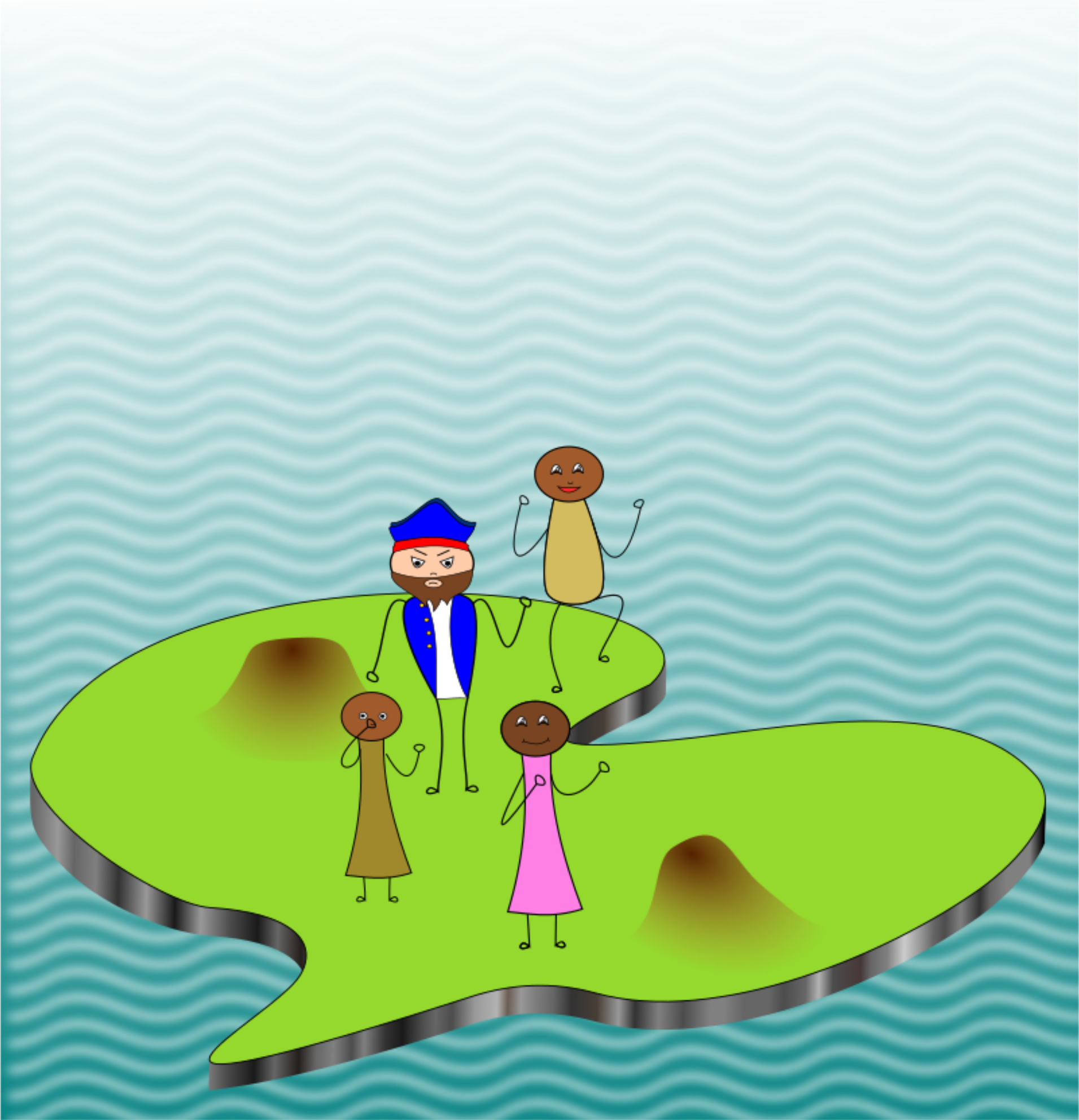
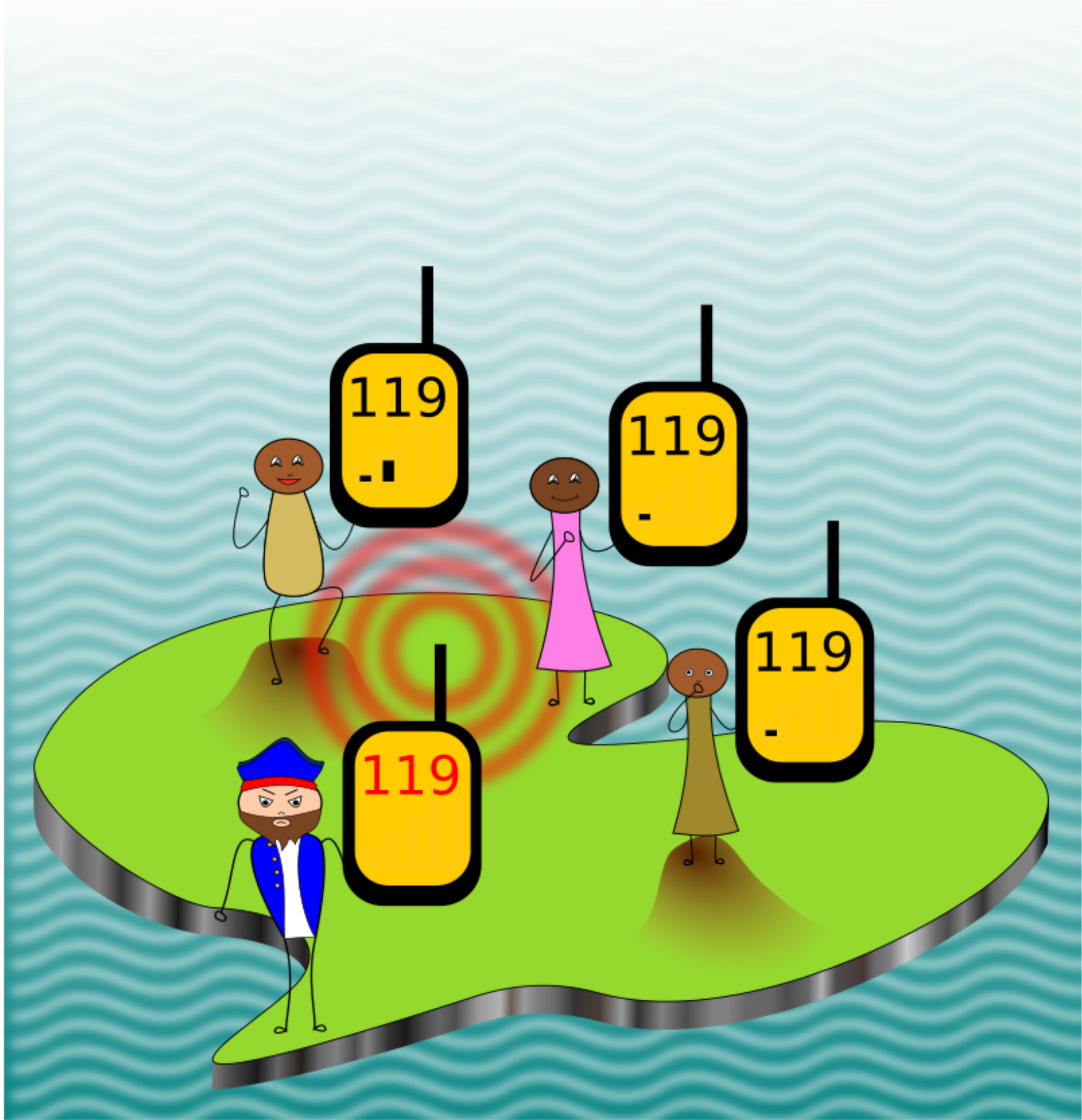
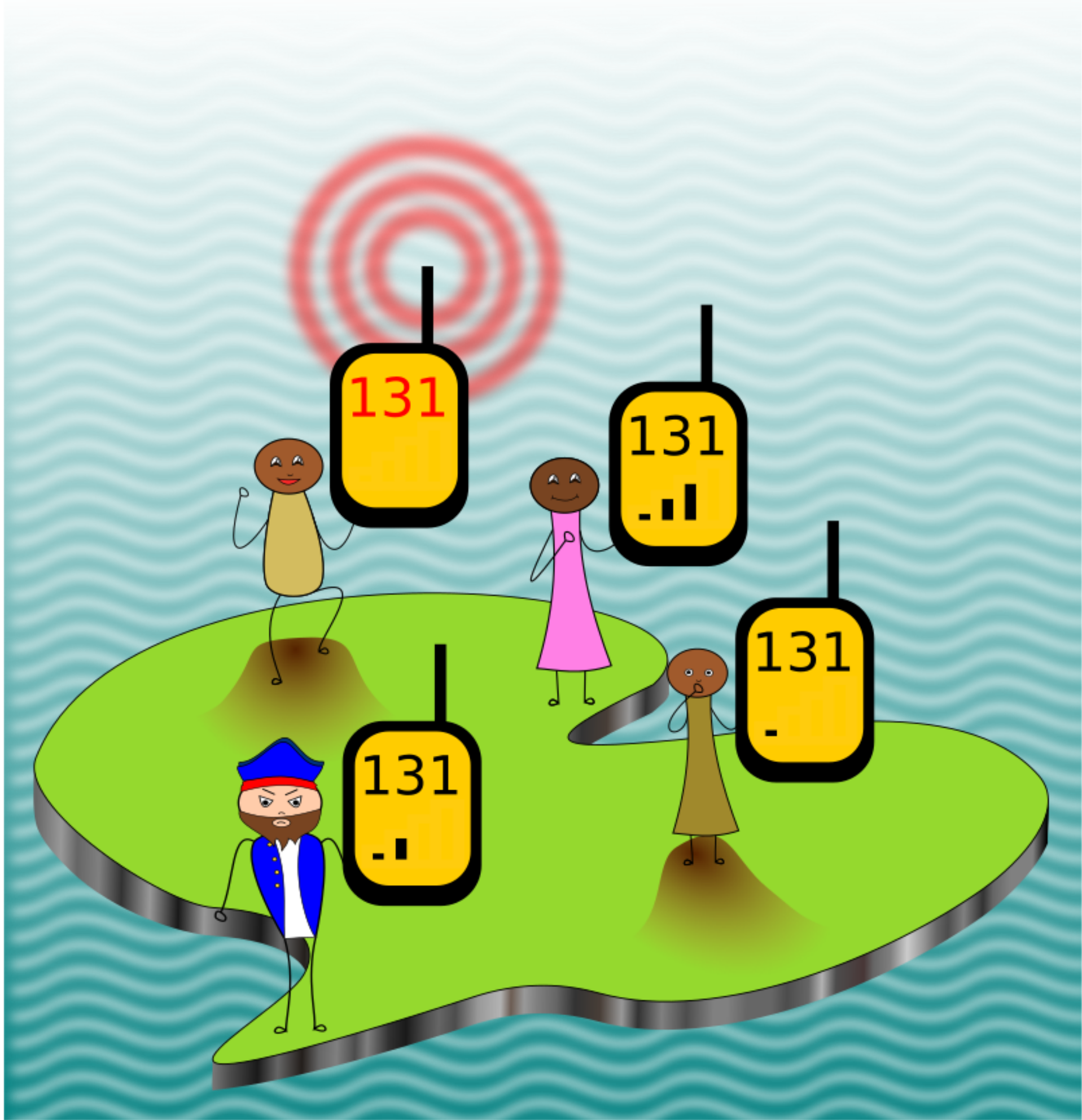


# NUKLEÁRNÍ MAGNETICKÁ REZONANCE

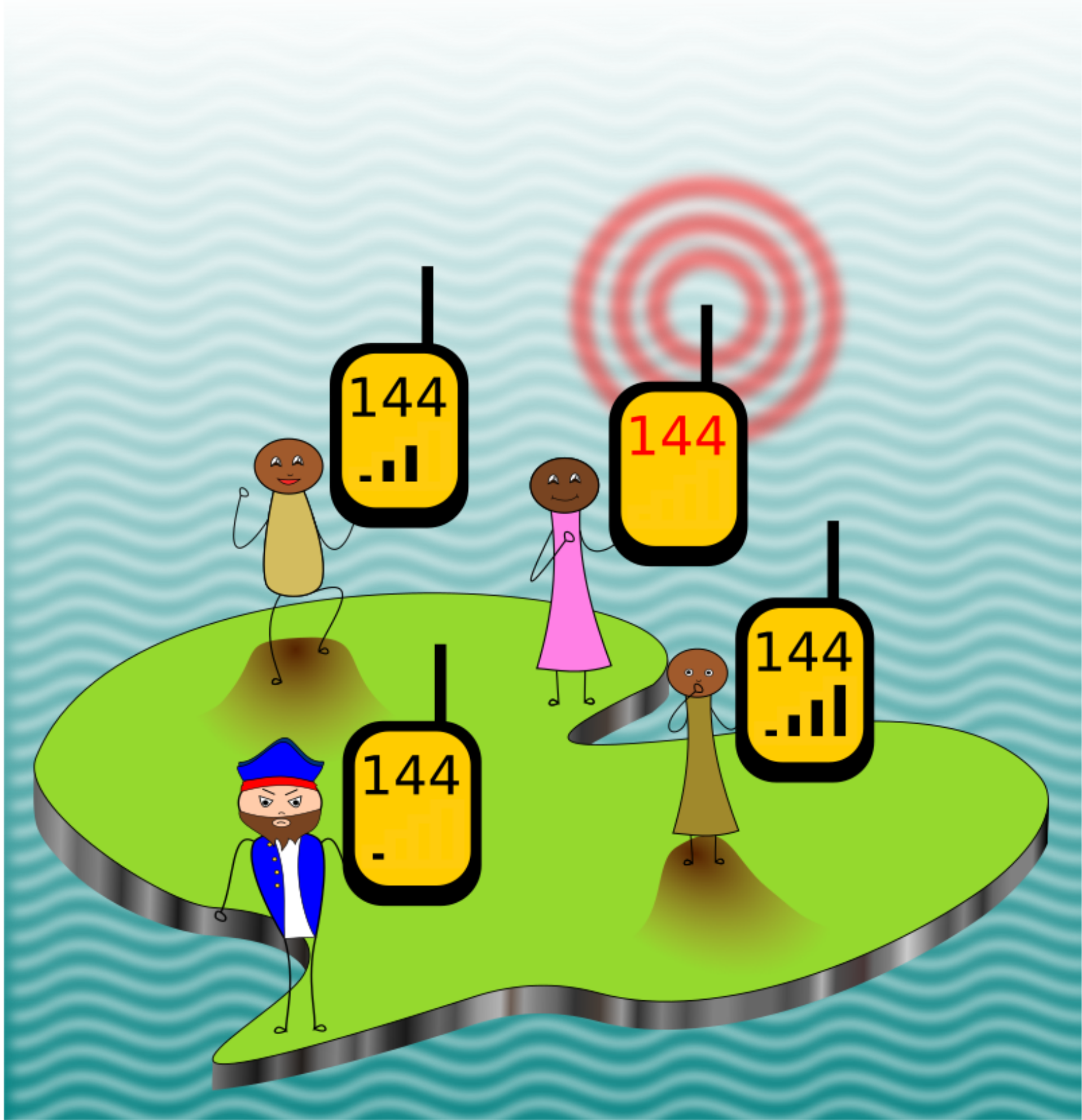


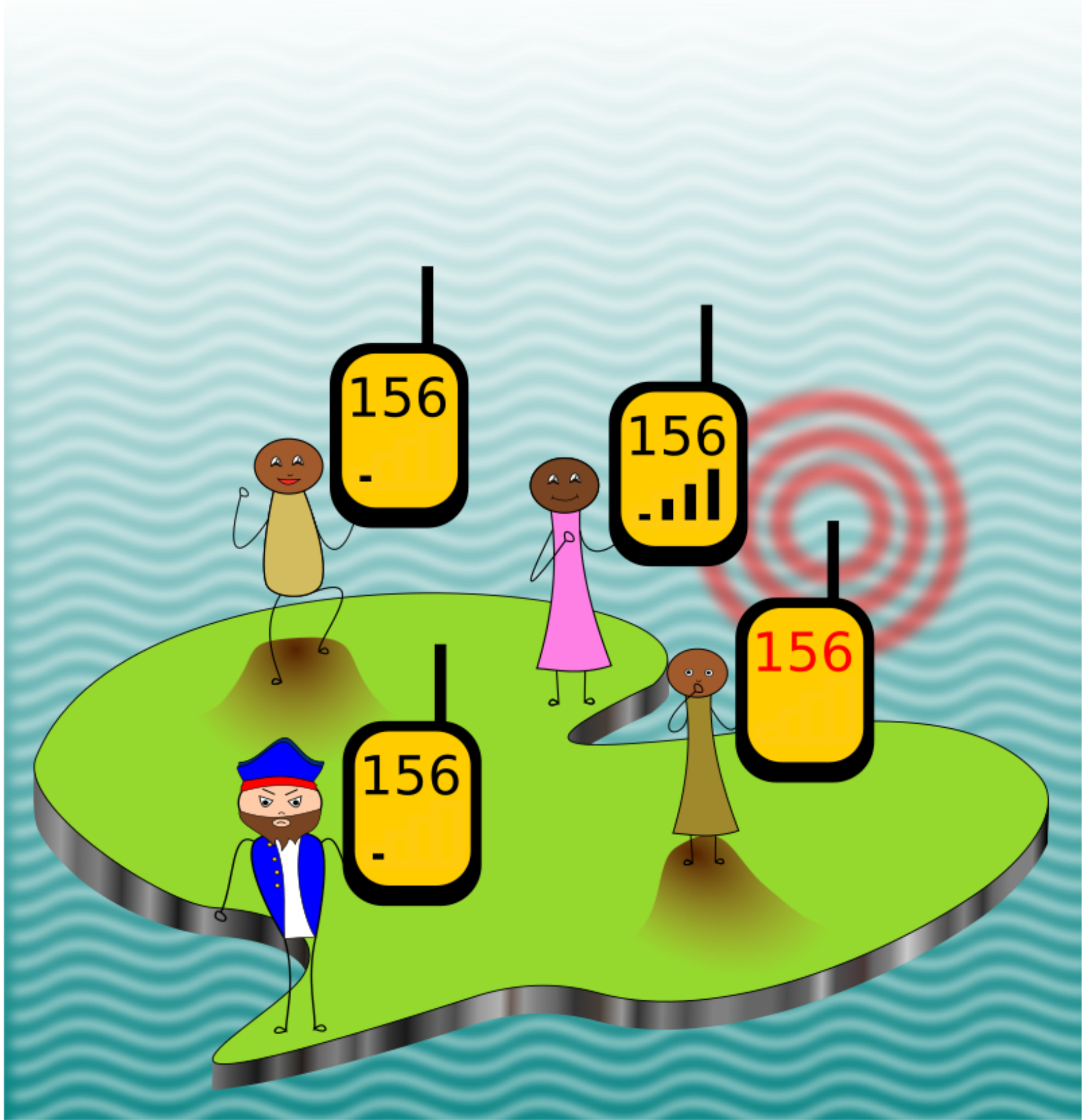












	$S$	$\frac{10^{-9}\gamma}{\text{rad s}^{-1}\text{T}^{-1}}$	% v přírodě
$e^-$	1/2	-182,000	100
$^1\text{H}$	1/2	0,277	99,98
$^2\text{H}$	<b>1</b>	0,042	<b>0,02</b>
$^{13}\text{C}$	1/2	0,067	<b>1,1</b>
$^{14}\text{N}$	<b>1</b>	0,019	99,6
$^{15}\text{N}$	1/2	-0,027	<b>0,4</b>
$^{17}\text{O}$	<b>5/2</b>	-0,036	<b>0,04</b>
$^{19}\text{F}$	1/2	0,252	100
$^{31}\text{P}$	1/2	0,108	100
$^{129}\text{Xe}$	1/2	-0,075	24,4

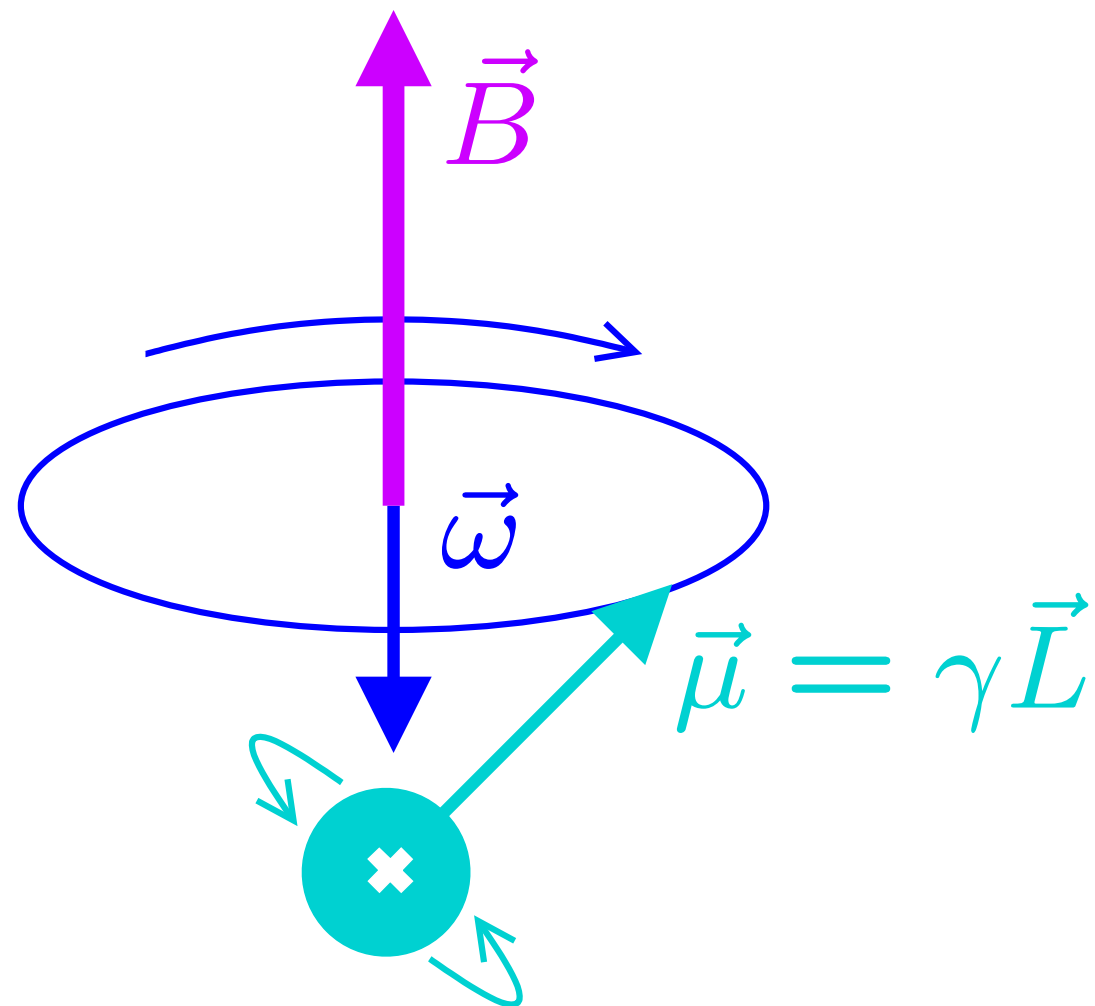
Počet stacionárních stavů =  $2S + 1$

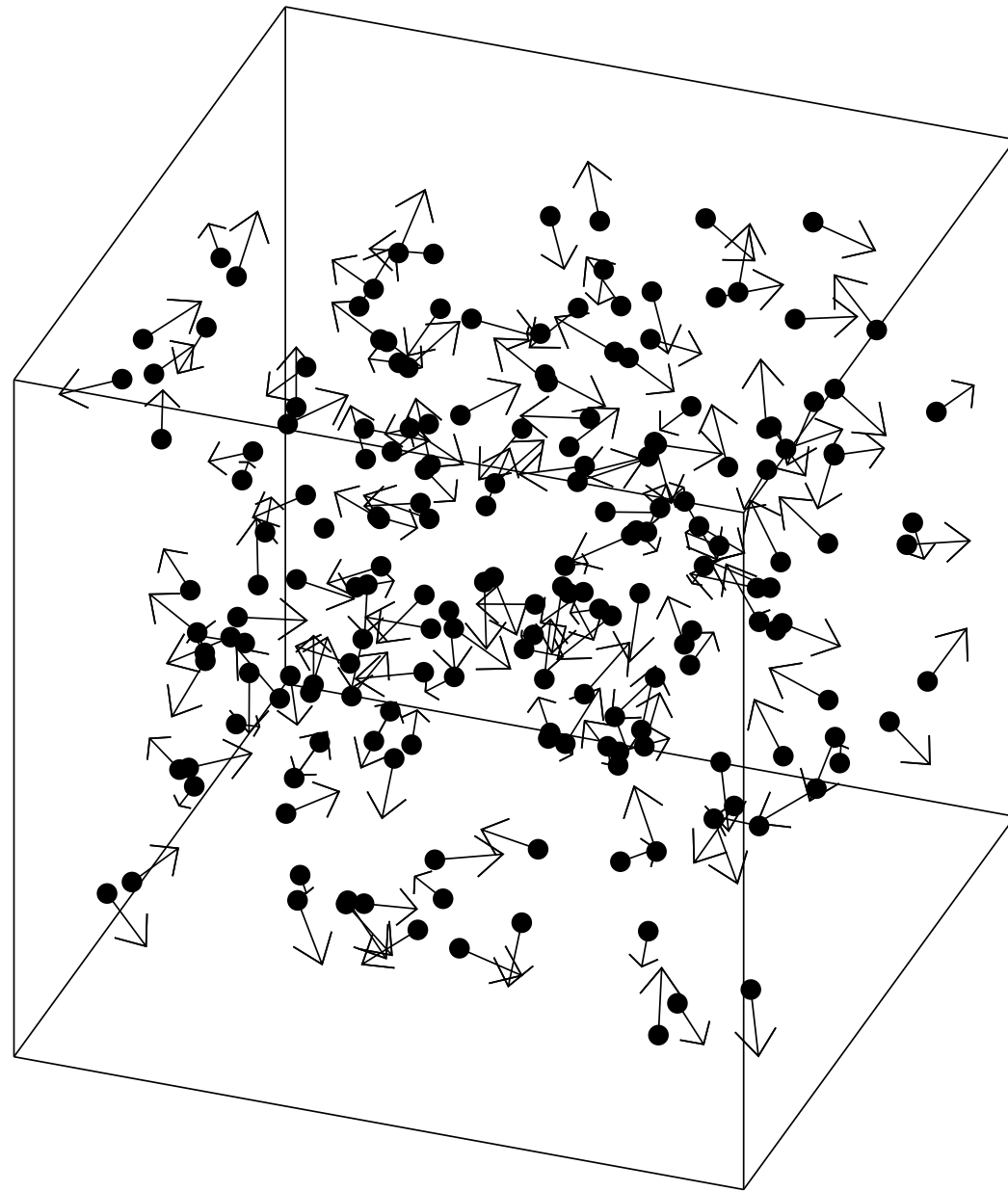
kvadrupolární jádra (příliš rychle se vrací do rovnováhy)

vzácné izotopy (vyžadují obohacení proteinů během exprese)

