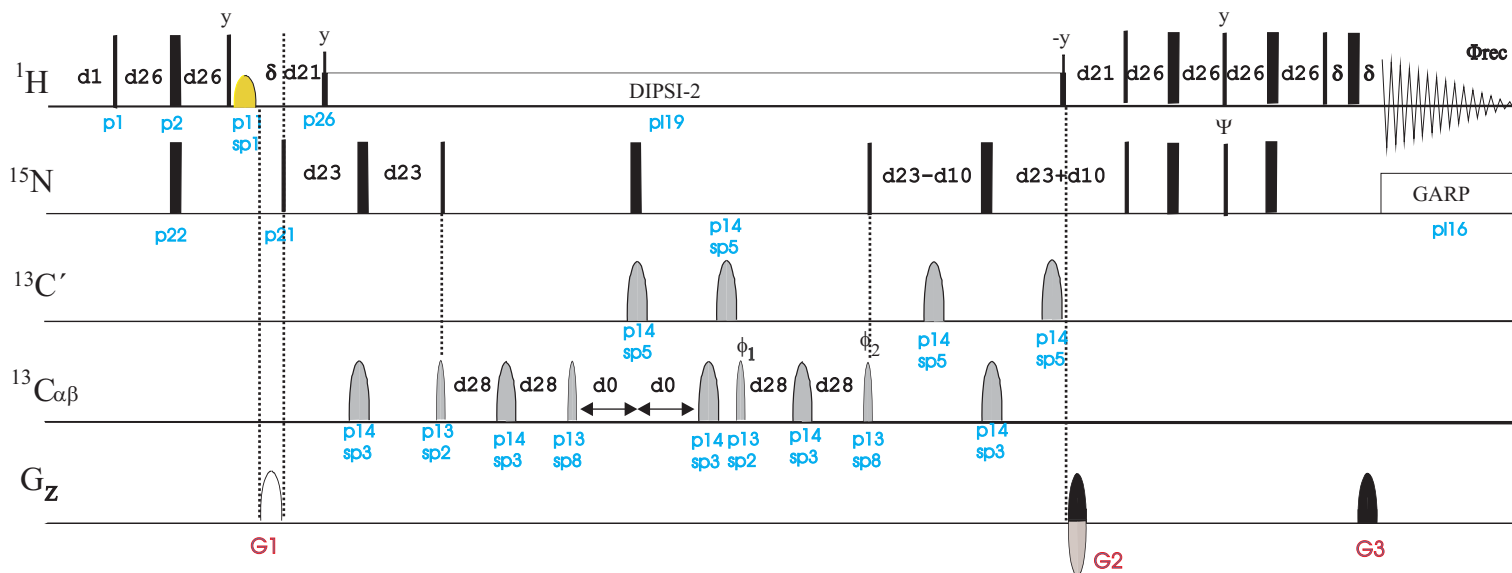
- with ^2H -decoupling (**trhncacbgp2h3d** | TRHNCACBGP2H3D)
- with gradient echo-antiecho (**trhncacbetgp3d** | TRHNCACBETGP3D)
- with gradient echo-antiecho and with ^2H -decoupling (**trhncacbetgp2h3d** | TRHNCACBETGP2H3D)

Also see CBCANH, CBCACONH, intra-HNCACB, sequential-HNCACB

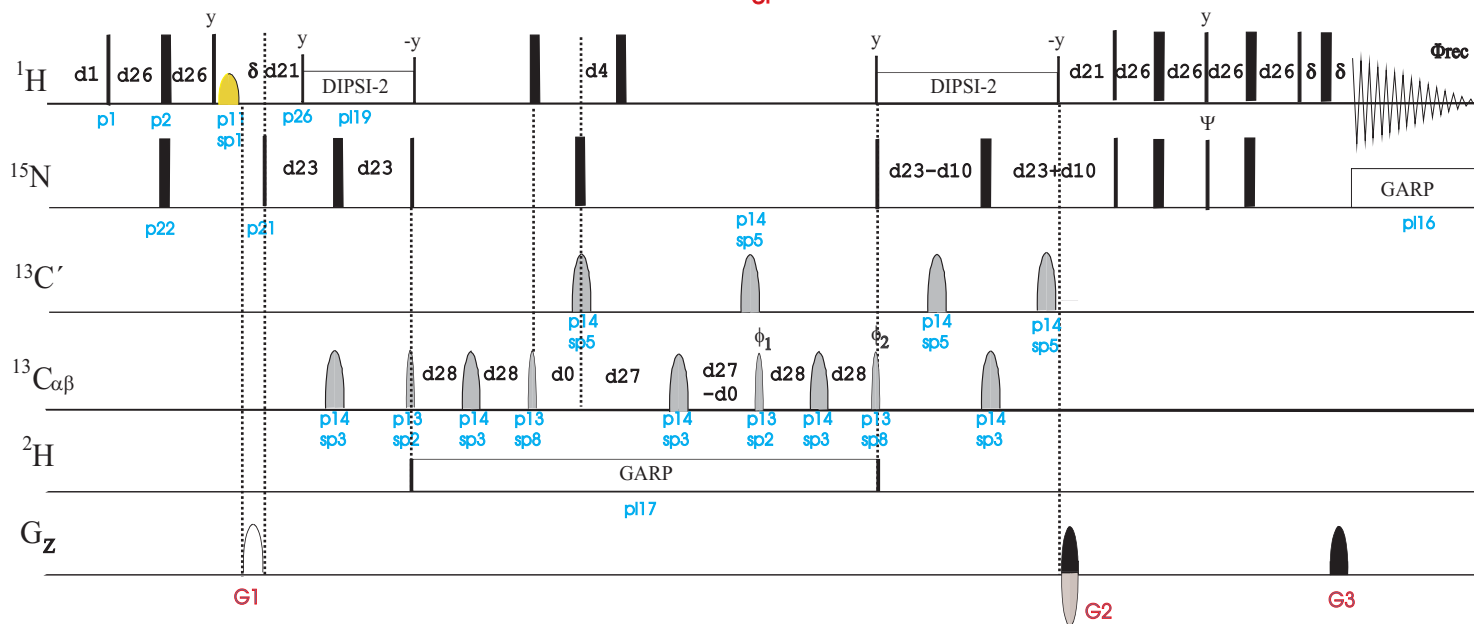


$$\begin{aligned} d26 &= 1/4J(\text{NH}) = 2.3\text{m} \\ d21 &= 1/2J(\text{NH}) = 5.5\text{m} \\ d23 &= 1/4J(\text{NCO}) = 12.4\text{m} \\ d28 &= 1/4J(\text{CACB}) = 3.6\text{m} \end{aligned}$$

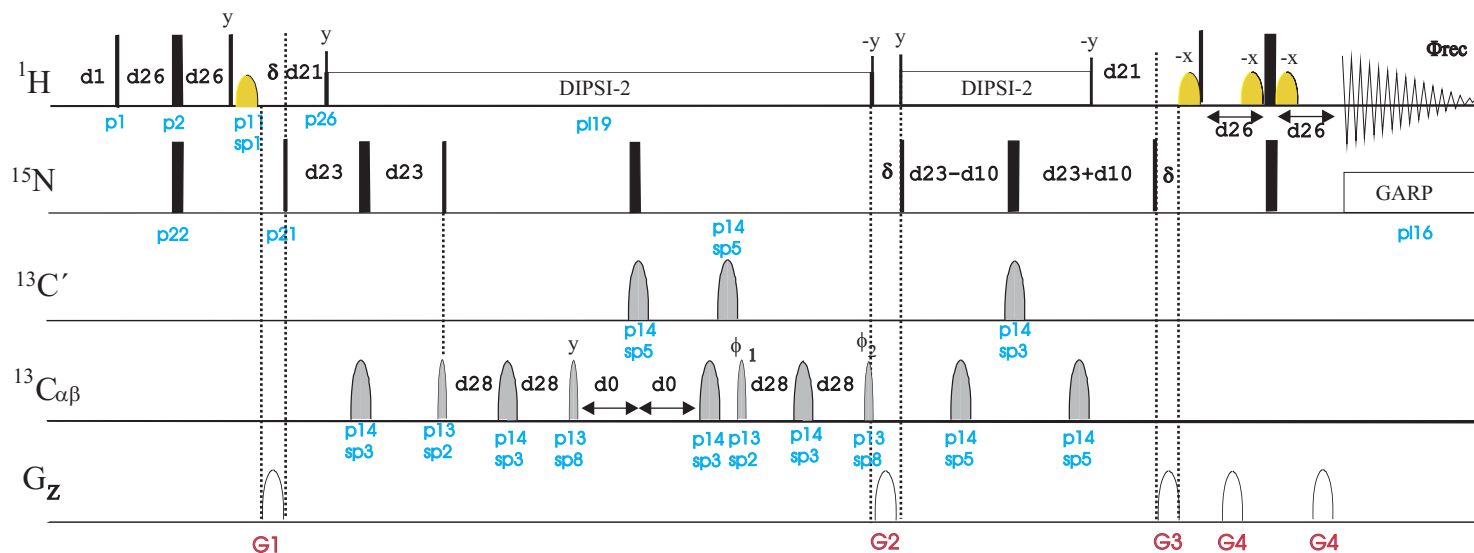
hncacbgp3d



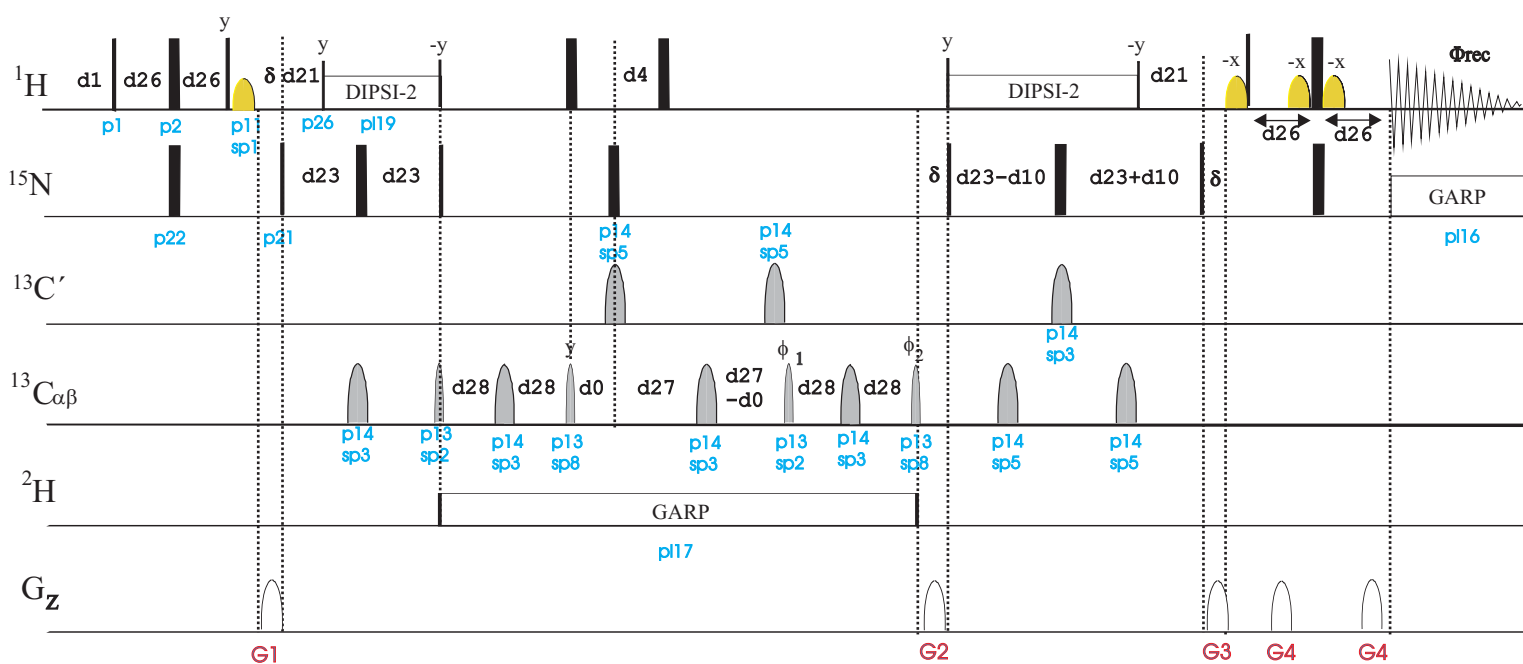
hncacbgp2h3d

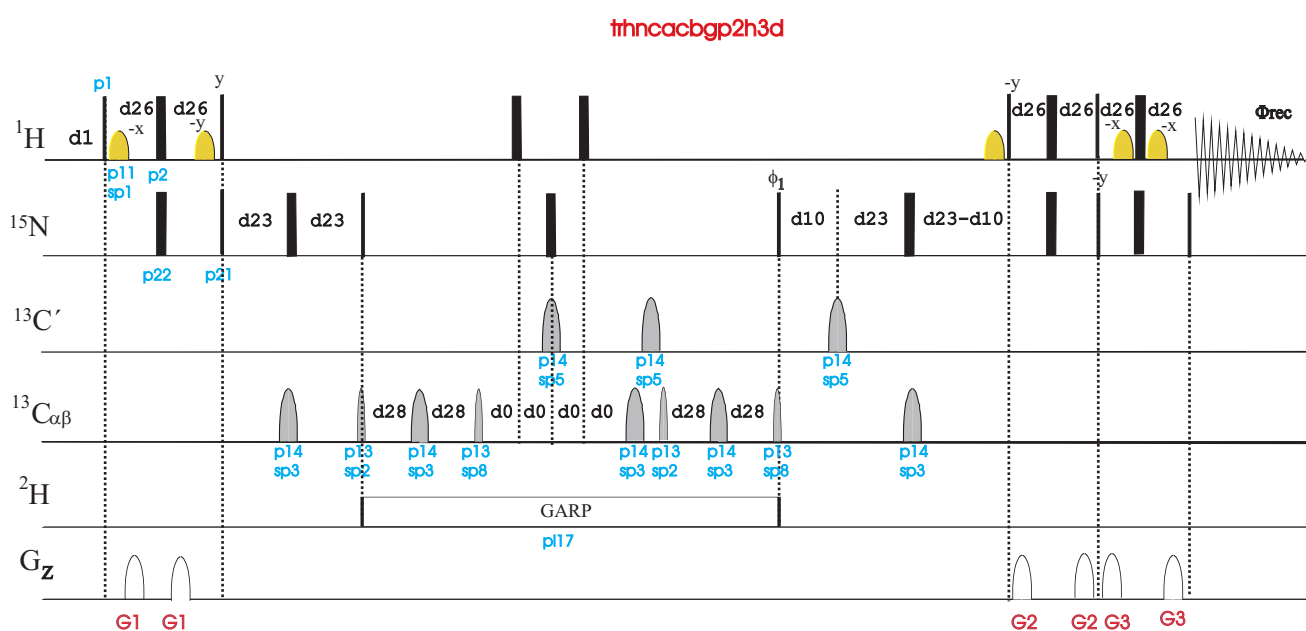
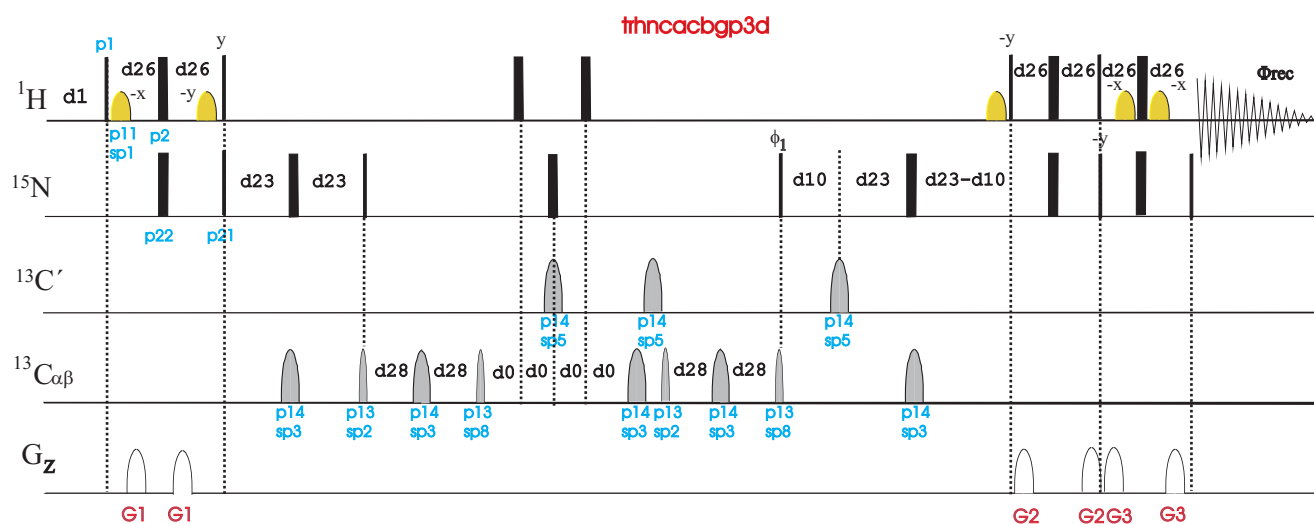


hncacbgpwg3d



hncacbgpwg2h3d







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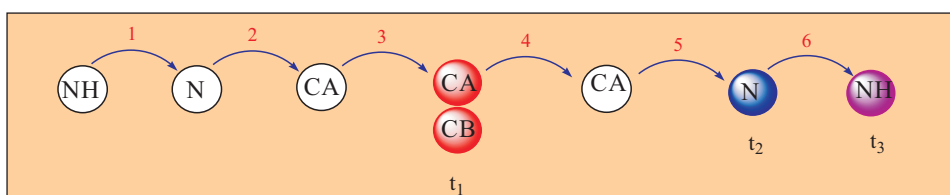
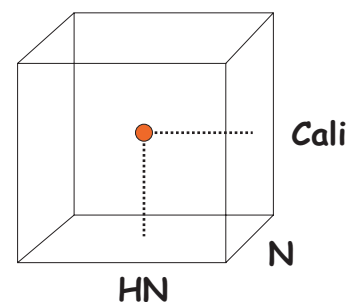
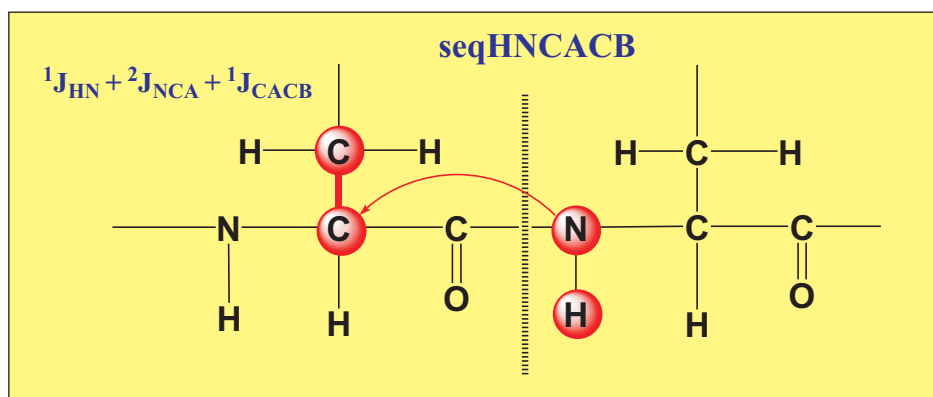
3D SEQUENTIAL HNCACB

3D sequential-HNCACB experiment

3D Sequential HNCACB using TROSY (**seqtrhncacb3d** | SEQTRHNCACB3D)

- with ^2H -decoupling (**seqtrhncacb2h3d** | SEQTRHNCACB2H3D)
- Using gradient echo-antiecho (**seqtrhncacbet3d** | SEQTRHNCACBET3D)
- Using gradient echo-antiecho and with ^2H -decoupling (**seqtrhncacbet2h3d** | SEQTRHNCACBET2H3D)

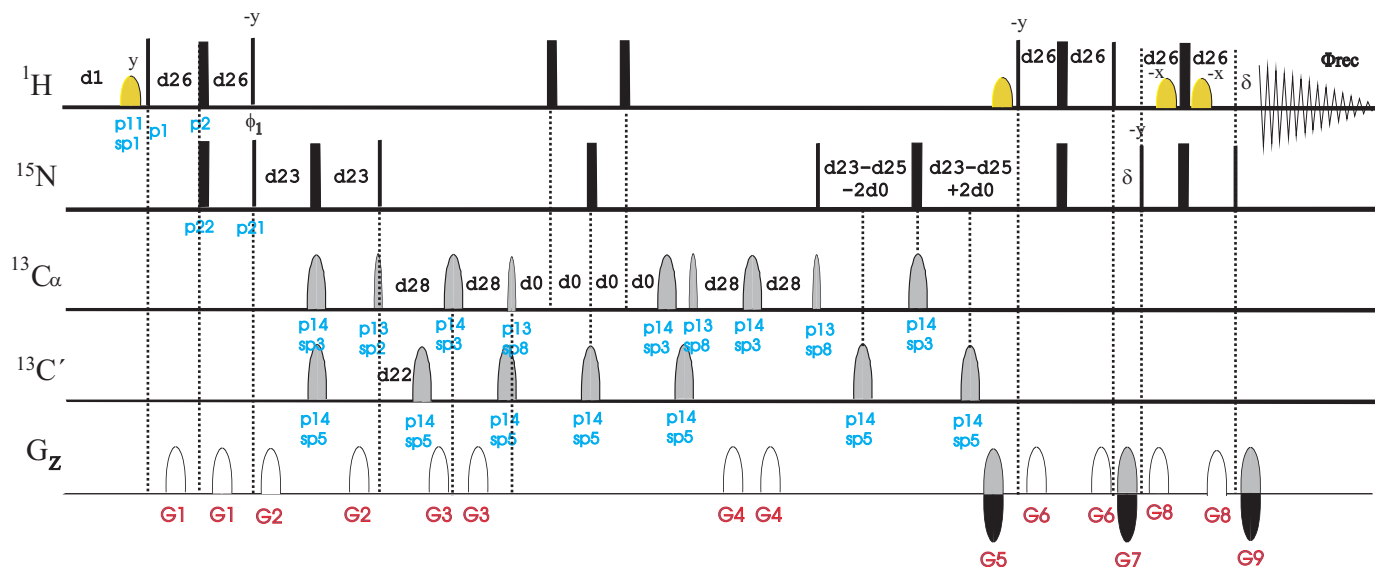
Also see: HNCACB, intra-HNCACB, HNCOCACB



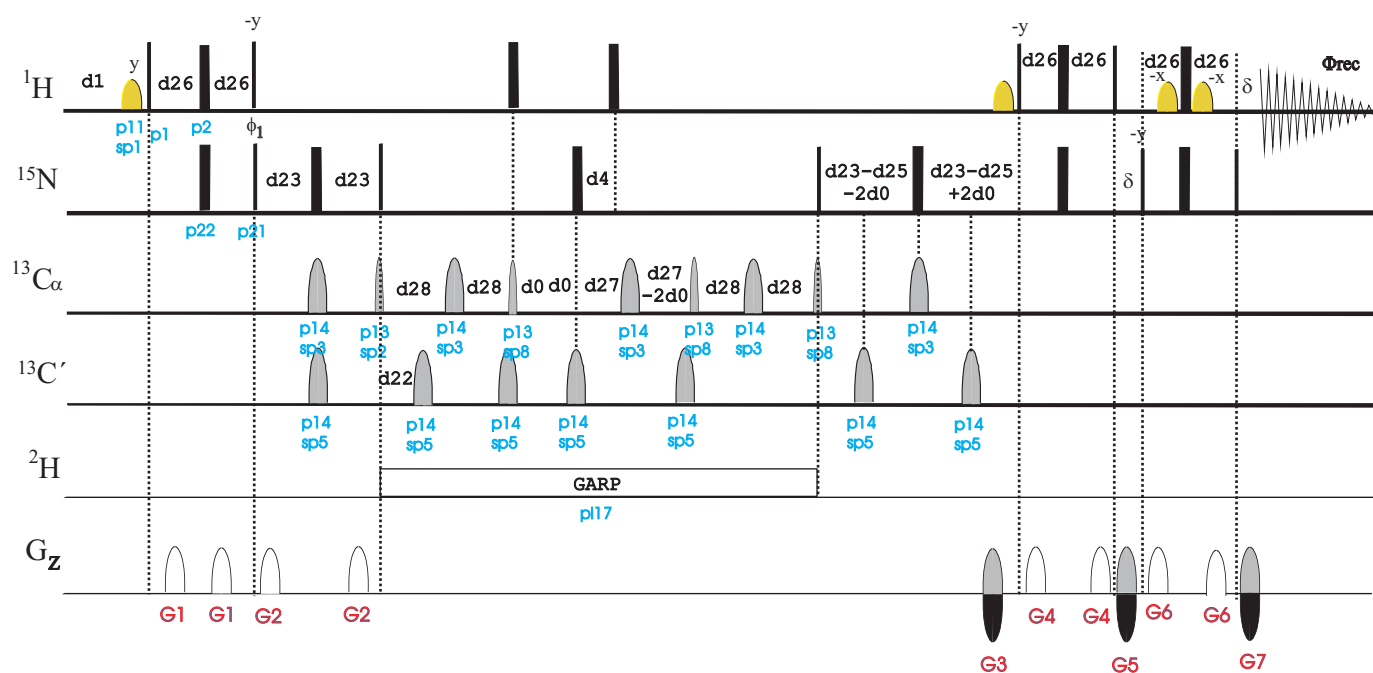
$d_{26} = 1/4J(\text{NH}) = 2.3\text{m}$
 $d_{23} = 1/4J(\text{NCA}) = 12\text{m}$
 $d_{22} = 1/4J(\text{CACO}) = 4.5\text{m}$
 $d_{28} = 1/8J(\text{CACB}) = 5\text{m}$
 $d_{25} = 1/4J(\text{NH}) = 2.3\text{m}$

[illegible]

seqtrhncacbetgp3d



seqtrhncacbetgp2h3d



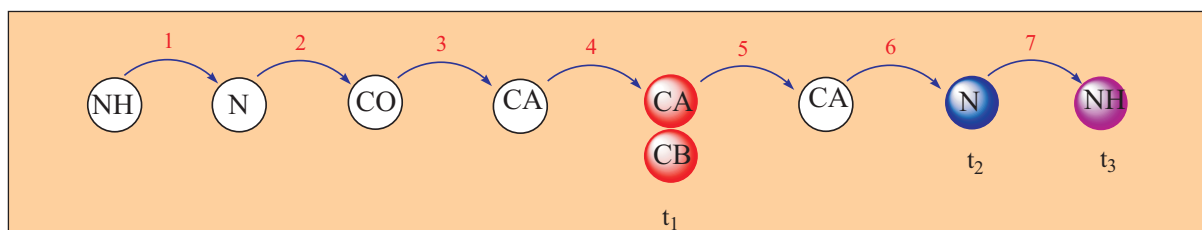
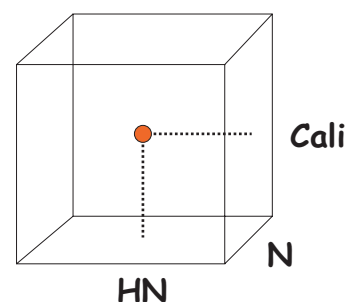
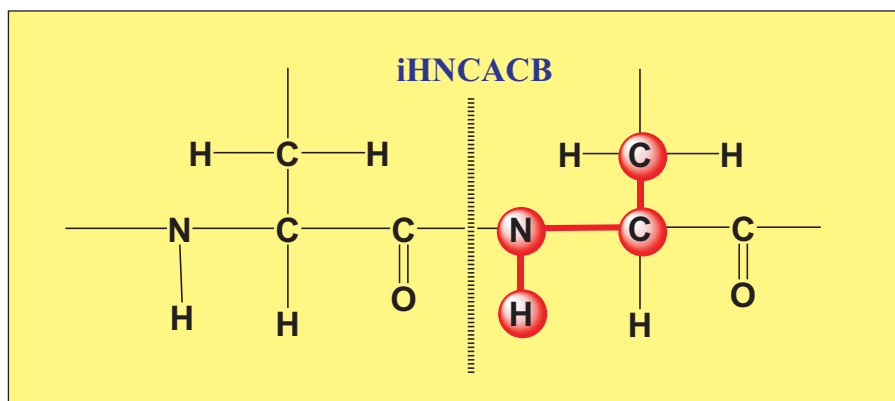
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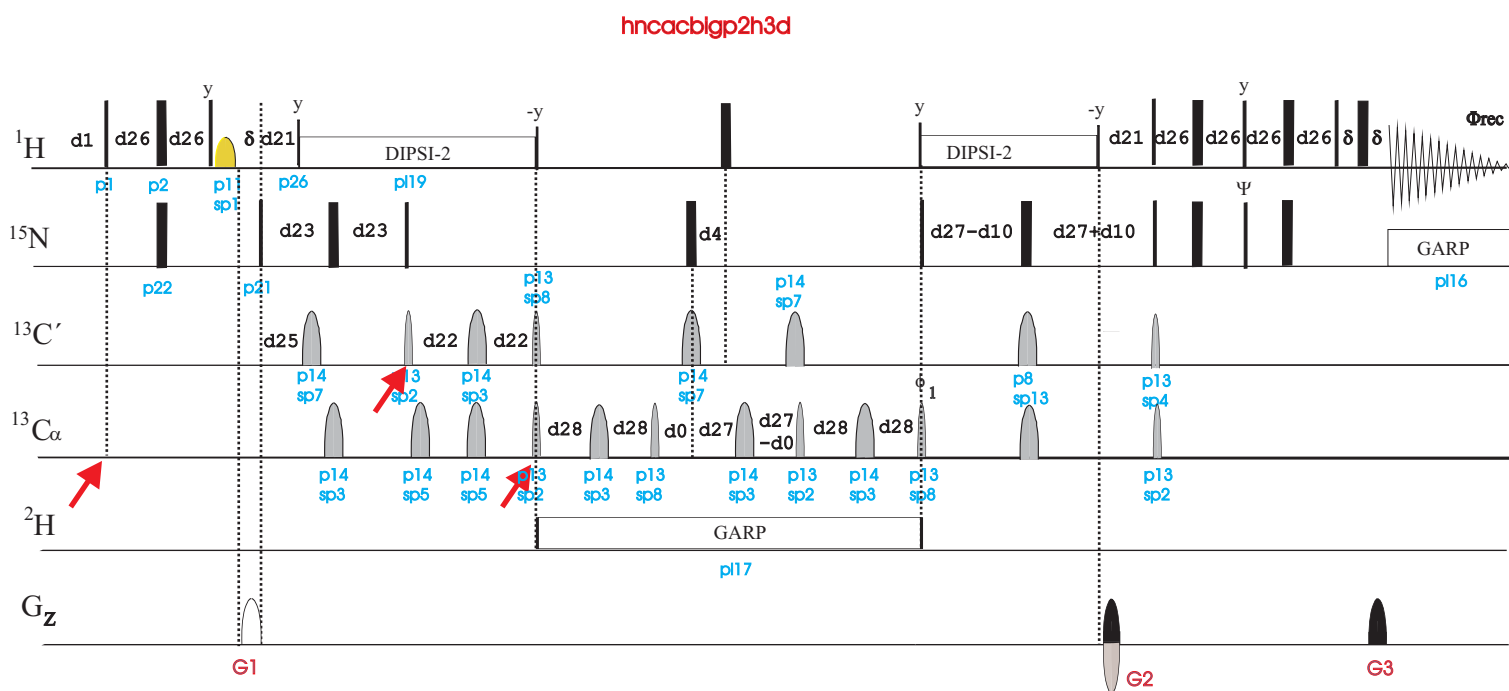
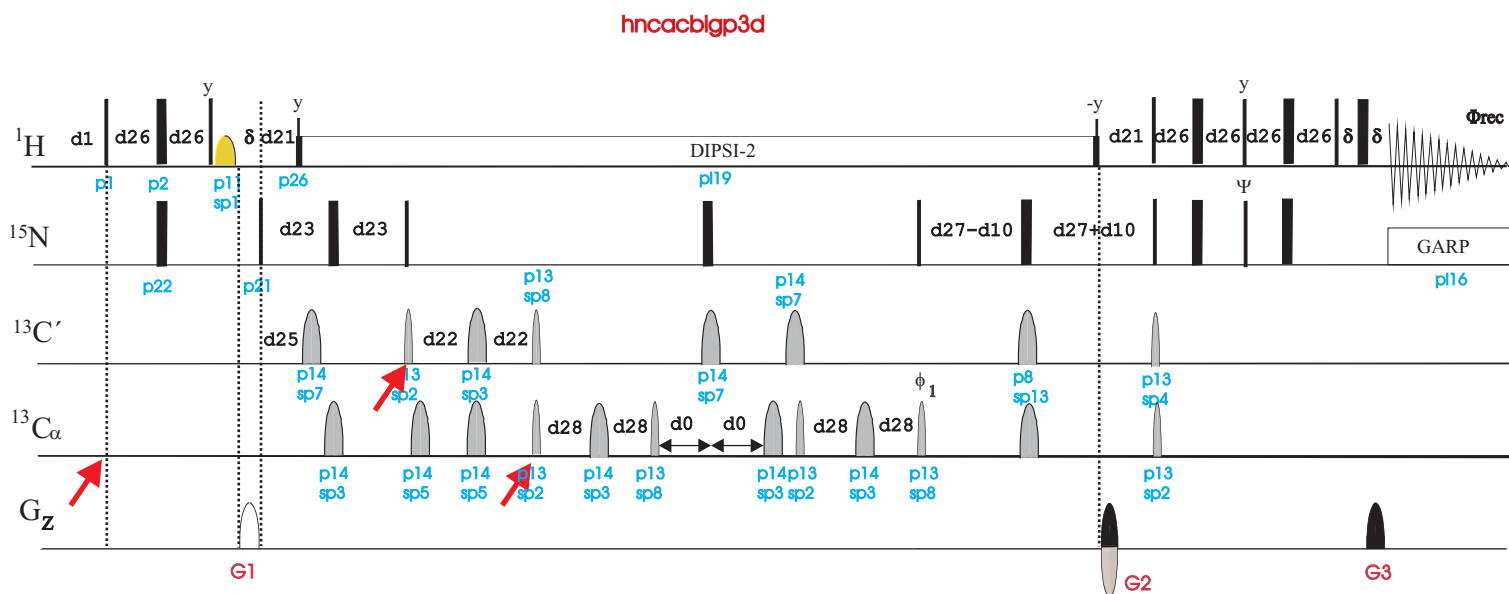
3D Intra-HNCACB

3D intra-HNCACB experiment

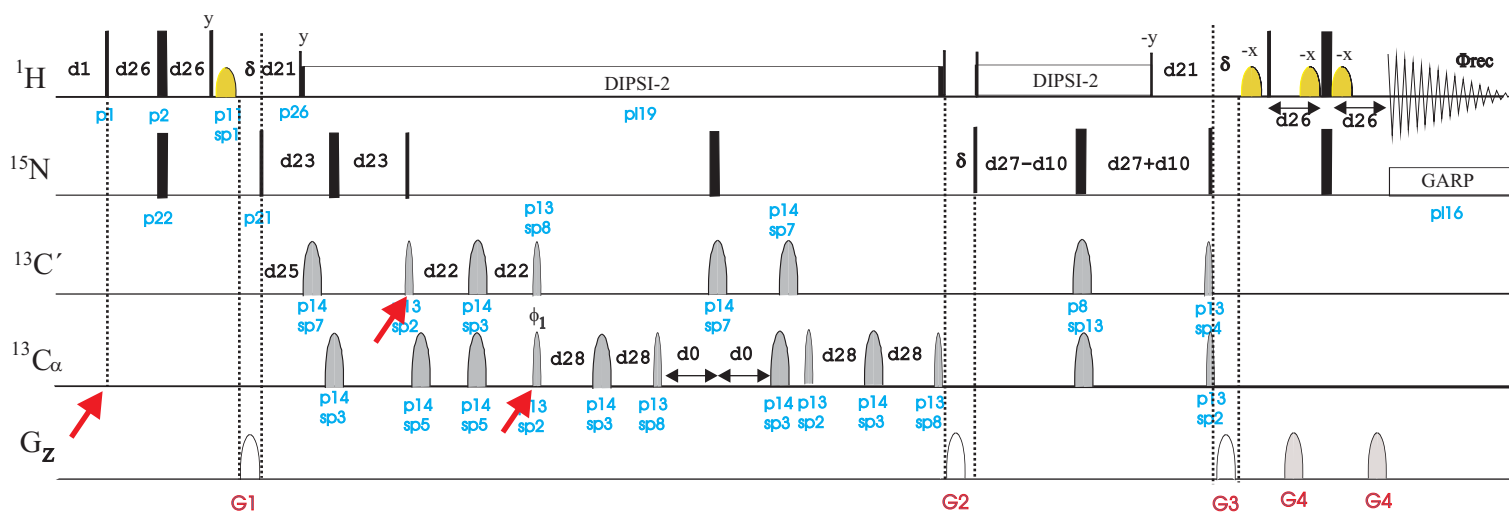
- 3D Intra-HNCACB using PEP (**hncacbigp3d** | HNCACBIGP3D)
 - with ^2H -decoupling (**hncacbigp2h3d** | HNCACBIGP2H3D)
- 3D Intra-HNCACB using WATERGATE (**hncacbigpwg3d** | HNCACBIGPWG3D)
 - with ^2H -decoupling (**hncacbigpwg2h3d** | HNCACBIGPWG2H3D)
- 3D Intra-HNCACB using TROSY (**trhncacbigp3d** | TRHNCACBIGP3D)
 - with ^2H -decoupling (**trhncacbigp2h3d** | TRHNCACBIGP2H3D)
 - With gradient echo-antiecho (**trhncacbietgp3d** | TRHNCACBIETGP3D)
 - With gradient echo-antiecho and with ^2H -decoupling (**trhncacbietgp2h3d** | TRHNCACBIETGP2H3D)



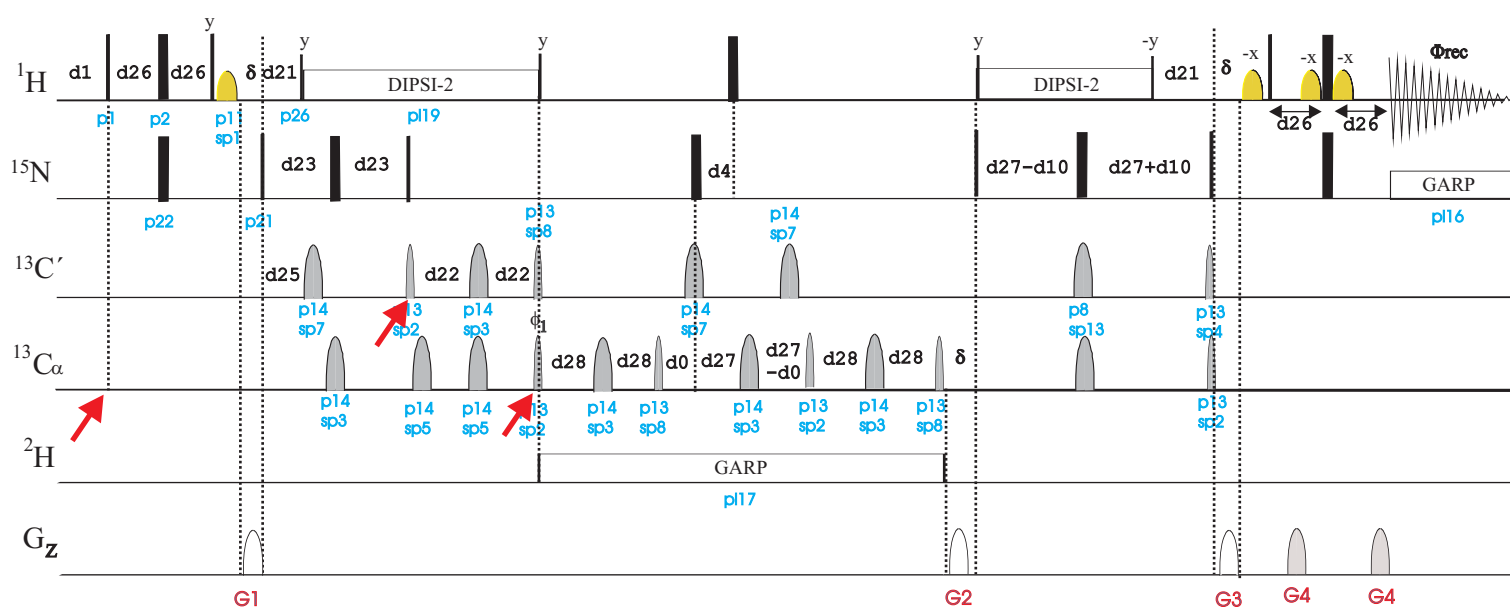
$d_{26}=1/4J(\text{NH})=2.3\text{m}$
 $d_{21}=1/2J(\text{NH})=5.5\text{m}$
 $d_{23}=1/4J(\text{NCA})=26\text{m}$
 $d_{22}=1/4J(\text{CACO})=4.2\text{m}$
 $d_{27}=1/4J(\text{NCA})+1/4J(\text{NCO})=15.8\text{m}$
 $d_{25}=1/4J(\text{NCO})=16.5\text{m}$

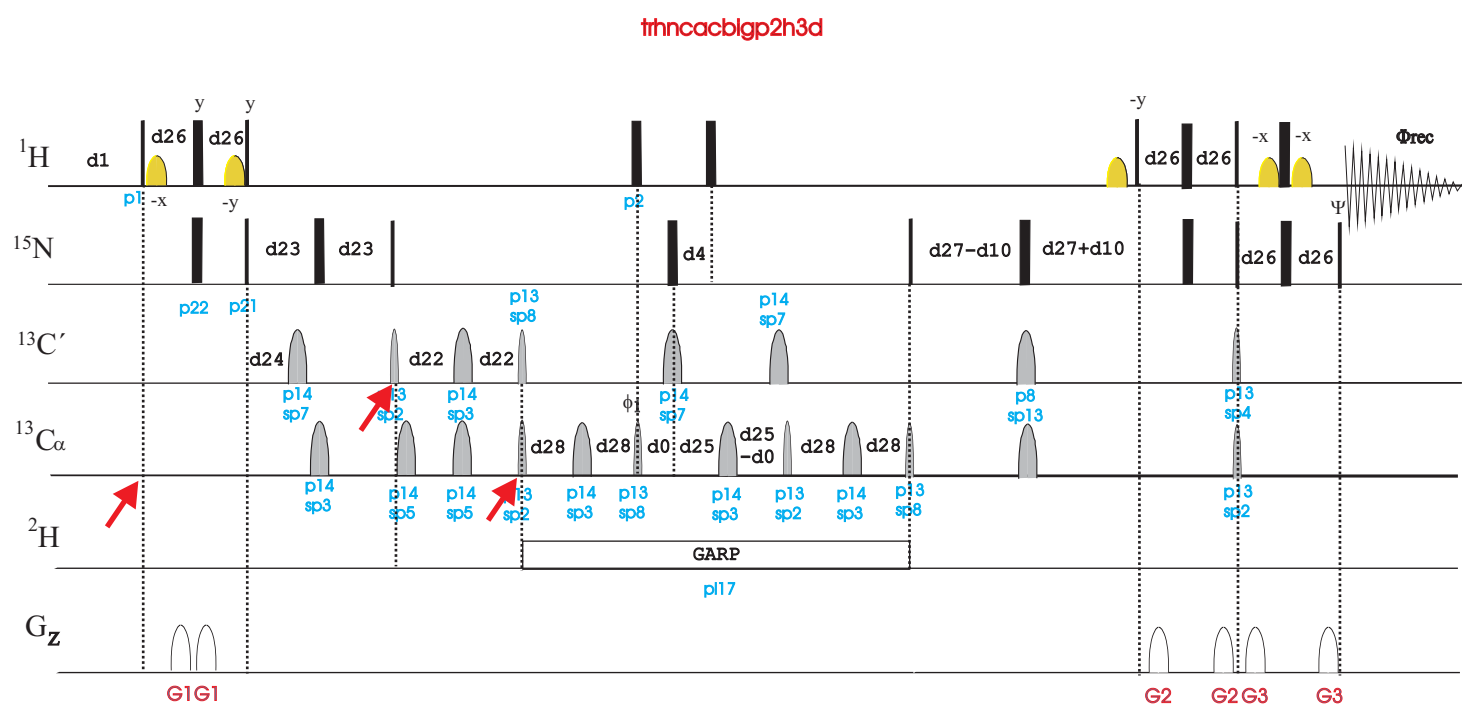
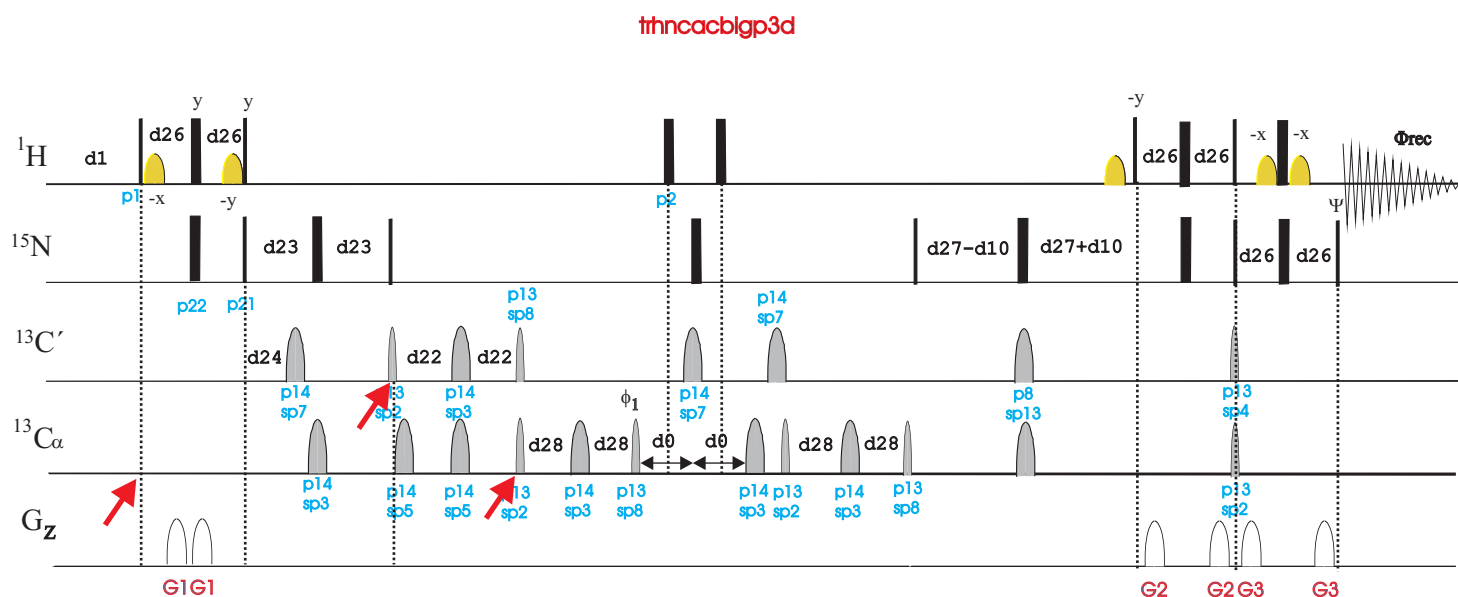


hncacblgpwg3d



hncacblgpwg2h3d



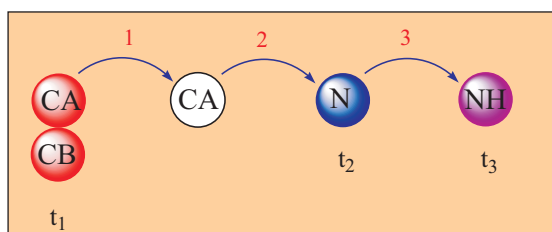
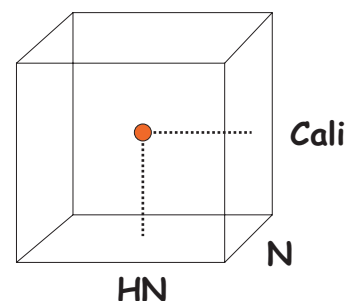
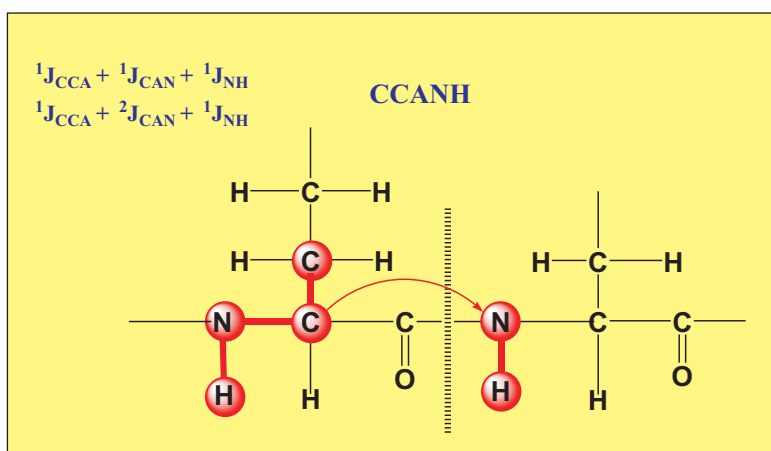


BRUKER PULSE PROGRAM CATALOGUE

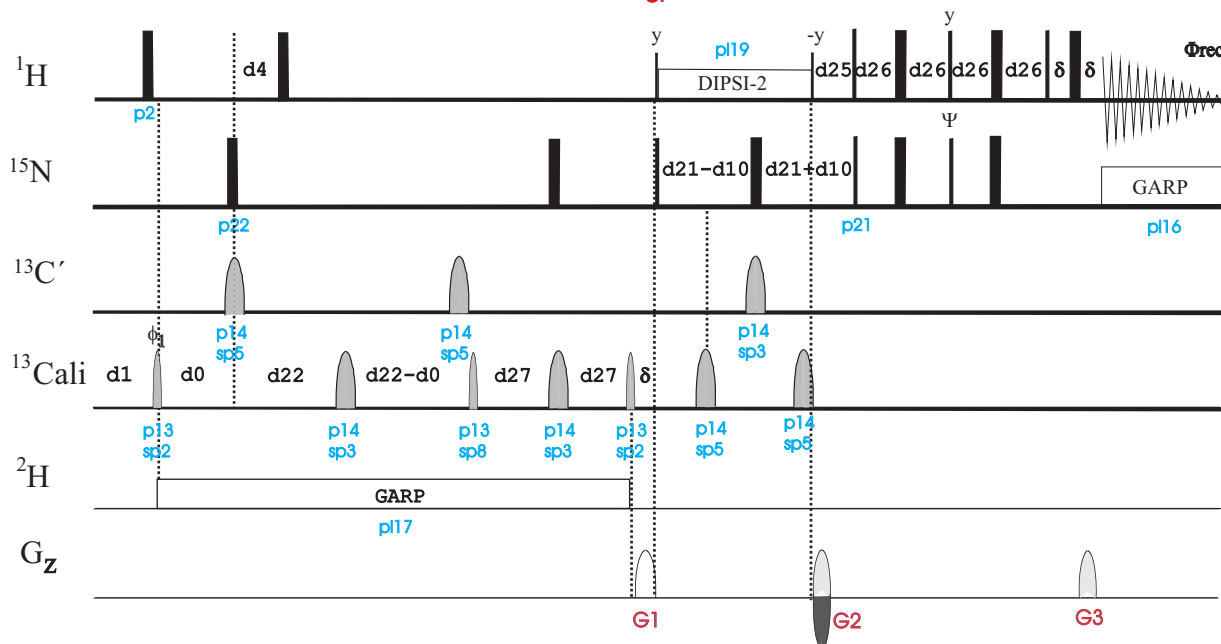
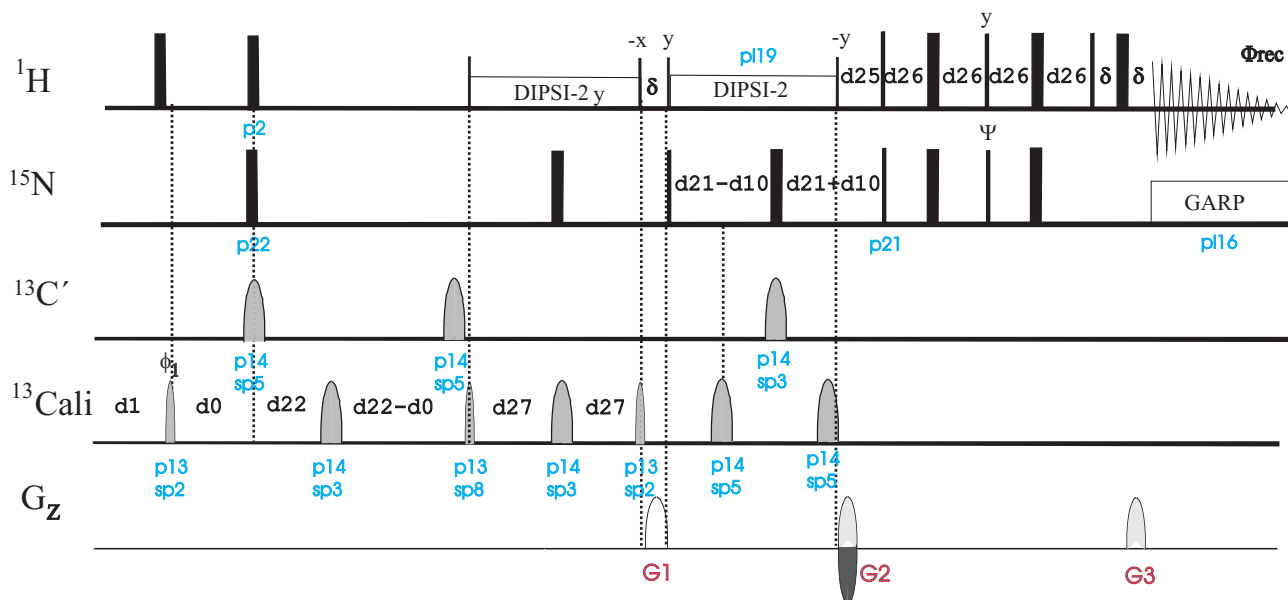
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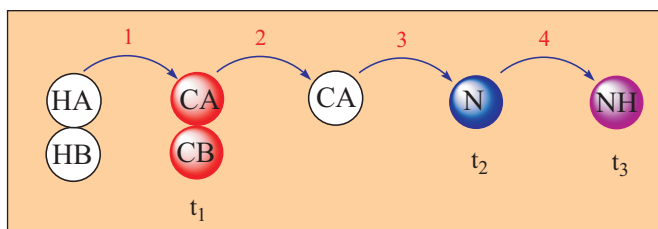
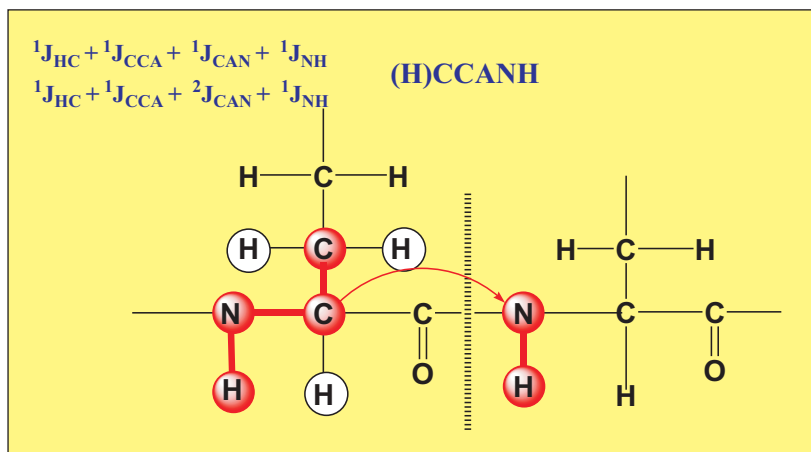
3D CCANH
3D ((H)CCANH

- 3D CCANH using PEP (**ccanhgp3d** | CCANHGP3D)
- 3D CCANH using PEP with ^2H -decoupling (**ccanhgp2h3d** | CCANHGP2H3D)
- 3D (H)CCANH using PEP and ^1H -NOE (**ccanhgp3d.2** | CCANHGP3D.2)

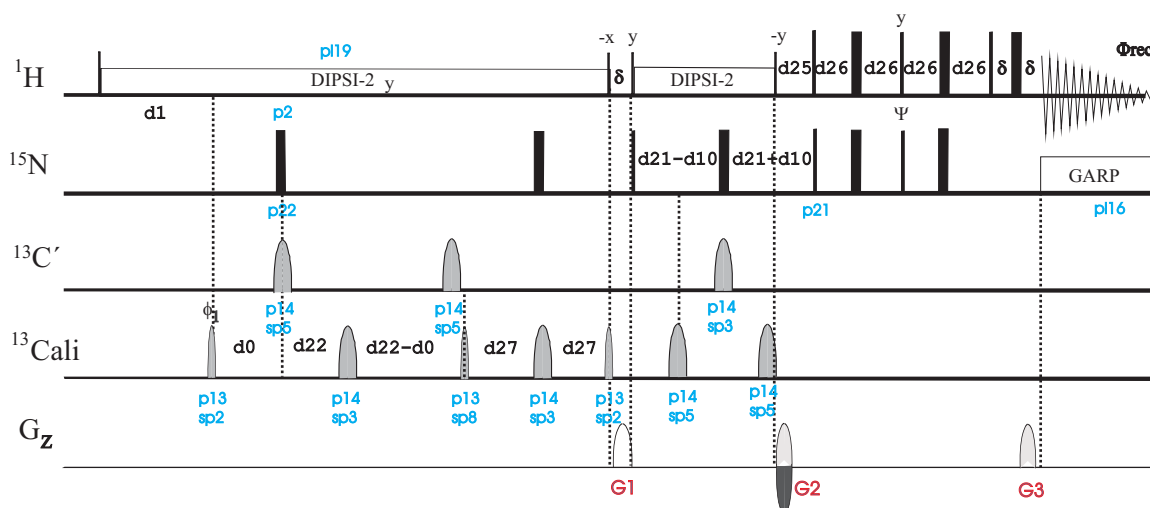


$d21 = 1/4J(\text{NCO}) = 12.4\text{m}$
 $d22 = 1/4J(\text{CC}) = 3.6\text{m}$
 $d25 = 1/2J(\text{NH}) = 5.5\text{m}$
 $d26 = 1/4J(\text{NH}) = 2.3\text{m}$
 $d27 = 1/4J(\text{CACO}) = 11\text{m}$





ccanhgp3d.2



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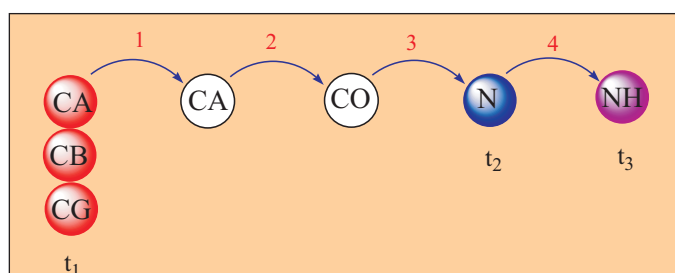
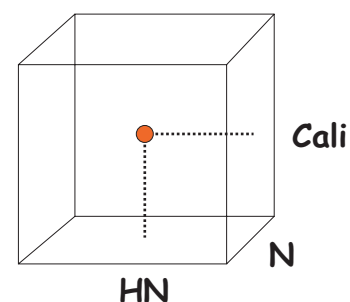
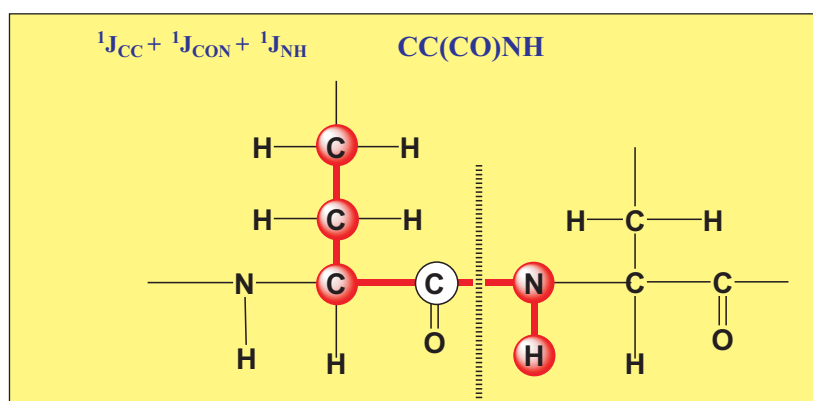
3D CC(CO)NH
3D CCA(CO)NH
3D (H)CCA(CO)NH

3D CC(CO)NH experiment

- 3D CC(CO)NH using PEP (**ccconhgp3d** | CCCONHGP3D)
- 3D CC(CO)NH using PEP with ^2H -decoupling (**ccconhgp2h3d** | CCCONHGP2H3D)

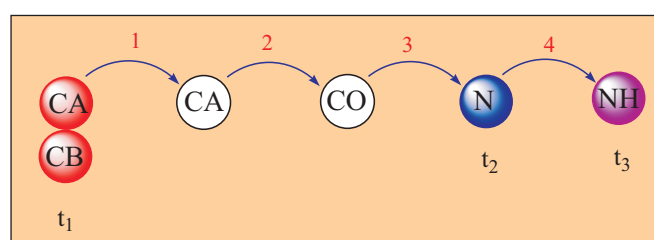
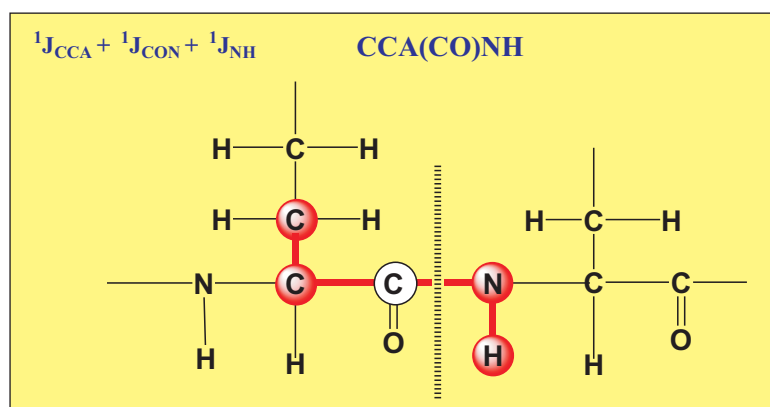
3D CCA(CO)NH experiment

- 3D CCA(CO)NH using PEP (**ccaconhgp3d** | CCACONHGP3D)
- 3D CCA(CO)NH using PEP with ^2H -decoupling (**ccaconhgp2h3d** | CCACONHGP2H3D)
- 3D (H)CCA(CO)NH using PEP and ^1H -NOE (**ccaconhgp3d.2** | CCACONHGP3D.2)

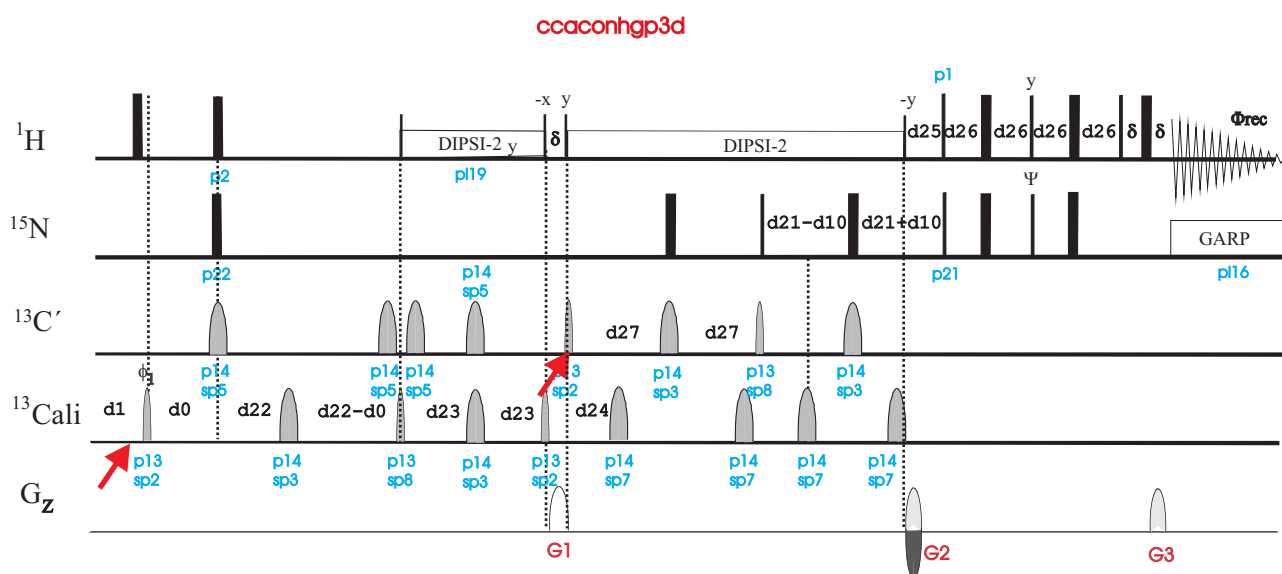


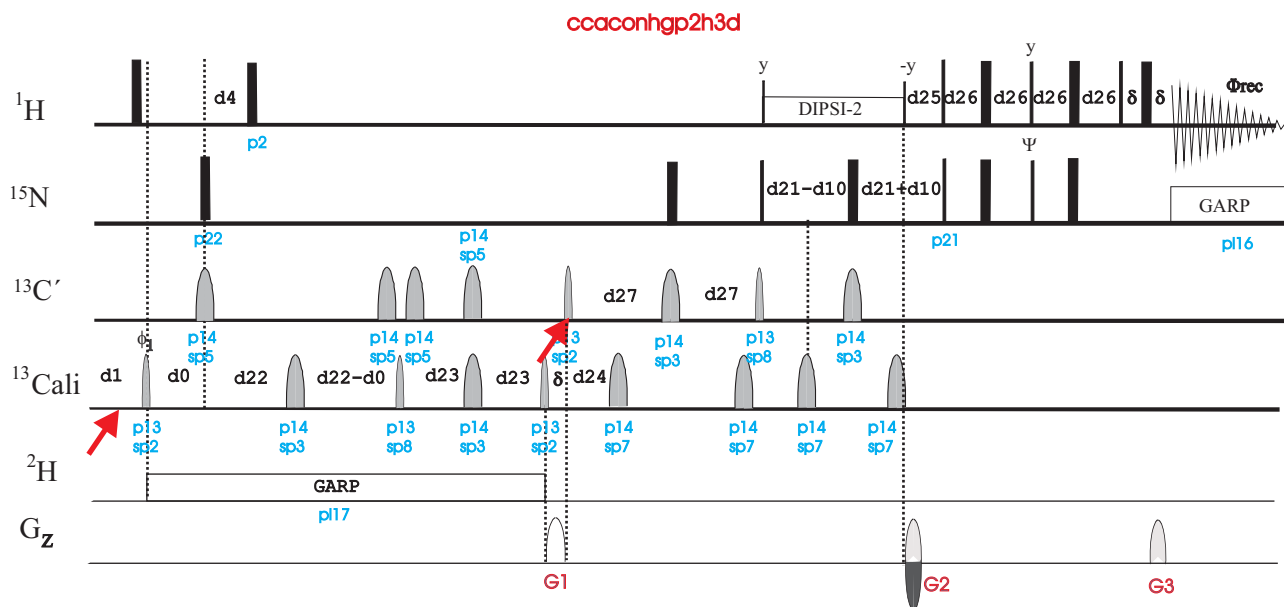
$d15 = 1/J(\text{CC})$
 $d21 = 1/4J(\text{CACO}) = 3.6\text{m}$
 $d22 = 1/2J(\text{CACO}) = 4.4\text{m}$
 $d23 = 1/4J(\text{NCO}) = 12.4\text{m}$
 $d25 = 1/2J(\text{NH}) = 5.5\text{m}$
 $d26 = 1/4J(\text{NH}) = 2.3\text{m}$
 $d4 = 1/4J(\text{CH}) = 1.7\text{m}$

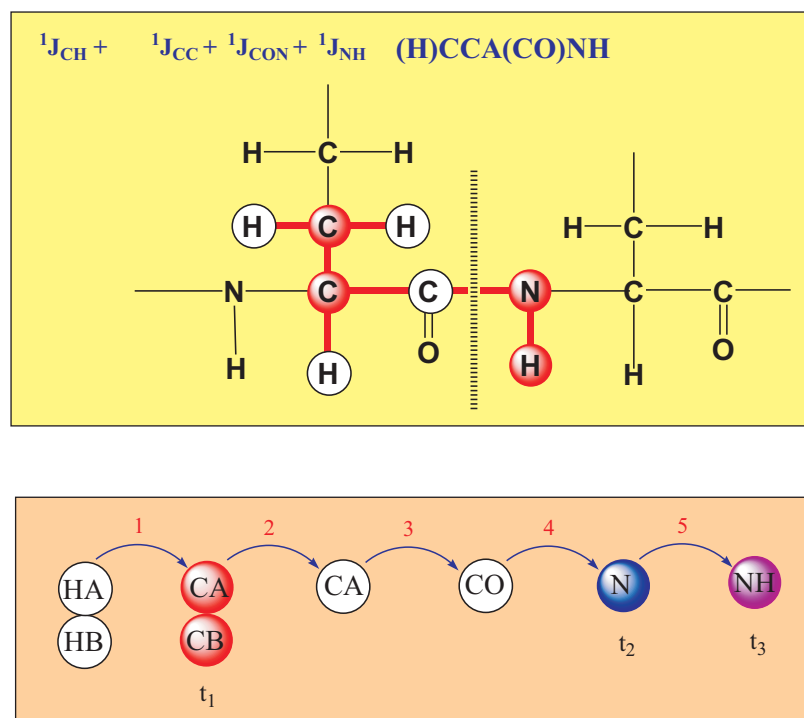




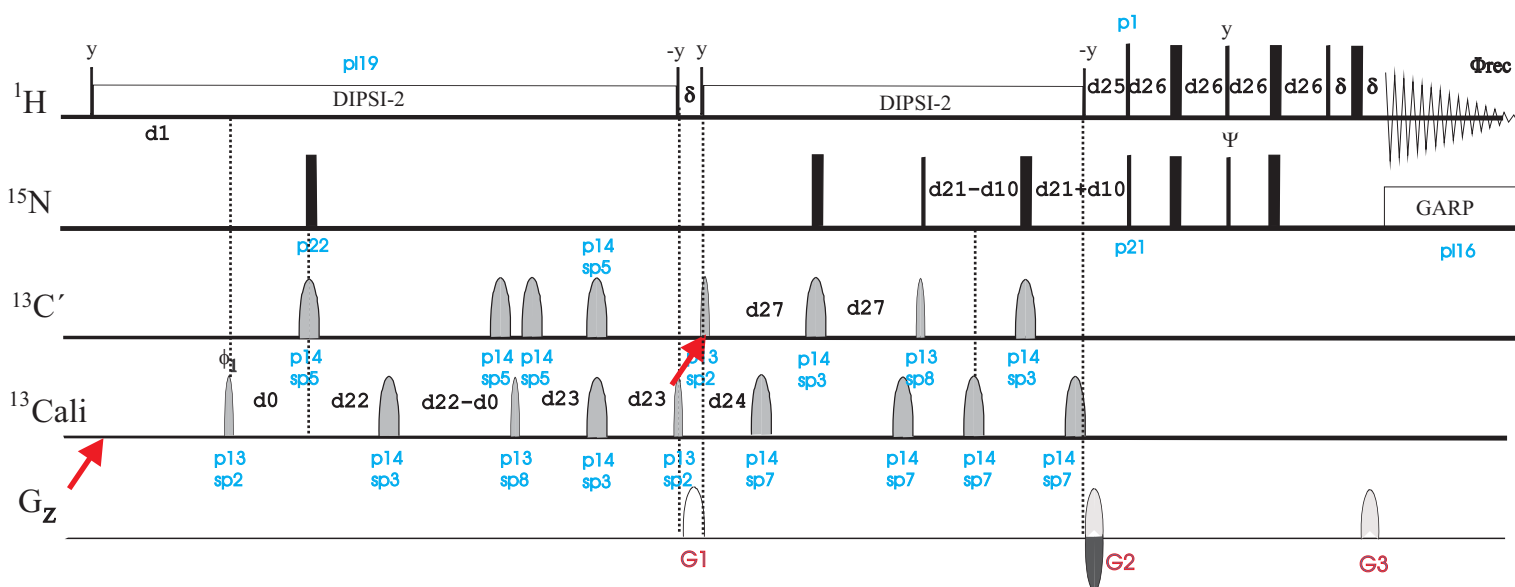
$d21 = 1/4J(NCO) = 12.4m$
 $d22 = 1/4J(CC) = 3.6m$
 $d23 = 1/4J(CBCA) = 3.6m$
 $d24 = 1/2J(CBCA) = 4.4m$
 $d25 = 1/2J(NH) = 5.5m$
 $d26 = 1/4J(NH) = 2.3m$
 $d27 = 1/4J(CACO) = 12.4m$







ccaconhgp3d.2



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3D (H)CC(CO)NH EXPERIMENTS

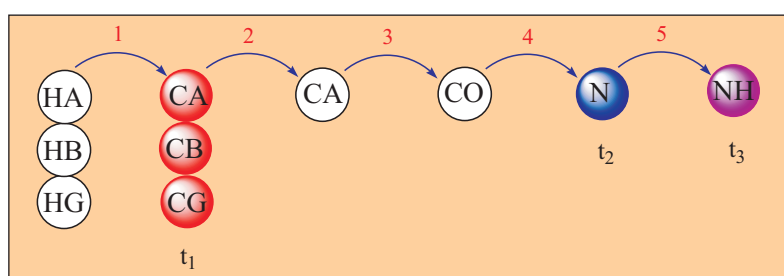
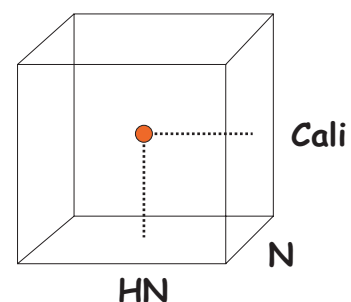
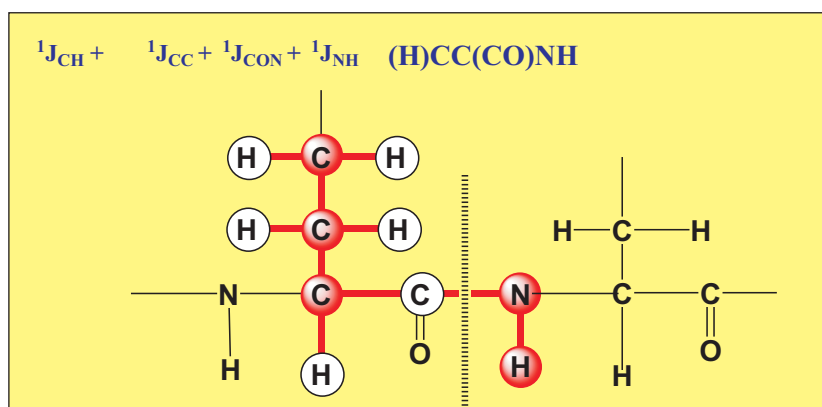
3D (H)CC(CO)NH experiment

3D (H)CC(CO)NH using PEP (**hccconhgp3d3** | HCCCONHGP3D3)

3D (H)CC(CO)NH using WATERGATE (**hccconhgpwg3d3** | HCCCONHGPWG3D3)

3D (H)CC(CO)NH using TROSY (**trhccconhgp3d3** | TRHCCCONHGP3D3)

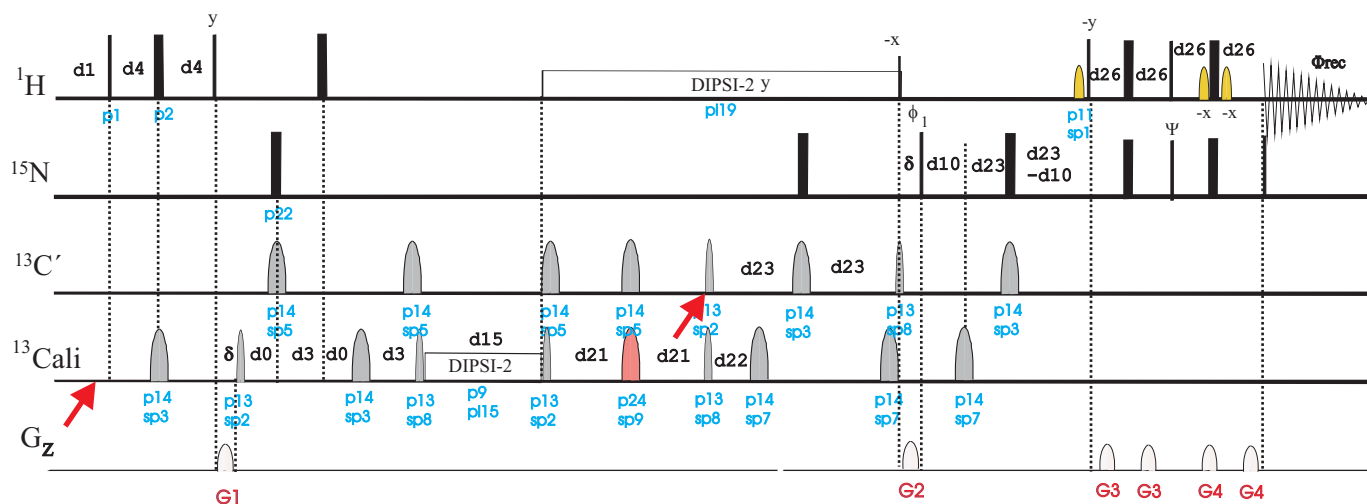
- With gradient echo-antiecho (**trhccconhetgp3d3** | TRHCCCONHETGP3D3)
- With additional gradient (**trhccconhgp3d3.2** | TRHCCCONHGP3D3.2)
- With additional gradient and with gradient echo-antiecho (**trhccconhetgp3d3.2** | TRHCCCONHETGP3D3.2)



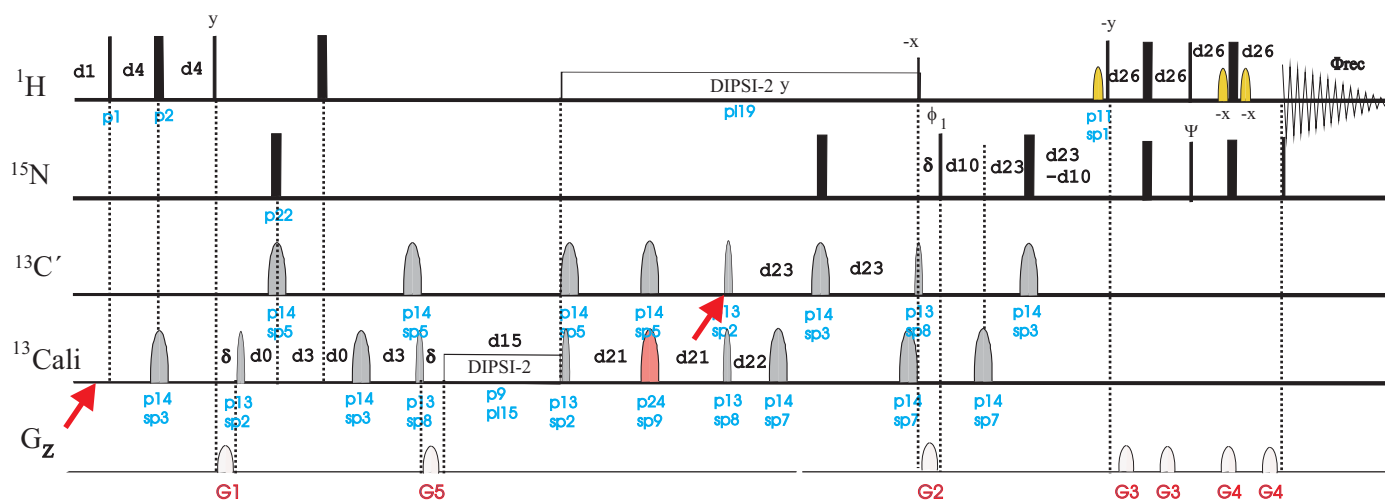
$d3 = 1/6J(CH) = 1.1m$
 $d4 = 1/4J(CH) = 1.7m$
 $d21 = 1/4J(CACO) = 3.6m$
 $d22 = 1/2J(CACO) = 4.4m$
 $d23 = 1/4J(NCO) = 12.4m$
 $d25 = 1/2J(NH) = 5.5m$
 $d26 = 1/4J(NH) = 2.3m$

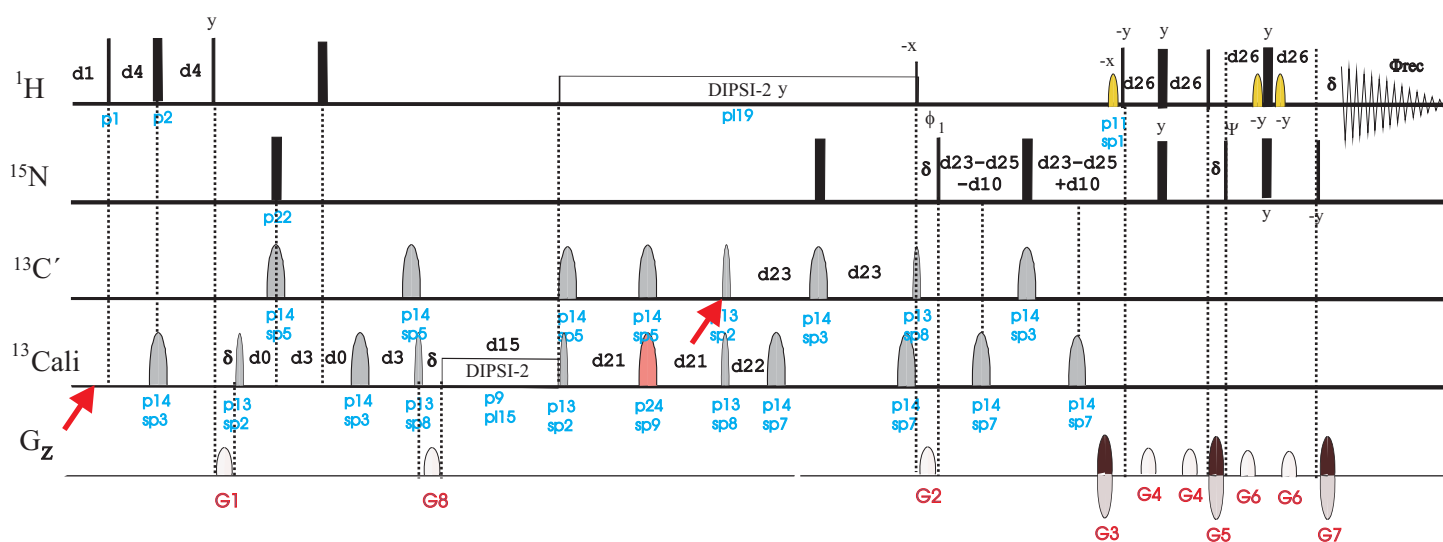
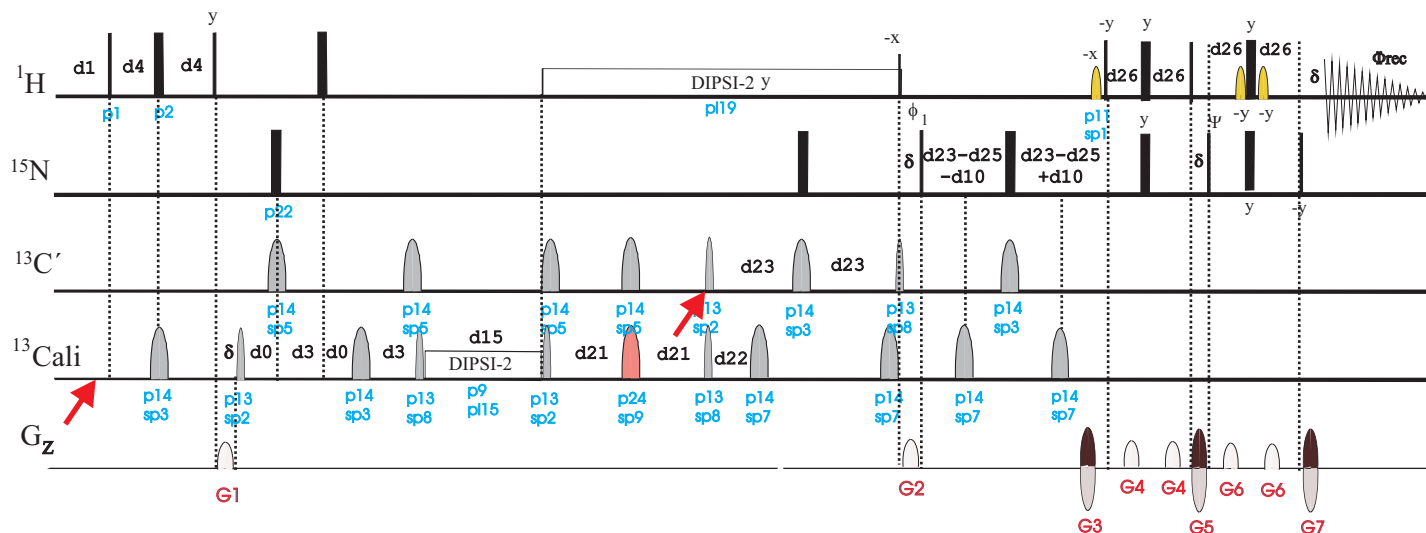


trhccconhgp3d3



trhccconhgp3d3.2





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3D H(CC)(CO)NH EXPERIMENTS

3D H(CC)(CO)NH experiment

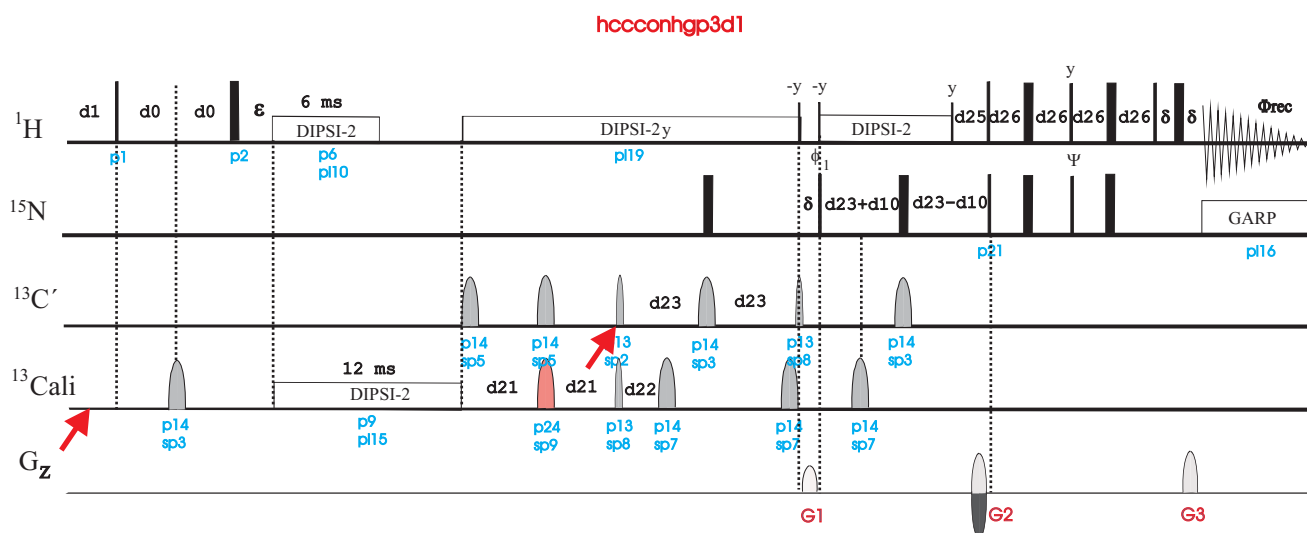
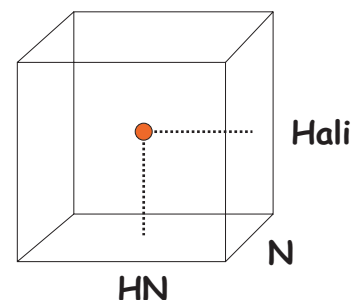
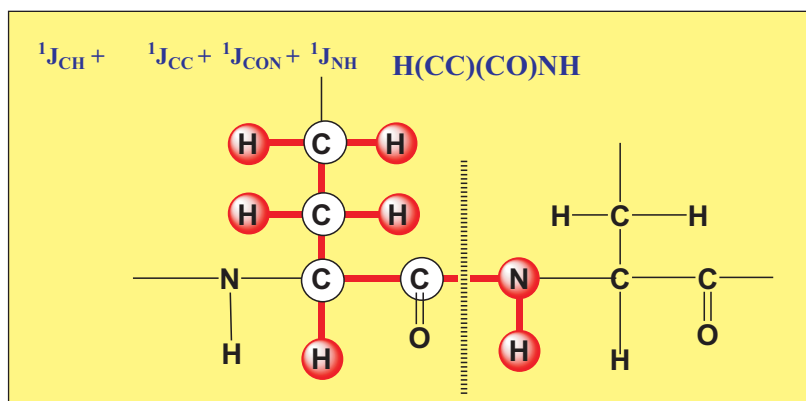
3D H(CC)(CO)NH using PEP (**hccconhgp3d2** | HCCCONHGP3D2)

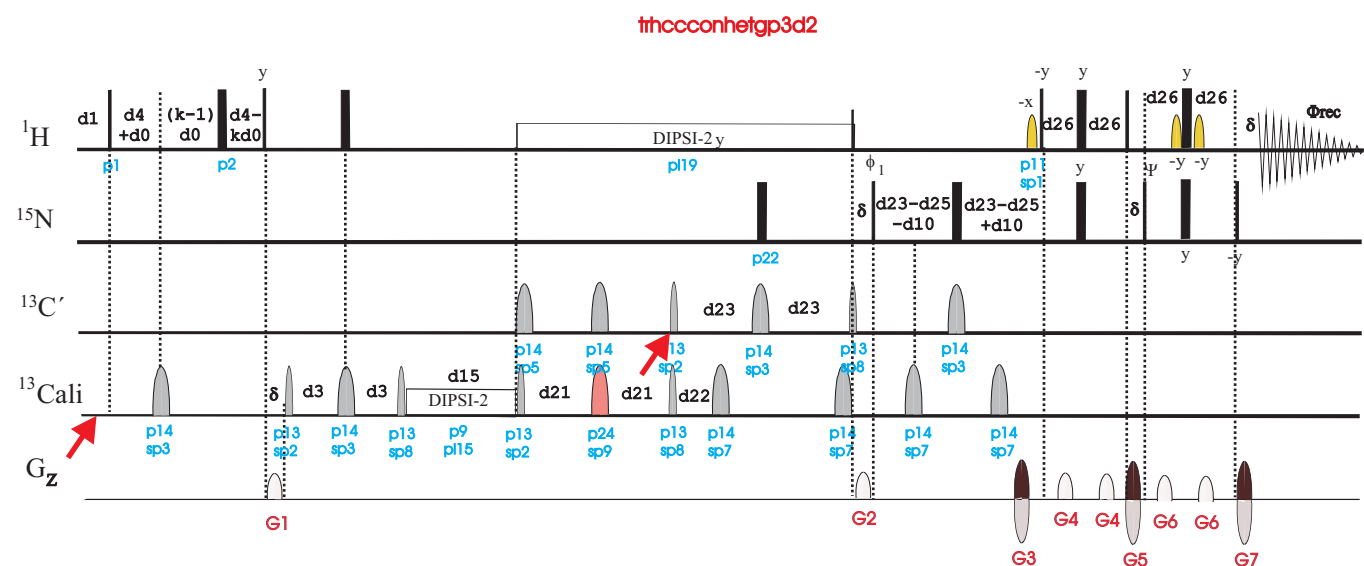
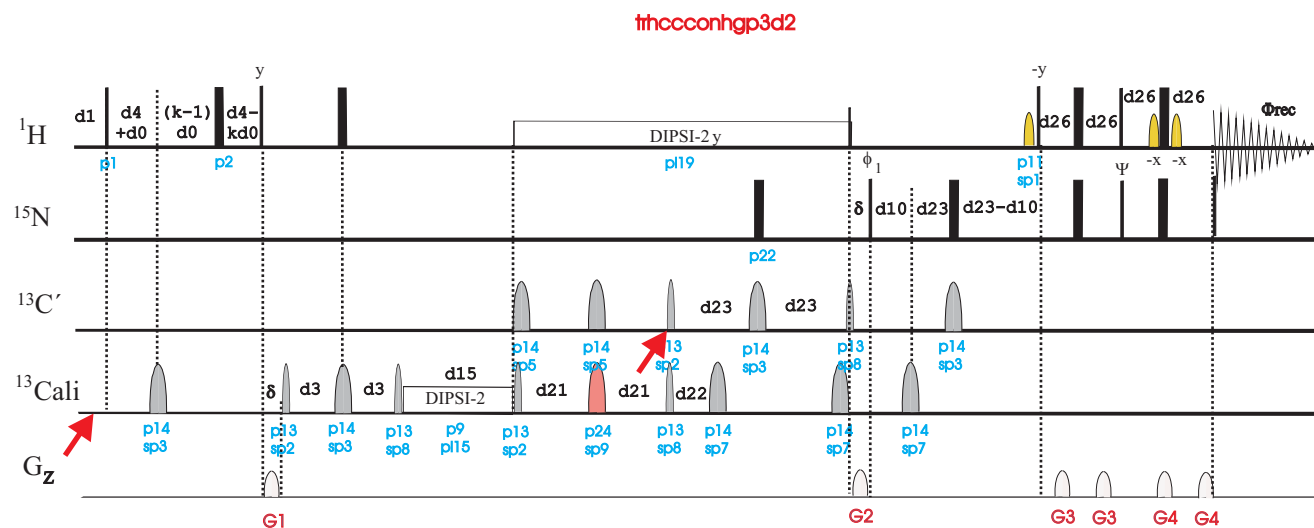
- with ^1H - ^{13}C CP transfer (**hccconhgp3d1** | HCCCONHGP3D1)

3D H(CC)(CO)NH using WATERGATE (**hccconhgpwg3d2** | HCCCONHGPWG3D2)

3D H(CC)(CO)NH using TROSY (**trhccconhgp3d2** | TRHCCCONHGP3D2)

- With gradient echo-antiecho (**trhccconhetgp3d2** | TRHCCCONHETGP3D2)



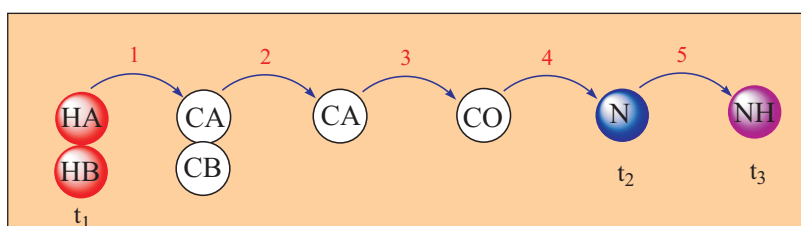
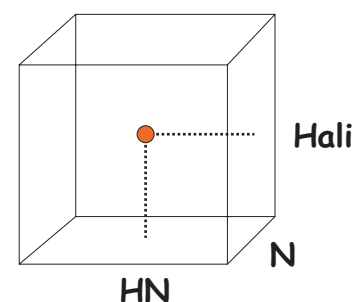
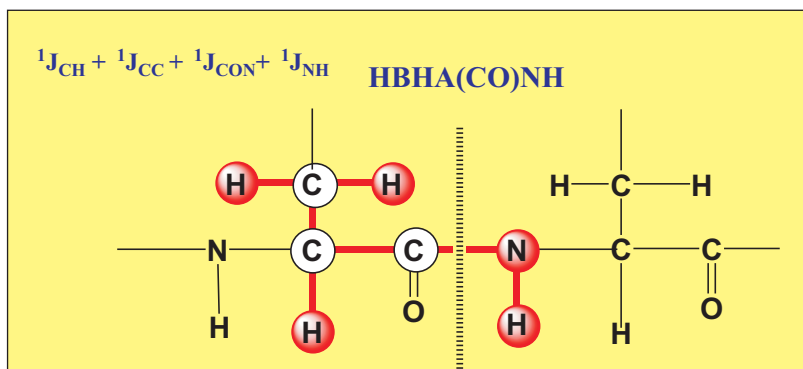


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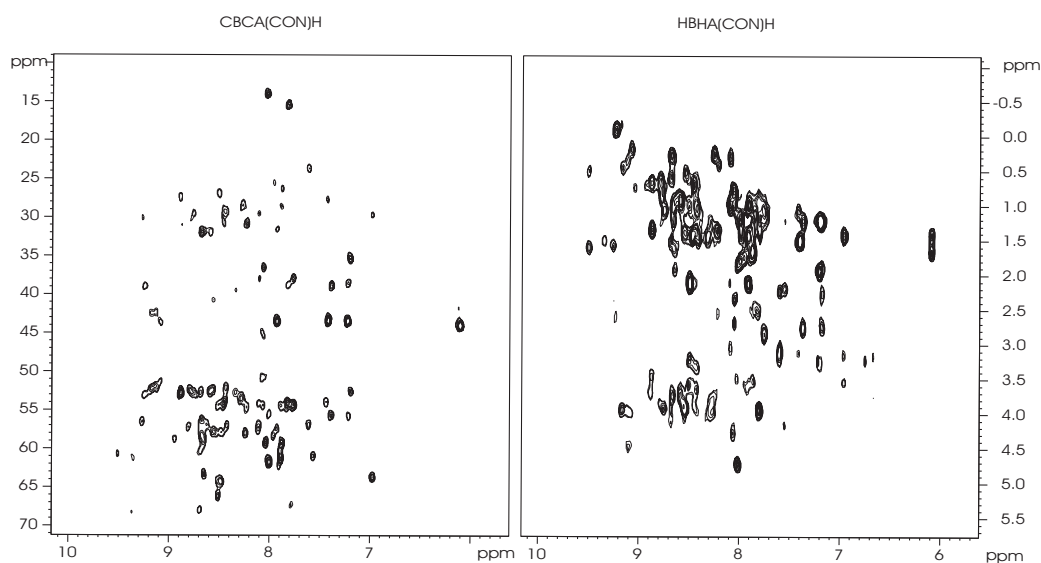
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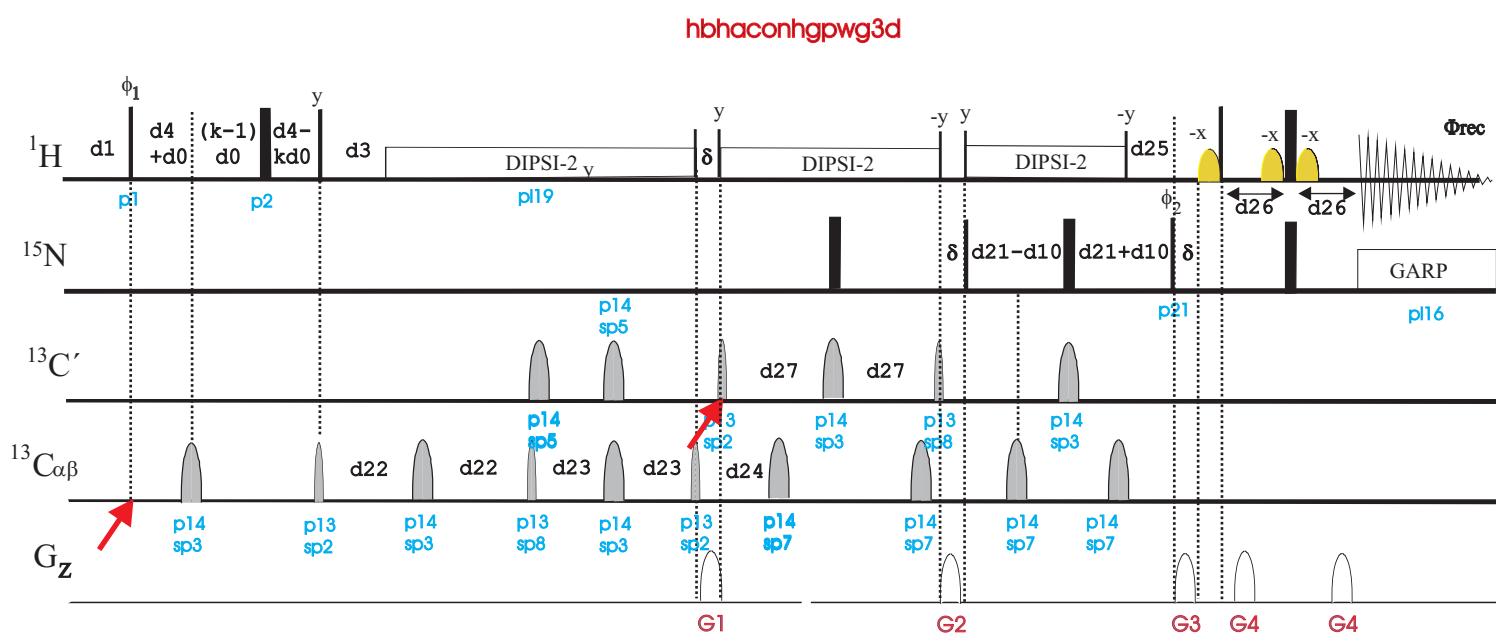
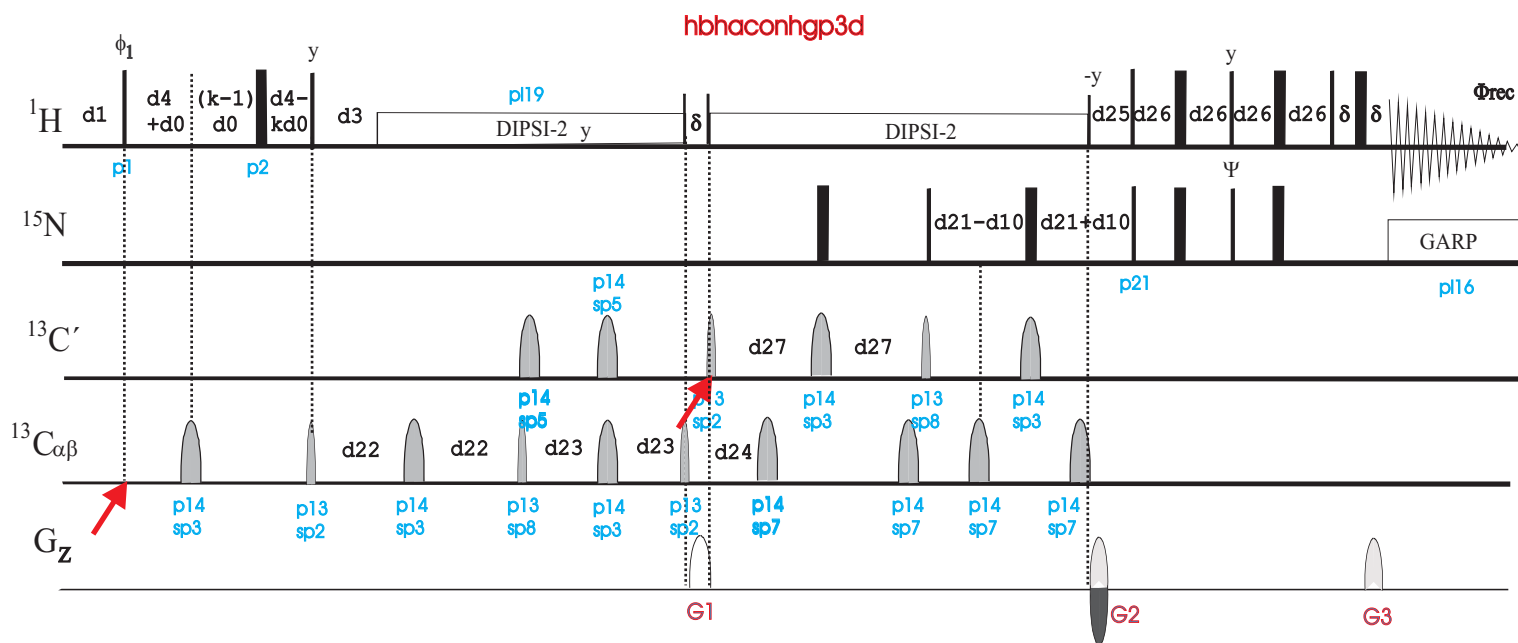
3D HBHA(CO)NH

