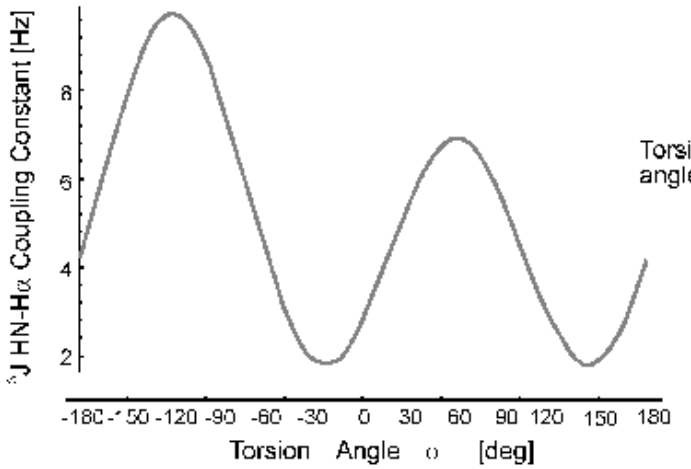
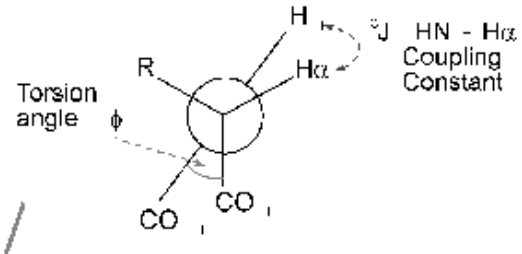
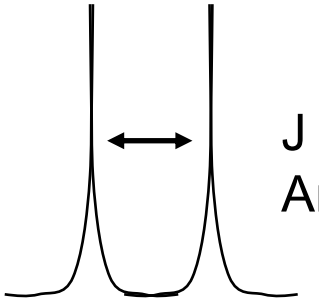
Magnitude of Chemical Coupling Determined by Conformation

