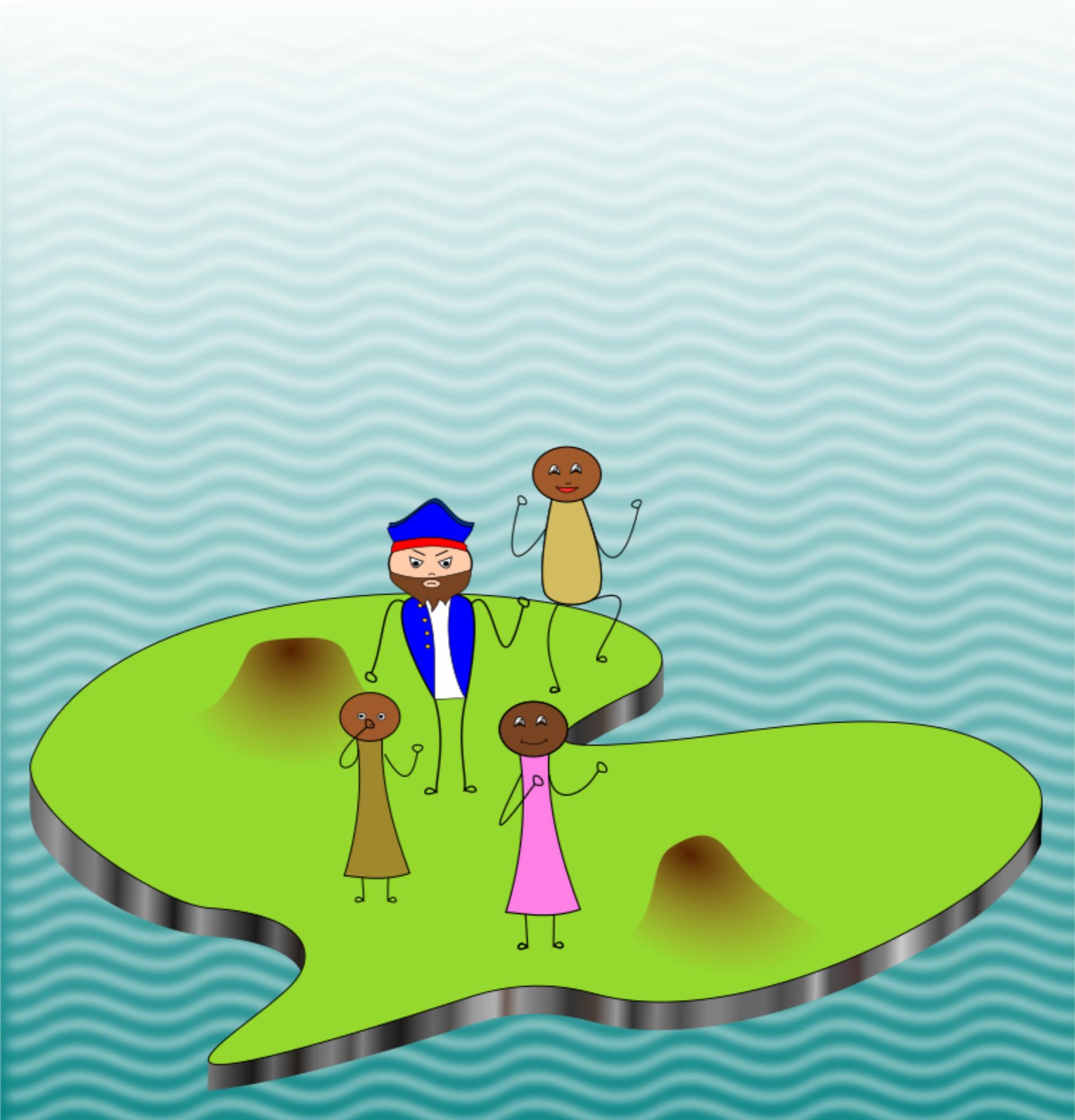
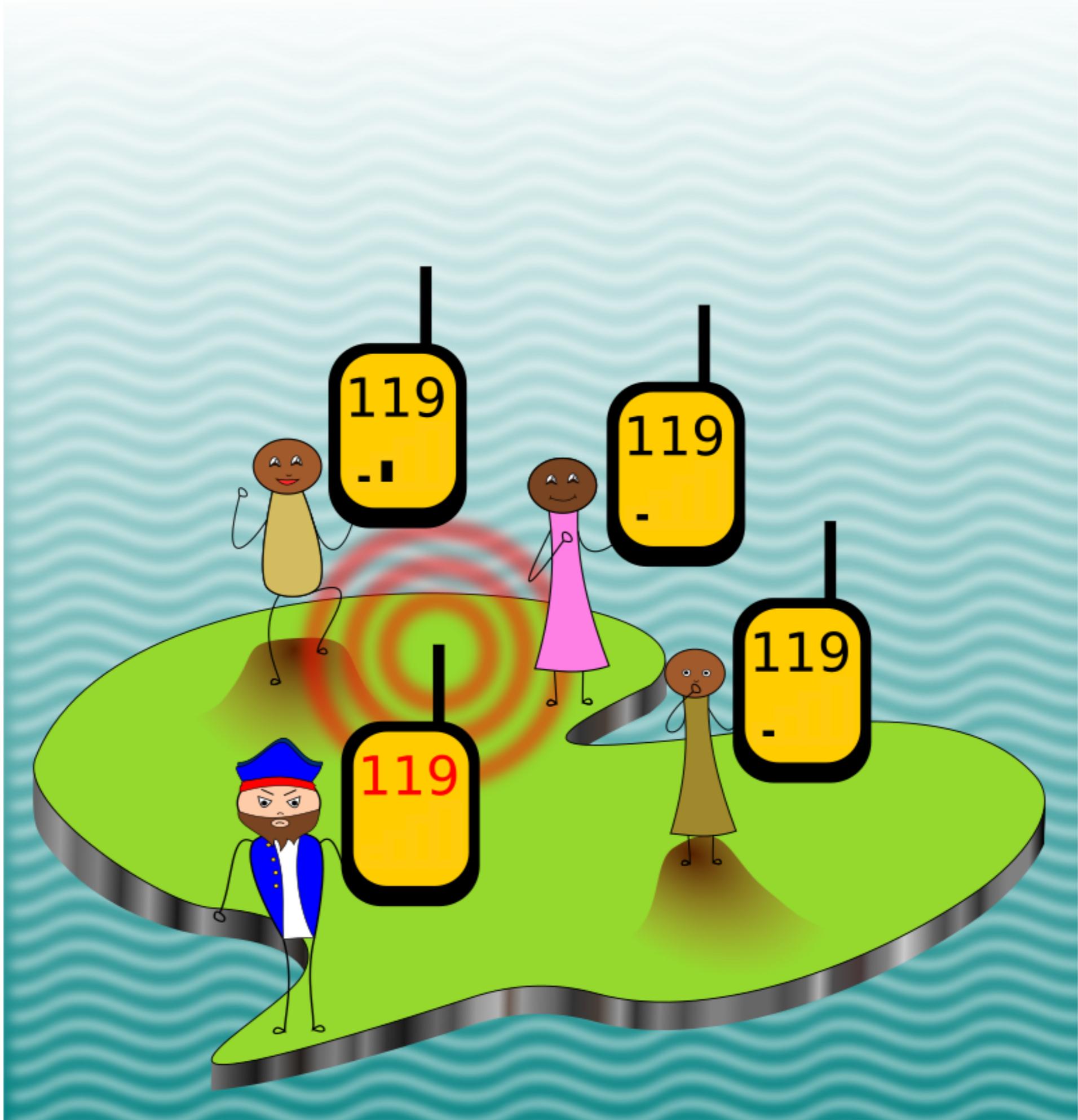
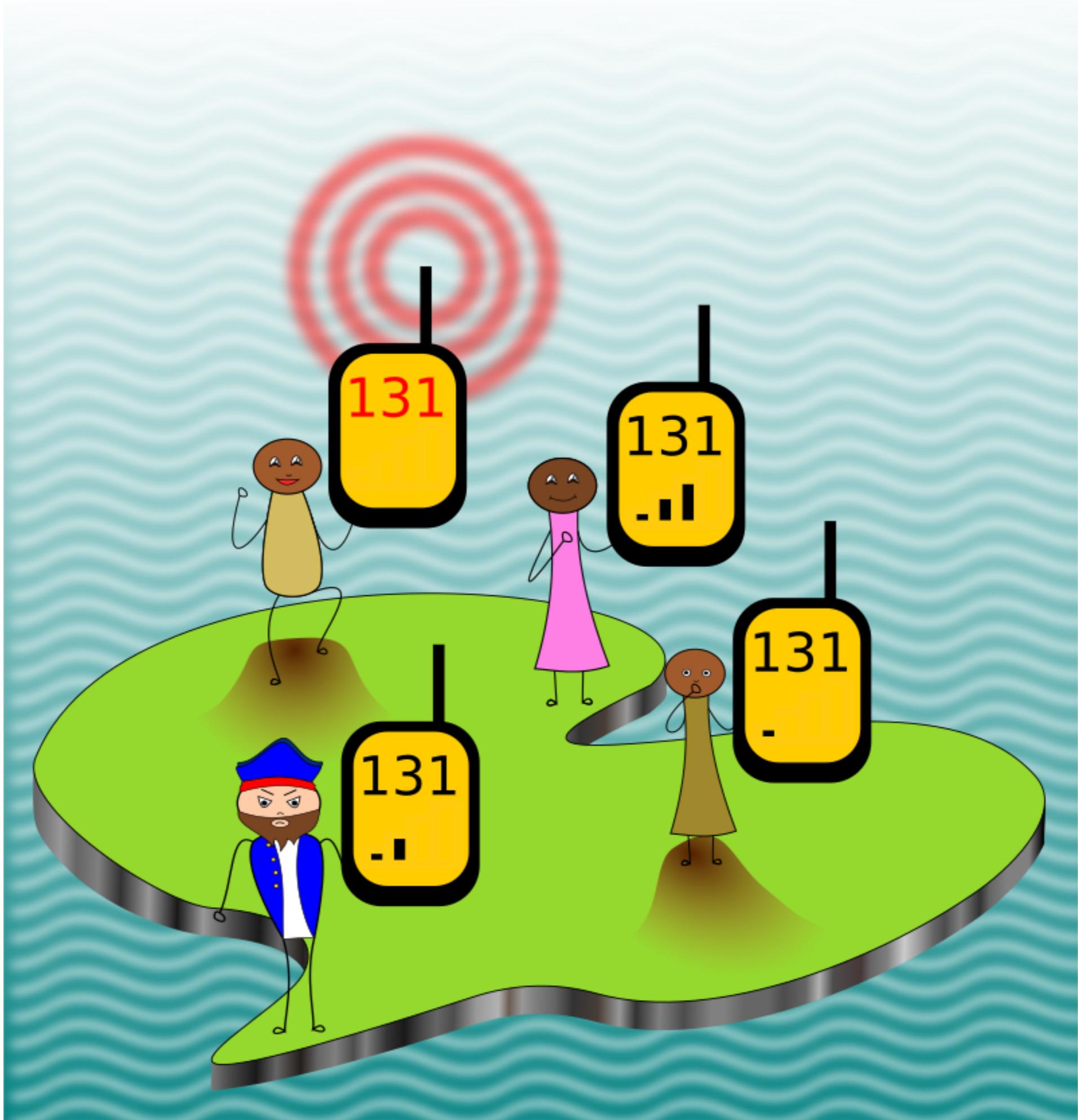
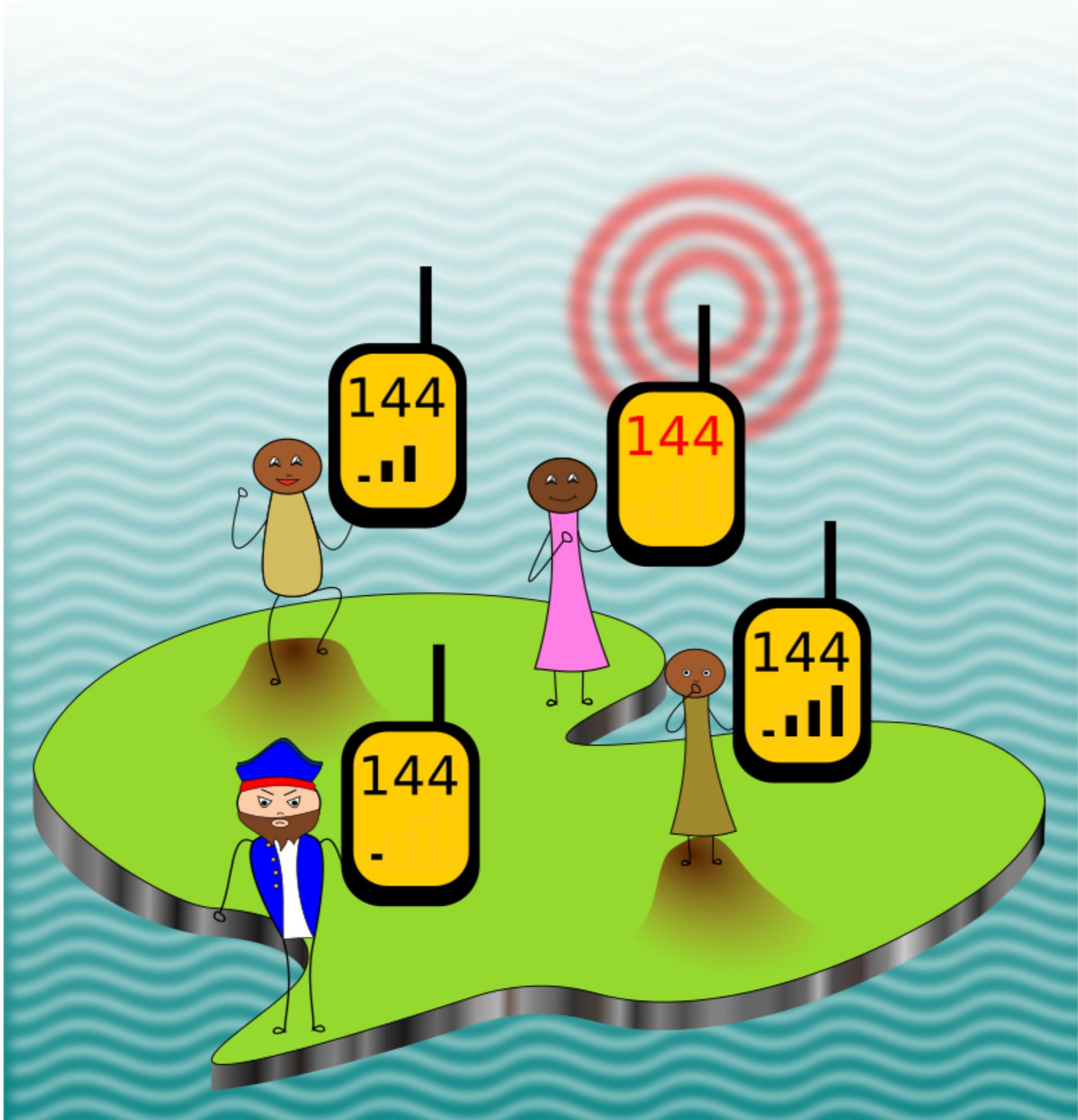


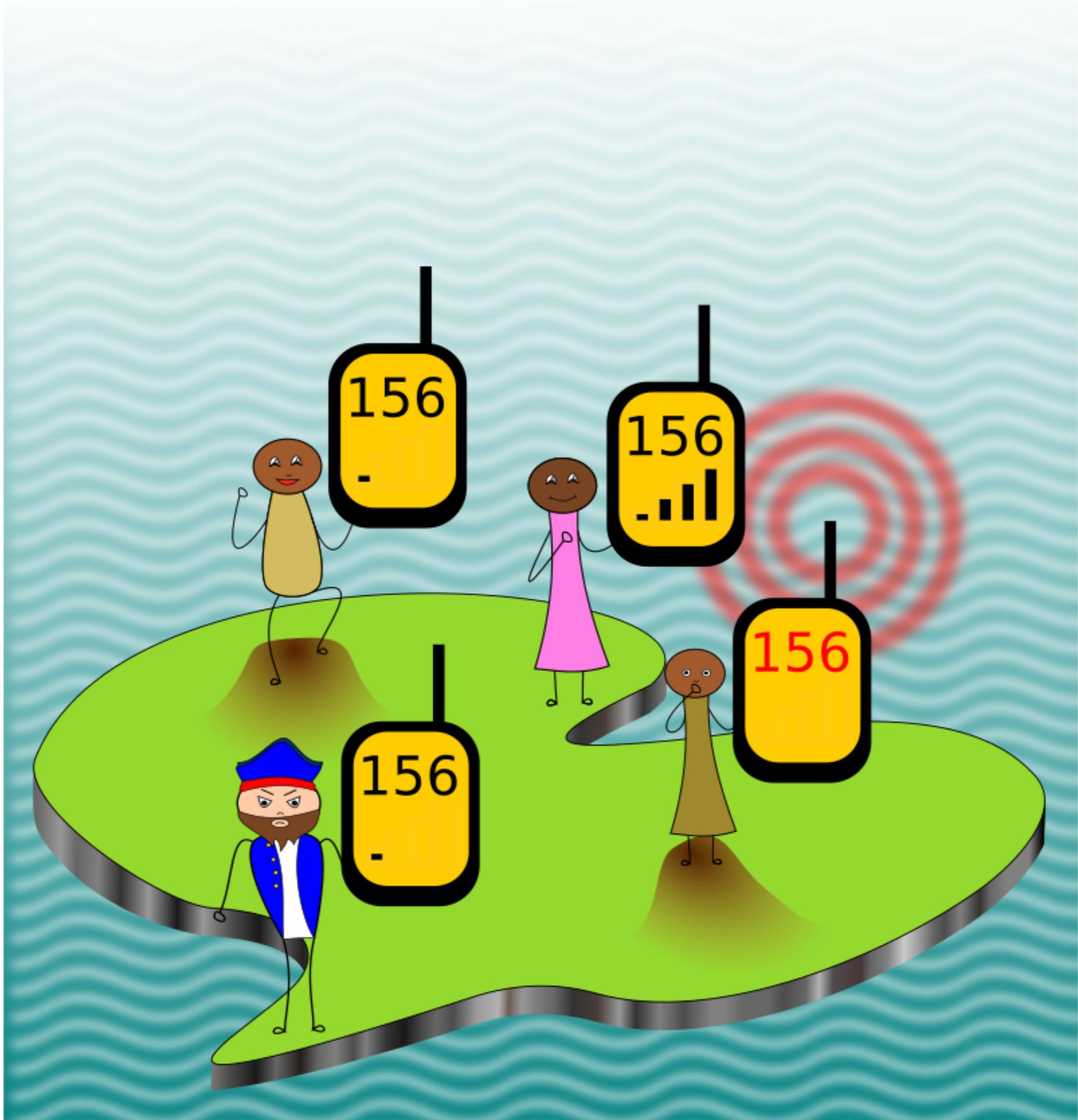
NUKLEÁRNÍ MAGNETICKÁ REZONANCE











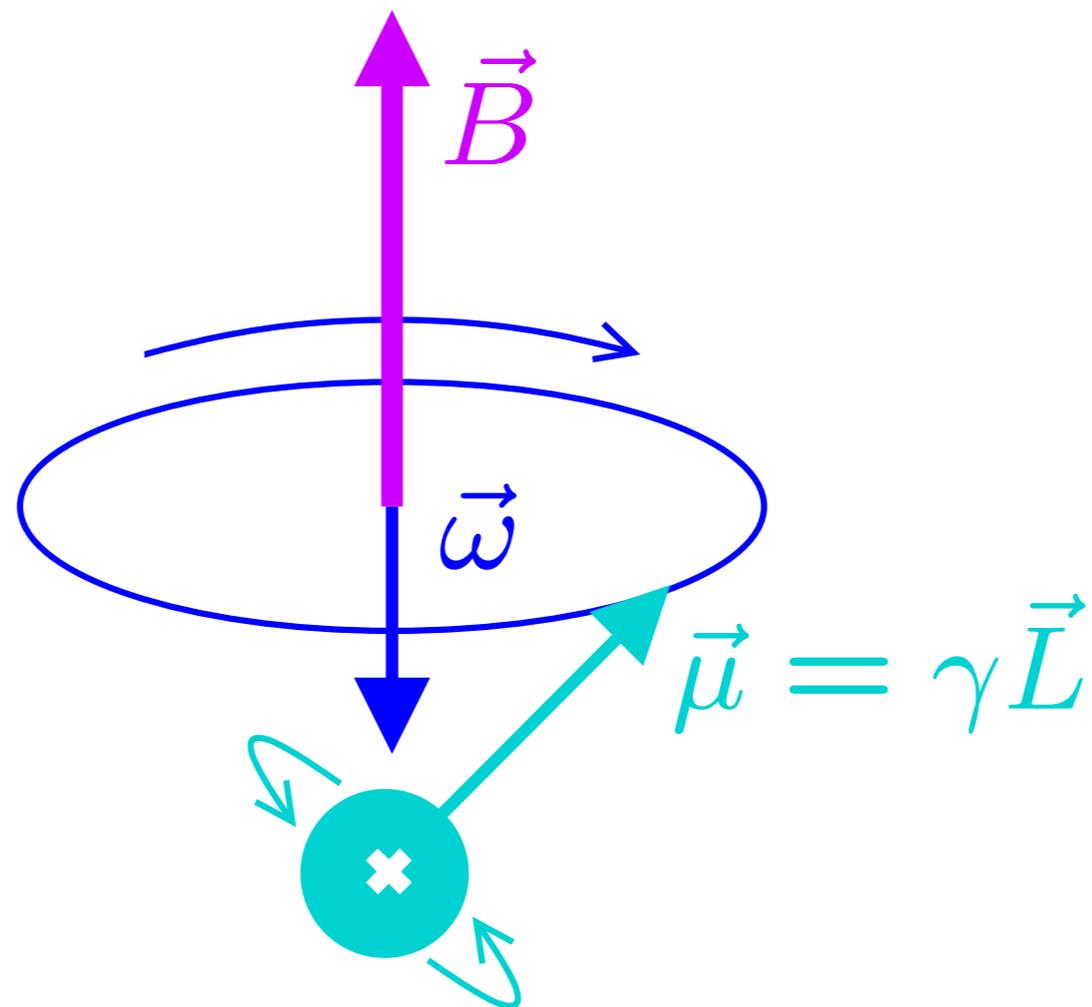
	S	$\frac{10^{-9}\gamma}{\text{rad s}^{-1}\text{T}^{-1}}$	% v přírodě
e^-	1/2	-182,000	100
^1H	1/2	0,277	99,98
^2H	1	0,042	0,02
^{13}C	1/2	0,067	1,1
^{14}N	1	0,019	99,6
^{15}N	1/2	-0,027	0,4
^{17}O	5/2	-0,036	0,04
^{19}F	1/2	0,252	100
^{31}P	1/2	0,108	100
^{129}Xe	1/2	-0,075	24,4

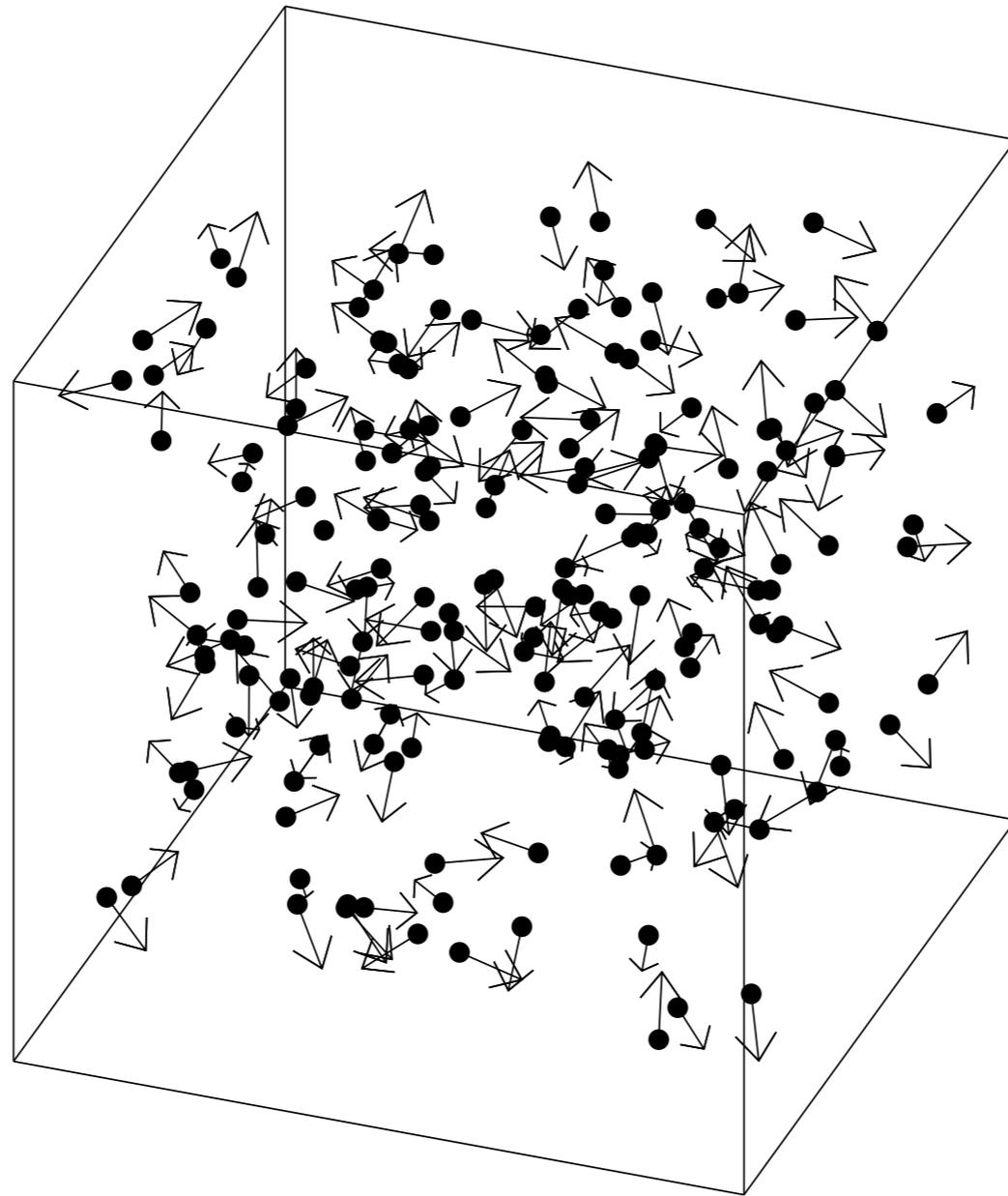
Počet stacionárních stavů = $2S + 1$

kvadrupolární jádra (příliš rychle se vrací do rovnováhy)

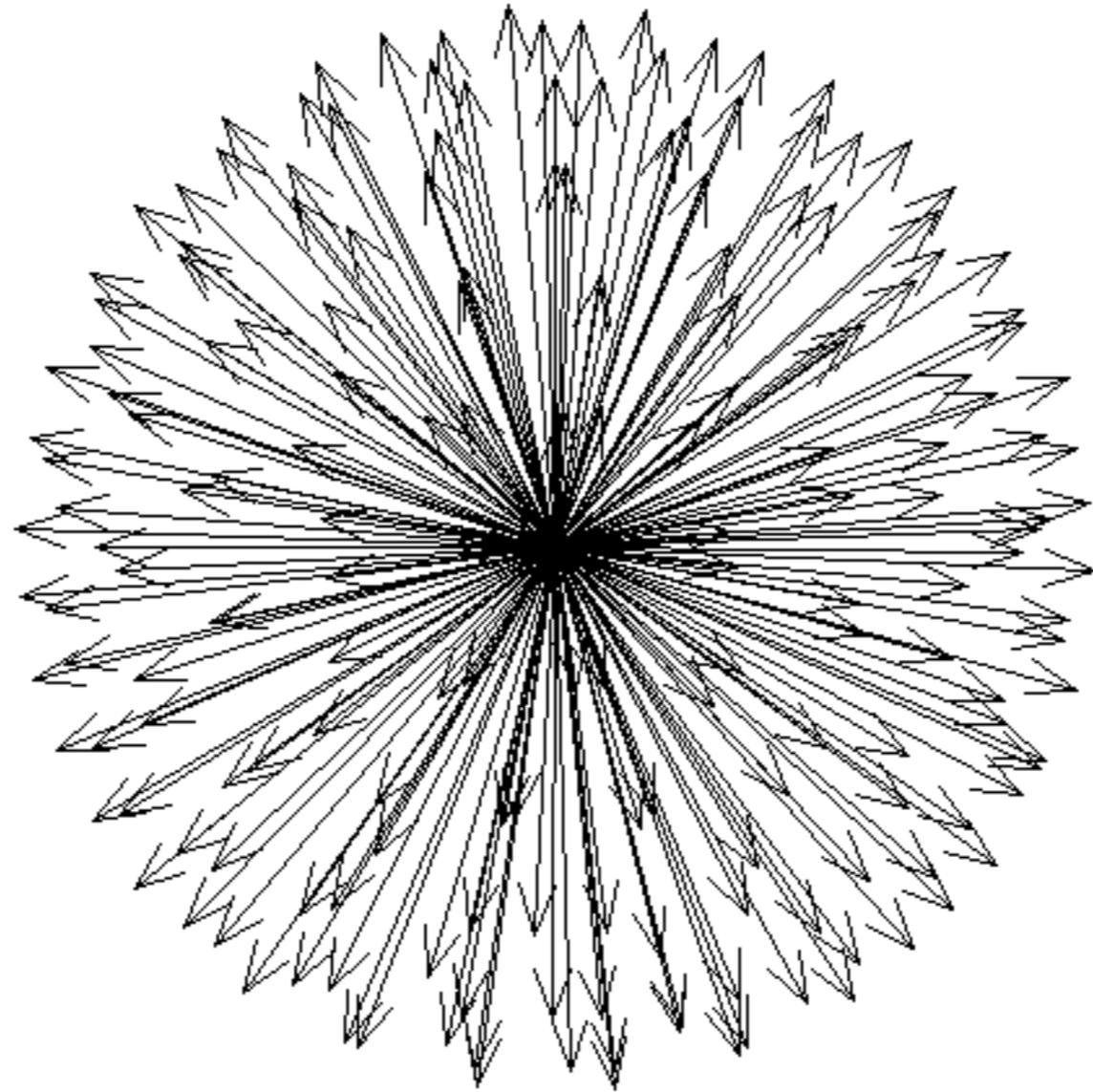
vzácné izotopy (vyžadují obohacení proteinů během exprese)

