

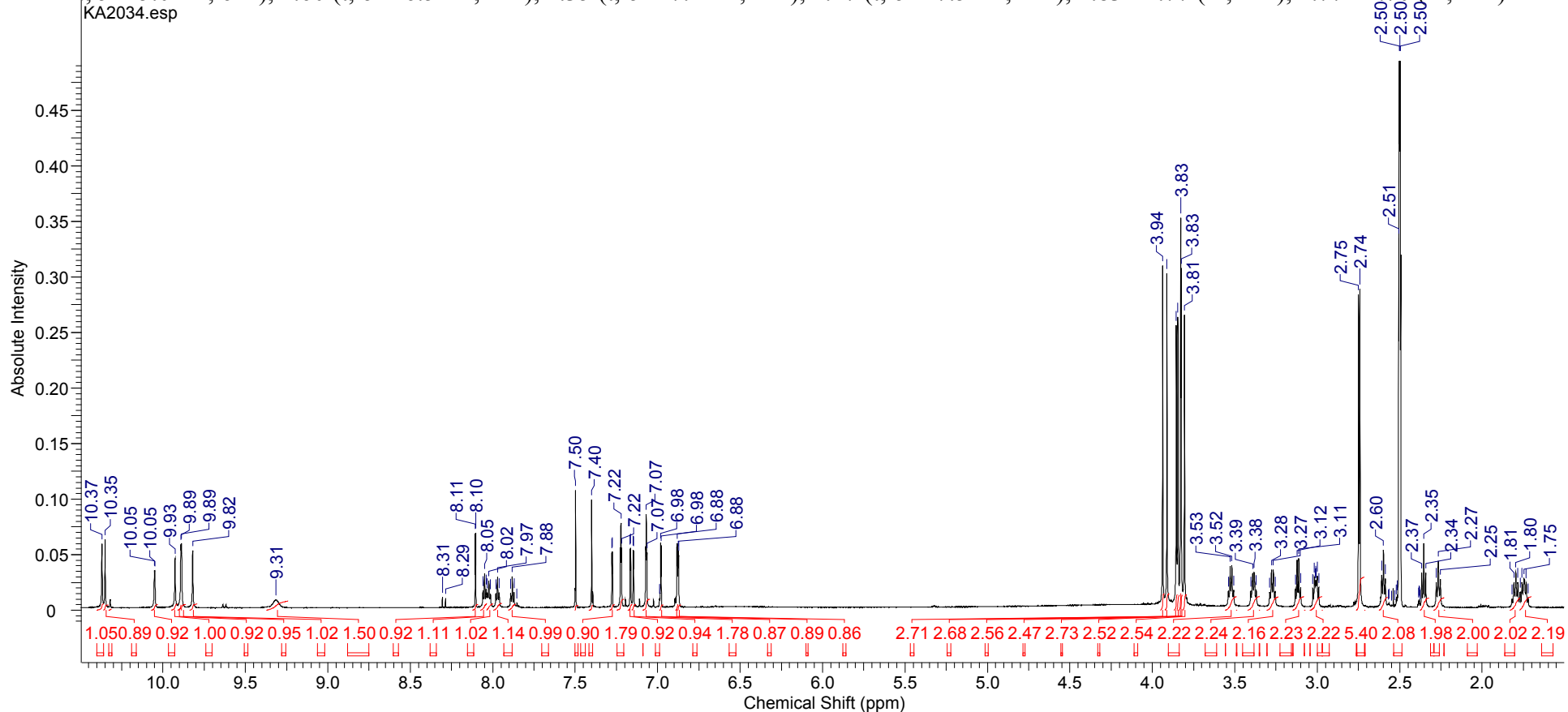
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# KA2034

KA2034

<b>Acquisition Time (sec)</b>	3.3280	<b>Comment</b>	Gradient Shimming		<b>Date</b>	Jul 5 2012	
<b>Date Stamp</b>	Jul 5 2012	<b>File Name</b>	\\stf.umsl.edu\deptshare\sh_nmrdata\Agilent600\bashkin\KA2031_070512.fid\fid				
<b>Frequency (MHz)</b>	599.78	<b>Nucleus</b>	1H	<b>Number of Transients</b>	64	<b>Original Points Count</b>	32000
<b>Points Count</b>	32768	<b>Pulse Sequence</b>	s2pul	<b>Receiver Gain</b>	48.00	<b>Solvent</b>	DMSO-d6
<b>Spectrum Offset (Hz)</b>	3599.5090	<b>Spectrum Type</b>	STANDARD	<b>Sweep Width (Hz)</b>	9615.38	<b>Temperature (degree C)</b>	25.000

<sup>1</sup>H NMR (600MHz, DMSO-d<sub>6</sub>) δ = 10.37 (s, 1 H), 10.35 (s, 1 H), 10.05 (d, *J* = 1.2 Hz, 1 H), 9.93 (s, 1 H), 9.89 (s, 1 H), 9.89 (s, 1 H), 9.82 (s, 1 H), 9.31 (br. s., 1 H), 8.10 (d, *J* = 1.8 Hz, 1 H), 8.05 (t, *J* = 5.9 Hz, 1 H), 8.02 (t, *J* = 5.7 Hz, 1 H), 7.97 (t, *J* = 6.2 Hz, 1 H), 7.88 (t, *J* = 6.2 Hz, 1 H), 7.50 (s, 1 H), 7.40 (s, 1 H), 7.28 (d, *J* = 1.8 Hz, 1 H), 7.25 - 7.21 (m, 2 H), 7.17 (d, *J* = 1.8 Hz, 1 H), 7.15 (d, *J* = 1.8 Hz, 1 H), 7.09 - 7.05 (m, 2 H), 6.98 (d, *J* = 2.1 Hz, 1 H), 6.88 (d, *J* = 1.8 Hz, 1 H), 6.87 (d, *J* = 1.8 Hz, 1 H), 3.94 (s, 3 H), 3.91 (s, 3 H), 3.85 (s, 3 H), 3.84 (s, 3 H), 3.83 (s, 3 H), 3.83 (s, 3 H), 3.81 (s, 3 H), 3.52 (q, *J* = 6.7 Hz, 2 H), 3.42 - 3.35 (m, 2 H), 3.27 (q, *J* = 6.6 Hz, 2 H), 3.12 (q, *J* = 6.5 Hz, 2 H), 3.04 - 2.97 (m, 2 H), 2.75 (d, *J* = 5.0 Hz, 6 H), 2.60 (t, *J* = 6.5 Hz, 2 H), 2.35 (t, *J* = 7.2 Hz, 2 H), 2.27 (t, *J* = 7.5 Hz, 2 H), 1.83 - 1.77 (m, 2 H), 1.77 - 1.70 (m, 2 H)