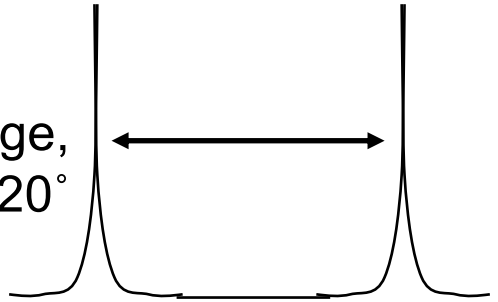




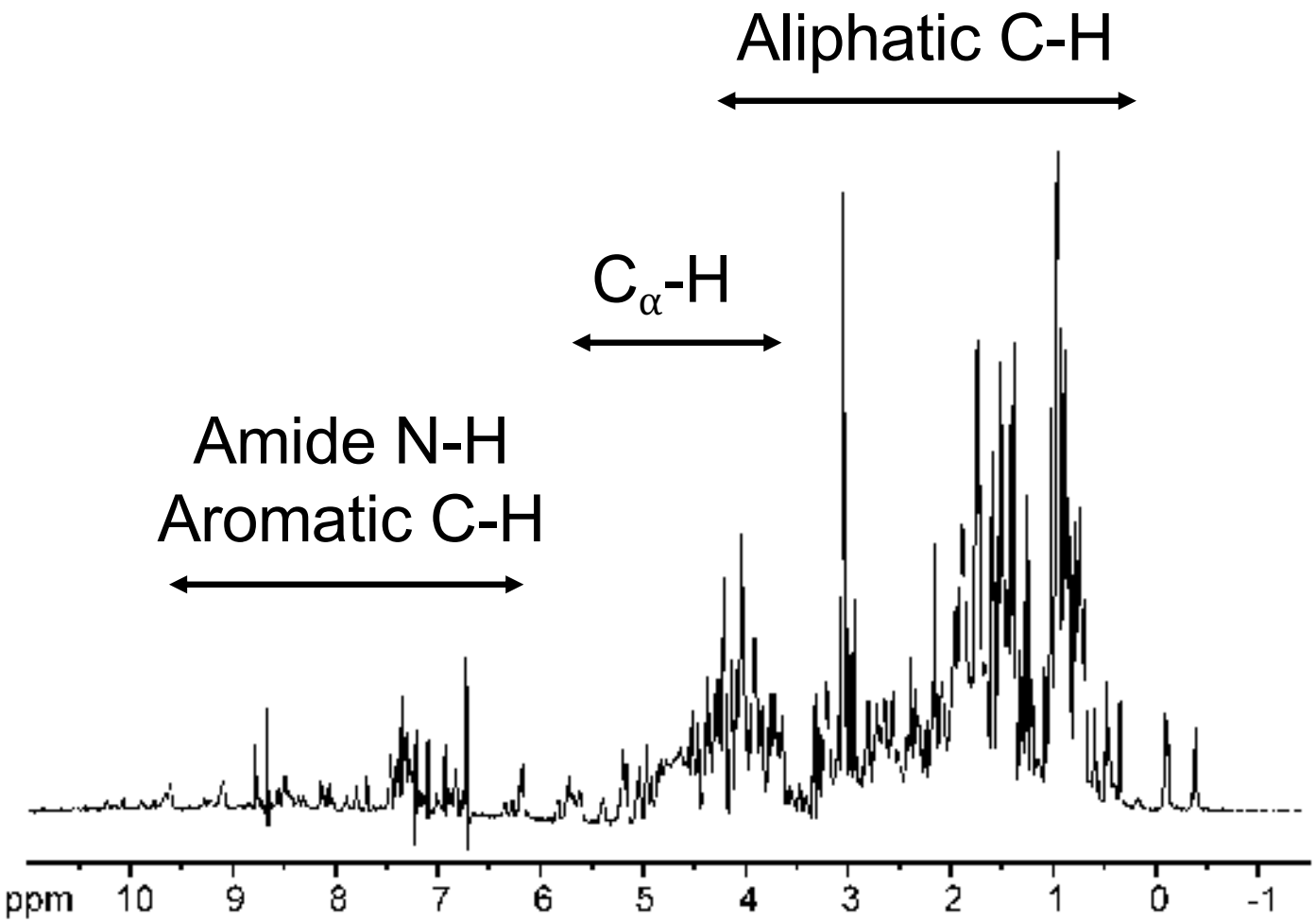


J is small,
Angle ≈ 150˚

J is large,
Angle ≈ -120˚



1-D NMR Spectrum

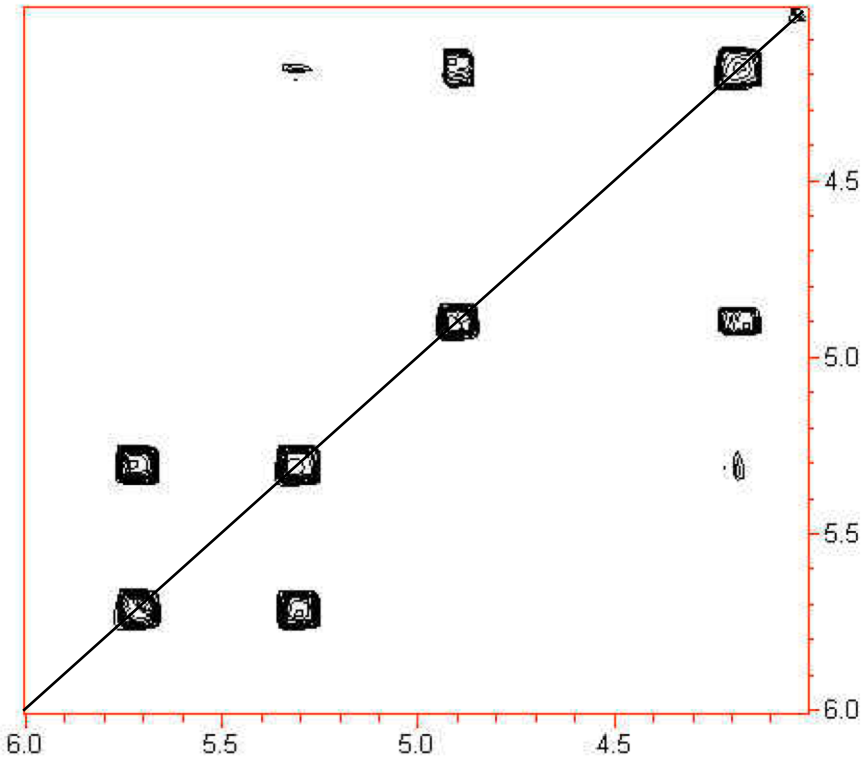


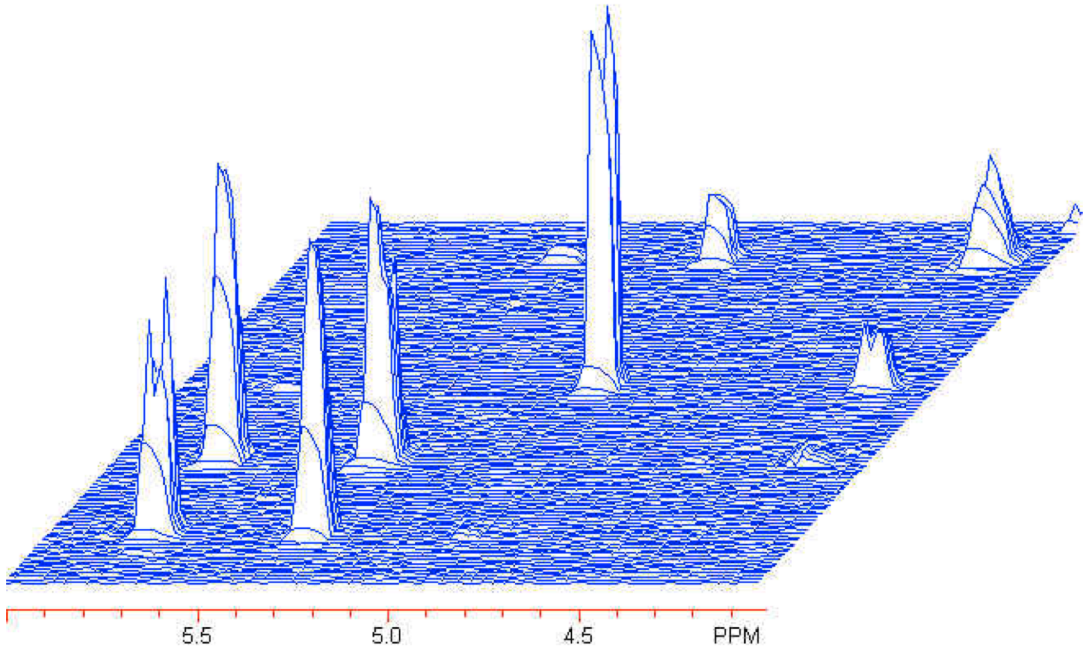