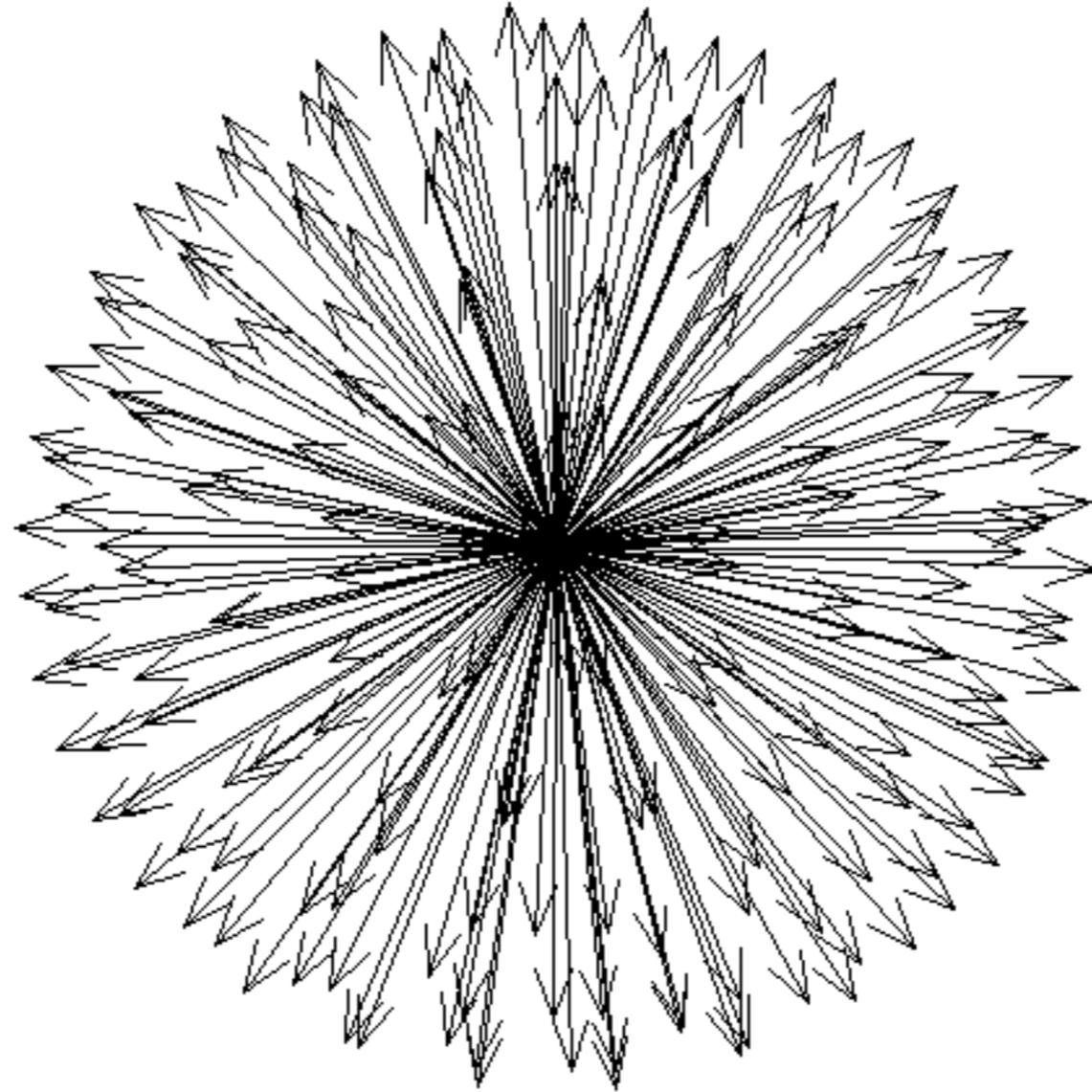
Úhlová rychlost precese $\vec{\omega} = -\gamma \vec{B}$



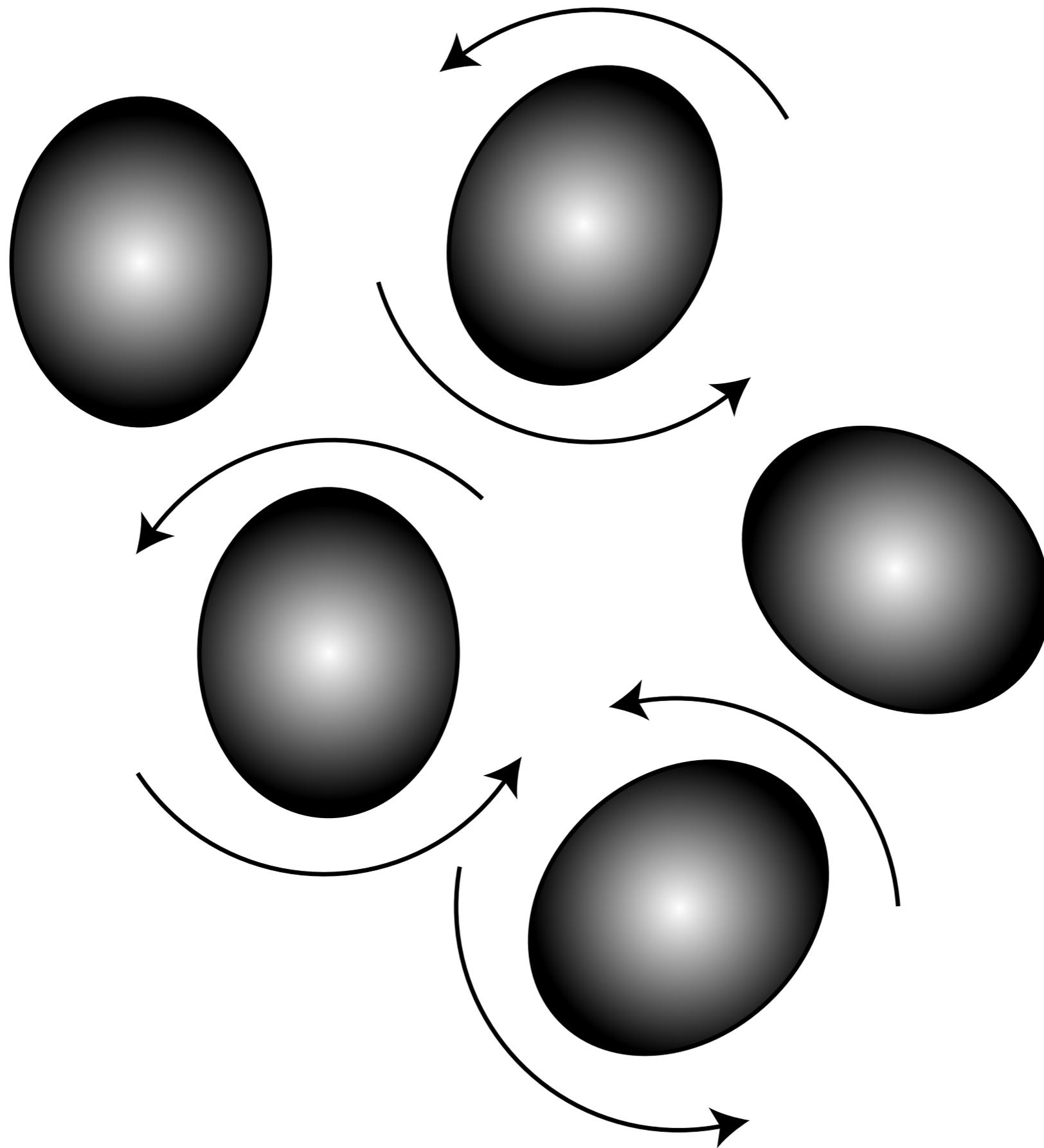


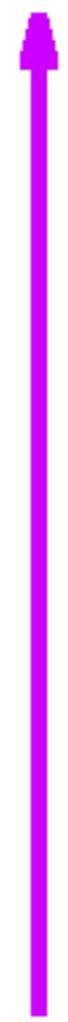
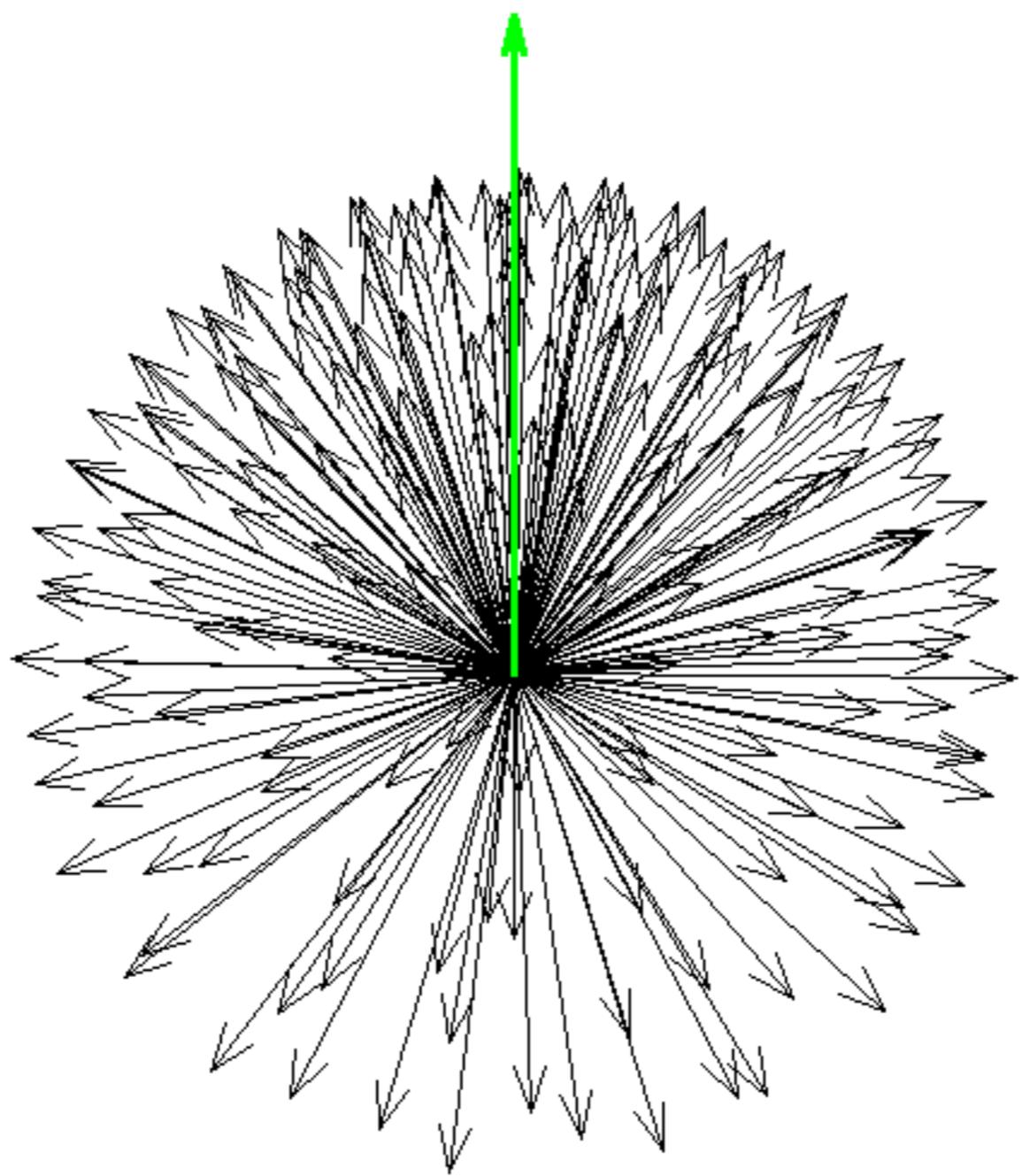
$$\vec{M} = (\vec{\mu}_1 + \vec{\mu}_2 + \vec{\mu}_3 + \vec{\mu}_4 + \vec{\mu}_5 + \vec{\mu}_6 + \dots) / V \quad \text{Magnetizace}$$



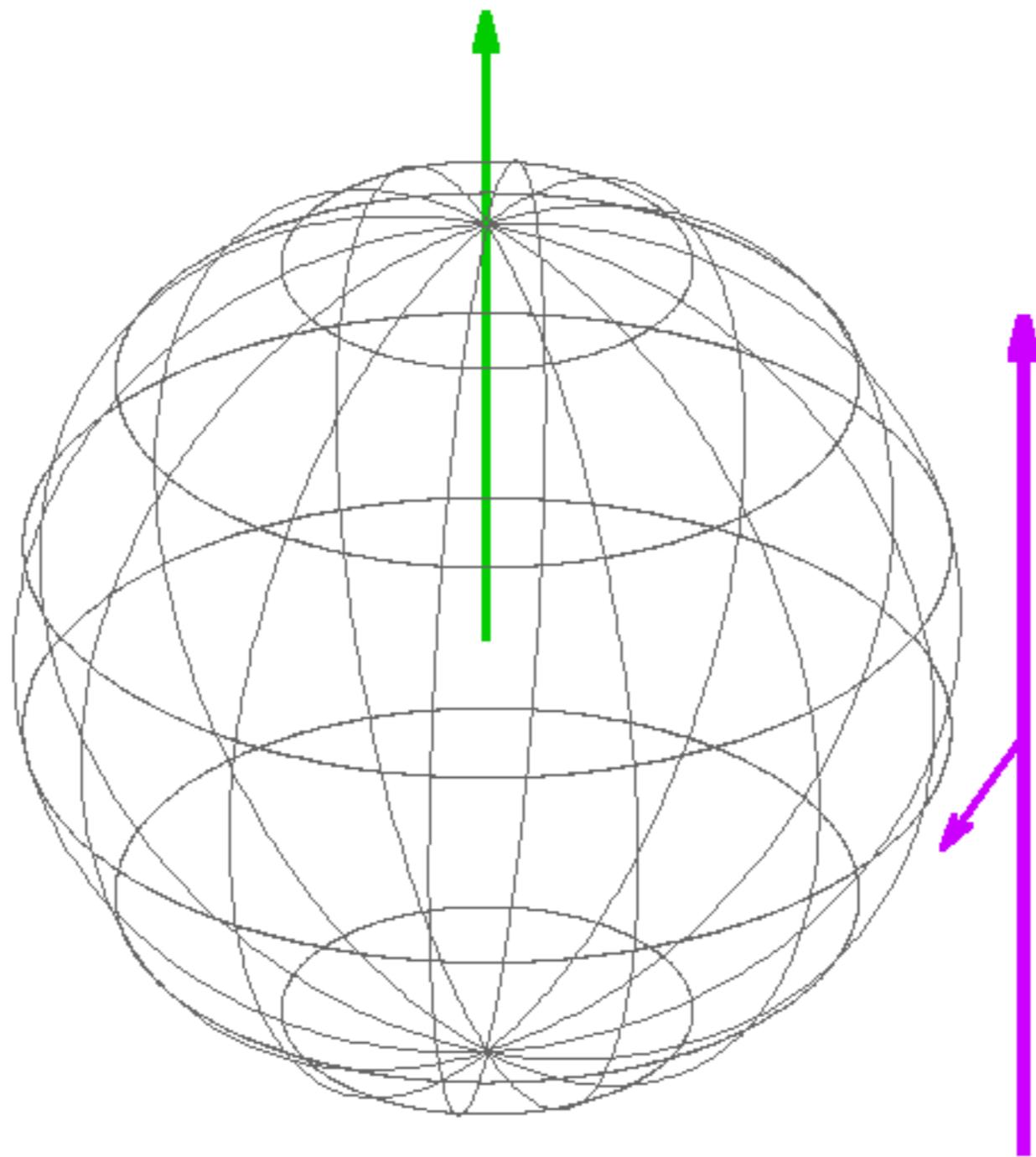


Magnetické momenty v magnetickém poli

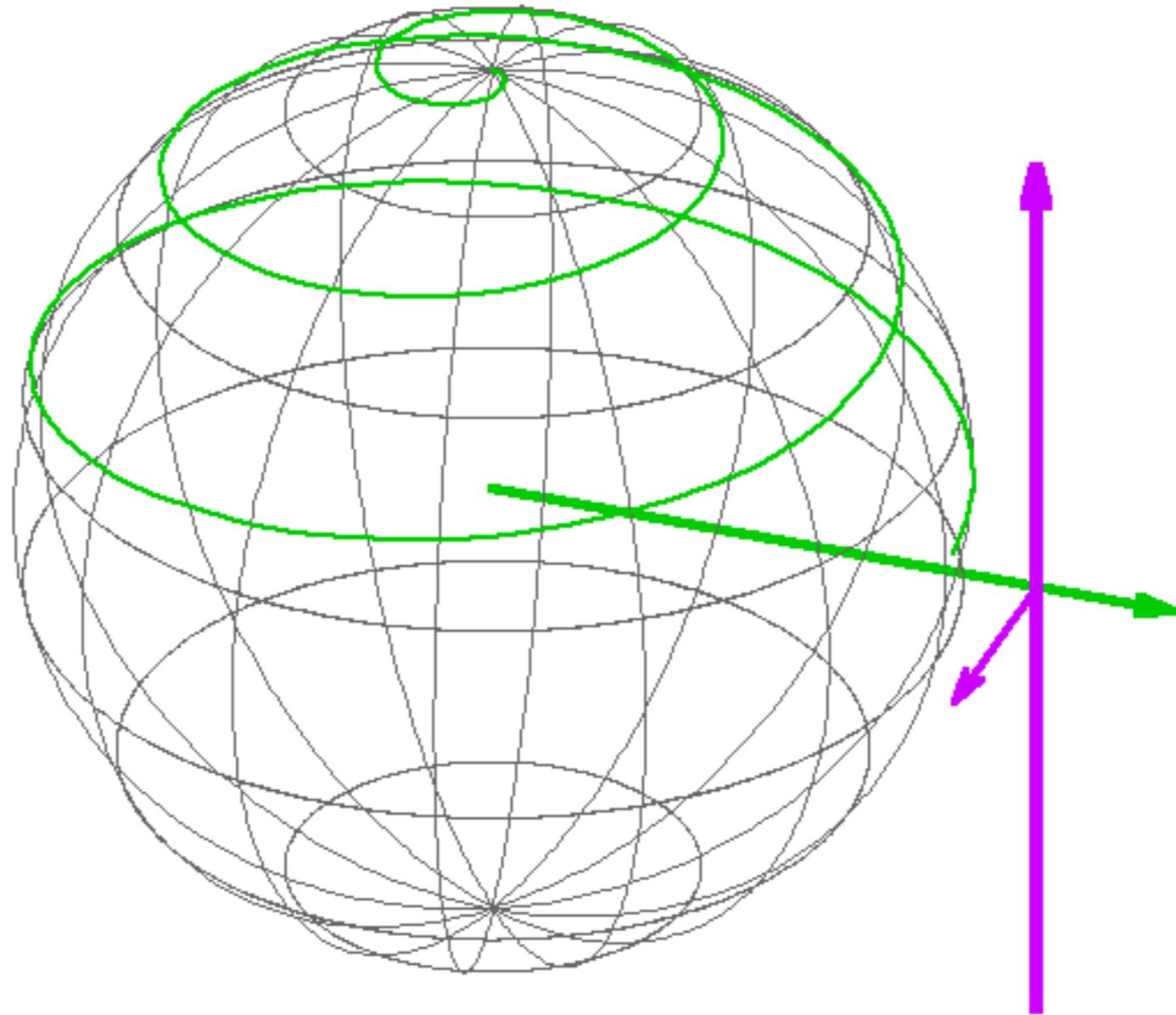


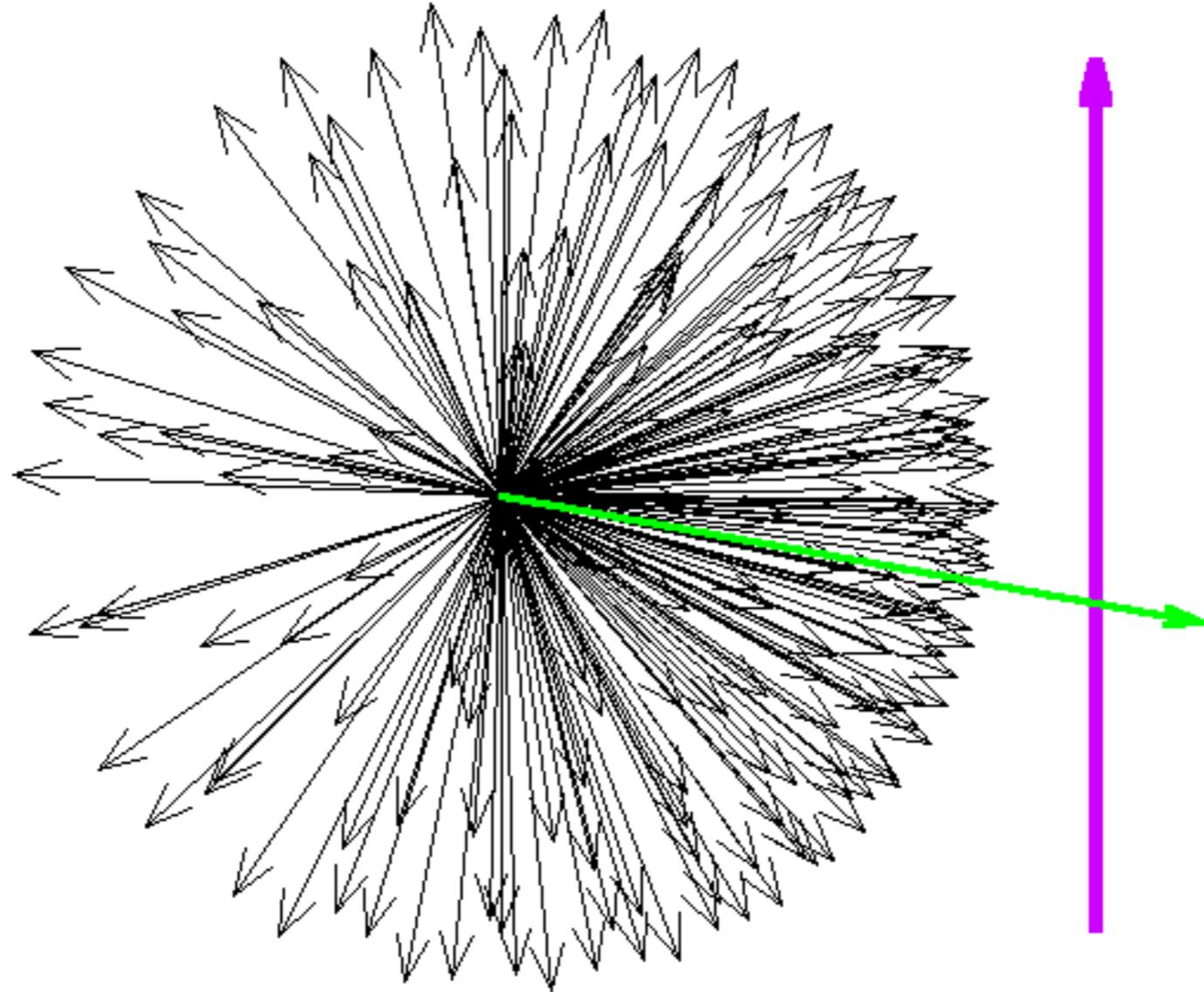


Vertikálně polarizované magnetické momenty
ve vertikálním magnetickém poli

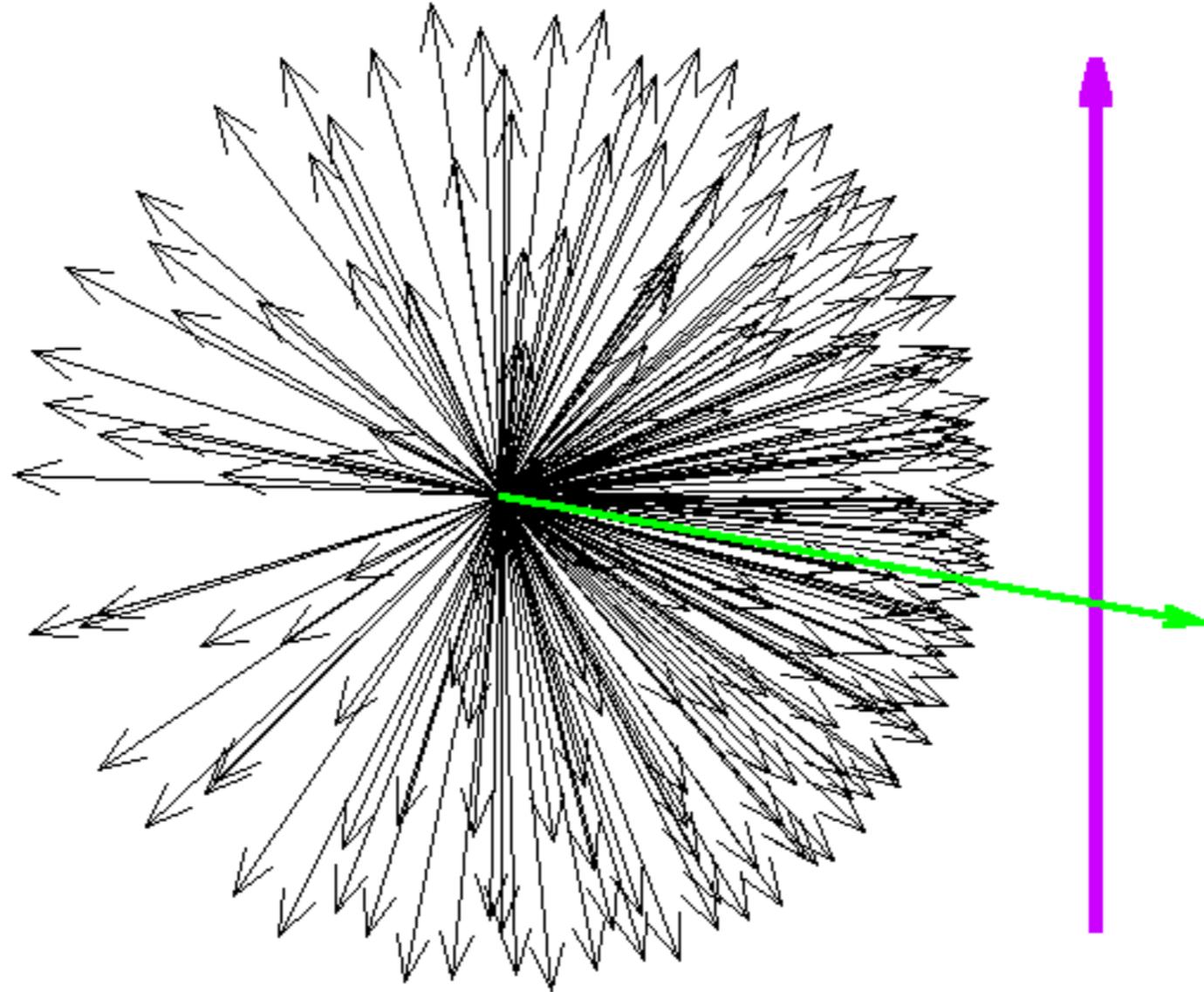


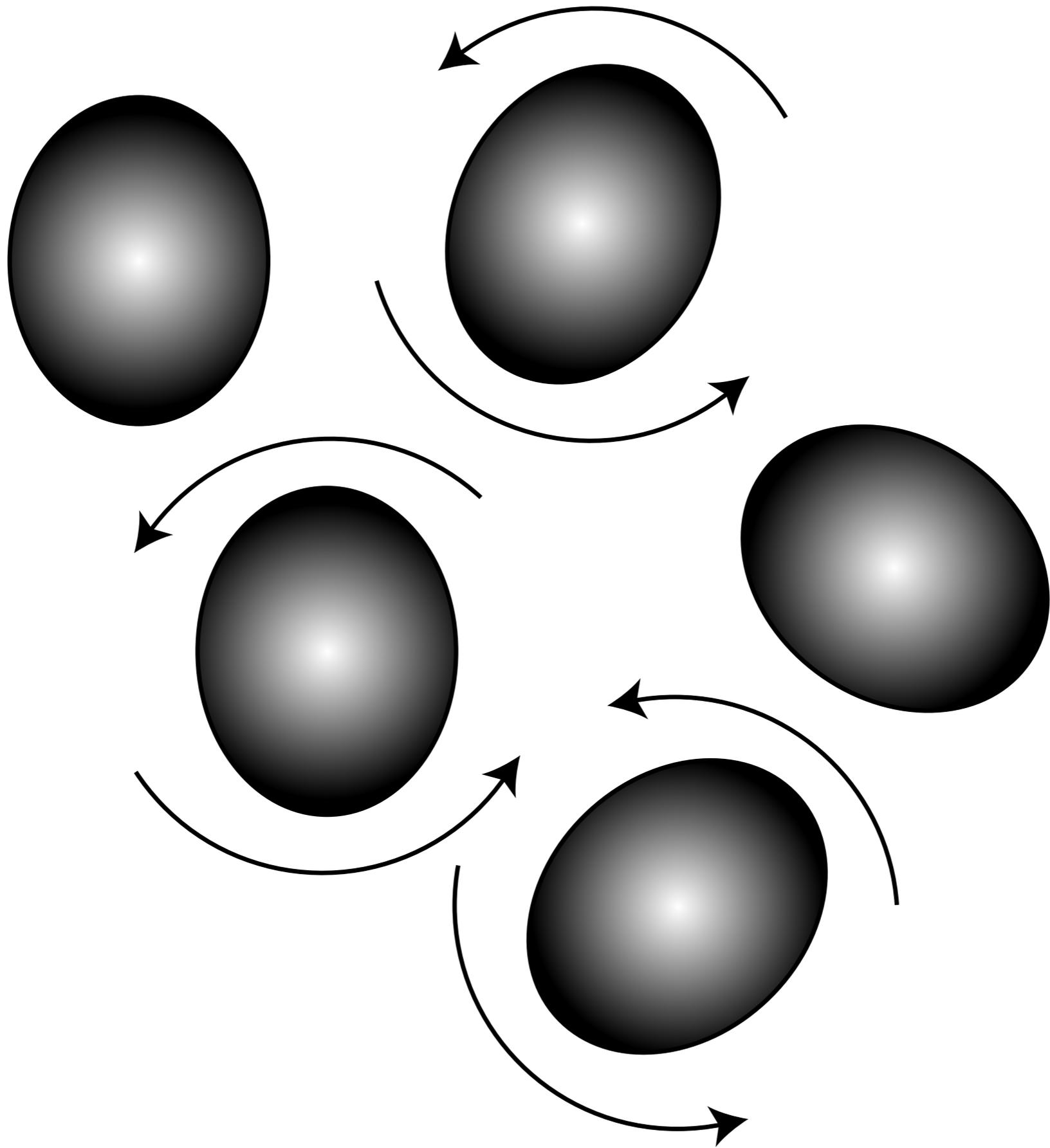
Sklopení vektoru magnetizace

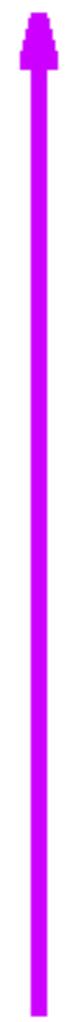
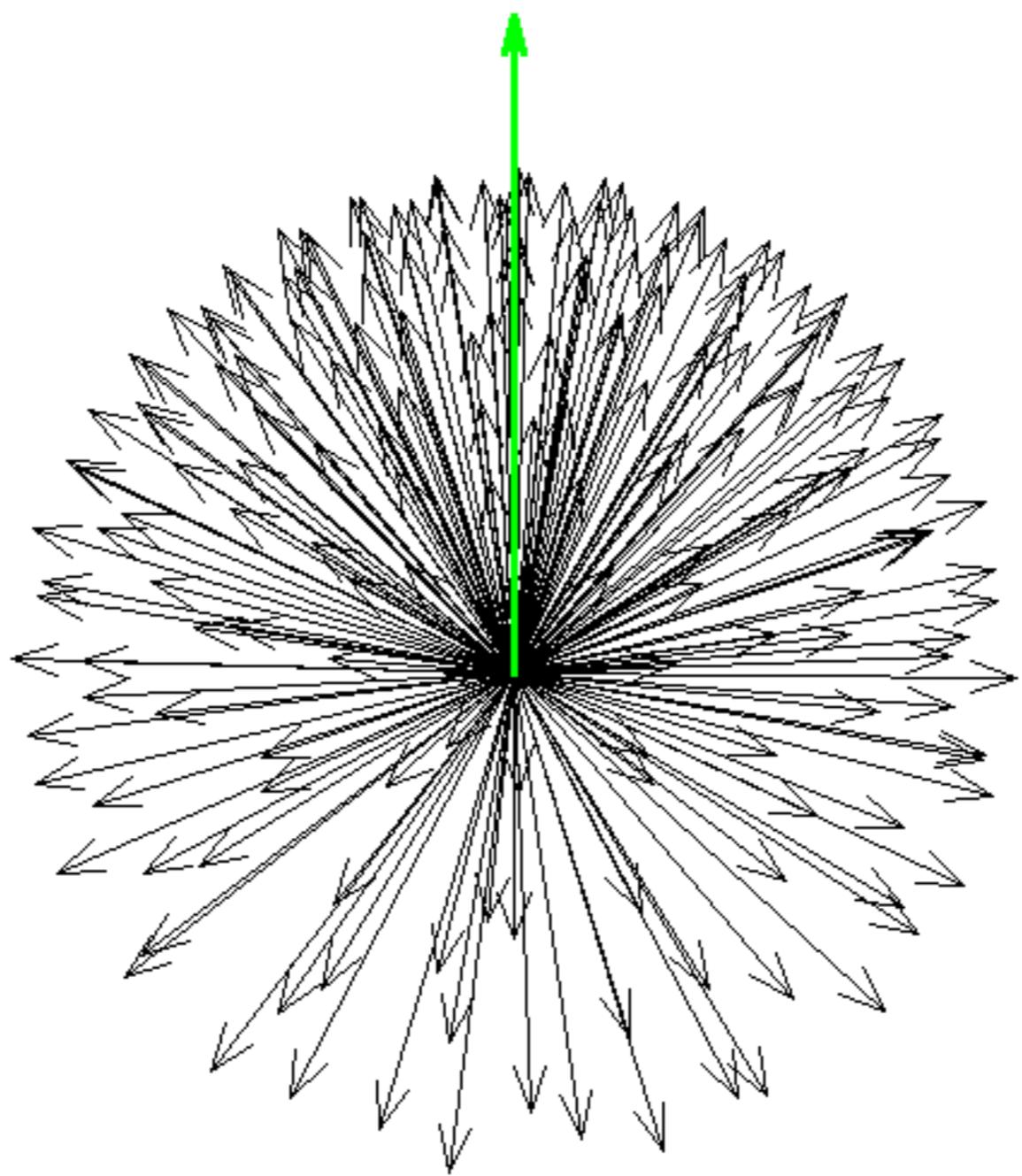


