

Supplement 1:**Parameters for NOESYPR1D experiments (1Dimensional ¹H NMR spectra with solvent suppression)**

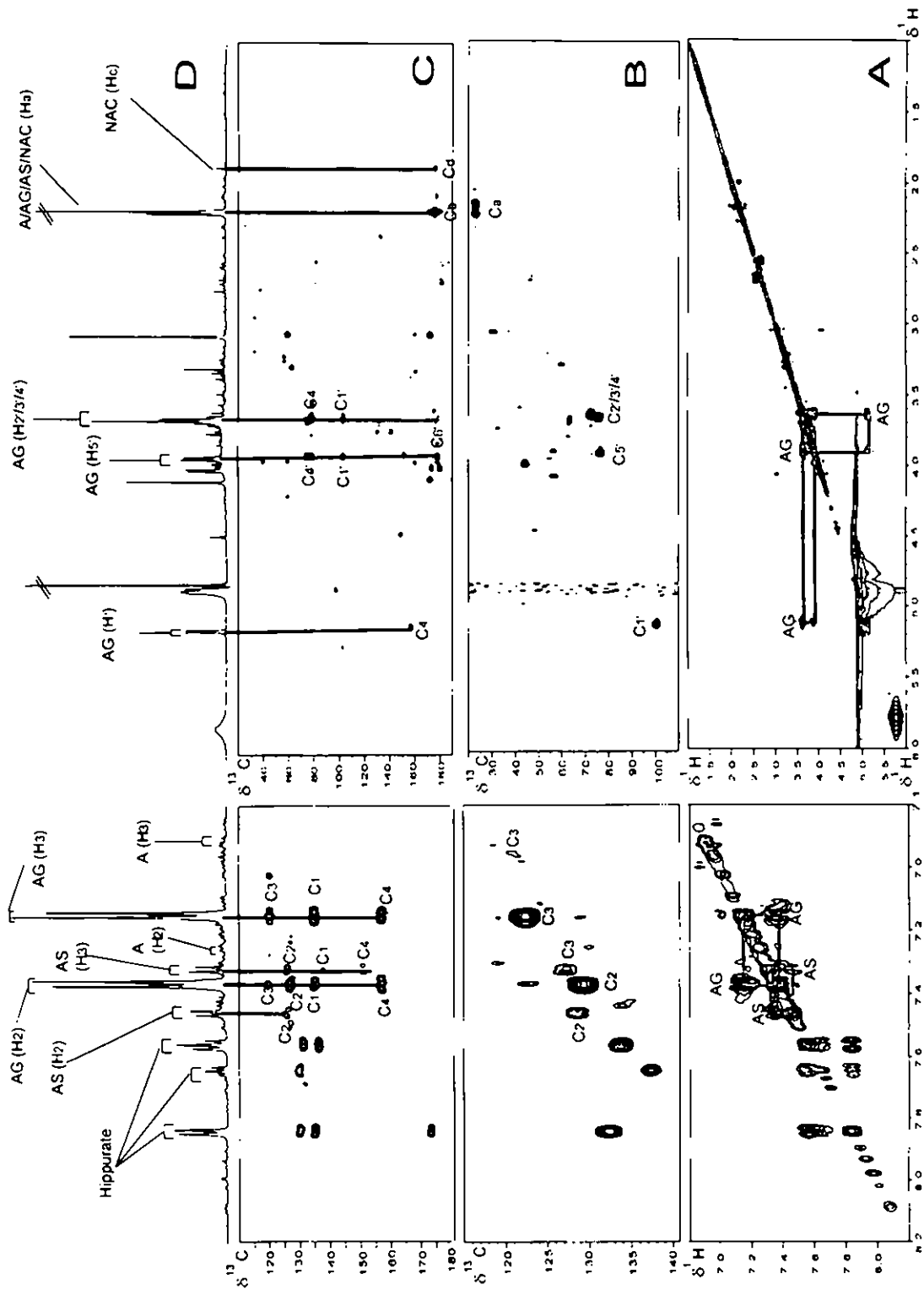
F2 - Acquisition Parameters		----- CHANNEL f1 -----	
PROBHD	5 mm FI	NUC1	¹ H
PULPROG	noesypr1d	P1	7.75 μsec
TD	32768	PL1	1.00 dB
SOLVENT	D2O	PL9	55.00 dB
NS	64	SFO1	600.2928245 MHz
DS	8	F2 - Processing parameters	
SWH	12019.23 Hz	SI	65536
FIDRES	0.366798 Hz	SF	600.2199568 MHz
AQ	1.3631988 sec	WDW	no
RG	228.1	SSB	0
DW	83.2 μsec	LB	0.3 Hz
DE	7.00 μsec	GB	0.0
TE	300.0 K	PC	1.00
D1	2.00000000 sec		
D8	0.10000000 sec		
D11	0.03000000 sec		
d12	0.00002000 sec		
MCREST	0.00000000 sec		
MCWRK	0.01500000 sec		

