Example of a data save frame for tabulating assigned chemical shifts.

Points: 1) Links to experiments and software and directly or indirectly to samples

2) One per sample conditions

3) Data can be stored as a text block

4) Ambiguity codes used instead of over loading atom nomenclature with ambiguity information

5) More than one save frame of this category can exist per entry

6) Author defined and IUPAC atom nomenclature supported (also PDB)

7) Figure of merit value included

save\_assigned\_chem\_shift\_list\_1

\_Assigned\_chem\_shift\_list.Sf\_category assigned\_chemical\_shifts \_Assigned\_chem\_shift\_list.Sf\_framecode assigned\_chem\_shift\_list\_1 \_Assigned\_chem\_shift\_list.Entry\_ID 17325

\_Assigned\_chem\_shift\_list.ID 1

\_Assigned\_chem\_shift\_list.Sample\_condition\_list\_ID 1 \_Assigned\_chem\_shift\_list.Sample\_condition\_list\_label $sample\_conditions\_1 \_Assigned\_chem\_shift\_list.Chem\_shift\_reference\_ID 1 \_Assigned\_chem\_shift\_list.Chem\_shift\_reference\_label $chemical\_shift\_reference\_1 \_Assigned\_chem\_shift\_list.Details .

\_Assigned\_chem\_shift\_list.Text\_data\_format .

\_Assigned\_chem\_shift\_list.Text\_data .

loop\_

\_Chem\_shift\_experiment.Experiment\_ID

\_Chem\_shift\_experiment.Experiment\_name

\_Chem\_shift\_experiment.Sample\_ID

\_Chem\_shift\_experiment.Sample\_label

\_Chem\_shift\_experiment.Sample\_state

\_Chem\_shift\_experiment.Entry\_ID

\_Chem\_shift\_experiment.Assigned\_chem\_shift\_list\_ID

1 '2D 1H-15N HSQC' . . . 17325 1

2 '3D HNCACB' . . . 17325 1

3 '3D CBCA(CO)NH' . . . 17325 1

4 '3D HNCO' . . . 17325 1

stop\_

loop\_

\_Chem\_shift\_software.Software\_ID

\_Chem\_shift\_software.Software\_label

\_Chem\_shift\_software.Method\_ID

\_Chem\_shift\_software.Method\_label

\_Chem\_shift\_software.Entry\_ID

\_Chem\_shift\_software.Assigned\_chem\_shift\_list\_ID

3 $CCPNmr\_Analysis . . 17325 1

stop\_

loop\_

\_Atom\_chem\_shift.ID

\_Atom\_chem\_shift.Assembly\_atom\_ID

\_Atom\_chem\_shift.Entity\_assembly\_ID

\_Atom\_chem\_shift.Entity\_ID

\_Atom\_chem\_shift.Comp\_index\_ID

\_Atom\_chem\_shift.Seq\_ID

\_Atom\_chem\_shift.Comp\_ID

\_Atom\_chem\_shift.Atom\_ID

\_Atom\_chem\_shift.Atom\_type

\_Atom\_chem\_shift.Atom\_isotope\_number

\_Atom\_chem\_shift.Val

\_Atom\_chem\_shift.Val\_err

\_Atom\_chem\_shift.Assign\_fig\_of\_merit

\_Atom\_chem\_shift.Ambiguity\_code

\_Atom\_chem\_shift.Ambiguity\_set\_ID

\_Atom\_chem\_shift.Occupancy

\_Atom\_chem\_shift.Resonance\_ID

\_Atom\_chem\_shift.Auth\_entity\_assembly\_ID

\_Atom\_chem\_shift.Auth\_asym\_ID

\_Atom\_chem\_shift.Auth\_seq\_ID

\_Atom\_chem\_shift.Auth\_comp\_ID

\_Atom\_chem\_shift.Auth\_atom\_ID

\_Atom\_chem\_shift.Details

\_Atom\_chem\_shift.Entry\_ID

\_Atom\_chem\_shift.Assigned\_chem\_shift\_list\_ID

1 . 1 1 2 2 PRO HA H 1 4.420 0.02 . 1 . . . . . 2 Pro HA . 17325 1 2 . 1 1 2 2 PRO HB2 H 1 2.288 0.02 . 2 . . . . . 2 Pro HB2 . 17325 1 3 . 1 1 2 2 PRO HB3 H 1 1.919 0.02 . 2 . . . . . 2 Pro HB3 . 17325 1 4 . 1 1 2 2 PRO HG2 H 1 1.984 0.02 . 2 . . . . . 2 Pro HG2 . 17325 1 5 . 1 1 2 2 PRO HG3 H 1 1.995 0.02 . 2 . . . . . 2 Pro HG3 . 17325 1 6 . 1 1 2 2 PRO HD2 H 1 3.551 0.02 . 2 . . . . . 2 Pro HD2 . 17325 1 7 . 1 1 2 2 PRO HD3 H 1 3.558 0.02 . 2 . . . . . 2 Pro HD3 . 17325 1 8 . 1 1 2 2 PRO C C 13 177.102 0.100 . 1 . . . . . 2 Pro C . 17325 1 9 . 1 1 2 2 PRO CA C 13 63.150 0.100 . 1 . . . . . 2 Pro CA . 17325 1 10 . 1 1 2 2 PRO CB C 13 32.241 0.100 . 1 . . . . . 2 Pro CB . 17325 1 11 . 1 1 2 2 PRO CG C 13 26.744 0.100 . 1 . . . . . 2 Pro CG . 17325 1 12 . 1 1 2 2 PRO CD C 13 49.499 0.100 . 1 . . . . . 2 Pro CD . 17325 1

