Protein structure
(PDB Format or PDB ID code)

Protein sequence
(plain or FASTA Format)

Amino Acid Sequence

User provided shifts
(Sparky, ShiftX or CSV Format)

Shift prediction via
ShiftX, ShiftX2, SHIFTS,
Sparta, Sparta+, shAIC
or CamShift

Average shifts extracted
from BioMagResBank

Chemical Shifts
for Nuclei

Inter-residue correlation

Intra-residue correlation

Double quantum correlation

Through space correlation

Chain

Model

Residue range

Residue types

Secondary structure

Labelling pattern

Predicted Spectra

Clone function

Spectra for Visualization

Upload Experimental
Spectrum
(Bruker, Agilent or
NMRPipe Format)

Intensity Comparison
Predicted / Experimental

Legend

Activity Flow

Data Flow

Peakr status

Computation

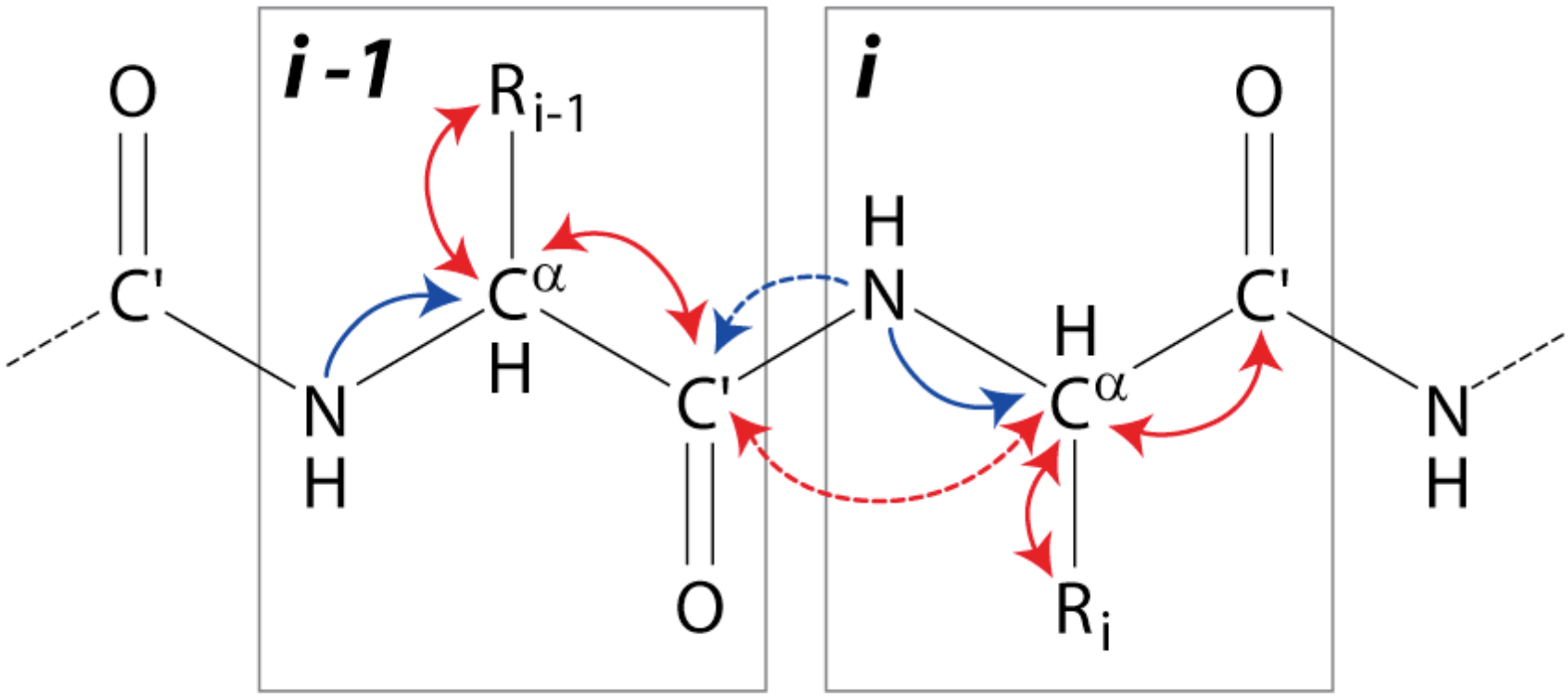
User input data

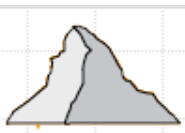
External software

External database

Correlations

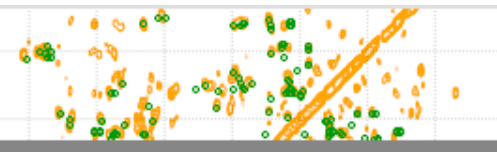
Residue selection


i -1
i
O
C'
N
H
R_{i-1}
C^{α}
H
C'
O
H
N
H
C^{α}
C'
O
N
H
R_i



Peakr

predicting 2D solid-state NMR spectra



Prediction | Upload | Team | Help | Contact

Spectra

Protein

Protein Name: 1D3Z

Protein Sequence:
MQIFVKTLTGKTITLEVEPSDTIENVKAKIQDKEGIPPDQQRLI
FAGKQLEDGRTLSDYNIQKESTLHLVLRLRGG

PDB File upload: Choose Files | No file chosen — 1D3Z.pdb ✓

or get PDB by name:

If a sequence and a pdb file are provided, the sequences will be aligned and the longer sequence will be used.

