IconNMR parameters sets – AVNEO400

Abbreviations

pulprog: pulse program; **ns**: number of scans; **sw**: spectral width; **o1p**: transmitter frequency offset (middle point of the spectrum); **td**: size of FID; **F2**: direct (horizontal) dimension in 2D NMR (^{1}H); **F1**: indirect (vertical) dimension in 2D NMR (^{1}H, ^{13}C or ^{15}N); **d1**: relaxation delay; **d8**: NOESY mixing time; **d9**: TOCSY mixing time; **p15**: ROESY spinlock time; **expt**: experiment time (if default parameters are used).

1D experiments

an_1H_nrot
Normal ^{1}H using 30° pulse, pulprog=zg30, ns=8, sw=16ppm, o1p=6ppm, d1=1s, expt=1min 2s, no sample rotation.

an_1H_wrot
Normal ^{1}H using 30° pulse, pulprog=zg30, ns=8, sw=16ppm, o1p=6ppm, d1=1s, expt=1min 2s, with sample rotation (20Hz).

an_1H_quant
Quantitative ^{1}H using 90° pulse, pulprog=zg, ns=16, sw=16ppm, o1p=6ppm, d1=5s (CHECK! Must be at least 5 times the longest T_1), expt=3min 5s, no sample rotation.

an_1H_quant_13C_dec
Quantitative ^{1}H using 90° pulse and inverse-gated ^{13}C decoupling, pulprog=zgig, ns=16, sw=18ppm, o1p=4.5ppm, d1=60s (CHECK! Must be at least 5 times the longest T_1 but not shorter than 60s), expt=16min 37s, no sample rotation.

an_1H_H2O_noesygppr1d
^{1}H with water suppression (1D NOESY with presaturation), pulprog=noesygppr1d, ns=8, sw=16ppm, o1p=4.7ppm (optimized), d1=4s, expt=1min 51s.

an_1H_H2O_noesygppr1d_comp
Combination of **an_1H_nrot** and **an_1H_H2O_noesygppr1d**, ns=8, sw=16ppm, o1p can be set manually based on normal ^{1}H measured before the water suppression experiment. Requires additional training.

an_1H_H2O_zggppeso
^{1}H with water suppression (SOGGY), pulprog=zggppeso, ns=8, sw=16ppm, o1p=4.7ppm (optimized), d1=4s, expt=1min 51s. Lock solvent must be H_2O+D_2O or H_2O+D_2O_salt.

an_1H_H2O_zggppeso_pr
^{1}H with water suppression (SOGGY with presaturation during d1), pulprog=zggppeso_pr, ns=8, sw=16ppm, o1p=4.7ppm (optimized), d1=4s, expt=1min 51s. Lock solvent must be H_2O+D_2O or H_2O+D_2O_salt.

an_1H_H2O_quant_13C_dec
^{1}H with water suppression (SOGGY) and inverse-gated ^{13}C decoupling, pulprog=zggppeso_ig, ns=16, sw=18ppm, o1p=4.7ppm (optimized), d1=60s (CHECK! Must be at least 5 times the longest T_1 but not shorter than 60s), expt=16min 37s. Lock solvent must be H_2O+D_2O or H_2O+D_2O_salt.

an_13C
Qualitative ^{13}C using 30° pulse and power-gated ^{1}H decoupling, pulprog=zgpg30, ns=256, sw=235ppm, o1p=110ppm, d1=2s, expt=14min 53s.

an_13C_quant_zgig
Quantitative ^{13}C using 90° pulse and inverse-gated ^{1}H decoupling, pulprog=zgig, ns=256, sw=235ppm, o1p=110ppm, d1=10s (CHECK! Must be at least 5 times the longest T_1), expt=50min 11s.

an_13C_quant_zgig30
Quantitative ^{13}C using 30° pulse and inverse-gated ^{1}H decoupling, pulprog=zgig30, ns=256, sw=235ppm, o1p=110ppm, d1=3s (CHECK! Must be at least 3 times the longest T_1), expt=28min 11s.

an_13C_UDEFT
Qualitative ^{13}C using UDEFT pulse sequence and ^{1}H decoupling, pulprog=udeft, ns=128, sw=235ppm, o1p=110ppm, d1=4s, expt=10min 54s.

an_13C_UDEFT_pg
Qualitative ^{13}C using UDEFT pulse sequence and power-gated ^{1}H decoupling, pulprog=udeft_pg, ns=128, sw=235ppm, o1p=110ppm, d1=4s, expt=10min 55s.

an_13C_DEPT135
^{13}C DEPT135 experiment, pulprog=deptsp135, ns=256, sw=235ppm, o1p=110ppm, d1=2s, expt=15min 2s.