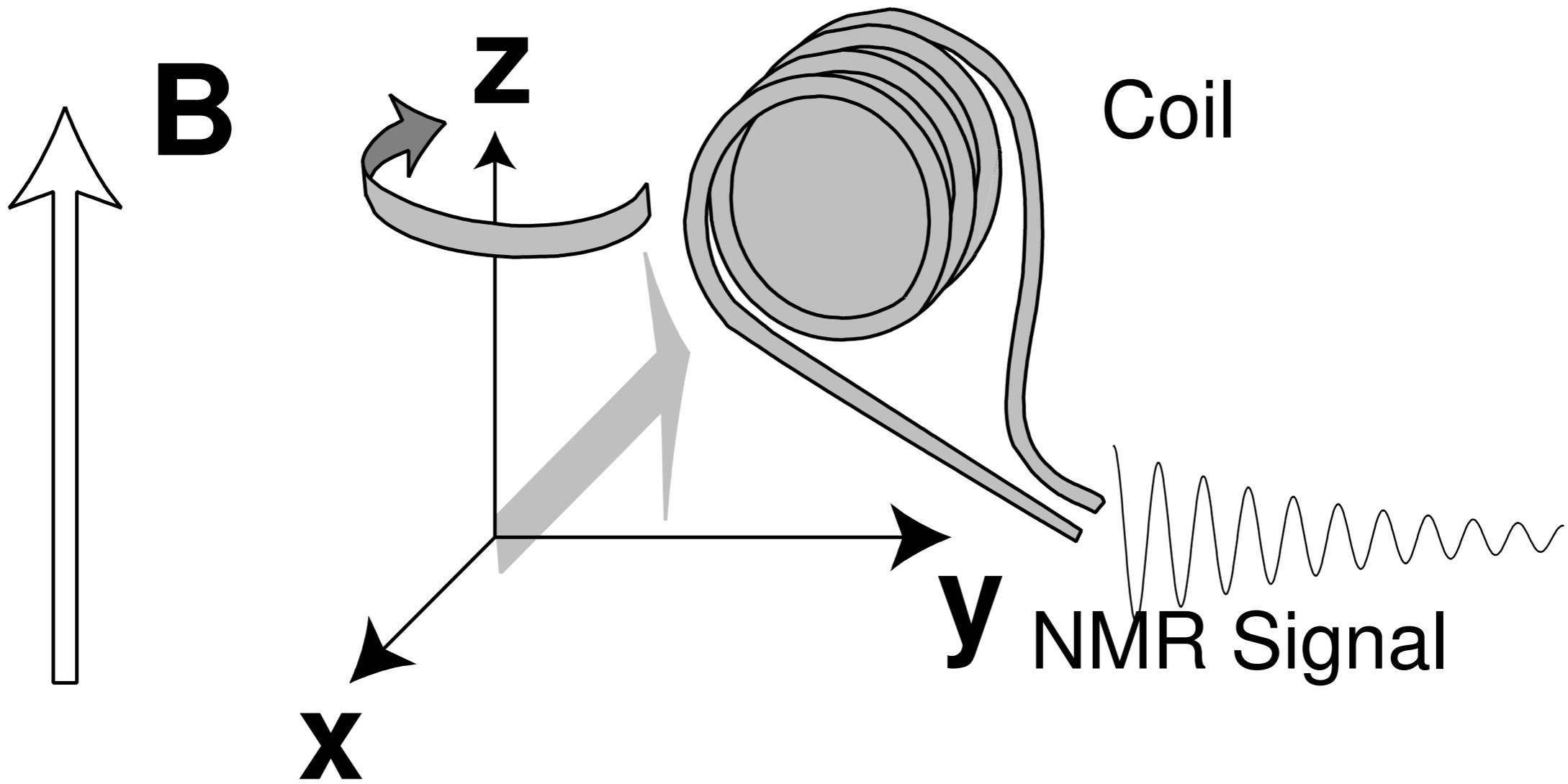


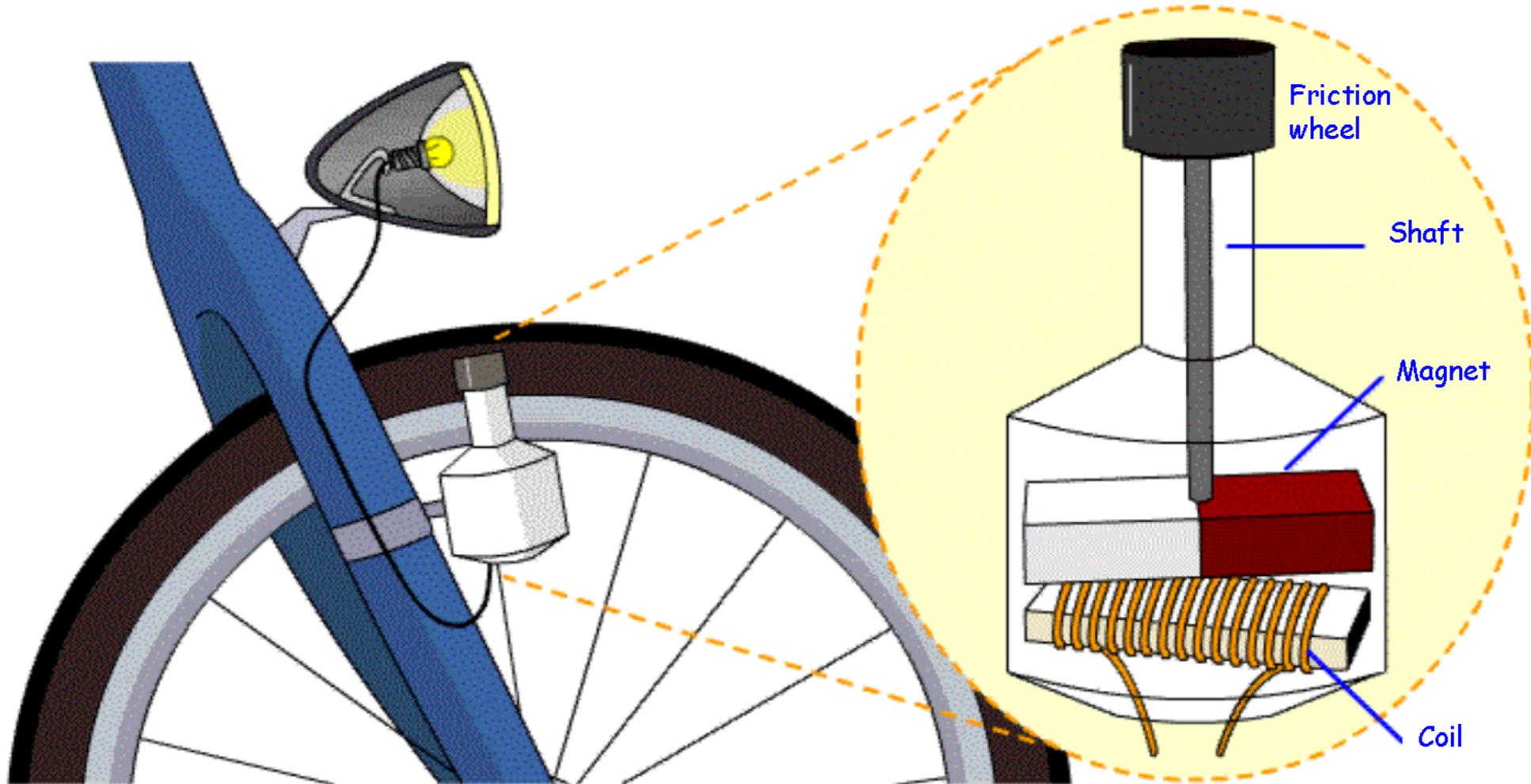
Horizontálně polarizované koherentní
magnetické momenty
ve vertikálním magnetickém poli

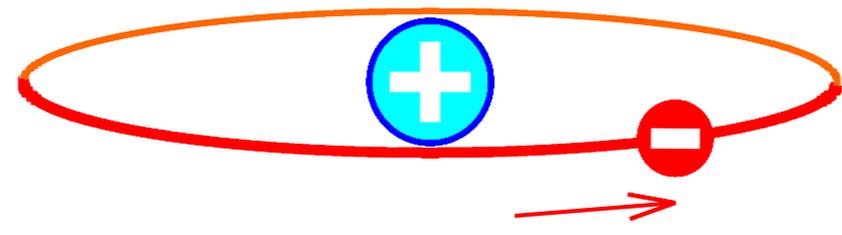


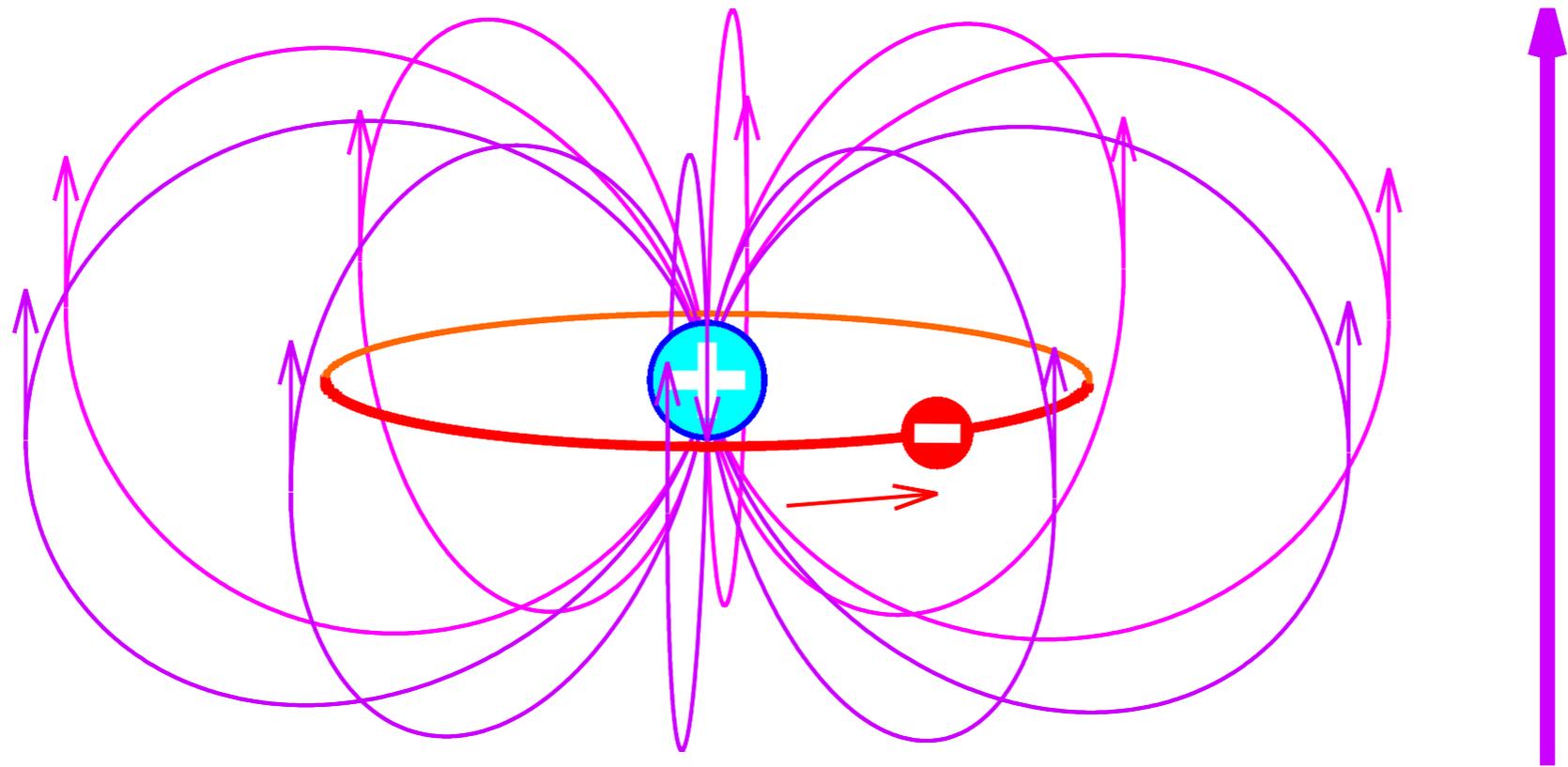


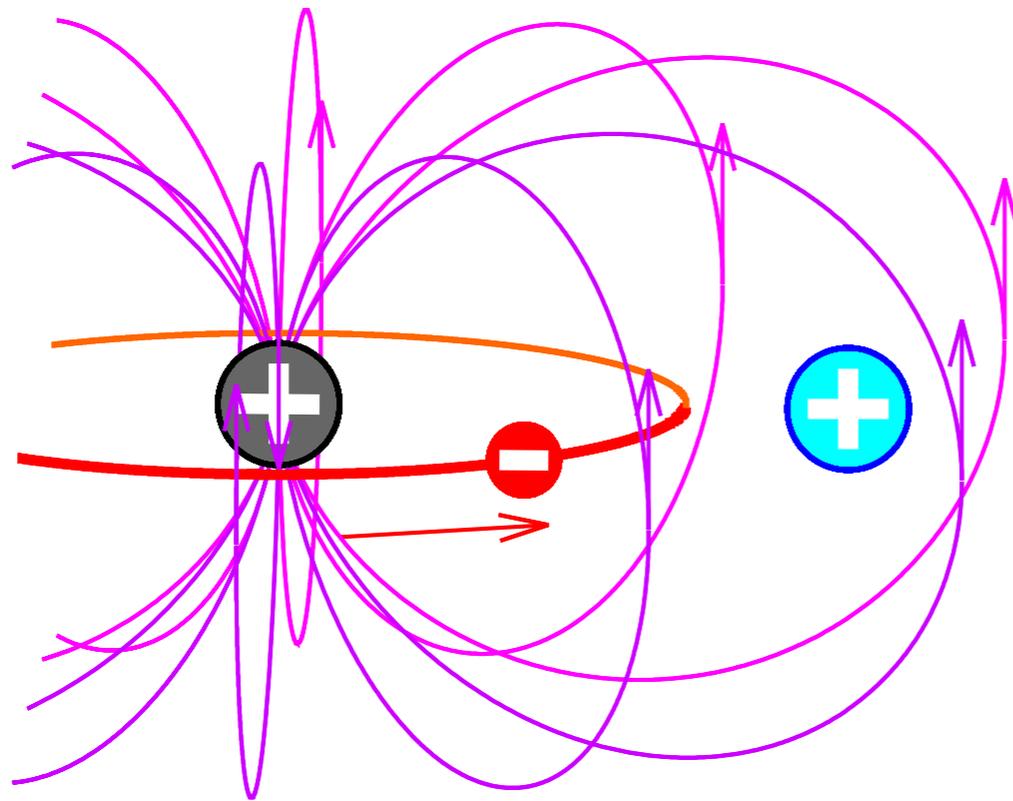


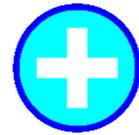
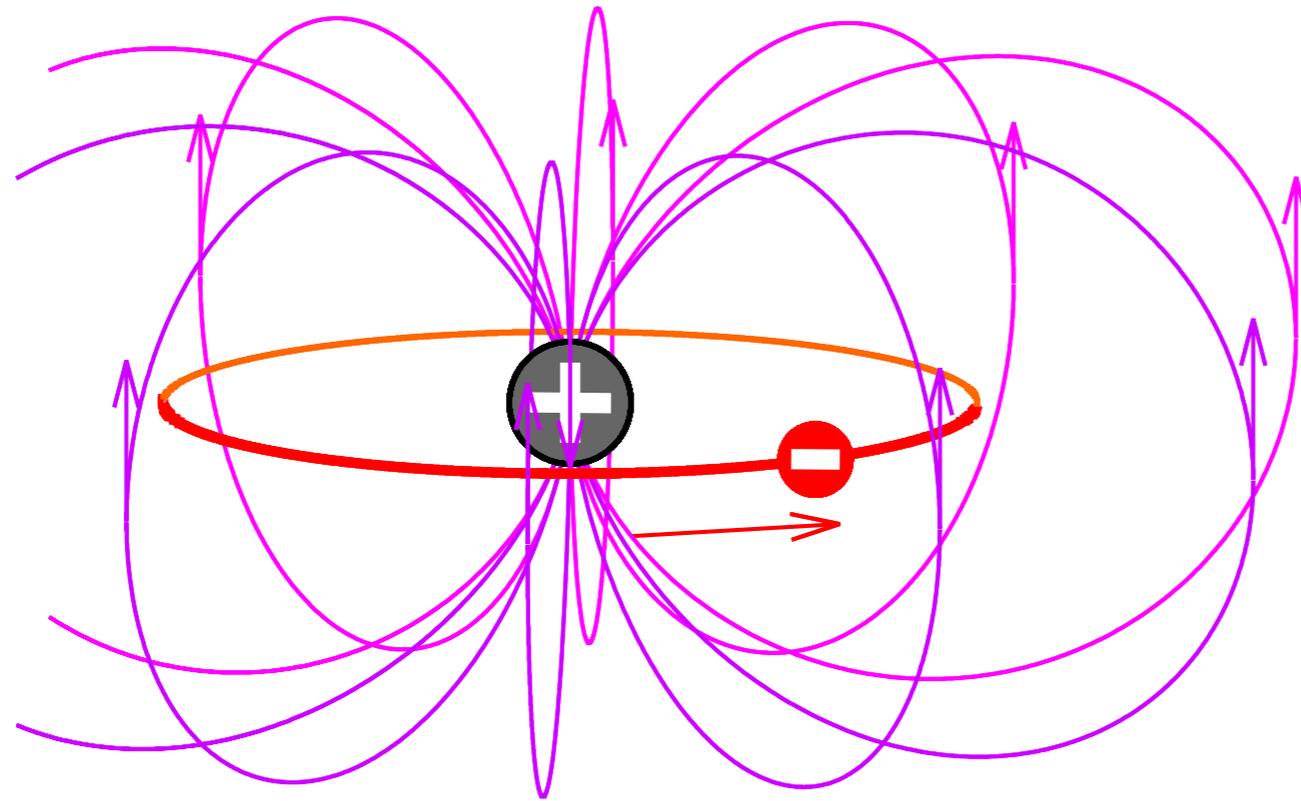


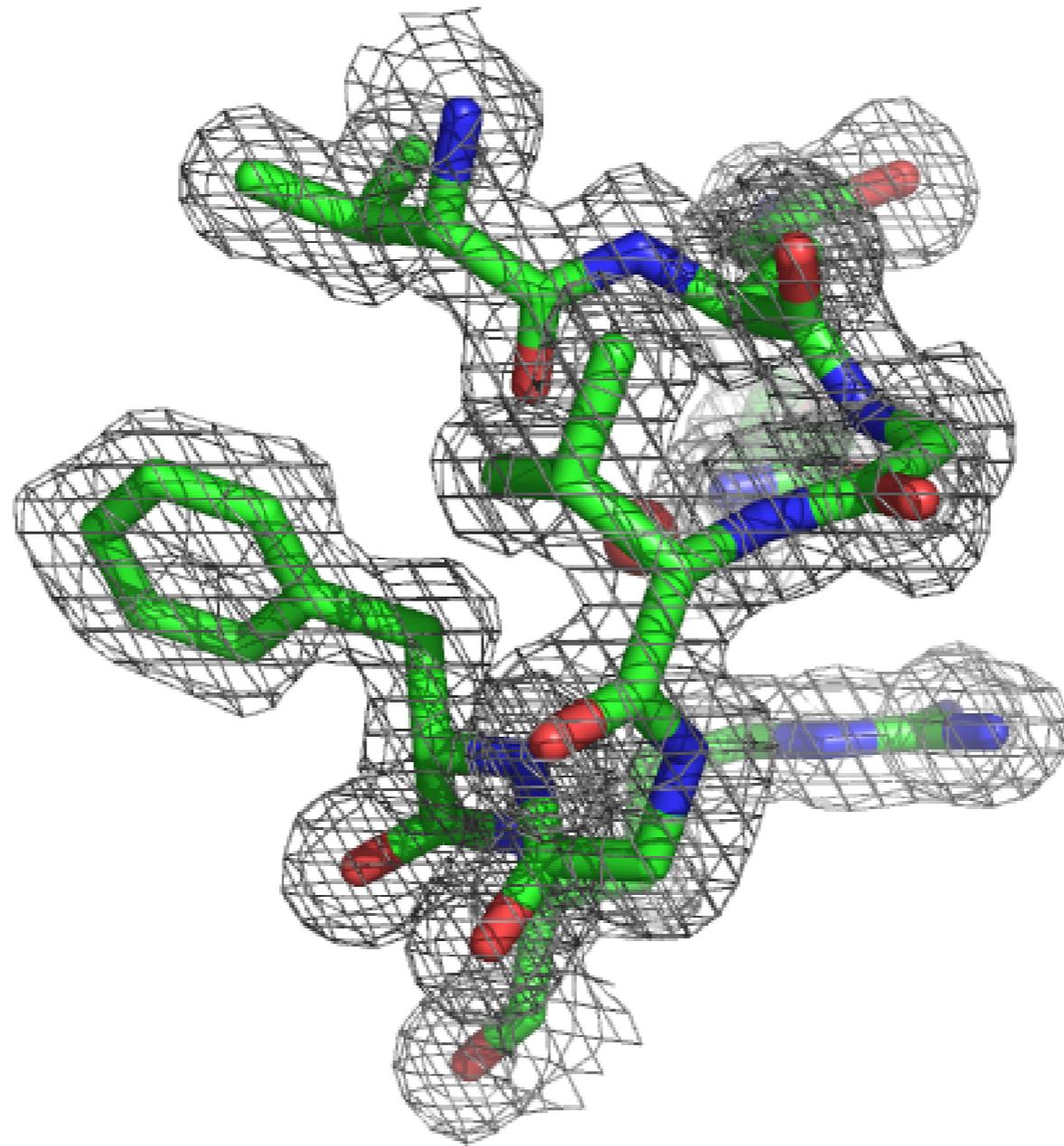


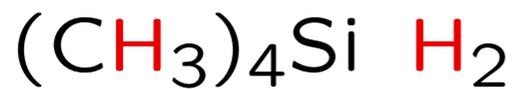
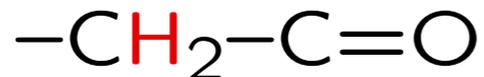
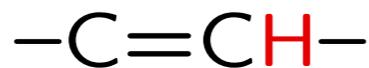
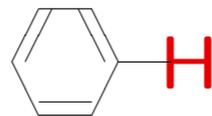
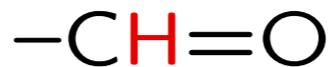










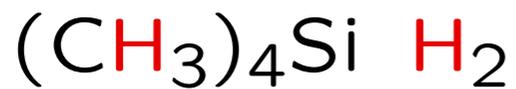
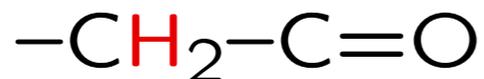
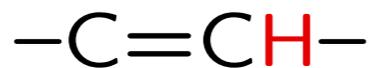
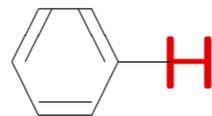
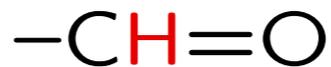


499.9985

499.9990

499.9995

500.0000 MHz

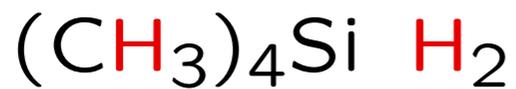
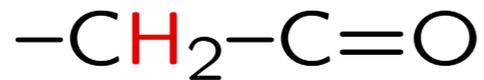
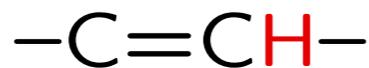
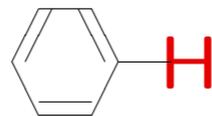