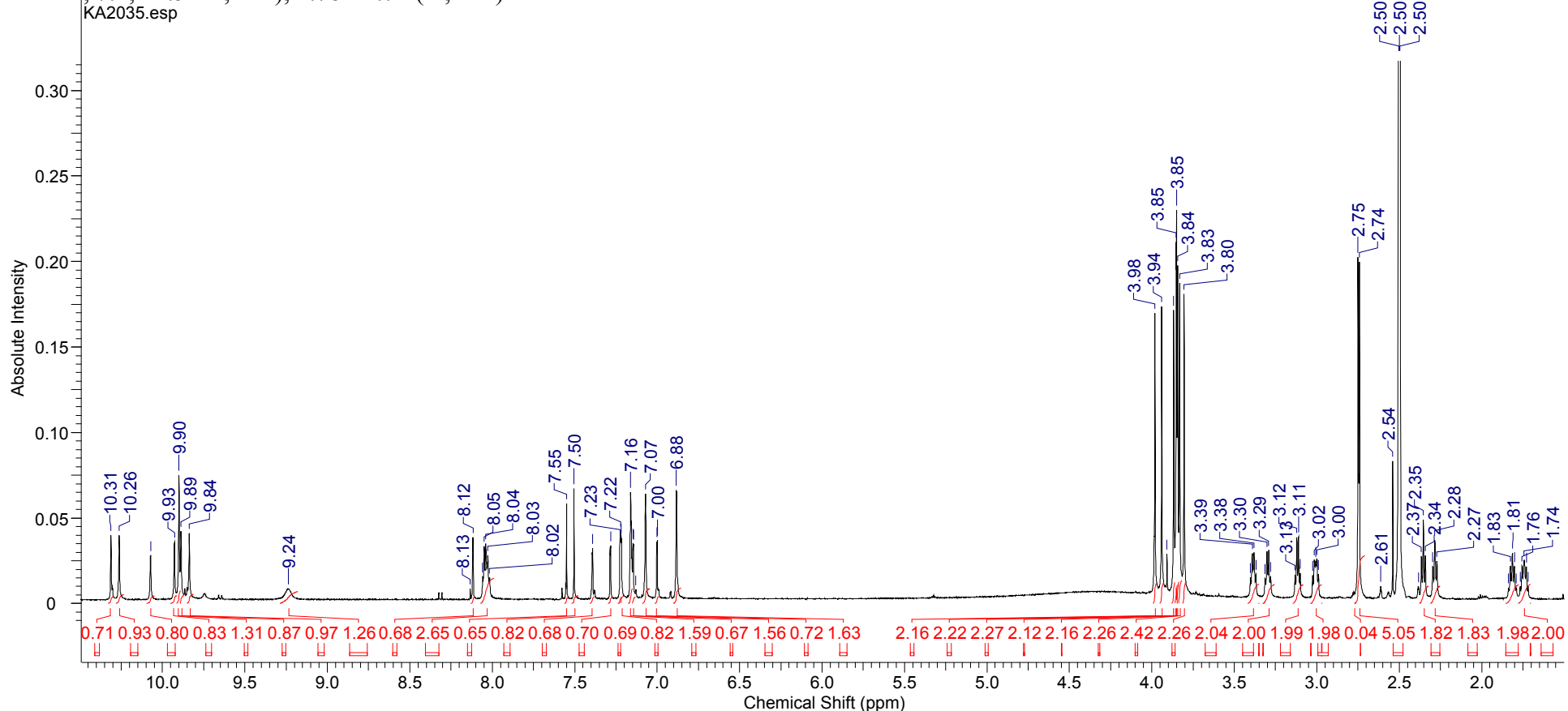


# KA2035

KA2035

<b>Acquisition Time (sec)</b>	1.7039	<b>Comment</b>	Gradient Shimming		<b>Date</b>	Dec 19 2012	
<b>Date Stamp</b>	Dec 19 2012	<b>File Name</b>	\\stl.umsl.edu\deptshare\sh_nmrdata\Agilent600\bashkin\KA2051E_20121219_01\PROTON_01.fid\fid				
<b>Frequency (MHz)</b>	599.78	<b>Nucleus</b>	1H	<b>Number of Transients</b>	64	<b>Original Points Count</b>	16384
<b>Points Count</b>	16384	<b>Pulse Sequence</b>	s2pul	<b>Receiver Gain</b>	50.00	<b>Solvent</b>	DMSO-d6
<b>Spectrum Offset (Hz)</b>	3608.5234	<b>Spectrum Type</b>	STANDARD	<b>Sweep Width (Hz)</b>	9615.38	<b>Temperature (degree C)</b>	24.000

$^1\text{H}$  NMR (600MHz, DMSO-d<sub>6</sub>)  $\delta$  = 10.31 (s, 1 H), 10.26 (s, 1 H), 10.07 (s, 1 H), 9.93 (s, 1 H), 9.90 (s, 2 H), 9.89 (s, 1 H), 9.84 (s, 1 H), 9.24 (br. s., 1 H), 8.12 (d,  $J$  = 1.8 Hz, 1 H), 8.07 - 7.99 (m, 4 H), 7.55 (s, 1 H), 7.50 (s, 1 H), 7.39 (d,  $J$  = 1.8 Hz, 1 H), 7.28 (d,  $J$  = 1.8 Hz, 1 H), 7.22 (d,  $J$  = 1.8 Hz, 1 H), 7.22 (d,  $J$  = 1.8 Hz, 1 H), 7.17 - 7.15 (m, 2 H), 7.15 (d,  $J$  = 1.8 Hz, 1 H), 7.07 (s, 2 H), 7.00 (d,  $J$  = 1.8 Hz, 1 H), 6.88 (d,  $J$  = 1.2 Hz, 2 H), 3.98 (s, 3 H), 3.94 (s, 3 H), 3.87 (s, 3 H), 3.85 (s, 3 H), 3.85 (s, 3 H), 3.84 (s, 3 H), 3.83 (s, 3 H), 3.80 (s, 3 H), 3.42 - 3.35 (m, 2 H), 3.30 (q,  $J$  = 6.8 Hz, 2 H), 3.12 (q,  $J$  = 6.5 Hz, 2 H), 3.03 - 2.97 (m, 2 H), 2.75 (d,  $J$  = 4.7 Hz, 6 H), 2.35 (t,  $J$  = 7.3 Hz, 2 H), 2.28 (t,  $J$  = 7.6 Hz, 2 H), 1.85 - 1.78 (m,  $J$  = 7.1, 7.1, 14.5 Hz, 2 H), 1.78 - 1.71 (m, 2 H)

