Chemical Shift Validation Report

February 26, 2025 – 5:53am EST

Entry ID	:	51537
Title	:	1H and 13C chemical shifts for retroenantio Ctn[15-34] in DPC micelles
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Deposited on	:	2022-07-28

The following versions of software and data were used in the production of this report:

PyNMRSTAR	:	3.3.0
RCI	:	1.1
ShiftChecker	:	1.2
LACS	:	VARLACSVER
AVS	:	VARAVSVER

1 Summary

The biological assembly is a monomer with one Entity.

1.1 Entity information

1.1.1 Entity 1

Type	:	polymer
Polymer type	:	polypeptide(D)
Name	:	entity_1
Sequence length	:	21
Sequence	:	FPITVGIVMPKKFIKKLRKK X

1.2 Chemical shift list information

There are 2 chemical shift lists reproted. The summary of the chemical shift data is given below

Saveframe name	assigned_chemical_shifts_1
Saveframe ID	1
Ionic Strength	0 M
PH	3.0 pH
Pressure	1 atm
Temperature	298 K
Number of shifts	271
Number of shift outliers	0
Assignment completeness	88.0%

Saveframe name	assigned_chemical_shifts_2
Saveframe ID	2
Ionic Strength	0 M
PH	3.0 pH
Pressure	1 atm
Temperature	308 K
Number of shifts	271
Number of shift outliers	0
Assignment completeness	88.0%

2 Completeness

Completeness information for Entity 1. It is a polypeptide(D) polymer. 3 out of 3 methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	57/97 (58.8%)	38/39 (97.4%)	19/40 (47.5%)	0/18 (0.0%)
Sidechain	194/208 (93.3%)	132/138 (95.7%)	62/63 (98.4%)	0/9 (0.0%)
Aromatic	20/20 (100.0%)	10/10 (100.0%)	10/10 (100.0%)	0/0 (0.0%)
Overall	283/325 (87.1%)	180/187 (96.3%)	91/113 (80.5%)	0/27 (0.0%)

Completeness information for Entity 1. It is a polypeptide(D) polymer. 0 out of 3 methyl groups (LEU and VAL) were assigned stereospecifically.

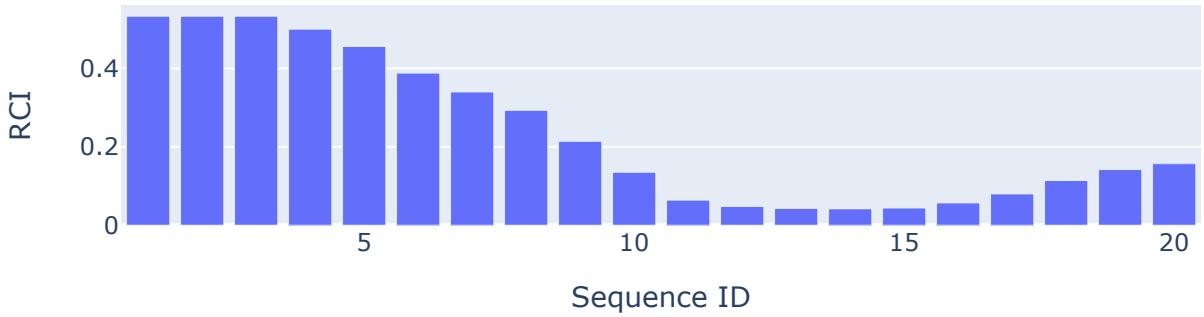
	Total	^{1}H	^{13}C	^{15}N
Backbone	57/97 (58.8%)	38/39 (97.4%)	19/40 (47.5%)	0/18 (0.0%)
Sidechain	194/208 (93.3%)	132/138 (95.7%)	62/63 (98.4%)	0/9 (0.0%)
Aromatic	20/20 (100.0%)	10/10 (100.0%)	10/10 (100.0%)	0/0 (0.0%)
Overall	289/325 (88.9%)	180/187 (96.3%)	91/113 (80.5%)	0/27 (0.0%)

