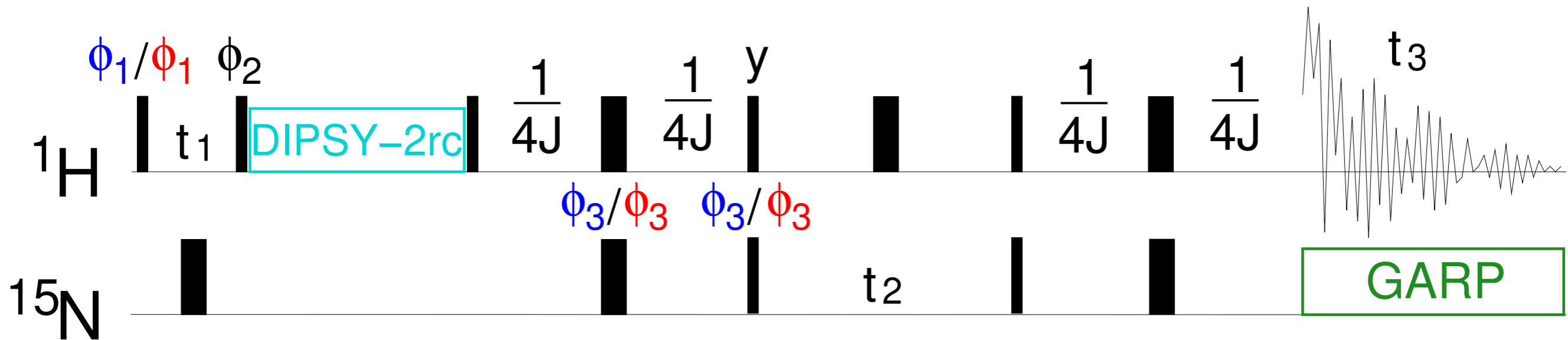


LECTURE 8

TOCSY-HSQC



$\phi_1 = X, X, -X, -X, X, X, -X, -X$

$\phi_1 = Y, Y, -Y, -Y, Y, Y, -Y, -Y$

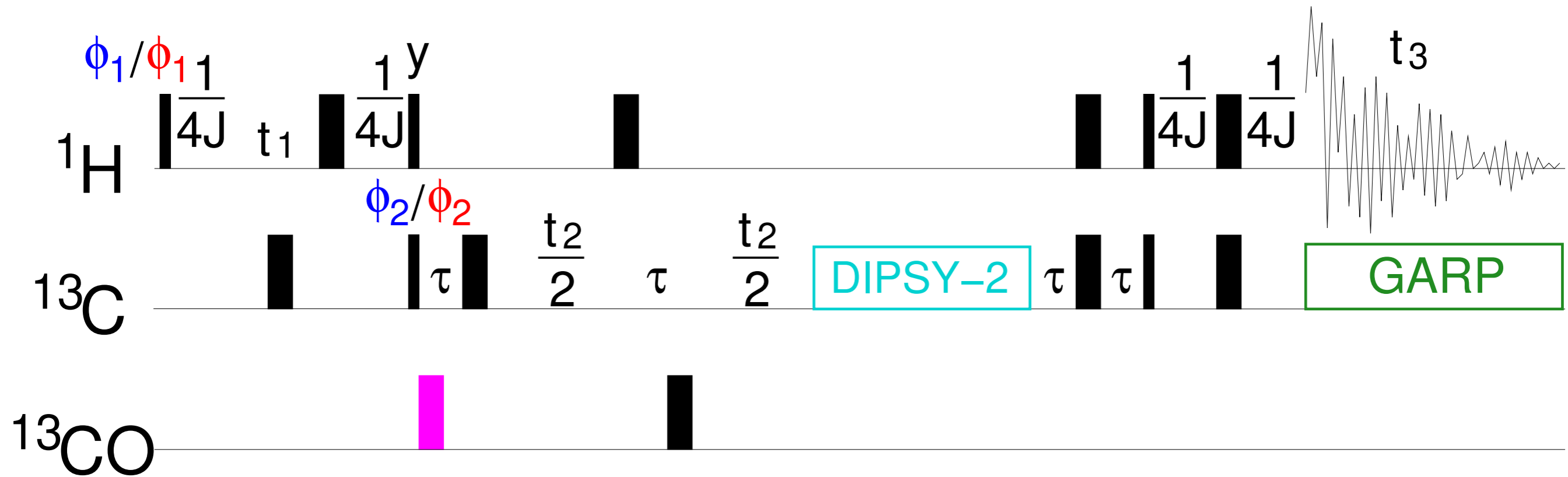
$\phi_2 = X, X, X, X, -X, -X, -X, -X$