an_13C_DEPTQ135
^{13}C DEPTQ135 experiment, pulprog=deptqgpsp, ns=256, sw=235ppm, o1p=110ppm, d1=2s, expt=15min 4s.

an_19F_ndec
Qualitative ^{19}F without ^{1}H decoupling, pulprog=zg30, ns=16, sw=300ppm, o1p=-55ppm, d1=2s, expt=46s.

an_31P_ndec
Qualitative ^{31}P without ^{1}H decoupling, pulprog=zg30, ns=16, sw=400ppm, o1p=0ppm, d1=2s, expt=50s.

an_31P_wdec
Qualitative ^{31}P with ^{1}H decoupling, pulprog=zgpg30, ns=16, sw=400ppm, o1p=0ppm, d1=2s, expt=51s.

an_31P_quant_zgig30
Quantitative ^{31}P with ^{1}H decoupling, pulprog=zgig30, ns=128, sw=400ppm, o1p=0ppm, d1=5s (CHECK! Must be at least 5 times the longest T_1), expt=12min 31s.

an_31P_quant_lignin_zgig
Quantitative ^{31}P with ^{1}H decoupling, optimized for lignin samples, pulprog=zgig, ns=128, sw=185ppm, o1p=67.5ppm, d1=5s (CHECK! Must be at least 5 times the longest T_1), expt=13min 52s.

2D experiments

All 2D experiments are composite experiments in which F2 (^{1}H) projection is measured before the 2D experiment. F2 projection is automatically added to the 2D spectrum.

an_COSY
$^{1}H,^{1}H$ COSY, sw optimized F2 and F1, pulprog=cosygpppqf, td(F2)=1K, td(F1)=128, ns=2, sw=11ppm (optimized), o1p=5.25ppm (optimized), d1=2s, expt=9min 50s.

an_COSY_sw_11
$^{1}H,^{1}H$ COSY, fixed F2 and F1, pulprog=cosygpppqf, td(F2)=1K, td(F1)=128, ns=2, sw=11ppm, o1p=5.25ppm, d1=2s, expt=9min 50s.

an_COSY_sw_13
$^{1}H,^{1}H$ COSY, fixed F2 and F1, pulprog=cosygpppqf, td(F2)=1K, td(F1)=128, ns=2, sw=13ppm, o1p=6ppm, d1=2s, expt=9min 44s.

an_COSY_H2O_pr_sw_13
$^{1}H,^{1}H$ COSY with water suppression (presaturation during d1), fixed F2 and F1, pulprog=cosygpprqf, td(F2)=1K, td(F1)=128, ns=2, sw=13ppm, o1p=4.7ppm (optimized), d1=4s, expt=18min 46s.

an_CLIP-COSY
$^{1}H,^{1}H$ CLIP-COSY, sw optimized F2 and F1, pulprog=clipcosy, td(F2)=1K, td(F1)=128, ns=2, sw=11ppm (optimized), o1p=5.25ppm (optimized), d1=2s, expt=10min 4s.

an_CLIP-COSY_sw_11
$^{1}H,^{1}H$ COSY, fixed F2 and F1, pulprog=clipcosy, td(F2)=1K, td(F1)=128, ns=2, sw=11ppm, o1p=5.25ppm, d1=2s, expt=10min 4s.

an_CLIP-COSY_sw_13
$^{1}H,^{1}H$ COSY, fixed F2 and F1, pulprog=clipcosy, td(F2)=1K, td(F1)=128, ns=2, sw=13ppm, o1p=6ppm, d1=2s, expt=9min 59s.

an_TOCSY
$^{1}H,^{1}H$ TOCSY, sw optimized F2 and F1, pulprog=dipsi2gpphzs, td(F2)=1K, td(F1)=128, ns=8, sw=11ppm (optimized), o1p=5.25ppm(optimized), d1=2s, d9=80ms, expt=38min 55s.

an_TOCSY_sw_11
^{1}H,^{1}H TOCSY, fixed F2 and F1, pulprog=dipsi2gpphzs, td(F2)=1K, td(F1)=128, ns=8, sw=11ppm, o1p=5.25ppm, d1=2s, d9=80ms, expt=38min 55s.

an_TOCSY_sw_13
^{1}H,^{1}H TOCSY, fixed F2 and F1, pulprog=dipsi2gpphzs, td(F2)=1K, T td(F1)=128, ns=8, sw=13ppm, o1p=6ppm, d1=2s, d9=80ms, expt=38min 35s.