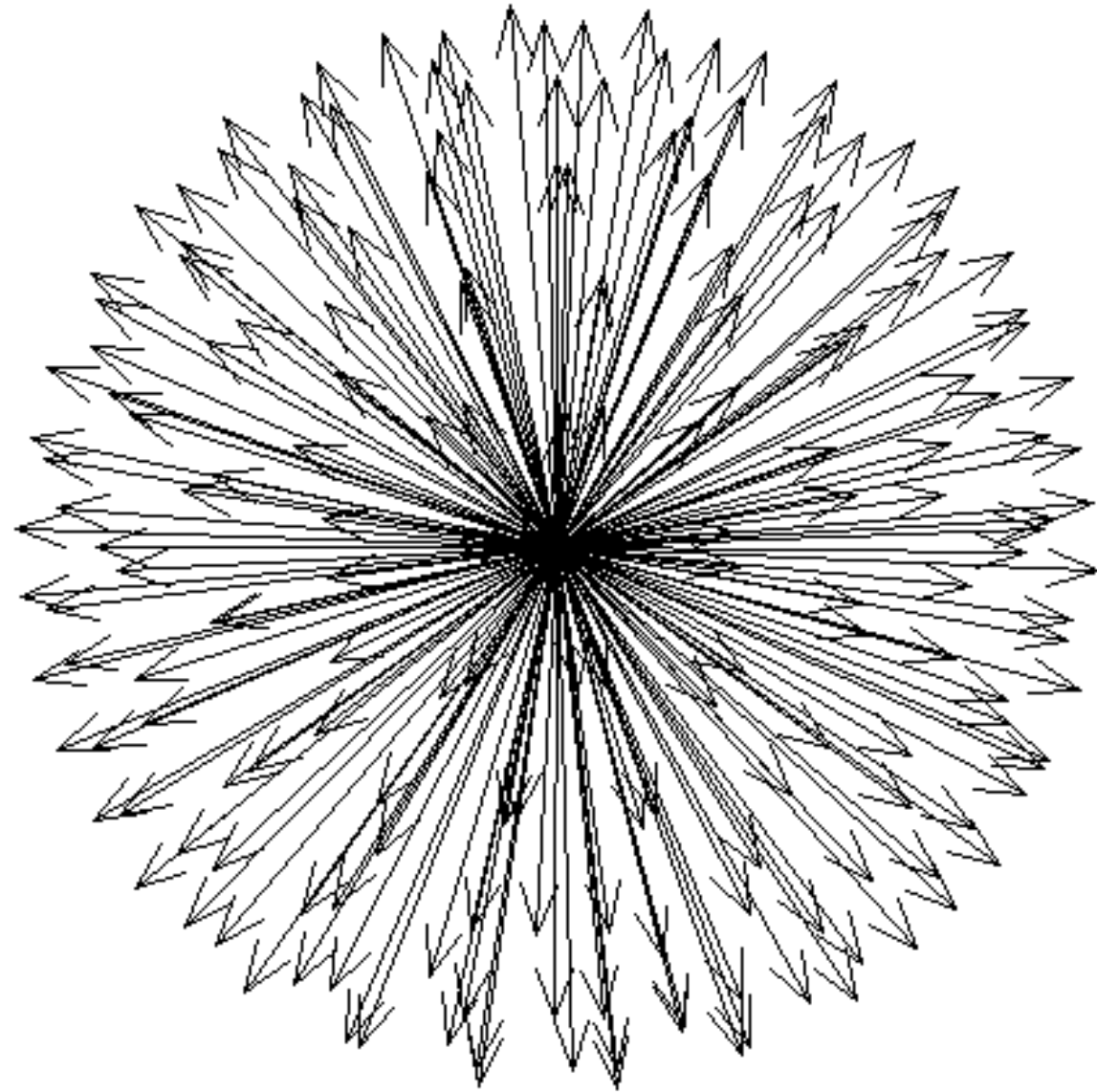


Úhlová rychlost precese  $\vec{\omega} = -\gamma \vec{B}$

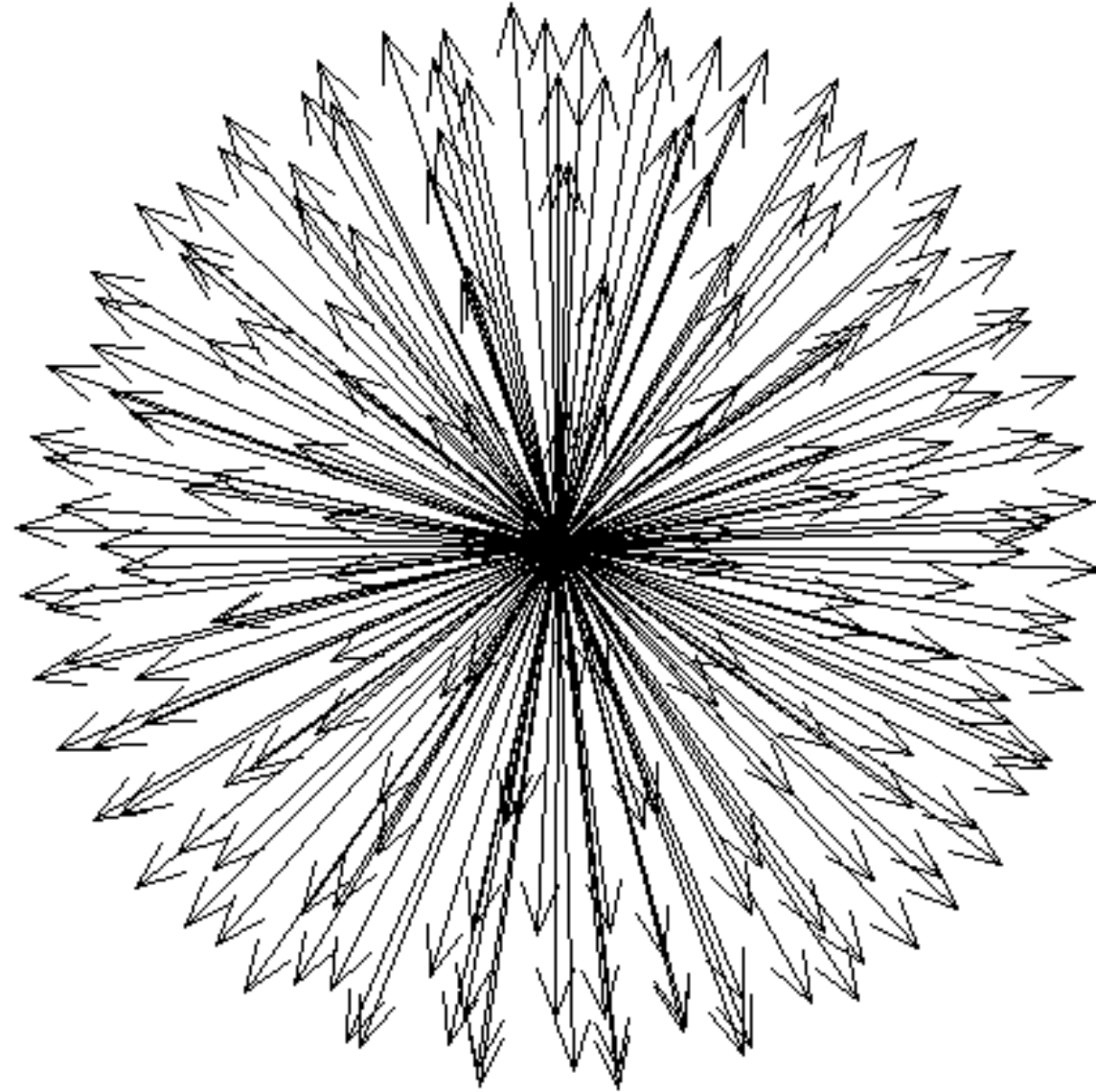




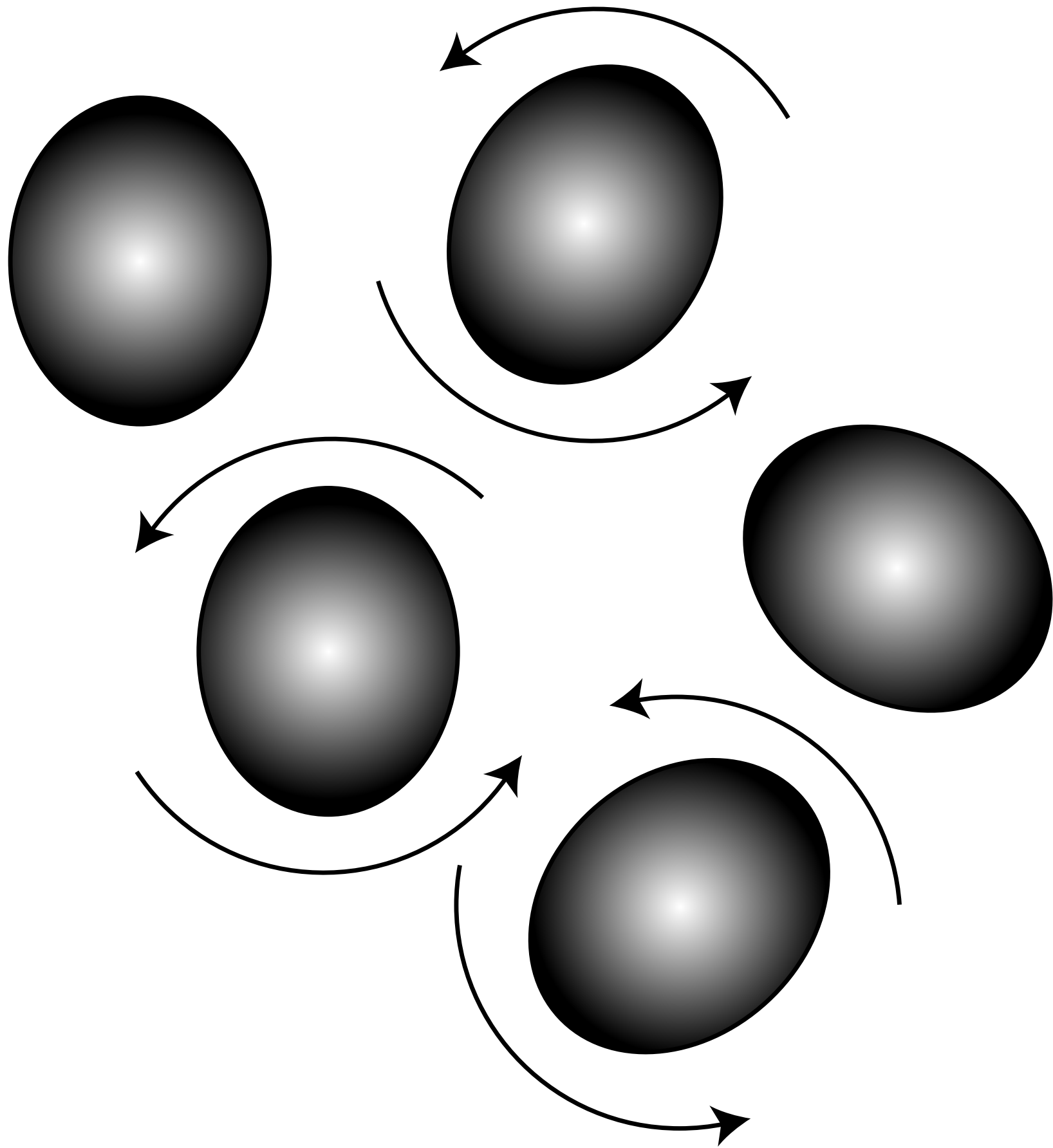
$$\vec{M} = (\vec{\mu}_1 + \vec{\mu}_2 + \vec{\mu}_3 + \vec{\mu}_4 + \vec{\mu}_5 + \vec{\mu}_6 + \dots) / V \quad \text{Magnetizace}$$



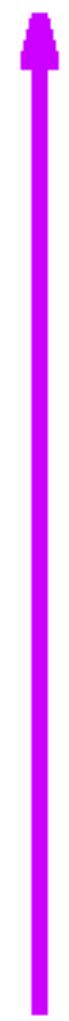
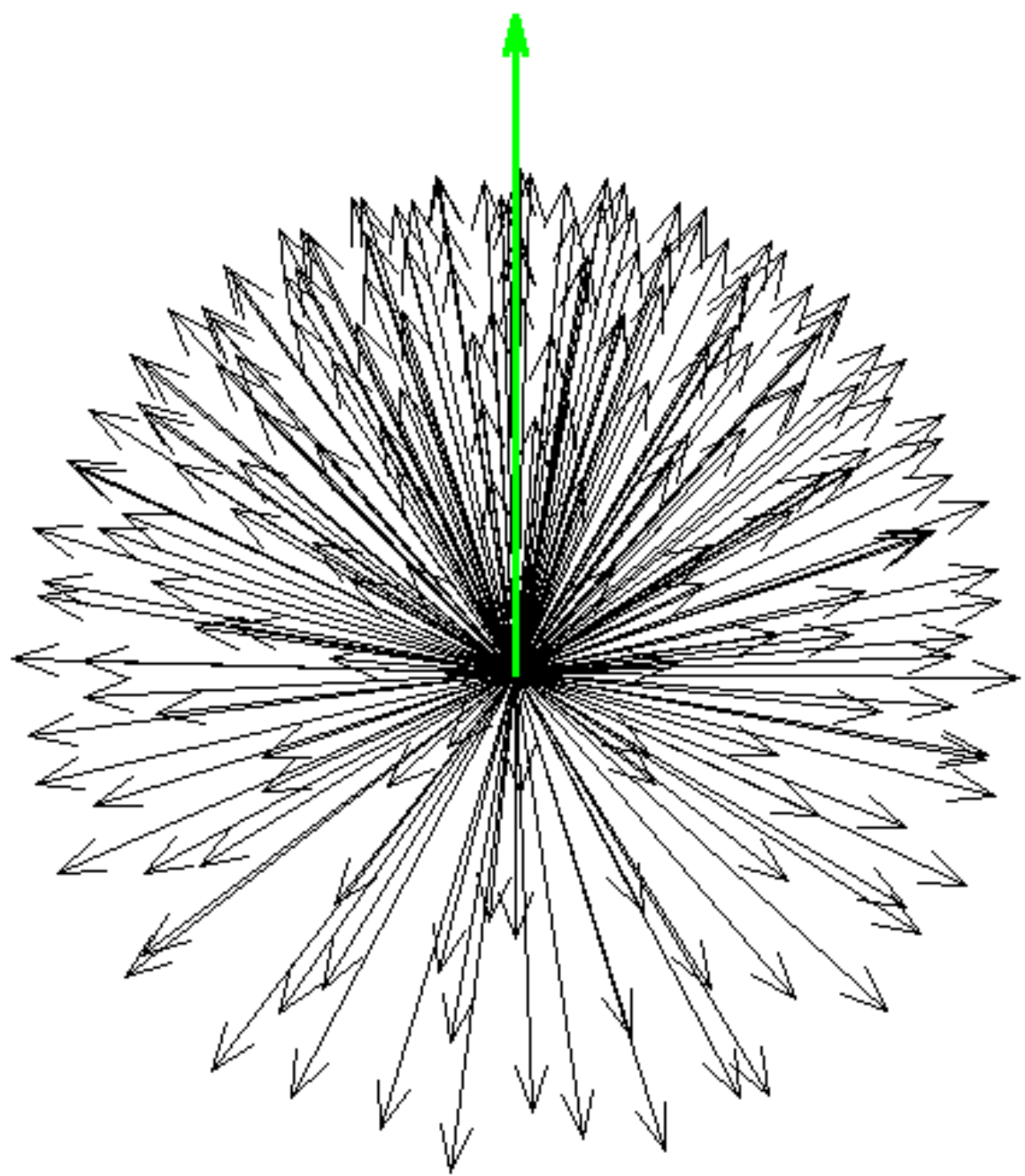




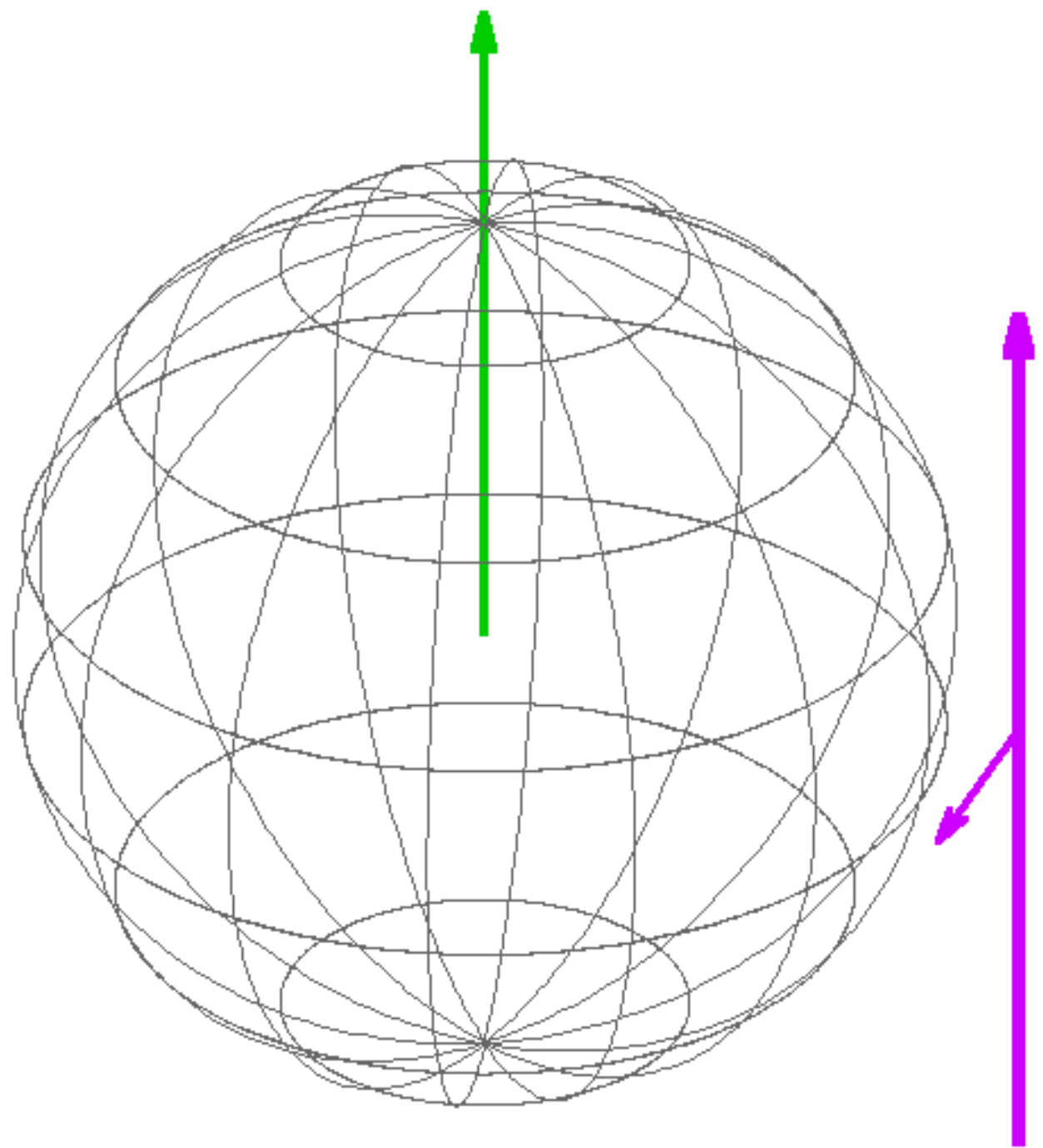
Magnetické momenty v magnetickém poli





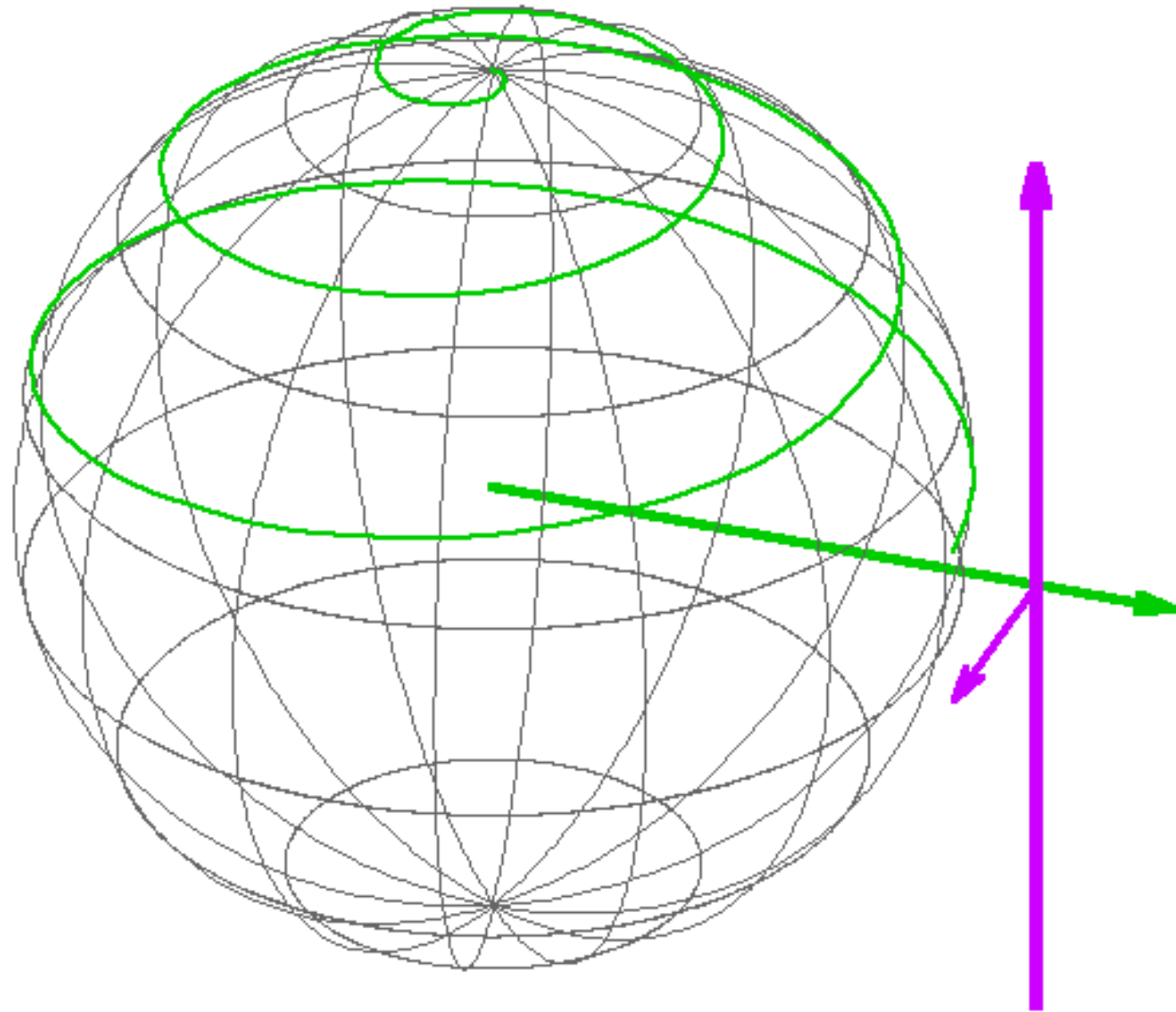


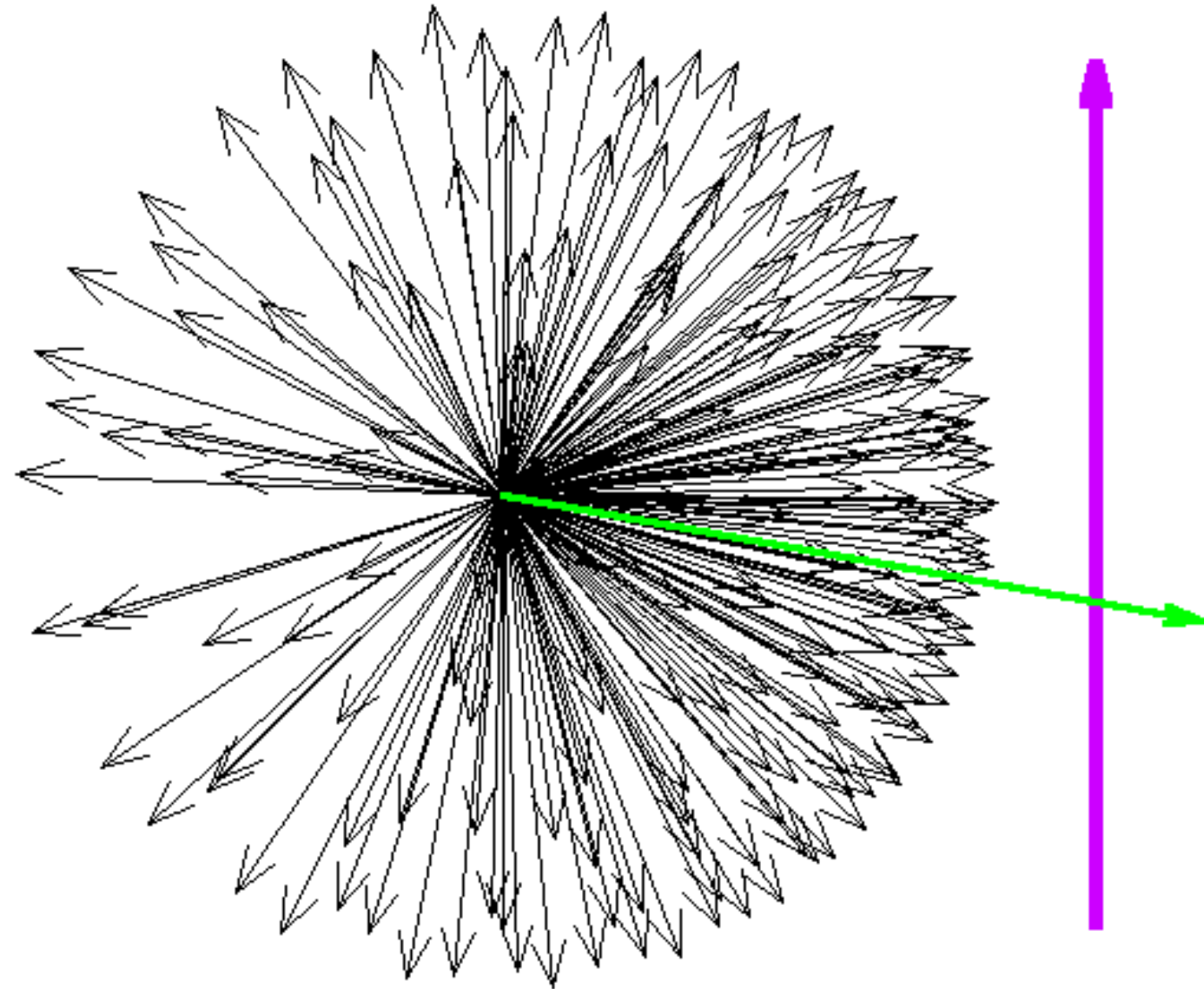
Vertikálně polarizované magnetické momenty  
ve vertikálním magnetickém poli





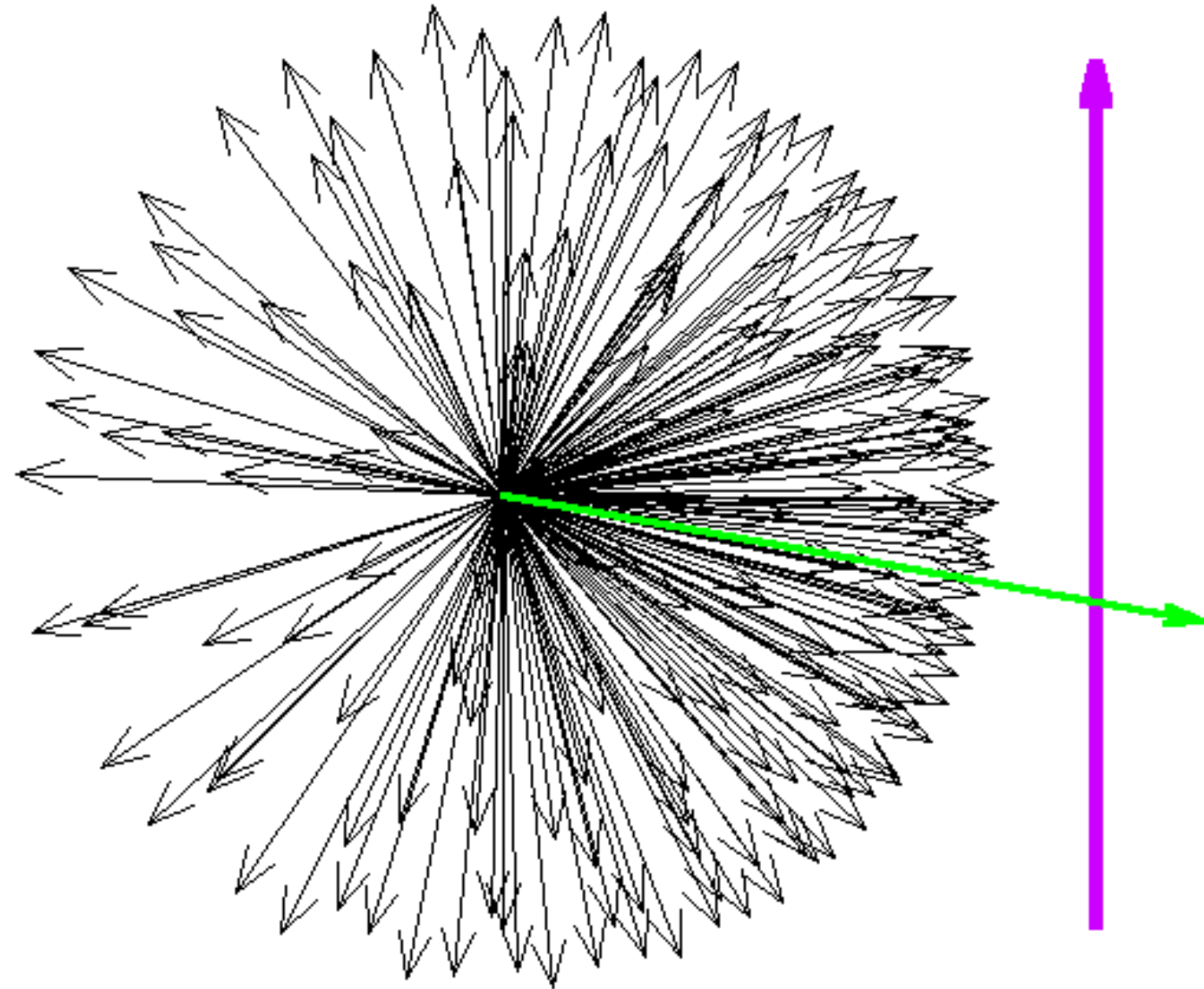
Sklopení vektoru magnetizace

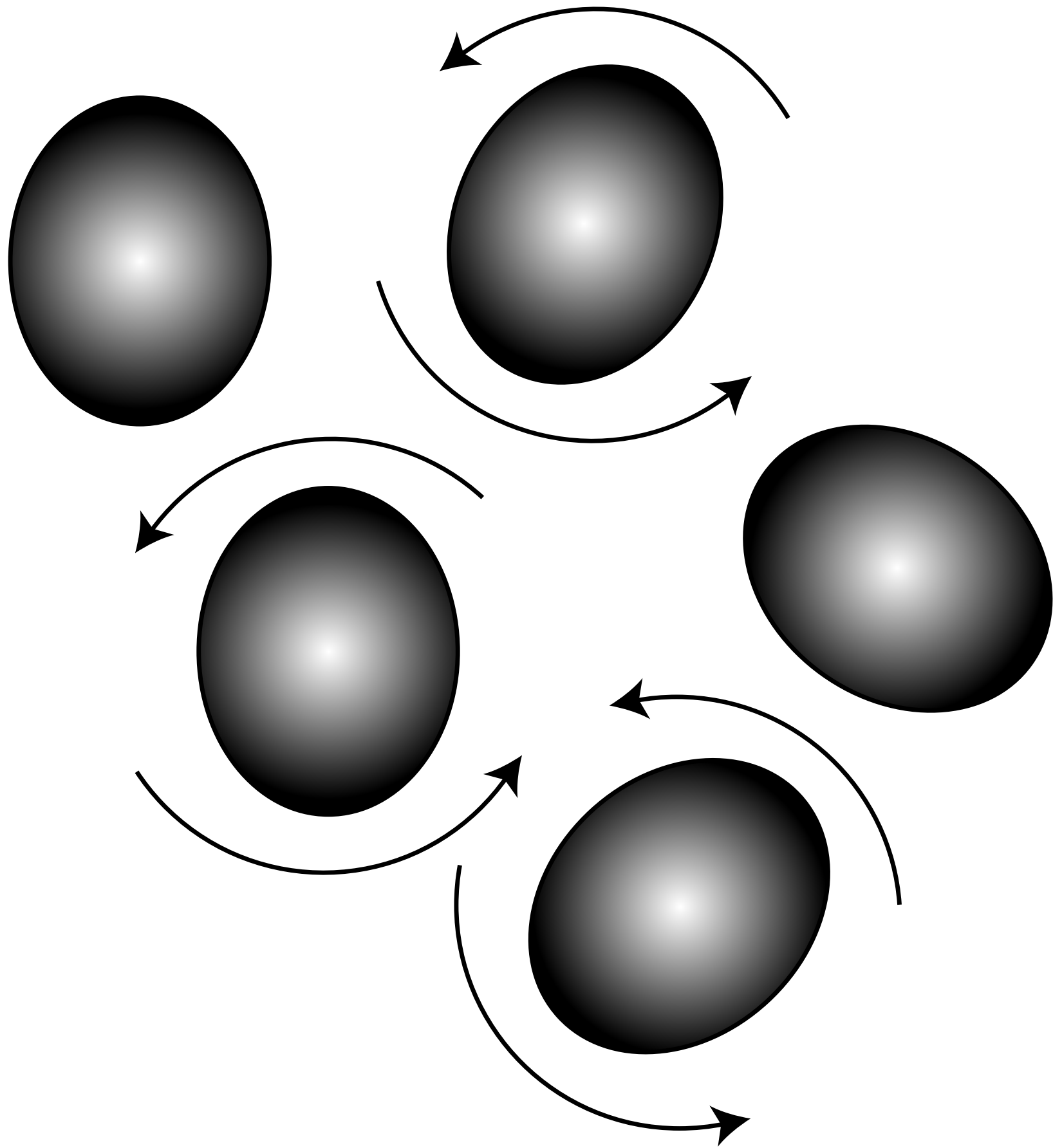


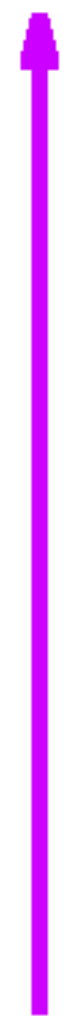
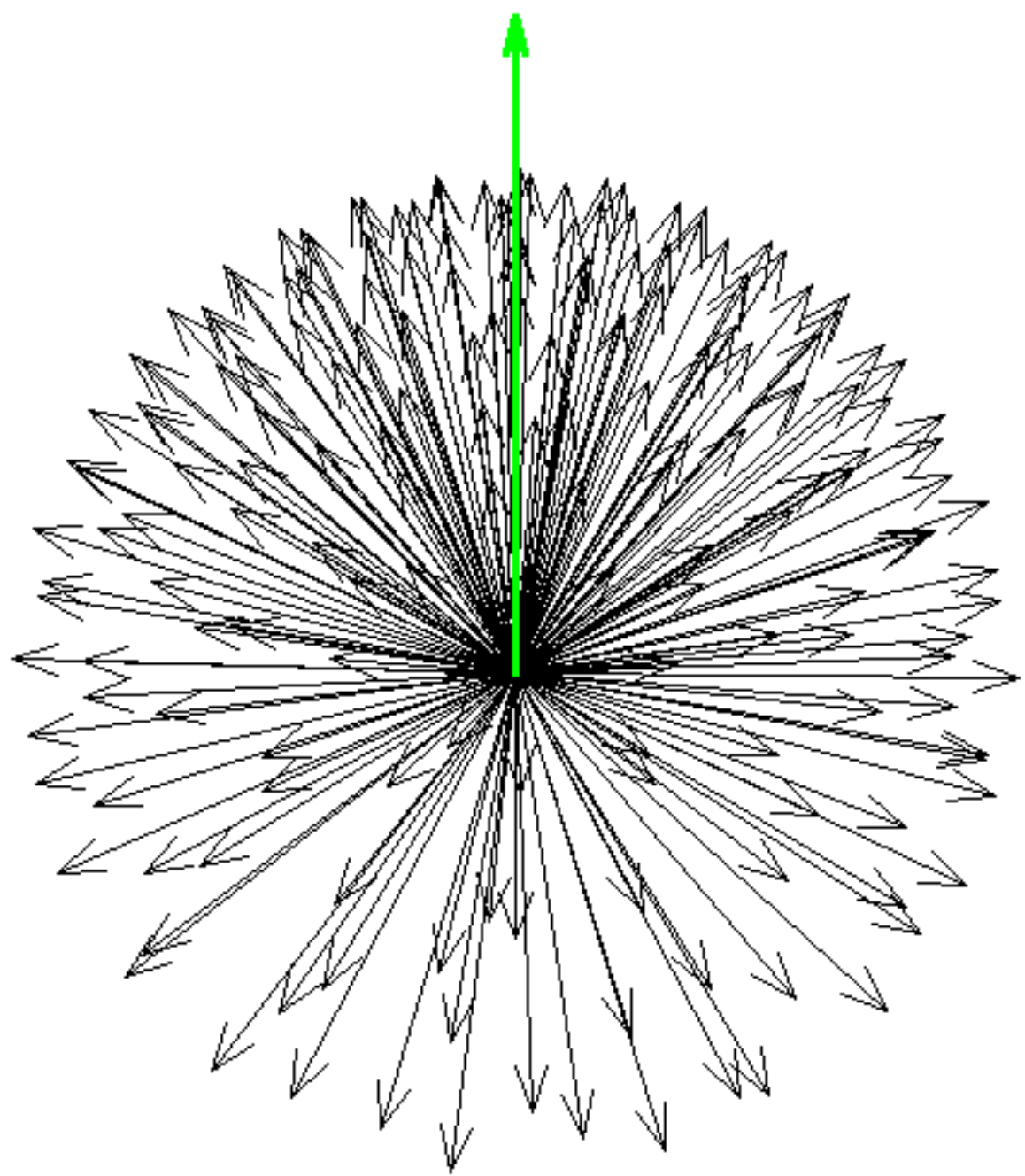


