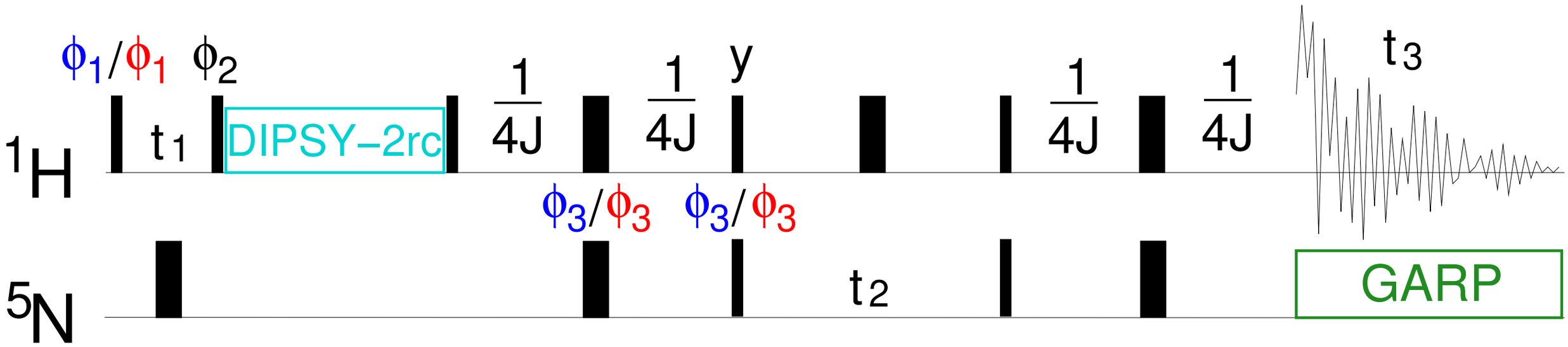
LECTURE 7

TOCSY-HSQC

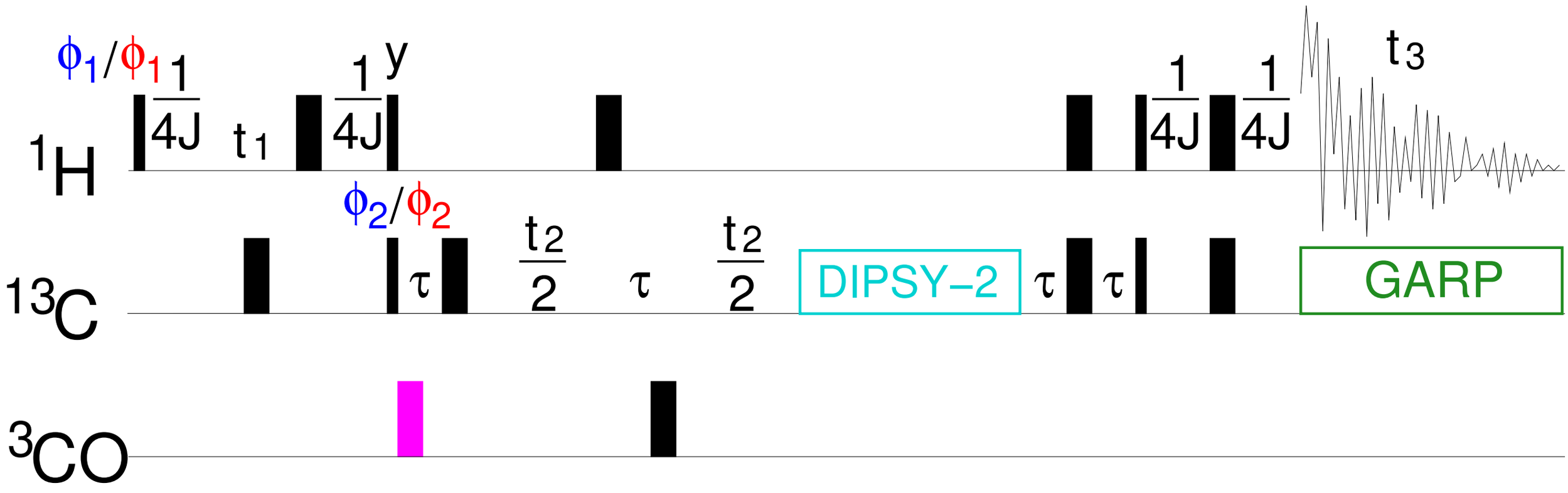


ϕ_1=x,x,–x,–x,x,x,–x,–x ϕ_3=x,–x,x,–x,x,–x,x,–x

ϕ_1=y,y,–y,–y,y,y,–y,–y ϕ_3=y,–y,y,–y,y,–y,y,–y

ϕ_2=x,x,x,x,–x,–x,–x,–x receiver phase: x,–x,–x,x,–x,x,x,–x

HC(C)H-TOCSY

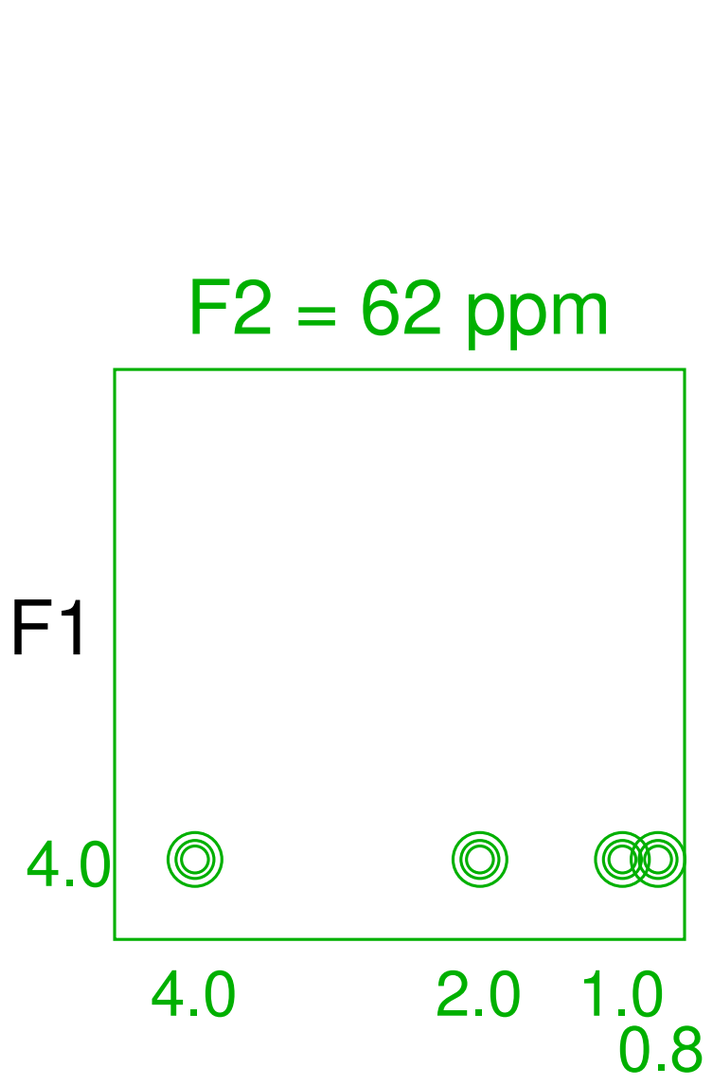


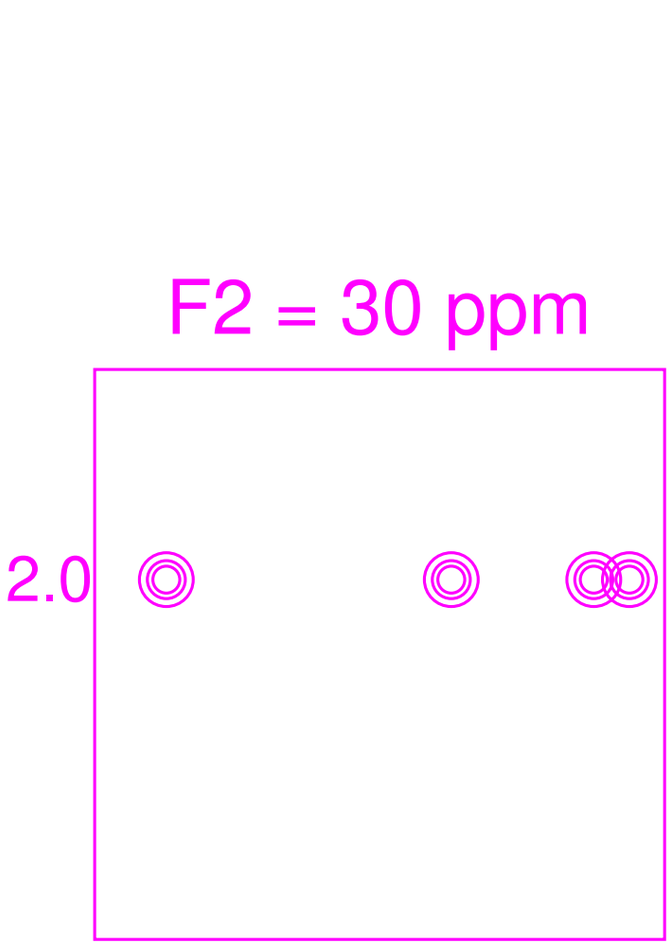
ϕ_1=x,–x,x,–x,x,–x,x,–x ϕ_2=x,x,–x,–x,x,x,–x,–x

