Chemical Shift Validation Report

November 29, 2022 – 5:11am EST

Entry ID	:	30478
Title	:	NMR solution structure of wild type hFABP1 in the presence of GW7647
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Deposited on	:	2018-06-11

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 complex.

1.1 Entity information

1.1.1 Entity 1

Type	:	polymer
Polymer type	:	polypeptide(L)
Name	:	entity_1
Sequence length	:	135
Sequence	:	HHHHHHVAMSFSGKYQLQSQ ENFEAFMKAIGLPEELIQKG KDIKGVSEIVQNGKHFKFTI TAGSKVIQNEFTVGEECELE TMTGEKVKTVVQLEGDNKLV TTFKNIKSVTELNGDIITNT MTLGDIVFKRISKRI

1.1.2 Entity 2

Type	:	non-polymer
Polymer type	:	.
Name	:	entity_2VN
Sequence length	:	1
Sequence	:	.

1.2 Chemical shift list information

There is 1 chemical shift list reproted. The summary of the chemical shift data is given below

Saveframe name	assigned_chemical_shifts_1
Saveframe ID	1
Ionic Strength	70 mM
PH	5.5 pH
Pressure	1 atm
Temperature	308 K
Number of shifts	1526
Number of shift outliers	1
Assignment completeness	81.8%

2 Completeness

Completeness information for Entity 1. It is a polypeptide(L) polymer. 0 out of 19 methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	523/684 (76.5%)	266/280 (95.0%)	130/270 (48.1%)	127/134 (94.8%)
Sidechain	919/1036 (88.7%)	626/675 (92.7%)	277/330 (83.9%)	18/35 (51.4%)
Aromatic	84/146 (57.5%)	42/73 (57.5%)	42/59 (71.2%)	0/14 (0.0%)
Overall	1526/1866 (81.8%)	934/1028 (90.9%)	449/659 (68.1%)	145/183 (79.2%)

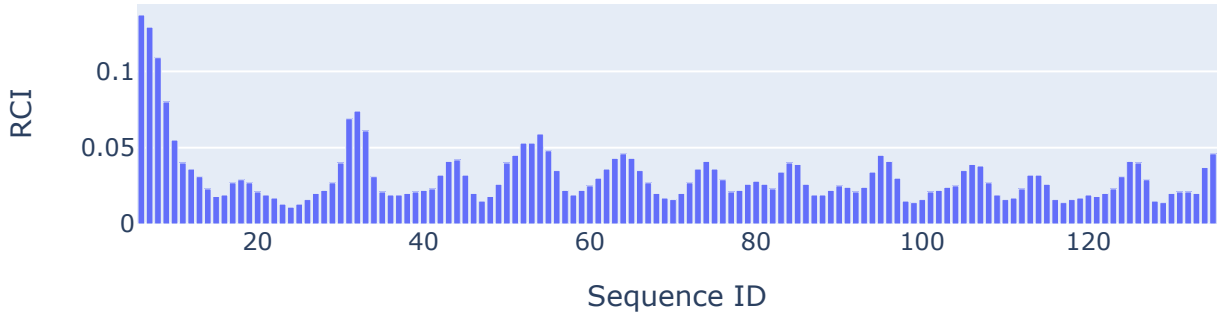
3 Statistically unusual chemical shifts

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts

Entity	Seq	Res	Atom	Shift (ppm)	Expected range (ppm)	Z-score
1	51	GLN	HG3	0.826	0.91 – 3.68	-5.31

