NMR-STAR Data File Structure Outline

data\_<string> # For a BMRB entry the ‘<string>’ would be a BMRB accession code.

save\_<save\_frame\_name1> # The save frame name must be unique within a STAR file.

\_Category1.Sf\_category <save\_frame\_category1> # Each save frame has a specific category designation.

\_Category1.Sf\_framecode <save\_frame\_name1> # The tag value is the save frame name.

\_Category1.Entry\_ID 1234 # An entry\_ID value is included in each tag category.

\_Category1.ID 1 # A unique integer identifier is assigned to each save frame of a specific category

\_Category1.Item1 <value1>

save\_

save\_<save\_frame\_name2>

\_Category2.Sf\_category <save\_frame\_category2>

\_Category2.Sf\_framecode <save\_frame\_name2>

\_Category2.Entry\_ID 1234

\_Category2.ID 1

\_Category2.Item1 <value2>

loop\_ # The data in a loop\_ construct can be formatted as a table, although this is not required.

\_Category3.Item1

\_Category3.Item2

\_Category3.Entry\_ID

\_Category3.Category2\_ID

<item1\_value\_1.1> <item2\_value\_1.1> 1234 1

<item1\_value\_1.2e> <item2\_value\_1.1> 1234 1

stop\_ # The stop\_ keyword is used to close all loop constructs.

save\_

save\_<save\_frame\_name3> # Multiple save frames of the same category are allowed for most categories.

\_Category2.Sf\_category <save\_frame\_category2>

\_Category2.Sf\_framecode <save\_frame\_name3>

\_Category2.Entry\_ID 1234

\_Category2.ID 2

\_Category2.Item1 <value3>

loop\_

\_Category3.Item1

\_Category3.Item2

\_Category3.Entry\_ID

\_Category3.Category2\_ID

<item1\_value\_2.1> <item2\_value\_2.1> 1234 2

<item1\_value\_2.2> <item2\_value\_2.2> 1234 2

stop\_

save\_

save\_<save\_frame\_name4>

\_Category4.Sf\_category <save\_frame\_category3>

\_Category4.Sf\_framecode <save\_frame\_name4>

\_Category4.Entry\_ID 1234

\_Category4.ID 1

\_Category4.Sample\_conditions\_ID 1 # Save frame containing experimental data are usually linked to a specific

# set of sample conditions.

\_Category4.Sample\_conditions\_label $save\_frame\_name # The STAR method for referencing save frames is supported.

loop\_

\_Category5.Item1

\_Category5.Item2

\_Category5.Entry\_ID

\_Category5.Category4\_ID

<item1\_value\_3.1> <item2\_value\_3.1> 1234 1

<item1\_value\_3.2> <item2\_value\_3.2> 1234 1

stop\_

loop\_ # A save frame may contain more than one ‘loop\_’ construct but the tag categories must be unique.

\_Category6.Item1

\_Category6.Item2

\_Category6.Entry\_ID

\_Category6.Category4\_ID

<item1\_value\_4.1> <item2\_value\_4.1> 1234 1

<item1\_value\_4.2> <item2\_value\_4.2> 1234 1

stop\_

save\_

**Figure 4.** NMR-STAR data file structure