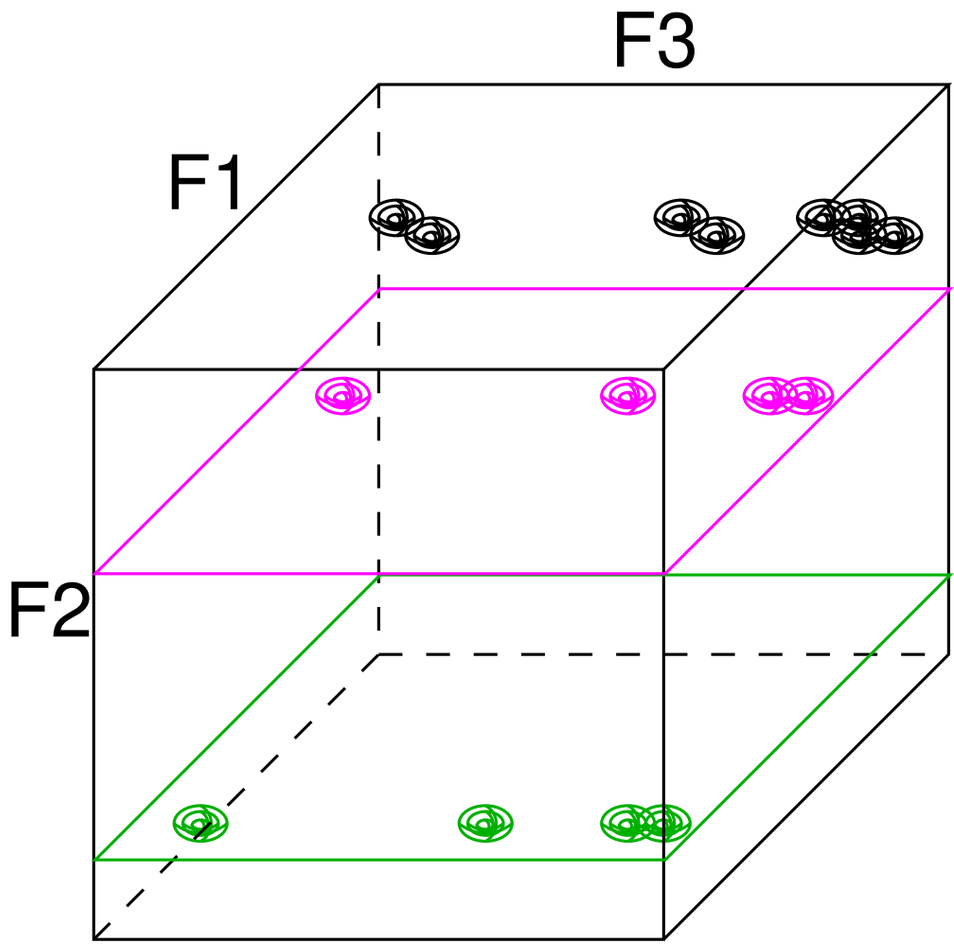
ϕ_1=y,–y,y,–y,y,–y,y,–y ϕ_2=y,y,–y,–y,y,y,–y,–y