$\phi_3 = X, -X, X, -X, X, -X, X, -X$

$\phi_3 = Y, -Y, Y, -Y, Y, -Y, Y, -Y$

receiver phase: $X, -X, -X, X, -X, X, X, -X$

HC(C)H-TOCSY

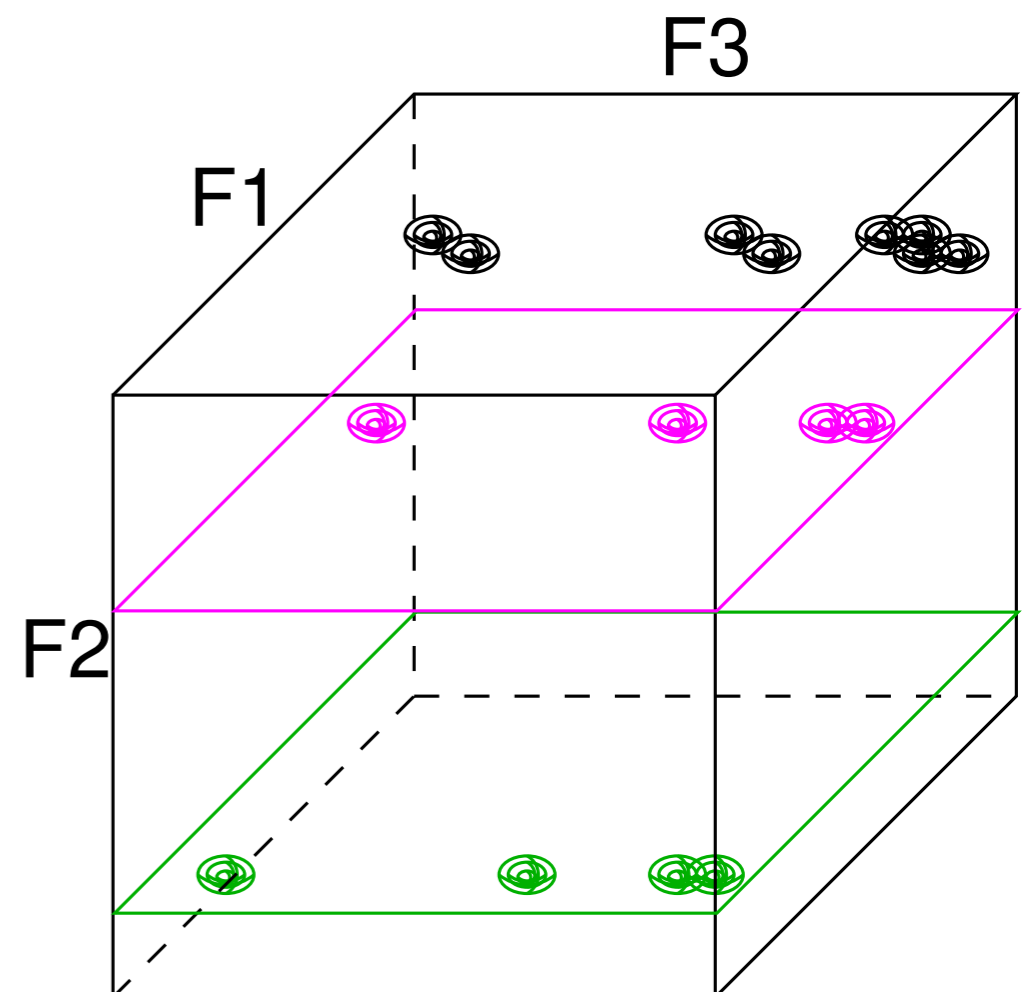
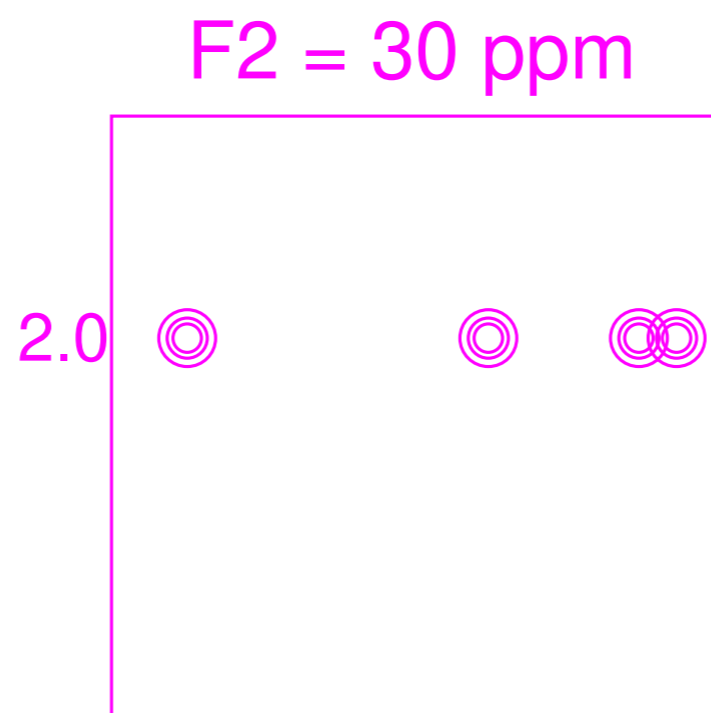
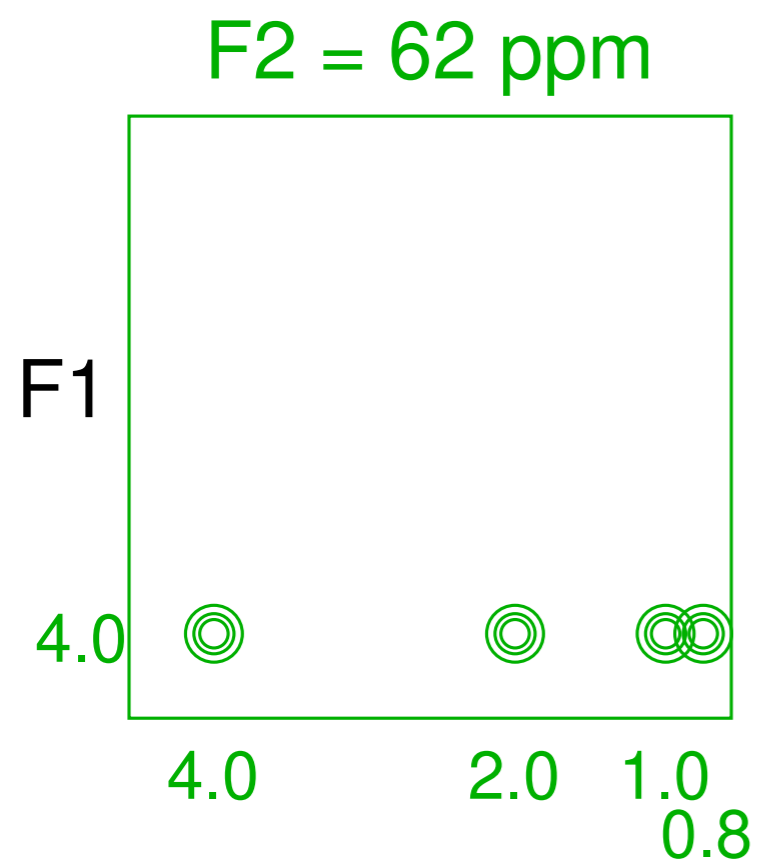