- 3D HBHA(CO)NH using PEP (**hbhaconhgp3d** | HBHACONHGP3D)
- 3D HBHA(CO)NH using WATERGATE (**hbhaconhgpwg3d** | HBHACONHGPWG3D)
- 3D HBHA(CO)NH using TROSY (**trhbhaconhgp3d** | TRHBHACONHGP3D)
- 3D HBHA(CO)NH using TROSY and gradient echo-antiecho (**trhbhaconhetgp3d** | TRHBHACONHETGP3D)

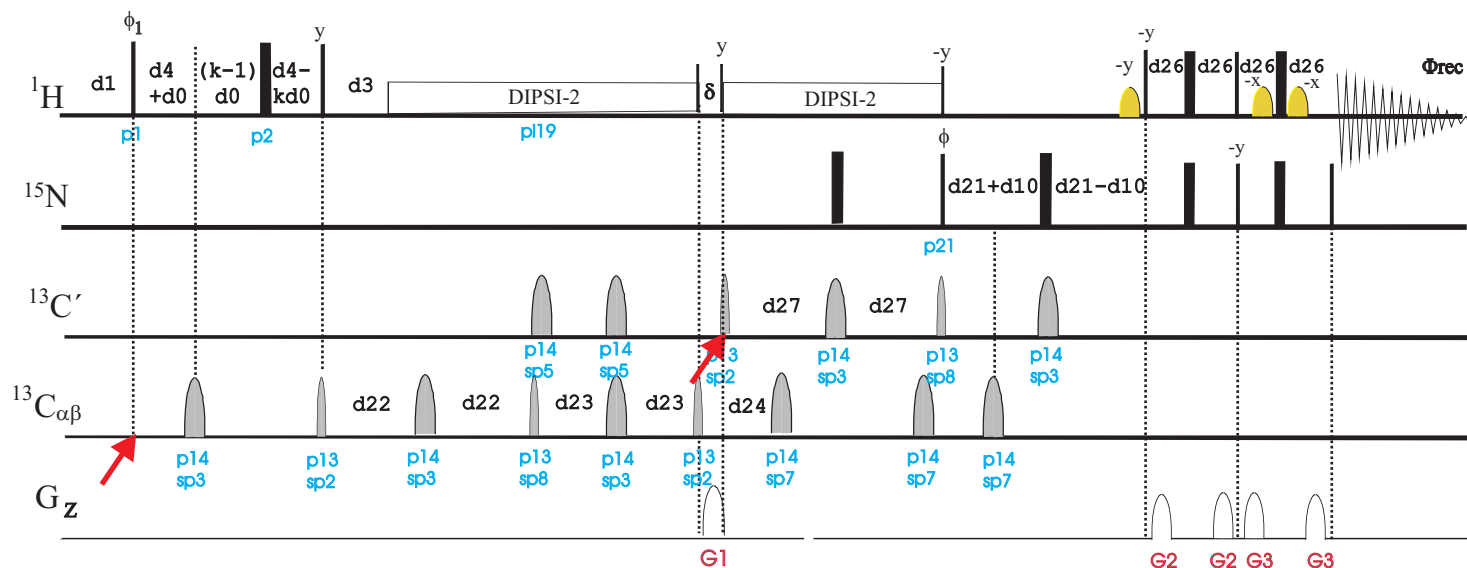


$d4 = 1/4J(CH) = 1.8m$
 $d3 = 1/6J(CH) = 2.2m$
 $d21 = 1/4J(NCO) = 12.4m$
 $d22 = 1/4J(CACB) = 3.6m$
 $d23 = 1/4J(CACO) = 3.6m$
 $d24 = 1/2J(CACO) = 4.4m$
 $d25 = 1/2J(NH) = 5.5m$
 $d26 = 1/4J(NH) = 2.3m$
 $d27 = 1/4J(NCO) = 12.4m$

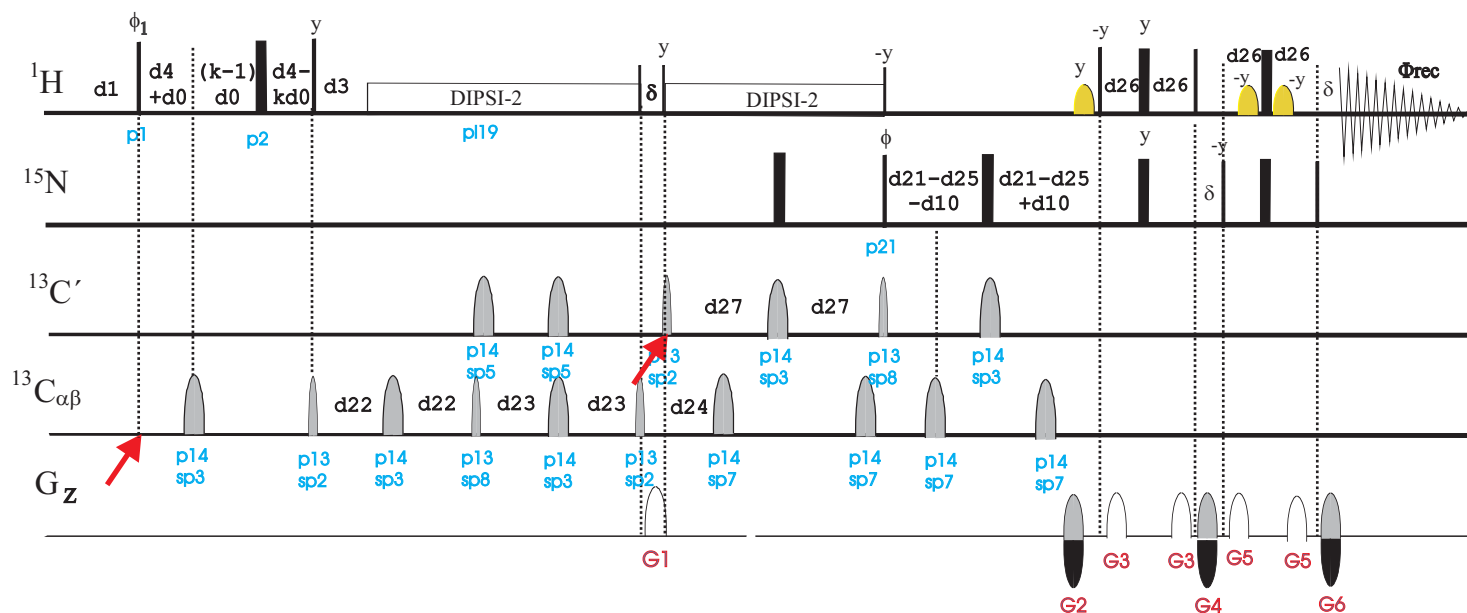




trhbhaconhgp3d



trhbhaconhetgp3d

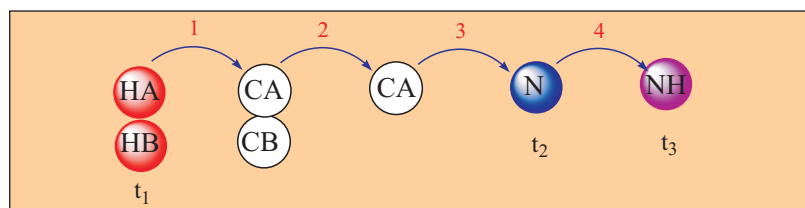
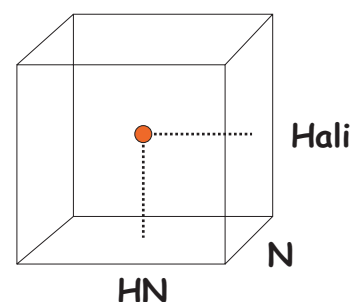
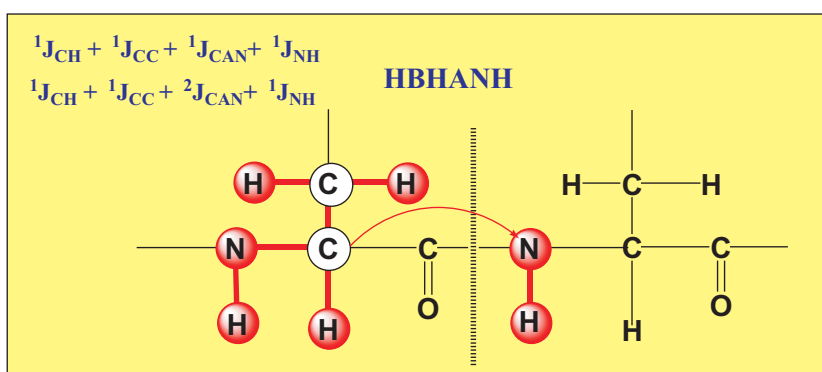


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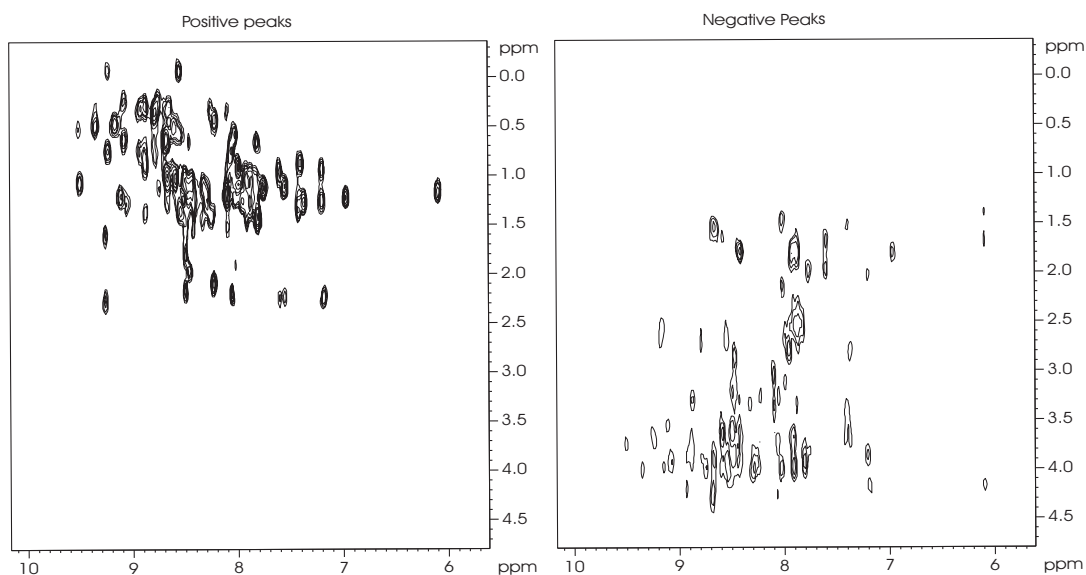
3D HBHANH

- 3D HBHANH using PEP (**hbhanhgp3d**) | HBHANHGP3D)
- 3D HBHANH using WATERGATE (**hbhanhgpwg3d**) | HBHANHGPWG3D)
- 3D HBHANH using TROSY (**trhbhanhgp3d**) | TRHBHANHGP3D)
- 3D HBHANH using TROSY and gradient echo-antiecho (**trhbhanhetgp3d**) | TRHBHANHETGP3D)

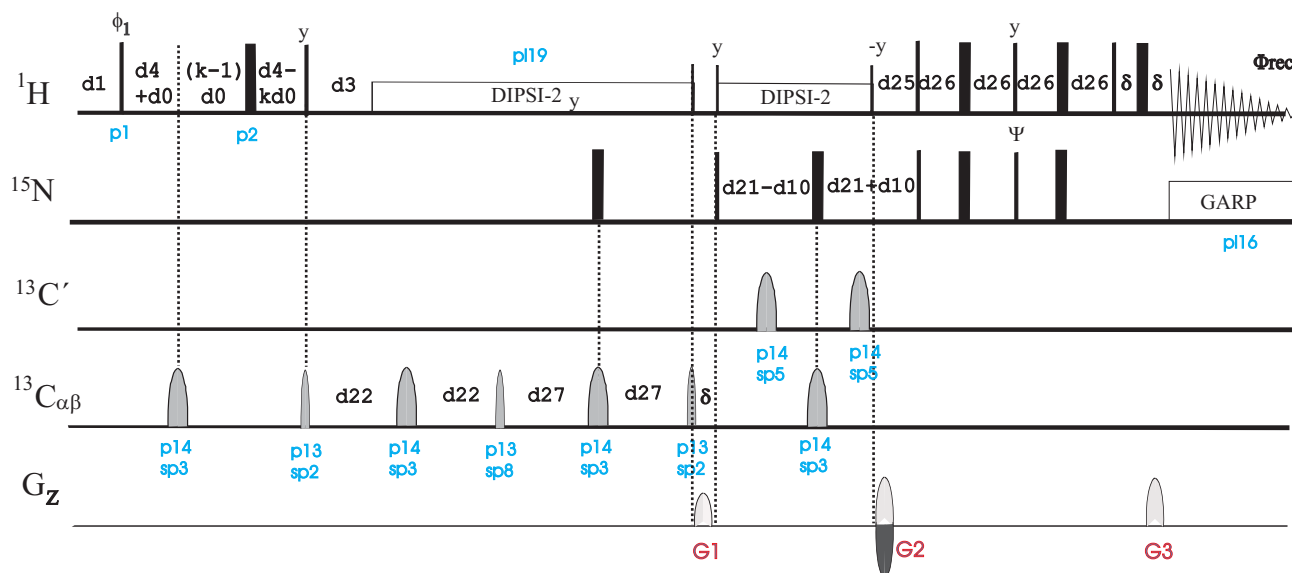


$d4 = 1/4J(CH) = 1.8m$
 $d3 = 1/6J(CH) = 2.2m$
 $d21 = 1/4J(NCO) = 12.4m$
 $d22 = 1/4J(CACB) = 3.6m$
 $d25 = 1/2J(NH) = 5.5m$
 $d26 = 1/4J(NH) = 2.3m$
 $d27 = 1/4J(NCO) = 12.4m$

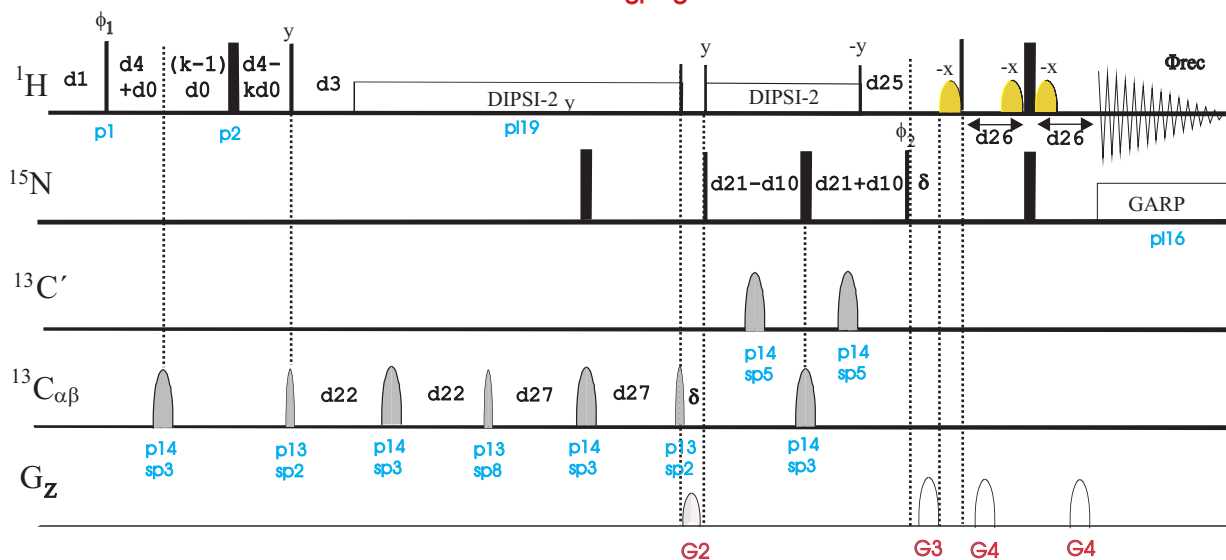
HBHA(N)H

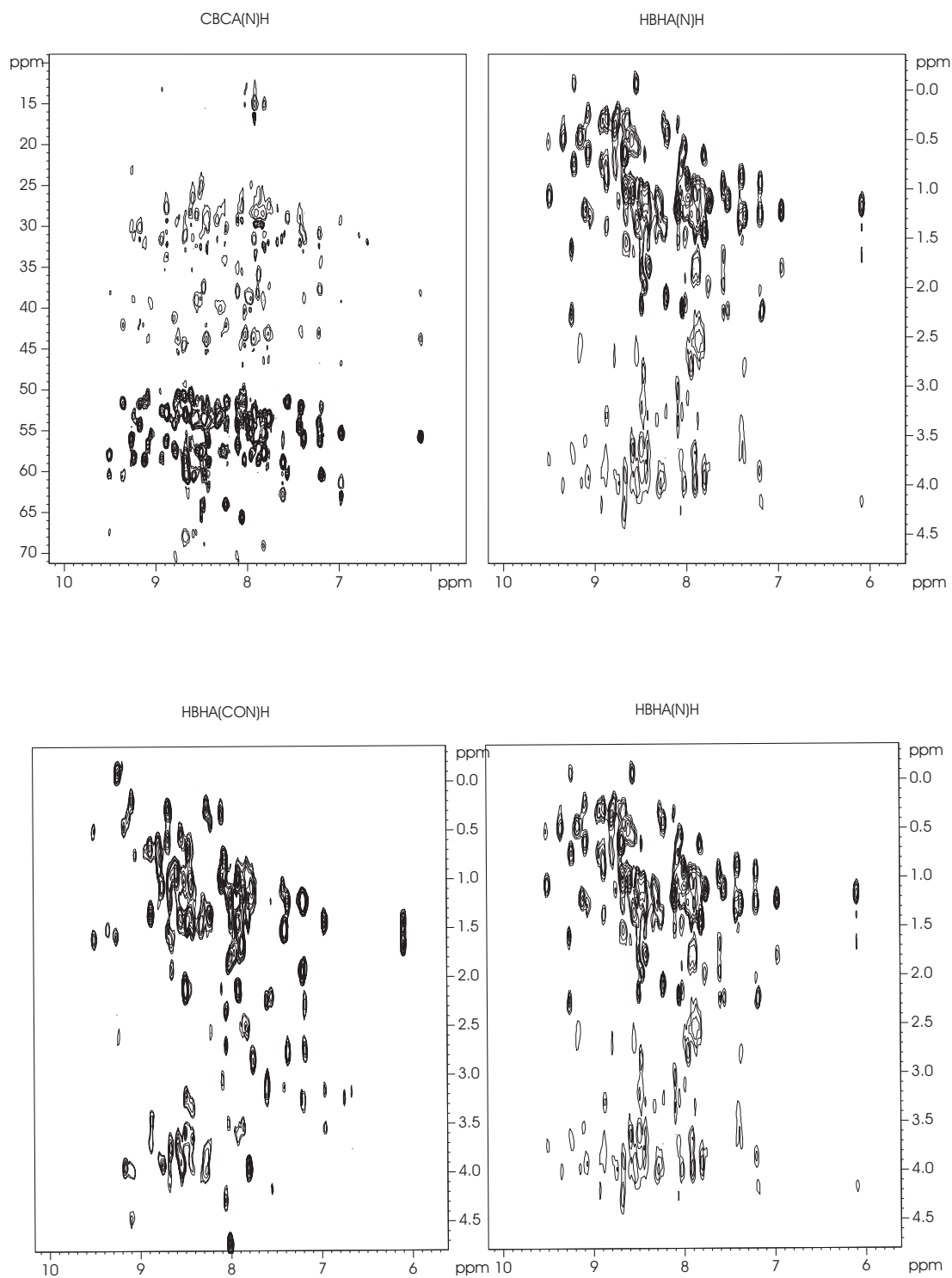


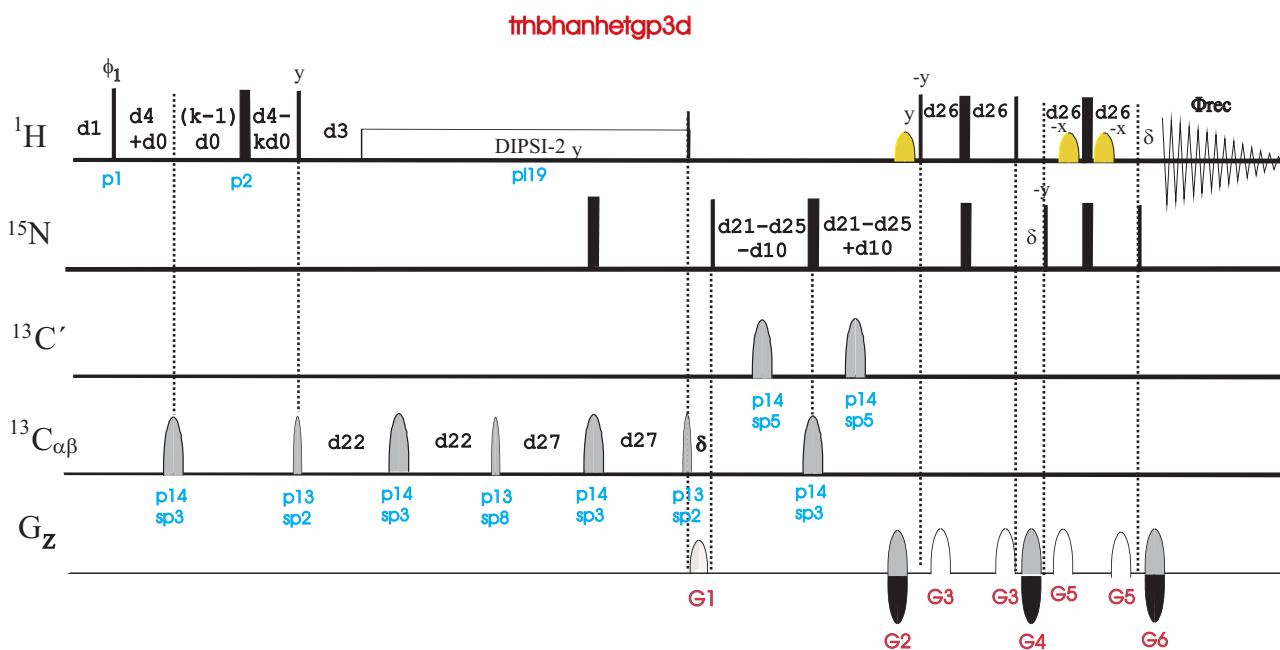
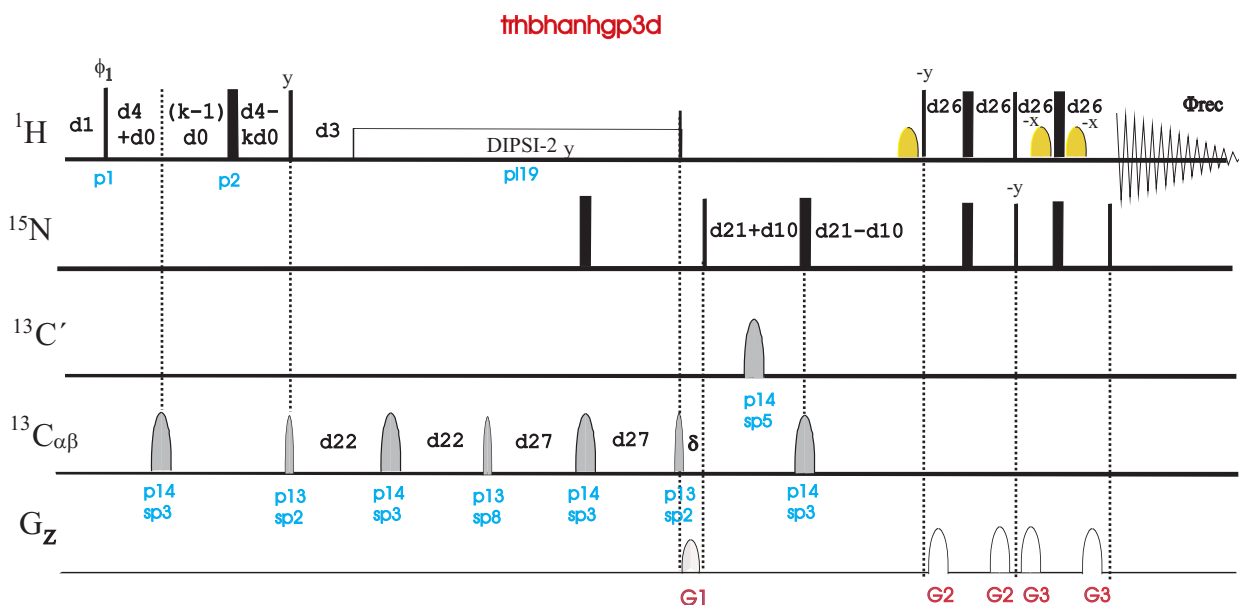
hbhanhgp3d



hbhanhgpwg3d



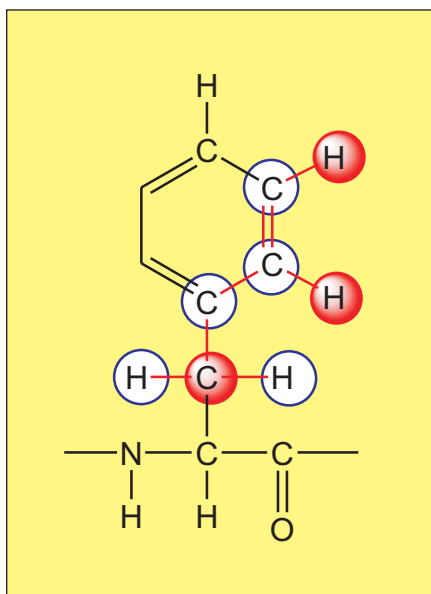




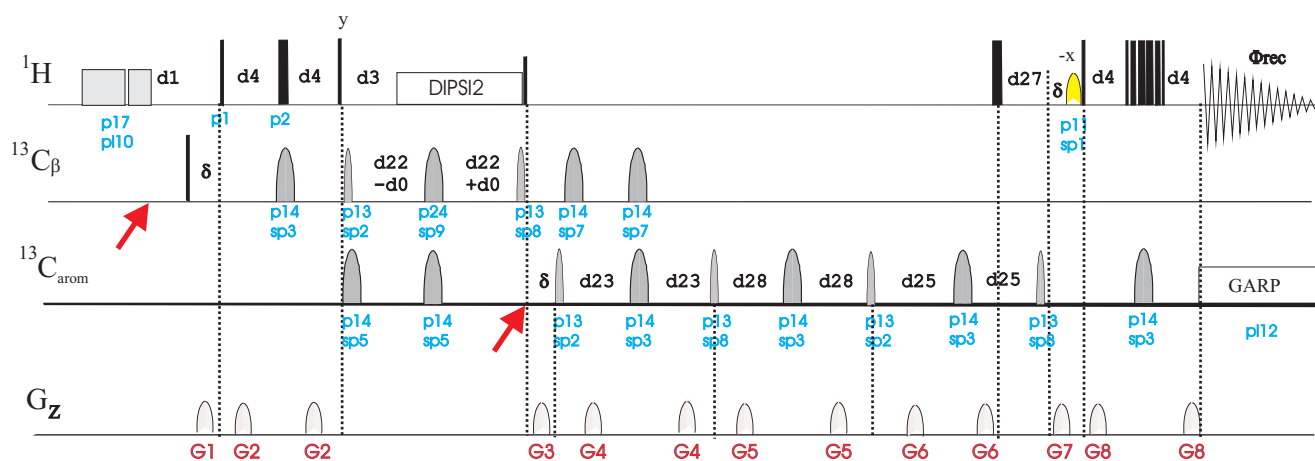
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PROTEIN NMR
AROMATIC RESIDUES



hbcbcgdccehegip



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2D & 3D CARBON-DETECTED
EXPERIMENTS

Main Features of carbon-detected experiments

Experiment Description

Shorter pulse sequences.

No need for solvent suppression techniques.

Avoid radiation damping.

Applied in spectra with low dispersion and on samples with low proton density.

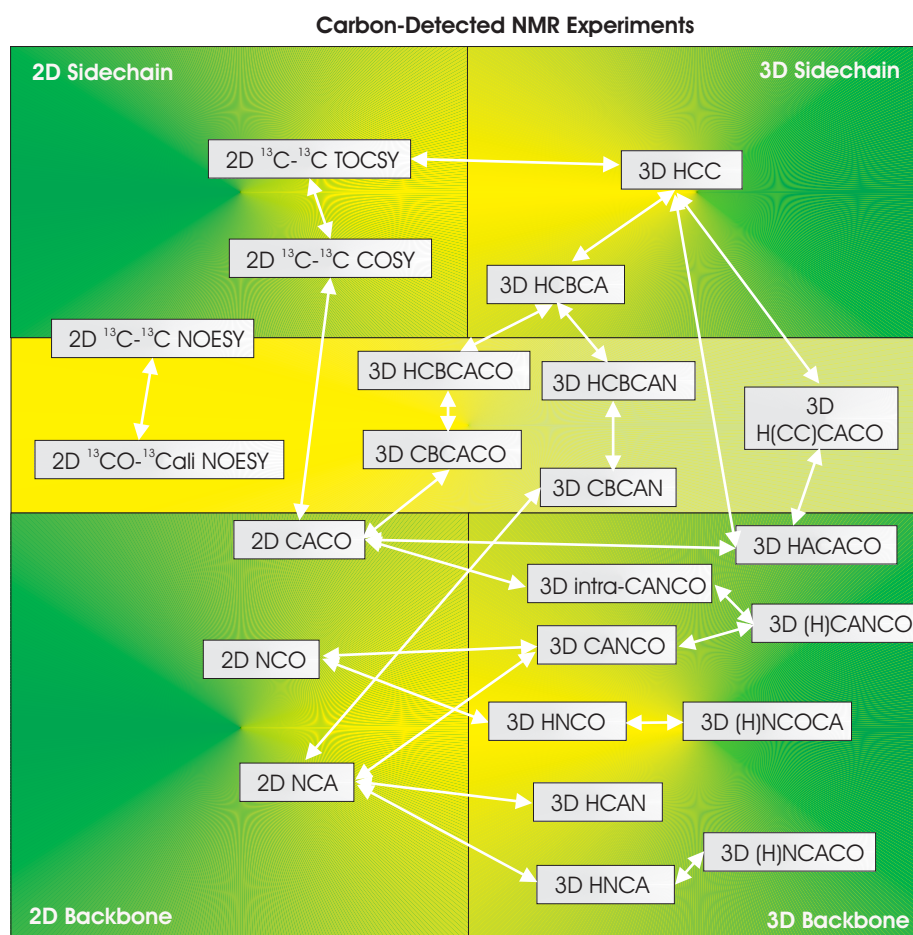
Excellent chemical shift dispersion for carbonyl CO nuclei.

Sample Requirements

Usually applied on doubly-labelled $^{13}\text{C}/^{15}\text{N}$ -labeled protein. Particular interesting in proteins showing fast relaxation properties such a paramagnetic or very large proteins. Also useful for labeled nucleic acids having low proton densities and low spectral dispersion.

Hardware Requirements

Carbon-detected experiments are best performed on a sensitivity-optimized cryoprobe dedicated for ^{13}C detection but it is not mandatory. In most cases, it is also necessary triple-resonance (^1H , ^{13}C , ^{15}N) and z-gradient capabilities.



Experimental details for carbon-detected experiments

Offsets

¹H at 4.7ppm (o2p)
¹⁵N at 118ppm (o3p)
¹³CO at 173ppm (cnst21)
¹³CA at 55 ppm (cnst22)
¹³Cali at 39ppm (cnst23)

Decoupling/Mixing

From f2 channel: ¹H CPD with 3.0KHz Waltz-16 (pcpd2 at pl12)
From f3 channel: ¹⁵N CPD with 1KHz GARP-4 (pcpd3 at pl16)

¹³C TOCSY with 10KHz FLOPSY-16 (pl10)

Spectral Widths

18-24ppm for CO
42 ppm for ¹⁵N
48 ppm for CA
75-80 ppm for Cali

Typical ¹³C pulses from F1 channel (For 600MHz spectrometer)

p11 sp23: 90° Cali/CO on- resonance (320us (Q5 and Q5tr))
P12 sp24: 180° Cali/CO on-resonance (256us (Q3))
p11 sp25: retro 90° Cali/CO on-resonance (320us (Q5 and Q5tr))
p12 sp26: 180° CO/Cali off-resonance with respect to Cali/CO (256us (Q3))
p12 sp27: 180° CO/CA off-resonance with respect to CA/CO (256us (Q3))
p25 sp28: 180° Selective CA on-resonance (1 ms (Q3))
p12 sp29: 180° Cali off-resonance with respect to CA (256us (Q3))
p30 sp30: Simultaneous 180° CA and CO (symmetrically modulated)

p8 sp13: 180° adiabatic for inversion (500us(Chirp))
p24 sp7: 180° adiabatic for refocusing (2000us(Composite chirp))

Very Important!!!: In all pulse programs the syntax

prosol relations= <triple_c>

**is included for automated acquisition/set-up using edprosol/getprosol.
This file is defined in the following directory:**

\$TOPSPINHOME/conf/instr/spect/prosol/relations/triple_c

Complete list of available carbon-detected 2D & 3D NMR experiments

2D Carbon-Detected Experiments:

2D CC COSY

- Conventional (**c_cosy**)
- Constant-time (**c_cosy_ct** / **c_cosy2_ct**)

2D CC NOESY

- Conventional (**c_ccnoesy**)
- 2D CC NOESY (**c_ccnoesy2**)
- Constant-time (**c_ccnoesy_ct**)

2D CC TOCSY

- Conventional (**c_ccflopsy16**)
- With DIPAP for virtual decoupling (**c_ccflopsy16_ia**)
- Constant-time (**c_ccflopsy16_ct**)
- Constant-time with DIPAP for virtual decoupling (**c_ccflopsy16_ctia**)

2D CACO

- Using HSQC (**c_caco**)
- with IPAP for virtual decoupling (**c_caco_ia**)
- with S3E for virtual decoupling (**c_caco_s3**)
- Using HMQC (**c_coca_mq** | **c_coca_mq.2**)

2D COCA

- Using HSQC (**c_coca**)
- with DIPAP for virtual decoupling (**c_coca_ia**)

2D CON

- Using HMQC (**c_con_mq**)
- Using HSQC (**c_con_sq**)
- Using HSQC with IPAP for virtual decoupling (**c_con_iasq**)
- Using HMQC with IPAP for virtual decoupling (**c_con_mqia**)

2D CAN

- Using HMQC (**c_can_mq**)
- Using HMQC (**c_can_mq.2**)
- Using HSQC with DIPAP for virtual decoupling (**c_can_iasq**)

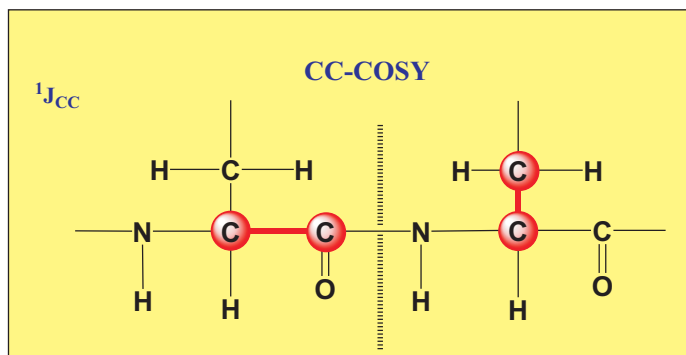
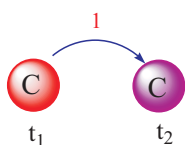
3D Carbon-Detected Experiments

- 3D HCC CT-TOCSY (**c_hccflopsy16_3d**)
- 3D HCBCA
 - With CA detection (**c_hcbca_3d**)
 - With CA detection and with DIPAP for virtual decoupling (**c_hcbca_ia3d**)
- 3D HCB(CA)CO
 - With CO detection (**c_hcbcac0_3d**)
 - With CO detection and with IPAP for virtual decoupling (**c_hcbcac0_ia3d**)
 - With CO detection and with S³E for virtual decoupling (**c_hcbcac0_s33d**)
- 3D CBCACO
 - With CO detection (**c_cbcaco_3d**)
 - With CO detection and with IPAP for virtual decoupling (**c_cbcaco_ia3d**)
- 3D (H)CBCAN
 - With CA detection (**c_hcbcan_3d**)
 - With CA detection with DIPAP for virtual decoupling (**c_hcbcan_ia3d**)
- 3D HCACO
 - With CO detection (**c_hcac0_3d**)
 - With CO detection and with IPAP for virtual decoupling (**c_hcac0_ia3d**)
 - With CO detection and with S3E for virtual decoupling (**c_hcac0_s33d**)
 - With CO detection and using HMQC (**c_hacaco_3d**)
- 3D HCAN
 - With CA detection (**c_hcan_3d**)
 - With CA detection and with DIPAP for virtual decoupling (**c_hcan_ia3d**)
- 3D CANCO
 - With CO detection (**c_canco_3d**)
 - With CO detection and with IPAP for virtual decoupling (**c_canco_ia3d**)
 - With CO detection and with IPAP for virtual decoupling (**c_canco_ia3d.2**)
 - (H)CANCO starting from HA and with CO detection (**c_hcanco_3d**)
 - (H)CANCO starting from HA and with CO detection and with IPAP for virtual decoupling (**c_hcanco_ia3d**)
- 3D intra-CANCO
 - With CO detection (**c_cancoi_3d**)
 - With CO detection and with IPAP for virtual decoupling (**c_cancoi_ia3d**)
 - Intra-(H)CANCO starting from HA and with CO detection (**c_hcancoi_3d**)
 - Intra-(H)CANCO starting from HA and with CO detection and with IPAP for virtual decoupling (**c_hcancoi_ia3d**)
- 3D HNCA
 - With CA detection (**c_hnca_3d**)
 - With CA detection and with DIPAP for virtual decoupling (**c_hnca_ia3d**)
- 3D HNCO
 - With CO detection (**c_hnco_3d**)
 - With CO detection and with IPAP for virtual decoupling (**c_hnco_ia3d**)
- 3D (H)NCACO
 - With CO detection (**c_hncaco_3d**)
 - With CO detection and with IPAP for virtual decoupling (**c_hncaco_ia3d**)
 - With CO detection and with S³E for virtual decoupling (**c_hncaco_s33d**)
- 3D (H)NCOCA
 - With CA detection (**c_hncoca2_3d**)
 - With CA detection and with DIPAP for virtual decoupling (**c_hncoca2_ia3d**)
 - (H)N(CO)CACO with CO detection (**c_hncoca_3d**)
 - (H)N(CO)CACO with CO detection and with IPAP for virtual decoupling (**c_hncoca_ia3d**)

2D ^{13}C - ^{13}C COSY Experiment

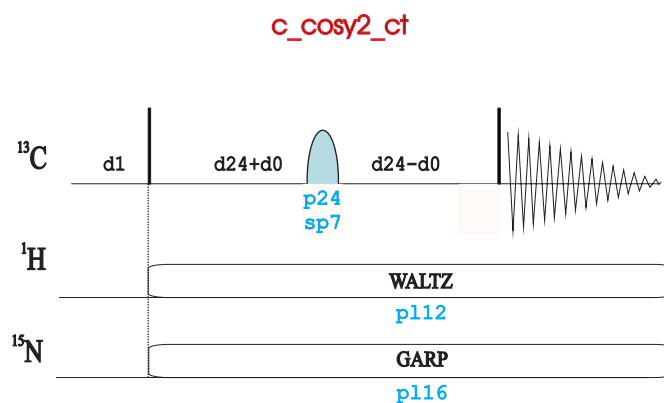
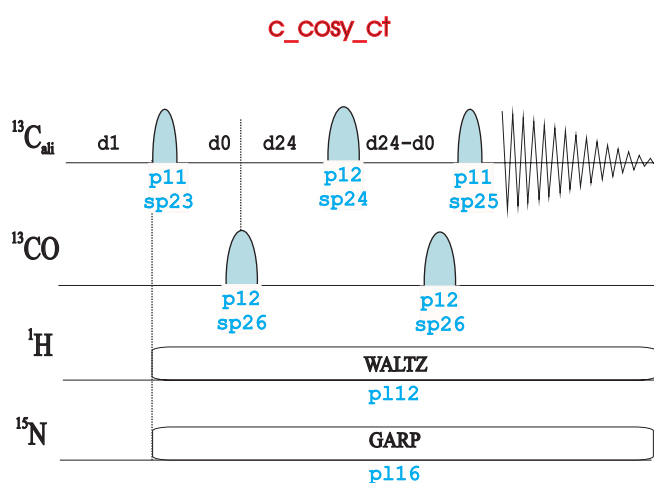
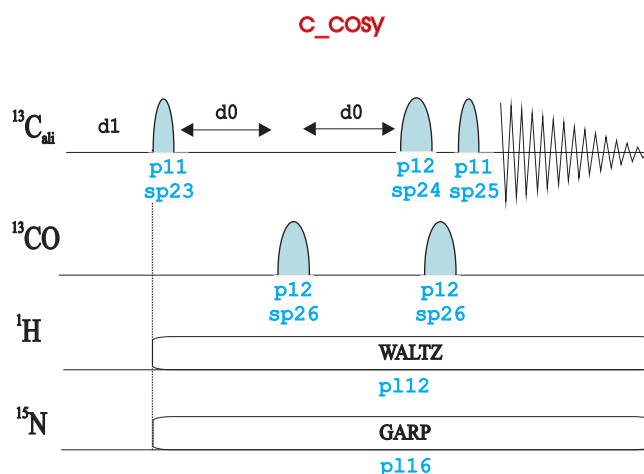
Experiment Description

The 2D CC COSY experiment allows to obtain a homonuclear CC correlation map to trace out through-bond carbon-carbon connectivities in ^{13}C -labeled proteins



Related Experiments

2D COCA
2D CC and 3D HCC TOCSY



Involved delays:

$$d24 = 1/4J(\text{CC}) = 5\text{ms}$$

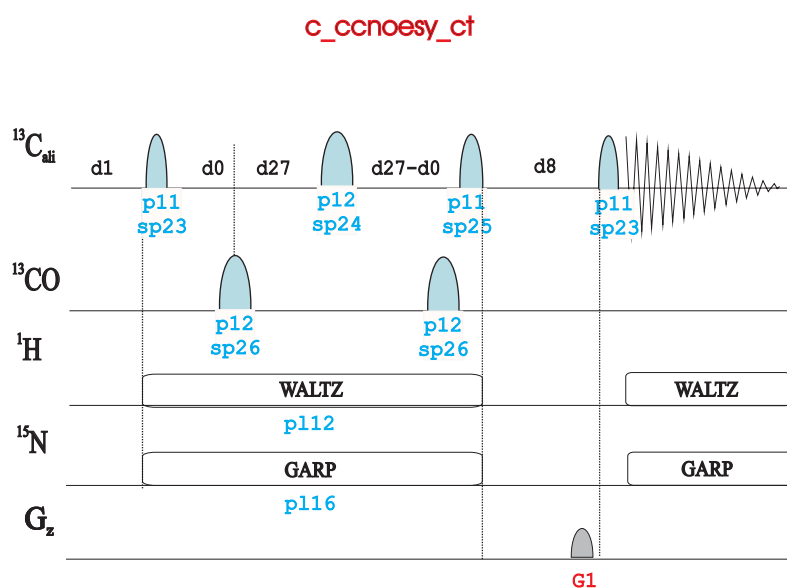
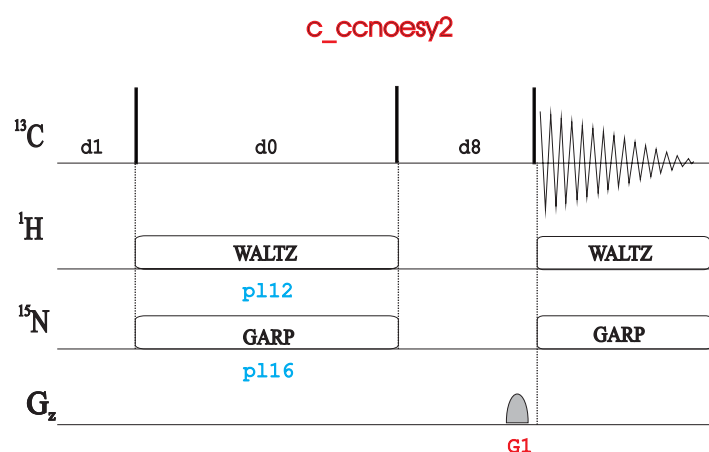
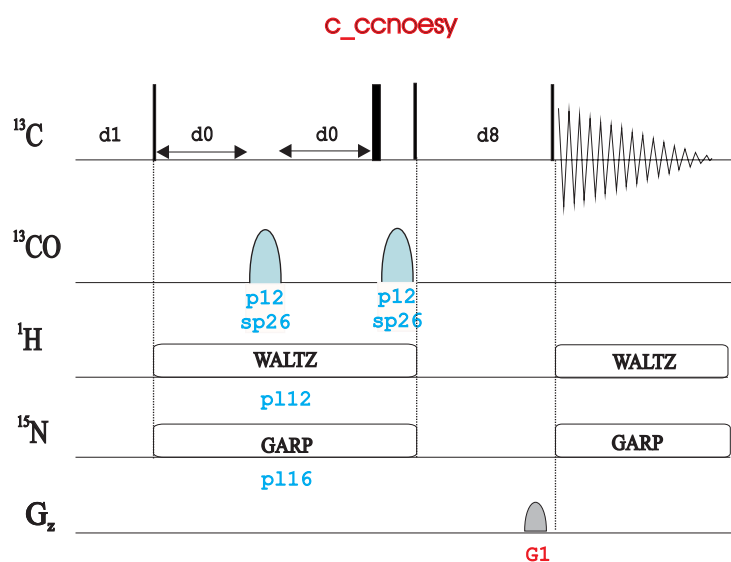
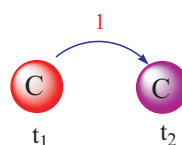
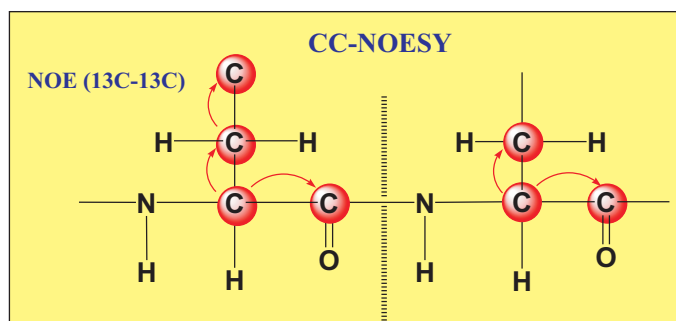
2D ^{13}C - ^{13}C NOESY Experiment

Experiment Description

The 2D CC NOESY experiment allows to obtain a homonuclear CC correlation map to trace out through-space carbon-carbon interactions in ^{13}C -labeled proteins

Related Experiments

2D CC COSY and 2D CC TOCSY



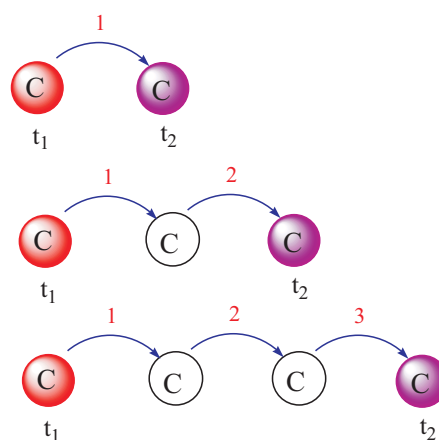
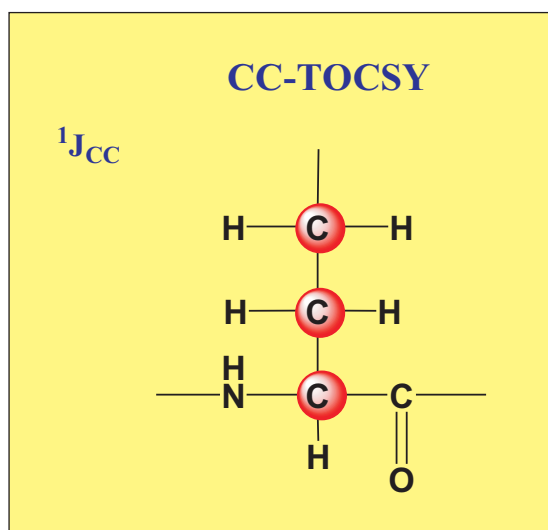
Involved delays:

d8=NOE mixing time
d27=1/2J(CACB)=13.3ms

2D ^{13}C - ^{13}C TOCSY Experiment

Experiment Description

The 2D CC TOCSY experiment is a ^{13}C -start, ^{13}C -detected TOCSY scheme that allows to trace out through-bond CC connectivities via $1J(\text{CC})$ in ^{13}C -labeled proteins. Homonuclear CC splitting in the acquisition dimension can be removed by selective homonuclear decoupling during acquisition or virtually using the DIPAP approach (05JMR404).



NMR Spectrum

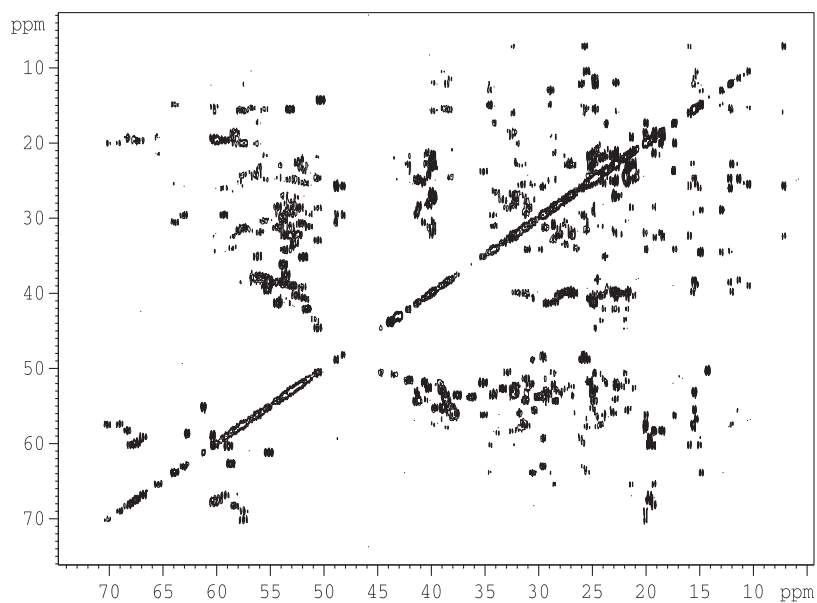
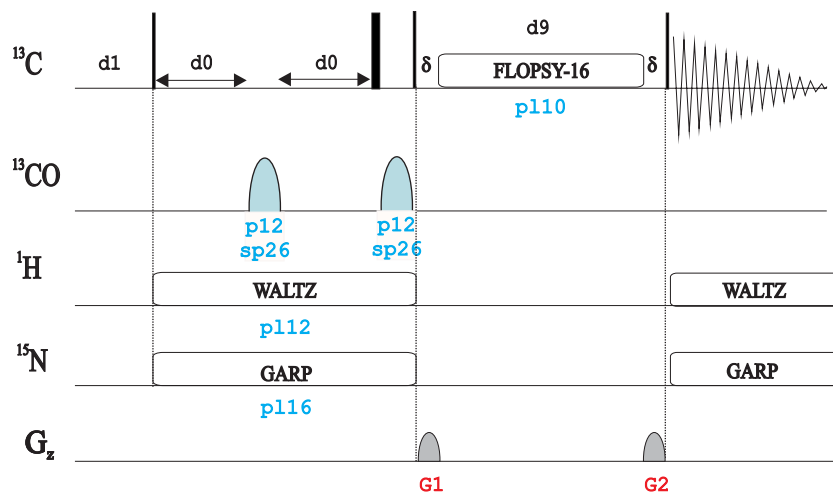
The experiment provides a 2D correlation map in which each cross-peak displays a doublet in the acquisition dimension due to $1J(\text{CC})$ coupling.

Related Experiments

2D CC COSY and 2D CC NOESY
3D carbon-detected HCC TOCSY

3D HCCH-type experiments

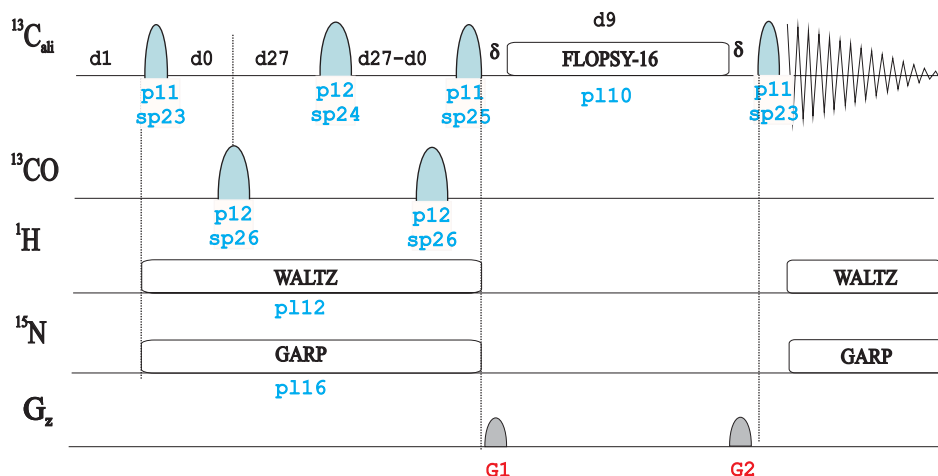
c_ccflopsy16



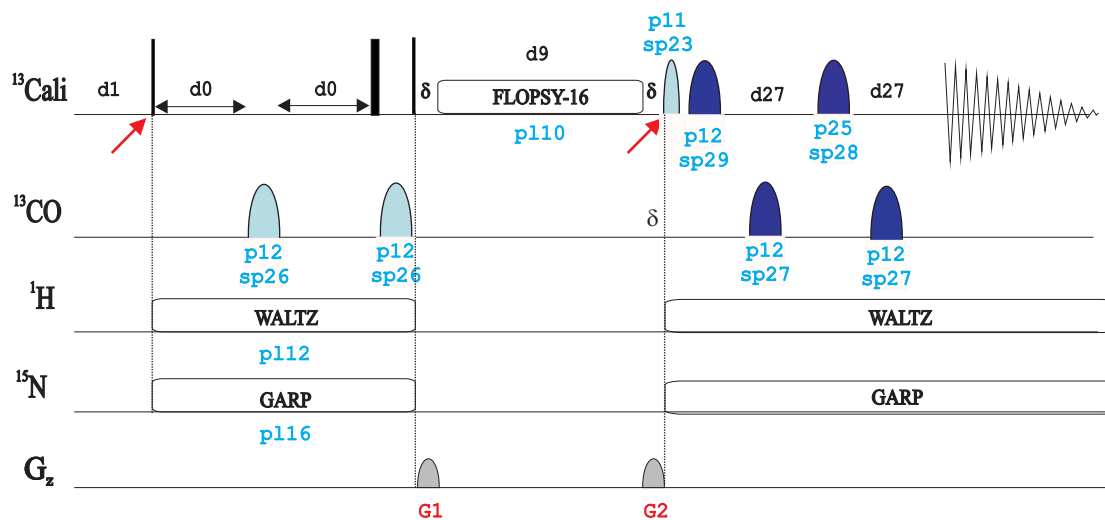
Involved delays:

$d9 = \text{TOCSY mixing time}$
 $d27 = 1/2J(\text{CACB}) = 13.3\text{ms}$
 or $= 1/8J(\text{CACB}) = 3.6\text{ms}$ (DIPAP)
 $d22 = 1/4J(\text{COCA}) = 4.5\text{ms}$
 $d23 = 1/2J(\text{CACB}) = 13.3\text{ms}$ (DIPAP)

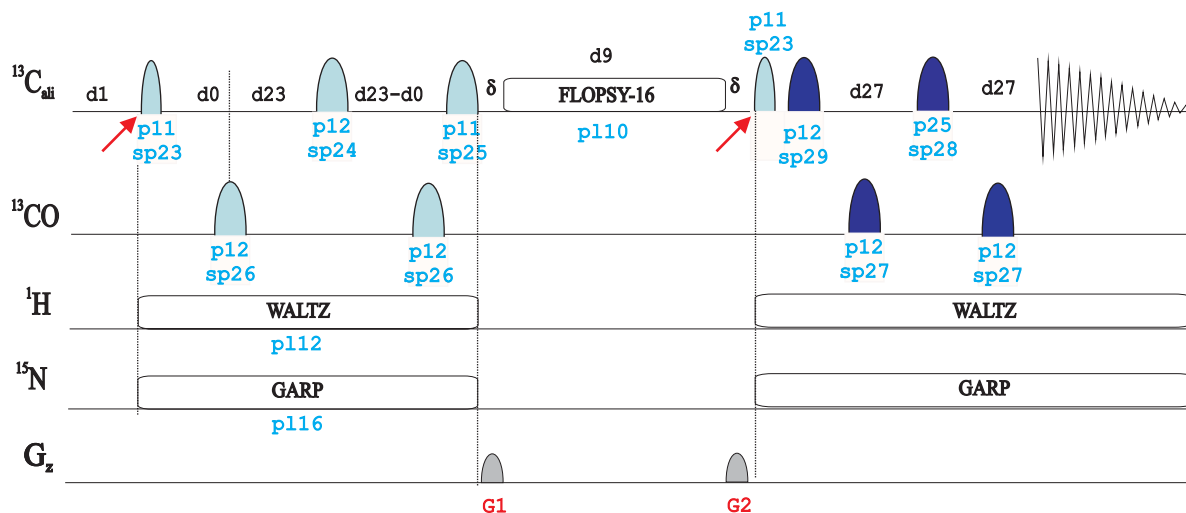
c_ccflopsy16_ct



c_ccflopsy16_la



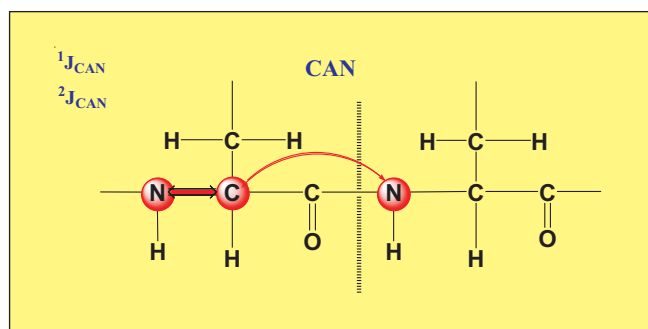
c_ccflopsy16_ctla



2D CAN Experiment

Experiment Description

The 2D CAN experiment is a CA-detected experiment that allows the correlation between the chemical shifts of the CA(i) carbon with the Nitrogen of the same (i) and the next (i+1) residue in doubly-labeled $^{13}\text{C}/^{15}\text{N}$ proteins. Homonuclear CO-CA splitting in the acquisition dimension can be removed by homonuclear decoupling during acquisition or virtually using the IPAP approach (05JMR404).

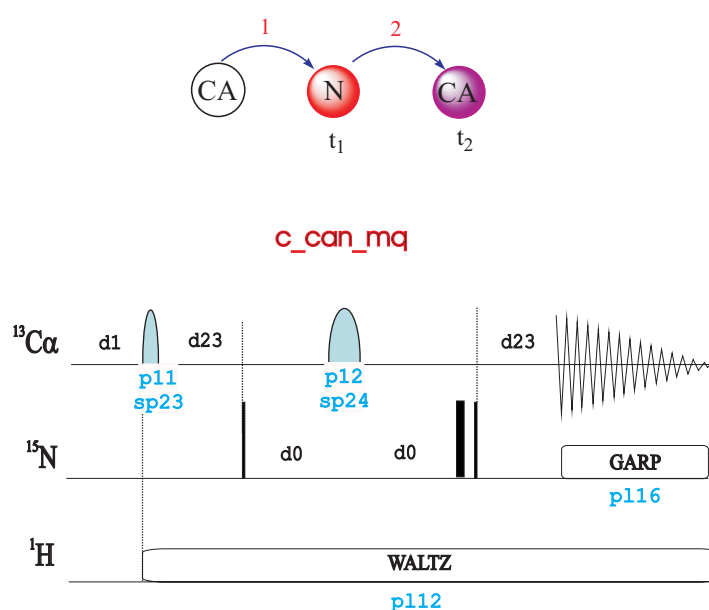


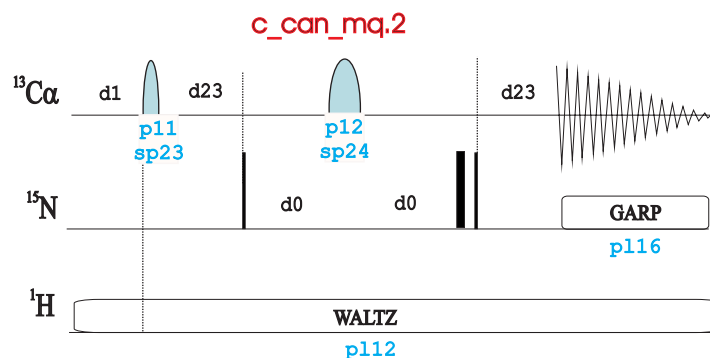
NMR Spectrum

The experiment provides a 2D correlation map in which each CA in the acquisition dimension is correlated to two different N chemical shifts.

Related Experiments

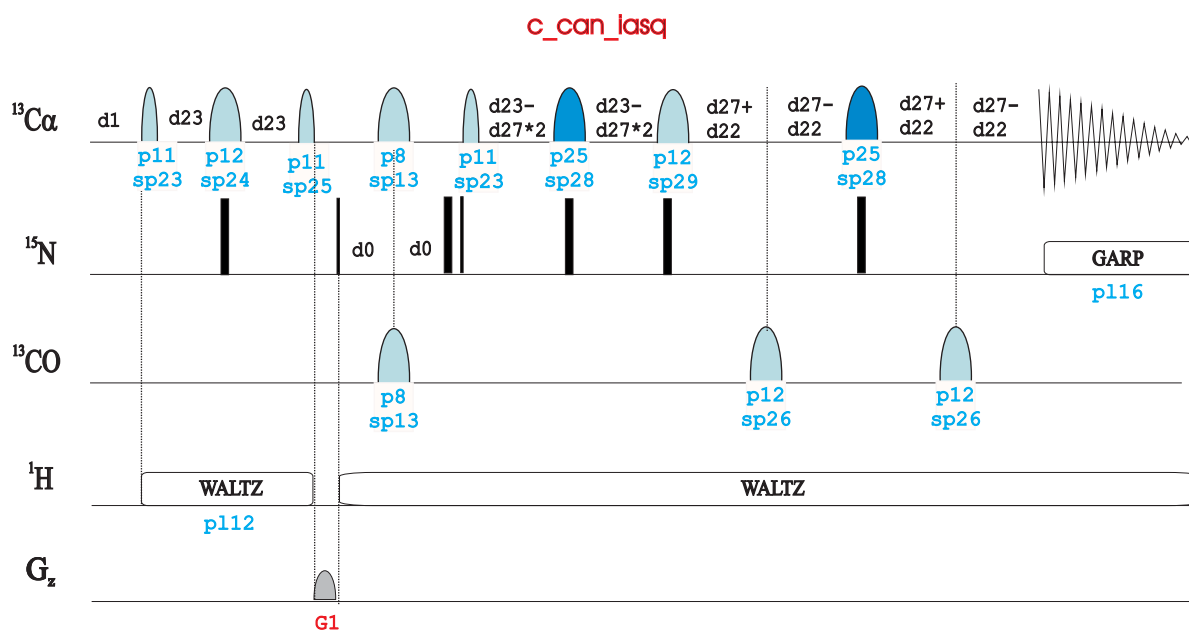
3D HCAN





Involved delays:

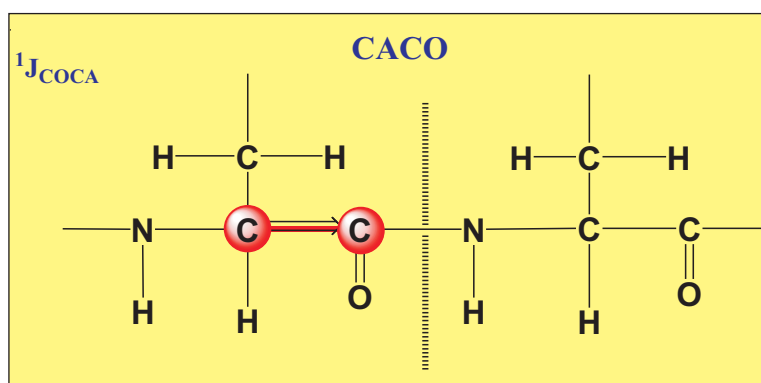
$d27 = 1/8J(CACB) = 3.6\text{ms}$
 $d22 = 1/4J(COCA) = 4.5\text{ms}$
 $d23 = 1/2J(CAN) = 25\text{ms}$ (in mq experiments)
 or $= 1/4J(CAN) = 12.4\text{ms}$ (in sq experiments)



2D CACO Experiment

Experiment Description

The 2D CACO experiment is a CO-detected that allows the correlation between the chemical shifts of the CA and CO carbons of the same residue in ^{13}C -labeled proteins. Homonuclear CO-CA splitting in the acquisition dimension can be removed by homonuclear decoupling during acquisition or virtually using the IPAP approach (05JMR404).



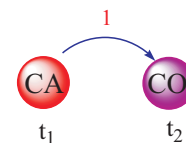
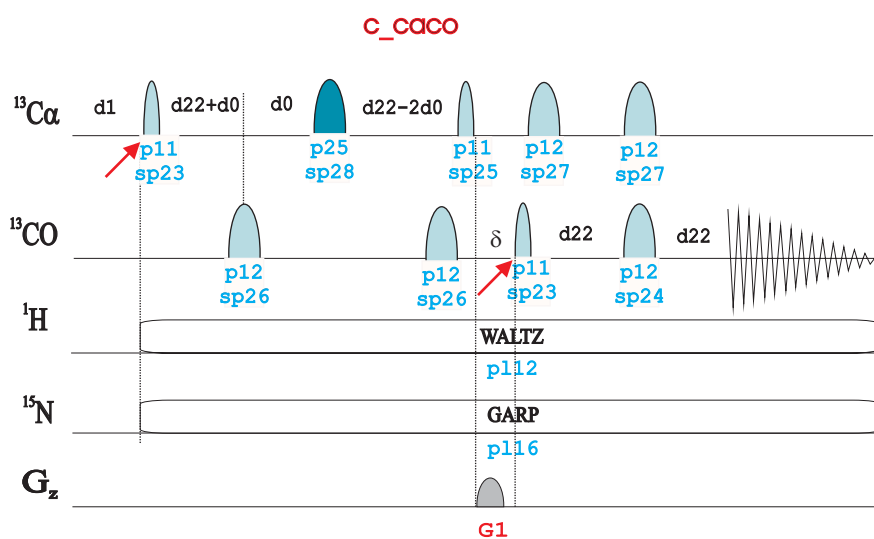
The CACO experiment can be driven in a out-and-stay way (c_caco) or using a out-and-back transfer (c_coca_mq).

NMR Spectrum

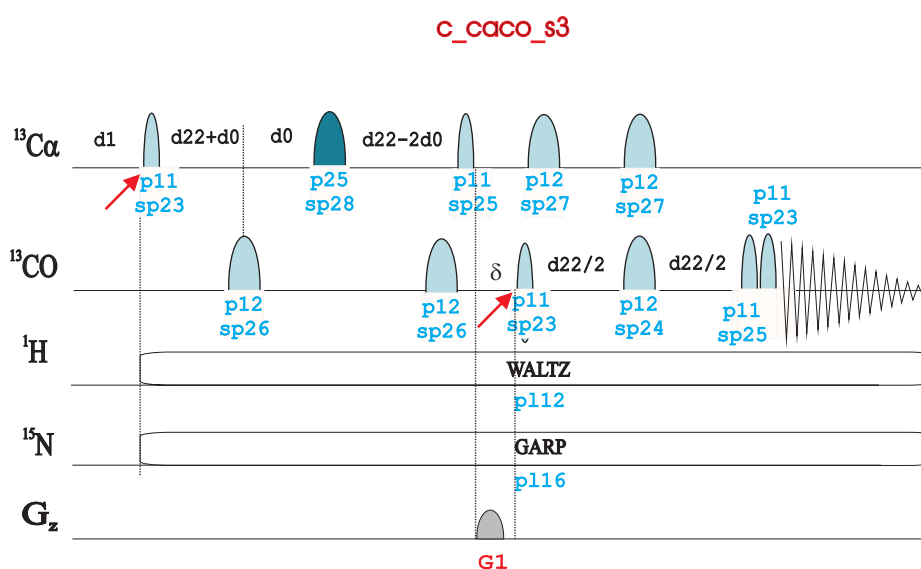
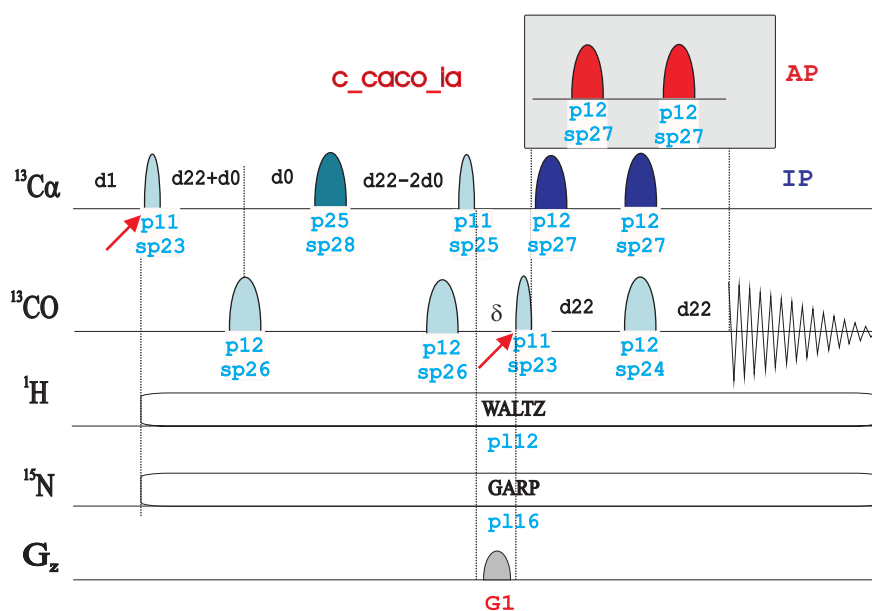
The experiment provides a 2D correlation map in which each cross-peak displays a doublet in the acquisition dimension due to $^1J(\text{CACO})$ coupling

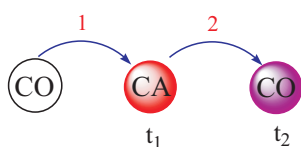
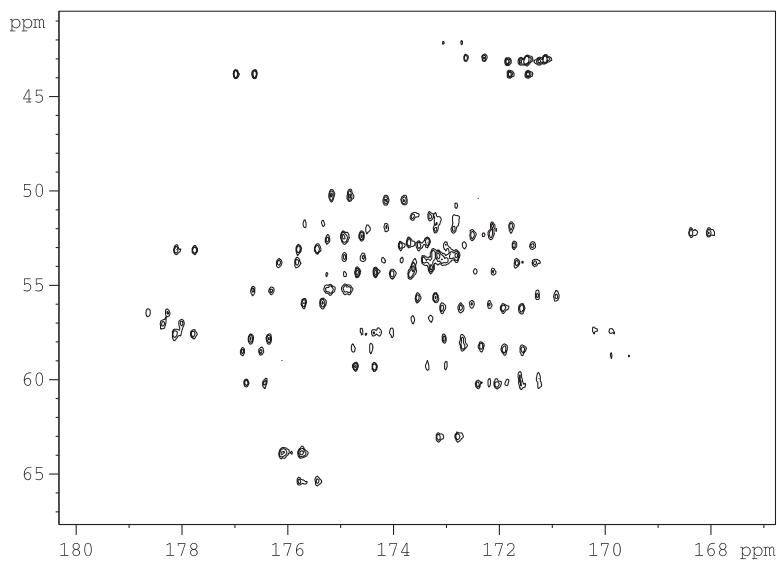
Related Experiments

2D COCA
3D HCACO

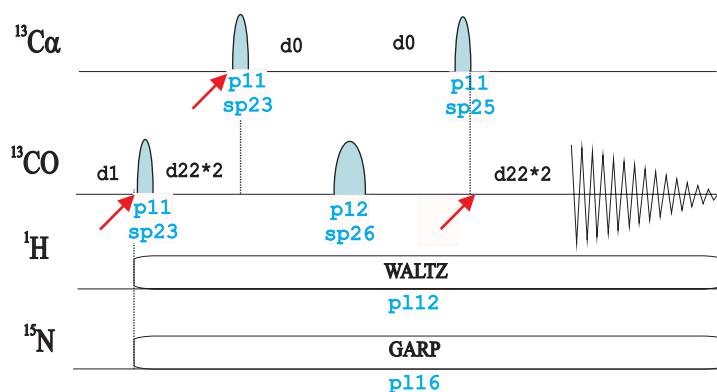


$$d22 = 1/4J(\text{COCA}) = 4.5\text{ms}$$

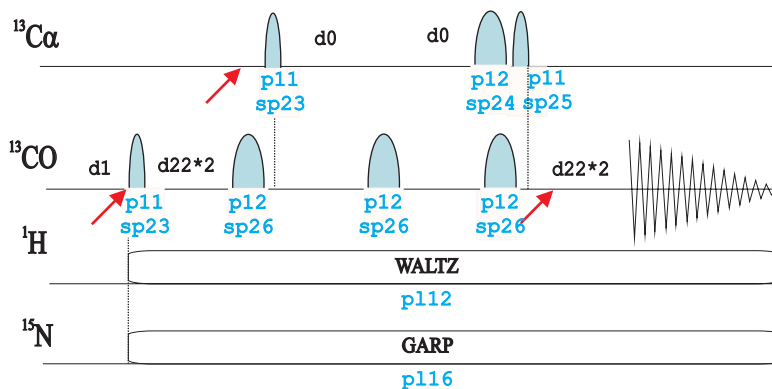




c_coca_mq



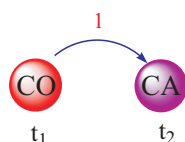
c_coca_mq.2



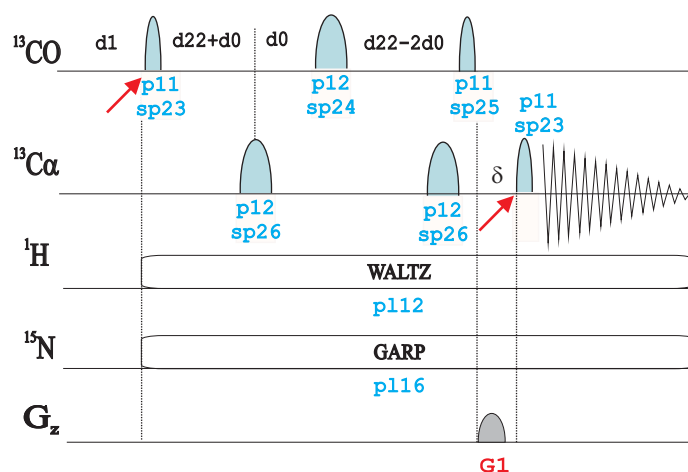
2D COCA Experiment

Experiment Description

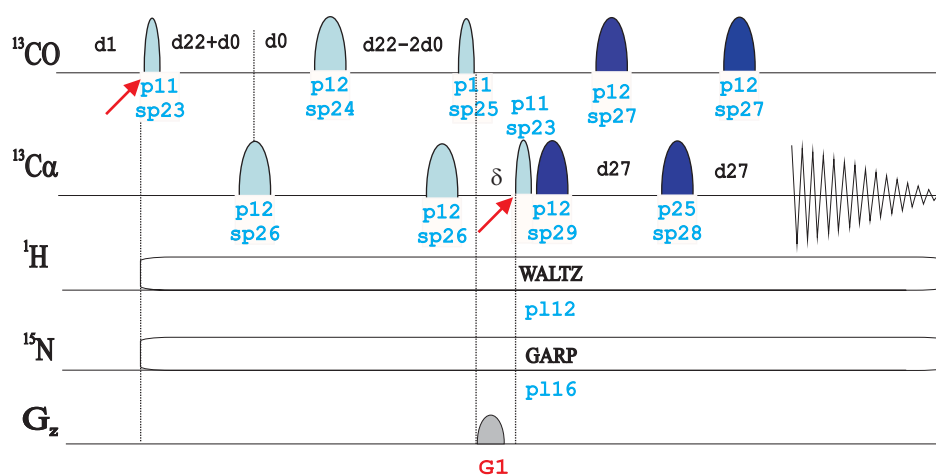
The 2D COCA experiment is the equivalent CA-detected experiment of the CO-detected CACO experiment



c_coca



c_coca_la

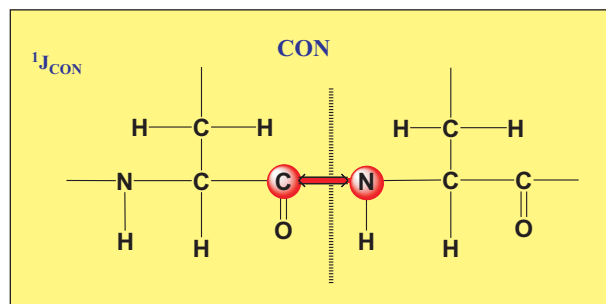


$d27 = 1/8J(CACB) = 3.6\text{ms}$
 $d22 = 1/4J(COCA) = 4.5\text{ms}$

2D CON Experiment

Experiment Description

The 2D CON experiment is a CO-detected experiment that allows the correlation between the chemical shifts of the carbonyl CO carbon and the amide N of the next residue in doubly $^{13}\text{C}/^{15}\text{N}$ -labeled proteins. Homonuclear CO-CA splitting (55Hz) in the acquisition dimension can be removed by homonuclear decoupling during acquisition or virtually using the IPAP approach (05JMR404).

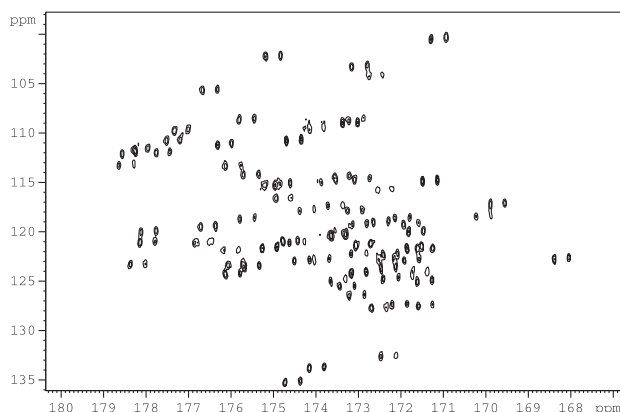


Related Experiments

3D HNCO

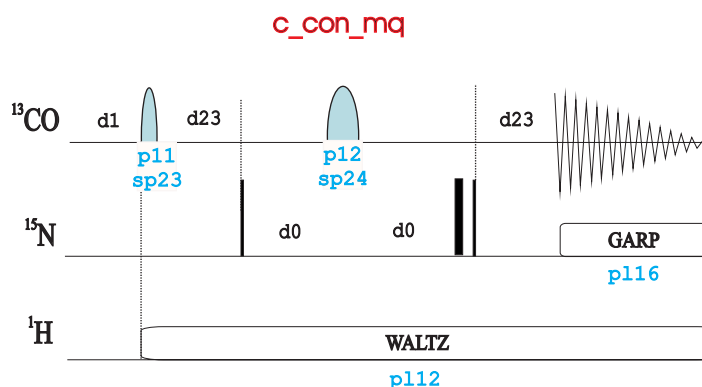
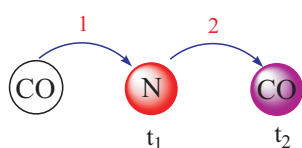
NMR Spectrum

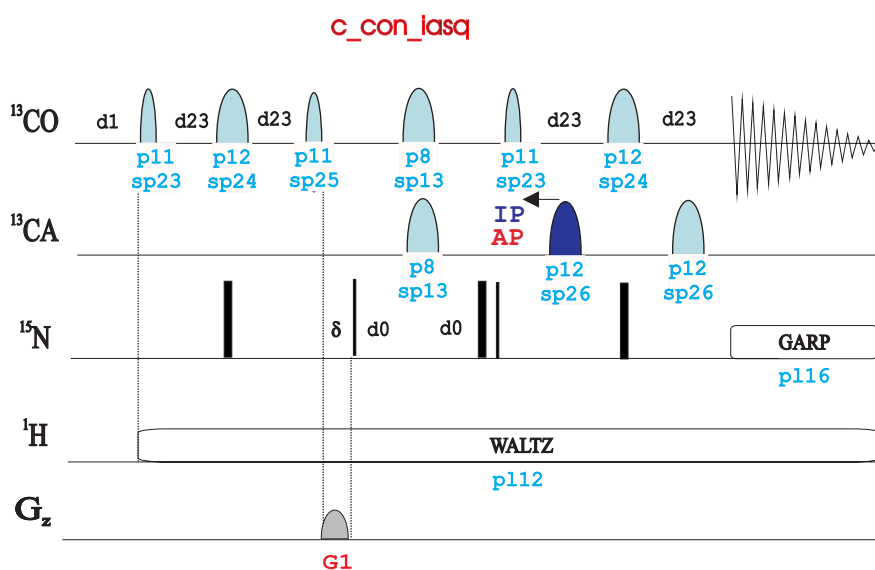
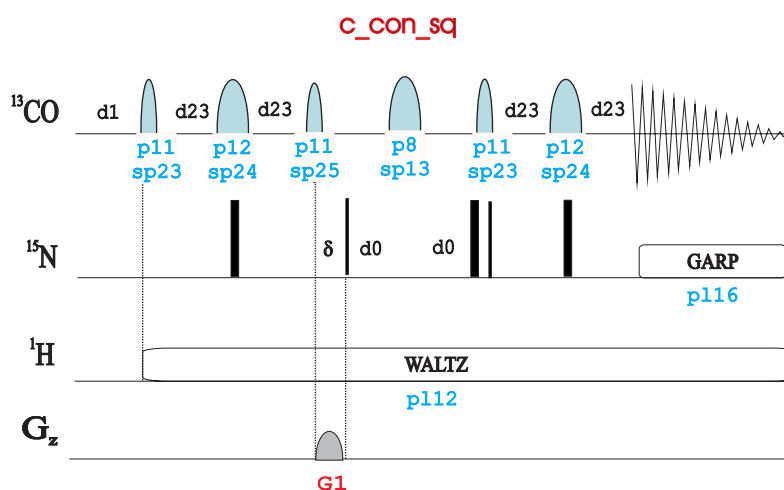
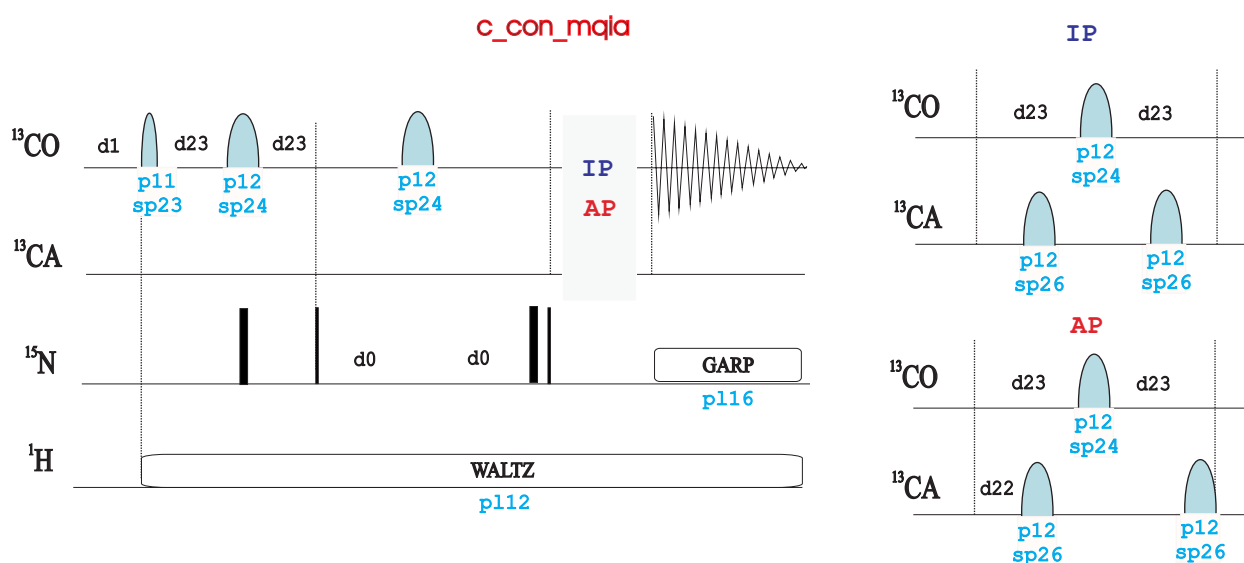
The experiment provides a 2D correlation map in which each cross-peak corresponds to the CO-N bond connectivity



Involved delays:

$d23 = 1/2J(\text{NCO}) = 25\text{ms}$ (in mq experiments)
or $= 1/4J(\text{NCO}) = 12.5\text{ms}$ (in sq experiments)
 $d22 = 1/4J(\text{COCA}) = 4.5\text{ms}$

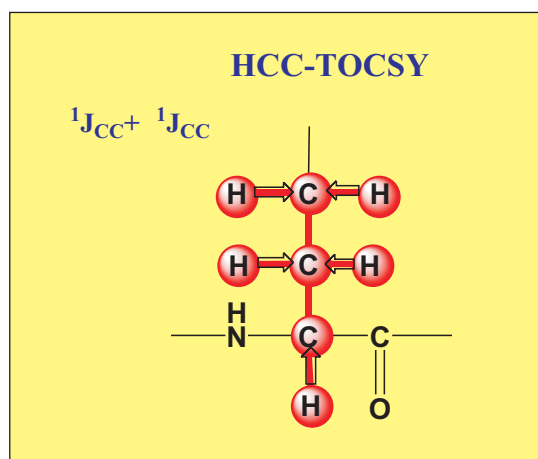




3D HCC-TOCSY Experiment

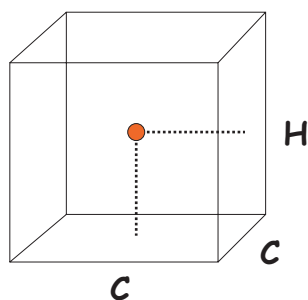
Experiment Description

The 3D HCC-TOCSY experiment is a C-detected experiment that allows the correlation between all sidechain ^1H and aliphatic ^{13}C of the same residues in ^{13}C -labeled proteins.



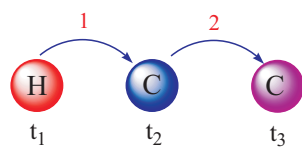
NMR Spectrum

The experiment provides a 3D correlation map in which each cross-peak correspond to a HC-C connectivity.

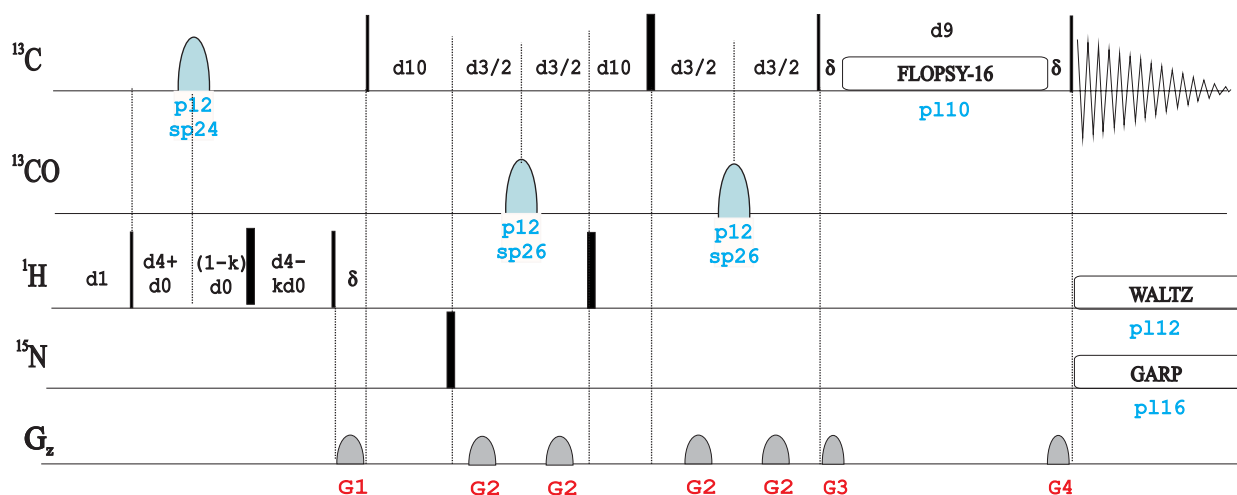


Related Experiments

2D CC COSY and CC-TOCSY experiment

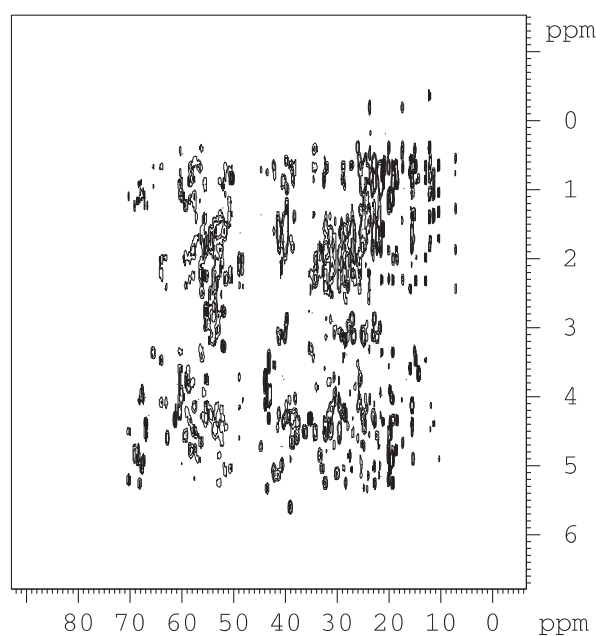
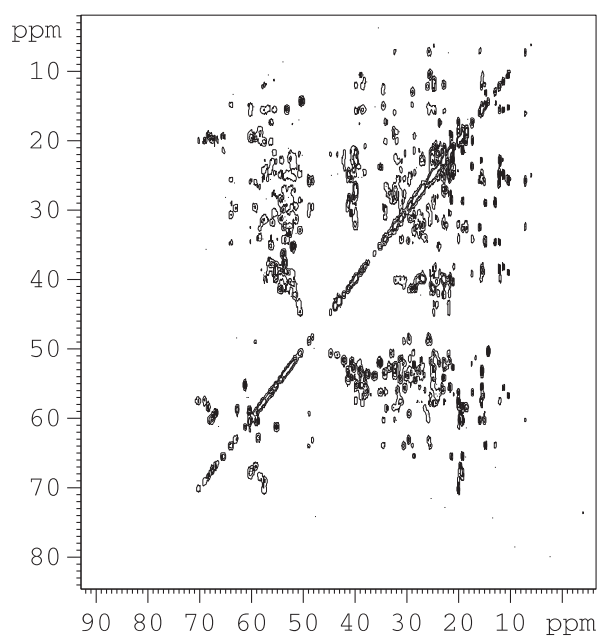


c_hccflopsy16_3d



2D (H)CC

2D H(C)C



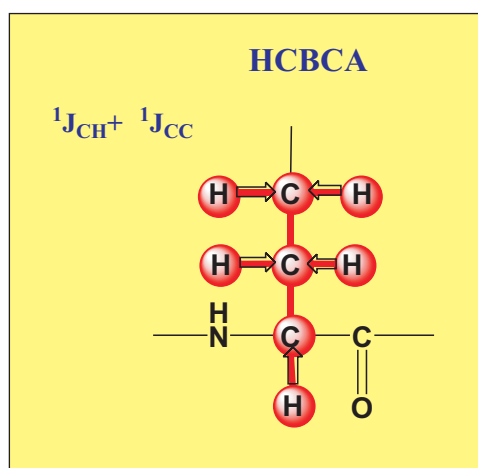
Involved delays:

d9 is the TOCSY mixing time
d3=1/6J(CH)=0.95ms
d4=1/4J(CH)=1.8ms

3D HCBCA Experiment

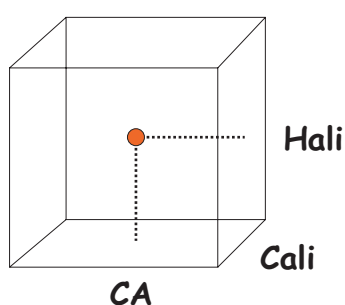
Experiment Description

The 3D HCBCA experiment is a carbon-detected experiment that allows to obtain the sidechain H, CB and CA connectivities in ^{13}C -labeled proteins. Homonuclear CO-CA splitting in the acquisition dimension can be removed by homonuclear decoupling during acquisition or virtually using the IPAP approach (05JMR404).



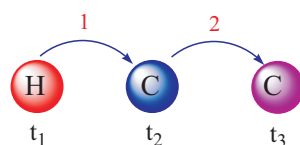
NMR Spectrum

The experiment provides a 3D correlation map in which each cross-peak displays a doublet in the acquisition dimension due to $^1J(\text{CACO})$ coupling

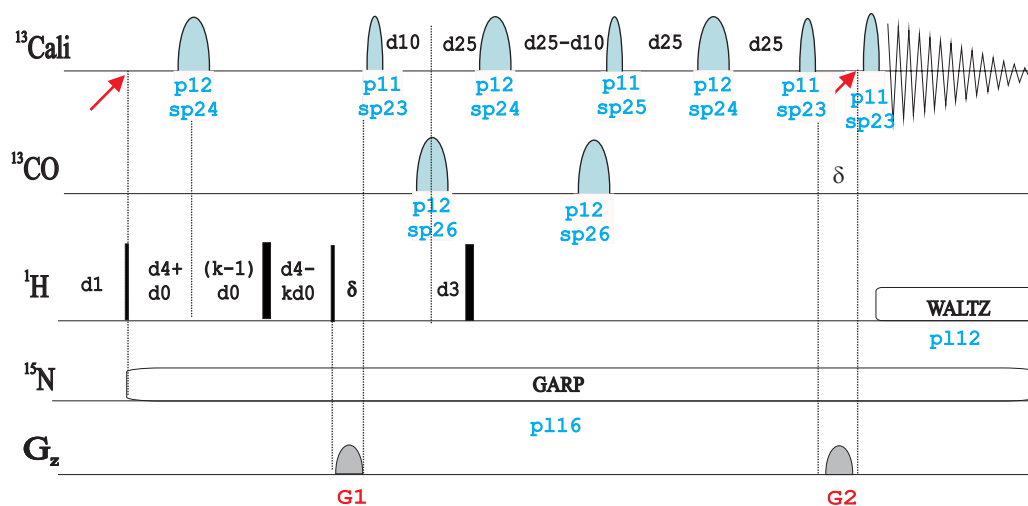


Related Experiments

2D CC TOCSY
3D HCC TOCSY



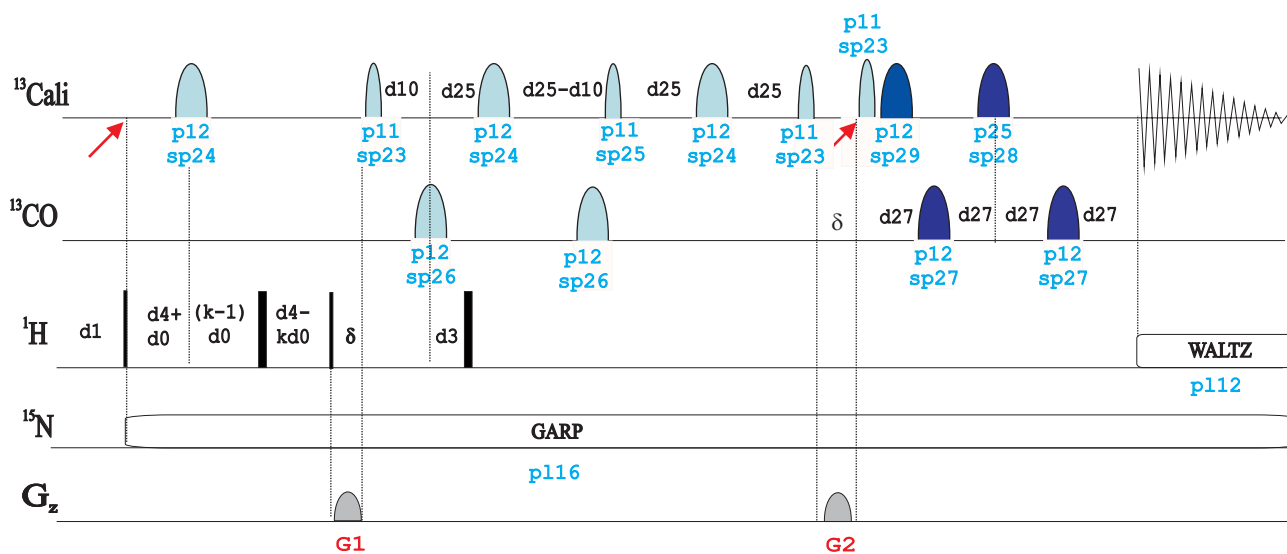
c_hcbca_3d



Involved delays:

$d25 = 1/8J(CACB) = 4.0\text{ms}$
 $d22 = 1/4J(COCA) = 4.5\text{ms}$
 $d27 = 1/4J(CACB) = 7.2\text{ms}$
 $d3 = 1/6J(CHA) = 1.1\text{ms}$
 $d4 = 1/4J(CHA) = 1.8\text{ms}$

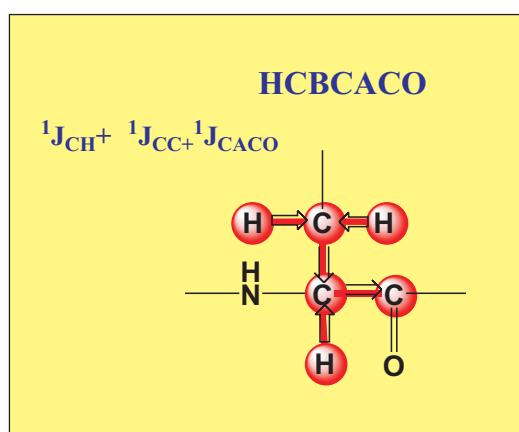
c_hcbca_la3d



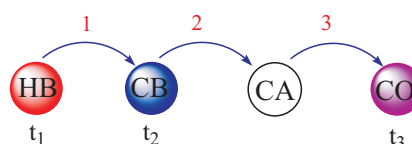
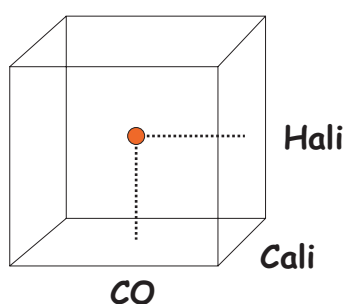
3D HCBCACO Experiment

Experiment Description

The 3D HCBCACO experiment is a CO-detected that allows the correlation between the chemical shifts of the sidechain protons and the CB, CA and CO carbons of the same residue in ^{13}C -labeled proteins. Homonuclear CO-CA splitting in the acquisition dimension can be removed by homonuclear decoupling during acquisition or virtually using the IPAP approach (05JMR404).