an_TOCSY_H2O_es_sw_13
^{1}H,^{1}H TOCSY with water suppression (excitation sculpting), fixed F2 and F1, pulprog=dipsi2esgpphzs, td(F2)=1K, td(F1)=128, ns=8, sw=13ppm, o1p=4.7ppm (optimized), d1=2s, d9=80ms, expt=38min 44s.

an_NOESY
^{1}H,^{1}H NOESY, sw optimized F2 and F1, pulprog=noesygpphzs, td(F2)=1K, td(F1)=128, ns=2, sw=11ppm (optimized), o1p=5.25ppm (optimized), d1=2s, d8=500ms, expt=11min 56s.

an_NOESY_sw_11
^{1}H,^{1}H NOESY, fixed F2 and F1, pulprog=noesygpphzs, td(F2)=1K, td(F1)=128, ns=2, sw=11ppm, o1p=5.25ppm, d1=2s, d8=500ms, expt=11min 56s.

an_NOESY_sw_13
^{1}H,^{1}H NOESY, fixed F2 and F1, pulprog=noesygpphzs, td(F2)=1K, td(F1)=128, ns=2, sw=13ppm, o1p=6ppm, d1=2s, d8=500ms, expt=11min 51s.

an_NOESY_H2O_es_sw_13
^{1}H,^{1}H NOESY with water suppression (excitation sculpting), fixed F2 and F1, pulprog=noesyesgpphzs, td(F2)=1K, td(F1)=128, ns=8, sw=13ppm, o1p=4.7ppm (optimized), d1=2s, d8=500ms, expt=45min 19s.

an_EASY-ROESY
^{1}H,^{1}H EASY-ROESY, sw optimized F2 and F1, pulprog=roesyadjsph, td(F2)=1K, td(F1)=128, ns=8, sw=11ppm (optimized), o1p=5.25ppm (optimized), d1=2s, p15=500ms, expt=46min 5s.

an_EASY-ROESY_sw_11
^{1}H,^{1}H EASY-ROESY, fixed F2 and F1, pulprog=roesyadjsph, td(F2)=1K, td(F1)=128, ns=8, sw=11ppm, o1p=5.25ppm, d1=2s, p15=500ms, expt=46min 5s.

an_EASY-ROESY_sw_13
^{1}H,^{1}H EASY-ROESY, fixed F2 and F1, pulprog=roesyadjsph, td(F2)=1K, td(F1)=128, ns=8, sw=13ppm, o1p=6ppm, d1=2s, p15=500ms, expt=45min 45s.

an_EASY-ROESY_H2O_es_sw_13
^{1}H,^{1}H EASY-ROESY with water suppression (excitation sculpting), fixed F2 and F1, pulprog=roesyadesjsph, td(F2)=1K, td(F1)=128, ns=8, sw=13ppm, o1p=4.7ppm (optimized), d1=2s, p15=500ms, expt=45min 54s.

an_HSQC
$^{1}H,^{13}C$ HSQC with adiabatic ^{13}C decoupling, sw optimized F2 and fixed F1, pulprog=hsqcetgpsisp.2, td(F2)=1K, td(F1)=128, ns=2, sw(F2)=11ppm (optimized), o1p(F2)=5.25ppm (optimized), sw(F1)=165ppm, o2p(F1)=80ppm, d1=2s, expt=9min 44s.

an_HSQC_sw_11-165
$^{1}H,^{13}C$ HSQC with adiabatic ^{13}C decoupling, fixed F2 and F1, pulprog=hsqcetgpsisp.2, td(F2)=1K, td(F1)=128, ns=2, sw(F2)=11ppm, o1p(F2)=5.25ppm, sw(F1)=165ppm, o2p(F1)=80ppm, d1=2s, expt=9min 44s.

an_HSQC_sw_13-215
$^{1}H,^{13}C$ HSQC with adiabatic ^{13}C decoupling, fixed F2 and F1, pulprog=hsqcetgpsisp.2, td(F2)=1K, td(F1)=128, ns=2, sw(F2)=13ppm, o1p(F2)=6ppm, sw(F1)=215ppm, o2p(F1)=105ppm, d1=2s, expt=9min 39s.

an_HSQC_lignin_sw_11-215
$^{1}H,^{13}C$ HSQC with adiabatic ^{13}C decoupling, optimized for lignin samples, fixed F2 and F1, pulprog=hsqcetgpsisp.2, td(F2)=1K, td(F1)=256, ns=36, sw(F2)=11ppm, o1p(F2)=6ppm, sw(F1)=215ppm, o2p(F1)=105ppm, d1=2s, expt=5h 28min 54s.