receiver phase: x,–x,–x,x,–x,x,x,–x

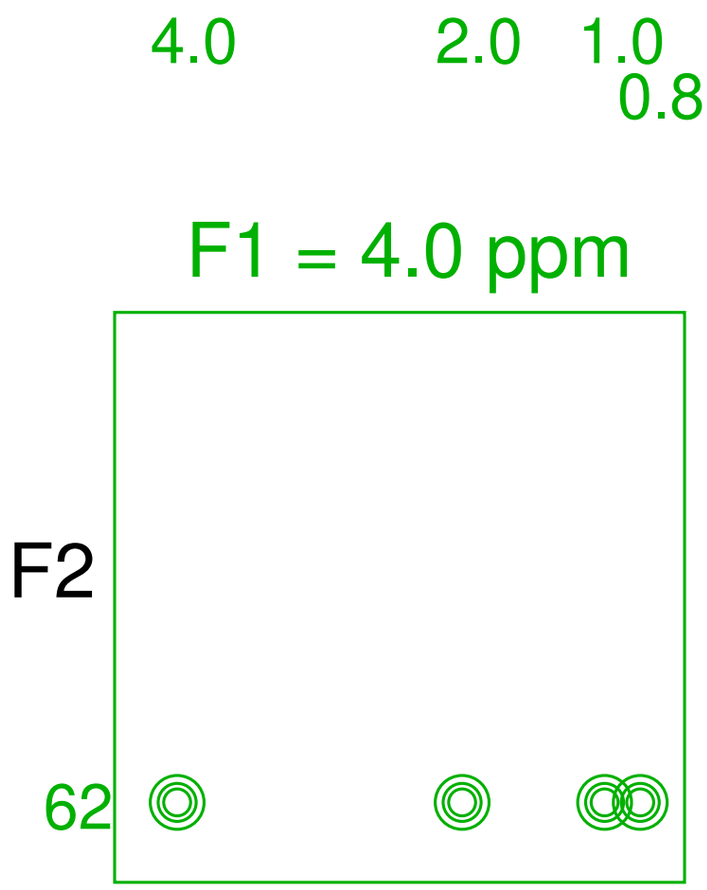
a

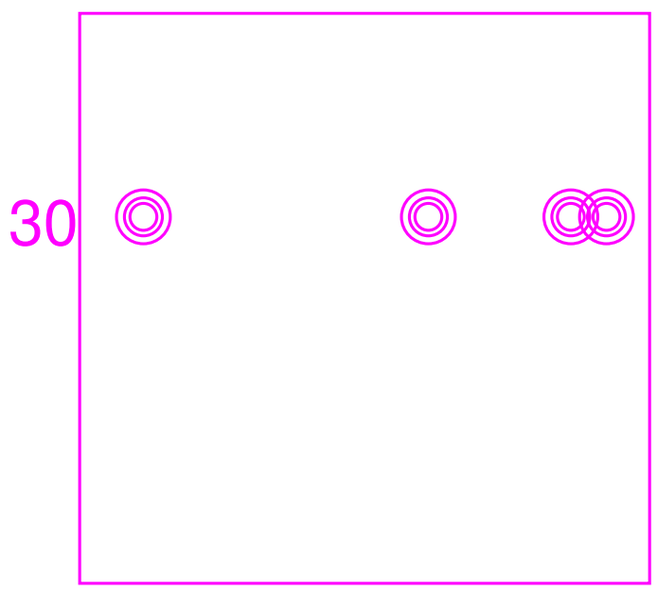


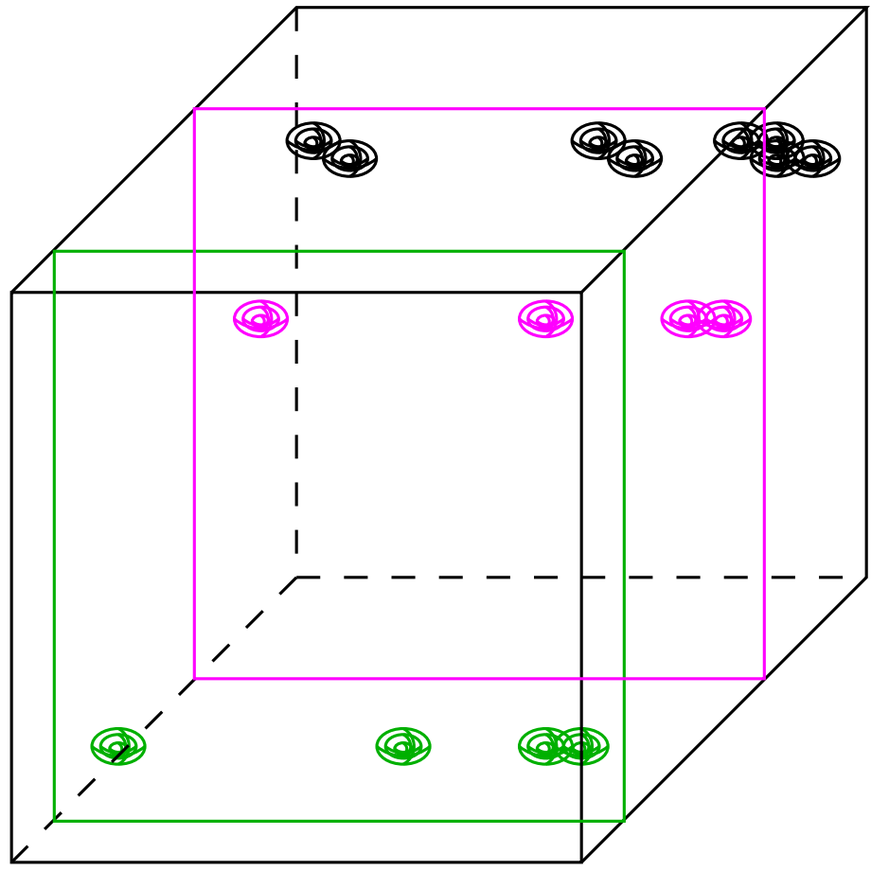




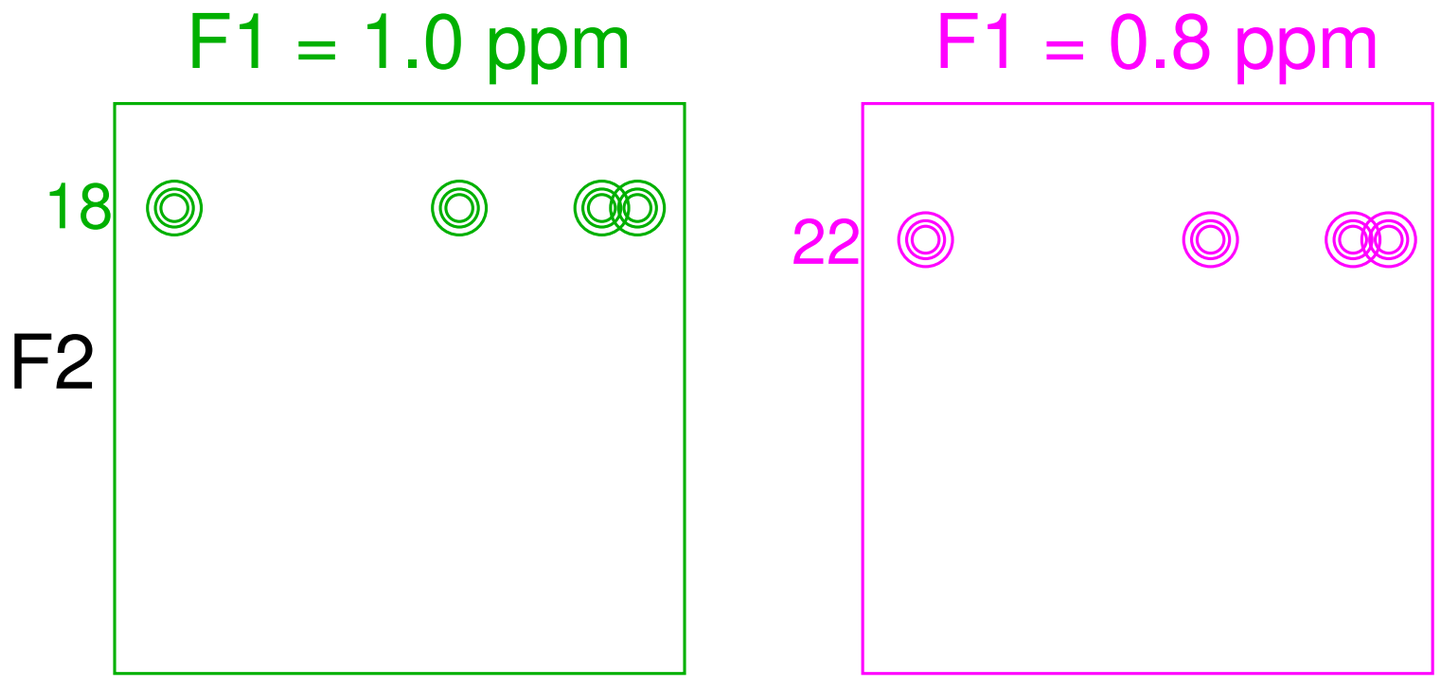
b

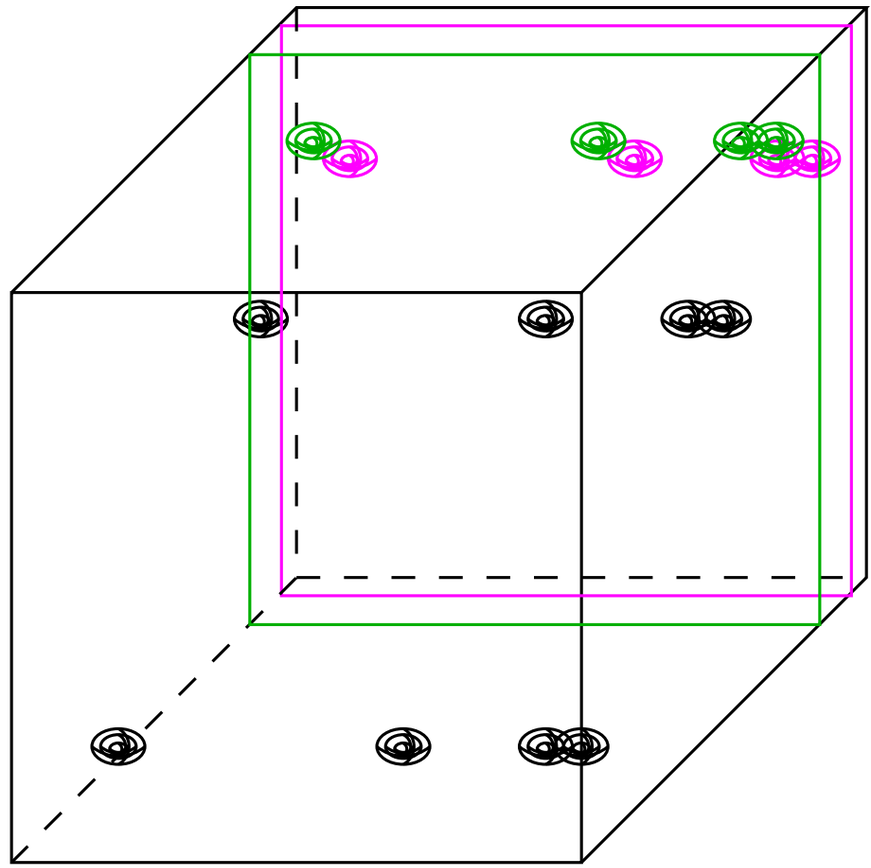




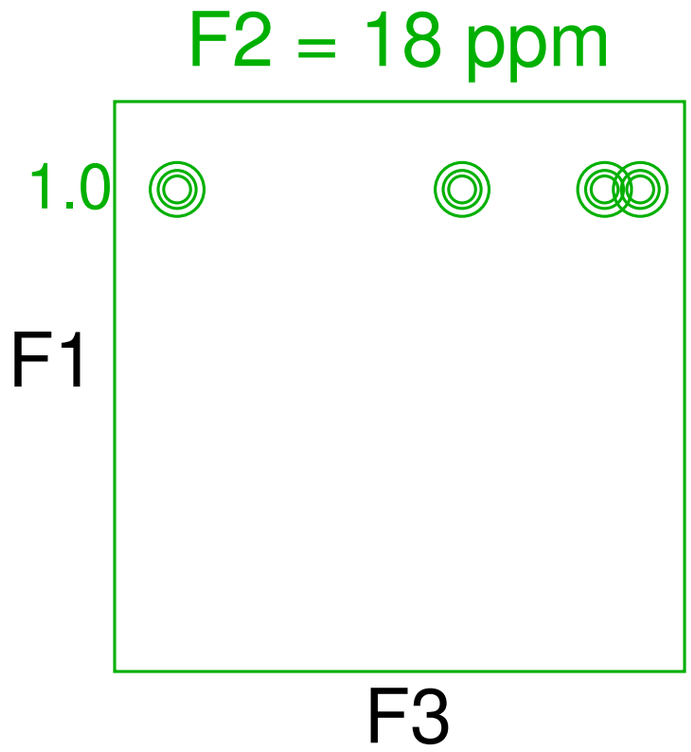