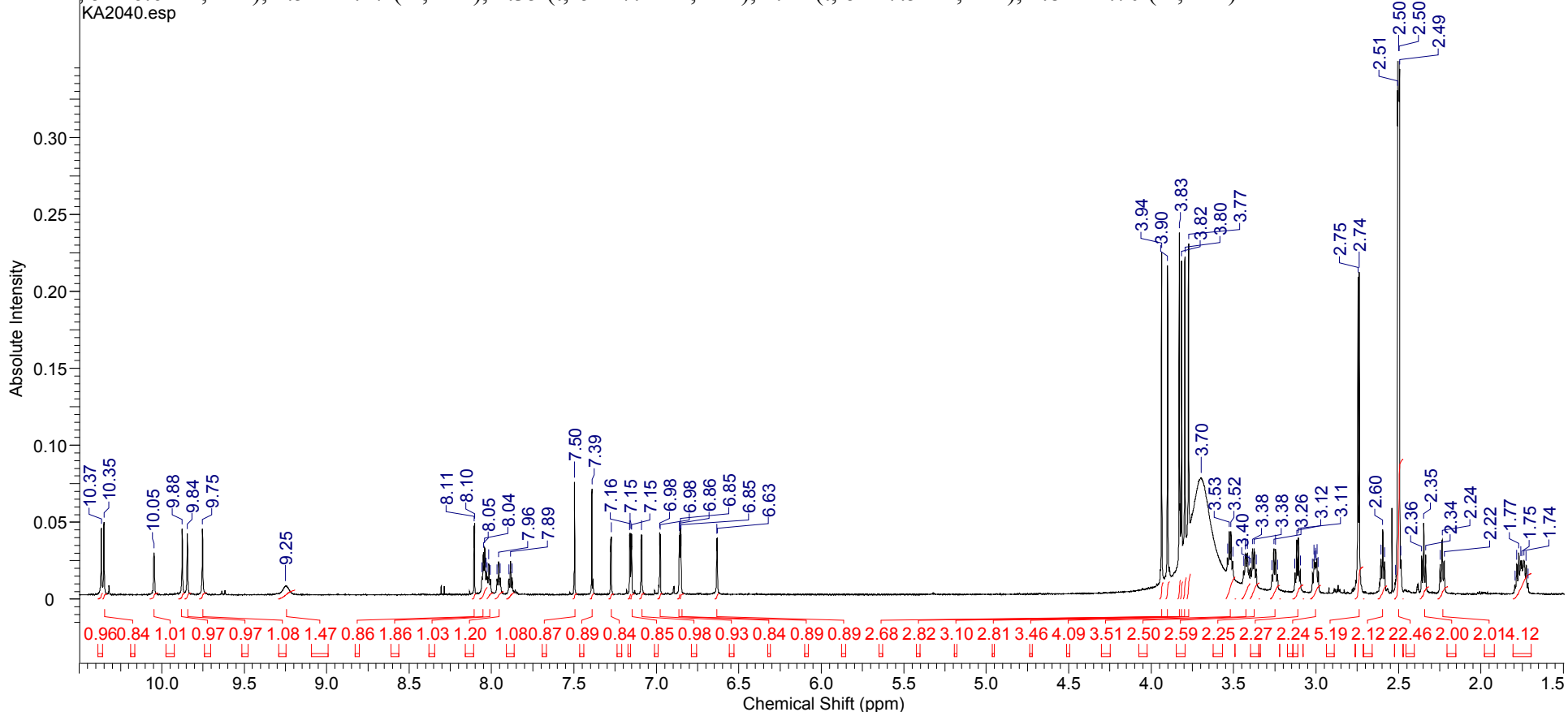


# KA2040

KA2040

<b>Acquisition Time (sec)</b>	3.3280	<b>Comment</b>	Gradient Shimming		<b>Date</b>	Jul 6 2012	
<b>Date Stamp</b>	Jul 6 2012	<b>File Name</b>	\\stf.umsl.edu\deptshare\sh_nmrdata\Agilent600\bashkin\ka2040C-070612.fid\fid				
<b>Frequency (MHz)</b>	599.78	<b>Nucleus</b>	1H	<b>Number of Transients</b>	64	<b>Original Points Count</b>	32000
<b>Points Count</b>	32768	<b>Pulse Sequence</b>	s2pul	<b>Receiver Gain</b>	46.00	<b>Solvent</b>	DMSO-d6
<b>Spectrum Offset (Hz)</b>	3600.6829	<b>Spectrum Type</b>	STANDARD	<b>Sweep Width (Hz)</b>	9615.38	<b>Temperature (degree C)</b>	25.000

$^1\text{H}$  NMR (600MHz, DMSO- $d_6$ )  $\delta$  = 10.37 (s, 1 H), 10.35 (s, 1 H), 10.05 (s, 1 H), 9.88 (s, 1 H), 9.84 (s, 1 H), 9.75 (s, 1 H), 9.25 (br. s., 1 H), 8.10 (d,  $J$  = 1.5 Hz, 1 H), 8.07 - 8.03 (m, 2 H), 8.02 (t,  $J$  = 5.7 Hz, 1 H), 7.96 (t,  $J$  = 6.0 Hz, 1 H), 7.89 (t,  $J$  = 6.0 Hz, 1 H), 7.50 (s, 1 H), 7.39 (s, 1 H), 7.28 (d,  $J$  = 1.8 Hz, 1 H), 7.16 (d,  $J$  = 1.8 Hz, 1 H), 7.15 (d,  $J$  = 1.8 Hz, 1 H), 7.09 (d,  $J$  = 1.8 Hz, 1 H), 6.98 (d,  $J$  = 2.1 Hz, 1 H), 6.86 (d,  $J$  = 1.8 Hz, 1 H), 6.85 (d,  $J$  = 1.8 Hz, 1 H), 6.63 (d,  $J$  = 1.5 Hz, 1 H), 3.94 (s, 3 H), 3.90 (s, 3 H), 3.83 (s, 3 H), 3.82 (s, 3 H), 3.80 (s, 3 H), 3.77 (s, 3 H), 3.55 - 3.49 (m, 2 H), 3.45 - 3.40 (m, 2 H), 3.40 - 3.35 (m, 2 H), 3.28 - 3.22 (m, 2 H), 3.14 - 3.08 (m, 2 H), 3.04 - 2.97 (m, 2 H), 2.74 (d,  $J$  = 5.0 Hz, 6 H), 2.60 (t,  $J$  = 6.6 Hz, 2 H), 2.52 - 2.47 (m, 2 H), 2.35 (t,  $J$  = 7.2 Hz, 2 H), 2.24 (t,  $J$  = 7.5 Hz, 2 H), 1.81 - 1.70 (m, 4 H)