99.997 %

99.998 %

99.999 %

100.000 %

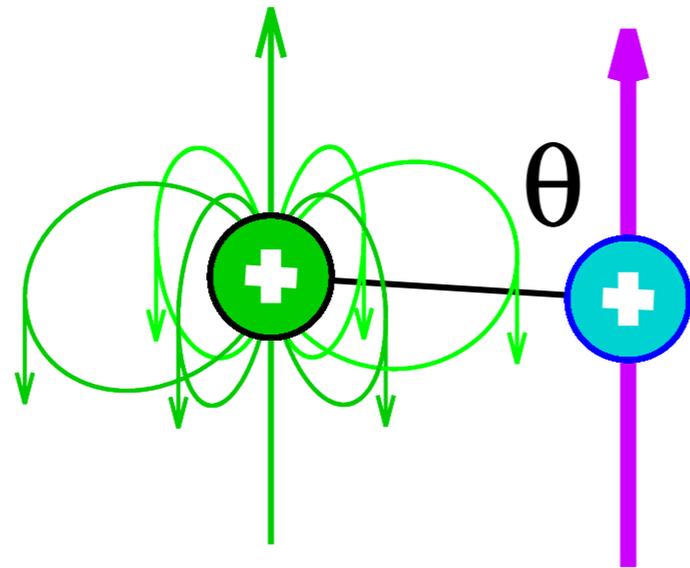


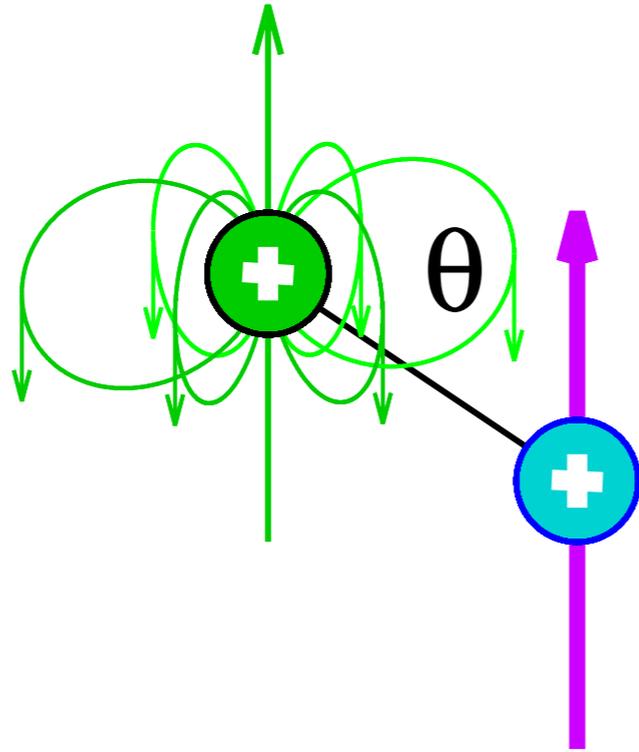
0 ppm

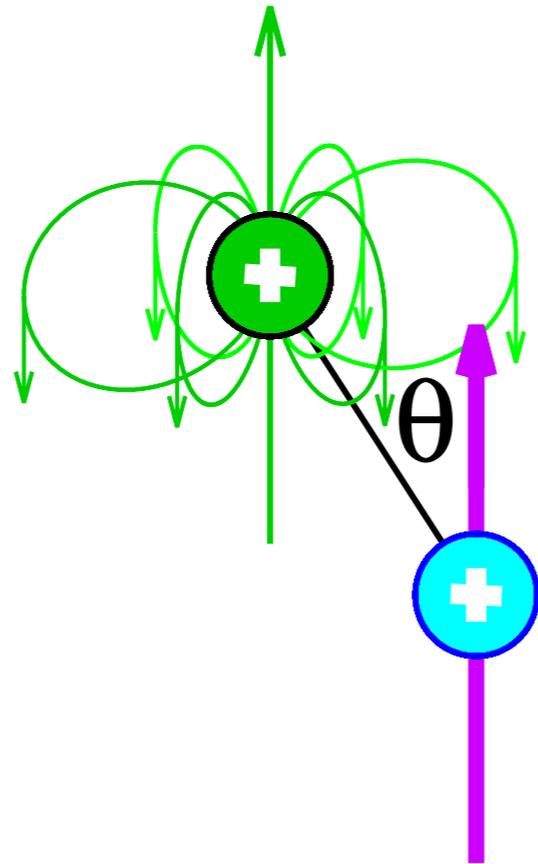
10 ppm

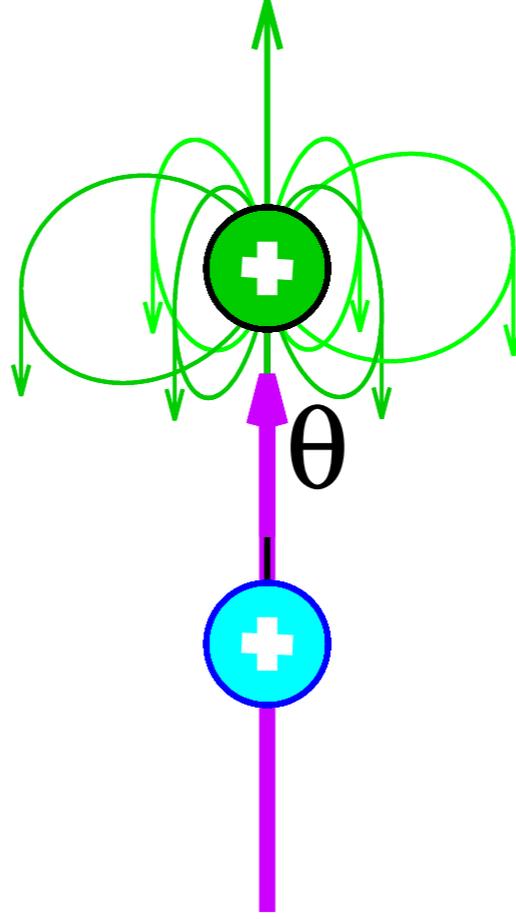
20 ppm

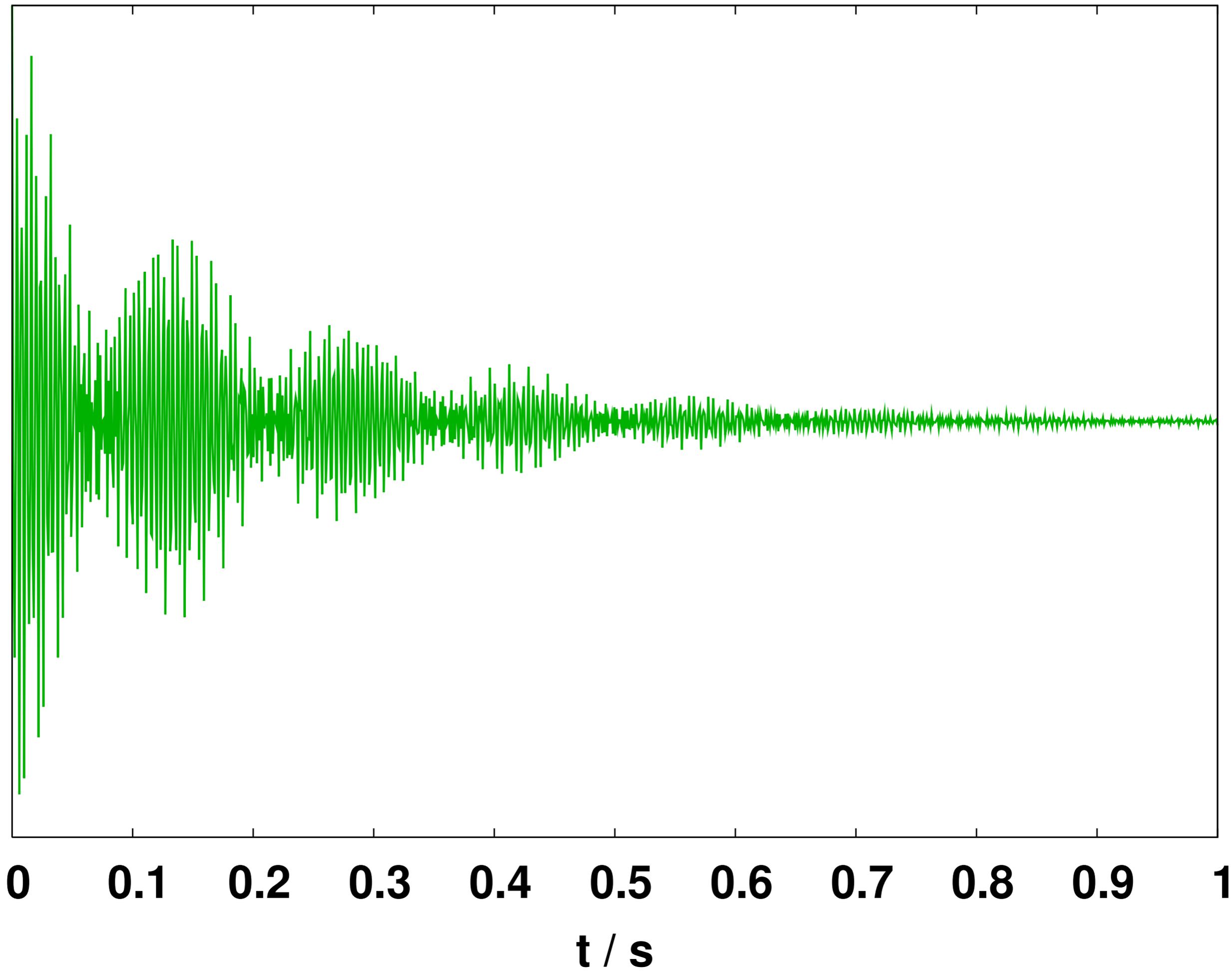
30 ppm

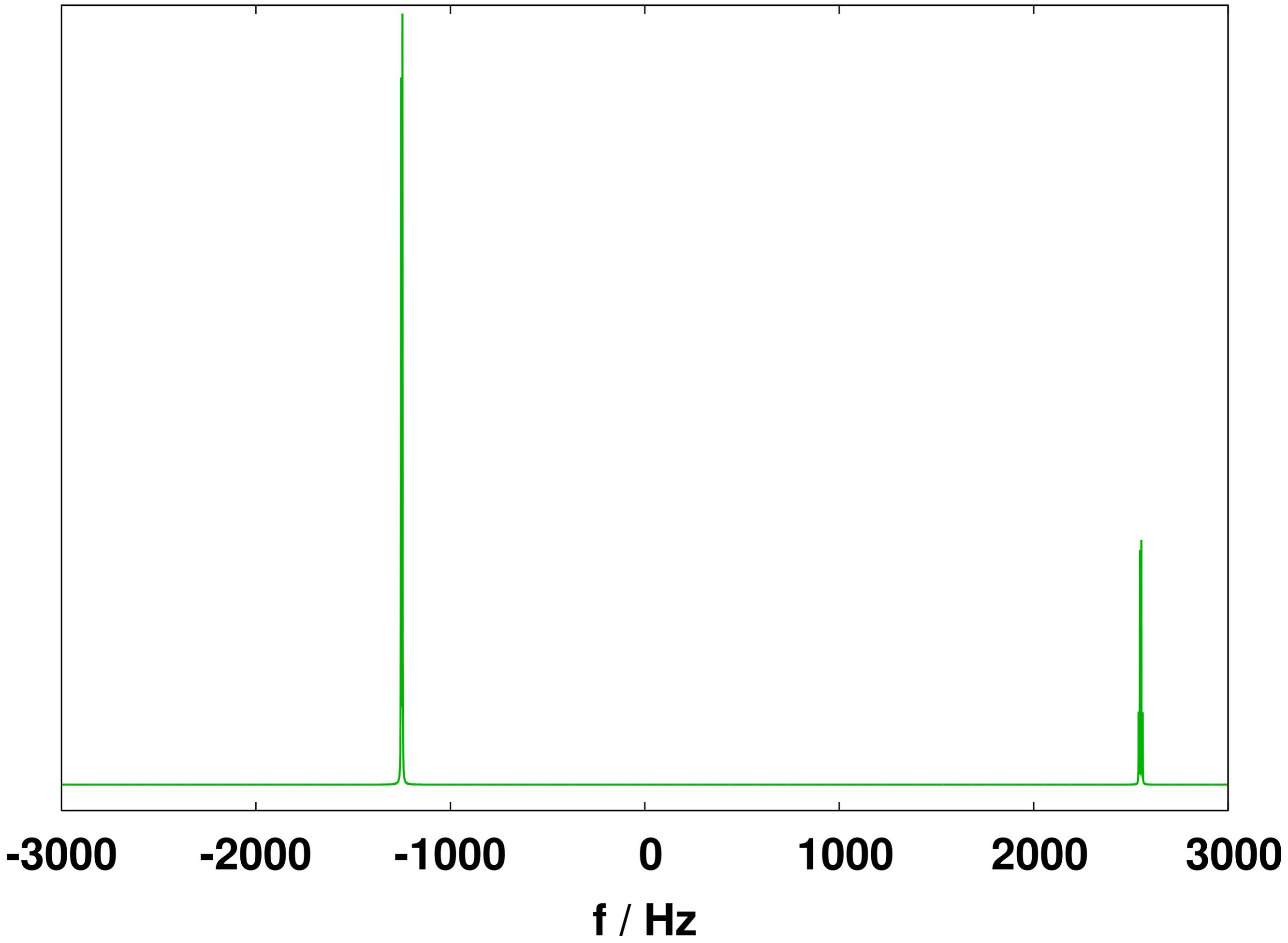


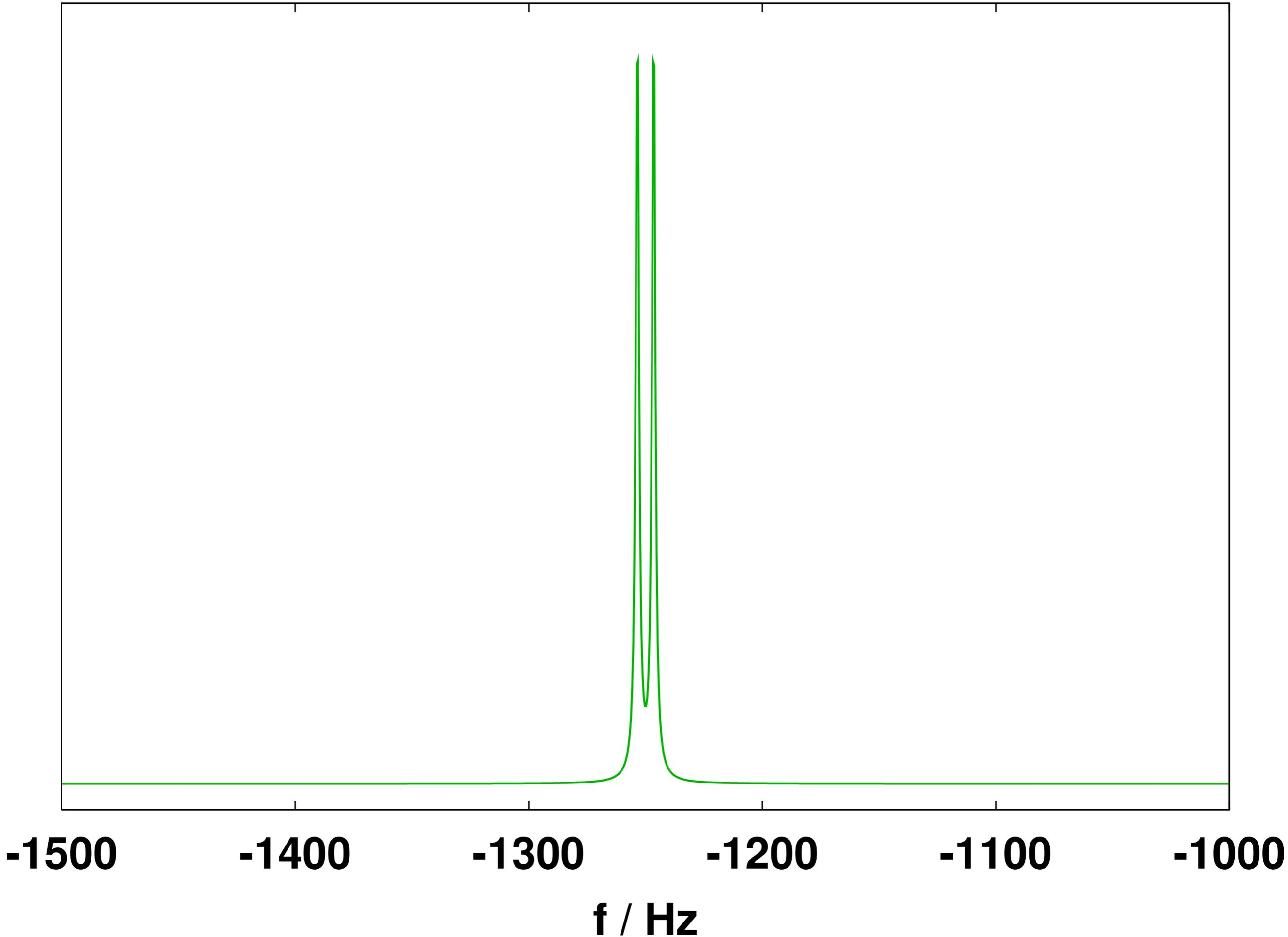


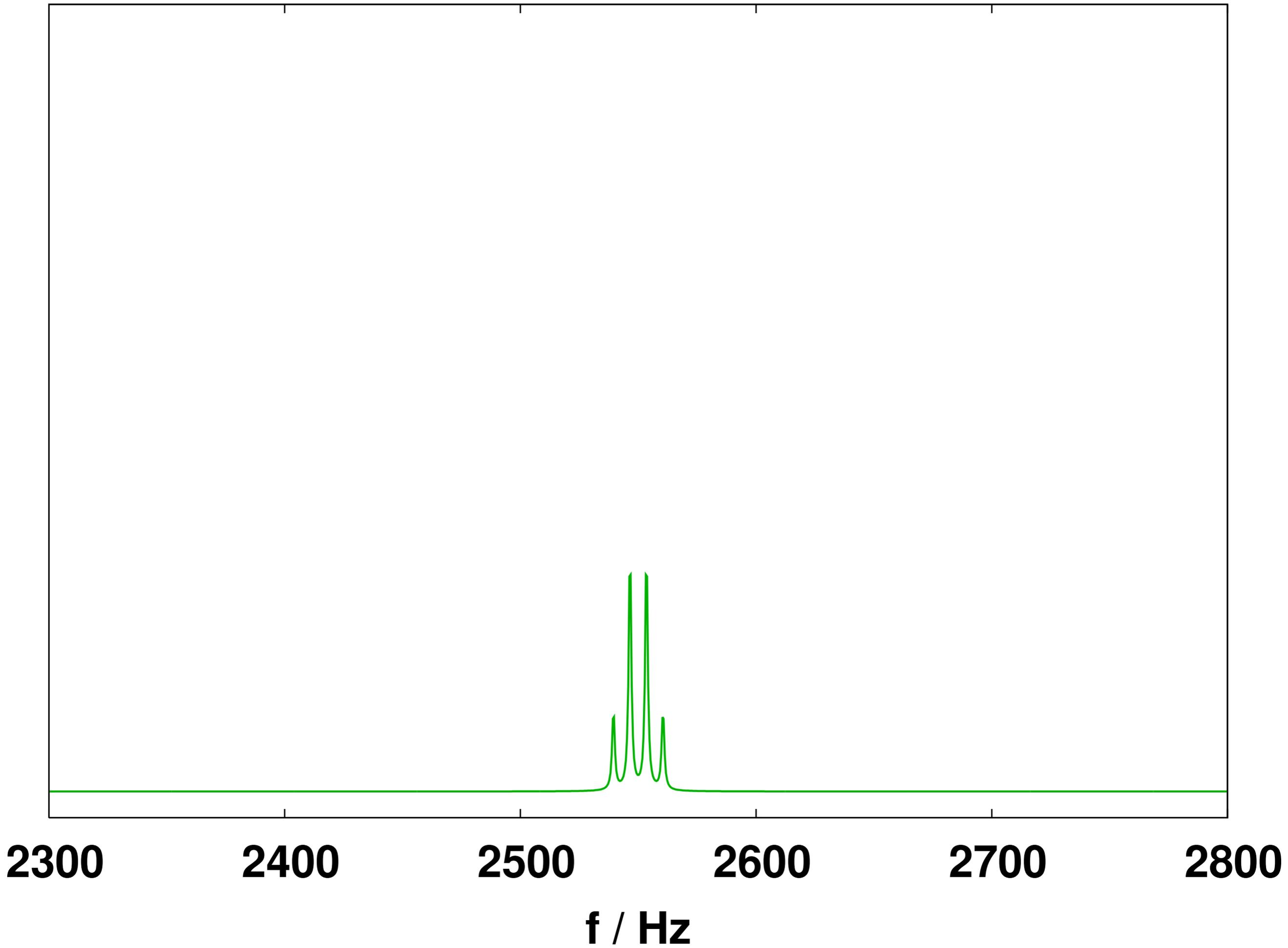


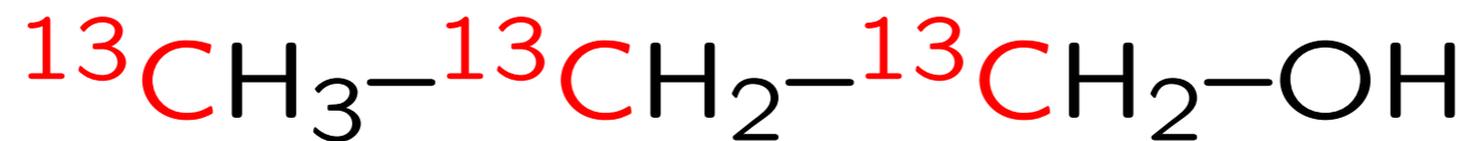
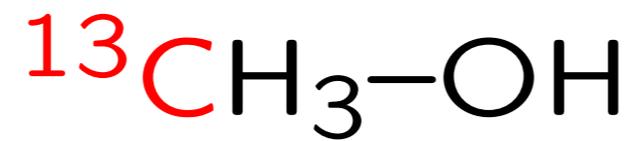


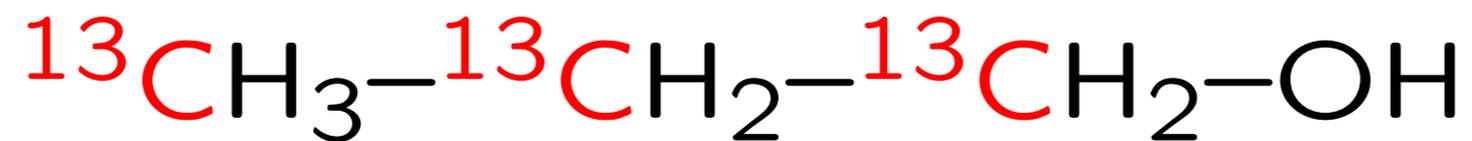
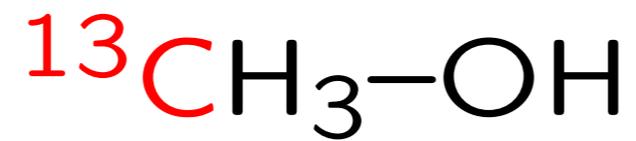