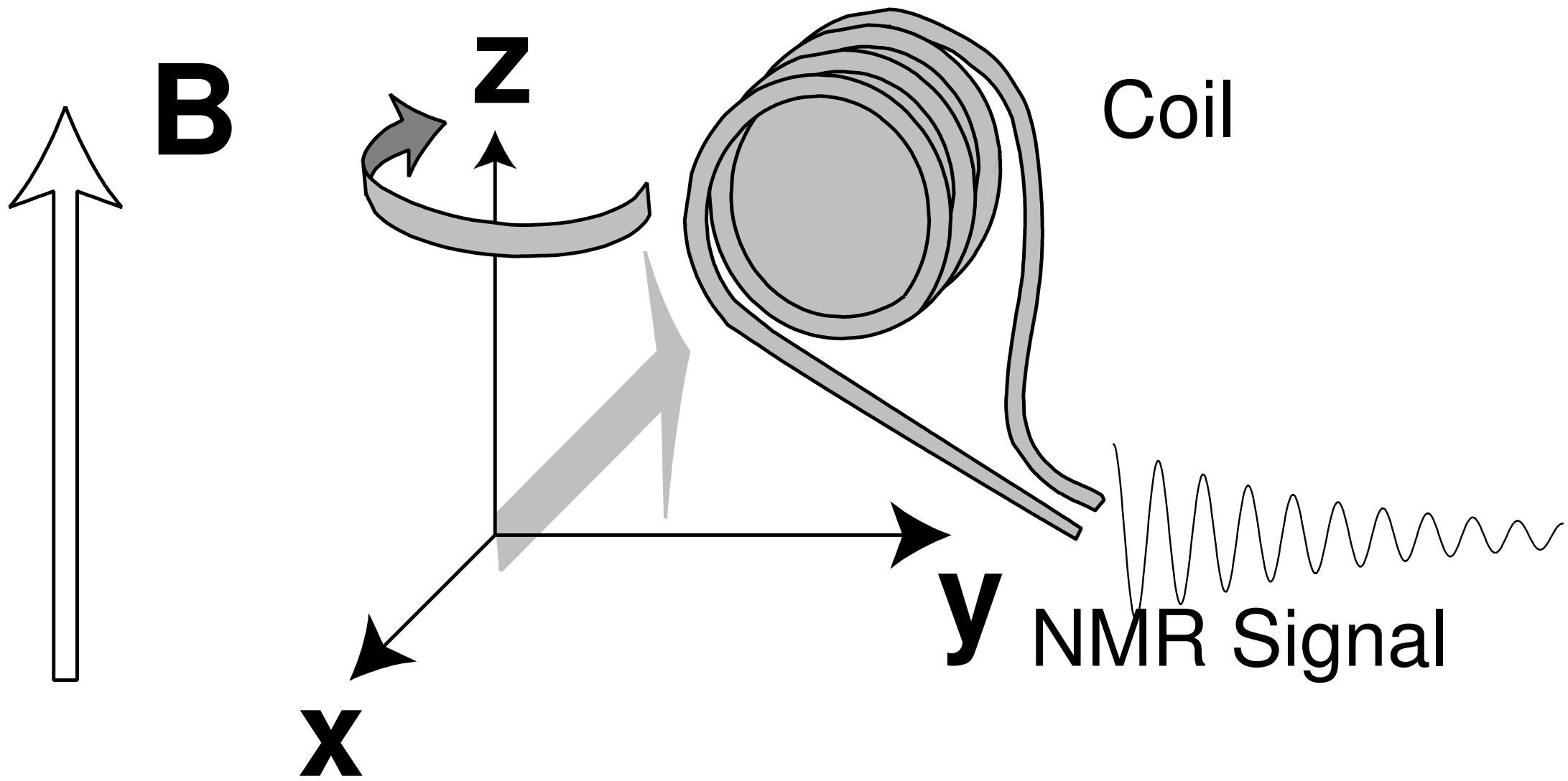
Horizontálně polarizované koherentní  
magnetické momenty  
ve vertikálním magnetickém poli

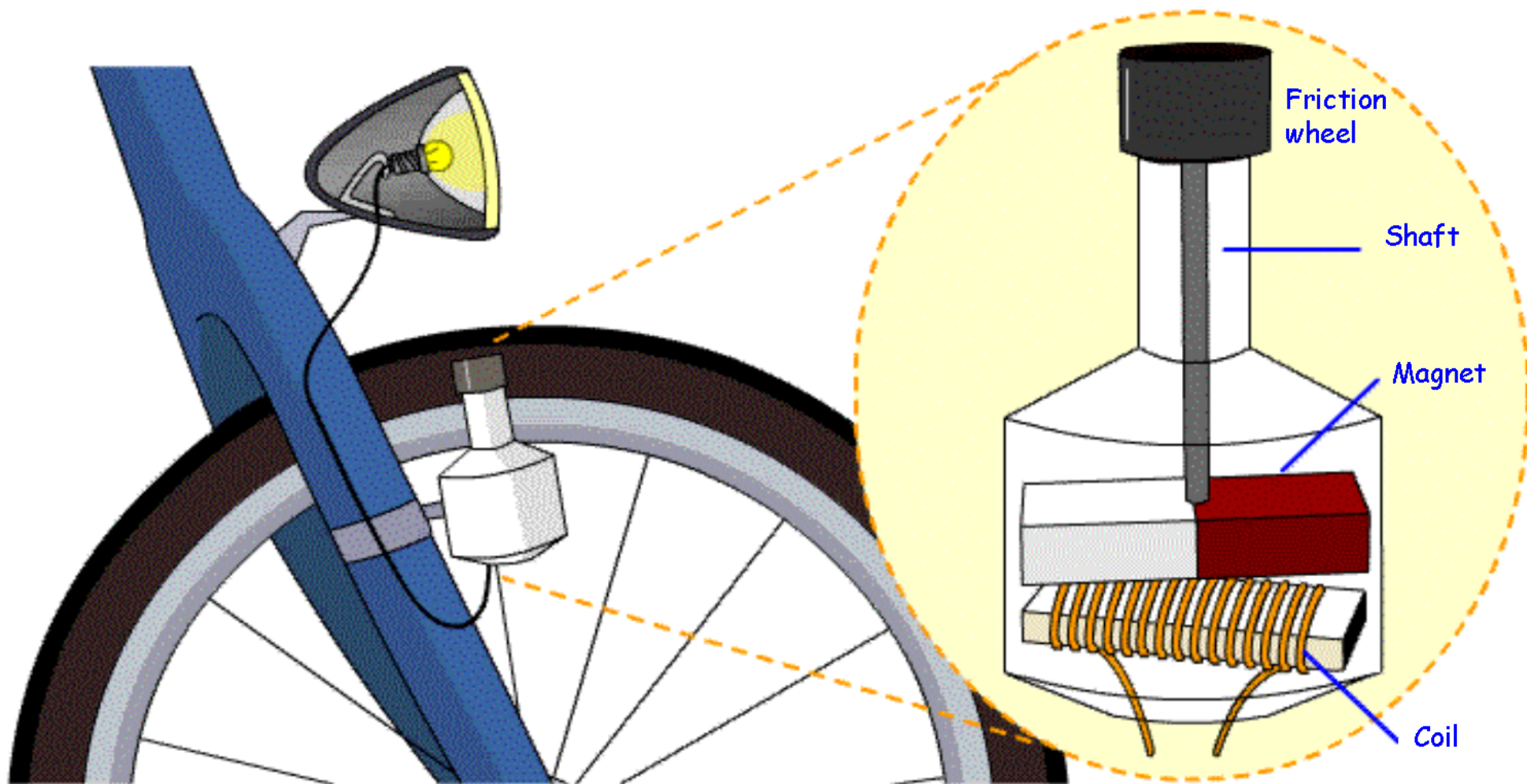


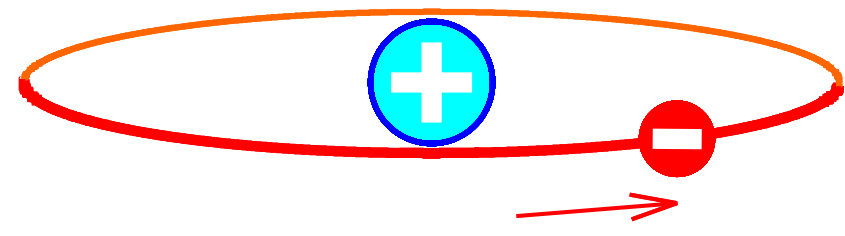




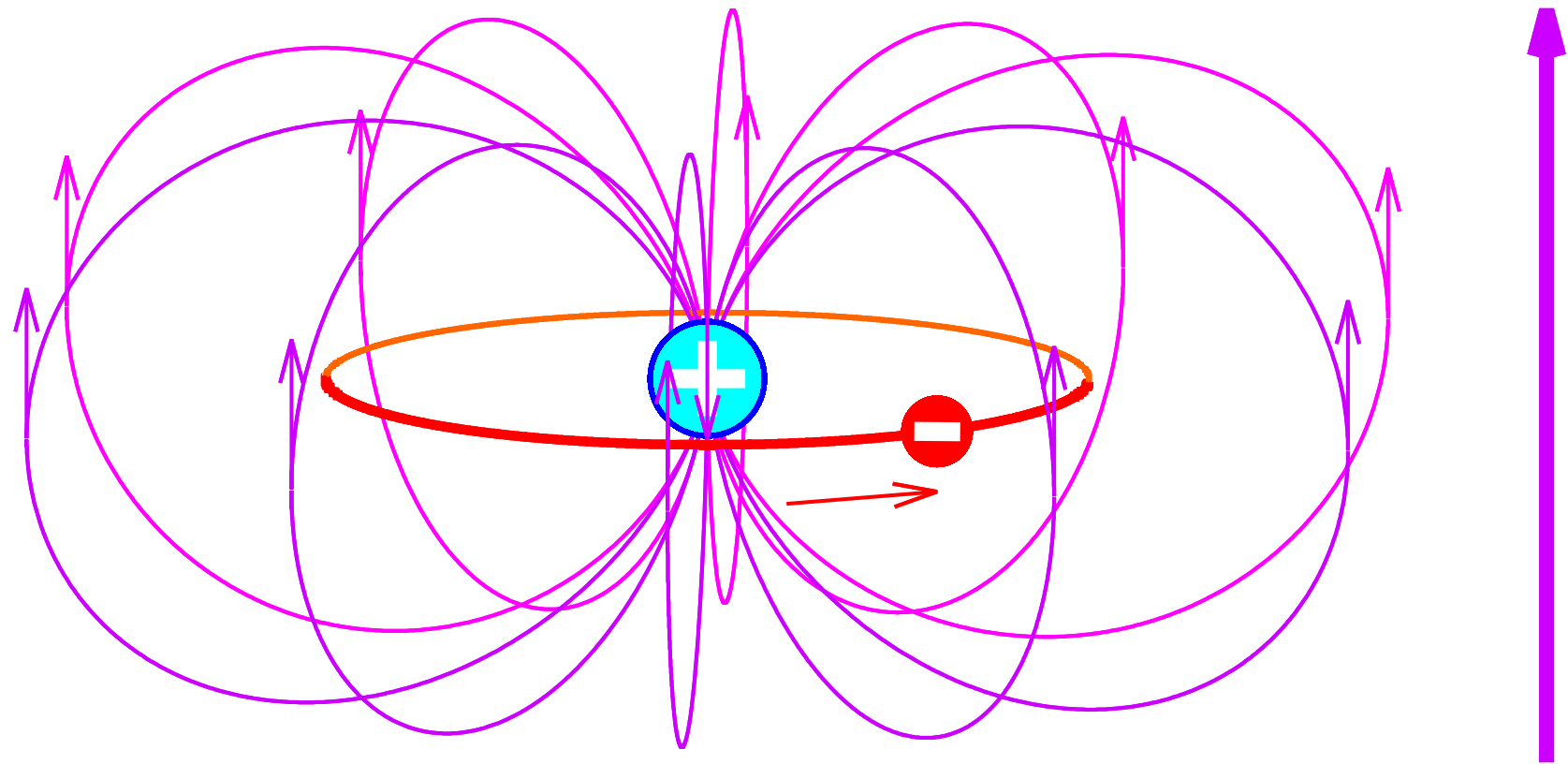


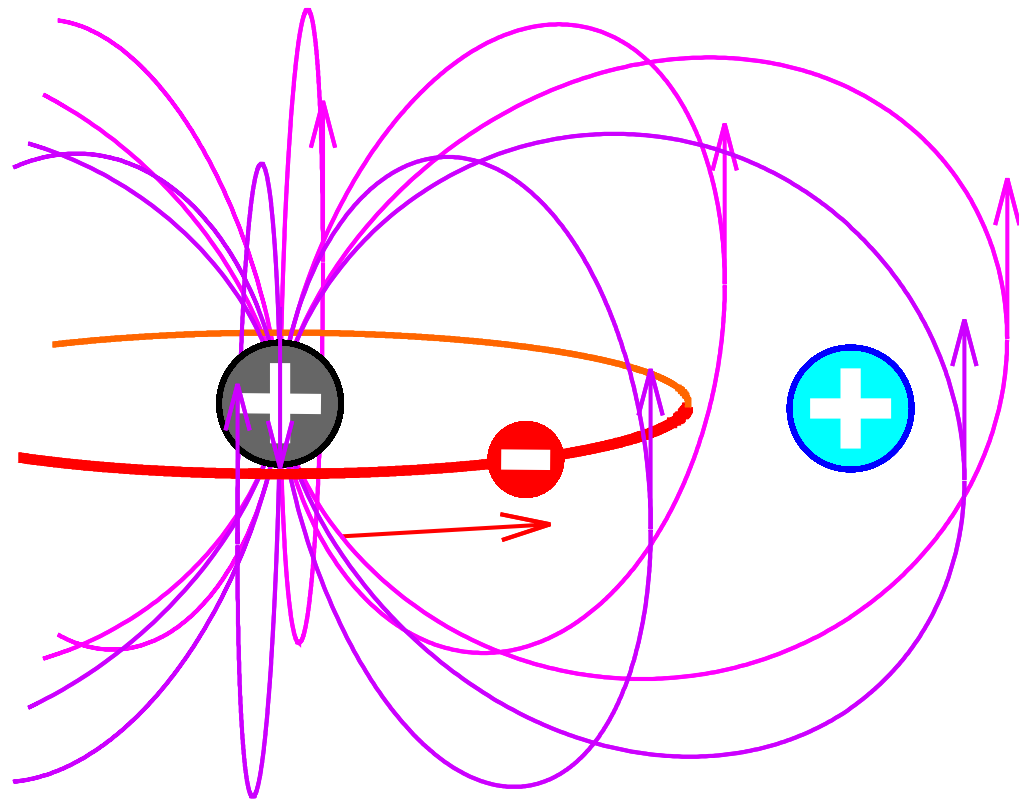


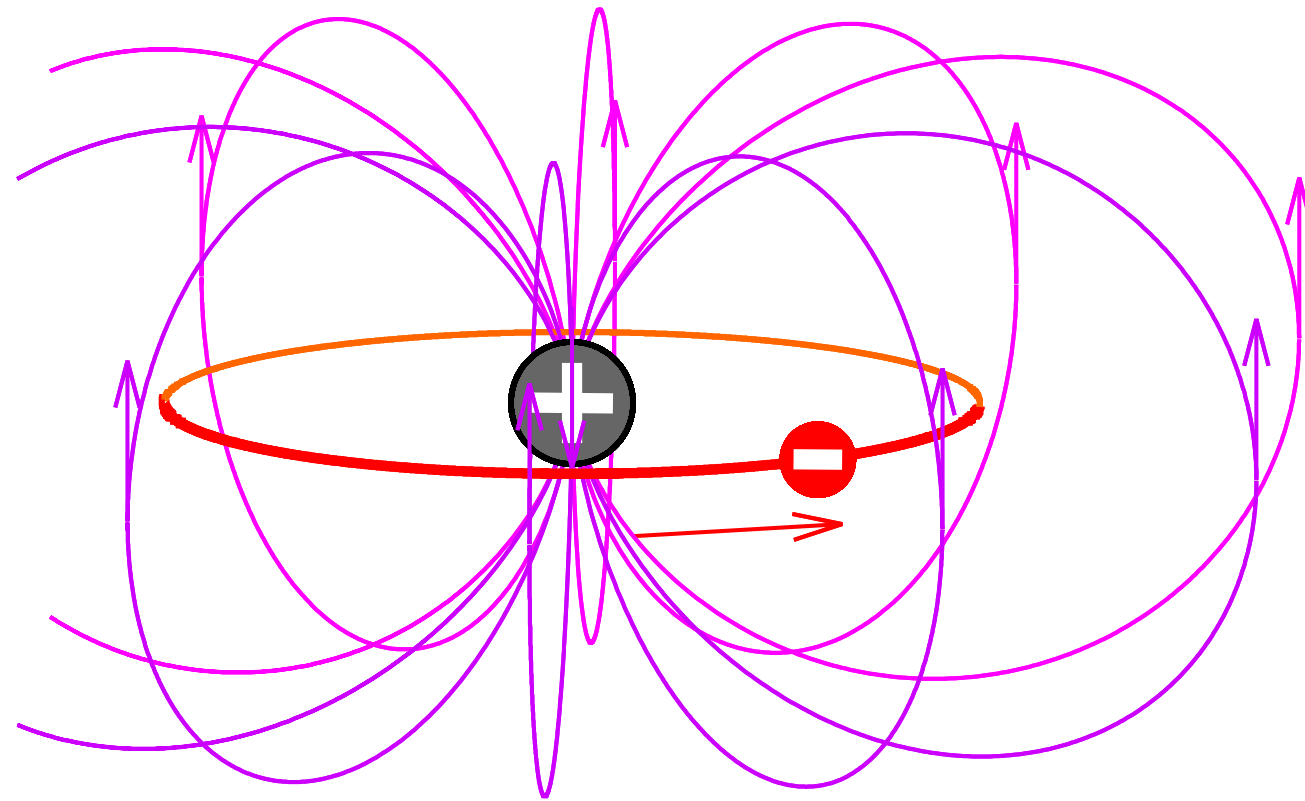


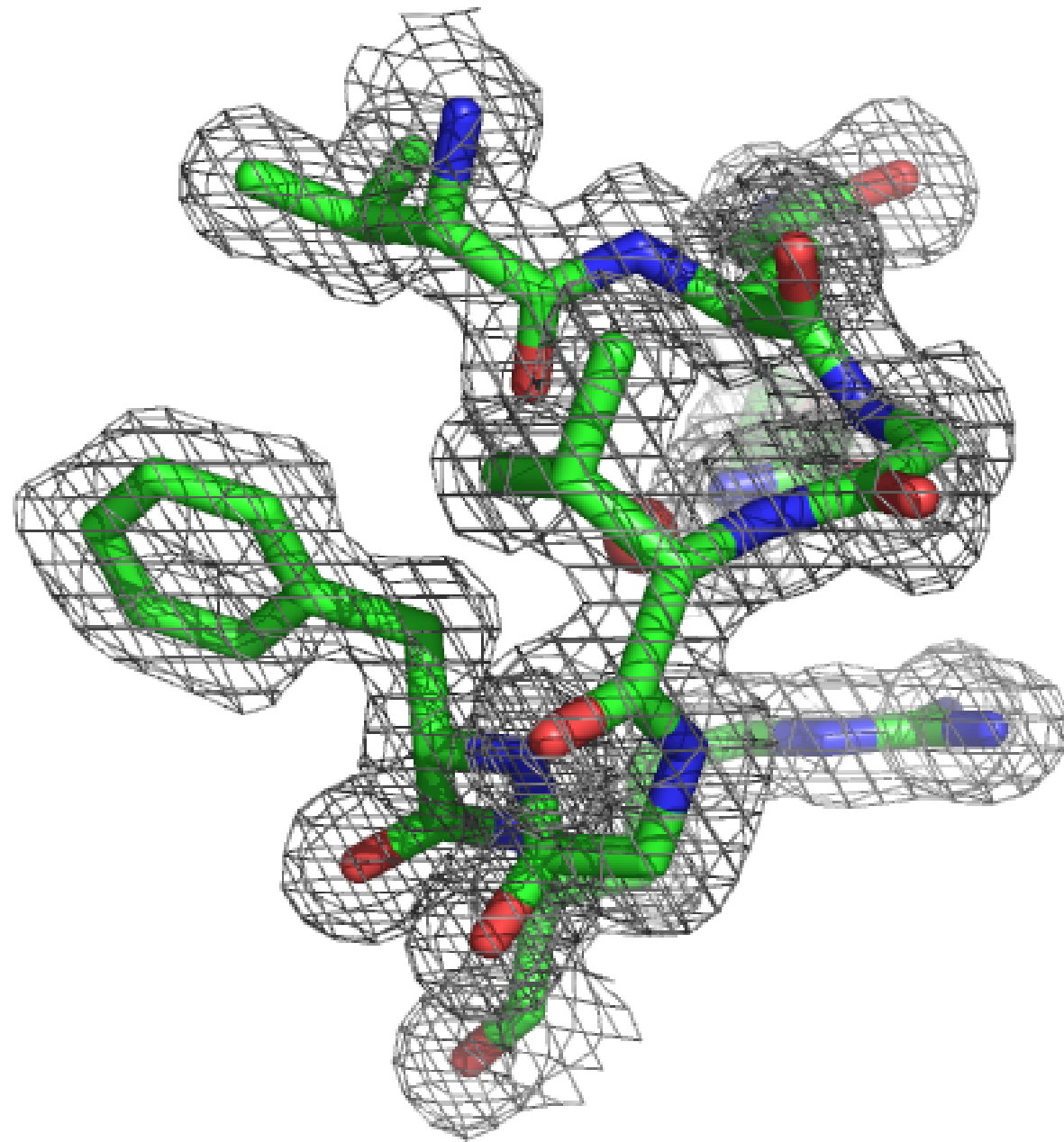


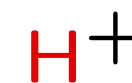
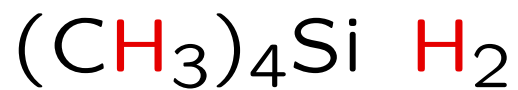
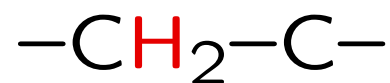
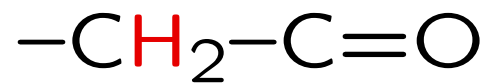
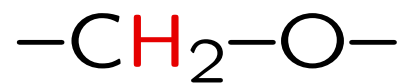
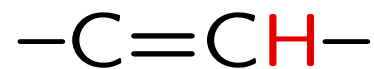
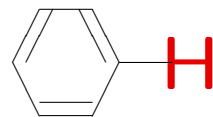










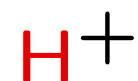
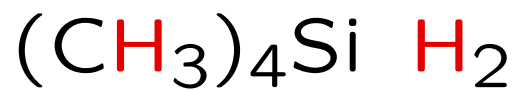
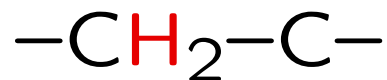
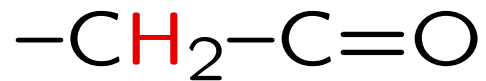
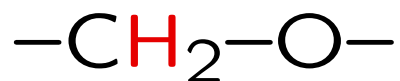
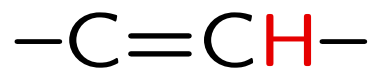
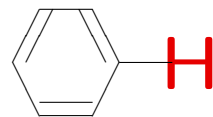


499.9985

499.9990

499.9995

500.0000 MHz



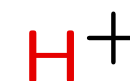
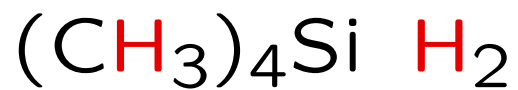
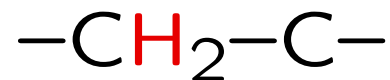
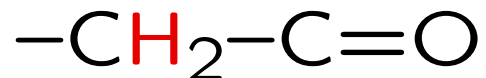
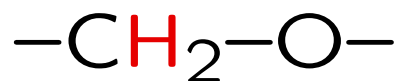
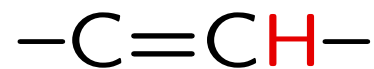
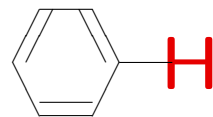
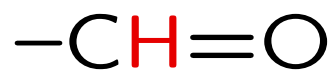
99.997 %

