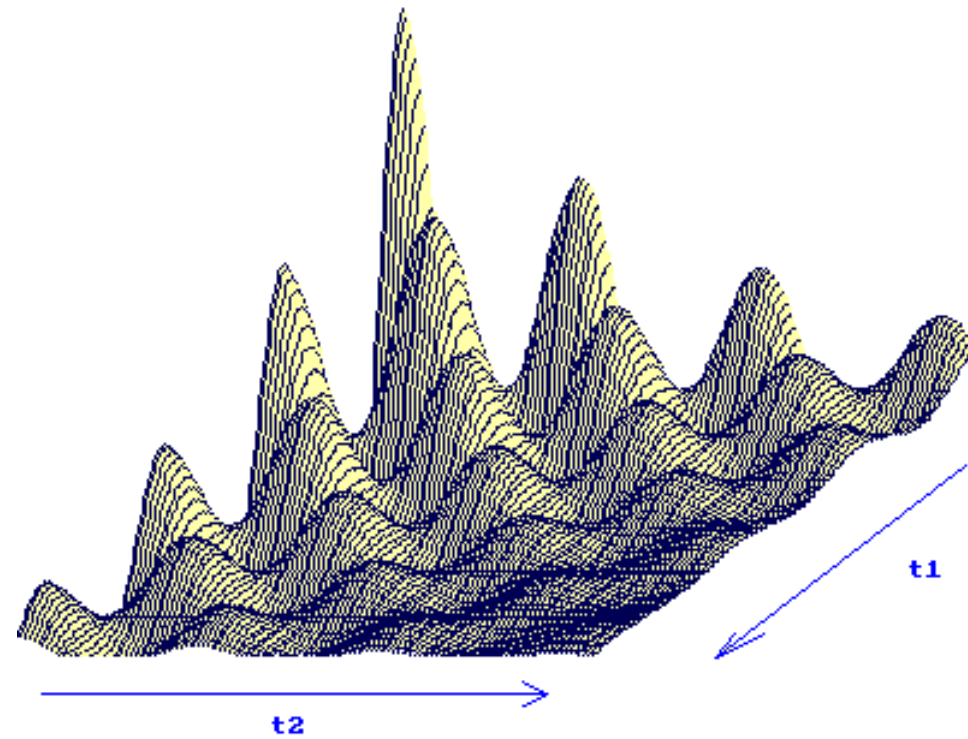


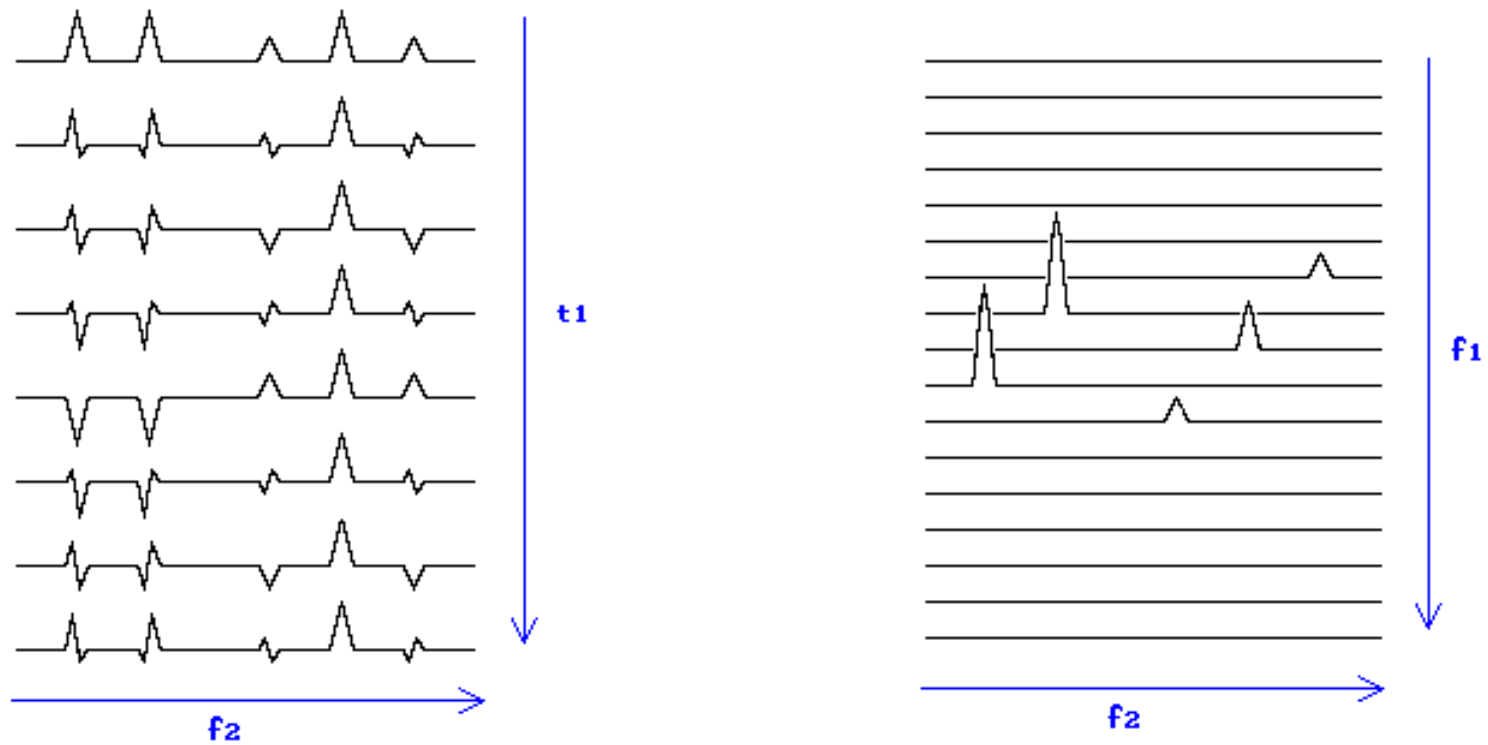
Zweidimensionale NMR Beispiele

2-D Experiment (Acronym)	Information	
	f_1	f_2
Homonuclear J resolved	J	δ
Heteronuclear J resolved	J_{AX}	δ_X
Homoculclear correlated spectroscopy (COSY)	δ_A	δ_A
Heteronuclear correlated spectroscopy (HETCOR)	δ_A	δ_X
Nuclear Overhauser Effect (2D-NOE)	δ_H, J_{HH}	δ_H, J_{HH}
2D-INADEQUATE	$\delta_A + \delta_X$	δ_X

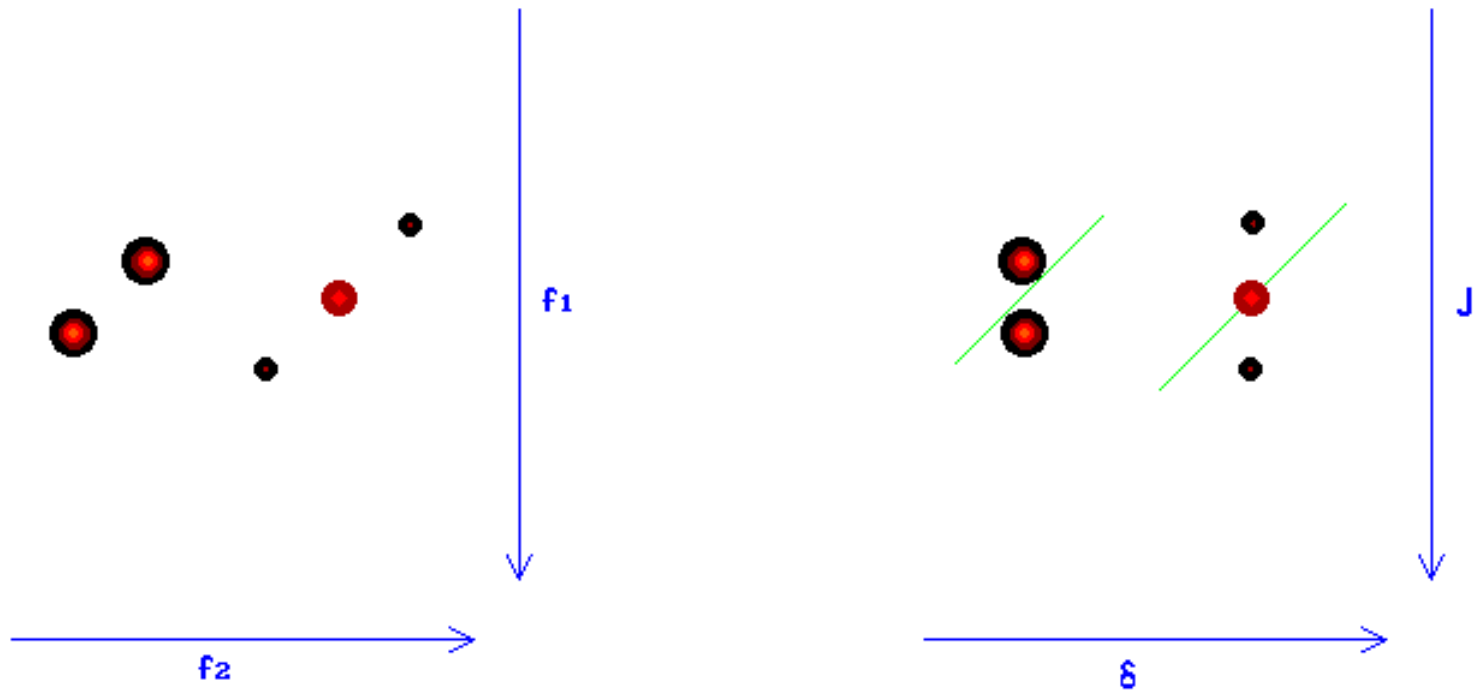
NMR J-aufgelöst



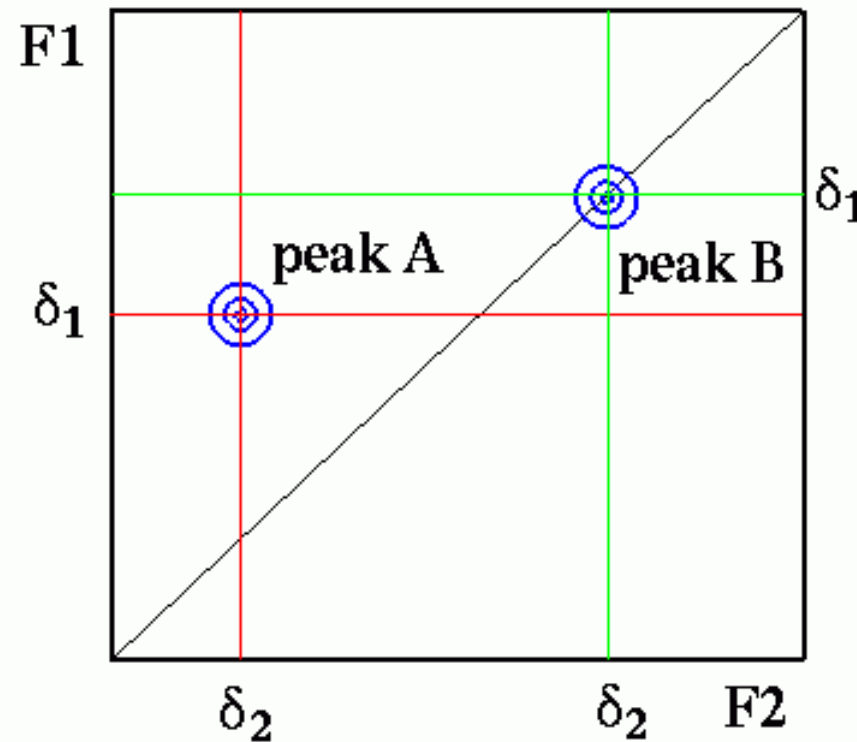
NMR J-aufgelöst



NMR J-aufgelöst



NMR Pulse



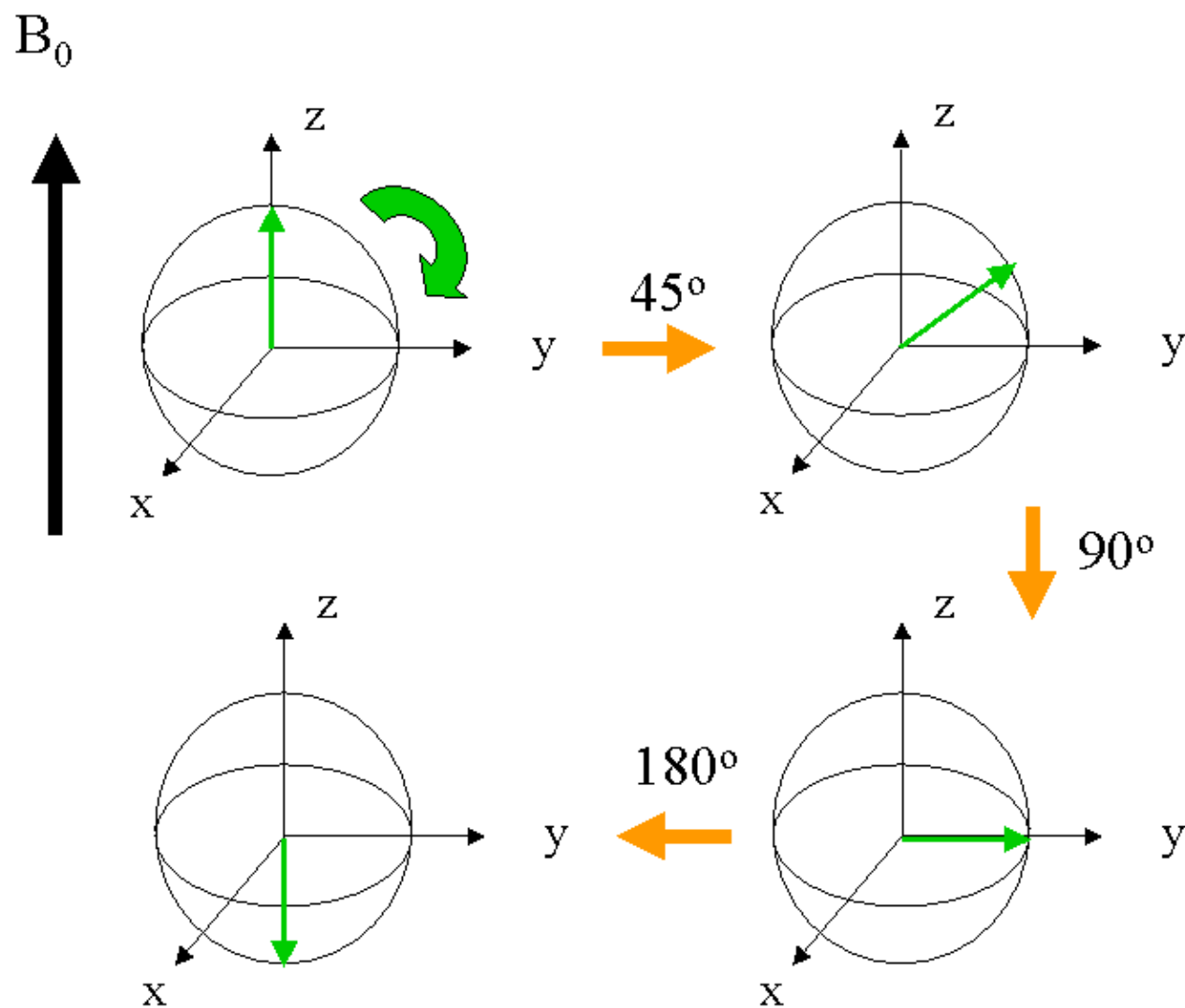
peak A :

$$\delta_1 \neq \delta_2$$

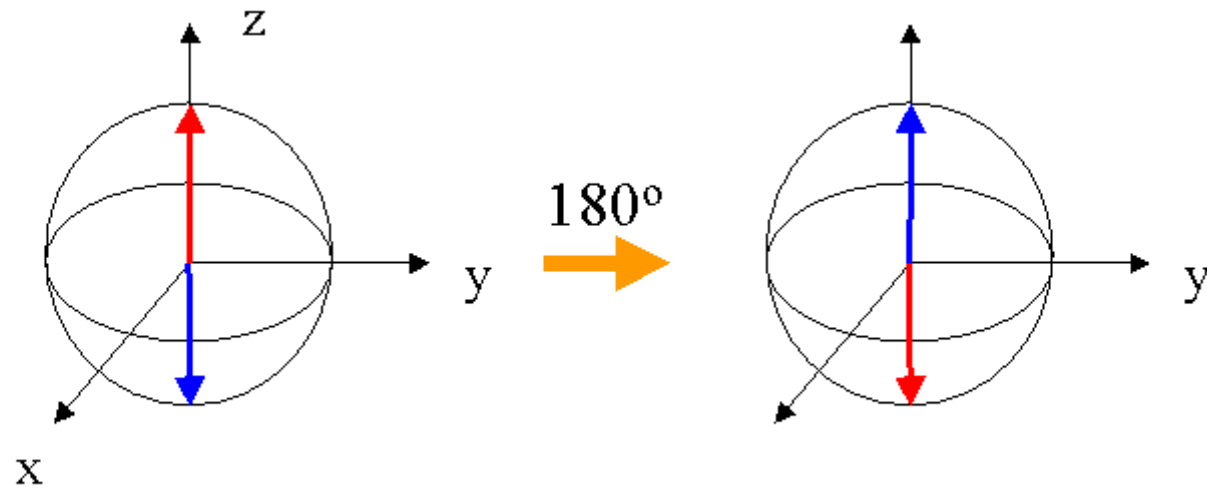
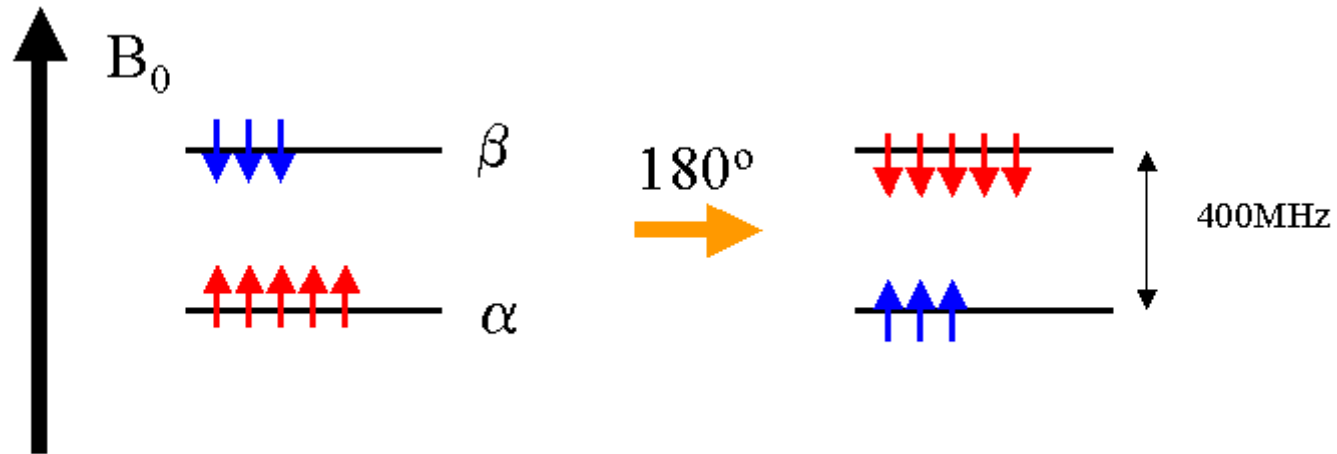
peak B :