255 . 1 1 27 27 TRP H H 1 7.890 0.02 . 1 . . . . . 27 Trp H . 17325 1 256 . 1 1 27 27 TRP HA H 1 4.885 0.02 . 1 . . . . . 27 Trp HA . 17325 1 257 . 1 1 27 27 TRP HB2 H 1 3.012 0.02 . 2 . . . . . 27 Trp HB2 . 17325 1 258 . 1 1 27 27 TRP HB3 H 1 3.166 0.02 . 2 . . . . . 27 Trp HB3 . 17325 1 259 . 1 1 27 27 TRP HD1 H 1 7.143 0.02 . 1 . . . . . 27 Trp HD1 . 17325 1 260 . 1 1 27 27 TRP HE1 H 1 10.017 0.02 . 1 . . . . . 27 Trp HE1 . 17325 1 261 . 1 1 27 27 TRP HE3 H 1 7.11 0.02 . 5 1 . . . . 27 Trp HE3 . 17325 1 262 . 1 1 27 27 TRP HZ2 H 1 7.410 0.02 . 1 . . . . . 27 Trp HZ2 . 17325 1 263 . 1 1 27 27 TRP HZ3 H 1 7.055 0.02 . 1 . . . . . 27 Trp HZ3 . 17325 1 264 . 1 1 27 27 TRP HH2 H 1 7.168 0.02 . 1 . . . . . 27 Trp HH2 . 17325 1 265 . 1 1 27 27 TRP C C 13 174.108 0.100 . 1 . . . . . 27 Trp C . 17325 1 266 . 1 1 27 27 TRP CA C 13 54.622 0.100 . 1 . . . . . 27 Trp CA . 17325 1 267 . 1 1 27 27 TRP CB C 13 29.095 0.100 . 1 . . . . . 27 Trp CB . 17325 1 268 . 1 1 27 27 TRP CD1 C 13 126.9 0.100 . 1 . . . . . 27 Trp CD1 . 17325 1 269 . 1 1 27 27 TRP CE3 C 13 120.6 0.100 . 1 . . . . . 27 Trp CE3 . 17325 1 270 . 1 1 27 27 TRP CZ2 C 13 114.7 0.100 . 1 . . . . . 27 Trp CZ2 . 17325 1 271 . 1 1 27 27 TRP CZ3 C 13 122.1 0.100 . 1 . . . . . 27 Trp CZ3 . 17325 1 272 . 1 1 27 27 TRP CH2 C 13 124.7 0.100 . 1 . . . . . 27 Trp CH2 . 17325 1 273 . 1 1 27 27 TRP N N 15 121.901 0.100 . 1 . . . . . 27 Trp N . 17325 1 274 . 1 1 27 27 TRP NE1 N 15 128.891 0.100 . 1 . . . . . 27 Trp NE1 . 17325 1 287 . 1 1 30 30 TRP H H 1 7.606 0.02 . 1 . . . . . 30 Trp H . 17325 1 288 . 1 1 30 30 TRP HA H 1 4.612 0.02 . 1 . . . . . 30 Trp HA . 17325 1 289 . 1 1 30 30 TRP HB2 H 1 3.276 0.02 . 2 . . . . . 30 Trp HB2 . 17325 1 290 . 1 1 30 30 TRP HB3 H 1 3.345 0.02 . 2 . . . . . 30 Trp HB3 . 17325 1 291 . 1 1 30 30 TRP HD1 H 1 7.195 0.02 . 1 . . . . . 30 Trp HD1 . 17325 1 292 . 1 1 30 30 TRP HE1 H 1 10.186 0.02 . 1 . . . . . 30 Trp HE1 . 17325 1 293 . 1 1 30 30 TRP HE3 H 1 7.06 0.02 . 5 1 . . . . 30 Trp HE3 . 17325 1 294 . 1 1 30 30 TRP HZ2 H 1 7.424 0.02 . 1 . . . . . 30 Trp HZ2 . 17325 1 295 . 1 1 30 30 TRP HZ3 H 1 7.115 0.02 . 1 . . . . . 30 Trp HZ3 . 17325 1 296 . 1 1 30 30 TRP HH2 H 1 7.249 0.02 . 1 . . . . . 30 Trp HH2 . 17325 1 297 . 1 1 30 30 TRP C C 13 176.719 0.100 . 1 . . . . . 30 Trp C . 17325 1 298 . 1 1 30 30 TRP CA C 13 57.687 0.100 . 1 . . . . . 30 Trp CA . 17325 1 299 . 1 1 30 30 TRP CB C 13 28.616 0.100 . 1 . . . . . 30 Trp CB . 17325 1 300 . 1 1 30 30 TRP CD1 C 13 126.9 0.100 . 1 . . . . . 30 Trp CD1 . 17325 1 301 . 1 1 30 30 TRP CE3 C 13 120.6 0.100 . 1 . . . . . 30 Trp CE3 . 17325 1 302 . 1 1 30 30 TRP CZ2 C 13 114.7 0.100 . 1 . . . . . 30 Trp CZ2 . 17325 1 303 . 1 1 30 30 TRP CZ3 C 13 122.1 0.100 . 1 . . . . . 30 Trp CZ3 . 17325 1 304 . 1 1 30 30 TRP CH2 C 13 124.7 0.100 . 1 . . . . . 30 Trp CH2 . 17325 1 305 . 1 1 30 30 TRP N N 15 116.231 0.100 . 1 . . . . . 30 Trp N . 17325 1 306 . 1 1 30 30 TRP NE1 N 15 129.938 0.100 . 1 . . . . . 30 Trp NE1 . 17325 1

stop\_

save\_