$\phi_1 = X, -X, X, -X, X, -X, X, -X$ $\phi_2 = X, X, -X, -X, X, X, -X, -X$

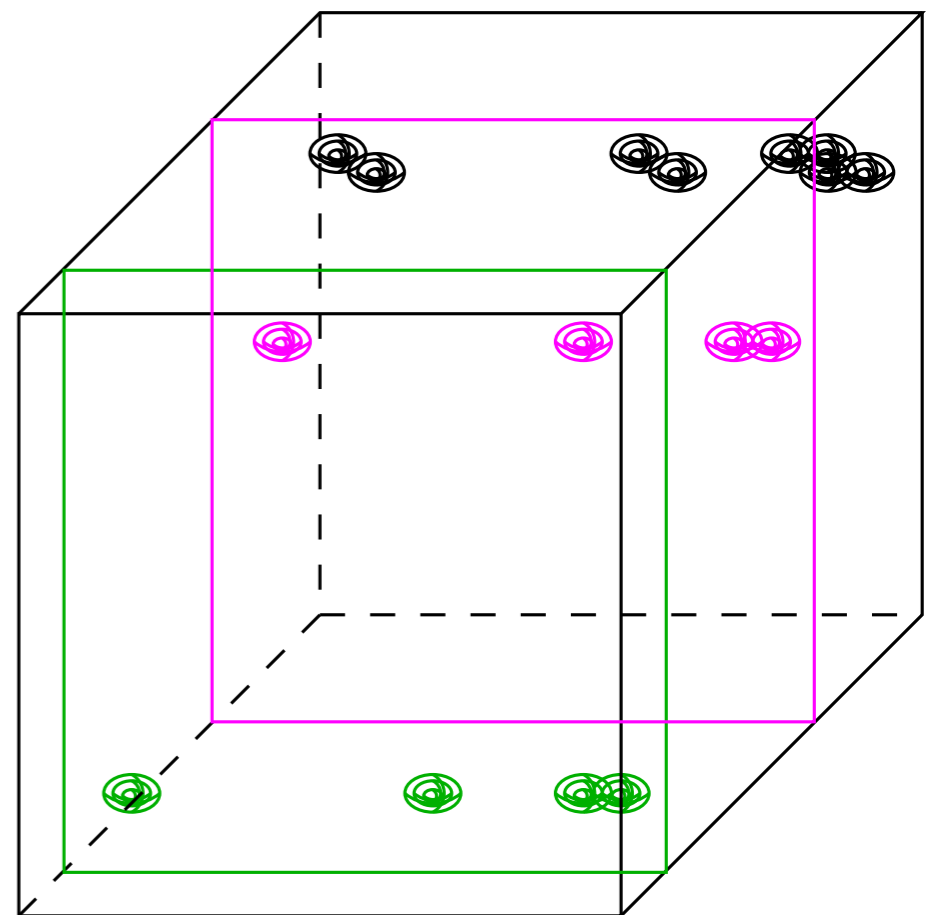
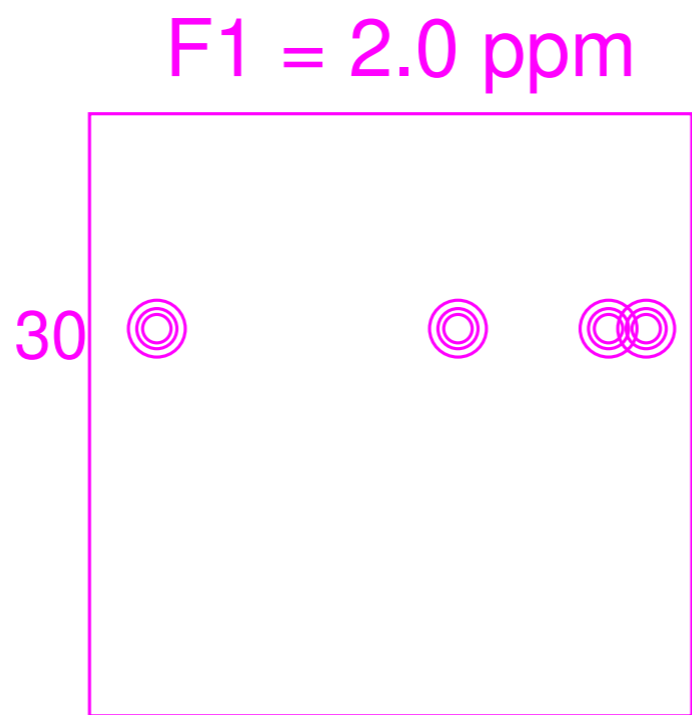
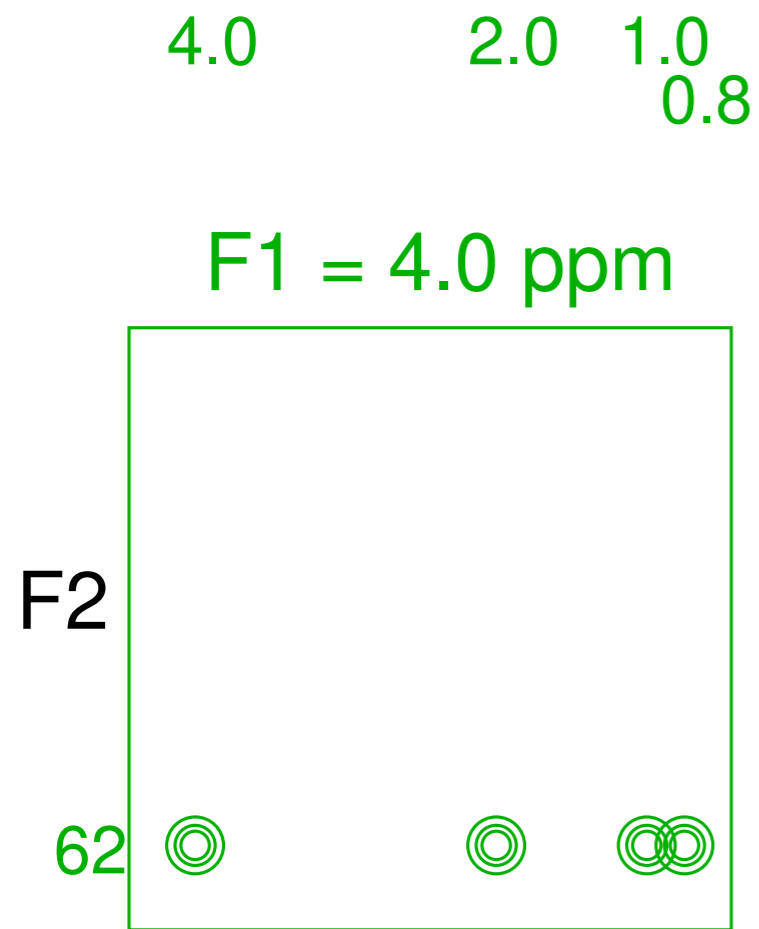
$\phi_1 = y, -y, y, -y, y, -y, y, -y$ $\phi_2 = y, y, -y, -y, y, y, -y, -y$