$$\delta_1 = \delta_2$$

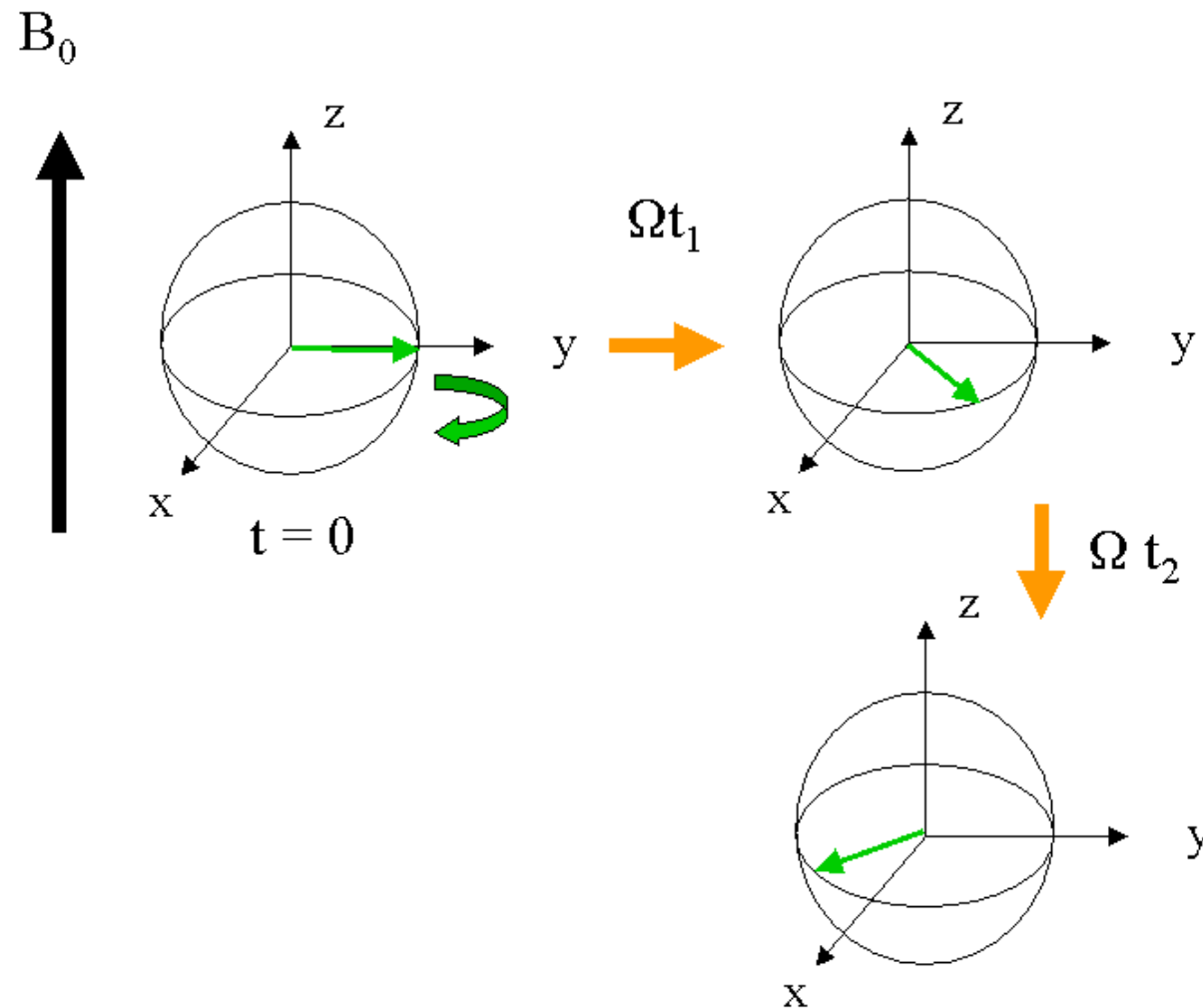
NMR Pulse



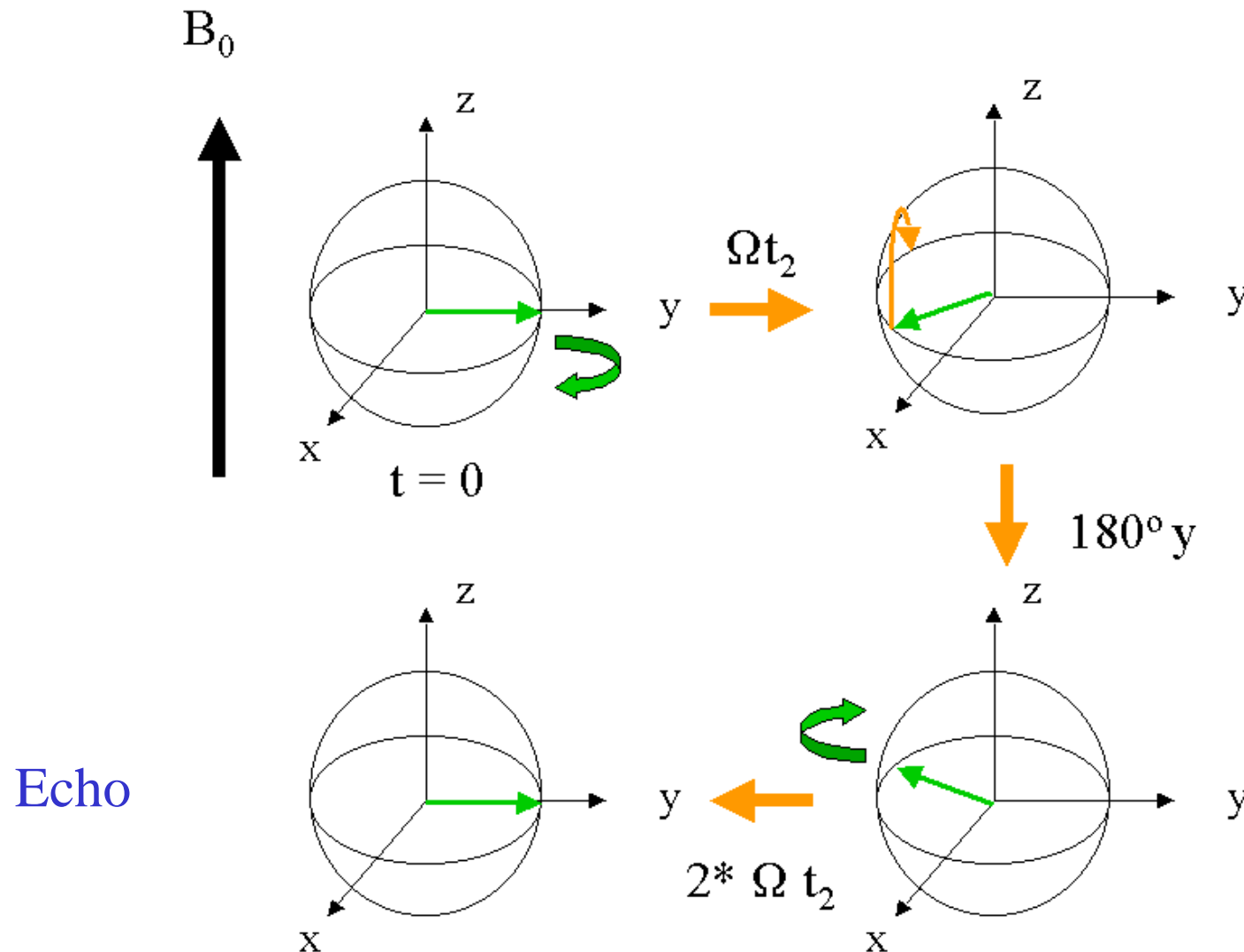
NMR Pulse



Evolution unter chemischer Verschiebung

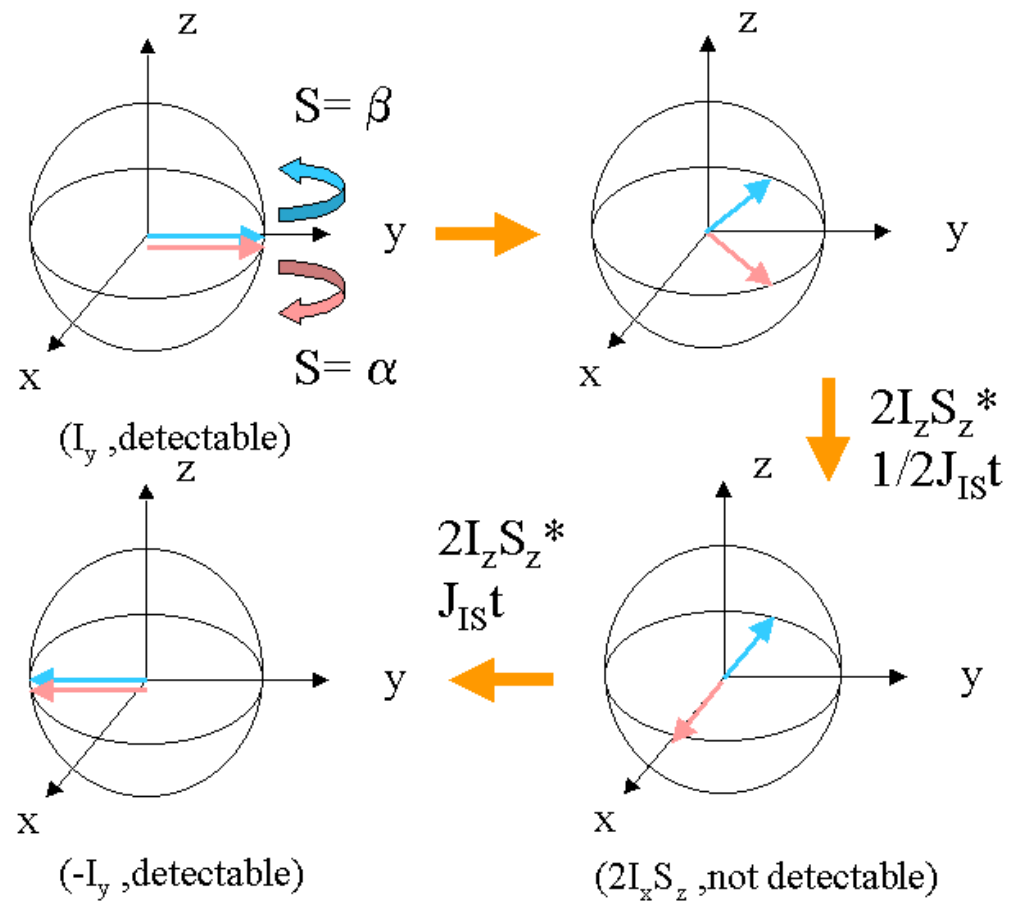
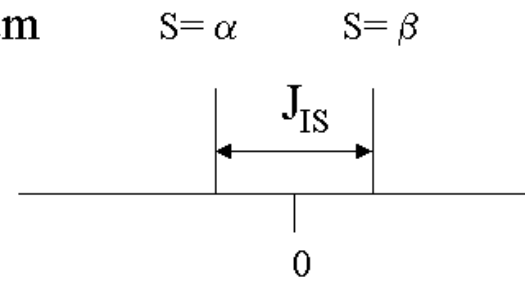


Evolution unter chemischer Verschiebung

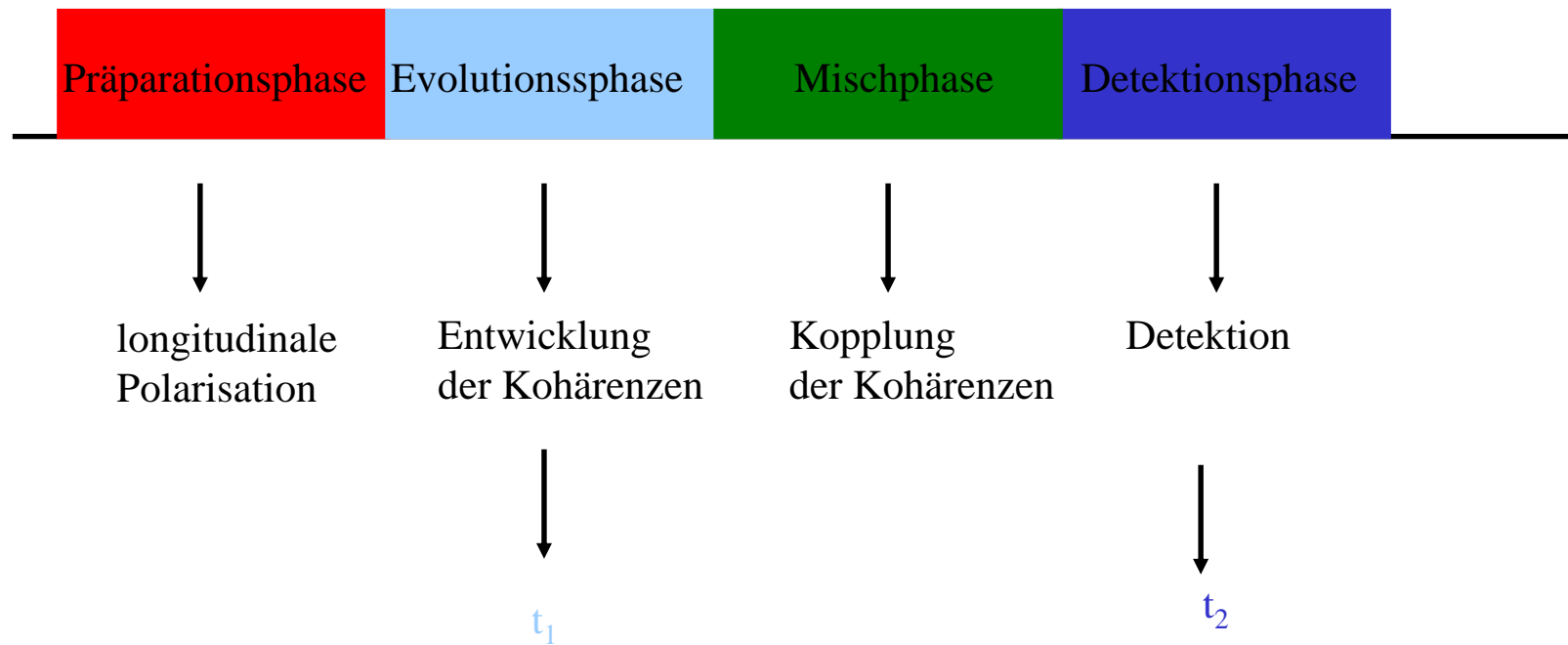


Evolution unter J-Kopplung

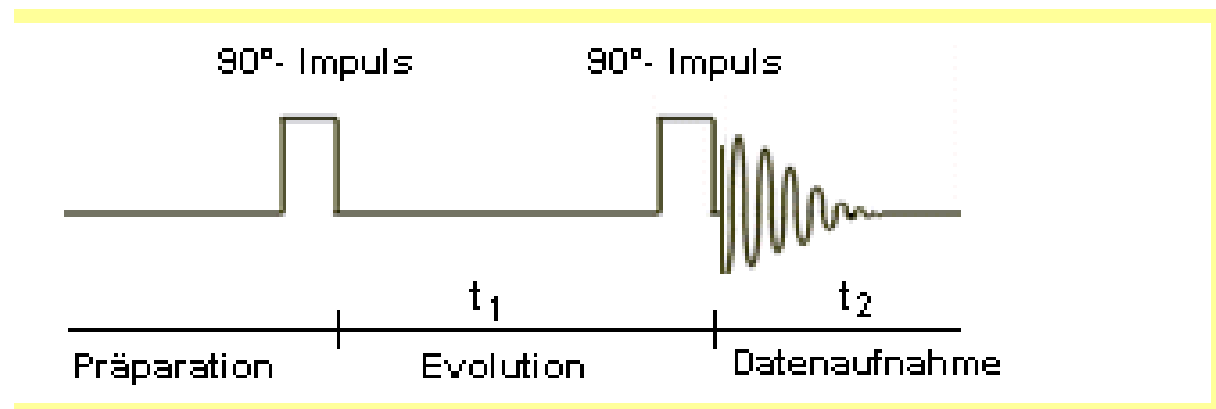
I-Spectrum



NMR COSY (COrelated SpectroscopY)