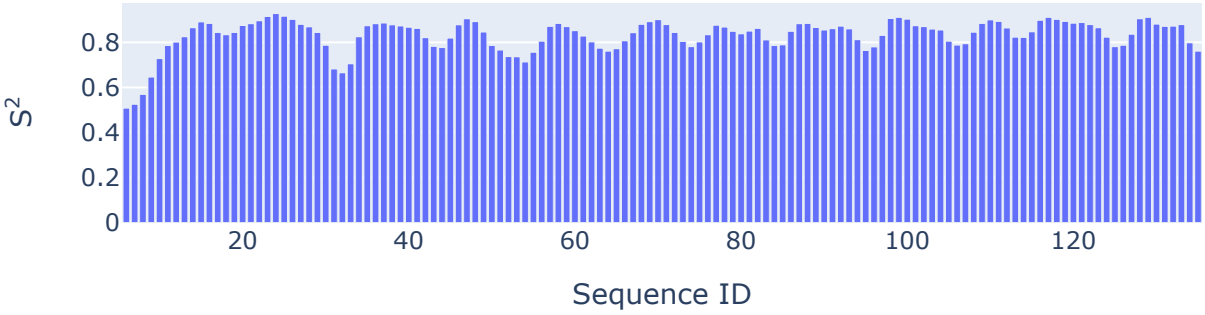
4 RCI

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

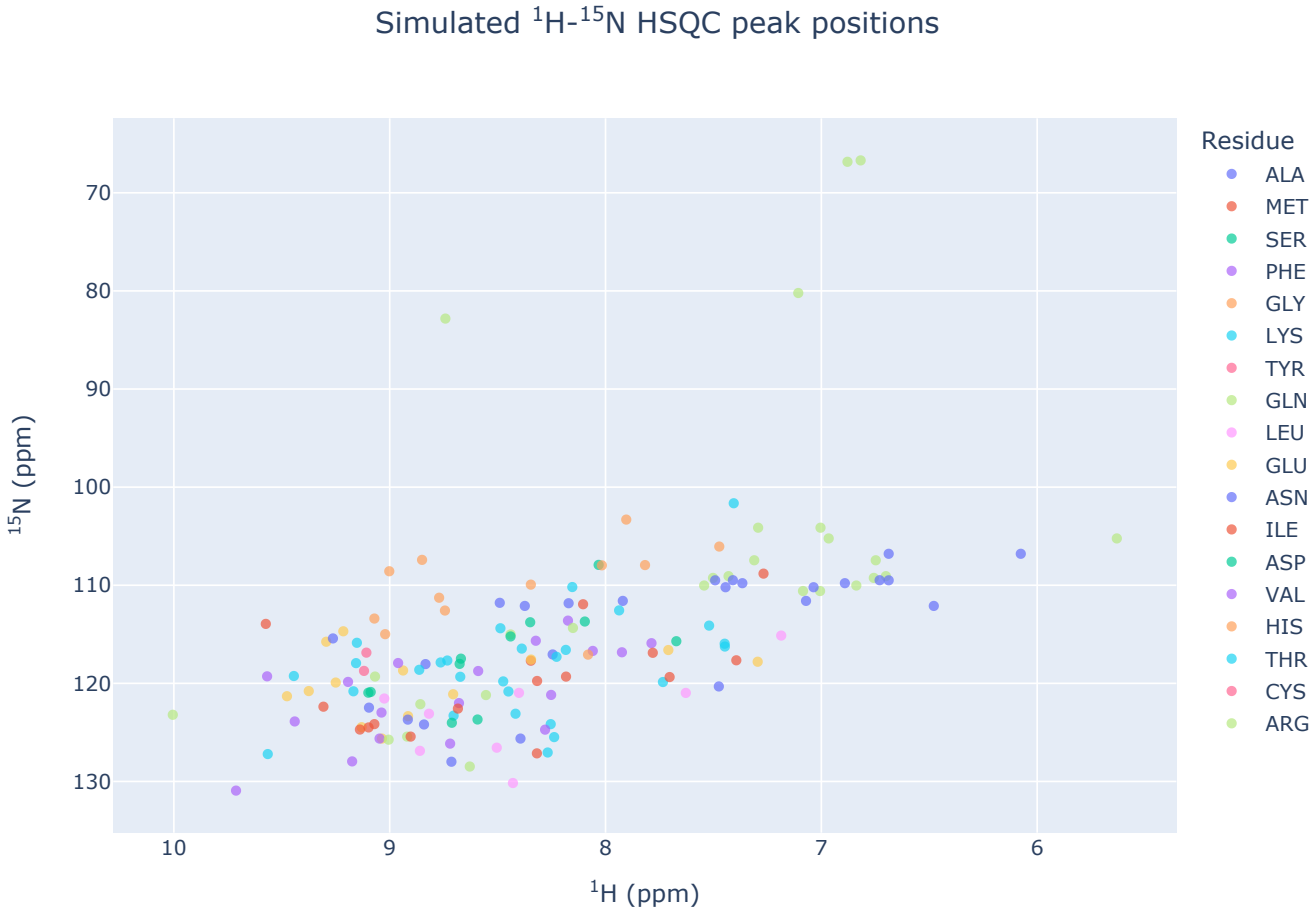


5 Order parameter

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



6 Simulated peak positions



7 LACS

Place holder for LACS results

8 Analysis data

place holder for the numerical values and tables.