receiver phase: $x, -x, -x, x, -x, x, x, -x$

a

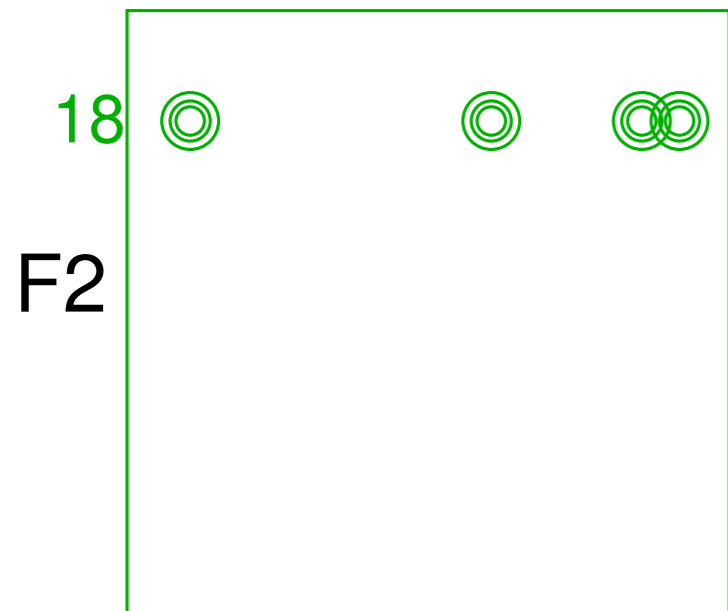


b

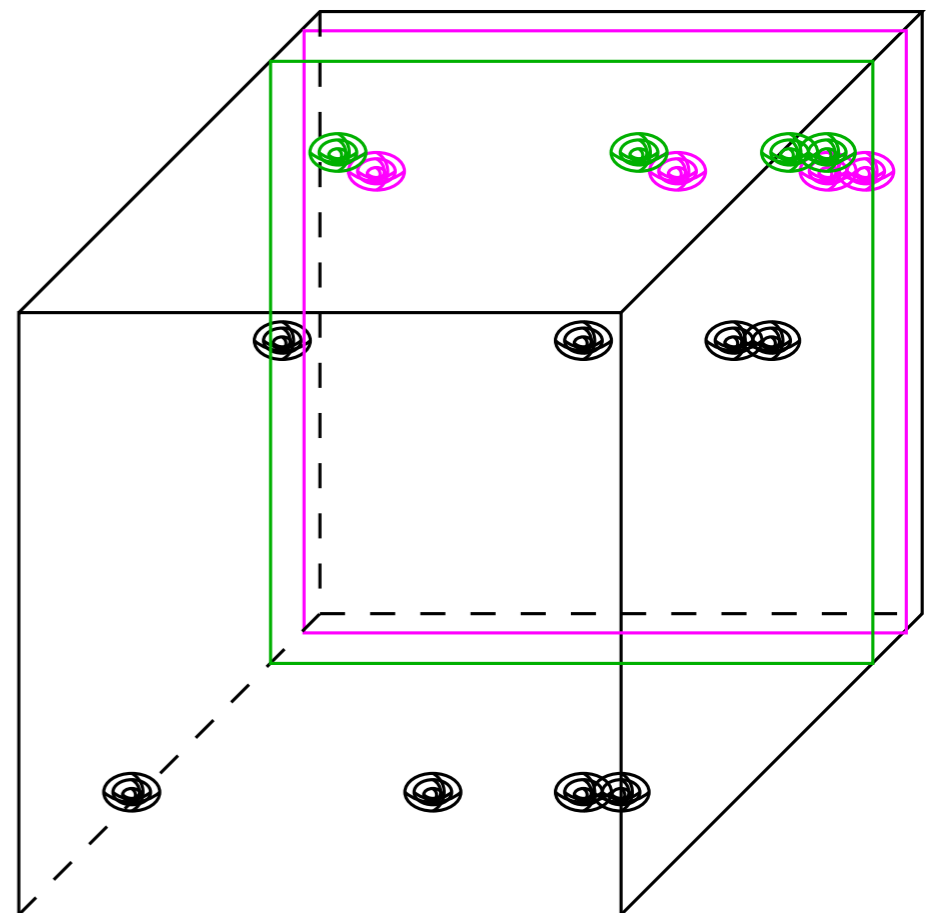
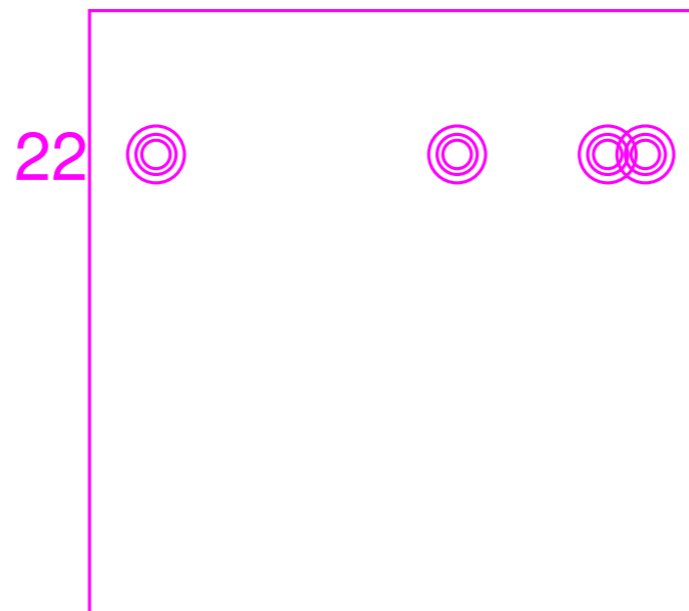