Ovčáci čtveráci

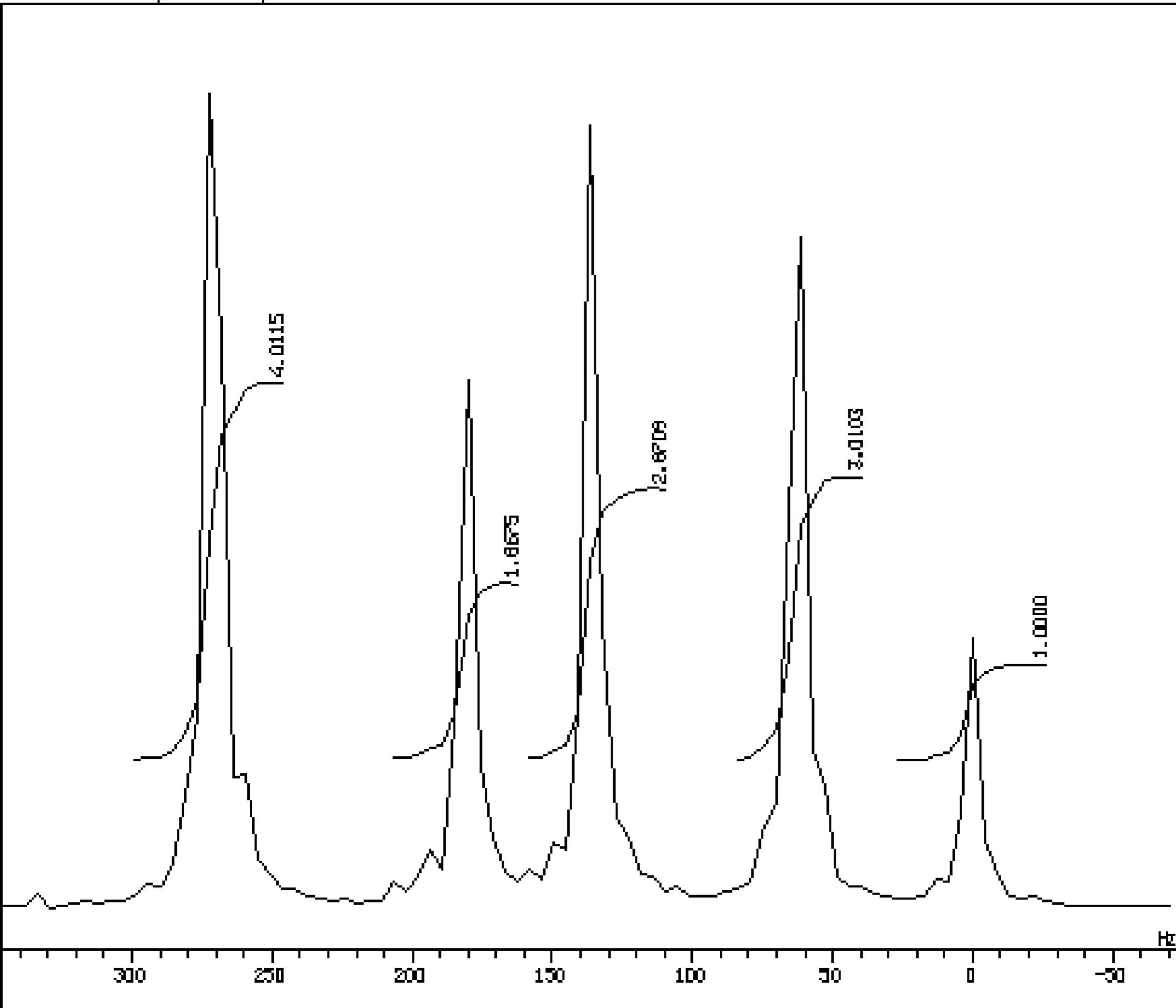
Prší, prší

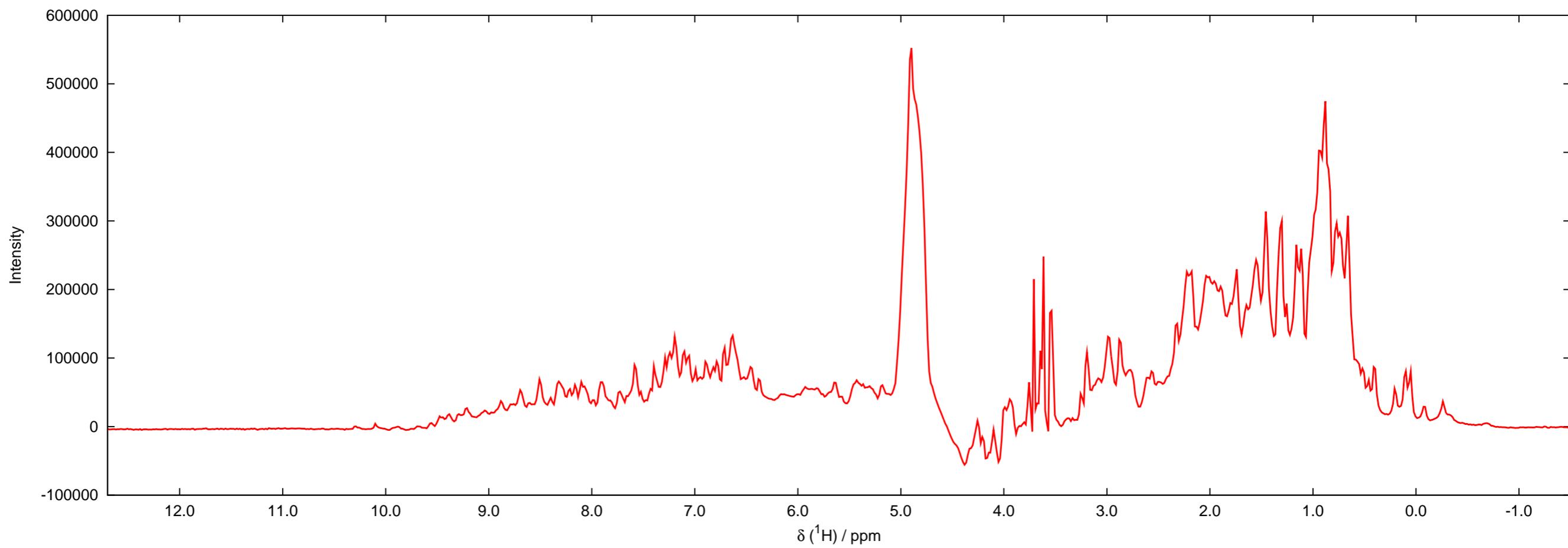
Kočka leze dírou

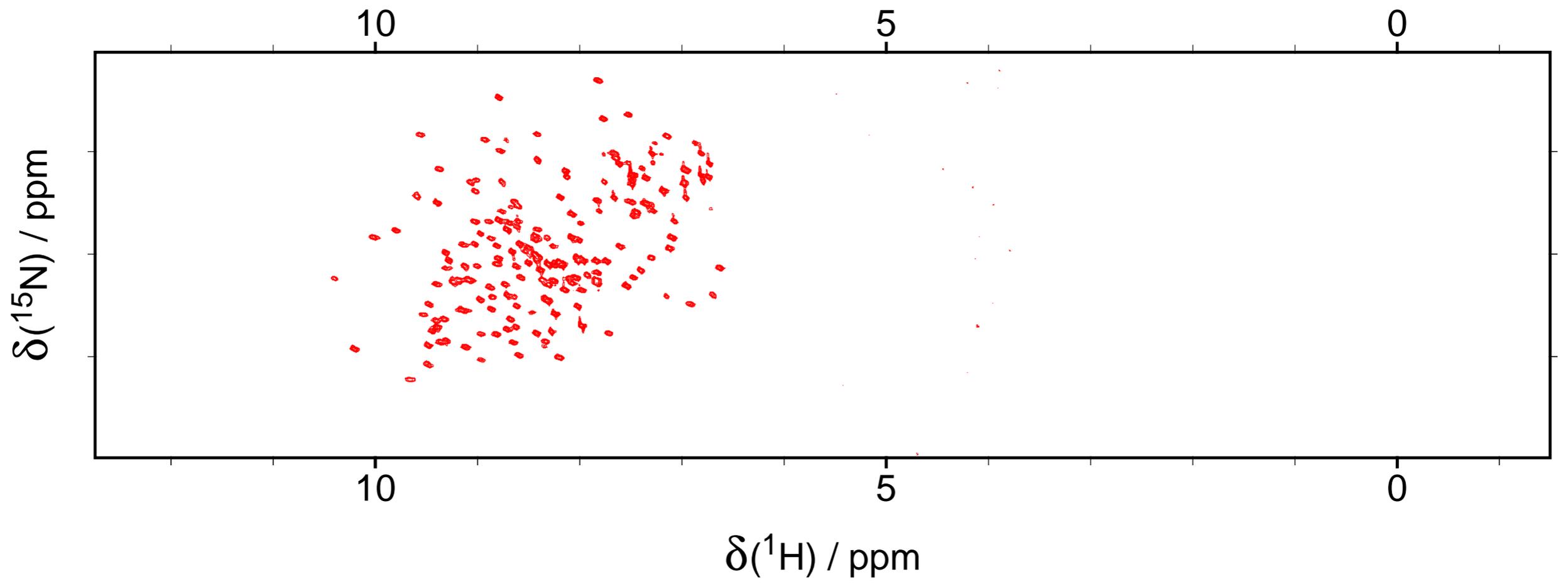
Acetaldehyd

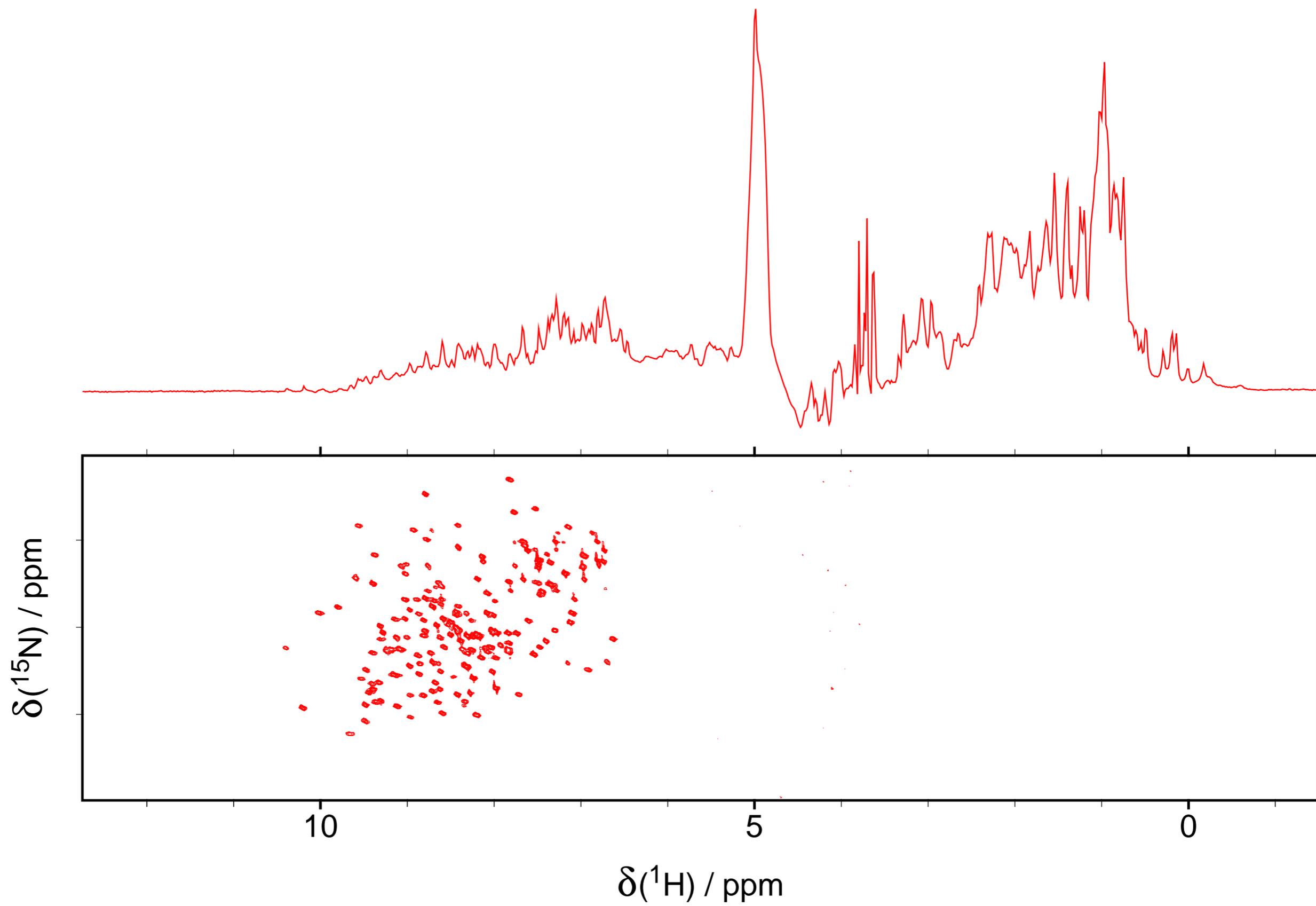
Hänschen klein

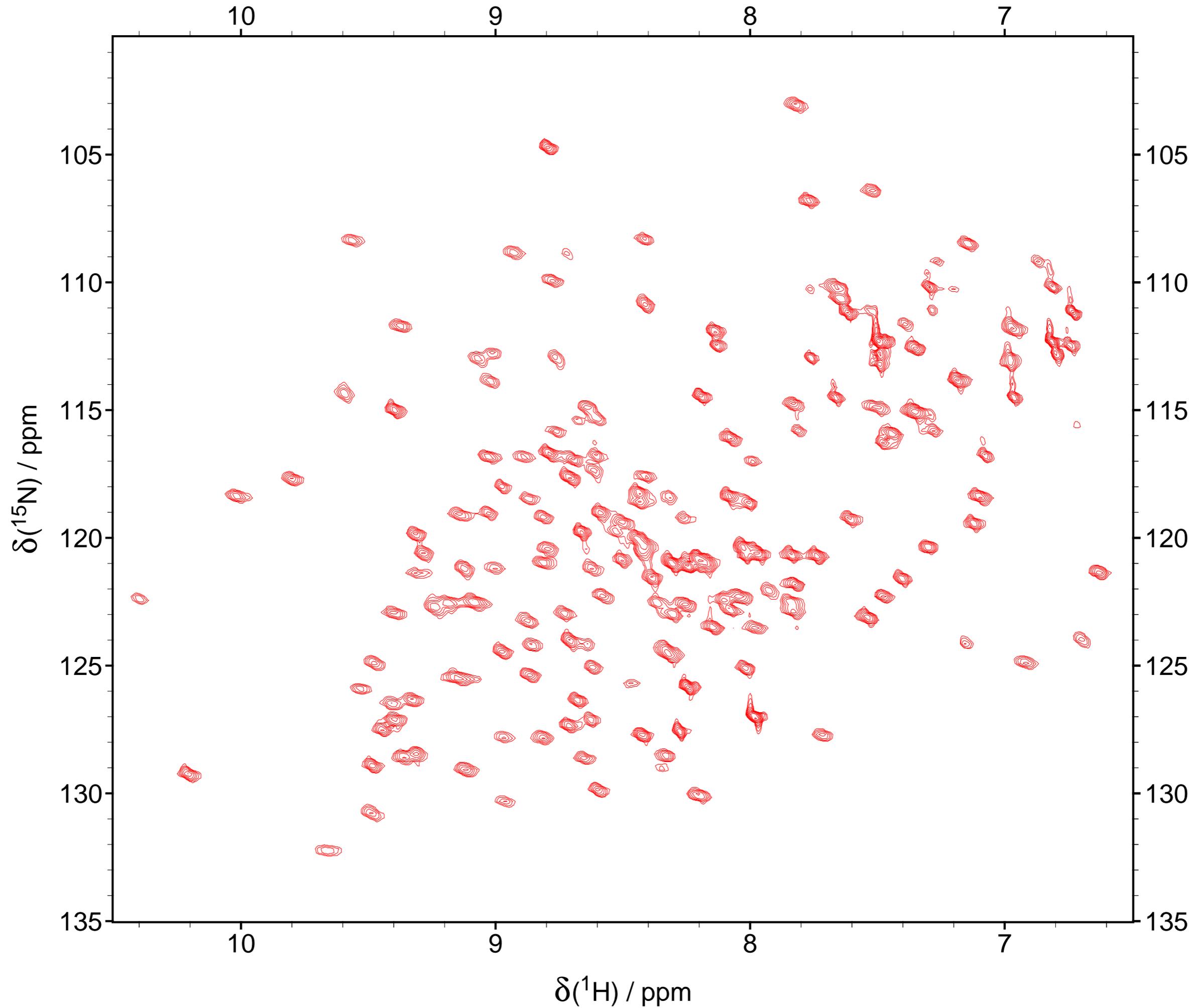
SFILE : HANS
 EXMOD : HANS
 IRMOD : NON
 POINT : 2048
 SAMPD : 2048
 FREQU : 9000.90 Hz
 FILTR : 4500 Hz
 SCANS : 1
 QUANTY : 0
 ACQTH : 0.7275 sec
 PD : 2.7231 sec
 RGAIN : 10
 PW1 : 1.00 usec
 OBNUC : 1H
 OBFRQ : 500.00 MHz
 OBSET : 160200.00 Hz
 IRNUC : 13C
 IRFRQ : 125.65 MHz
 IRSET : 127958.00 Hz
 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
 GF : 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

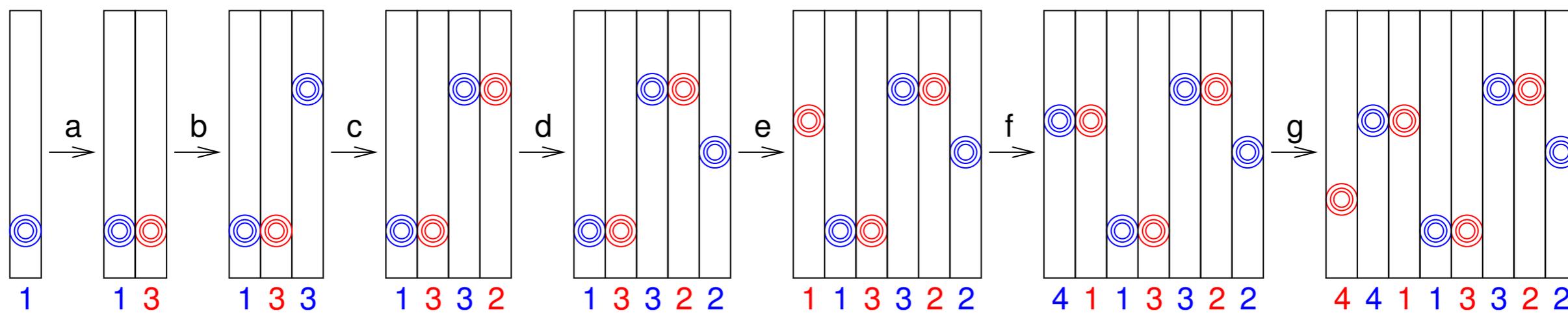
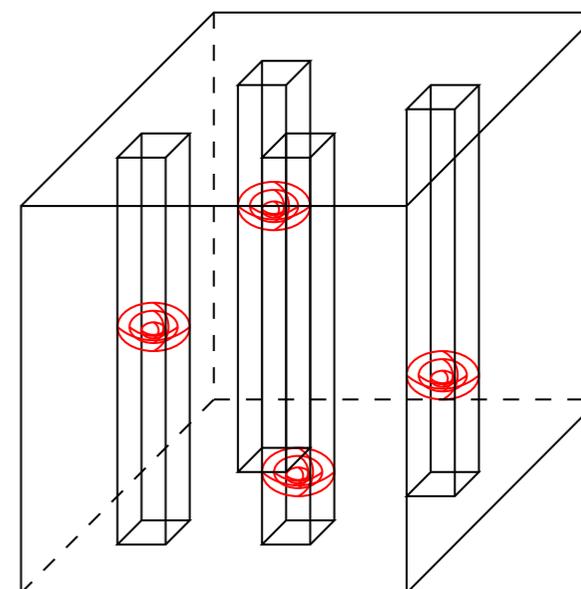
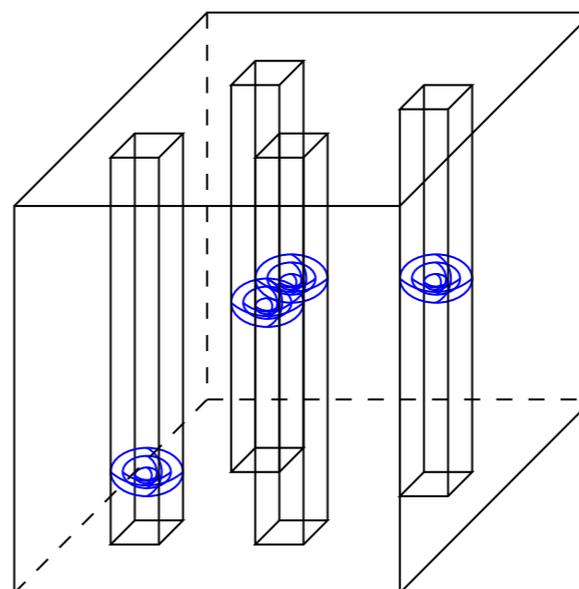
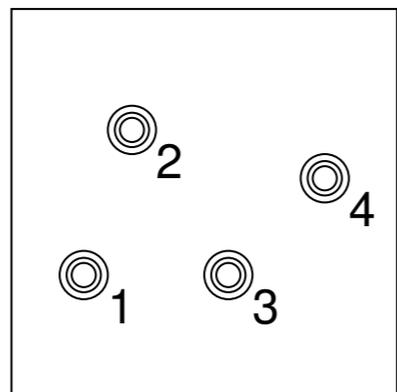
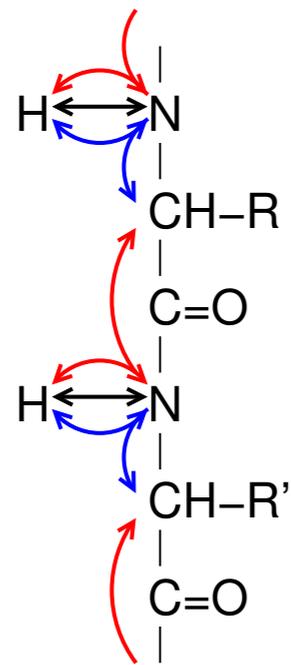