NMR Spectrum



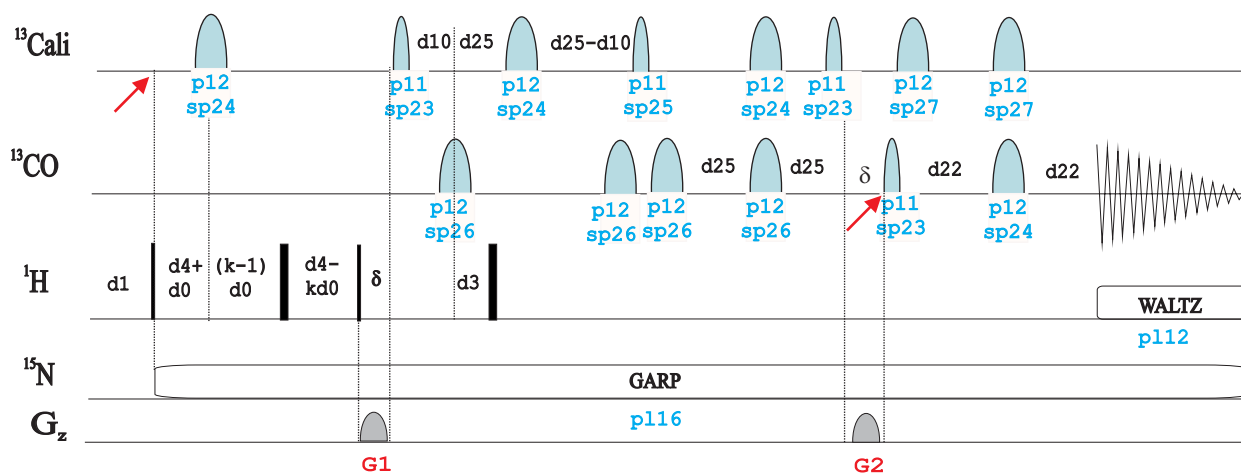
Related Experiments

2D CC TOCSY
3D HCC TOCSY and HCBCA experiments

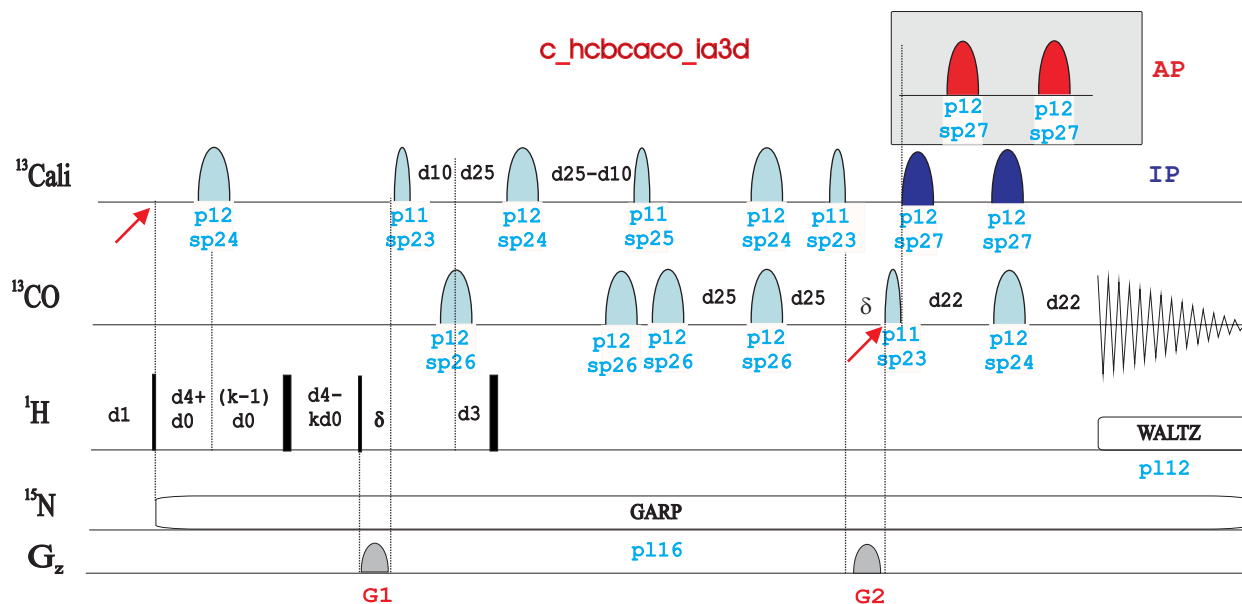
Involved delays:

$d_{25} = 1/8J(\text{CACB}) = 4.0\text{ms}$
 $d_{22} = 1/4J(\text{COCA}) = 4.5\text{ms}$
 $d_3 = 1/6J(\text{CHA}) = 1.1\text{ms}$
 $d_4 = 1/4J(\text{CHA}) = 1.8\text{ms}$

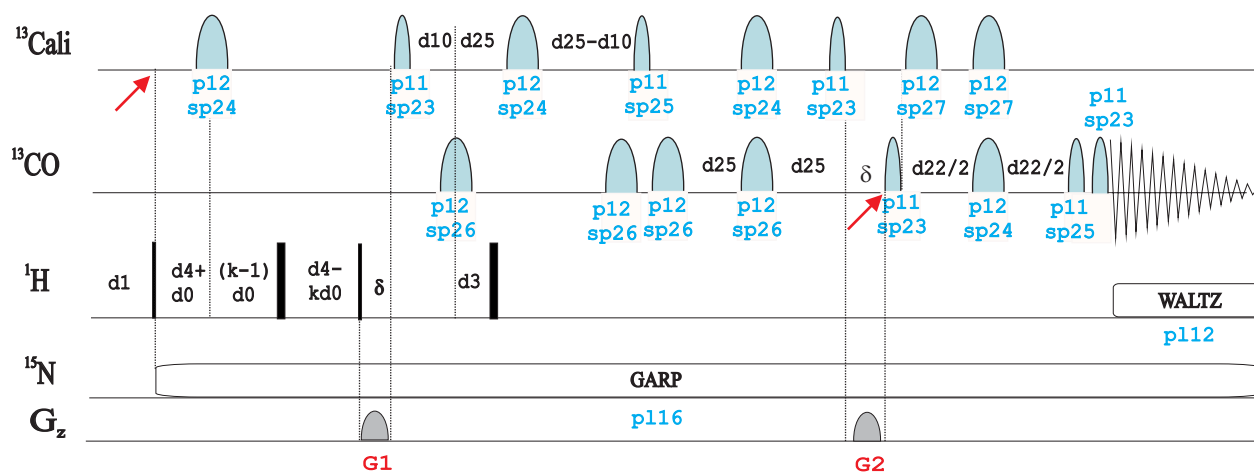
c_hcbbcaco_3d



c_hcbbcaco_la3d



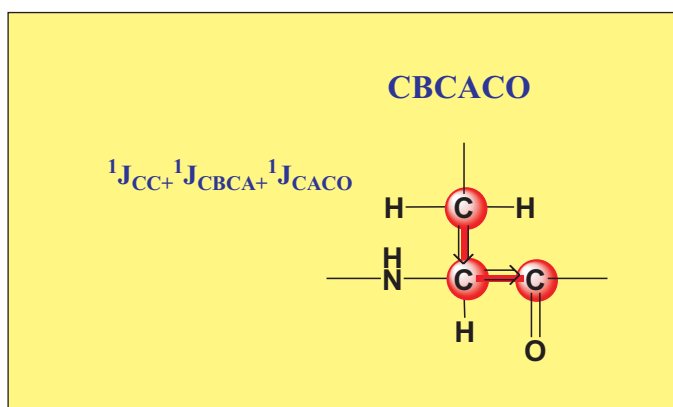
c_hcbbcaco_s33d



3D CBCACO Experiment

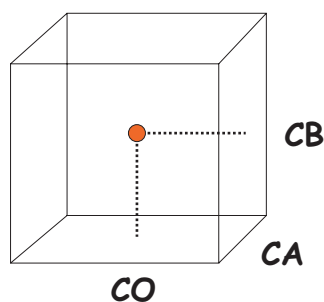
Experiment Description

The 3D CBCACO experiment is a CO-detected experiment that allows the correlation between the chemical shifts of the sidechain CB, CA and CO carbons of the same residue in ^{13}C -labeled proteins. Homonuclear CO-CA splitting in the acquisition dimension can be removed by homonuclear decoupling during acquisition or virtually using the IPAP approach (05JMR404)



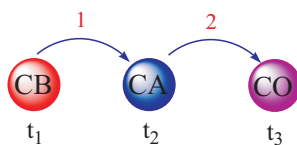
NMR Spectrum

The experiment provides a 3D correlation map in which each cross-peak displays a doublet in the acquisition dimension due to $^1J(\text{CACO})$ coupling

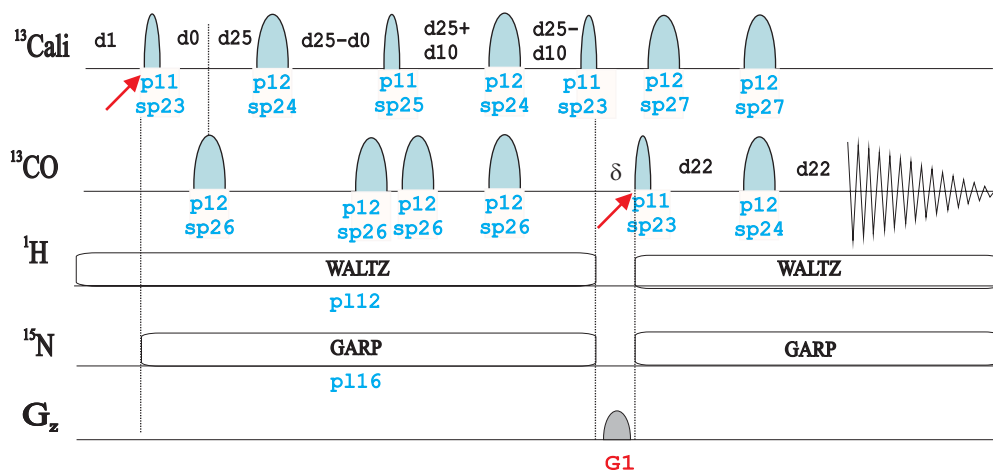


Related Experiments

2D CC COSY and TOCSY
2D CACO
3D HCACO



c_cbcaco_3d

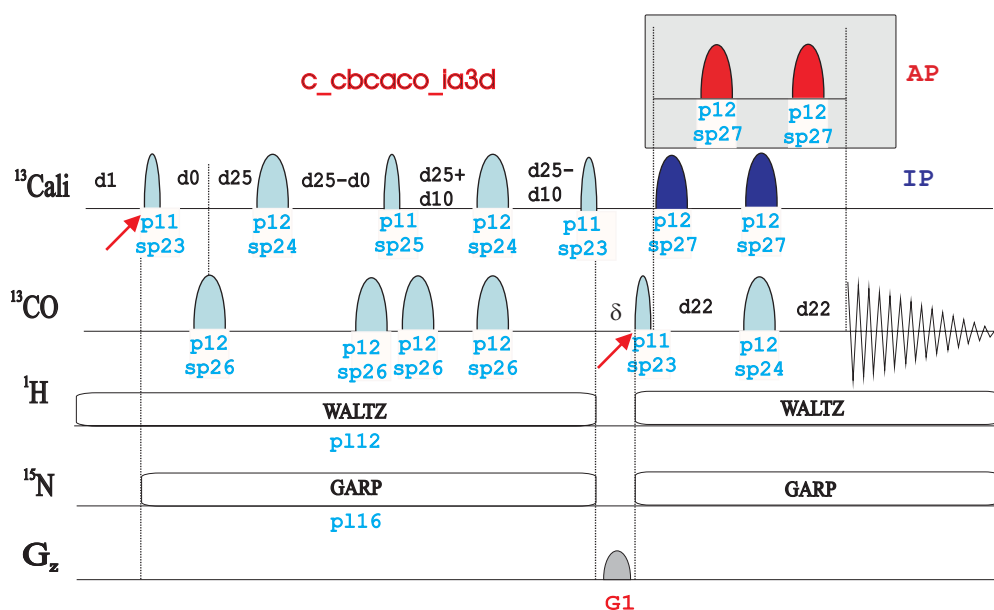


Involved delays:

$$d22 = 1/4J(\text{COCA}) = 4.5\text{ms}$$

$$d25 = 1/8J(\text{CACB}) = 5.0\text{ms}$$

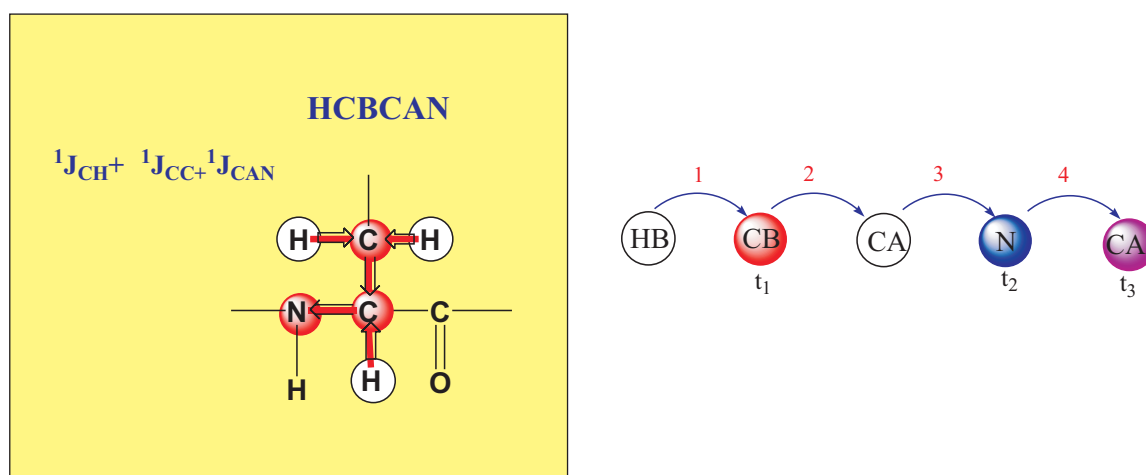
c_cbcaco_la3d



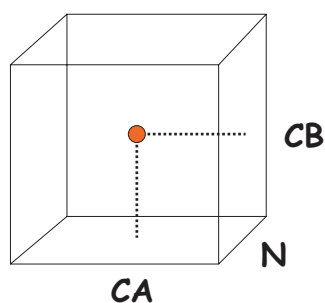
3D HCBCAN Experiment

Experiment Description

The 3D (H)CBCAN experiment is a CA-detected experiment that allows to assign intra-residue CA, CB and N chemical shifts in doubly-labeled $^{13}\text{C}/^{15}\text{N}$ proteins. Homonuclear CO-CA splitting in the acquisition dimension can be removed by homonuclear decoupling during acquisition or virtually using the IPAP approach (05JMR404).



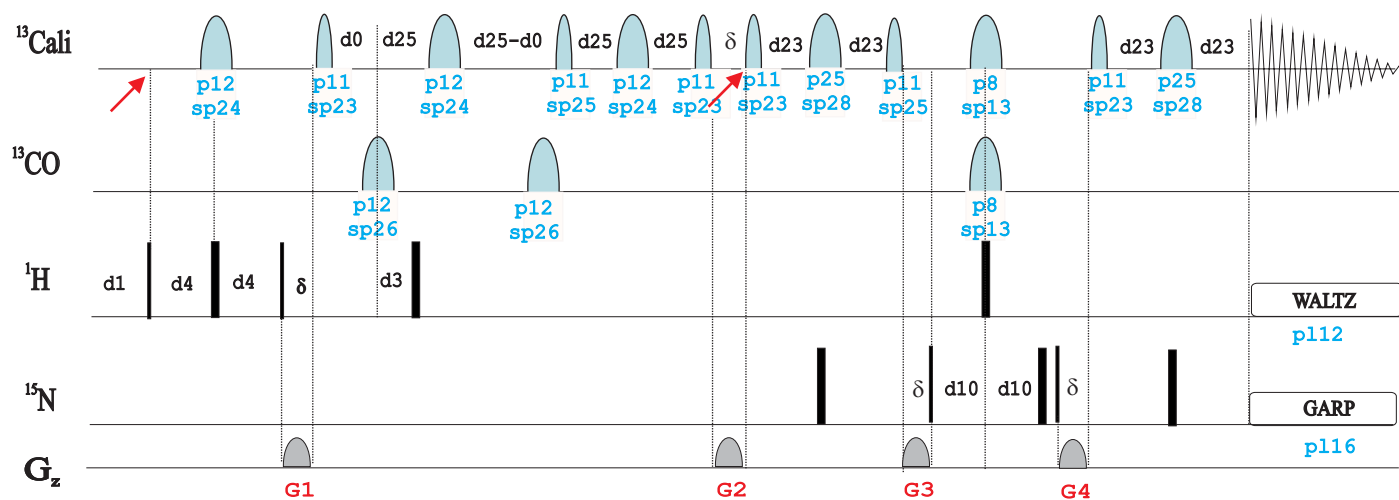
NMR Spectrum



Related Experiments

3D HCC TOCSY

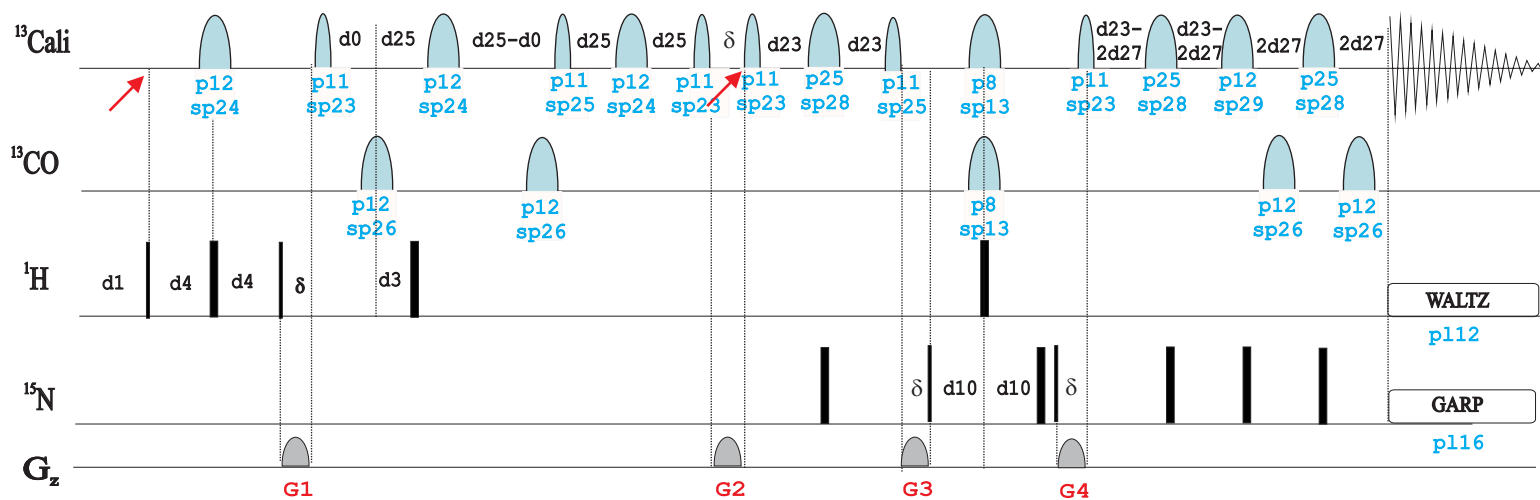
c_hcscan_3d



Involved delays:

$d22 = 1/4J(\text{COCA}) = 4.5\text{ms}$
 $d25 = 1/8J(\text{CACB}) = 4.0\text{ms}$
 $d23 = 1/4J(\text{NCA}) = 12.4\text{ms}$
 $d27 = 1/8J(\text{CACB}) = 3.6\text{ms}$
 $d3 = 1/6J(\text{CHA}) = 1.1\text{ms}$
 $d4 = 1/4J(\text{CHA}) = 1.8\text{ms}$

c_hcscan_la3d



3D HCACO Experiment

Experiment Description

The 3D HCACO experiment is a CO-detected experiment that allows the correlation between the chemical shifts of the CA and CO carbons of the same residue in ^{13}C -labeled proteins. Homonuclear CO-CA splitting in the acquisition dimension can be removed by homonuclear decoupling during acquisition or virtually using the IPAP approach (05JMR404).

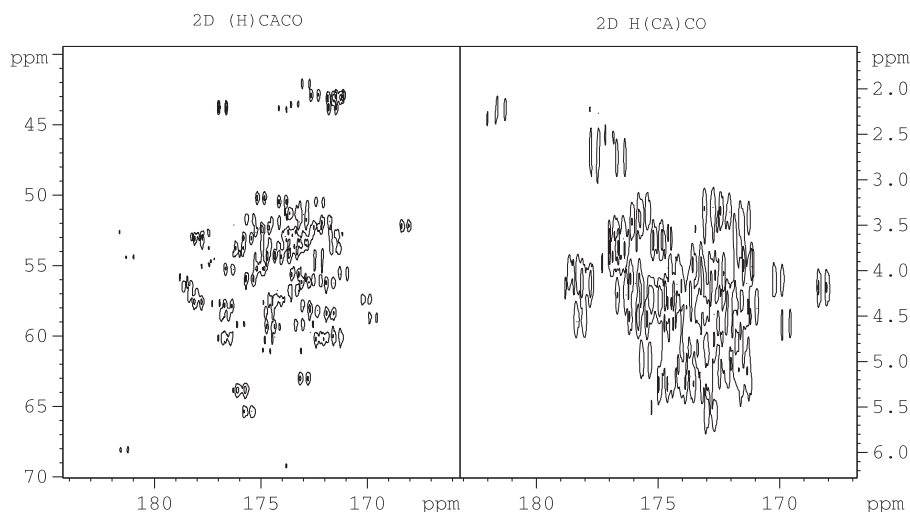
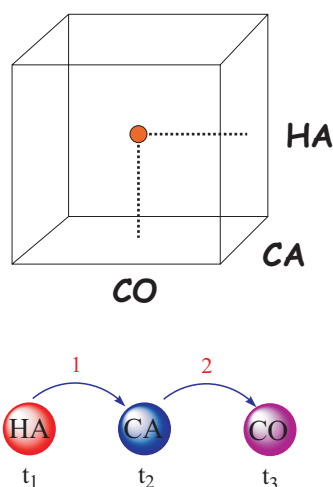
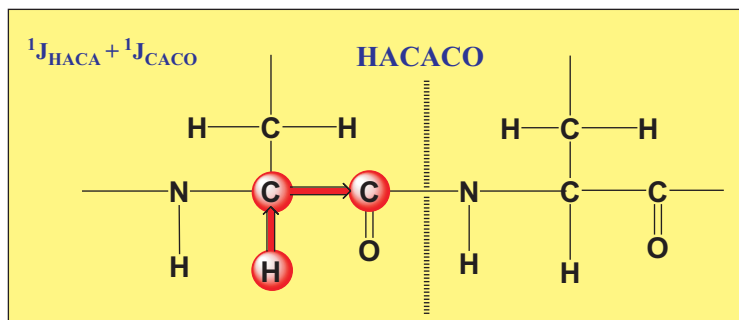
Related Experiments

2D COCA

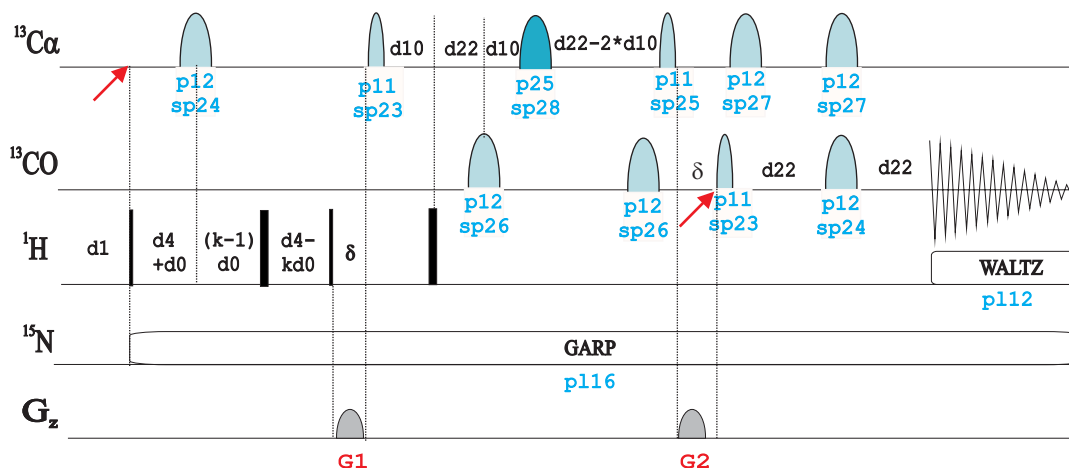
3D ^1H -detected HCACO

NMR Spectrum

The experiment provides a 3D correlation map in which each cross-peak displays a doublet in the acquisition dimension due to $^1\text{J}(\text{CACO})$ coupling

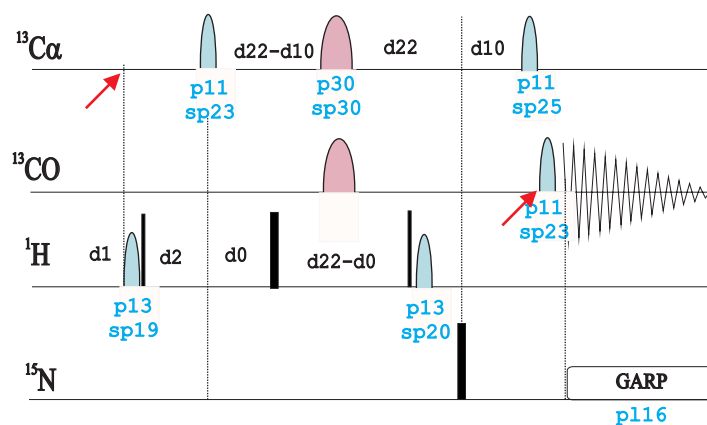


c_hcaco_3d



Involved delays:

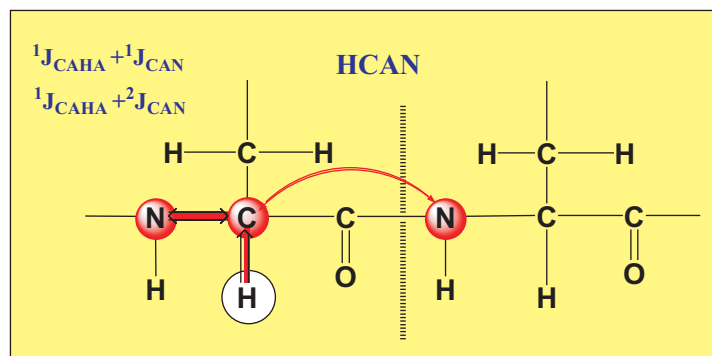
$d22 = 1/4J(\text{COCA}) = 4.5\text{ms}$
 $d2 = 1/2J(\text{CHA}) = 3.2\text{ms}$
 $d3 = 1/6J(\text{CHA}) = 1.1\text{ms}$
 $d4 = 1/4J(\text{CHA}) = 1.8\text{ms}$



3D HCAN Experiment

Experiment Description

The 3D HCAN experiment is a CA-detected experiment that correlates the CA-HA of a given residue with the N chemical shift of the same and the next residue in doubly-labeled $^{13}\text{C}/^{15}\text{N}$ proteins.

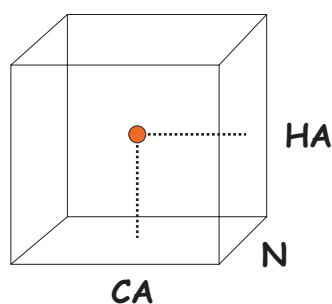


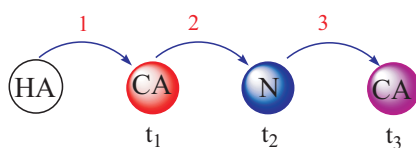
Related Experiments

2D CAN
3D HNCA

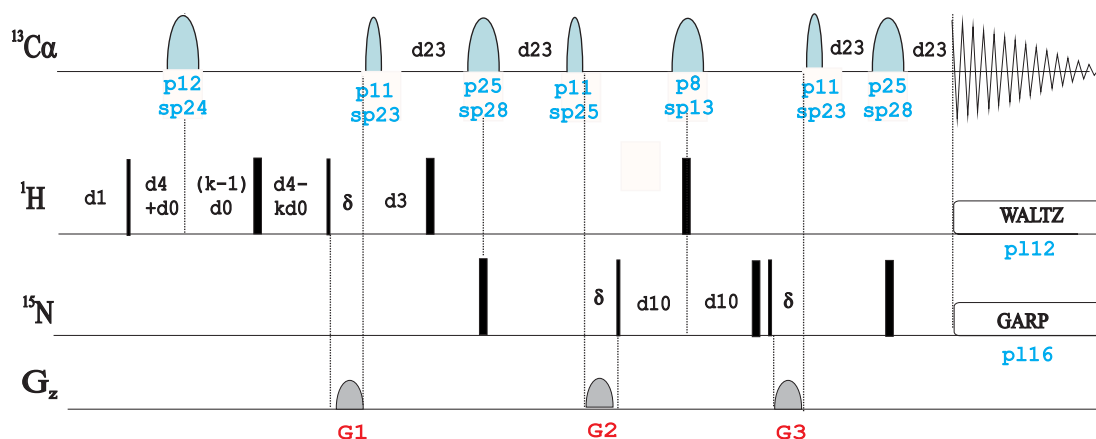
NMR Spectrum

A 3D H,N,C map is obtained





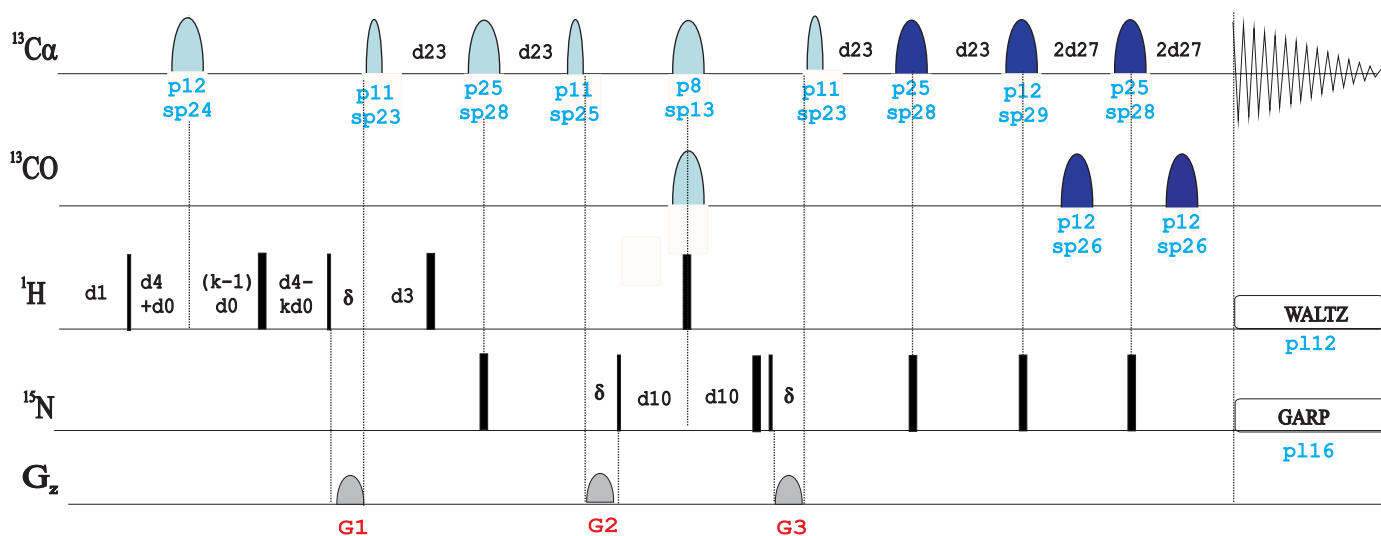
c_hcan_3d



Involved delays:

$d23 = 1/4J(NCA) = 12.4\text{ms}$
 $d22 = 1/4J(COCA) = 4.5\text{ms}$
 $d27 = 1/8J(CACB) = 3.6\text{ms}$
 $d3 = 1/6J(CHA) = 1.1\text{ms}$
 $d4 = 1/4J(CHA) = 1.8\text{ms}$

c_hcan_la3d

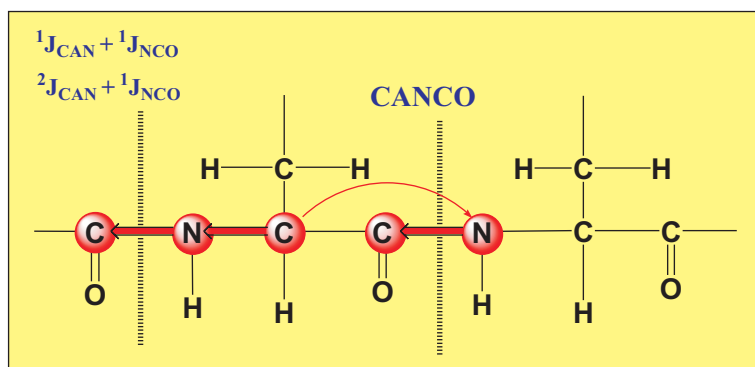


3D CANCO Experiment

Experiment Description

The 3D CANCO experiment is a CO-detected experiment that allows the correlation between the chemical shifts of the CA and the CO of the same and the previous residues and the N of the same and the next residue in doubly-labeled $^{13}\text{C}/^{15}\text{N}$ proteins.

Homonuclear CO-CA splitting in the acquisition dimension can be removed by homonuclear decoupling during acquisition or virtually using the IPAP approach (05JMR404).

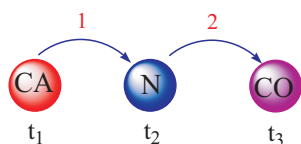
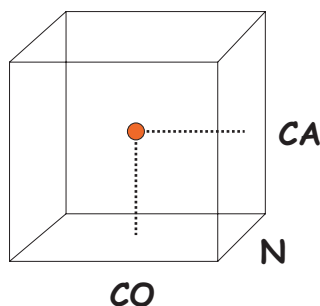


Related Experiments

3D HNCACO experiment
3D intra-CANCO and (H)CANCO experiments

NMR Spectrum

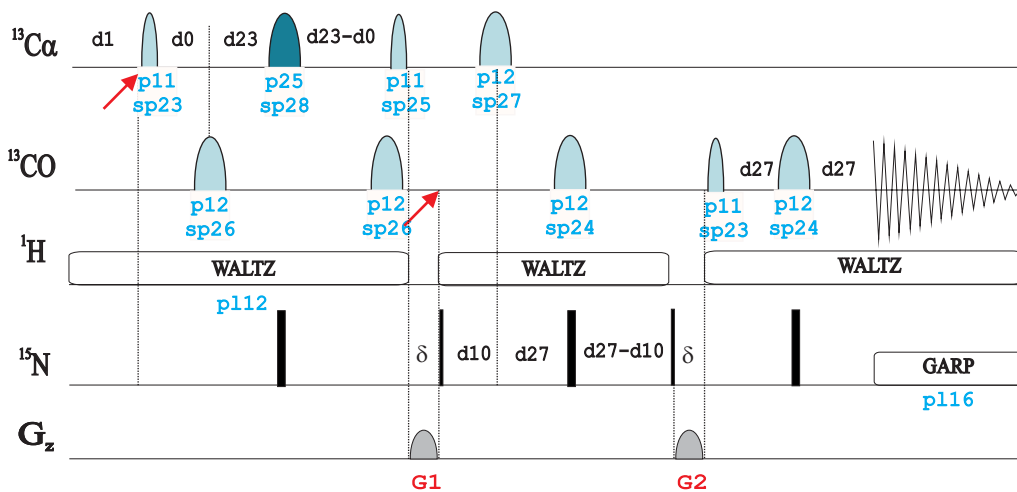
The experiment provides a 3D correlation map in which each CA nucleus displays two different connectivities



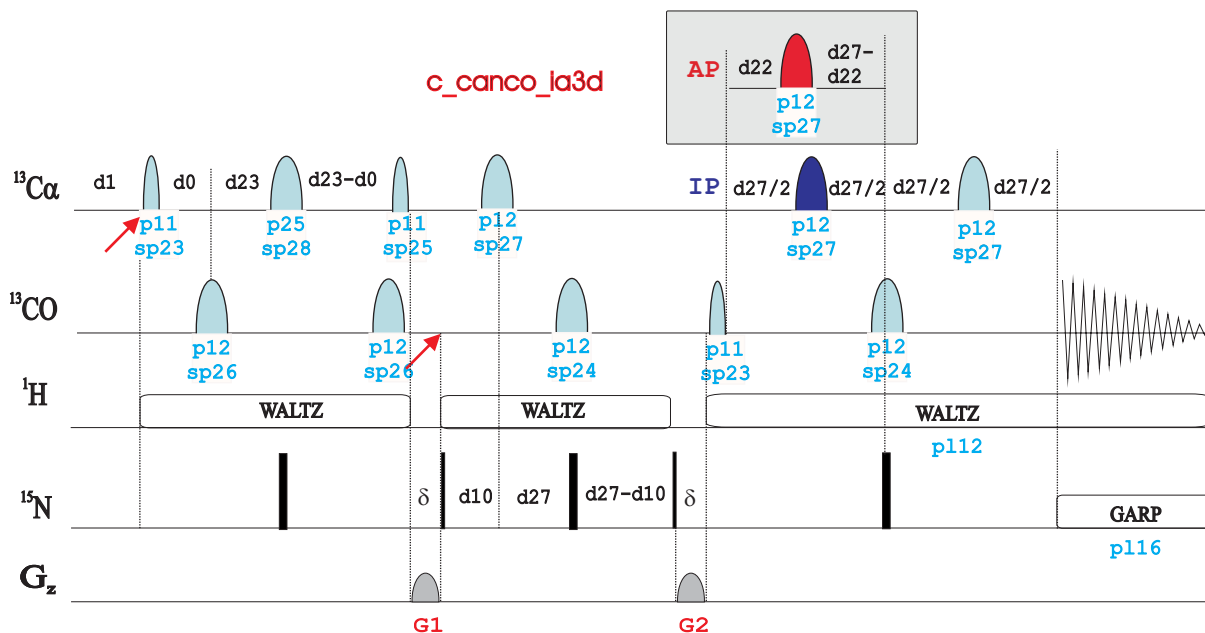
Involved delays:

$d_{23} = 1/4J(\text{NCA}) = 12.4\text{ms}$
 $d_{22} = 1/4J(\text{COCA}) = 4.5\text{ms}$
 $d_{27} = 1/4J(\text{NCO}) = 16.0\text{ms}$
 $d_3 = 1/6J(\text{CHA}) = 1.1\text{ms}$
 $d_4 = 1/4J(\text{CHA}) = 1.8\text{ms}$

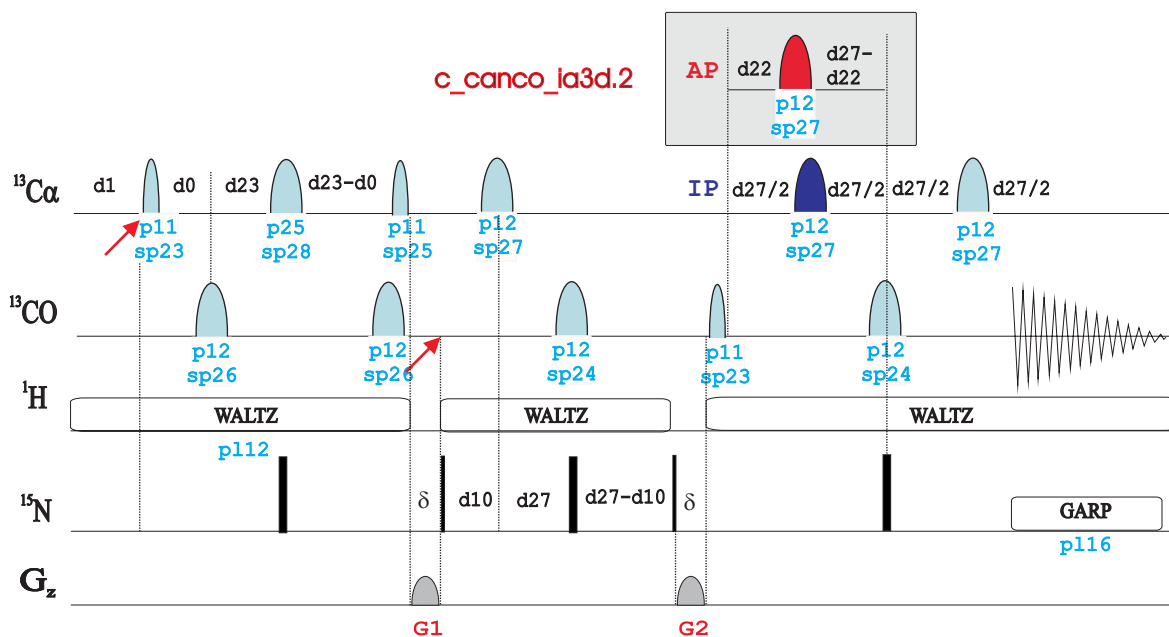
c_canco_3d



c_canco_la3d



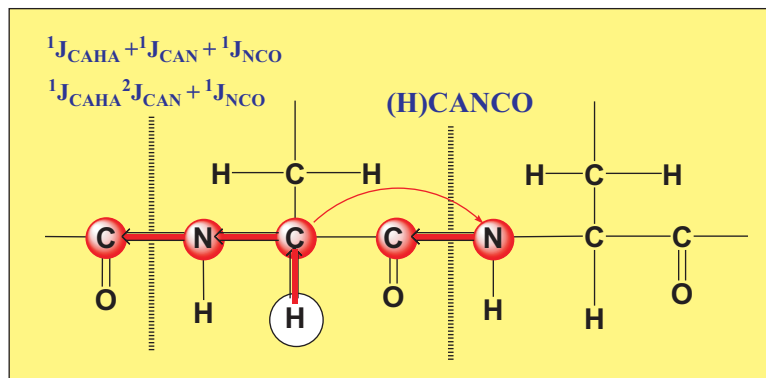
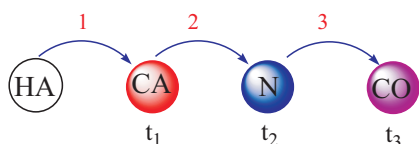
c_canco_la3d.2



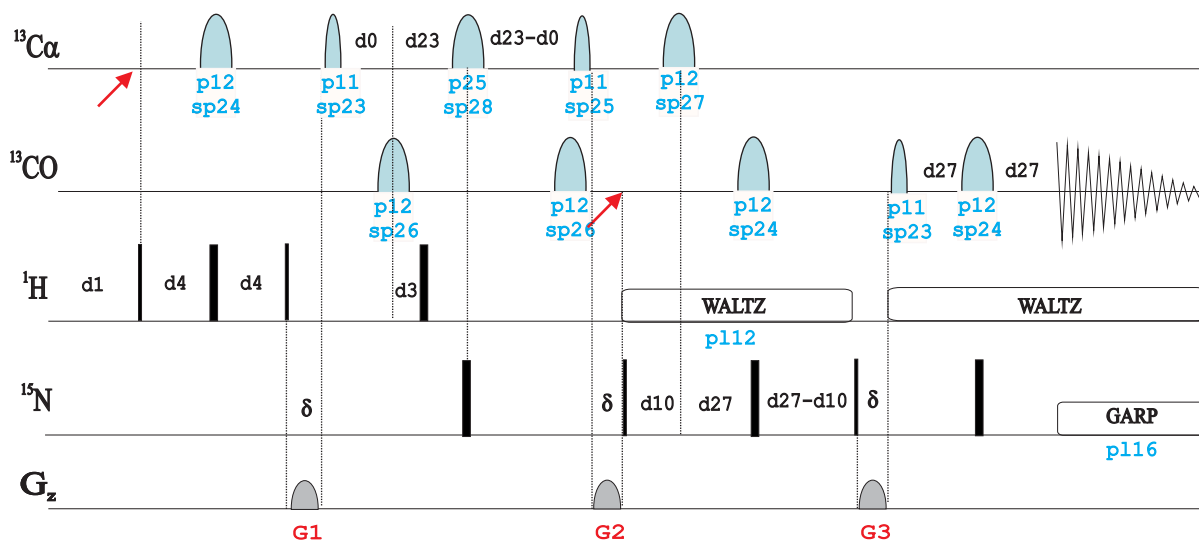
3D (H)CANCO Experiment

Experiment Description

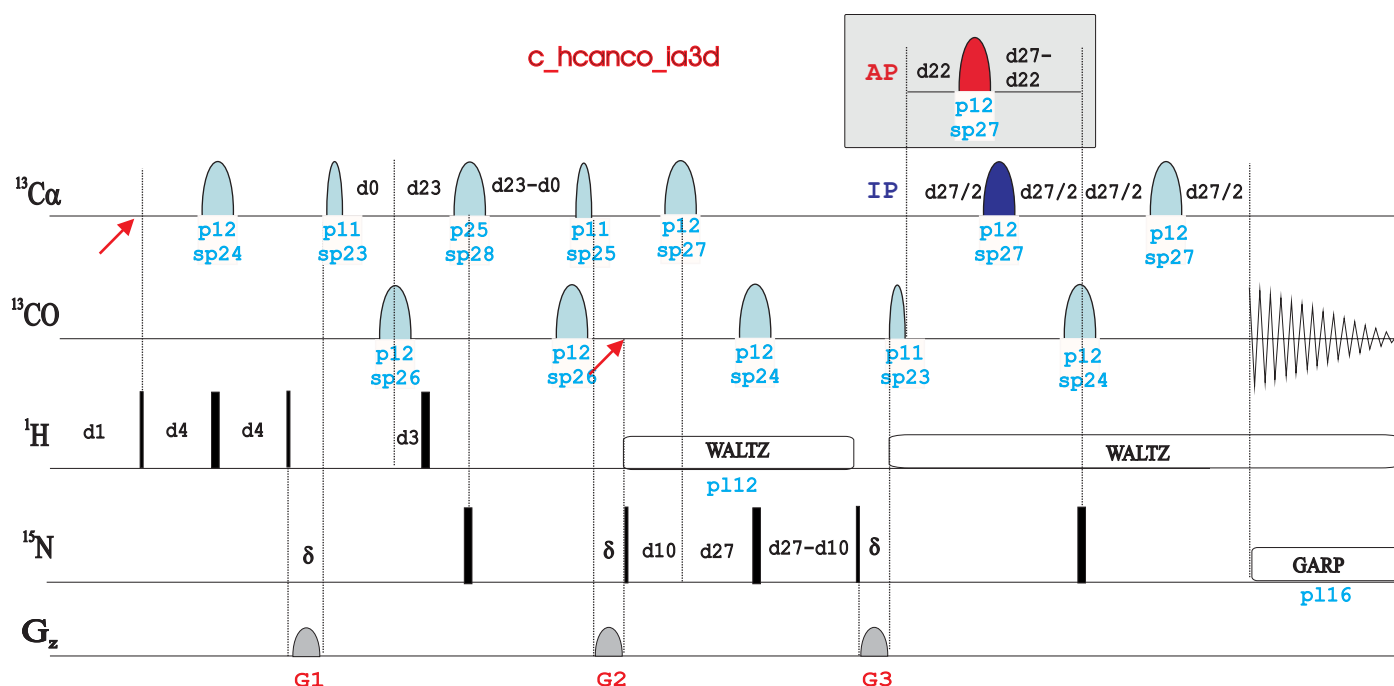
Variant of the CANCO experiment that starts from the HA protons.



c_hcanco_3d



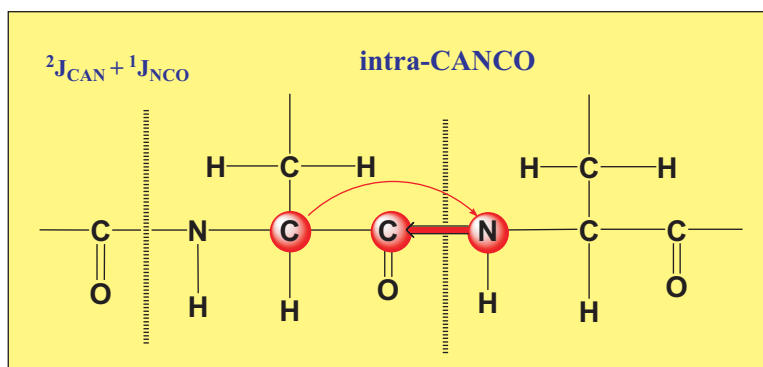
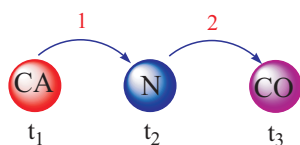
c_hcanco_la3d



3D intra-CANCO Experiment

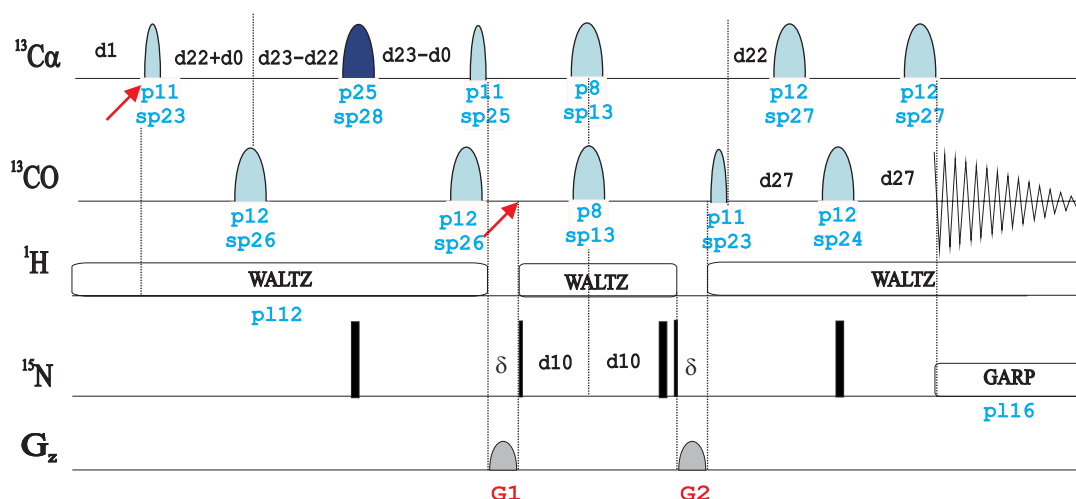
Experiment Description

Variant of the CANCO experiment that provides exclusively intra-residue CANCO connectivities

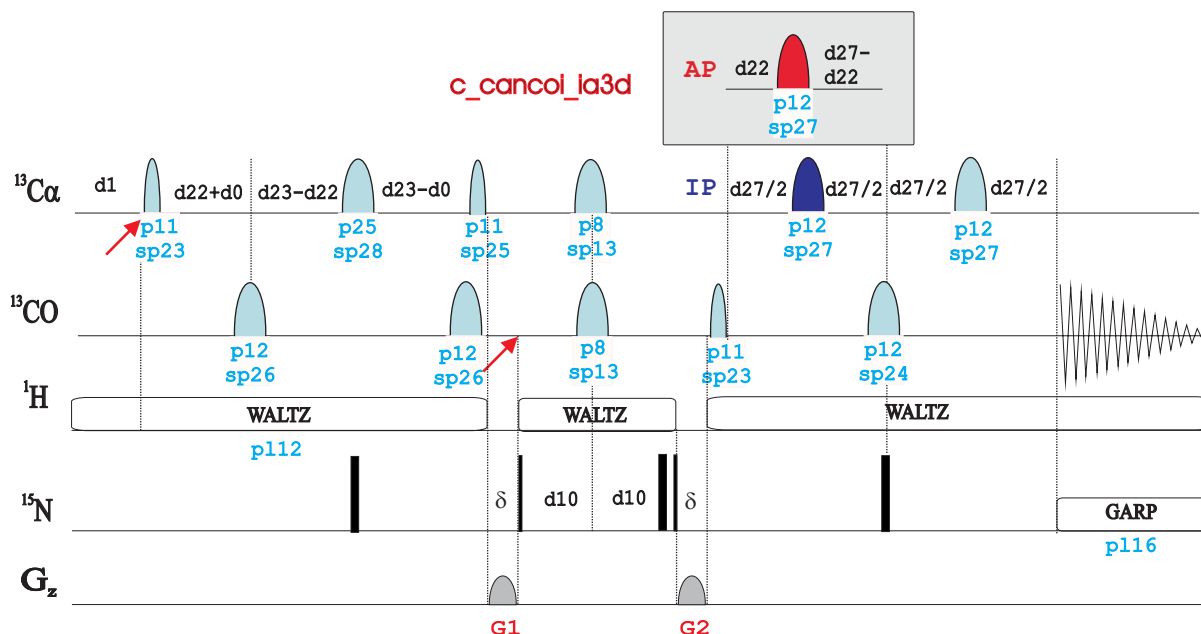


$d23 = 1/4J(\text{NCA}) = 12.4\text{ms}$
 $d22 = 1/4J(\text{COCA}) = 4.5\text{ms}$
 $d27 = 1/4J(\text{NCO}) = 16.0\text{ms}$
 $d3 = 1/6J(\text{CHA}) = 1.1\text{ms}$
 $d4 = 1/4J(\text{CHA}) = 1.8\text{ms}$

c_cancel_3d



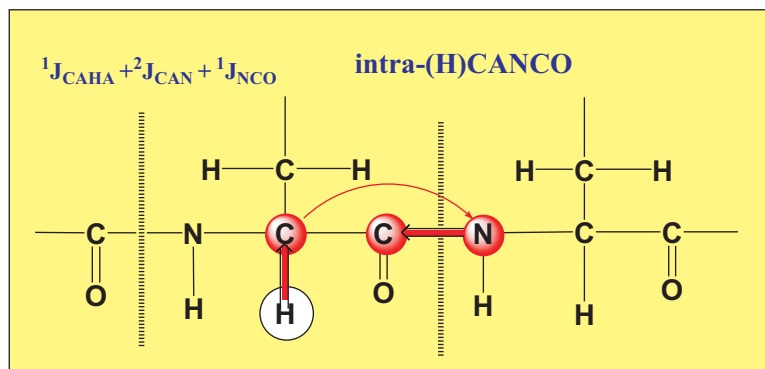
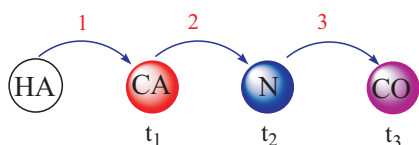
c_cancel_la3d



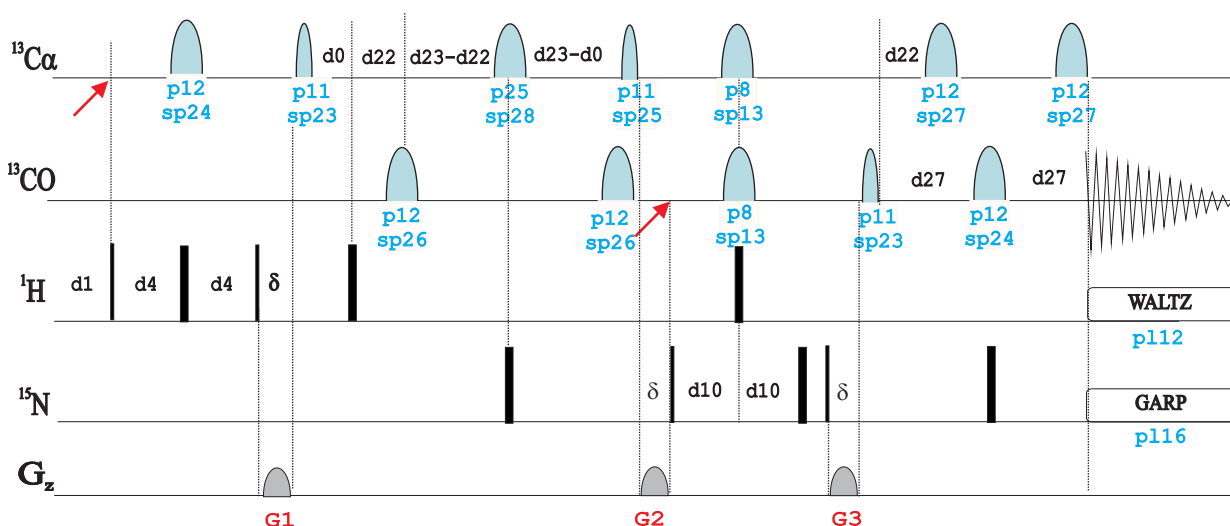
3D intra-(H)CANCO Experiment

Experiment Description

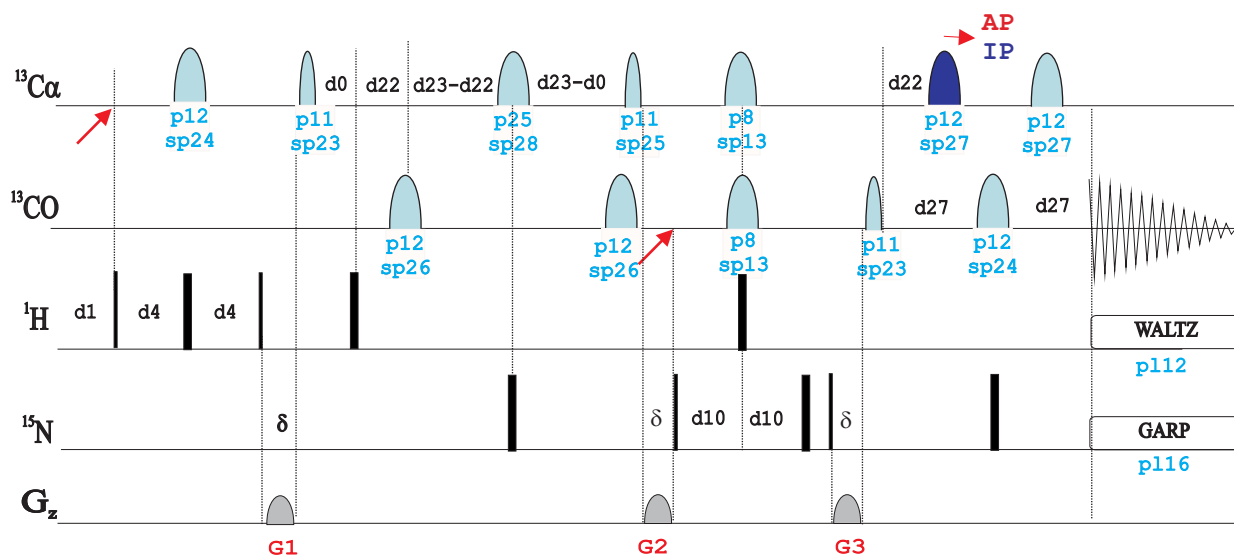
Variant of the intra-CANCO experiment that starts from the HA protons.



c_hcancol_3d



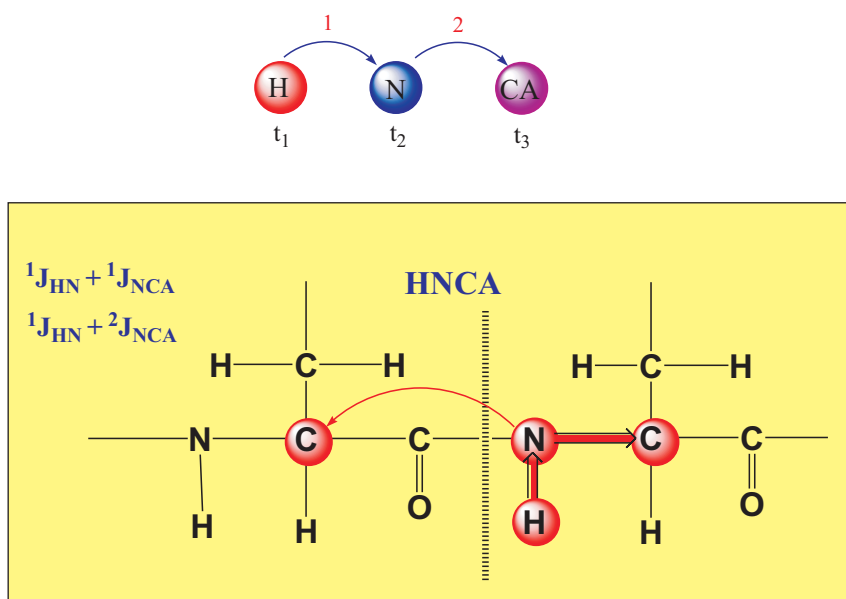
c_hcancol_la3d



3D CA-detected HNCA Experiment

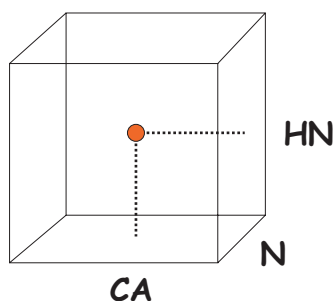
Experiment Description

The 3D CA-detected HNCA experiment is an out-and-stay version of the conventional HNCA experiment

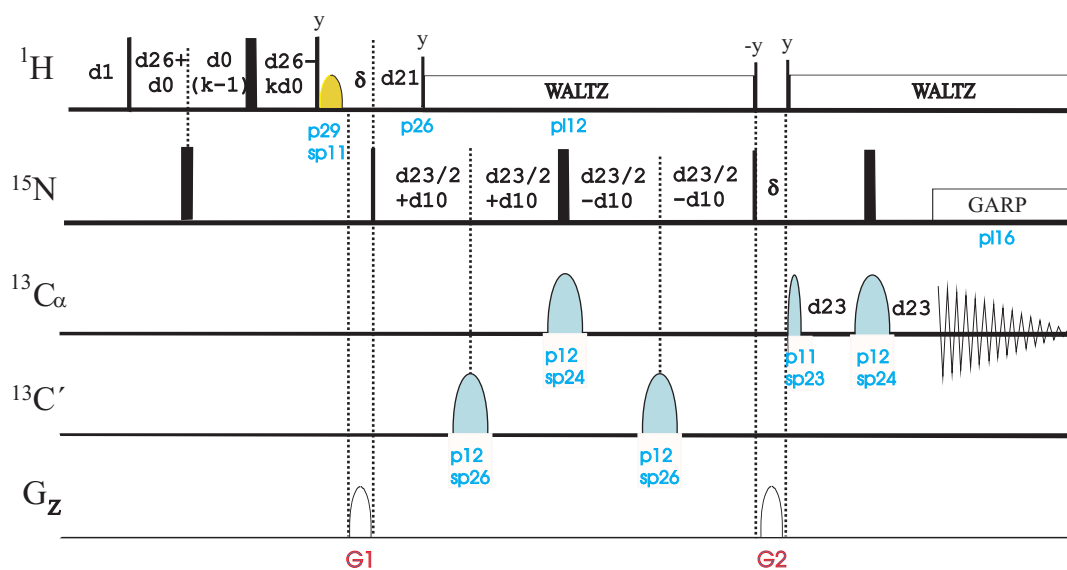


NMR Spectrum

The experiment provides the same 3D HNCA correlation map



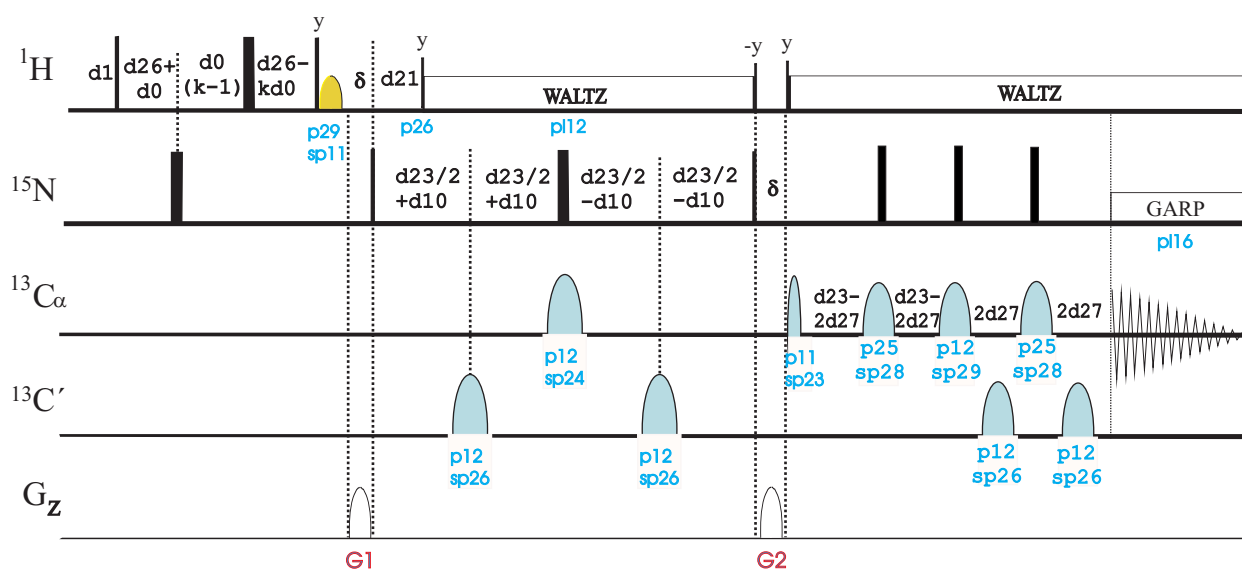
c_hnca_3d



Involved delays:

$d21 = 1/2J(\text{NH}) = 5.5\text{ms}$
 $d22 = 1/4J(\text{COCA}) = 4.5\text{ms}$
 $d23 = 1/4J(\text{NCA}) = 12.4\text{ms}$
 $d26 = 1/4J(\text{NH}) = 2.3\text{ms}$
 $d27 = 1/8(\text{CACB}) = 3.6\text{ms}$

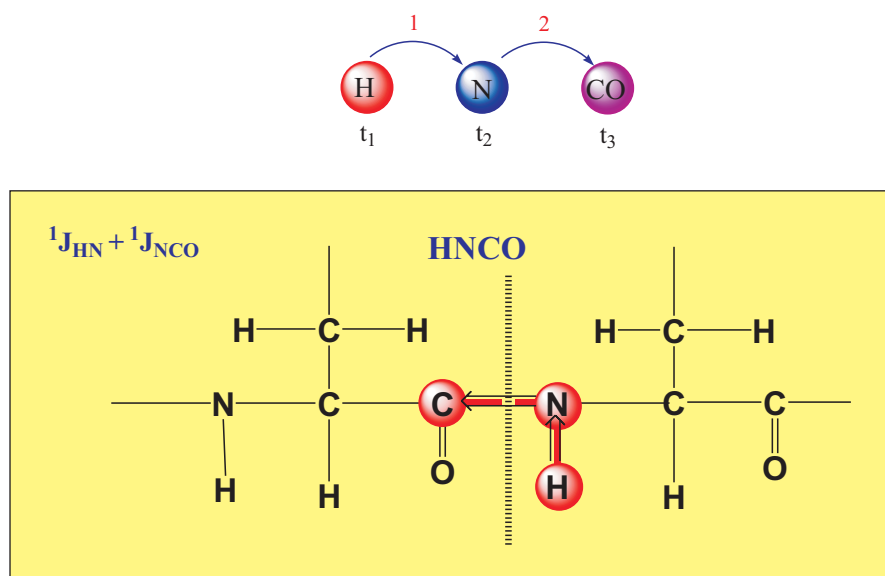
c_hnca_la3d



3D CO-detected HNCO Experiment

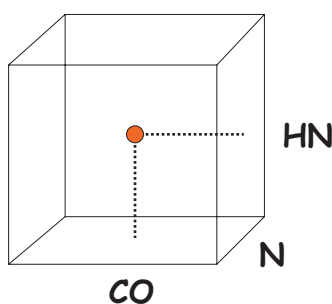
Experiment Description

The 3D CO-detected HNCO experiment is an out-and-stay version of the conventional HNCO experiment

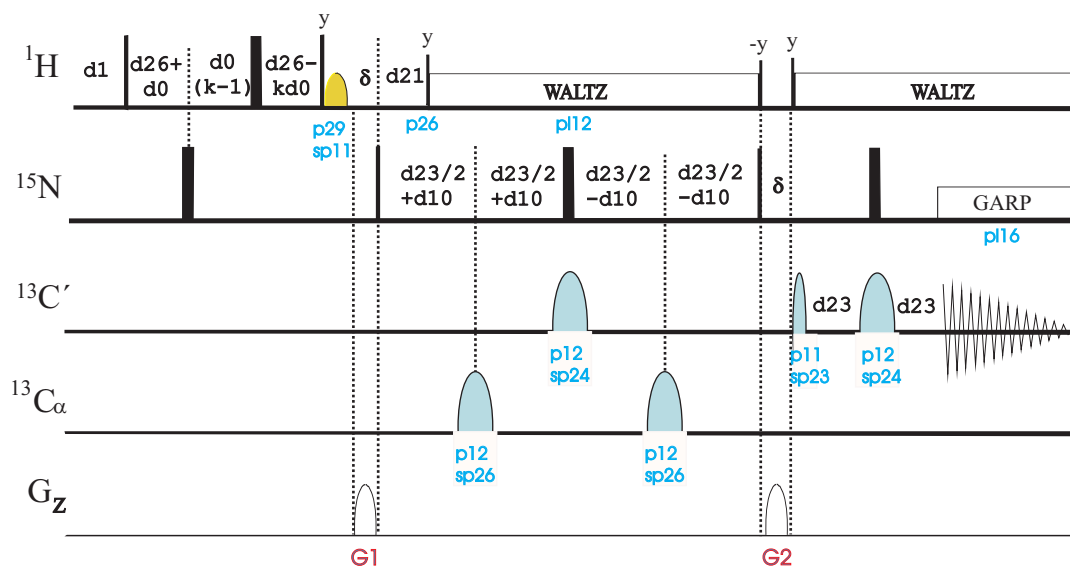


NMR Spectrum

The experiment provides the same 3D HNCO correlation map



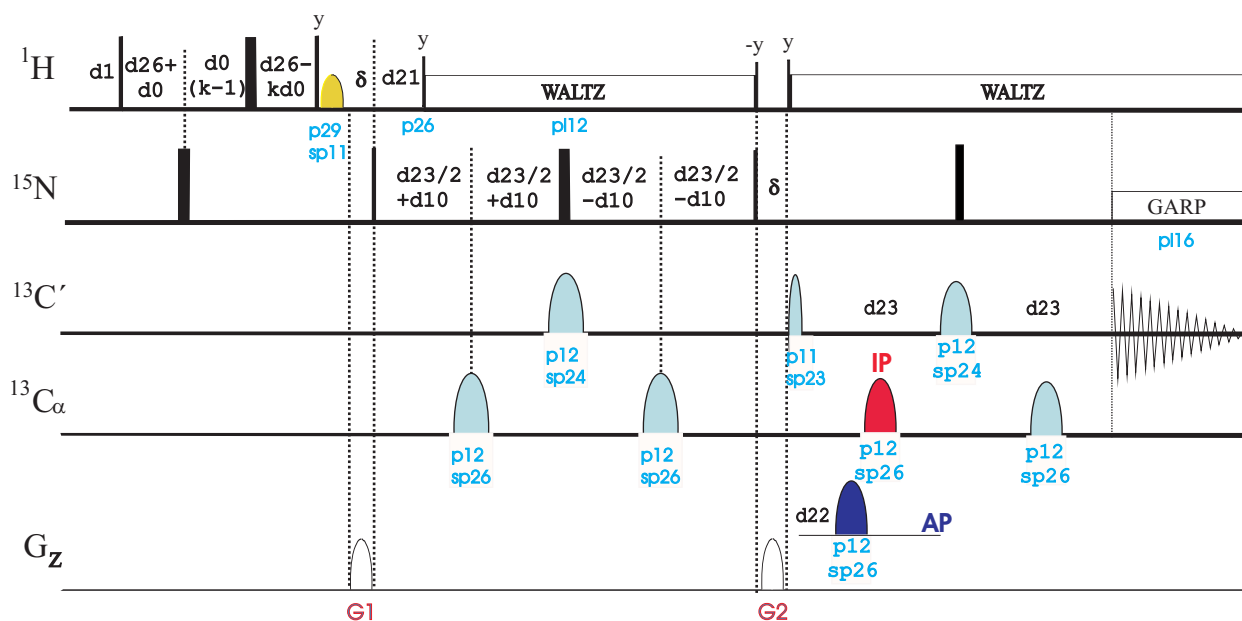
c_hnco_3d



Involved delays:

$d21 = 1/2J(\text{NH}) = 5.5\text{ms}$
 $d22 = 1/4J(\text{COCA}) = 4.5\text{ms}$
 $d23 = 1/4J(\text{NCA}) = 12.4\text{ms}$
 $d27 = 1/8(\text{CACB}) = 3.6\text{ms}$

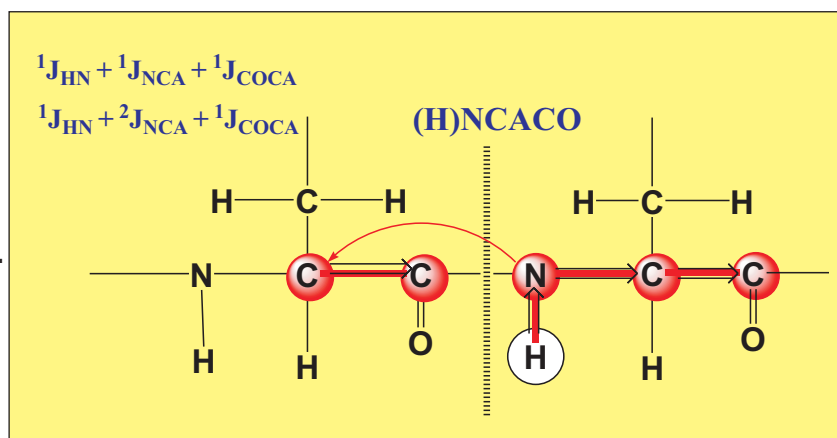
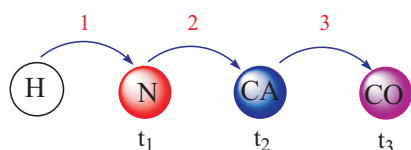
c_hnco_la3d



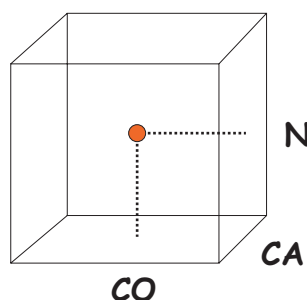
3D CO-detected (H)NCACO Experiment

Experiment Description

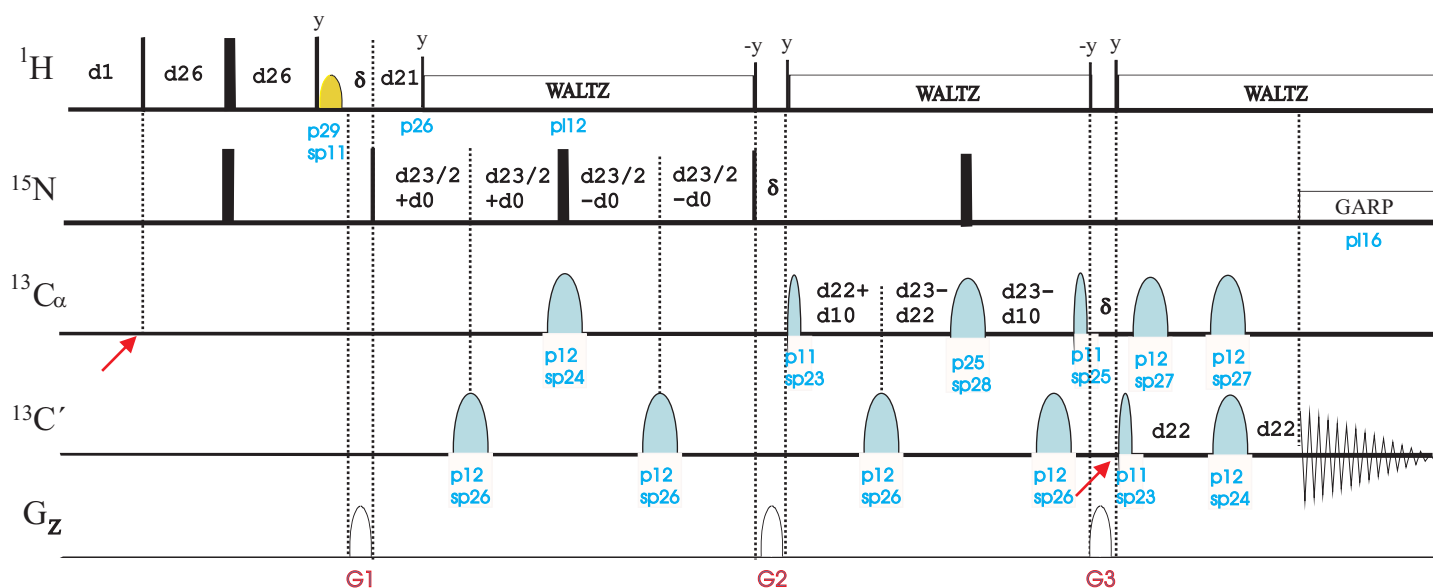
The 3D CO-detected HNCACO experiment is an out-and-stay version of the conventional ^1H -detected HNCACO experiment. Each nitrogen is correlated to CA and CO carbons of the same and the previous residue.



NMR Spectrum



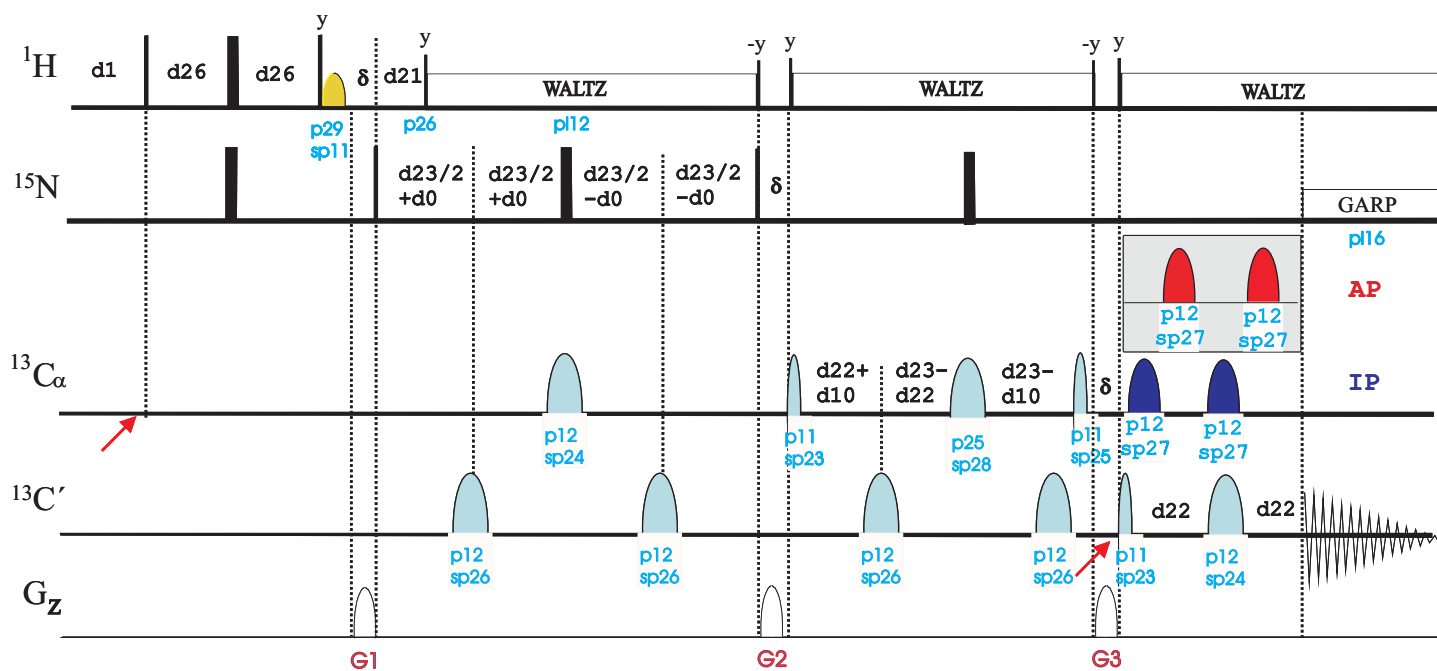
c_hncaco_3d



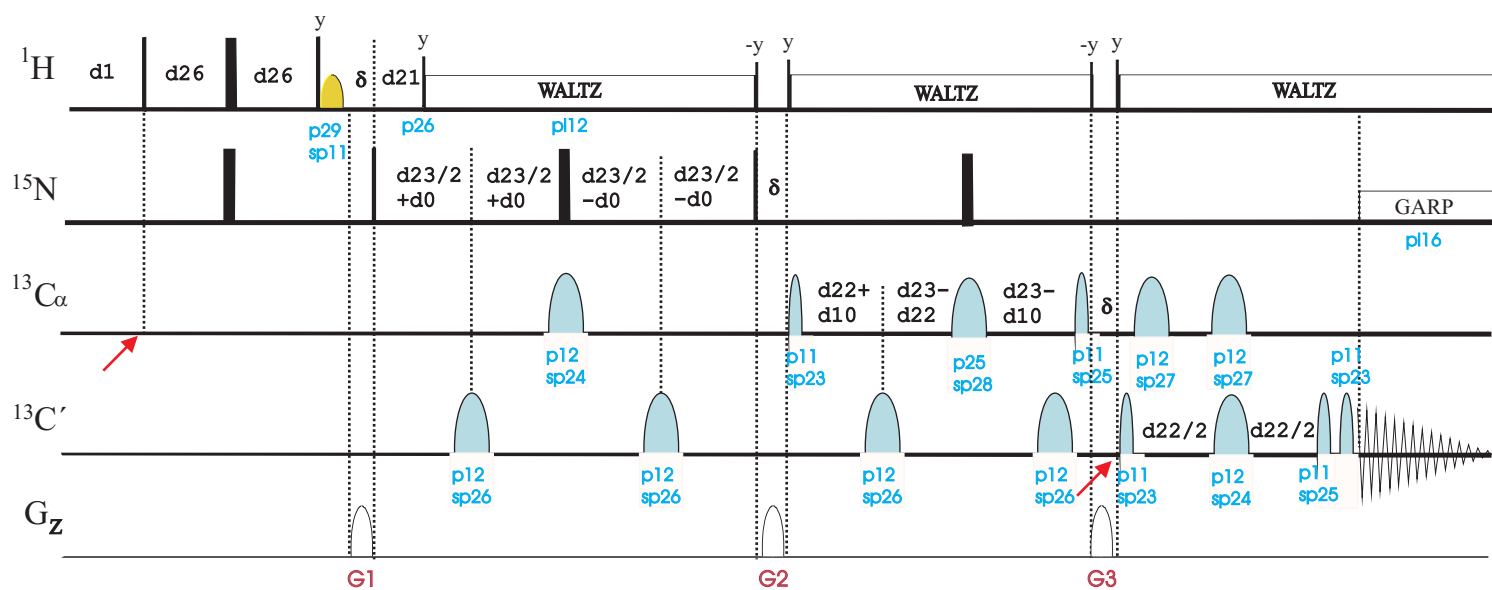
Involved delays:

$d21 = 1/2J(\text{NH}) = 5.5\text{ms}$
 $d22 = 1/4J(\text{COCA}) = 4.5\text{ms}$
 $d23 = 1/4J(\text{NCA}) = 12.4\text{ms}$
 $d26 = 1/4J(\text{NH}) = 2.3\text{ms}$

c_hncaco_la3d



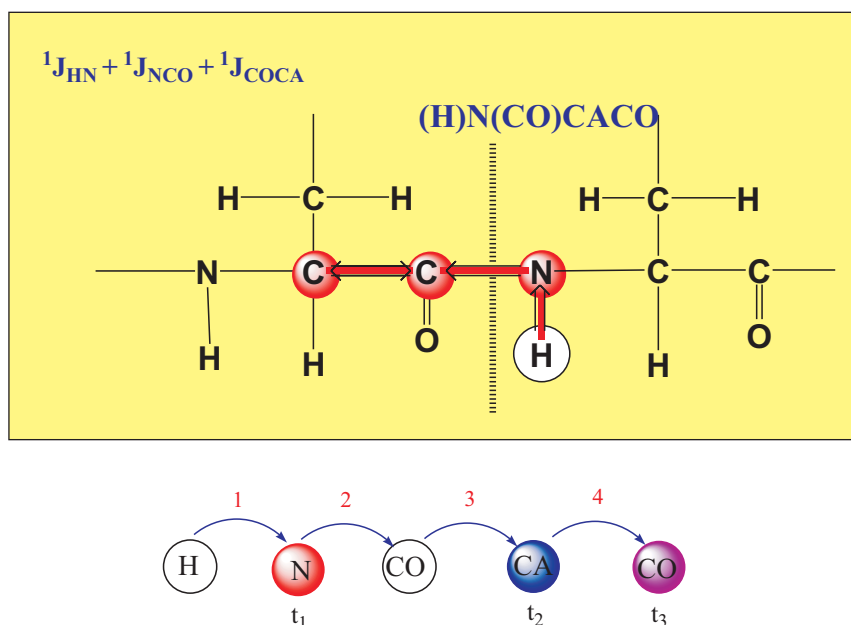
c_hncaco_s33d



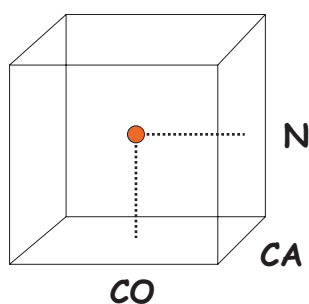
3D CO-detected (H)NCOCA Experiment

Experiment Description

The 3D (H)N(CO)CACO is the CO-detected equivalent of the HNCOCA experiment, in which a nitrogen nucleus is correlated to the CO and CA carbons of the previous residue.



NMR Spectrum

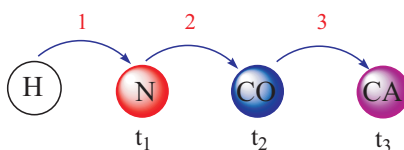
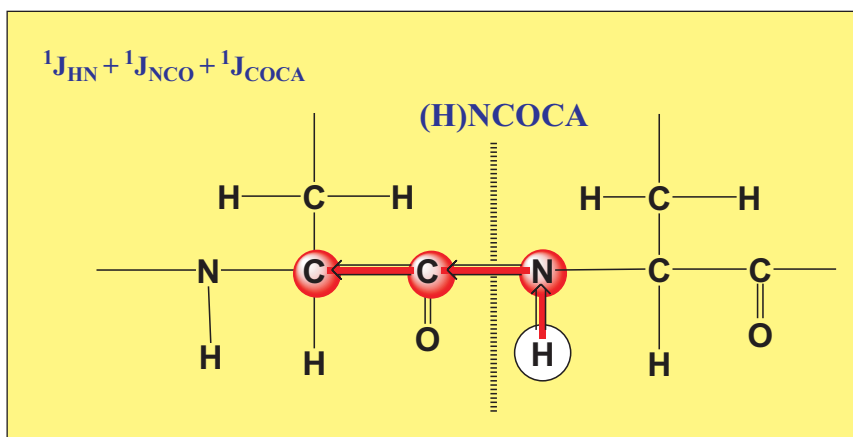


$d_{21} = 1/2J(\text{NH}) = 5.5\text{ms}$
 $d_{22} = 1/4J(\text{COCA}) = 4.5\text{ms}$
 $d_{23} = 1/4J(\text{NCO}) = 12.4\text{ms}$
 $d_{26} = 1/4J(\text{NH}) = 2.3\text{ms}$

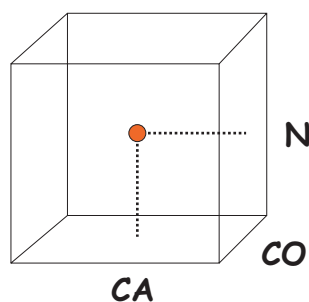
3D CA-detected (H)NCOCA Experiment

Experiment Description

The 3D CA-detected HNCOCA experiment is an out-and-stay version of the conventional ^1H -detected HNCOCA experiment. Each nitrogen is correlated to CA and CO carbons of the same and the previous residue.



NMR Spectrum



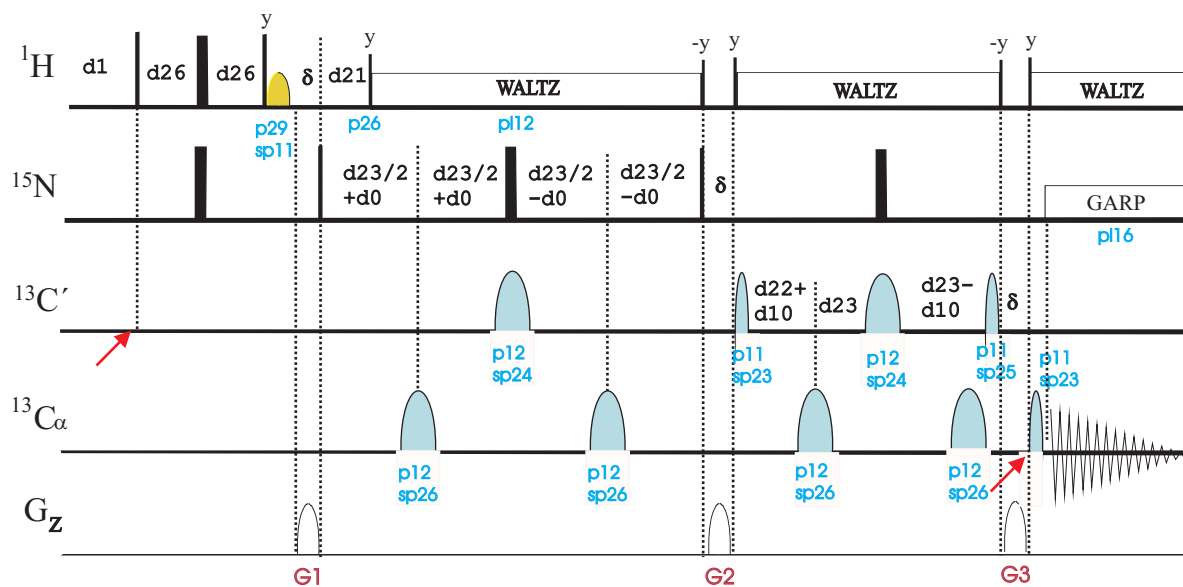
Related Experiments

^1H -detected HNCOCA
CO-detected (H)NCOCA
CANCO and i-CANCO

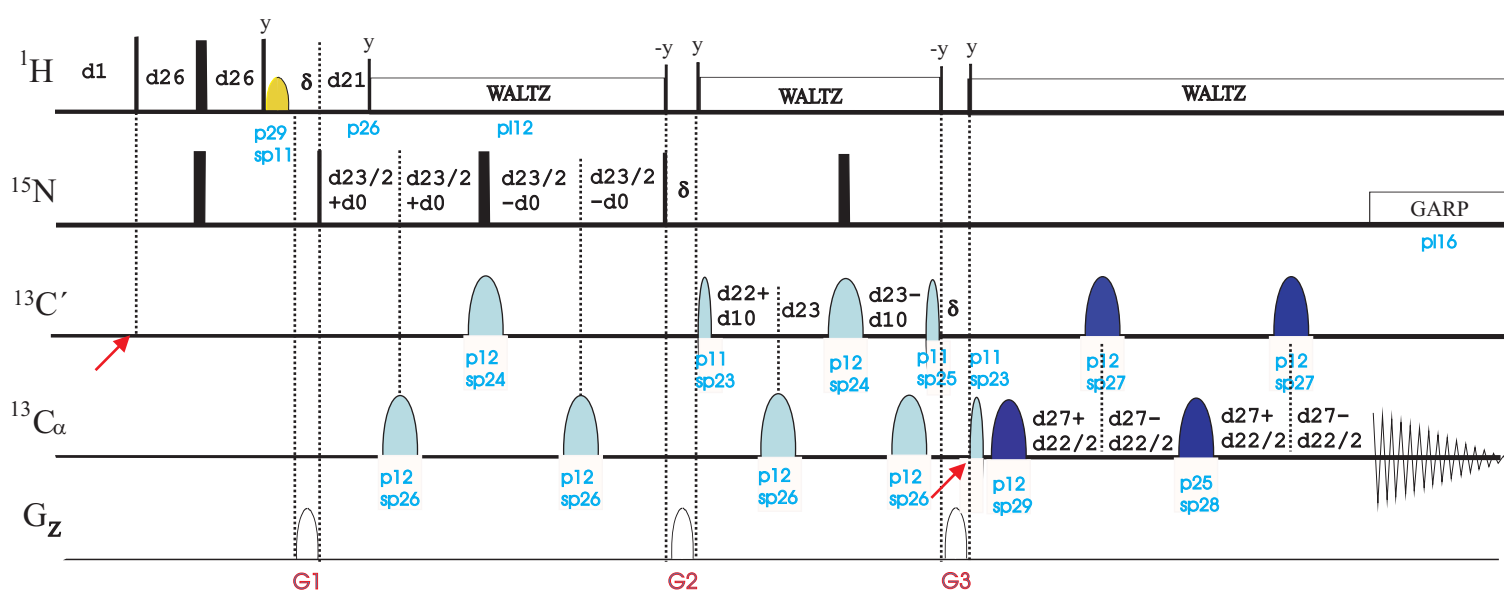
Involved delays:

$d21 = 1/2J(NH) = 5.5\text{ms}$
 $d22 = 1/4J(COCA) = 4.5\text{ms}$
 $d23 = 1/4J(NCA) = 12.4\text{ms}$
 $d26 = 1/4J(NH) = 2.3\text{ms}$
 $d27 = 1/8(CACB) = 3.6\text{ms}$

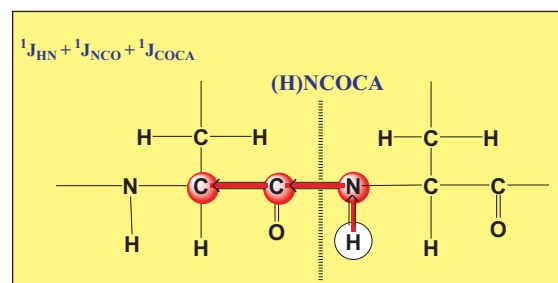
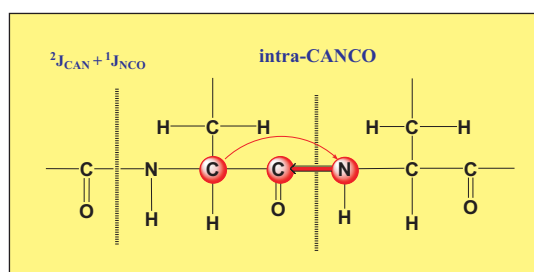
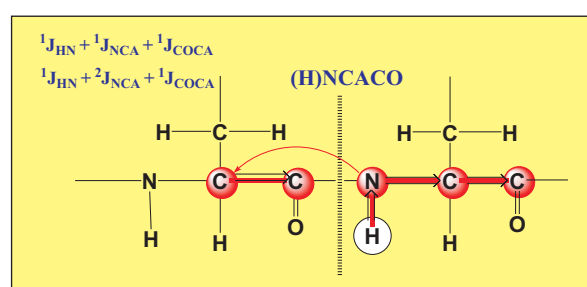
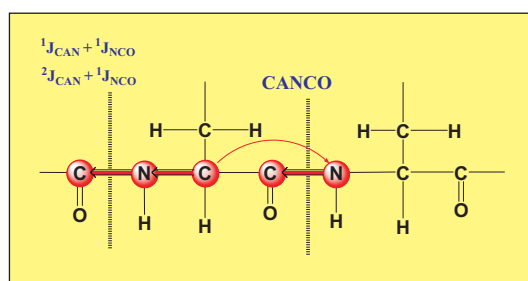
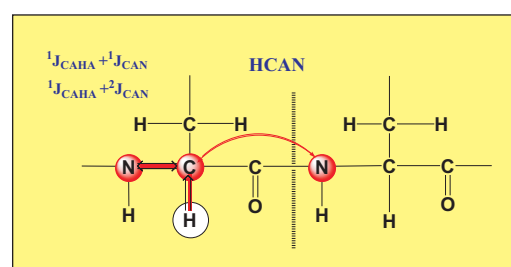
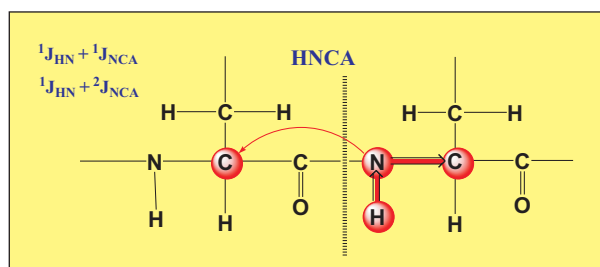
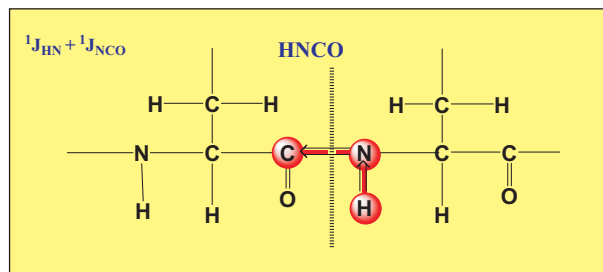
c_hncoca2_3d



c_hncoca2_la3d



Summary of C-detected backbone CN experiments



BRUKER PULSE PROGRAM CATALOGUE

NMRGuide

2D HSQC EXPERIMENTS FOR
THE MEASUREMENT OF T₁, T₂, T₁RHO
RELAXATION TIMES AND
HETERONUCLEAR NOEs.

2D HSQC experiments for ^{13}C Relaxation Measurements (from f2 channel)

Heteronuclear ^{13}C - ^1H NOEs:

Phase sensitive ge-2D ^1H - ^{13}C HSQC to measure heteronuclear ^{13}C - ^1H NOEs using PEP
(**hsqcnoegpsi** | HSQCNOEGPSI)

Phase sensitive ge-2D ^1H - ^{13}C HSQC to measure heteronuclear ^{13}C - ^1H NOEs using PEP and refocusing adiabatic ^{13}C pulses (**hsqcnoegpsi.2** | HSQCNOEGPSI)

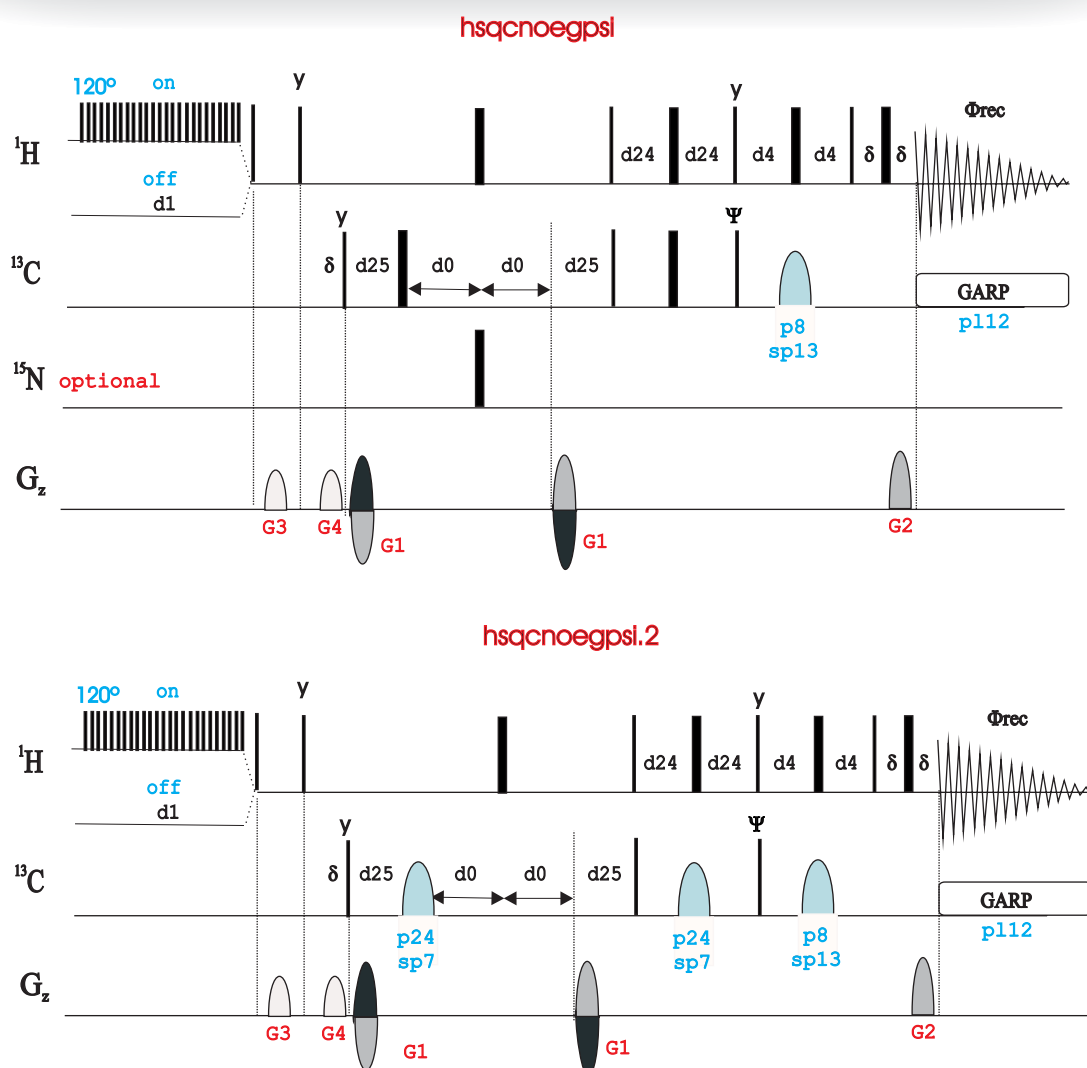
$T_1(\text{C})$:

Phase-sensitive ge-2D ^1H - ^{13}C HSQC to measure ^{13}C T_1 relaxation times using PEP, 180° ^1H pulses and acquired as pseudo-3D (**hsqct1etgpsi3d**).