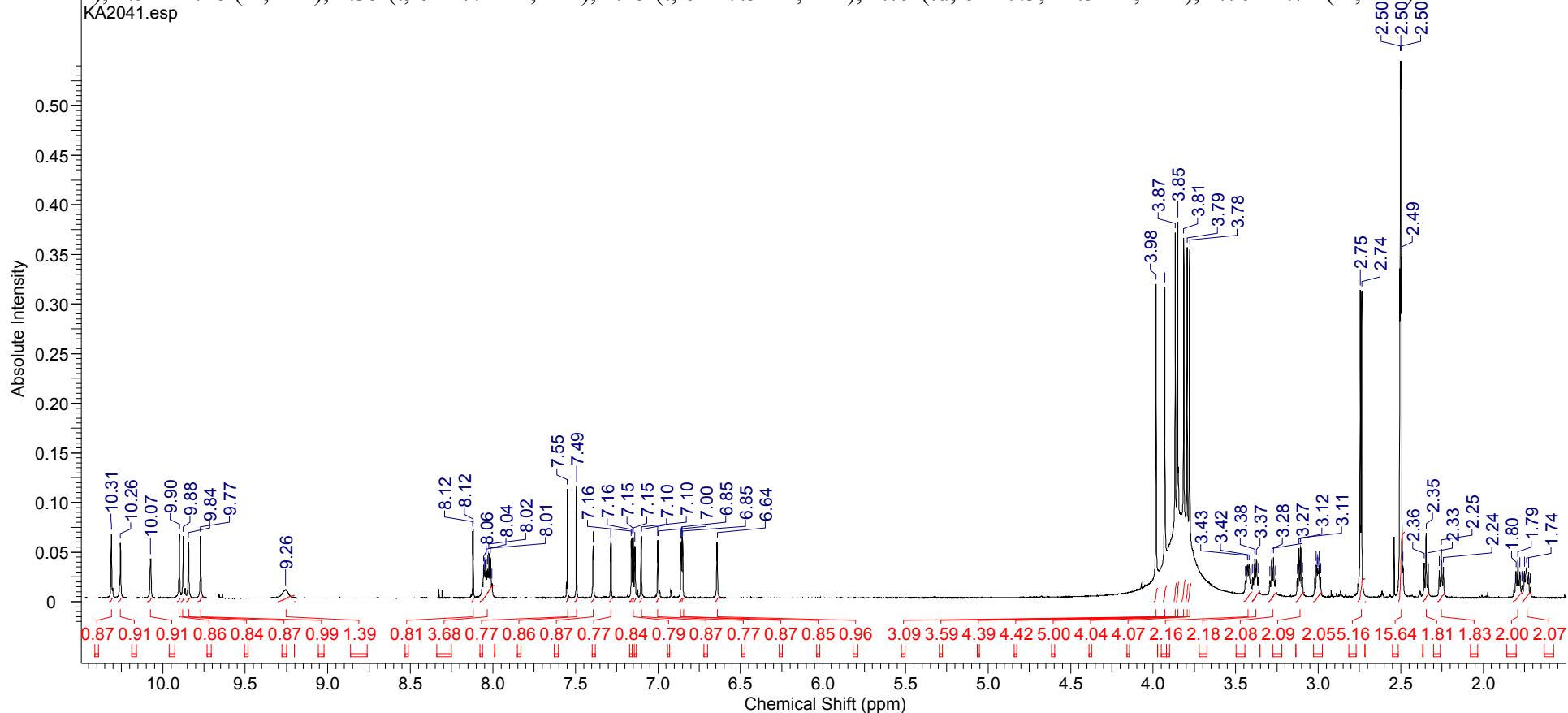


# KA2041

KA2041

<b>Acquisition Time (sec)</b>	3.3280	<b>Comment</b>	Gradient Shimming		<b>Date</b>	Jul 6 2012	
<b>Date Stamp</b>	Jul 6 2012	<b>File Name</b>	\\stl.umsl.edu\deptshare\sh_nmrdata\Agilent600\bashkin\ka2041C-070612.fid\fid				
<b>Frequency (MHz)</b>	599.78	<b>Nucleus</b>	1H	<b>Number of Transients</b>	64	<b>Original Points Count</b>	32000
<b>Points Count</b>	32768	<b>Pulse Sequence</b>	s2pul	<b>Receiver Gain</b>	44.00	<b>Solvent</b>	DMSO-d6
<b>Spectrum Offset (Hz)</b>	3608.8994	<b>Spectrum Type</b>	STANDARD	<b>Sweep Width (Hz)</b>	9615.38	<b>Temperature (degree C)</b>	25.000

$^1\text{H}$  NMR (600MHz, DMSO-d<sub>6</sub>)  $\delta$  = 10.31 (s, 1 H), 10.26 (s, 1 H), 10.07 (d,  $J$  = 0.9 Hz, 1 H), 9.90 (s, 1 H), 9.88 (s, 1 H), 9.84 (s, 1 H), 9.77 (s, 1 H), 9.26 (br. s., 1 H), 8.12 (d,  $J$  = 1.8 Hz, 1 H), 8.08 - 7.99 (m, 4 H), 7.55 (s, 1 H), 7.49 (s, 1 H), 7.39 (d,  $J$  = 1.5 Hz, 1 H), 7.28 (d,  $J$  = 1.8 Hz, 1 H), 7.16 (d,  $J$  = 1.8 Hz, 1 H), 7.15 (d,  $J$  = 1.8 Hz, 1 H), 7.14 (d,  $J$  = 1.8 Hz, 1 H), 7.10 (d,  $J$  = 1.8 Hz, 1 H), 7.00 (d,  $J$  = 1.8 Hz, 1 H), 6.86 (d,  $J$  = 1.8 Hz, 1 H), 6.85 (d,  $J$  = 2.1 Hz, 1 H), 6.64 (d,  $J$  = 1.8 Hz, 1 H), 3.98 (s, 3 H), 3.93 (s, 3 H), 3.87 (s, 3 H), 3.85 (s, 3 H), 3.81 (s, 3 H), 3.79 (s, 3 H), 3.78 (s, 3 H), 3.45 - 3.40 (m, 2 H), 3.40 - 3.35 (m, 2 H), 3.28 (q,  $J$  = 6.7 Hz, 2 H), 3.11 (q,  $J$  = 6.5 Hz, 2 H), 3.03 - 2.98 (m, 2 H), 2.74 (d,  $J$  = 5.0 Hz, 6 H), 2.51 - 2.48 (m, 2 H), 2.35 (t,  $J$  = 7.2 Hz, 2 H), 2.25 (t,  $J$  = 7.5 Hz, 2 H), 1.79 (td,  $J$  = 7.3, 14.5 Hz, 2 H), 1.76 - 1.71 (m, 2 H)