Parameters for TOCSY experiments

F2 - Acquisition Parameters		===== CHANNEL f1 =====	
PROBHD	5 mm TXI ¹ H-13	NUC1	¹ H
PULPROG	mlevphpr	P1	10.65 μ sec
TD	2048	p5	26.68 μ sec
SOLVENT	D ₂ O	P6	40.00 μ sec
NS	56	p7	80.00 μ sec
DS	8	P17	2500.00 μ sec
SWH	6313.131 Hz	PL1	0.00 dB
FIDRES	3.082584 Hz	PL9	54.00 dB
AQ	0.1622516 sec	PL10	12.00 dB
RG	228.1	SFO1	600.2928250 MHz
DW	79.200 μ sec	F1 - Acquisition parameters	
DE	6.50 μ sec	ND0	1
TE	300.0 K	TD	120
d0	0.00006855 sec	SFO1	600.2928 MHz
D1	1.20000005 sec	FIDRES	52.526527 Hz
D9	0.09500000 sec	SW	10.500 ppm
d11	0.03000000 sec	FnMODE	TPPI
d12	0.00002000 sec	F2 - Processing parameters	
d13	0.00000400 sec	SI	2048
FACTOR1	6	SF	600.2899643 MHz
IN0	0.00015865 sec	WDW	SINE
II	36	SSB	2
MCREST	0.00000000 sec	LB	0.00 Hz
MCWRK	0.01500000 sec	GB	0
SCALEF	6	PC	1.00
		F1 - Processing parameters	
		SI	2048
		MC2	TPPI
		SF	600.2899657 MHz
		WDW	SINE
		SSB	2
		LB	0.00 Hz
		GB	0

Parameters for HSQC experiments

F2 - Acquisition Parameters		----- GRADIENT CHANNEL -----	
PROBHD	5 mm TX1 H-13	GPNAM1	SINE.100
PULPROG	hsqcetgppr	GPNAM2	SINE.100
TD	2048	GPX1	0.00 %
SOLVENT	D ₂ O	GPX2	0.00 %
NS	280	GPY1	0.00 %
DS	16	GPY2	0.00 %
SWH	6313.131 Hz	GPZ1	80.00 %
FIDRES	3.082584 Hz	GPZ2	20.10 %
AQ	0.1622516 sec	P16	1500.00 usec
RG	5792.6		
DW	79.200 μsec	F1 - Acquisition parameters	
DE	7.00 μsec	ND0	2
TE	300.0 K	TD	100
CNST2	145.0000000	SFO1	150.9573 MHz
d0	0.00000300 sec	FIDRES	301.886780 Hz
D1	1.20000005 sec	SW	199.982 ppm
d4	0.00172414 sec	FnMODE	Echo-Antiecho
d11	0.03000000 sec		
d13	0.00000400 sec	F2 - Processing parameters	
D16	0.00020000 sec	SI	2048
DELTA	0.00172730 sec	SF	600.2899613 MHz
DELTA1	0.00021614 sec	WDW	QSINE
IN0	0.00001656 sec	SSB	2
MCREST	0.00000000 sec	LB	0.00 Hz
MCWRK	0.00600000 sec	GB	0
STICNT	50	PC	1.40
		F1 - Processing parameters	
----- CHANNEL f1 -----		SI	2048
NUC1	¹ H	MC2	echo-antiecho
P1	10.65 μsec	SF	150.9430146 MHz
p2	21.30 μsec	WDW	QSINE
P28	1.00 μsec	SSB	2
PL1	0.00 dB	LB	0.00 Hz
PL9	54.00 dB	GB	0
SFO1	600.2928250 MHz		
----- CHANNEL f2 -----			
CPDPRG2	garp		
NUC2	¹³ C		
P3	13.20 μsec		
p4	26.40 μsec		
PCPD2	65.00 μsec		
PL2	0.00 dB		
PL12	13.80 dB		
SFO2	150.9573206 MHz		