99.998 %

99.999 %

100.000 %



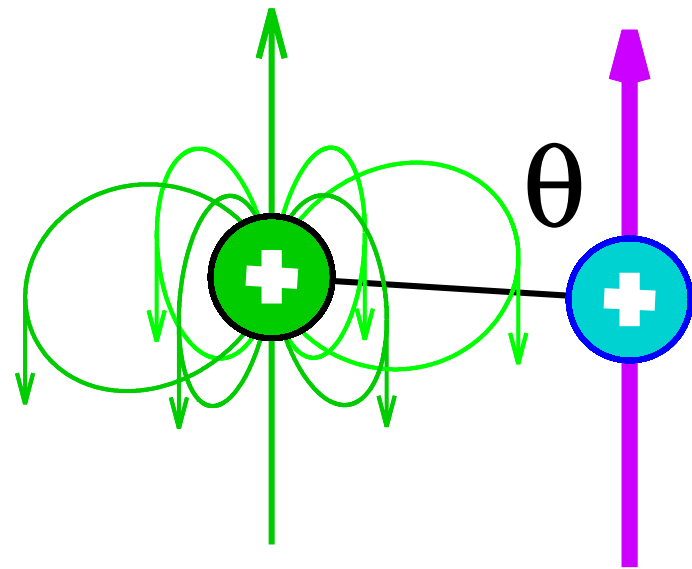


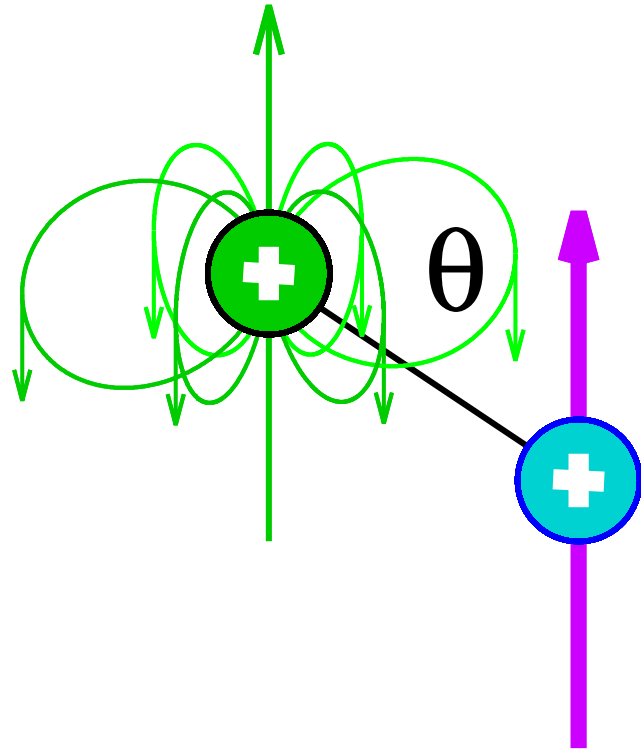
0 ppm

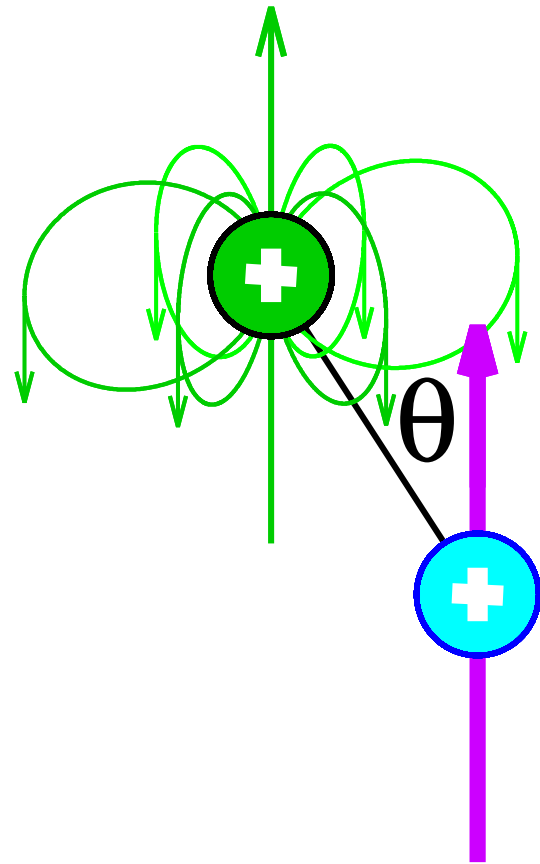
10 ppm

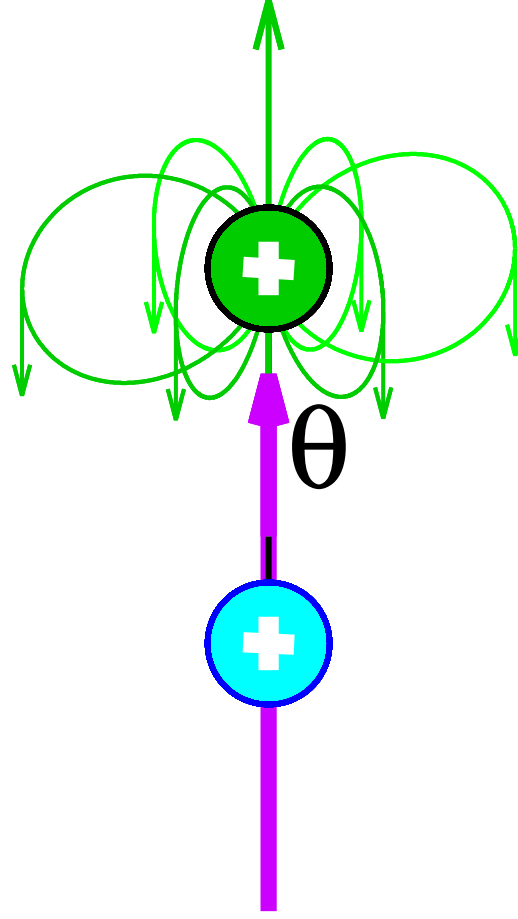
20 ppm

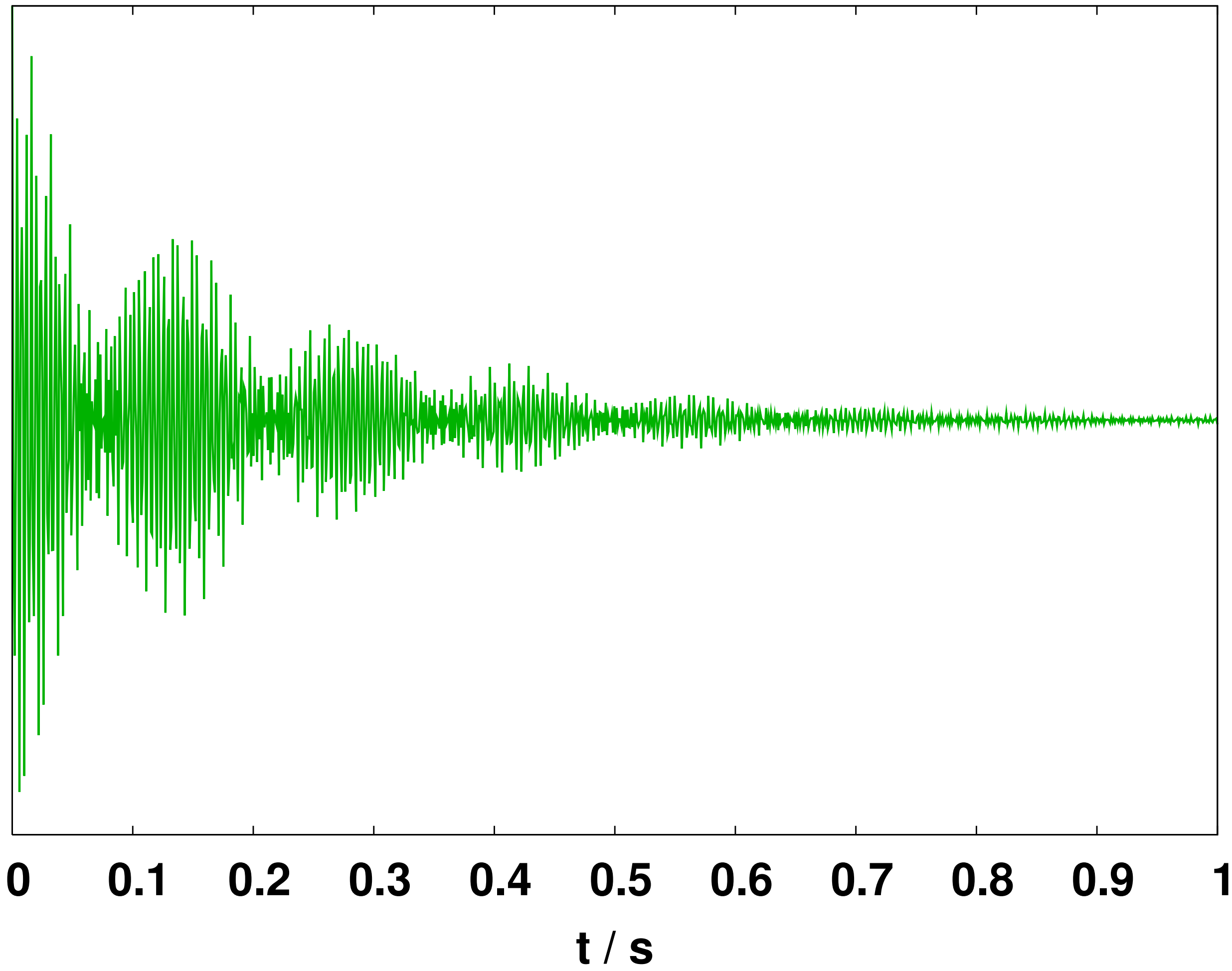
30 ppm



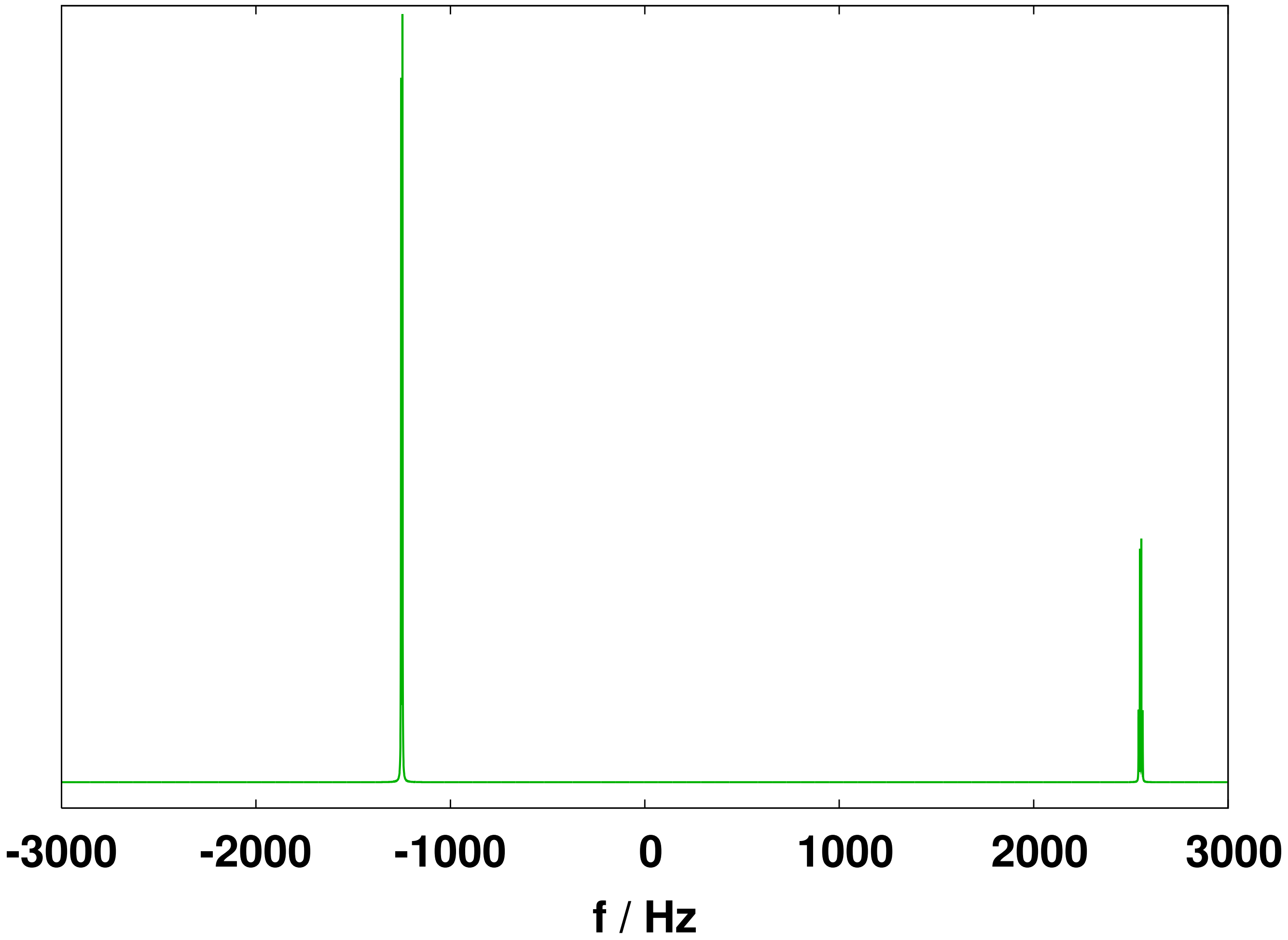


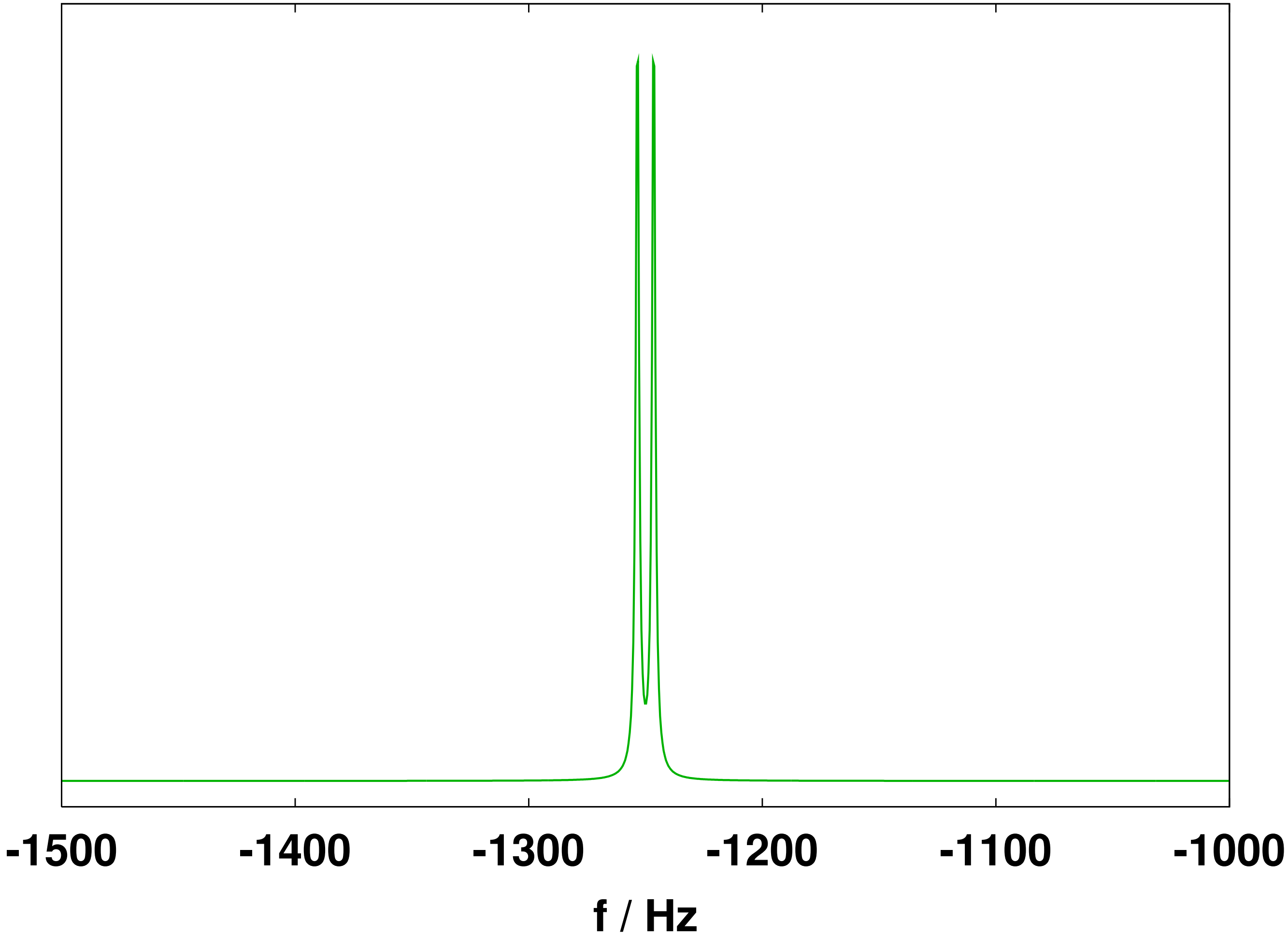


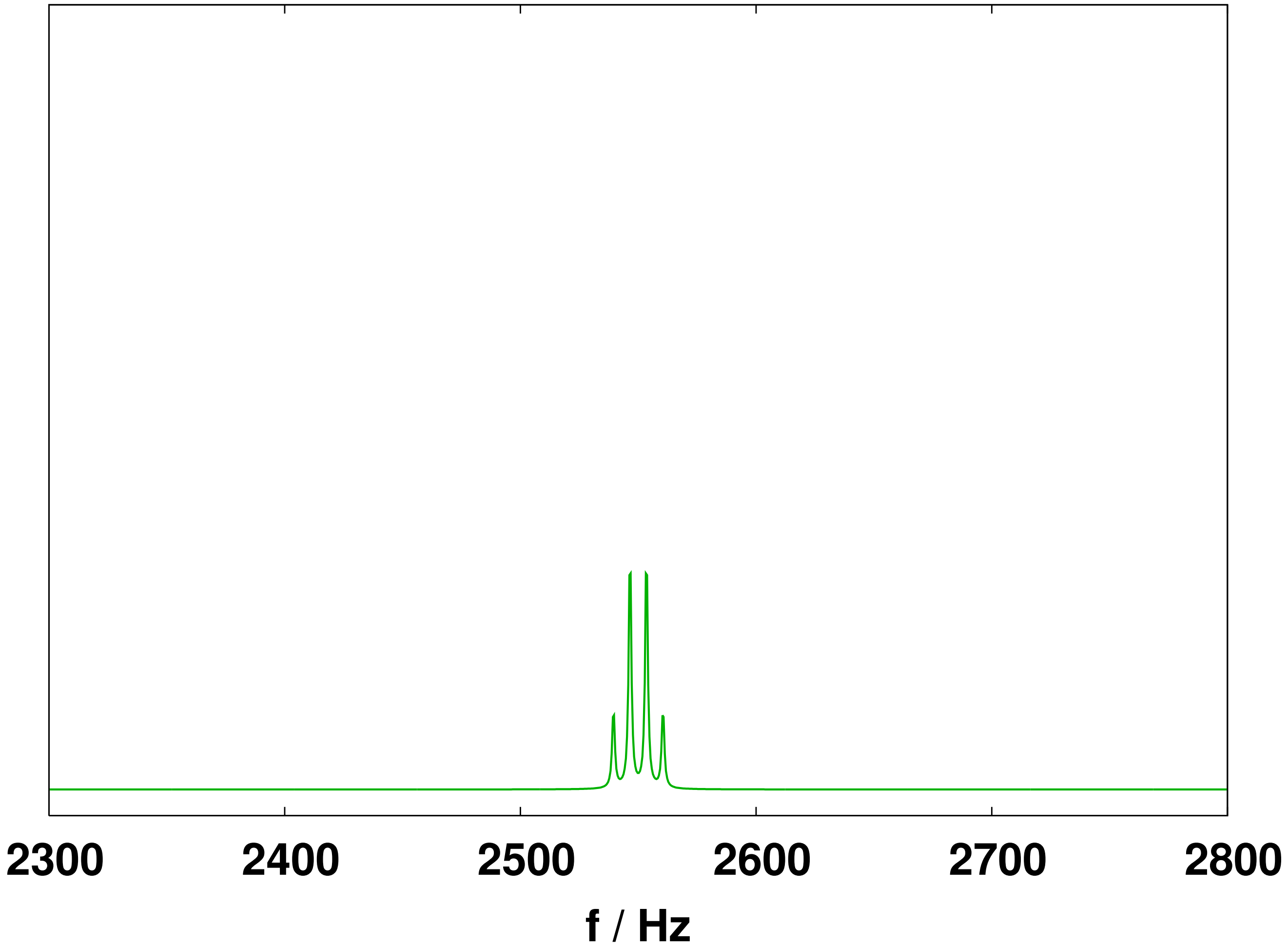


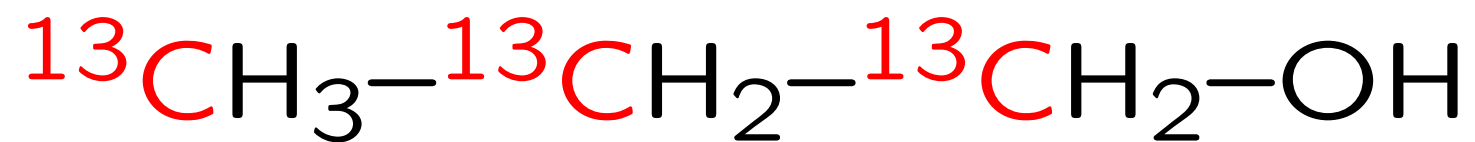
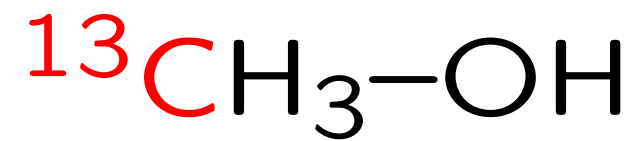


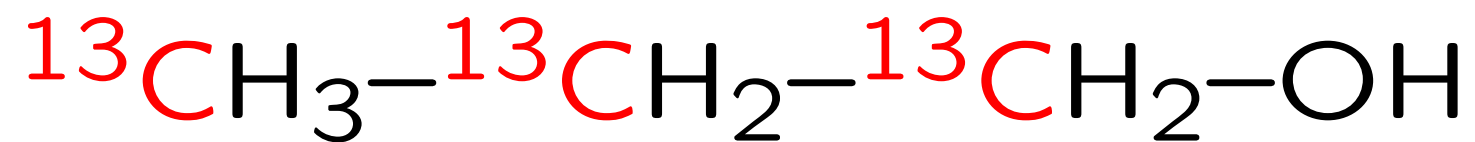
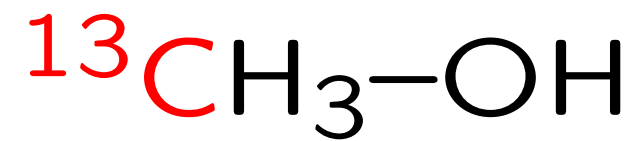