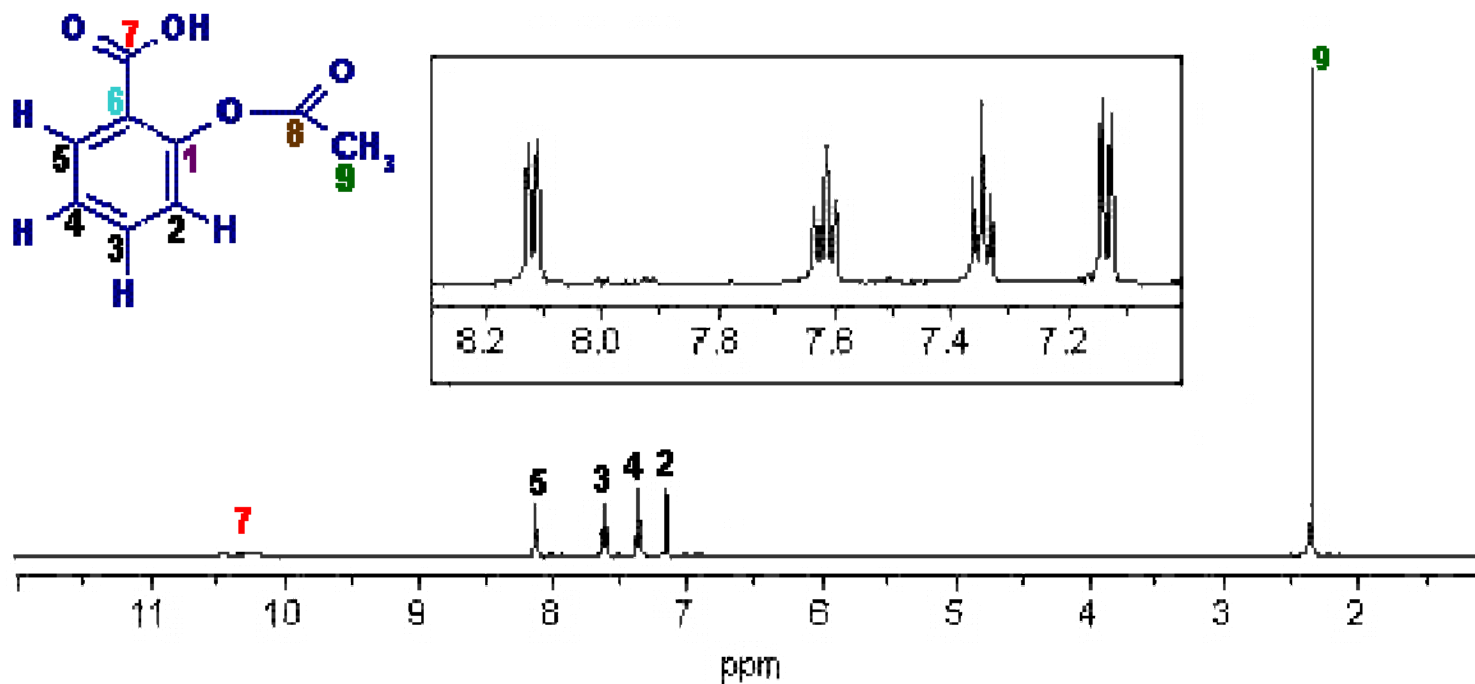


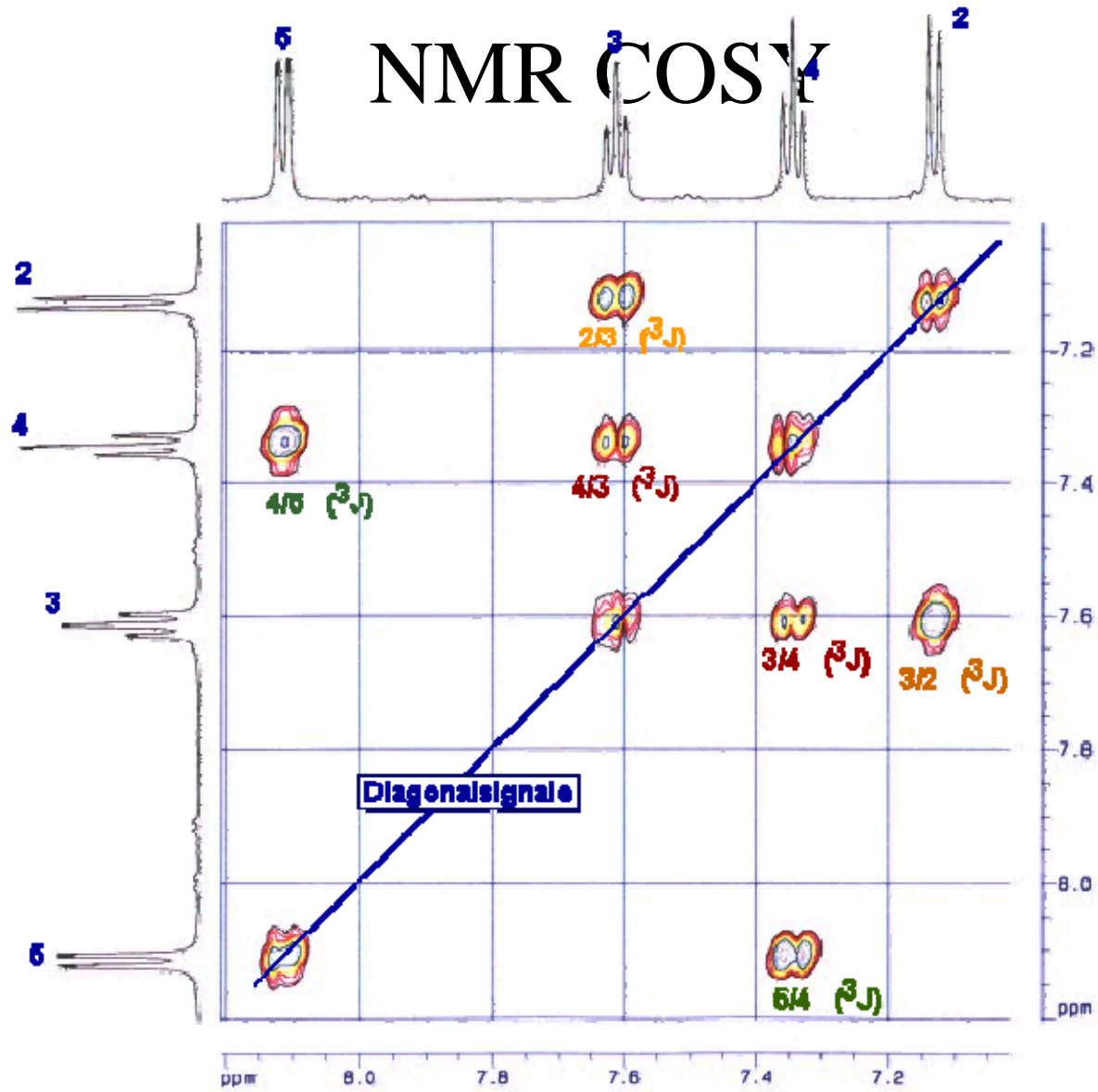
NMR COSY

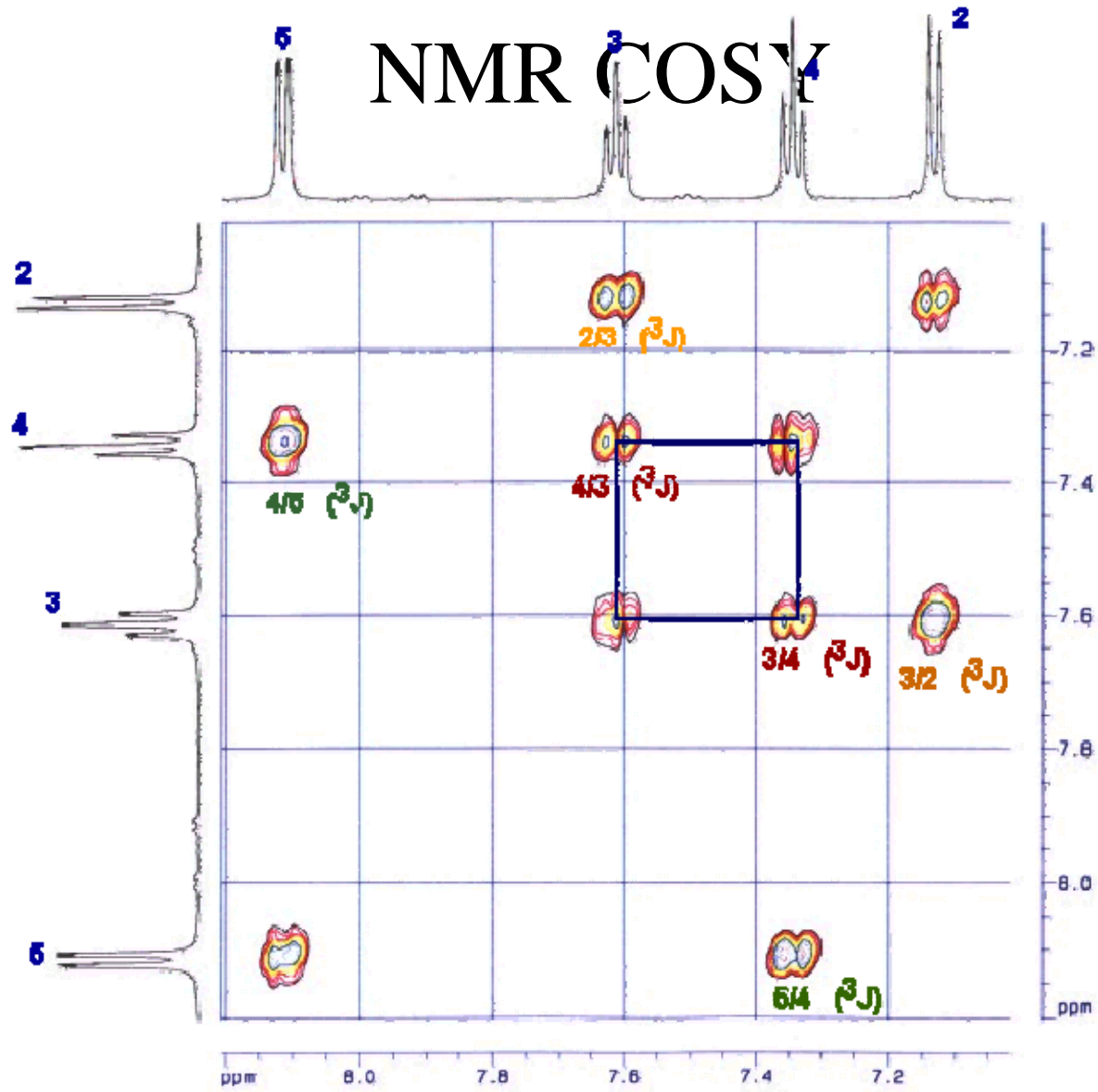


$$S(\omega_1, \omega_2) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} S(t_1, t_2) \exp(-i\omega t_1) \exp(-i\omega_2 t_2) dt_1 dt_2$$