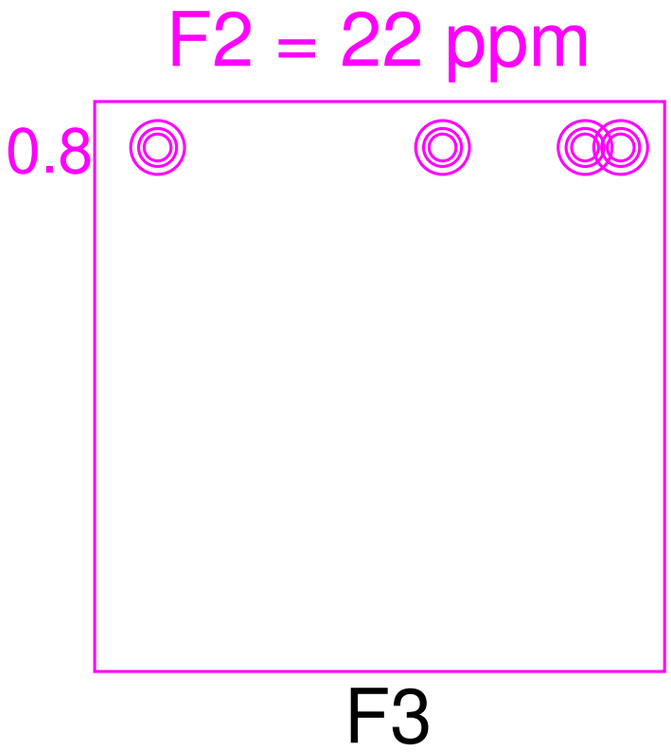
c

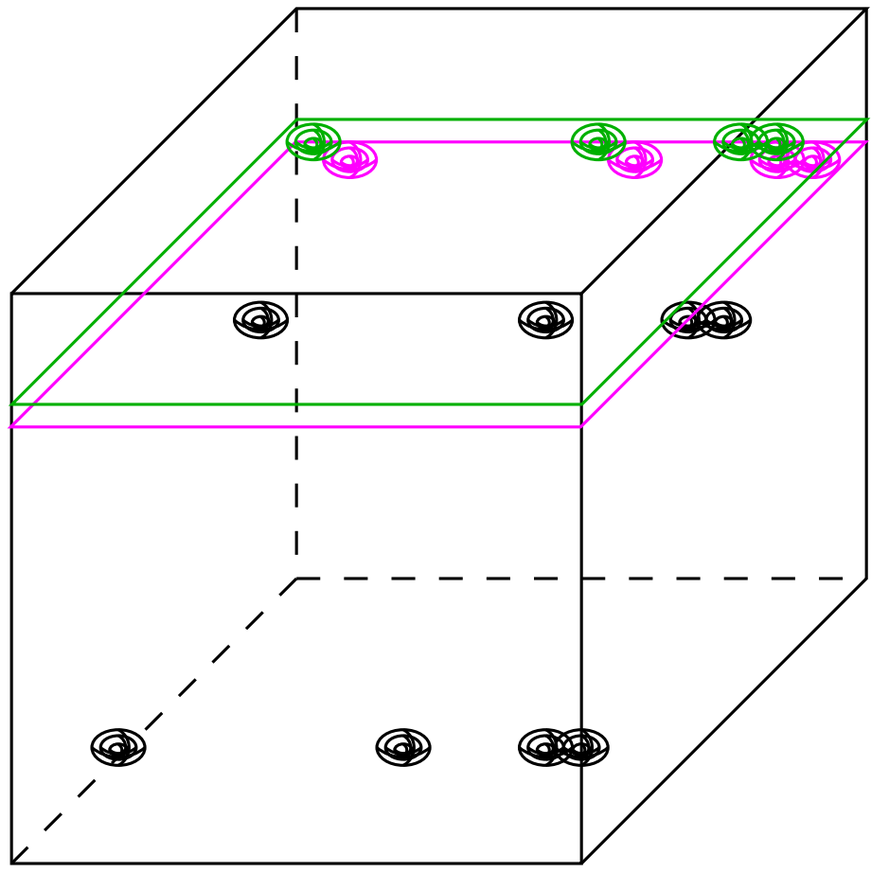




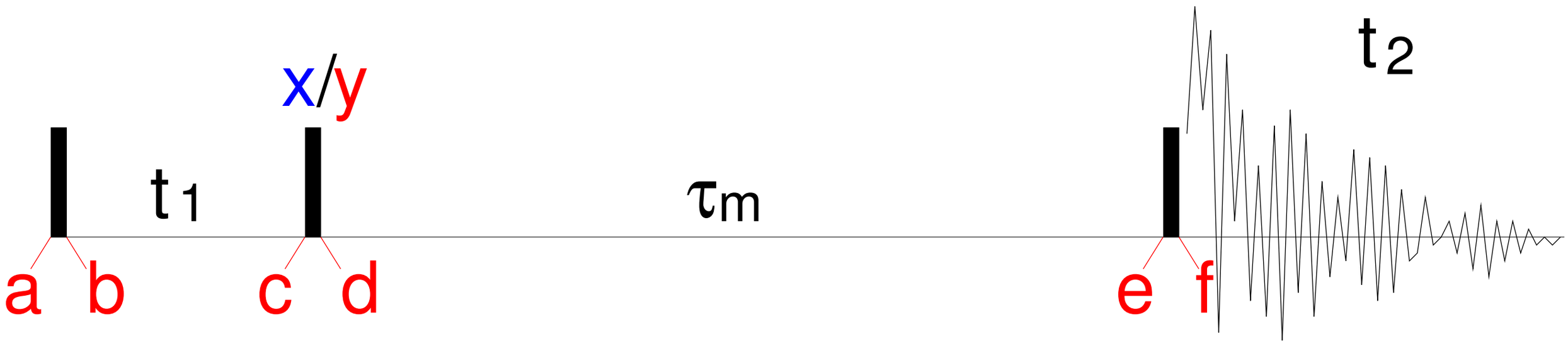
d

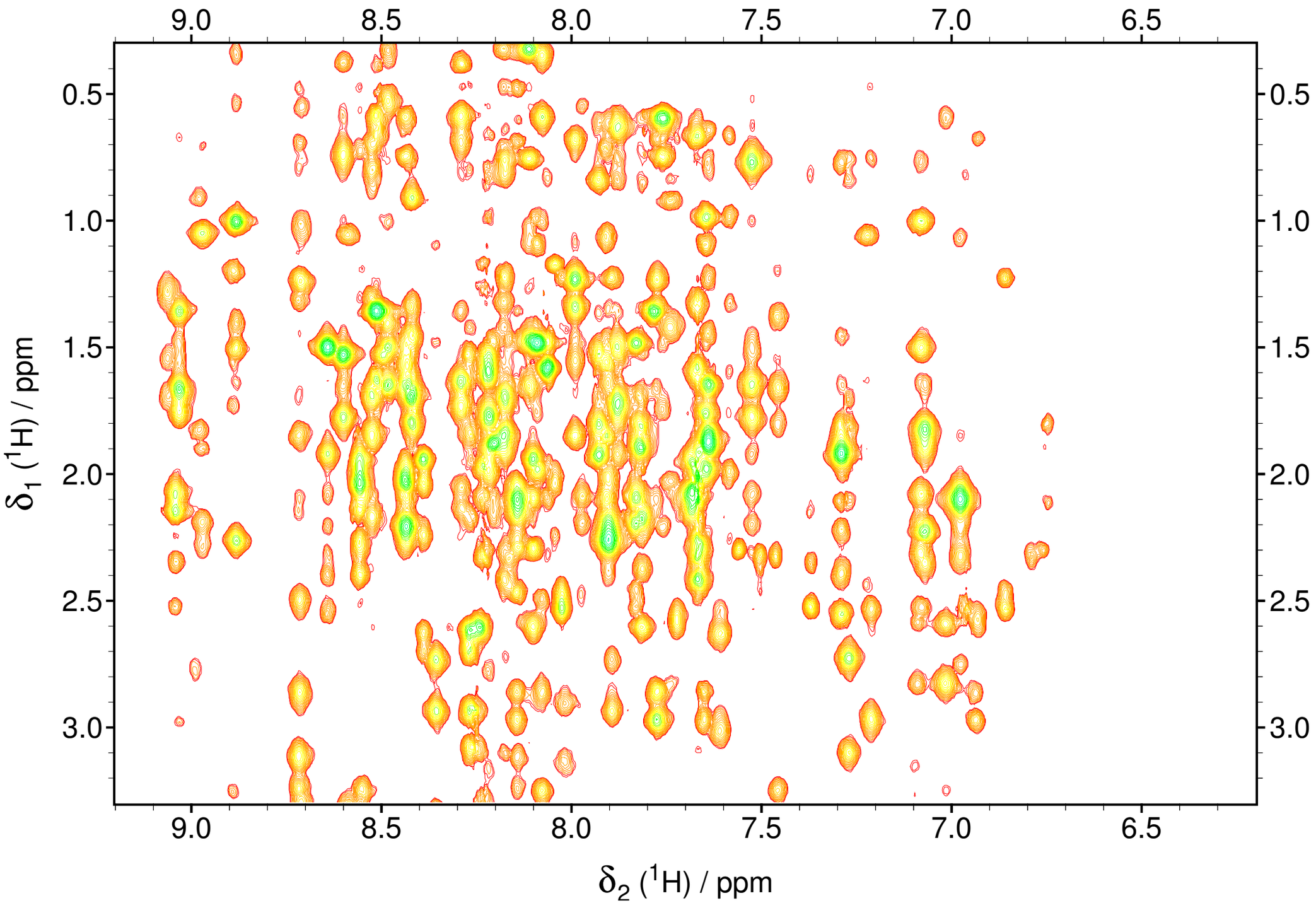




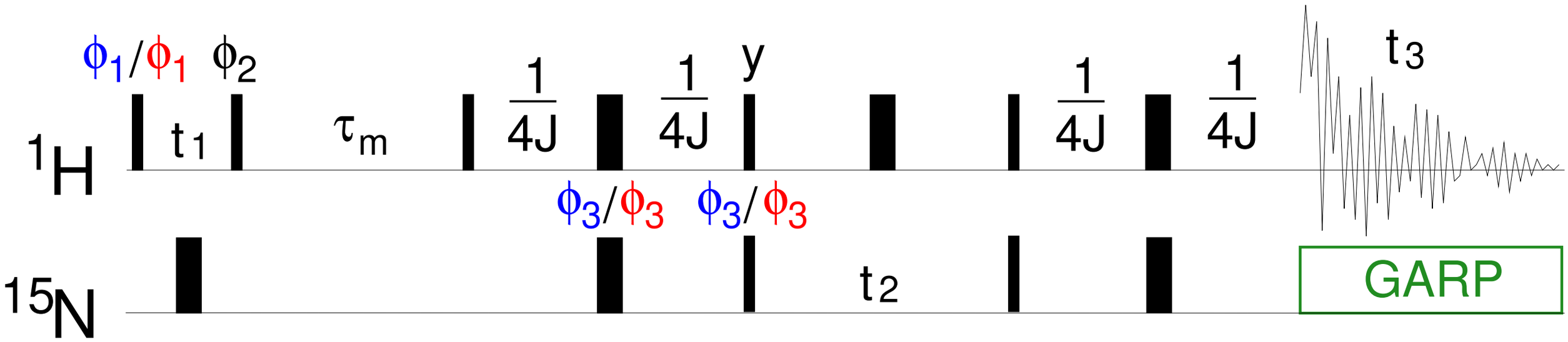


NOESY




9.0
8.5
8.0
7.5
7.0
6.5
0.5
1.0
1.5
2.0
2.5
3.0
δ1 (1H) / ppm
δ2 (1H) / ppm

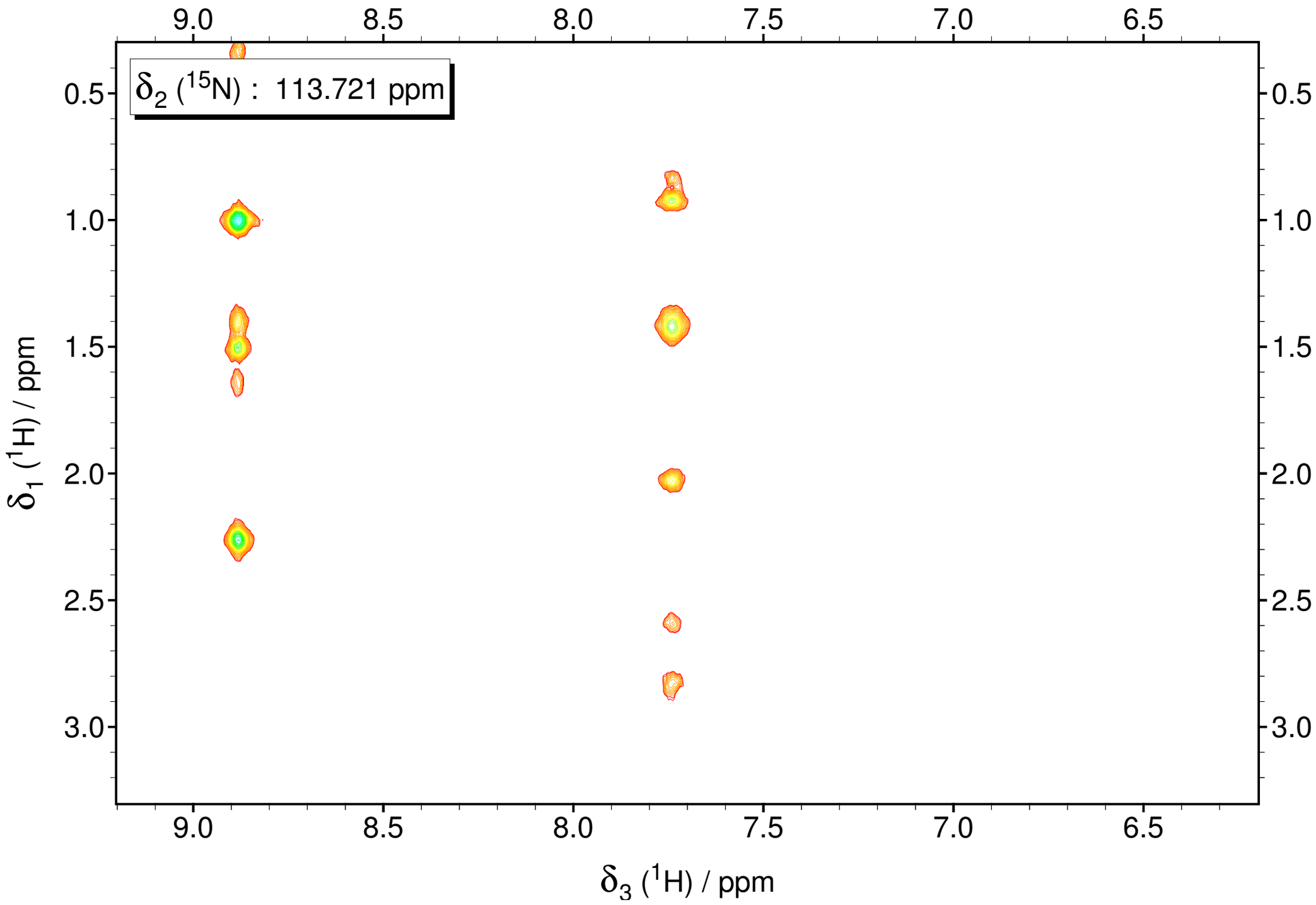