C

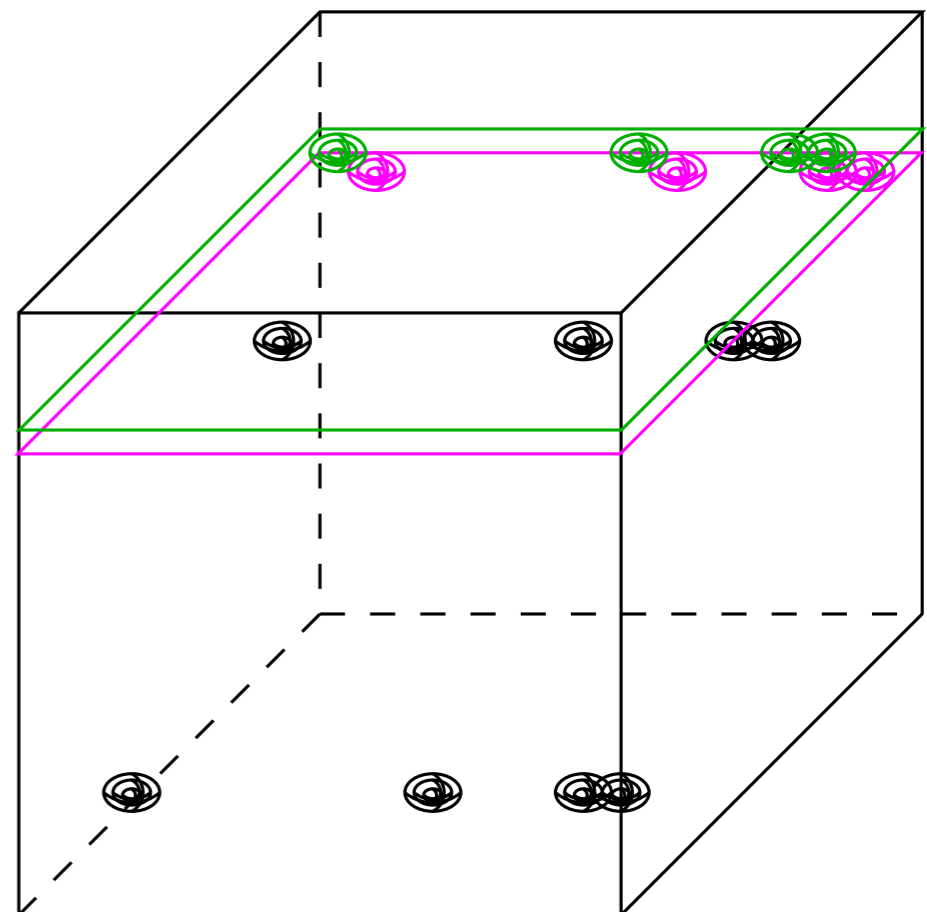
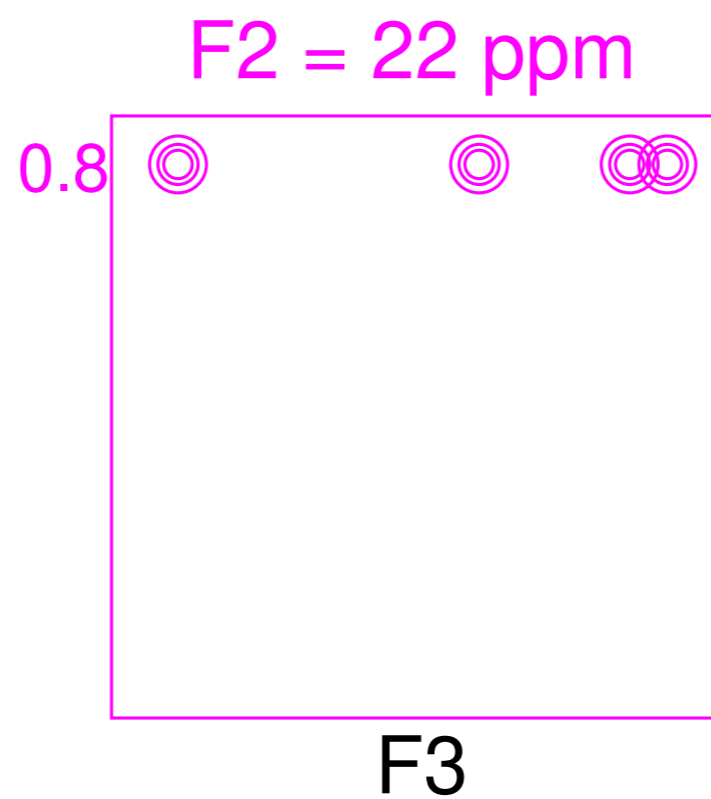
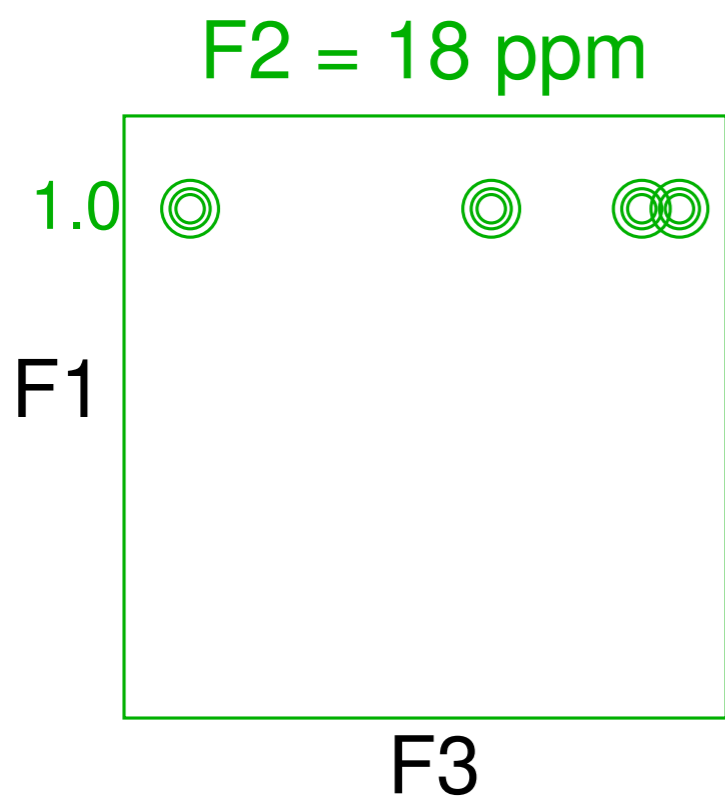
F1 = 1.0 ppm