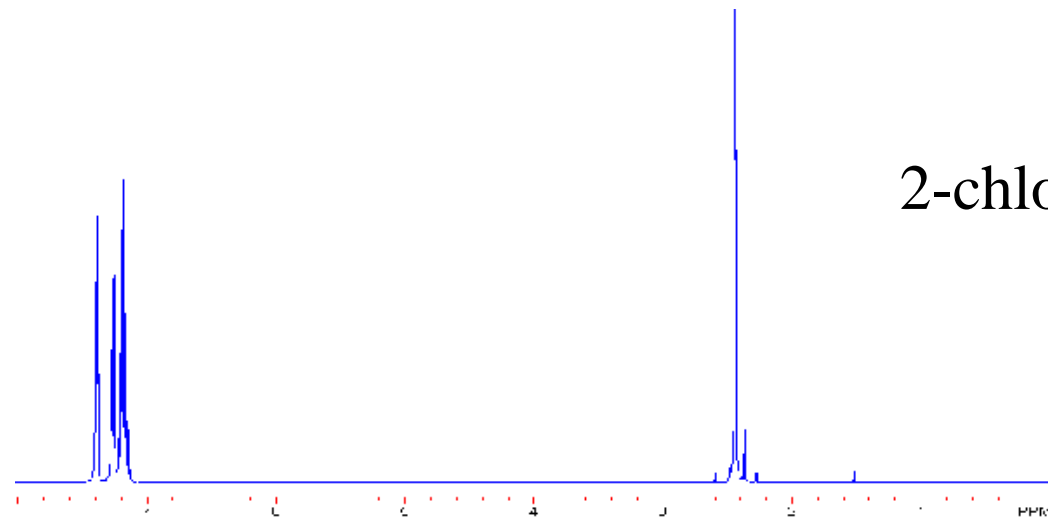
NMR COSY



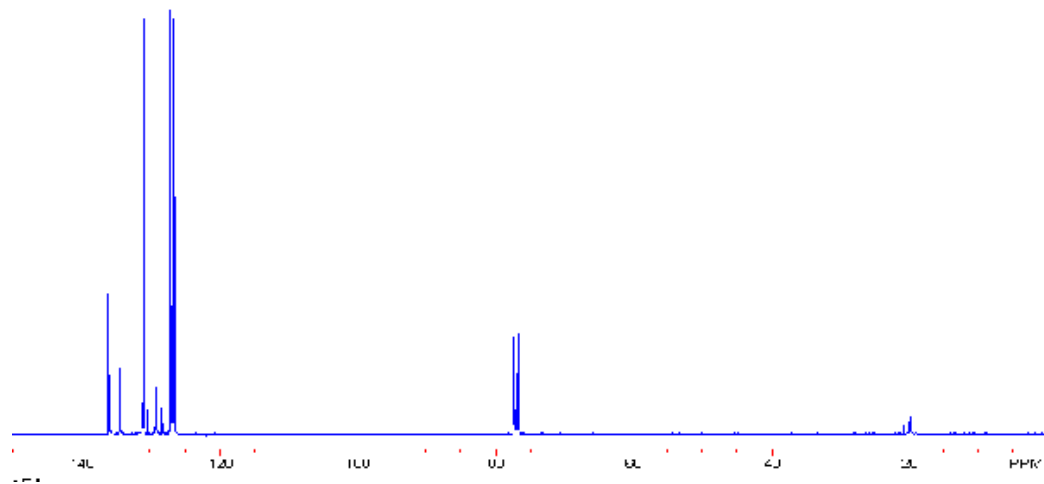




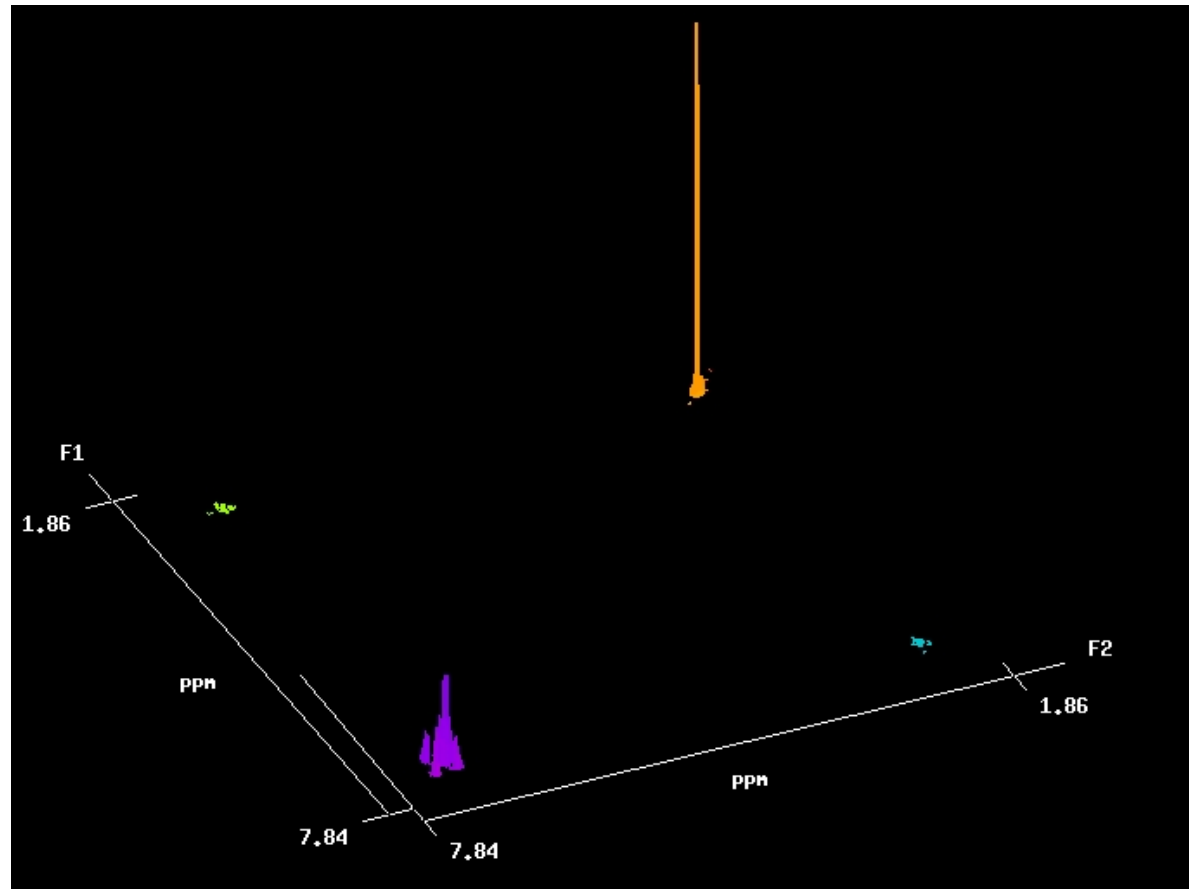
1D-Spektren



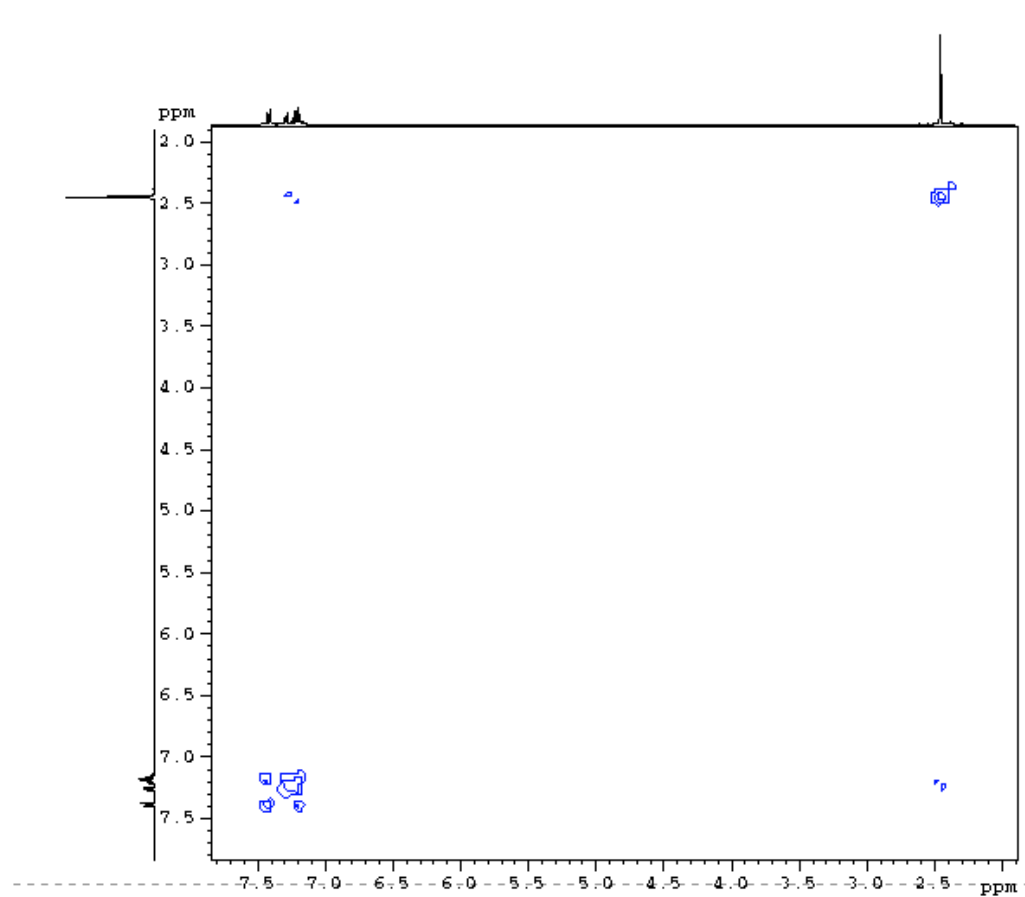
2-chlorotoluene



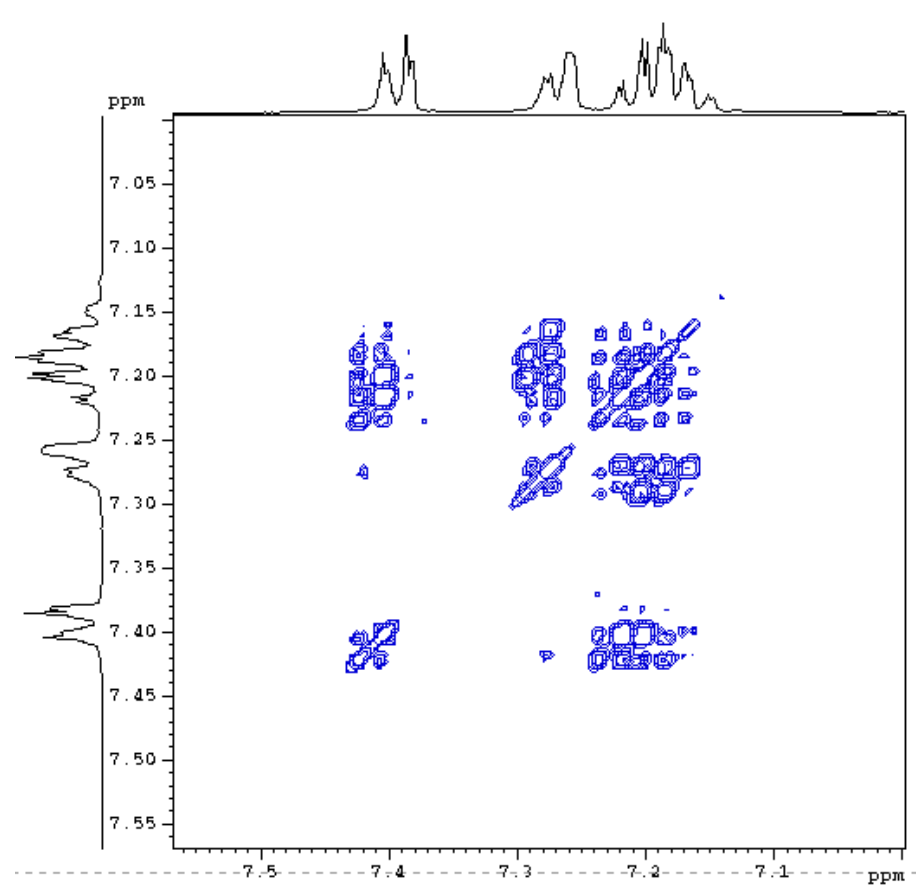
COSY Stacked-Plot



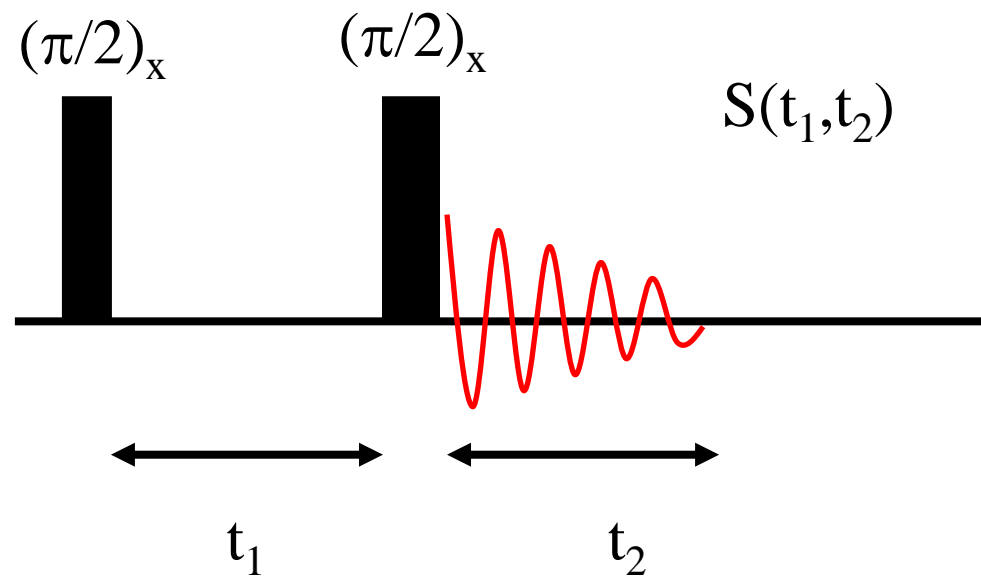
COSY Contour-Plot



COSY Contour-Plot

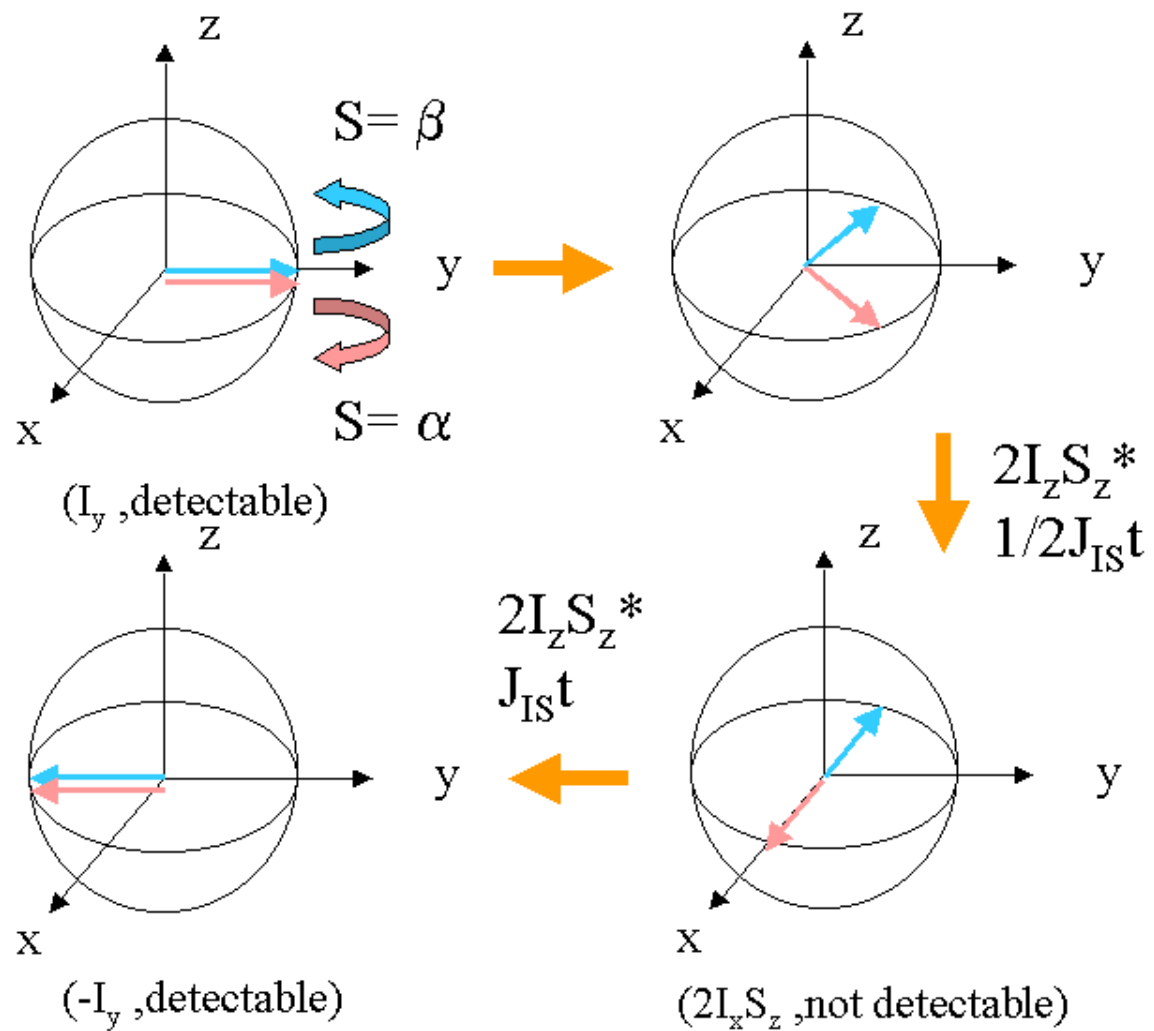


NMR COSY

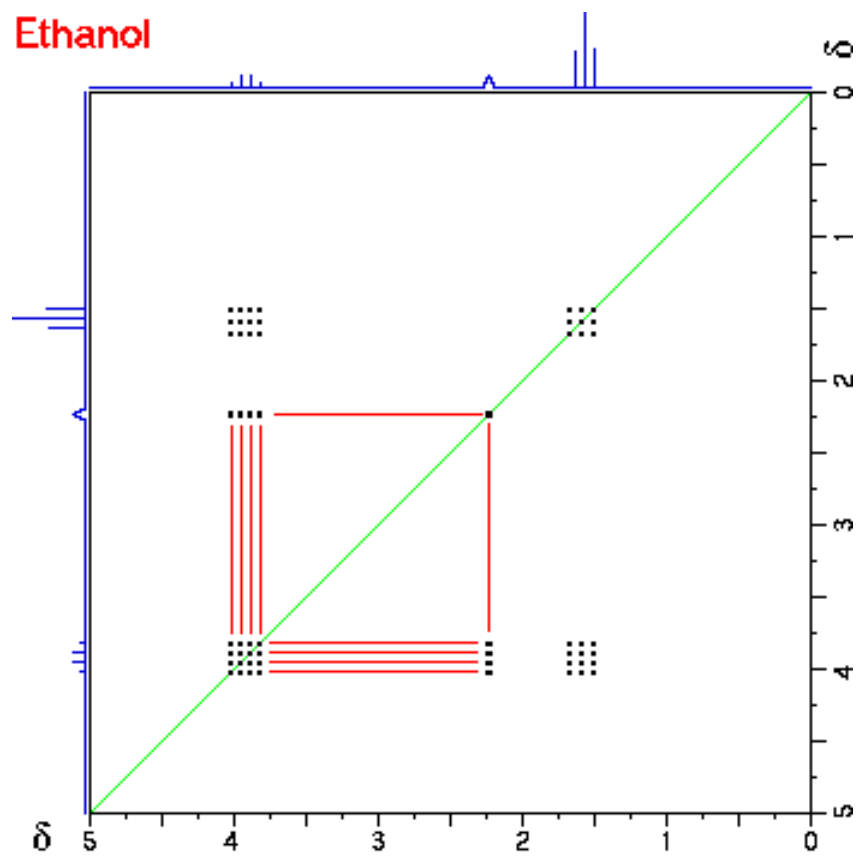
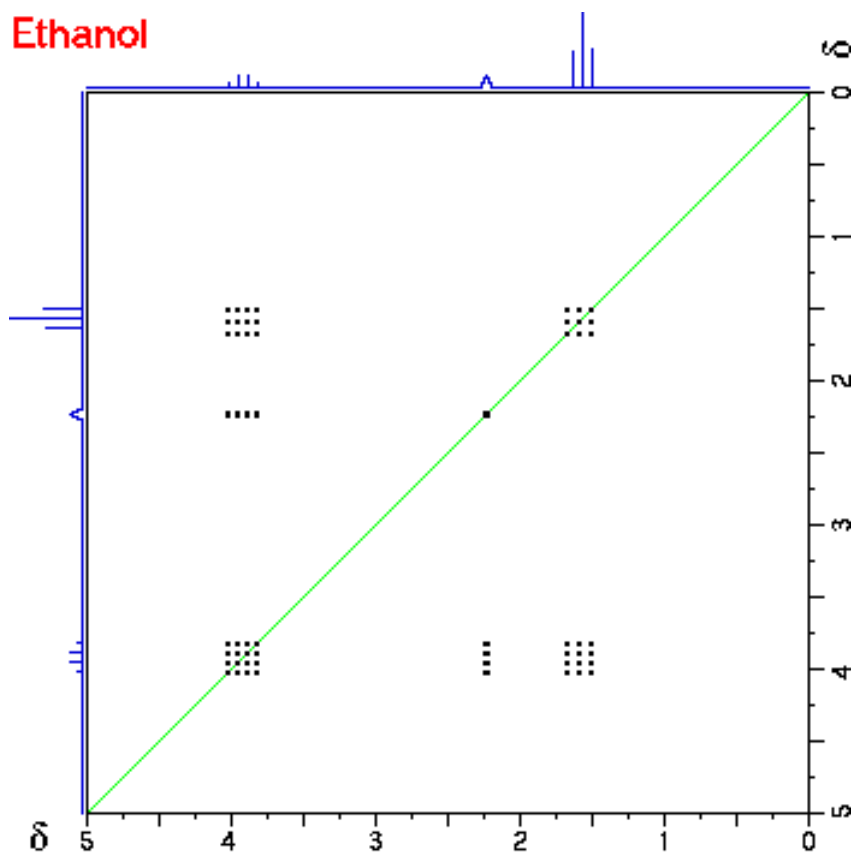


$$90^\circ_x - t_1 - 90^\circ_x - \text{FID}(t_2)$$

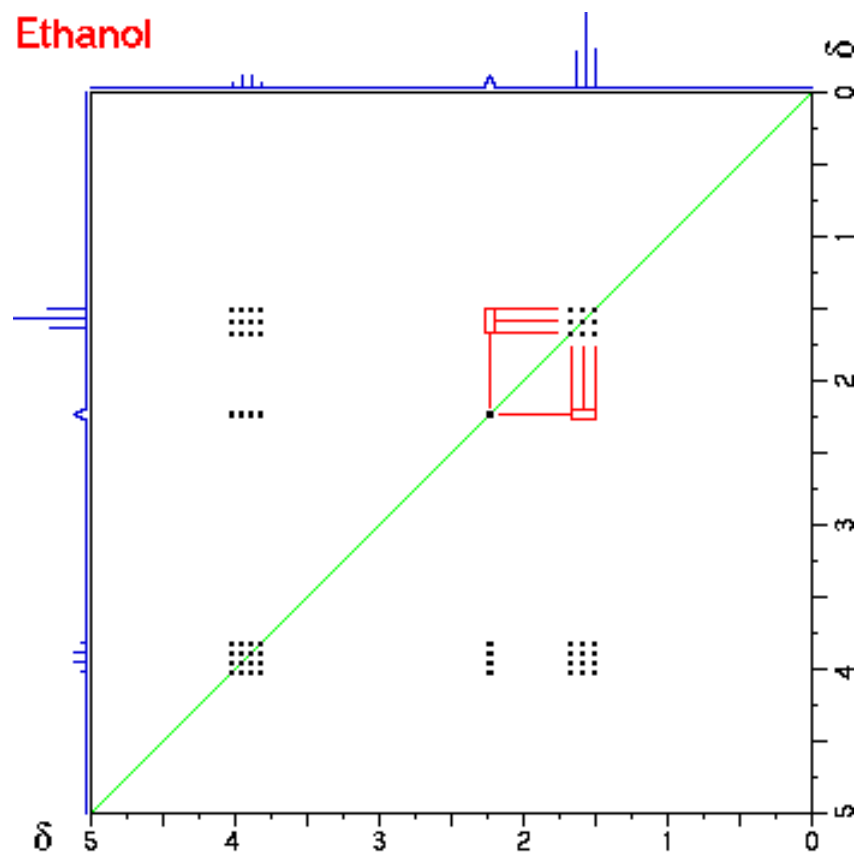
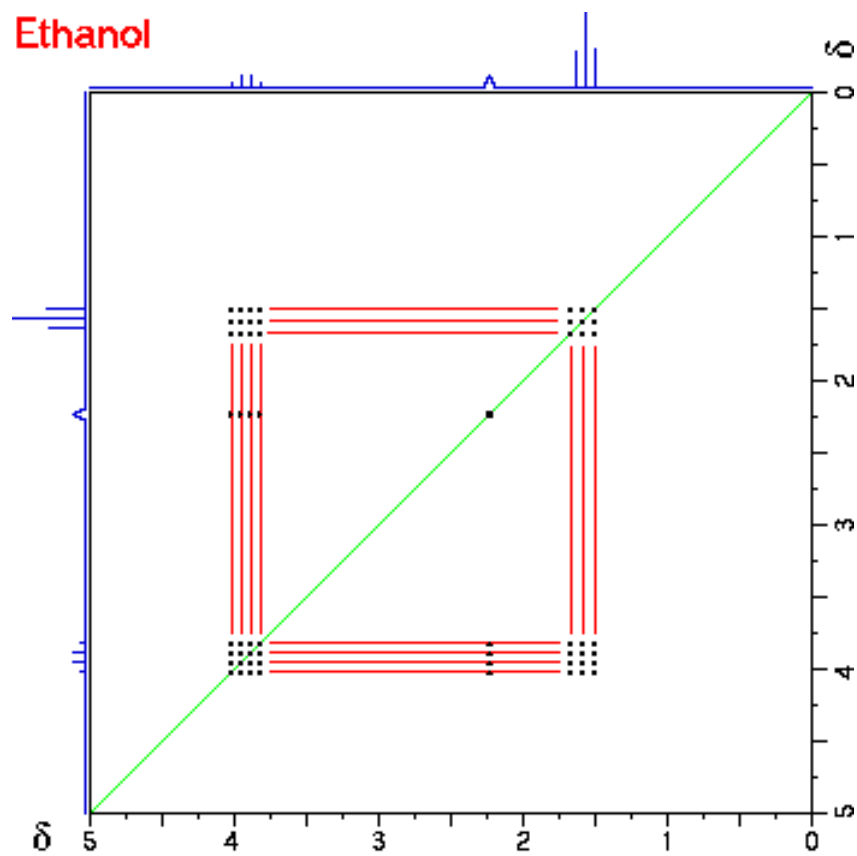
NMR COSY