Spread the Signal With a Magnet

NMR lab at UWisconsin (left to right): 750 MHz, 800 MHz & 900 MHz

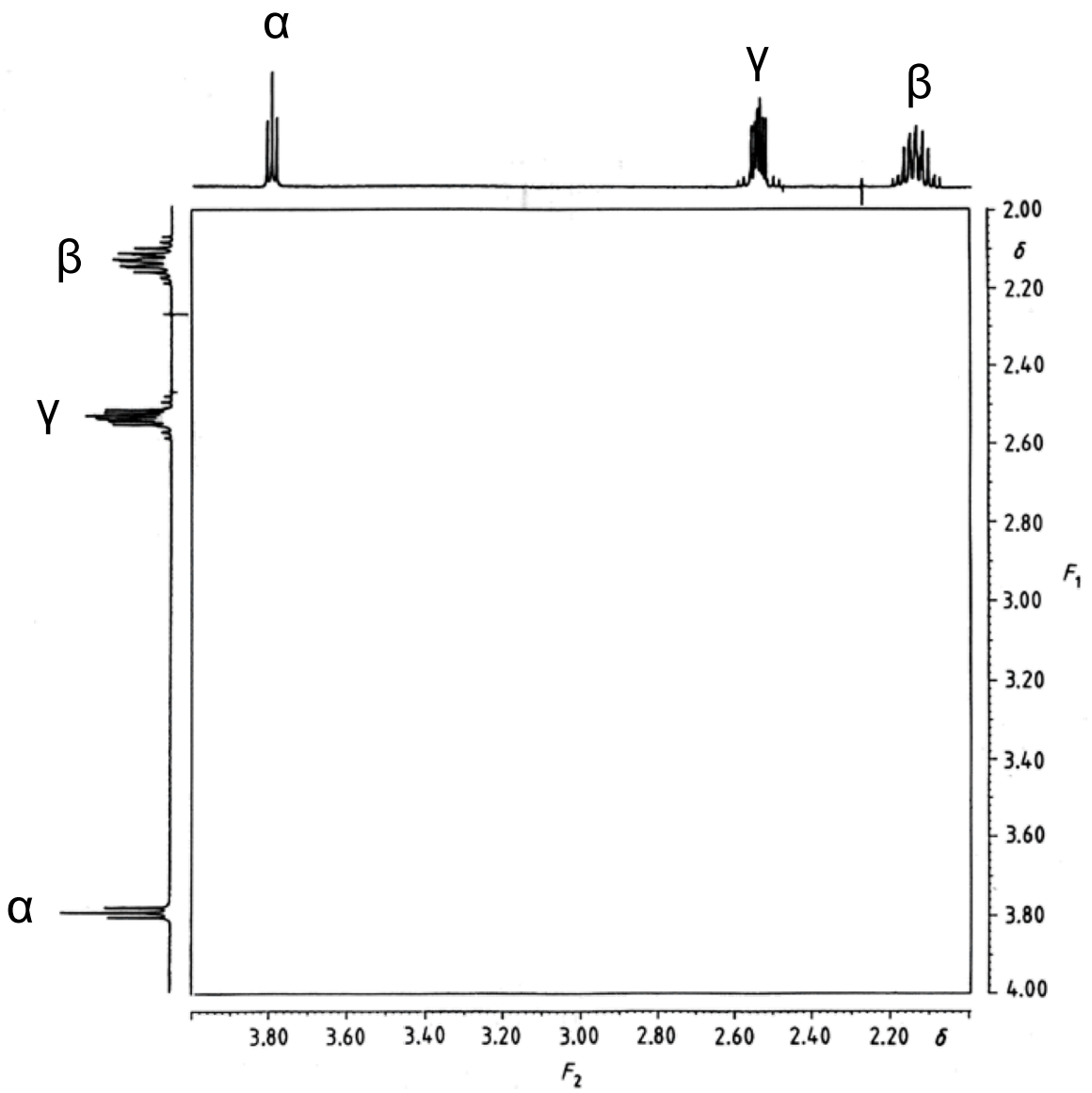
Manhattan: 1D vs. 2D

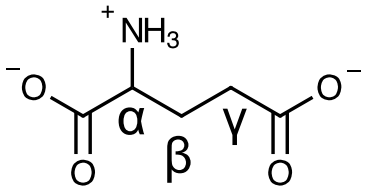
2D NMR in 3D