Phase-sensitive ge-2D ^1H - ^{13}C HSQC to measure ^{13}C T_1 relaxation times using PEP, 180° ^1H pulses, refocusing adiabatic ^{13}C pulses and acquired as pseudo-3D (**hsqct1etgpsi3d.2**).

$T_2(\text{C})$:

Phase-sensitive ge-2D ^1H - ^{15}N HSQC to measure ^{13}C T_2 relaxation times using PEP and refocusing adiabatic ^{13}C pulses (**hsqct2etgpsi3d.2**)



[illegible]

2D HSQC experiments for ^{15}N Relaxation Measurements (from f3 channel)

Heteronuclear ^{15}N - ^1H NOEs:

Phase sensitive ge-2D ^1H - ^{15}N HSQC to measure heteronuclear ^{15}N - ^1H NOEs using PEP
(**hsqcnoef3gpsi** | **HSQCNOEF3GPSI**)

Phase sensitive ge-2D ^1H - ^{15}N HSQC to measure heteronuclear ^{15}N - ^1H NOEs using TROSY
(**trnoef3gpsi** | **TRNOEF3GPSI**)

$T_1(\text{N})$:

Phase-sensitive ge-2D ^1H - ^{15}N HSQC to measure ^{15}N T_1 relaxation times using PEP:

Using 1H-decoupling (**hsqct1etf3gpsi** | **HSQCT1ETF3GPSI**)

Using 1H-decoupling acquired as pseudo-3D (**hsqct1etf3gpsi3d** | **HSQCT1ETF3GPSI3D**)

Using 180 1H pulses (**hsqct1etf3gpsi.2** | **HSQCT1ETF3GPSI.2**)

Using 180 1H pulses acquired as pseudo-3D (**hsqct1etf3gpsi3d.2** | **HSQCT1ETF3GPSI3D.2**)

Phase sensitive ge-2D ^1H - ^{15}N HSQC to measure ^{15}N T_1 relaxation times using TROSY (**trt1etf3gpsi** | **TRT1ETF3GPSI**)

$T_2(\text{N})$:

Phase-sensitive ge-2D ^1H - ^{15}N HSQC to measure ^{15}N T_2 relaxation times using PEP (**hsqct2etf3gpsi** | **HSQCT2ETF3GPSI**):

Acquired as pseudo-3D (**hsqct2etf3gpsi3d** | **HSQCT2ETF3GPSI3D**)

Phase sensitive ge-2D ^1H - ^{15}N HSQC to measure ^{15}N T_2 relaxation times using PEP and Relaxation-dispersion (**hsqcrexetf3gpsi3d** | **HSQCTREXETF3GPSI3d**)

Phase sensitive ge-2D ^1H - ^{15}N HSQC to measure ^{15}N T_2 relaxation times using TROSY (**trt2etf3gpsi** | **TRT2ETF3GPSI**)

$T_{1\rho}(\text{N})$:

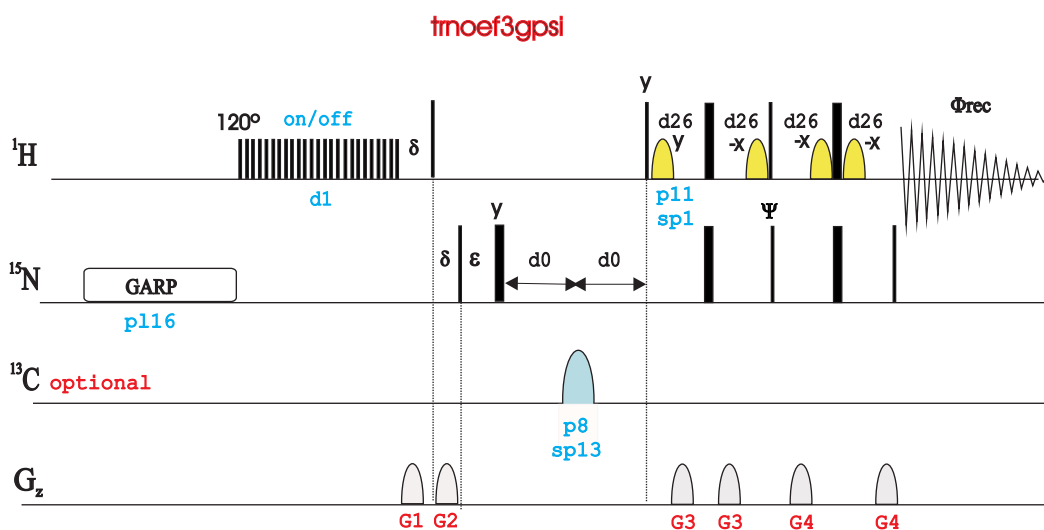
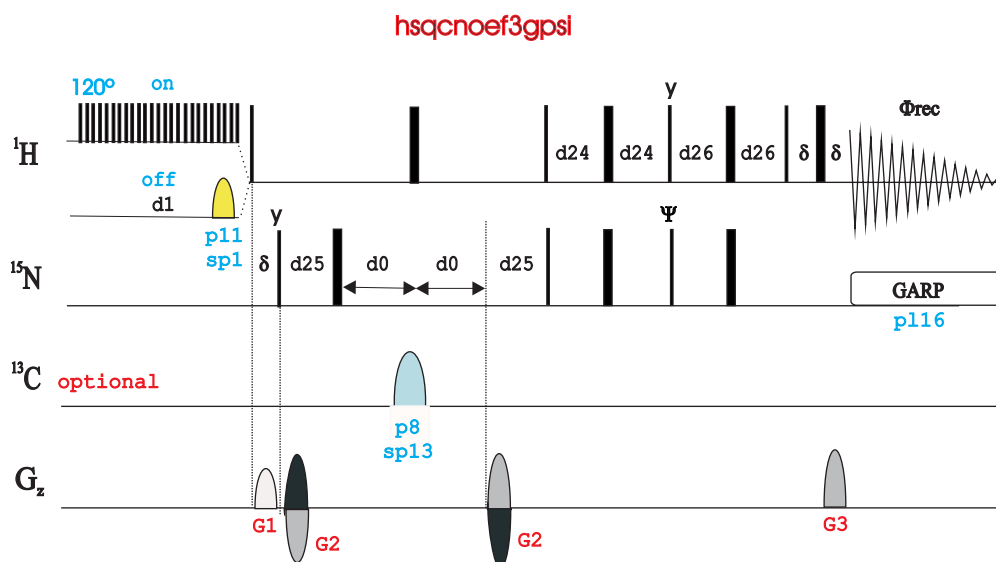
Phase-sensitive ge-2D ^1H - ^{15}N HSQC to measure ^{15}N $T_{1\rho}$ relaxation times using PEP
(**hsqctretf3gpsi** | **HSQCTRETF3GPSI**):

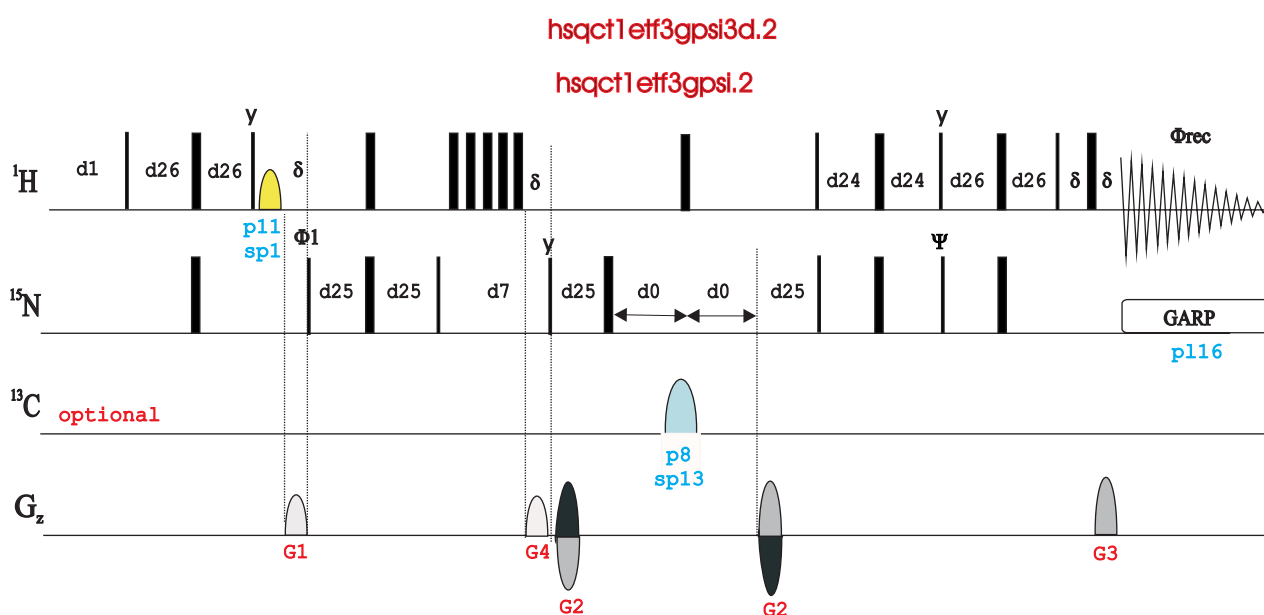
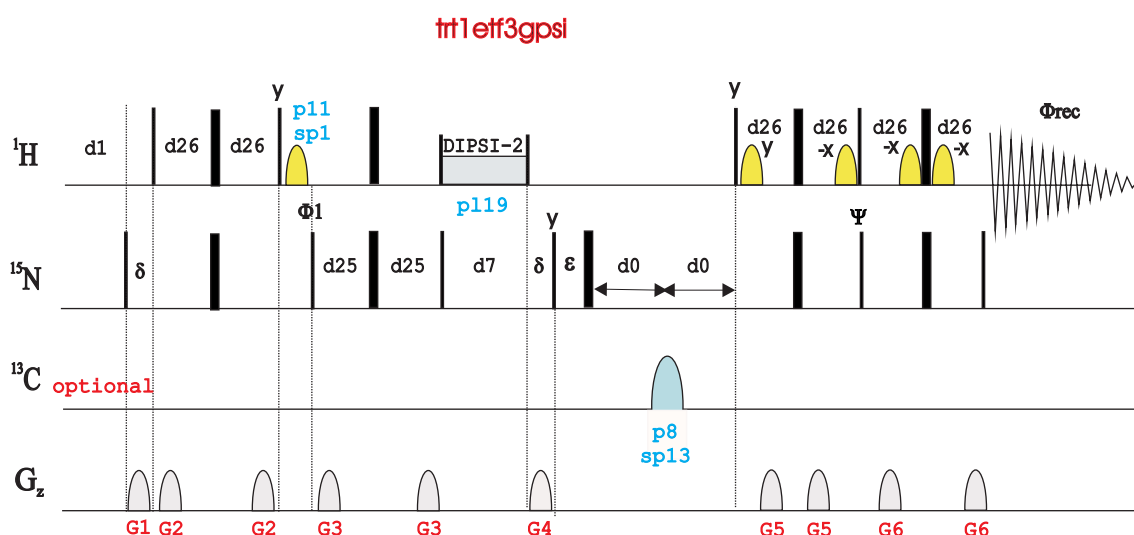
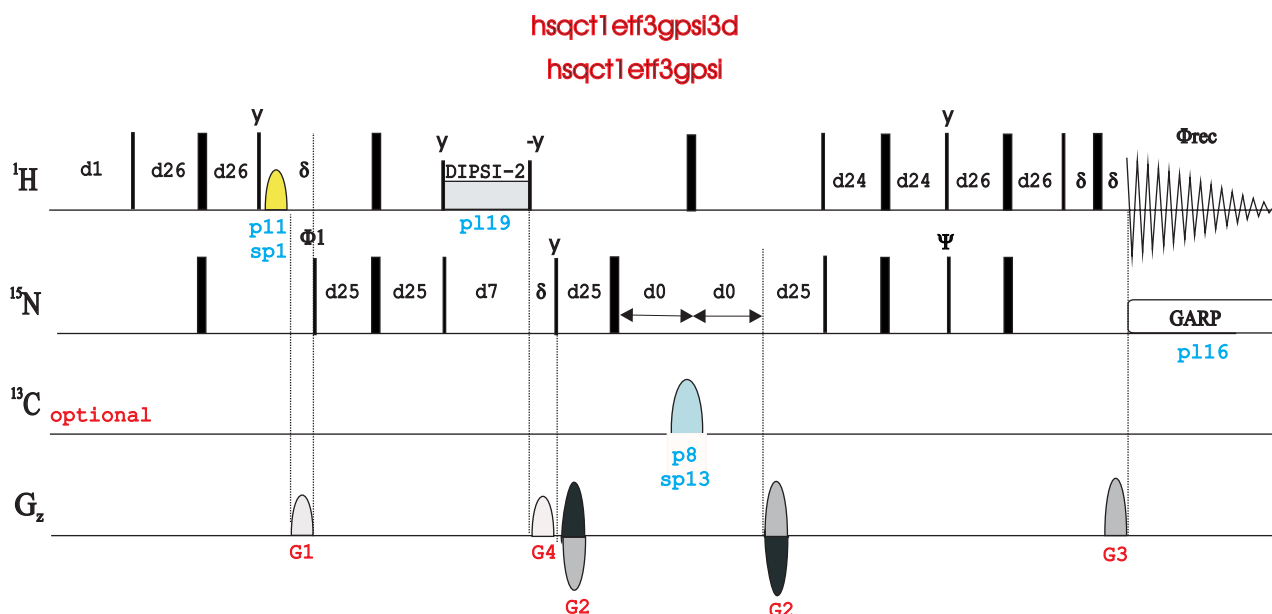
Acquired as pseudo-3D (**hsqctretf3gpsi3d** | **HSQCTRETF3GPSI3D**)

Phase-sensitive ge-2D ^1H - ^{15}N HSQC to measure ^{15}N $T_{1\rho}$ relaxation times using PEP with adiabatic ramping (**hsqctretf3gpsi3d.2** | **HSQCTRETF3GPSI3D.2**)

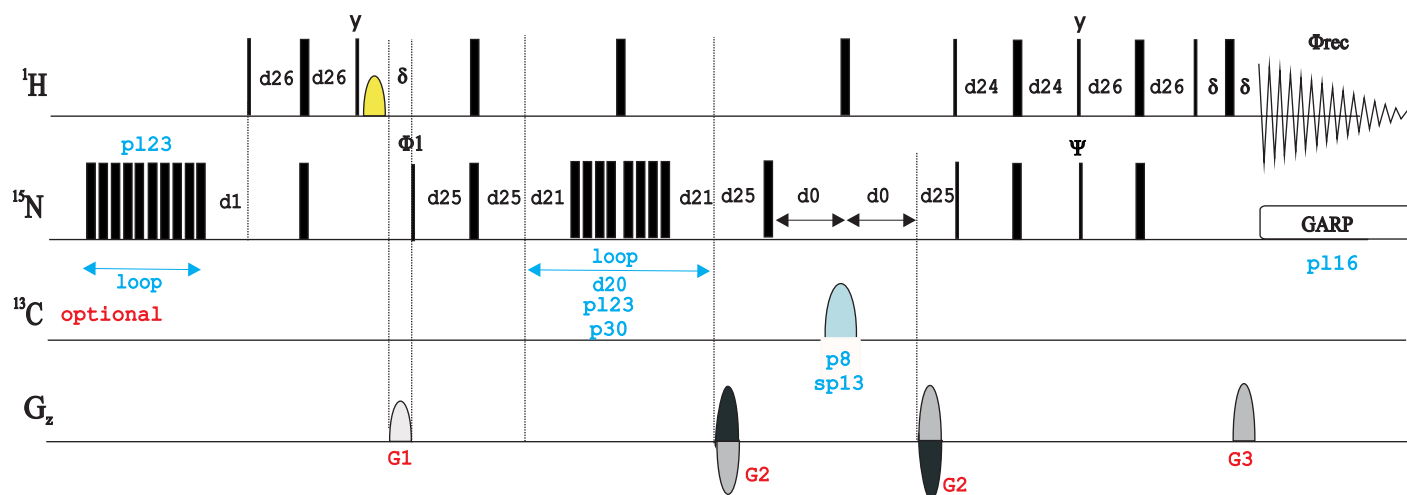
Cross-correlation:

Phase-sensitive ge-2D ^1H - ^{15}N HSQC to measure N-15 / H-1 cross correlation (**hsqcccf3gp phwg**)

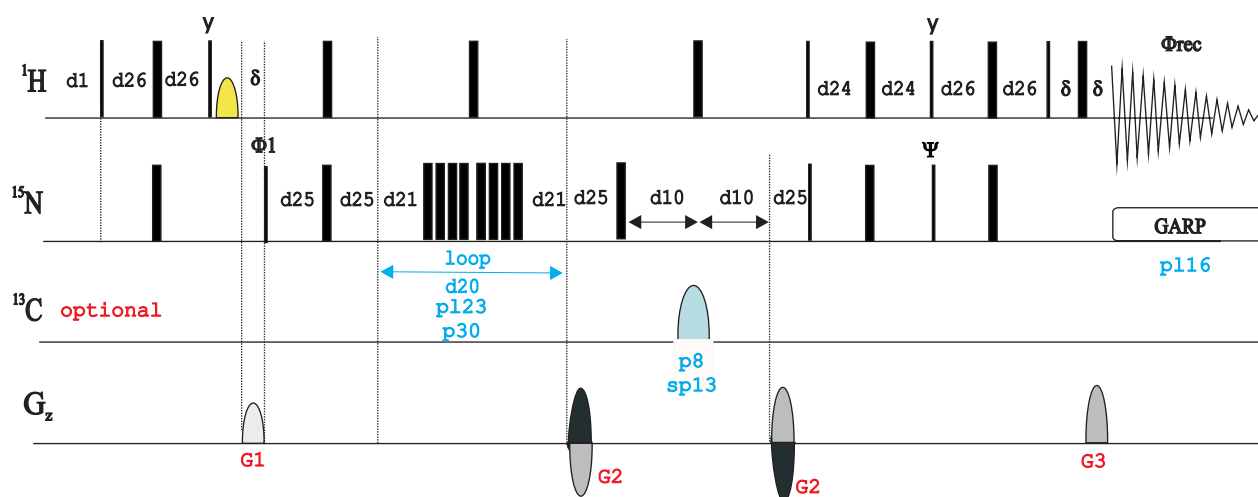




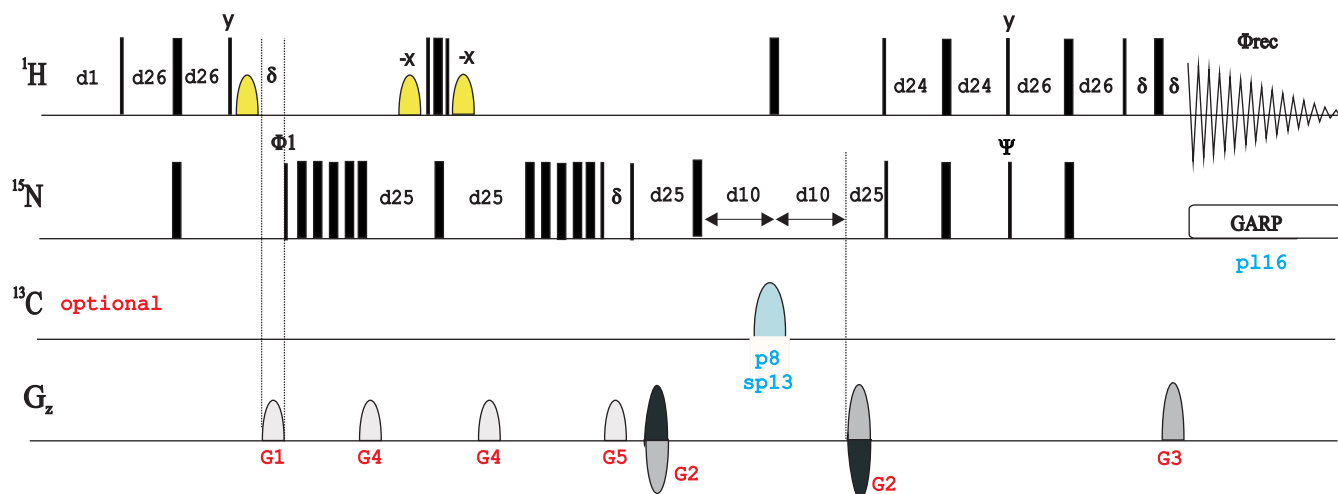
hsqct2etf3gpsl



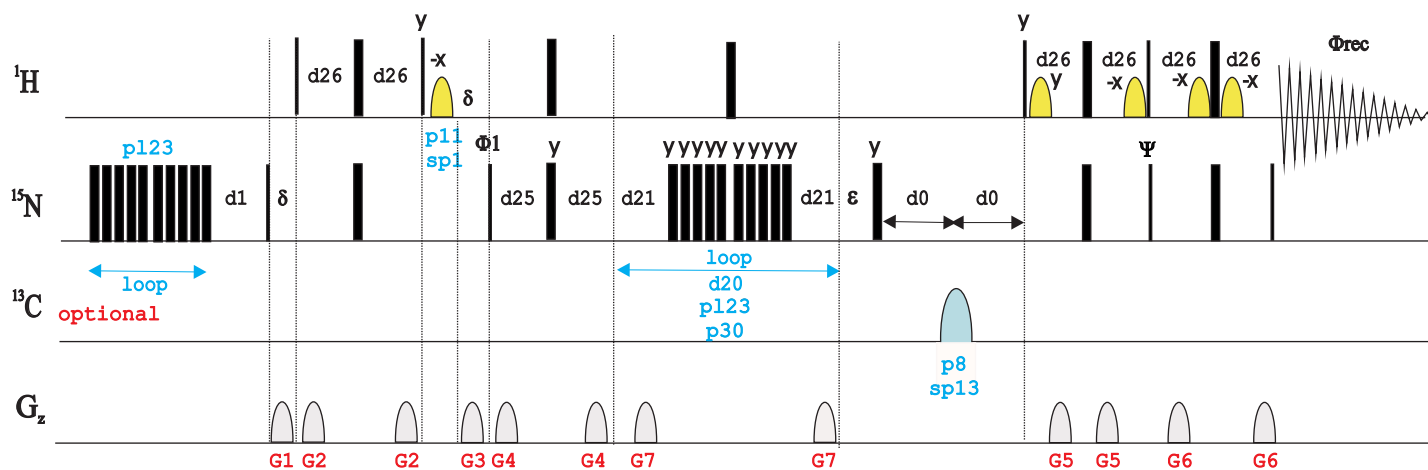
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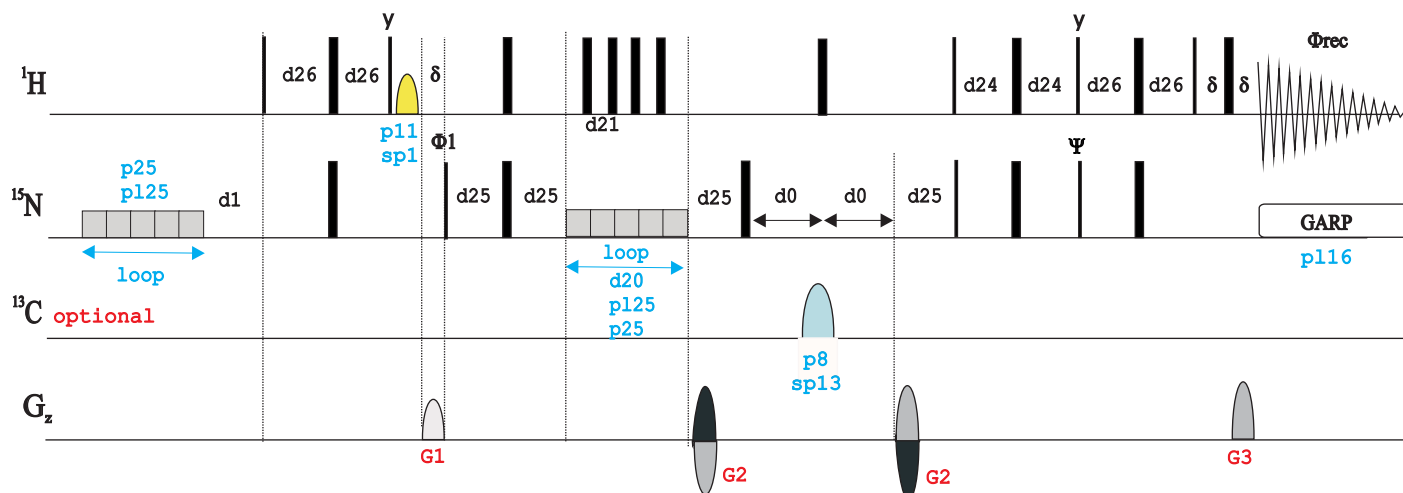
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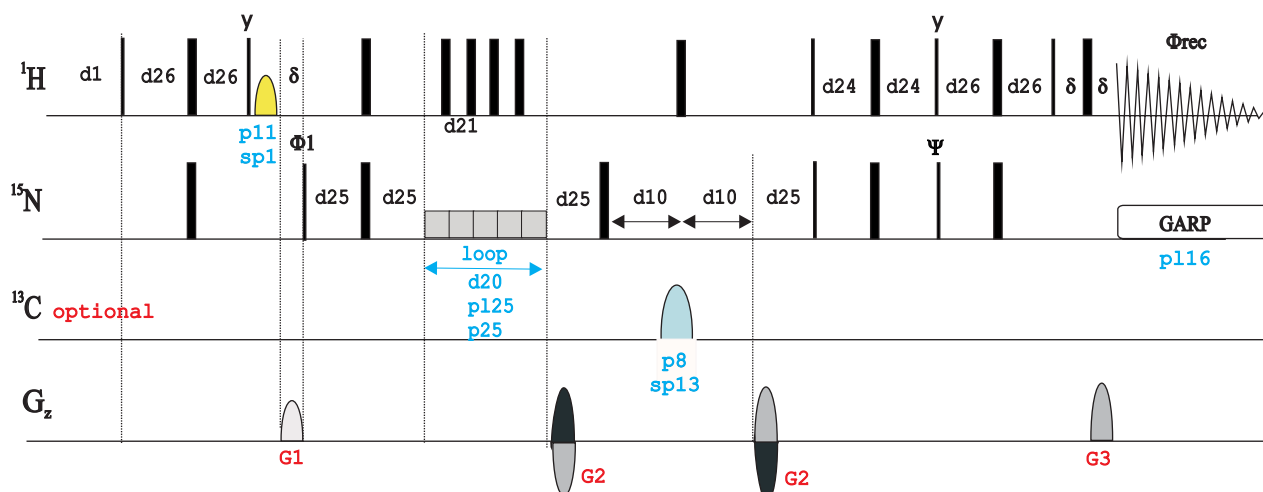
trf2etf3gpsl



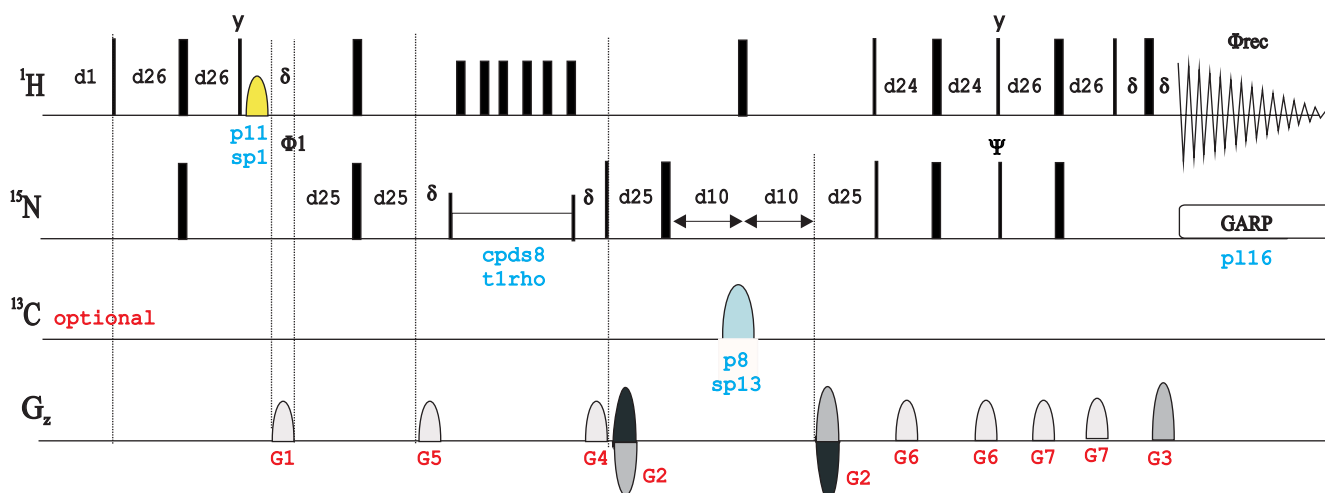
hsqctretf3gpsl

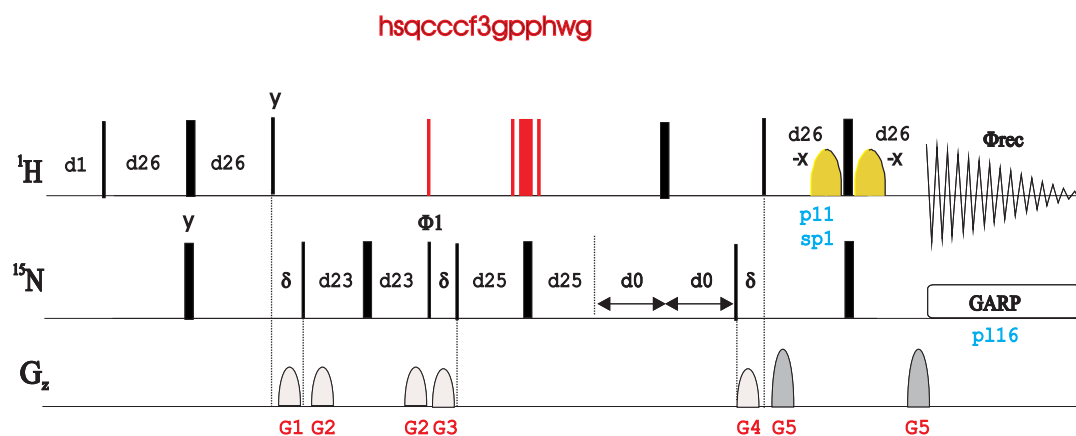


hsqctretf3gpsl3d



hsqctretf3gpsl3d.2





BRUKER PULSE PROGRAM CATALOGUE

NMRGuide

3D HNCO EXPERIMENTS FOR
THE MEASUREMENT OF T₁, T₂ AND T₁RHO
RELAXATION TIMES.

3D HNCO experiments for ^{15}N Relaxation Measurements

Heteronuclear ^{15}N - ^1H NOEs:

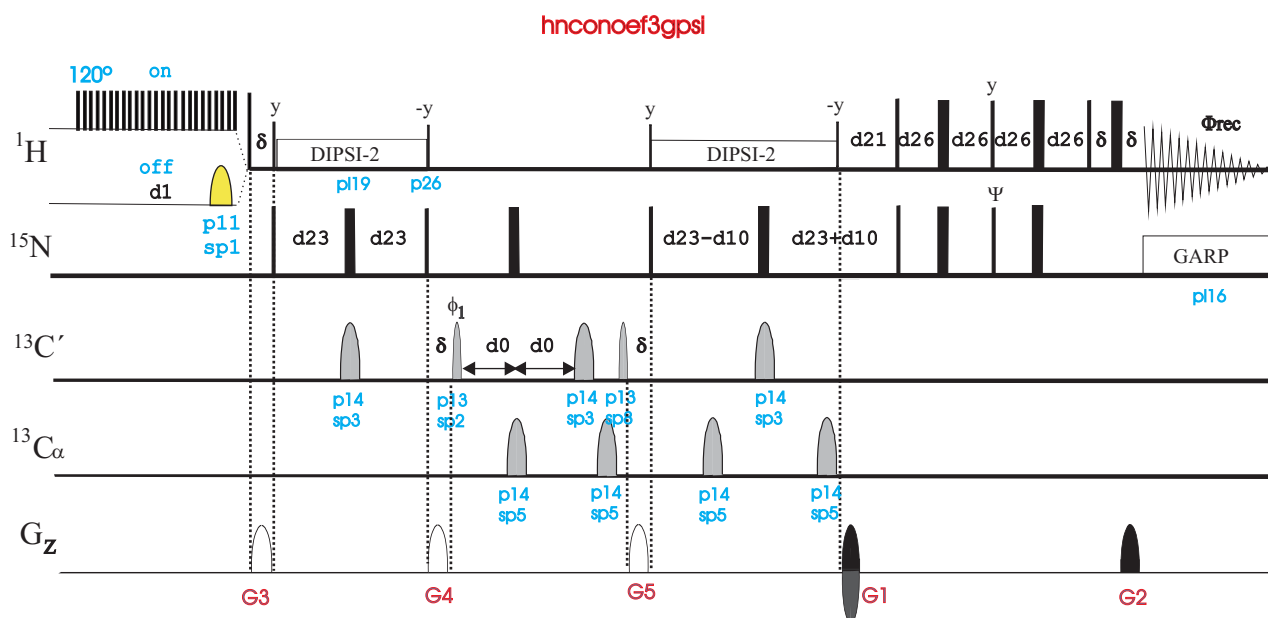
3D HNCO to measure heteronuclear ^{15}N - ^1H NOEs using PEP (**hnconoef3gpsi**)

$T_1(\text{N})$:

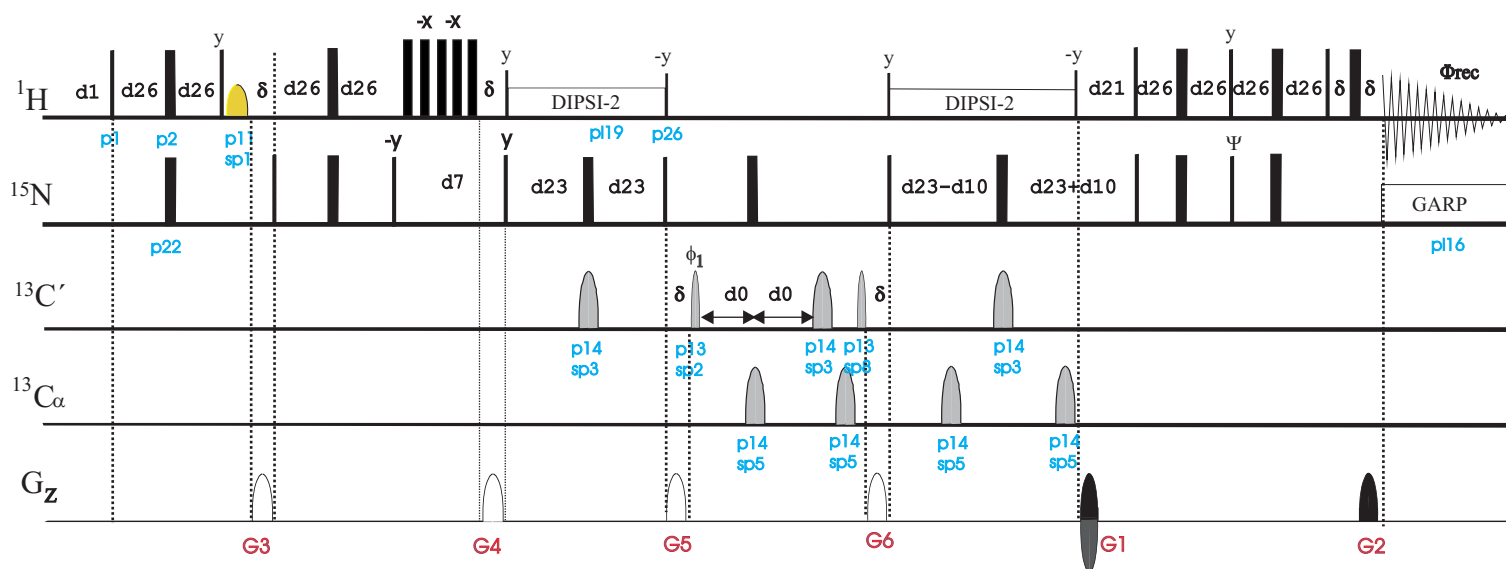
3D HNCO to measure ^{15}N T_1 relaxation times using PEP (**hncot1f3gpsi**)

$T_2(\text{N})$:

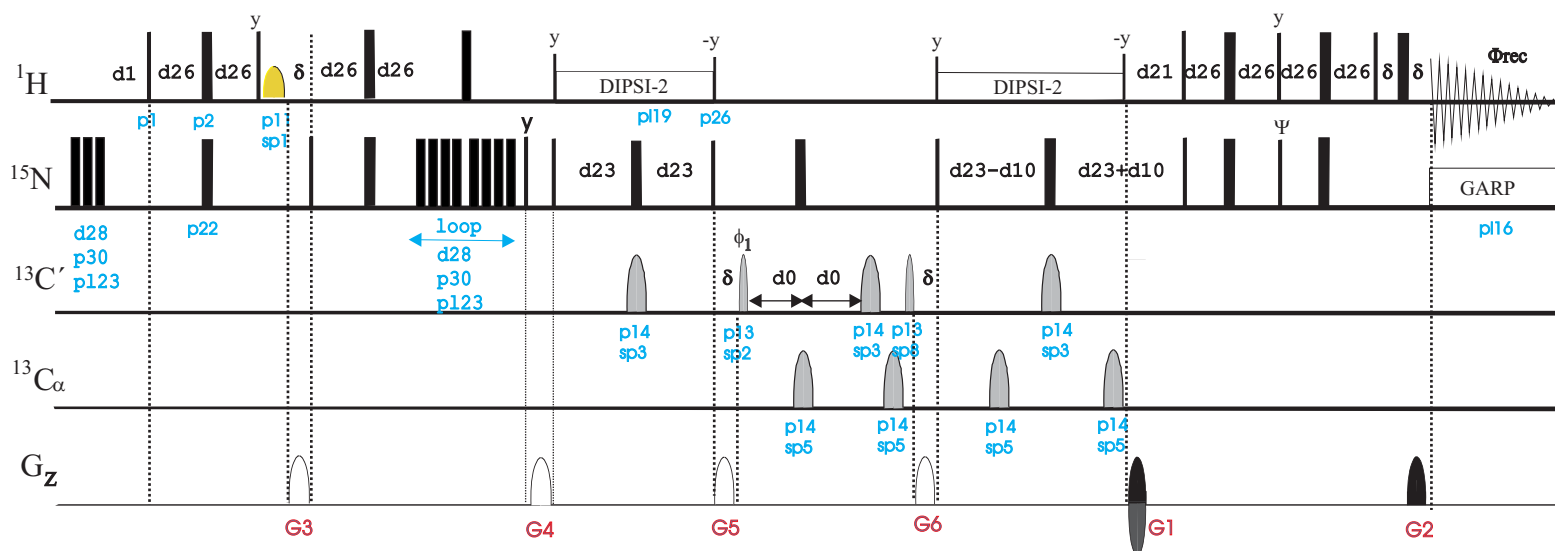
3D HNCO to measure ^{15}N T_2 relaxation times using PEP (**hncot2f3gpsi**)



hncot1f3gpsl



hncot2f3gpsl



BRUKER PULSE PROGRAM CATALOGUE

NMRGuide

PROTEIN NMR
COUPLING CONSTANTS

Protein NMR Coupling Constants

[Tutorials: J Backbone](#)
[Tutorials: J Sidechain](#)
[Tutorials: J Miscellaneous](#)

NMR Experiments

[Introduction](#)
[Determination](#)
[J-Resolved](#)
[Spin-State Selective](#)
[E.COSY](#)
[TROSY/antiTROSY](#)
[J-scaling](#)
[J-Quantitative](#)
[DQ-ZQ](#)

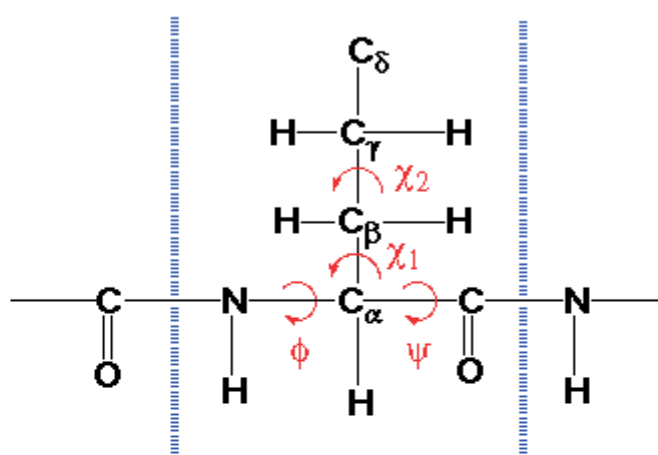
Scalar Couplings (J)

[One-bond](#)
[Two-bond](#)
[Three-bond](#)
[Backbone Three-bond \$\phi\$](#)
[Backbone Three-bond \$\omega\$](#)
[Backbone Three-bond \$\psi\$](#)
[Sidechain Three-bond \$\chi_1\$](#)
[Sidechain Three-bond \$\chi_2\$](#)

Dipolar Couplings (D)

[Introduction](#)
[Anisotropic Media](#)
[NMR Experiments](#)
[Structure Calculation](#)

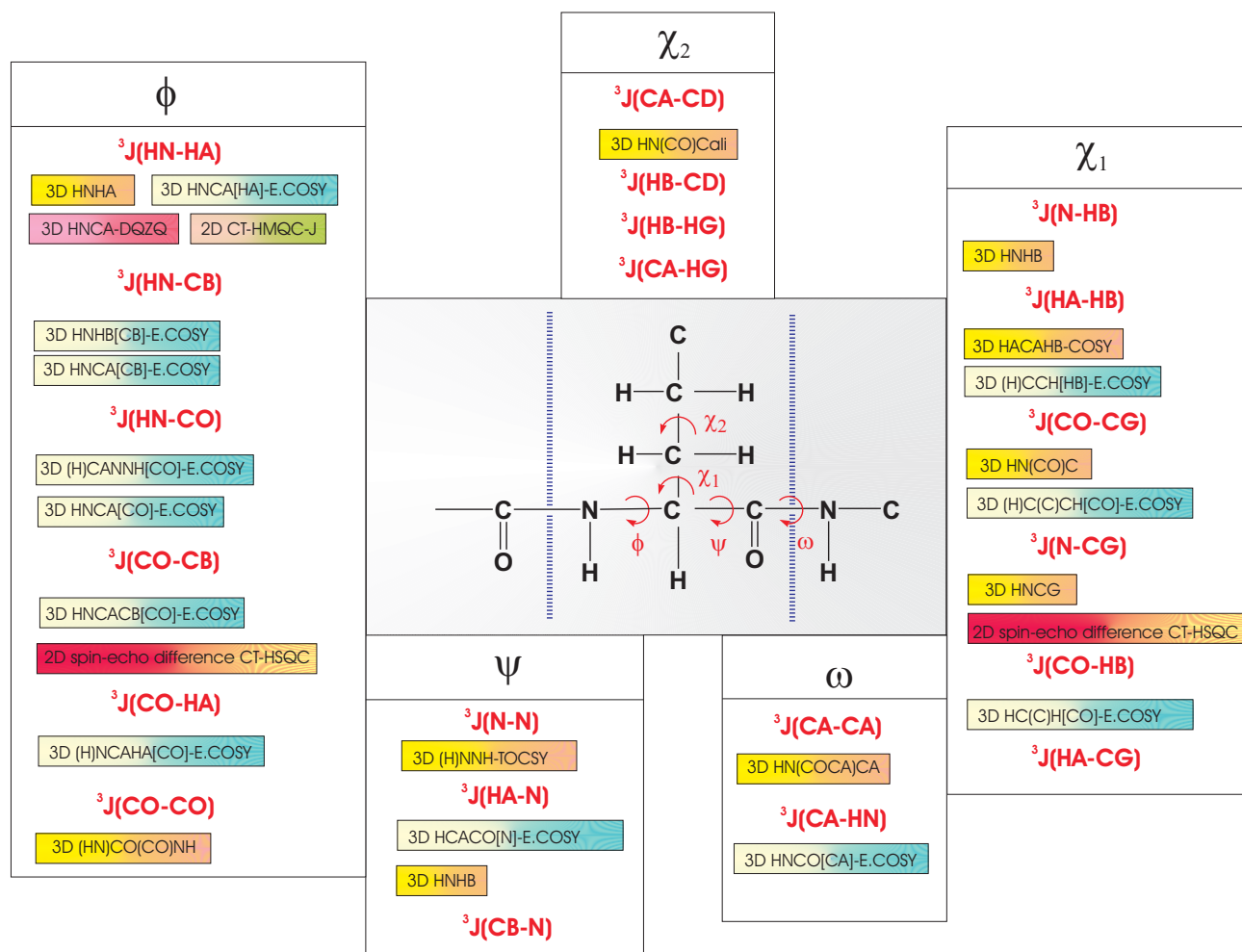
[Cross-Hydrogen Bond \(\$^hJ\$ \)](#)
[Introduction](#)
[NMR Experiments](#)
[Applications](#)



Applications

[2D Experiments](#) | [3D Double-Resonance Experiments](#)
[3D Triple-Resonance Experiments](#)

General Reading: [76PROG41](#), [B03ZER147](#)



Phi Backbone Coupling Constant

3D HNHA experiment (**hnhagp3d** | HNHAGP3D) - 3J(HN-HA) via quantitative-J
 3D HNCA[HA,CB]-E.COSY (**hncacosgp3d** | HNCAECOSGP3D) - 3J[H(N)-HA] and 3J[H(N)-CB] via E.COSY
 3D HNCA[HA]-E.COSY (**hncacosgp3d2** | HNCAECOSGP3D2) - 3J[H(N)-HA] via E.COSY
 3D DQ/ZQ HNCA (**hncadqzqgp3d** | HNCADQZQGP3D) - 3J[H(N)-HA] and 3J[H(N)-CB] via DQ/ZQ
 2D CT-HMQC-J (**hmqcjgp** | HMQCJGP) - 3J[H(N)-HA] via J-modulation
 3D HNHB[CB]-E.COSY (**hnhbecosgp3d** | HNHBECOSGP3D) - 3J[H(N)-CB] via E.COSY
 3D HNCA[CB]-E.COSY (**hncajcgp3d** | HNCAJCGP3D) - 3J[H(N)-CB] via E.COSY
 3D (H)CANNH[CO]-E.COSY (**hcannhgp3d** | HCANNHGP3D) - 3J[H(N)-CO] via E.COSY
 3D HNCA[CO]-E.COSY (**hncacosygp3d** | HNCACOSYGP3D) - 3J[H(N)-CO] via E.COSY
 3D HNCACB[CO]-E.COSY (**hncacbgpjc3d** | HNCACBGPJC3D) - 3J[CO-CB] via E.COSY
 2D spin-echo difference CT-HSQC (**hsqcctetgpcjlr** | HSQCCTETGPGJCLR) - 3J[CO-CB] via spin-echo difference
 3D (H)NCAHA[CO]-E.COSY (**hncahagp3d** | HNCAHAGP3D) - 3J[HA-CO] via E.COSY
 3D (HN)CO(CO)NH (**hncocogp3d** | HNCOCOGP3D) - 3J[CO-CO] via quantitative-J

Psi Backbone Coupling Constant

3D (H)NNH-TOCSY (**hnnhdigp3d** | HNNHDIGP3D) - 3J[N-N] via quantitative-J
 3D HCACO[N]-E.COSY (**hcacogpjc3d** | HCACOGPJC3D) - 3J[HA-N] via E.COSY
 3D HNHB (**hnhbgp3d** | HNHBGP3D) - 3J[HN-HA] and 3J[HN-HB] via quantitative-J

Omega Backbone Coupling Constant

3D HN(COCA)CA (**hncocacagp3d** | HNCOCACAGP3D) - 3J[CA-CA] via quantitative-J
 3D HNCO[CA]-E.COSY (**hncoccosgp3d** | HNCOCOSGP3D) - 3J[H(N)-CA] via E.COSY

Chi1 Sidechain Coupling Constant

3D HNHB (**hnhbgp3d** | HNHBGP3D) - 3J[HN-HA] and 3J[HN-HB] via quantitative-J
 3D HACAHB-COSY (**hacahbcosygp3d** | HACAHCOSYGP3D) - 3J[HA-HB] via quantitative-J
 3D HN(CO)C (**hncocgp3d** | HNCOCGP3D) - 3J[CG-CO] via quantitative-J
 3D HC(C)H[HA]-E.COSY (**hcchecosgp3d** | HCCHECOSGP3D) - 3J[HA-HB] via E.COSY
 3D HC(C)H[CO]-E.COSY (**hcchcosygp3d** | HCCHCOSYGP3D) - 3J[CO-HB] via E.COSY
 3D (H)C(C)CH[CO]-E.COSY (**hccccosygp3d** | HCCCCOSYGP3D) - 3J[CG-CO] via E.COSY
 3D HNCG (**hncggp3d.1** | HNCGGP3D.1) - 3J[N-CG] via quantitative-J
 3D HNCG (**hncggp3d.2** | HNCGGP3D.2) - 3J[N-CG] via quantitative-J
 2D spin-echo difference CT-HSQC (**hsqcetfpgpjcsl** | HSQCETFPFGPGJCSL) - 3J[N-CG] via spin-echo difference

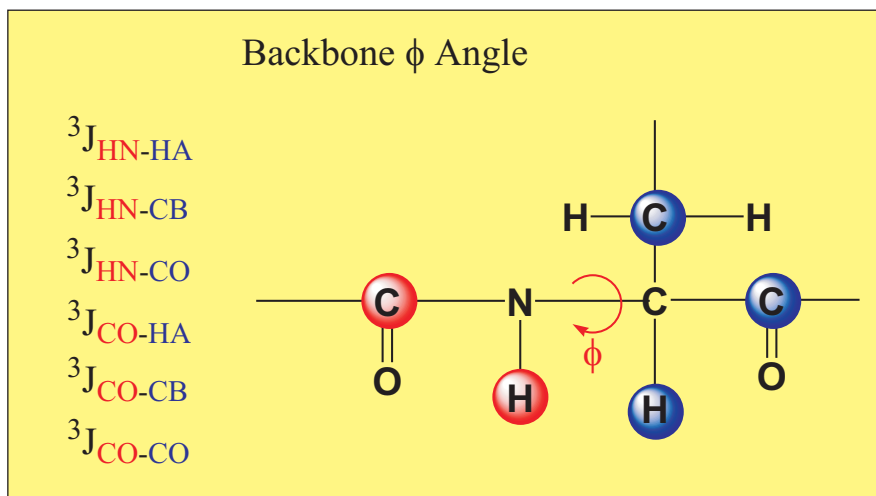
Chi2 Sidechain Coupling Constant

3D HN(CO)CACali (**hncocacgp3d** | HNCOCACGP3D) - 3J[CA-CD] via quantitative-J

BRUKER PULSE PROGRAM CATALOGUE

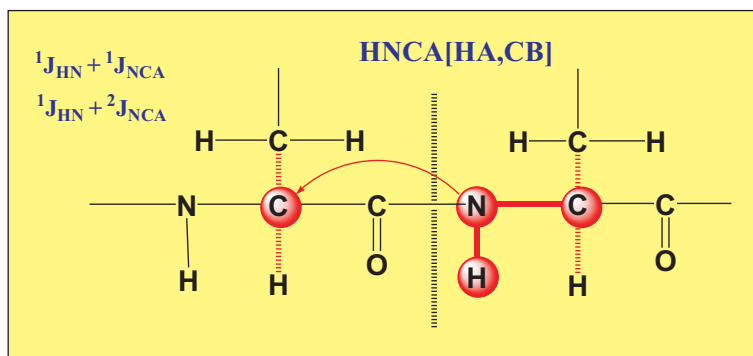
NMRGuide

PROTEIN NMR
COUPLING CONSTANTS
PHI BACKBONE ANGLE



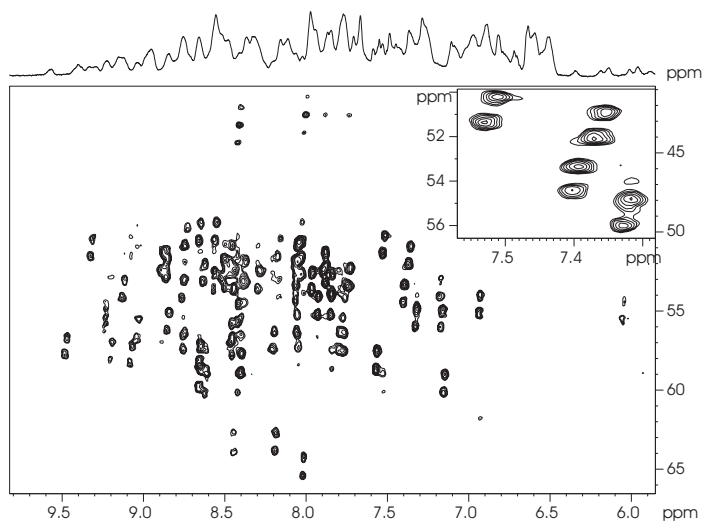
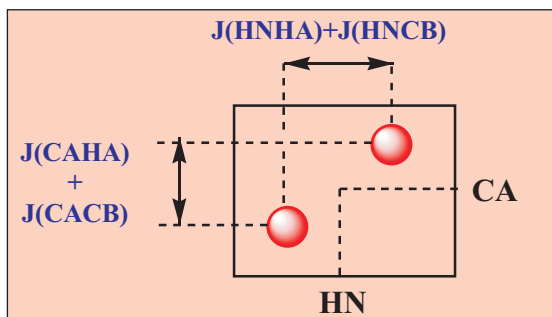
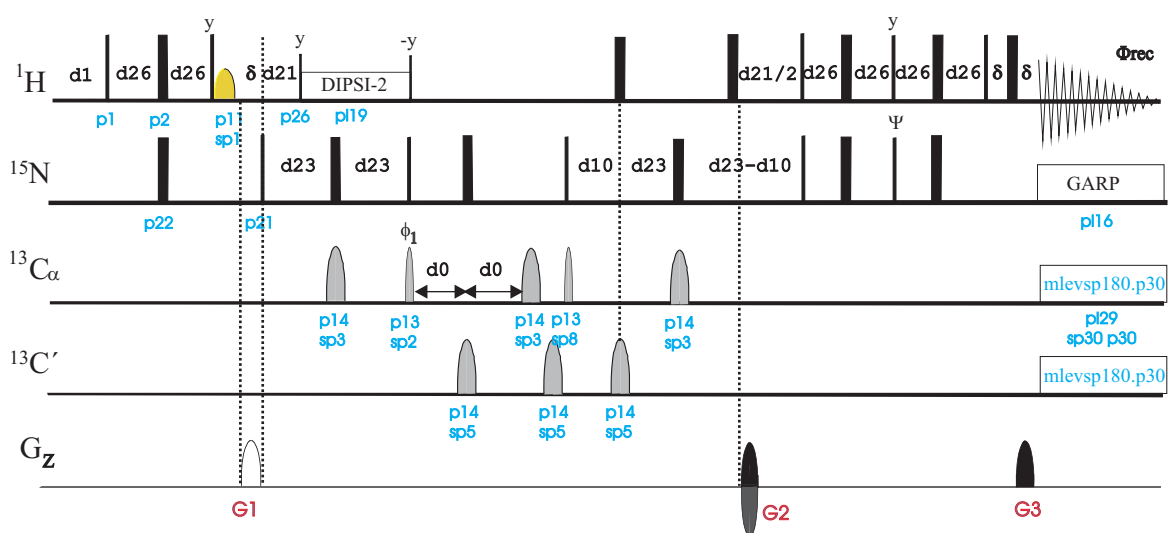
Phi Backbone Coupling Constant

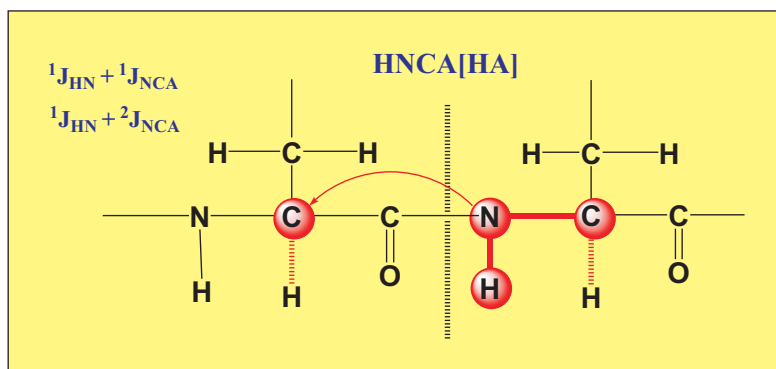
3D HNHA experiment (**hnhagp3d** | HNHAGP3D) - $3J(\text{HN-HA})$ via quantitative-J
 3D HNCA[HA,CB]-E.COSY (**hnaecosgp3d** | HNAECOSGP3D) - $3J[\text{H(N)-HA}]$ and $3J[\text{H(N)-CB}]$ via E.COSY
 3D HNCA[HA]-E.COSY (**hnaecosgp3d2** | HNAECOSGP3D2) - $3J[\text{H(N)-HA}]$ via E.COSY
 3D DQ/ZQ HNCA (**hncadqzqgp3d** | HNCADQZQGP3D) - $3J[\text{H(N)-HA}]$ and $3J[\text{H(N)-CB}]$ via DQ/ZQ
 2D CT-HMQC-J (**hmqcjgp** | HMQCJGP) - $3J[\text{H(N)-HA}]$ via J-modulation
 3D HNHB[CB]-E.COSY (**hnhbecosgp3d** | HNHBECOSGP3D) - $3J[\text{H(N)-CB}]$ via E.COSY
 3D HNCA[CB]-E.COSY (**hncajcgp3d** | HNAJC GP3D) - $3J[\text{H(N)-CB}]$ via E.COSY
 3D (H)CANNH[CO]-E.COSY (**hcannhgp3d** | HCANNHGP3D) - $3J[\text{H(N)-CO}]$ via E.COSY
 3D HNCA[CO]-E.COSY (**hncacosygp3d** | HNCACOSYGP3D) - $3J[\text{H(N)-CO}]$ via E.COSY
 3D HNCACB[CO]-E.COSY (**hncacbgpjc3d** | HNCACBGJPC3D) - $3J[\text{CO-CB}]$ via E.COSY
 2D spin-echo difference CT-HSQC (**hsqcctetgpjclr** | HSQCCTETGPJCLR) - $3J[\text{CO-CB}]$ via spin-echo difference
 3D (H)NCAHA[CO]-E.COSY (**hncahagp3d** | HNCAHAGP3D) - $3J[\text{HA-CO}]$ via E.COSY
 3D (HN)CO(CO)NH (**hncocogp3d** | HNCOCOGP3D) - $3J[\text{CO-CO}]$ via quantitative-J



J(HN-HA)
J(HN-CB)
E.COSY

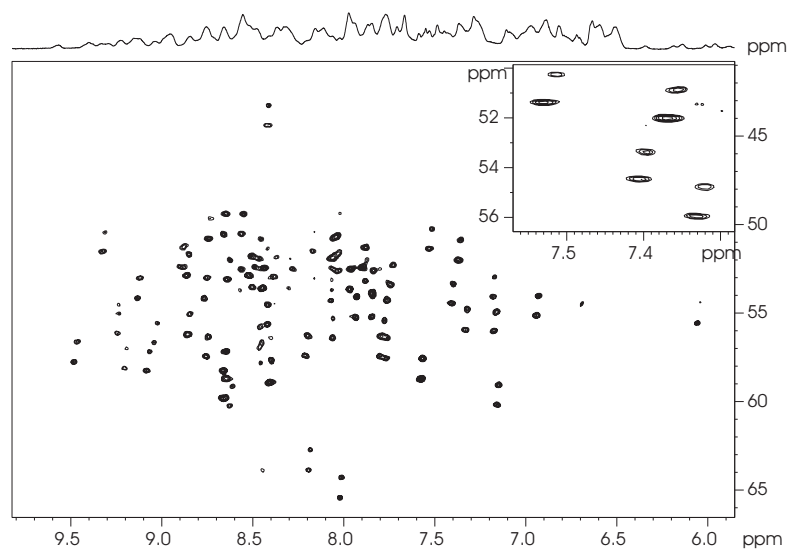
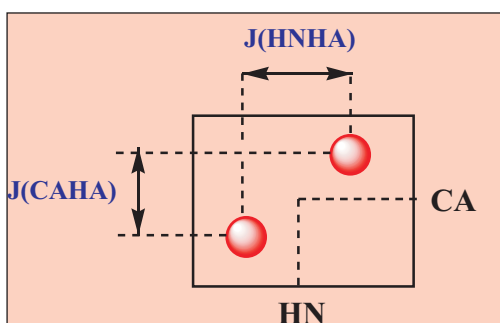
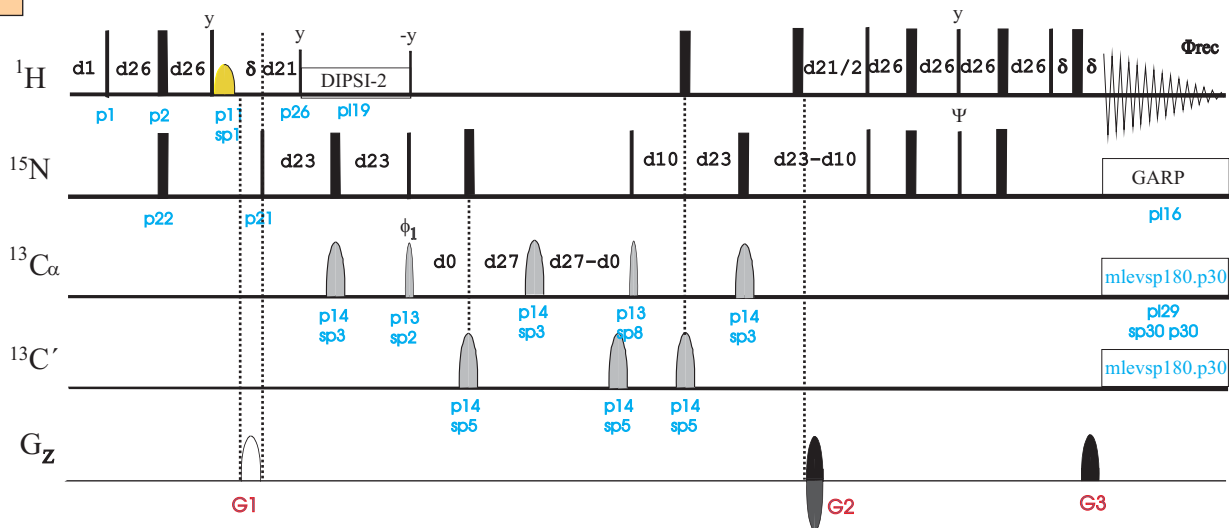
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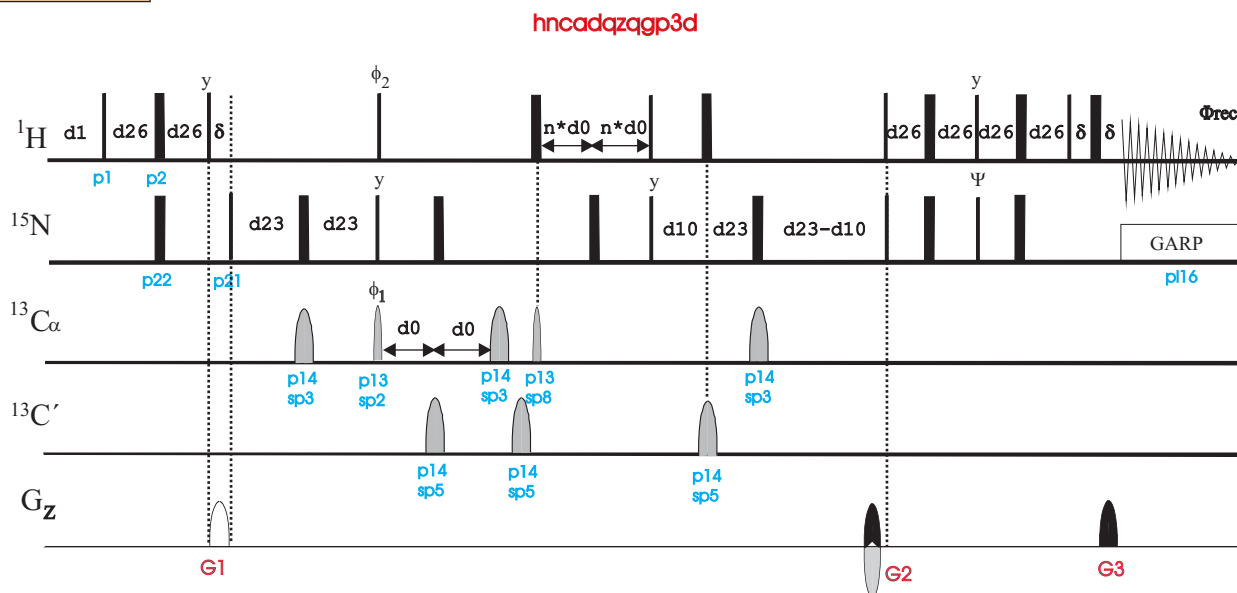


J(HN-HA)
E.COSY

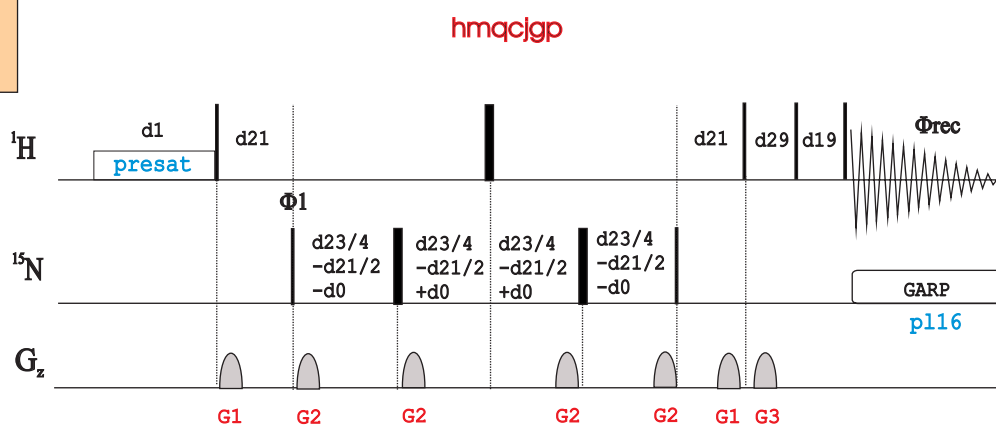
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J(HN-HA)
DQ/ZQ

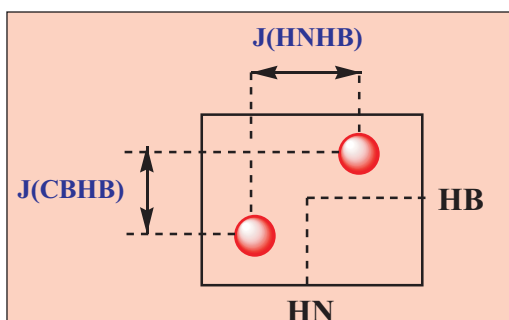
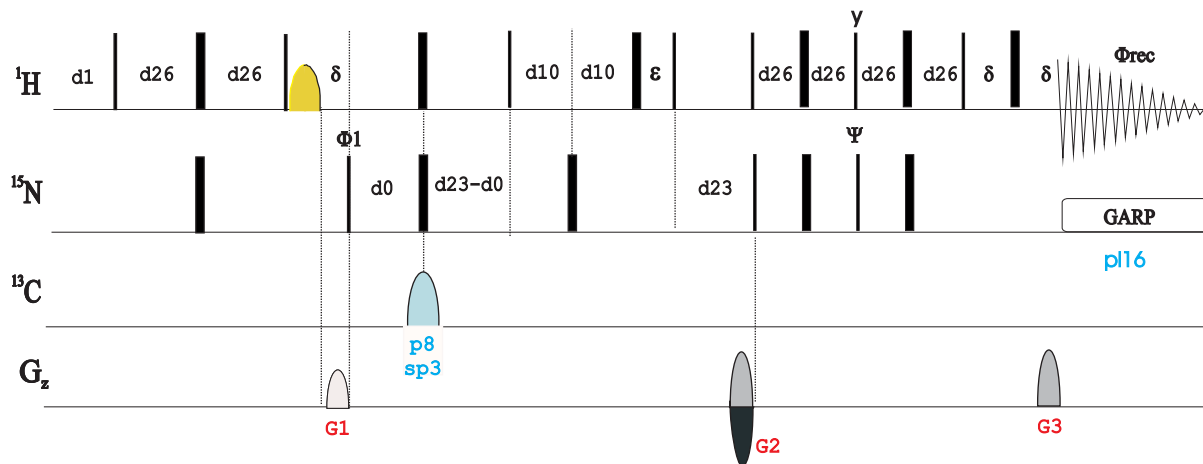


J(HN-HA)
J-modulation



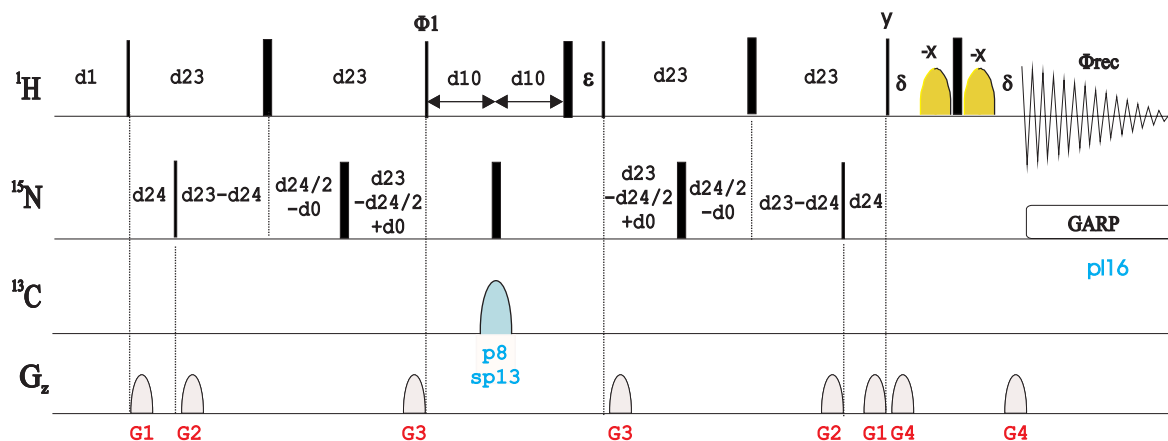
J(HN-CB)
E.COSY

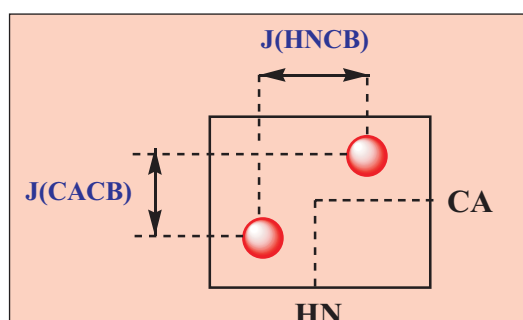
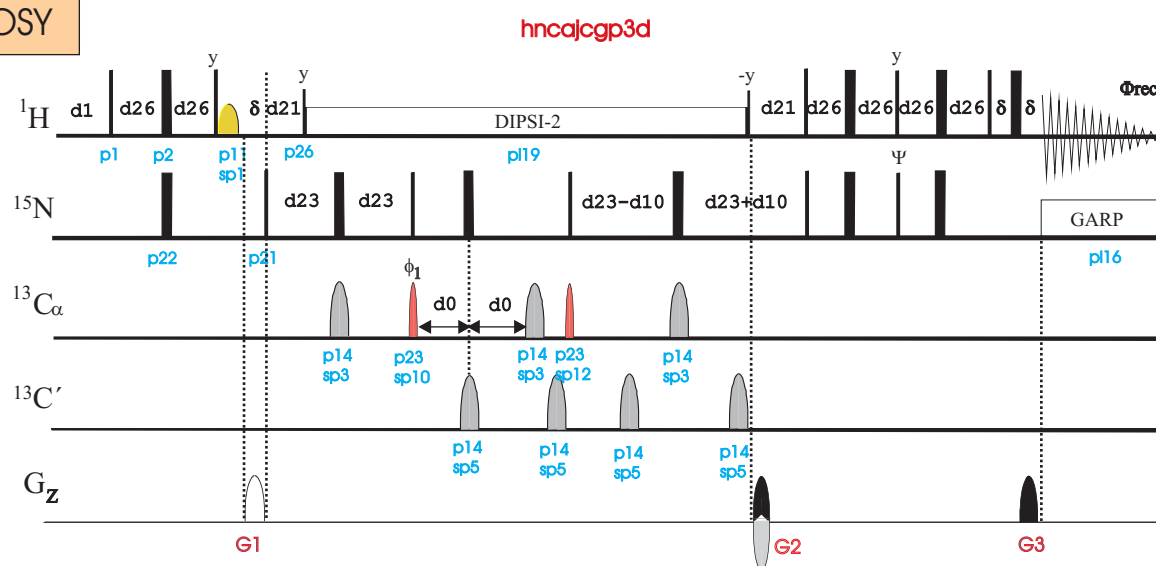
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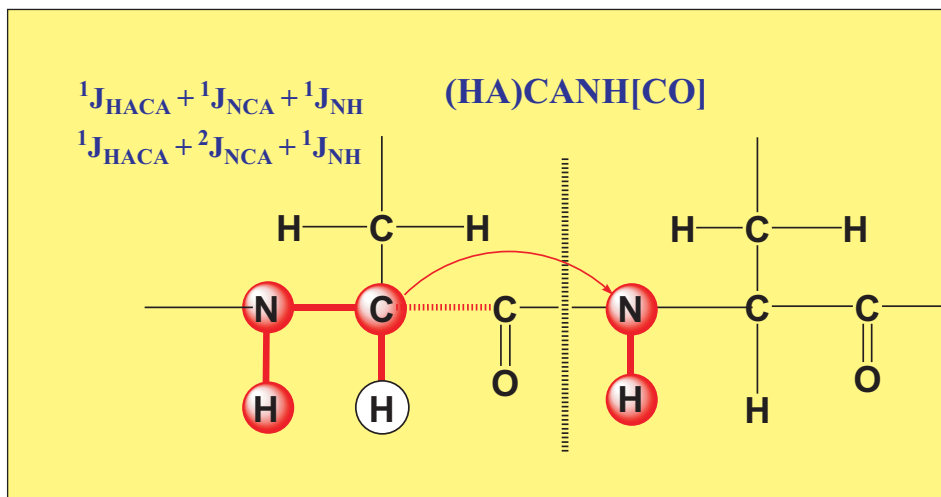


J(HN-HA)
J-quantitative

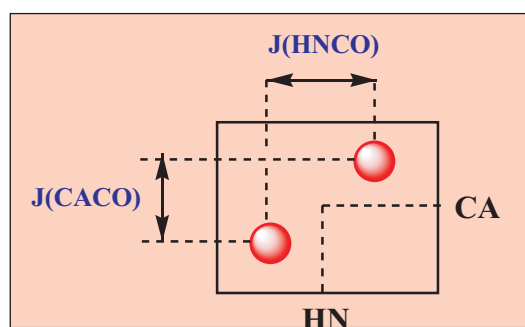
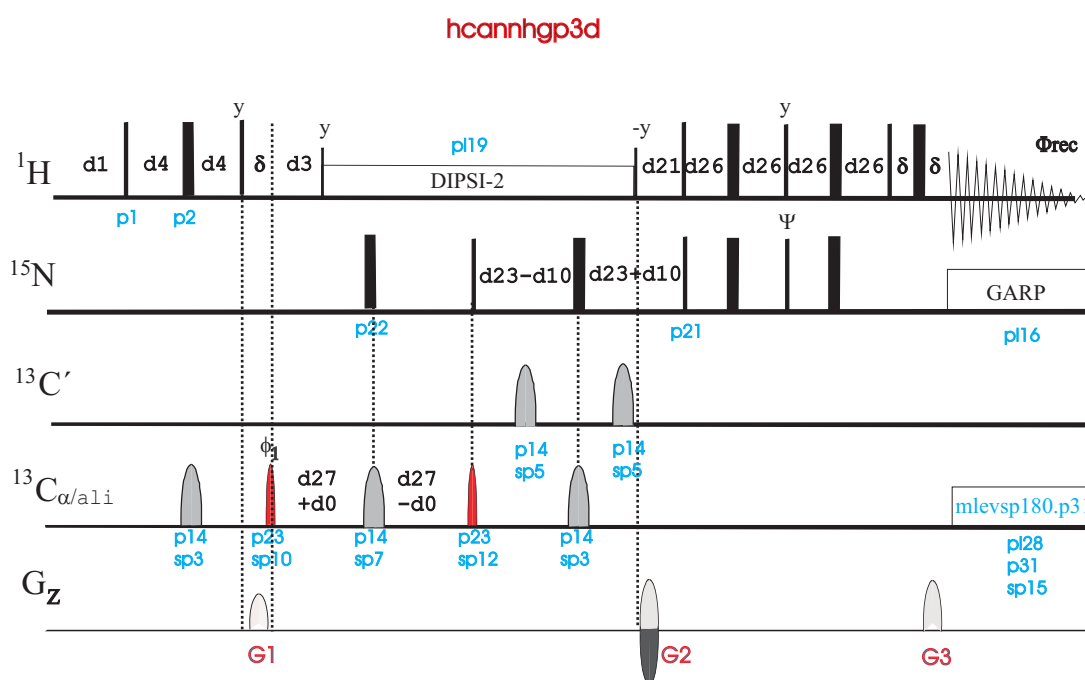
hnhagp3d

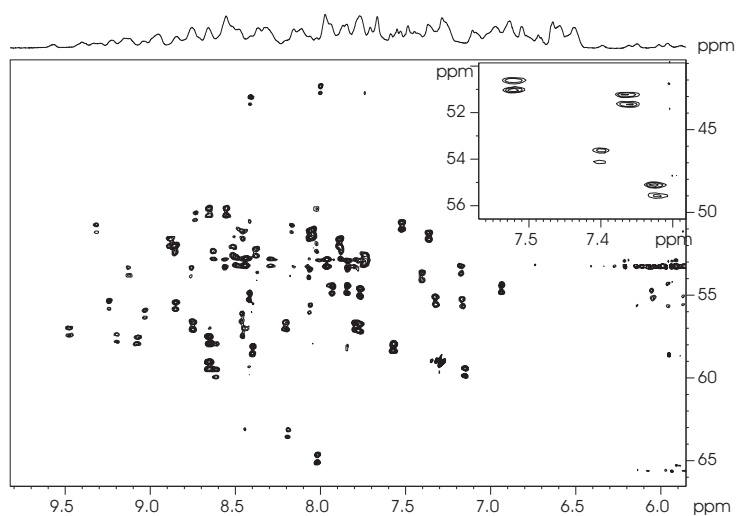
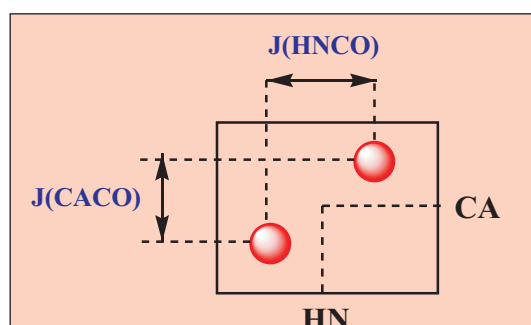


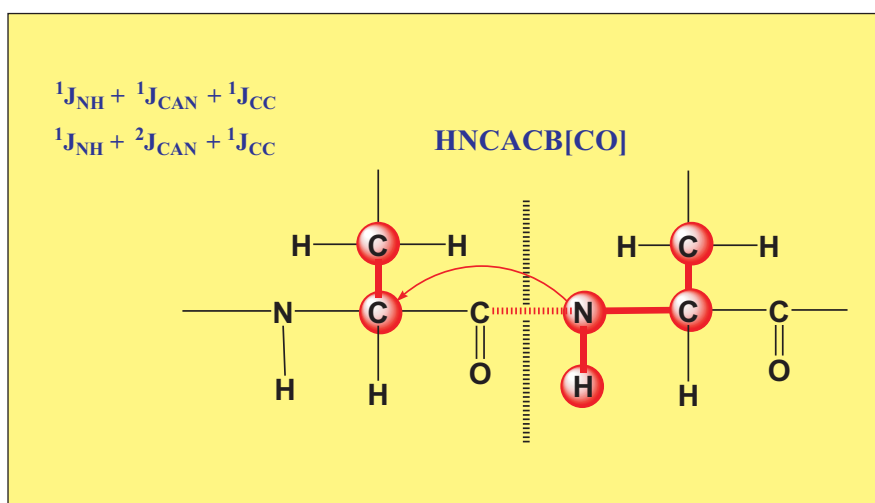




J(HN-CO)
E.COSY

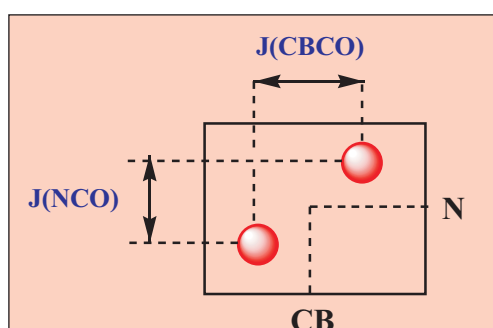
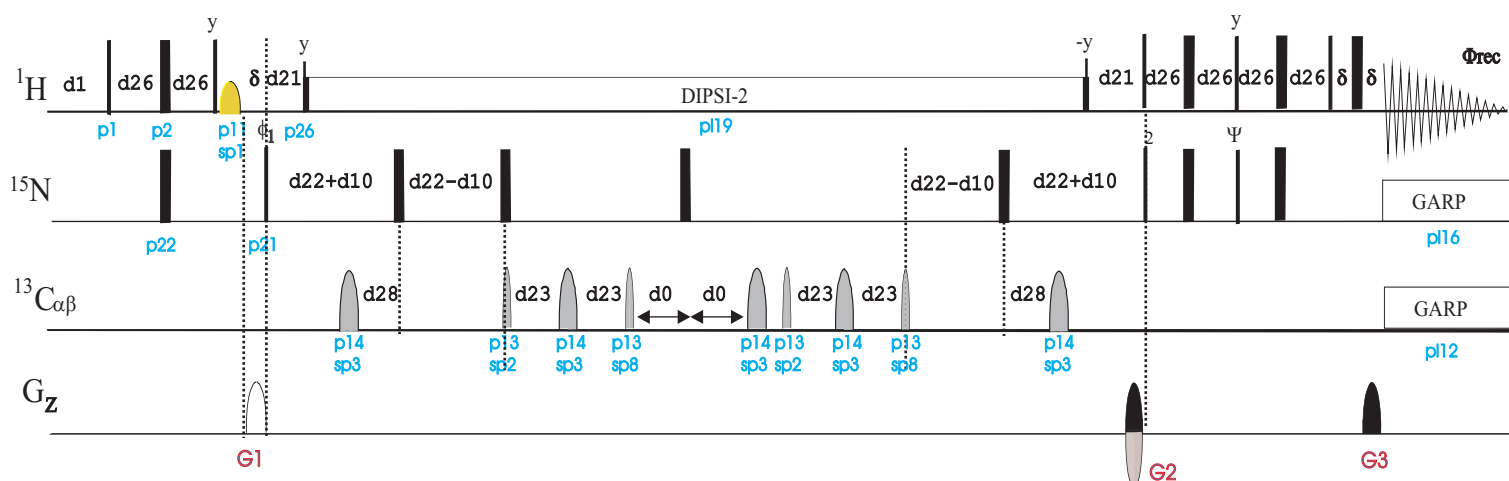






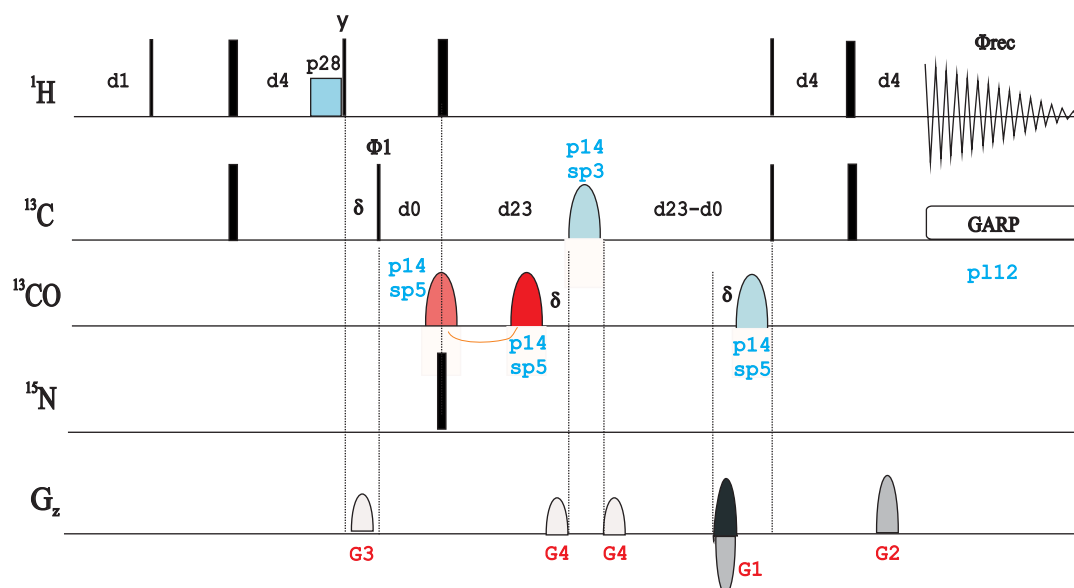
J(CO-CB)
E.COSY

hncacbgpjc3d



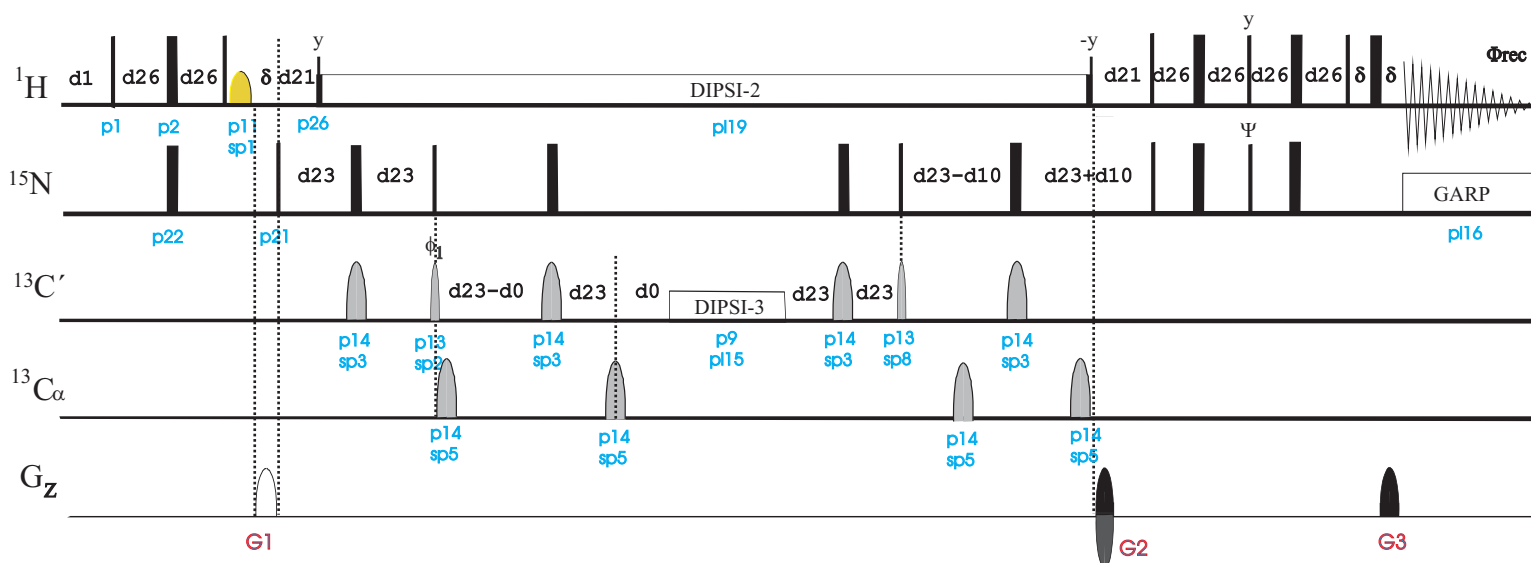
J(CO-CB)
spin-echo difference

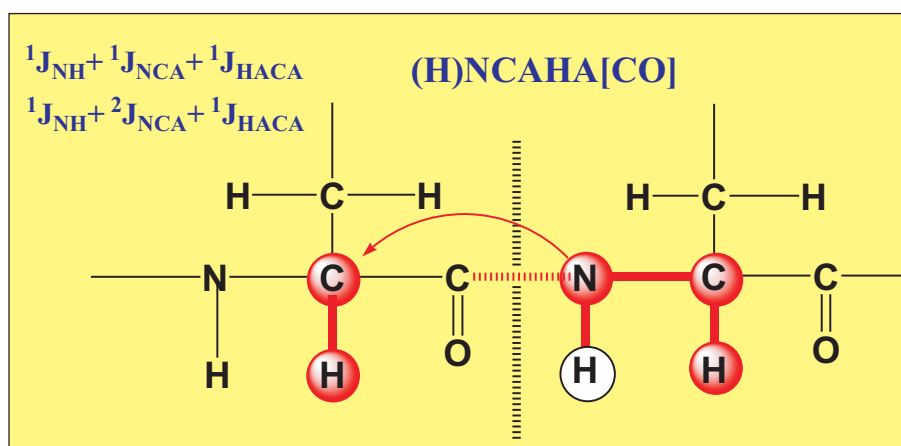
hsqcctetgpgjclr



J(CO-CO)
J-quantitative

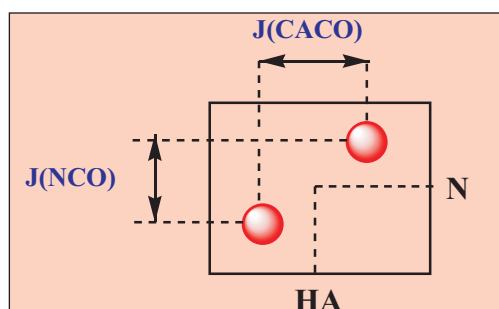
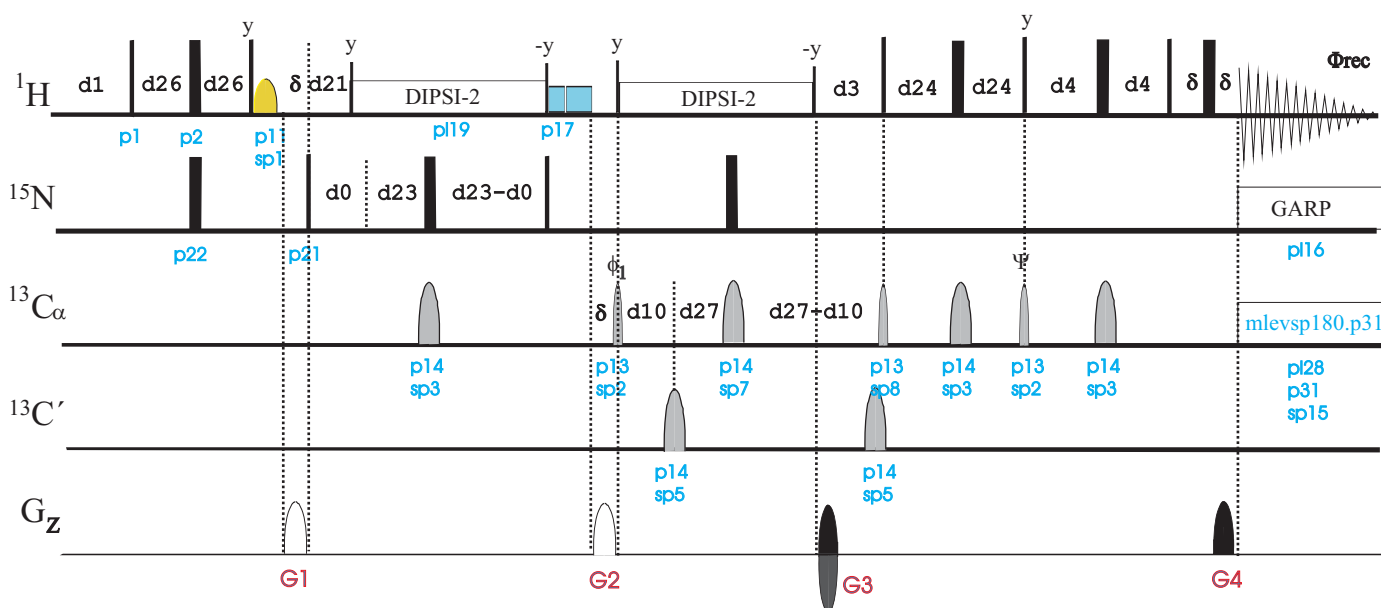
hncocogp3d





J(HA-CO)
E.COSY

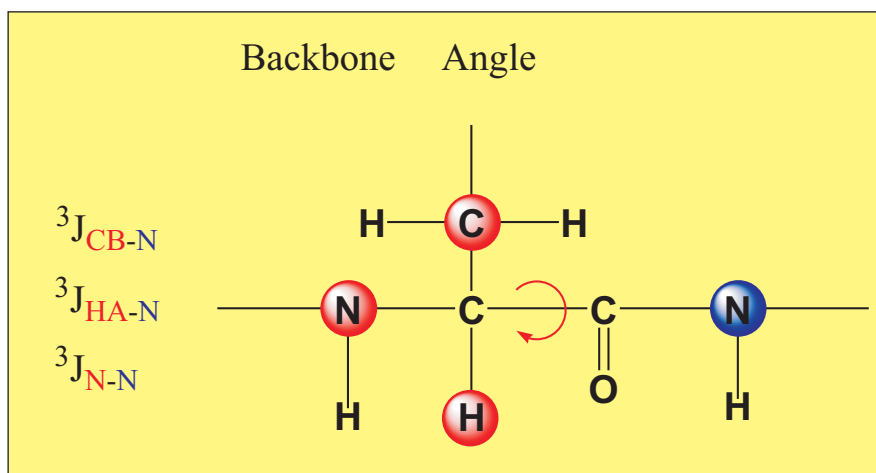
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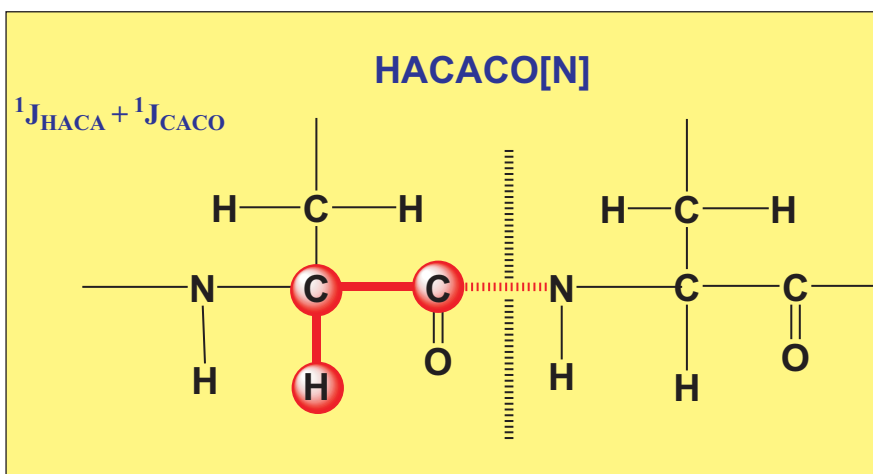
NMRGuide

PROTEIN NMR
COUPLING CONSTANTS
PSI BACKBONE ANGLE



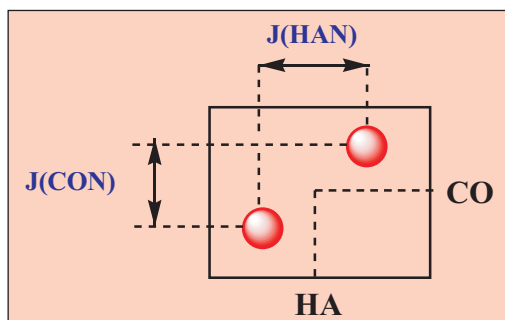
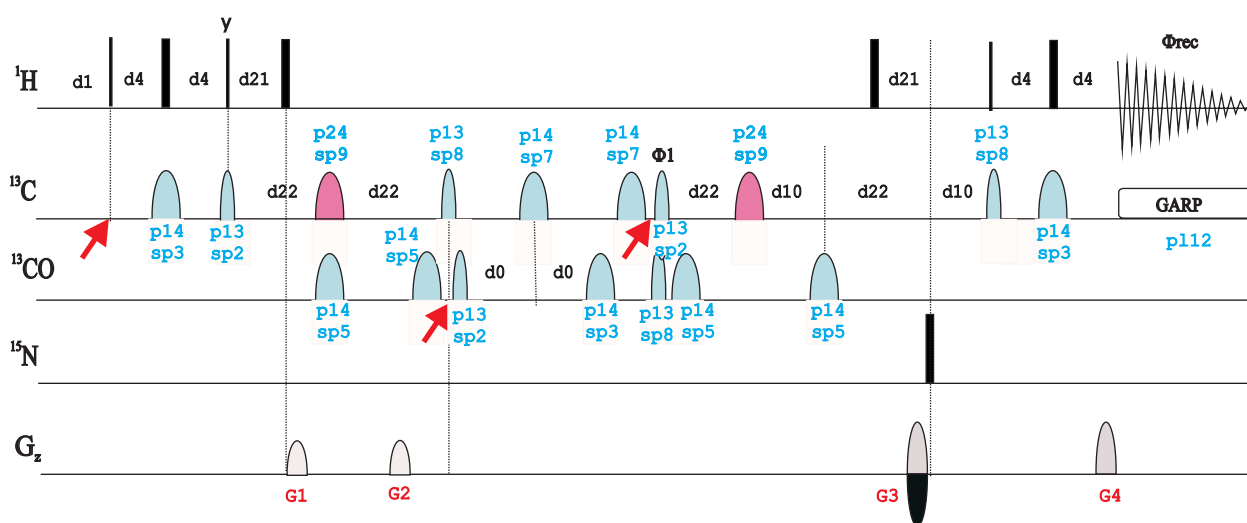
Psi Backbone Coupling Constant

3D (H)NNH-TOCSY (**hnnhdigp3d** | **HNNHDIGP3D**) - $3J[\text{N-N}]$ via quantitative-J
 3D HCACO[N]-E.COSY (**hcacogpjc3d** | **HCACOGPJC3D**) - $3J[\text{HA-N}]$ via E.COSY
 3D HNHB (**hnhbgp3d** | **HNHBGP3D**) - $3J[\text{HN-HA}]$ and $3J[\text{HN-HB}]$ via quantitative-J