3 Statistically unusual chemical shifts

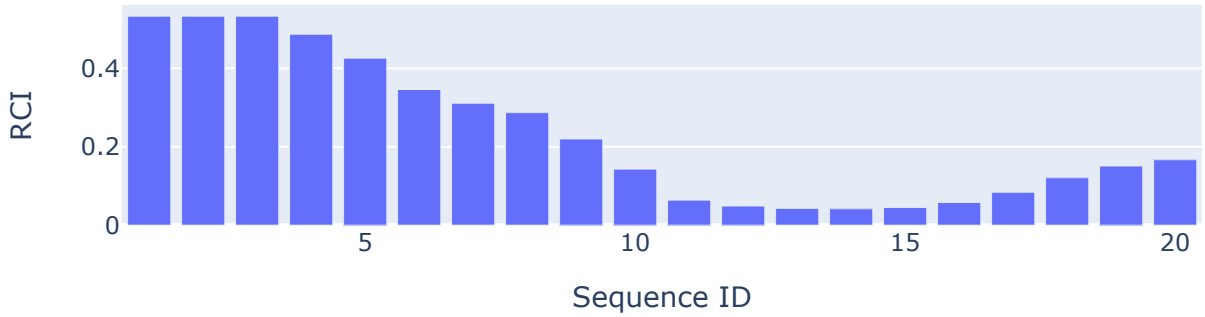
There are no chemical shift outliers.

4 RCI

RCI plot for the chemical shifts from the save frame *assigned_chemical_shifts_1*

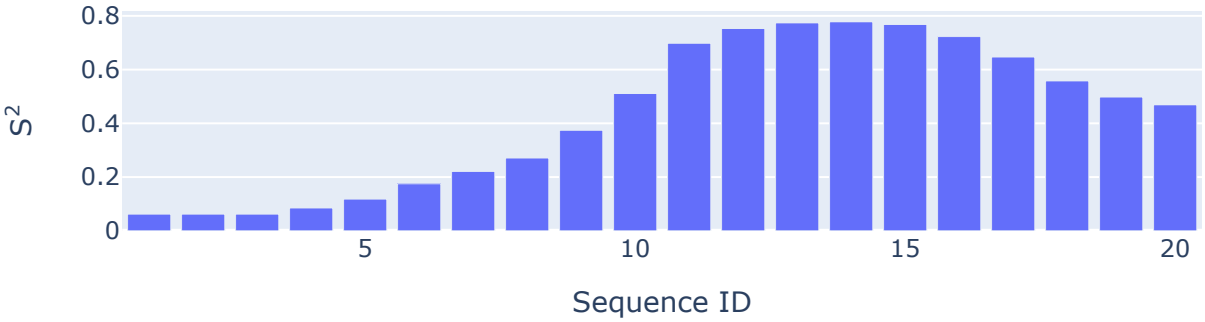


RCI plot for the chemical shifts from the save frame *assigned_chemical_shifts_2*

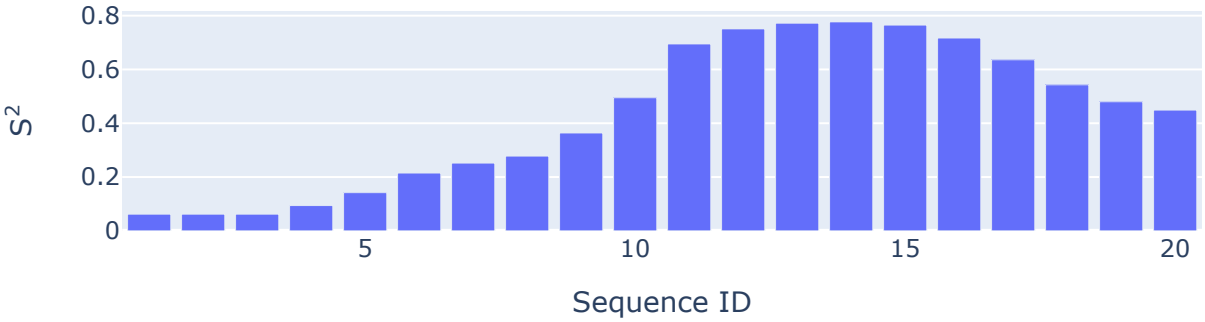


5 Order parameter

Order parameter plot for the chemical shifts from the save frame *assigned_chemical_shifts_1*



Order parameter plot for the chemical shifts from the save frame *assigned_chemical_shifts_2*



6 Simulated peak positions

Not enough data to simulate spectum

7 LACS

Place holder for LACS results

8 Analysis data

place holder for the numerical values and tables.