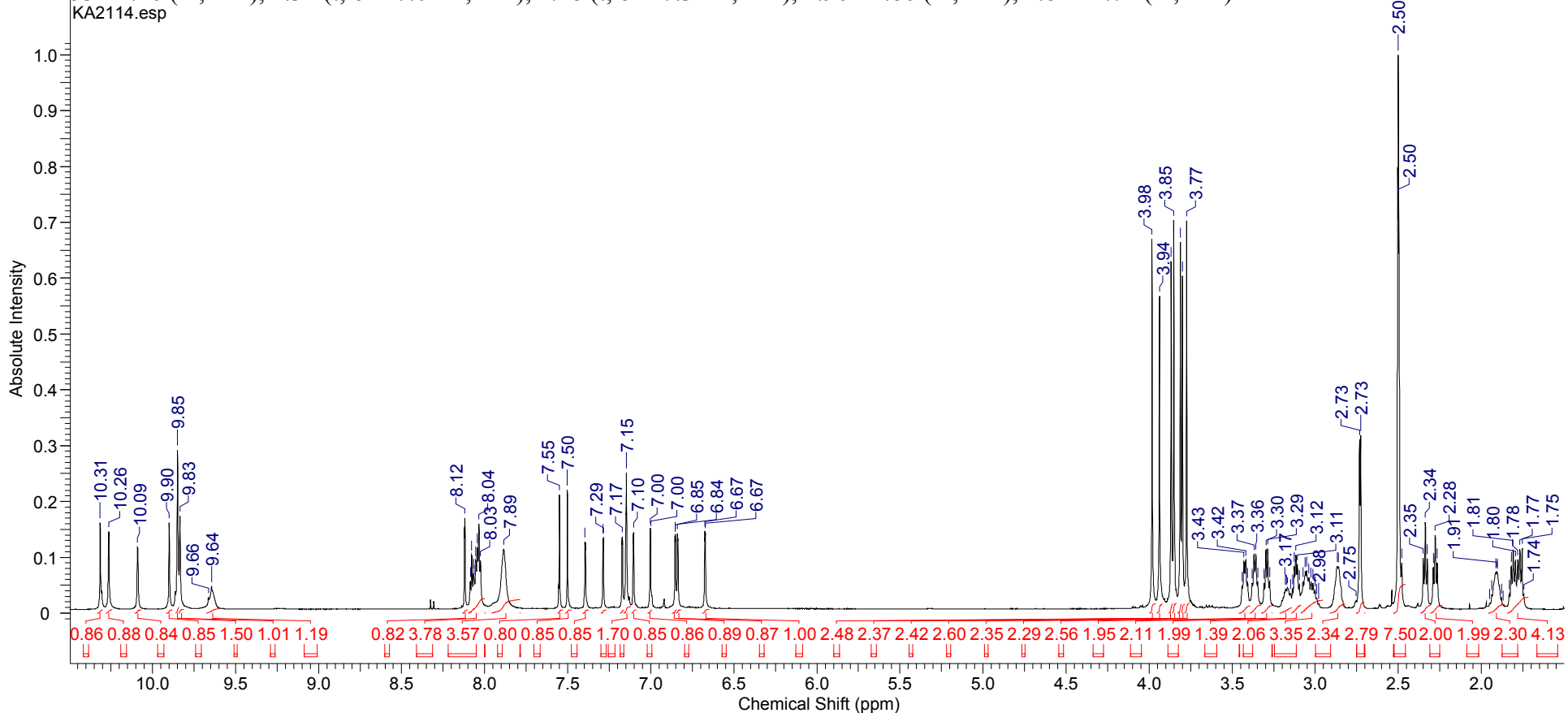


# KA2114

KA2114

<b>Acquisition Time (sec)</b>	1.7039	<b>Comment</b>	Gradient Shimming		<b>Date</b>	Apr 4 2013	
<b>Date Stamp</b>	Apr 4 2013	<b>File Name</b>	\\stl.umsl.edu\deptshare\sh_nmrdata\Agilent600\bashkin\ka2114d_20130404_01\PROTON_01.fid\fid				
<b>Frequency (MHz)</b>	599.78	<b>Nucleus</b>	1H	<b>Number of Transients</b>	128	<b>Original Points Count</b>	16384
<b>Points Count</b>	16384	<b>Pulse Sequence</b>	s2pul	<b>Receiver Gain</b>	30.00	<b>Solvent</b>	DMSO-d6
<b>Spectrum Offset (Hz)</b>	3609.6973	<b>Spectrum Type</b>	STANDARD	<b>Sweep Width (Hz)</b>	9615.38	<b>Temperature (degree C)</b>	24.000

$^1\text{H}$  NMR (600MHz, DMSO-d<sub>6</sub>)  $\delta$  = 10.31 (s, 1 H), 10.26 (s, 1 H), 10.09 (s, 1 H), 9.90 (s, 1 H), 9.85 (s, 2 H), 9.83 (s, 1 H), 9.68 - 9.60 (m, 1 H), 8.12 (d,  $J$  = 1.2 Hz, 1 H), 8.10 - 8.00 (m, 5 H), 7.89 (br. s., 4 H), 7.55 (s, 1 H), 7.50 (s, 1 H), 7.39 (d,  $J$  = 1.2 Hz, 1 H), 7.29 (d,  $J$  = 1.8 Hz, 1 H), 7.17 (d,  $J$  = 1.2 Hz, 1 H), 7.15 (d,  $J$  = 1.8 Hz, 2 H), 7.10 (d,  $J$  = 1.8 Hz, 1 H), 7.00 (d,  $J$  = 1.8 Hz, 1 H), 6.85 (d,  $J$  = 1.2 Hz, 1 H), 6.84 (d,  $J$  = 1.2 Hz, 1 H), 6.67 (d,  $J$  = 1.8 Hz, 1 H), 3.98 (s, 3 H), 3.94 (s, 3 H), 3.87 (s, 3 H), 3.85 (s, 3 H), 3.81 (s, 3 H), 3.80 (s, 3 H), 3.77 (s, 3 H), 3.46 - 3.39 (m, 2 H), 3.39 - 3.33 (m, 2 H), 3.29 (q,  $J$  = 6.7 Hz, 2 H), 3.21 - 3.14 (m, 1 H), 3.14 - 3.09 (m, 2 H), 3.09 - 2.95 (m, 3 H), 2.91 - 2.82 (m, 2 H), 2.73 (d,  $J$  = 4.7 Hz, 3 H), 2.53 - 2.46 (m, 2 H), 2.34 (t,  $J$  = 7.0 Hz, 2 H), 2.28 (t,  $J$  = 7.3 Hz, 2 H), 1.96 - 1.86 (m, 2 H), 1.84 - 1.72 (m, 4 H)