an_HSQC_edit
Multiplicity edited $^{1}H,^{13}C$ HSQC with adiabatic ^{13}C decoupling, sw optimized F2 and fixed F1, pulprog=hsqcedetgpsisp2.3, td(F2)=1K, td(F1)=128, ns=2, sw(F2)=11ppm (optimized), o1p(F2)=5.25ppm (optimized), sw(F1)=165ppm, o2p(F1)=80ppm, d1=2s, expt=9min 46s.

an_HSQC_edit_sw_11-165
Multiplicity edited $^{1}H,^{13}C$ HSQC with adiabatic ^{13}C decoupling, fixed F2 and F1, pulprog=hsqcedetgpsisp2.3, td(F2)=1K, td(F1)=128, ns=2, sw(F2)=11ppm, o1p(F2)=5.25ppm, sw(F1)=165ppm, o2p(F1)=80ppm, d1=2s, expt=9min 46s.

an_HSQC_edit_sw_13-215
Multiplicity edited $^{1}H,^{13}C$ HSQC with adiabatic ^{13}C decoupling, fixed F2 and F1, pulprog=hsqcedetgpsisp2.3, td(F2)=1K, td(F1)=128, ns=2, sw(F2)=13ppm, o1p(F2)=6ppm, sw(F1)=215ppm, o2p(F1)=105ppm, d1=2s, expt=9min 40s.

an_HSQC_H2O_pr_sw_13-215
$^{1}H,^{13}C$ HSQC with adiabatic ^{13}C decoupling and water suppression (presaturation during d1), fixed F2 and F1, pulprog=hsqcetgpprsisp2.2, td(F2)=1K, td(F1)=128, ns=2, sw(F2)=13ppm, o1p(F2)=4.7ppm (optimized), sw(F1)=215ppm, o2p(F1)=105ppm, d1=2s, expt=9min 44s.

an_HMBC
$^{1}H,^{13}C$ HMBC without ^{13}C decoupling, sw optimized F2 and fixed F1, pulprog=hmbcetgpl3nd, td(F2)=4K, td(F1)=128, ns=4, sw(F2)=11ppm (optimized), o1p(F2)=5.25ppm (optimized), sw(F1)=235ppm, o2p(F1)=110ppm, d1=2s, expt=22min 25s.

an_HMBC_sw_11-235
$^{1}H,^{13}C$ HMBC without ^{13}C decoupling, fixed F2 and F1, pulprog=hmbcetgpl3nd, td(F2)=4K, td(F1)=128, ns=4, sw(F2)=11ppm, o1p(F2)=5.25ppm, sw(F1)=235ppm, o2p(F1)=110ppm, d1=2s, expt=22min 25s.

an_HMBC_sw_13-235
$^{1}H,^{13}C$ HMBC without ^{13}C decoupling, fixed F2 and F1, pulprog=hmbcetgpl3nd, td(F2)=4K, td(F1)=128, ns=4, sw(F2)=13ppm, o1p(F2)=5.25ppm, sw(F1)=235ppm, o2p(F1)=110ppm, d1=2s, expt=21min 46s.

an_HMBC_H2O_pr_sw_13-235
$^{1}H,^{13}C$ HMBC without ^{13}C decoupling and with water suppression (presaturation during d1 and gradients), fixed F2 and F1, pulprog=hmbcetgpl2nd.2_pr, td(F2)=4K, td(F1)=128, ns=4, sw(F2)=13ppm, o1p(F2)=4.7ppm (optimized), sw(F1)=235ppm, o2p(F1)=115ppm, d1=2s, expt=21min 57s.

an_HSQC-TOCSY_sw_13-215
$^{1}H,^{13}C$ HSQC-TOCSY with adiabatic ^{13}C decoupling, fixed F2 and F1, pulprog=hsqcdietgpsisp.2, td(F2)=1K, td(F1)=128, ns=2, sw(F2)=13ppm, o1p(F2)=6ppm, sw(F1)=215ppm, o2p(F1)=105ppm, d1=2s, d9=15ms expt=9min 42s.

an_1H-15N_HSQC_sw_11-400
$^{1}H,^{15}C$ HSQC with ^{15}N decoupling, fixed F2 and F1, pulprog=hsqcetgpsi2, td(F2)=1K, td(F1)=128, ns=8, sw(F2)=11ppm, o1p(F2)=5.25ppm, sw(F1)=400ppm, o2p(F1)=190ppm, d1=2s, expt=37min 5s.

an_1H-15N_HMBC_sw_11-400
$^{1}H,^{15}C$ HMBC without ^{15}N decoupling, fixed F2 and F1, pulprog=hmbcgpndqf, td(F2)=4K, td(F1)=128, ns=16, sw(F2)=11ppm, o1p(F2)=5.25ppm, sw(F1)=400ppm, o2p(F1)=190ppm, d1=2s, expt=1h 28min 29s.