2D COSY Spectrum of Glutamate



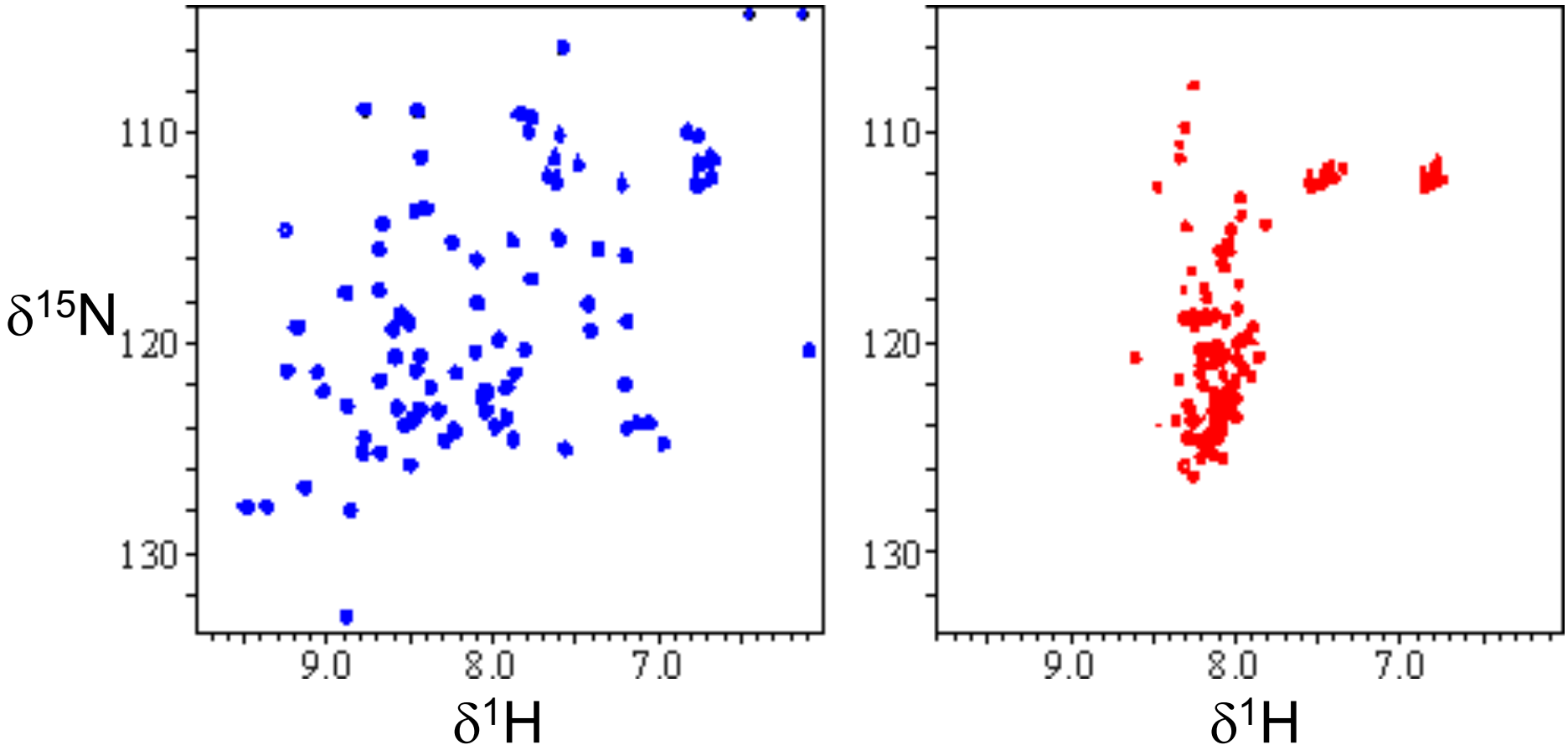


http://131.104.156.23/Lectures/CHEM_207/CHM_207_NMR.htm

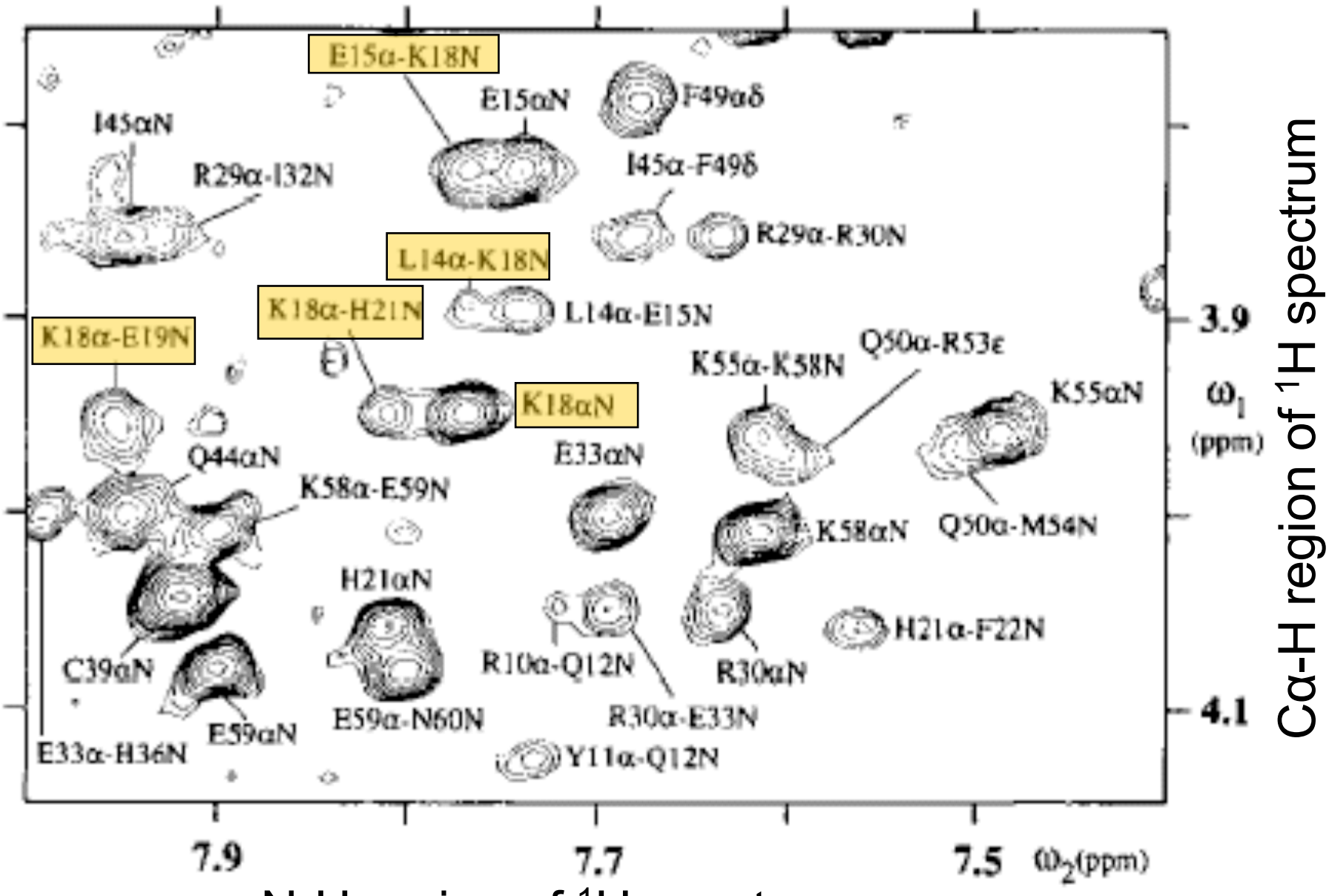
HSQC Spectrum

Folded/Disperse

Unfolded/Non-disperse