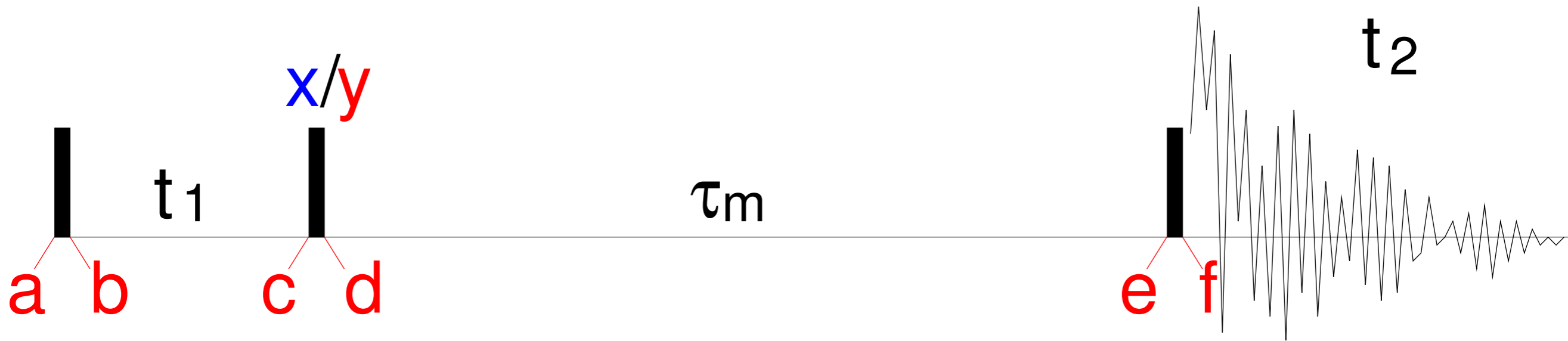
F1 = 0.8 ppm

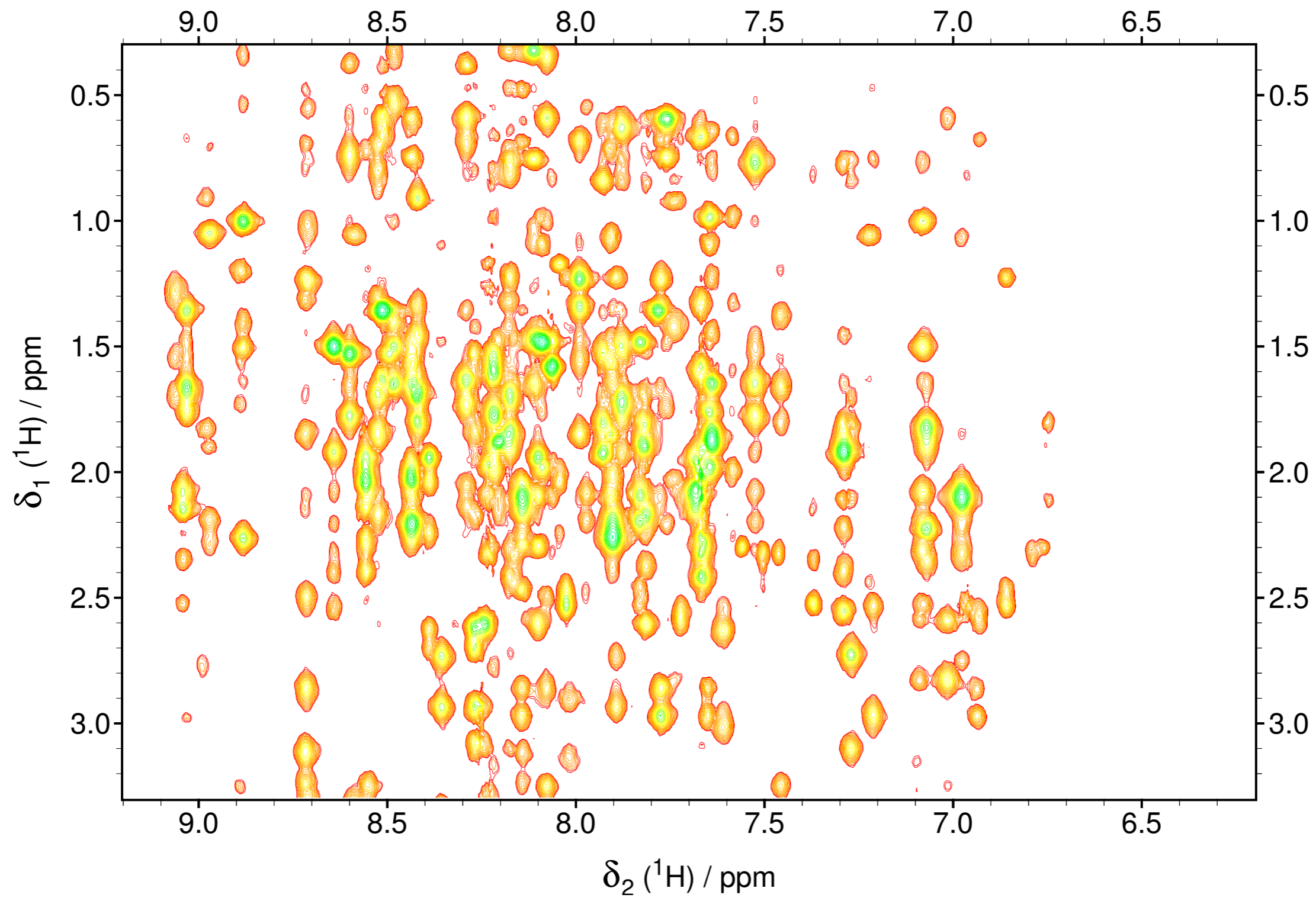


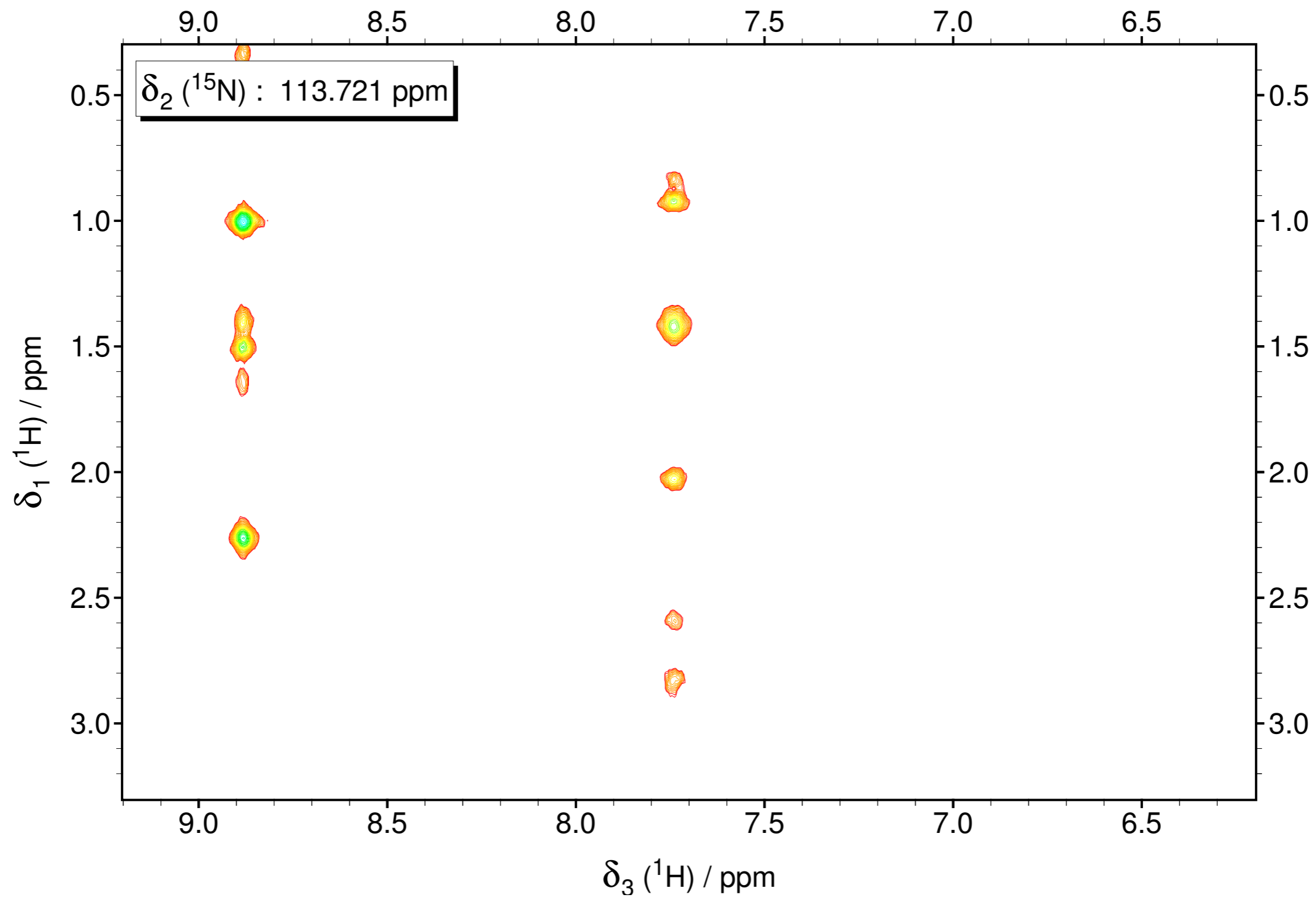
d

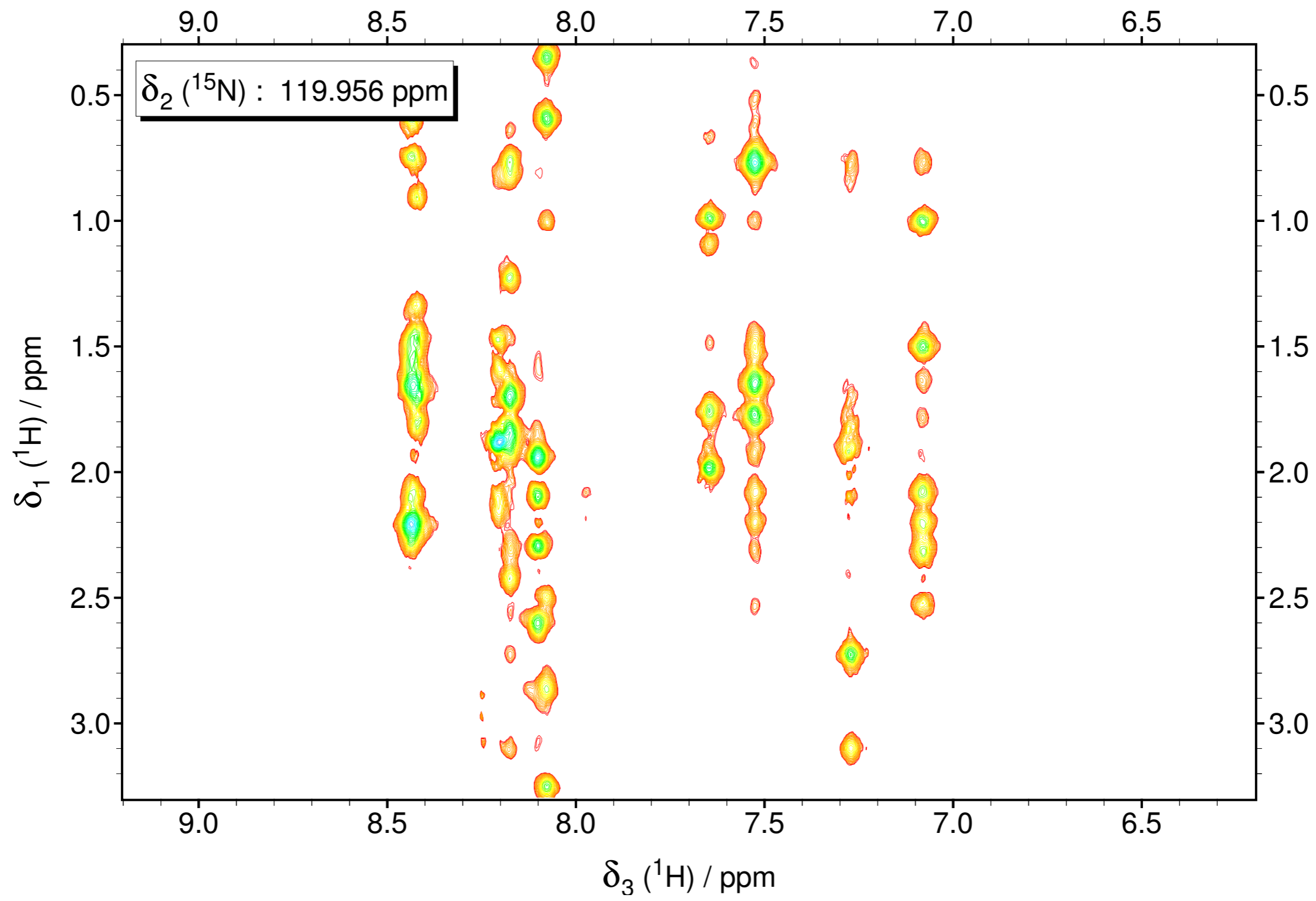


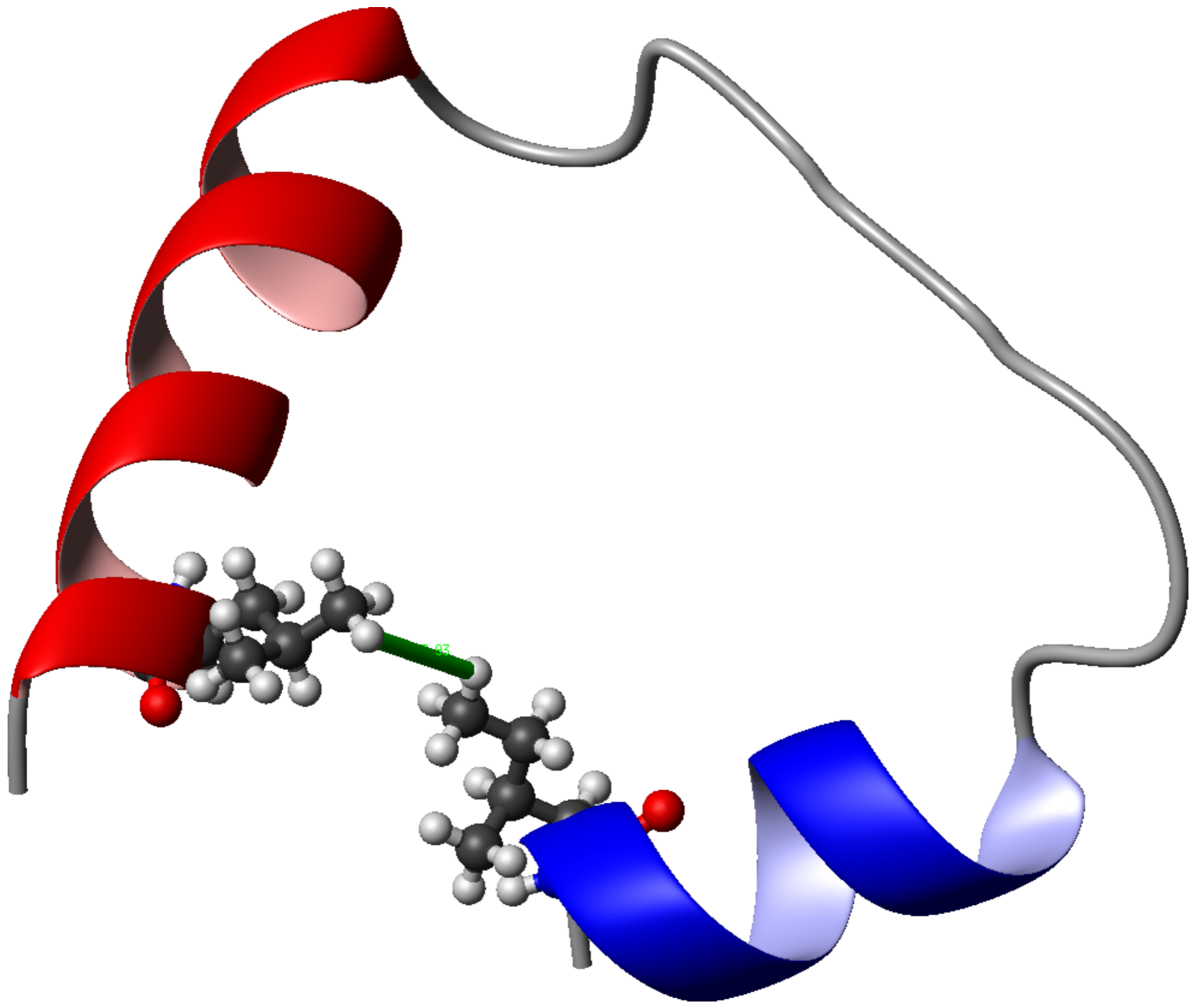