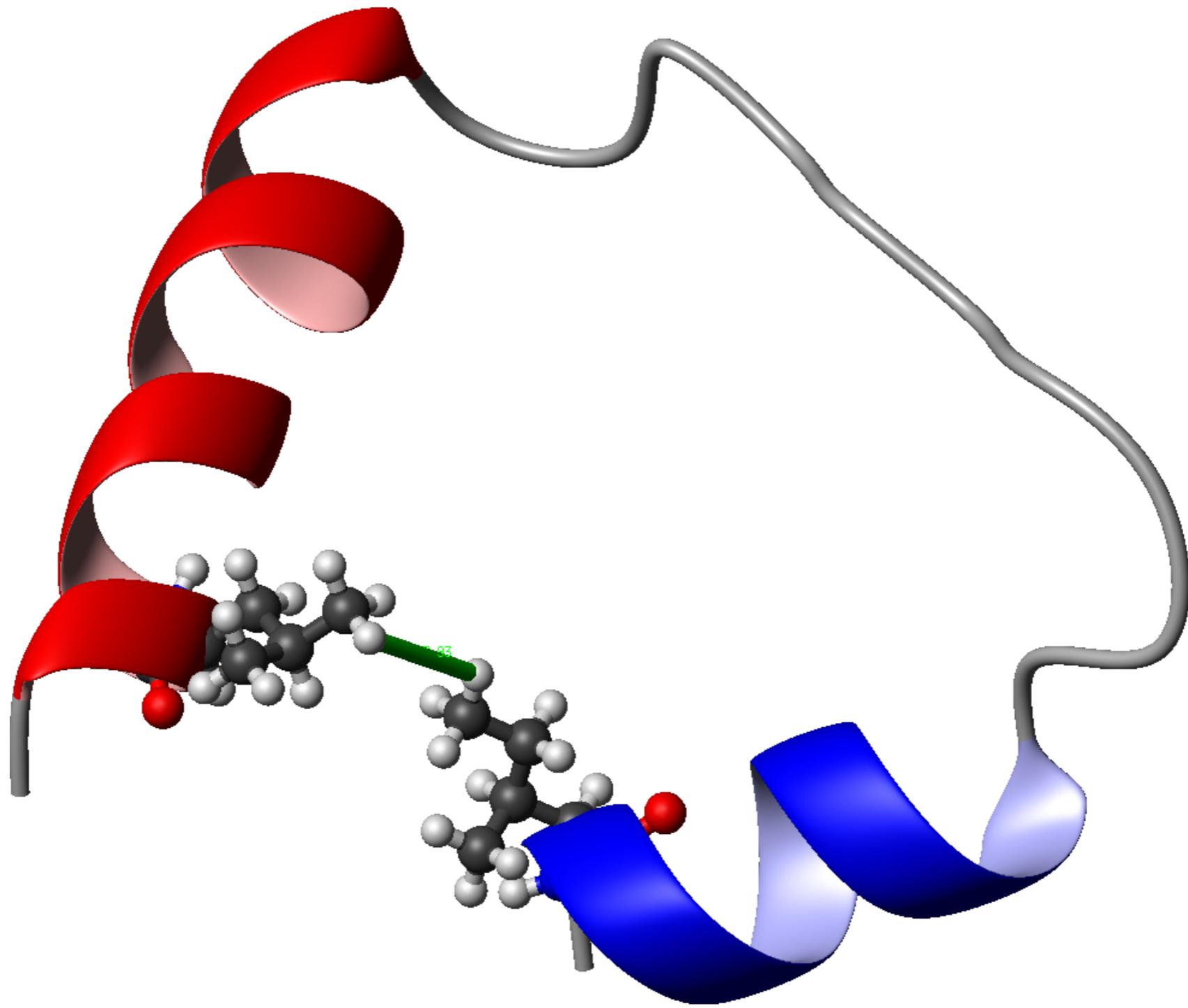


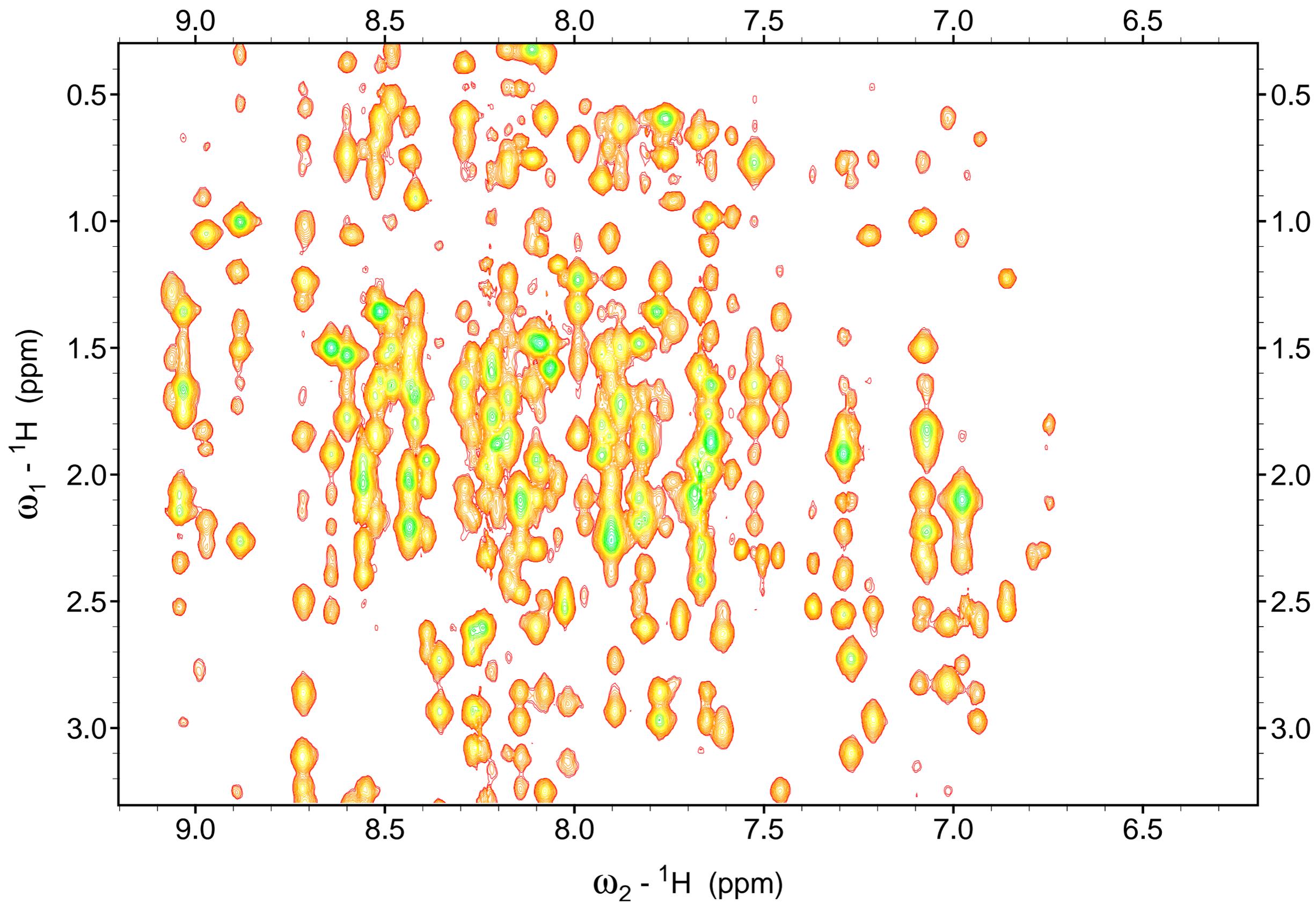


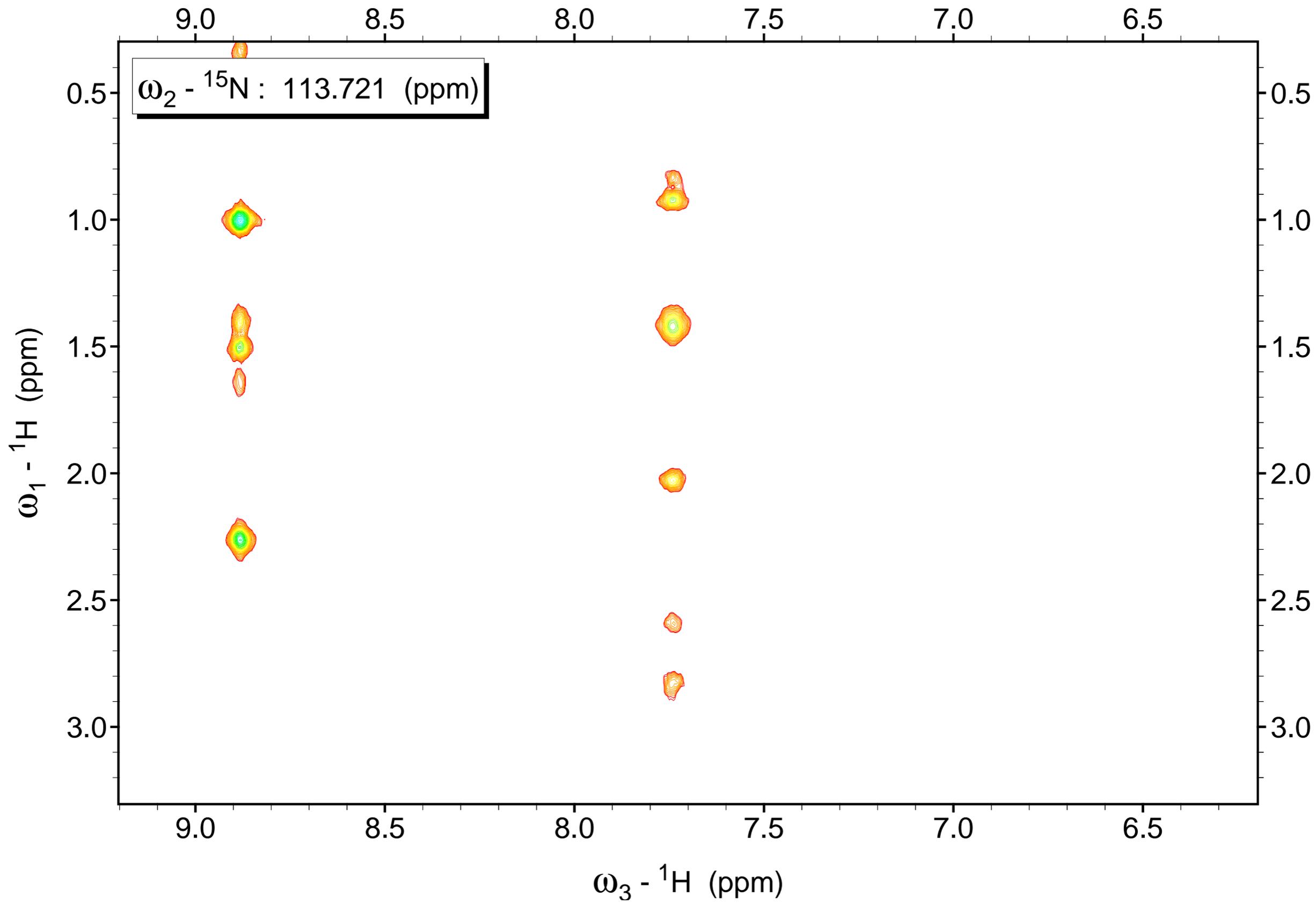


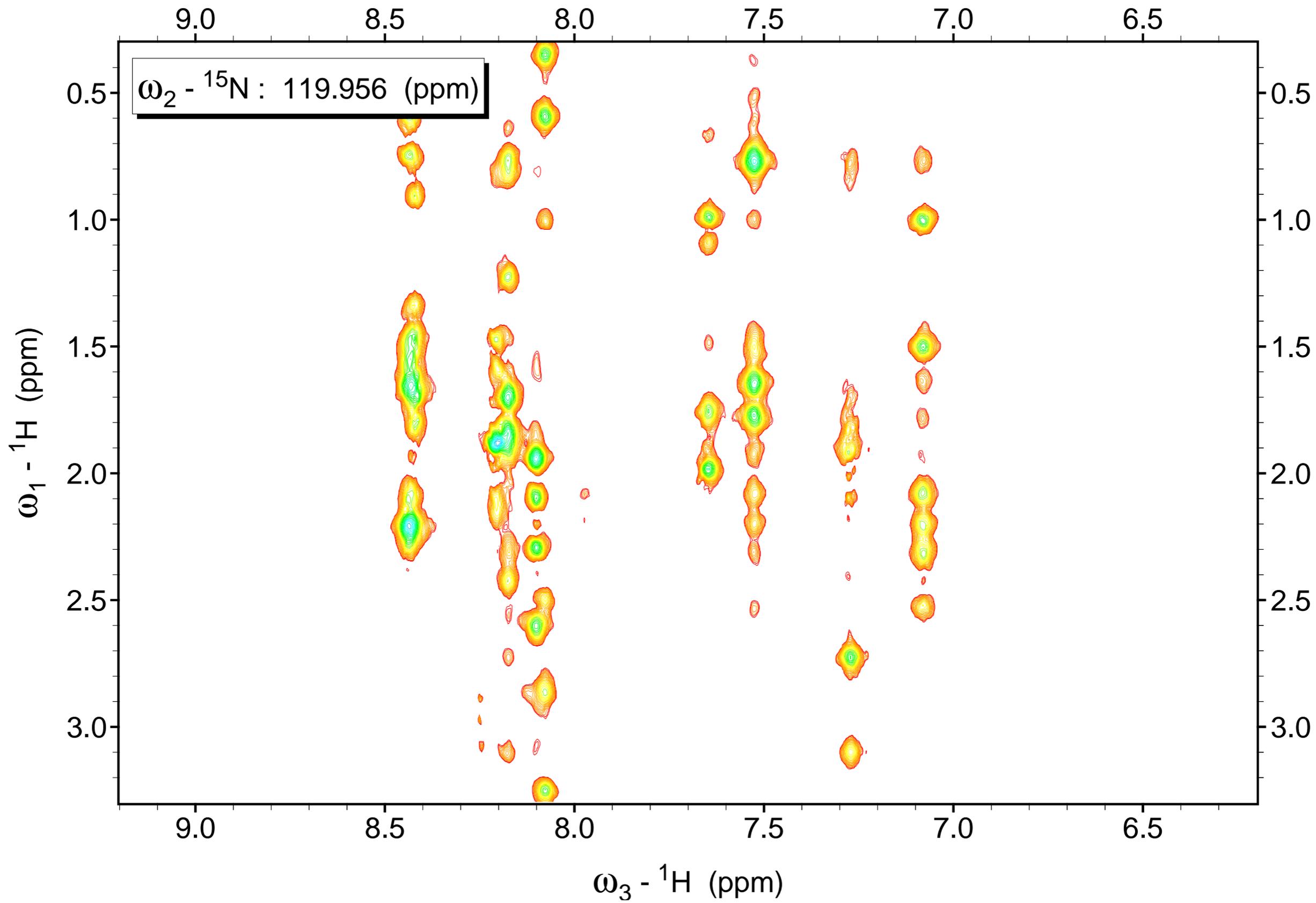


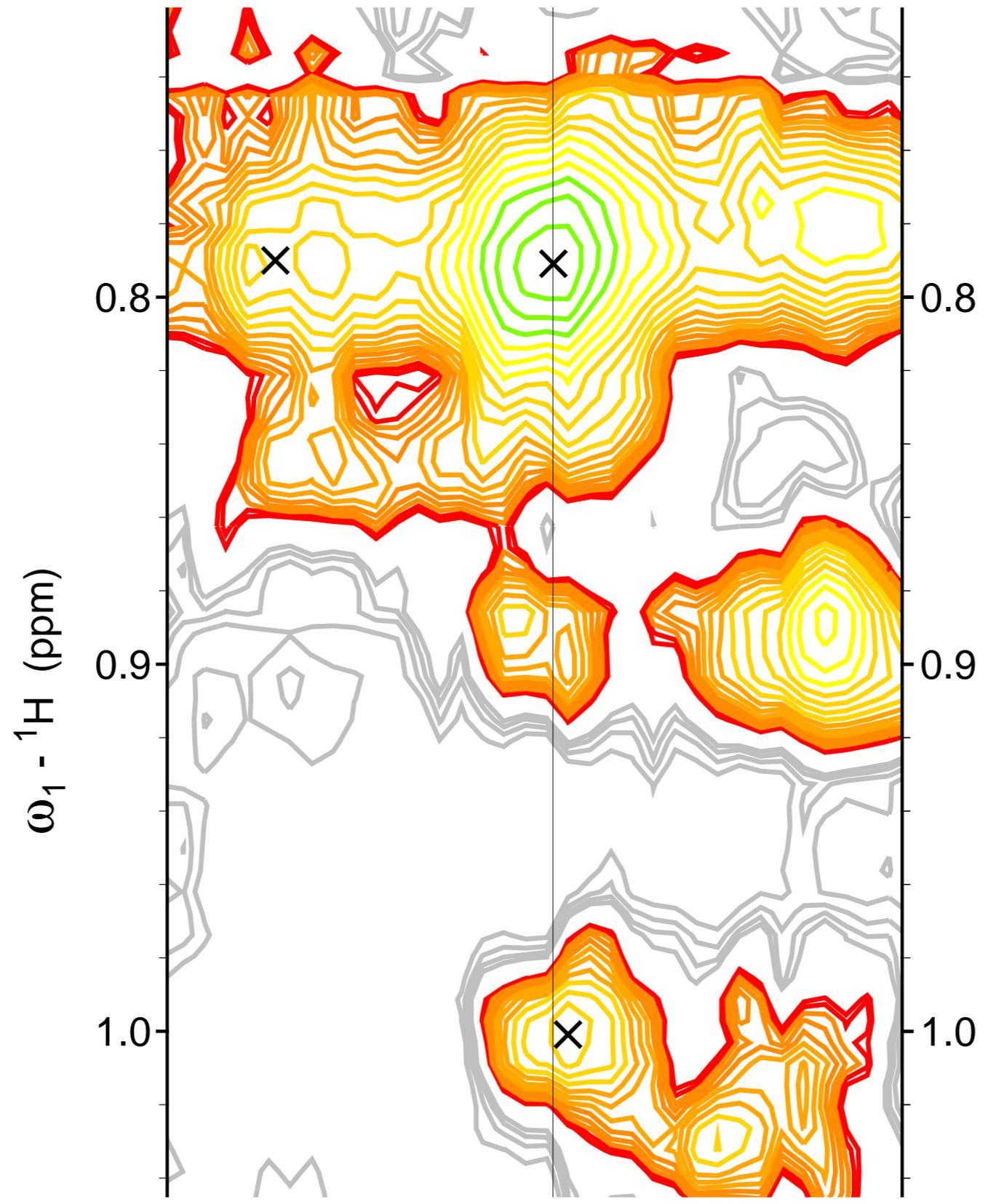


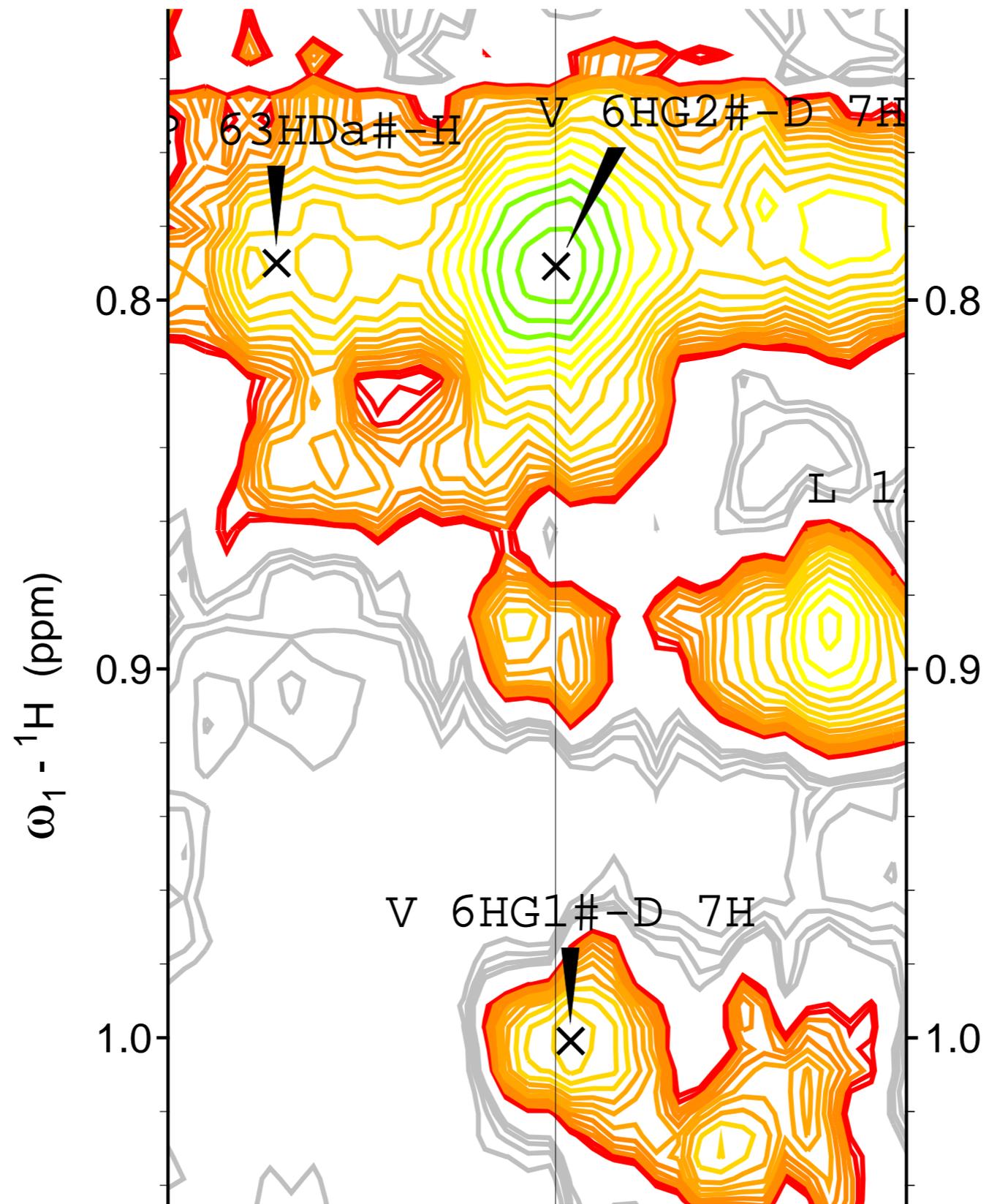








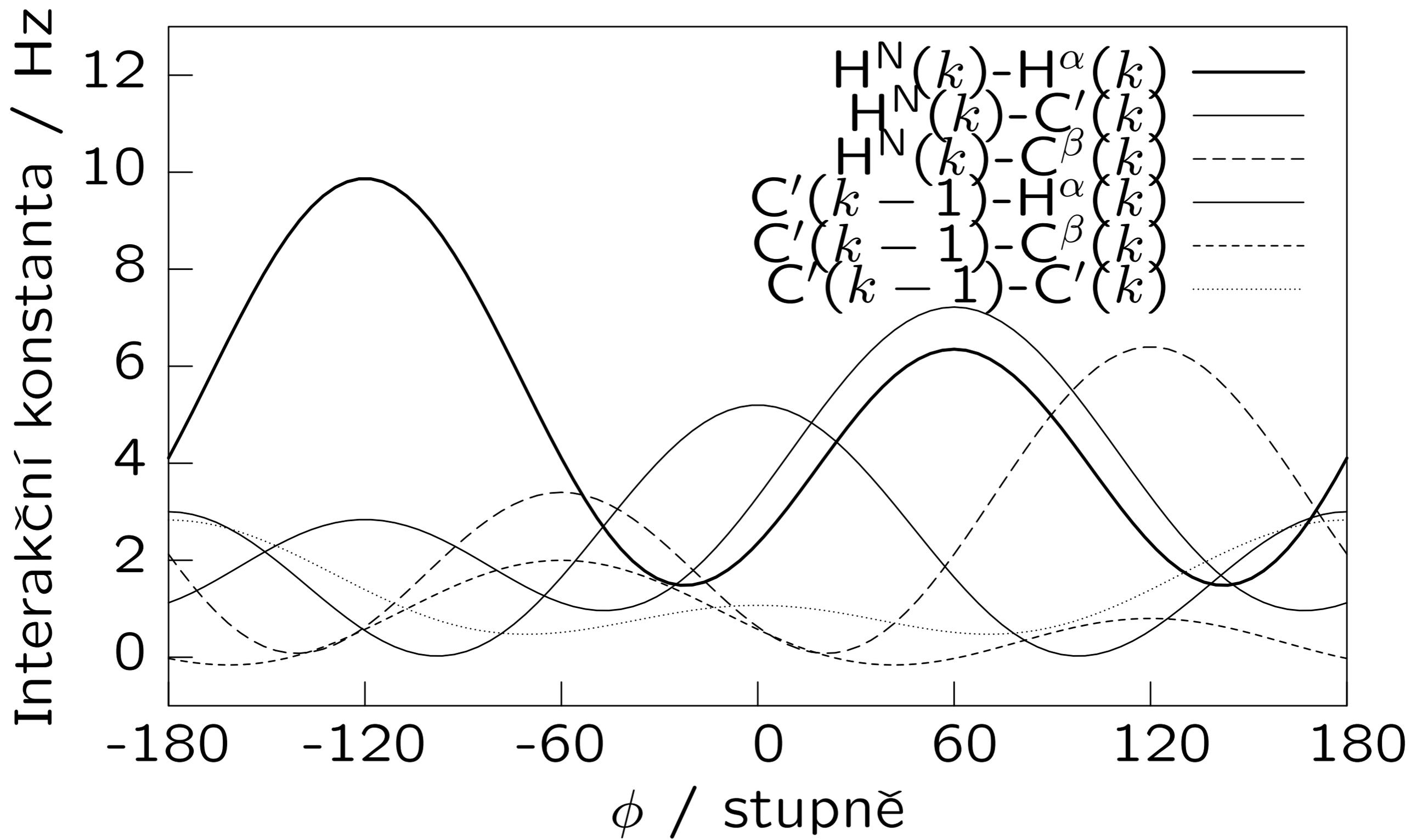




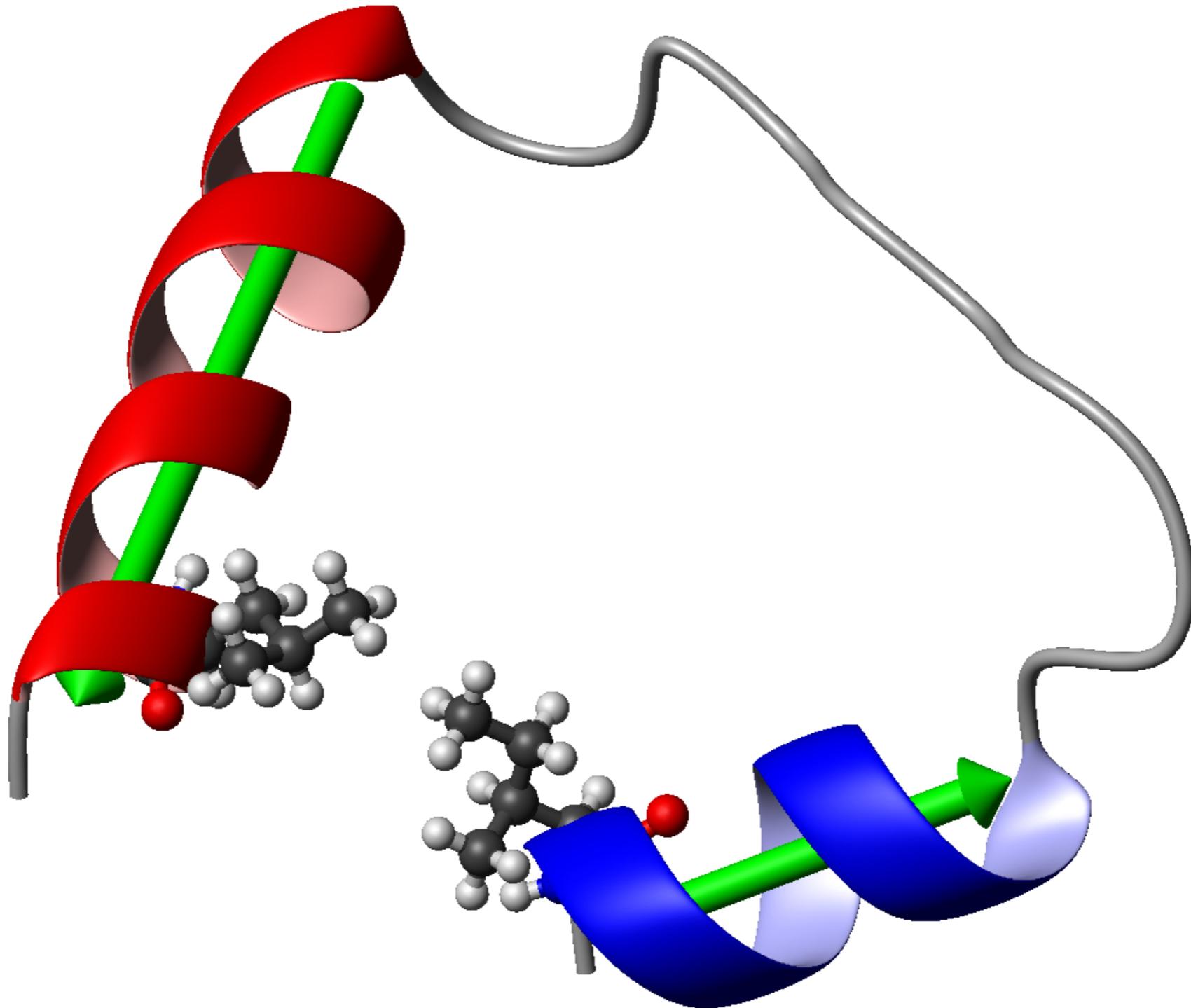
$$\frac{S}{S_{\text{ref}}} = \left(\frac{r_{\text{ref}}}{r}\right)^6 \quad (1)$$

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

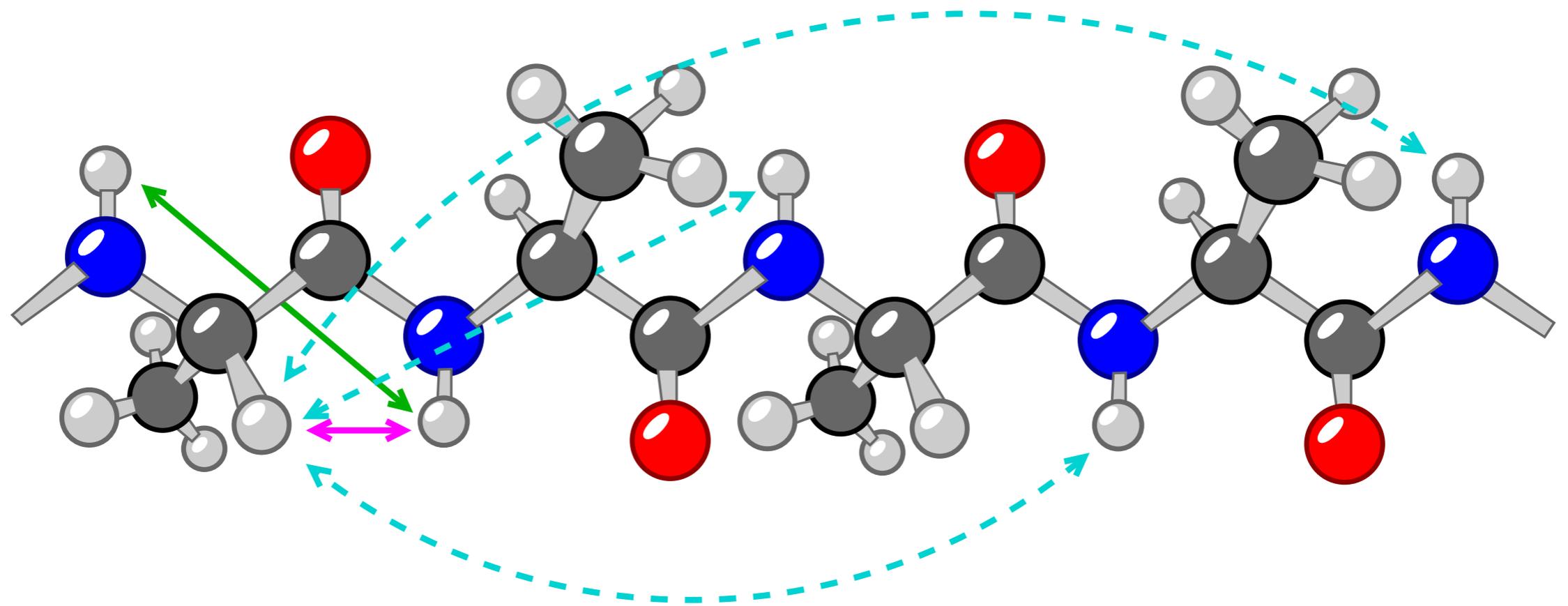
Referenční protony		vzdálenost
geminální v methylenu	$\text{H}-\text{C}-\text{H}$	0,17 nm
vicinální v aromatickém kruhu	$\text{H}-\text{C}=\text{C}-\text{H}$	0,25 nm
<i>meta</i> v aromatickém kruhu	$\text{H}-\text{C}=\text{CH}-\text{C}-\text{H}$	0,42 nm

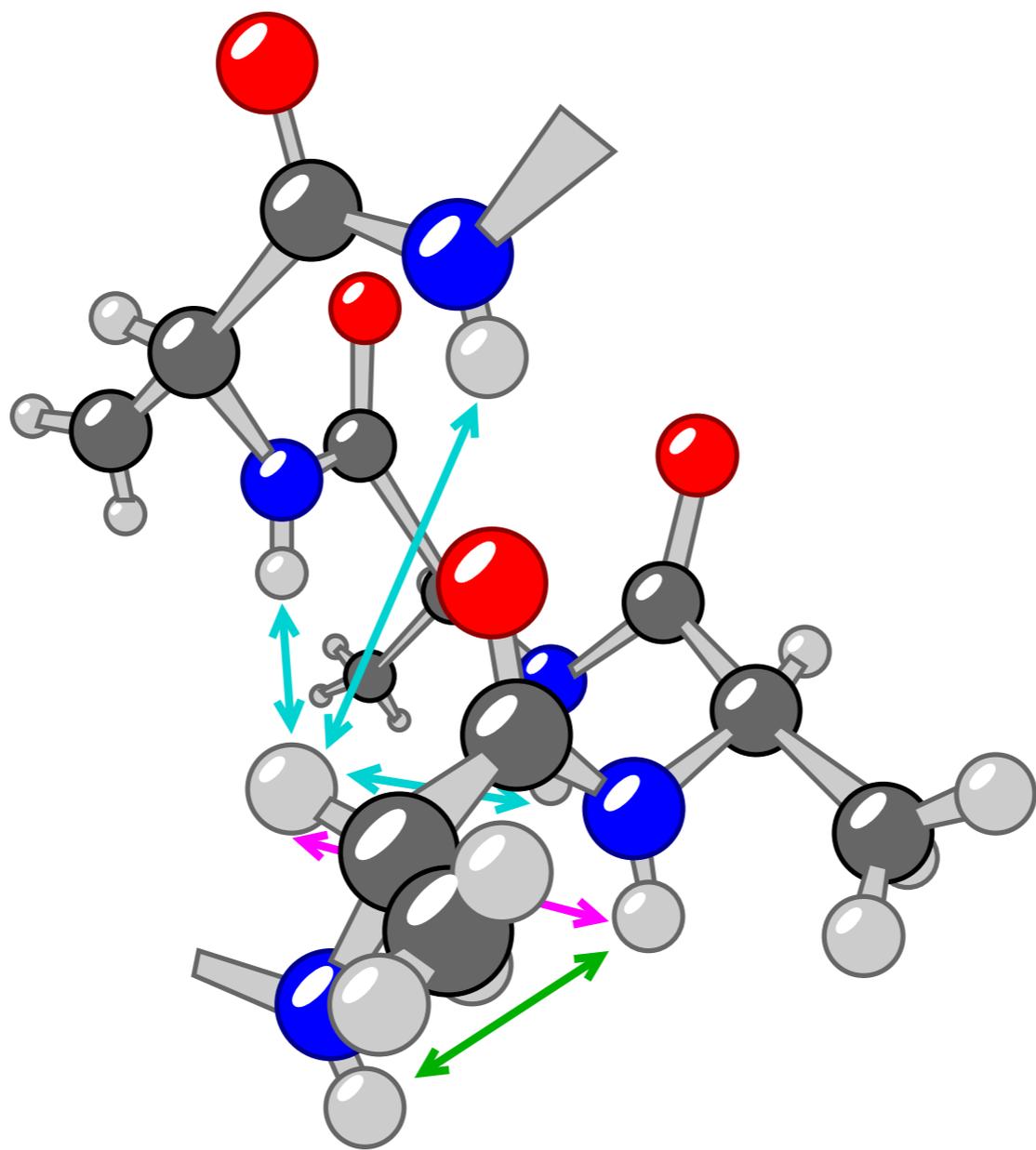


Zbytkové dipólové interakce $\propto \langle 3 \cos^2 \theta - 1 \rangle \Rightarrow$ orientace



Data	β -list	α -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



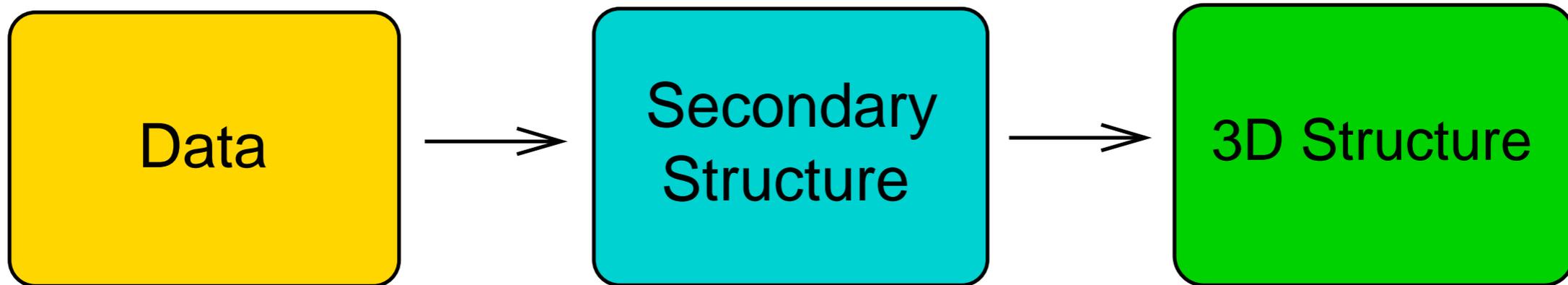


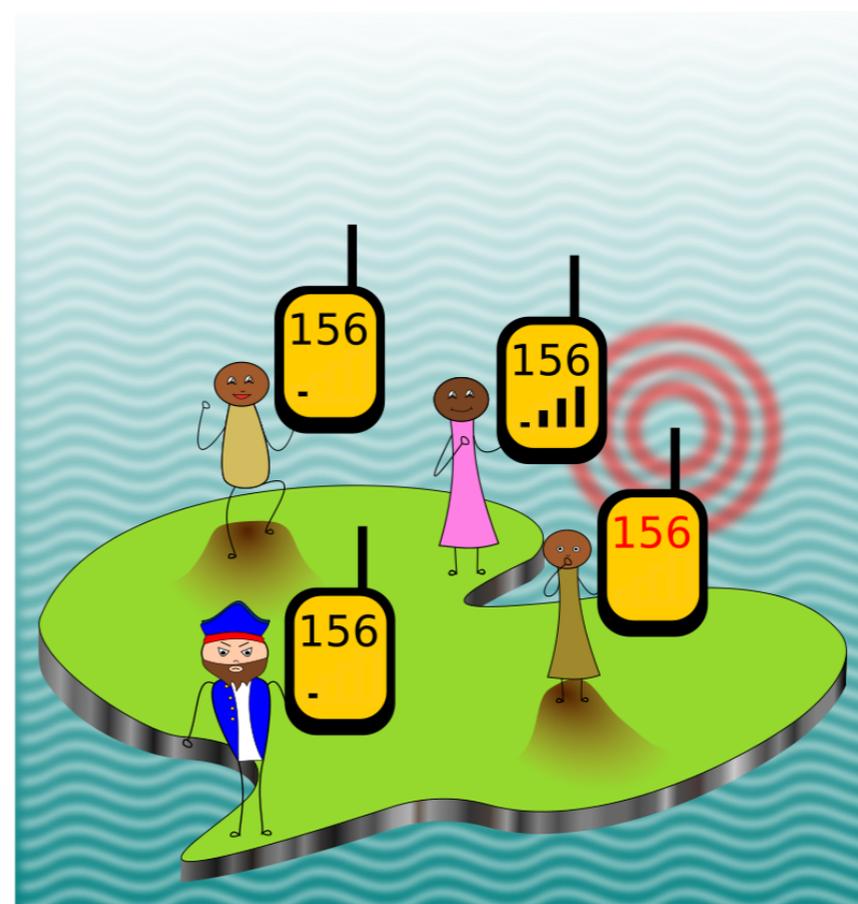
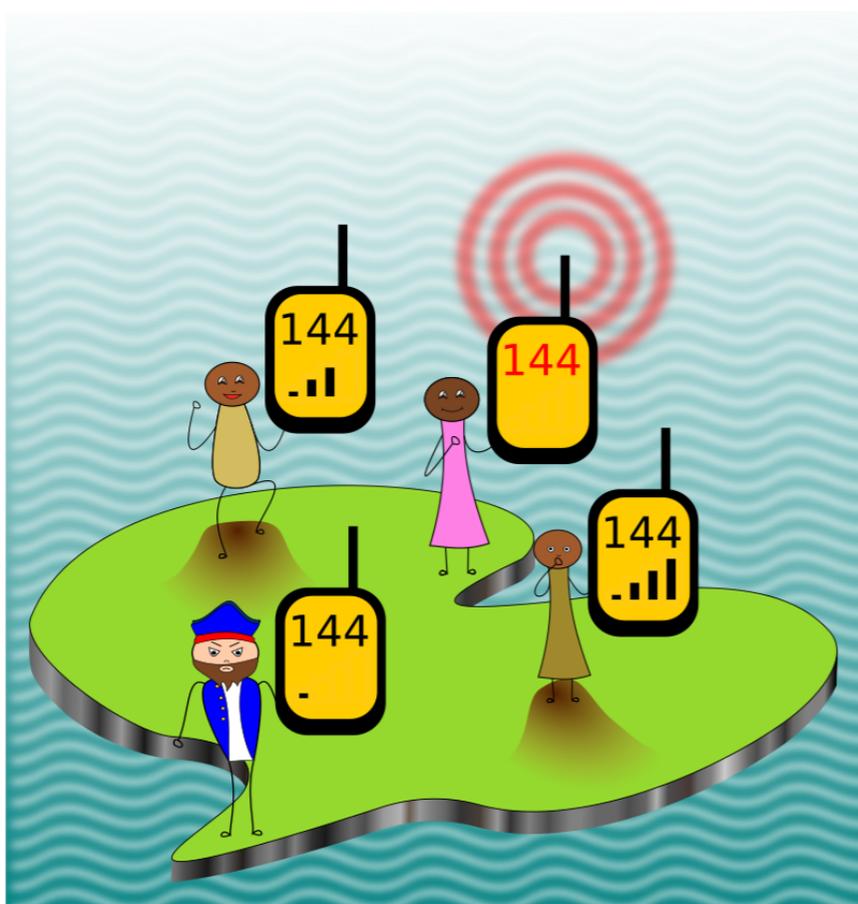
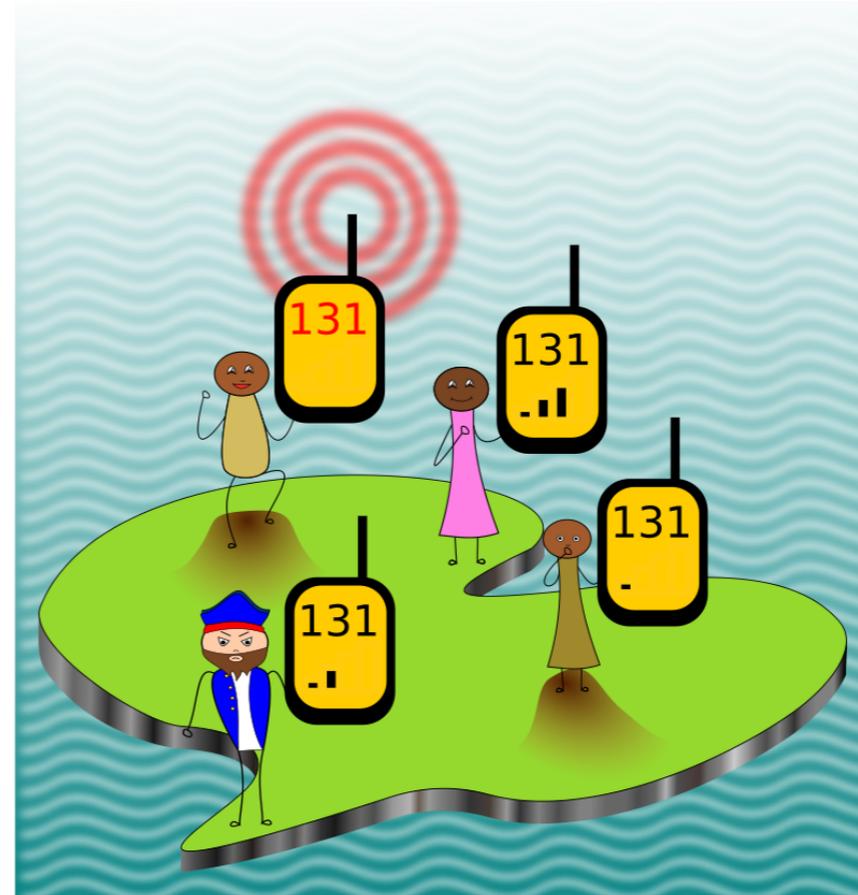
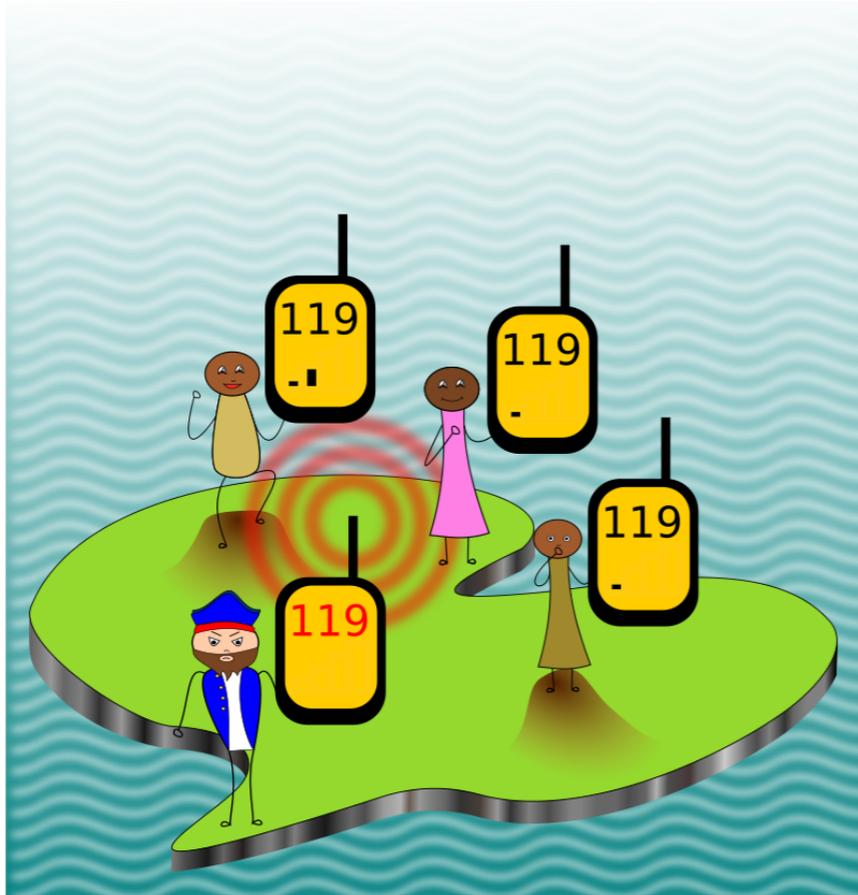
α -helix