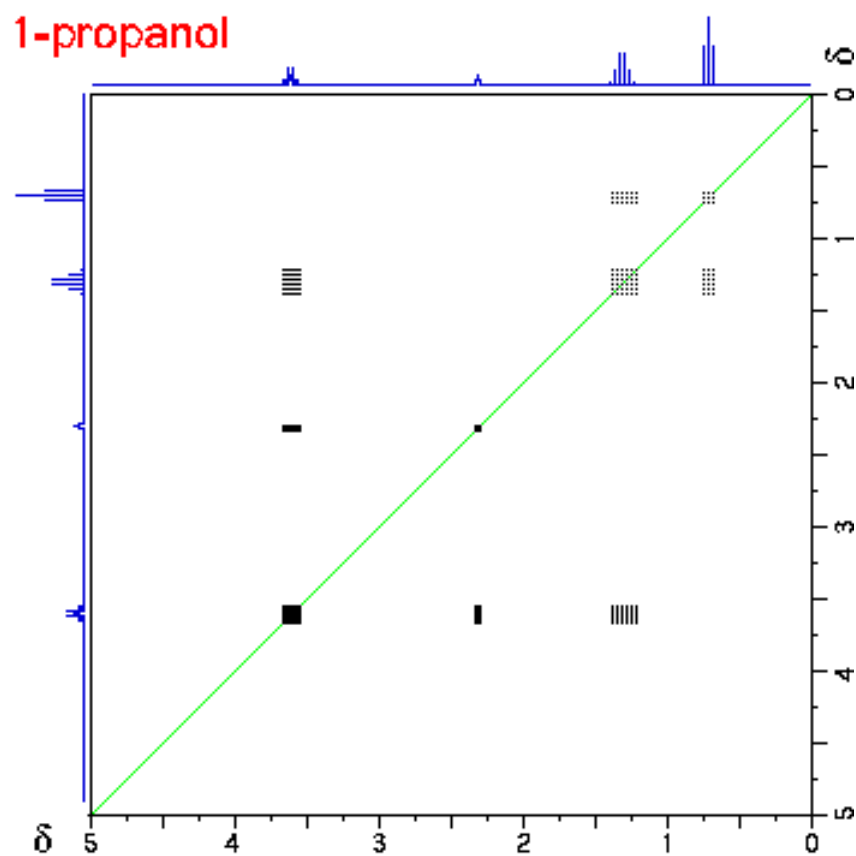
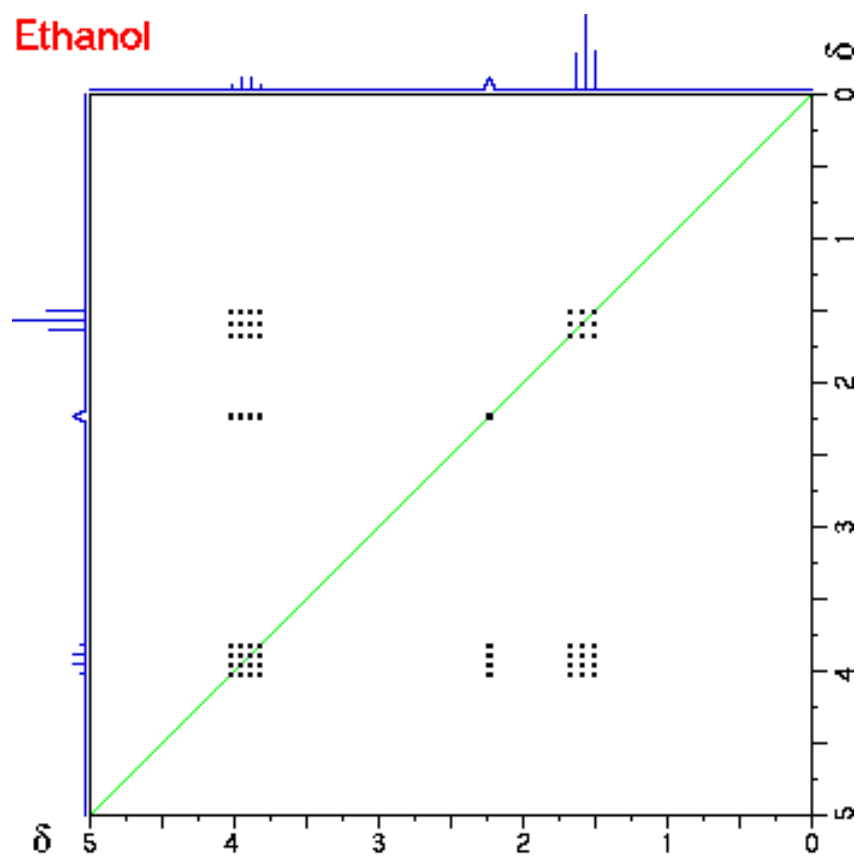
NMR COSY Ethanol



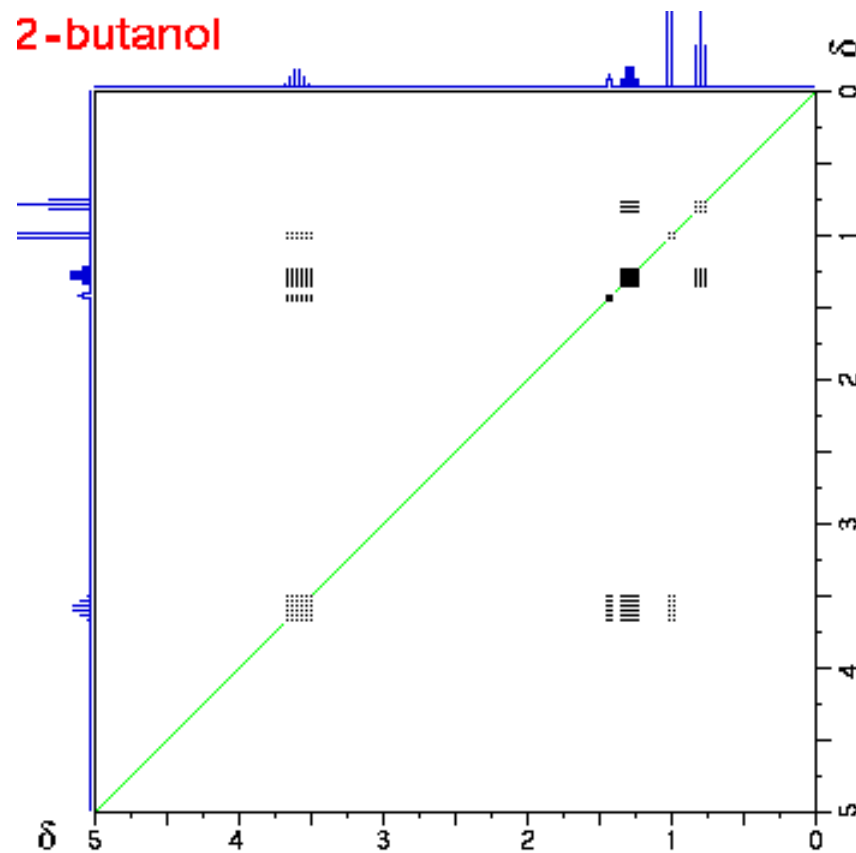
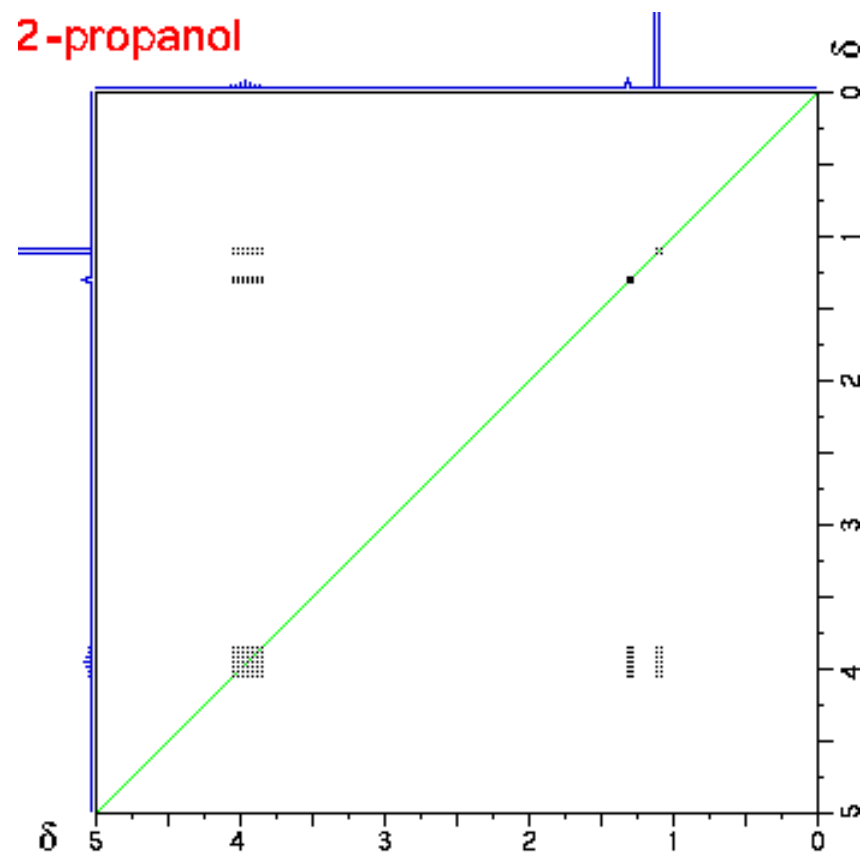
NMR COSY Ethanol



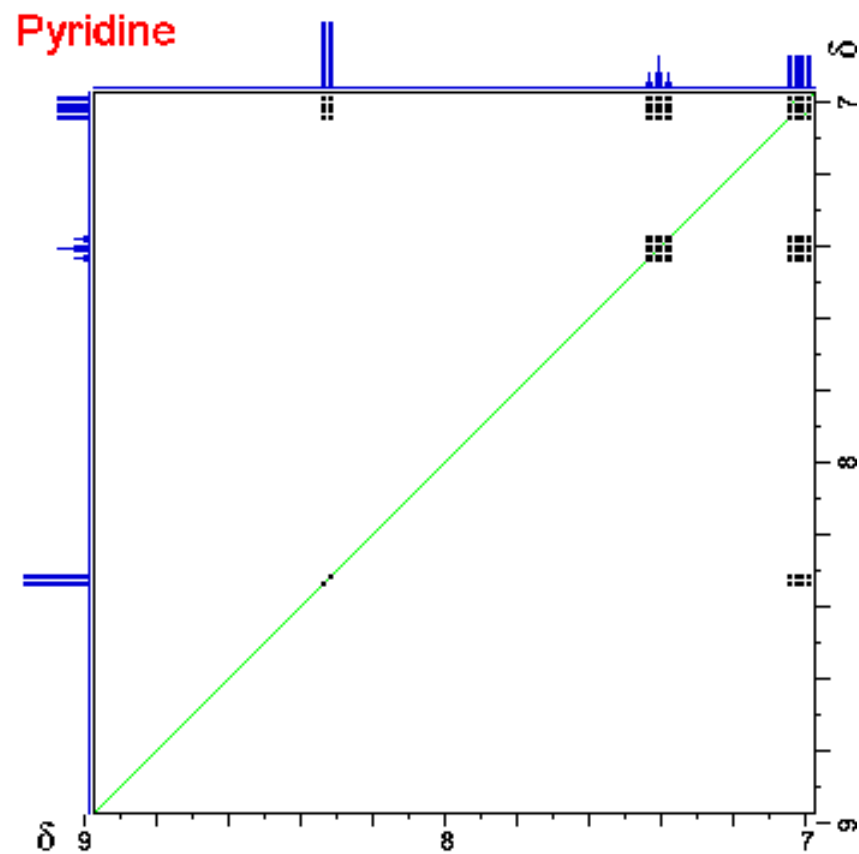
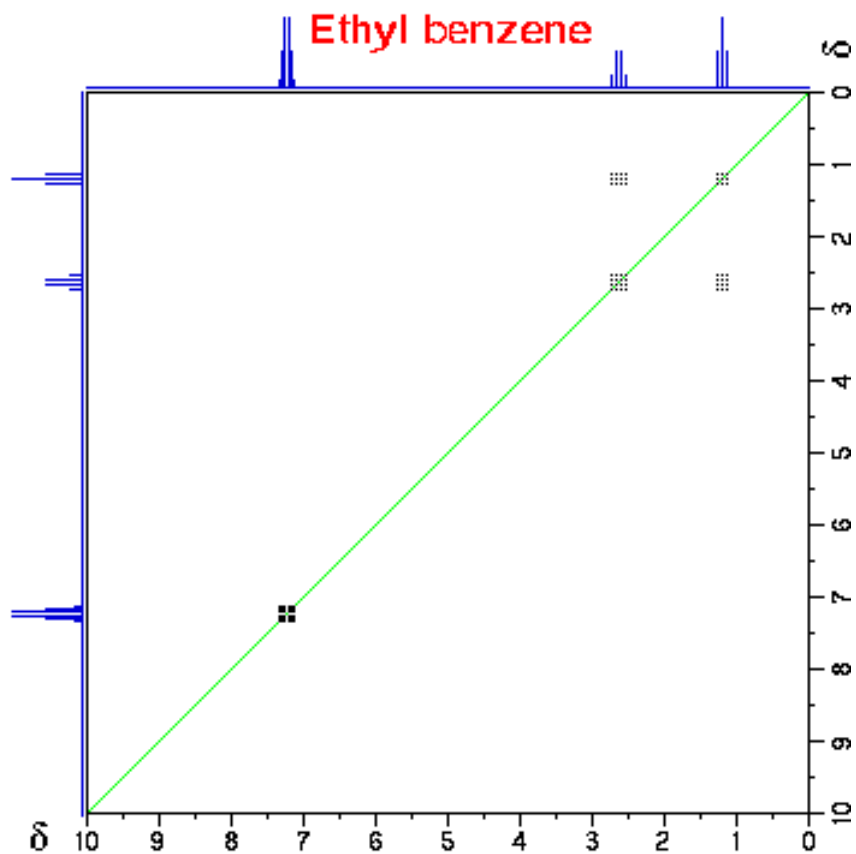
NMR COSY Ethanol + 1-Propanol



