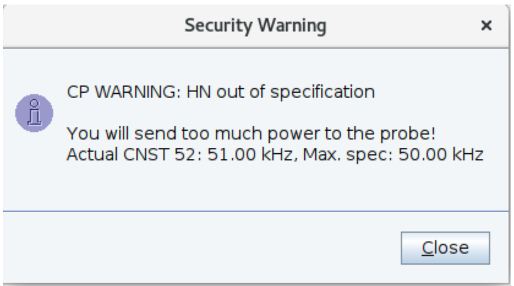
Listing S5 : Security checks – How does it work?

Each pulse sequence within the solid-state NMRlib module is associated with a jython script named as "experiment_p.py". This script allows the user to define selectively which parameters will be verified for this specific experiment.
In order to perform the safety checks, the safety script will compare : the parameter value within the topspin experiment with the safety table adapted by the user for his probes.
This safety table, so-called "Security_table_SSNMRlib.txt", is located in : "/NMRlib/py" and contains all the maximum values authorized for each probe.
An extract of this file is shown below.

SIZE	PULSE_TYPE	ELEMENT	DEFINITION	CNST_NAME	MAX_kHz	PULSE	DURATION	UNIT	SPNAM	MIDPOINT_RAMP	SEQ_DETECTION
0.7	HP	1H	1H_HP	-	-	P1	15	us	-	-	1H
0.7	HP	1H	1H_HP	-	-	P2	15	us	-	-	13C
0.7	HP	1H	1H_HP	-	-	P2	15	us	-	-	15N
0.7	HP	13C	13C_HP	-	-	P1	15	us	-	-	13C
0.7	HP	13C	13C_HP	-	-	P2	15	us	-	-	1H
0.7	HP	13C	13C_HP	-	-	P3	15	us	-	-	15N
0.7	HP	15N	15N_HP	-	-	P1	15	us	-	-	15N
0.7	HP	15N	15N_HP	-	-	P3	15	us	-	-	13C
0.7	HP	15N	15N_HP	-	-	P3	15	us	-	-	1H
0.7	HP	2H	2H_HP	-	-	P4	25	us	-	-	1H
0.7	HP	2H	2H_HP	-	-	P4	25	us	-	-	13C
0.7	HP	2H	2H_HP	-	-	P4	25	us	-	-	15N
0.7	HP	13C	13C_HP_for_CP	-	-	P21	5	us	-	-	1H
0.7	HP	13C	13C_HP_for_CP	-	-	P21	5	us	-	-	13C
0.7	HP	13C	13C_HP_for_CP	-	-	P21	5	us	-	-	15N
0.7	HP	1H	1H_HP_for_CP	-	-	P22	4	us	-	-	1H
0.7	HP	1H	1H_HP_for_CP	-	-	P22	4	us	-	-	13C
0.7	HP	1H	1H_HP_for_CP	-	-	P22	4	us	-	-	15N
0.7	HP	15N	15N_HP_for_CP	-	-	P23	6	us	-	-	1H
0.7	HP	15N	15N_HP_for_CP	-	-	P23	6	us	-	-	13C
0.7	HP	15N	15N_HP_for_CP	-	-	P23	6	us	-	-	15N
0.7	HP	2H	2H_HP_for_CP	-	-	P24	25	us	-	-	1H
0.7	HP	2H	2H_HP_for_CP	-	-	P24	25	us	-	-	13C
0.7	HP	2H	2H_HP_for_CP	-	-	P24	25	us	-	-	15N
0.7	CP	HN	RF_Field_1H	CNST42	190	P45	6000	us	42	62	-
0.7	CP	HN	RF_Field_15N	CNST52	55	P45	6000	us	-	-	-
0.7	CP	HC	RF_Field_13C	CNST31	70	P43	6000	us	-	-	-
0.7	CP	HC	RF_Field_1H	CNST41	190	P43	6000	us	41	61	-
0.7	CP	HCA	RF_Field_13C	CNST31	70	P43	6000	us	-	-	-
0.7	CP	HCA	RF_Field_1H	CNST41	190	P43	6000	us	41	61	-
0.7	CP	HCO	RF_Field_13C	CNST31	70	P43	6000	us	-	-	-
0.7	CP	HCO	RF_Field_1H	CNST41	190	P43	6000	us	41	61	-
0.7	CP	HACA	RF_Field_13CA	CNST35	70	P34	7000	us	-	-	-
0.7	CP	HACA	RF_Field_1HA	CNST45	190	P34	7000	us	45	57	-
0.7	CP	NCO	RF_Field_13CO	CNST33	70	P53	10000	us	-	-	-
0.7	CP	NCO	RF_Field_15N	CNST53	55	P53	10000	us	53	63	-
0.7	CP	NCA	RF_Field_13CA	CNST34	70	P35	10000	us	-	-	-
0.7	CP	NCA	RF_Field_15N	CNST54	55	P35	10000	us	54	60	-
0.7	CP	sim_HCN	RF_Field_13C	CNST31	70	P43	6000	us	-	-	-
0.7	CP	sim_HCN	RF_Field_1H	CNST41	190	P43	6000	us	41	61	-
0.7	CP	sim_HCN	RF_Field_15N	CNST51	55	P43	6000	us	-	-	-