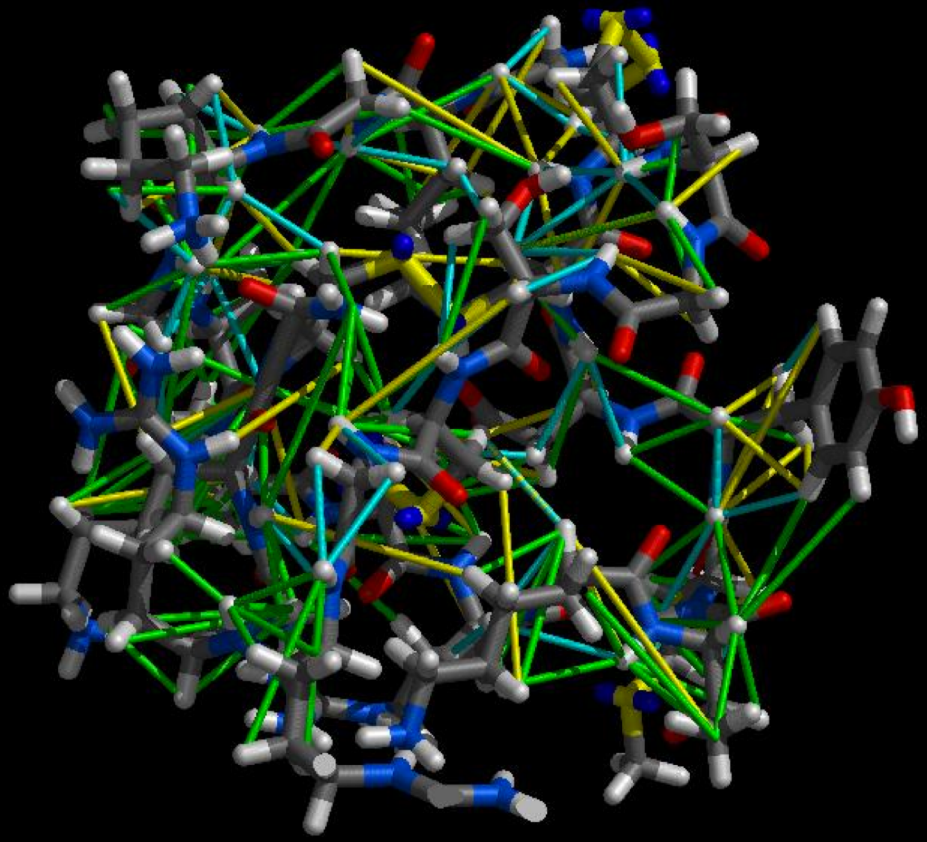


Sample NOESY Spectrum



N-H region of ^{1}H spectrum

Cα-H region of ^{1}H spectrum



http://www.cgl.ucsf.edu/midas-images/noeshow.jpeg

Guide to Structure Quality

REVIEW ARTICLE

Macromolecular NMR spectroscopy for the non-spectroscopist

Table 1. A guide for judging the 'resolution' of NMR-derived protein structures.

Assessment criterion	Very high resolution	High resolution	Medium resolution	Low resolution
Restraints per residue[a]	> 18	14–18	10–15	< 10
Backbone rmsd (Å)[b]	< 0.3	0.3–0.5	0.5–0.8	> 0.8
Heavy-atom rmsd (Å)[b]	< 0.75	0.75–1.0	1.0–1.5	> 1.5
Ramachandran				
Plot quality (%)[c]	> 95	85–95	75–85	< 75
Example PDB file	1TVJ [63]	2IL8 [65]	2FE0 [66]	1LMM [67]