NOESY-HSQC

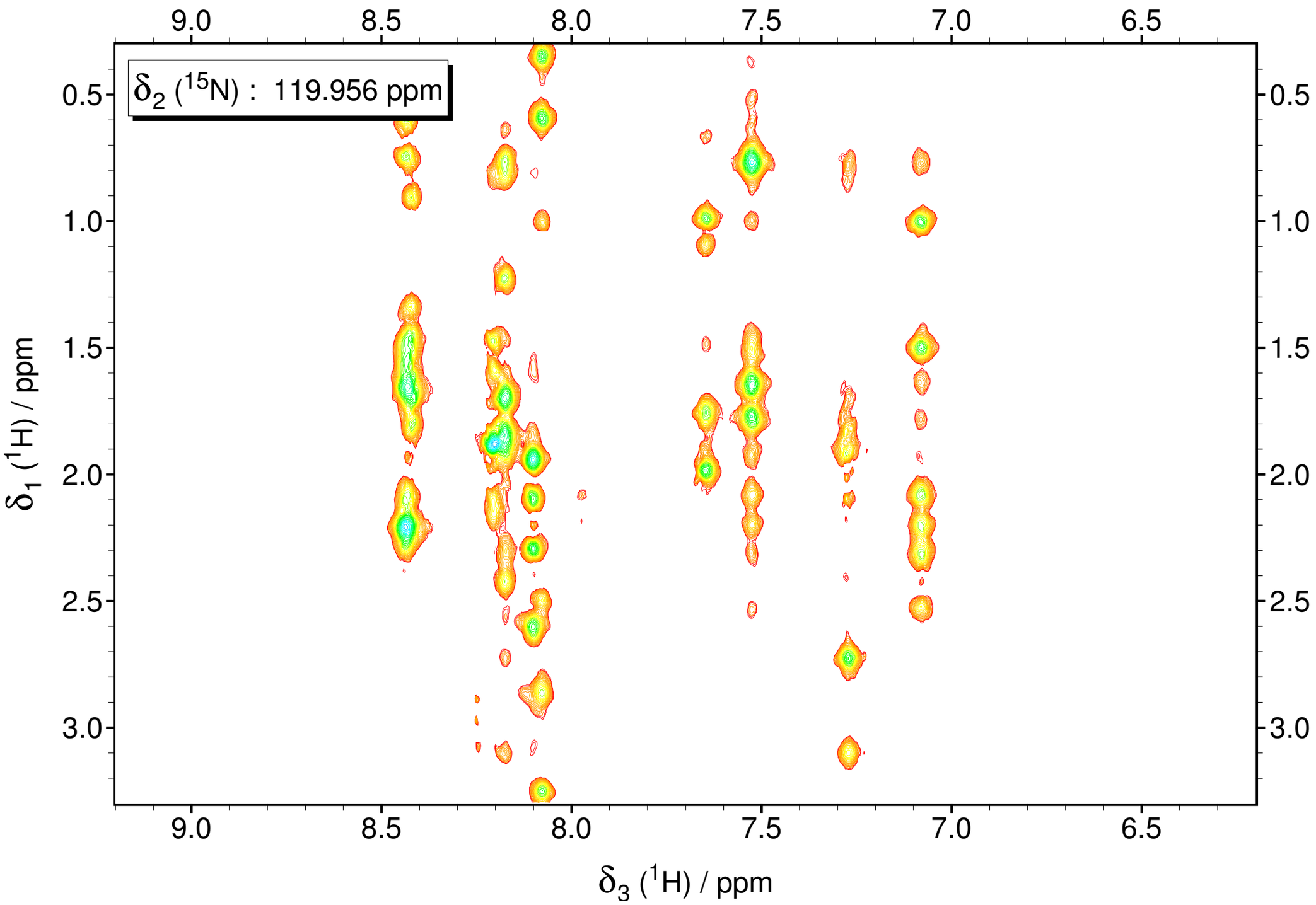


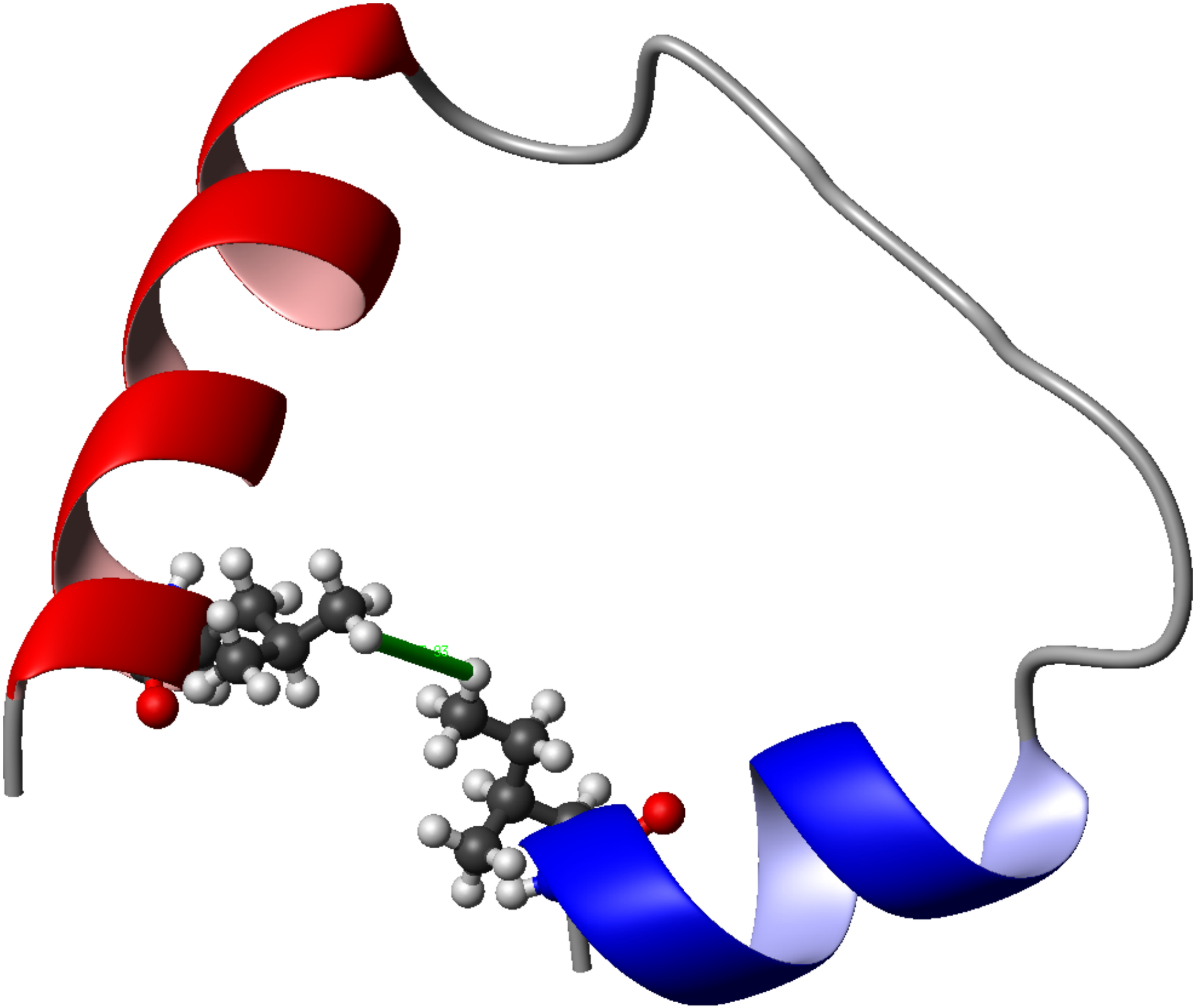
ϕ_1=x,x,–x,–x,x,x,–x,–x ϕ_3=x,–x,x,–x,x,–x,x,–x

ϕ_1=y,y,–y,–y,y,y,–y,–y ϕ_3=y,–y,y,–y,y,–y,y,–y

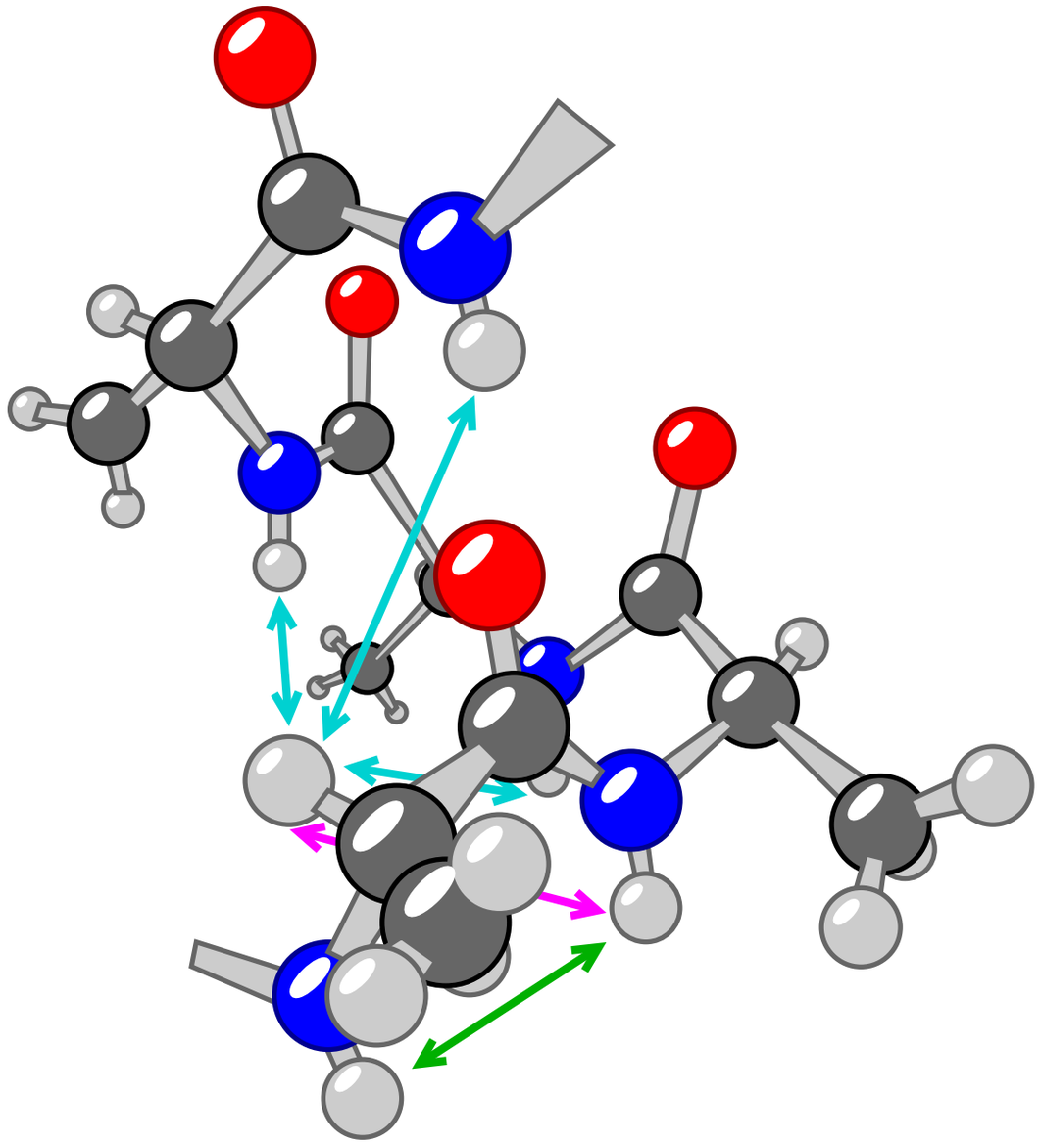
ϕ_2=x,x,x,x,–x,–x,–x,–x receiver phase: x,–x,–x,x,–x,x,x,–x