The security check is automatically performed when an experiment is loaded from NMRlib. Moreover, if the user wants to change a parameter inside topspin, a "security button" can be hit, at any time, in order to re-do all the checks.
If a problem appears, a pop-up is generated showing the actual problematic topspin value and the specification in order to alert the user. This warning is also written in the topspin terminal.




```
############ Security checking #############
PULSE PROGRAM : av_hNH_cp_cp_miss.IBS
Security table : /home/avallet/NMRlib/py/Security_table_SSNMRlib.txt
P21, P22, P23 & P24 are used for the power calculation
Hard Pulse P1 for the nucleus 1H:   2.75 us, spec:   15.00 us: Ok.
Hard Pulse P2 for the nucleus 13C:   2.93 us, spec:   15.00 us: Ok.
Hard Pulse P3 for the nucleus 15N:   3.80 us, spec:   15.00 us: Ok.
Hard Pulse P21 for the nucleus 13C:   2.93 us, spec:    6.00 us: Ok.
Hard Pulse P22 for the nucleus 1H:   2.75 us, spec:    5.00 us: Ok.
Hard Pulse P23 for the nucleus 15N:   3.80 us, spec:    7.00 us: Ok.
D1 :   0.89 sec, spec:    0.60 sec: Ok
CP HN CNST 42:  15.00 kHz, spec:  120.00 kHz: Ok
CP HN duration P  45: 1000.00 us, spec:  6000.00 us: Ok
CP HN SPNAM 42 ramp50100.100 :  max RF on CNST 42:  18.75 kHz, max spec: 120.00 kHz : Ok
WARNING CP HN CNST 52:  51.00 kHz, spec:   50.00 kHz
Water suppression CNST24:  10.00 kHz, spec:   30.00 kHz: Ok
CP duration D30 for water suppression:  0.16 sec, spec:    0.20 sec: Ok
Decoupling CNST 12:   10.00 kHz, Max spec: 120.00 kHz: Ok
CNST 12: Decoupling time during indirect dimension F 1:  0.0263 sec, Max spec: 0.0300 sec: Ok
Decoupling CNST 13:    5.00 kHz, Max spec:  30.00 kHz: Ok
Decoupling on CNST 13 during the aquisition:  0.0150 sec, Max spec: 0.0300 sec: Ok
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In this way, each pulse sequence has its own personalized security which is adapted for its use and to the probe specification :

For each pulse sequence :

- All the parameters (water suppression elements, pulse, duration & RF power) within the pulse sequence are checked according to the probe.
- In a ramped RF shape, for CP or DREAM/BSH, the maximum value of the ramp is taken into account. To this end, the maximum value in the shape file is extracted, and the corresponding kHz value is calculated.
- The safety check verifies that midpoint of the ramp that is stored in a constant (e.g. cnst62 = 95 for a 90-to-100 ramp) and used for calculating the power level of the ramp, is indeed the mean of that ramp. This is done by explicitly verifying the ramp in the shape file.
- In CP experiments, the values of the two corresponding RF fields is checked. If the values are too far from Hartmann-Hahn conditions a popup window informs the user. This may point to mis-calibration of the reference pulses, as the CP power levels are calculated from them.
- If a list is used in the pulse sequence (e.g. the spin-lock duration in an $R_{1\rho}$ experiment), the safety check retrieves all the values within this list and determines the maximal value. This ensures that all values are within the safety limits.
- If an element is repeated multiple times, the safety check will verify the total duration, i.e. the duration of the unit element times the number of repeats.
- The decoupling times are retrieved automatically for the whole direct and indirect dimensions, i.e. the maximum evolution time (t_{1max}) is considered.

In addition, for the calibrations :

- As the parameter optimization array is define within the python script, negative values are automatically discarded.
- In a parameter optimization, the safety check verifies that none of the experiments of the array exceeds the allowed safety limits.
- Clicking the button of a calibration experiment generally starts the acquisition automatically. However, if a safety problem is detected, the calibration is not launched automatically.