Ovčáci čtveráci

Prší, prší

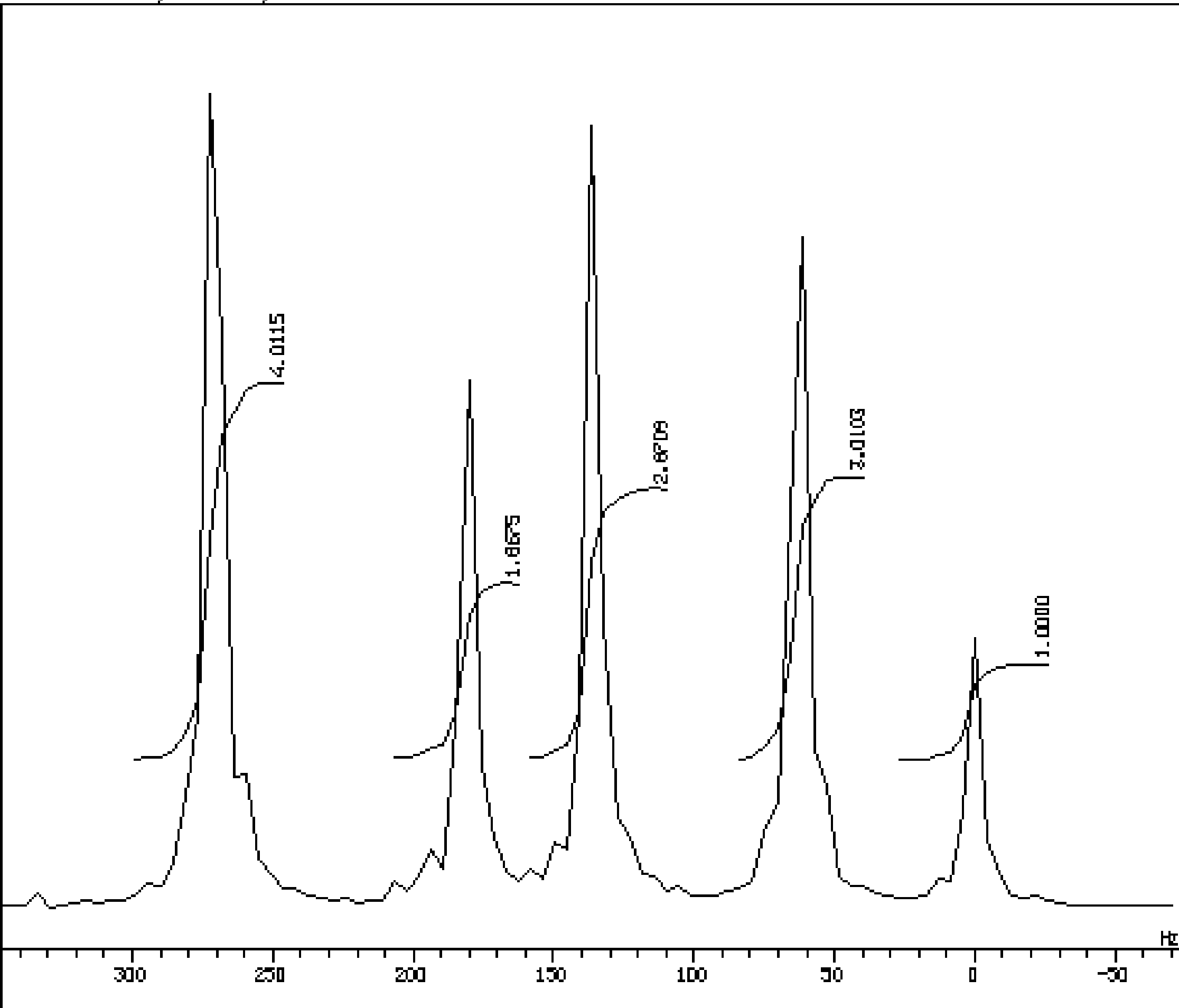
Kočka leze dírou

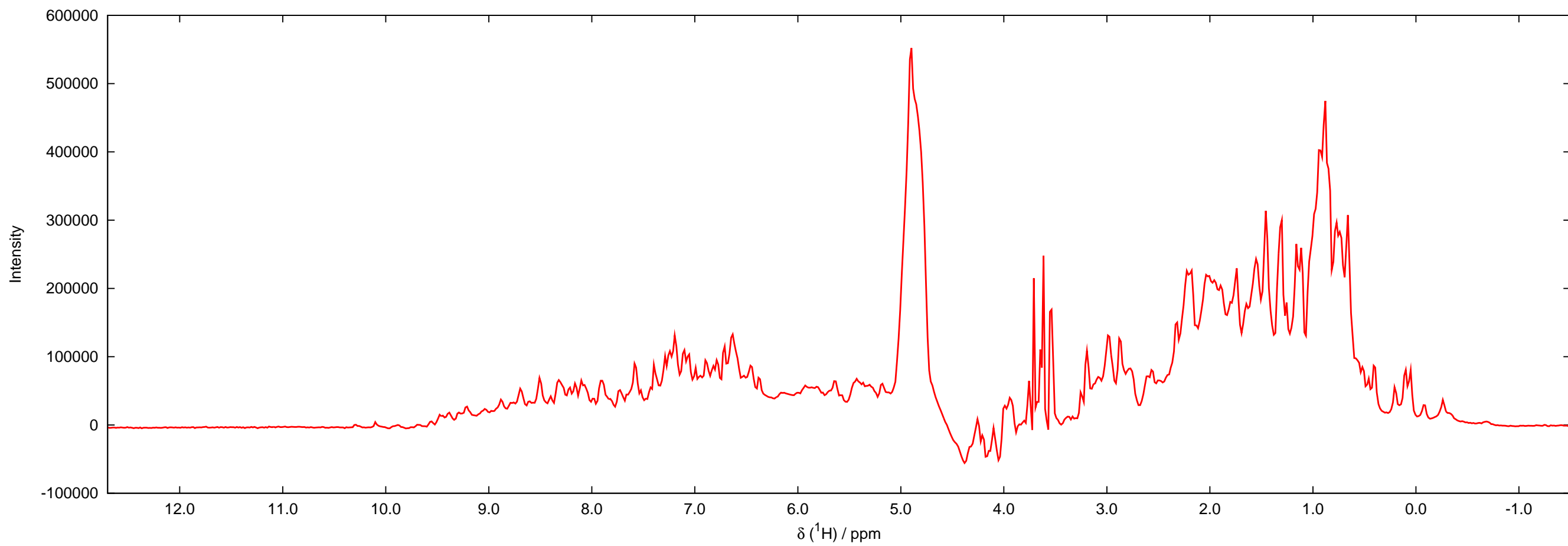


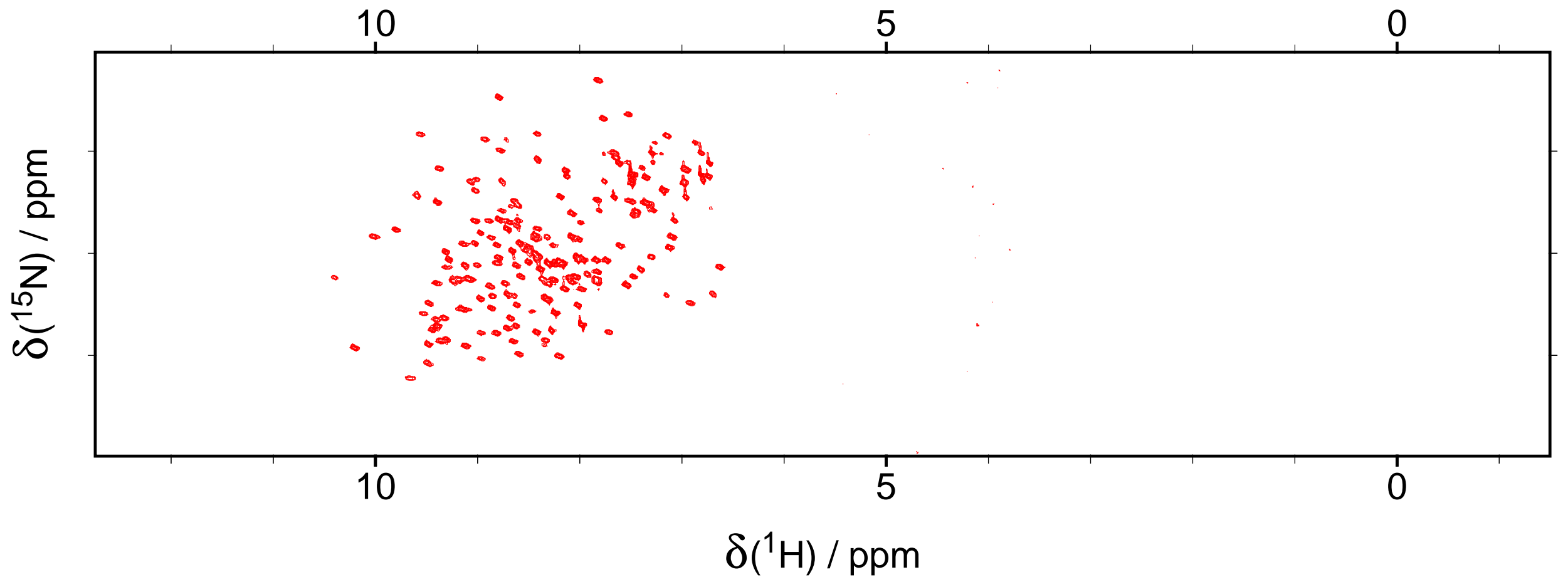
Acetaldehyd

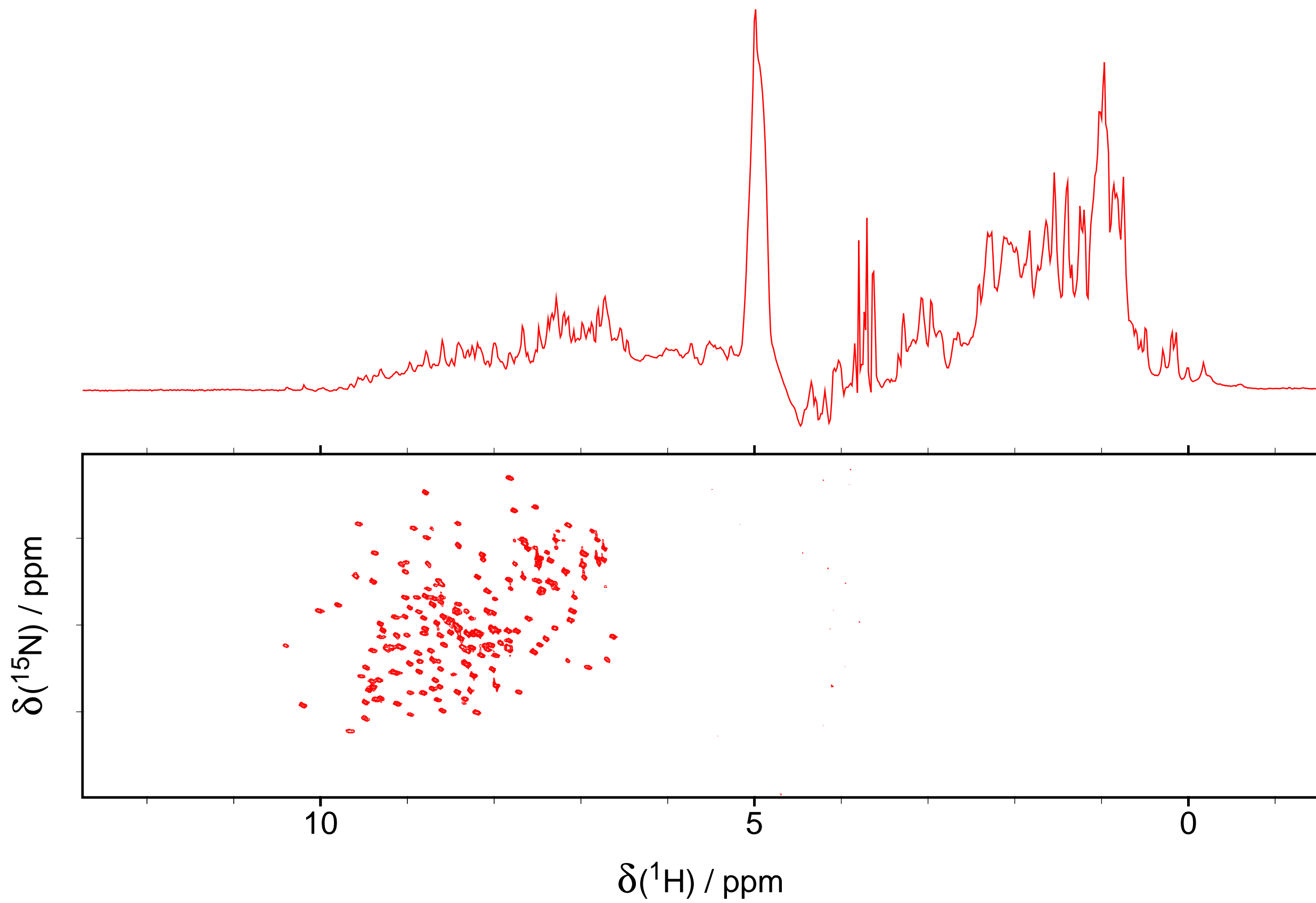
Hänschen klein

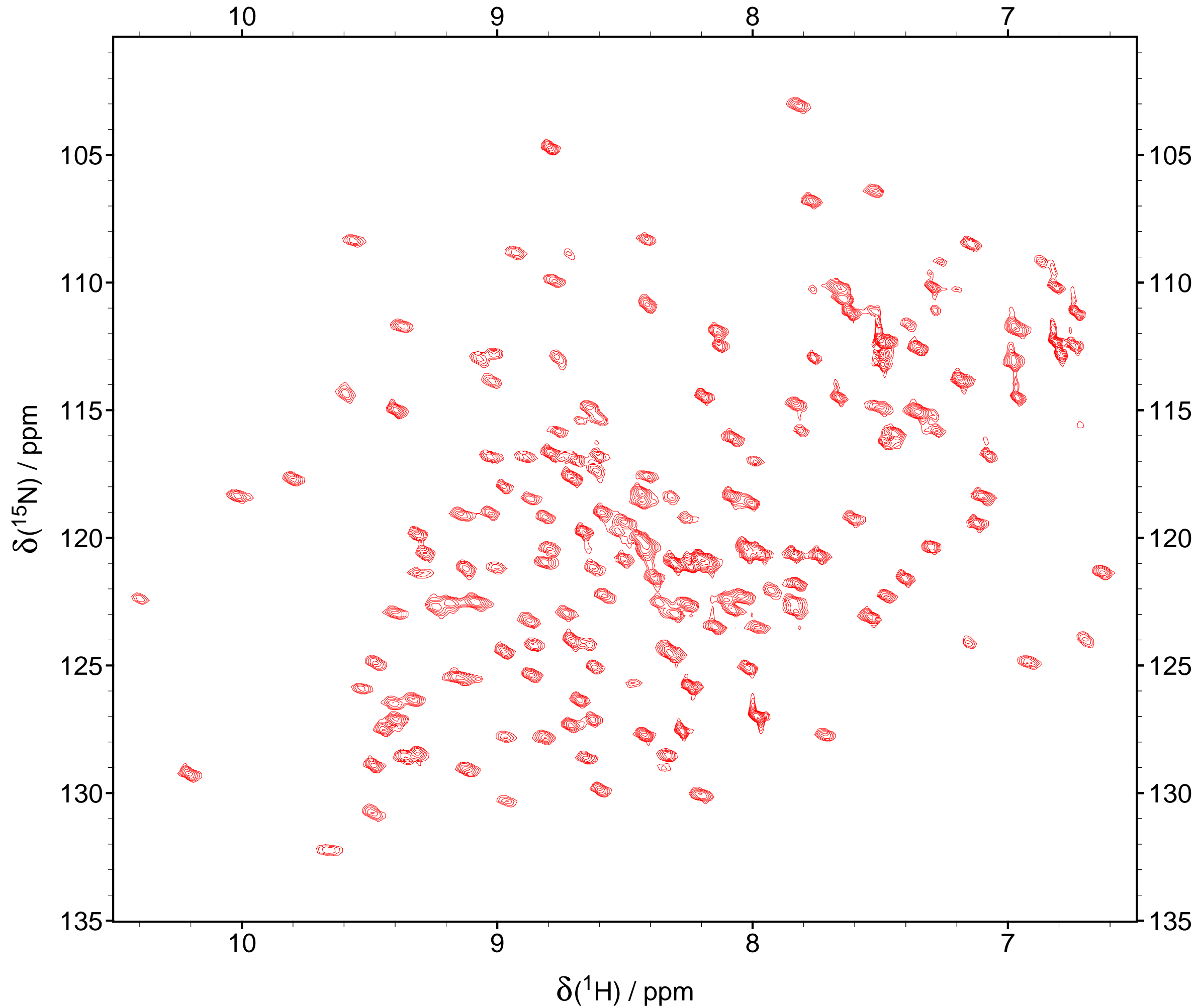
SFILE : HANS  
 EXMOD : HANS  
 IRMOD : NON  
 POINT : 2048  
 SAMPD : 2048  
 FREQU : 9000.90 Hz  
 FILTR : 4500 Hz  
 SCANS : 1  
 QUANTY : 0  
 ACQTH : 0.7275 sec  
 PD : 2.7231 sec  
 RGAIN : 10  
 PW1 : 1.00 usec  
 OBNUC : 1H  
 OBFRQ : 500.00 MHz  
 OBSET : 160200.00 Hz  
 IRNUC : 13C  
 IRFRQ : 125.65 MHz  
 IRSET : 127958.00 Hz  
 IRATN : 511  
 IRRPW : 50.0 usec  
 IRBP1 : 50  
 IRBP2 : 6  
 IRNS : 0  
 TRNUC : 1H  
 TRFRQ : 500.00 MHz  
 TRSET : 162410.00 Hz  
 TRATN : 511  
 TRRPW : 50.0 usec  
 TRBP1 : 30  
 TRBP2 : 6  
 TRNS : 0  
 CTEMP : 24.1 c  
 CSPED : 11 Hz  
 SLVNT : C6D6  
 RESOL : 4.39 Hz  
 NNUC : 8  
 BF : 0.10 Hz  
 CF : 0.00 Hz  
 PF : 840 cp  
 ABSFO : -92.11 deg  
 ABSF1 : 0.00 deg  
 T1 : 0.00 s  
 T2 : 0.00 s  
 T3 : 90.00 s  
 T4 : 100.00 s  
 REFVL : 0.00 ppm  
 T19F : 902  
 XE : 421.92 Hz  
 XS : -676.83 Hz  
 Y6 : 0.001

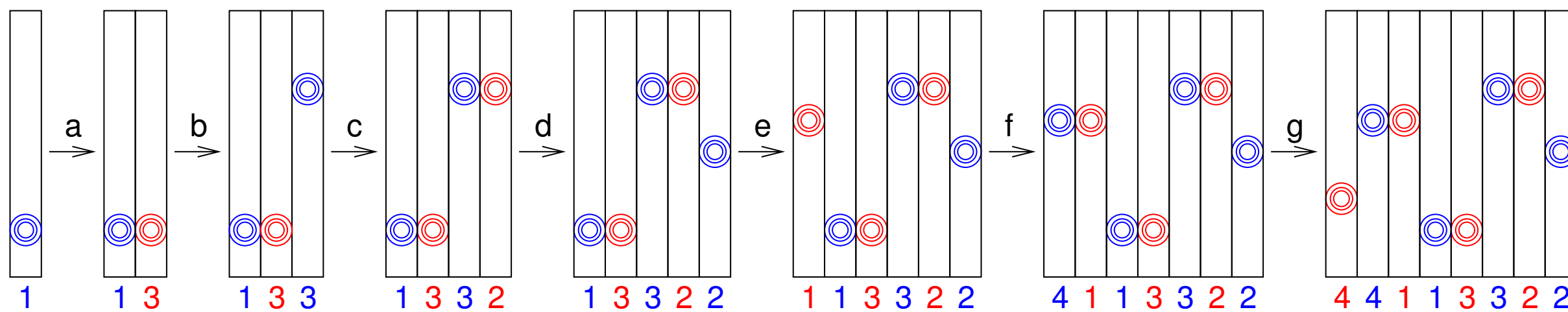
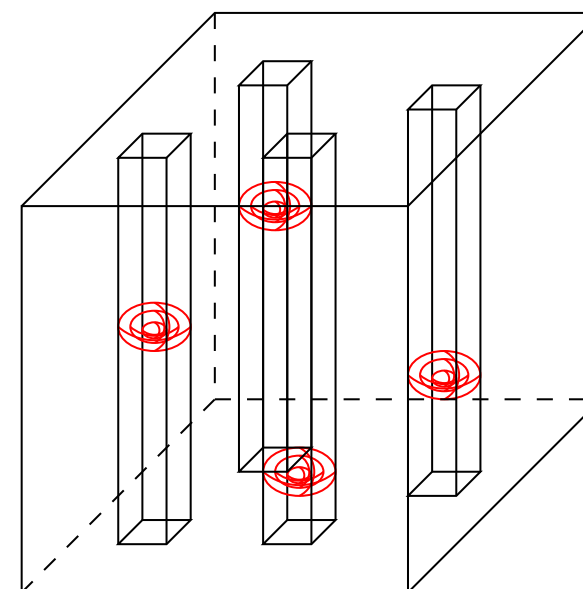
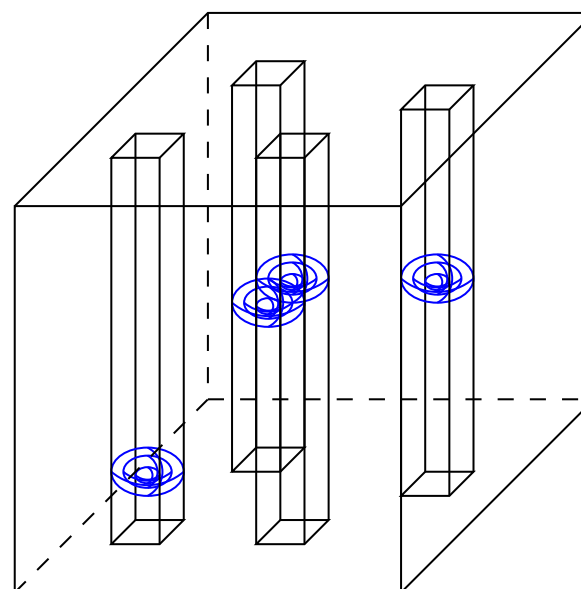
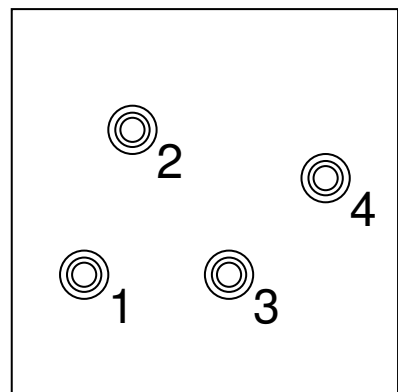
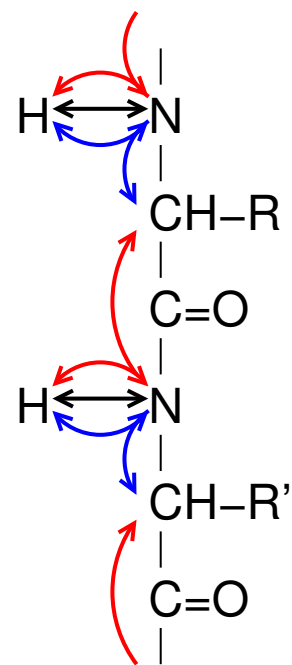