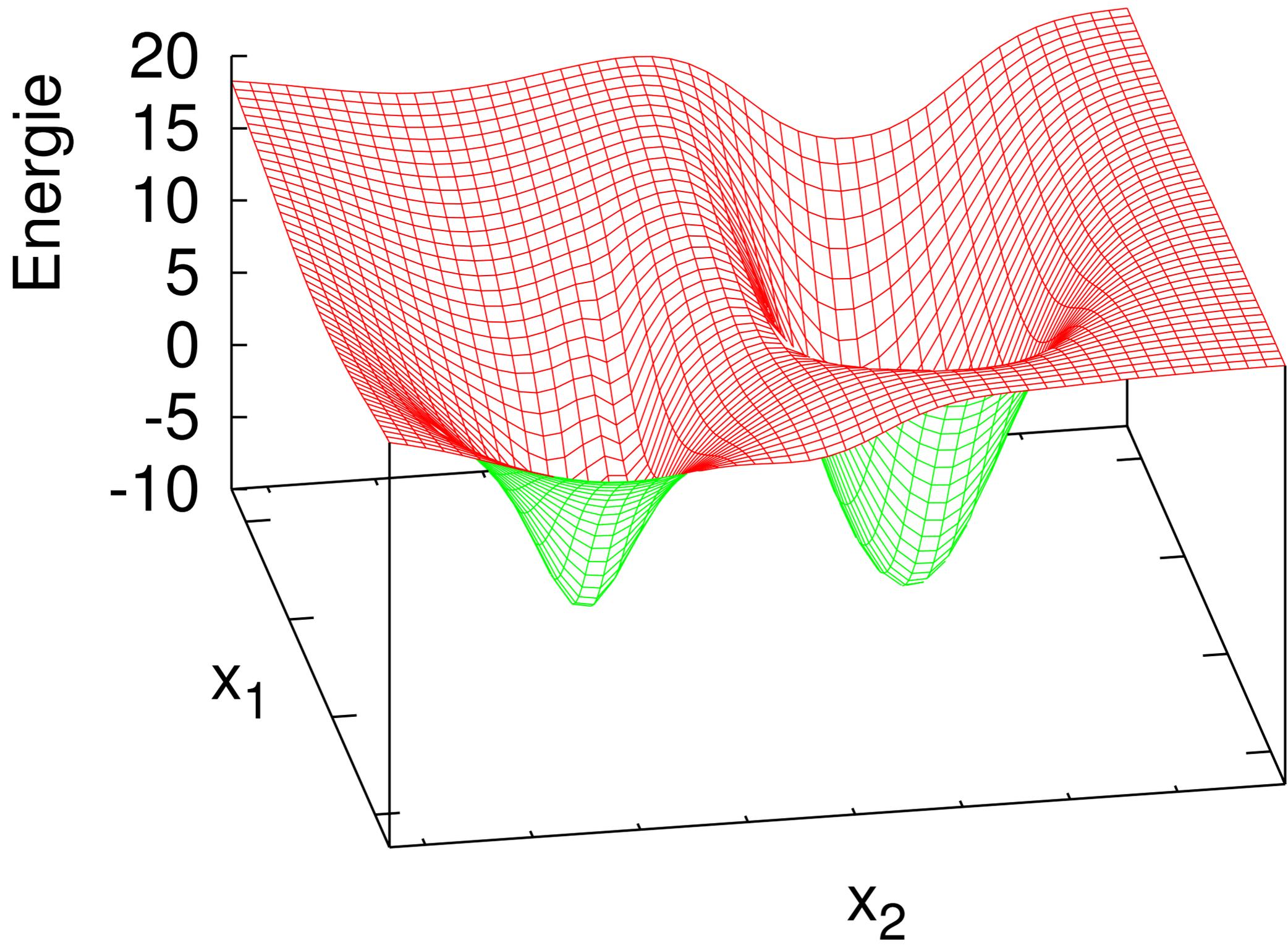
3_{10} -helix

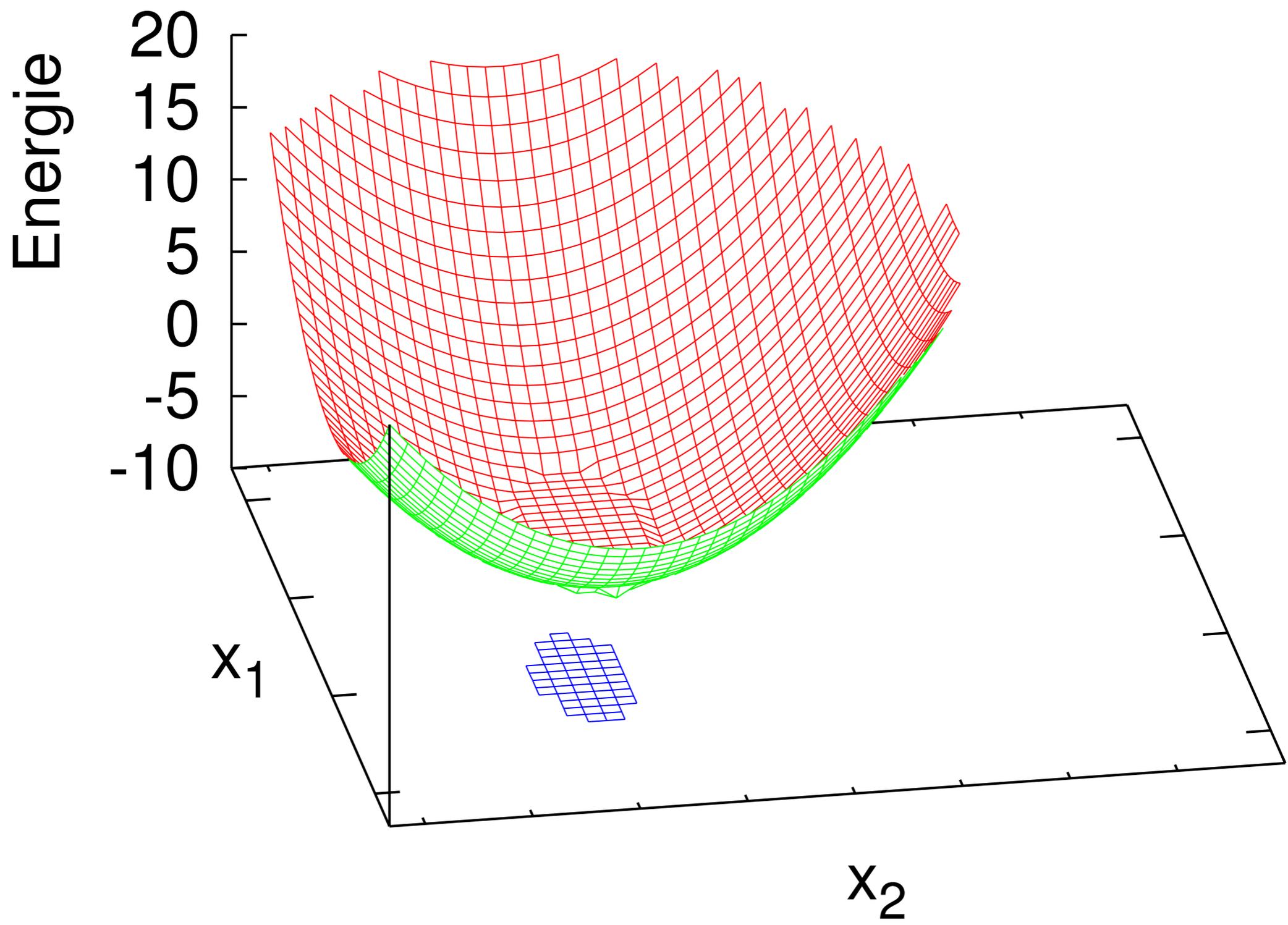
antiparallel β -sheet

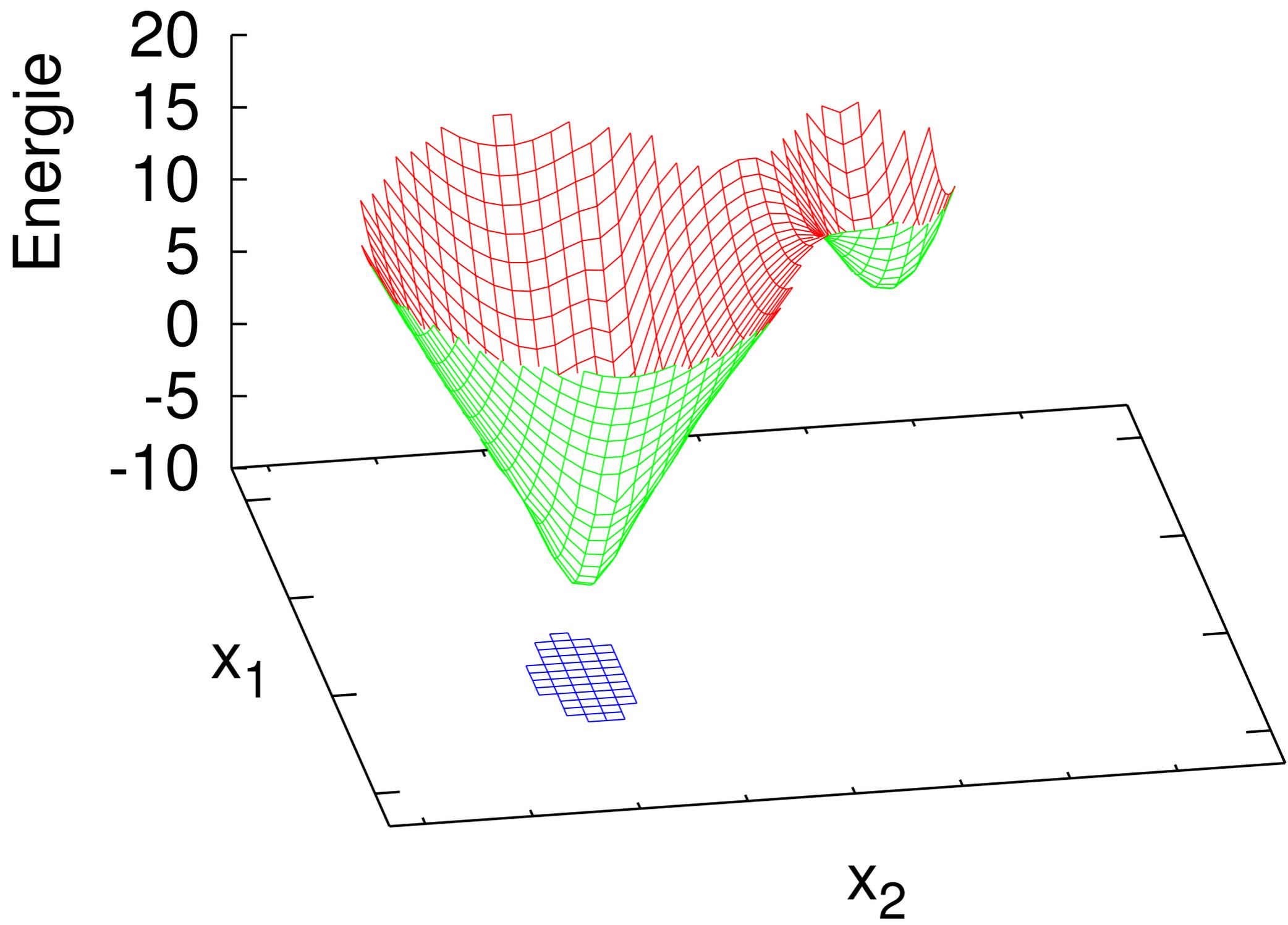
parallel β -sheet

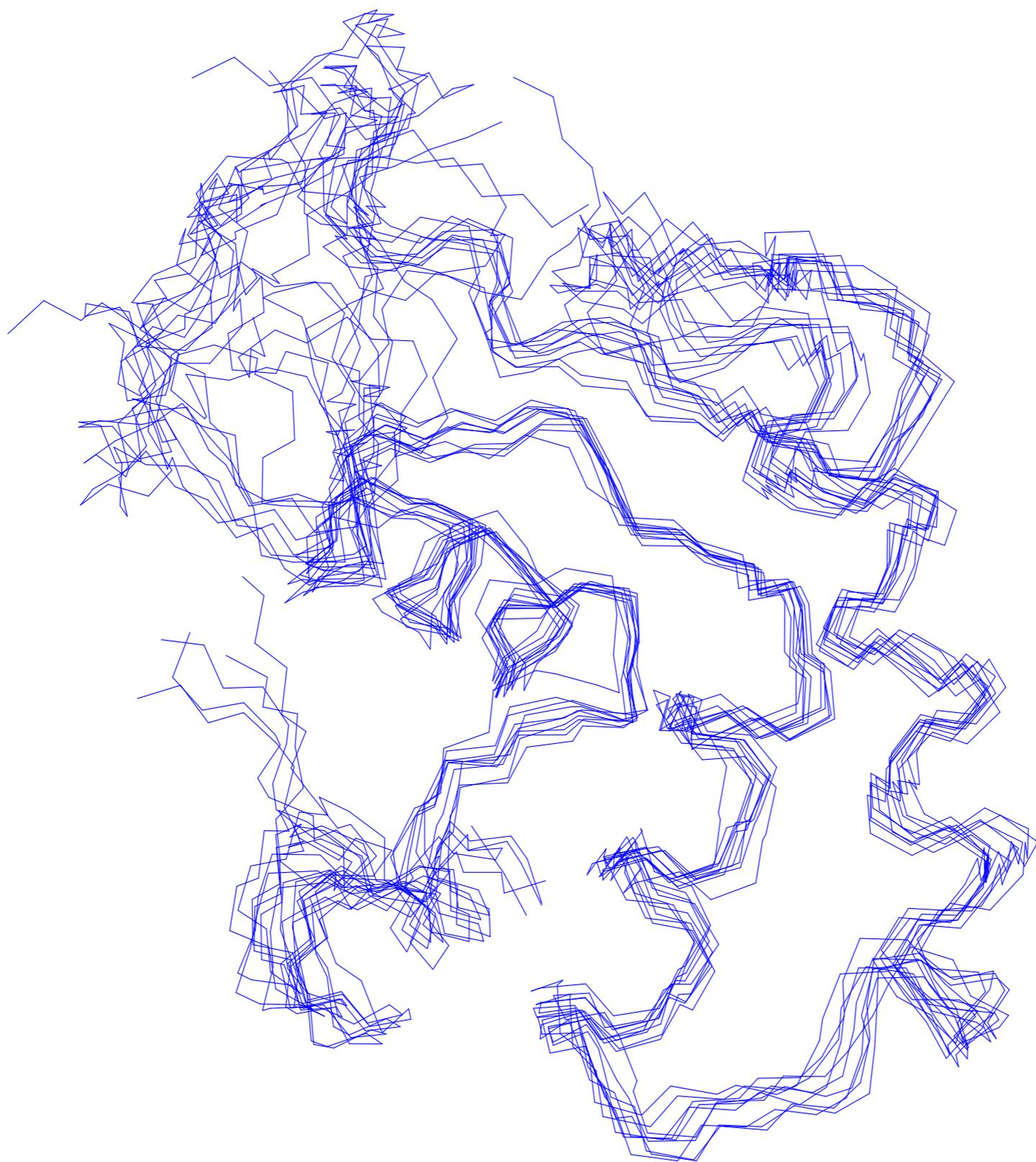


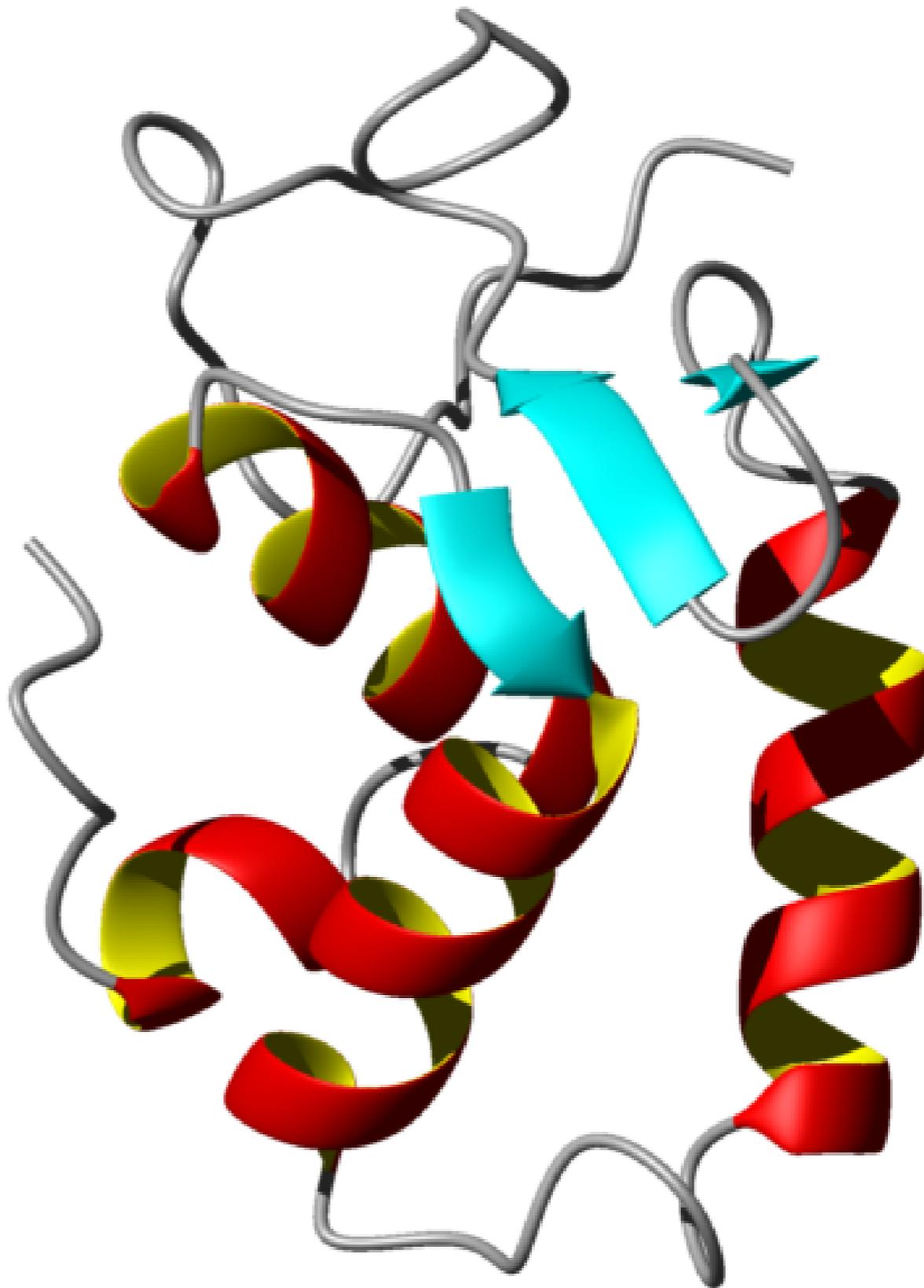






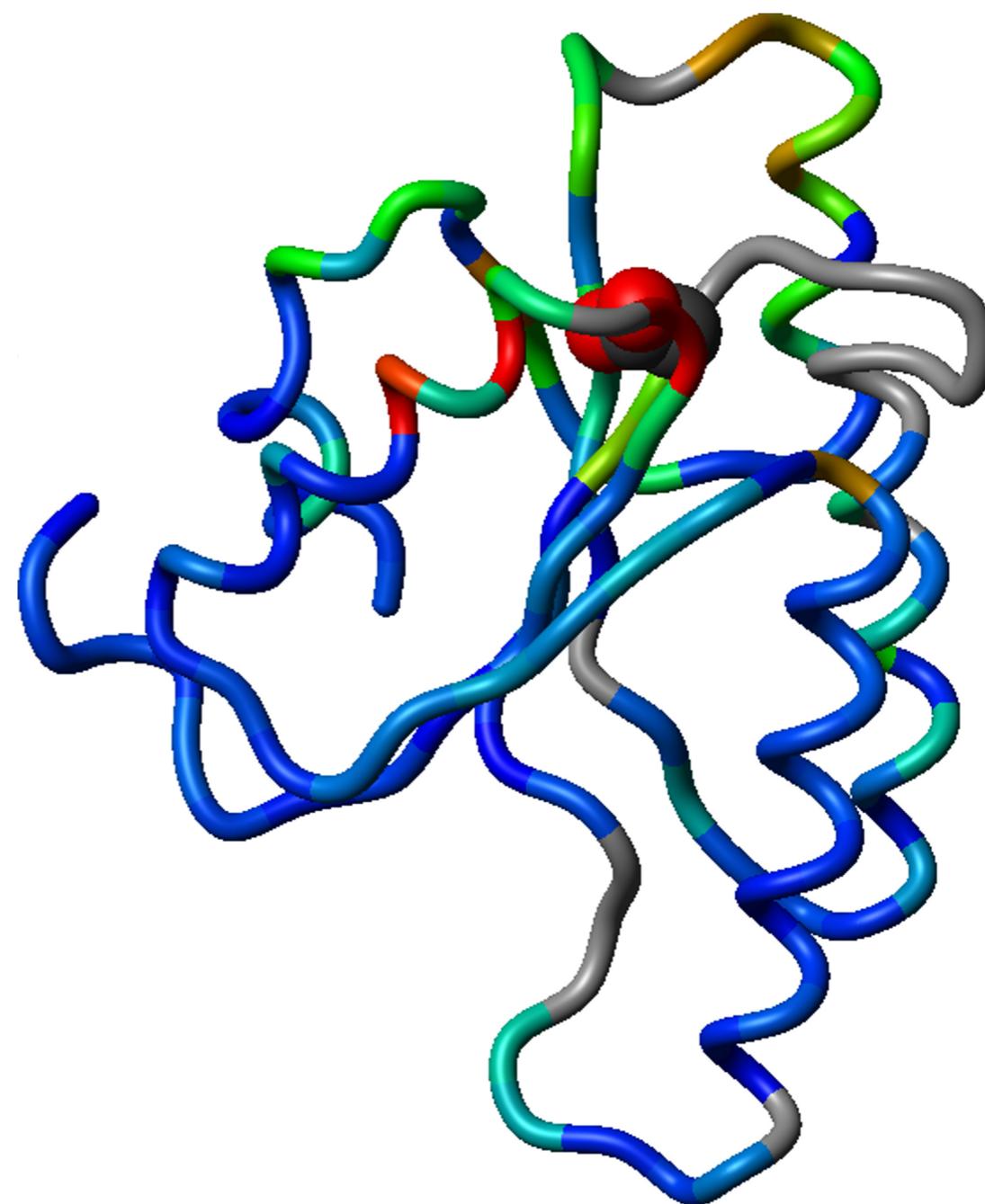
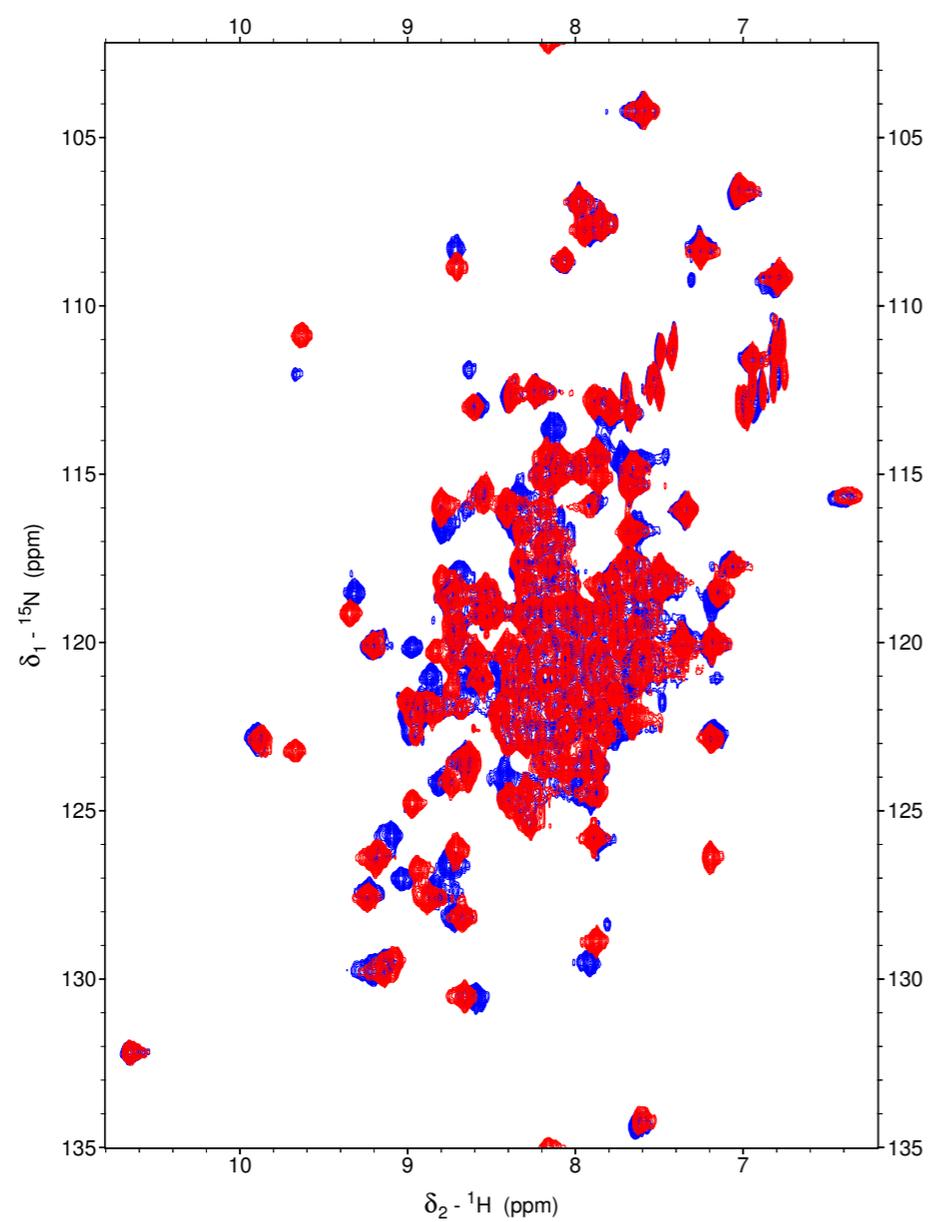






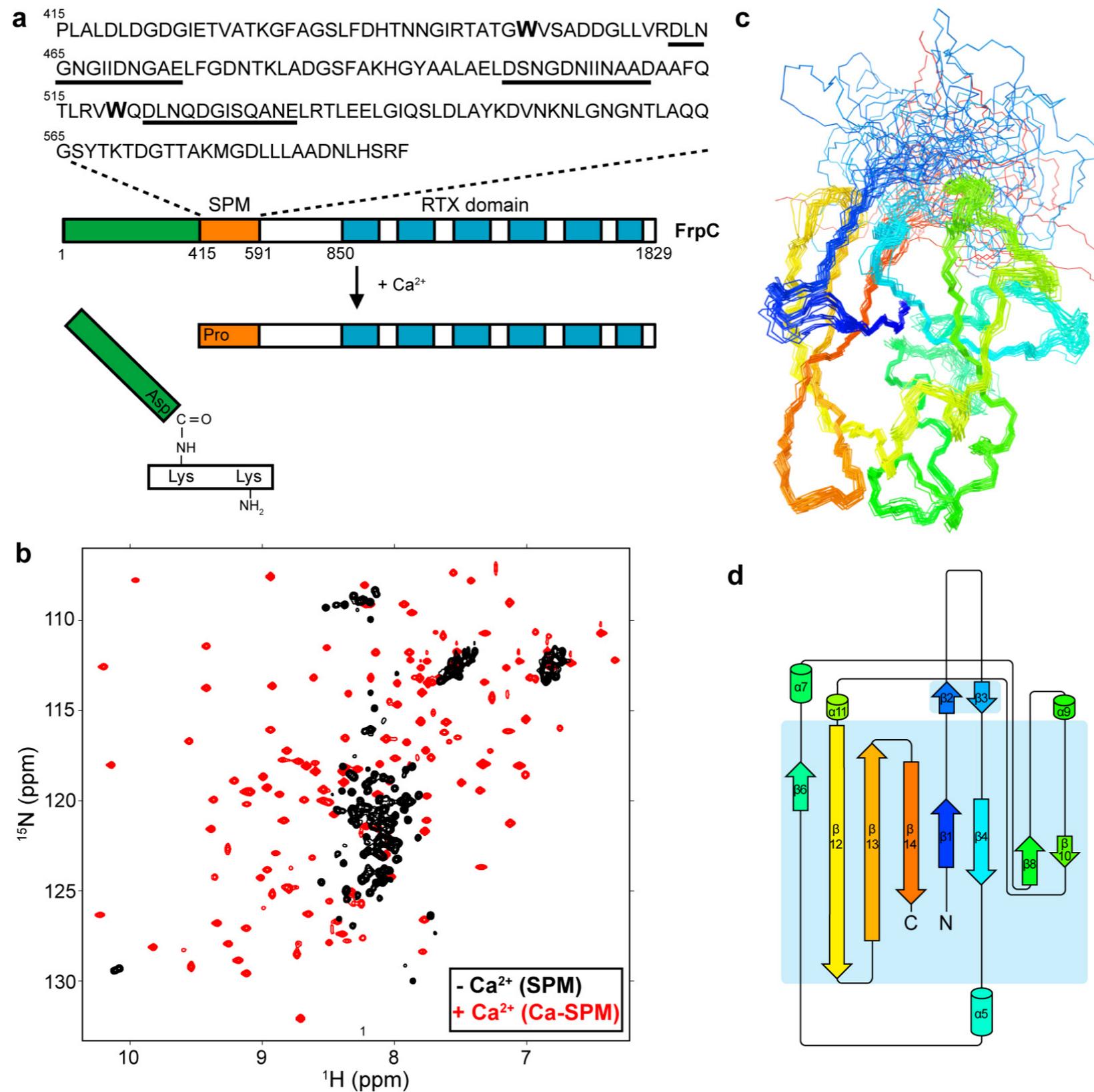
Příklady využití NMR

Rychlé určení vazebného místa

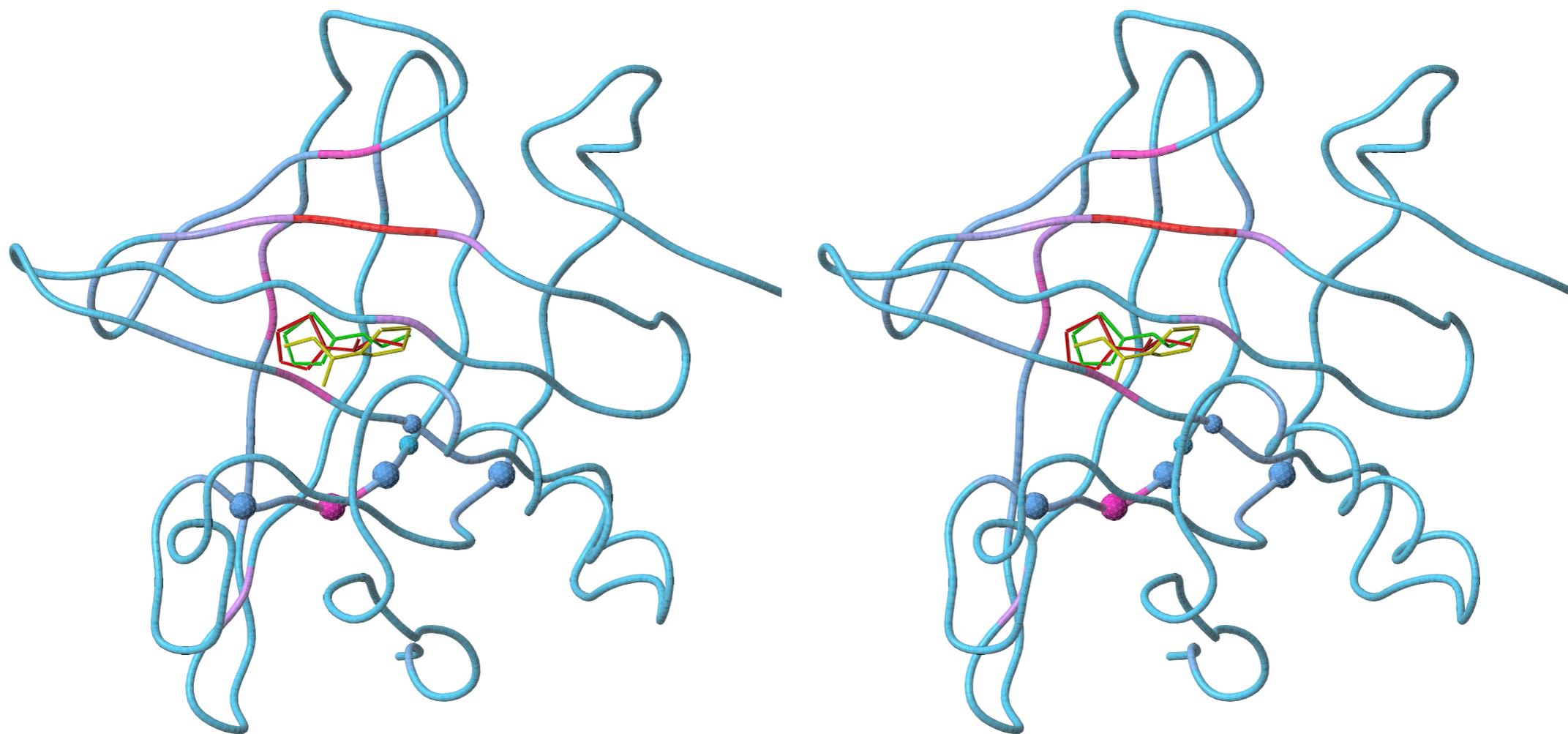


Pekárová et al., *Plant. J.* **67** (2011) 827–839.