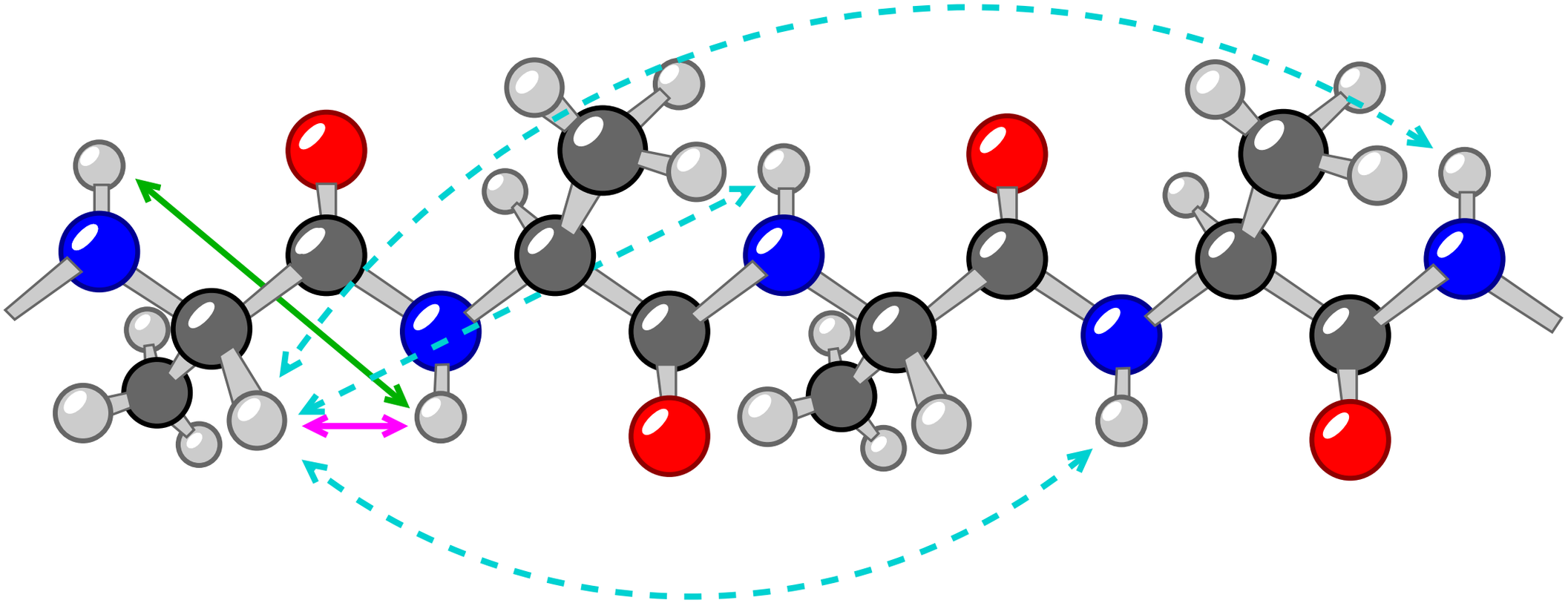

δ_2 (^{15}N) : 113.721 ppm
9.0
8.5
8.0
7.5
7.0
6.5
0.5
1.0
1.5
2.0
2.5
3.0
δ_1 (^{1}H) / ppm
δ_3 (^{1}H) / ppm


δ_2 (^{15}N) : 119.956 ppm
9.0
8.5
8.0
7.5
7.0
6.5
0.5
1.0
1.5
2.0
2.5
3.0
δ_1 (^{1}H) / ppm
δ_3 (^{1}H) / ppm

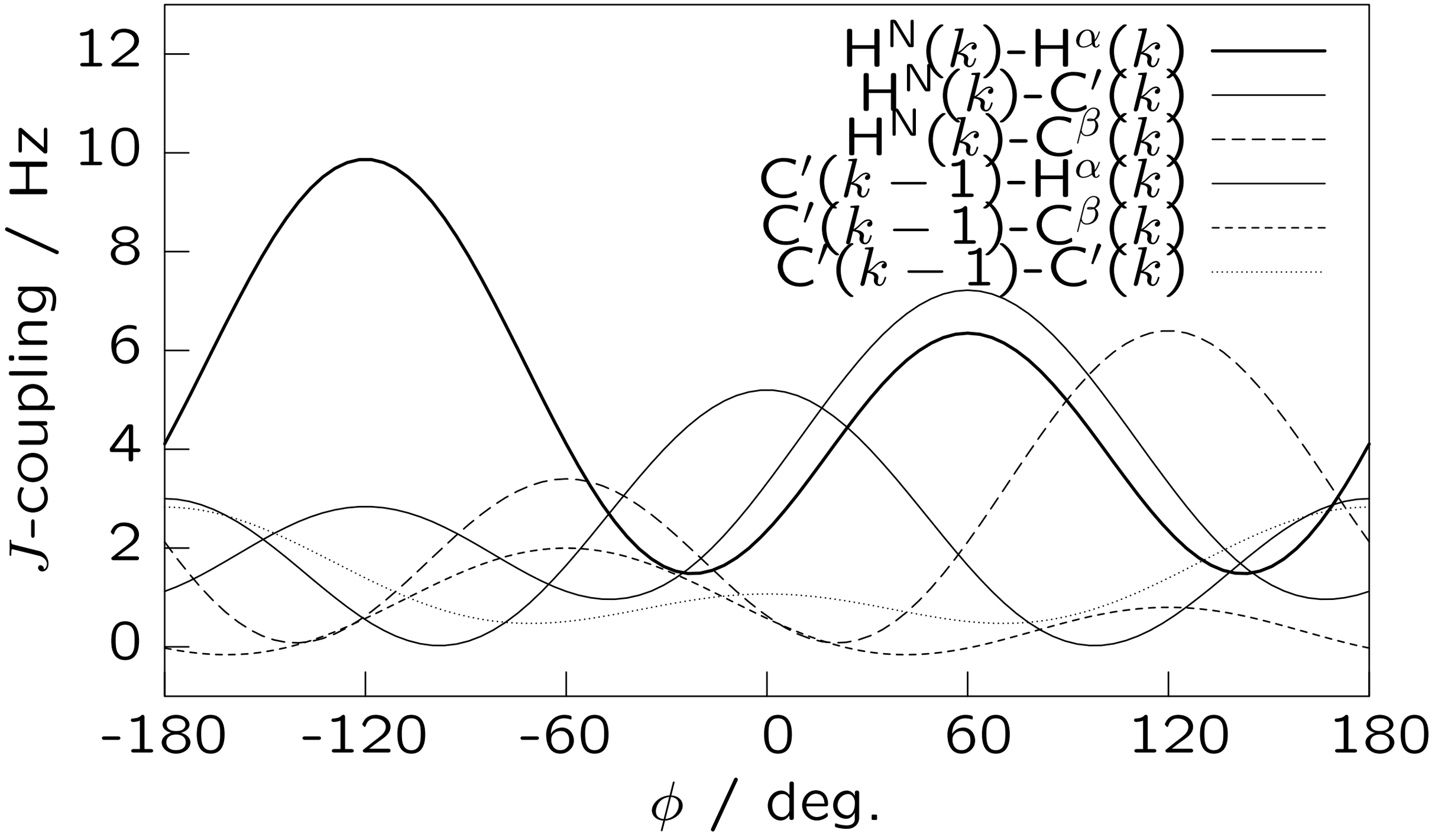


geminal protons in methylene H–C–H	0.17 nm
vicinal protons in aromatic ring H–C=C–H	0.25 nm
H_i^{α} and H_{i+3}^{N} protons in α-helix	0.34 nm
meta protons in aromatic ring H–C=CH–C–H	0.42 nm