NOESY



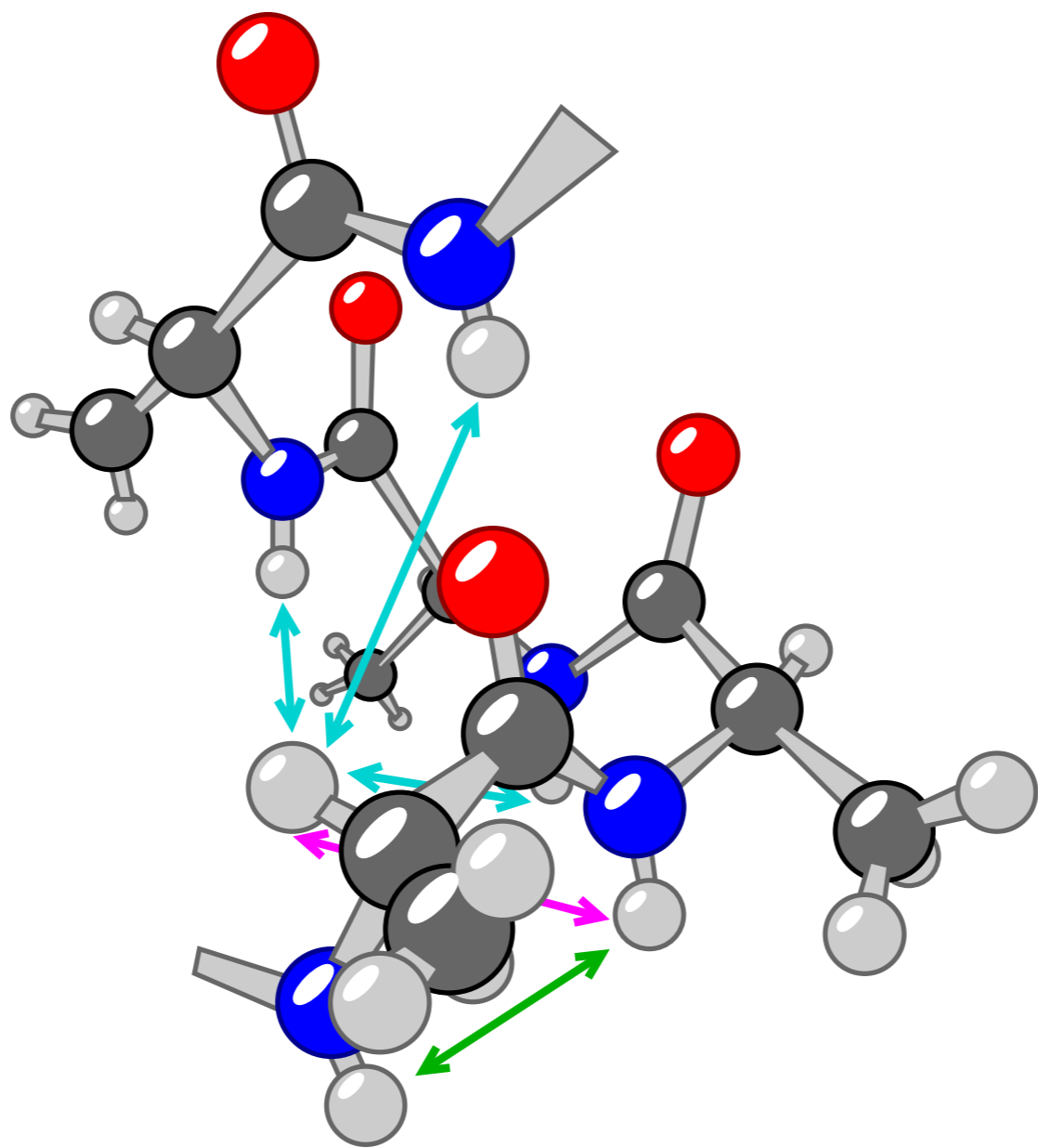


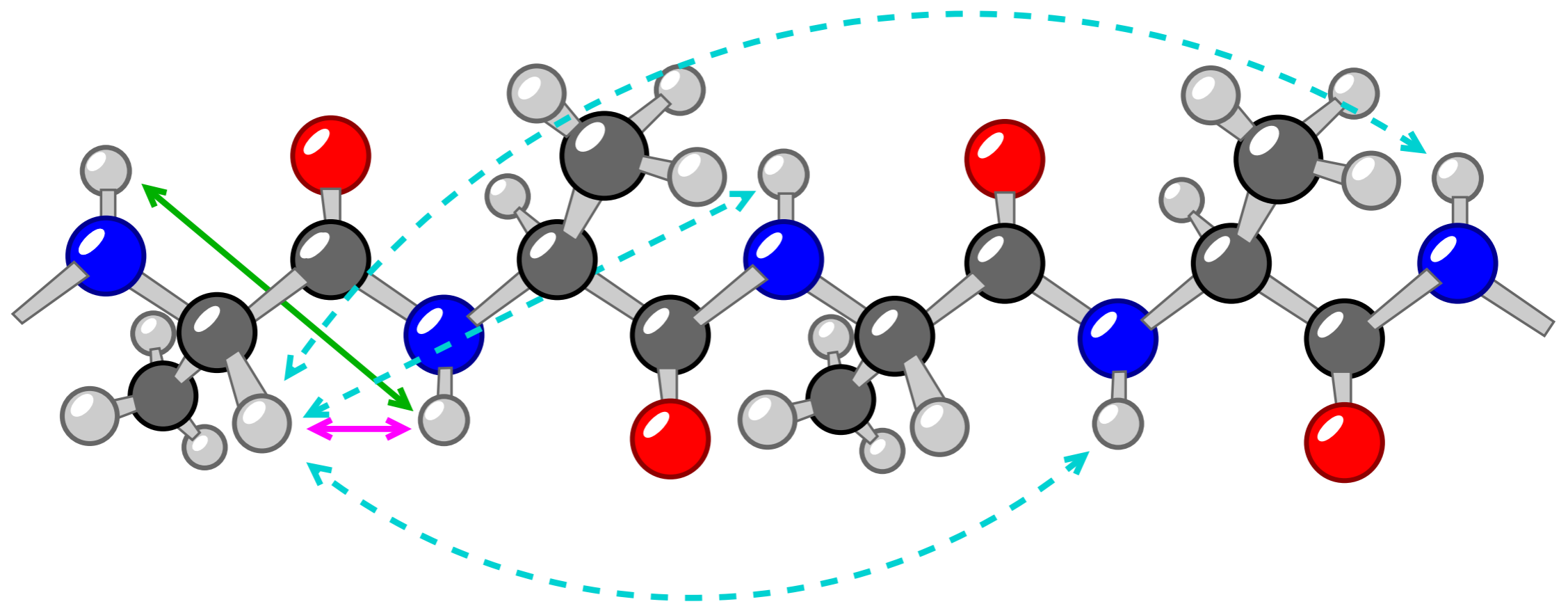






geminal protons in methylene	$\text{H}-\text{C}-\text{H}$	0.17 nm
vicinal protons in aromatic ring	$\text{H}-\text{C}=\text{C}-\text{H}$	0.25 nm
H_i^α and $\text{H}_{i+3}^{\text{N}}$ protons in α -helix		0.34 nm
<i>meta</i> protons in aromatic ring	$\text{H}-\text{C}=\text{CH}-\text{C}-\text{H}$	0.42 nm





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