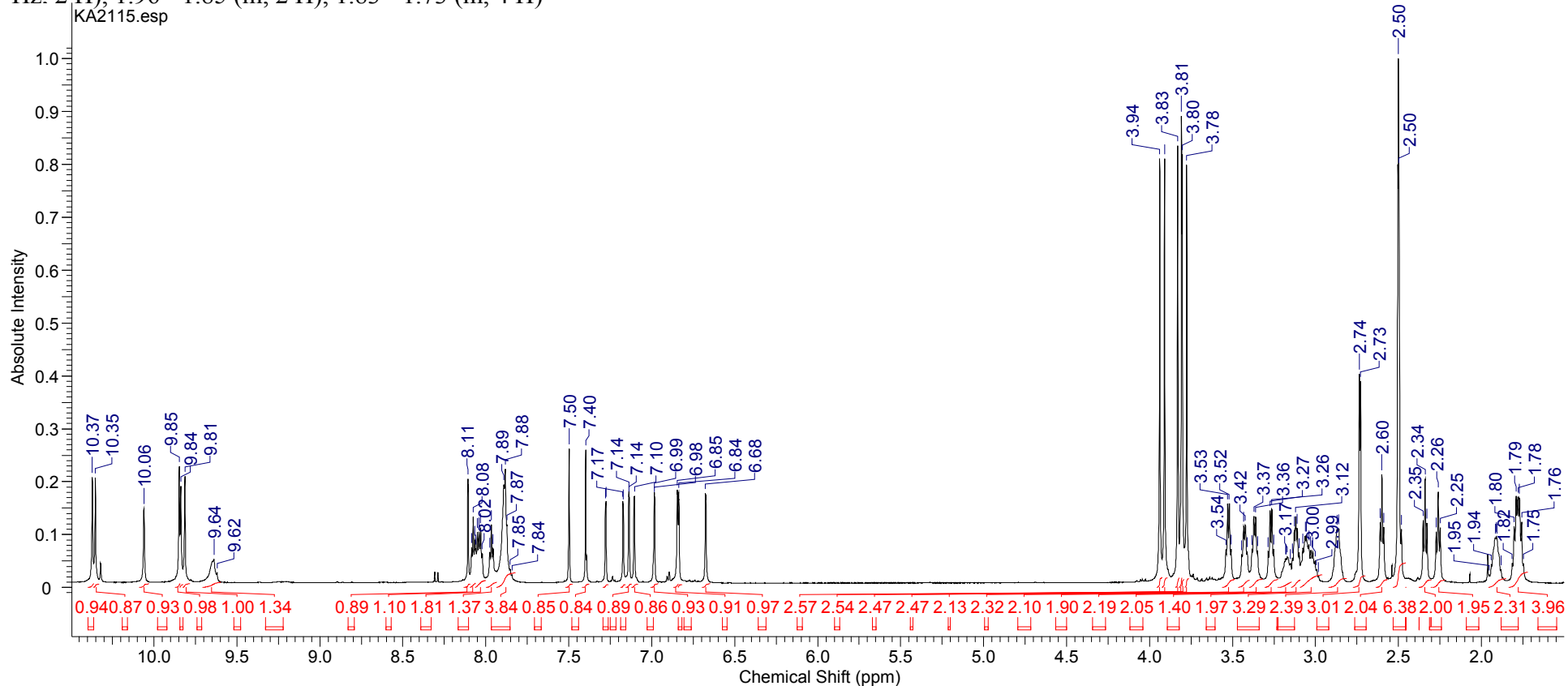


# KA2115

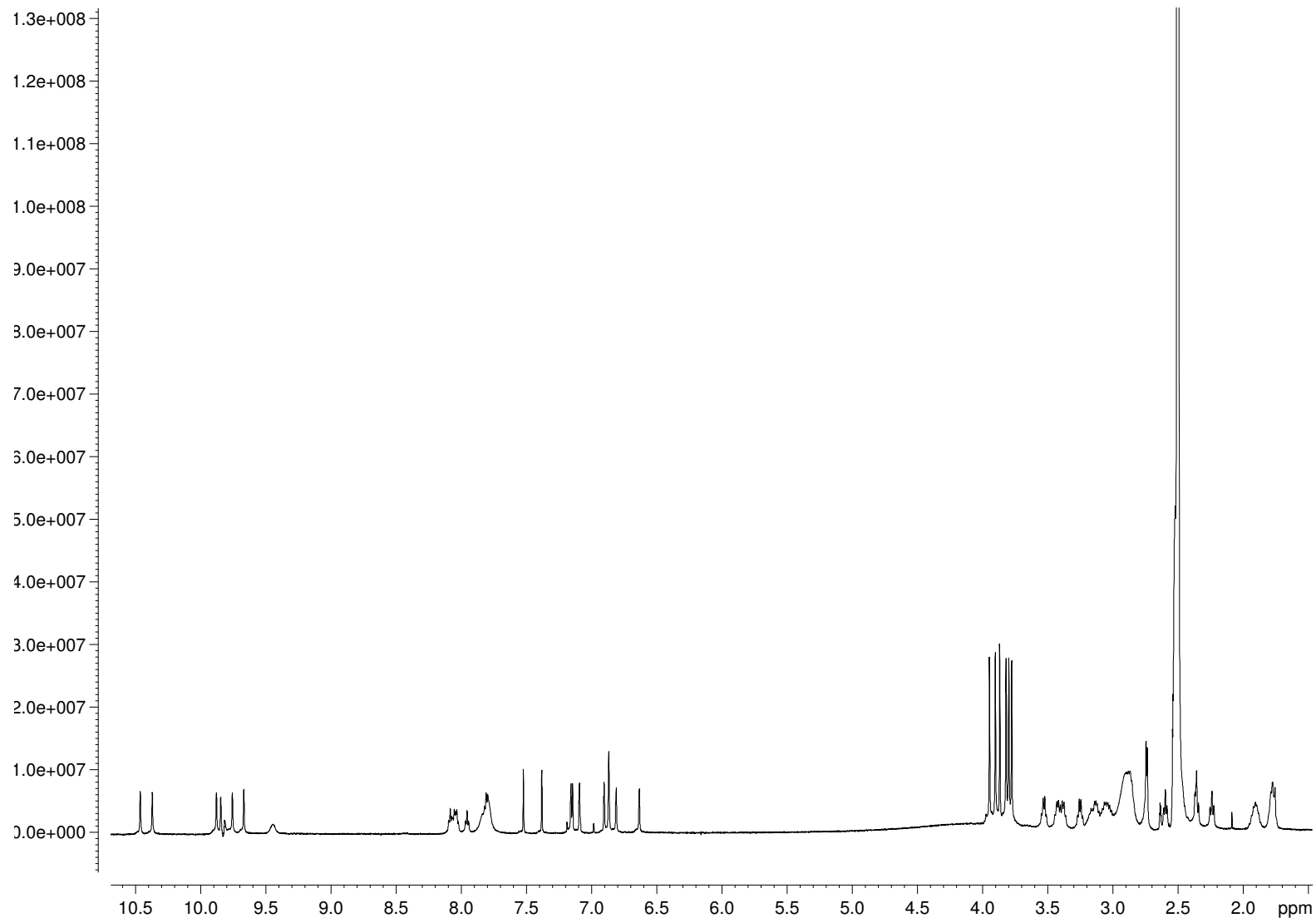
KA2115

<b>Acquisition Time (sec)</b>	1.7039	<b>Comment</b>	Gradient Shimming		<b>Date</b>	Apr 26 2013	
<b>Date Stamp</b>	Apr 26 2013	<b>File Name</b>	\\stl.umsl.edu\deptshare\sh_nmrdata\Agilent600\BASHKIN\ka2115a-proton_042613.fid\fid				
<b>Frequency (MHz)</b>	599.78	<b>Nucleus</b>	1H	<b>Number of Transients</b>	64	<b>Original Points Count</b>	16384
<b>Points Count</b>	16384	<b>Pulse Sequence</b>	s2pul	<b>Receiver Gain</b>	30.00	<b>Solvent</b>	DMSO-d6
<b>Spectrum Offset (Hz)</b>	3609.6973	<b>Spectrum Type</b>	STANDARD	<b>Sweep Width (Hz)</b>	9615.38	<b>Temperature (degree C)</b>	25.000

$^1\text{H}$  NMR (600MHz, DMSO-d<sub>6</sub>)  $\delta$  = 10.37 (s, 1 H), 10.35 (s, 1 H), 10.06 (s, 1 H), 9.85 (s, 1 H), 9.84 (s, 1 H), 9.81 (s, 1 H), 9.71 - 9.60 (m, 1 H), 8.11 (d,  $J$  = 1.2 