Chemical shifts

Add shifts using: Shift list + Prediction

Shifts from Sparky file

Upload Sparky file: Choose Files | No file chosen — ubq_shifts_sparky.txt ✓

Shifts from CSV file

Upload CSV file: Choose Files | No file chosen — No file selected

Prediction options

Add missing shifts with: ShiftX

Correlations

Correlation Type: C-C intraresidue

Correlation Name: C-C-intra

Depth: All

Number of Bonds: 2

Single Bond Distance: ☐

Create Spectrum | Reset form | or | Load Example

Added Spectra

Protein_Correlation Hide settings

Labelling 15N, 13C uniform Graded opacity

Chain n/a **Model** n/a **Start** 1 **End** 20

Amino Acids A D *E F G* H *I K L M* N *P Q* R *S T V* Y

Secondary structure *H* G *E* B T *C*

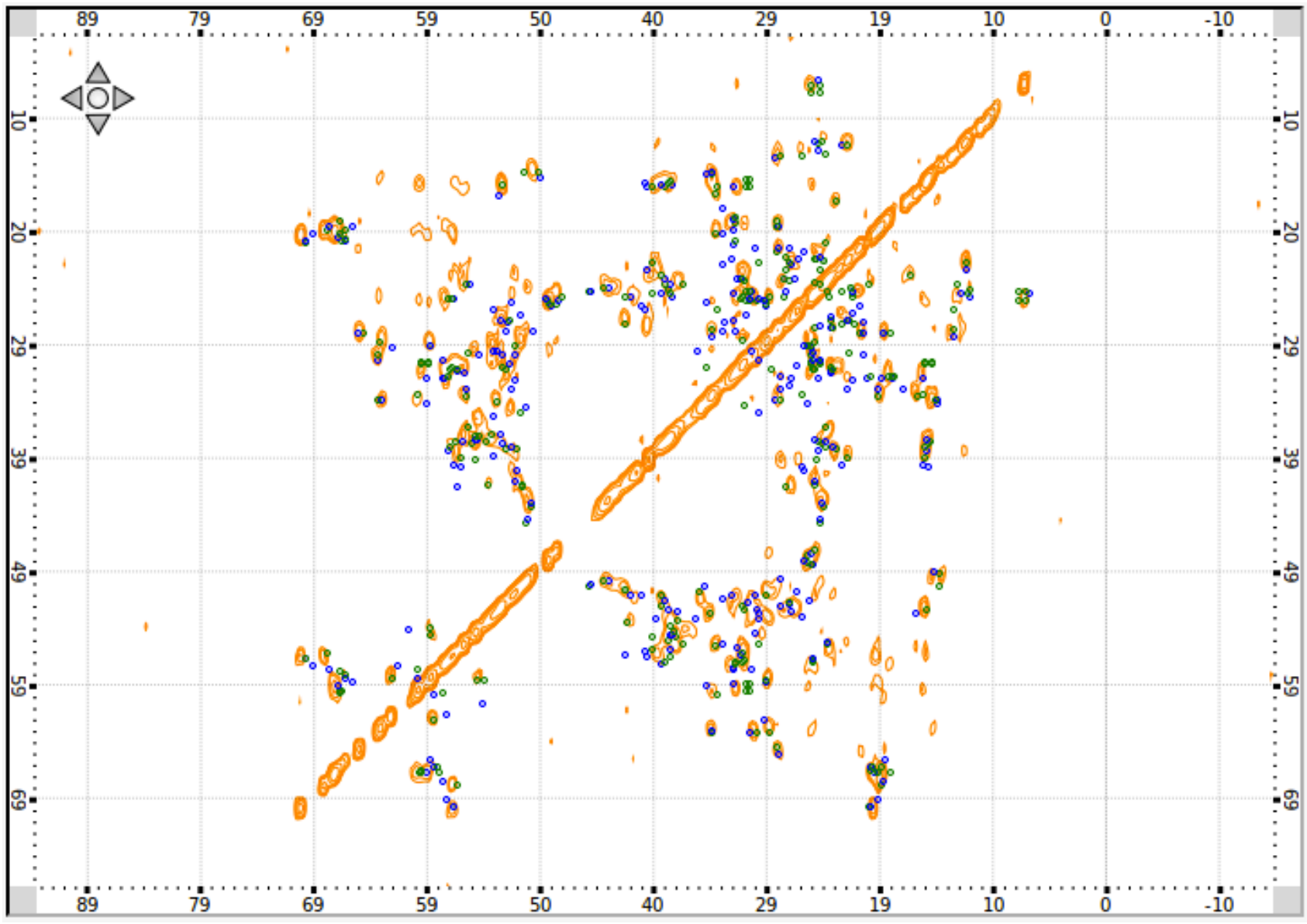
Protein_Correlation_1 Hide settings

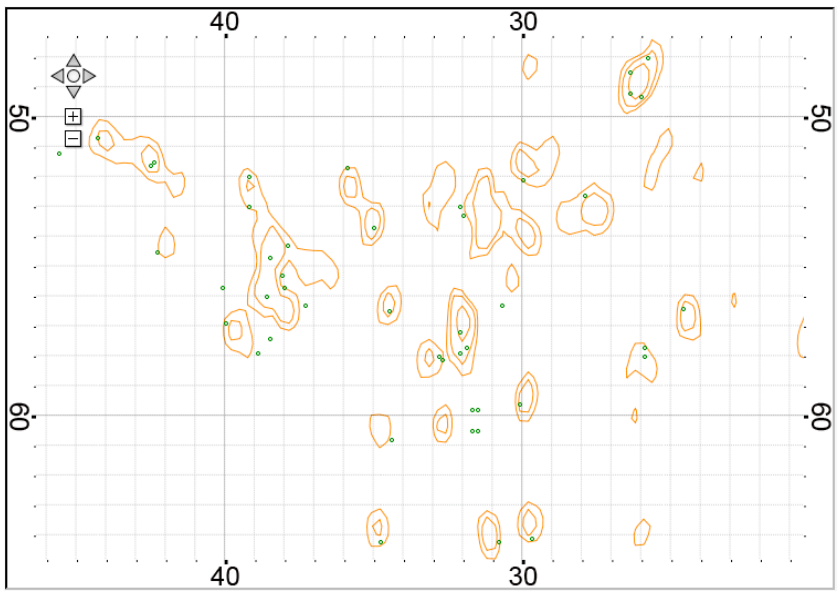
Labelling 15N, 13C uniform Graded opacity

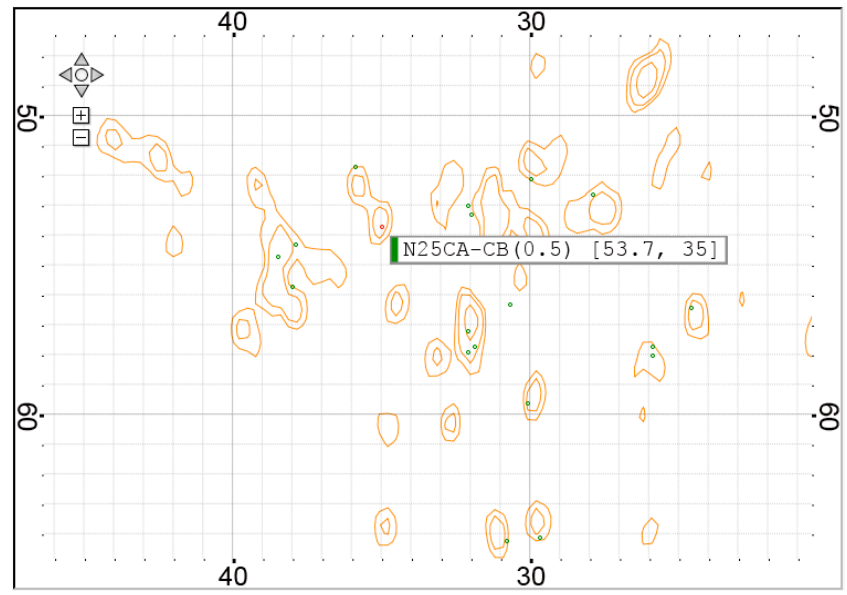
Chain n/a **Model** n/a **Start** 30 **End** 76

Amino Acids *A D E F G H I K L* M *N P Q R S T V Y*

Secondary structure *H* G *E* B T *C*


89
79
69
59
50
40
29
19
10
0
-10
10
20
29
39
49
59
69


40
30
50
60
40
30


N25CA-CB(0.5) [53.7, 35]
40
30
50
60
40
30