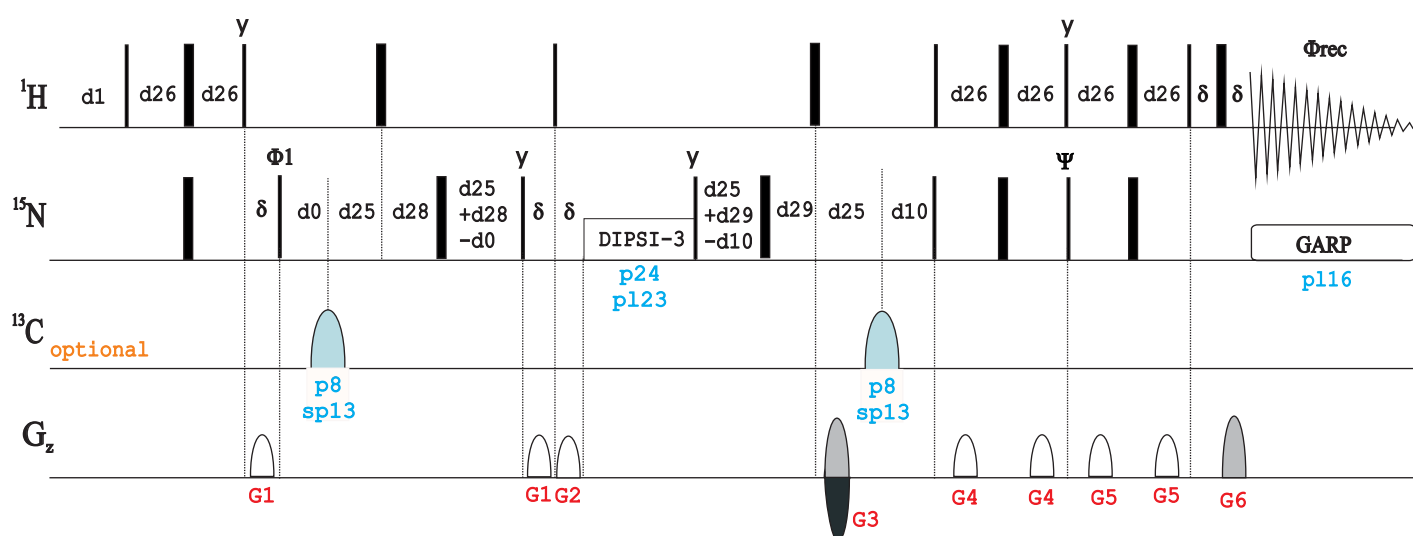


J(HA-N)
E.COSY

hcacogpjc3d



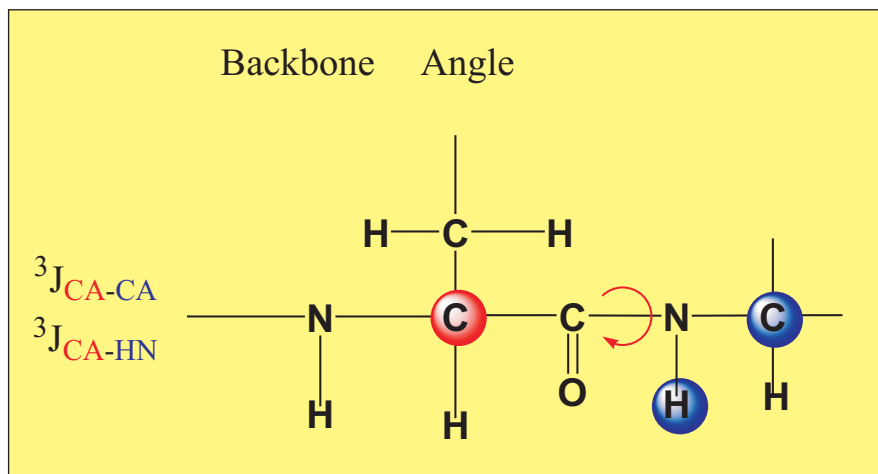
hnnhdigp3d



BRUKER PULSE PROGRAM CATALOGUE

NMRGuide

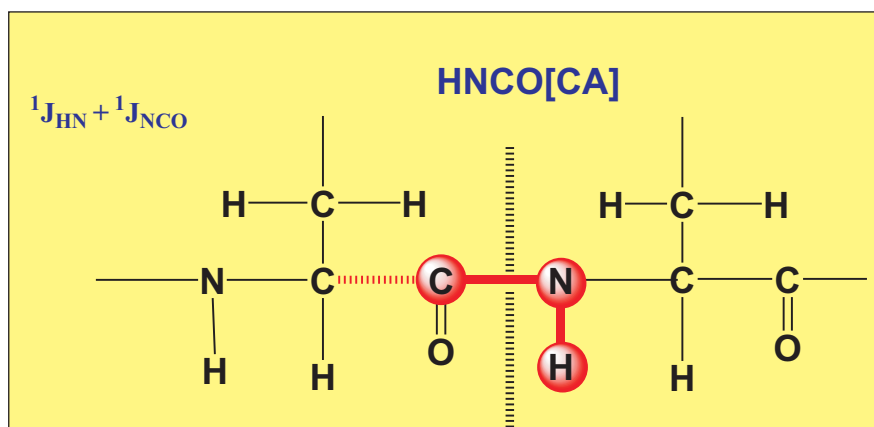
PROTEIN NMR
COUPLING CONSTANTS
OMEGA BACKBONE ANGLE



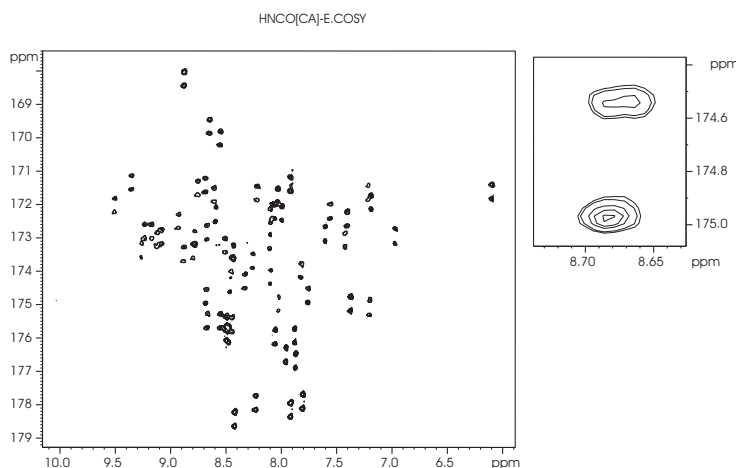
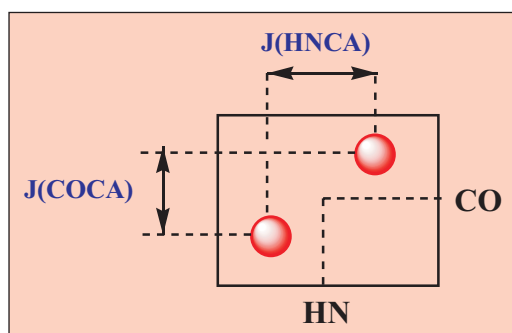
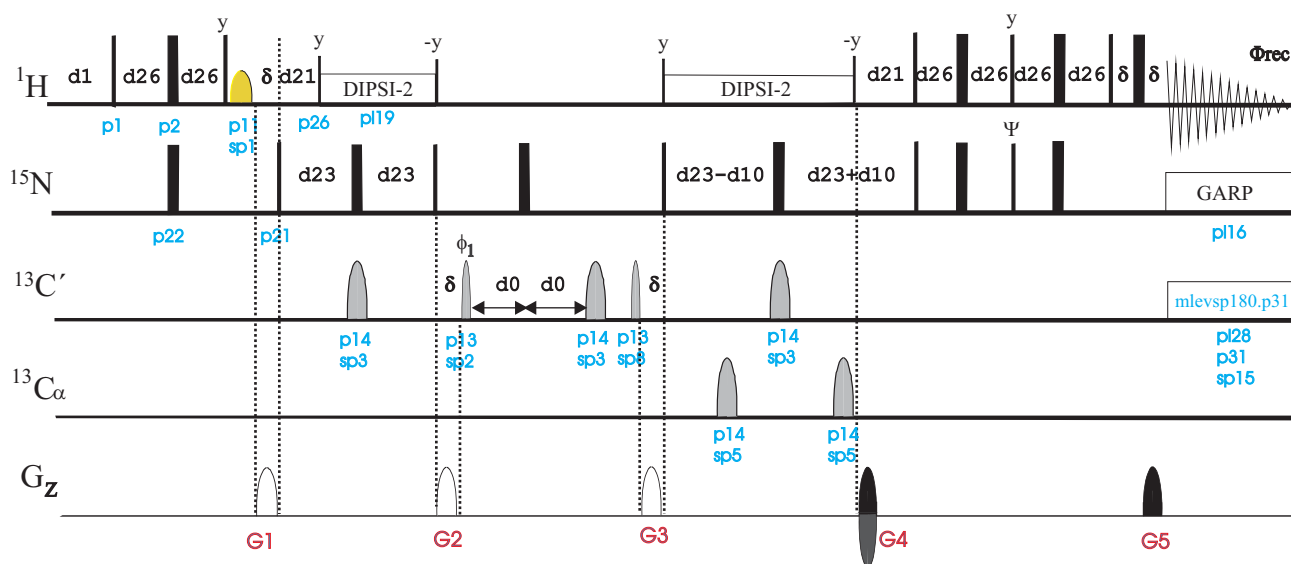
Omega Backbone Coupling Constant

3D HN(COCA)CA (**hncocacagp3d** | HNCOCACAGP3D) - $3J[\text{CA-CA}]$ via quantitative-J
3D HNCO[CA]-E.COSY (**hncocosg3d** | HNCOCOSGP3D) - $3J[\text{H(N)-CA}]$ via E.COSY

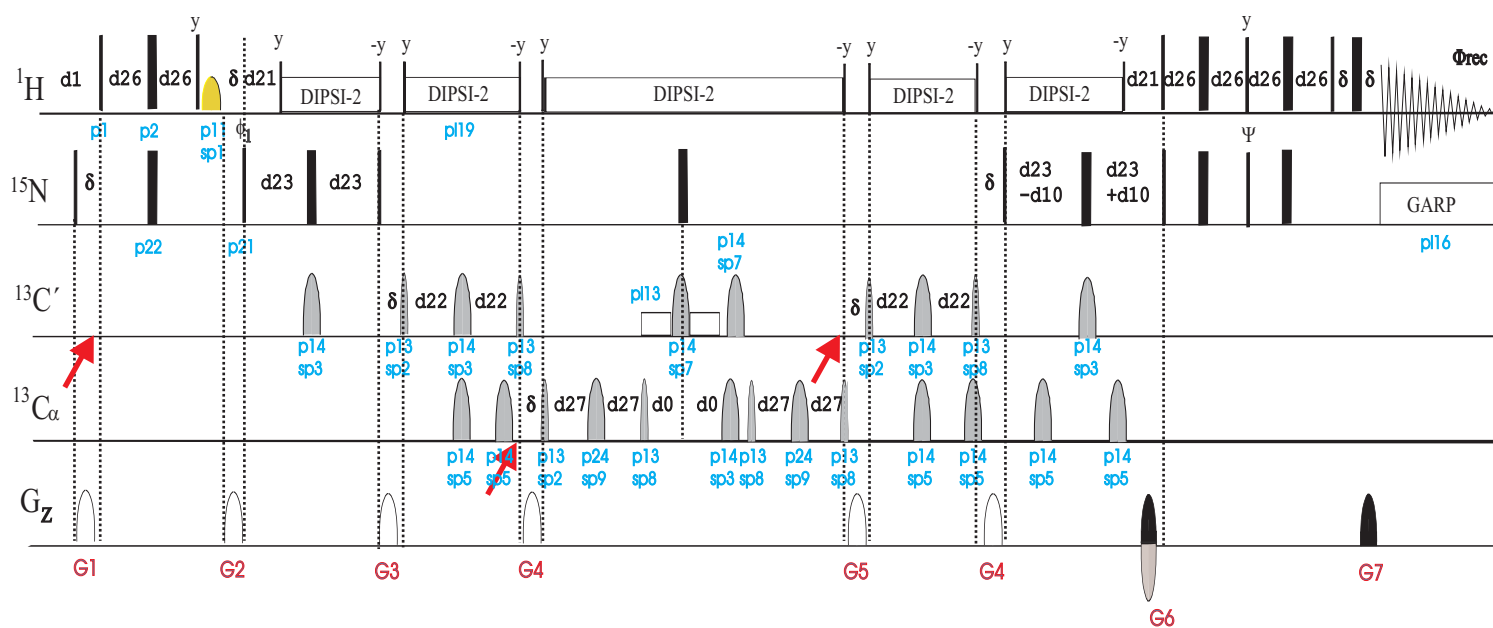
$J(\text{HN-CA})$
E.COSY



hncoecosgp3d



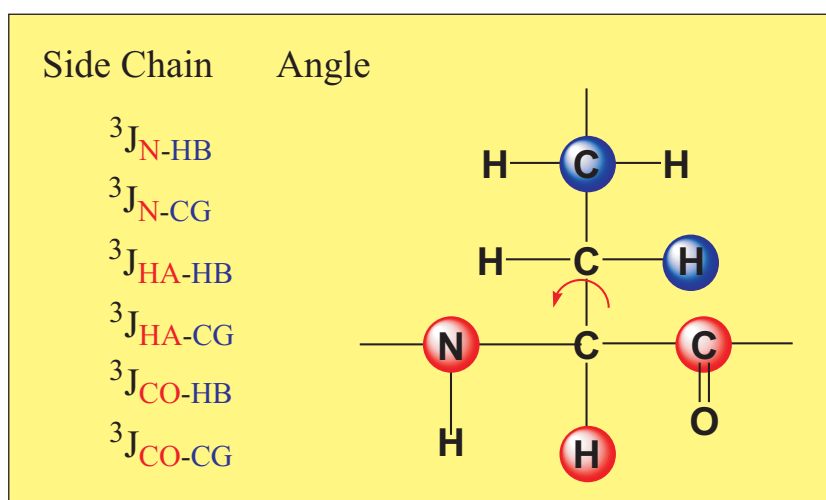
hncocacagp3d



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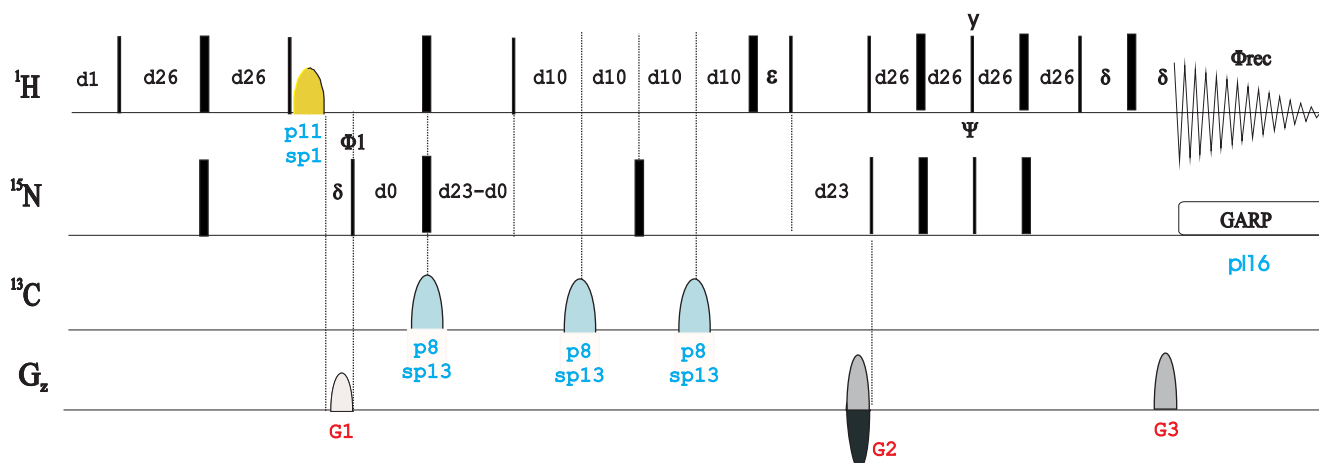
PROTEIN NMR
COUPLING CONSTANTS
CHI1 SIDECHAIN ANGLE



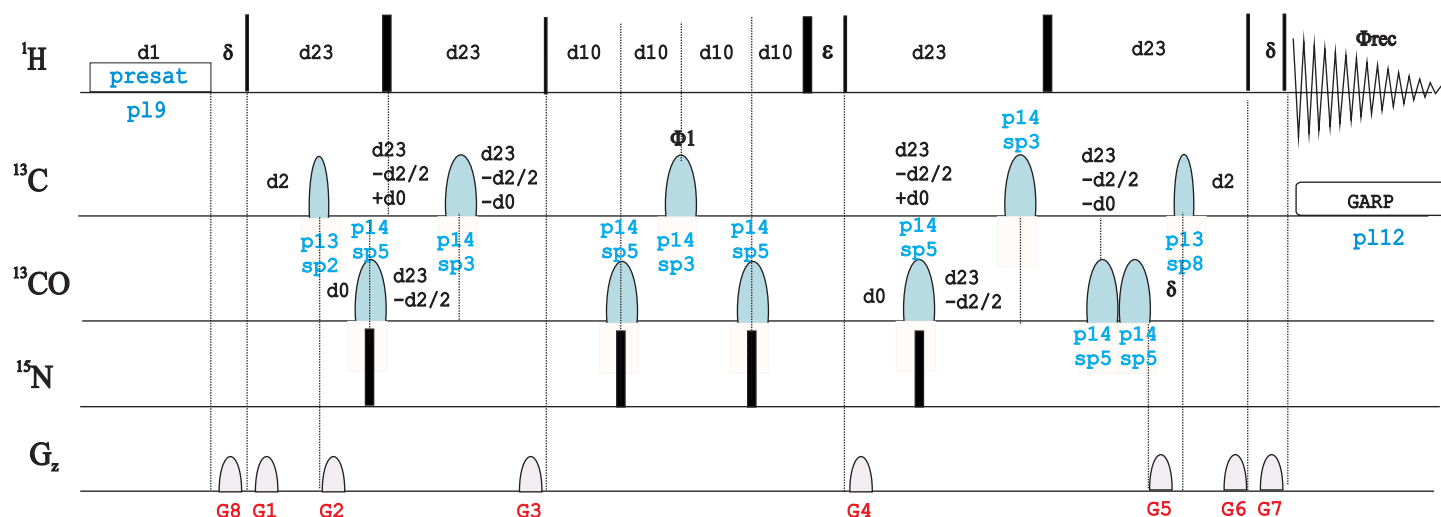
3D HNHB (**hnhb3d** | HNHBP3D) - $3J[\text{HN-HA}]$ and $3J[\text{HN-HB}]$ via quantitative-J
 3D HACAHB-COSY (**hacahbcosy3d** | HACAHBCOSYGP3D) - $3J[\text{HA-HB}]$ via quantitative-J
 3D HN(CO)C (**hncoc3d** | HNCOCGP3D) - $3J[\text{CG-CO}]$ via quantitative-J
 3D HC(C)H[HA]-E.COSY (**hcchecosy3d** | HCCHECOSYGP3D) - $3J[\text{HA-HB}]$ via E.COSY
 3D HC(C)H[CO]-E.COSY (**hcchcosy3d** | HCCHCOSYGP3D) - $3J[\text{CO-HB}]$ via E.COSY
 3D (H)C(C)CH[CO]-E.COSY (**hccccosy3d** | HCCCCOSYGP3D) - $3J[\text{CG-CO}]$ via E.COSY
 3D HNCG (**hncgg3d.1** | HNCGGP3D.1) - $3J[\text{N-CG}]$ via quantitative-J
 3D HNCG (**hncgg3d.2** | HNCGGP3D.2) - $3J[\text{N-CG}]$ via quantitative-J
 2D spin-echo difference CT-HSQC (**hsqcetfp3gpjcsi** | HSCQETFPFGPJCSI) - $3J[\text{N-CG}]$ via spin-echo difference

$J(\text{N-HB}), J(\text{N-HA})$
 J-quantitative

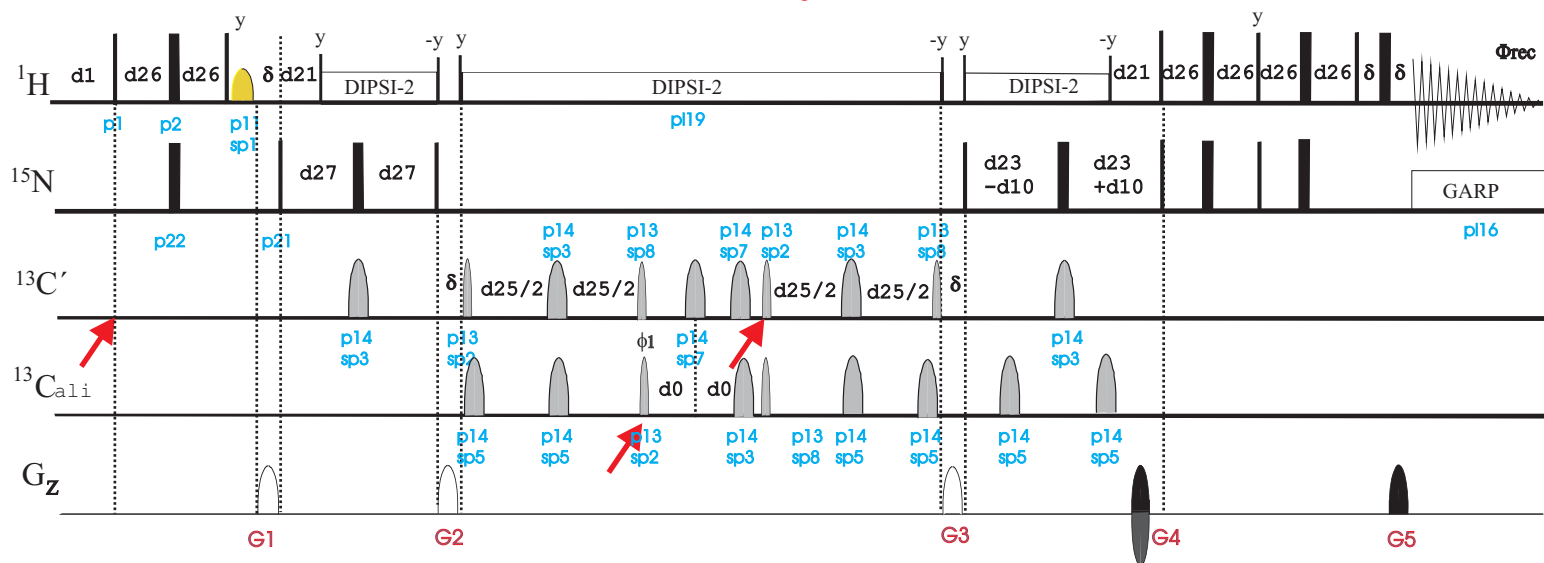
hnhb3d

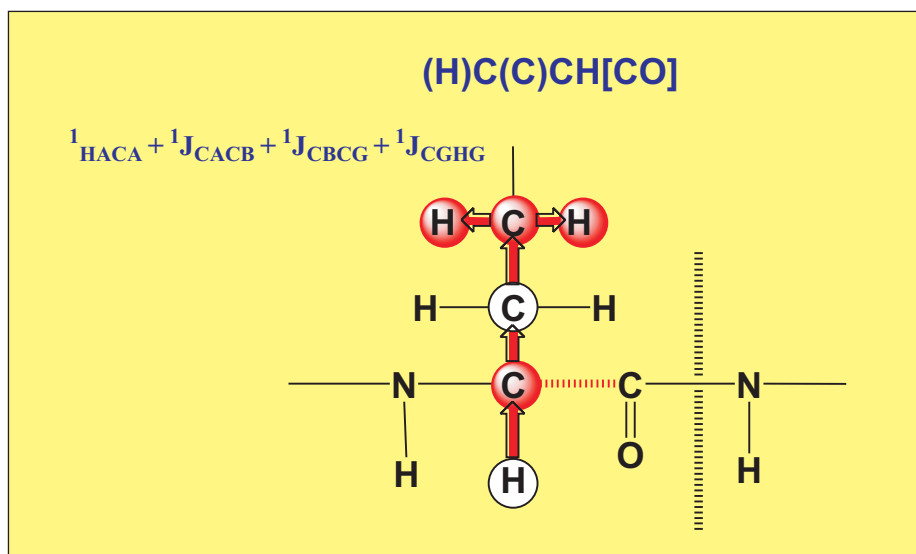


hacahbcosygp3d



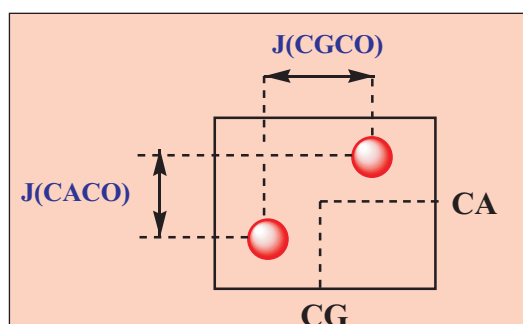
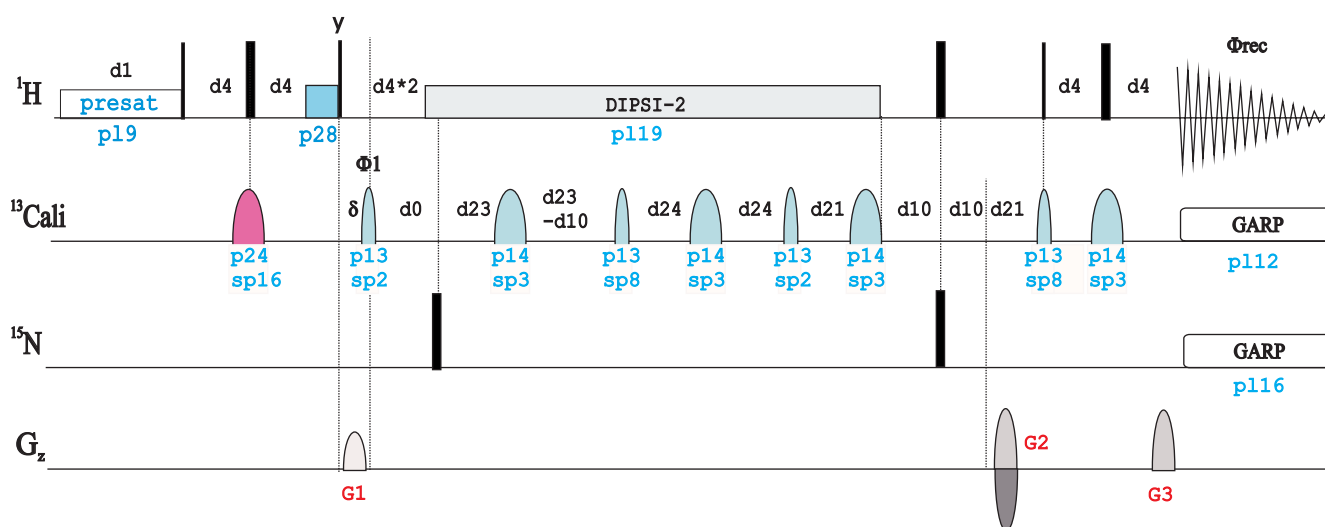
hncocgp3d



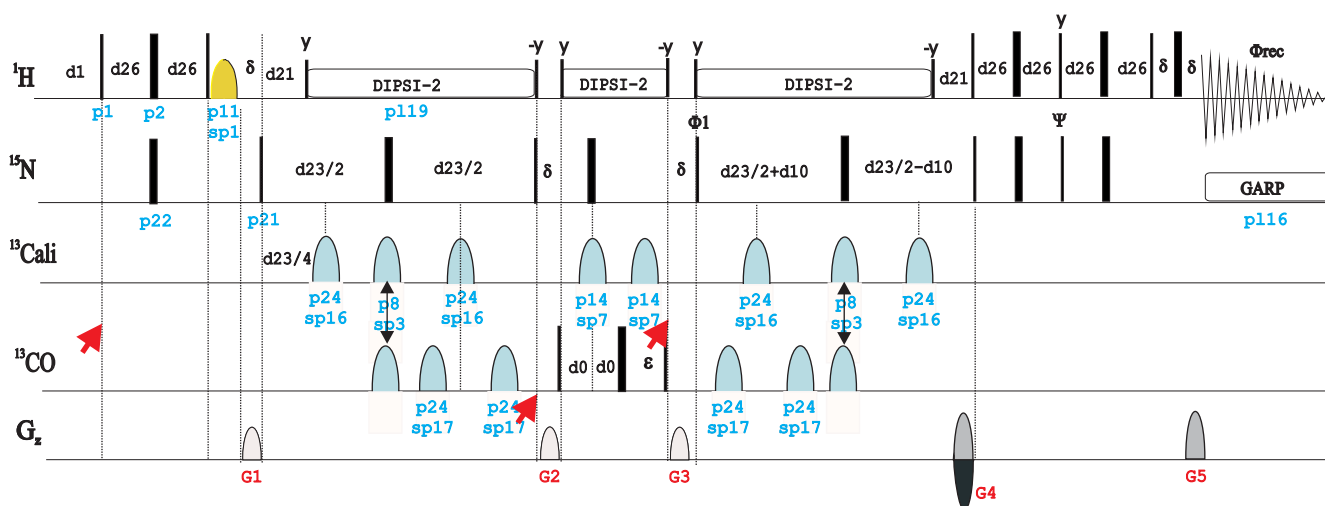


J(CG-CO)
E.COSY

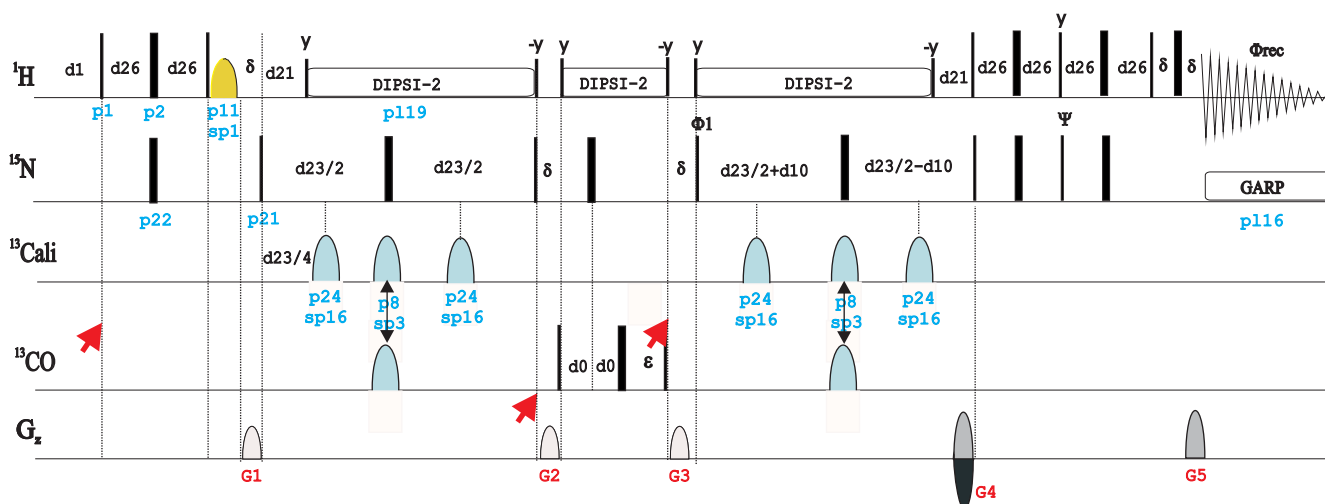
hccccosygp3d

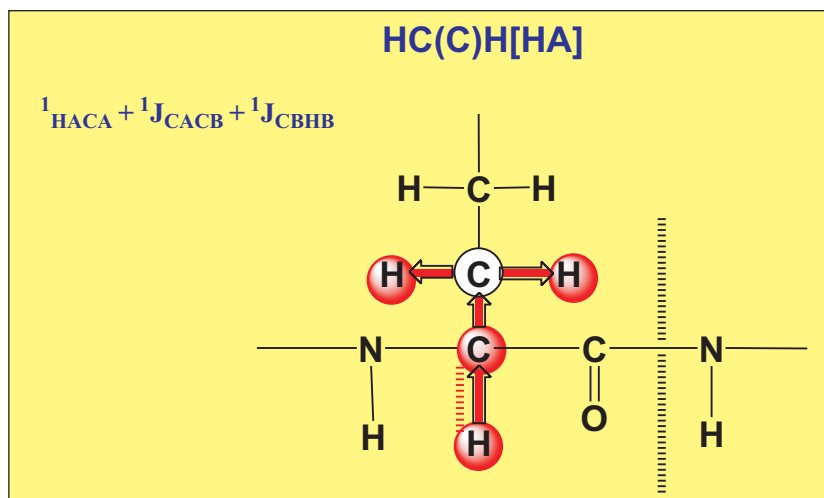


hncggp3d.1

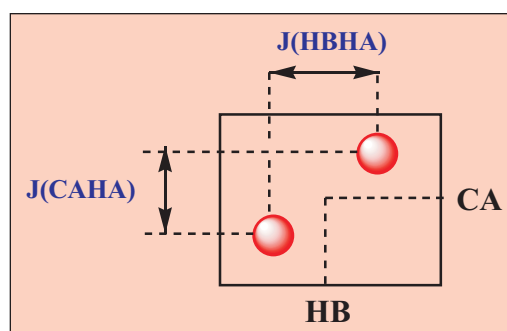
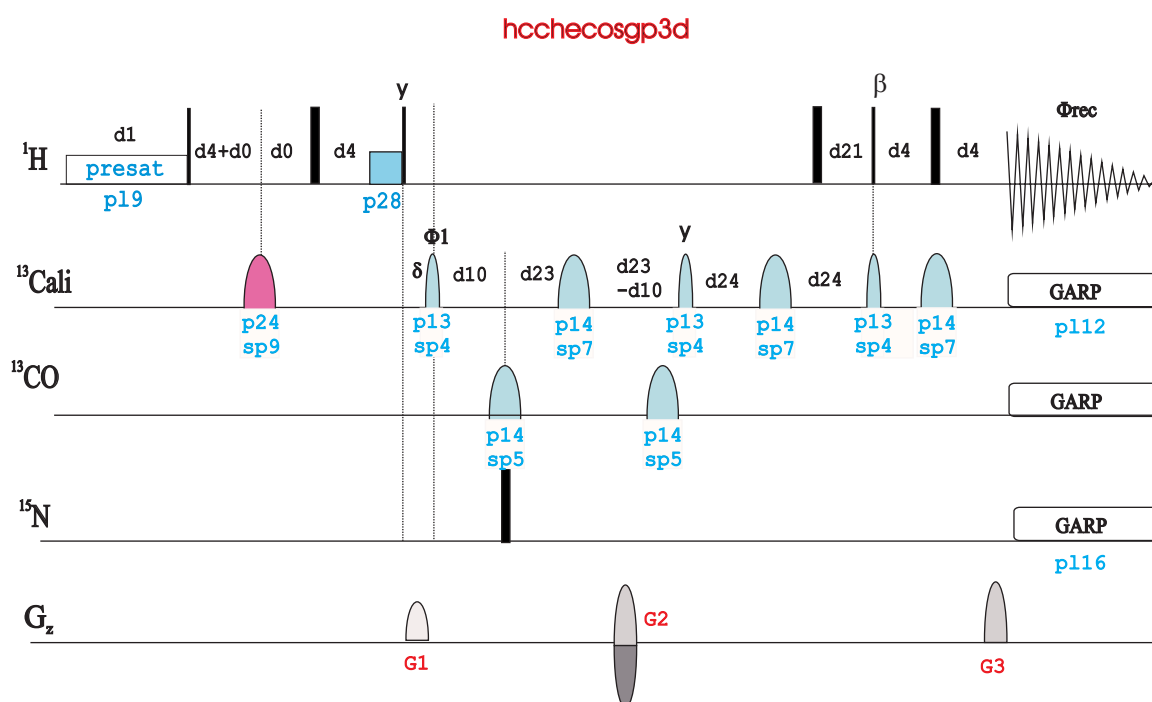


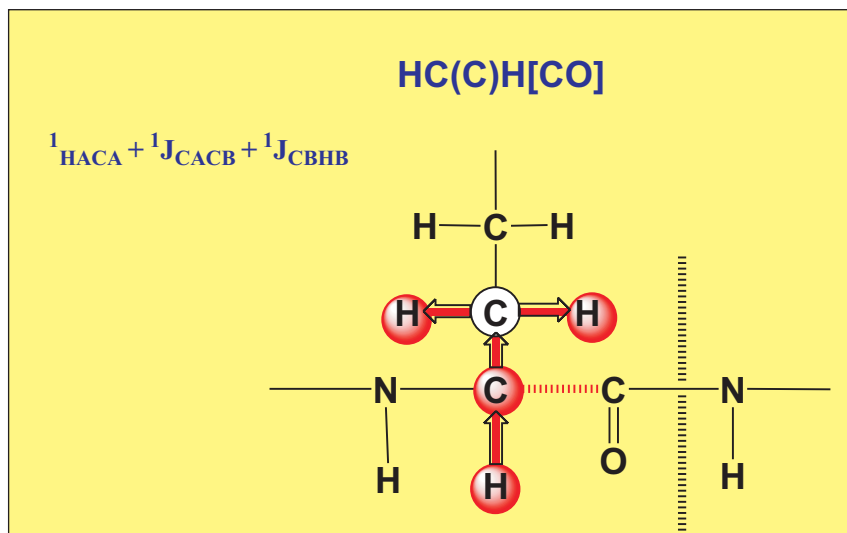
hncggp3d.2





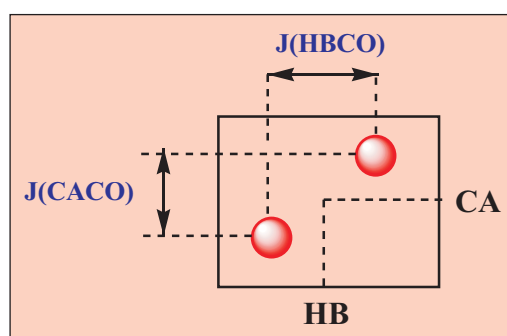
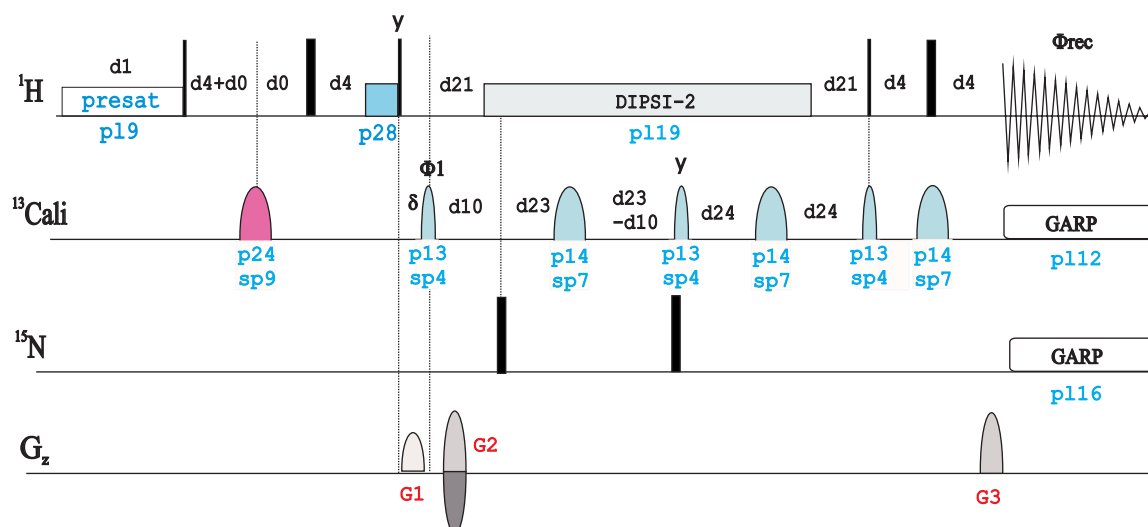
J(HB-HA)
E.COSY





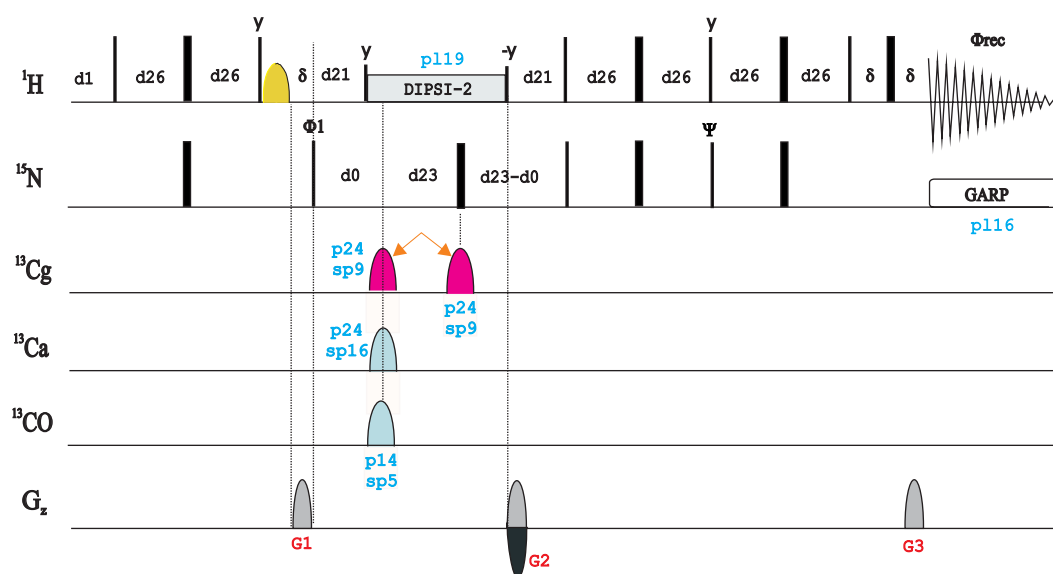
J(HB-CO)
E.COSY

hcchcosygp3d



**J(N-CG)
spin-echo difference**

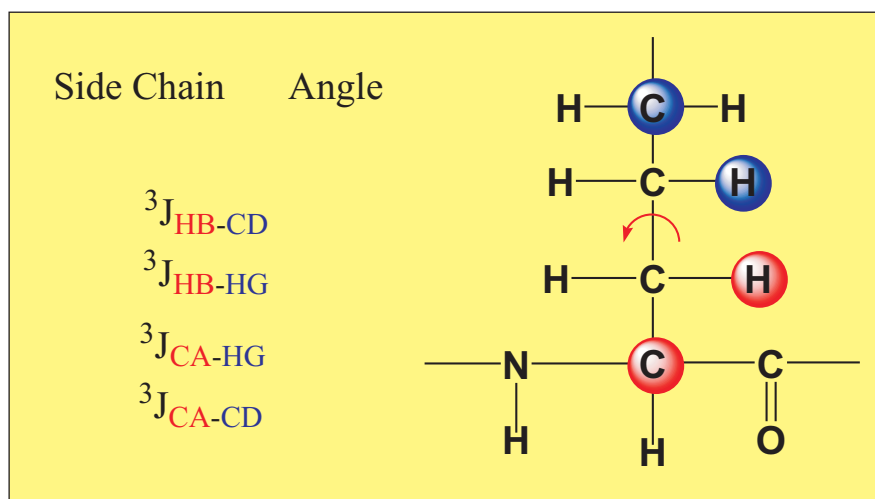
hsqcetf3gplcsi



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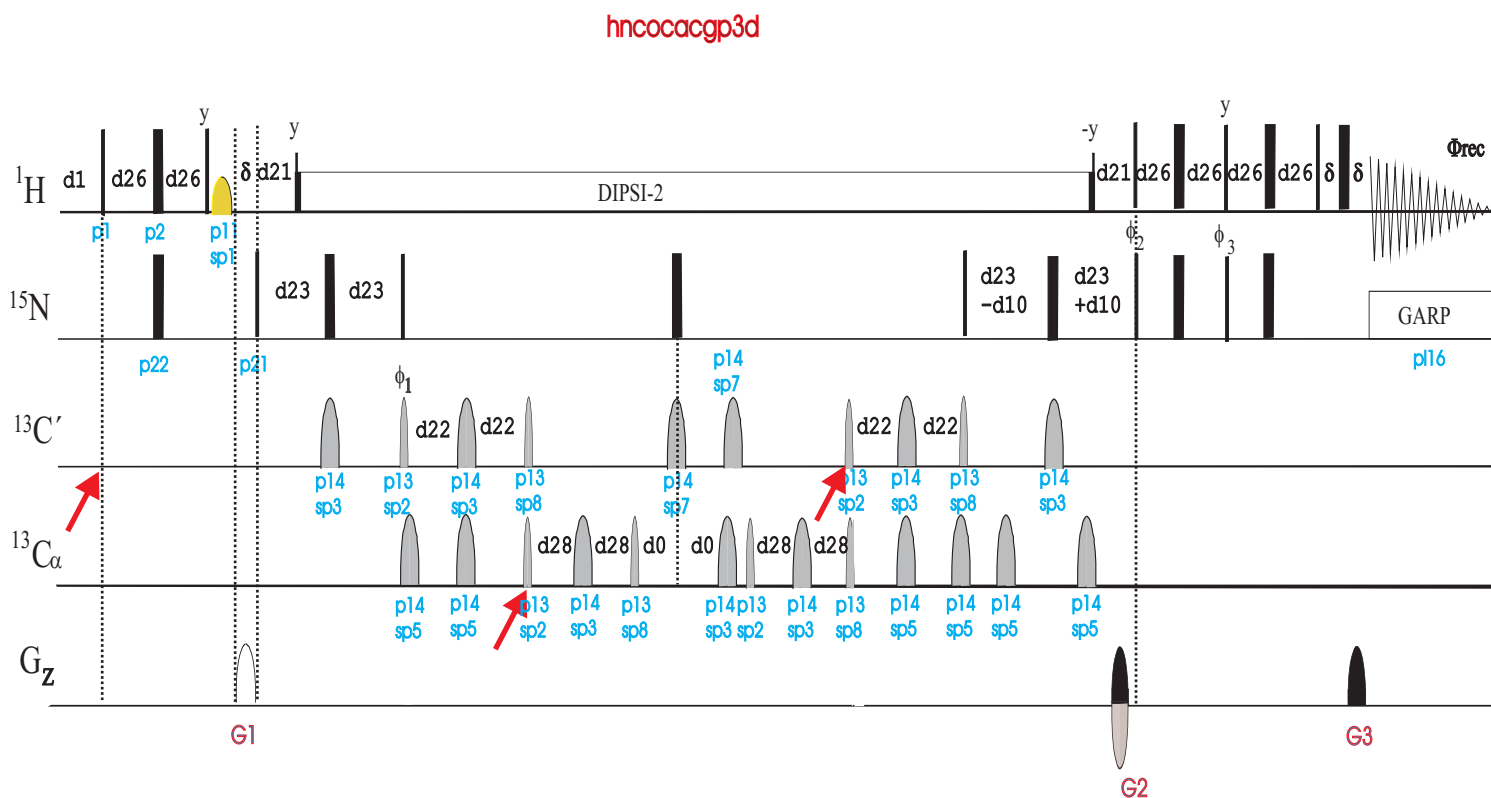
PROTEIN NMR
COUPLING CONSTANTS
CHI2 SIDECHAIN ANGLE



Chi2 Sidechain Coupling Constant

3D HN(CO)CACali (**hncocacgp3d** | HNCOCACGP3D) - $3J[\text{CA-CD}]$ via quantitative-J

$J(\text{CA-CD})$
J-quantitative

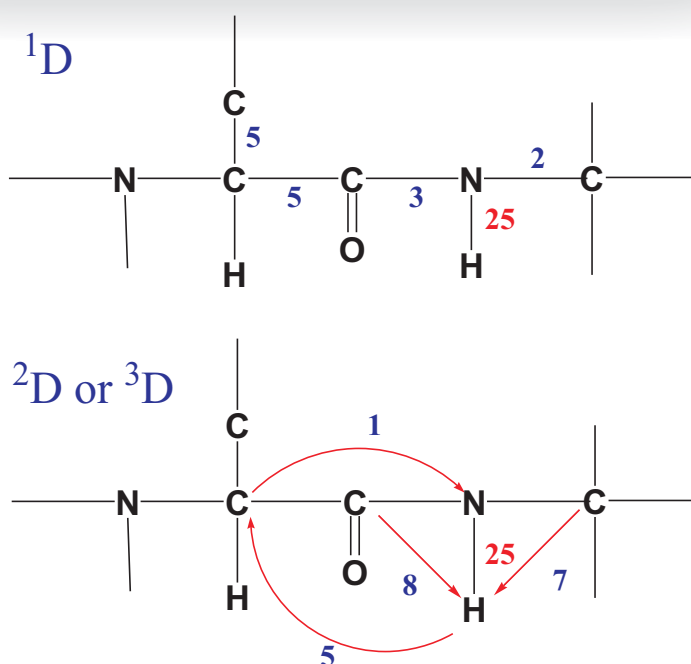


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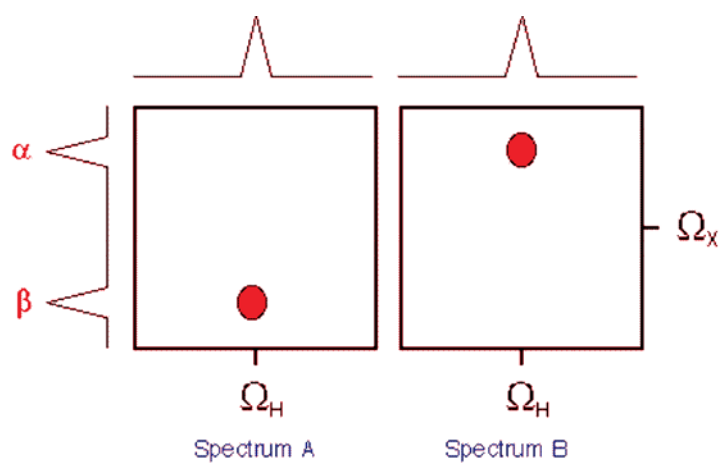
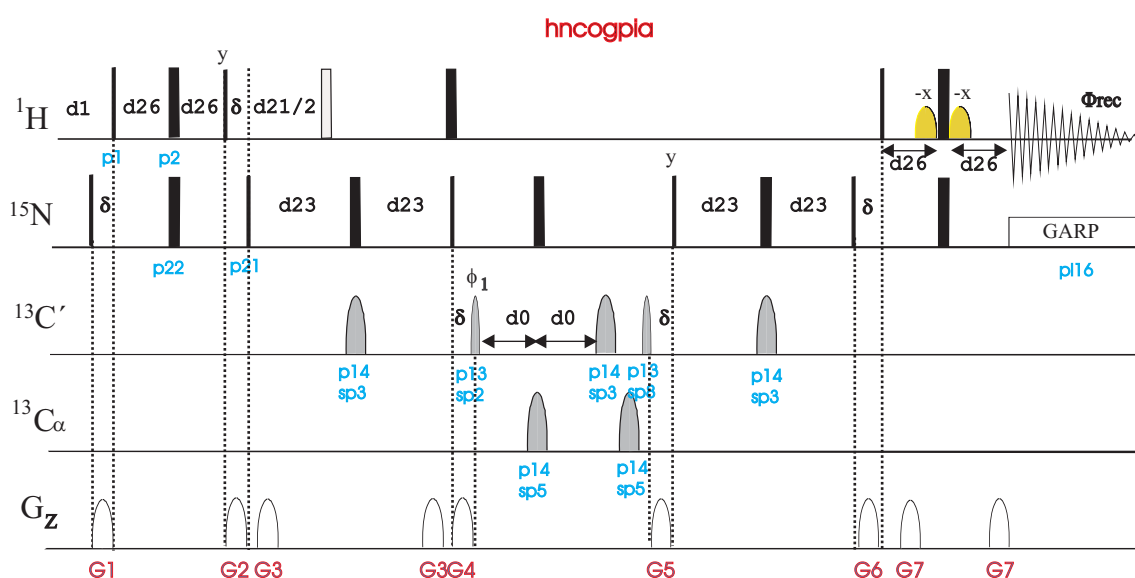
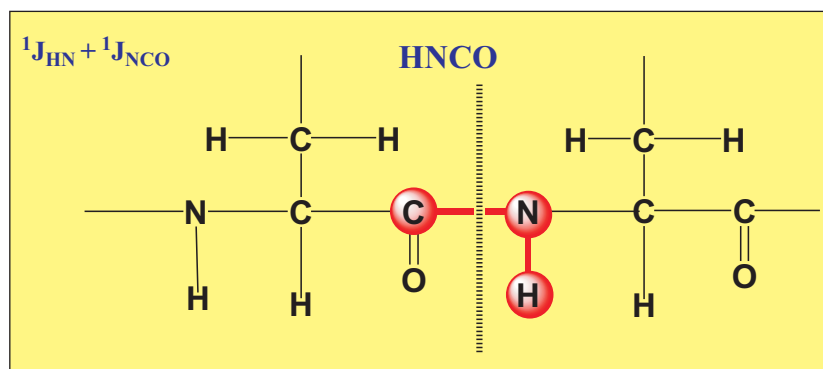
NMRGuide

PROTEIN NMR
COUPLING CONSTANTS
3D HNCO-J

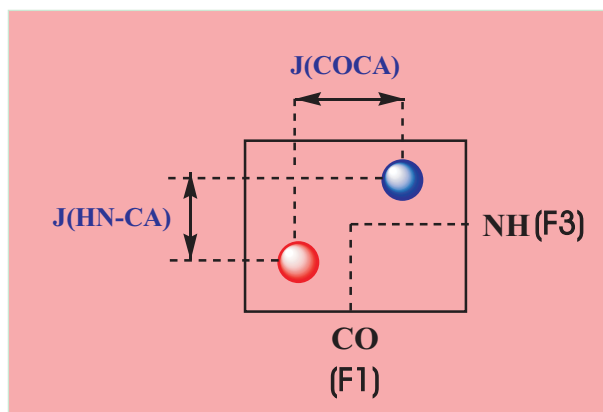
- 3D IPAP-HNCO to measure $^1J(\text{NH})$ (**hncogpia**)
- 3D IPAP-J-HNCO to measure $^1J(\text{CA-CO})$ and $^3J(\text{HN-CA})$:
Using PEP (**hncogprc3d1** | **HNCOGRPC3D1**)
Using WATERGATE (**hncogprcwg3d1** | **HNCOGRPCWG3D1**)
Using TROSY (**trhncogprc3d1** | **TRHNCOGRPC3D1**)
- 3D IPAP-J-HNCO to measure $^{12}J(\text{N-CA})$ and $^3J(\text{HN-CA})$:
Using PEP (**hncogprc3d2** | **HNCOGRPC3D2**)
Using WATERGATE (**hncogprcwg3d2** | **HNCOGRPCWG3D2**)
Using TROSY (**trhncogprc3d2** | **TRHNCOGRPC3D2**)
- 3D IPAP-J-HNCO to measure $^1J(\text{N-CO})$:
Using PEP (**hncogprc3d3** | **HNCOGRPC3D3**)
Using WATERGATE (**hncogprcwg3d3** | **HNCOGRPCWG3D3**)
Using TROSY (**trhncogprc3d3** | **TRHNCOGRPC3D3**)
- 3D J-HNCO (CA) to measure $^1J(\text{CA-CB})$:
Using PEP (**hncogprc3d4** | **HNCOGRPC3D4**)
Using WATERGATE (**hncogprcwg3d4** | **HNCOGRPCWG3D4**)
Using TROSY (**trhncogprc3d4** | **TRHNCOGRPC3D4**)
- 3D IPAP-J-HNCO (CA) to measure $^1J(\text{CA-HA})$ and $^1J(\text{CA-CB})$:
Using PEP (**hncogprc3d5** | **HNCOGRPC3D5**)
Using WATERGATE (**hncogprcwg3d5** | **HNCOGRPCWG3D5**)
Using TROSY (**trhncogprc3d5** | **TRHNCOGRPC3D5**)
- 3D IPAP-J-HNCO to measure $^1J(\text{H-N})$ and $^3J(\text{HN-CA})$:
Using PEP (**hncogprc3d6** | **HNCOGRPC3D6**)
Using WATERGATE (**hncogprcwg3d6** | **HNCOGRPCWG3D6**)
Using TROSY (**trhncogprc3d6** | **TRHNCOGRPC3D6**)



3D IPAP-HNCO: J(NH)

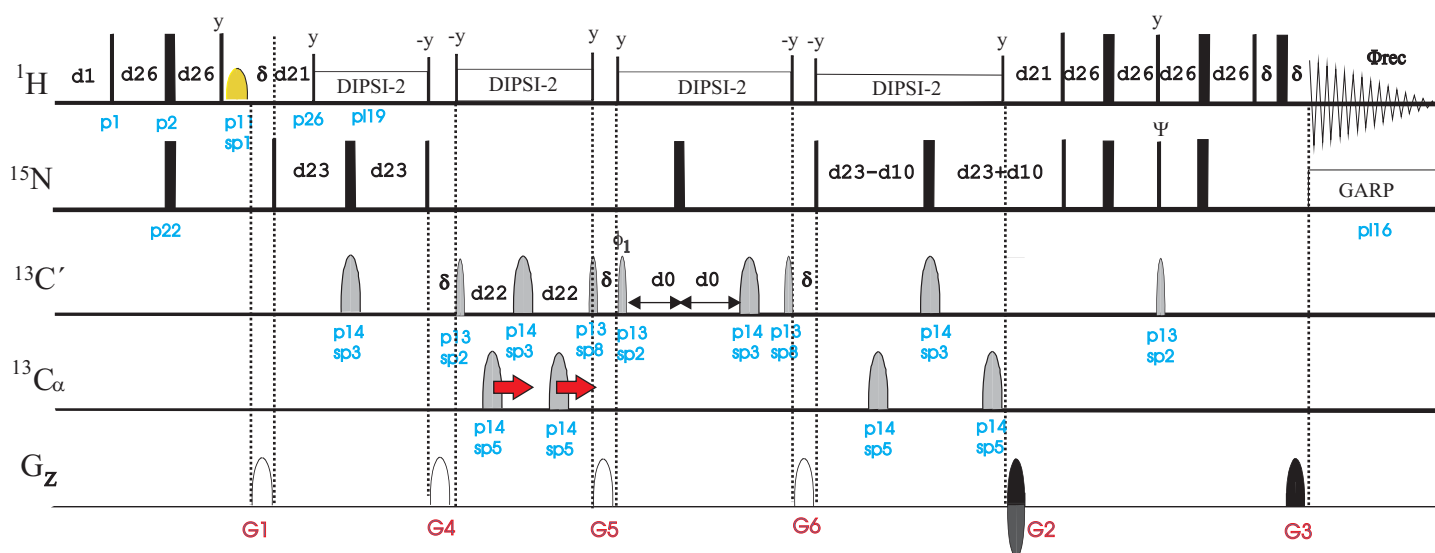


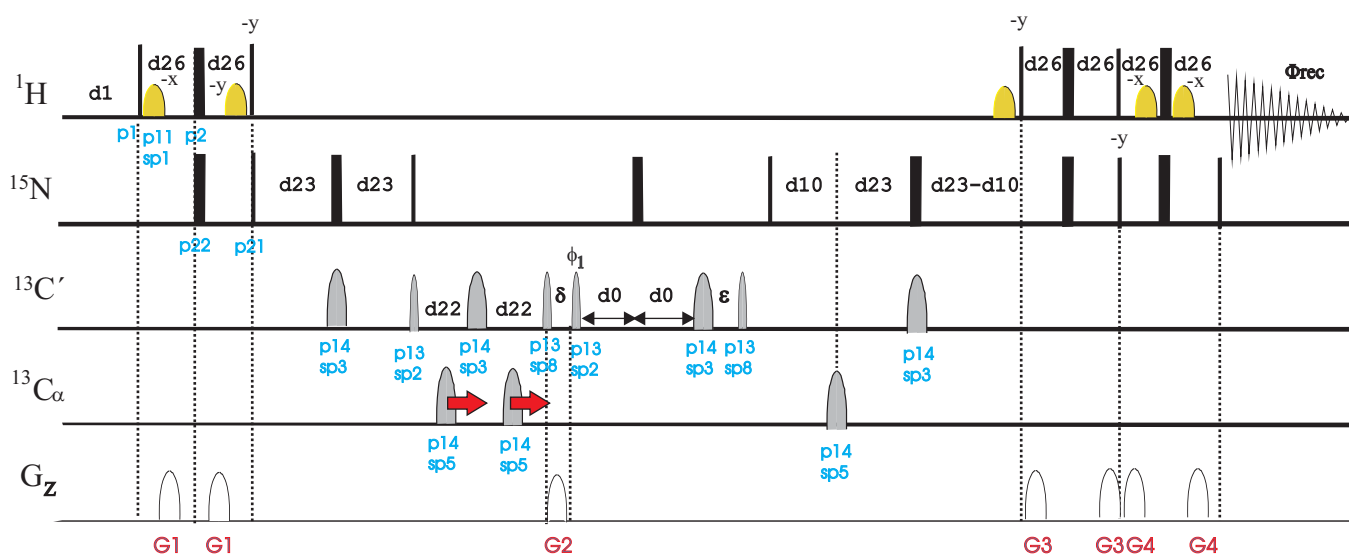
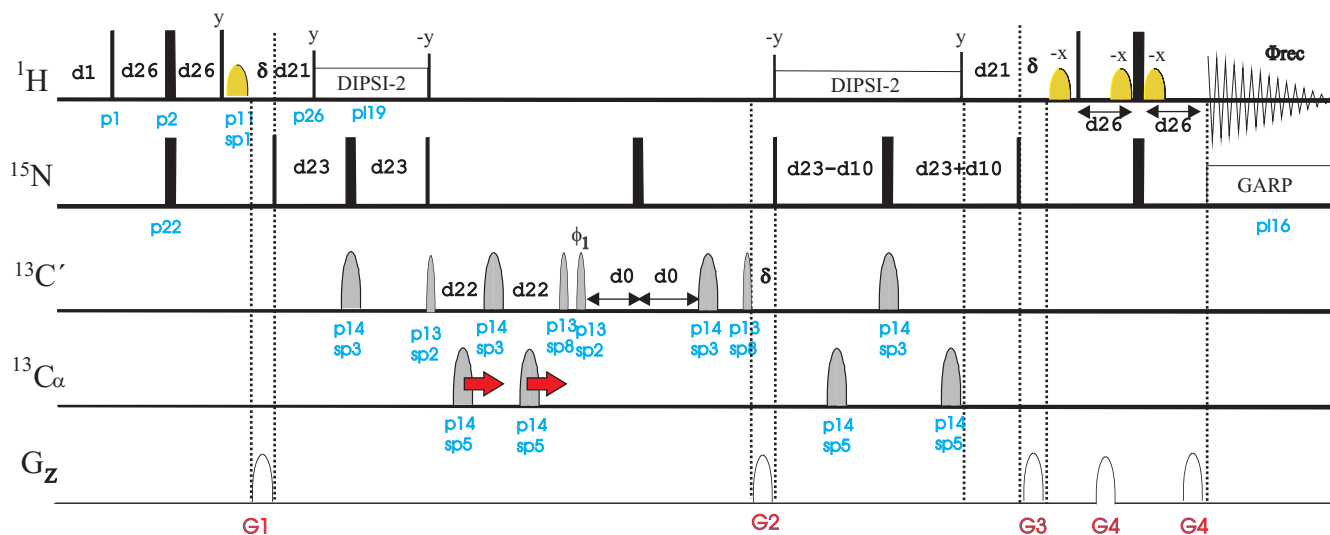
3D IPAP-J-HNCO: J(CA-CO) and J(HN-CA)



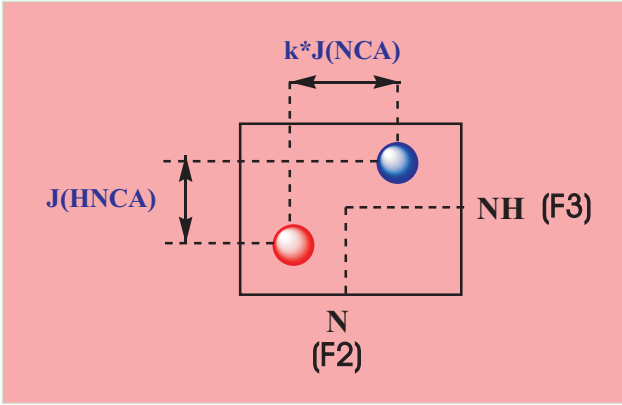
$$\begin{aligned} d26 &= 1/4J(\text{NH}) = 2.3\text{m} \\ d21 &= 1/2J(\text{NH}) = 5.5\text{m} \\ d23 &= 1/4J(\text{NCO}) = 12\text{m} \\ d22 &= 1/4J(\text{COCA}) = 4.3\text{m} \end{aligned}$$

hncogpr3d1

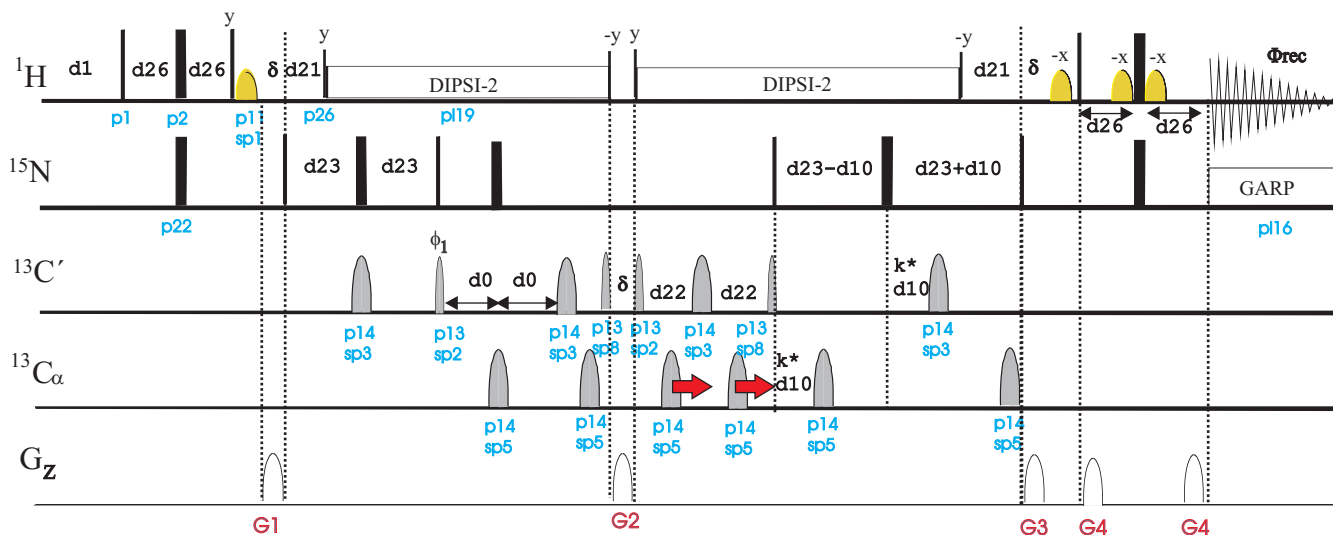




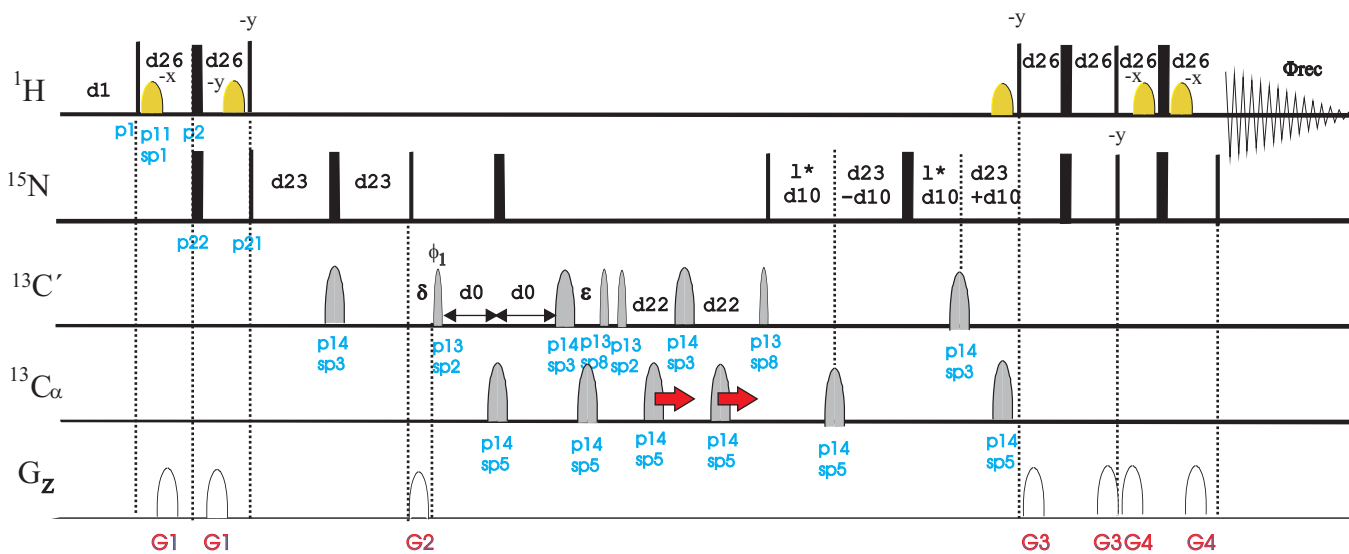
3D IPAP-J-HNCO: J(N-CA) and J(HN-CA)



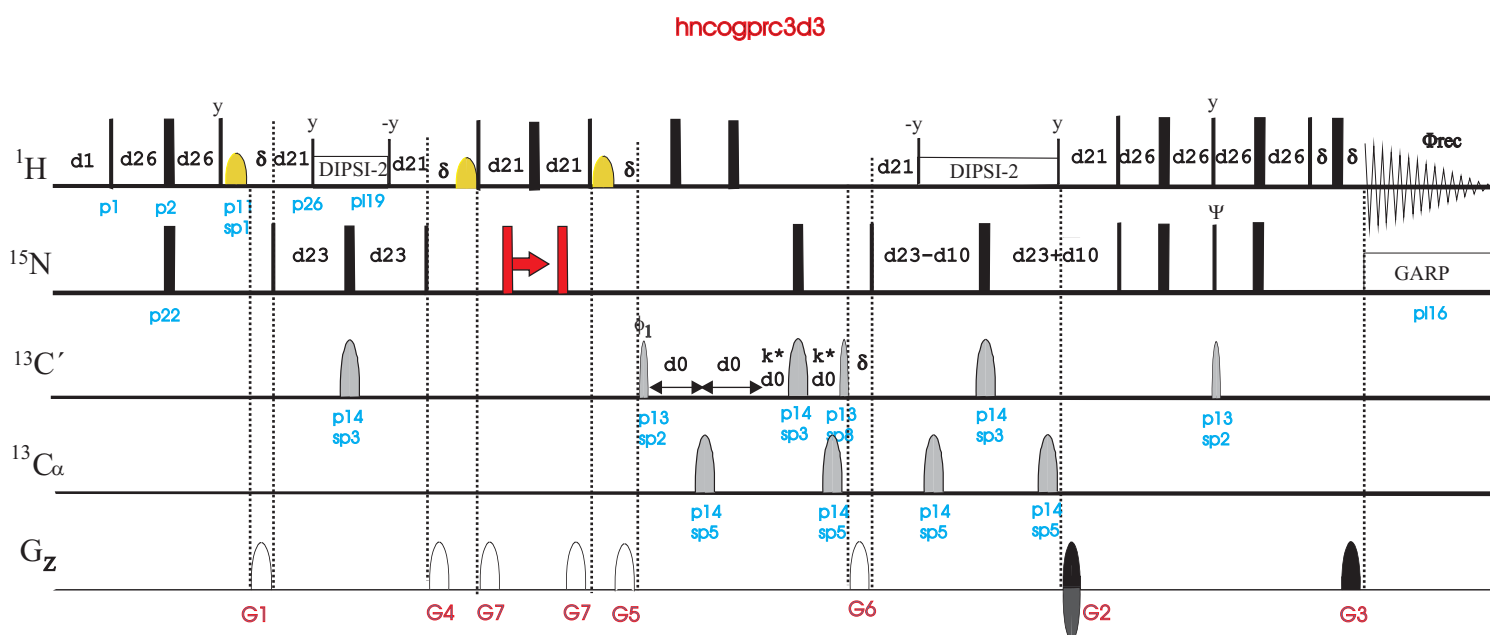
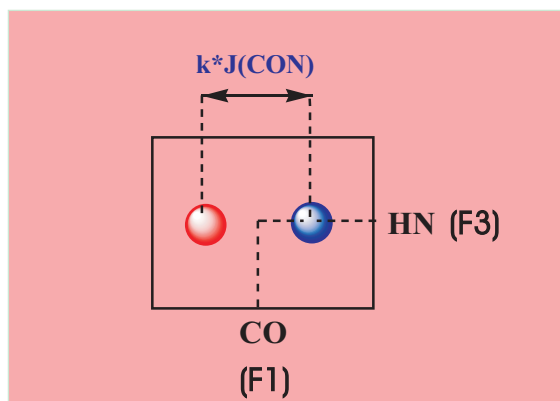
hncogprcw3d2



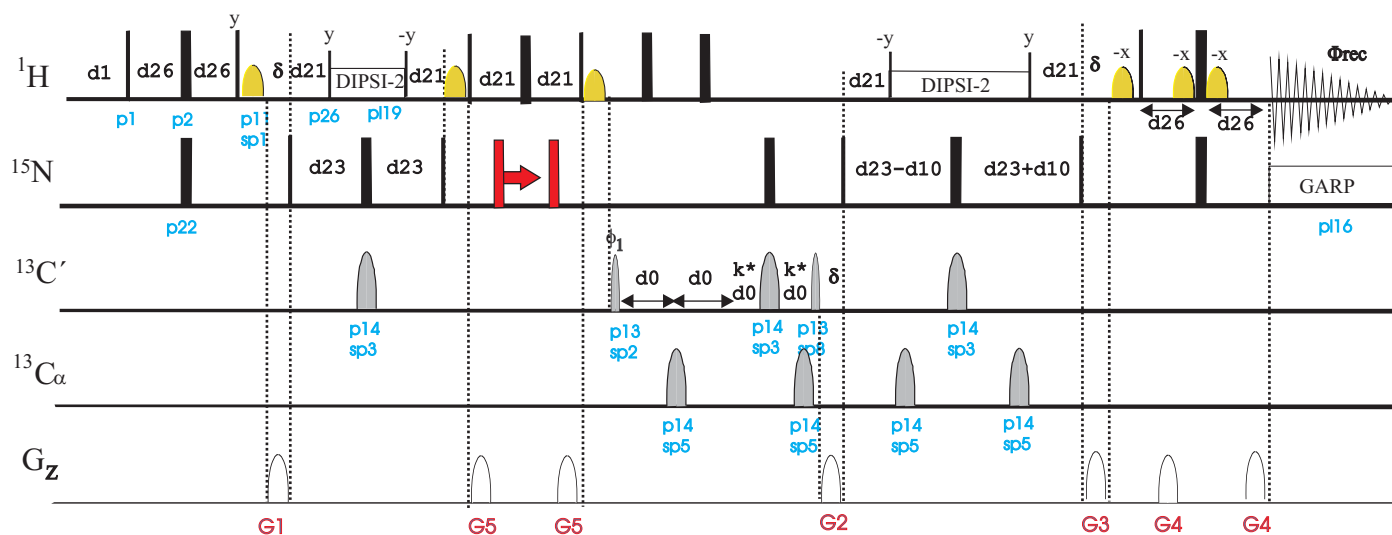
trhncogprc3d2



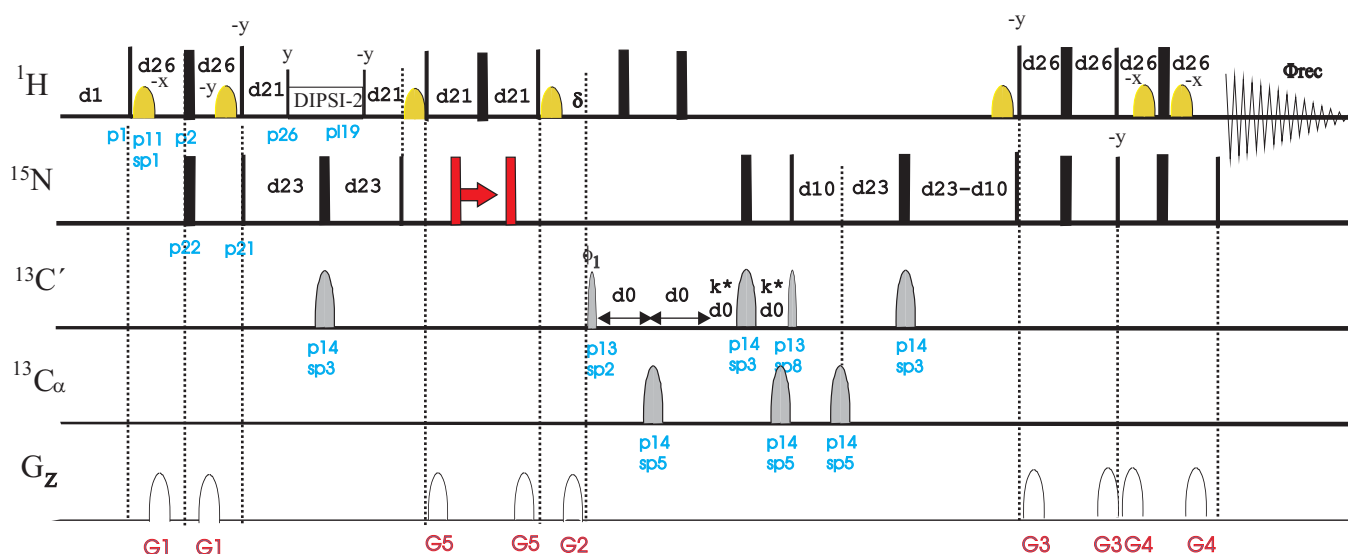
3D IPAP-J-HNCO: J(N-CO)



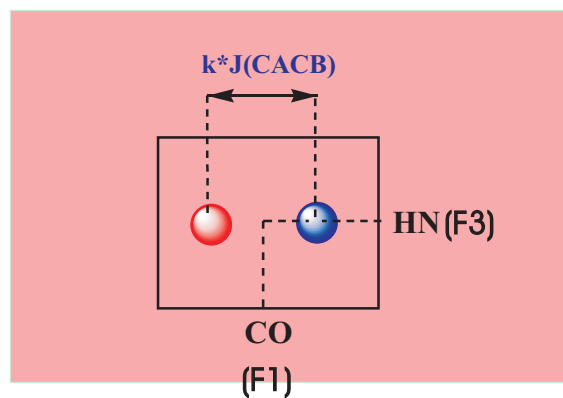
hncogprcw3d3



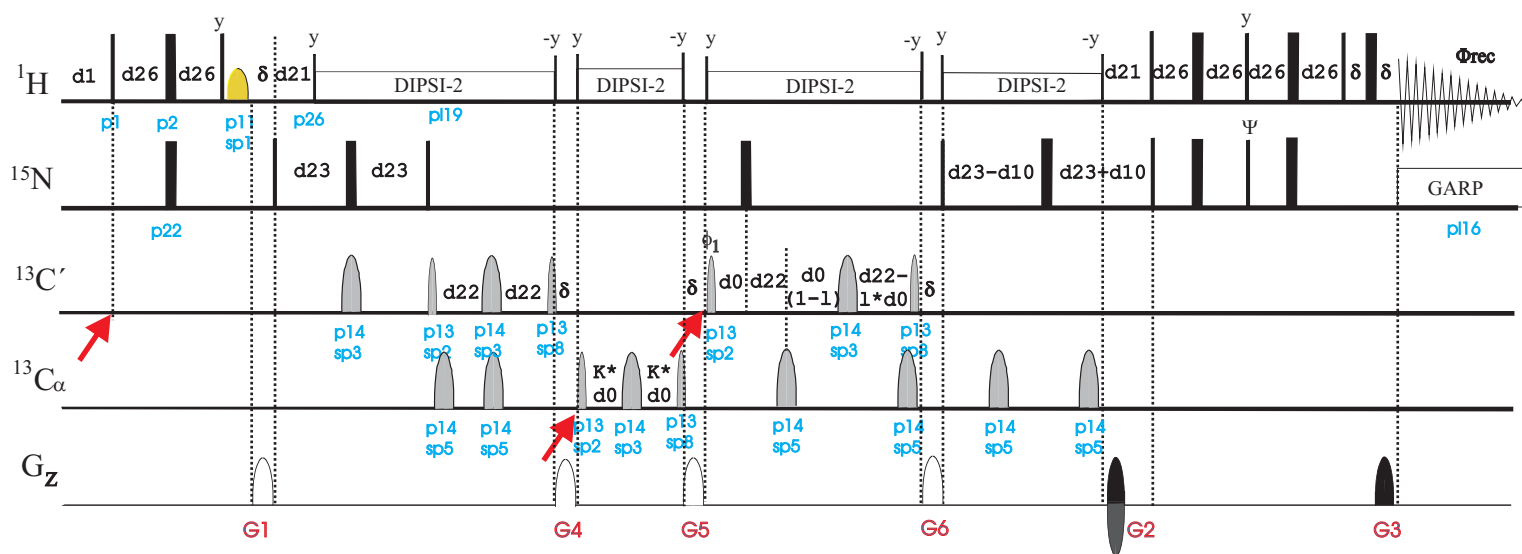
trhncogprc3d3

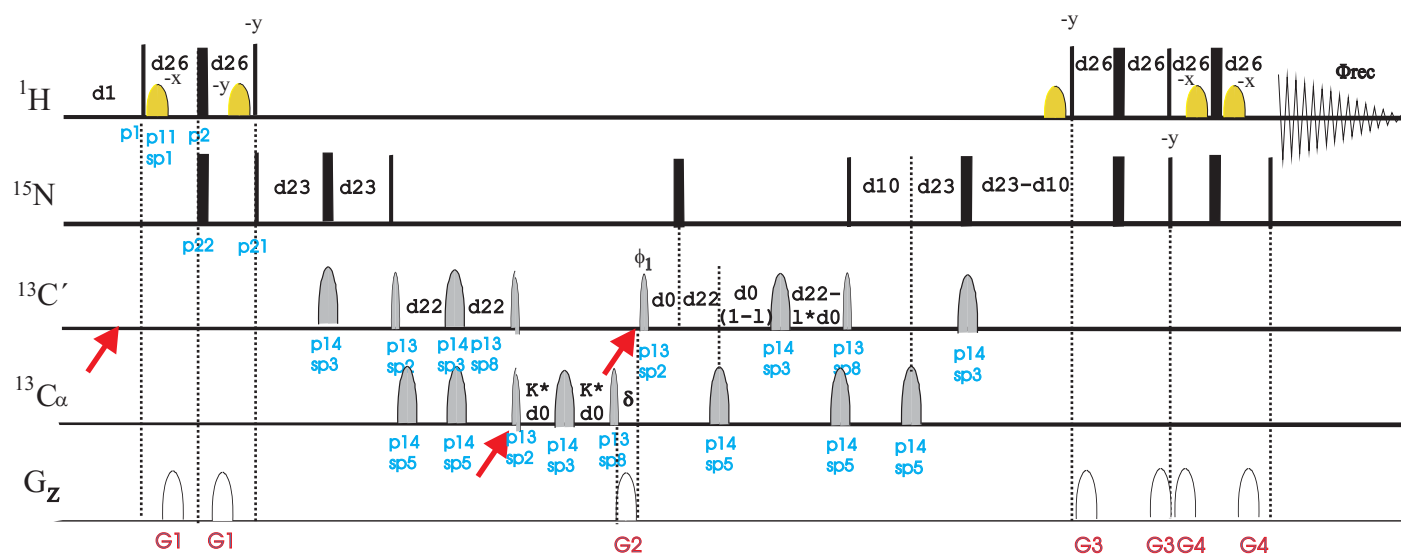
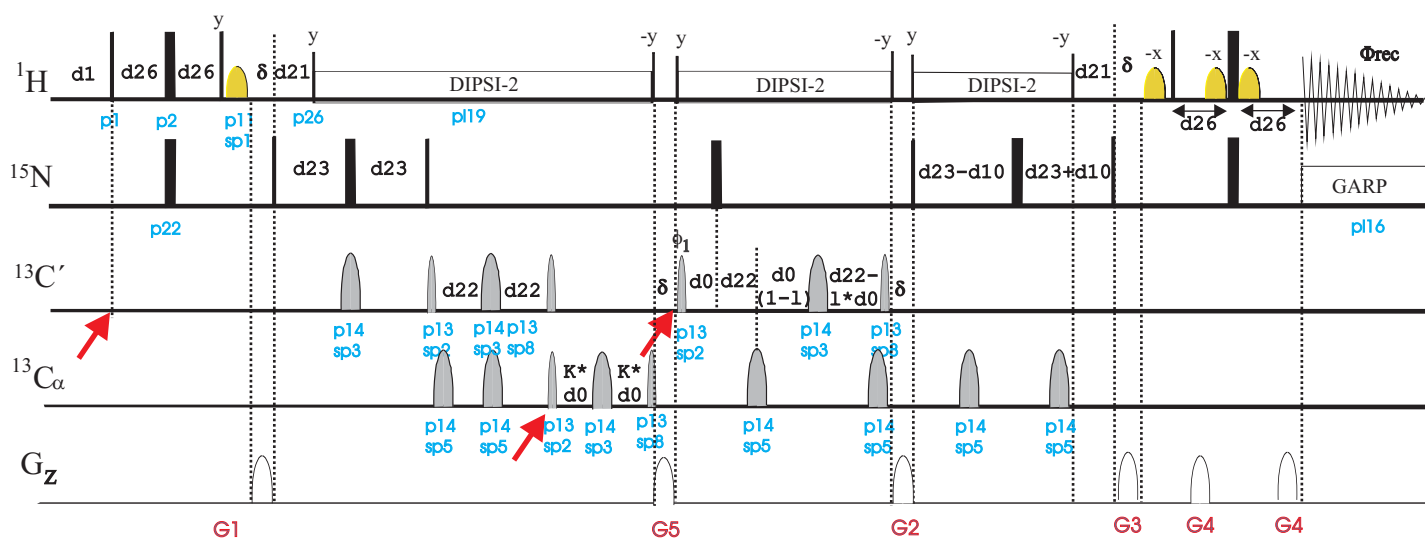


3D J-HNCO: J(CA-CB)

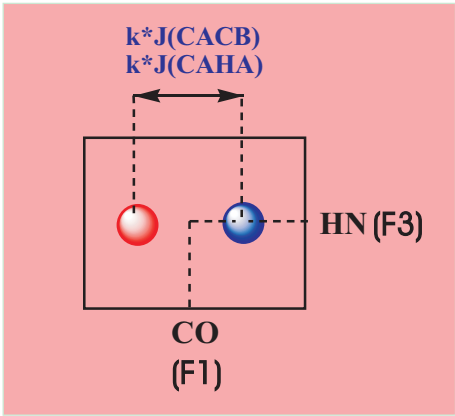


hncogprc3d4

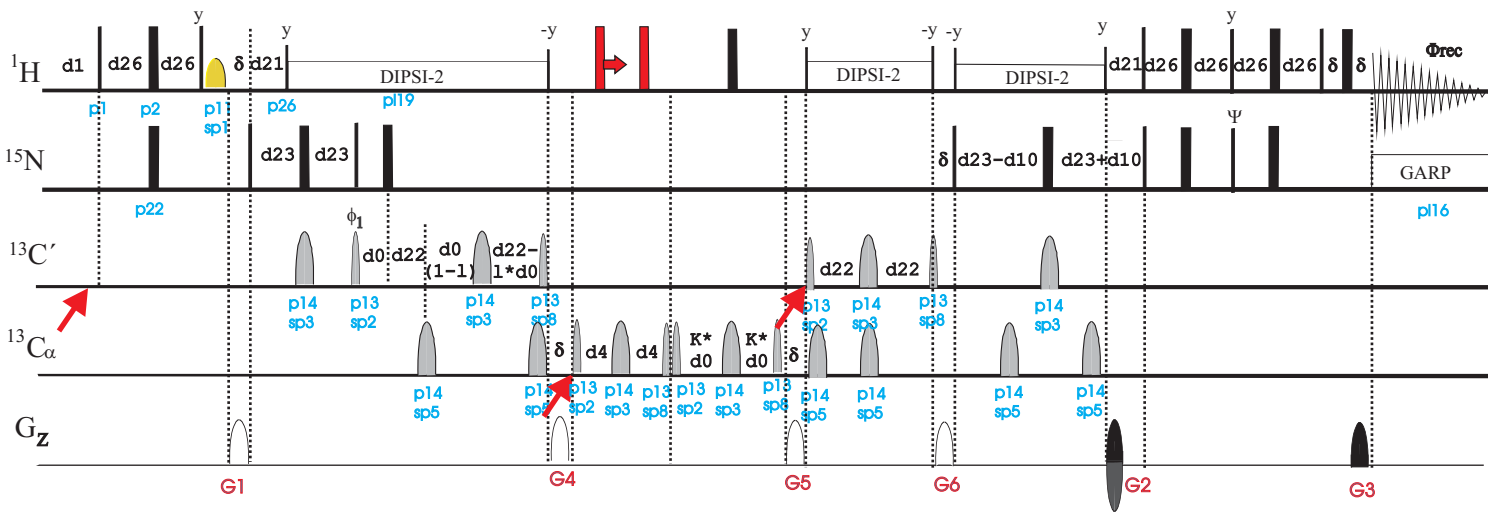




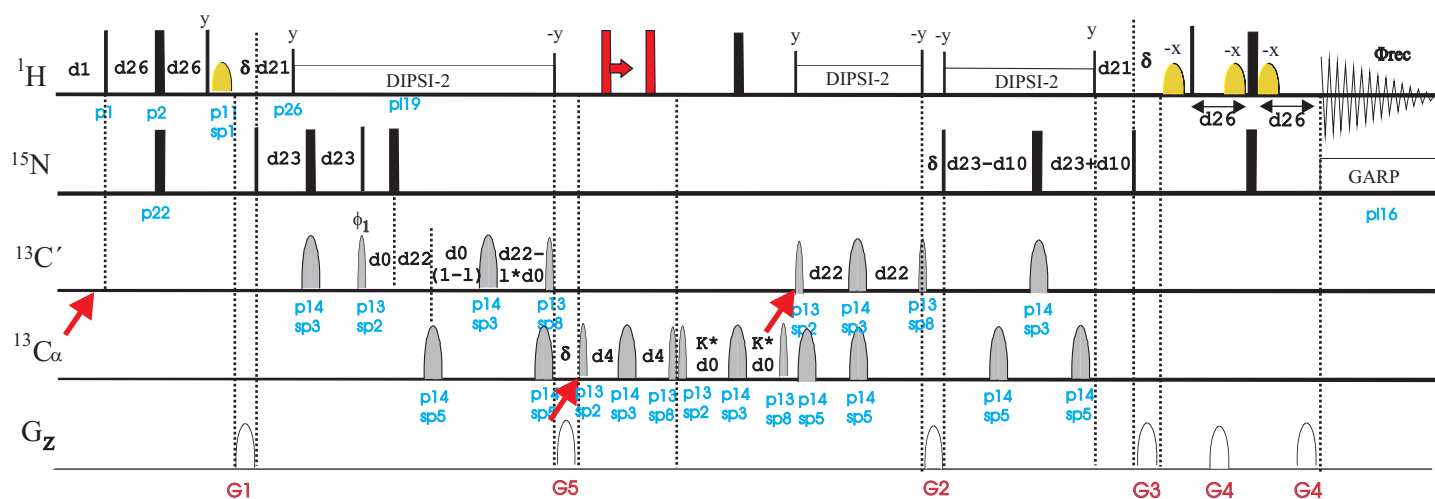
3D IPAP-J-HNCO: J(CA-HA) and J(CA-CB)



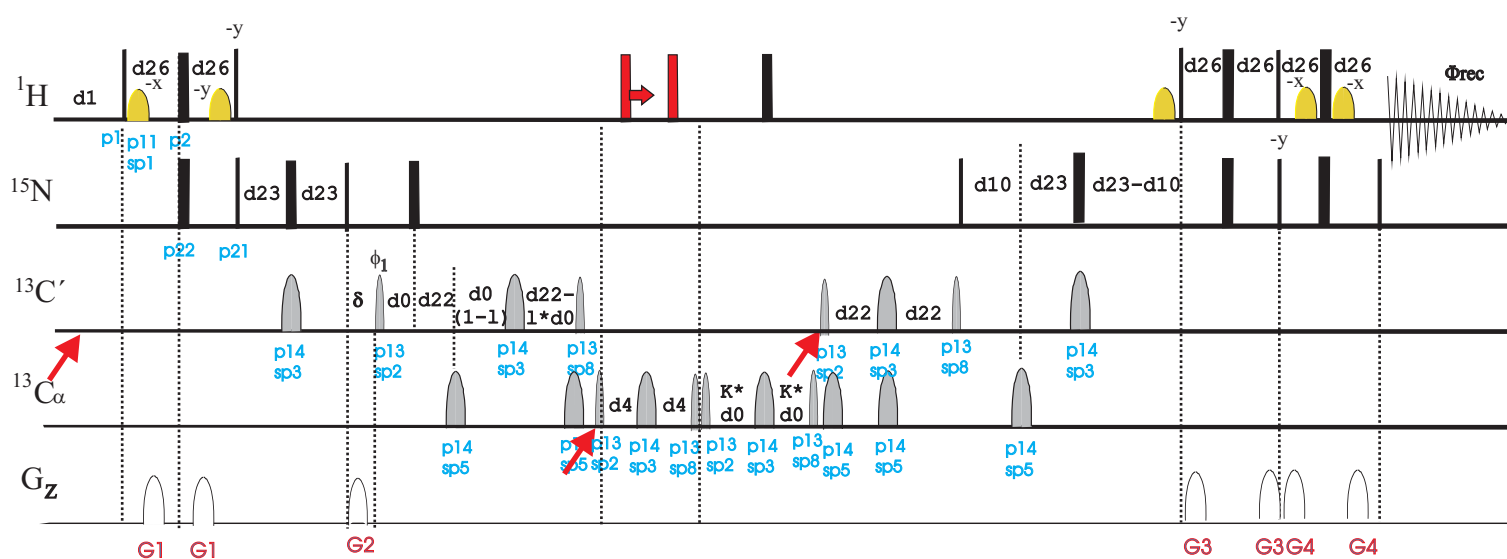
hncogprc3d5



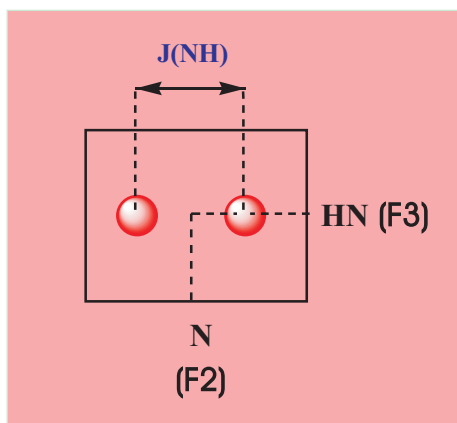
hncogprcw3d5



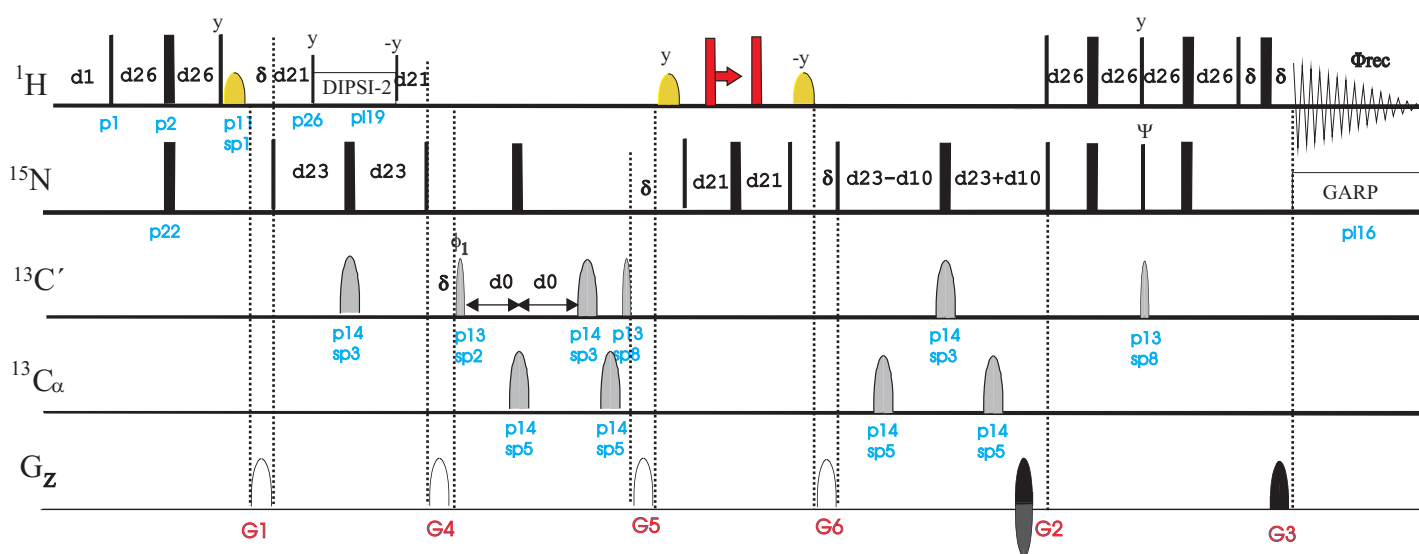
trhncogprc3d5



3D IPAP-J-HNCO: J(HN)



hncogprc3d6

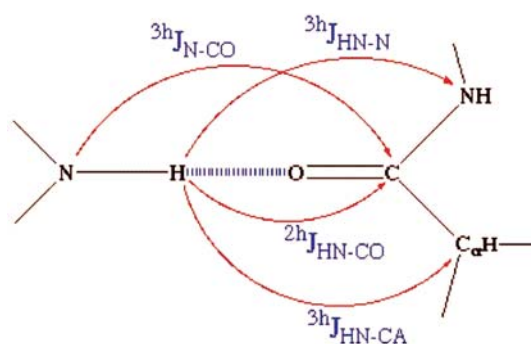


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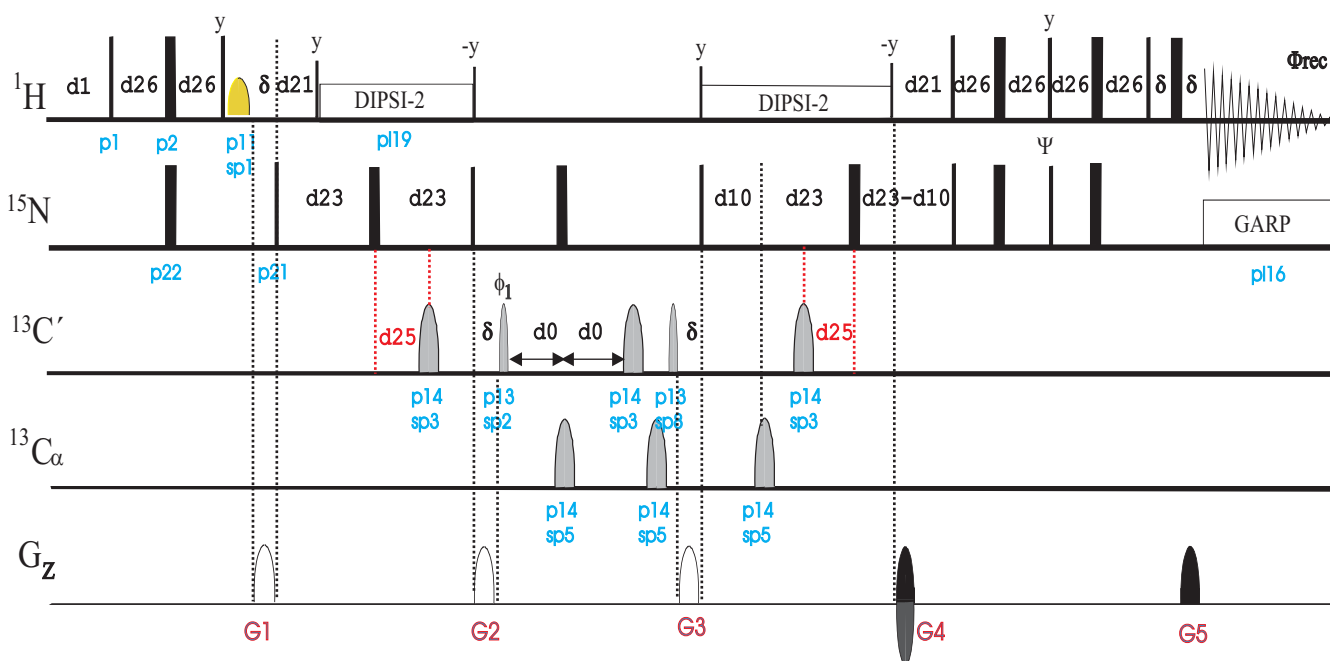
NMRGuide

PROTEIN NMR
COUPLING CONSTANTS
THROUGH-HYDROGEN BONDS

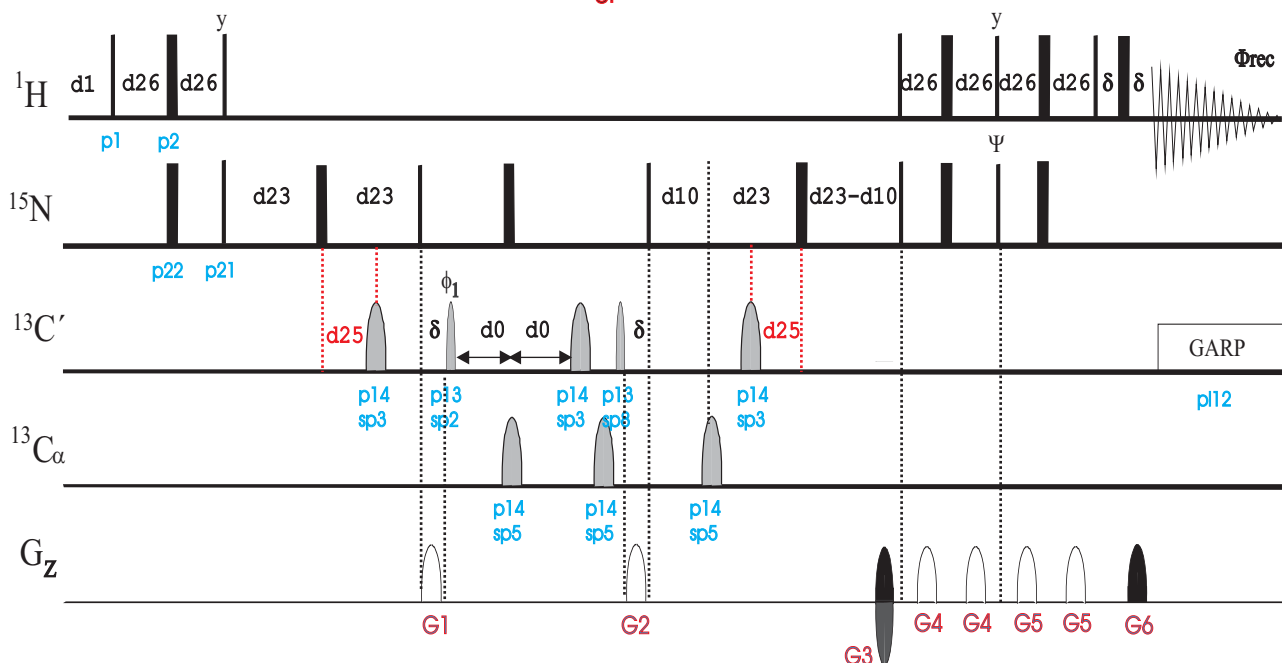
3D Hydrogen bond-HNCO
(**hncogphb3d** | **HNCOGPHB3D**)
3D Hydrogen bond-HNCO using TROSY
(**hncogphb3d2** | **HNCOGPHB3D2**)



hncogphb3d



hncogphb3d2



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NMRGuide

2D & 3D NUCLEIC-ACID
NMR EXPERIMENTS

Reading:

1. S.S. Wijmenga and B.N.M. van Buuren, "The use of NMR methods for conformational studies of nucleic acids, Prog. Nucl. Magn. Reson., 32, 287-387 (1998).
2. B. Fürtig, C. Richter, J. Wöhnert, and H. Scwalbe, "NMR of RNA", ChemBioChem, 4, 936-962(2003).