Hz, 1 H), 8.08 (t,  $J$  = 5.9 Hz, 1 H), 8.06 - 8.00 (m, 2 H), 7.97 (t,  $J$  = 5.9 Hz, 1 H), 7.93 - 7.82 (m, 5 H), 7.50 (s, 1 H), 7.40 (s, 1 H), 7.28 (d,  $J$  = 1.8 Hz, 1 H), 7.17 (d,  $J$  = 1.8 Hz, 1 H), 7.14 (d,  $J$  = 1.2 Hz, 1 H), 7.11 (d,  $J$  = 1.8 Hz, 1 H), 6.98 (d,  $J$  = 1.8 Hz, 1 H), 6.85 (d,  $J$  = 1.8 Hz, 1 H), 6.84 (d,  $J$  = 1.2 Hz, 1 H), 6.67 (d,  $J$  = 1.8 Hz, 1 H), 3.94 (s, 3 H), 3.91 (s, 3 H), 3.83 (s, 3 H), 3.81 (s, 3 H), 3.80 (s, 3 H), 3.78 (s, 3 H), 3.52 (q,  $J$  = 6.5 Hz, 2 H), 3.47 - 3.40 (m, 2 H), 3.40 - 3.32 (m, 2 H), 3.27 (q,  $J$  = 6.8 Hz, 2 H), 3.22 - 3.15 (m, 1 H), 3.15 - 3.09 (m, 2 H), 3.09 - 2.96 (m, 3 H), 2.92 - 2.82 (m,  $J$  = 5.9 Hz, 2 H), 2.73 (d,  $J$  = 4.7 Hz, 3 H), 2.60 (t,  $J$  = 6.5 Hz, 2 H), 2.53 - 2.46 (m, 2 H), 2.34 (t,  $J$  = 7.3 Hz, 2 H), 2.26 (t,  $J$  = 7.3 Hz, 2 H), 1.96 - 1.85 (m, 2 H), 1.83 - 1.73 (m, 4 H)

