Adosy_ste_setup_BBFO   Topspin 3.6   600MHz.   Fu Chen   October 2021

Usage: Optimize critical parameters for DOSY experiment for solution without solvent suppression at BBFO probe.

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Parameters to be optimized: P30, d20, RG and NS.

For standard D2O/Cu test sample, sine.100 gradient used, P30 1.0ms, d20 0.06s; D1 7s; NS 1

*****WARNNING:

DONOT increase P30 more than 2.5ms.

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General Instruction:

1. Create experiment #1: Set stable temperature (type edte), tune and shim well.
   - Run 1H NMR (Ah1): obtain o1p and sw
   - Remark: For 100% water, detune the probe by 10MHz, and calibrate 90.

2. Calibrate proton 90 degree pulse at #1. Obtain P1 and PL1 value for your sample.
   - Automation: type pulsecal
   - Manually: RPAR Ah1_90_water

3. Create experiment #2:
   - rpar Adosy_ste_setup_BBFO
   - getprosol

4. For Staff only:
   - Check the record for gadient calibration (gradpar cf with edhead gradient history).

5. Update o1p, sw and P1 (from step 1-2), NS 1, D1 7s to #2
   - Set d20 (default 60ms, typical 50-150ms)
   - Check to use the following default values as a starter {gpz6 2; gpz7 -17.13 (fixed); gradient pulse shape: SINE.100}

6. Optimize: P30 from 1ms (typical 1-2ms sample dependent)
   - Set a value of p30 between 1.3-1.5ms for water,
   - Demo sample (H2O/D2O with Cu+2). uses 1.0ms.
   - rga. and zg to collect and phase the first spectrum properly.

7. Do three measurements vary parameter gpz6:

- At #2, type i or iexpno to create #3
- Change gpz6 to 95 at #3
- At #2, type multizg, then type 2
- At #2 and #3, type efp;apk
- Compare peak intensities for #2 and #3 using multi-display; signals should decrease approx. 50 ratio.

8. Adjust P30 values:
   - If Signal decay too rapidly, return to #2 and #3, decrease the P30 value by 0.1ms; repeat multizg at step 7.
   - If Signal decay too slowly, return to #2 and #3, increase the P30 value by 0.1ms; repeat multizg at step 7.
   - Remark: P30 should not exceed 2.5ms. If P30 is out of its range, go to the next step.

9. If step 8 fails, adjust d20 by 0.1ms and repeat steps 7 & 8, then step 9 as needed.
   - d20 (default 60ms, typical 50-150ms)
   - The larger the P30 or/and D20, the faster the decay in intensities.

10. Optimize NS for your sample:
    - Set GPZ6 set to 95% with NS = 8
    - zg to collect a spectrum; check the sufficient intensities of the signal of interests by increasing NS = 8