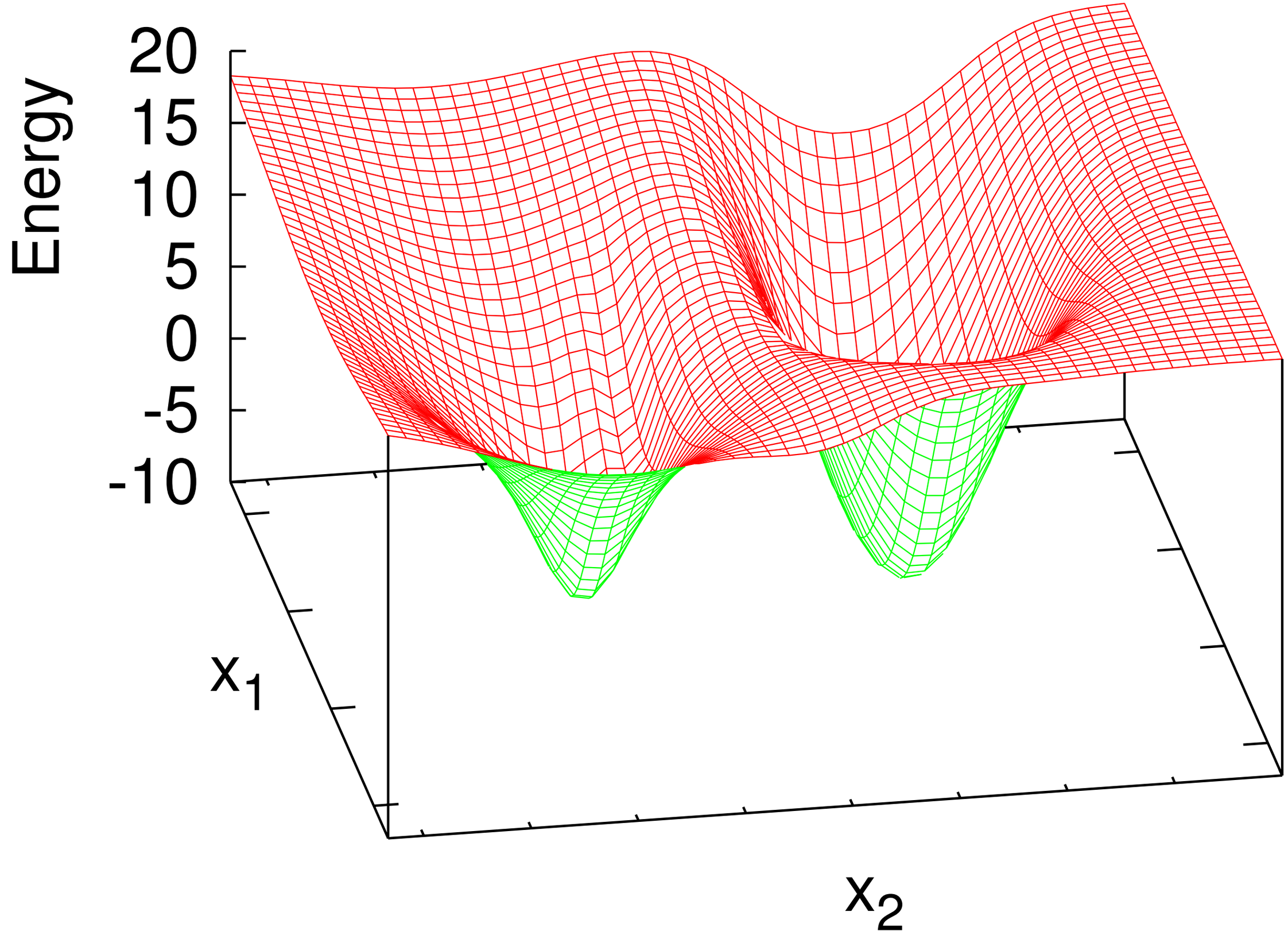


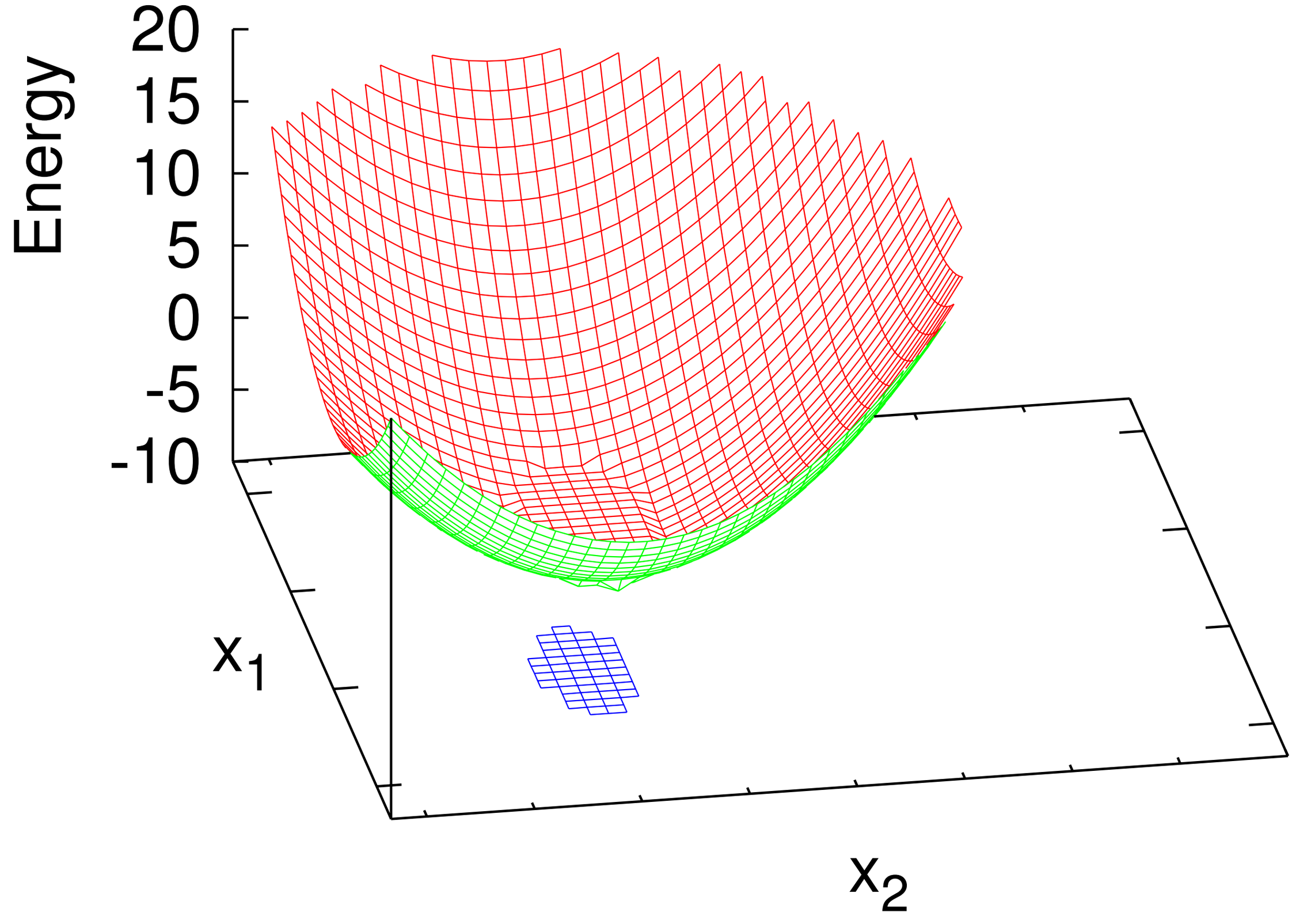


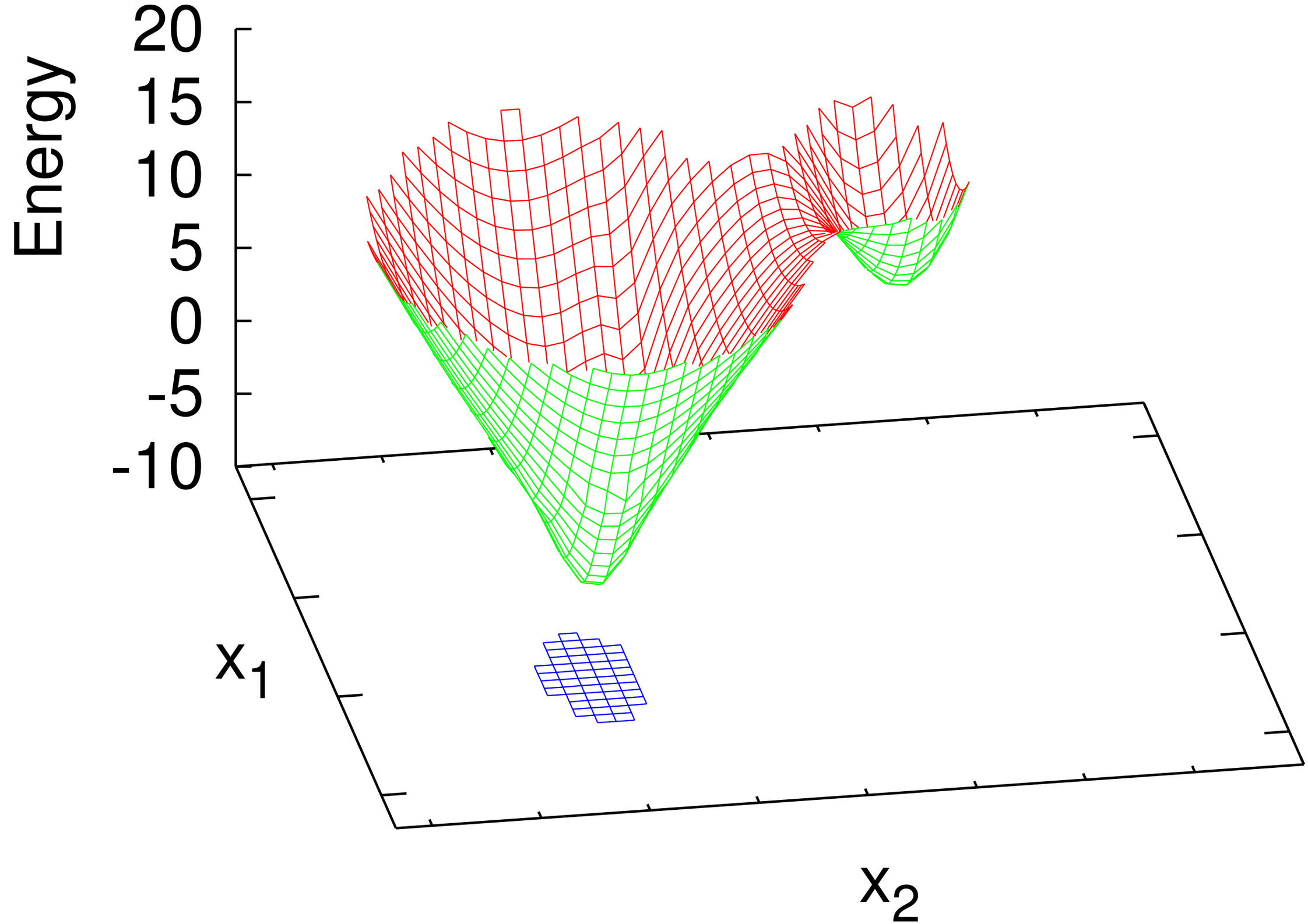
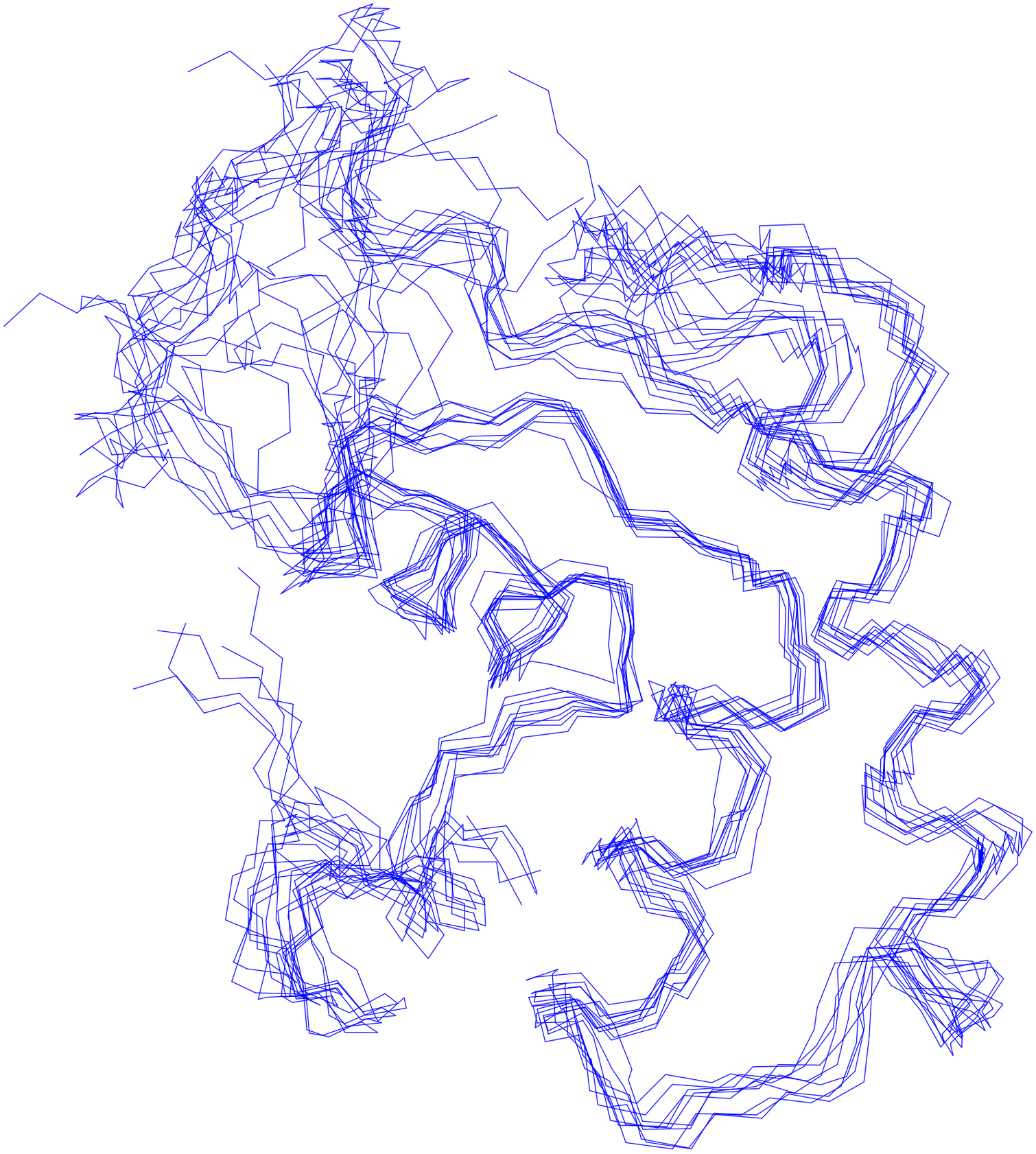
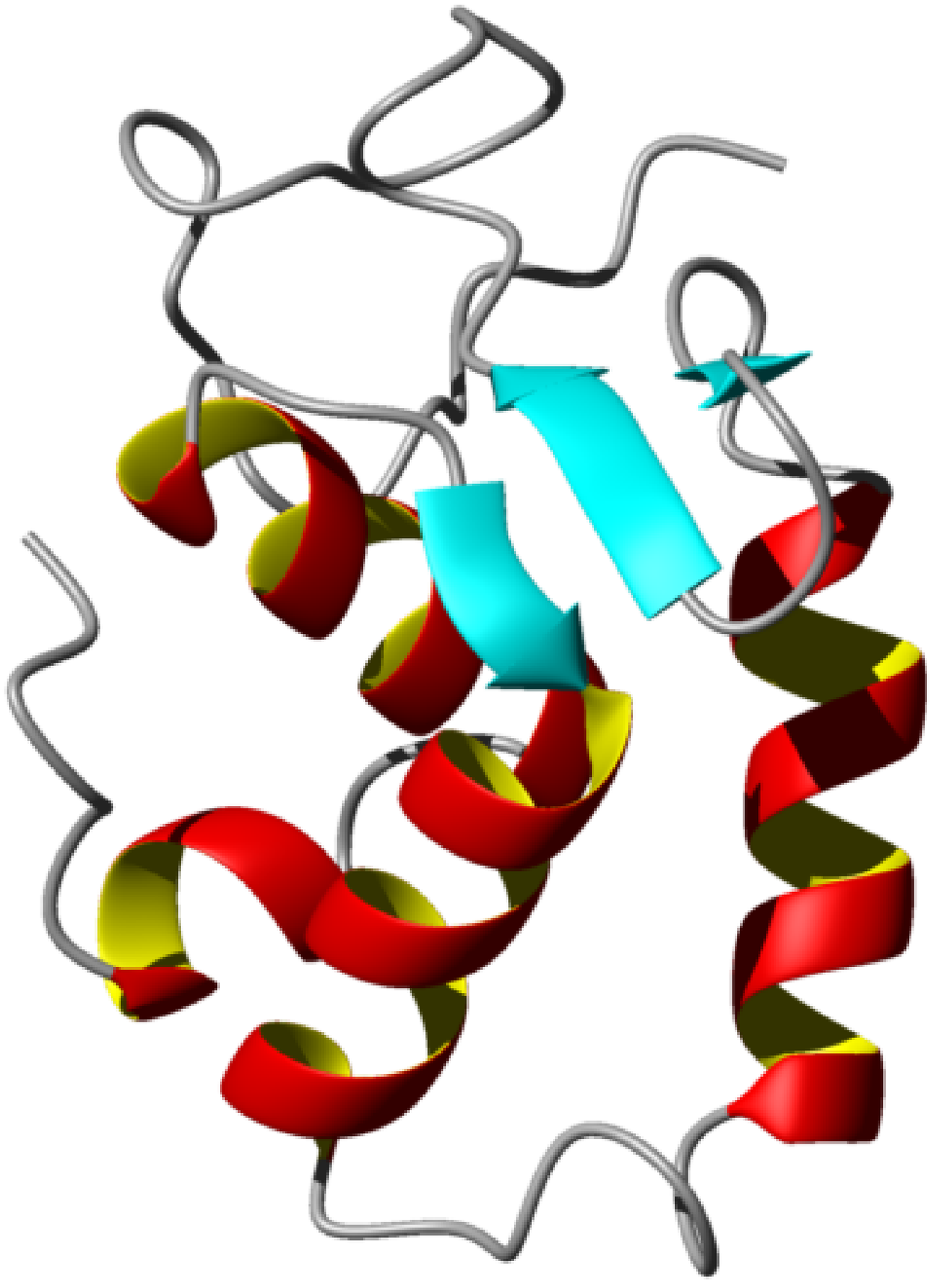
Data	β-sheet	α-helix
$\delta(\mathrm{CO})$, $\delta(\mathrm{C}^{\alpha})$	↓	↑
$\delta(\mathrm{C}^{\beta})$, $\delta(\mathrm{H}^{\alpha})$	↑	↓
$\lvert \mathrm{H}_i^{\alpha}\mathrm{H}_{i+1}^{\mathrm{N}} \rvert$	0.22 nm	0.35 nm
$\lvert \mathrm{H}_i^{\mathrm{N}}\mathrm{H}_{i+1}^{\mathrm{N}} \rvert$	0.40 nm	0.28 nm
$\lvert \mathrm{H}_i^{\alpha}\mathrm{H}_{i+2}^{\mathrm{N}} \rvert$	too far	0.42 nm
$\lvert \mathrm{H}_i^{\alpha}\mathrm{H}_{i+3}^{\mathrm{N}} \rvert$	too far	0.34 nm
$\lvert \mathrm{H}_i^{\alpha}\mathrm{H}_{i+4}^{\mathrm{N}} \rvert$	too far	0.42 nm
${}^3J(\mathrm{H}_i^{\mathrm{N}}\mathrm{H}_i^{\alpha})$	> 8 Hz	< 5 Hz