1. Sugar Assignment

H and H/C experiments

Sugar puckering

Measurement of J(CH) and J(HH)

2. Sequential assignment via phosphodiester linkage

H/P and H/C/P experiments

Measurement of J(PH) and J(PC)

NOE contacts

3. Sugar-to-base connectivities

H/C/N experiments

NOE contacts

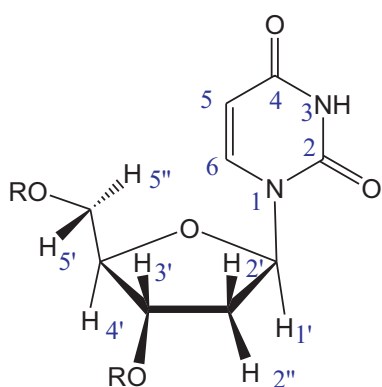
4. Intra-base assignment

H/N, H/C and H/C/N experiments

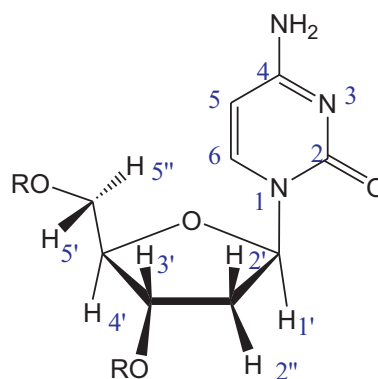
5. Base-pairing identification

Through-hydrogen-bond H/N experiments

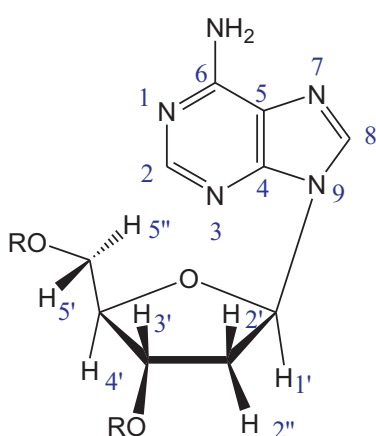
NOE contacts



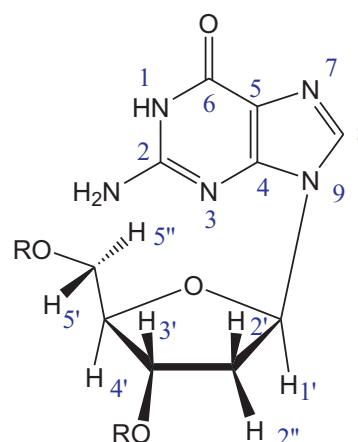
Uridine



Cytosine, C



Adenine, A



Guanine, G

	<u>N1</u>	<u>C2</u>	<u>N3(H)</u>	<u>C4</u>	<u>C5(H5)</u>	<u>C6(H6)</u>	<u>N(H₂)</u>			
<u>U</u>	142-146	154	156-162 (13-14)	169	102-107 (5.0-6.0)	137-144 (6.9-7.9)	-			
<u>C</u>	150-156	159	210	166-168	94-99 (5.0-6.0)	136-144 (6.9-7.9)	94-98 (6.7-7.0 & 8.1-8.8)			
	<u>N1(H)</u>	<u>C2(H2)</u>	<u>N3</u>	<u>C4</u>	<u>C5</u>	<u>C6</u>	<u>N7</u>	<u>C8(H8)</u>	<u>N9</u>	<u>N(H₂)</u>
<u>A</u>	214-216 (7-8)	152-156 (7-8)	220-226	149-151	119-121	157-158	224-232	137-142 (7.7-8.5)	166-172	82-84 (5-6 & 7.8)
<u>G</u>	146-149 (12-13.6)	156	167	152-154	117-119	161	228-238	131-138 (7.5-8.3)	166-172	72-76 (5-6 & 8-9)
	<u>C1'</u>	<u>C2'</u>	<u>C3'</u>	<u>C4'</u>	<u>C5'</u>					
<u>Sugar</u>	87-94 (5-6	70-78 4.4-5.0	70-78 4.4-5.0	82-86 3.8-4.3	63-68 3.8-4.3)					

Main Features of nucleic acid (NA) experiments

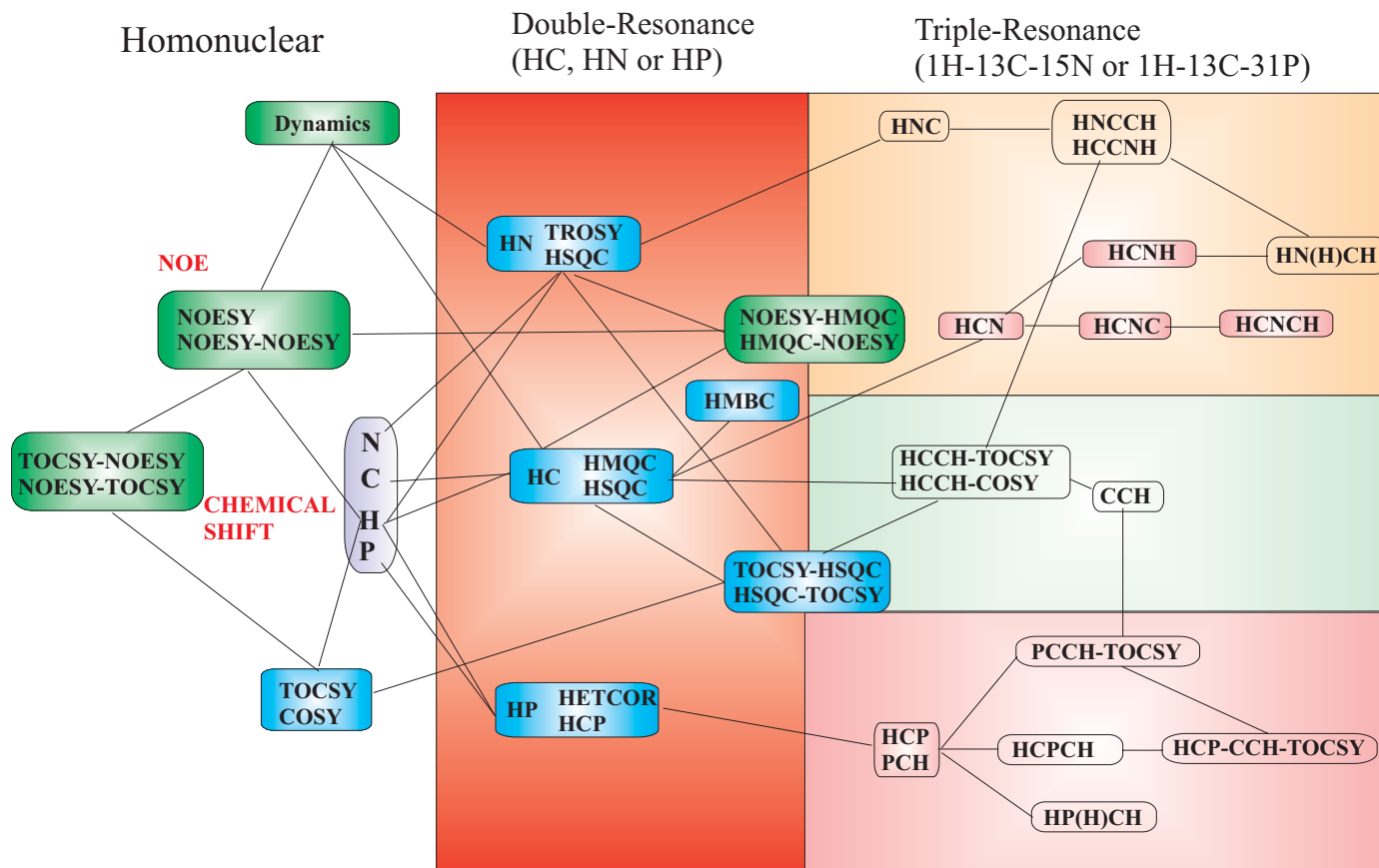
NAs usually present poor degeneracy and important conformational flexibility. Thus, ^1H NMR spectra of NAs can be difficult to analyze because of their low proton density and important resonance overlapping due to poor ^1H chemical shift dispersion. However, small NAs can be studied using the same 1D and 2D NMR experiments dedicated to study natural-abundance organic molecules. Higher NAs would require double- and triple-resonance NMR experiments involving low-sensitive ^{13}C or ^{15}N nuclei.

Sample Requirements

Unlabeled NAs can be analyzed with typical 1D and 2D NMR homo- and heteronuclear NMR experiments. In complex NAs, more sophisticated and specifically designed ^{15}N and Triple-resonance HCX experiments can require selective $^{13}\text{C}/^{15}\text{N}$ labeling or $^{13}\text{C}/^{15}\text{N}$ -doubly labeled samples.

Hardware Requirements

NAs experiments are best recorded on triple-resonance $^1\text{H}, ^{13}\text{C}, ^{15}\text{N}$ or $^1\text{H}, ^{13}\text{C}, ^{31}\text{P}$ inverse probeheads with z-gradients capabilities.



Experimental details for nucleic-acid experiments

Offsets

F1 channel: ^1H (o1p)
F2 channel: ^{13}C (o2p)
F3 channel: ^{15}N (o3p) in HN-type or HCN-type experiments
F3 channel: ^{31}P (o3p) in HP-type or HCP-type experiments

Mixing/Decoupling

From f2 channel:
 ^{13}C CPD with GARP (pcpd2=80us at pl12)
 ^{13}C - ^{13}C TOCSY with FLOPSY-16 (p9 at pl15)

From f3 channel:
 ^{15}N CPD with GARP (pcpd3=200us at pl16)
 ^{31}P CPD with GARP (pcpd3 at pl16)

Typical ^{13}C pulses from F2 channel

p13 sp2: 90° C on- resonance (320us , spnam2=Q5.1000)
P14 sp3: 180° C on-resonance (256us, spnam3= Q3.1000)
p13 sp8: retro- 90° C on-resonance (320us, spnam8= Q5tr.1000)
p14 sp5: 180° C off-resonance (256us, spnam5=Q3.1000)

p8 sp13: 180° adiabatic for inversion (500us using CHIRP , spnam13=Crp60,0.5,20.1)

Typical ^{15}N pulses from F3 channel

p30 sp9: 180° N1/N9 on- resonance (700us , spnam9=Q3.1000)

Very Important!!!: In all pulse programs the syntax

prosol relations= <triple_na>

is included for automated acquisition/set-up using edprosol/getprosol.
This file is defined in the following directory:

\$TOPSPINHOME/conf/instr/spect/prosol/relations/triple_na

Specific Nucleic Acid NMR

3D HC and HN NOESY Experiments:

3D ^1H - ^{13}C NOESY-CT-HSQC using echo-antiecho (**na_noesyhsqcctetgp3d**)
 3D ^1H - ^{13}C NOESY-HSQC using WATERGATE and refocusing of J(C5C6) during t_1 (**na_c6noesyhsqcgp3d**)
 3D ^1H - ^{15}N NOESY-HSQC using WATERGATE (**na_noesyhsqcf3gpwg3d** / **na_noesyhsqcf3gpwg3d.2**)

2D and 3D HCN-type Experiments:

HCN experiment

3D using echo-antiecho (**na_hcnetgps3d** | **NA_HCNETGPSI3D**)
 3D using echo-antiecho and selective pulses (**na_hcnetgpsisp3d** | **NA_HCNETGPSISP3D**)
 3D using MQ (**na_hcnmq3d**)
 3D using MQ and selective ^1H pulses (**na_hcnmqsp3d**)
 3D using TROSY (**na_trhcnph3d**)
 3D using TROSY and gradient selection (**na_trhcnetsi3d**)
 2D H(C)N using TROSY (**na_trhcnph**)
 2D H(C)N using TROSY and gradient selection (**na_trhcnnet**)
 2D H(C)N using MQ (**na_hcnmqgpphpr** | **NA_HCNMQGPPHPR**)

HCNCH experiment

2D H(CNC)H (**na_hcnchgpjrphsp** | **NA_HCNCHGJRPHSP**)
 3D H(C)N(C)H using MQ (**na_hcnchmqsp3d**)
 3D H(C)N(C)H using MQ and TROSY (**na_trhcnchmqsp3d**)
 3D H(C)N(C)H using MQ, TROSY and WATERGATE (**na_trhcnchmqspwg3d**)
 3D (H)CN(C)H using MQ, TROSY and WATERGATE (**na_trhcnchmqspwg3d2**)
 3D (HC)N(C)CH-COSY using MQ (**na_hcnchcomq3d**)
 3D (HC)N(C)CH-TOCSY using MQ (**na_hcnchdimq3d**)
 2D H(CN)H using WATERGATE (**na_hcnhgpph19** | **NA_HCNHGPPH19**)

3D TROSY-(H)CCH-COSY for intra-base correlation (**na_trhcchco3d**)

2D H(CN)C (**na_h68c68n19c42**)

HCCNH experiment

3D H(6/8)(CCC)NH (**na_hccnhdigp3d** | **NA_HCCNHDIGP3D**)
 3D H(CC)NH (**na_h5c5c4n3h_3d**, **na_h56c56c4n3h_3d**)
 3D (H)C(C)NH (**na_h56c56c4n3h_3d2**)
 2D H(NC6)C5 (**na_hnc6c5etgps3d**)
 3D (H)N(C)CH (**na_hncch3d**)

Observation HN-N hydrogen bonds:

2D HNN-COSY (**na_hnncosygpphgw** | **NA_HNNCOSYGPPHWG**)
 2D HNN-COSY using shaped ^{15}N 180° pulses (**na_hnncosygpphspwg**)
 2D HNN-COSY using TROSY and shaped ^{15}N 180° pulses (**na_trhnncosygpphspwg**)

2D and 3D HC Experiments to determine J(HH) and J(CH) :

3D H(C)CH-E.COSY experiment (**hcchecgp3d** | **NA_HCCHECGP3D**)
 3D HCC-TOCSY-CCH-COSY experiment (**na_hcchfwdigp3d** | **NA_HCCHFWDIGP3D**)
 3D HCC-TOCSY-CCH-E.COSY experiment (**na_hcchfwdiecg3d** | **NA_HCCHFWDIECGP3D**)
 3D HCC-TOCSY-CCH-E.COSY experiment using jump-and-return (11) (**na_hcchfwdiecgpr3d**)
 3D forward directed quantitative gamma HCC-TOCSY (**ghcchfwdigp3d** | **NA_GHCCHFWDIGP3D**)
 2D ^1H - ^{13}C HSQC for measuring J_{CH} in sugars (**na_hsqcetgpjcs3d** | **NA_HSQCETGPJCS3D**)

2D HP Experiments:

2D CT HH- $\{^3\text{P}\}$ -COSY with presaturation to measure $J(\text{H}3'-\text{P})$ (**hpcosyphpr** | **NA_HPCOSYPHPR**)

2D ^1H - ^3P HETCOR experiment

Using echo-antiecho (**na_xhcoetf3gp**)

Constant-time using echo-antiecho (**na_xhcoctetf3gp**)

Constant-time without gradient selection (**na_hpctco**)

Constant-time without gradient selection using jr (**na_hpctcojr**)

2D ^1H - ^3P HSQC experiment

Using CPMG (**na_hsqcetf3gpxy**)

Using CPMG and jump-and-return (**na_hsqcetf3gpjrphxy**)

2D ^1H - ^3P Hetero-TOCSY using cross-polarization (**na_hpd**)

2D ^1H - ^3P HSQC-NOESY using CPMG (**na_hsqcetf3gpnoxy**)

2D ^1H - ^3P Hetero-TOCSY-NOESY

Using cross-polarization (**na_hpdino**)

Using WATERGATE and cross-polarization (**na_hpdino19**)

Using cross-polarization (**na_hpdino3d**)

Using WATERGATE and cross-polarization (**na_hpdino193d**)

2D and 3D HCP Experiments:

HCP Experiment

3D HCP using sensitivity-enhancement (**na_hcpetgpsi3d** | **NA_HCPETGPSI3D**)

3D HCP-TOCSY

Using CC TOCSY and presaturation (**na_hcpdigp3d**)

Using CC TOCSY and jump-and-return (11) (**na_hcpdigpjr3d**)

Using CC TOCSY and echo-antiecho (**na_hcpdietgp3d**)

Using CC TOCSY and sensitivity-enhancement (**na_hcpdietgpsi3d** | **NA_HCPDIETGPSI3D**)

PHCH Experiment

3D P(H)CH using HMQC and echo-antiecho (**na_hpccoetf3gp3d**)

3D Constant-time P(H)CH using HMQC (**na_hpcctco3d**)

3D Constant-time P(H)CH using HMQC and echo-antiecho (**na_hpccoetf3gp3d**)

3D Hetero-TOCSY-COSY using HMQC and cross-polarization (**na_hpdico3d**)

PCH Experiment

2D P(C)H using HC INEPT transfer (**na_pcchco**)

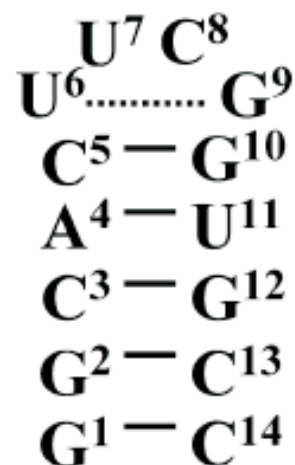
2D P(C)H using HC cross-polarization (**na_pcchdi**)

2D P(CCC)H using CC TOCSY and HC cross-polarization (**na_pcchdi2**)

2D quantitative HC(P) for determination of $J(\text{CP})$ (**na_hcpqetgpsi.1** | **NA_HCPQETGPSI.1** and **na_hcpqetgpsi.2** | **NA_HCPQETGPSI.2**)

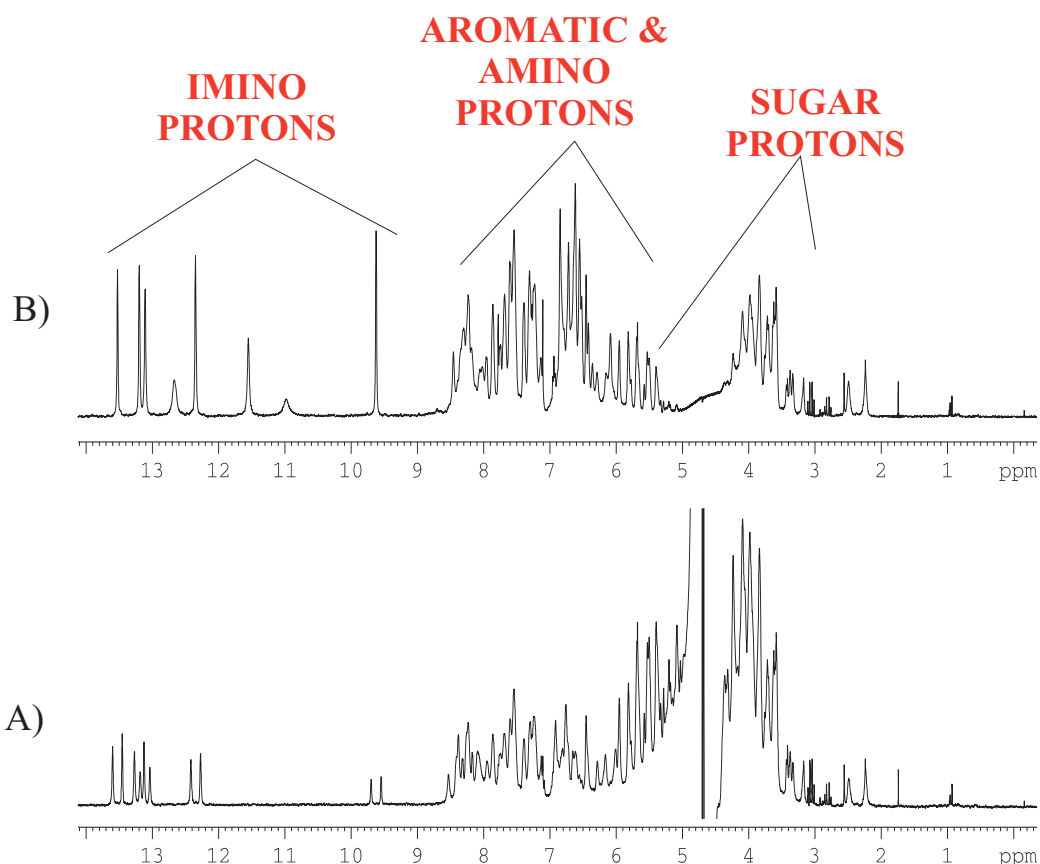
2D P-FIDS experiment to measure $J(\text{HP})$ and $J(\text{CP})$ (**pfidsetgpsi** | **NA_PFIDSETGPSI**)

All NMR spectra shown in this chapter correspond to a 1mM sample of doubly-labeled $^{13}\text{C}/^{15}\text{N}$ RNA 14-mer 5'-GGCACUUCGGUGCC-3' (commercially available from Silantes) dissolved in 90% $\text{H}_2\text{O}/10\%$ D_2O (courtesy from Dr. W. Bermel - Bruker Biospin, Kalshruhe). Experiments were recorded in a 600MHz AVANCE spectrometer equipped with a 5mm TXI probehead.

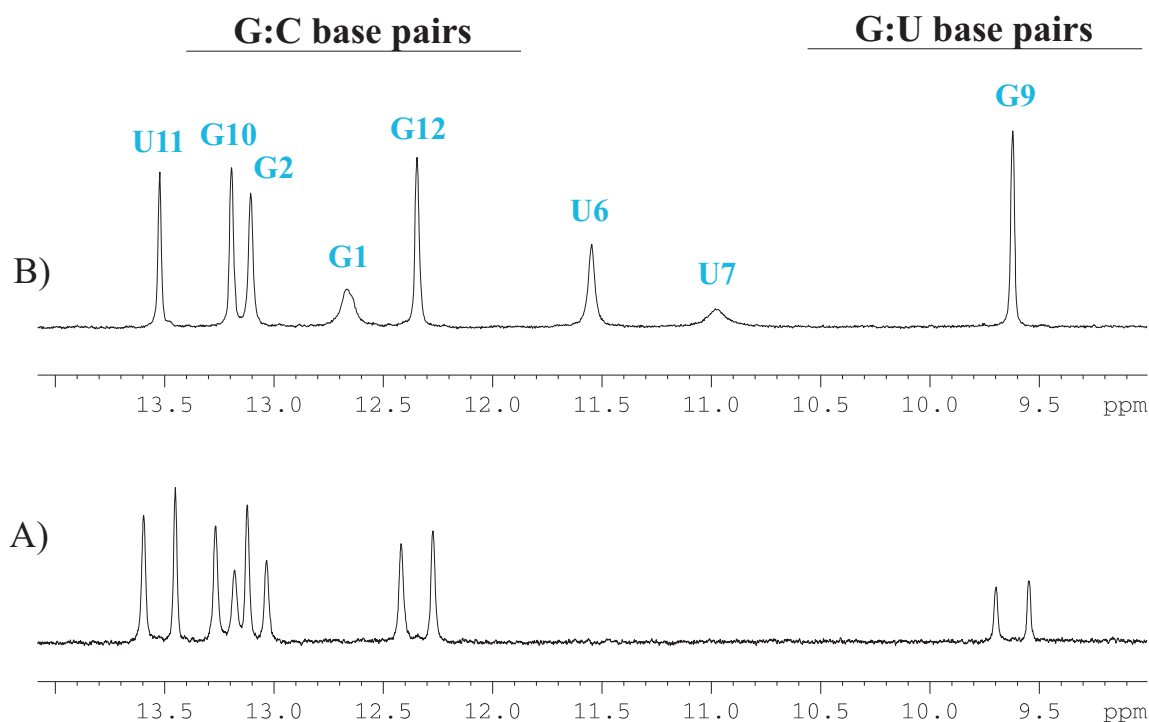


A) ^1H spectrum using presaturation (zgpr)

B) ^1H spectrum using water suppression using WATERGATE and heteronuclear ^{15}N decoupling during ^1H acquisition.



Expansions of the lowfield imino NH region.



Important classical 2D experiments to study NAs:

2D ^1H - ^1H COSY and TOCSY experiments for assignment of ribose spin systems
2D ^1H - ^1H NOESY experiment for intra- and inter-residue connectivities, and also for base pairing

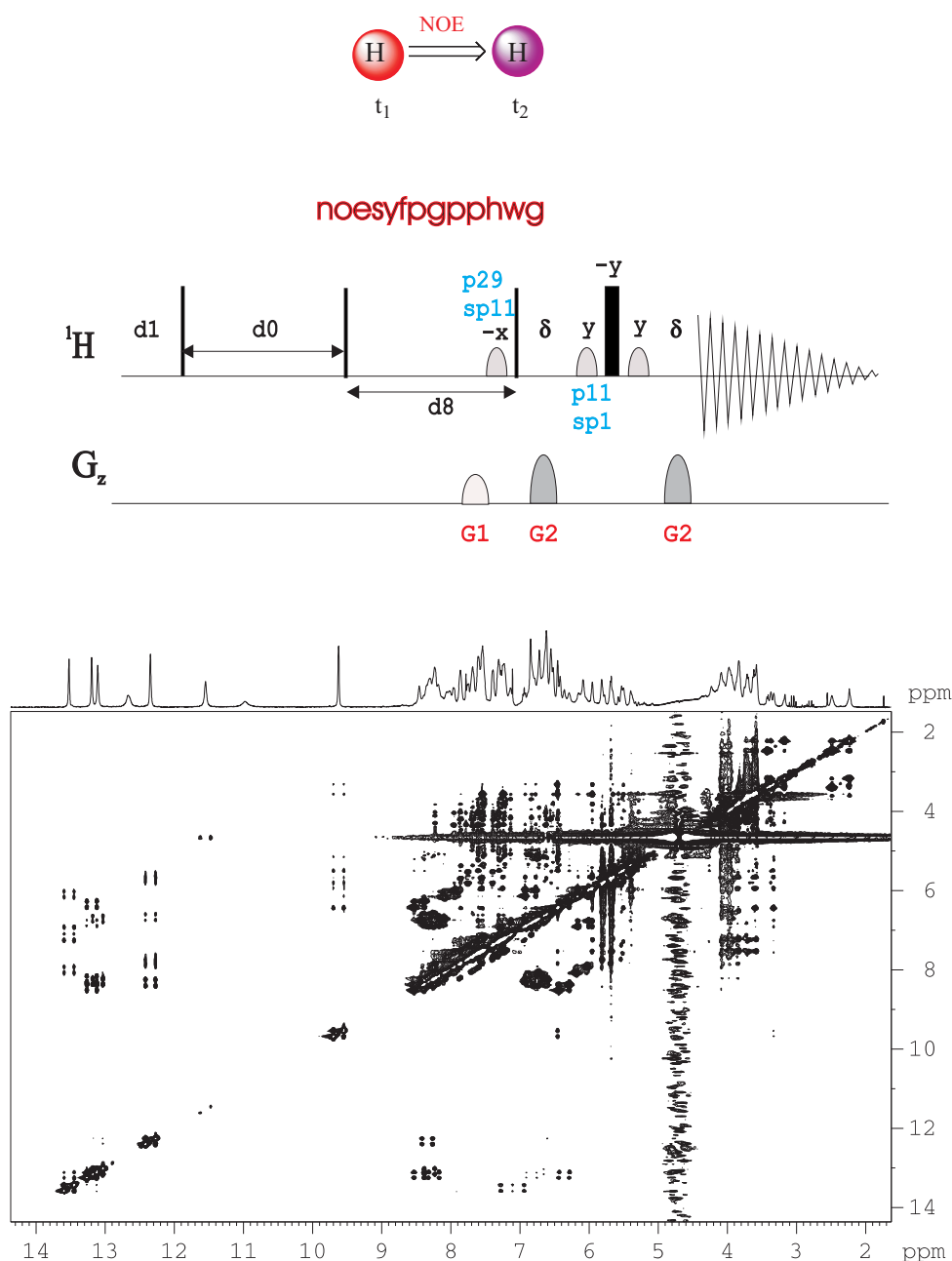
2D ^1H - ^{13}C and ^1H - ^{15}N HMQC i HSQC experiments to identify directly-attached CH and NH spin systems.

2D ^1H - ^{13}C HMBC and 2D long-range optimized HSQC to trace out two- and three-bond away proton-carbon and proton-nitrogen connectivities. Very useful for the assignment of non-protonated carbon and nitrogen in the base moiety.

2D NOESY Experiment

Experiment Description NOESY experiment is an important tool for conformational studies of nucleic acids. It can be run on unlabeled and labeled nucleic acids. Important NOE contacts for sequential assignments are imino-to-imino, imino-to-amino, and imino-to-nonexchangeable proton regions. Information on base pairing and hydrogen bonding can be also extracted from NOE imino cross-peaks.

See all available NOESY schemes in the 2D NOESY chapter or also 3D X-edited NOESY experiments.



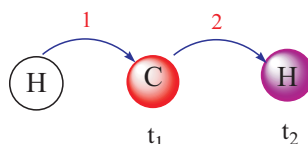
BRUKER PULSE PROGRAM CATALOGUE

NMRGuide

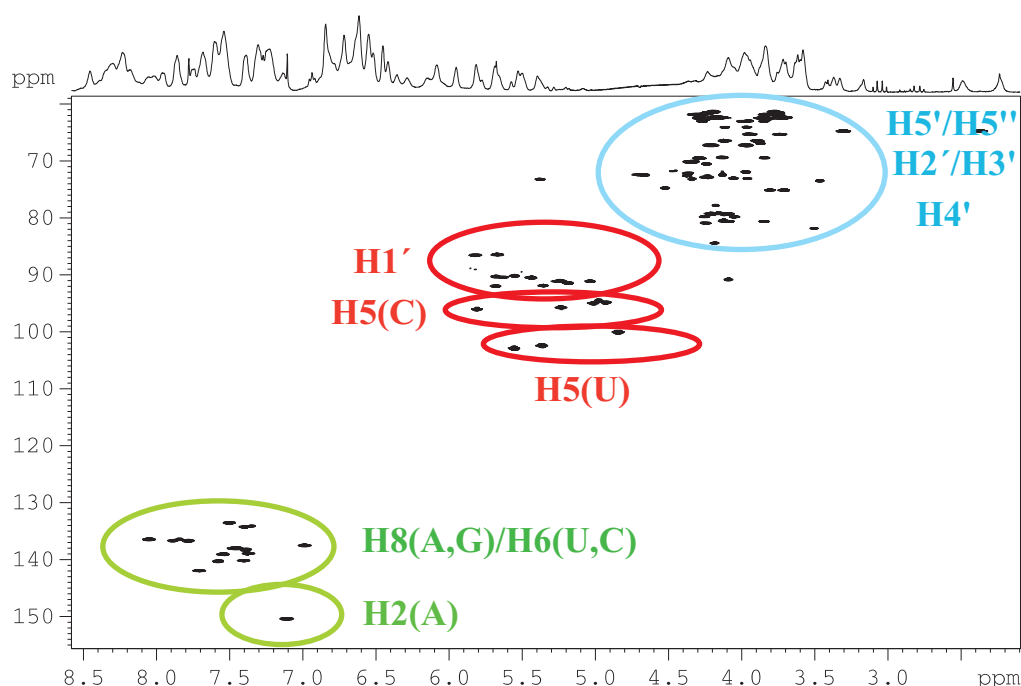
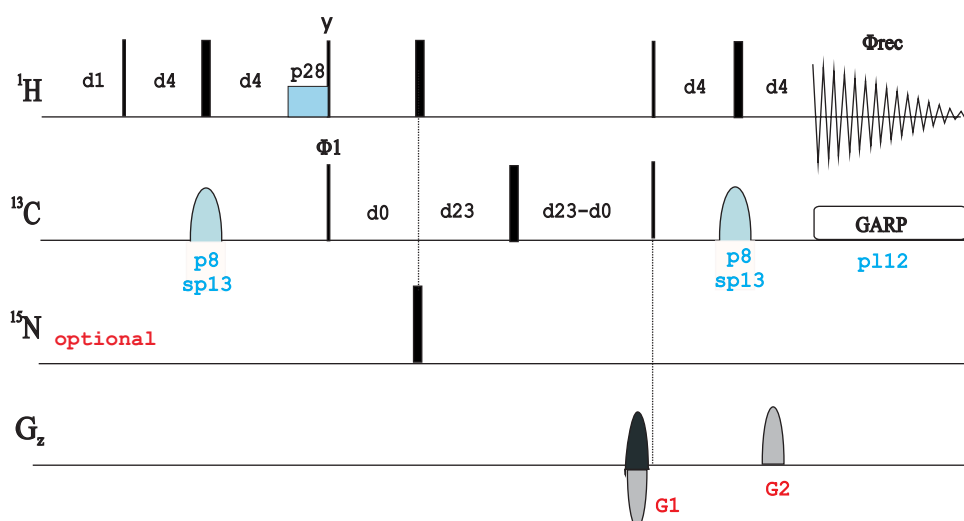
NUCLEIC-ACID NMR
2D & 3D HCN EXPERIMENTS

2D Constant-time HSQC/HMQC Experiment

Experiment Description: ^1H - ^{13}C correlation experiments can be recorded as usual for both unlabeled and ^{13}C -labeled NAs. IN the later, constant-time experiments are recommended to refocus $J(\text{CC})$ during the indirect F1 dimension. See the corresponding 2D HSQC and HMQC chapters for all available pulse programs.



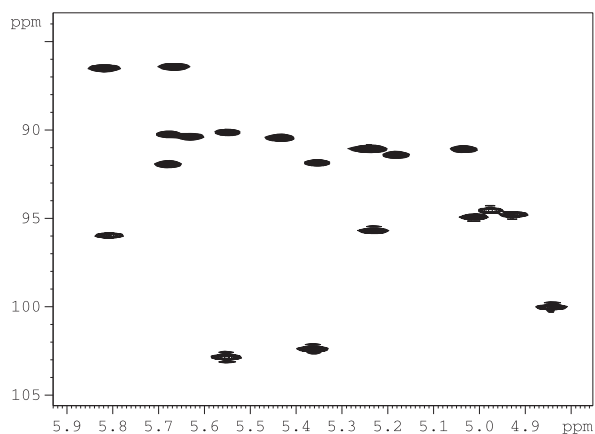
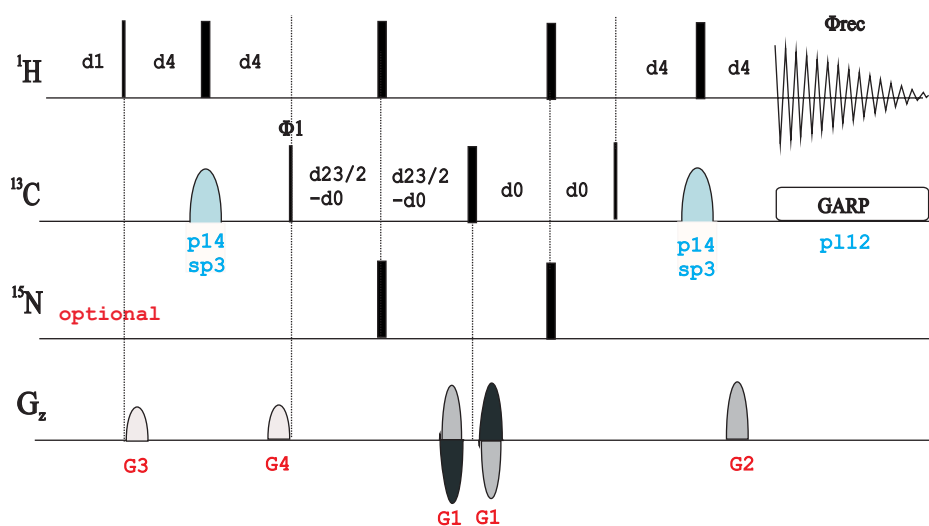
hsqcctetgsp.2



d1=1.5s
d4=1/4J(CH)=1.72ms
(optimized to cnst2=145Hz)
d23=CT(C) period=8.8ms

For a complete assignment,
See Fig. 6 in 04jb69-28

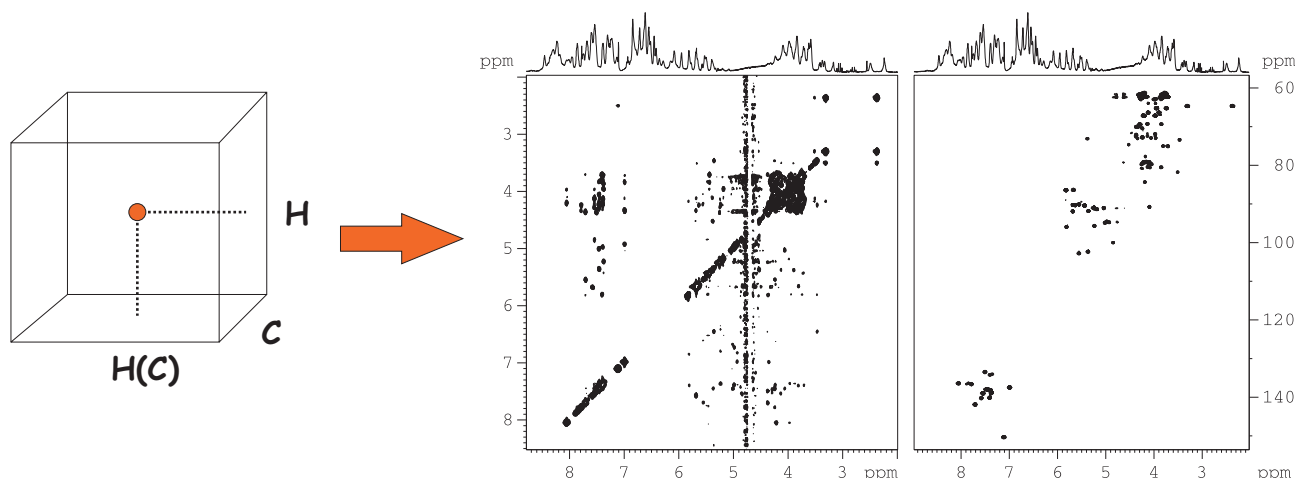
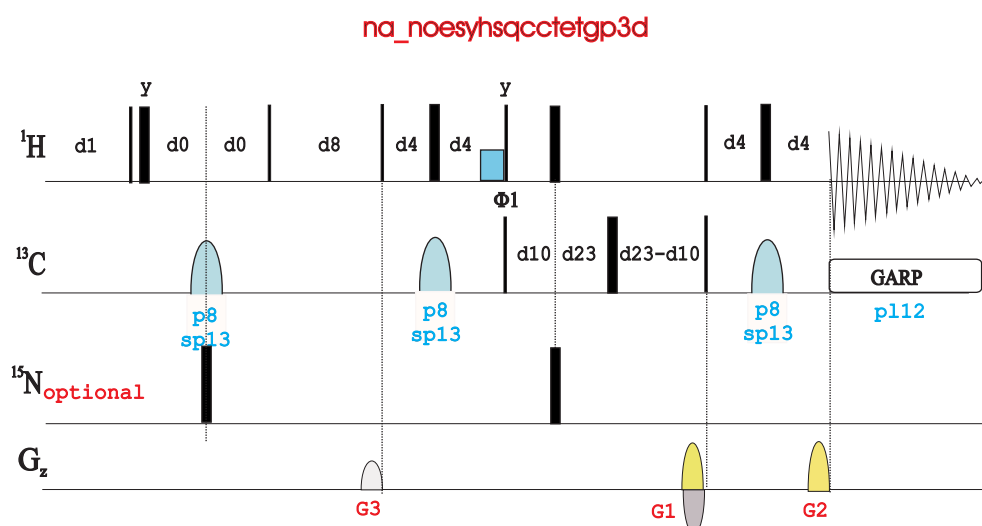
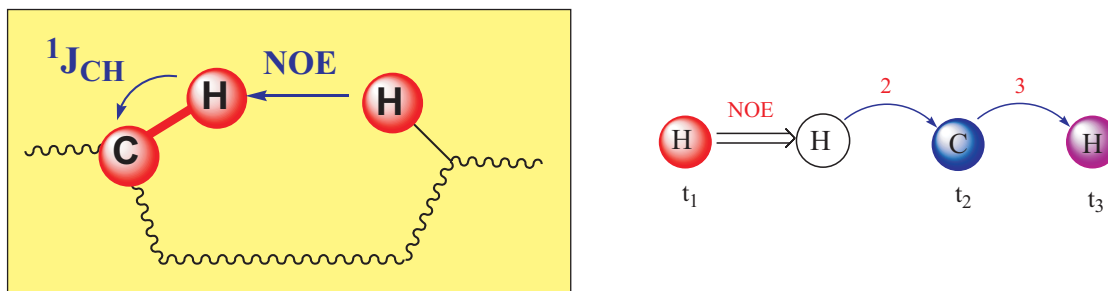
hmqcctetgp



d1=1.5s
d4=1/4J(CH)=1.72ms
 (optimized to **cnst2=145Hz**)
d23=CT(C) period=8.8ms

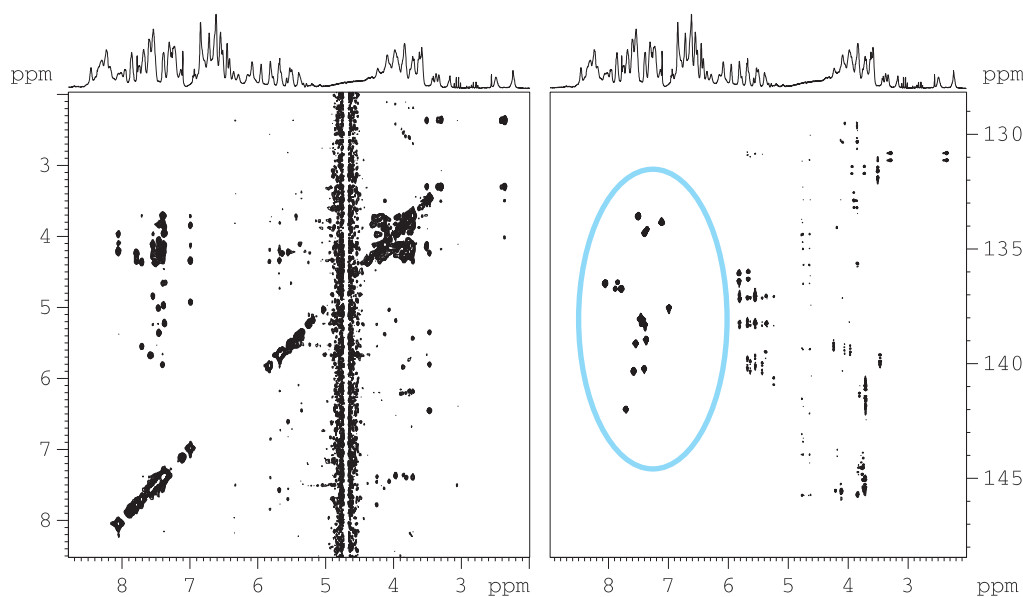
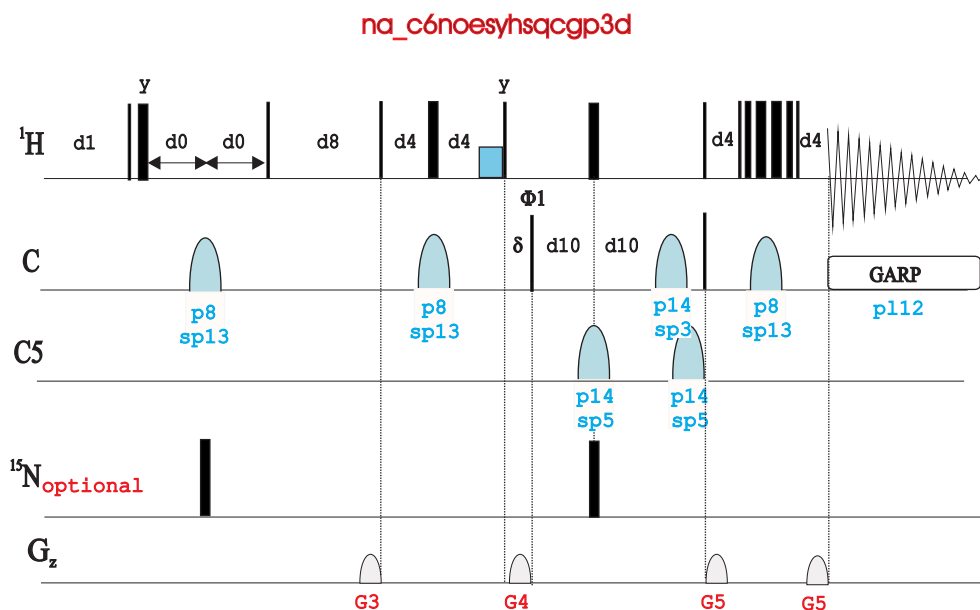
3D Constant-time ^1H - ^{13}C NOESY-HSQC Experiment

Experiment Description: Constant-time version of the 3D NOESY-HSQC experiment to be applied on ^{13}C -labeled NAs. Useful to remove $J(\text{CC})$ splitting from the indirect C dimension. The experiment allows to detect intra-residue ^1H - ^1H NOE contacts between individual sugar rings and their connected bases.



d1=1.5s
d8=NOESY mixing time=100ms
d4=1/4J(CH)=1.72ms
(optimized cnst2=145Hz)
d23=CT(C) period=8.8ms

Non-constant-time version of the 3D NOESY-HSQC experiment with selective refocusing of the H(C6C5) coupling constant by means of 180° ¹³C selective pulses (p14=1ms, spnam3=Q3)) on C5 during the indirect d10 period.

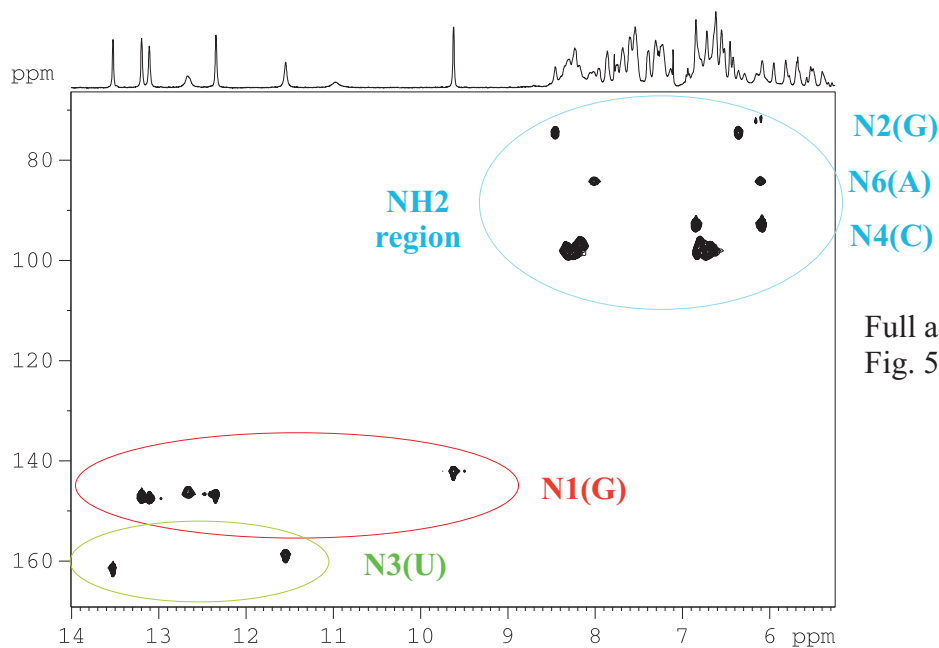
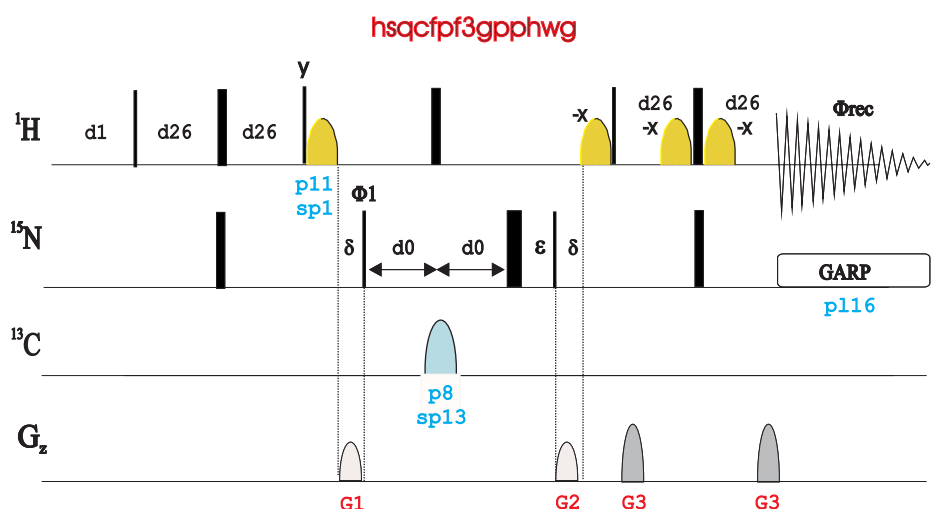
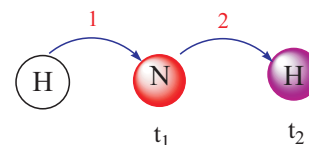


d1=1.5s
d8=NOESY mixing time=100ms
d4=1/4J(CH)=1.25ms (optimized to cnst2=200Hz)
SW in the C dimension reduced to 16.5ppm

2D ^1H - ^{15}N HSQC Experiment

Experiment Description

Assignment of exchangeable imino and amino protons with their directly-attached nitrogen nuclei in H₂O.

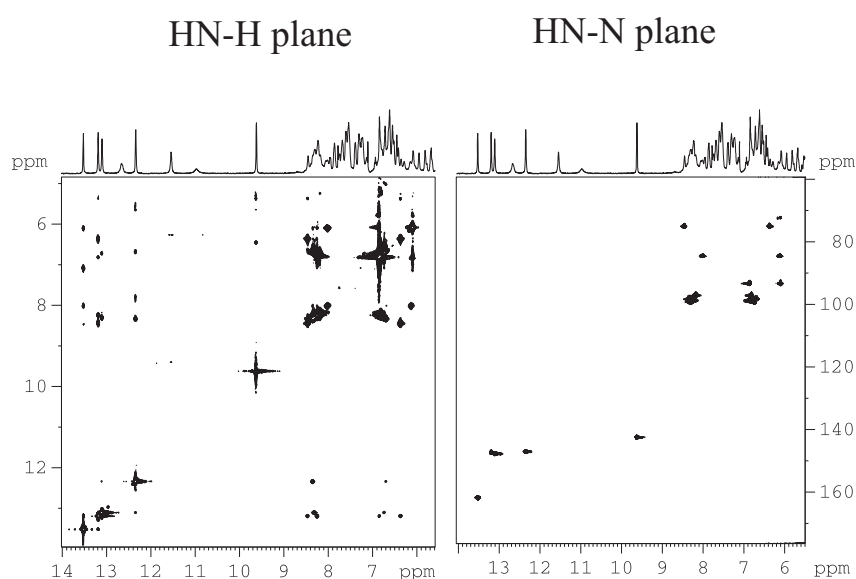
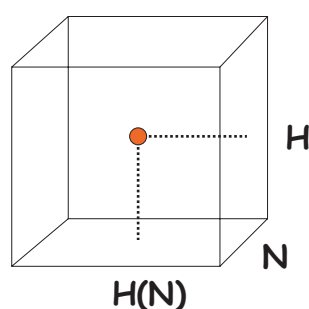
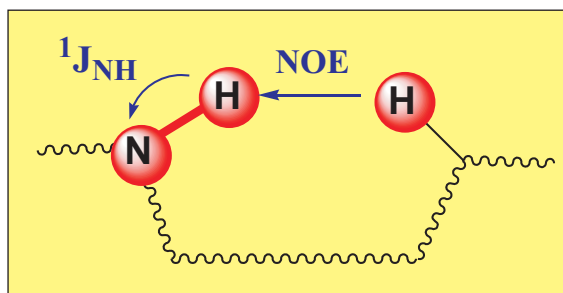


d1=1.5s
p11=90° water selective=1ms (Squa100.1000)
d26=1/4J(NH)=2.77ms
(optimized cnst4=90Hz)

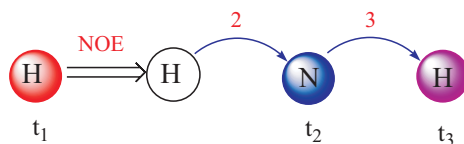
3D ^1H - ^{15}N NOESY-HSQC Experiment

Experiment Description

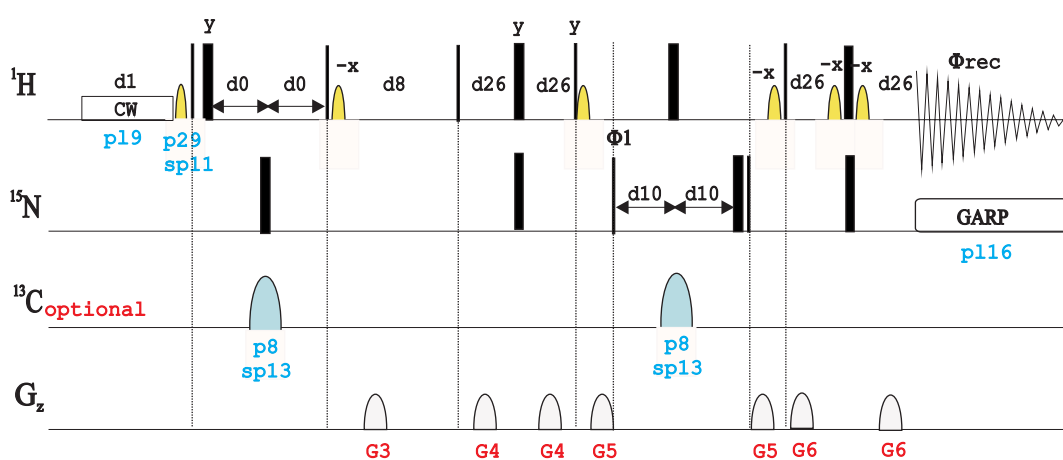
Sequential assignment of exchangeable imino and amino groups via NOE contacts. Three important connectivities: imino-to-imino, imino-to-amino, and amino-to-non exchangeable aromatic and sugar protons



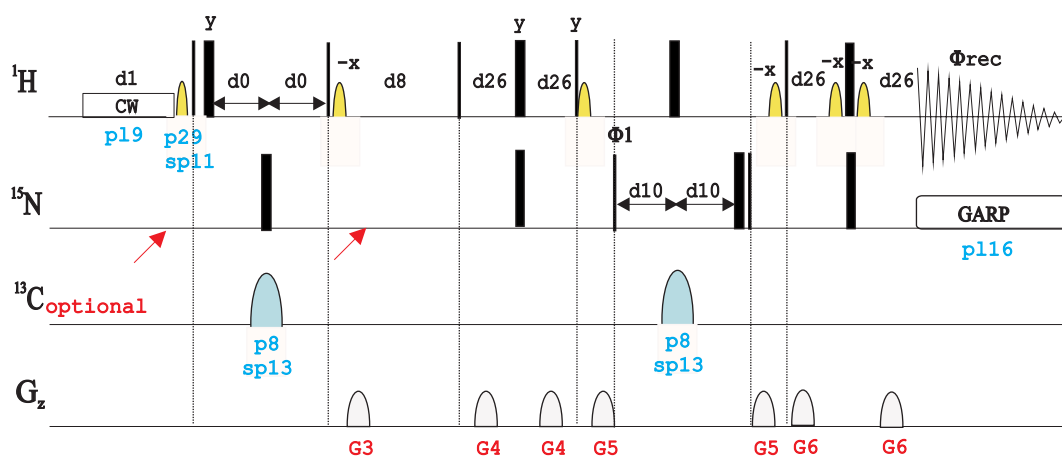
d1=1.5s
d8=NOE mixing time=100ms
p11=water selective=1ms (Squa100.1000)
p29=water selective=2ms (sinc1.1000)
d26=1/4J(NH)=2.77m
(optimized cnst4=90Hz)
ZGOPTNS=DLABEL_CN



na_noesyhsqcf3gpwg3d



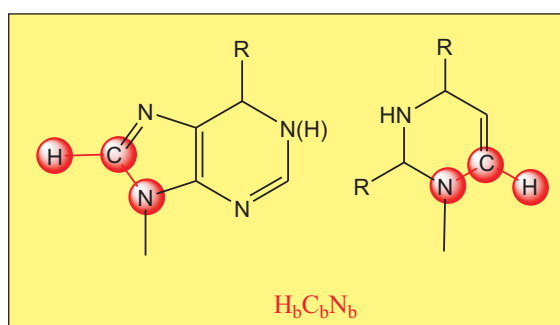
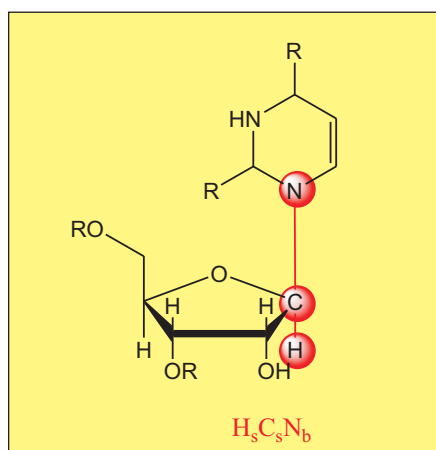
na_noesyhsqcf3gpwg3d.2



3D HCN Experiment

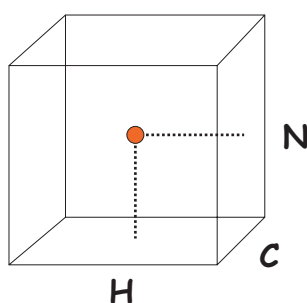
Experiment Description:

This experiment provides sugar-to-base and intrabase HCN connectivities in isotopically labeled nucleotides. Several 2D and 3D versions of this out-and-back HCN experiment incorporating SQC, MQC and TROSY effects are available.



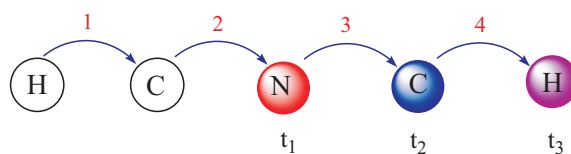
NMR Spectrum

The experiment provides a 3D correlation map. As a function of experimental conditions, both type of correlations can be observed in the same spectrum. Otherwise, selective HsCsNb or HbCbNb spectra can also be obtained.

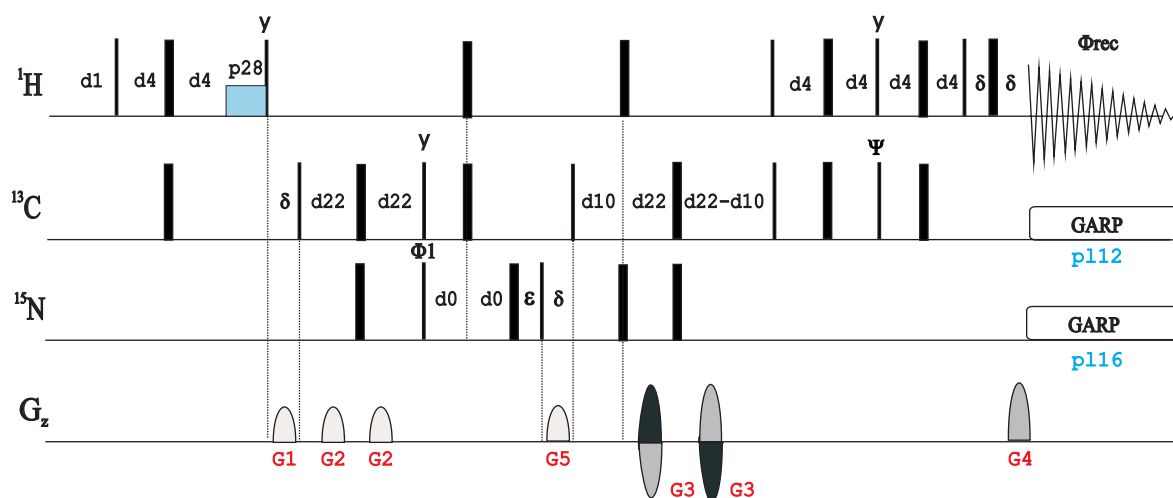


Related Experiments

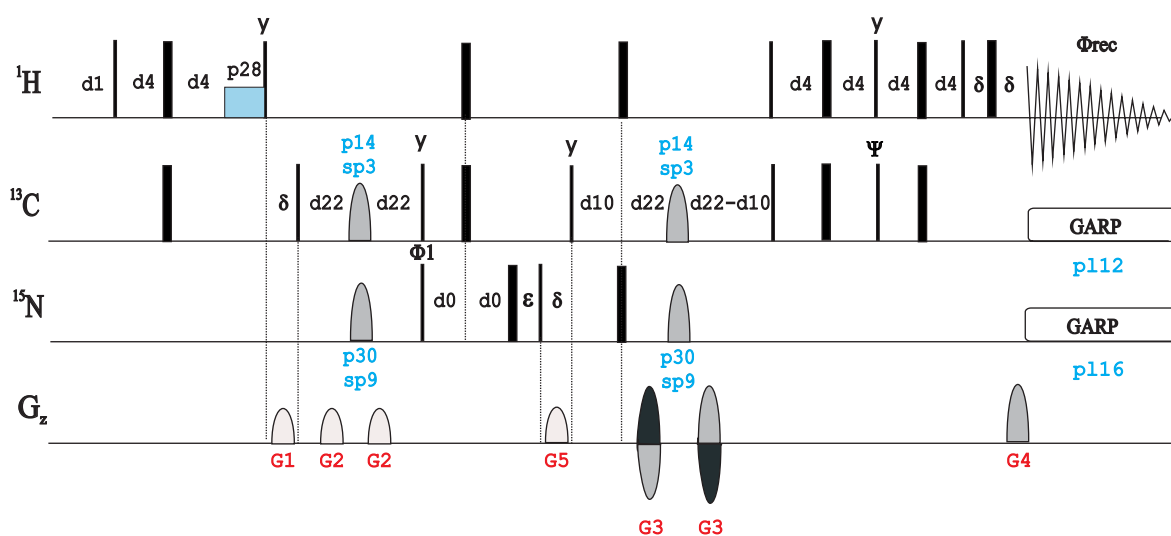
HCNCH
HCNH



na_hcnetgpsl3d

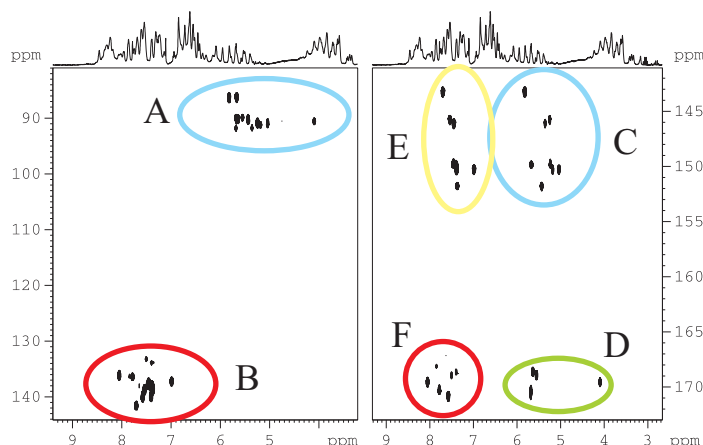


na_hcnetgpslsp3d

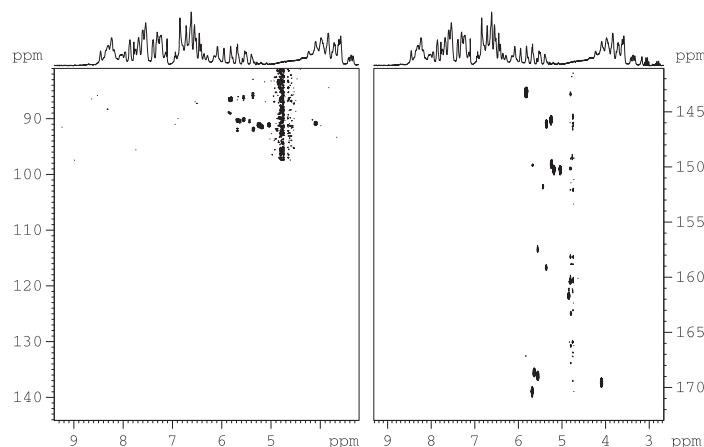


The 2D HC(N) plane can be separated in two areas: A) sugar area (blue) displaying the anomeric H1'-C1' correlations; and B) base area (red) displaying the olefinic H6C6(U,C) and H8C8(A,G) correlations.

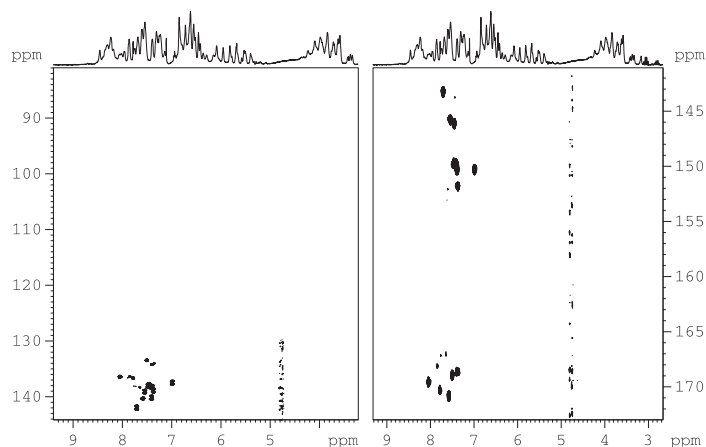
The 2D H(C)N plane displays four different sugar-to-base correlations C) H1'-to-N1(U,C) (blue area); D) H1'-to-N9(A,G) (green area); E) H6(U,C)-to-N1(U,C) (yellow area); and F) H8(A,G)-to-N9(A,G) (red area).



d1=1.5s
d4=1/4J(CH)=1.40ms for all J(HC) ,
 J(H8C8) and J(H6C6)
d22=1/4J(CN)=17.5ms for all J(N1C1'), J(N9C1'),
 J(N1C6), and J(N9C8)
p14=2.6ms (spnam3=q3_rna_c68c1.256)
o2p=113.45ppm
p30=700us(spnam9=Q3.1000)



d1=1.5s
d4=1/4J(CH)=1.56ms for J(H1'C1')
d22=1/4J(CN)=15ms for J(N1C1'), J(N9C1')
p14=1.0ms (spnam3=Q3.1000)
o2p=89.19ppm
p30=700us(spnam9=Q3.1000)
 Reduced SW in the C dimension=16.5ppm

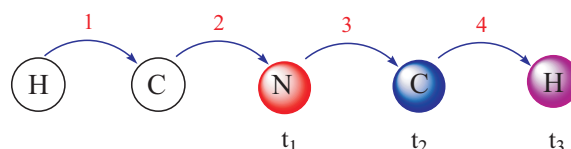


d1=1.5s
d4=1/4J(CH)=1.25ms for J(H8C8) and J(H6C6)
d22=1/4J(CN)=15ms for J(N1C6), and J(N9C8)
p14=1.0ms (spnam3=Q3.1000)
o2p=137.7ppm
p30=700us(spnam9=Q3.1000)
 Reduced SW in the C dimension=16.5ppm

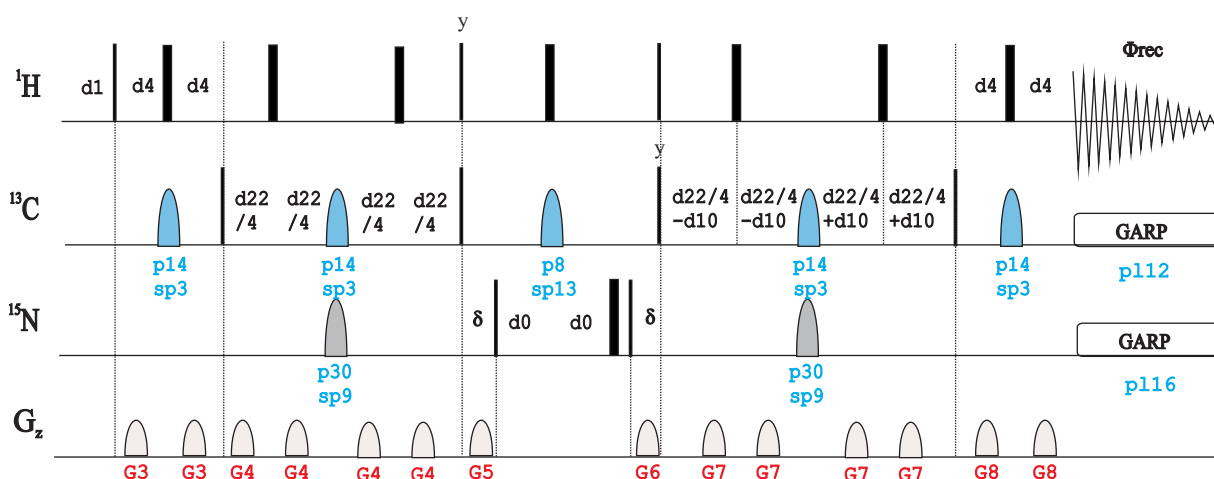
3D MQ-HCN Experiment

Experiment Description:

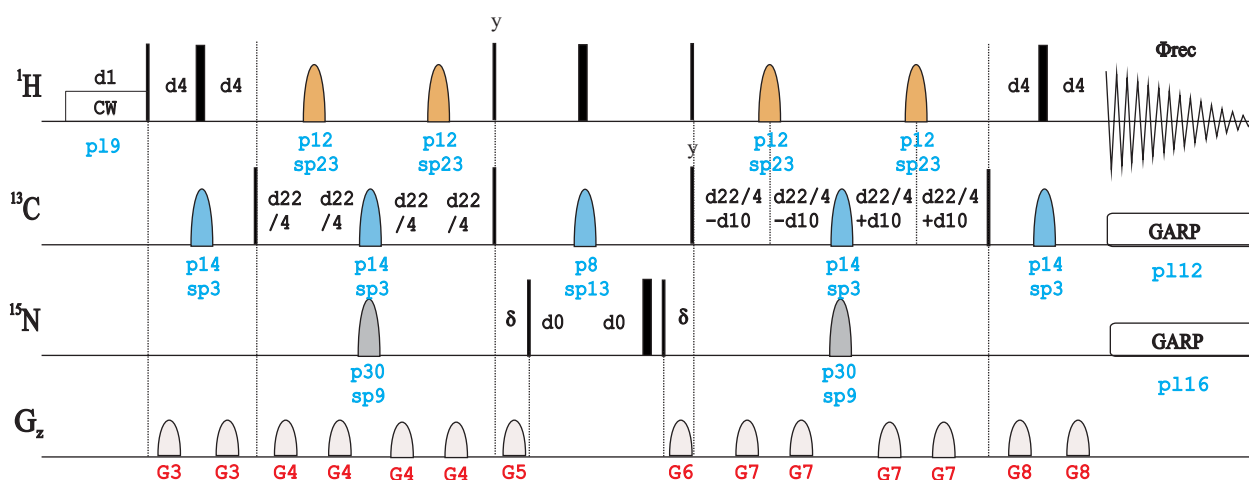
Version of the HCN experiment that involves multiple-quantum coherences (MQC) instead of SQC to enhance relaxation features.

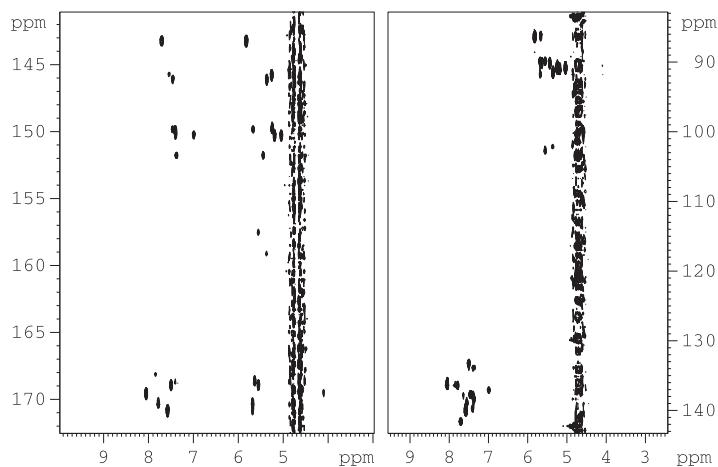


na_hcnmq3d

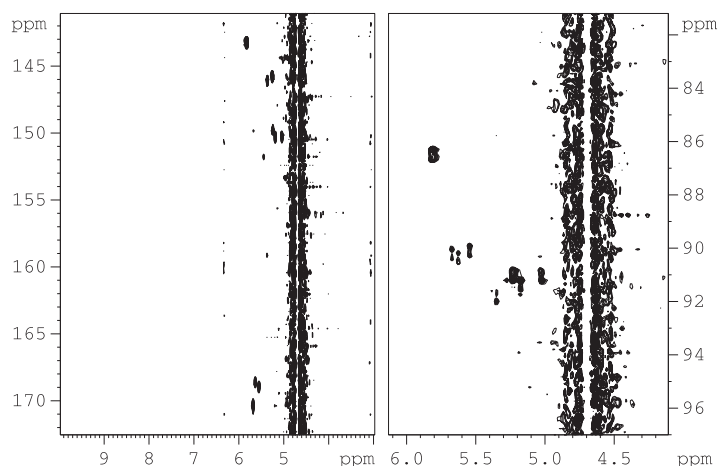


na_hcnmqsp3d

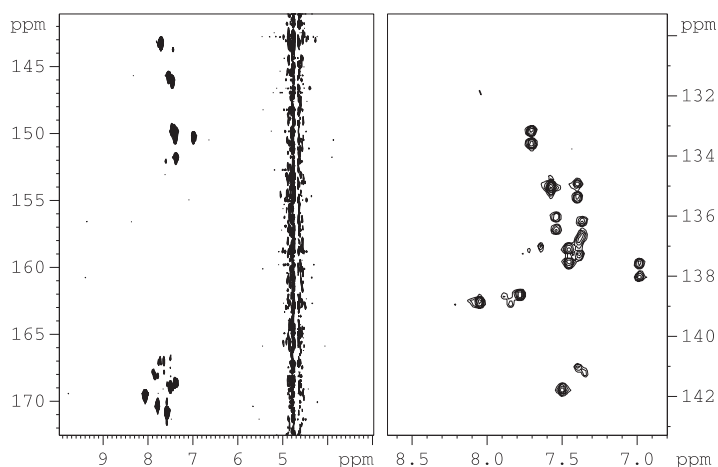




d1=1.5s
d4=1/4J(CH)=1.40ms for all J(H1'C1'), J(H8C8) and J(H6C6)
d22=1/4J(CN)=16.0ms for all J(N1C1'), J(N9C1'), J(N1C6), and J(N9C8)
p14=2.6ms (spnam3=q3_rna_c68c1.256)
o2p=113.45ppm
p30=700us(spnam9=Q3.1000)
p12=1.65ms (spnam23=reburp.1000)



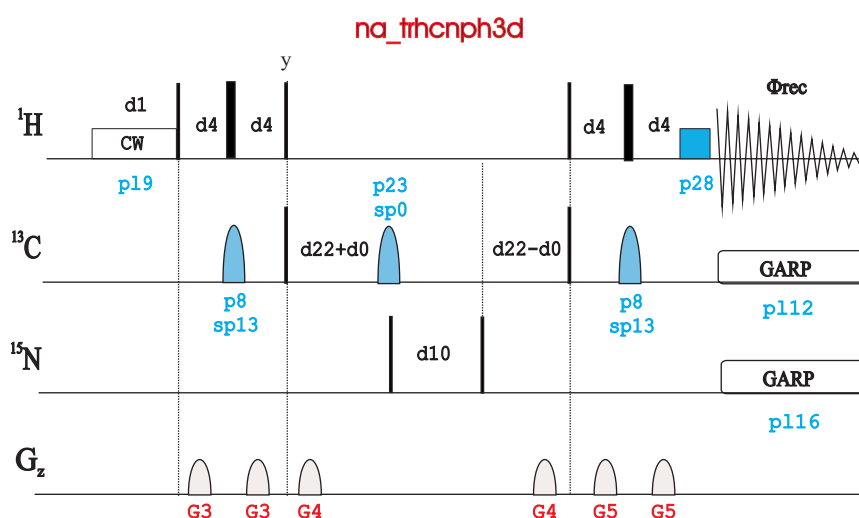
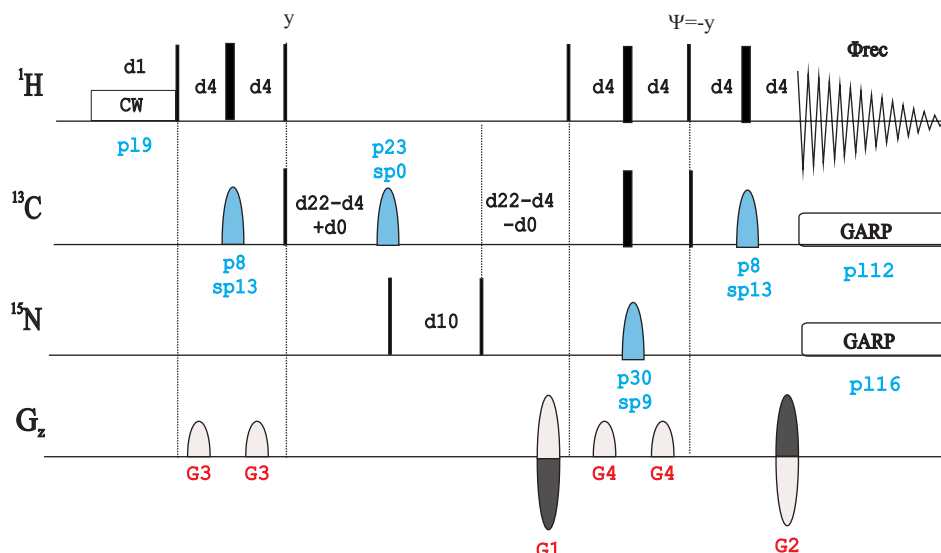
d1=1.5s
d4=1/4J(CH)=1.56ms for J(H1'C1')
d22=1/4J(CN)=16ms for J(N1C1'), J(N9C1')
p14=1.0ms (spnam3=Q3.1000)
o2p=89.19ppm
p30=700us(spnam9=Q3.1000)
p12=3.30ms (spnam23=reburp.1000)
Reduced SW in the C dimension=16.5ppm



d1=1.5s
d4=1/4J(CH)=1.25ms for J(H8C8) and J(H6C6)
d22=1/4J(CN)=16ms for J(N1C6), and J(N9C8)
p14=1.0ms (spnam3=Q3.1000)
o2p=137.7ppm
p30=700us(spnam9=Q3.1000)
p12=3.30ms (spnam23=reburp.1000)
Reduced SW in the C dimension=16.5ppm

Experiment Description:

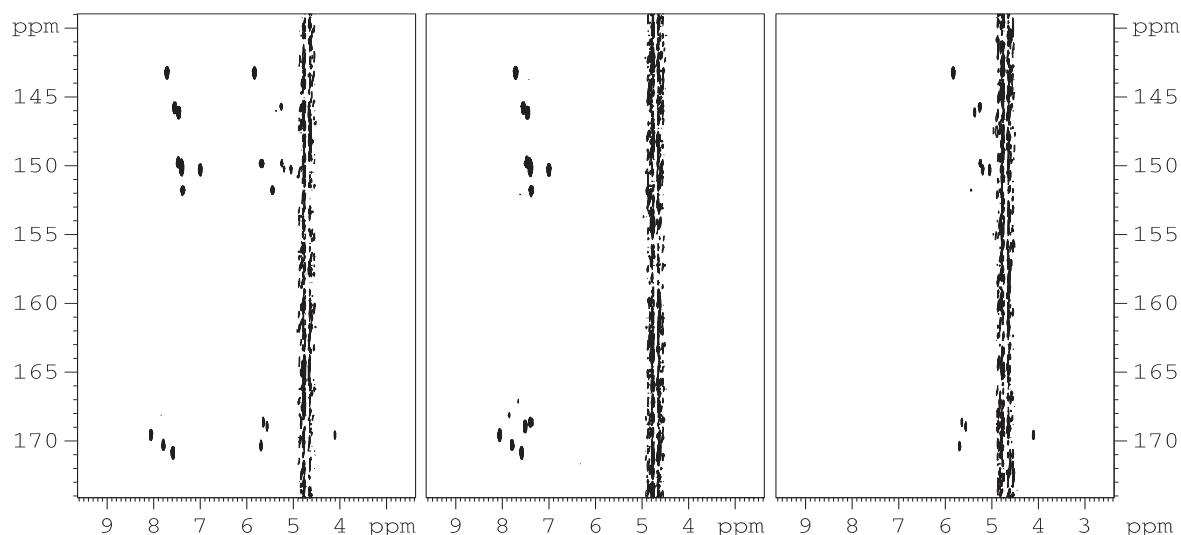
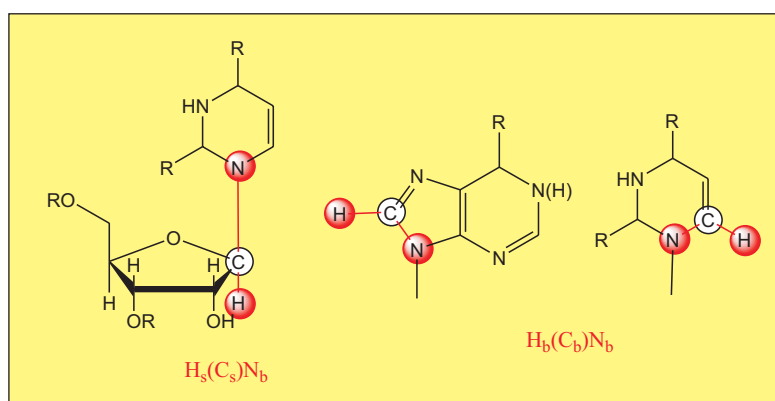
na trhcnet3d



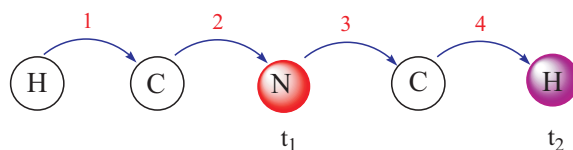
2D TROSY-H(C)N Experiment

Experiment Description:

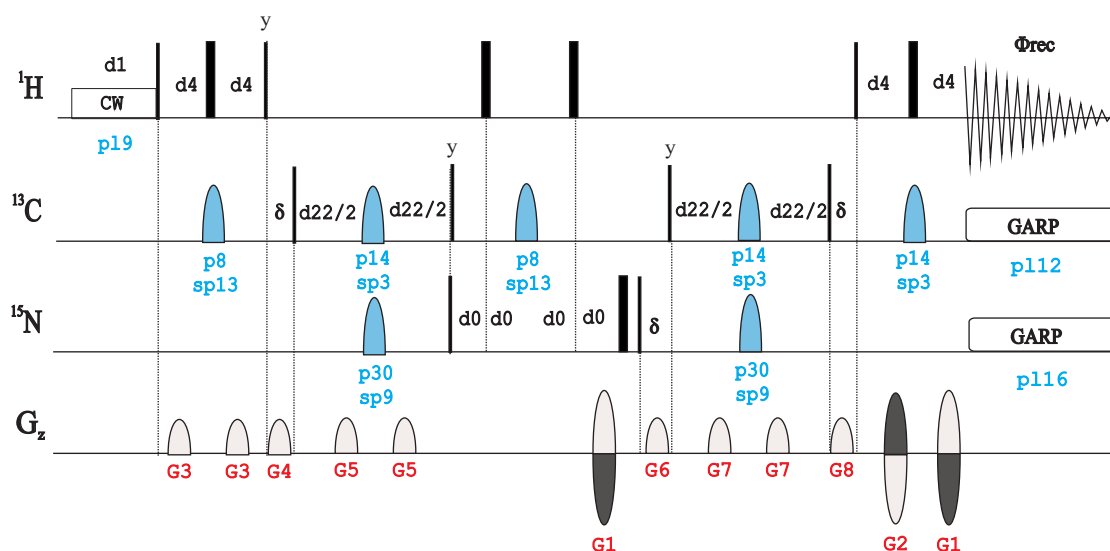
2D TROSY version of the HCN experiment in which the 2D H(C)N plane is obtained



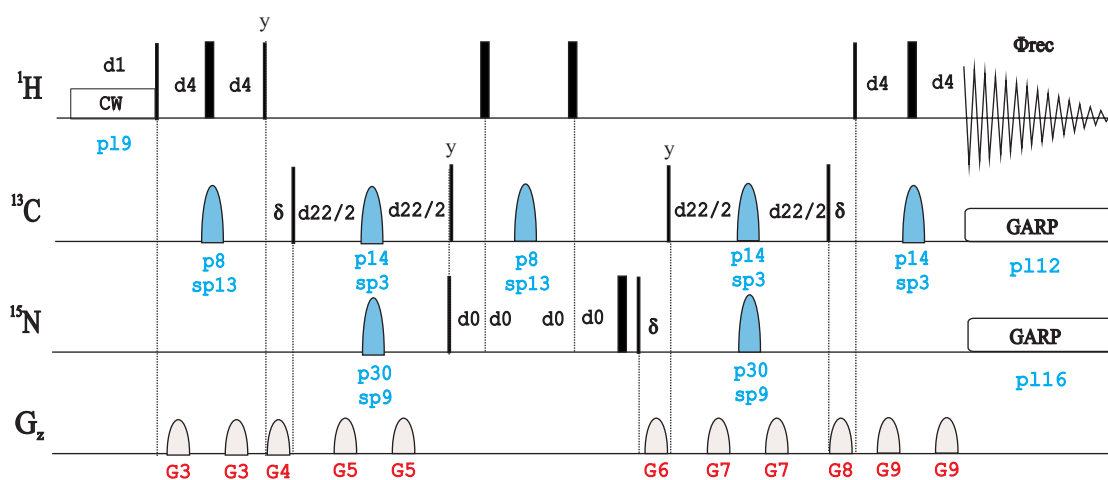
The same acquisition parameters as discussed
in the 3D HCN experiments



na_trhcnph



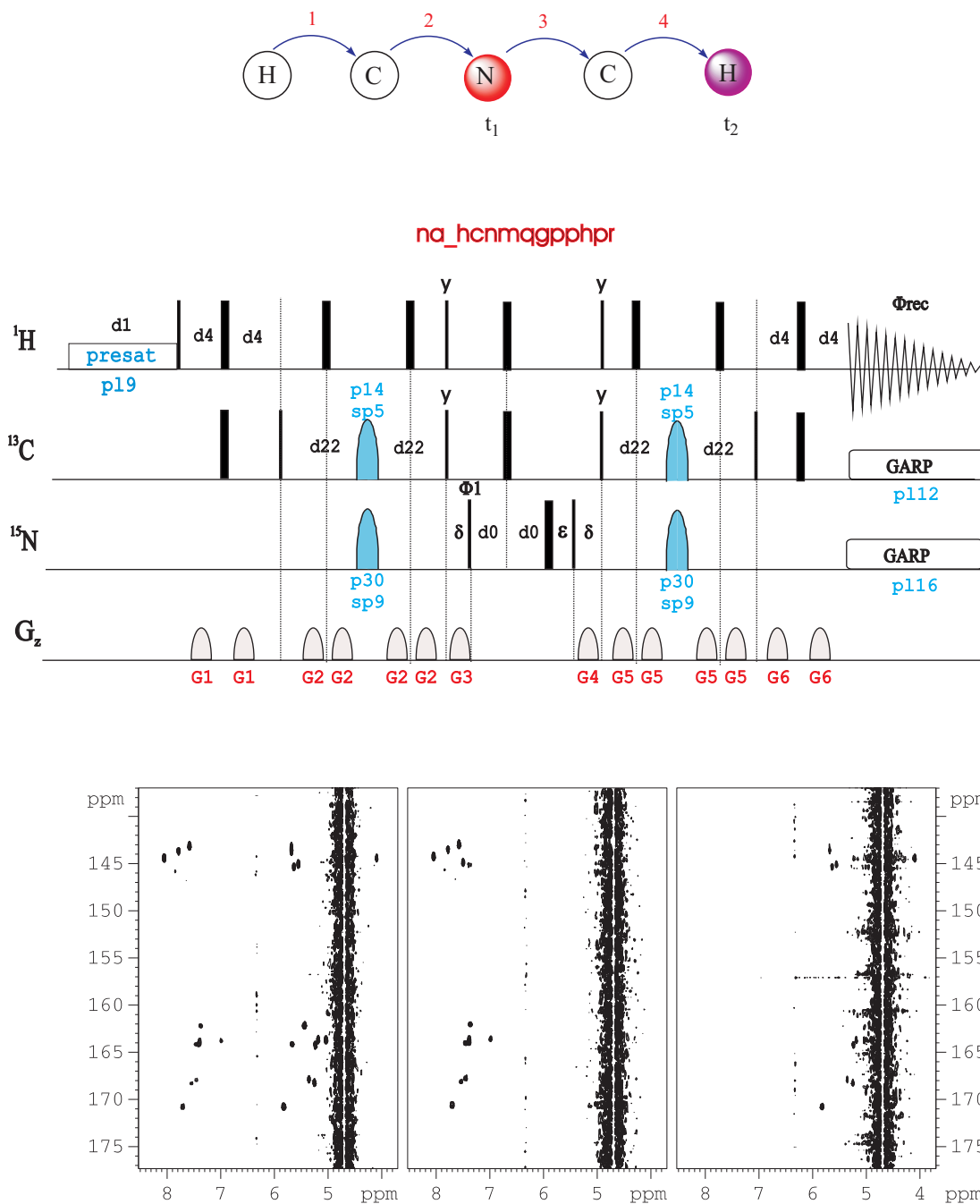
na_trhcnph



2D MQ-H(C)N Experiment

Experiment Description:

2D MQ version of the HCN experiment in which the 2D H(C)N plane is obtained

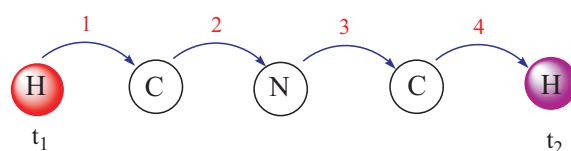
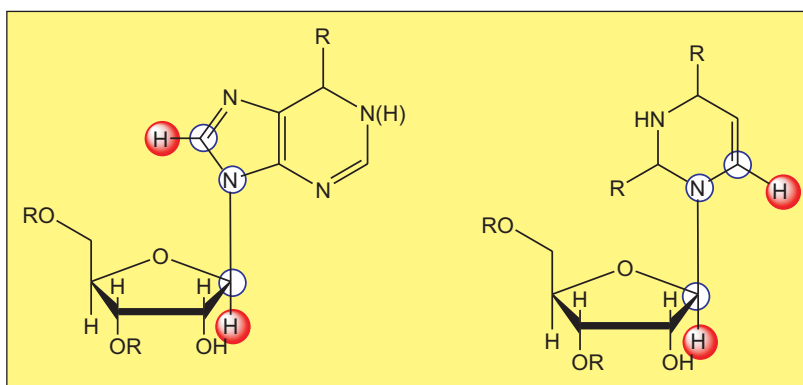


The same acquisition parameters as discussed
in the 3D HCN experiments

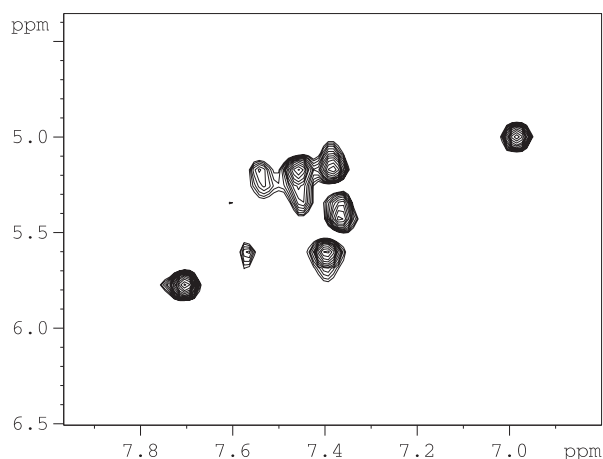
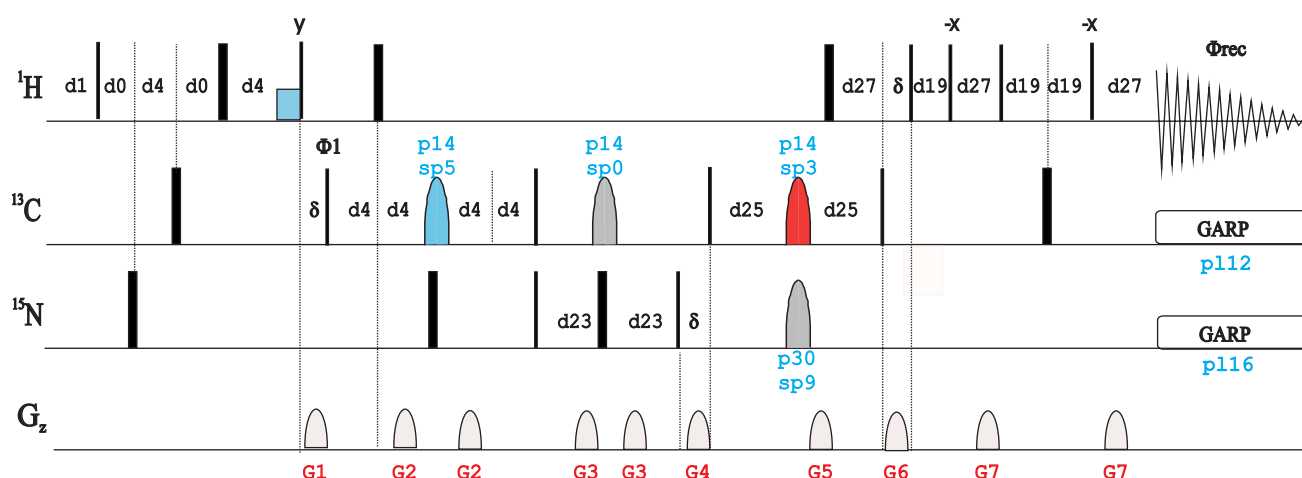
2D H(CNC)H Experiment

Experiment Description

2D version of the HCNCH experiment (93jacs12181) that allows to correlate the anomeric proton of the sugar ring with the H6/H8 of the connected base in isotopically labeled oligonucleotides.



na_hcnchgplrphsp

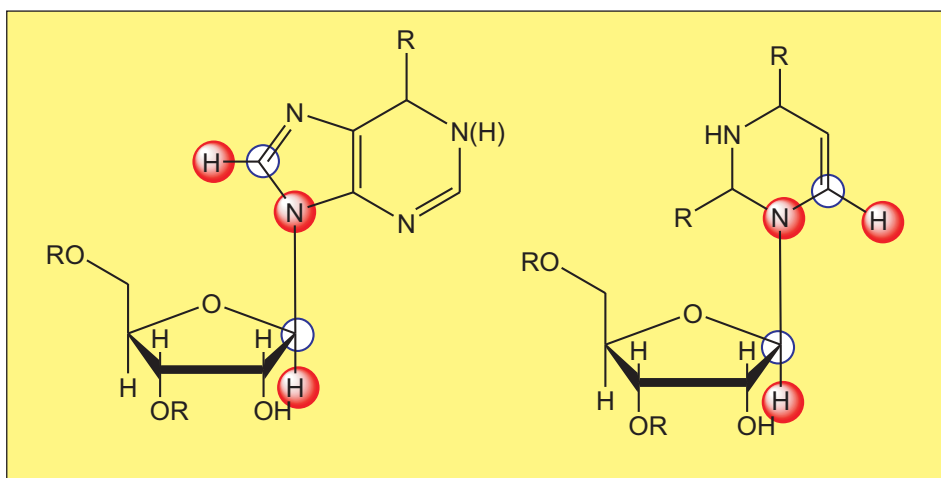


d1=1.5s
d4=1/4J(CH)=1.56ms
d23=1/4J(CN)=17ms
d25=1/4J(CN)=16ms
d27=1/4J(CH)=1.25ms
d19=134us
p14=1ms (spnam3=spnam5=Q3.1000
and spnam0=q3_rna_c68c1.1000)
o2p=113.5 ppm

3D H(C)N(C)H Experiment

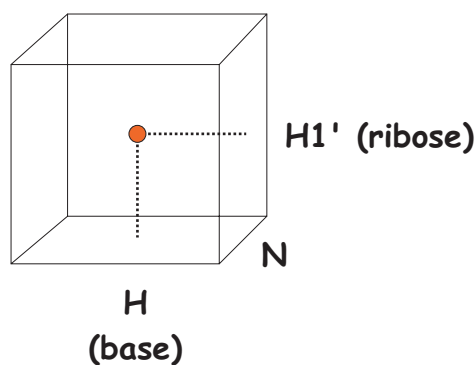
Experiment Description:

3D version of the HCNCH experiment (00jb291-16, 98jb373-12) that allows to correlate the two different HCN correlations observed in the HCN experiment. The experiment starts from the H1'-C1' ribose pair, N1/9 is allowed to evolve in an indirect dimension and finally the H6C6/H8C8 base proton is detected.



