Proposed updates and changes to the NEF standard – version 1.2:

1. Addition of a MANDATORY tag indicating database submission in _nef_chemical_shift loop

As the process of "assignment" involves the association of a label, initially "undefined" with the Peaks in an NMR spectrum; this association infers the Values of the Chemical-shift from the frequencies of the Peak's local maxima across the Peak's various dimensions. The same "Undefined"-Label could appear across multiple Peaks and in multiple spectra, thus connecting these peaks as involving the same molecular atom (or set of atoms, such as methyl protons).

It is possible that not all labels are identified at the time of submission, but it is desirable to retain such labels, e.g. in the NEF's role as an exchange format or for possible future analysis by other software programmes. Such chemical shift labels, however, would be (near) impossible for BMRB to validate.

A solution therefore would involve a tagging mechanism by which the depositors of a NEF file indicate which chemical shifts should be included in the submission to the BMRB database and validated.

V1.2 PROPOSAL:
_nef_chemical_shift.include_in_submission (true/false; MANDATORY, default value: false)

2. Addition of a NON-MANDATORY tag in a restraints saveframe indicating whether a particular restraint list has been used in calculations.

This change would enable the preservation of the data that has not been used in biomolecular structure calculations, such as restraints (and associated peaks) which were deemed problematic by the calculation program, or restraints that were predicted.

V1.2 PROPOSAL:
_nef_distance_restraint_list.calculation_used (true/false; NON-MANDATORY; default: false)