The mean and median correlation coefficient (together with 95% confidence interval) for the major acetaminophen metabolites as 1D STOCYSY 'driver' peaks (δ)

	N-acetyl-cysteine (NAC) δ 1.86	Acetaminophen (A) δ 7.25	Acetaminophen glucuronide (AG) δ 2.17	Acetaminophen sulfate (AS) δ 7.46
NAC	1.86	1, 1	0.61, 0.60 (0.50 - 0.72)	0.68, 0.68 (0.57 - 0.78)
	2.15	0.80, 0.80 (0.72 - 0.85)	0.84, 0.84 (0.71 - 0.92)	0.88, 0.88 (0.84 - 0.91)
	6.96	0.77, 0.77 (0.71 - 0.82)	0.73, 0.74 (0.60 - 0.83)	0.70, 0.70 (0.59 - 0.78)
A	2.16	0.76, 0.76 (0.62 - 0.88)	0.83, 0.83 (0.71 - 0.90)	0.88, 0.88 (0.83 - 0.92)
	6.91	0.69, 0.70 (0.63 - 0.76)	0.79, 0.80 (0.66 - 0.89)	0.76, 0.76 (0.69 - 0.84)
	7.25	0.74, 0.74 (0.62 - 0.84)	1, 1	0.85, 0.85 (0.78 - 0.9)
AG	2.17	0.61, 0.60 (0.50 - 0.72)	1, 1	0.88, 0.88 (0.84 - 0.92)
	3.62	0.77, 0.77 (0.71 - 0.83)	0.79, 0.79 (0.67 - 0.88)	0.83, 0.83 (0.79 - 0.86)
	3.89	0.57, 0.57 (0.49 - 0.65)	0.69, 0.70 (0.59 - 0.79)	0.72, 0.72 (0.61 - 0.82)
AS	5.1	0.70, 0.70 (0.61 - 0.78)	0.80, 0.80 (0.68 - 0.88)	0.87, 0.87 (0.81 - 0.91)
	7.13	0.69, 0.69 (0.61 - 0.77)	0.75, 0.75 (0.64 - 0.83)	0.80, 0.80 (0.75 - 0.85)
	7.36	0.72, 0.72 (0.64 - 0.79)	0.82, 0.83 (0.70 - 0.90)	0.89, 0.89 (0.84 - 0.92)
AS	2.18	0.73, 0.73 (0.64 - 0.81)	0.81, 0.81 (0.74 - 0.87)	0.94, 0.94 (0.91 - 0.96)
	7.31	0.69, 0.69 (0.62 - 0.77)	0.76, 0.76 (0.63 - 0.85)	0.90, 0.90 (0.86 - 0.93)
	7.46	0.68, 0.68 (0.57 - 0.78)	0.85, 0.85 (0.78 - 0.90)	1, 1

Shaded columns indicate the intra-molecular correlation coefficient.