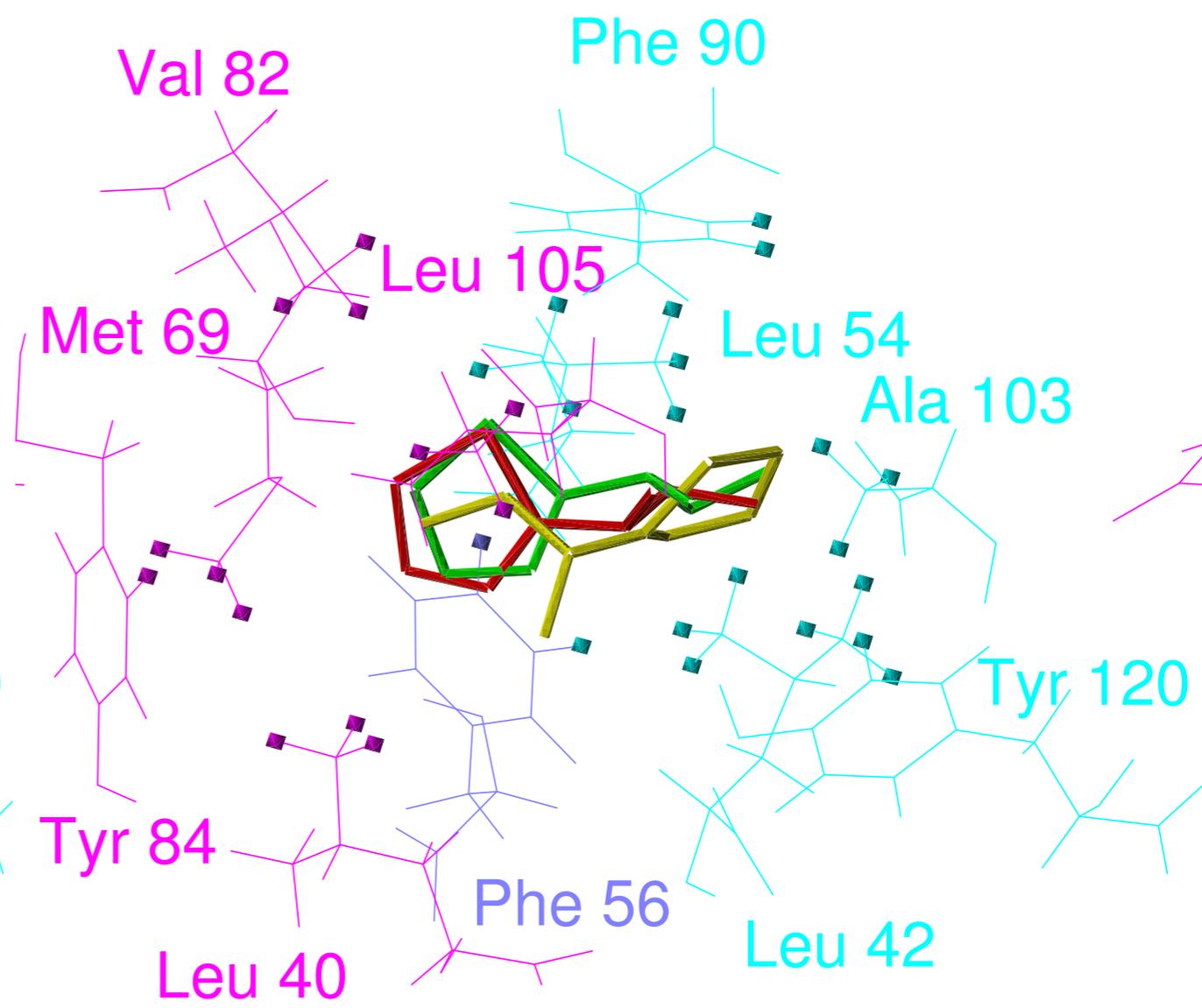
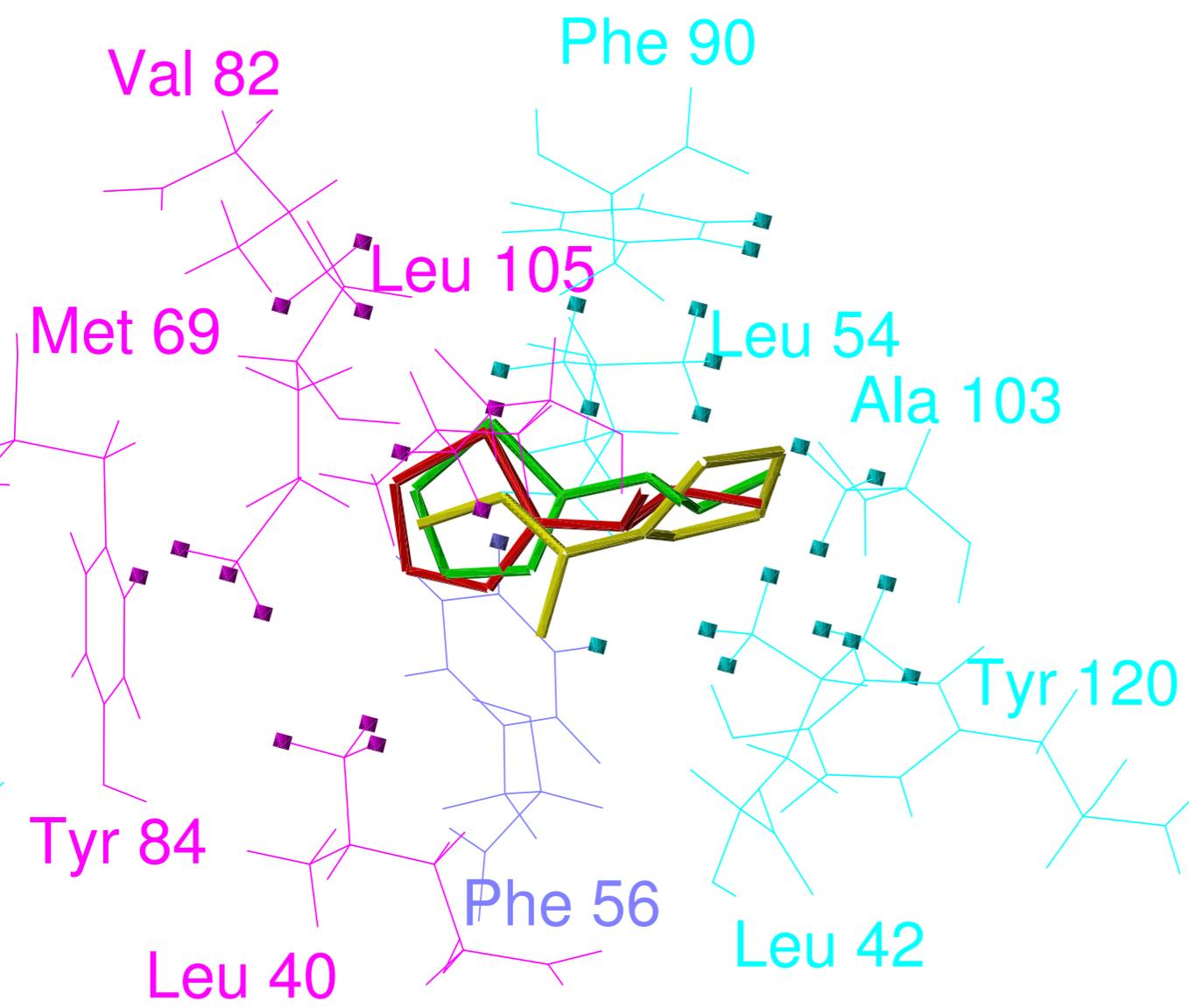
Určení struktury proteinu, který nekrystalizuje



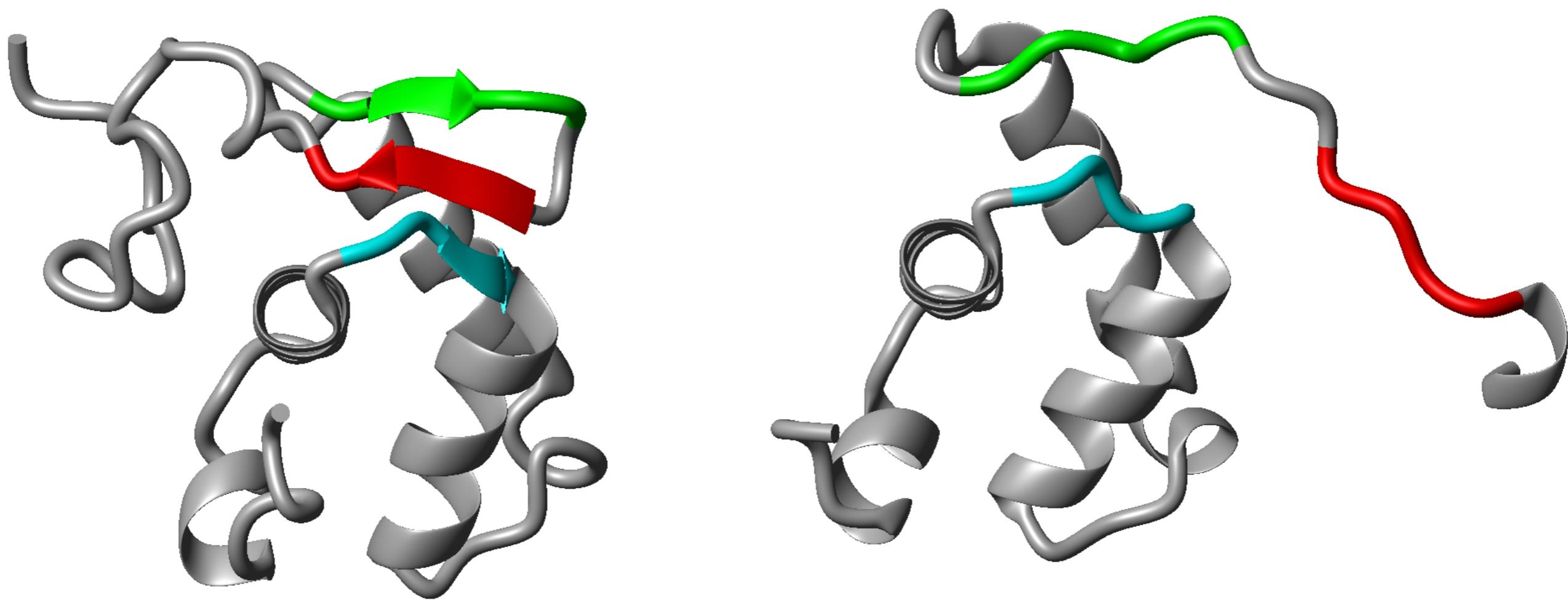
Oprava chybné krystalové struktury



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

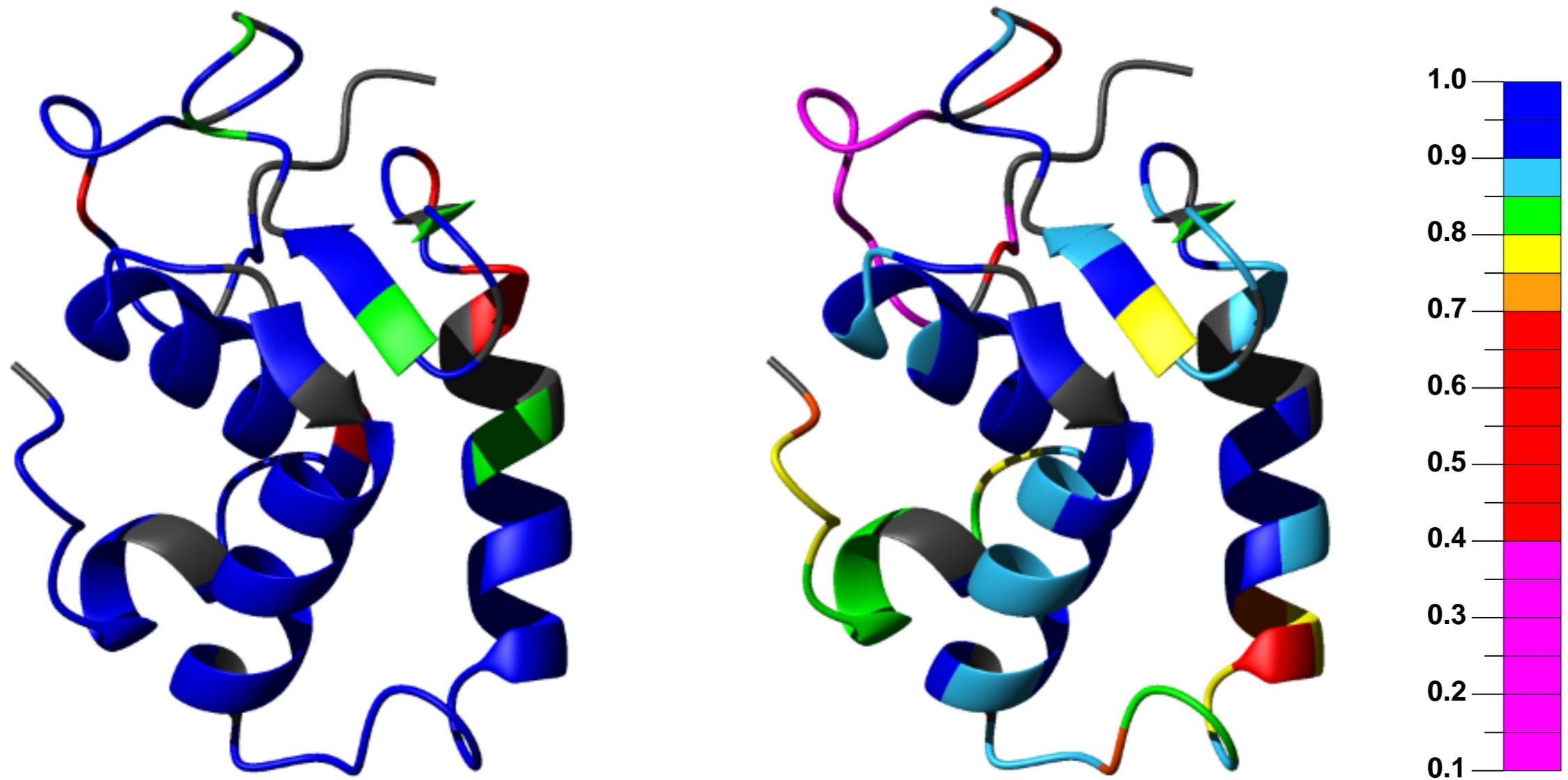


Určení struktury, která se liší v roztoku a krystalu



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

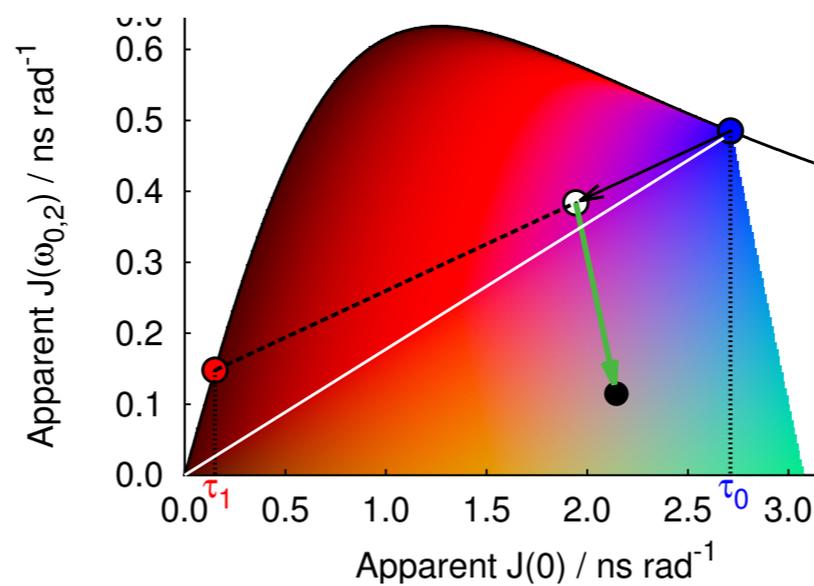
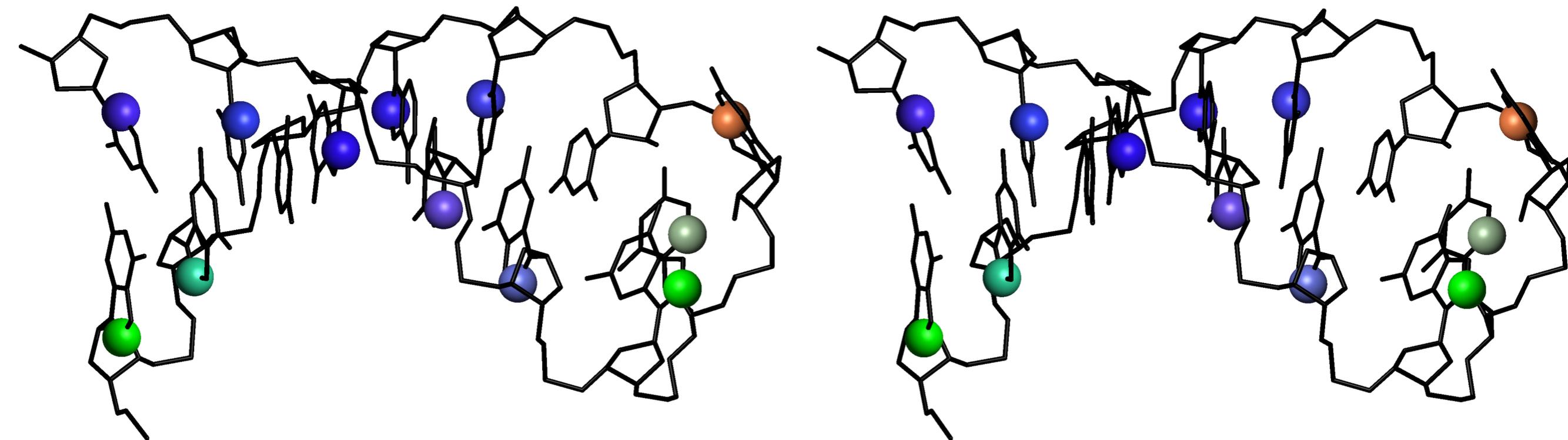
Studium pomalých (μs – ms) a rychlých (ps – ns) pohybů proteinu



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

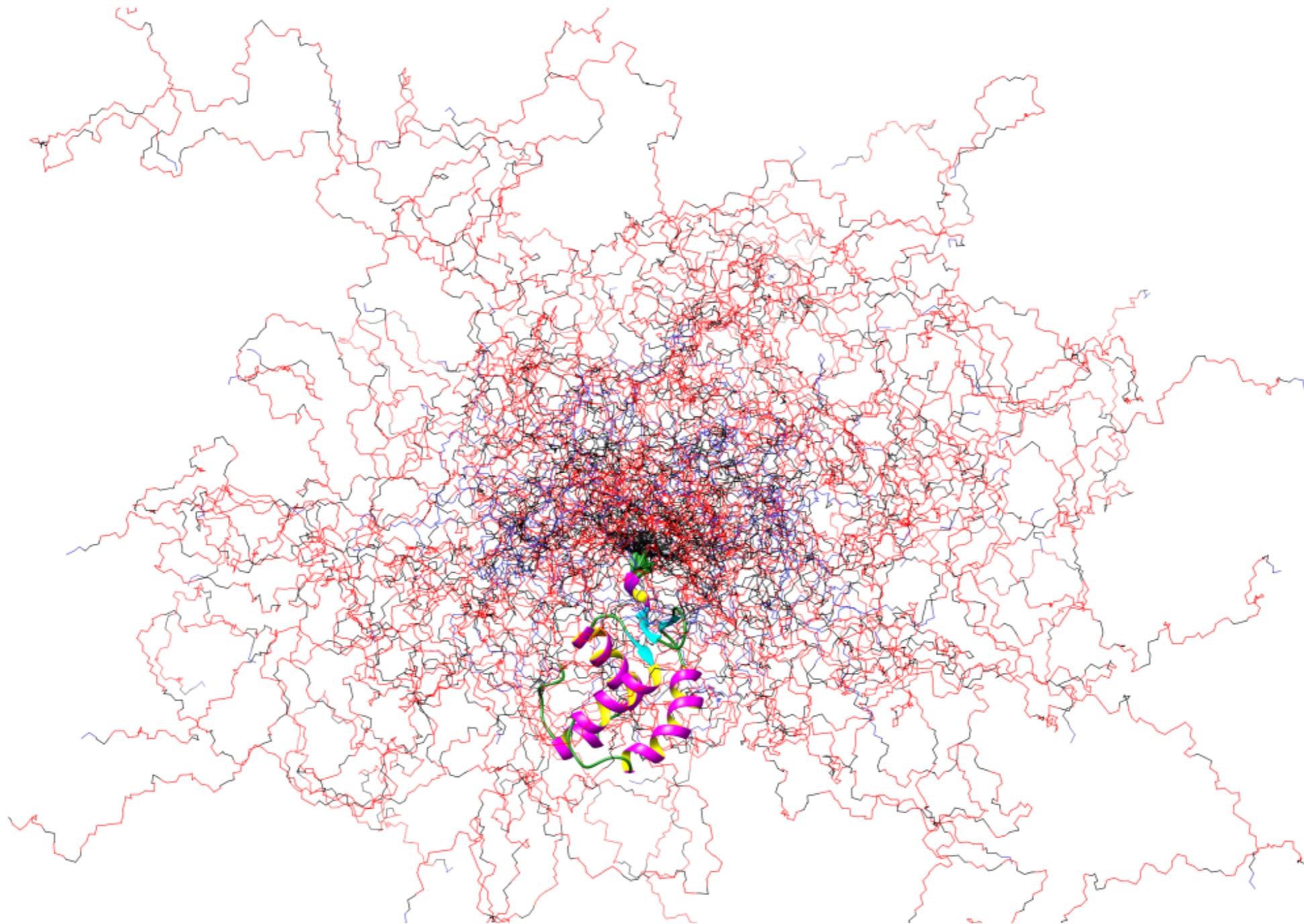
Kadeřávek et al., unpublished

Studium pomalých (μs – ms) a rychlých (ps – ns) pohybů DNA

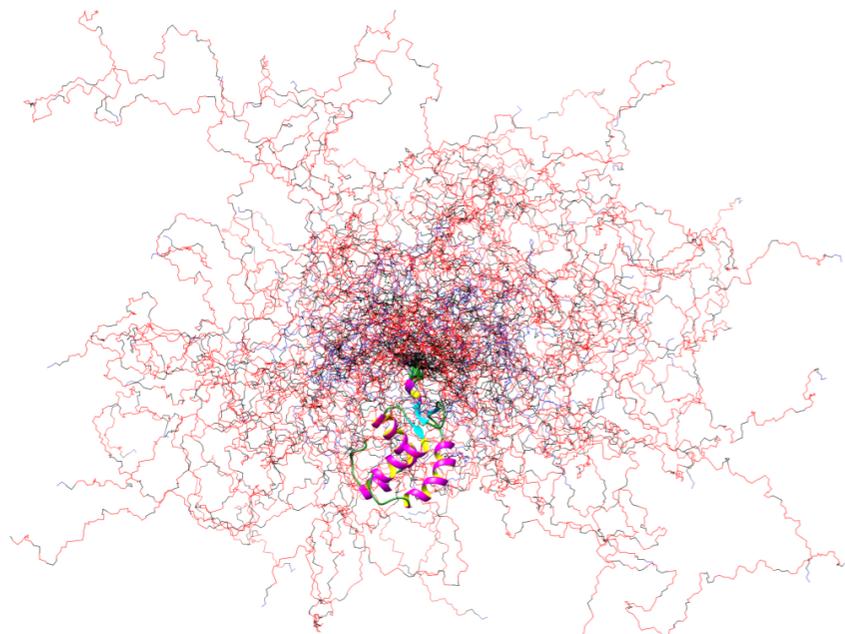


Kadeřávek et al., *J. Magn. Reson.* **266** (2016) 23–40.

Studium částečně neuspořádaného proteinu



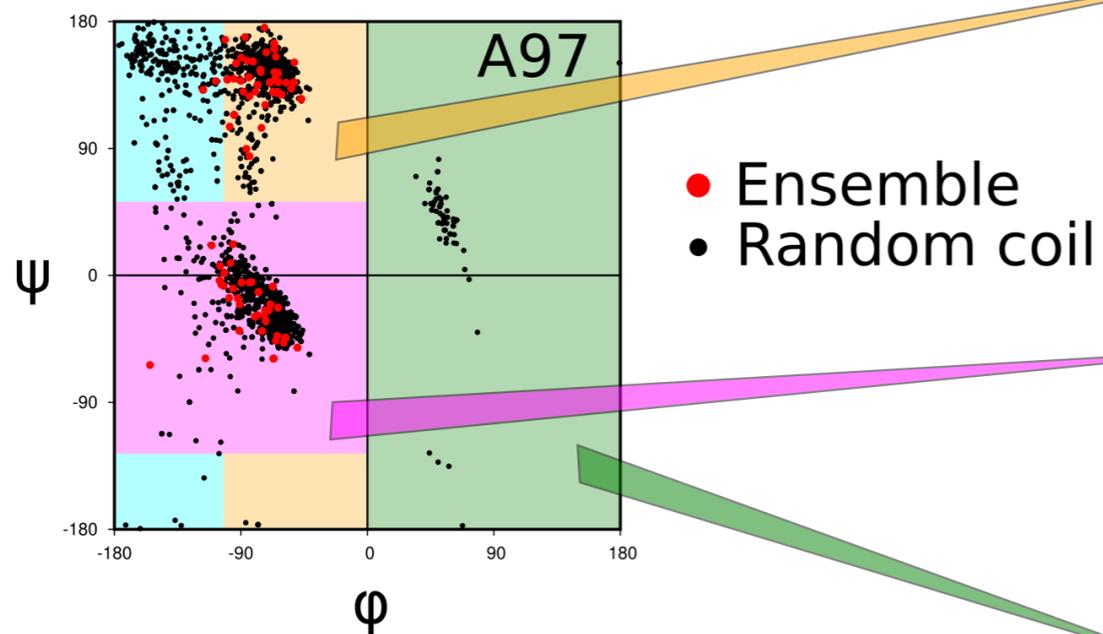
Kubáň et al., *J. Am. Chem. Soc.* **141** (2019) 16817–16828.



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