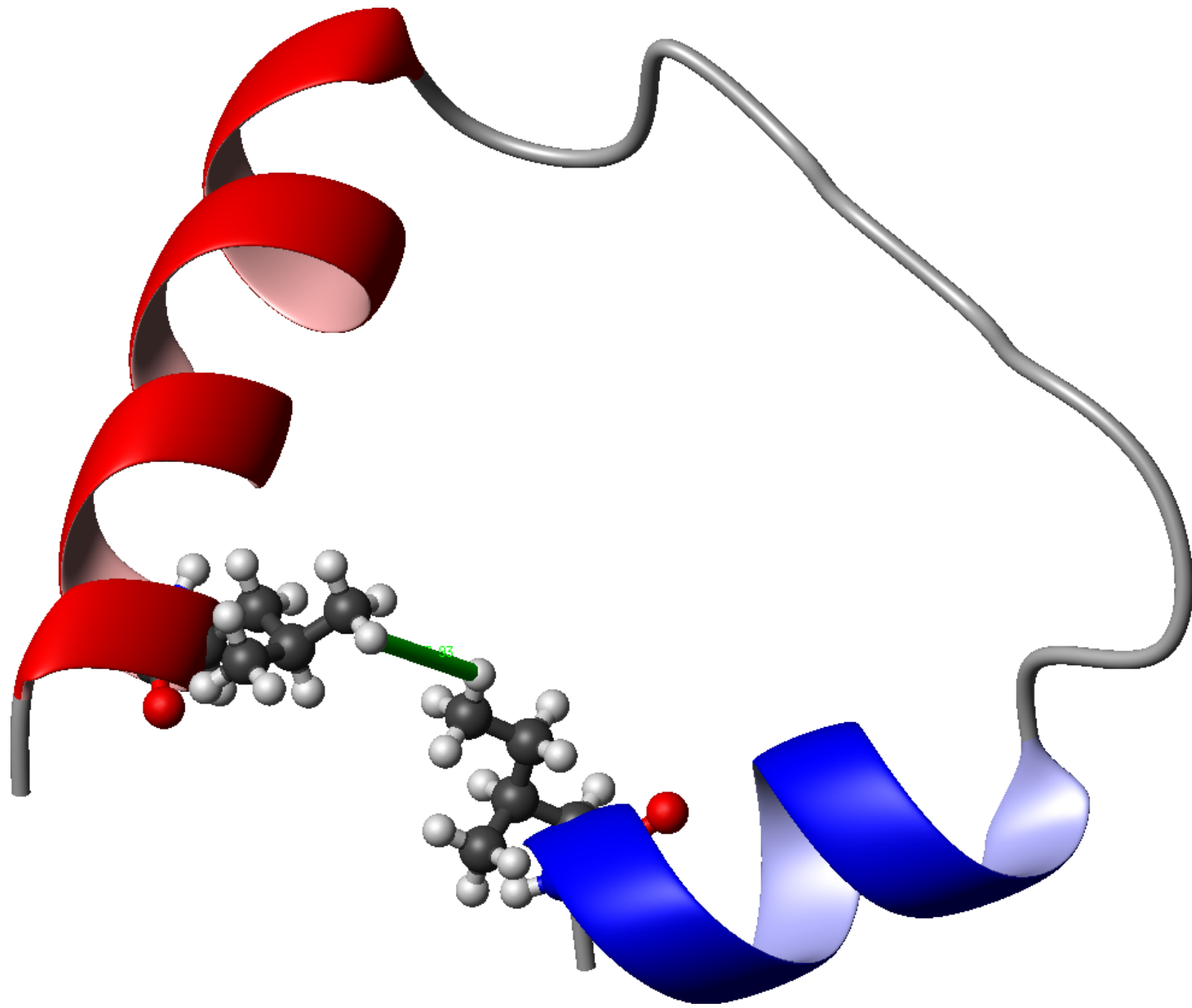


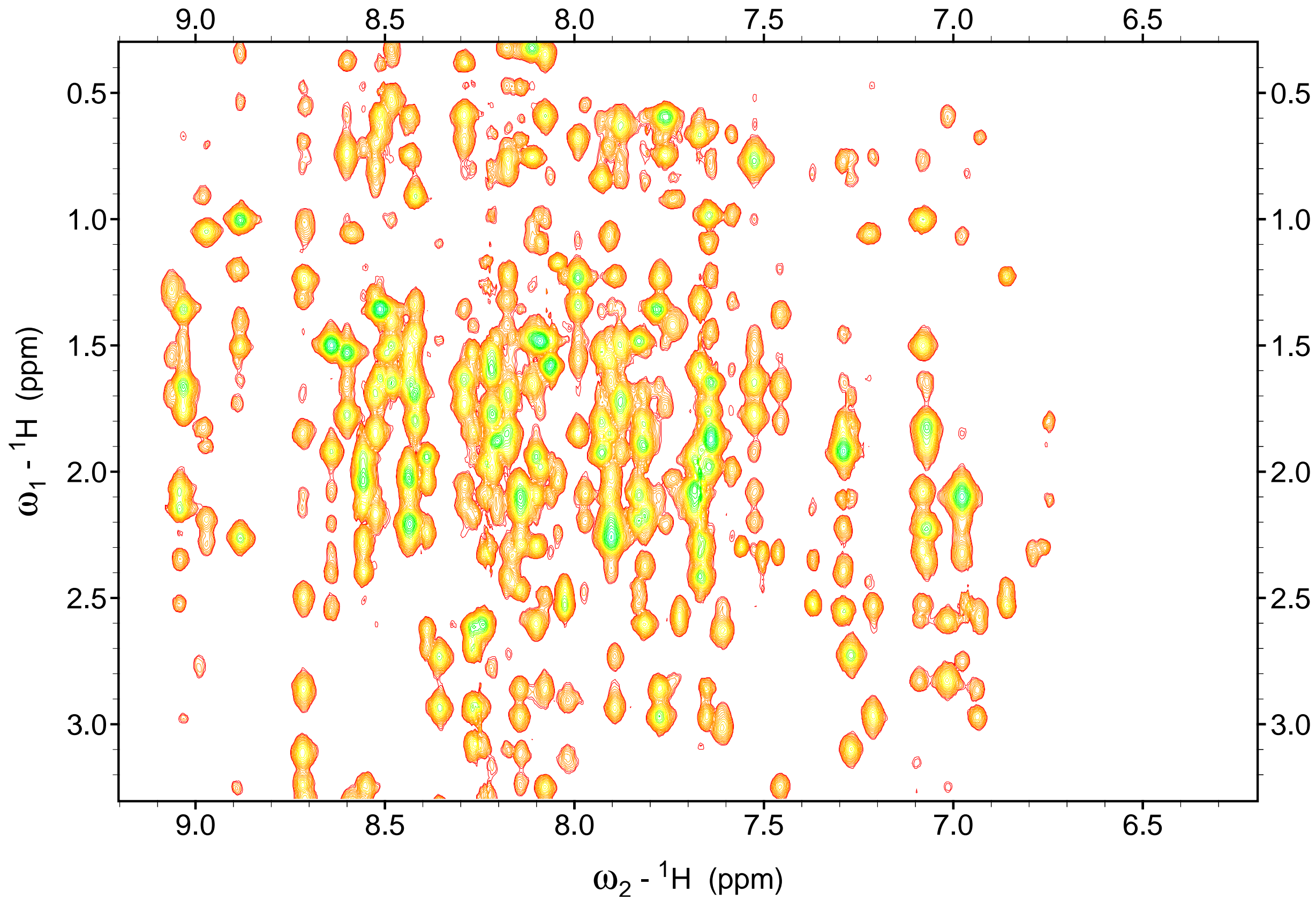


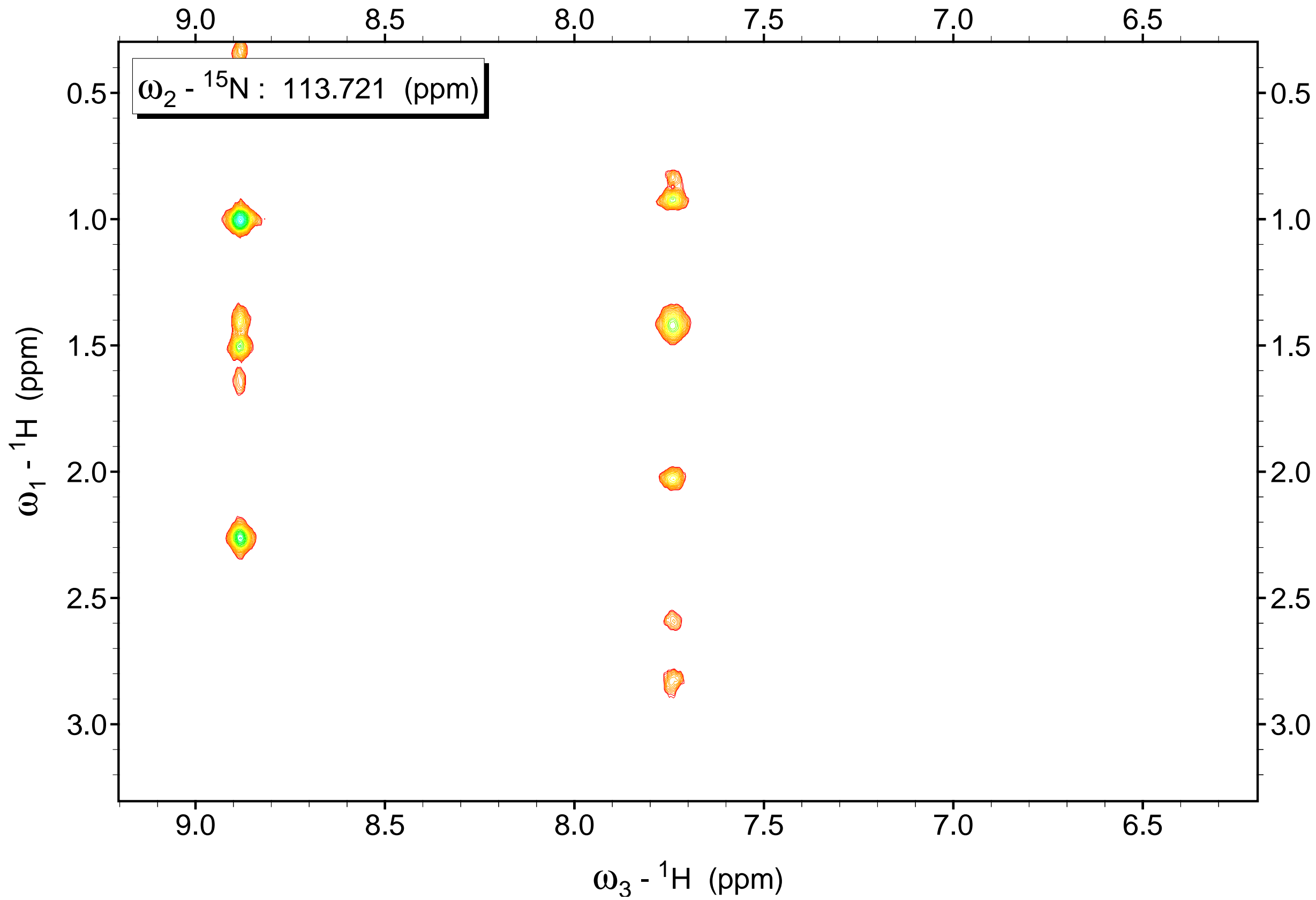


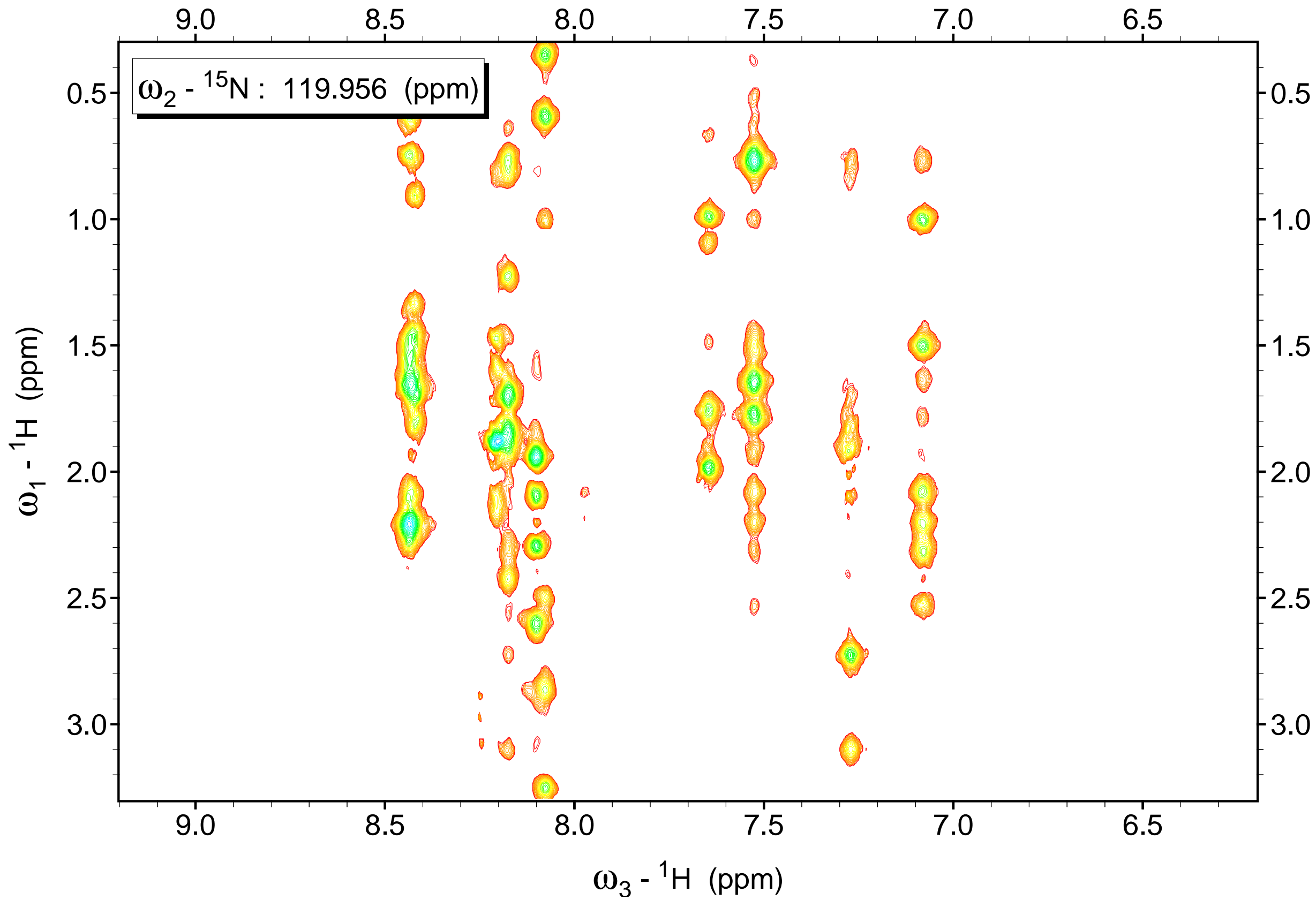


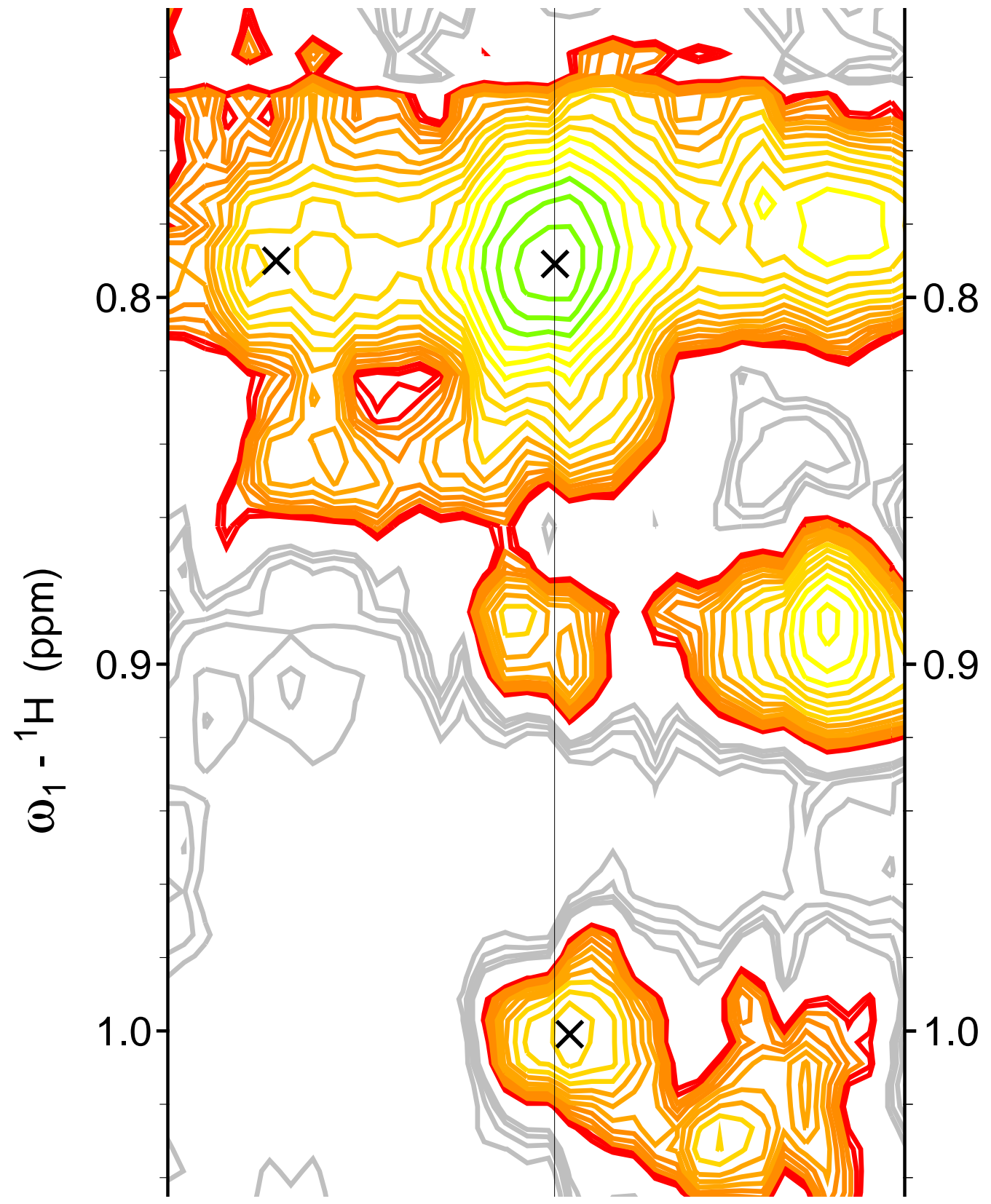


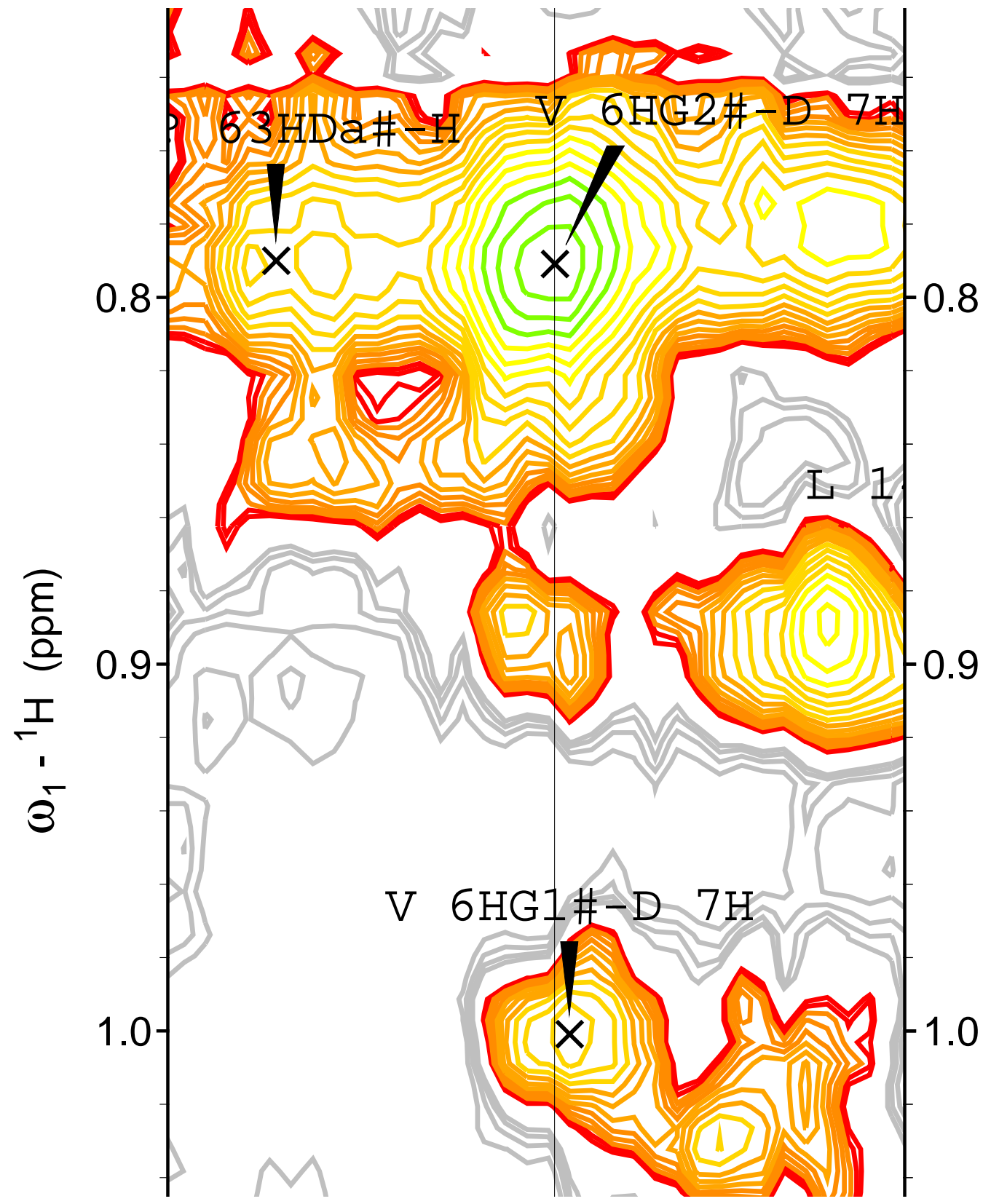








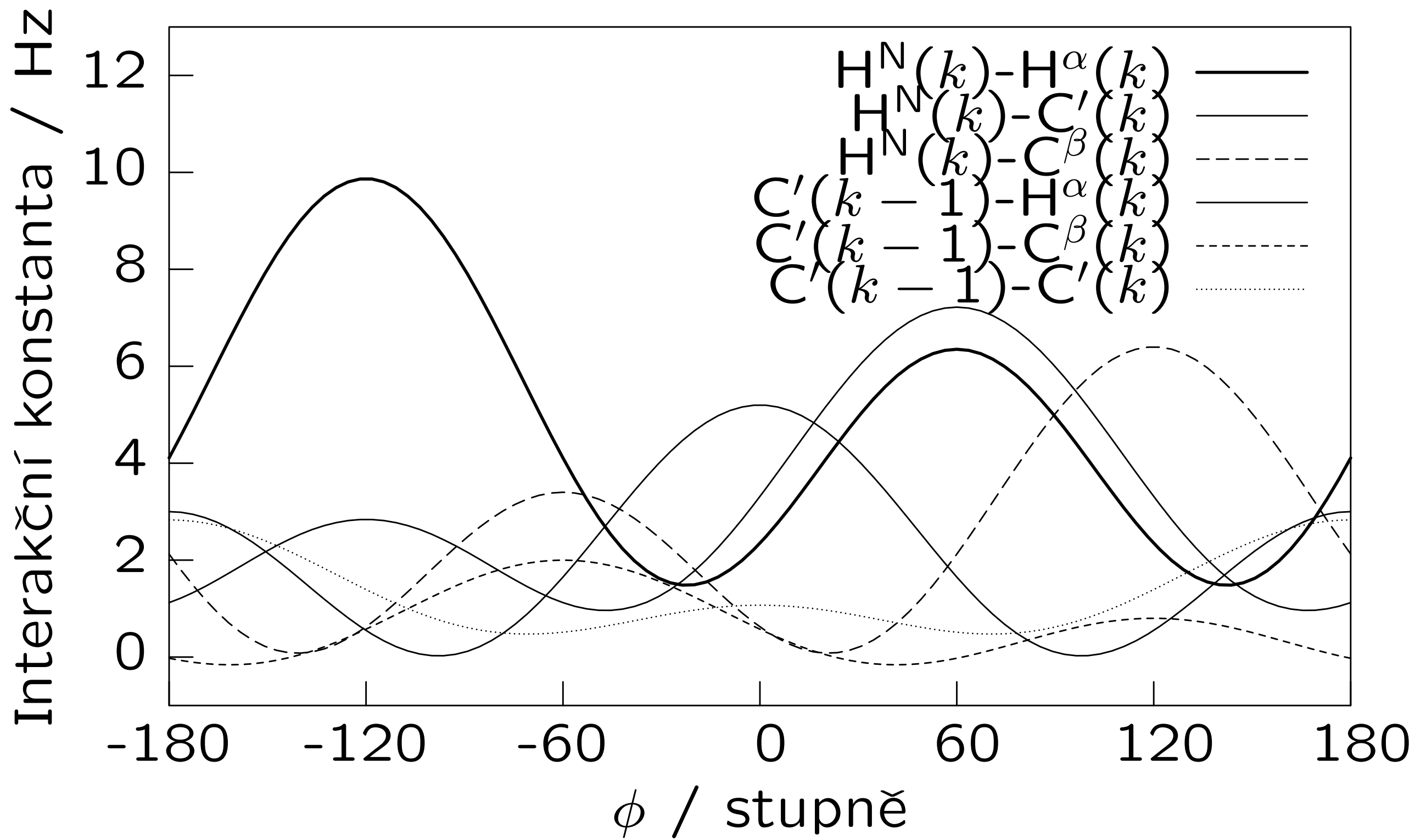




$$\frac{S}{S_{\text{ref}}} = \left(\frac{r_{\text{ref}}}{r}\right)^6 \quad (1)$$

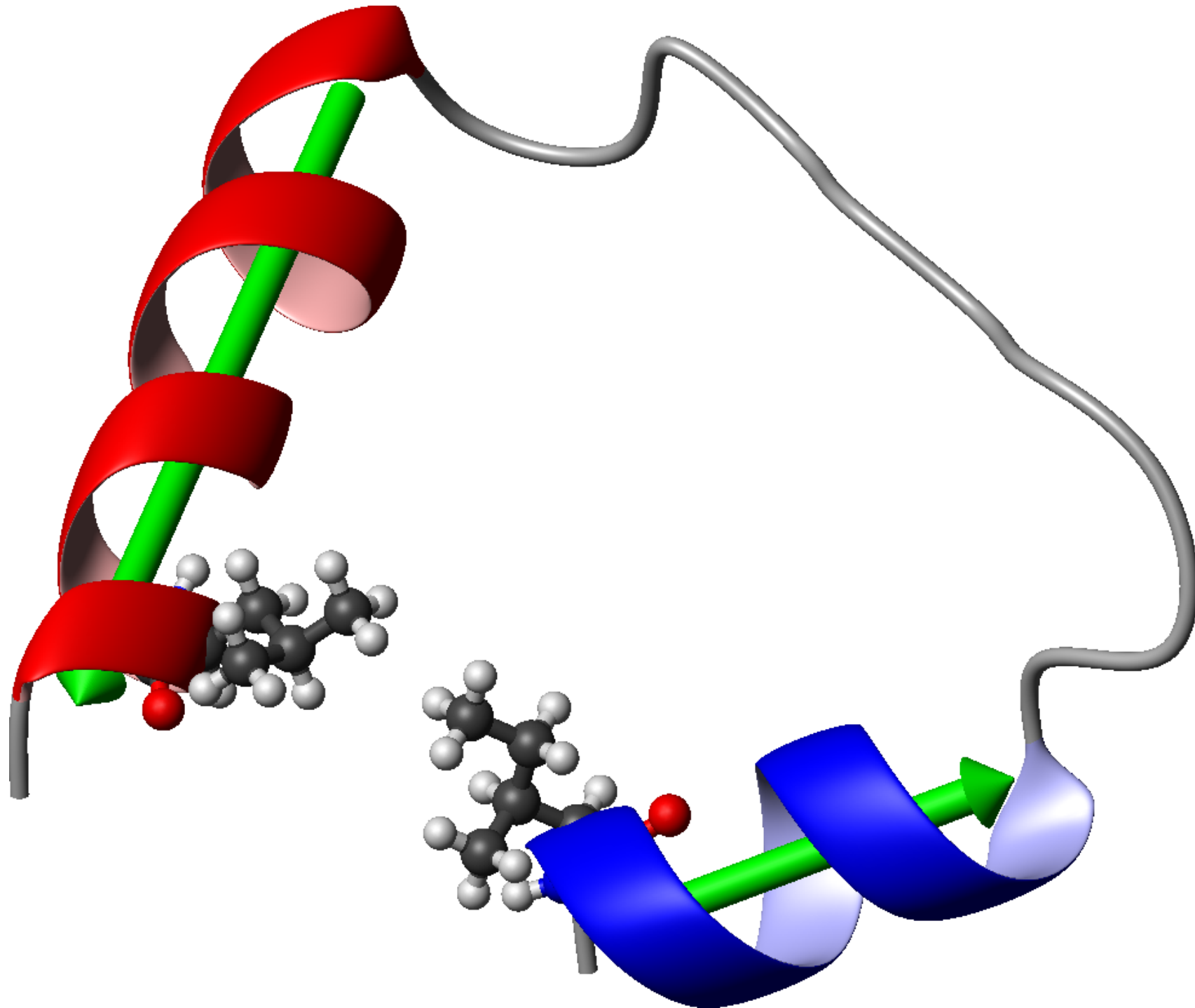
$$r = r_{\text{ref}} \sqrt[6]{\frac{S_{\text{ref}}}{S}} \quad (2)$$

Referenční protony		vzdálenost
geminální v methylenu	$\text{H}-\text{C}-\text{H}$	0,17 nm
vicinální v aromatickém kruhu	$\text{H}-\text{C}=\text{C}-\text{H}$	0,25 nm
<i>meta</i> v aromatickém kruhu	$\text{H}-\text{C}=\text{CH}-\text{C}-\text{H}$	0,42 nm

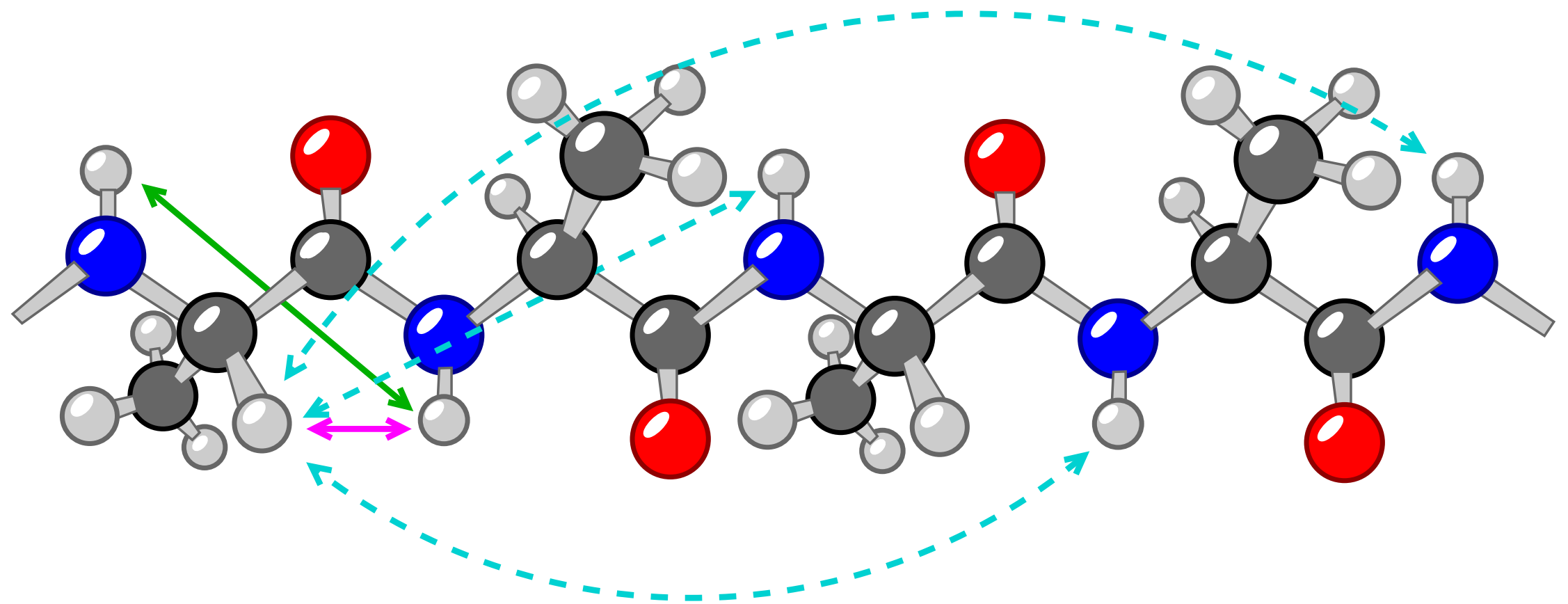


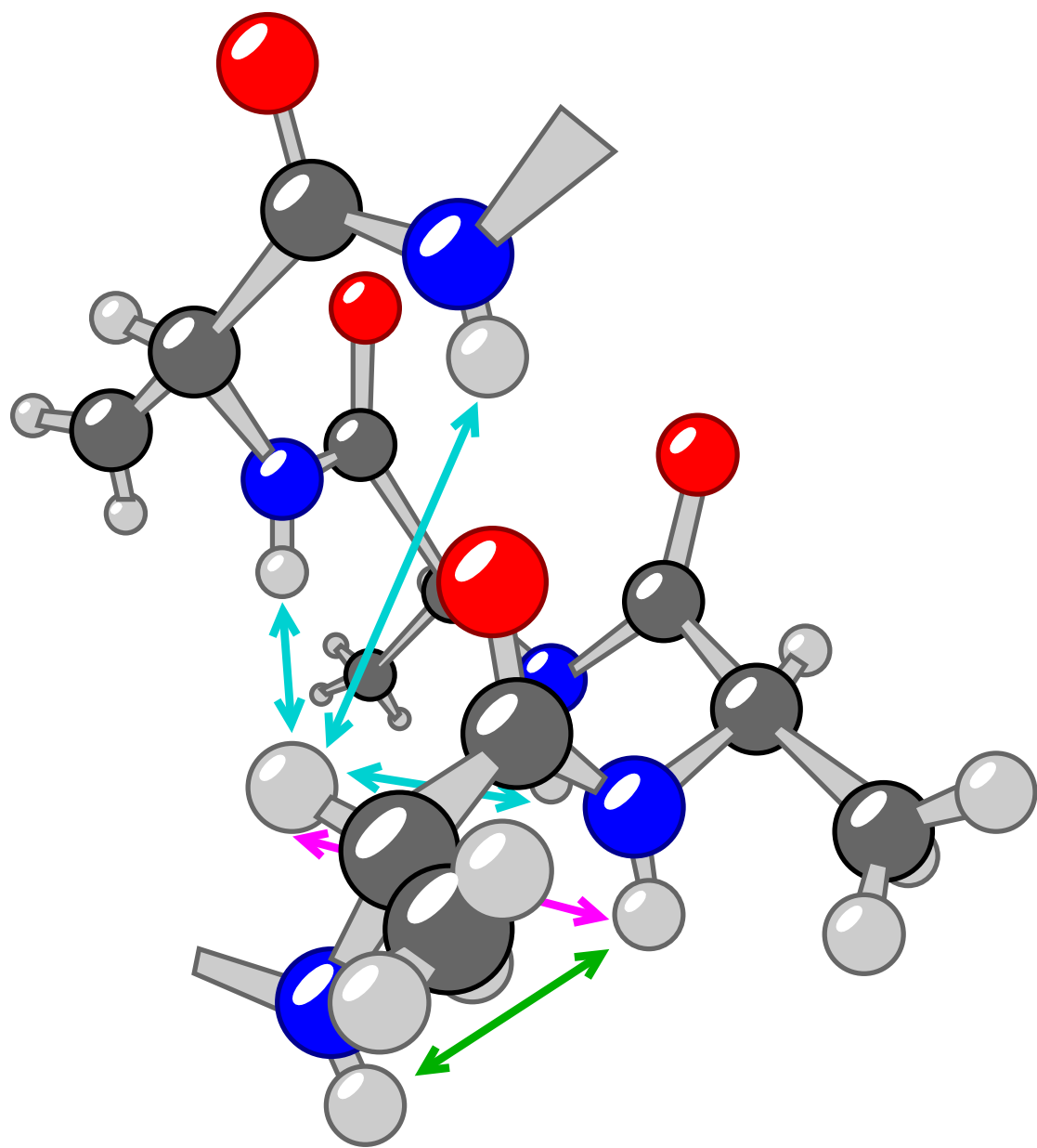


Zbytkové dipólové interakce  $\propto \langle 3 \cos^2 \theta - 1 \rangle \Rightarrow$  orientace



Data	$\beta$ -list	$\alpha$ -šroubovice
$\delta(C')$ , $\delta(C^\alpha)$	↓	↑
$\delta(C^\beta)$ , $\delta(H^\alpha)$	↑	↓
$ H_i^\alpha H_{i+1}^N $	0,22 nm	0,35 nm
$ H_i^N H_{i+1}^N $	0,40 nm	0,28 nm
$ H_i^\alpha H_{i+2}^N $	daleko	0,42 nm
$ H_i^\alpha H_{i+3}^N $	daleko	0,34 nm
$ H_i^\alpha H_{i+4}^N $	daleko	0,42 nm
${}^3J(H_i^N H_i^\alpha)$	> 8 Hz	< 5 Hz



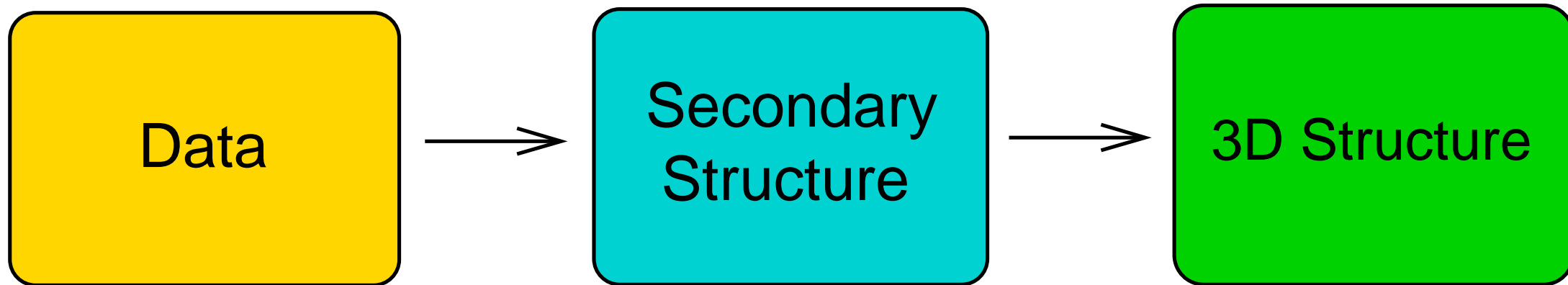


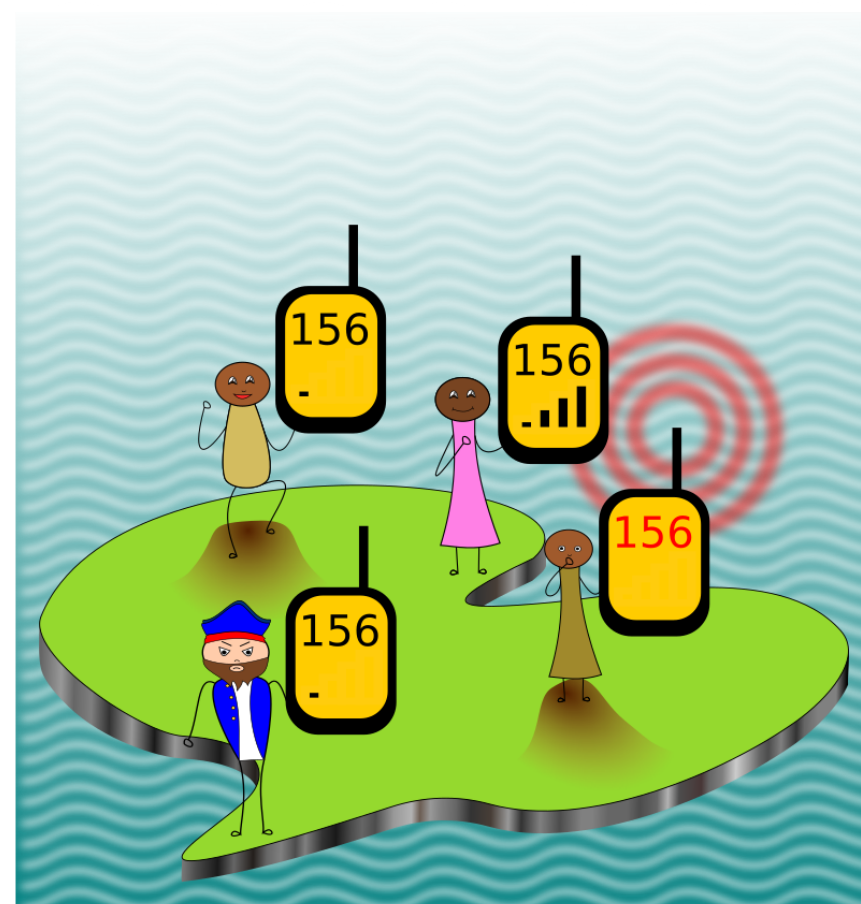
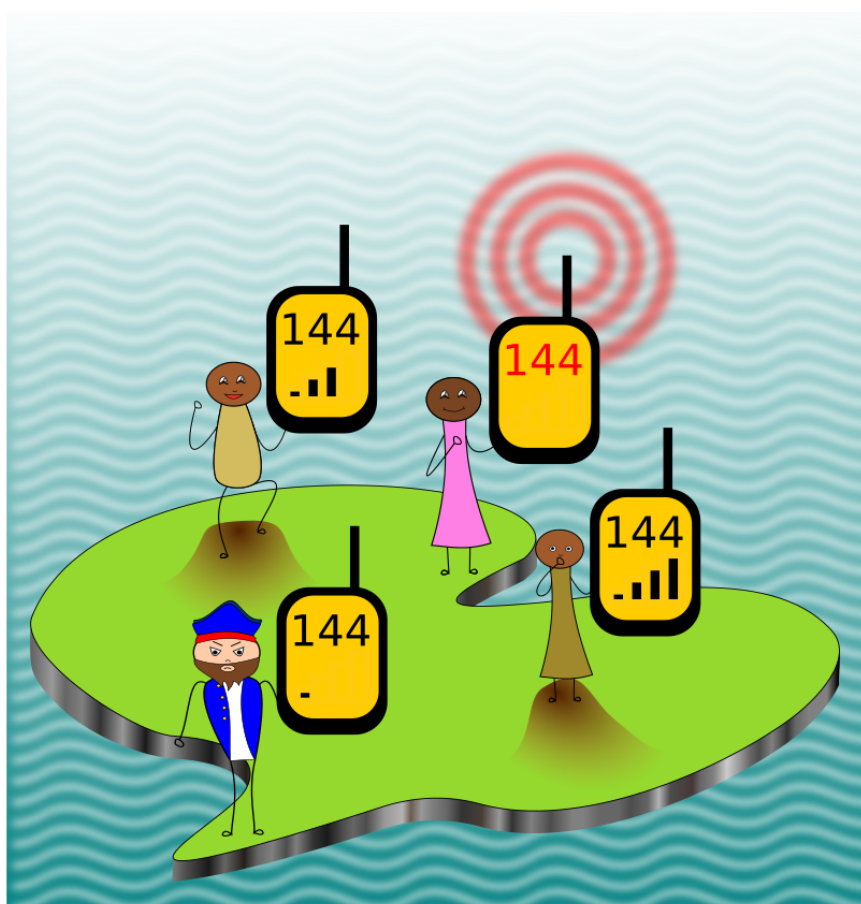
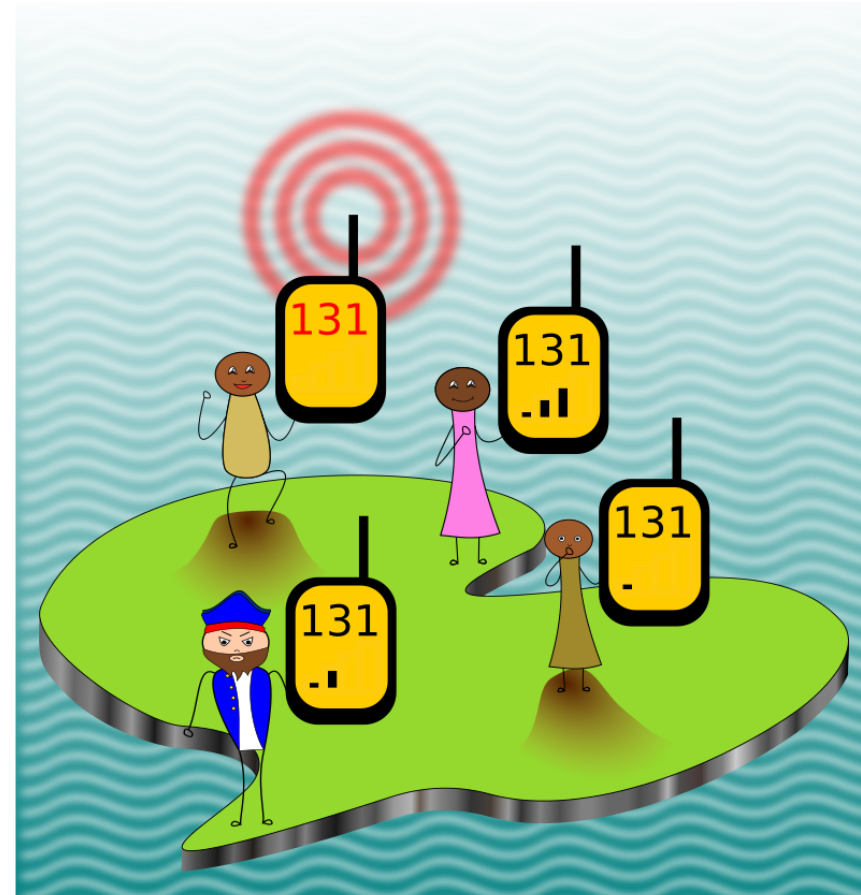
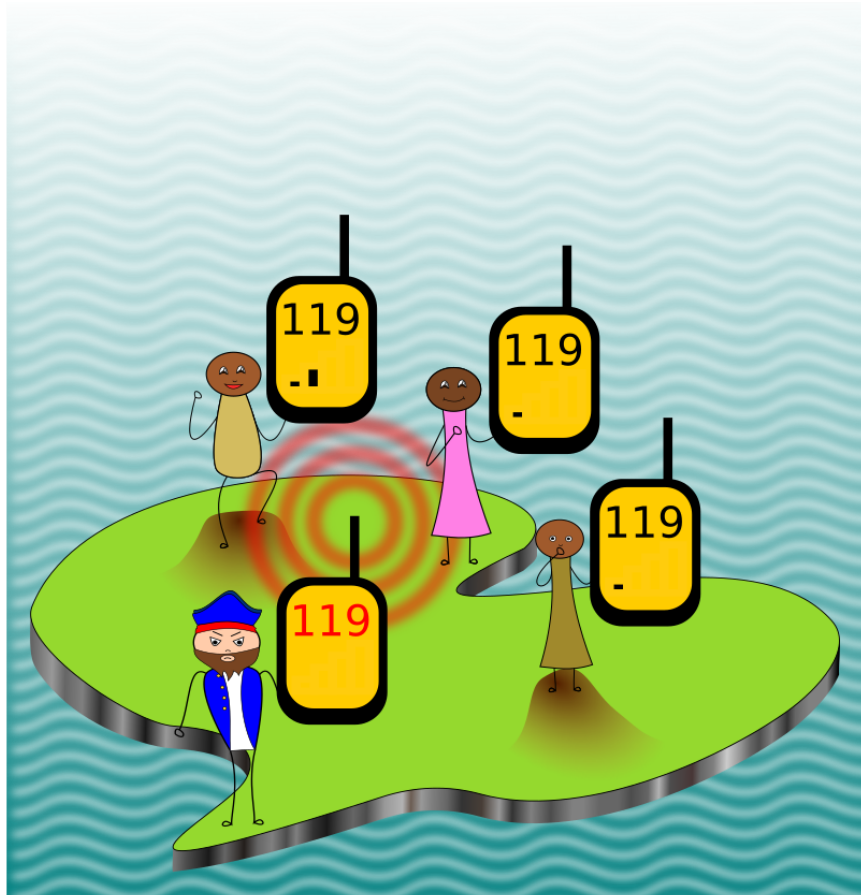
$\alpha$ -helix