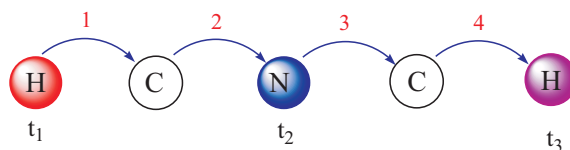
NMR Spectrum

The experiment provides a 3D correlation map

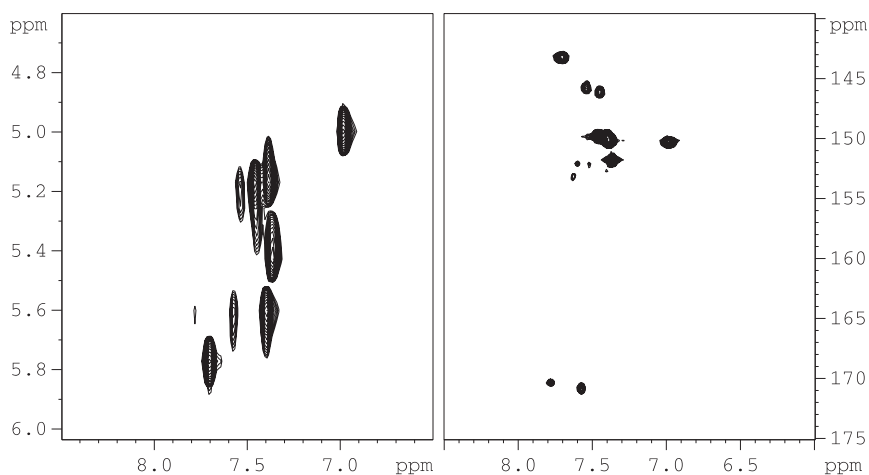
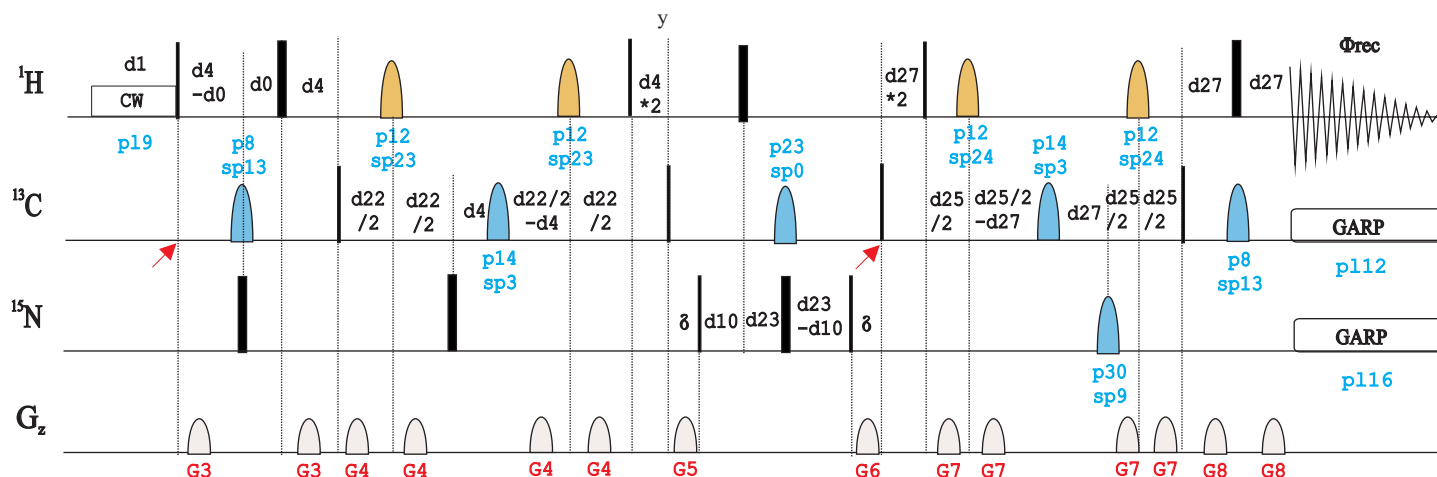


Related Experiments

HCN experiment

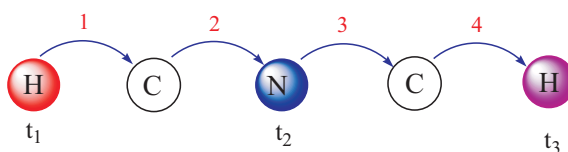


na_hcnchmqsp3d

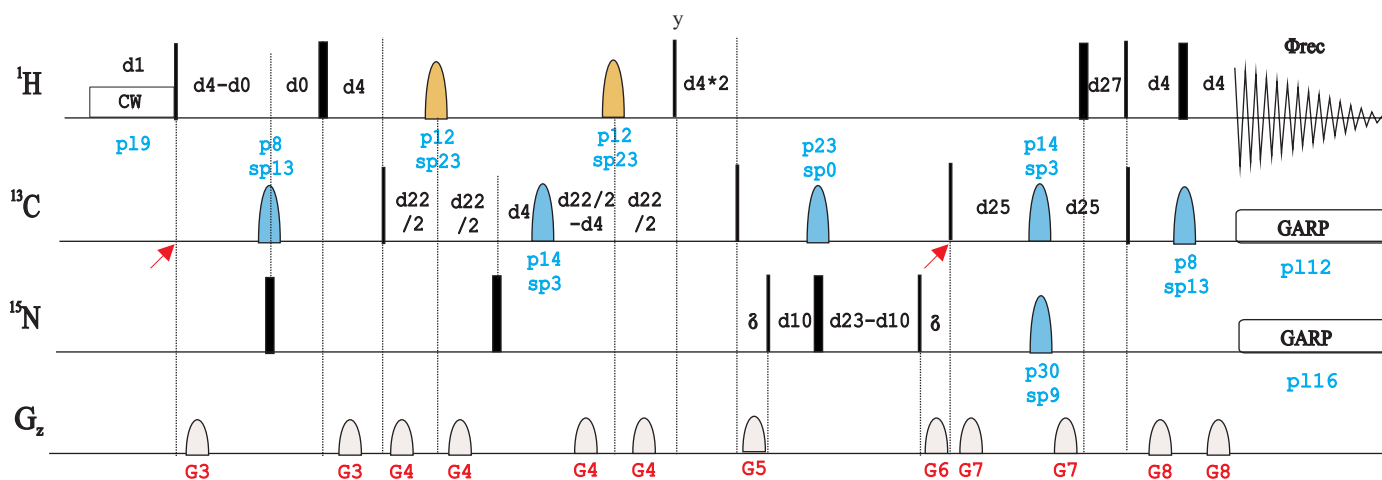


d1=1.5s
d4=1/4J(C1'H1')=1.6ms
d22=1/4J(C1'N)=18ms
d23=1/4J(C1'N, C6/8N)=17ms
d25=1/4J(C6/8N)=16ms
d27=1/4J(C6/8H6/8)=1.25ms
p12=3.3ms (spnam23=spnam24=reburp.1000)
p14=1ms (spnam3=spnam5=Q3.1000)
p23=0 (spnam0=q3_rna_c68c1.1000)
cnst21=89.19 (C1' chemical shift)
cnst22=137.7 (C6C(chemical shift)

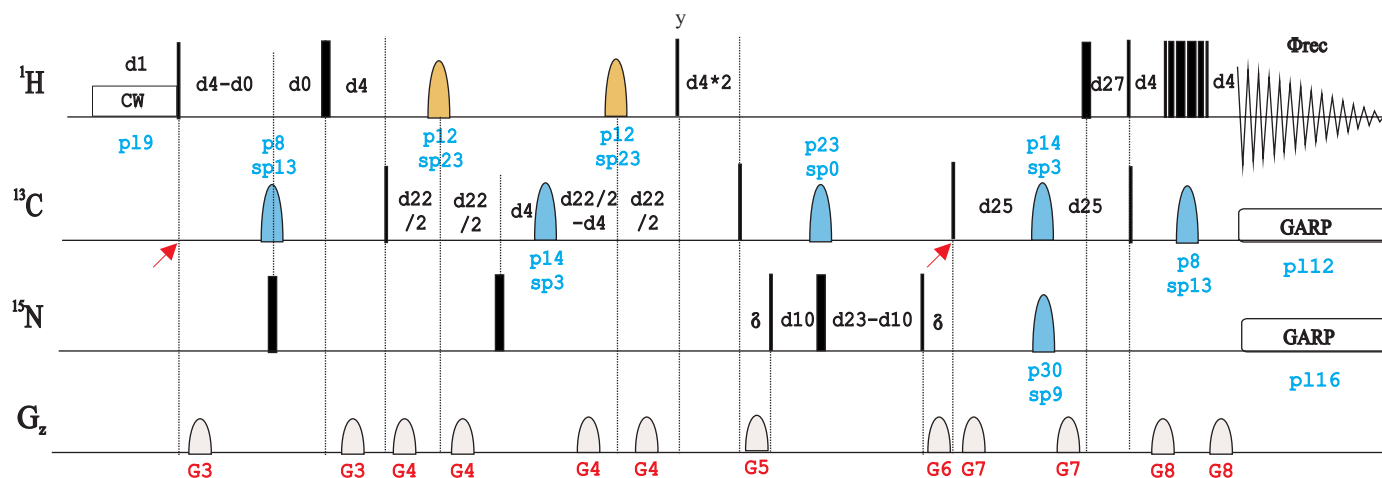
3D TROSY MQ-H(C)N(C)H Experiment



na_tthcnchmqsp3d



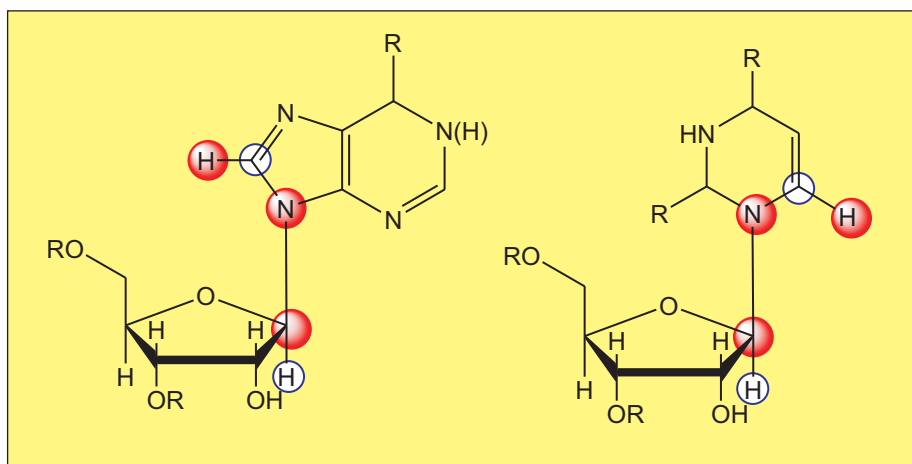
na_tthcnchmqspwg3d



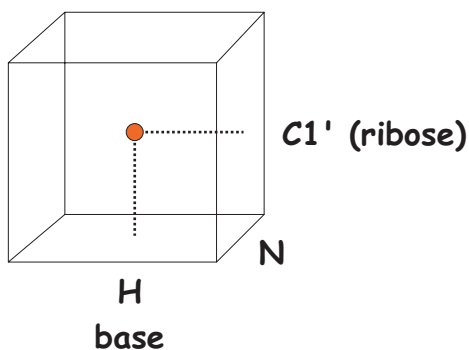
3D TROSY (H)CN(C)H Experiment

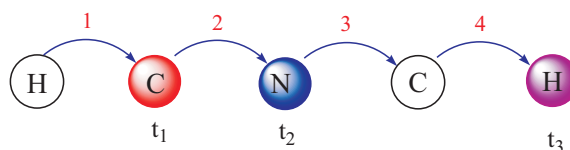
Experiment Description:

TROSY version of the 3D HCNCH experiment in which C1' chemical shift evolves instead of the H1' chemical shift.

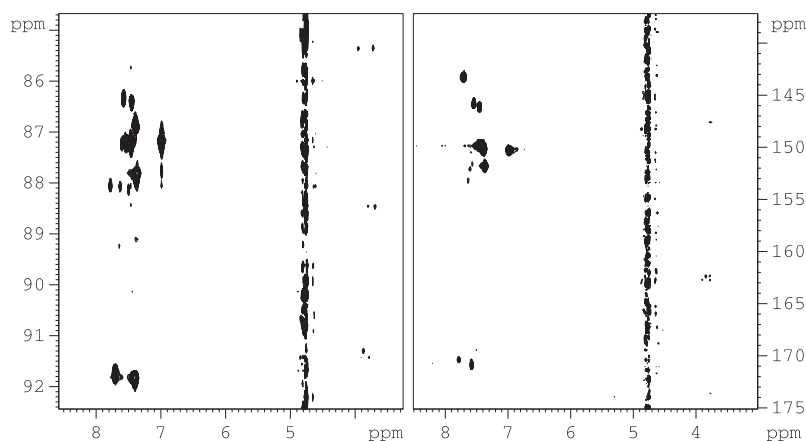
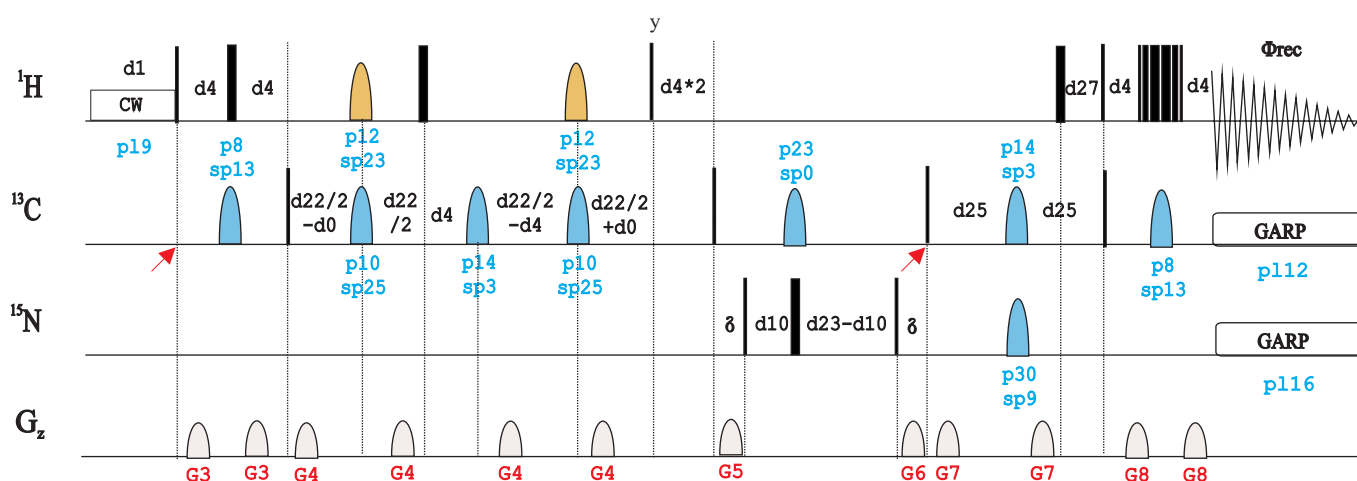


The experiment yields a 3D map correlation the sugar C1' carbon with the N1/N9 nitrogen and the H2/H8 protons of the connected base.





na_trhcnchmqspwg3d2

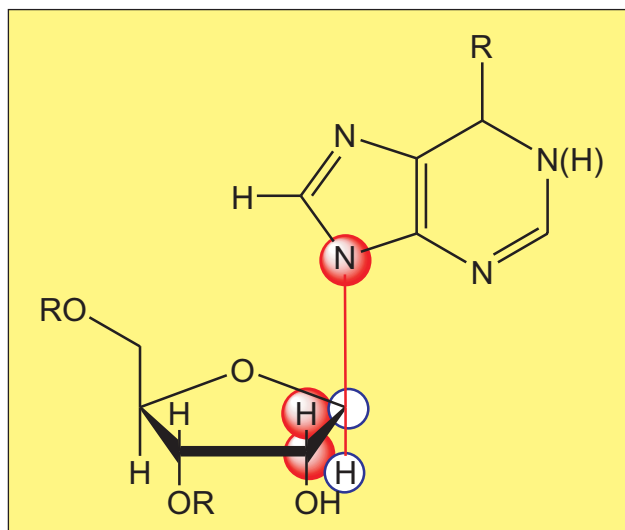


d1=1.5s
d4=1/4J(C1'H1')=1.6ms
d22=1/4J(C1'N)=18ms
d23=1/4J(C1'N, C6/8N)=17ms
d25=1/4J(C6/8N)=16ms
d27=1/4J(C6/8H6/8)=1.25ms
p12=3.3ms (spnam23=spnam24=reburp.1000)
p14=1ms (spnam3=spnam5=Q3.1000)
p23=0 (spnam0=q3_rna_c68c1.1000)
cnst21=89.19 (C1' chemical shift)
cnst22=137.7 (C6C8 chemical shift)
cnst23=72 (C2' chemical shift)

3D MQ-(HC)N(C)CH-COSY Experiment

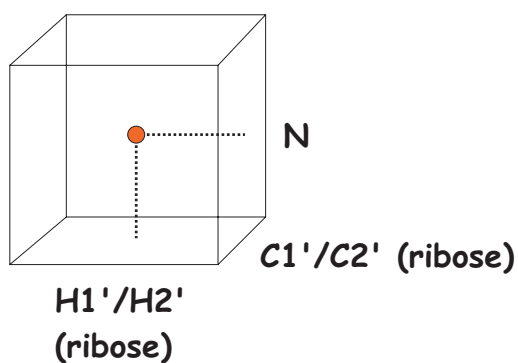
Experiment Description:

This experiment (HCN-CCH COSY) uses the good chemical shift dispersion of N1/N9 to assign the ribose spin system (00JMR147-145) via a C1' to C2' COSY transfer after an initial HCNC transfer.



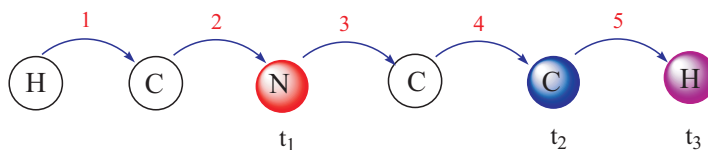
NMR Spectrum

The experiment provides a 3D correlation map

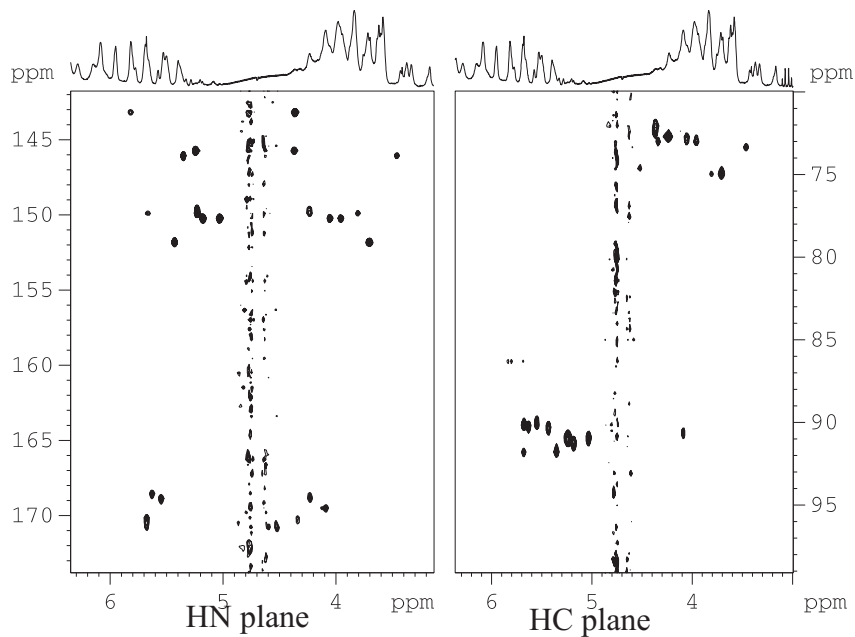
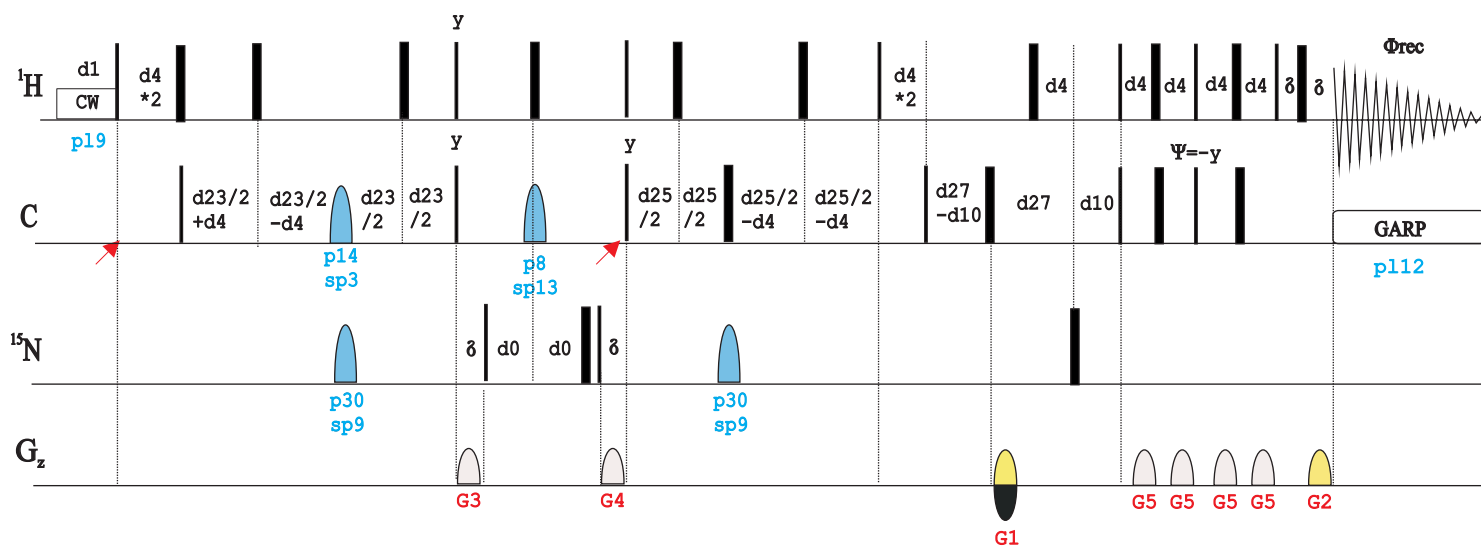


Related Experiments

HCN-CCH TOCSY



na_hnccchcomq3d

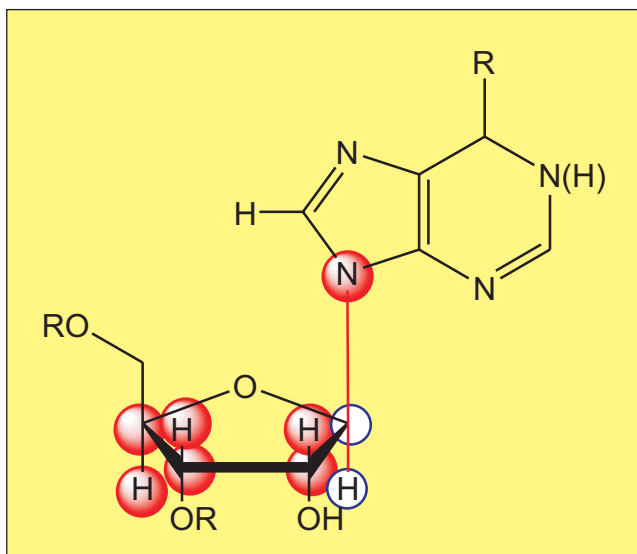


$d1=1.5\text{s}$
 $d4=1/4J(\text{C1}'\text{H1}')=1.56\text{ms}$
 $d23=1/4J(\text{C1}'\text{N})=18\text{ms}$
 $d25=1/4J(\text{C1}'\text{N})=15\text{ms}$
 $d27=1/8J(\text{C1}'\text{C2}')=3.25\text{ms}$
 $\text{cnst21}=\text{C1}' \text{ chemical shift}=90\text{ppm}$
 $\text{cnst23}=\text{C2}' \text{ chemical shift}=72 \text{ ppm}$
 $\text{o2p}=79\text{ppm}$
 $\text{p14}=1\text{ms} (\text{spnam3}=\text{Q3.1000})$
 $\text{o3p}=160 \text{ ppm}$
 $\text{p30}=700\text{us} (\text{spnam9}=\text{Q3.1000})$

3D MQ-(HC)N(C)CH-TOCSY Experiment

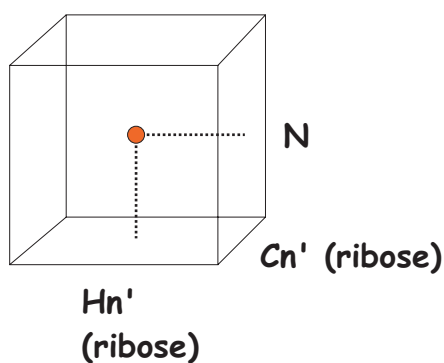
Experiment Description:

This experiment (HCN-CCH TOCSY) uses the good chemical shift dispersion of N1/N9 to assign the ribose spin system (00JMR147-145) via a C1' to Cn' TOCSY transfer after an initial HCNC transfer.



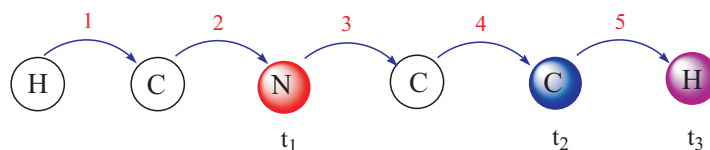
NMR Spectrum

The experiment provides a 3D correlation map

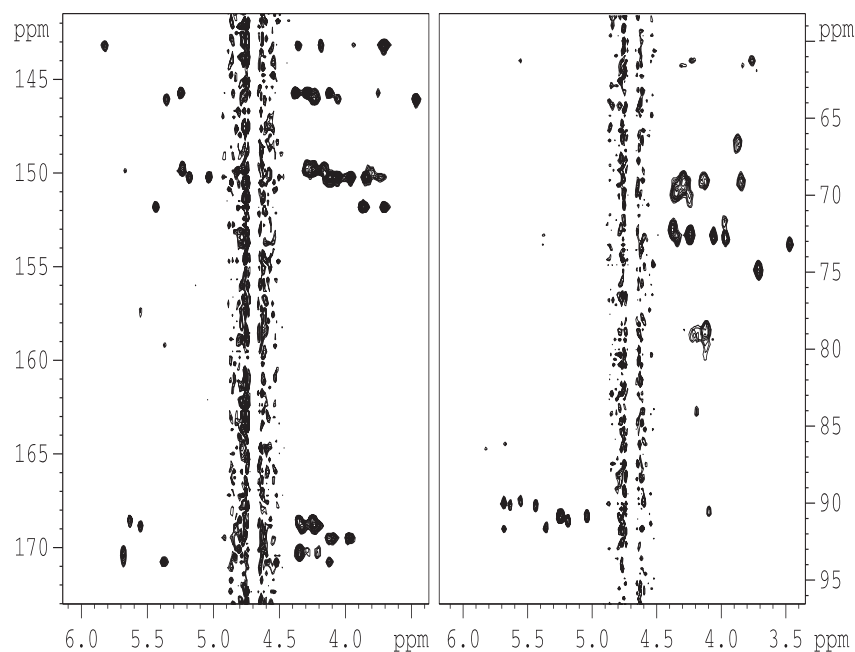
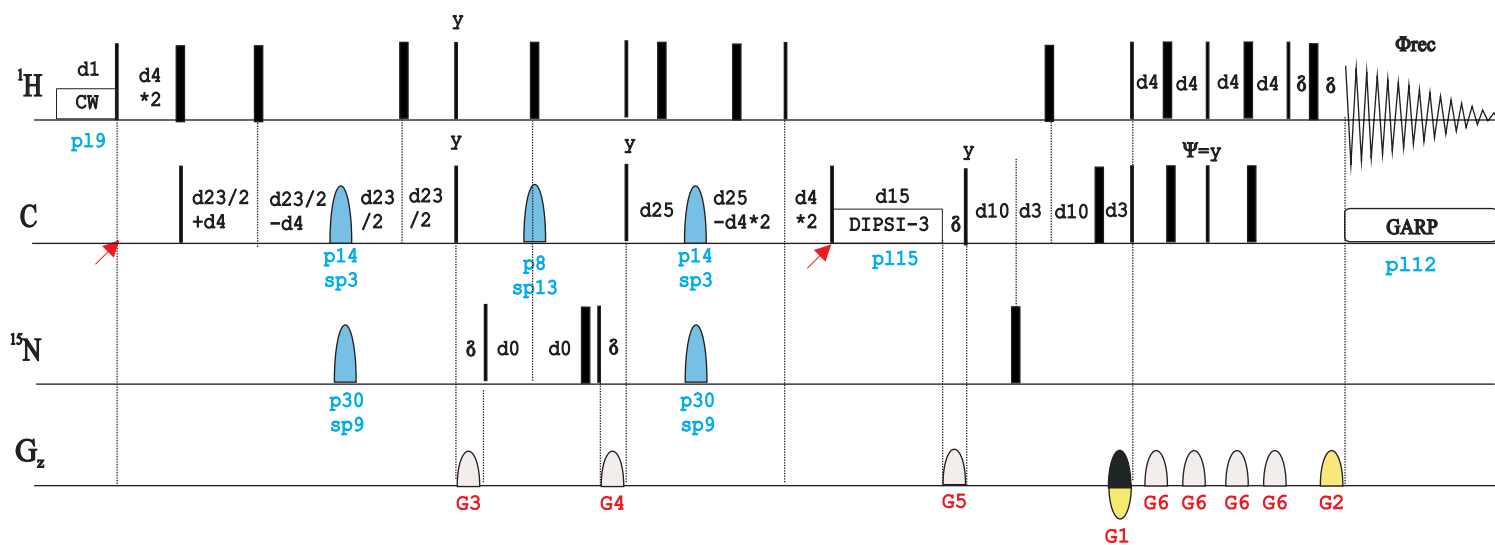


Related Experiments

HCN-CCH COSY



na_hnccchdlmq3d

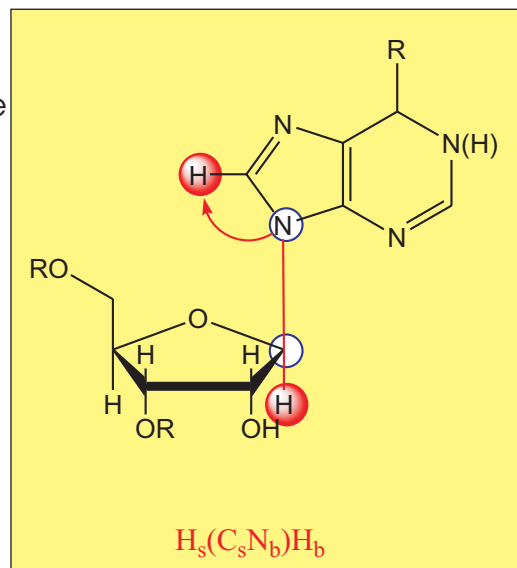
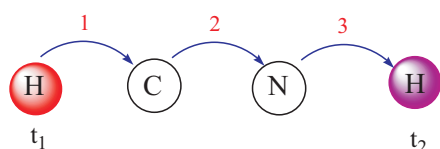


`d1=1.5s`
`d4=1/4J(C1'H1')=1.56ms`
`d3=1/4J(C'H')=0.95ms`
`d15=CC TOCSY= 12 ms`
`d23=1/4J(C1'N)=18ms`
`d24=1/8J(C'H')=0.78ms`
`d25=1/4J(C1'N)=15ms`
`d27=1/8J/C1'C2')=3.25ms`
`cnst21=C1' chemical shift=90ppm`
`cnst23=C2' chemical shift=72 ppm`
`o2p=79ppm`
`p14=1ms (spnam3=Q3.1000)`
`o3p=160 ppm`
`p30=700us (spnam9=Q3.1000)`

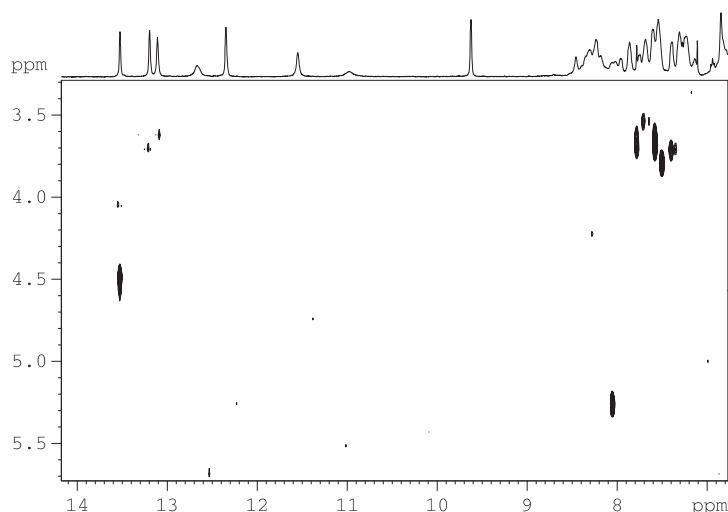
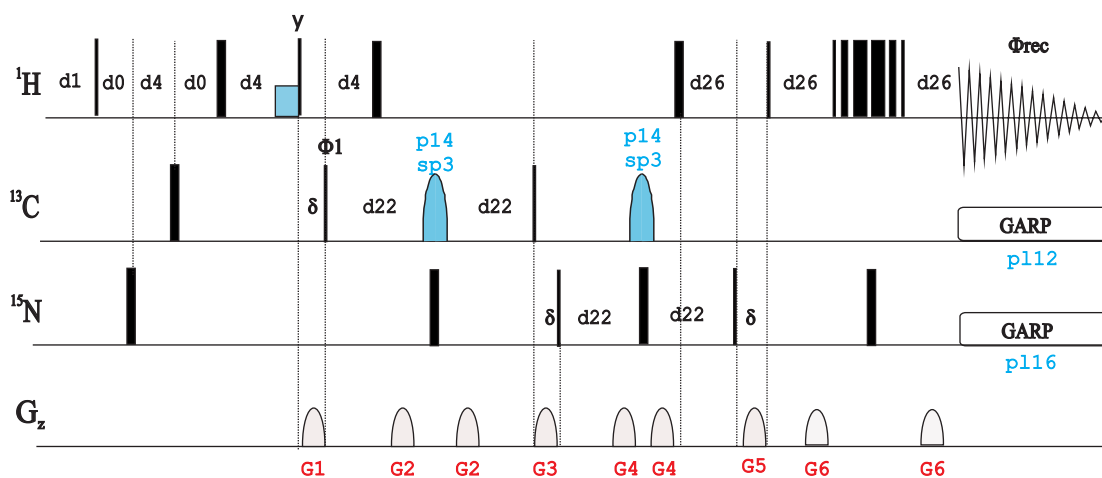
2D H(CN)H Experiment

Experiment Description:

Experiment alternative to the HCNCH experiment that allows to correlate the H1' ribose proton with the base H6/8 protons via $2J(N1/9-H6/8)$ coupling constant.



na_hcnhgpph19

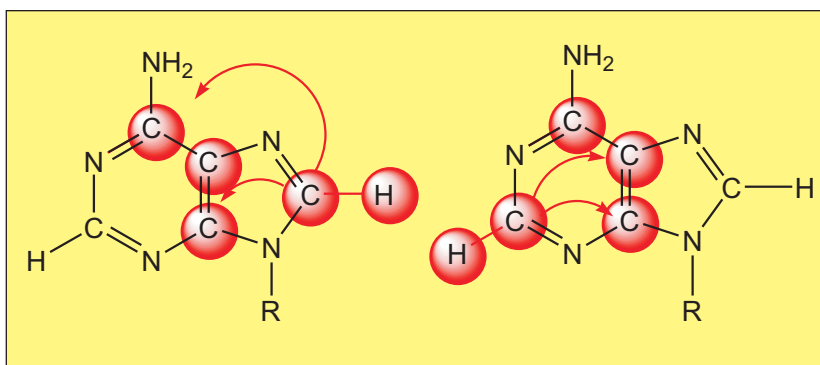


d1=1.5s
d4=1/4J(CH)=1.56ms
d22=1/4J(CN)=18.0ms
d26=1/4J(NH)=15ms (long-range)
p14=1ms (spnam3=Q3.1000)
o2p=89.19ppm

3D TROSY-(H)CCH-COSY Experiment

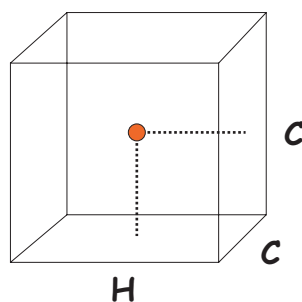
Experiment Description:

Experiment that correlates the adenine H2 and H8 protons in ^{13}C -labeled NAs molecules. The experiment provides ^{13}C chemical shifts of all carbon nuclei in the adenine base and also the long-range H8-C4/C5/C8 correlation in guanines (01jb173-20).



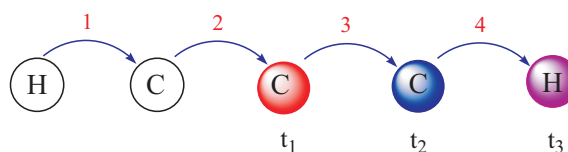
NMR Spectrum

The experiment provides a 3D correlation map

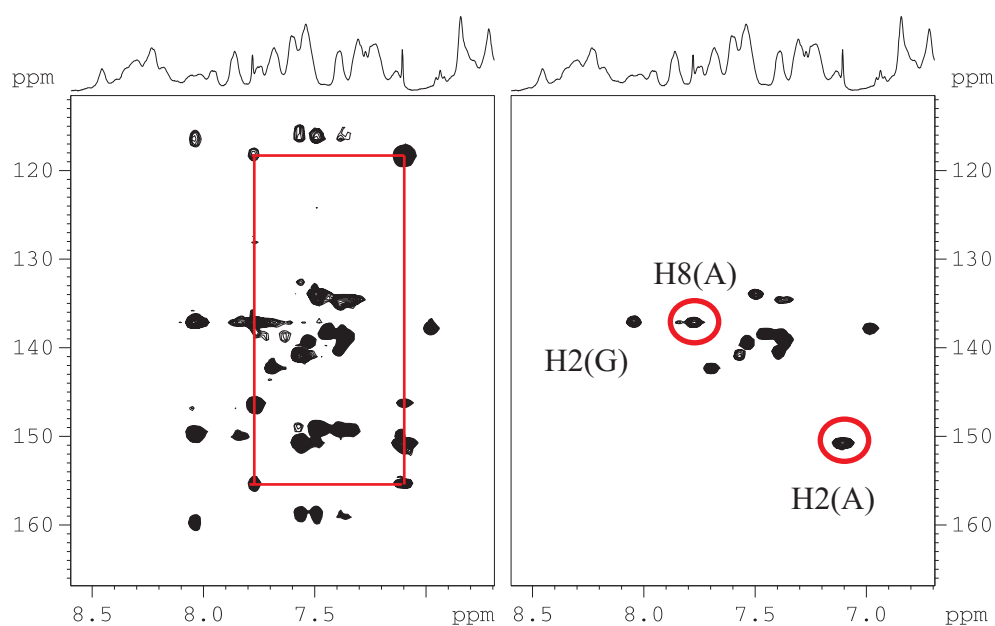
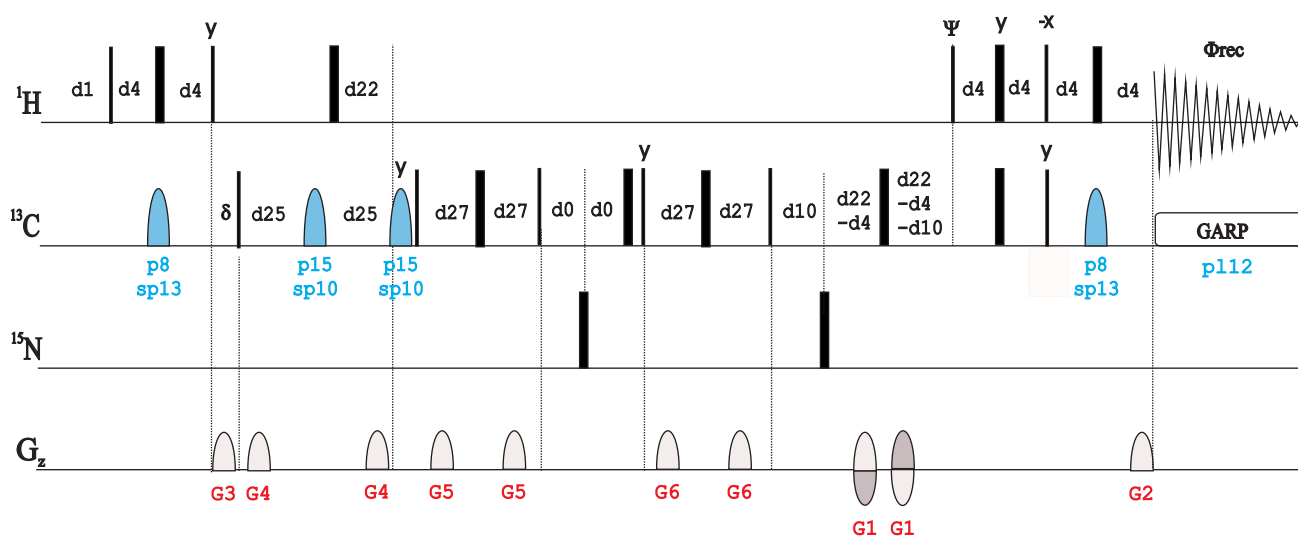


Related Experiments

2D ^1H - ^{13}C HMBC



na_trhchco3d

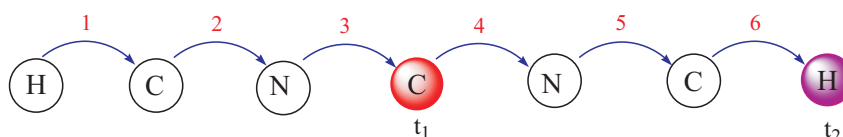
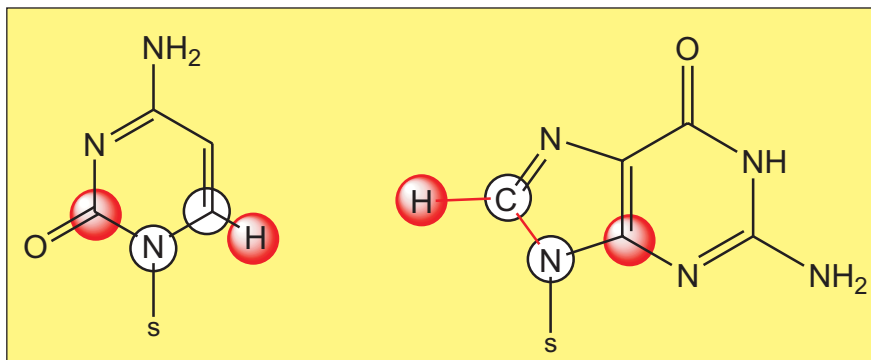


d1=1.5s
d4=1.25ms
cnst28=4.69 C5 offset
d22=1/4J(C2C5) and
1/4(C8C4/C6)=14.2ms
d25=1/2J(C5C6)=7.12ms
d27=1/4J(C5C4/C6)=1ms
o2p=140ppm
p15=90 pulse C5 off-resonance

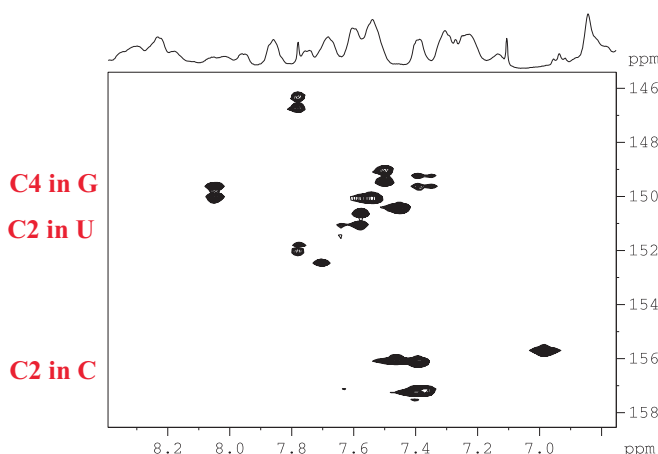
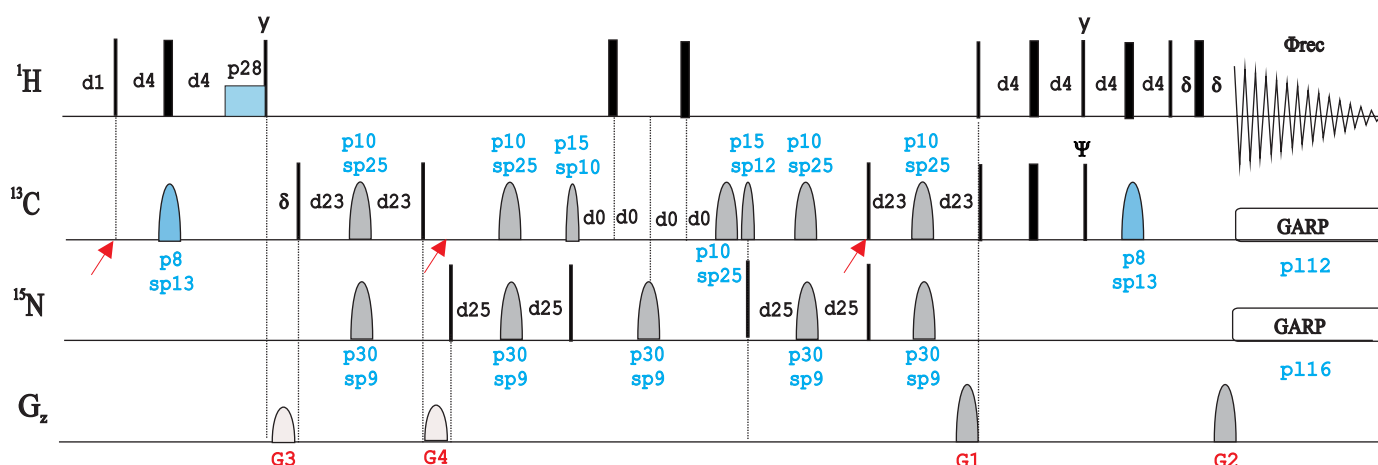
2D H(CN)C Experiment

Experiment Description:

The H(CN)C experiment (also referred as H(6/8)C(6/8)N(1/9)C(2/4)) correlates the aromatic H6/8 protons of the base with the non-protonated C2/4 carbons via the C6/8 and N1/9 centers (04jb69-28).



na_h68c68n19c42



d1=1.5s
d4=1/4J(CH)=1.25ms for J(H8C8) and J(H6C6)
d23=1/4J(CN)=15ms for J(N1C6), and J(N9C8)
d25=1/4J(CN)=15ms for J(N1C2), and J(N9C4)
o2p=cnst27=152ppm
cnst22=137.7=chemical shift C6(CU)/C8(AG)
p30=700us(spnam9=Q3.1000)
p10=
p15=
Reduced SW in the C dimension=16.5ppm

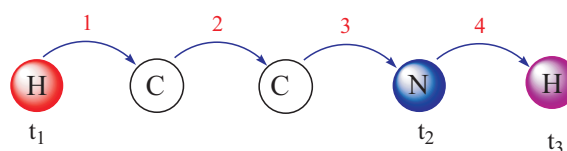
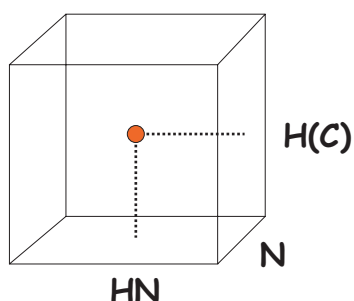
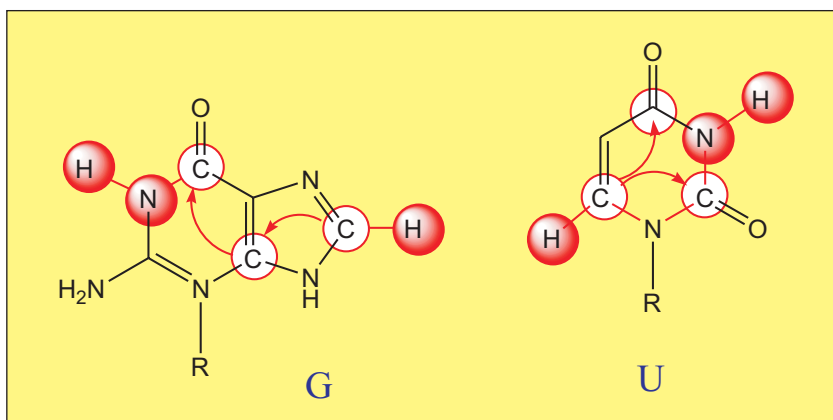
3D H(6/8)(CCC)NH Experiment

Experiment Description:

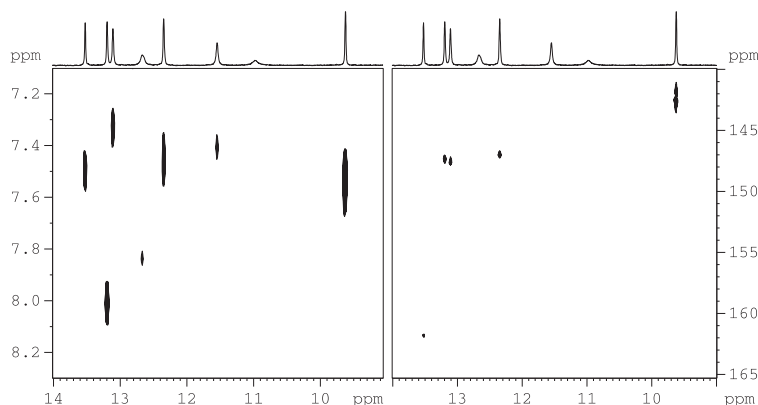
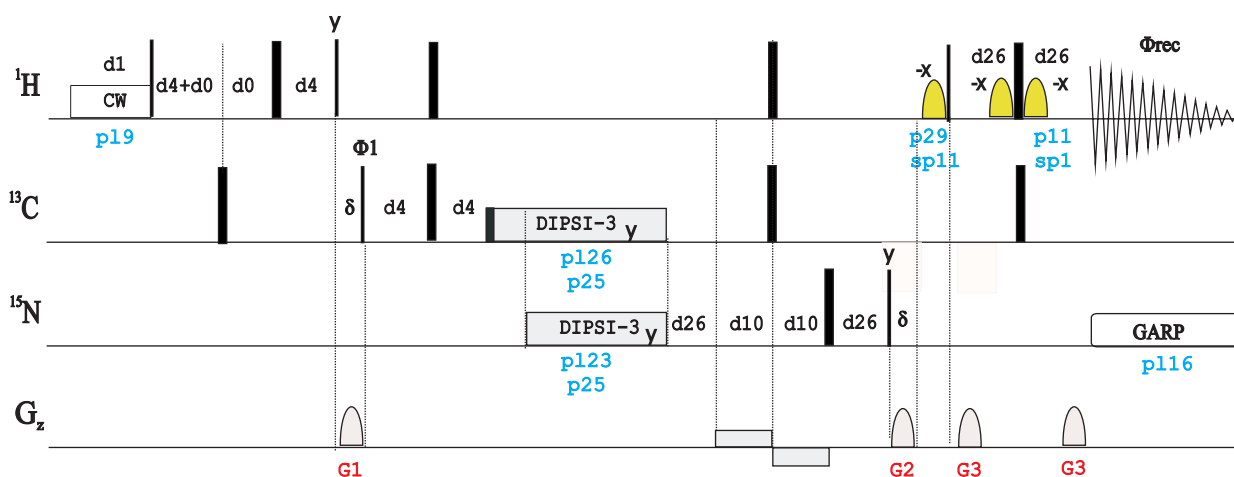
The HCCNH-TOCSY experiment allows the correlation between the exchangeable imino NH groups with H8 in guanines and H6 in uridines.

NMR Spectrum

The experiment provides a 3D correlation map



na_hccnhdlgpgw3d

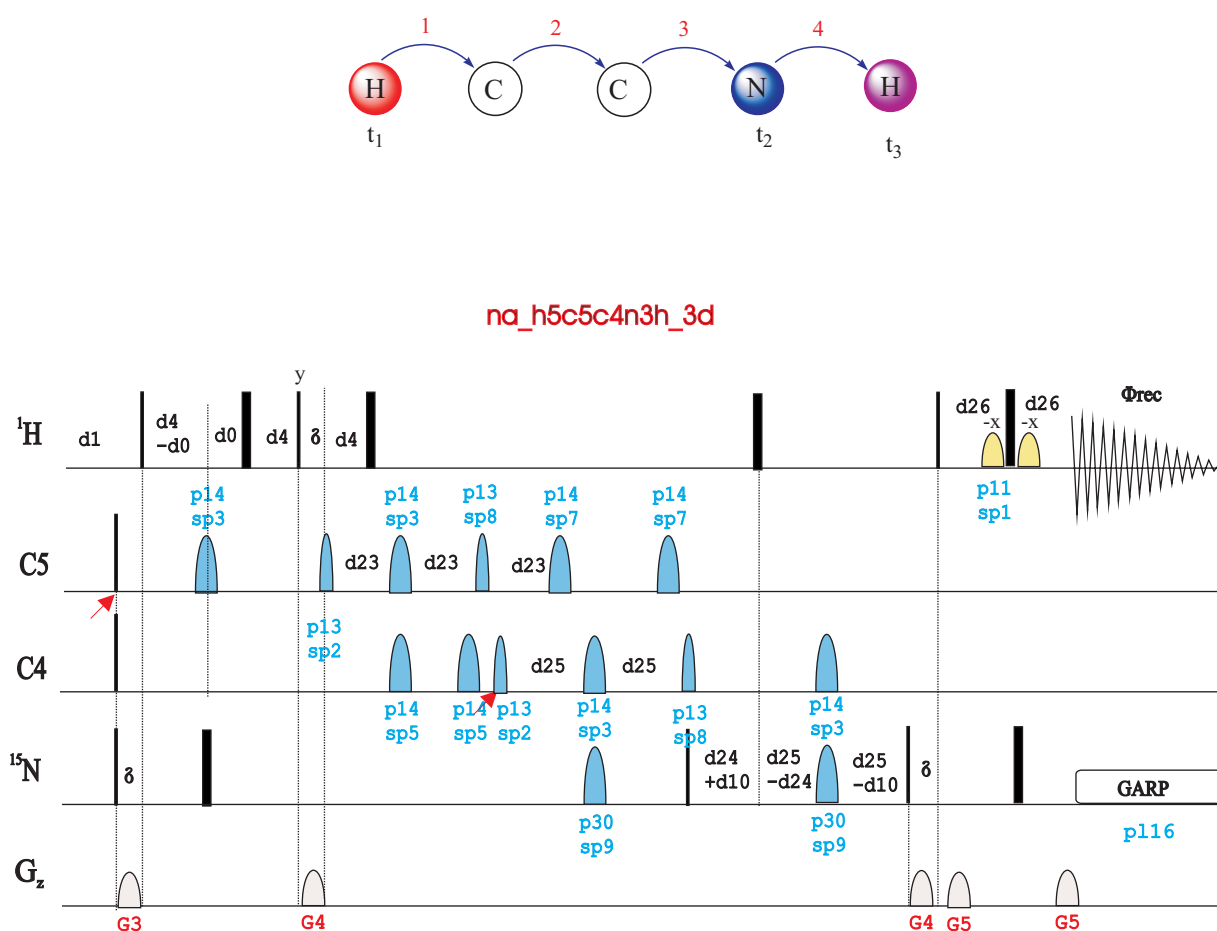


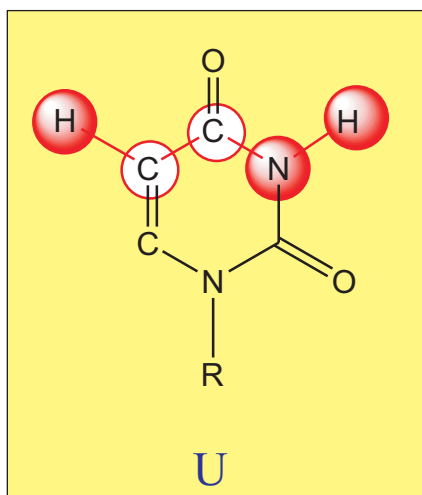
d1=1.5s
d4=1/4J(CH)=12.5ms
optimized for cnst2=200Hz
d26=1/4J(NH)=2.77ms
optimized for cnst4=90Hz
p29=p11=1ms (Squa100.1000)
p25=245us
l1=1
l1=3
o2p=149 ppm

3D H(CC)NH-COSY Experiment

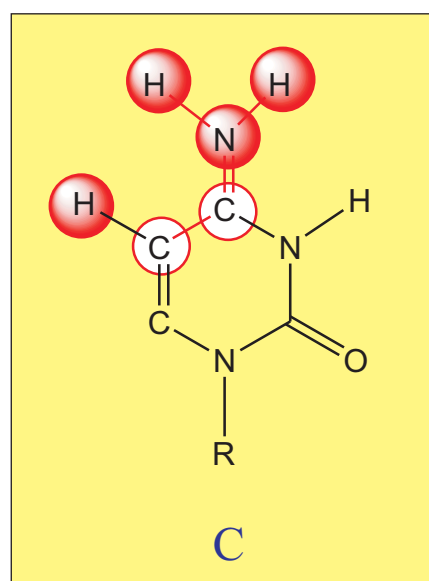
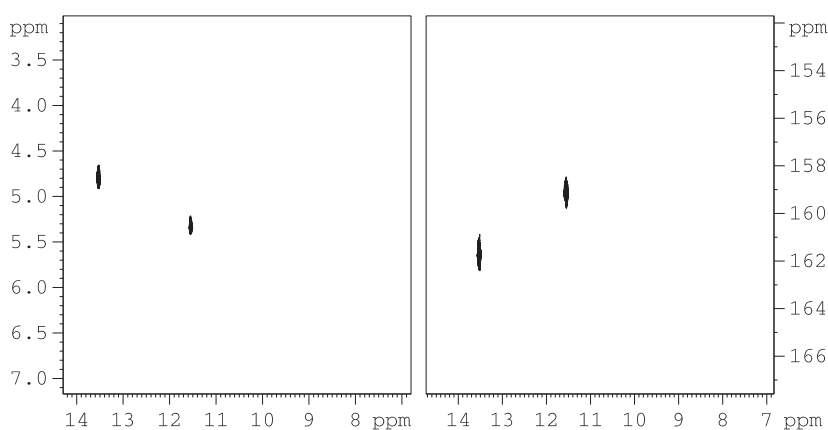
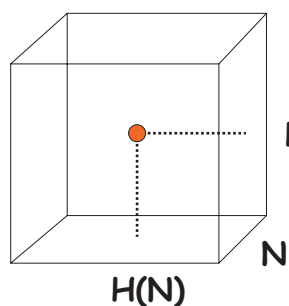
Experiment Description:

The HCCNH experiment allows the correlation of the exchangeable NH and NH₂ spin systems with the H5 and H6 protons in U and C via a CC COSY transfer (99JMR430-139). The experiment starts from the aromatic CH spin system and detects H(N). It can be separately optimized for imino NH or for amino NH₂ groups.

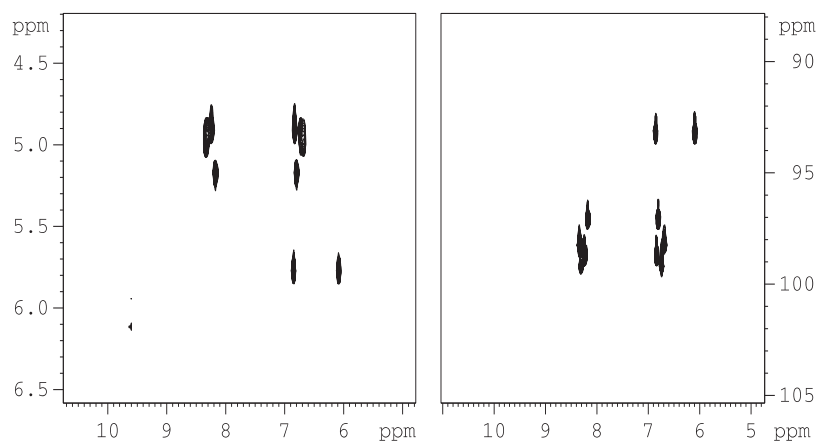




d1=1.5s
d4=1/4J(C5H5)=1.25ms
d23=1/4J(C5C4)=4.1ms
d24=1/4J(NH) for U=2.78ms
d25=1/4J(C4N)=10ms
d26=1/4J(NH)=2.5ms
p11=1 ms (spnam1=Squa100.1000)
p13=1ms (spnam2=Q5.1000 and spnam8=Q5tr.1000)
p14=1ms (spnam3/5/7=Q3.1000)
cnst24=C4(C/U) chemical shift=169ppm
cnst28=C5(C/U) chemical shift=105ppm
o3p=160ppm (for U)
p30=700us (spnam9=Q3.1000)



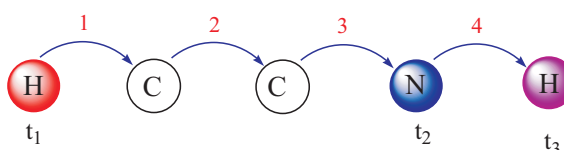
d1=1.5s
d4=1/4J(C5H5)=1.25ms
d23=1/4J(C5C4)=4.1ms
d24=1/8J(NH) for C=1.39ms
d25=1/4J(C4N)=10ms
d26=1/4J(NH)=2.5ms
p11=1 ms (spnam1=Squa100.1000)
p13=1ms (spnam2=Q5.1000 and spnam8=Q5tr.1000)
p14=1ms (spnam3/5/7=Q3.1000)
cnst24=C4(C/U) chemical shift=169ppm
cnst28=C5(C/U) chemical shift=105ppm
o3p=100ppm (for C)
p30=700us (spnam9=Q3.1000)



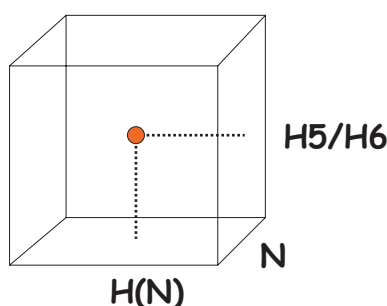
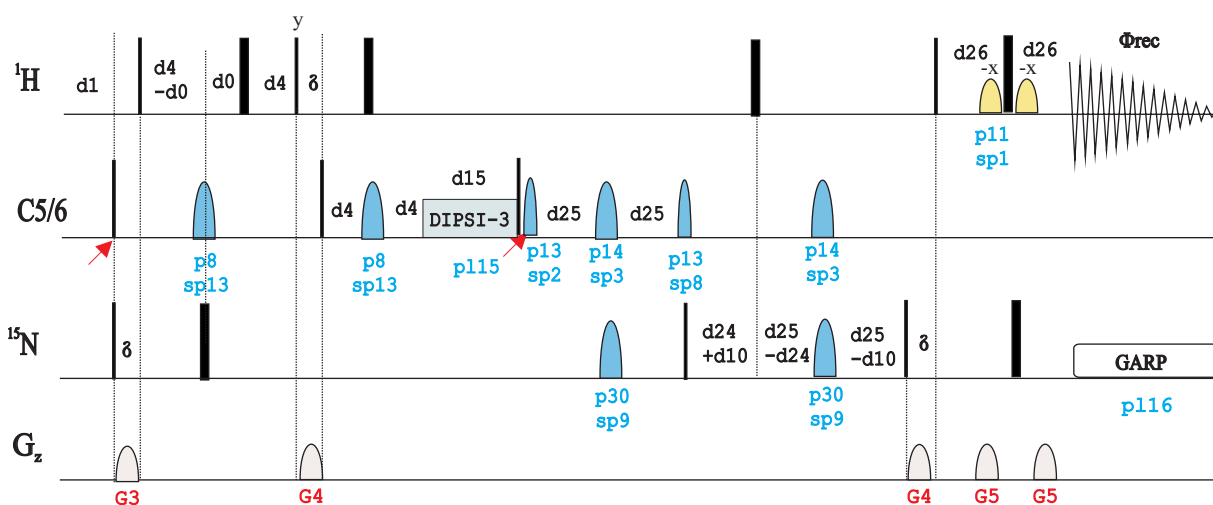
3D H(CC)NH-TOCSY Experiment

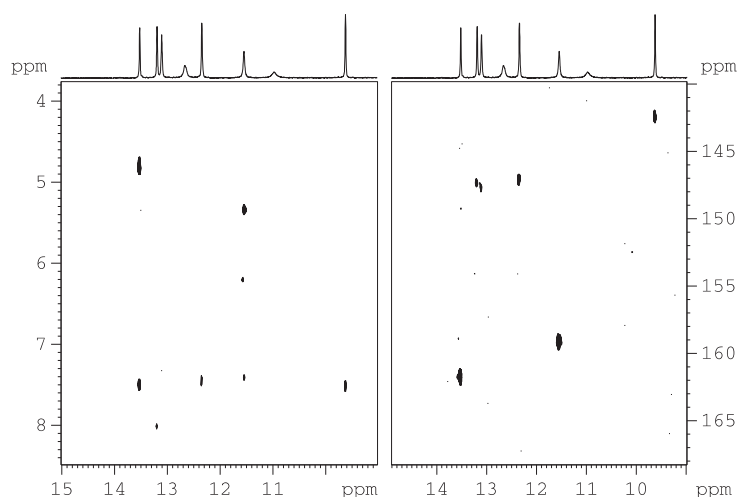
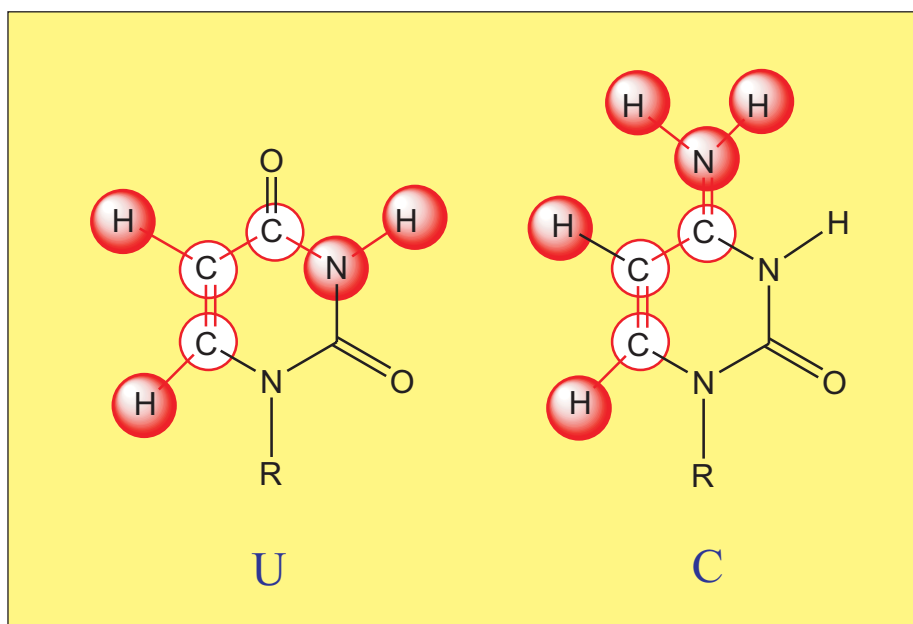
Experiment Description:

The HCCNH-TOCSY experiment allows the correlation of the exchangeable NH and NH spin systems with the H5 and H6 protons in U and C via a CC TOCSY transfer (03JB79-26). The experiment starts from the aromatic CH spin system and detects H(N). It can be separately optimized for imino NH or for amino NH₂ groups.

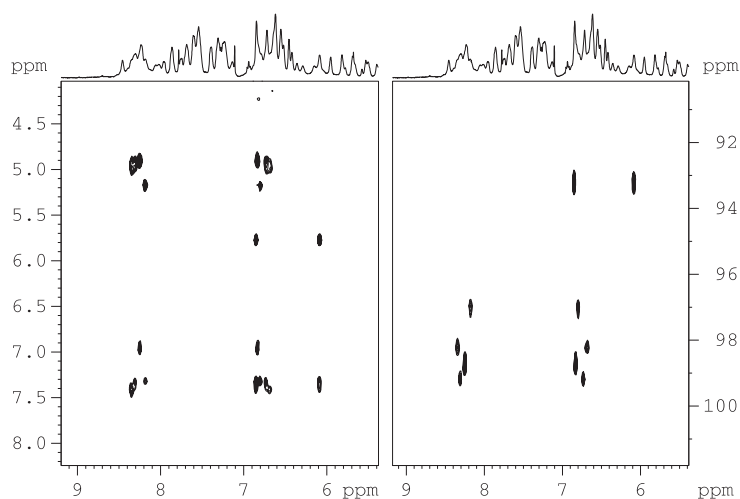


na_h56c56c4n3h_3d





$d_{24}=1/4J(\text{NH})$ for U=2.78ms
 $o_{3p}=160\text{ppm}$ (for U)



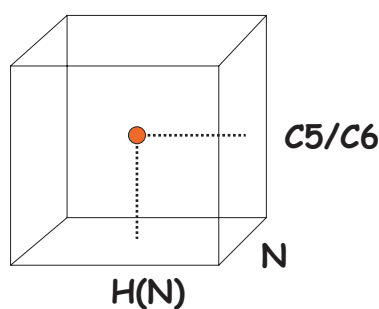
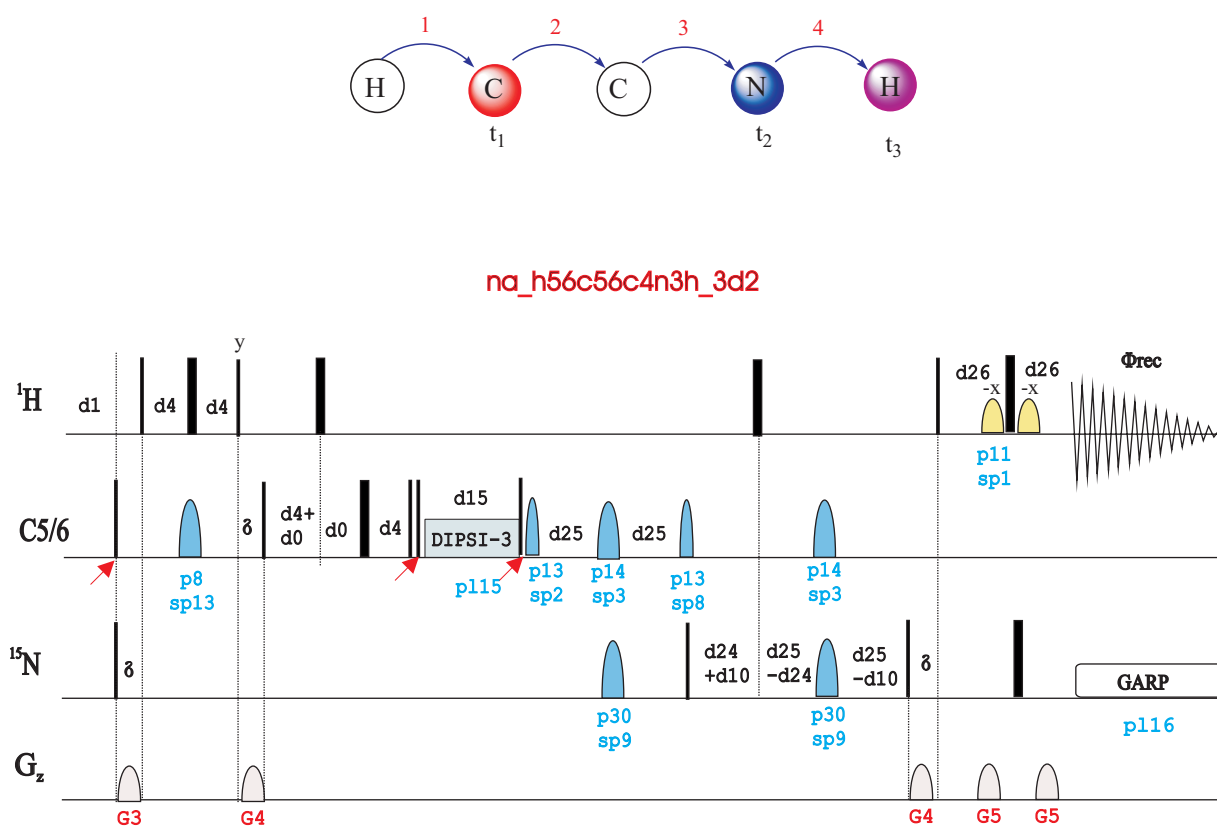
$d_1=1.5\text{s}$
 $d_4=1/4J(\text{C}5\text{H}5)=1.25\text{ms}$
 $d_{24}=1/4J(\text{NH})$ for U or $1/8J(\text{NH})$ for C
 $d_{25}=1/4J(\text{C}4\text{N})=10\text{ms}$
 $d_{26}=1/4J(\text{NH})=2.5\text{ms}$
 $d_{15}=\text{CC TOCSY}=19.5\text{ms}$
 $p_{13}=1\text{ms}$ (spnam2=Q5.1000 and spnam8=Q5tr.1000)
 $p_{14}=1\text{ms}$ (spnam3=Q3.1000)
 $p_{30}=700\text{us}$ (spnam9=Q3.1000)
 $cnst_{24}=169\text{ppm}$ (C4 in C/U)
 $cnst_{28}=105\text{ppm}$ (C5 in C/U)
 $o_{2p}=89.19\text{ppm}$
 $o_{3p}=160\text{ppm}$ (for U) or 100ppm (for C)

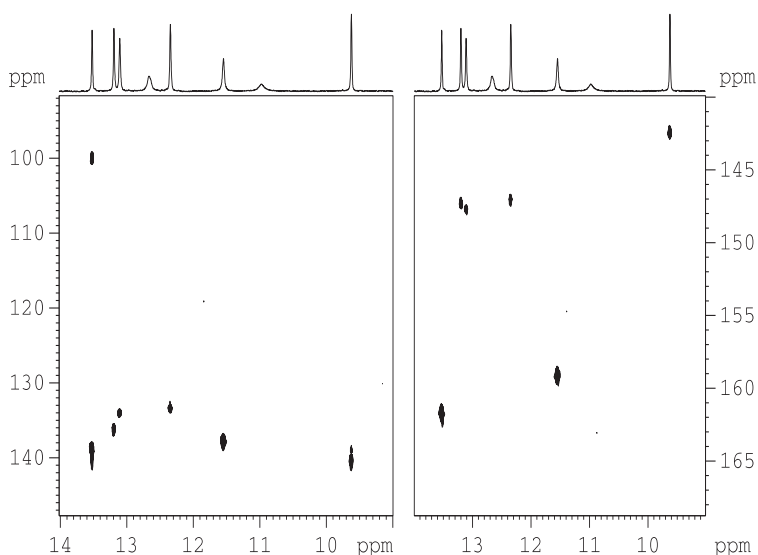
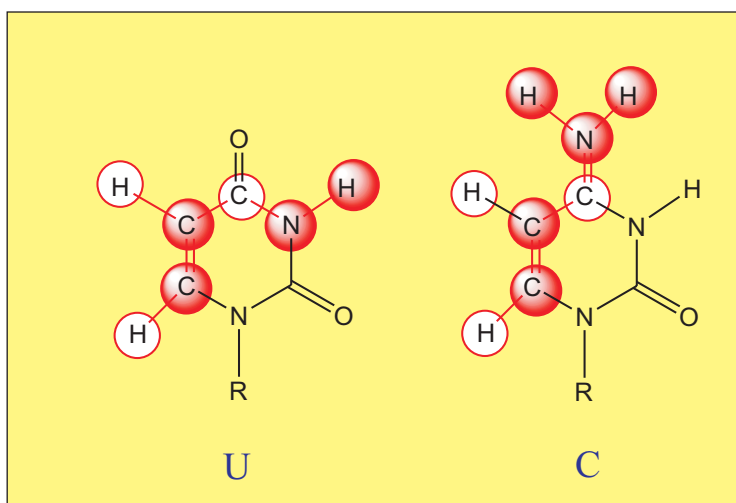
$d_{24}=1/8J(\text{NH})$ for U=1.39ms
 $o_{3p}=100\text{ppm}$ (for C)

3D (H)C(C)NH-TOCSY Experiment

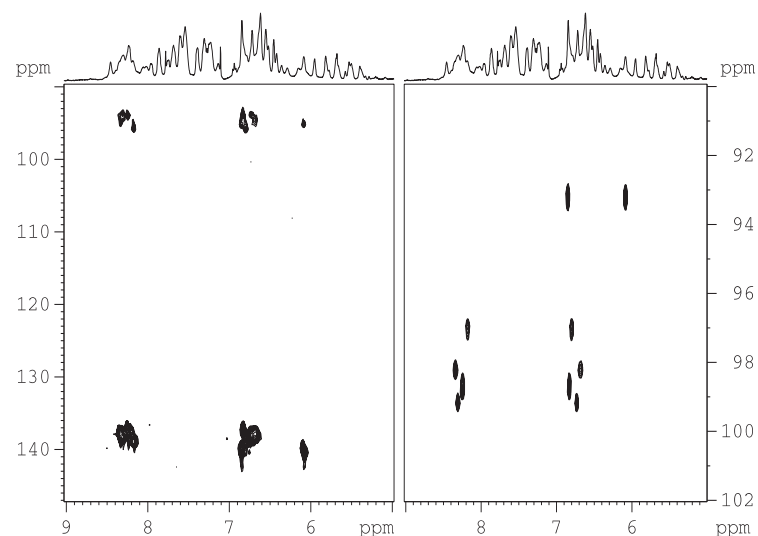
Experiment Description:

The HCCNH-TOCSY experiment allows the correlation of the exchangeable NH and NH spin systems with the C6 carbons in U and C via a CC TOCSY transfer (03JB79-26). The experiment starts from the aromatic CH spin system and detects H(N). It can be separately optimized for imino NH or for amino NH₂ groups.





d24=1/4J(NH) for U=2.78ms
o3p=160ppm (for U)



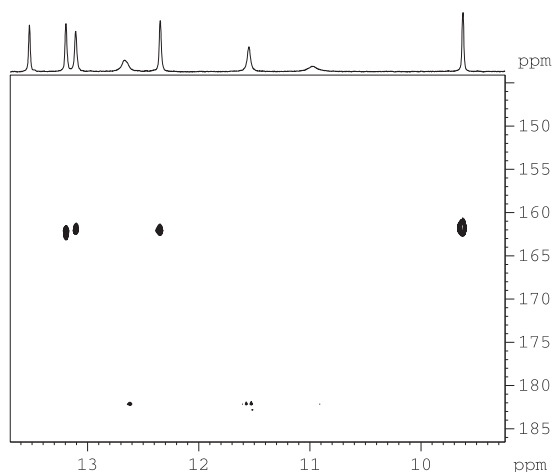
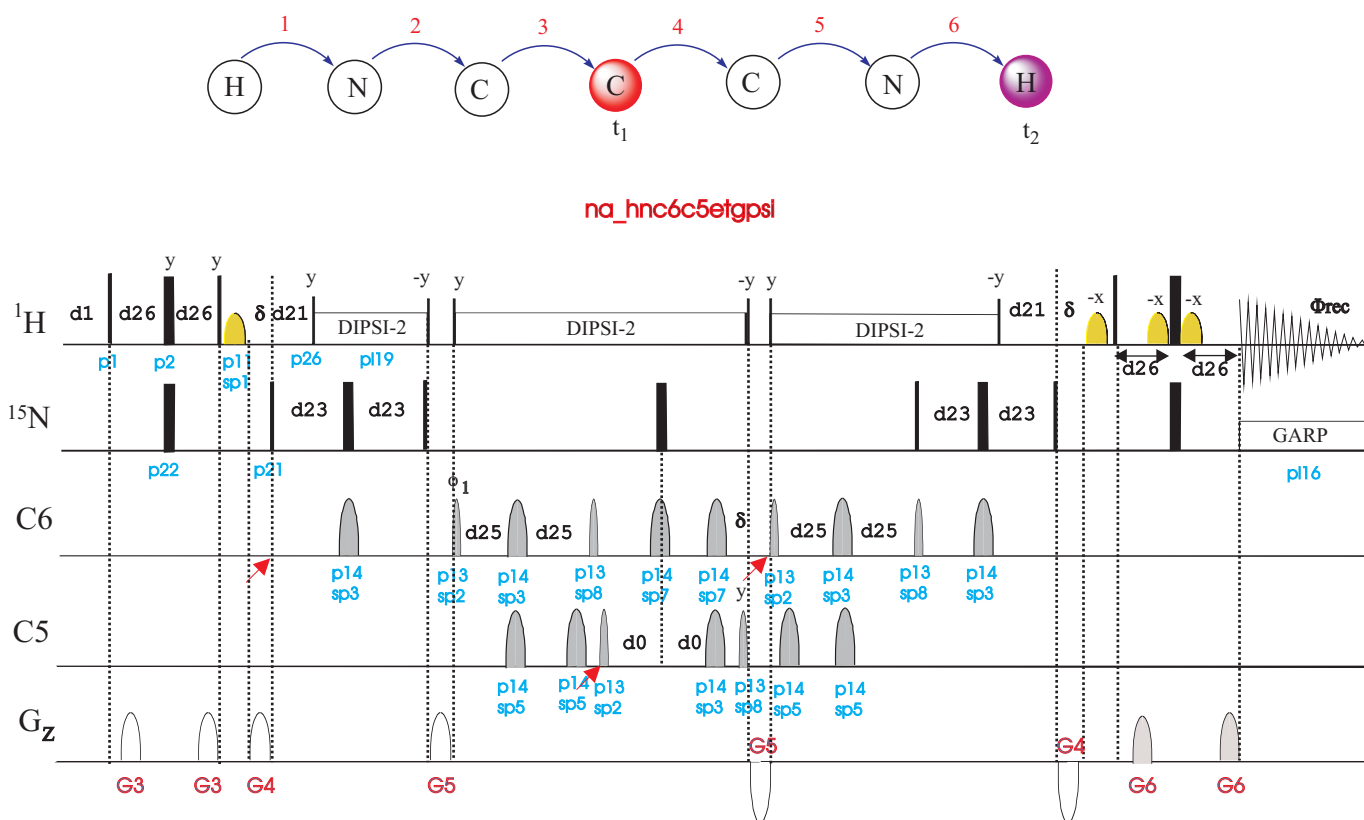
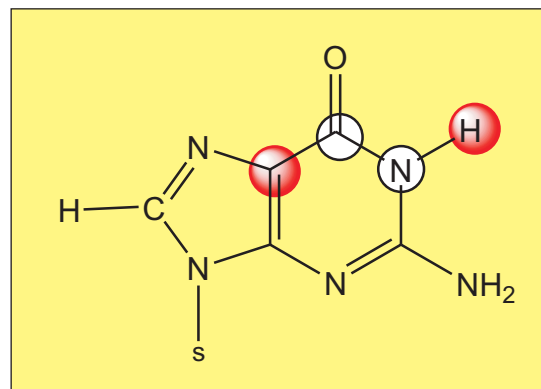
d1=1.5s
d4=1/4J(C5H5)=1.25ms
d25=1/4J(C4N)=10ms
d26=1/4J(NH)=2.5ms
d15=CC TOCSY=19.5ms
p13=1ms (spnam2=Q5.1000 and
spnam8=Q5tr.1000)
p14=1ms (spnam3=Q3.1000)
p30=700us (spnam9=Q3.1000)
cnst22=137ppm (C6 in C7U)
cnst24=169ppm (C4 in C/U)
cnst28=105ppm (C5 in C/U)
o2p=121.35ppm

d24=1/8J(NH) for C=1.39ms
o3p=100ppm (for C)

2D H(NC)C Experiment

Experiment Description:

The H(NC)C experiment allows the assignment of C5 carbon in G residues from imino NH proton via the C6 carbon (04jb69). The pulse scheme is a variant of the out-and-back HNCOCA experiment

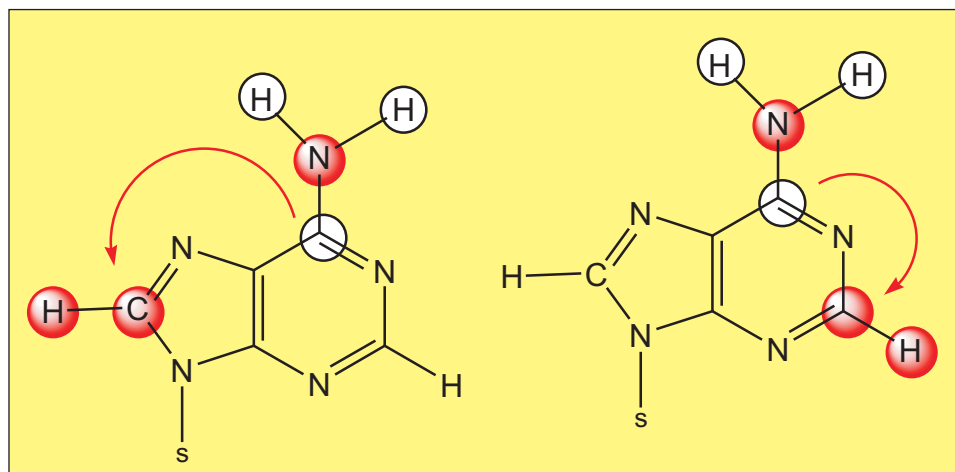


d1=1.5s
d26=1/4J(NH)=2.78ms
d23=1/4J(C6N)=25ms
d25=1/4J(C6C5)=2.8ms
d21=1/2J(NH)=5.56ms
p11=1s (spnam1=Squa100.1000)
p14=1ms (spnam3/5/7=Q3.1000)
p13=1ms (spnam2=Q5.1000 and spnam8=Q5tr.1000)
cnst25=C6(G) chemical shift=160ppm
cnst26=C5(G) chemical shift=119ppm
o2p=C5 chemical shift=165ppm
o3p=160ppm

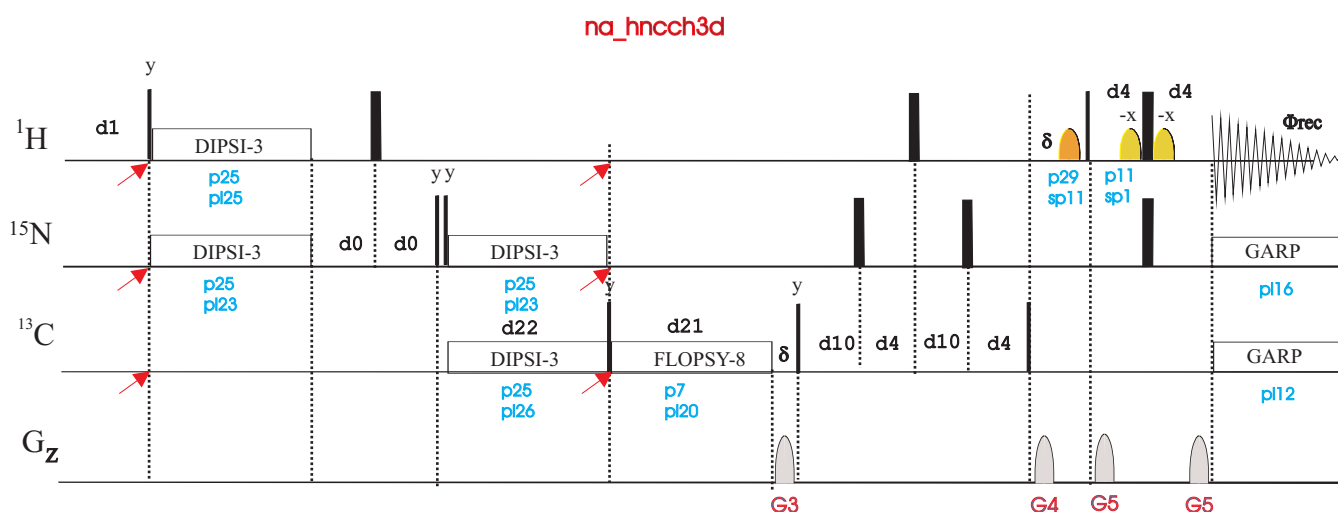
3D (H)N(C)CH Experiment

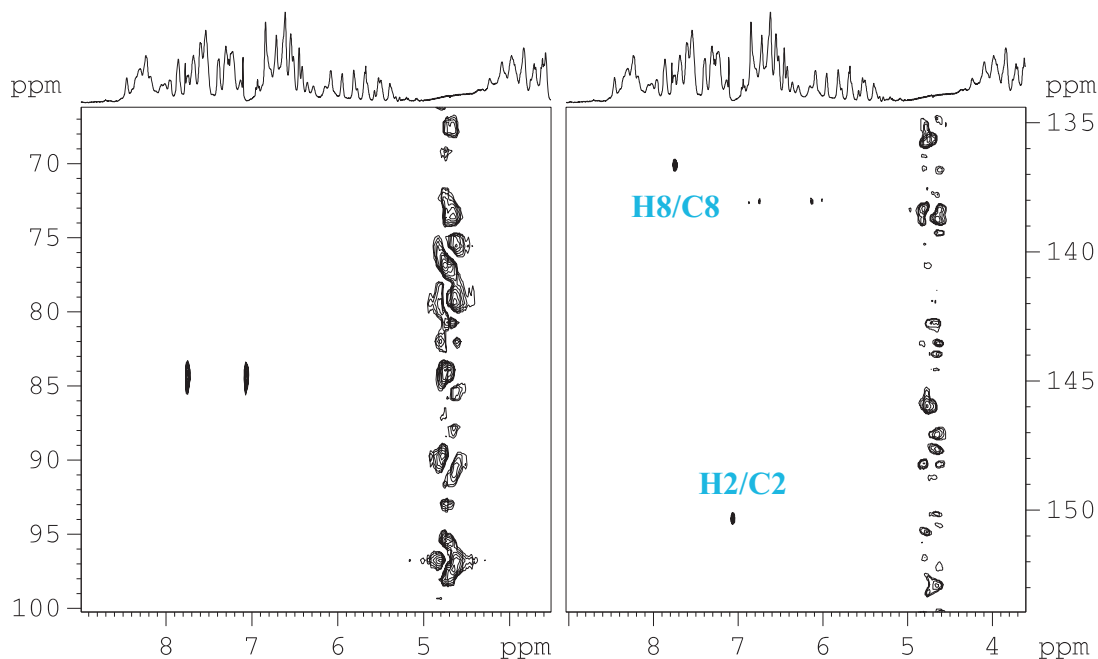
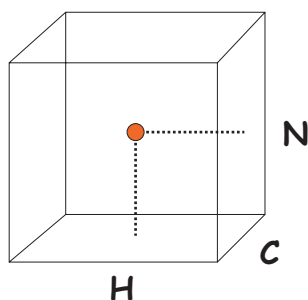
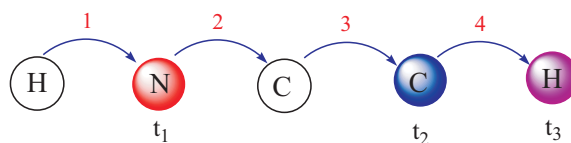
Experiment Description:

The 3D HNCCH experiment allows the correlation of the imino N nitrogen with the H2/C2 and H8/C8 spin systems in adenines (96jacs5316).



The experiment uses three different cross-polarization transfer schemes. First, a heteronuclear cross-polarization (HCP) transfer from ^1H to ^{15}N . Then, another HC transfer from N to C followed by a homonuclear TOCSY CC transfer



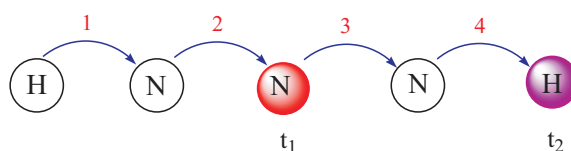
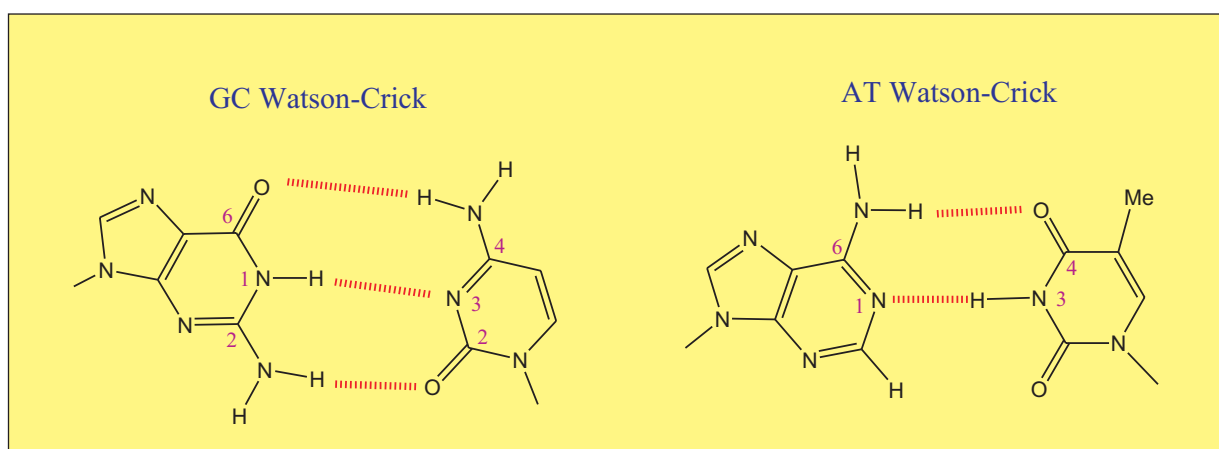
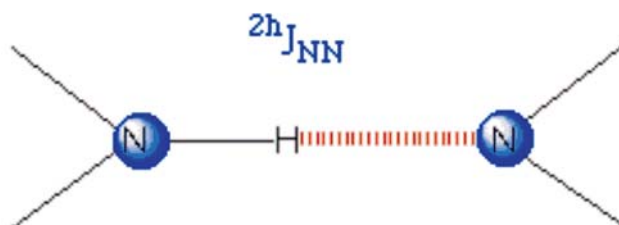


d1=1.5s
d4=1/4J(CH)=1.25ms
p11=p29=1s (spnam1=Squa100.1000)
p25=226us
d21=CC TOCSY=38ms
d22=CN TOCSY=45ms
o1p=cnst18=4.7ppm
cnst19=NH chemical shift
cnst25=C6 chemical shift=160ppm
o2p=cnst29=145 ppm (Caro)
o3p=cnst31=81ppm (NH2)

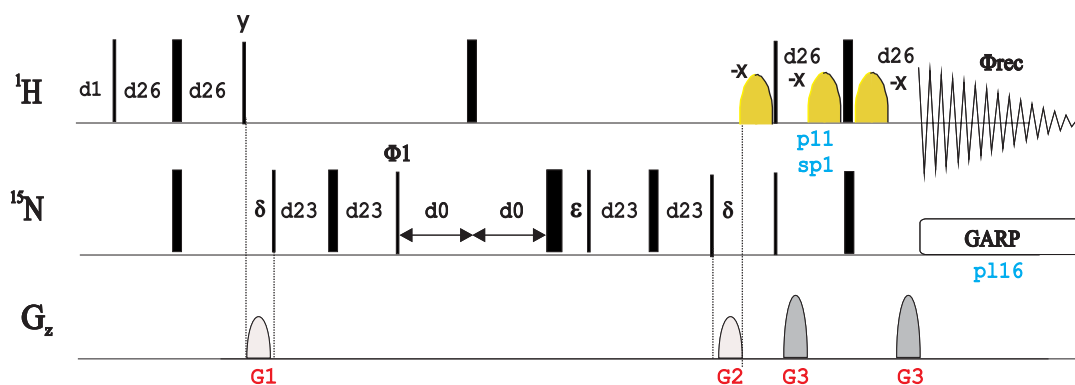
3D hydrogen-bond HNN Experiment

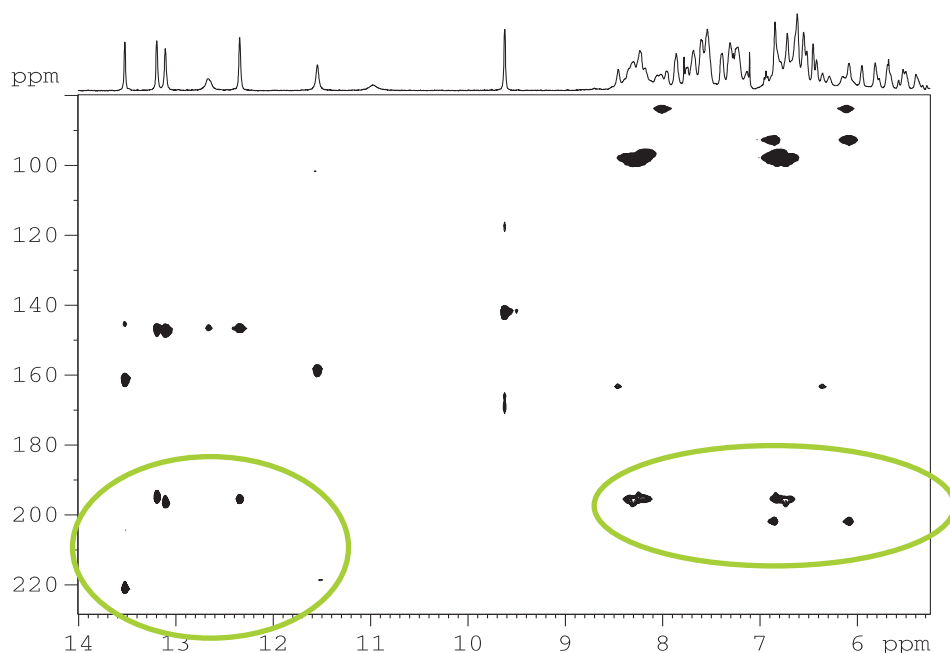
Experiment Description:

Experiment to detect hydrogen-bond NH-N connectivities (98jacs8293, 20NAR1585-28)



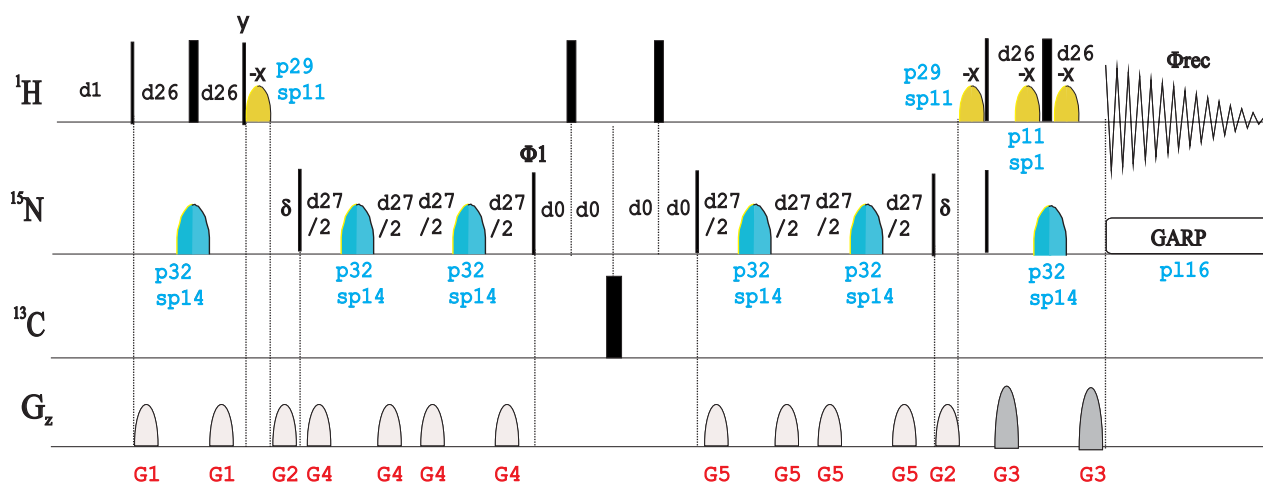
na_hnncosygpphwg



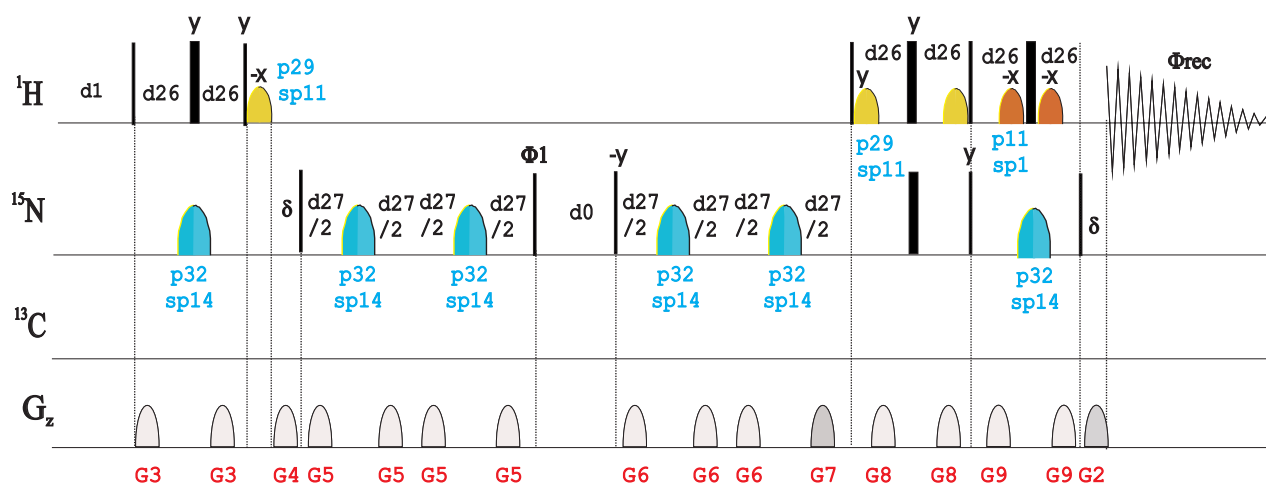


d1=1.5s
p11=90° water selective
=1ms (Squa100.1000)
d26=1/4J(NH)=2.25ms
d23=1/4J(NN)=15ms

na_hnncosygpphspwg



na_trhnncosygpphspwg



BRUKER PULSE PROGRAM CATALOGUE

NMRGuide

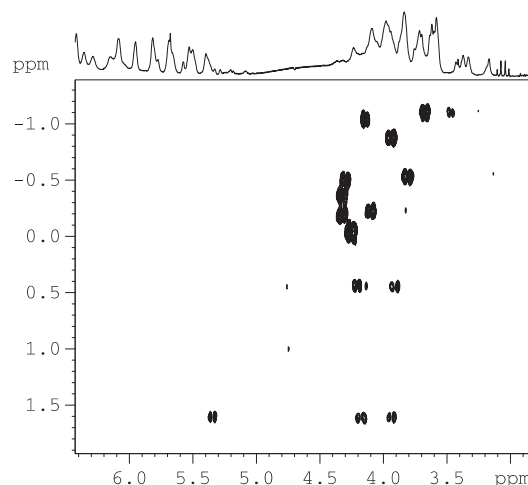
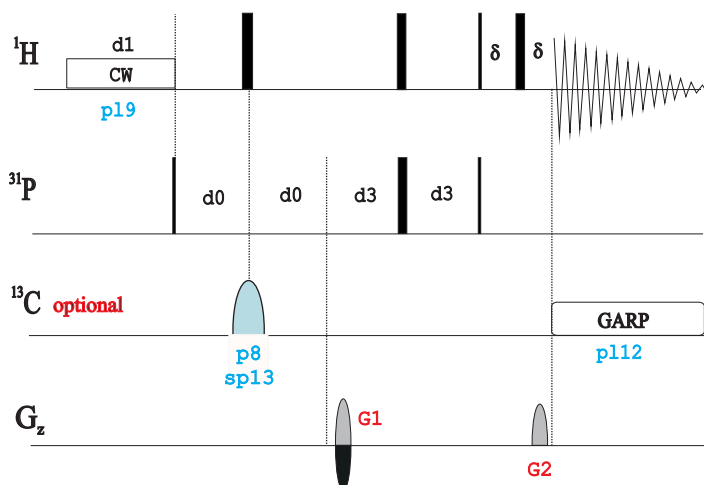
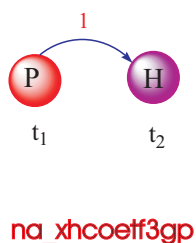
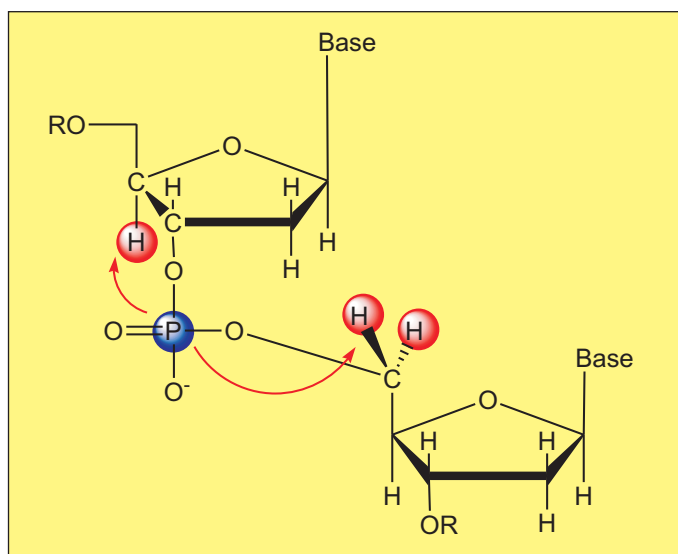
NUCLEIC-ACID NMR
2D & 3D HCP EXPERIMENTS

2D ^{31}P - ^1H HETCOR or HP COSY Experiment

Experiment Description

Experiment to achieve sequential backbone assignment via through-bond $J(\text{H}3'(i)\text{P}(i))$ and $J(\text{H}5'/\text{H}5''(i+1)\text{P}(i))$ connectivities in unlabeled and ^{13}C -labeled NAs.