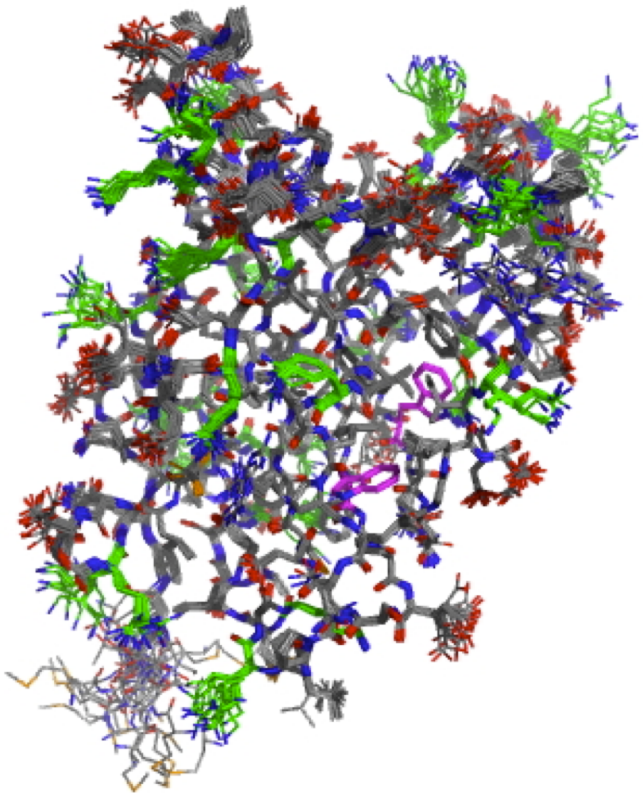
FEBS Journal **278** (2011) 687–703

Example of High Resolution

Table 1. Structural Statistics for the Ensemble of 20 Chick Cofilin Structures

Experimental Restraints	
Interproton distances (2533 total)[a]	
Intraresidue	465
Sequential	665
Medium range	459
Long range	944
Hydrogen bonds[b]	92
Dihedral angles (155 ϕ, 148 ψ, 62 χ_1)	365
Mean Rms Deviations from Experimental Restraints	
NOE distances (Å)	0.0321 ± 0.0004[c]
Dihedral angles (deg)	0.539 ± 0.021
Mean Rms Deviations from Idealized Geometry[d]	
Bonds (Å)	0.00323 ± 0.00003
Angles (deg)	0.454 ± 0.003
Rms Deviation to Mean Coordinate Structure (Å)	
Backbone atoms (residues 5–166)	0.25 ± 0.05
All heavy atoms (residues 5–166)	0.73 ± 0.04

Molecular Cell *24*, 511–522, November 17, 2006



http://www.rcsb.org/pdb/explore.do?structureId=1TVJ

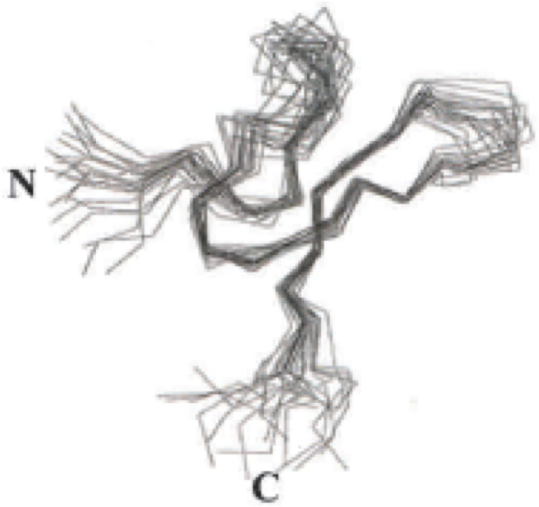
Example of Low Resolution

Table 1. *Structural statistics of the PcTx1 20 best structures obtained by distance geometry and minimization*

Coordinate precision[a]	
r.m.s. deviation (Å)	
Region 1–40	
Backbone	2.51 ± 0.51
All heavy atoms	3.58 ± 0.48
Region 6–35	
Backbone	1.68 ± 0.36
All heavy atoms	2.92 ± 0.48
Region 6–9, 18–25, 31–35	
Backbone	0.90 ± 0.22
All heavy atoms	1.95 ± 0.36
Statistics for structure determination	
r.m.s. deviation from experimental restraints	
NOE distances (Å)	0.029 ± 0.001
Dihedral angles (degrees)	0.14 ± 0.01
r.m.s. deviation over secondary structure	
Bonds (Å)	0.0033 ± 0.0001
Angles (degrees)	0.42 ± 0.02
Impropers (degrees)	0.26 ± 0.02
Procheck analysis	
Most favored and additional allowed (%)	92.5
Generously allowed (%)	7.5
Disallowed region (%)	0

Protein Science (2003), 12:1332–1343.

The structure of PcTx1 was determined by using 374 NOE-based distance restraints, including 195 intraresidue restraints, 111 sequential restraints, 24 medium-range restraints, and 44 long-range restraints.



http://www.rcsb.org/pdb/explore.do?structureId=1LMM