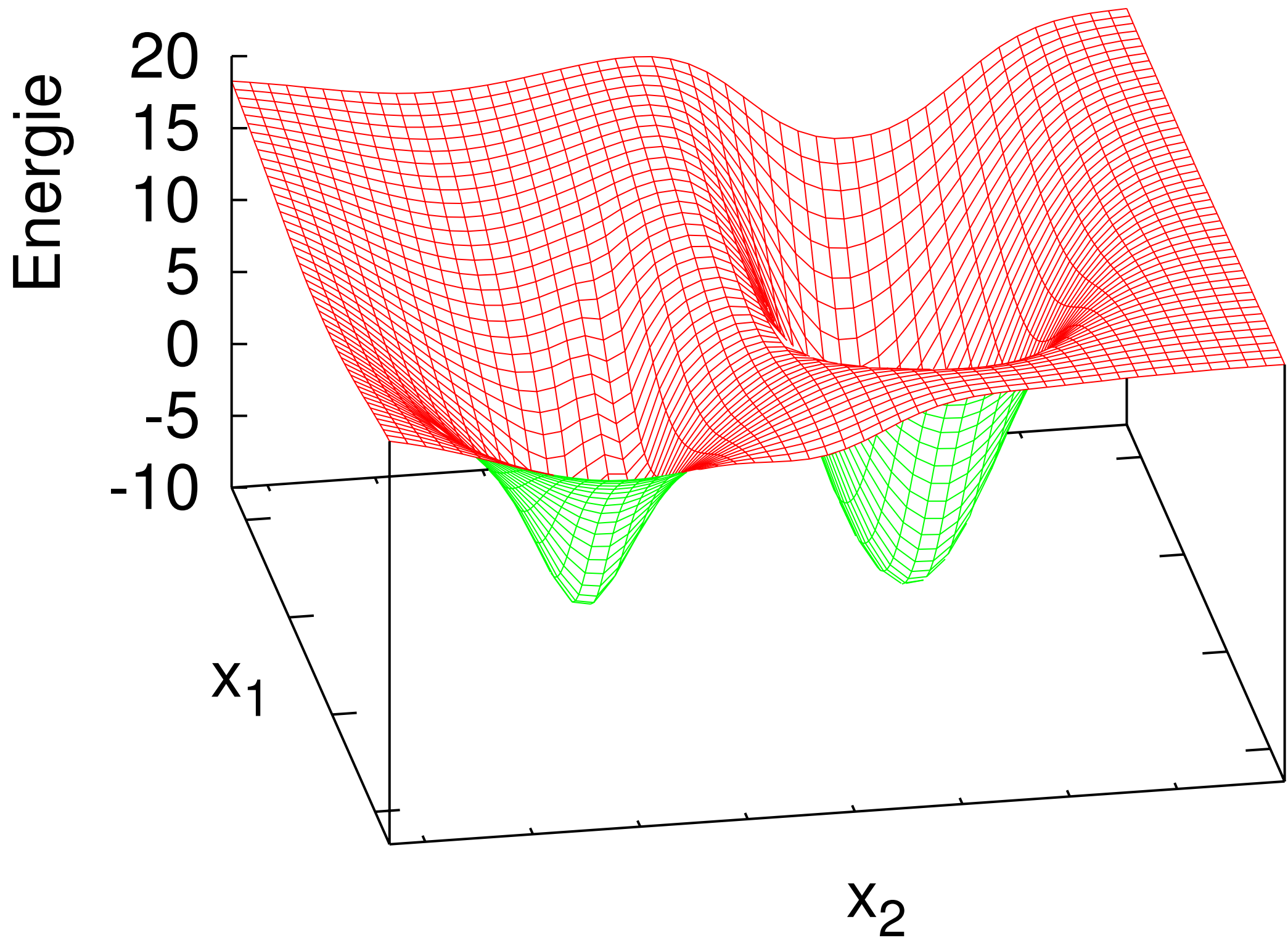
$3_{10}$ -helix

antiparallel  $\beta$ -sheet

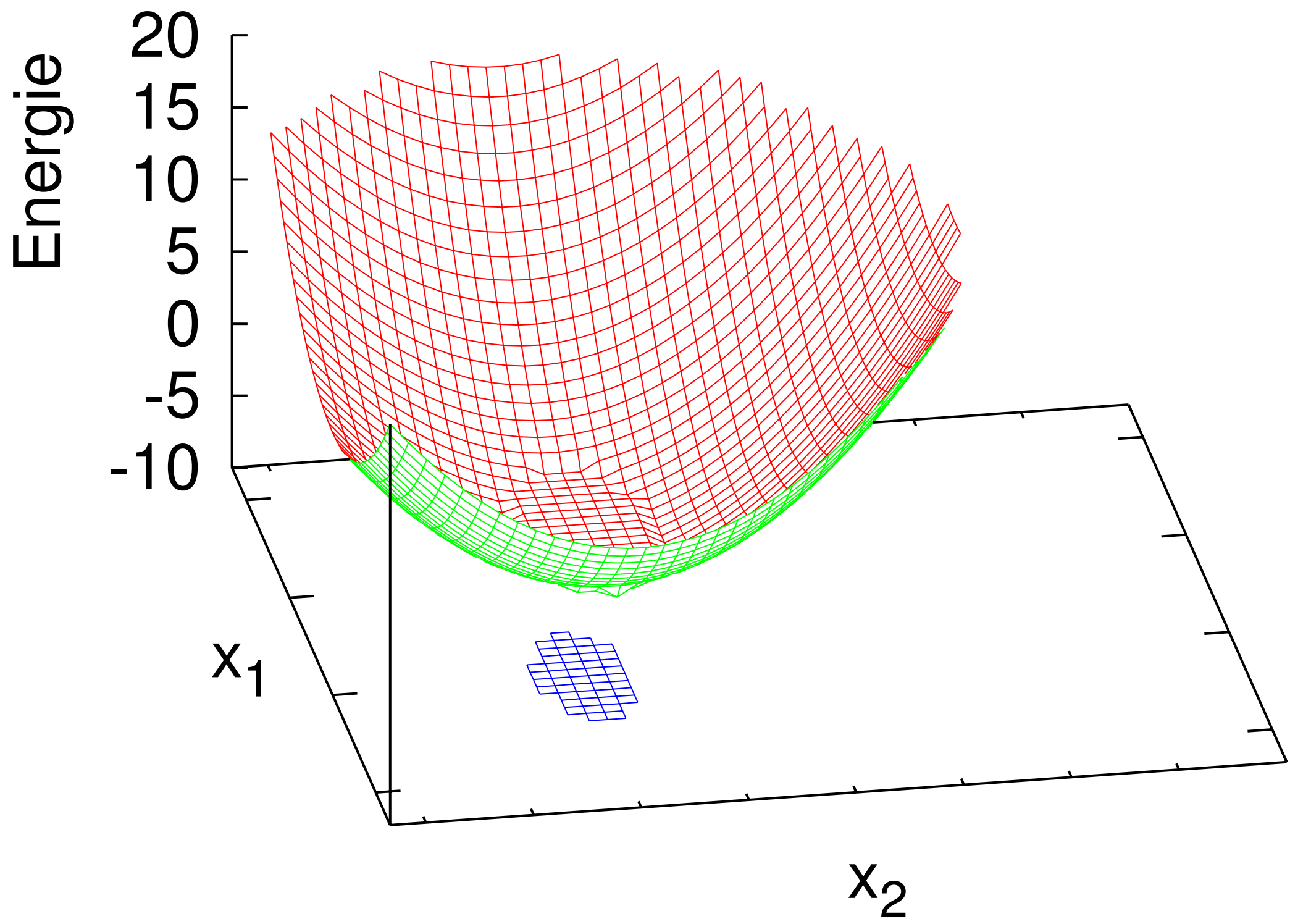
parallel  $\beta$ -sheet

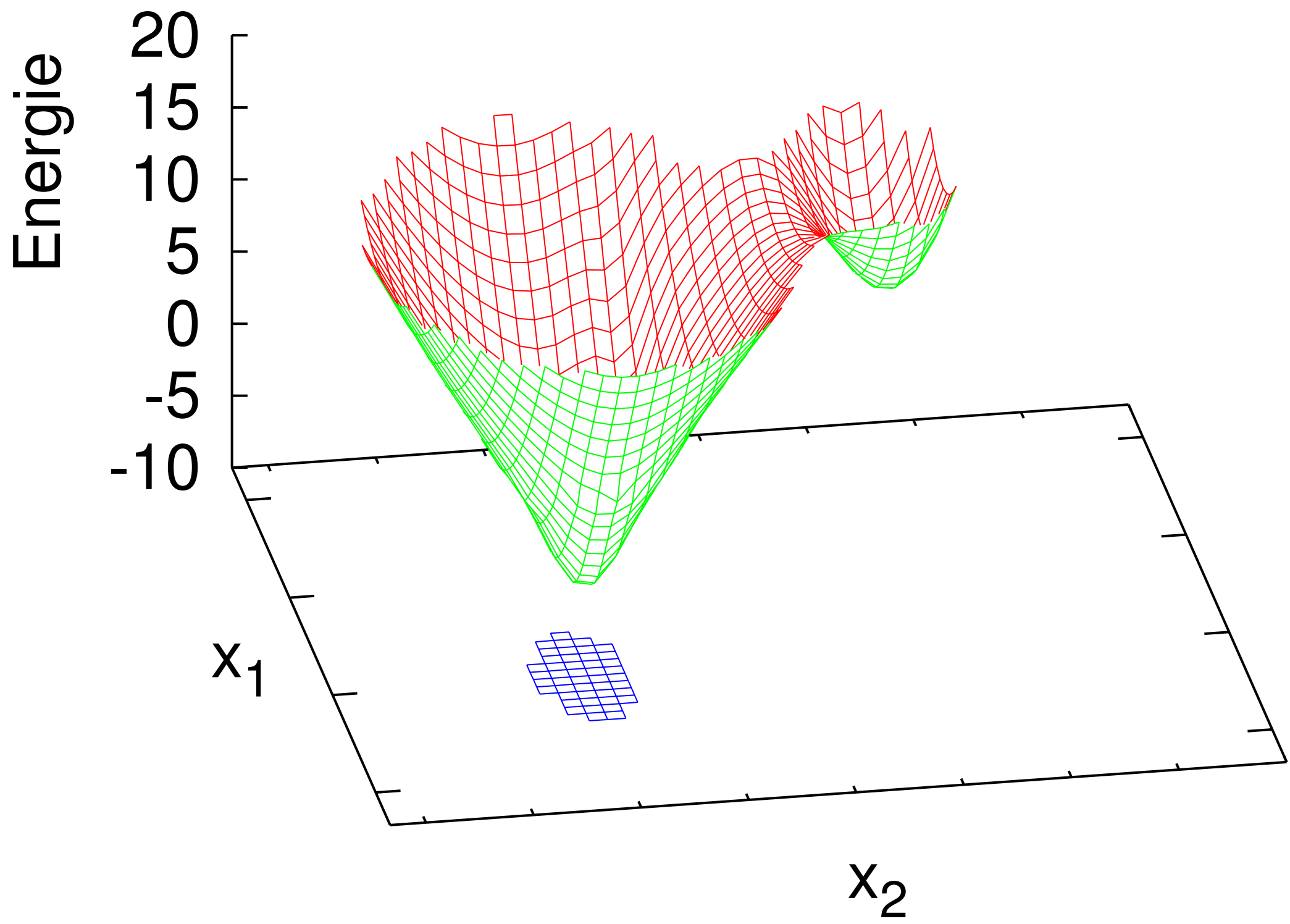


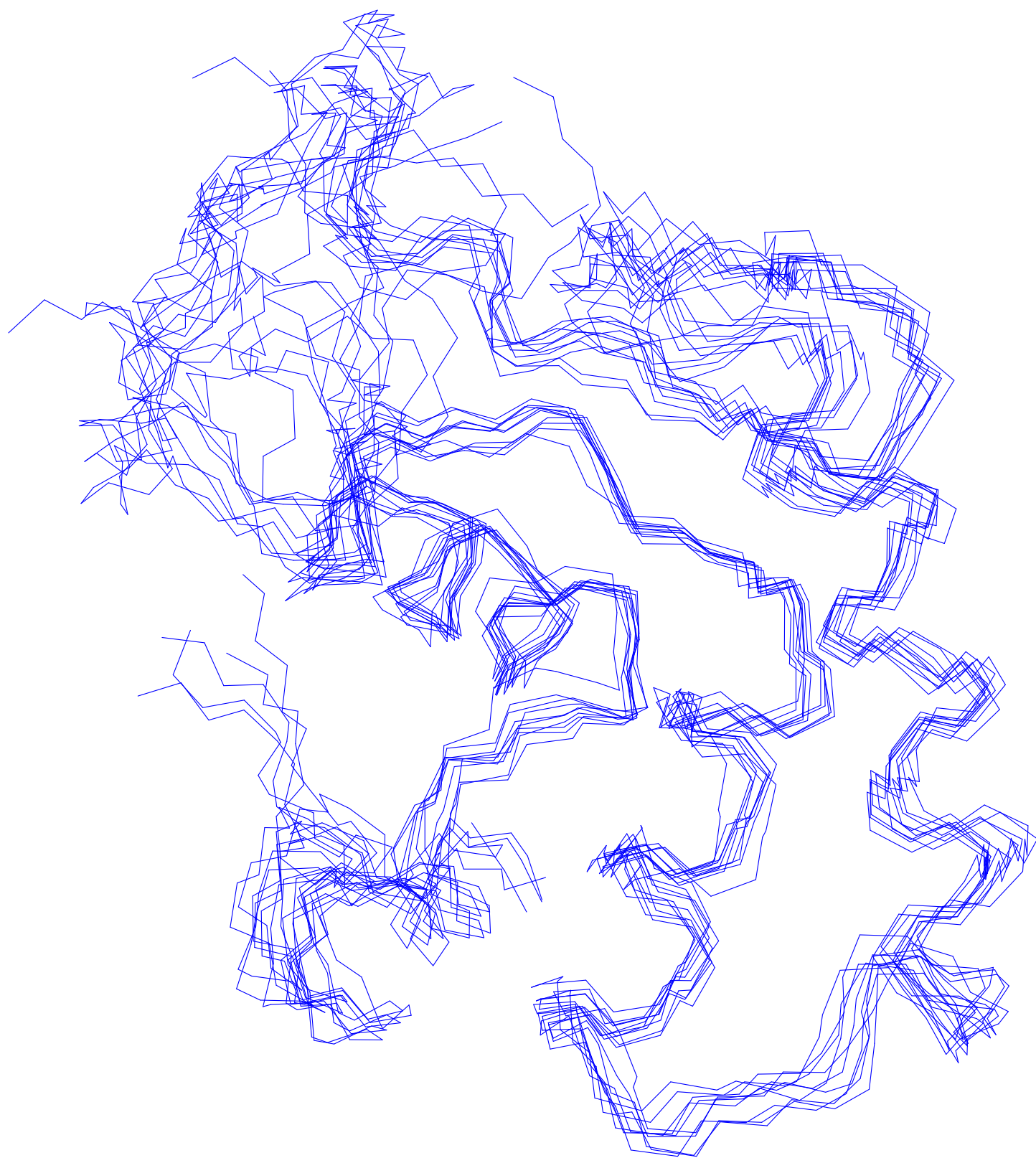


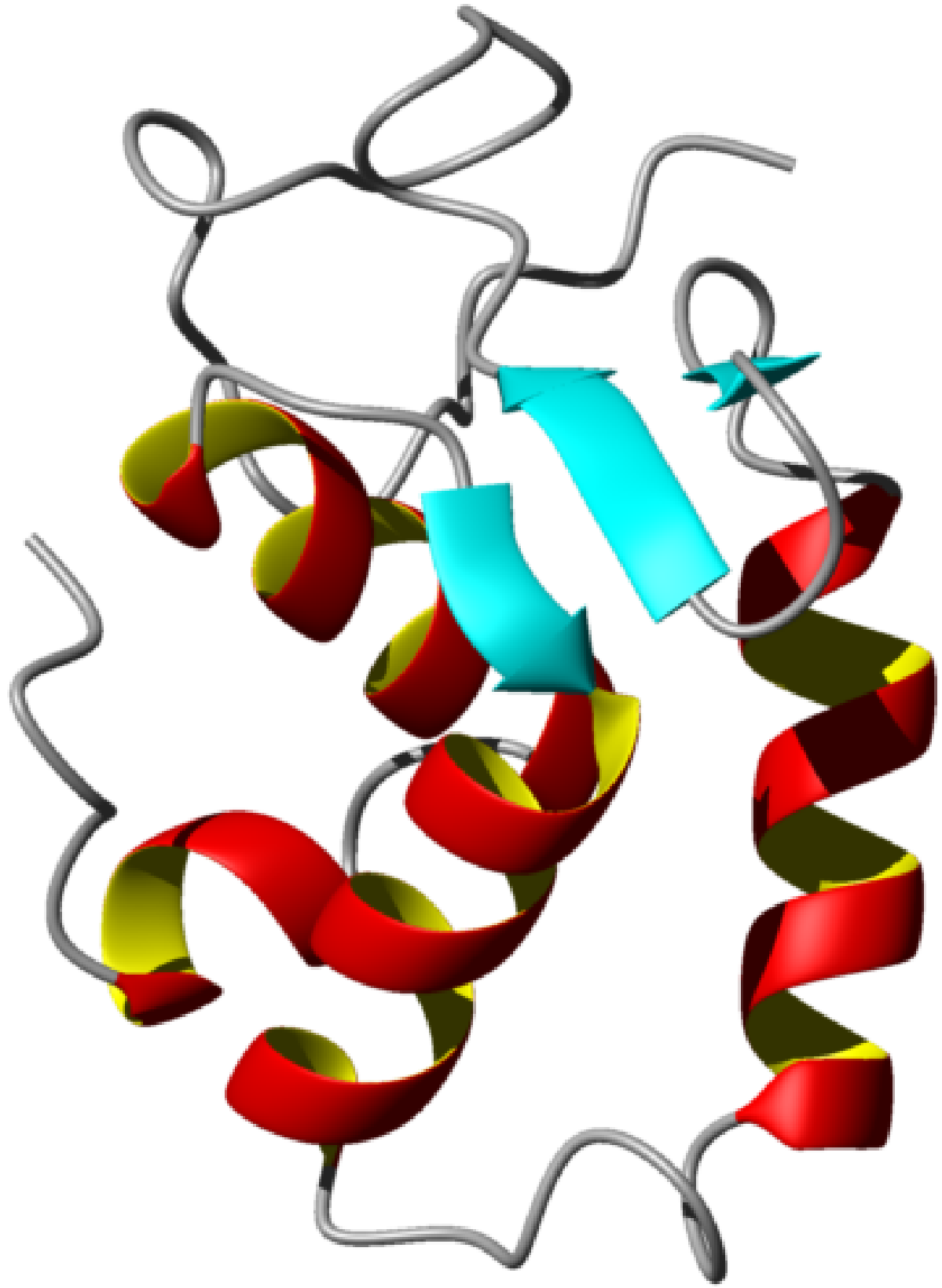
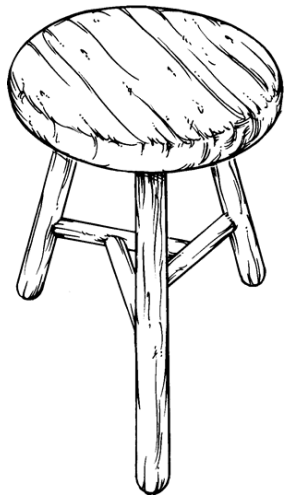






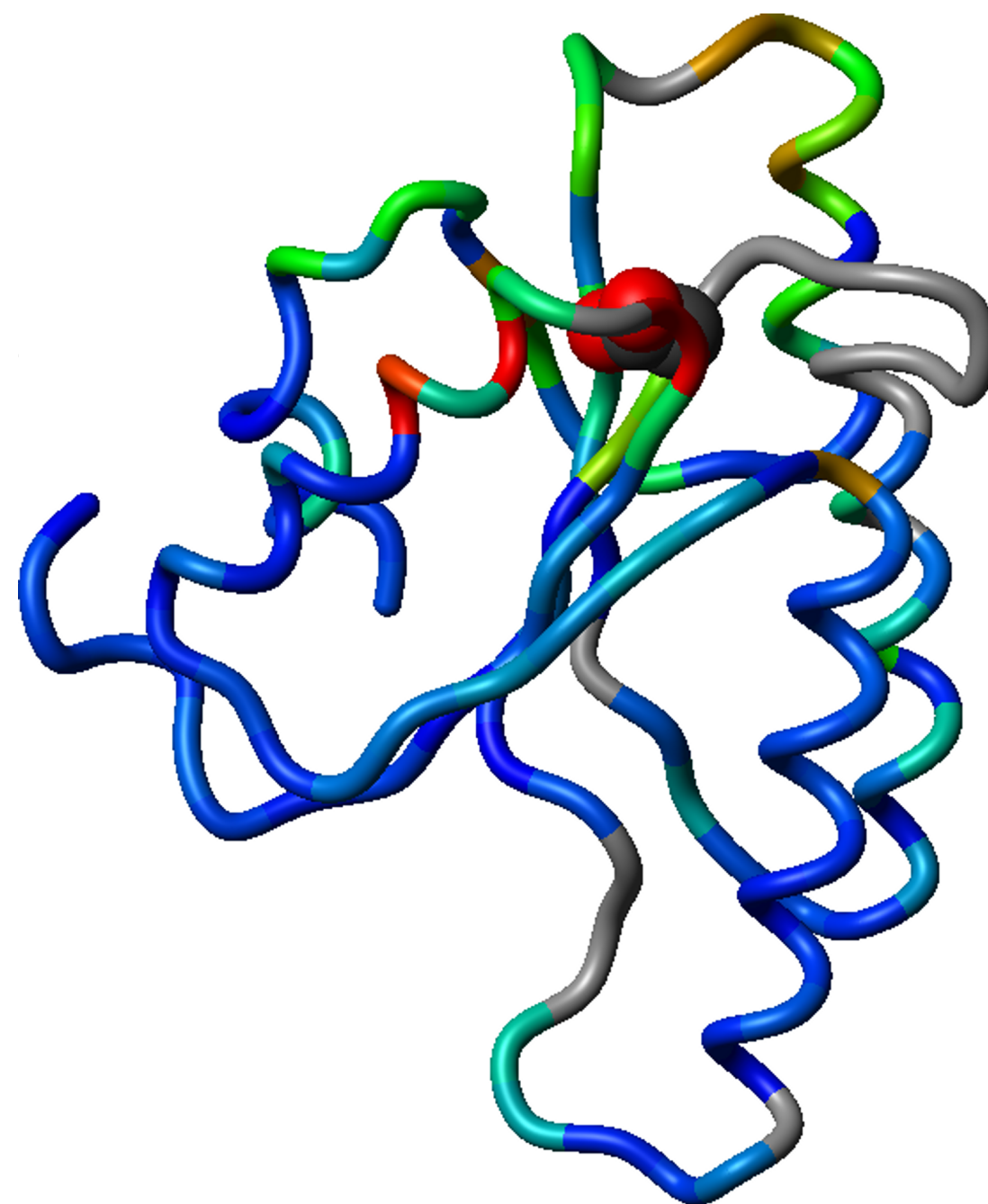
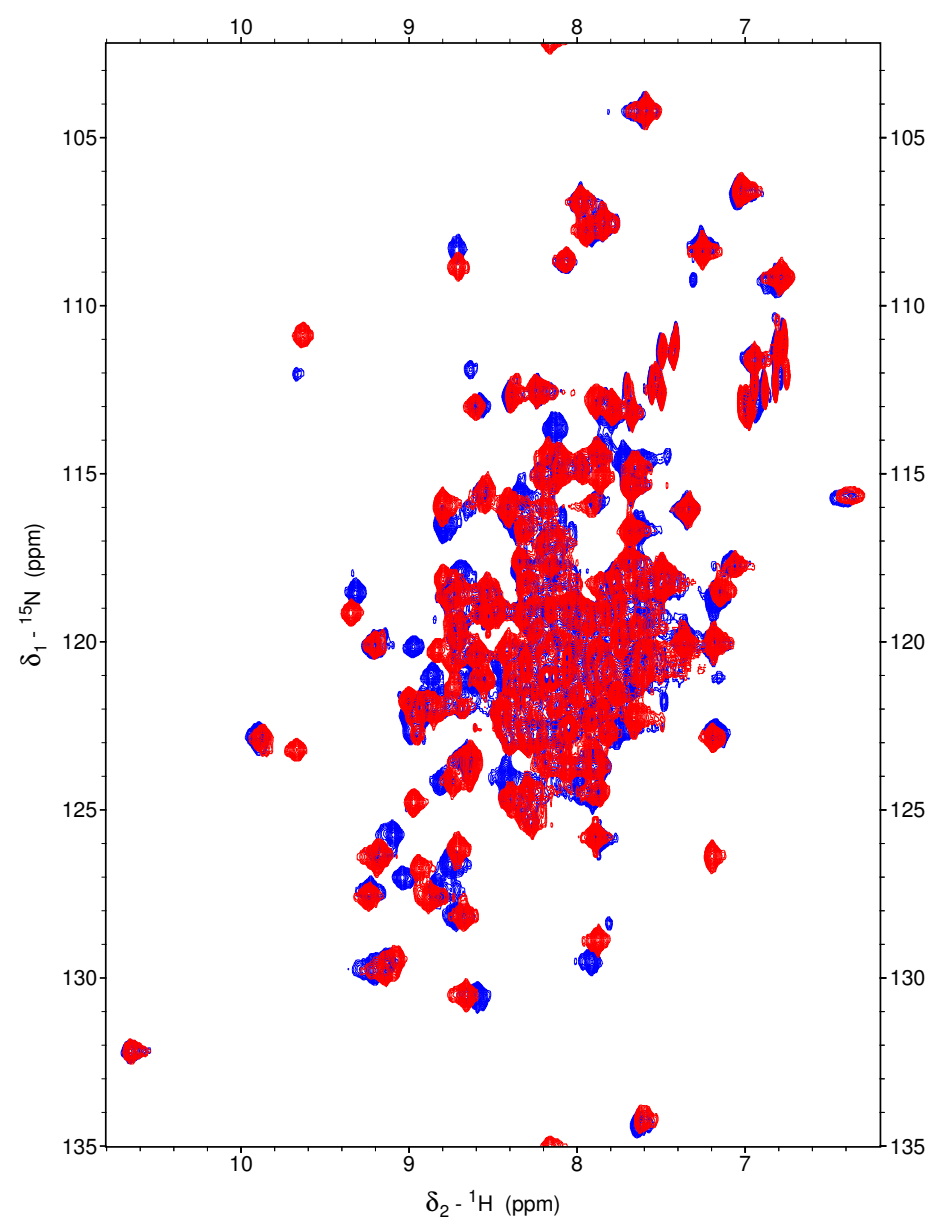






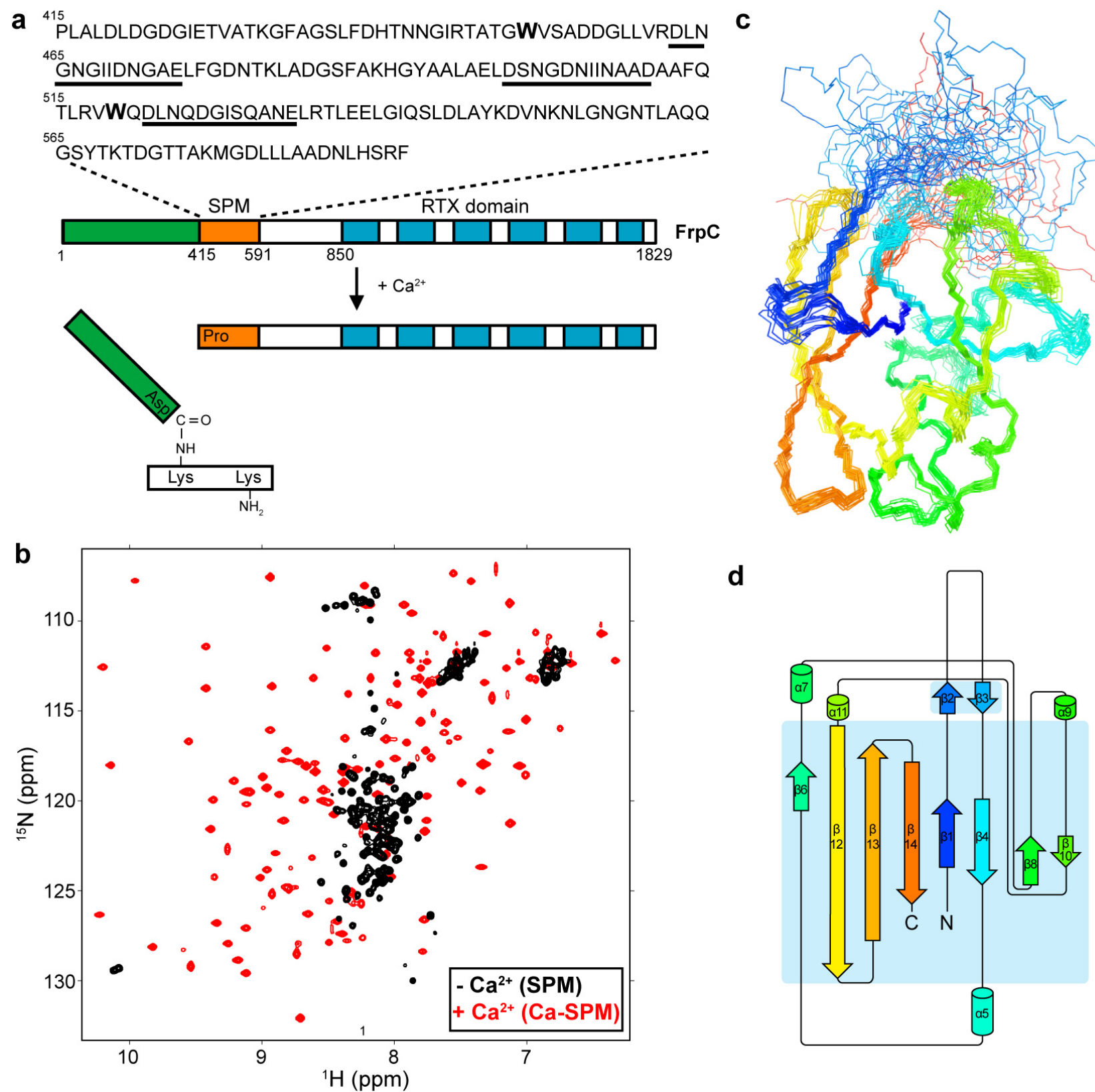
# **Příklady využití NMR**

# Rychlé určení vazebného místa



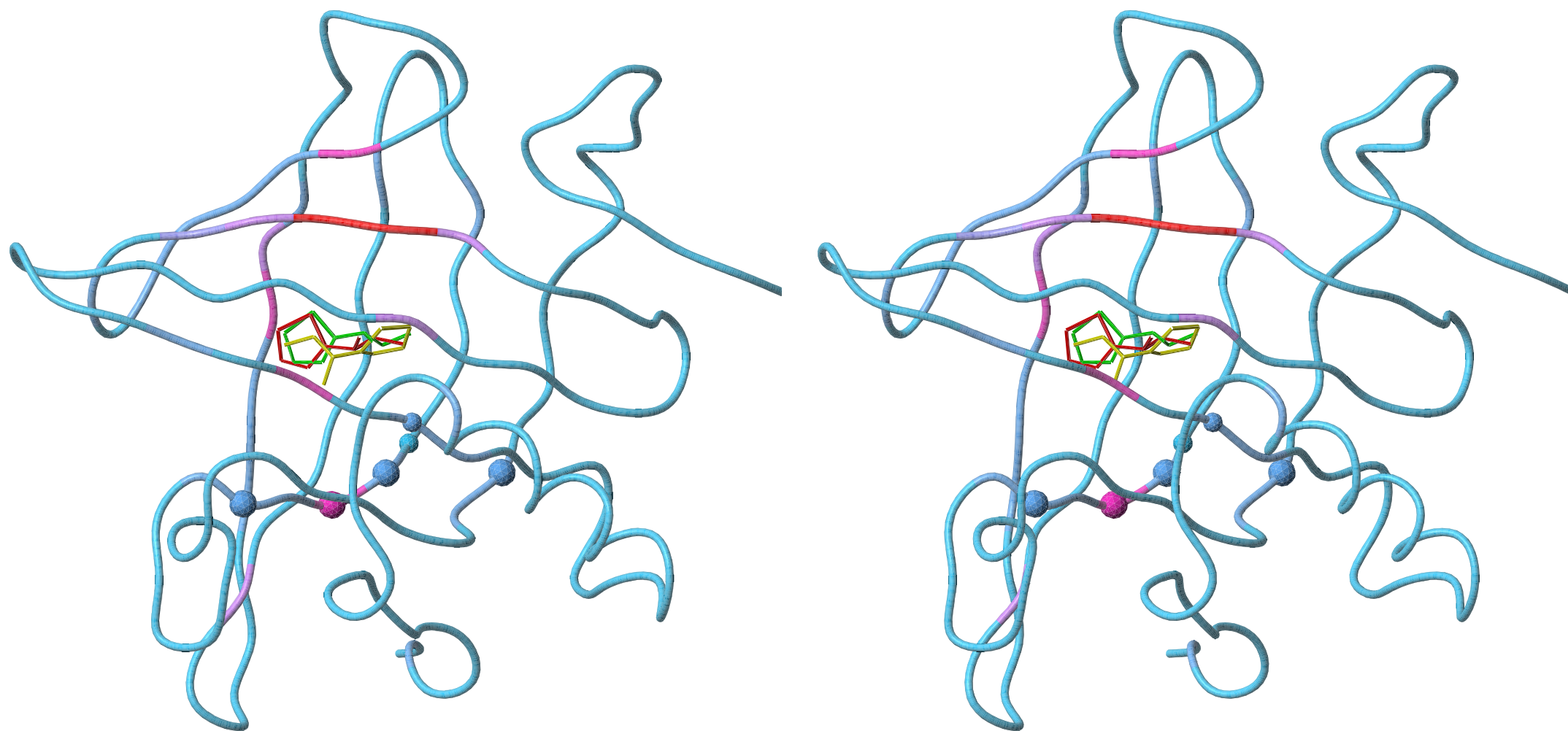
Pekárová et al., *Plant. J.* **67** (2011) 827–839.