The pulse sequence uses a direct ^{31}P -to- ^1H INEPT-like transfer and can be also driven in a constant-time mode..

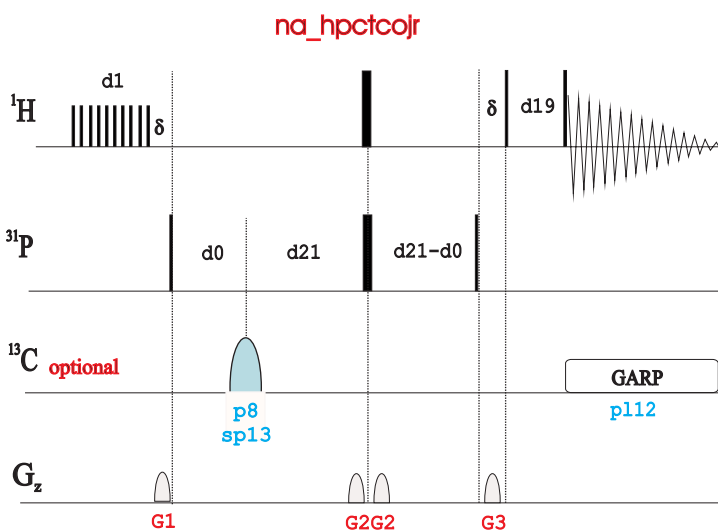
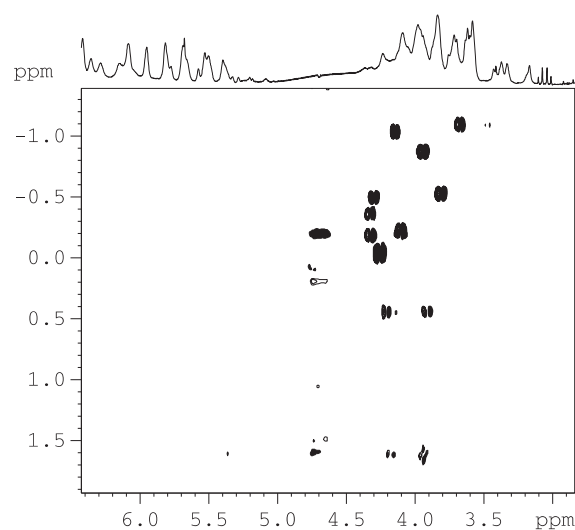
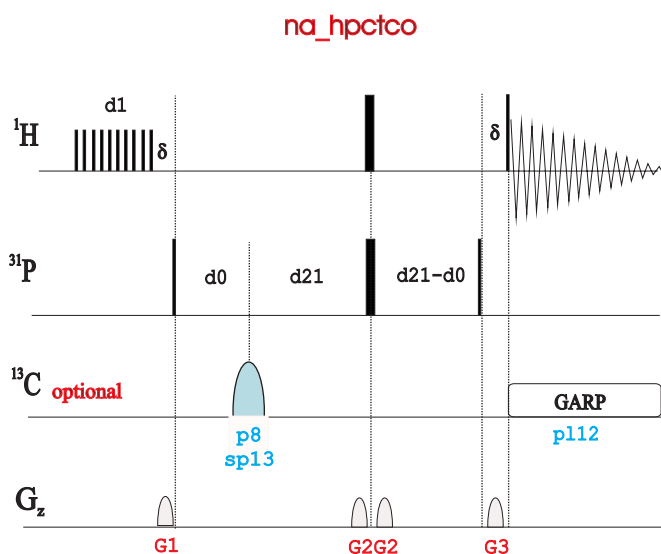
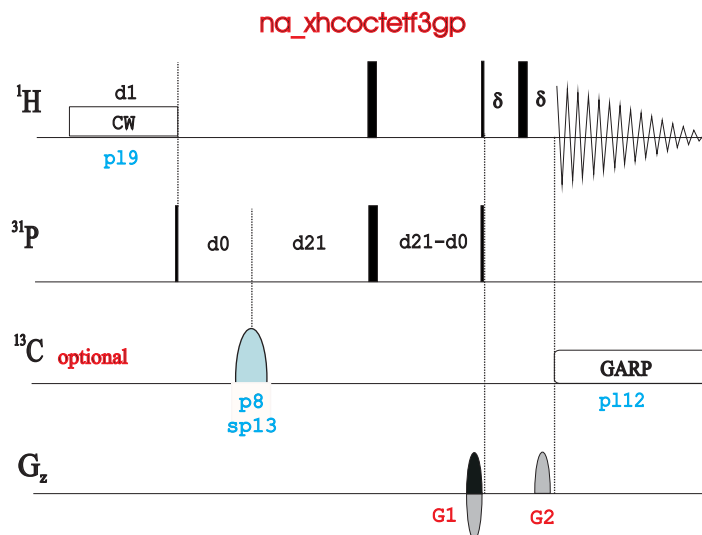
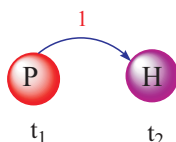


d1=1.5 s
d3=1/6J(PH)=16.6 ms
(optimized cnst2=10Hz with cnst11=6)
o3p=0 ppm
o2p=77 ppm

2D Constant-time HP COSY Experiment

Experiment Description:

Constant-time version of the ^1H - ^{31}P HETCOR or HP-COSY experiment

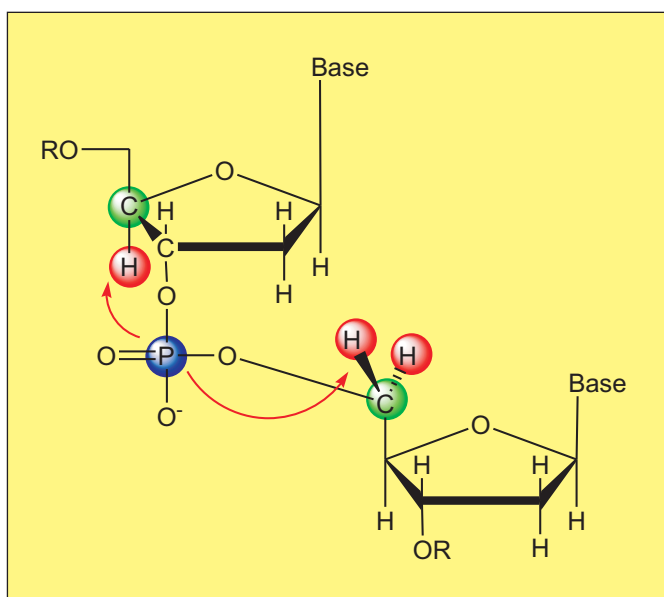


d1=1.5 s
d21=1/4J(PH)=22 ms
(optimized cnst4=11 Hz)
o3p=0 ppm
o2p=77 ppm

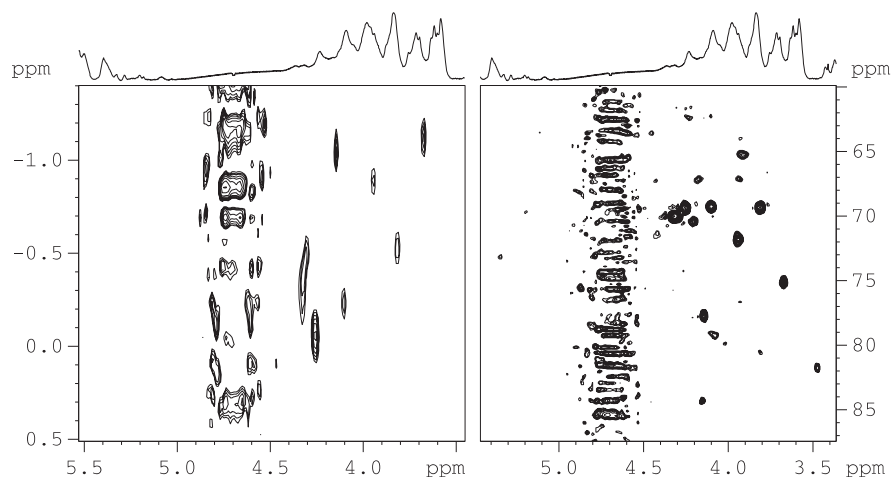
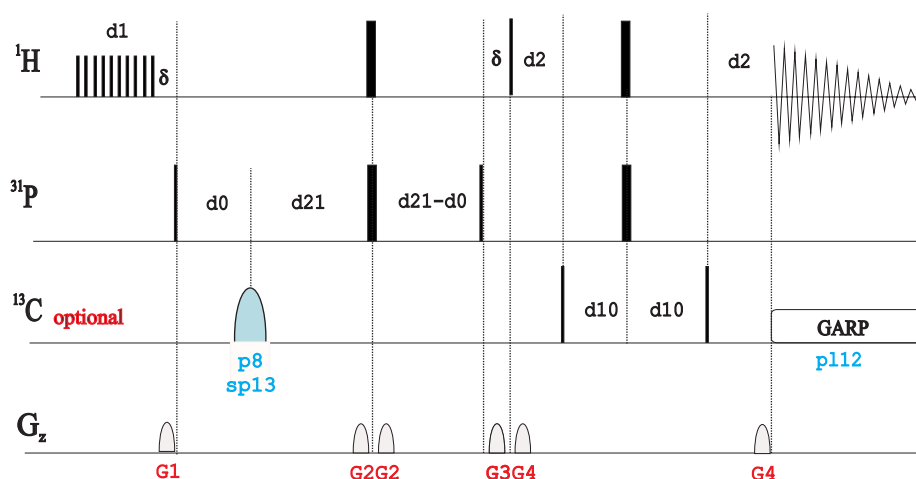
3D CT PHCH Experiment

Experiment Description

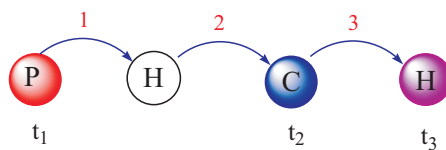
The 3D constant-time version of the P(H)CH experiment extends the backbone assignment of the HP experiment to C3'(i) and C5'(i+1) carbons by means a ^1H - ^{13}C HMQC building block.



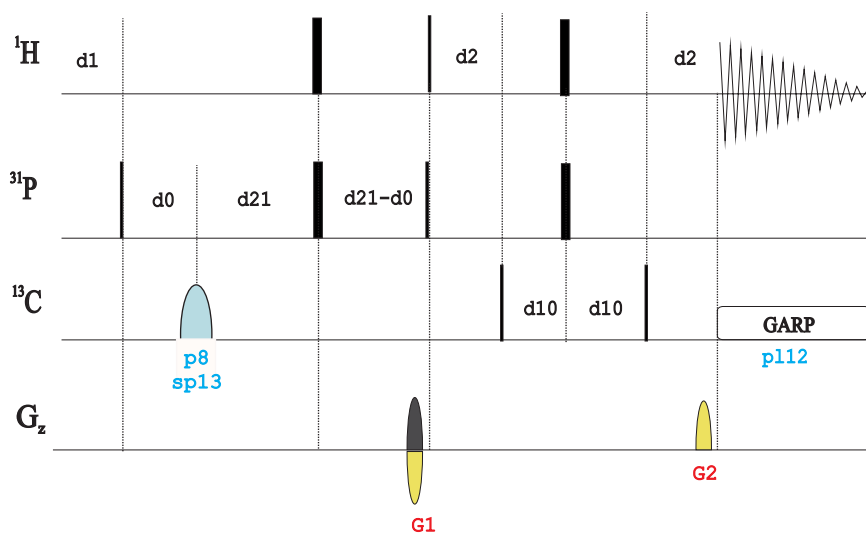
na_hpcctco3d



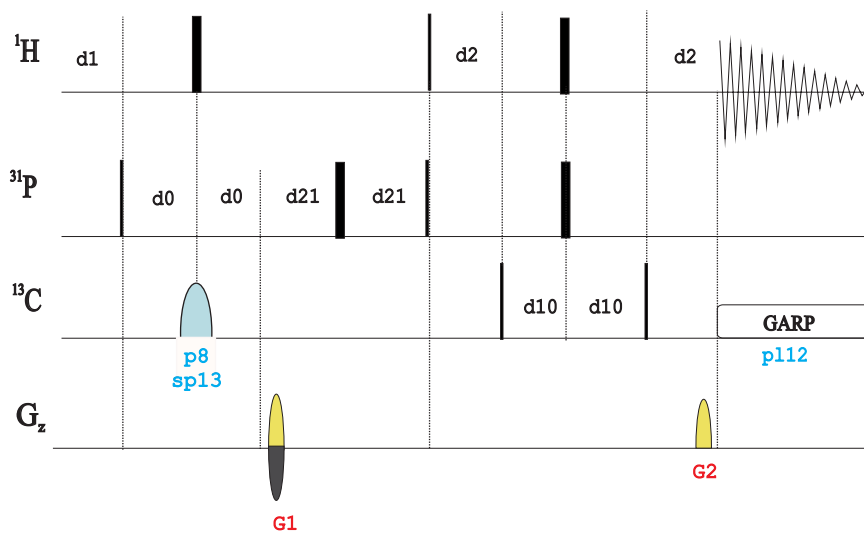
d1=1.5 s
d21=1/4J(PH)=22.7ms
(optimized cnst4=J(PH)=11Hz)
d2=1/2J(CH)=3.44ms
(optimized cnst2=J(CH)=145Hz)



na_hpccoctetf3gp3d



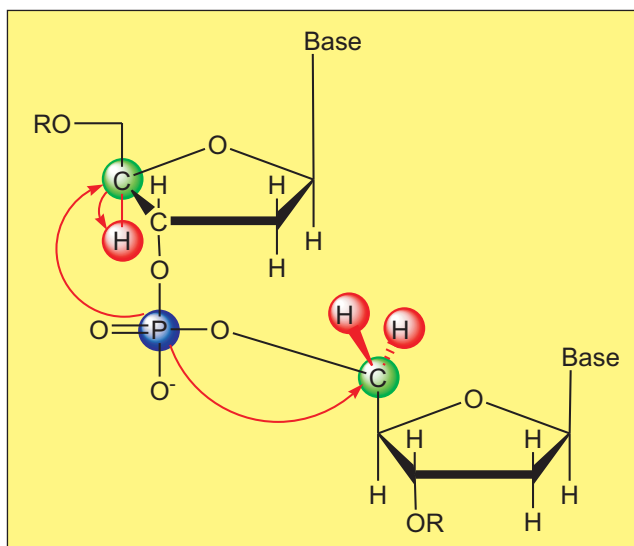
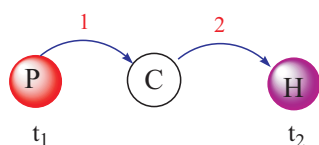
na_hpccoeftf3gp3d



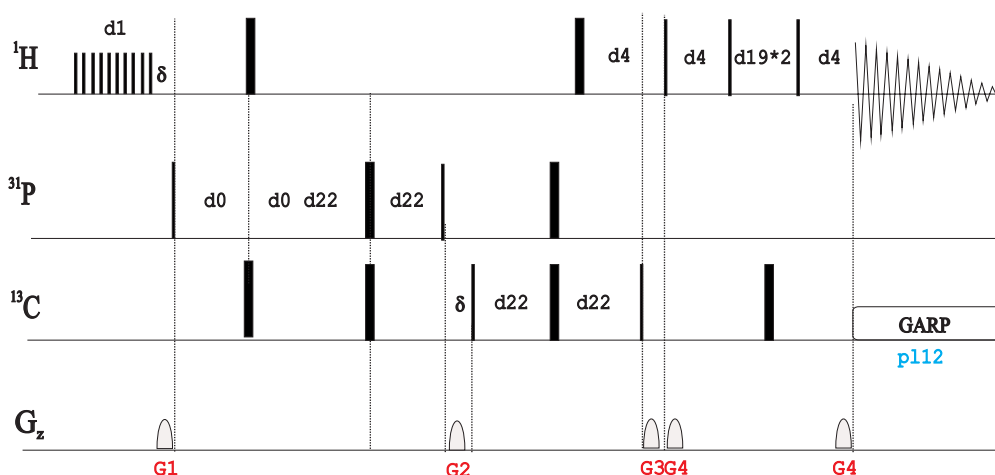
2D P(C)H Experiment

Experiment Description

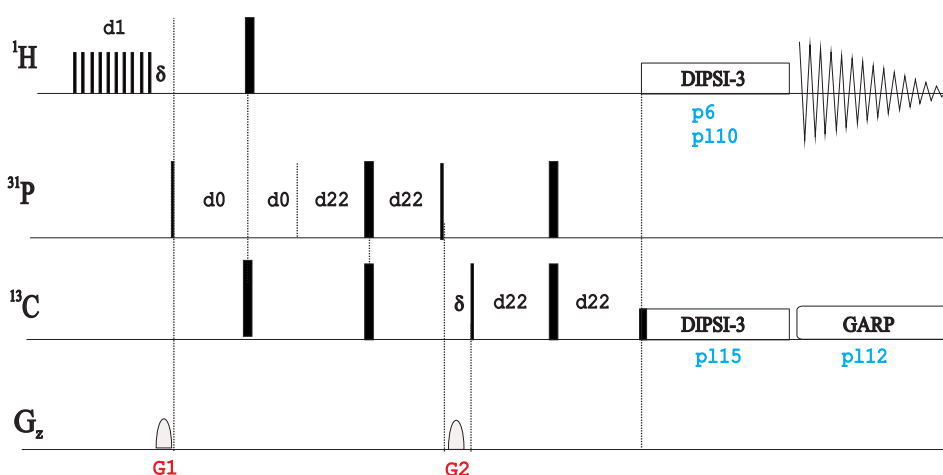
Experiment to achieve backbone PH assignment by through-bond coherence transfer P-to-C via $J(C4'(i)-P(i))$ and $J(C4'(i+1)-p(i))$ followed by an INEPT or cross-polarization C-to-H transfer.



na_pccchco



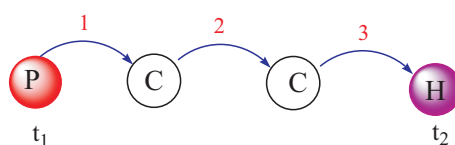
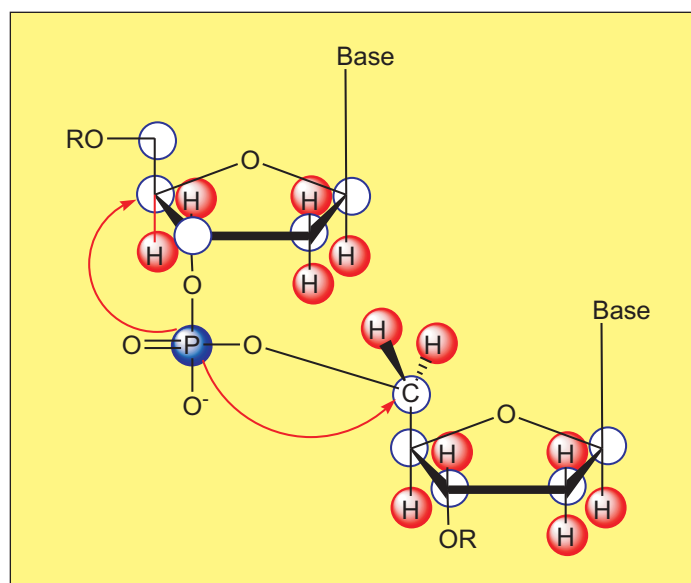
na_pccchdl



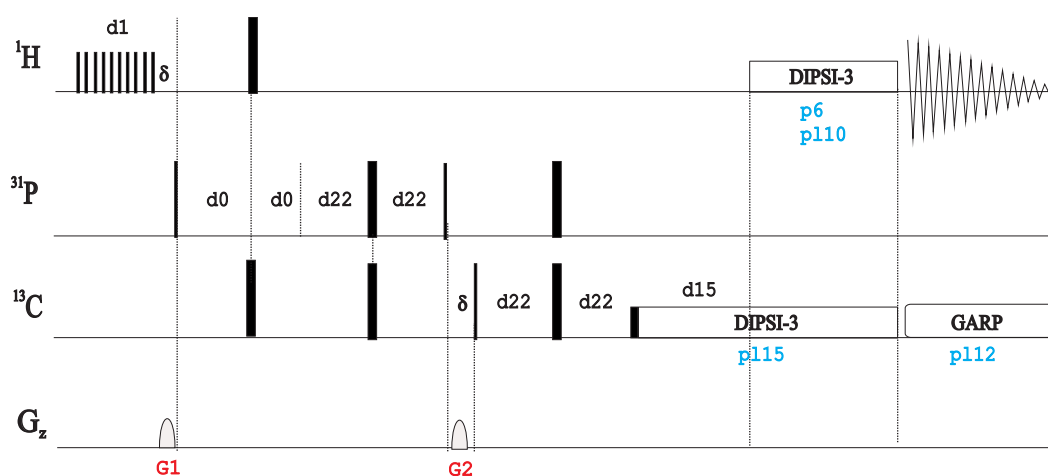
2D P(CC)H Experiment

Experiment Description

Extension of the P(C)H experiment in which after the P-to-C transfer, a C-C TOCSY transfer relays the information through all carbons of the ribose ring and, finally, a C-to-P cross-polarization scheme allows to detect all ribose protons.



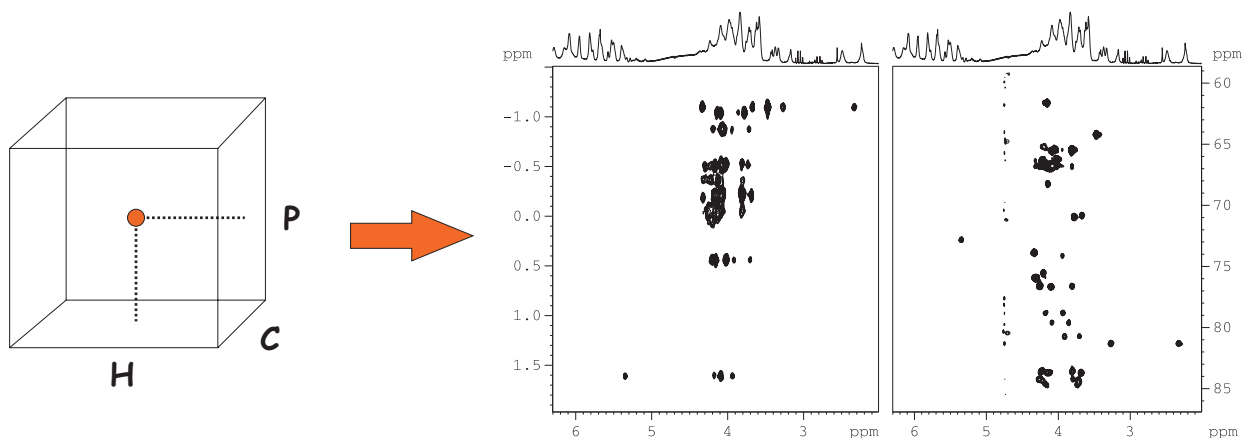
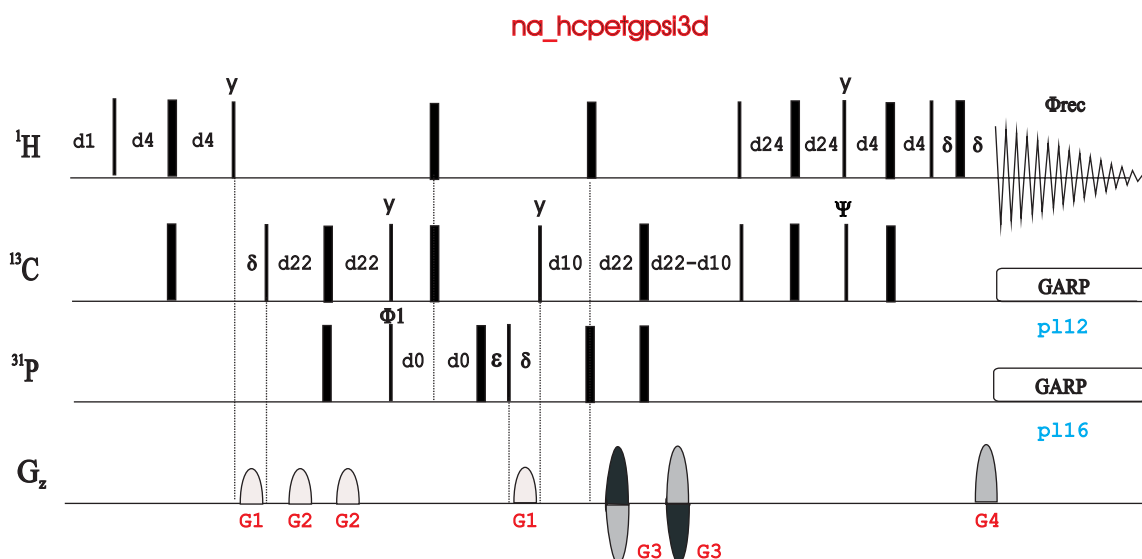
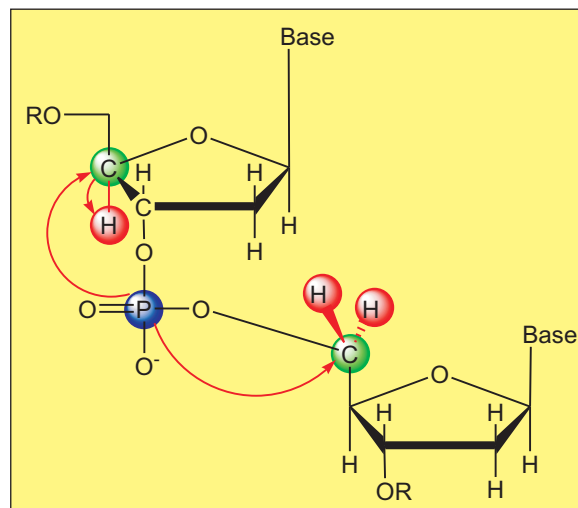
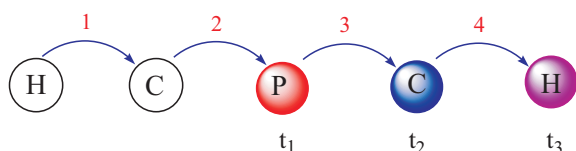
na_pcchd12



3D HCP Experiment

Experiment Description:

Out-and-back pulse scheme to correlate backbone P, C and H in a 3D experiment (94jacs6472).



d1=1.5 s
d4=1/4J(CH)=1.6 ms (optimized cnst2=J(CH)=155Hz)
d22=1/8J(CP)=12.5ms (optimized cnst5=J(CP)=10Hz)
d24=0.8 ms (optimized cnst11=8)

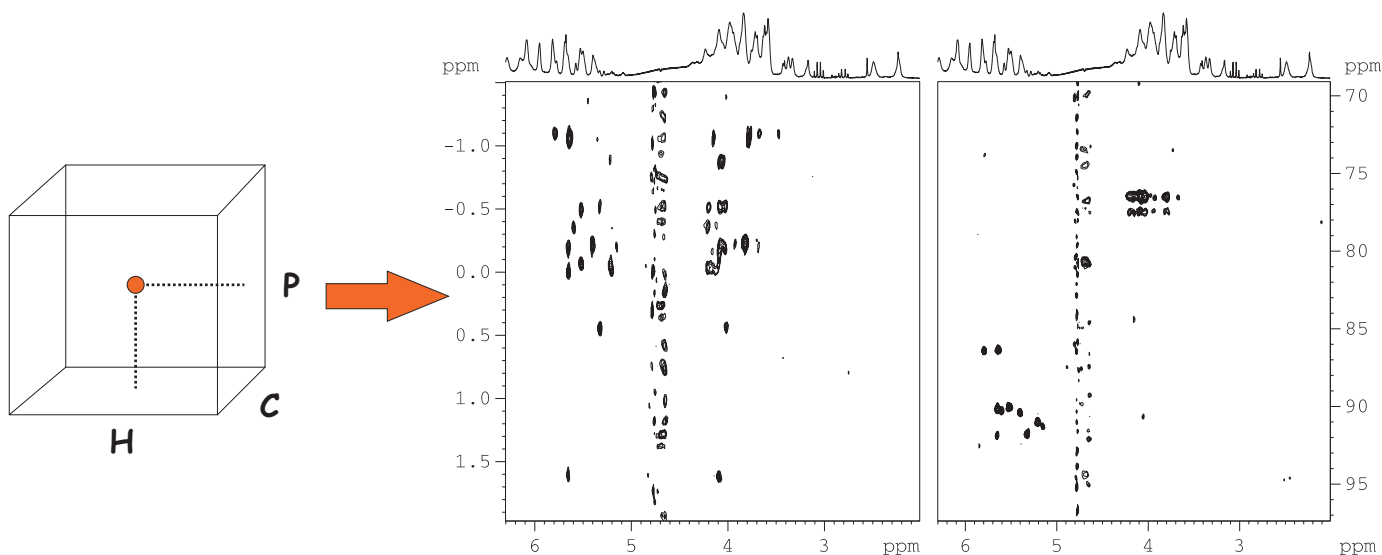
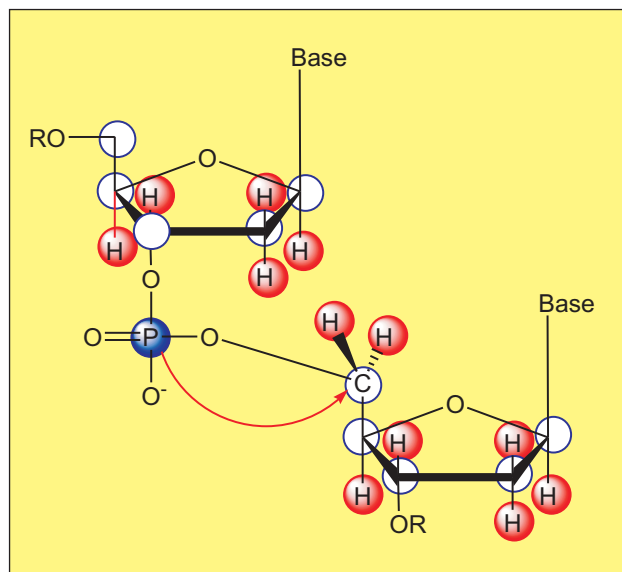
3D HCP-TOCSY Experiment

Experiment Description:

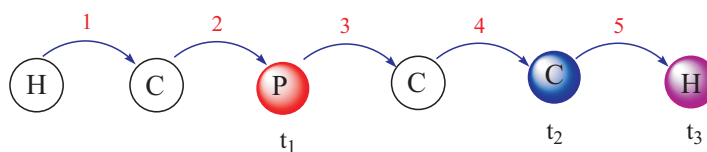
Variant of the 3D HCP experiment in which a CC TOCSY transfer has been included to involve all carbons and protons of the ribose ring (95JB87-5), in particular, the well dispersed anomeric H1' protons.

NMR Spectrum

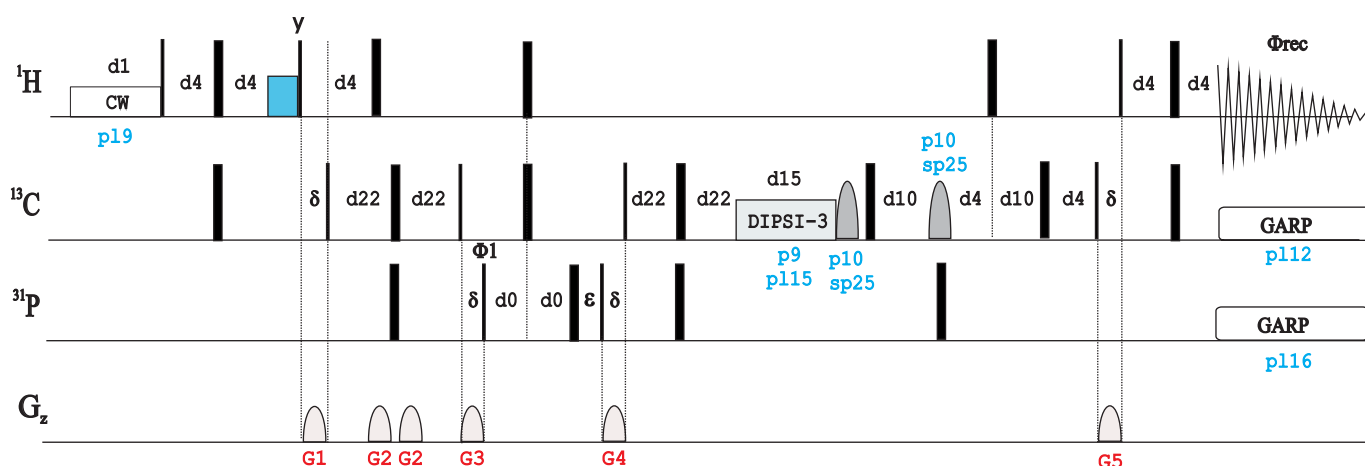
The out-and-back experiment provides a 3D ^1H , ^{13}C , ^{31}P correlation map



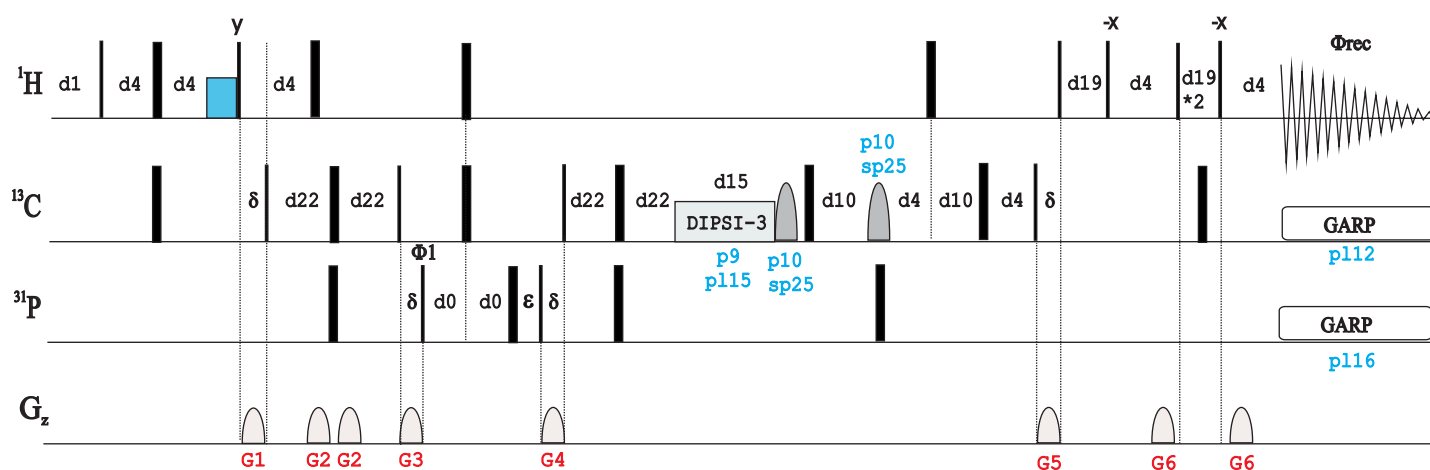
d1=1.5 s
d4=1/4J(CH)=1.6 ms
(optimized cnst2=J(CH)=155Hz)
d22=1/8J(CP)=12.5ms
(optimized cnst5=J(CP)=10Hz)
d15=CC TOCSY mixing=11 ms



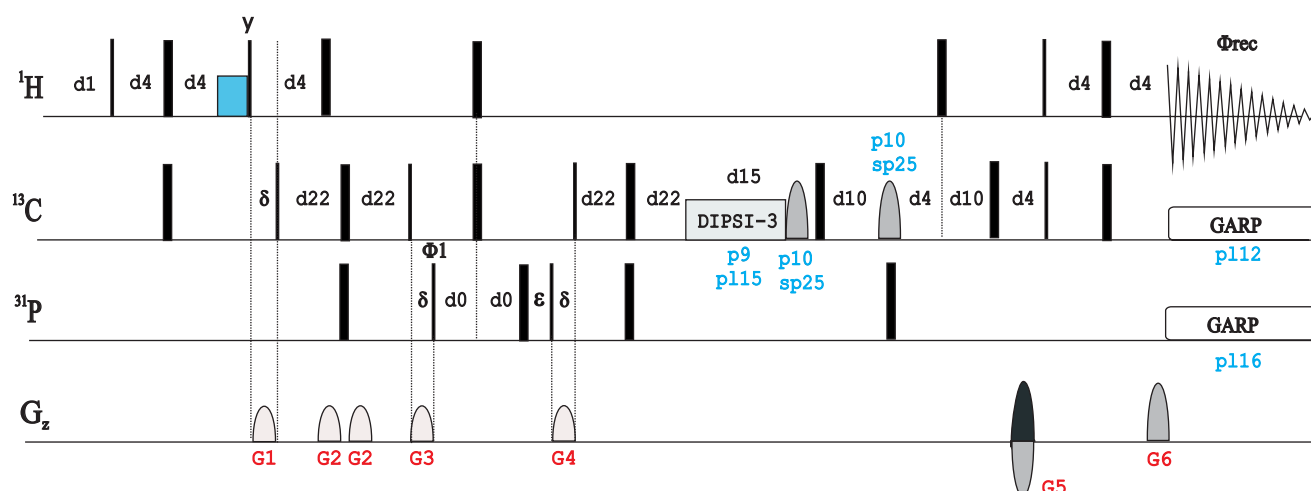
na_hcpdip3d



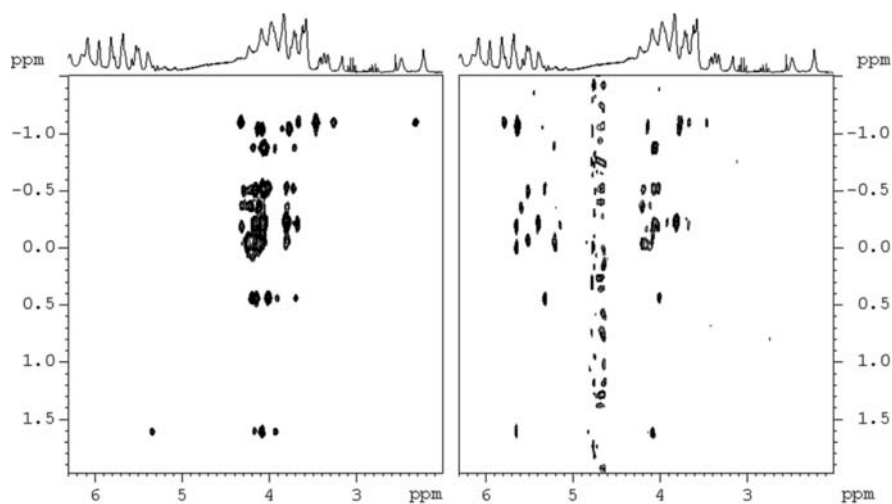
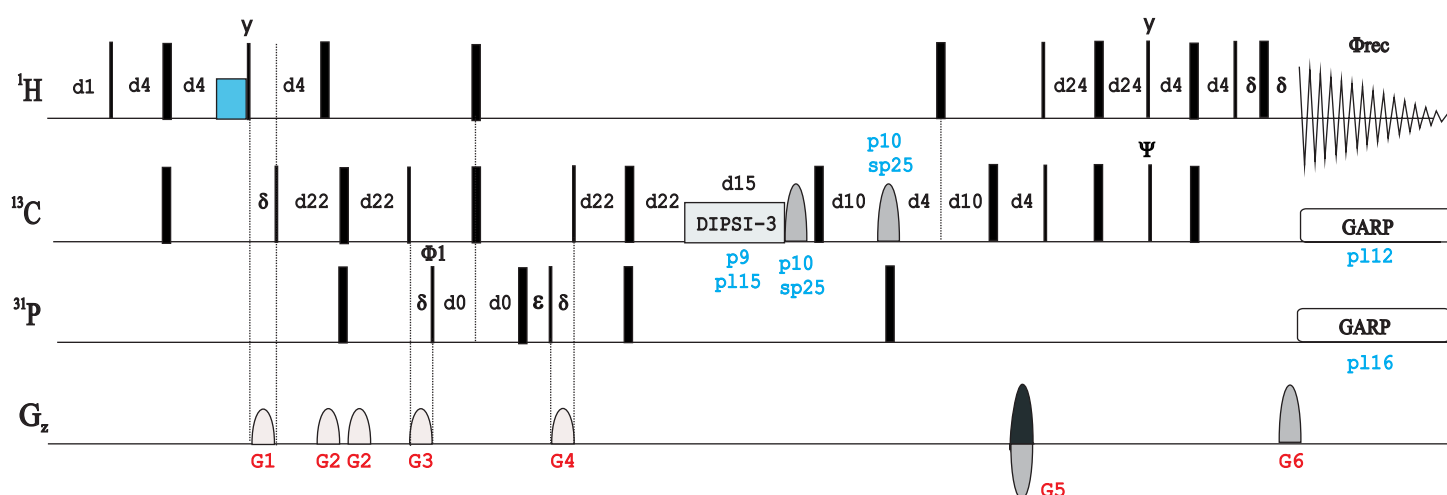
na_hcpdip3d



na_hcpdletgp3d

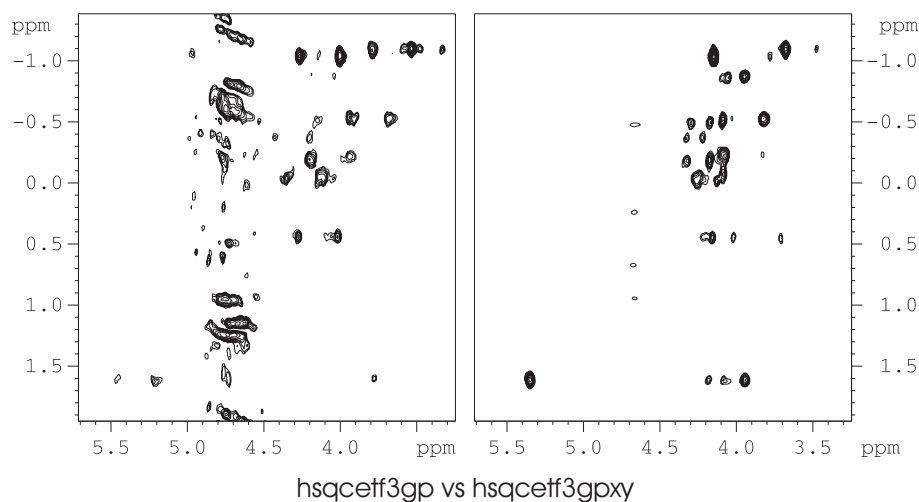
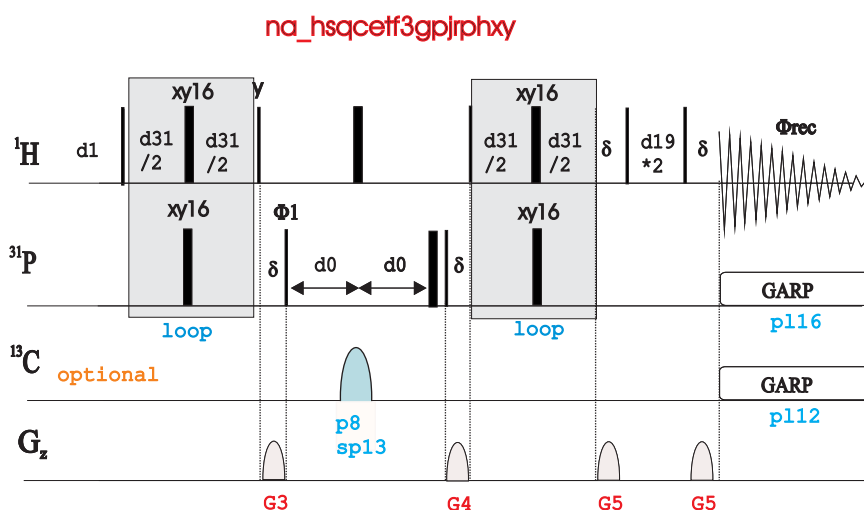
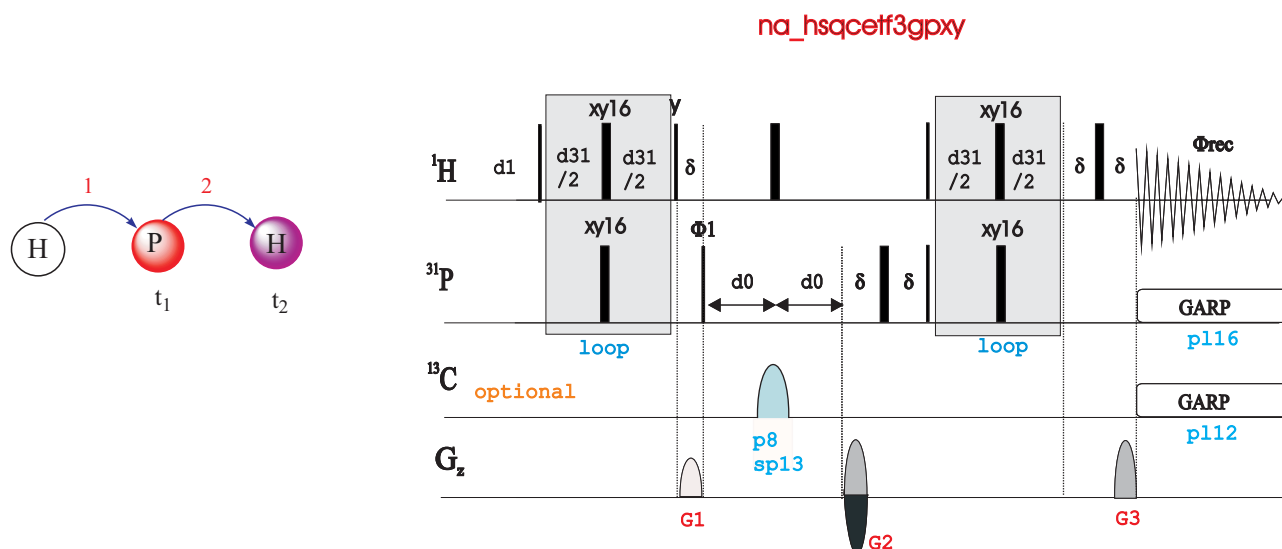


na_hcpdletgpsl3d



2D ^1H - ^{31}P HSQC using CPMG-XY16 Experiment

Experiment Description: Modified version of the long-range optimized ^1H - ^{31}P HSQC experiment in which a CPMG-XY16 pulse train is included to avoid ^1H - ^1H modulation and exchange processes (01jacs11306)

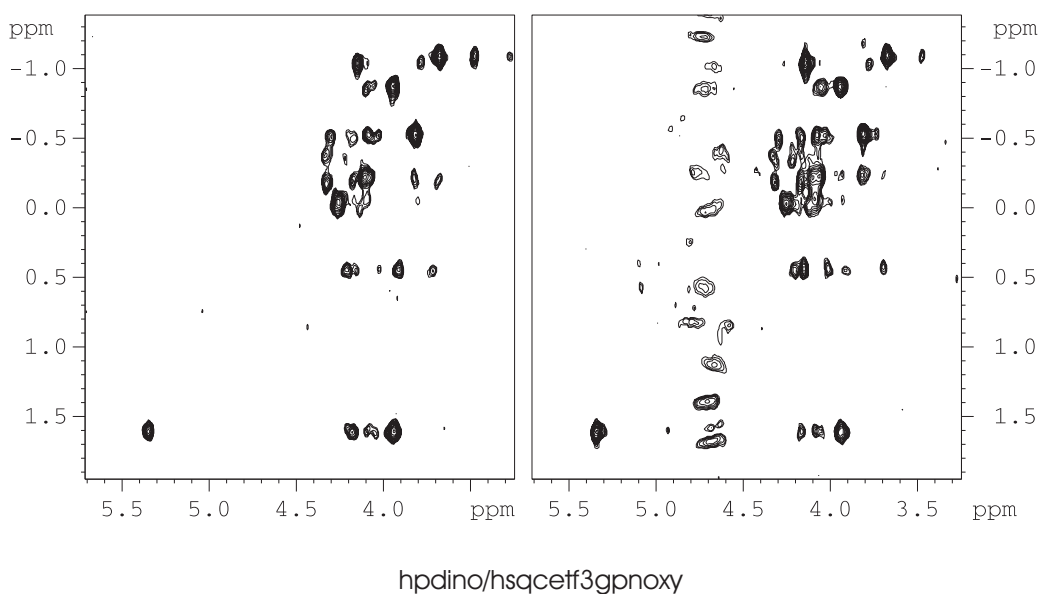
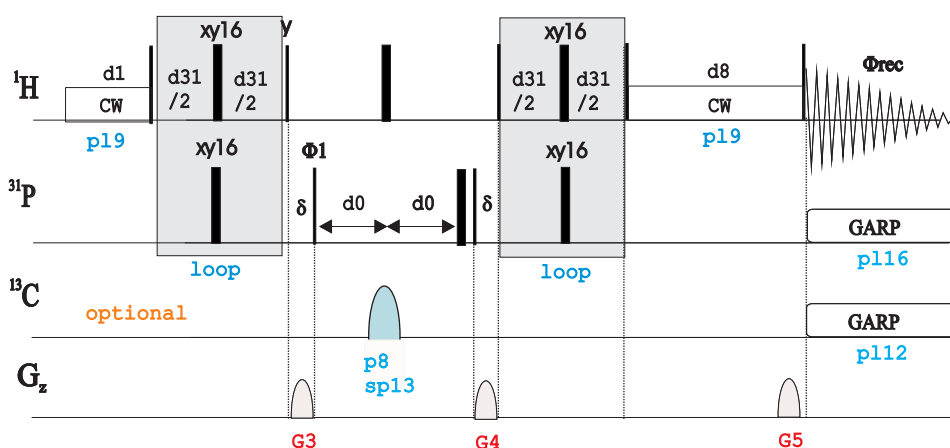
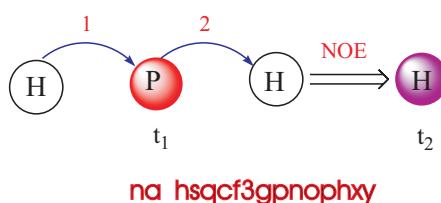


$d1 = 1.5$ s
 $d26 = 1/4J(\text{PH}) = 12.5$ ms
 (optimized $\text{cnst4} = J(\text{PH}) = J(20\text{Hz})$)
 $d21 = \text{delay in CY16-CPMG} = 100\mu\text{s}$

2D ^1H - ^{31}P HSQC-NOESY using CPMG-XY16 Experiment

Experiment Description:

Modified HSQC-NOESY pulse scheme involving CPMG-XY16 transfer during the INEPT periods (01jacs11306).

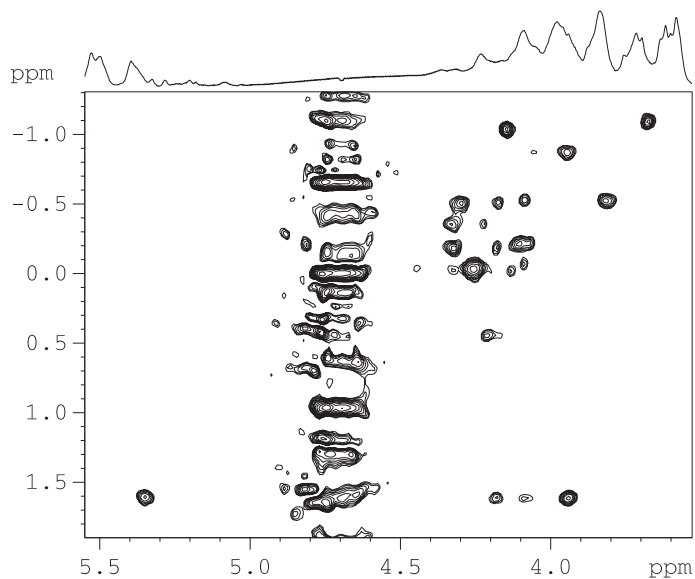
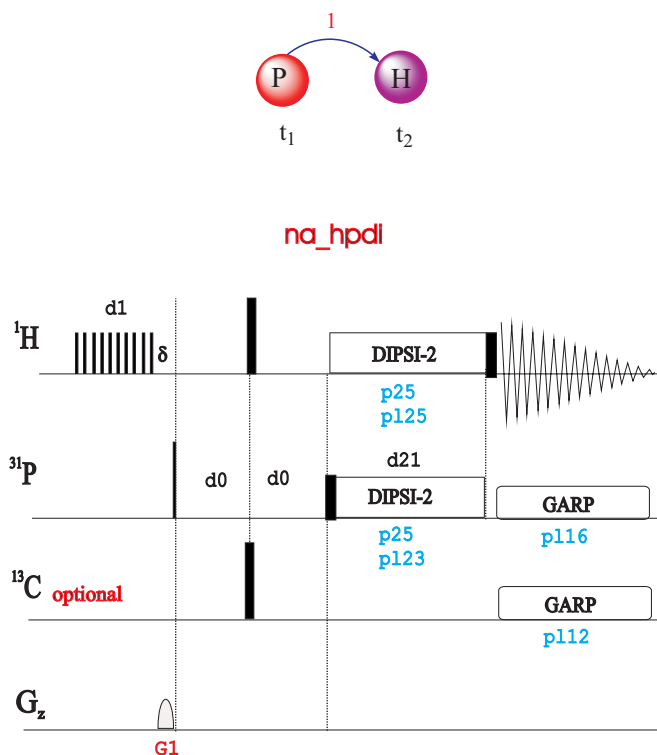


d1=1.5 s
d26=1/4J(PH)=12.5ms
(optimized cnst4=J(PH)=20Hz)
d21=delay in CY16-CPMG=100us
d8=NOE mixing time

2D ¹H-³¹P HeteroTOCSY Experiment

Experiment Description:

Experiment to correlate ³¹P and ¹H chemical shifts that uses Heteronuclear cross-polarization for magnetization transfer from ³¹P to ¹H via J(PH).

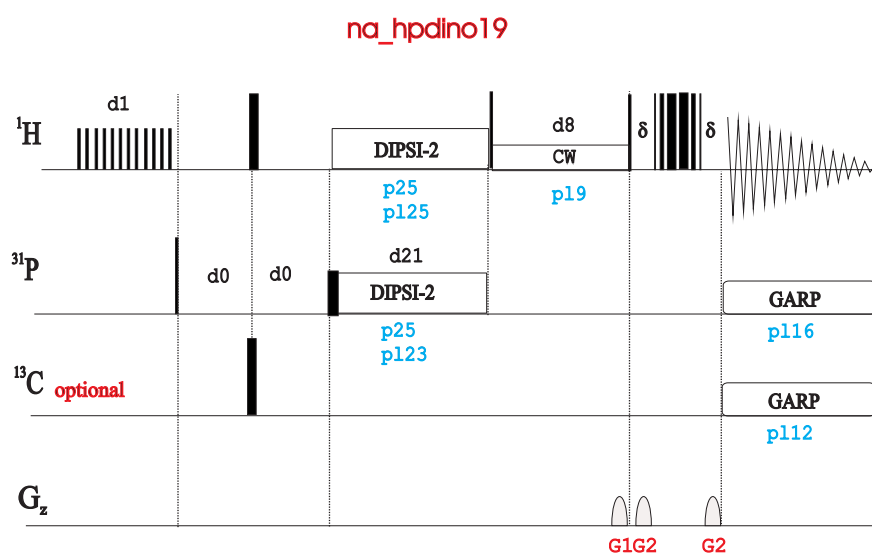
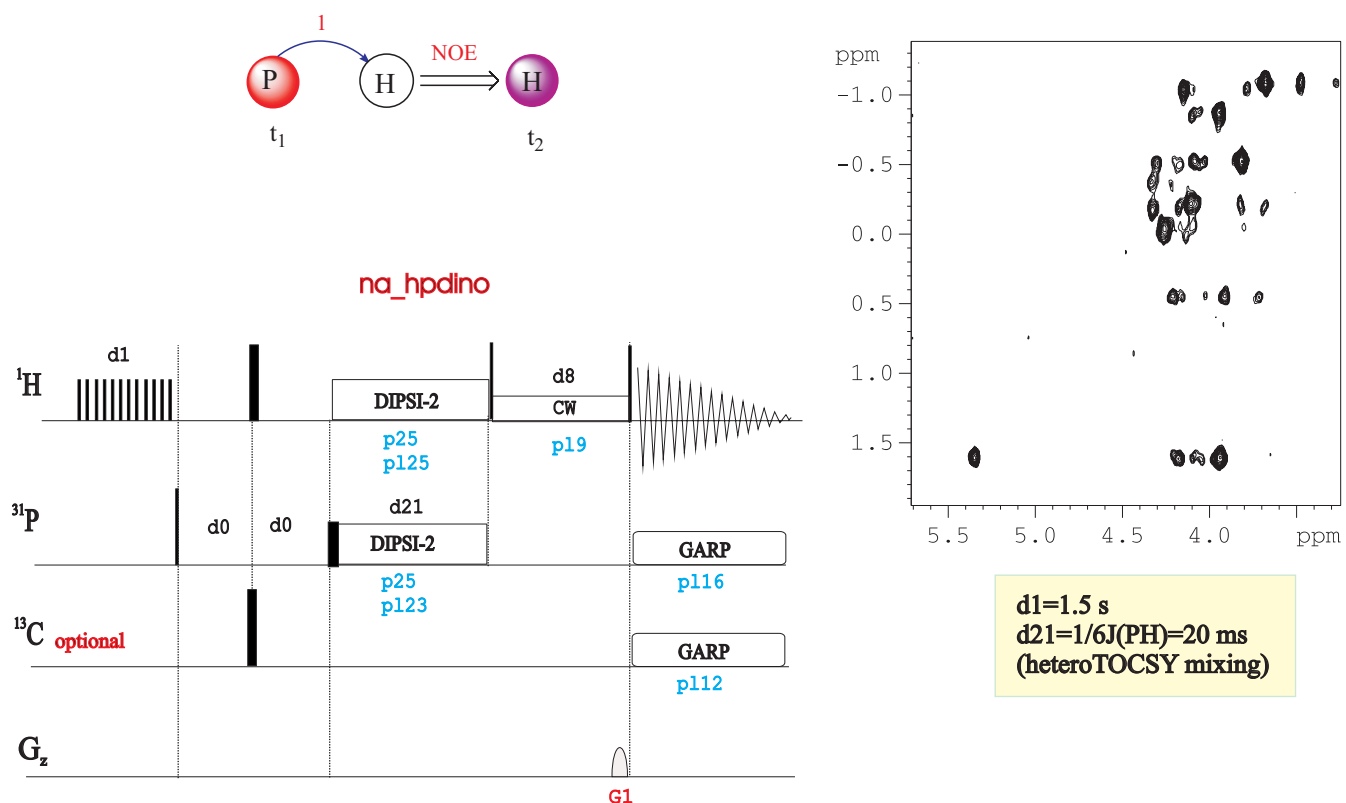


d1=1.5 s
d21=1/6J(PH)=20 ms
(heteroTOCSY mixing)

2D HeteroTOCSY-NOESY Experiment

Experiment Description

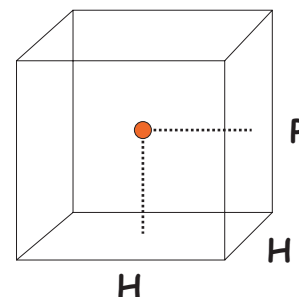
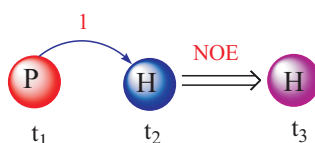
2D Cross-polarization version of a ^{31}P -edited NOESY experiment.



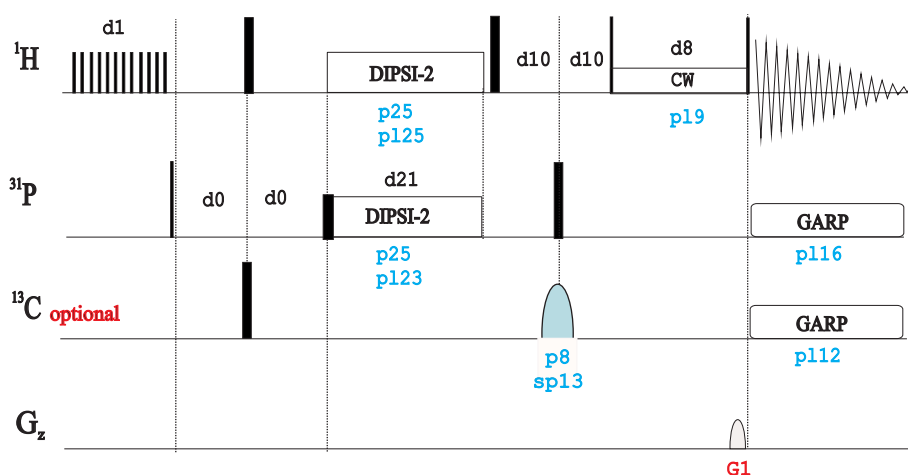
3D HeteroTOCSY-NOESY Experiment

Experiment Description

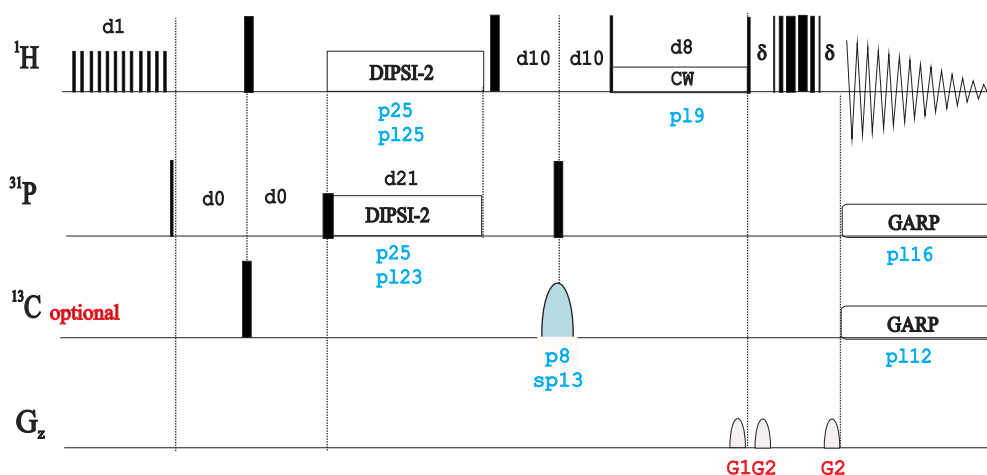
3D Cross-polarization version of a P-edited ^1H - ^1H NOESY experiment that provides a 3D P,H,H map.



na_hpdino3d



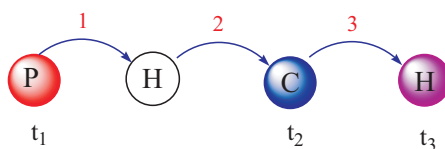
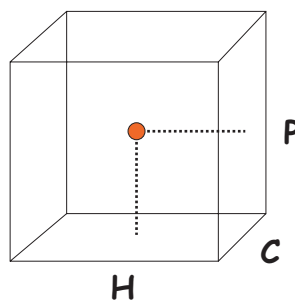
na_hpdino193d



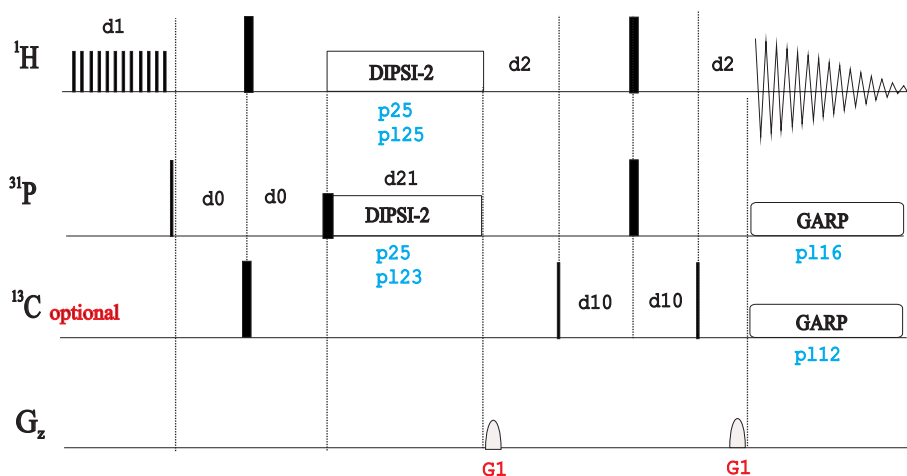
3D HeteroTOCSY-COSY Experiment

Experiment Description

3D version of the PHCH experiment that uses cross-polarization for P-to-H transfer. The experiment provides a 3D correlation P;C;H map.



na_hpdico3d

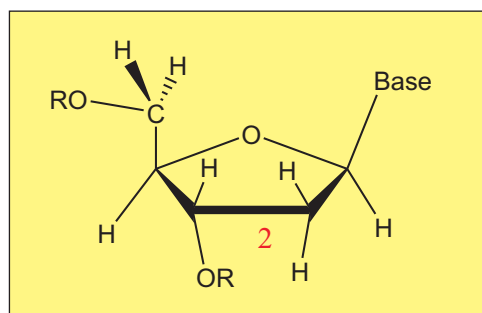
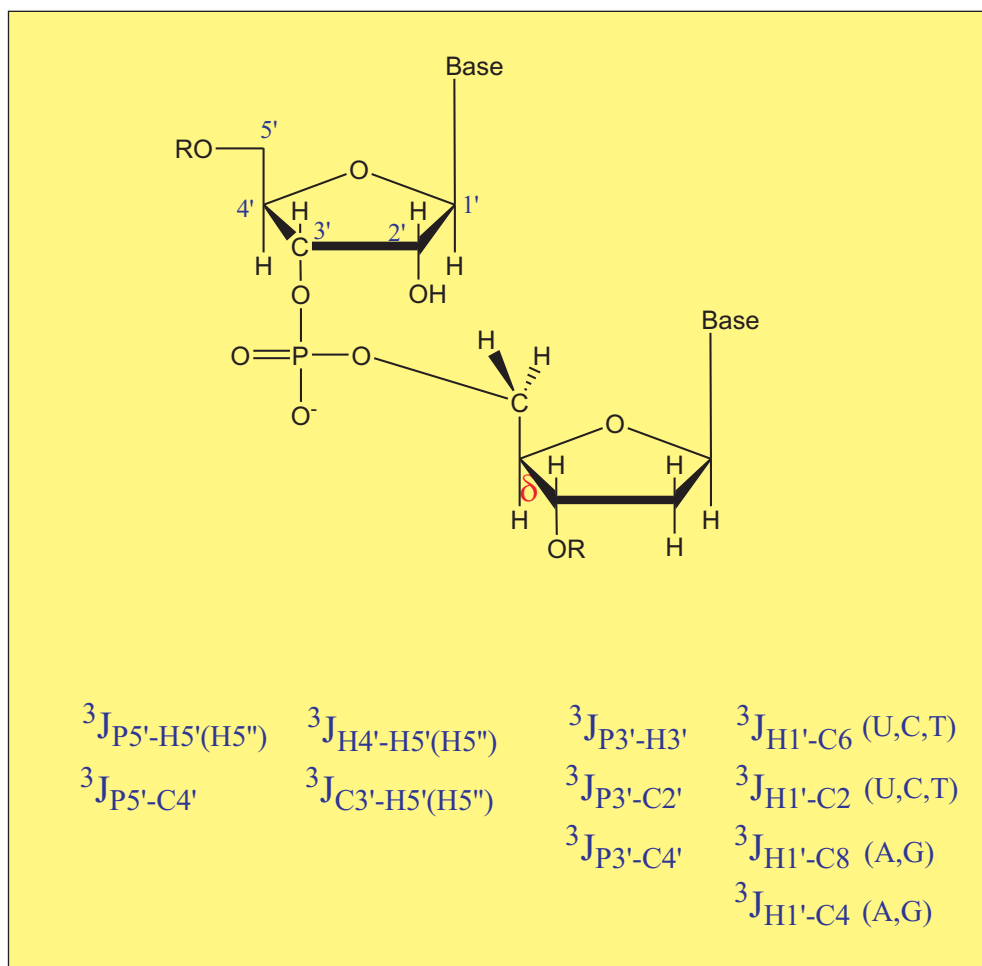


BRUKER PULSE PROGRAM CATALOGUE

NMRGuide

NUCLEIC-ACID NMR
EXPERIMENTS TO MEASURE J

Important Dihedral angles in nucleic acids:

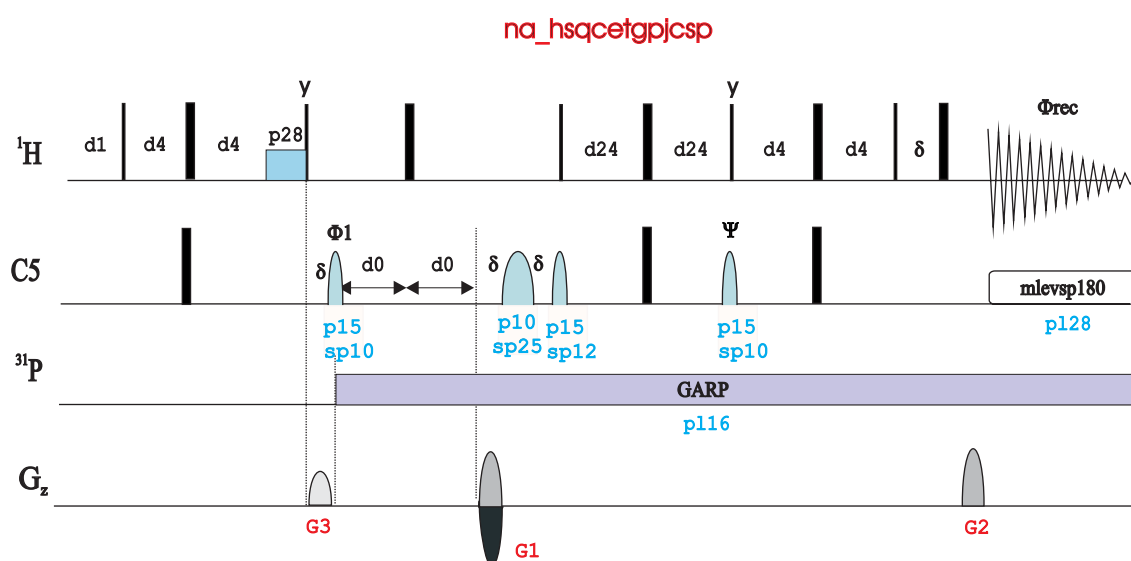


2D HSQC Experiment for measuring J(CH)

Experiment Description

Modified sensitivity-improved HSQC pulse scheme for the stereospecific assignment of H5'/H5'' diastereotopic protons in NAs by measurement of homonuclear J(H4'H5') and heteronuclear J(C4'H5') coupling constants (96jacs4388).

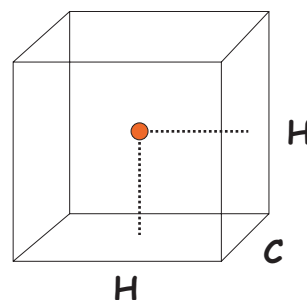
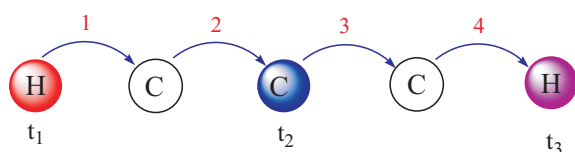
Also useful for measurement of J(C2'H1') via N in ¹³C/¹⁵N labeled NAs.



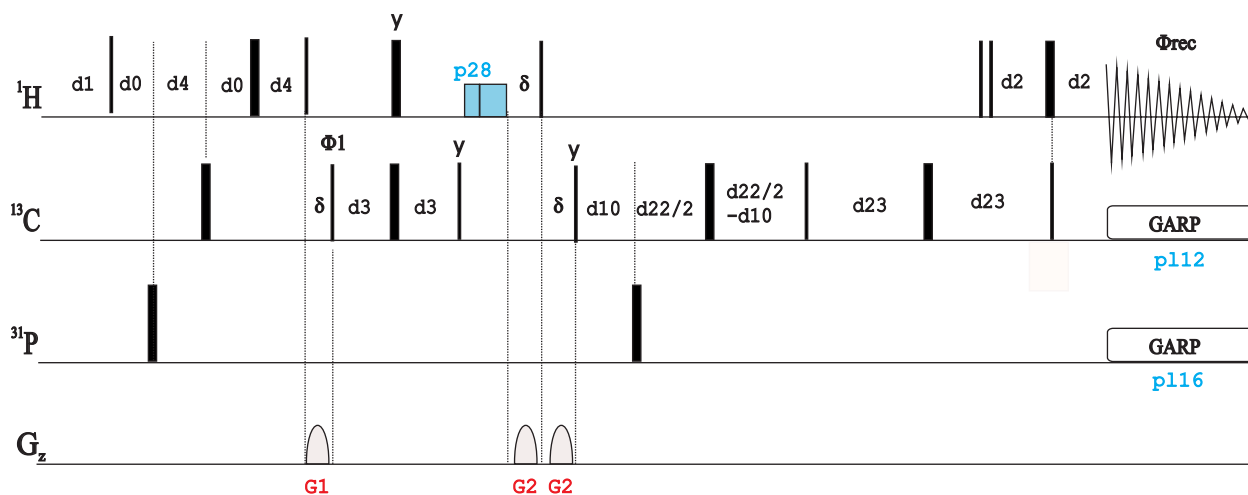
3D H(C)CH-E.COSY Experiment

Experiment Description:

Modified HCCH-COSY pulse scheme to measure $J(\text{CH})$ in ribose rings (93JMRB333-101, 94JB631).



hcchecgp3d



$d2 = 1/2J(\text{CH})$
 $d4 = 1/4J(\text{CH}) = 1.6\text{ms}$
 $d3 = 1/4J(\text{CH})$
 $d23 = 1/8J(\text{CC}) = 3.1\text{ms}$
 $d22 = \text{Constant-time C period.}$
 For all correlations $3/4J(\text{CC}) = 18.8\text{ms}$
 For C1' and C5' $1/2J(\text{CC}) = 12.5\text{ms}$

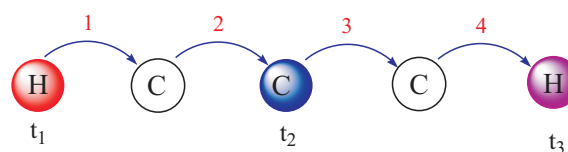
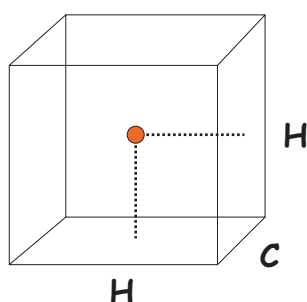
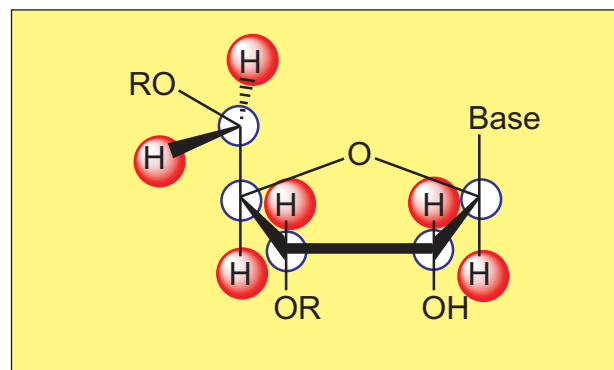
3D H(C)CH-TOCSY Experiment

Experiment Description

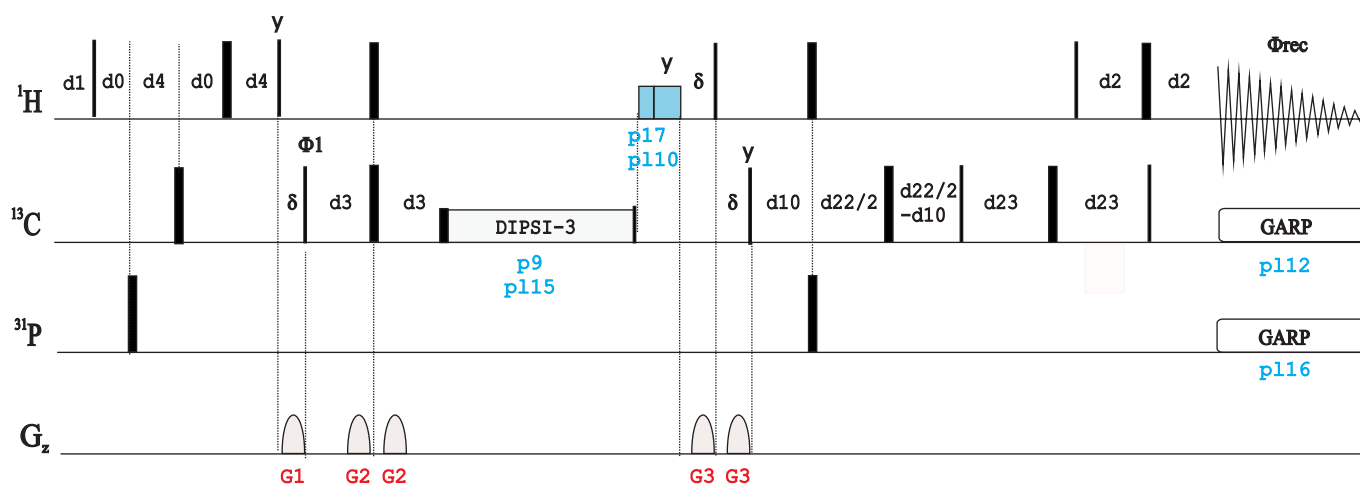
Specific HCCH-TOCSY experiment to identify all ^1H and ^{13}C nuclei belonging to the same sugar ring in ^{13}C -labeled NAs. Alternative to classical COSY and TOCSY experiment. Also see other HCCH-COSY and HCCH-TOCSY experiments.

NMR Spectrum

The experiment provides a 3D correlation map



na_hcchfwdlqp3d



$d2 = 1/2J(\text{CH})$
 $d4 = 1/4J(\text{CH}) = 1.6\text{ms}$
 $d3 = 1/4J(\text{CH})$
 $d23 = 1/8J(\text{CC}) = 3.1\text{ms}$
 $d22 = \text{Constant-time C period.}$
 For all correlations $3/4J(\text{CC}) = 18.8\text{ms}$
 For C1' and C5' $1/2J(\text{CC}) = 12.5\text{ms}$

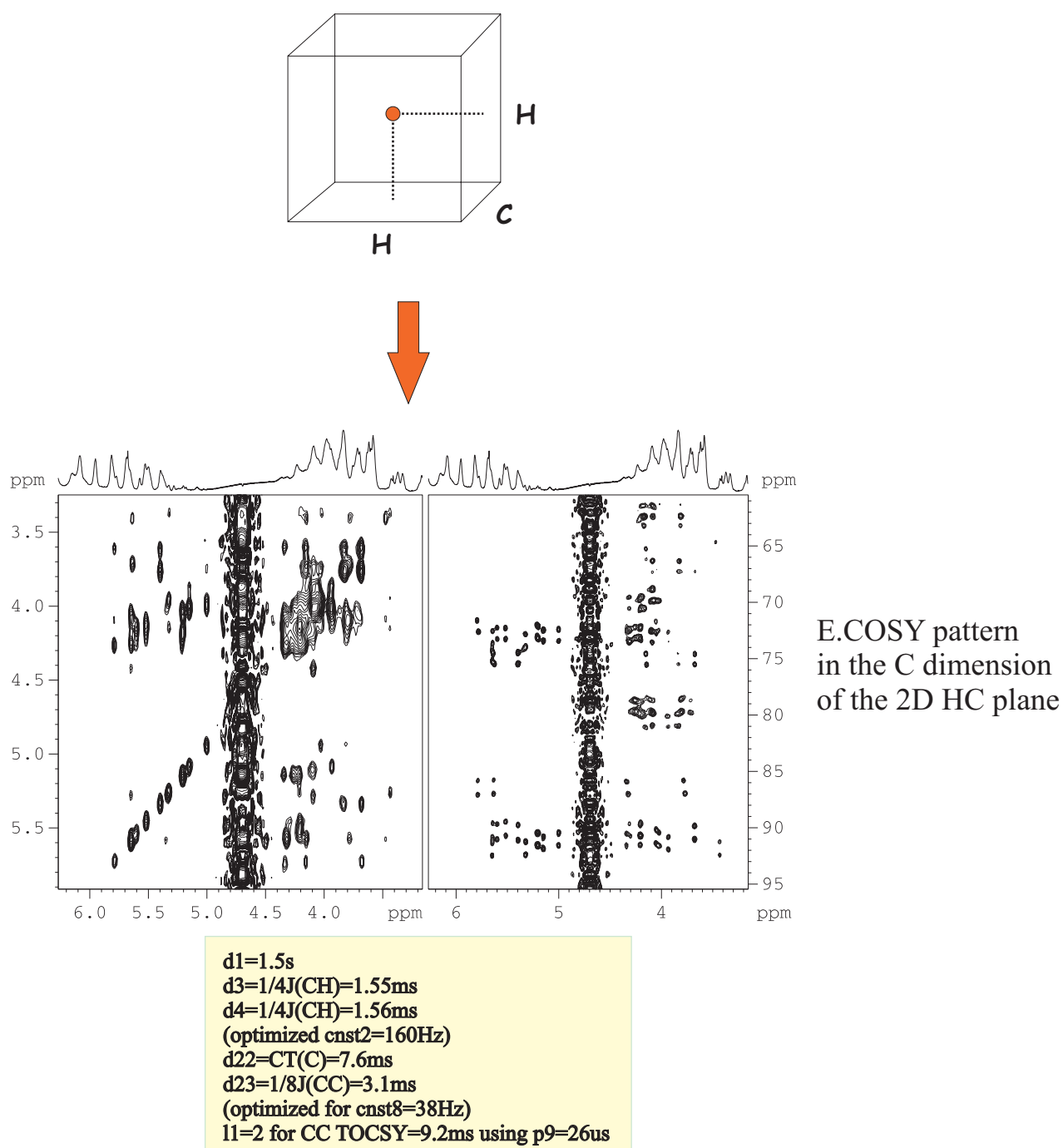
3D H(C)CH-TOCSY E.COSY Experiment

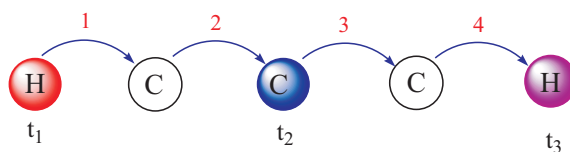
Experiment Description:

E.COSY version of the HCCH-TOCSY experiment to measure $J(H4'H5')$ coupling constants (96jacs4388)

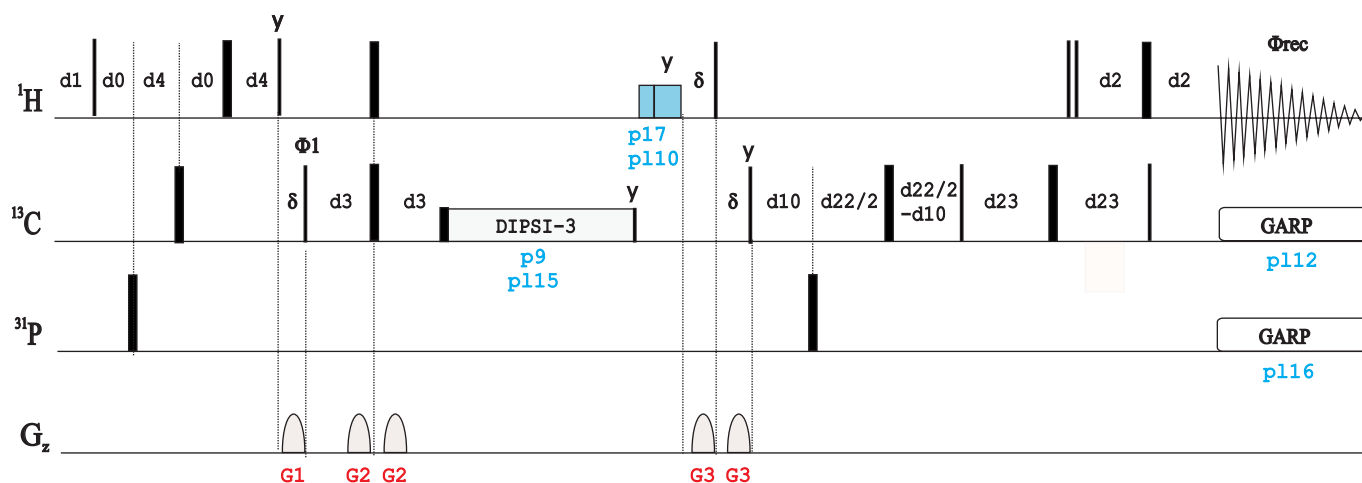
NMR Spectrum

The experiment provides a 3D correlation map

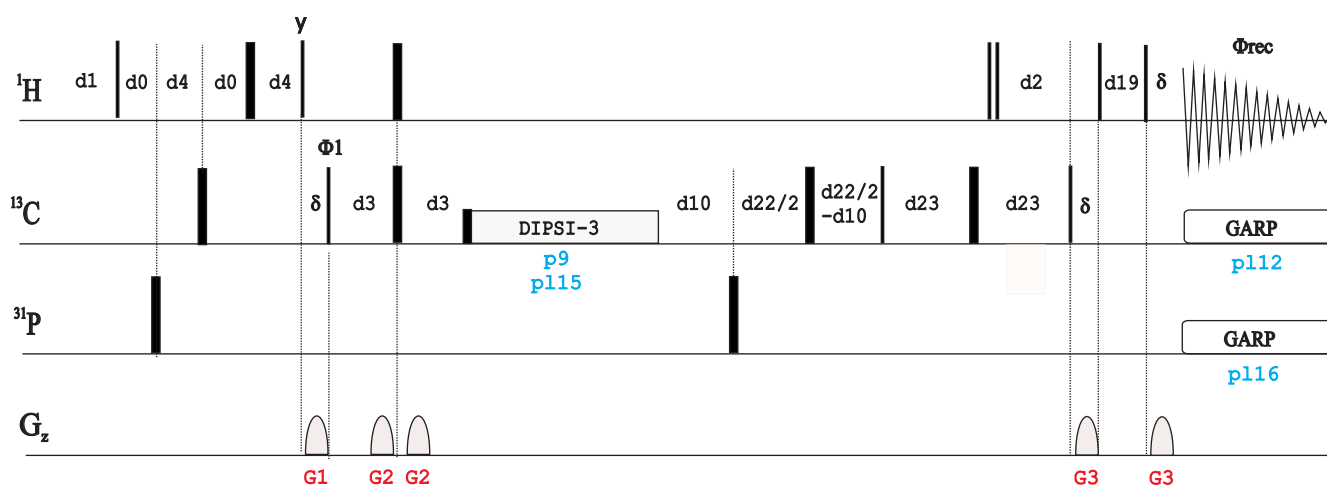




na_hcchfwdlecgp3d



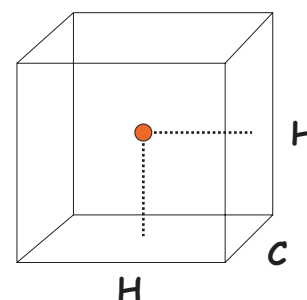
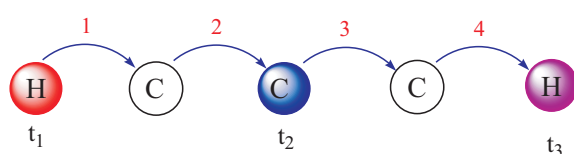
na_hcchfwdlecgpjr3d



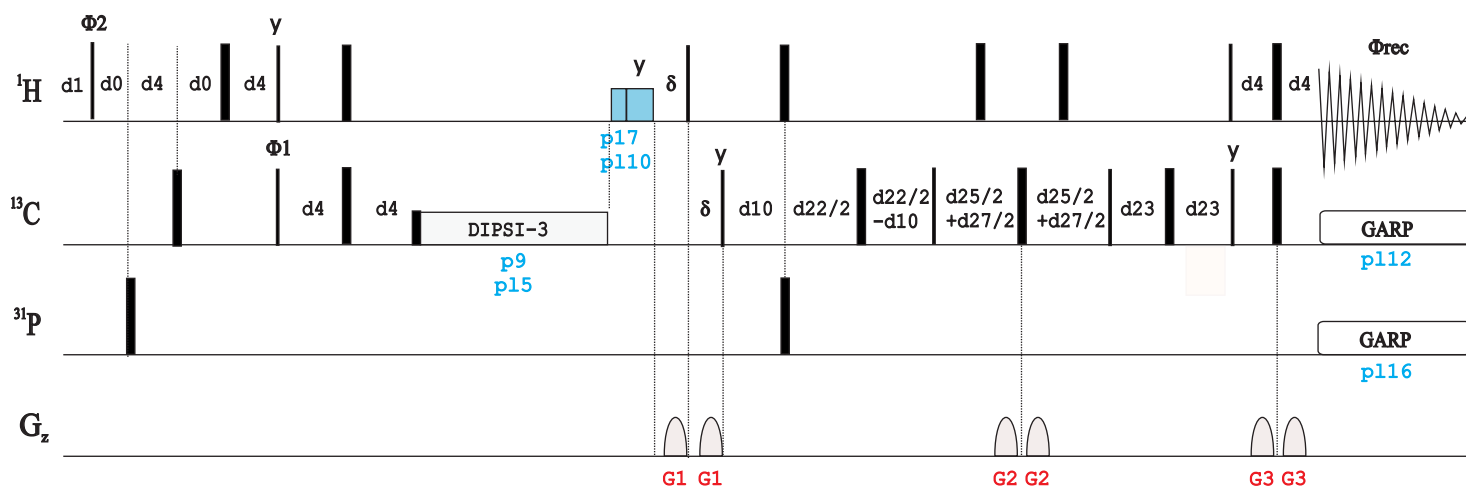
Forward-directed quantitative 3D H(C)CH-TOCSY Experiment

Experiment Description:

Modified HCCH-TOCSY version to measure $J(\text{HH})$ and $J(\text{CH})$ coupling constants
(99JACS1956 & 99JB241-15)



ghcchfwdlqp3d



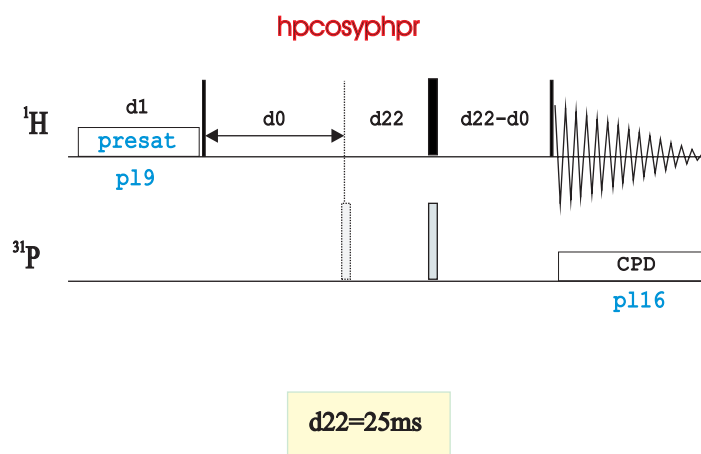
$d4 = 1/4J(\text{CH}) = 1.6\text{ms}$
 $d23 = 1/8J(\text{CC}) = 3.1\text{ms}$
 $d22 = \text{Constant-time C period.}$
 For all correlations $3/4J(\text{CC}) = 18.8\text{ms}$
 For C1' and C5' $1/2J(\text{CC}) = 12.5\text{ms}$
 $d25 = \text{development of cross-correlated relaxation} = 25\text{ms}$

For reference experiment $d27 = 1/2J(\text{CH}) = 3.1\text{ms}$
 For cross-peak experiment $d27 = 0$

2D Constant-time HH- $\{^{31}\text{P}\}$ COSY Experiment

Experiment Description

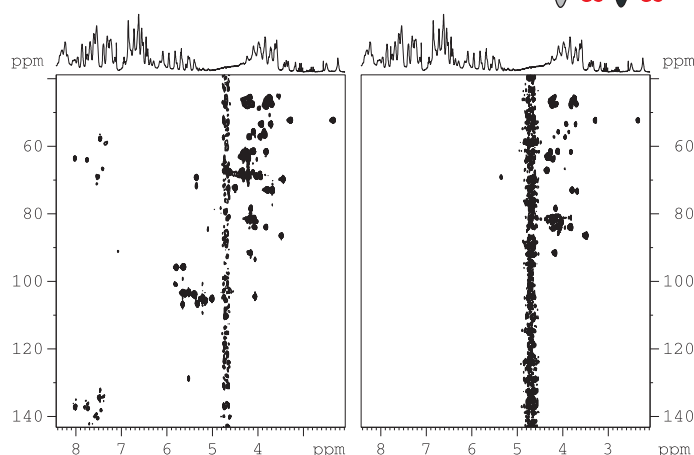
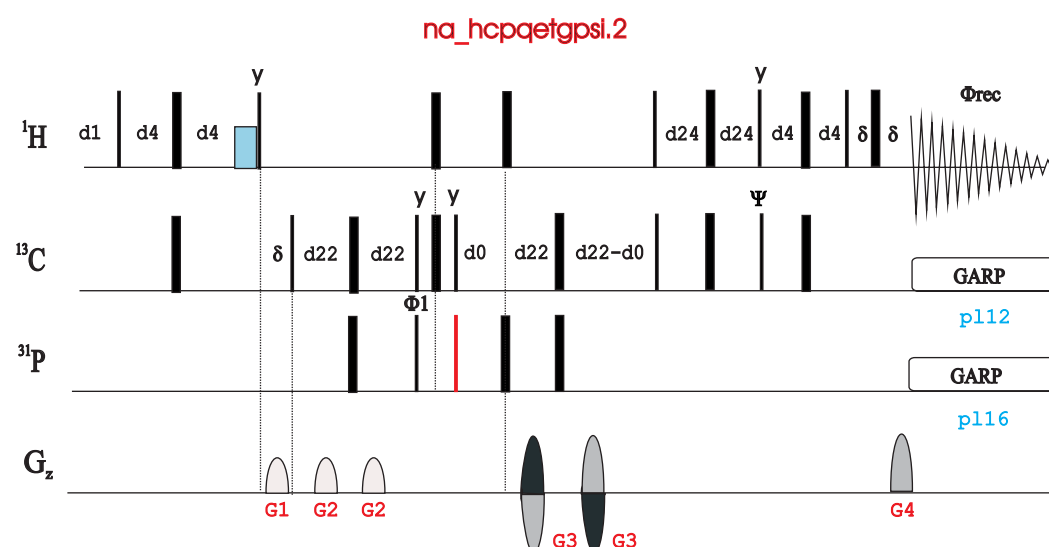
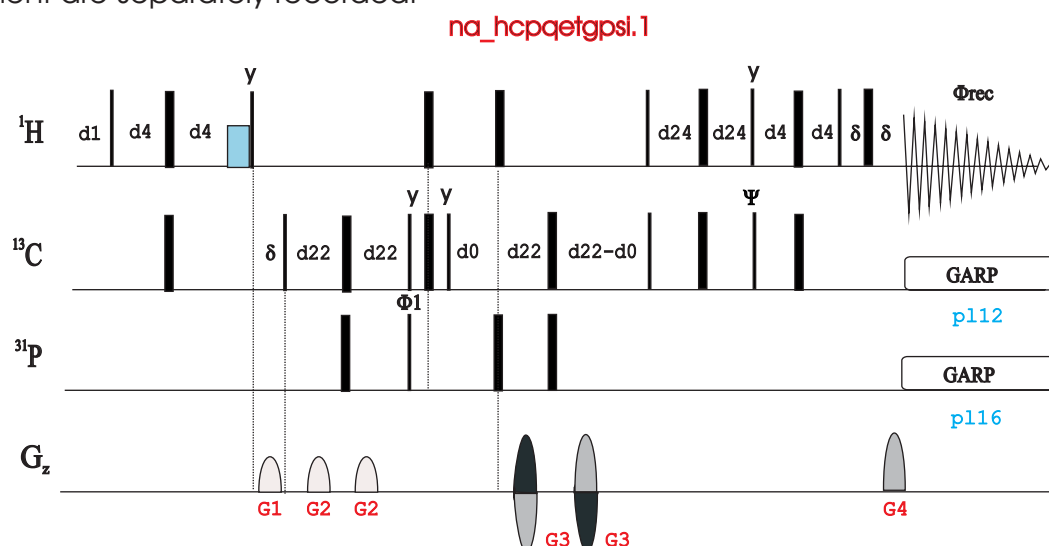
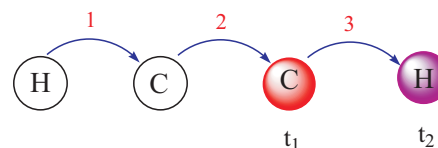
Constant-time ^1H - ^1H COSY experiment for the measurement of $J(\text{H3-P})$ coupling constants in NAs (98jmr164-134). Two experiments are recorded varying the position of the 180° ^{31}P pulse.



2D quantitative HC(P) Experiment

Experiment Description:

Modified 2D version of the put-and-back HCP experiment to measure $J(\text{CP})$ coupling constants (98jb223-12). Independent reference-peak and a cross-peak experiment are separately recorded.

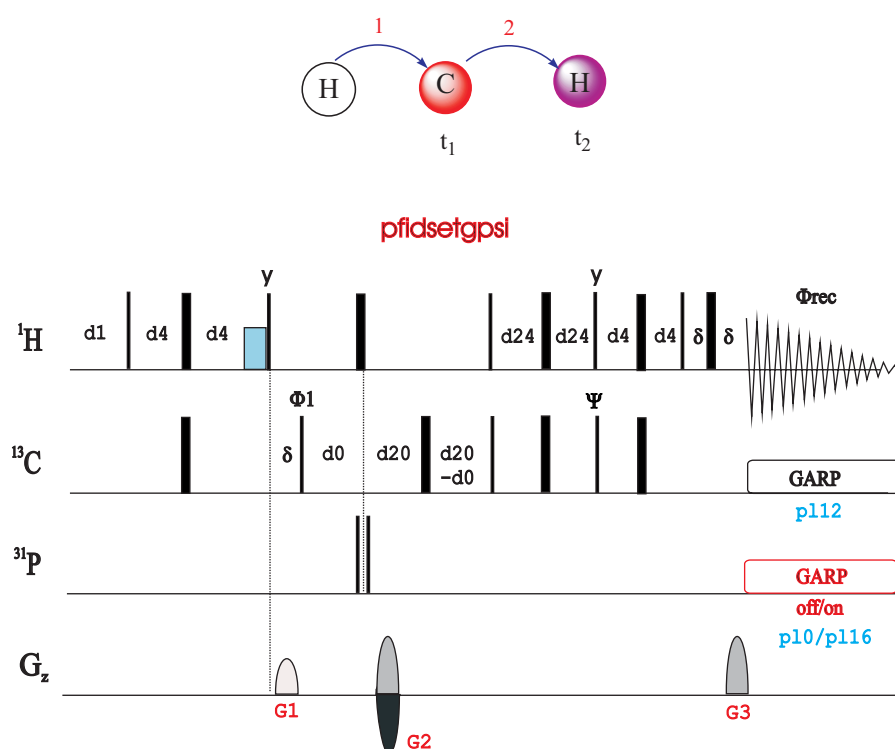


$d1=1.5s$
 $d4=1/4J(\text{CH})=1.6ms$
 $cnst2=J(\text{CH})$
 $cnst5=J(\text{CP})$
 $d22=CT(1/J(\text{CC}) \text{ for } J(\text{CC})=40\text{Hz and } 1/4J(\text{C4}'-\text{P})=12.5ms$
 $1/4J(\text{C5}'-\text{P})=25ms$

2D P-FIDS Experiment

Experiment Description:

Modified HSQC experiment to measure $J(\text{HP})$ and $J(\text{CP})$ in NAs (93jb479-3, 94jb631-4).
Two experiments are recorded with optional ^{31}P decoupling during ^1H acquisition.



$d4=1/4J(\text{CH})$
 $d24$ optimized as a function of CH_n multiplicity
 $d20=1/2J(\text{CC})=12.5\text{ms}$ or $3/2J(\text{CC})=37.5\text{ms}$