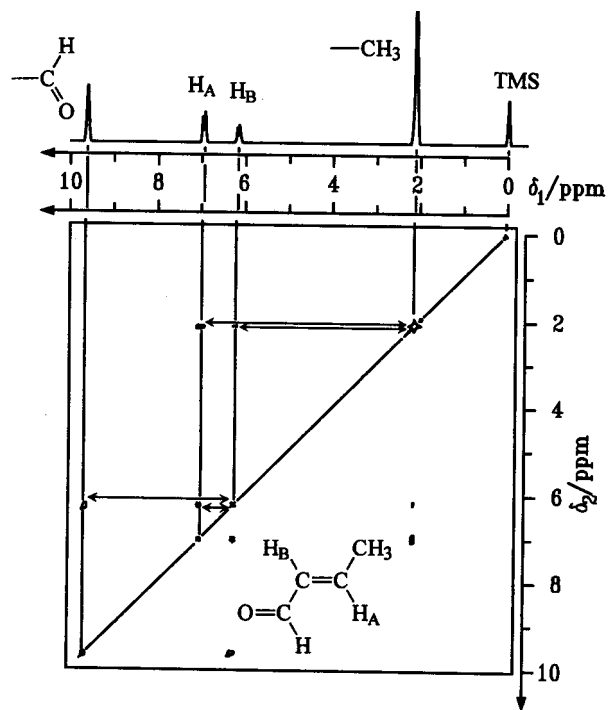
NMR COSY 2-Propanol + 2-Butanol



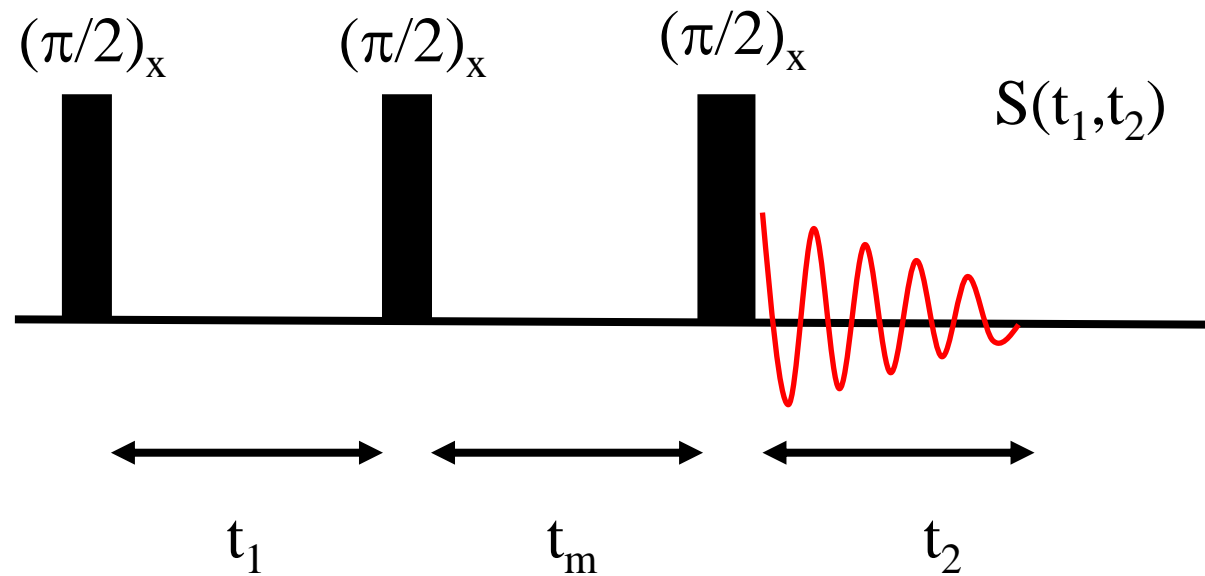
NMR COSY Ethylbenzol + Pyridin



NMR COSY trans-Crotonaldehyd

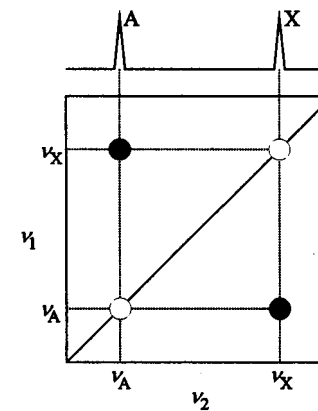
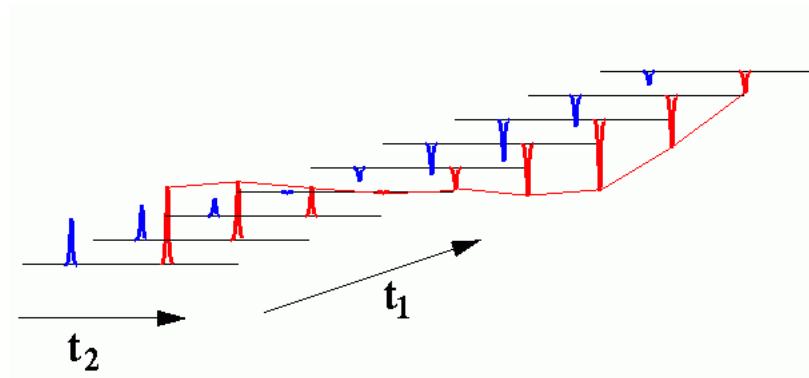
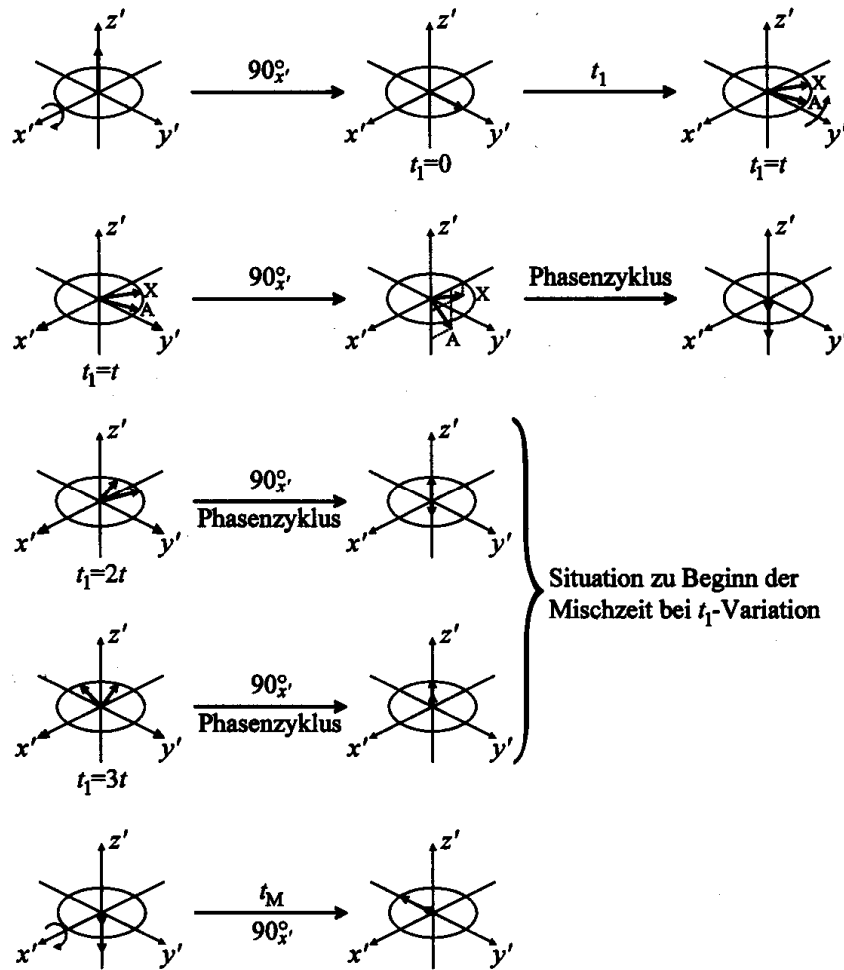


NMR NOESY Pulsfolge

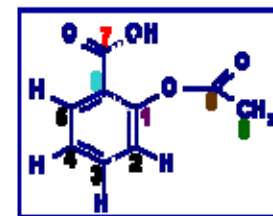
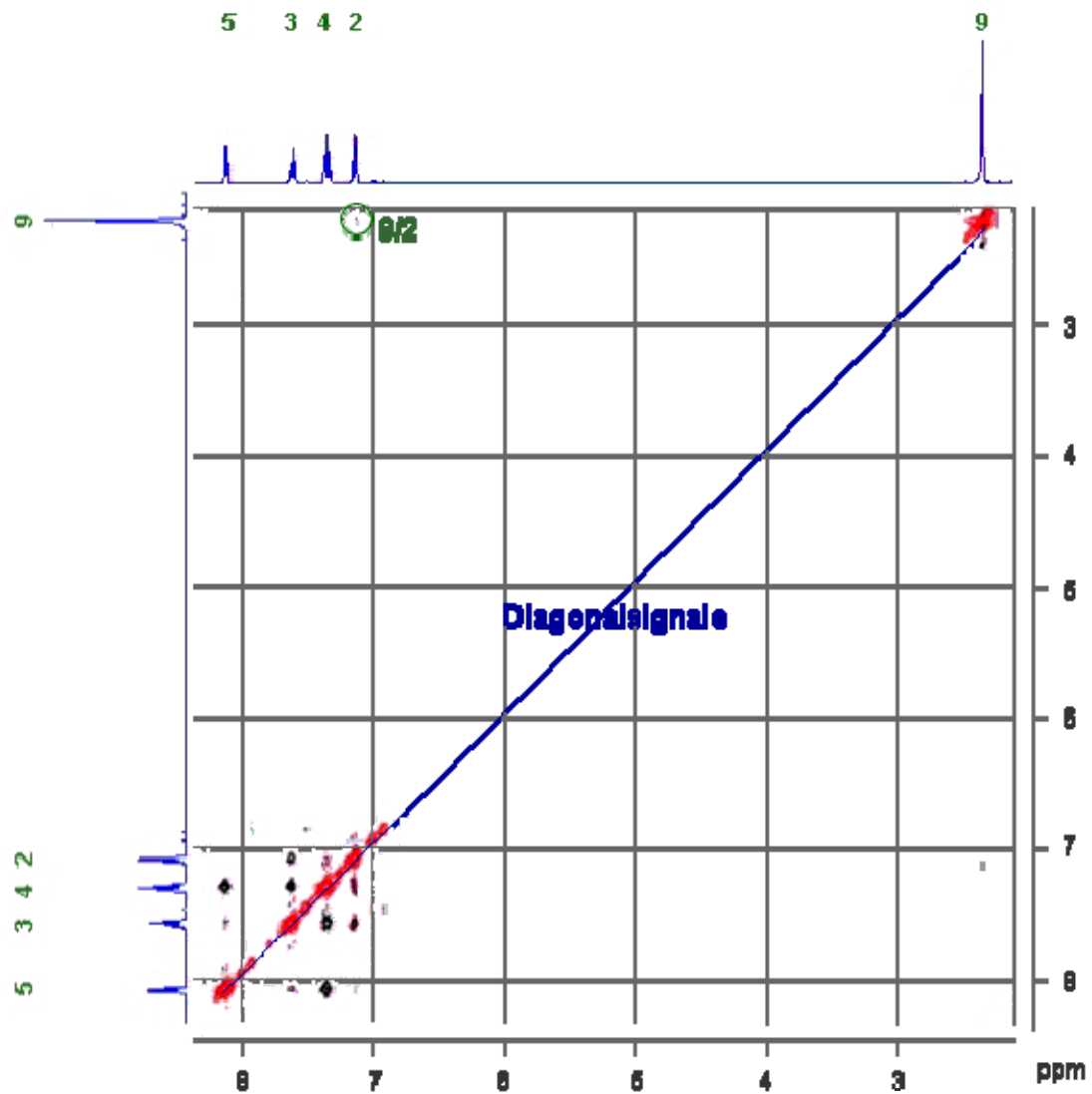


$$90^\circ_x - t_1 - 90^\circ_x - t_m - 90^\circ_x - \text{FID}(t_2)$$

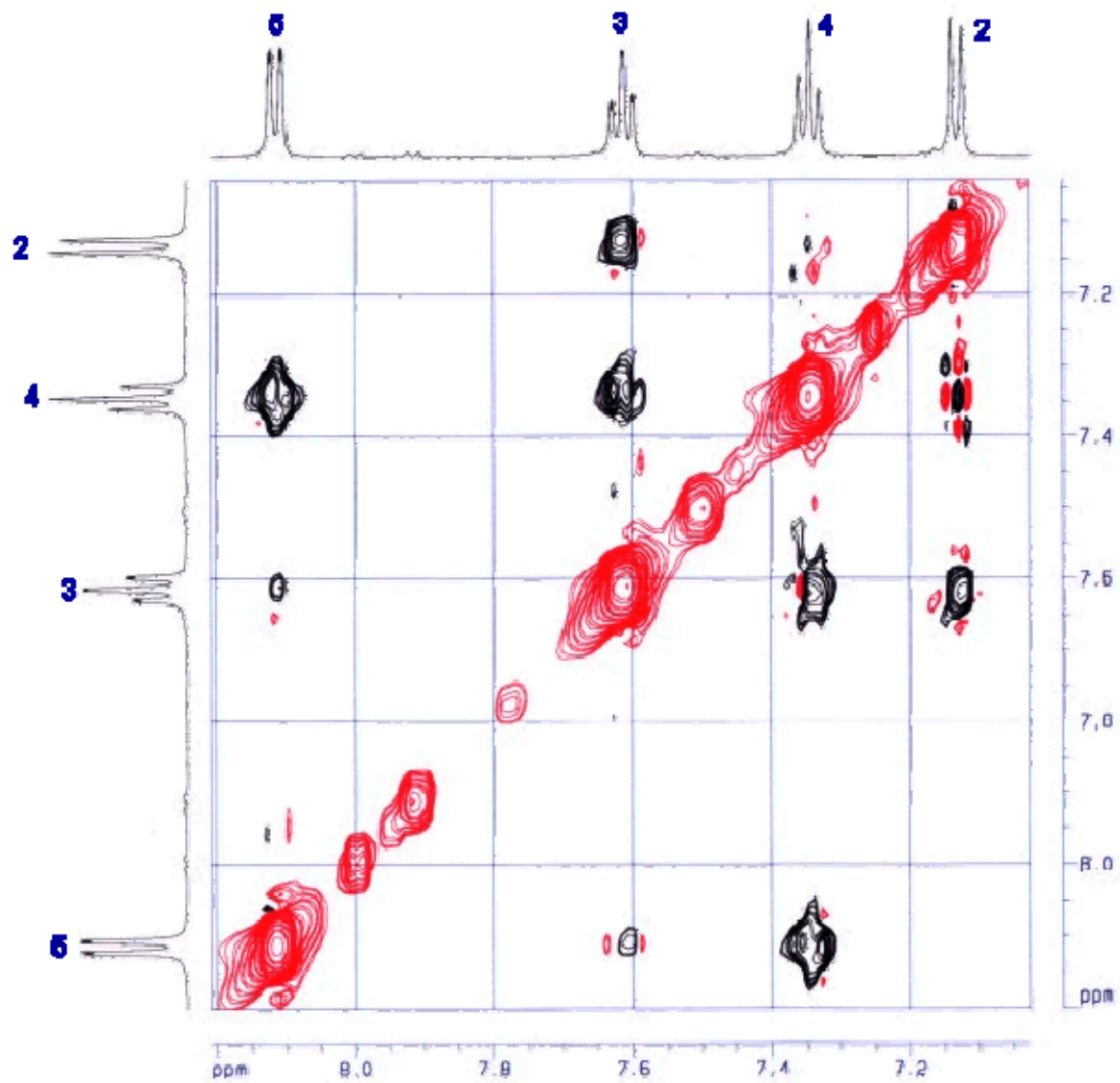
NMR NOESY Vektordiagramm



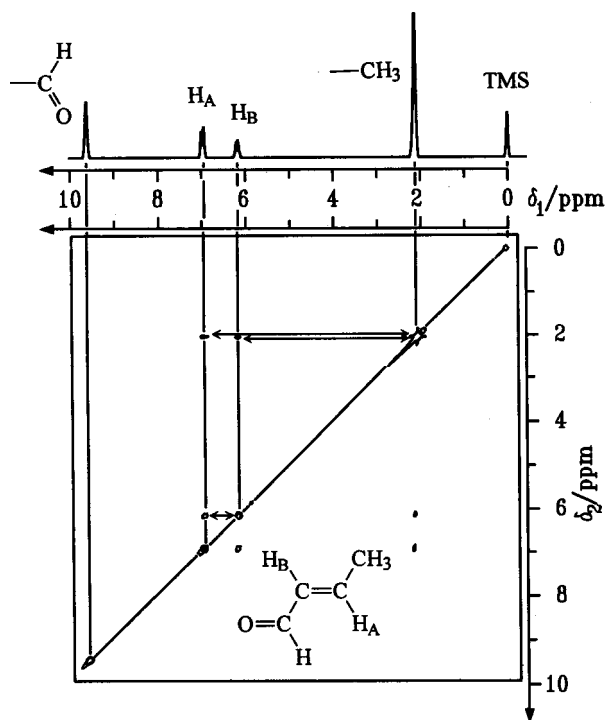
NMR NOESY Acetylsalicylsäure



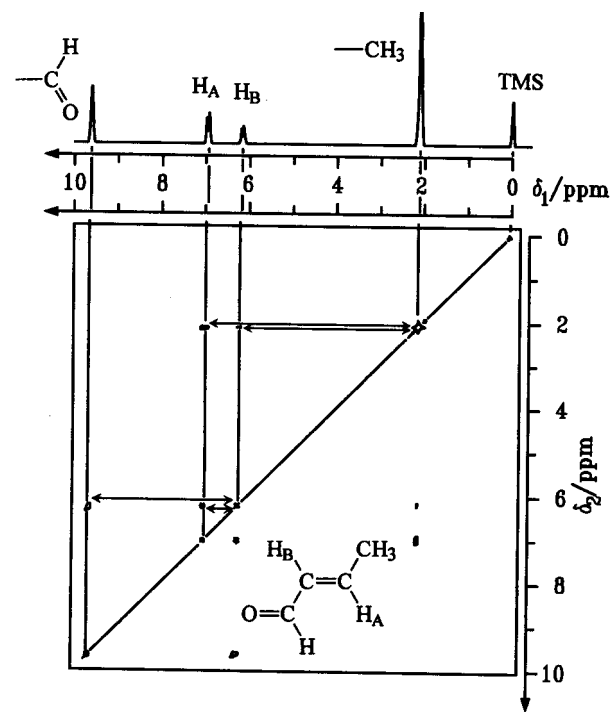
NMR NOESY Acetylsalicylsäure



NMR NOESY trans-Crotonaldehyd



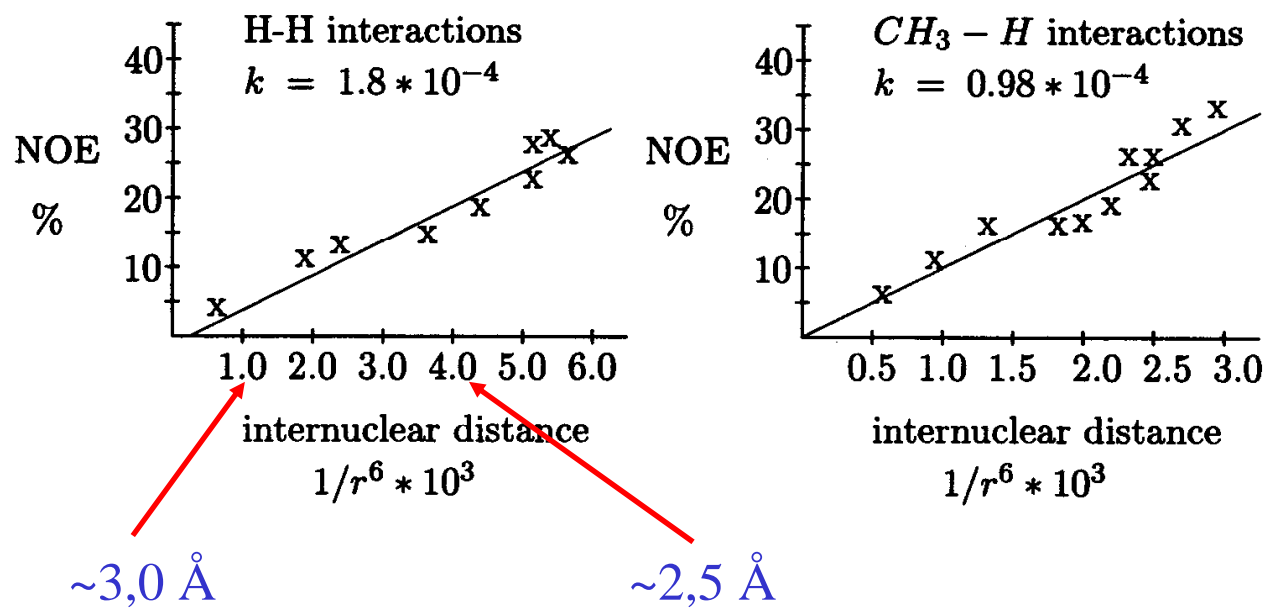
NOESY



COSY

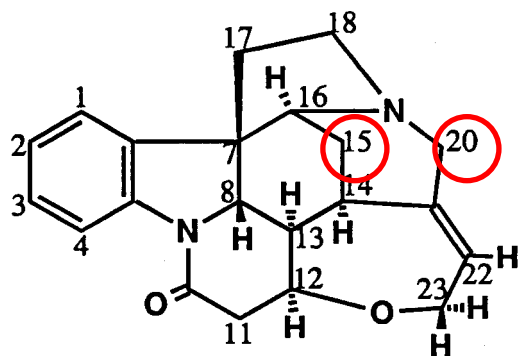
NMR NOESY

$$I = k \gamma_1^2 \gamma_2^2 r^{-6} \sum J(\omega)$$

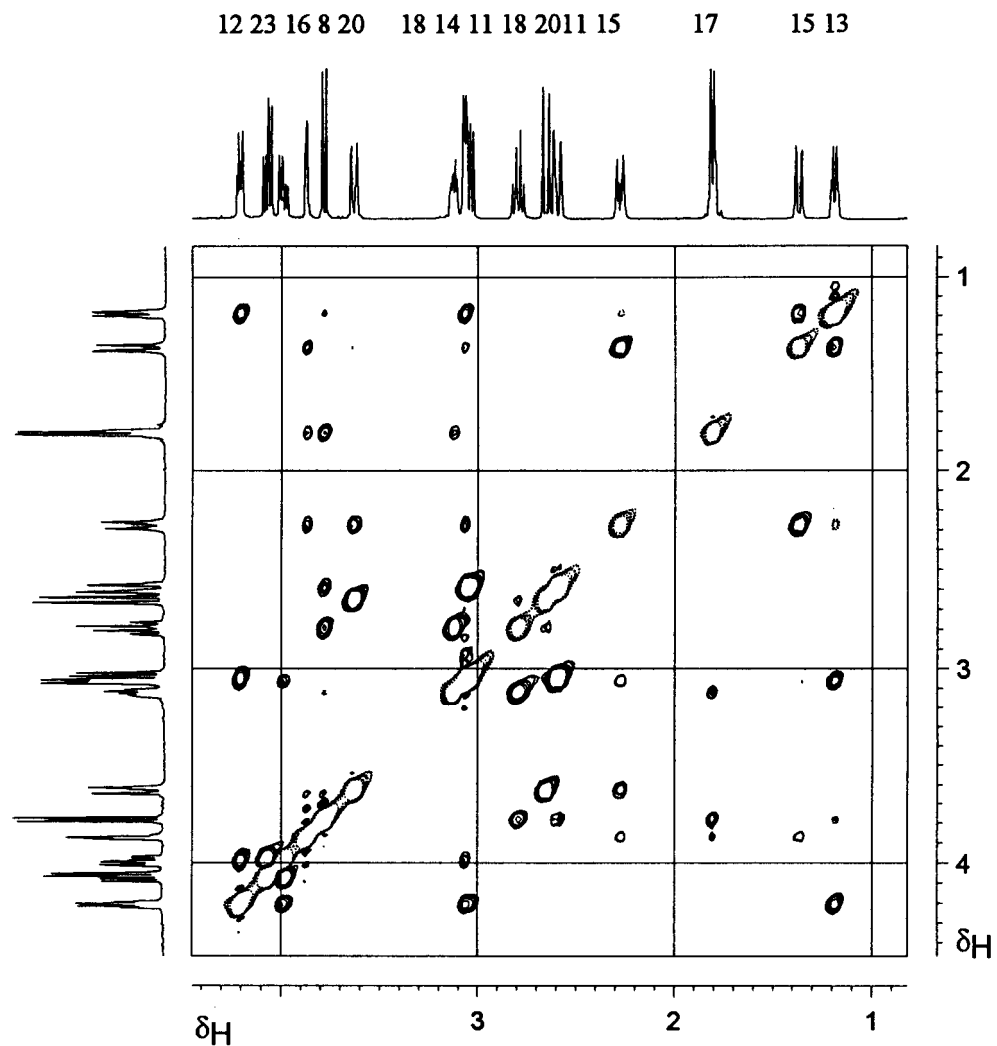


NMR NOESY

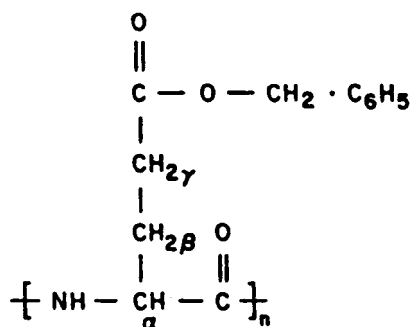
10% Strychnin in CDCl₃



12 23 16 8 20 18 14 11 18 20 11 15 17 15 13



NMR NOESY



Poly(γ -benzyl L-glutamate)