# Určení struktury proteinu, který nekrystalizuje



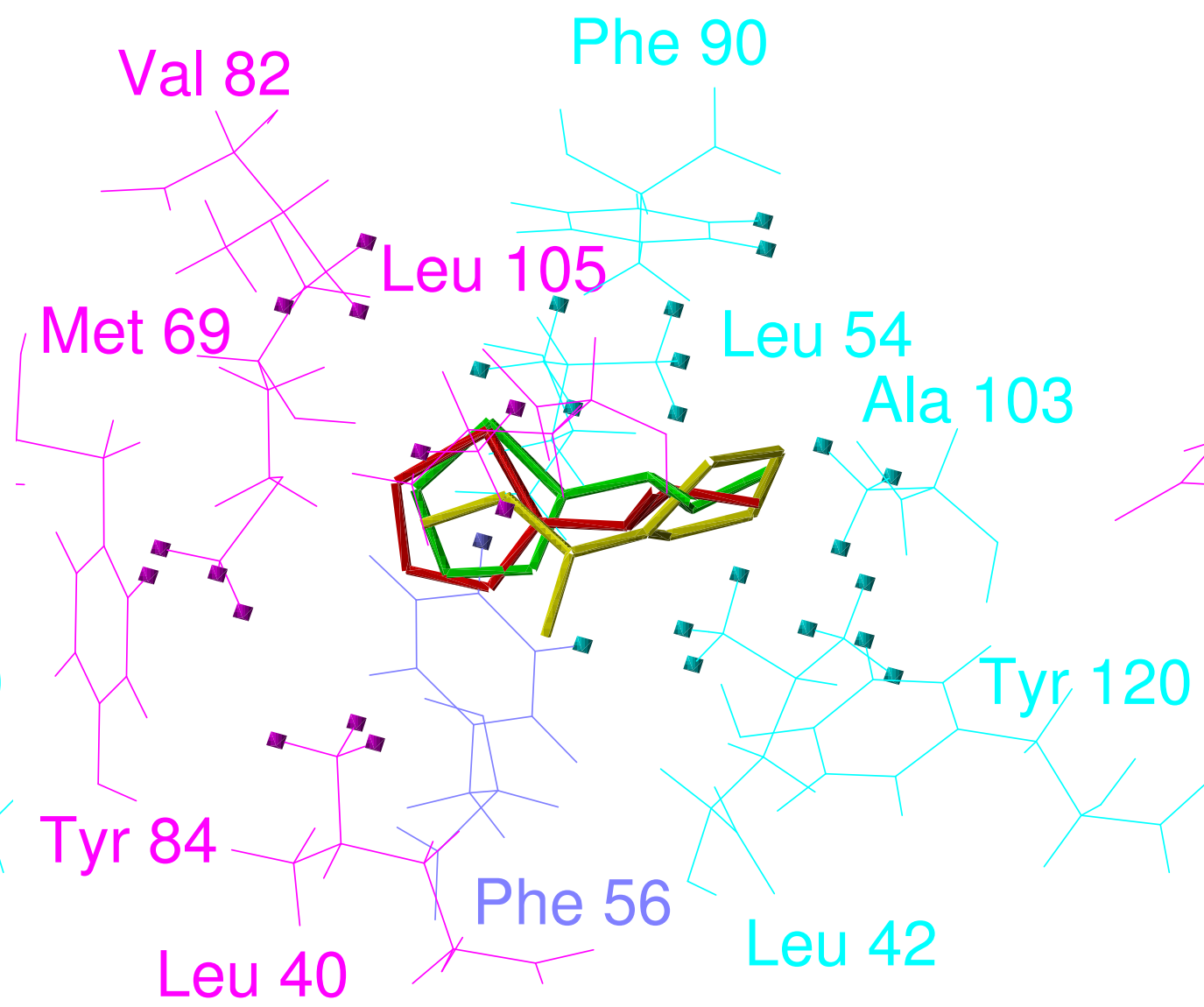
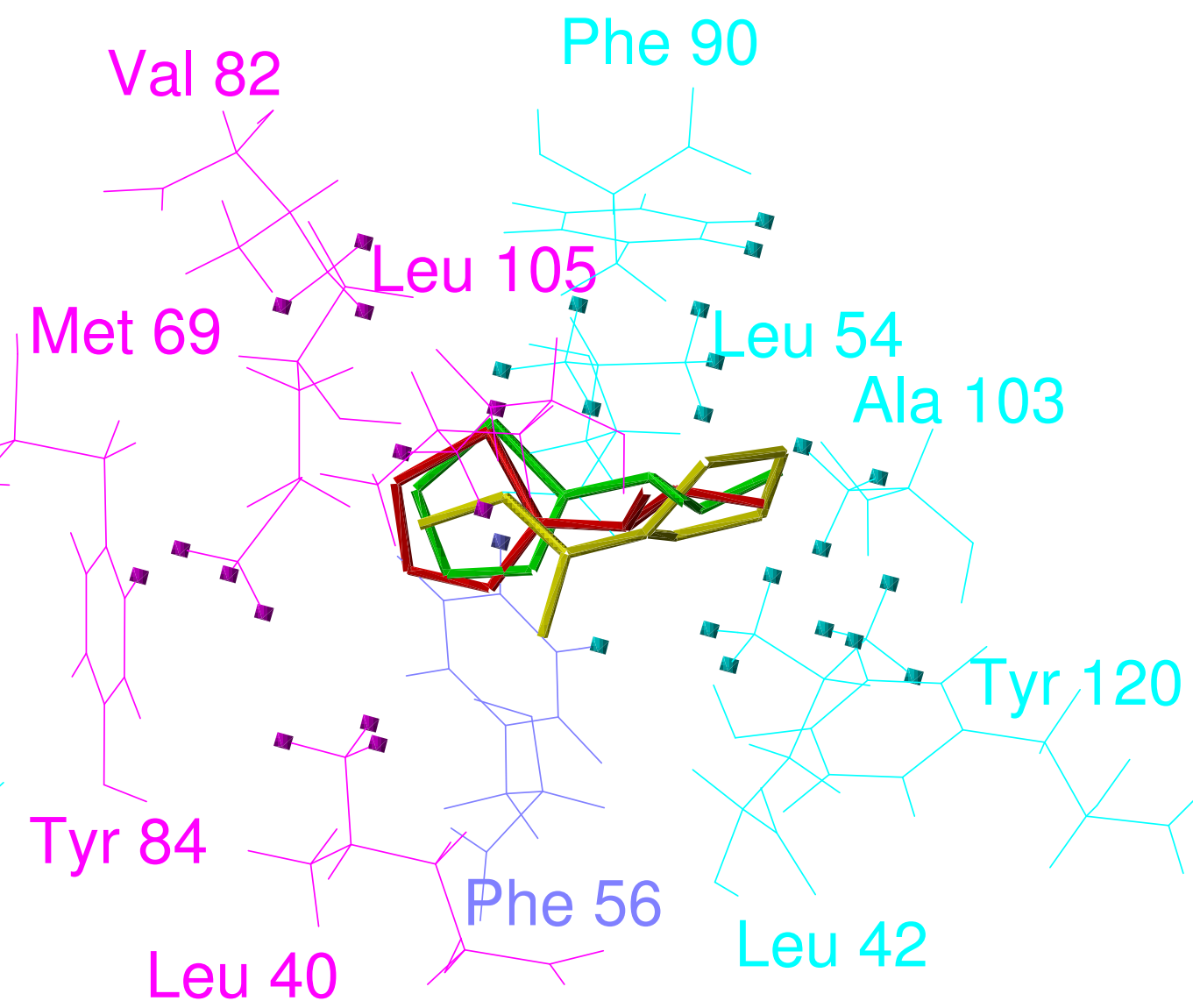


# Oprava chybné krystalové struktury

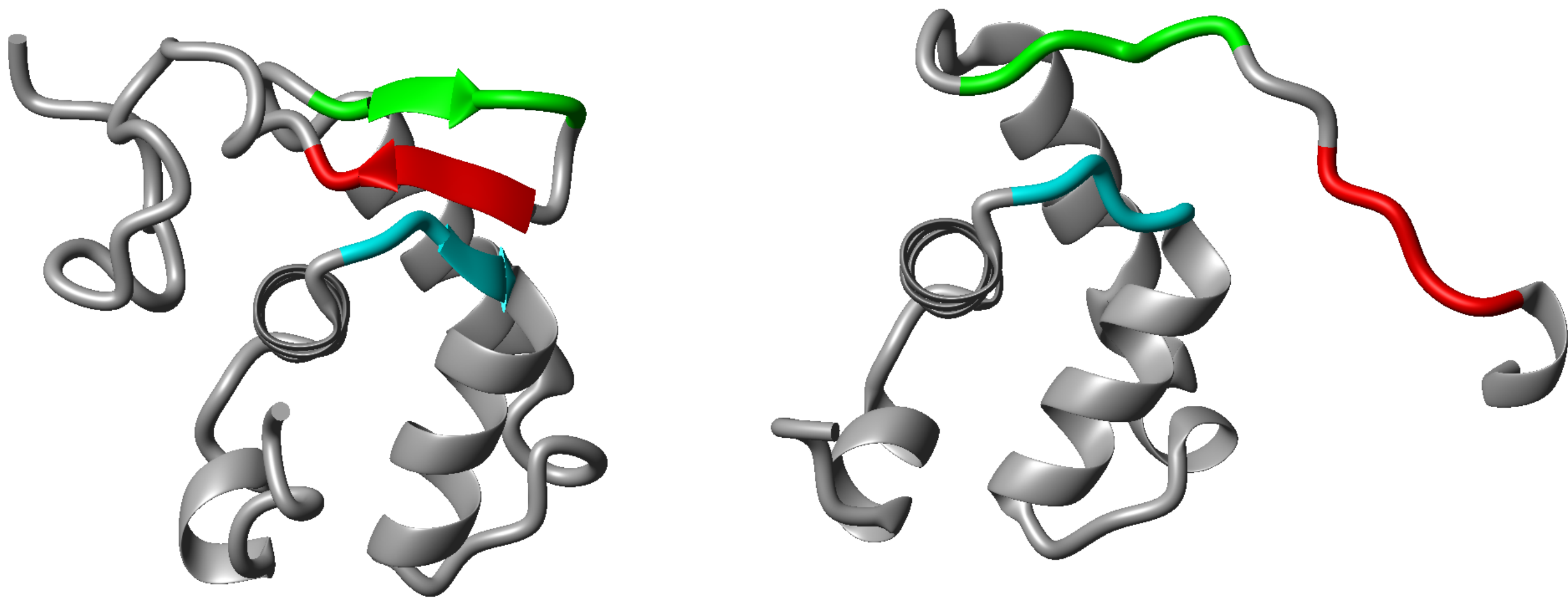


Žídek et al., *Biochemistry* **38** (1999) 9850–9861.



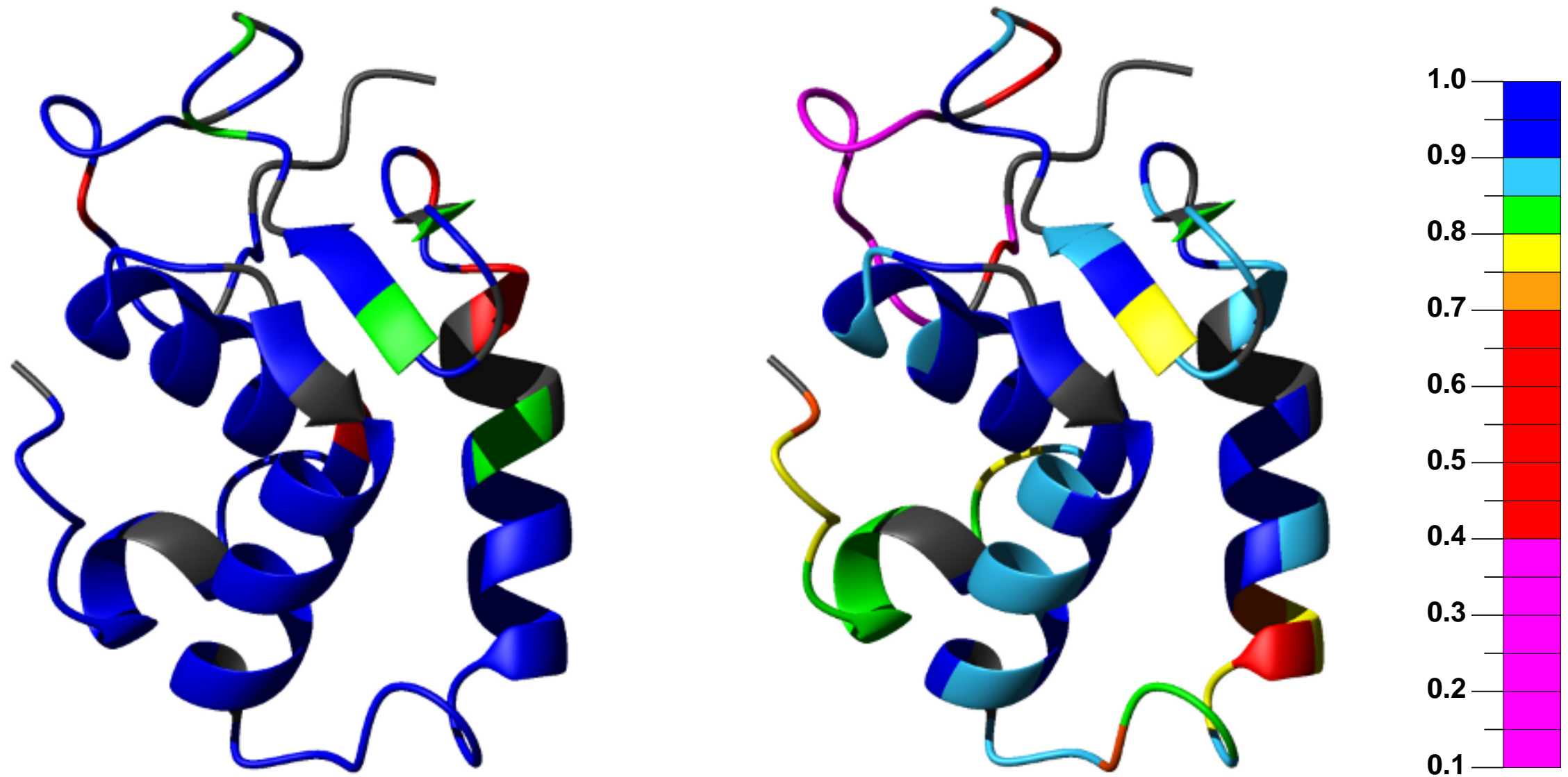


Určení struktury, která se liší v roztoku a krystalu



Demo et al., *J. Struct. Biol.* **187** (2014) 174–186.

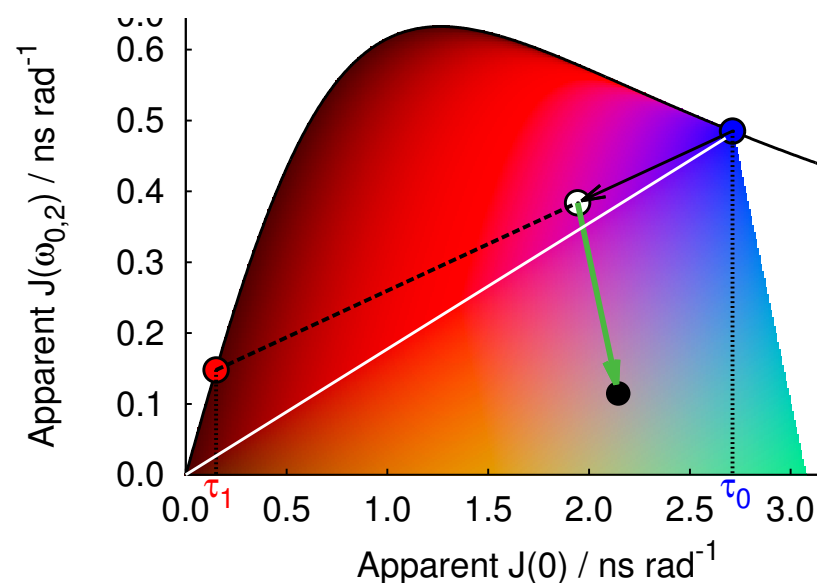
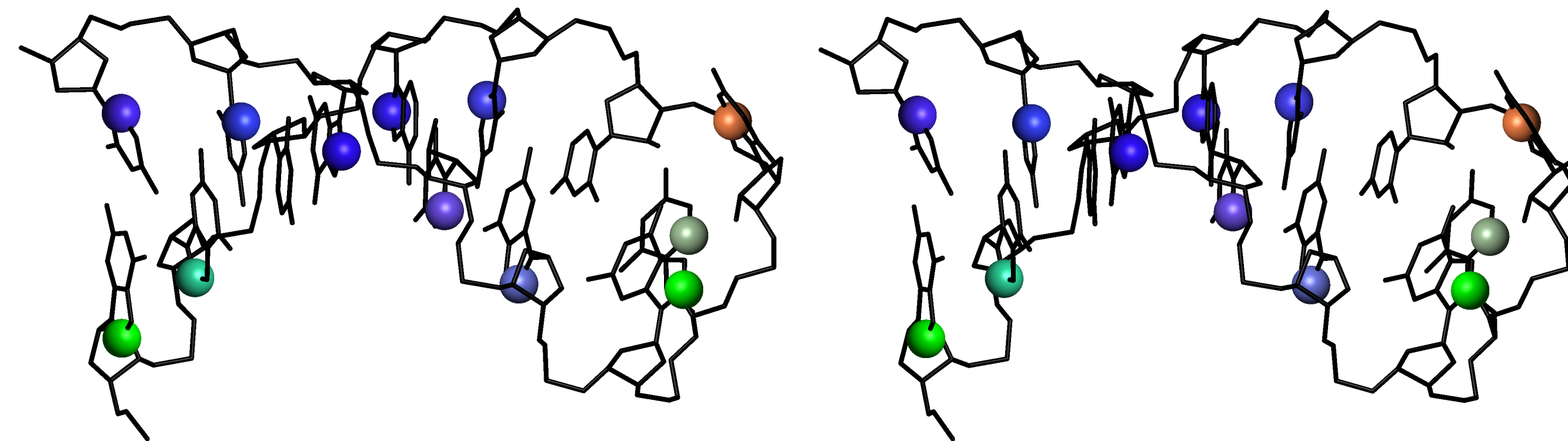
# Studium pomalých ( $\mu\text{s}$ – $\text{ms}$ ) a rychlých ( $\text{ps}$ – $\text{ns}$ ) pohybů proteinu



Papoušková et al., *ChemBioChem* **14** (2013) 1172–1179.

Kadeřávek et al., unpublished

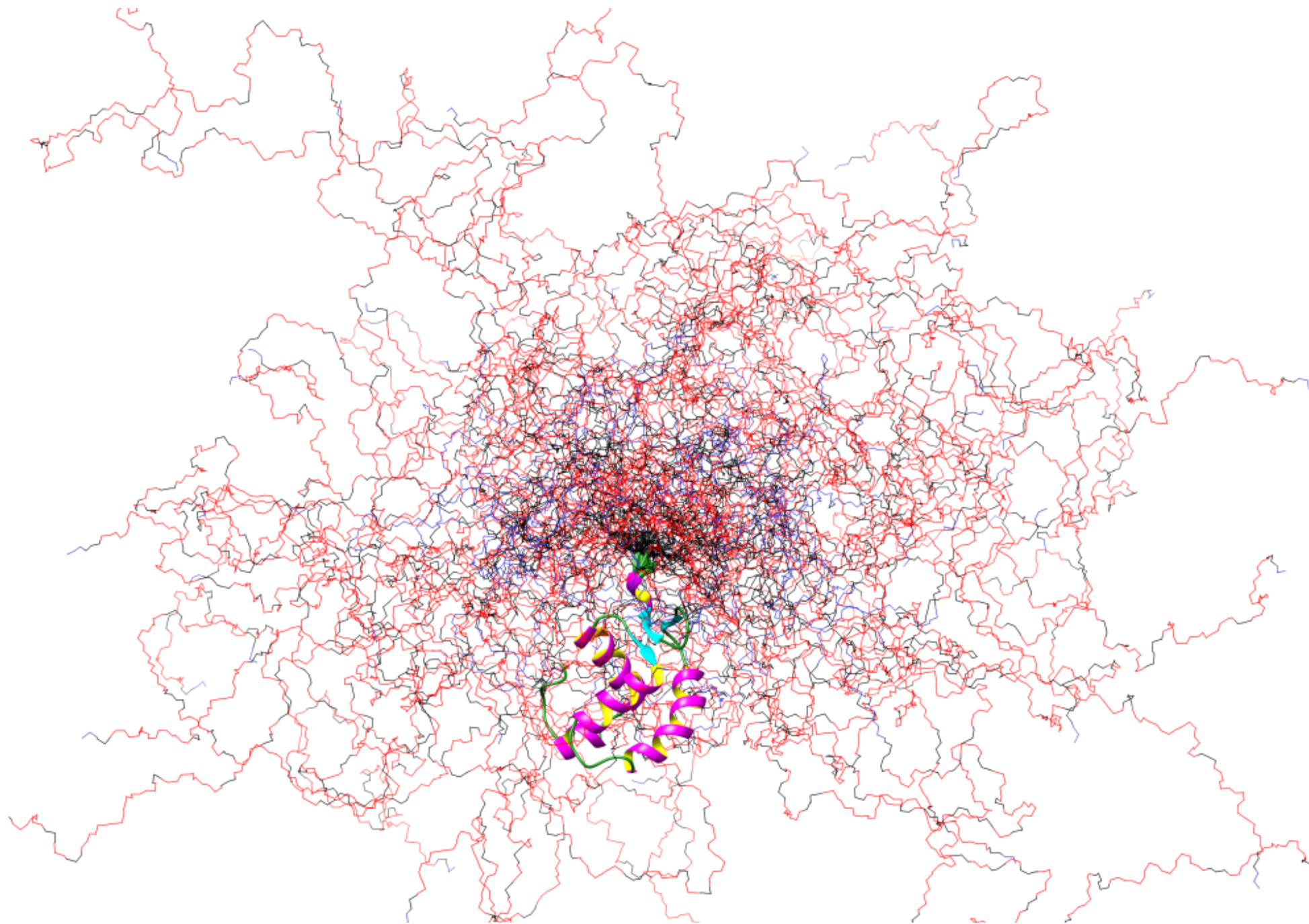
# Studium pomalých ( $\mu\text{s}$ – $\text{ms}$ ) a rychlých ( $\text{ps}$ – $\text{ns}$ ) pohybů DNA



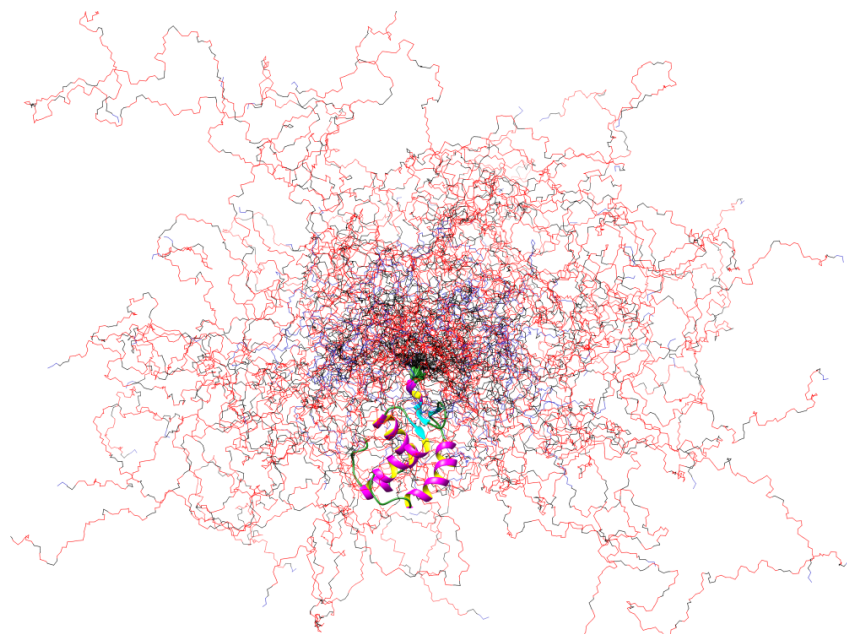
Kadeřávek et al., *J. Magn. Reson.* **266** (2016) 23–40.



# Studium částečně neuspořádaného proteinu



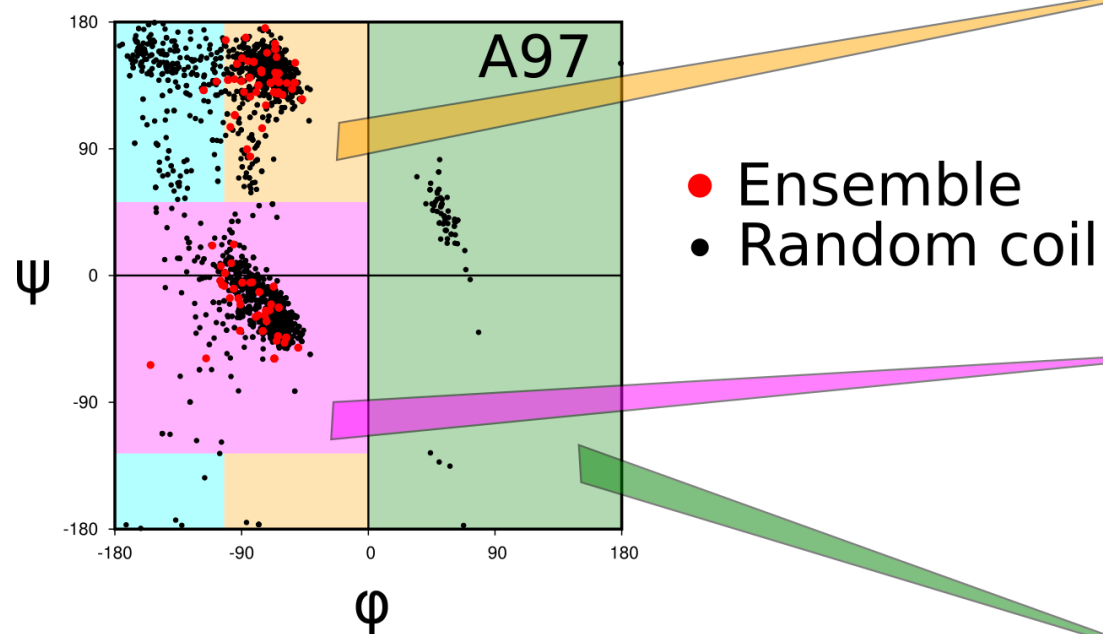
Kubáň et al., *J. Am. Chem. Soc.* **141** (2019) 16817–16828.



The final ensemble of 150 structures



Ramachandran plot for each residue



Each individual structure is meaningless as only local conformation contains information like CS or RDC.

Probability of secondary motives of the selected ensemble