$\mathrm{H}^{\mathrm{N}}(k)$-$\mathrm{H}^{\alpha}(k)$
$\mathrm{H}^{\mathrm{N}}(k)$-$\mathrm{C}'(k)$
$\mathrm{H}^{\mathrm{N}}(k)$-$\mathrm{C}^{\beta}(k)$
$\mathrm{C}'(k-1)$-$\mathrm{H}^{\alpha}(k)$
$\mathrm{C}'(k-1)$-$\mathrm{C}^{\beta}(k)$
$\mathrm{C}'(k-1)$-$\mathrm{C}'(k)$
J-coupling / Hz
12
10
8
6
4
2
0
-180
-120
-60
0
60
120
180
ϕ / deg.

TALOS prediction
^{3}J prediction
NOE prediction
CSI prediction
10 20 30 40 50 60 70 80 90
GIKQYSQEELKEMALVEIAHELFEEHKKPVPFQELLNEIASLLGVKKEEL GDRIAQFYTDLNIDGRFLALSDQTWGLRSWYPYDQLDEETQLEHHHHHH
TALOS
^{3}J(H$^\alpha$H^N)
NN$(i,i+1)$
αN$(i,i+1)$
αN$(i,i+2)$
αN$(i,i+3)$
αN$(i,i+4)$
CO CSI
C$^\alpha$ CSI
H$^\alpha$ CSI
C$^\beta$ CSI
consensus CSI


Energy
20
15
10
5
0
-5
-10
x1
x2


Energy
20
15
10
5
0
-5
-10
x1
x2


Energy
20
15
10
5
0
-5
-10
x1
x2