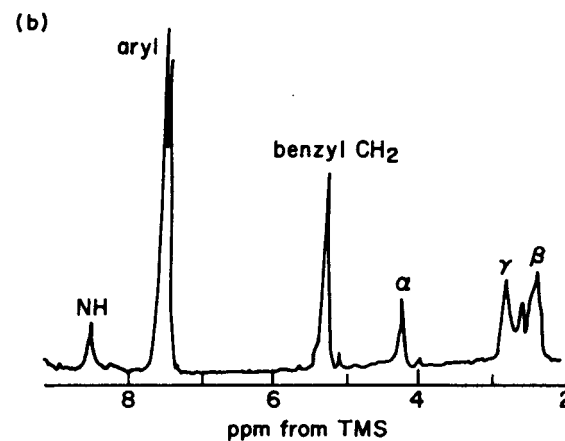
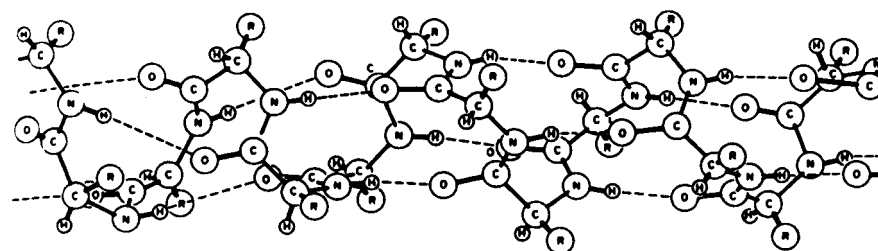
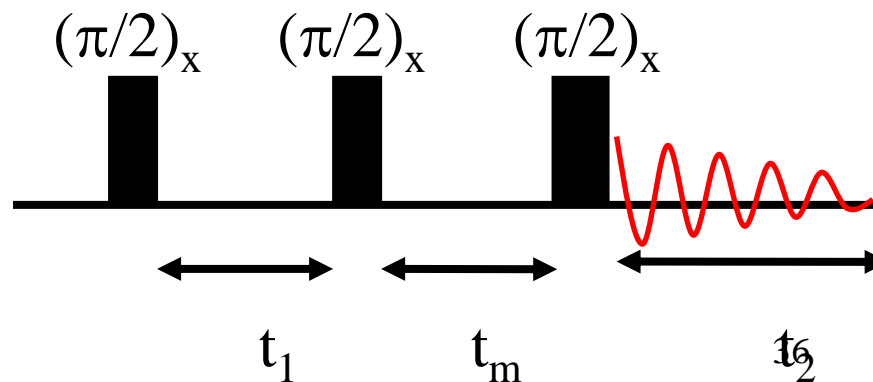
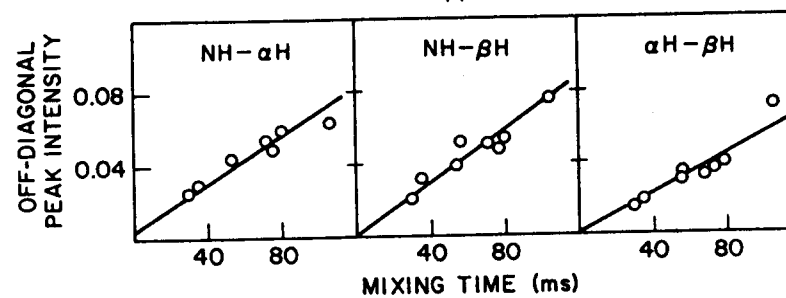
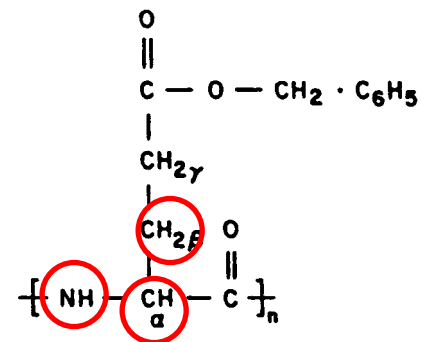
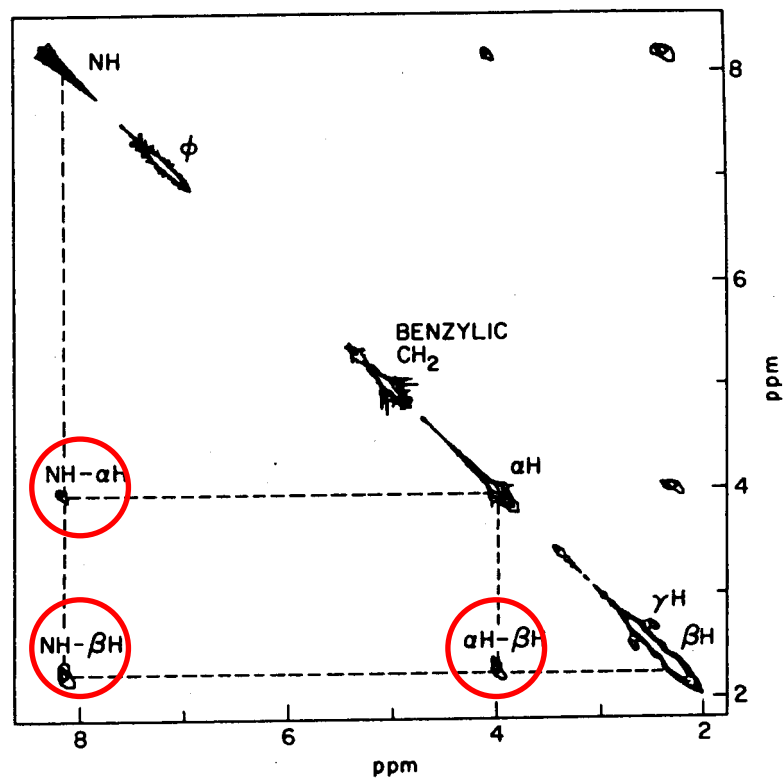
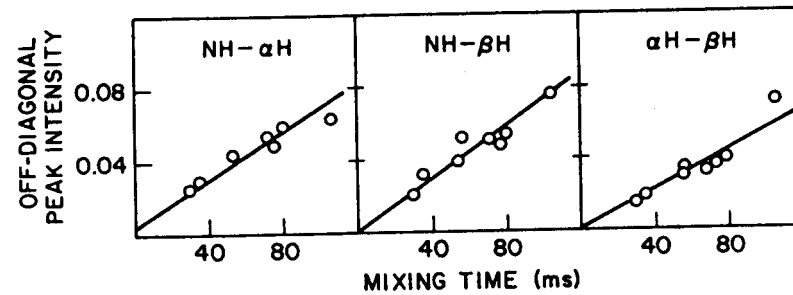


Figure 6. (a) Conformation of α -helix (14-mer). (b) 500-MHz proton spectrum of α -helical poly(γ -benzyl L-glutamate) (PBLG) in 95:5 (v/v) chloroform-trifluoroacetic acid. The trifluoroacetic acid serves to break up aggregates of α -helices, which themselves remain intact. (Mirau, P. A.; Bovey, F. A. *J. Am. Chem. Soc.* 1986, 108, 5130.)

NMR NOESY



NMR NOESY



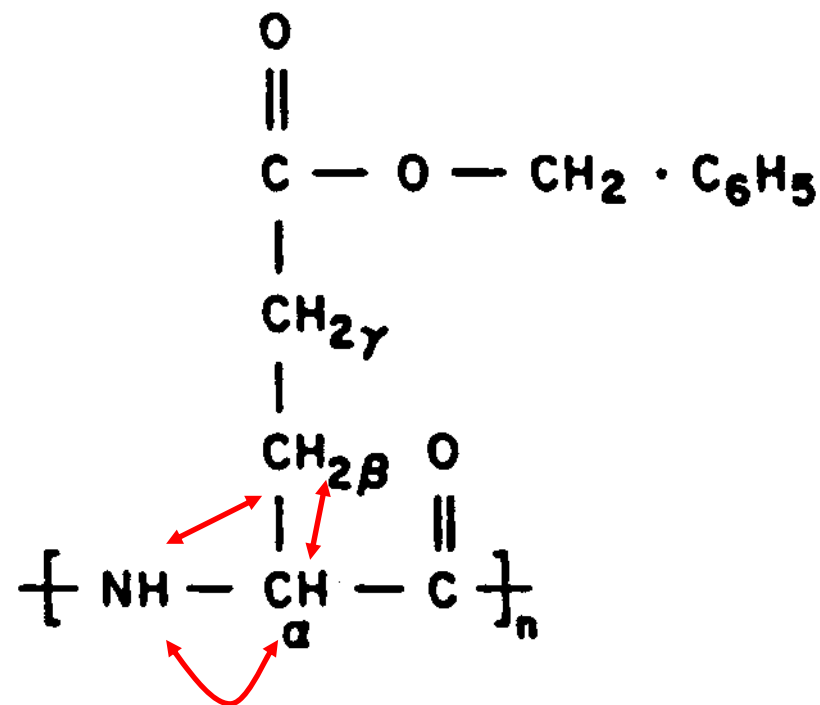
$$\frac{R_{II}}{R_{IS}} \approx \frac{-J(\omega_0) + 6J(\omega_2)}{J(\omega_0) + 3J(\omega_1) + 6J(\omega_2)} \quad J \propto \frac{\tau_c}{(1 + \omega^2 \tau_c^2)}$$

$$\text{Steigung} = \sigma = 5.7 \left[\frac{6\tau_c}{1 + 4\omega^2 \tau_c^2} - \tau_c \right] \times 10^{10} r_6^{HH}$$

NMR NOESY

Cross-Relaxation Rates, Calculated Interproton Distances and X-ray Distances for α -Helical PBLG

interaction	σ, s^{-1}	$r_{\text{HH}}, \text{\AA}$	
		from NOESY	expected for α -helix (X-ray)
NH- α H	0.54	2.20	2.48
NH- β H	0.55	2.20	2.26
α H- β H	0.72	2.10	2.20



NMR NOESY

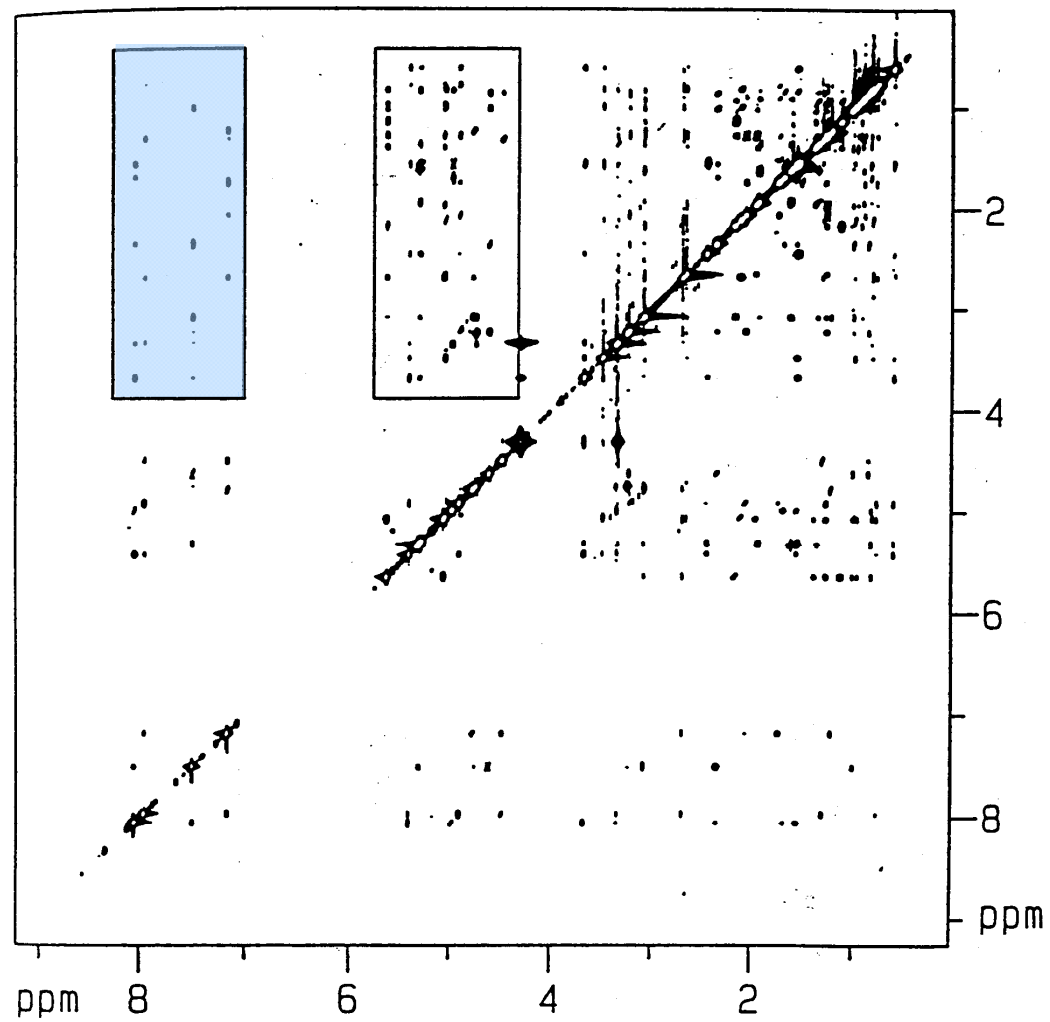
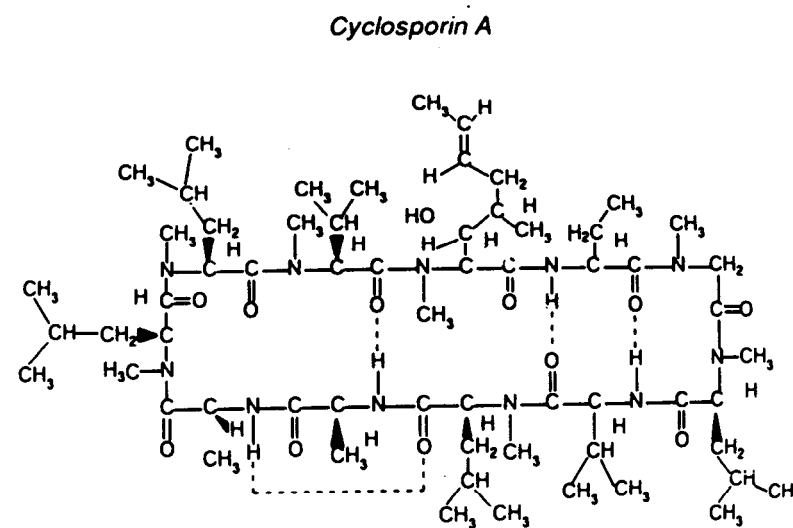
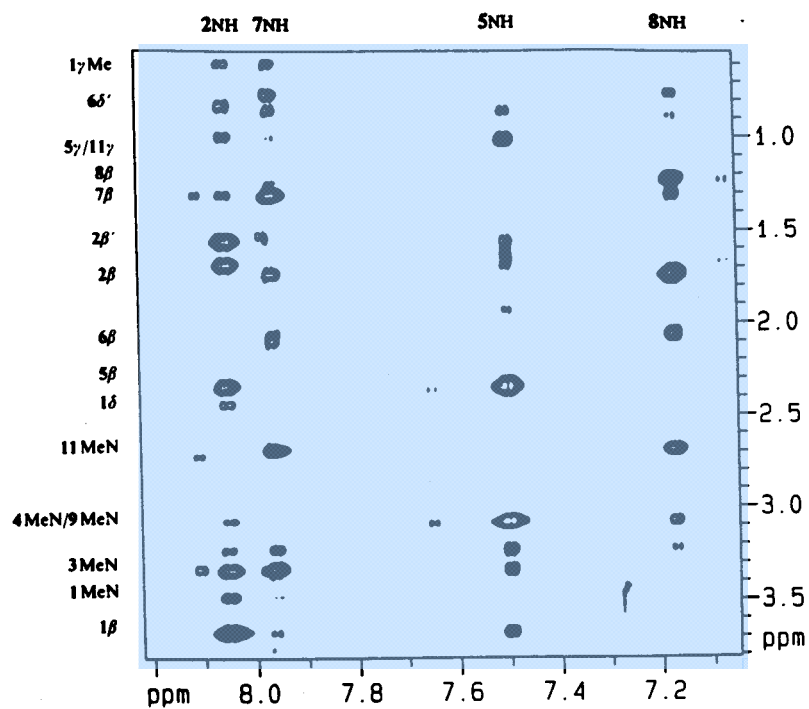
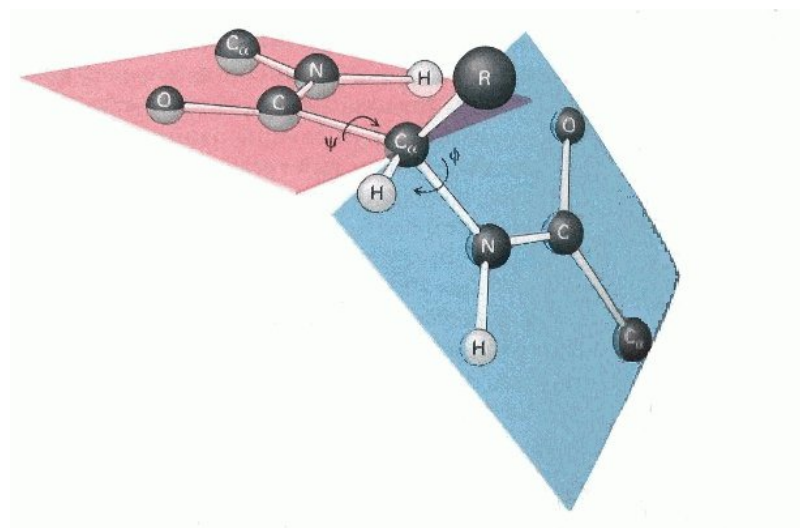
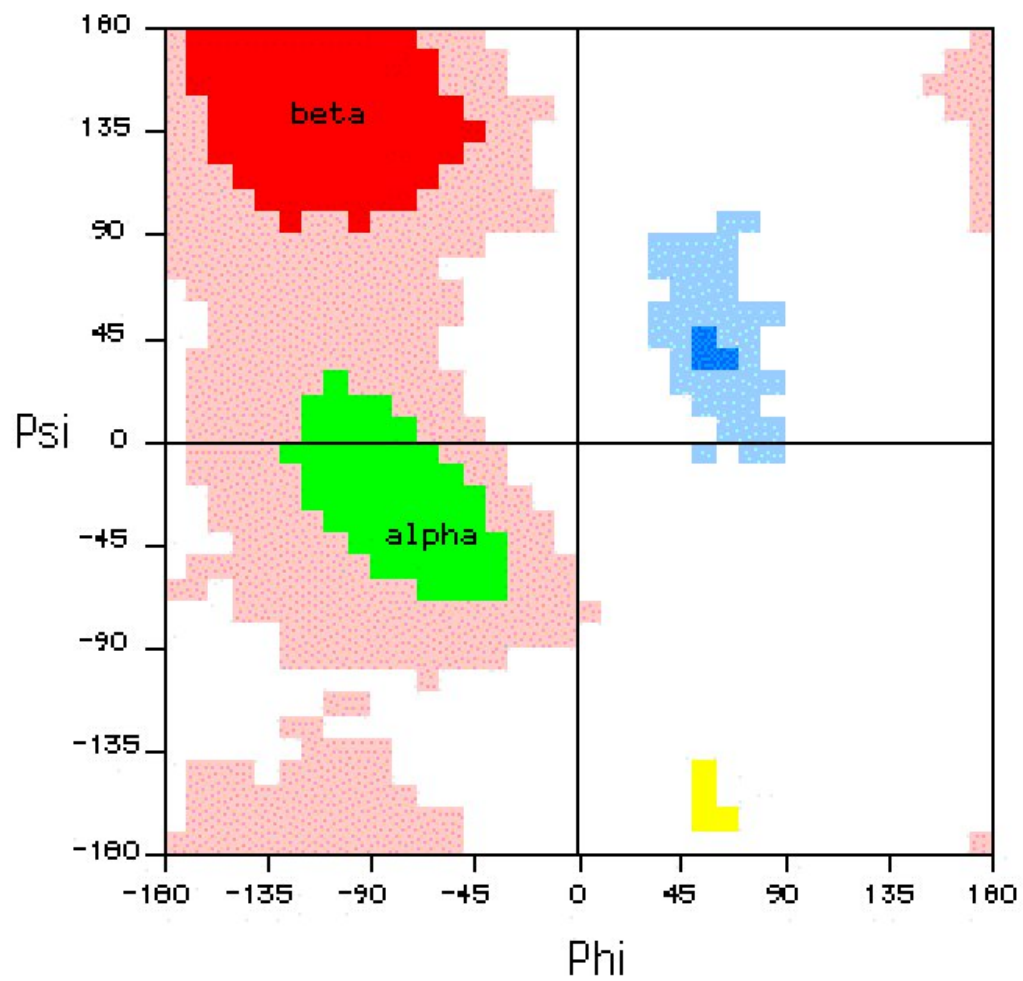


Fig. 1. 600-MHz NOESY spectrum of cyclosporin A at 252.5 K in $CDCl_3$ obtained with a mixing time of 200 ms. The indicated areas are expanded in Figs. 2 and 3, the left one in Fig. 2 and the right in Fig. 3.

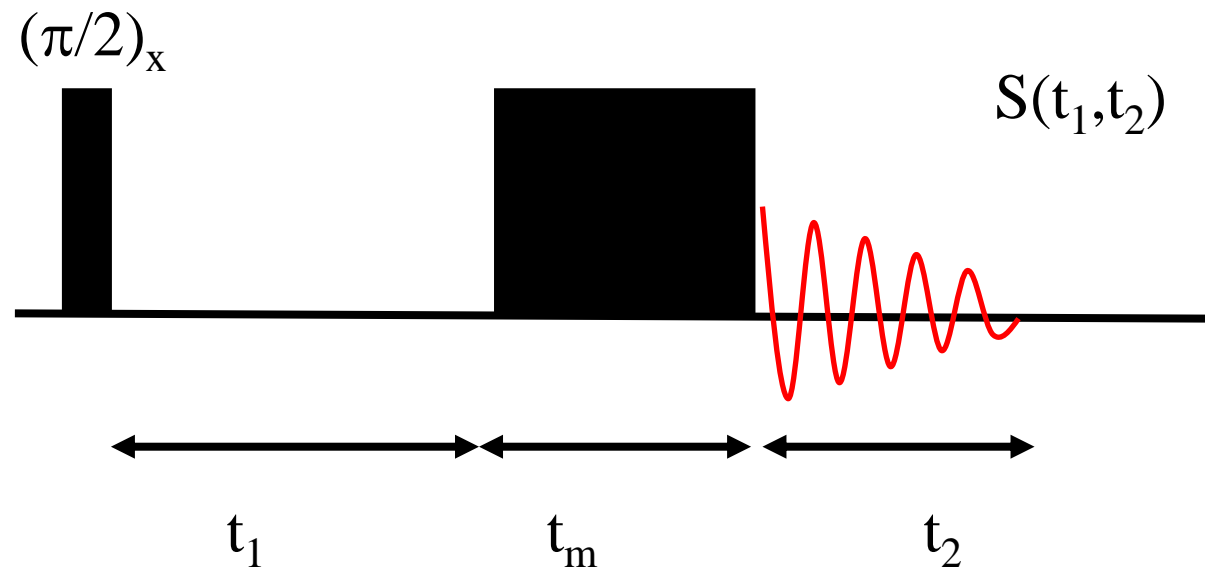
NMR NOESY



NMR NOESY



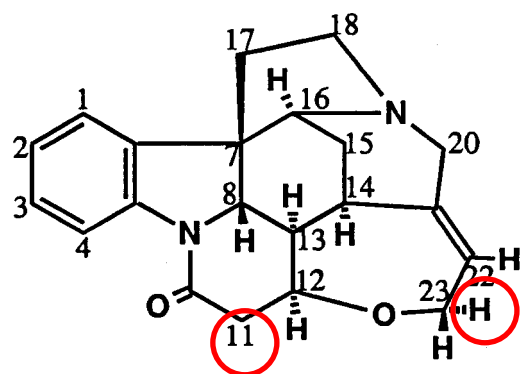
TOCSY (Total Correlation Spectroscopy)



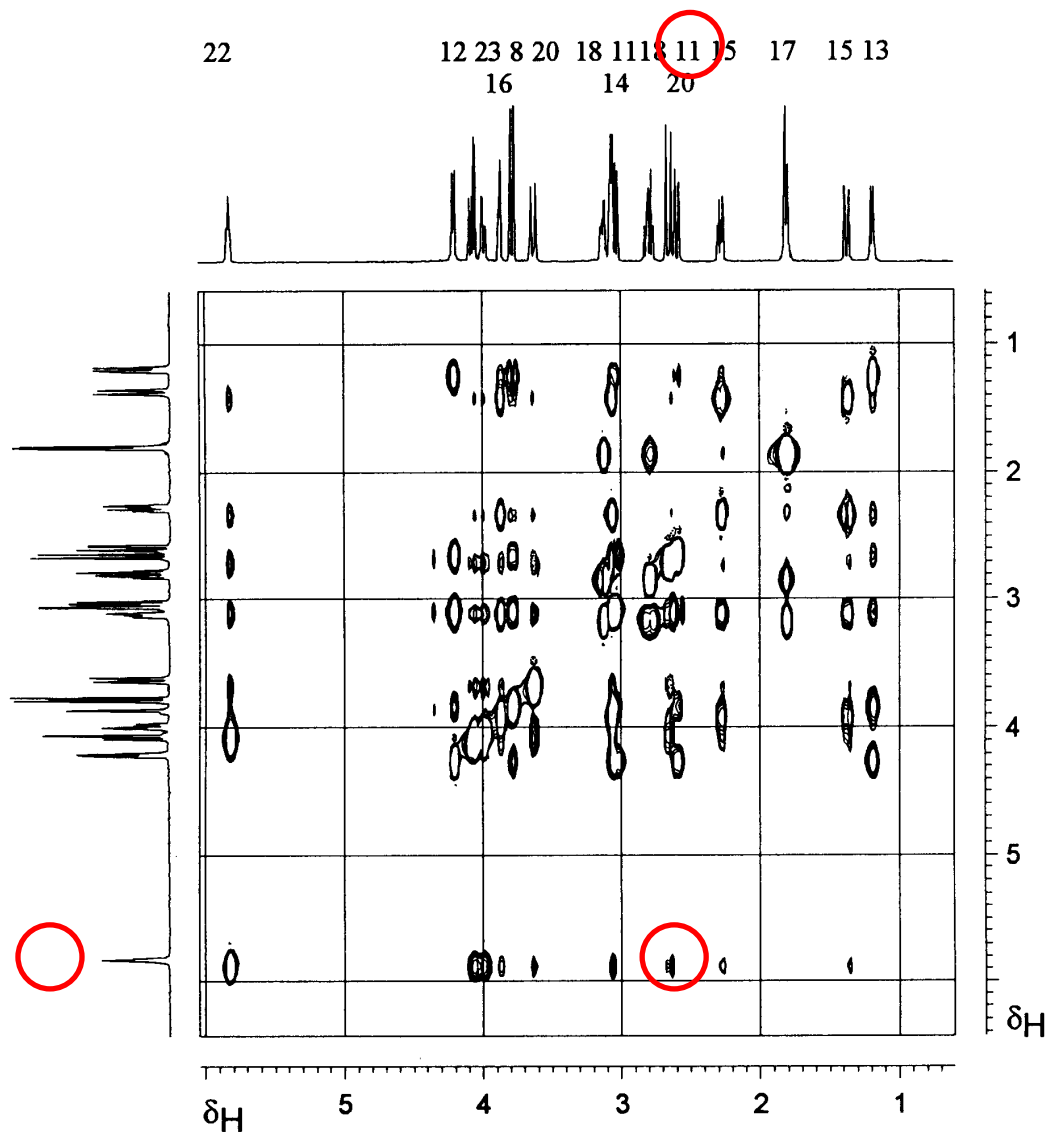
$$90^\circ_x - t_1 - 90^\circ_x - t_m - 90^\circ_x - \text{FID}(t_2)$$

NMR TOCSY

10% Strychnin in CDCl_3

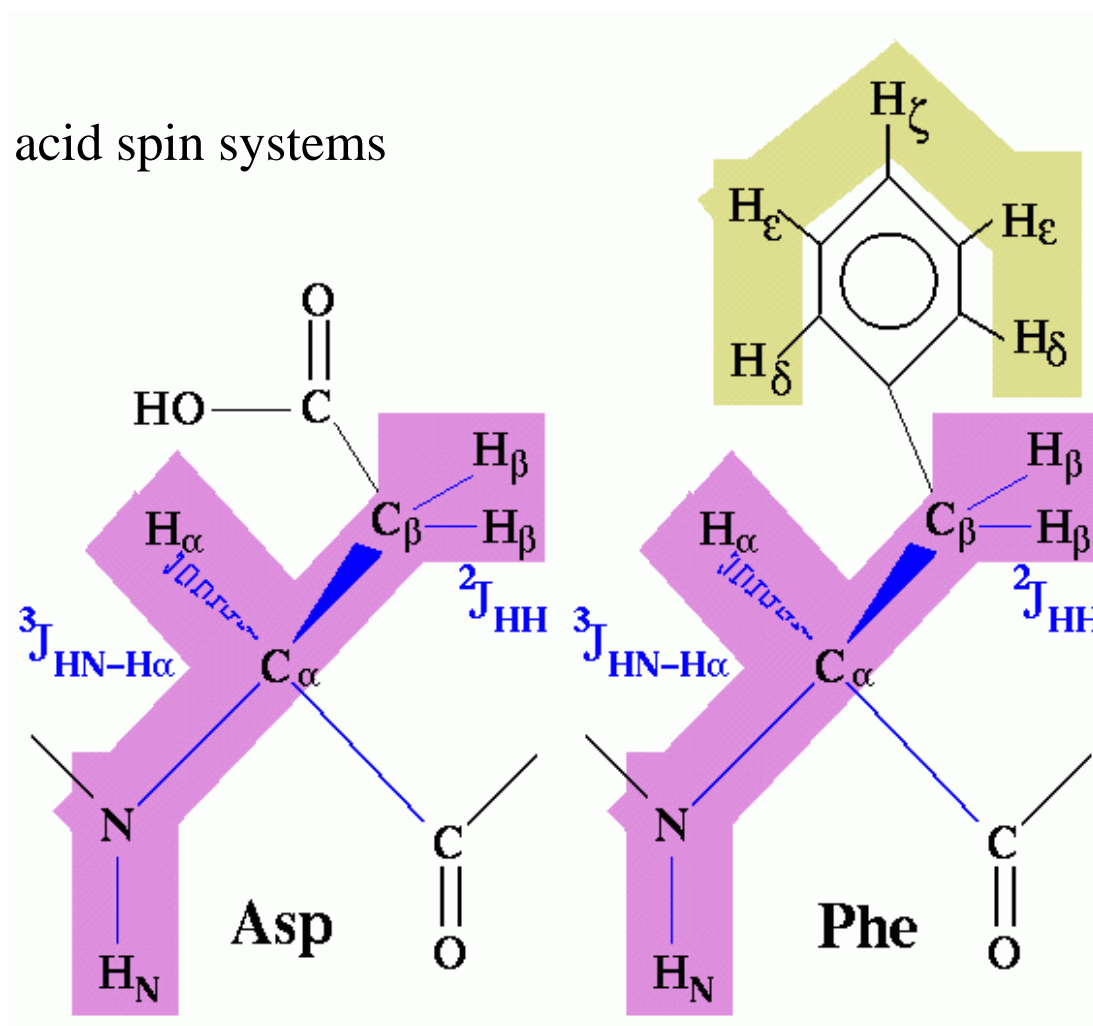


12 23 16 8 20 18 14 11 18 20 11 15 17 15 13

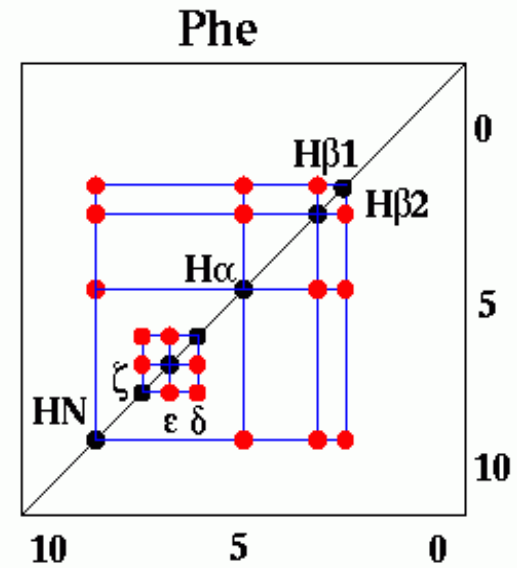
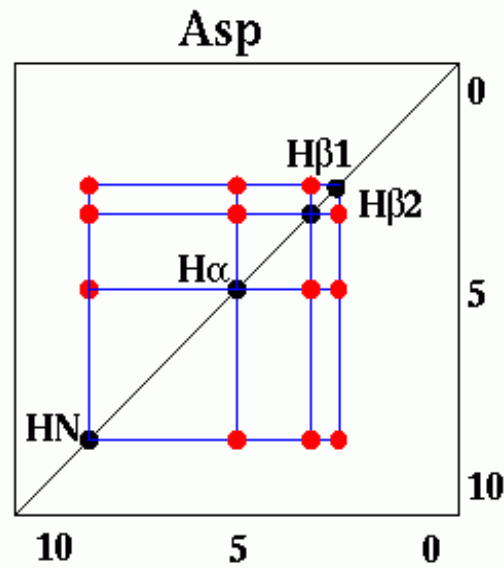
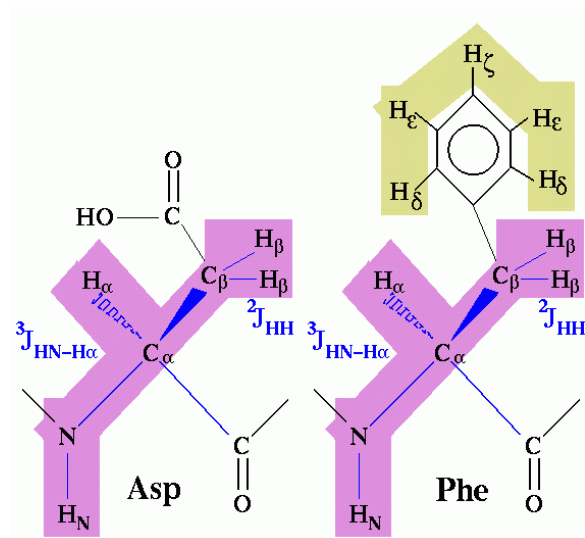


NMR TOCSY

Amino acid spin systems



NMR TOCSY



2D TOCSY Spectrum von Aspartinsäure und Phenylalanin