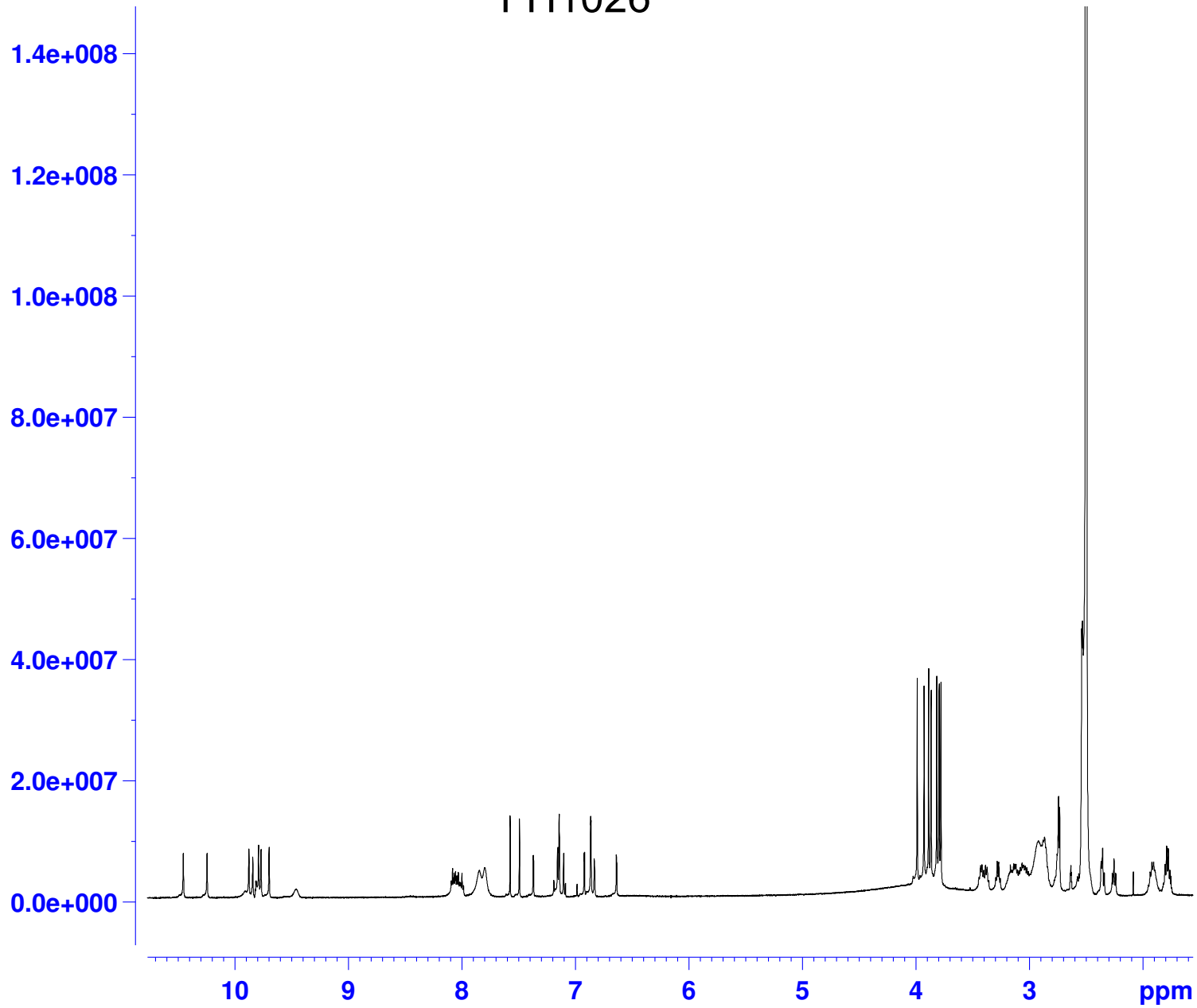


# FH1024



NAME	FH1024C
EXPNO	1
PROCNO	1
Date_	20120507
Time_	11.36
INSTRUM	spect
PROBHD	5 mm Multinu
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	2000
DS	2
SWH	10416.667 Hz
FIDRES	0.158946 Hz
AQ	3.1457779 sec
RG	2048
DW	48.000 usec
DE	68.57 usec
TE	300.0 K
D1	1.00000000 sec
P1	12.50 usec
SFO1	500.1330885 MHz
NUCLEUS	1H
SI	32768
SF	500.1300078 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

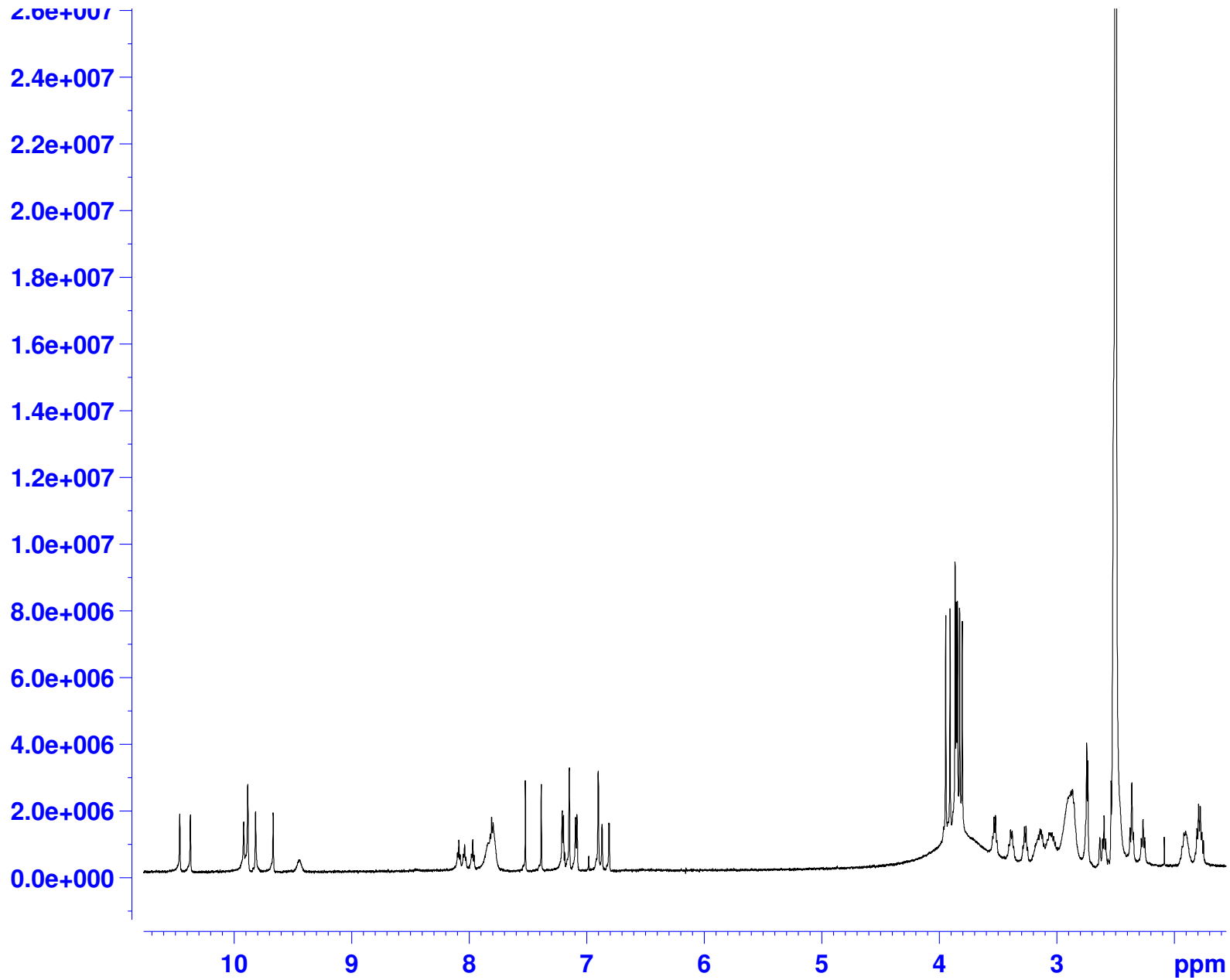
# FH1026



NAME	FH1026C
EXPNO	1
PROCNO	1
Date_	20120507
Time	14.08
INSTRUM	spect
PROBHD	5 mm Multinu
PULPROG	zg30
ID	65536
SOLVENT	DMSO
NS	1941
DS	2
SWH	10416.667 Hz
FIDRES	0.158946 Hz
AQ	3.1457779 sec
RG	2048
DW	48.000 usec
DE	68.57 usec
TE	300.0 K
D1	1.00000000 sec
P1	12.50 usec
SFO1	500.1330885 MHz
NUCLEUS	1H
SI	32768
SF	500.1300081 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



# FH1028

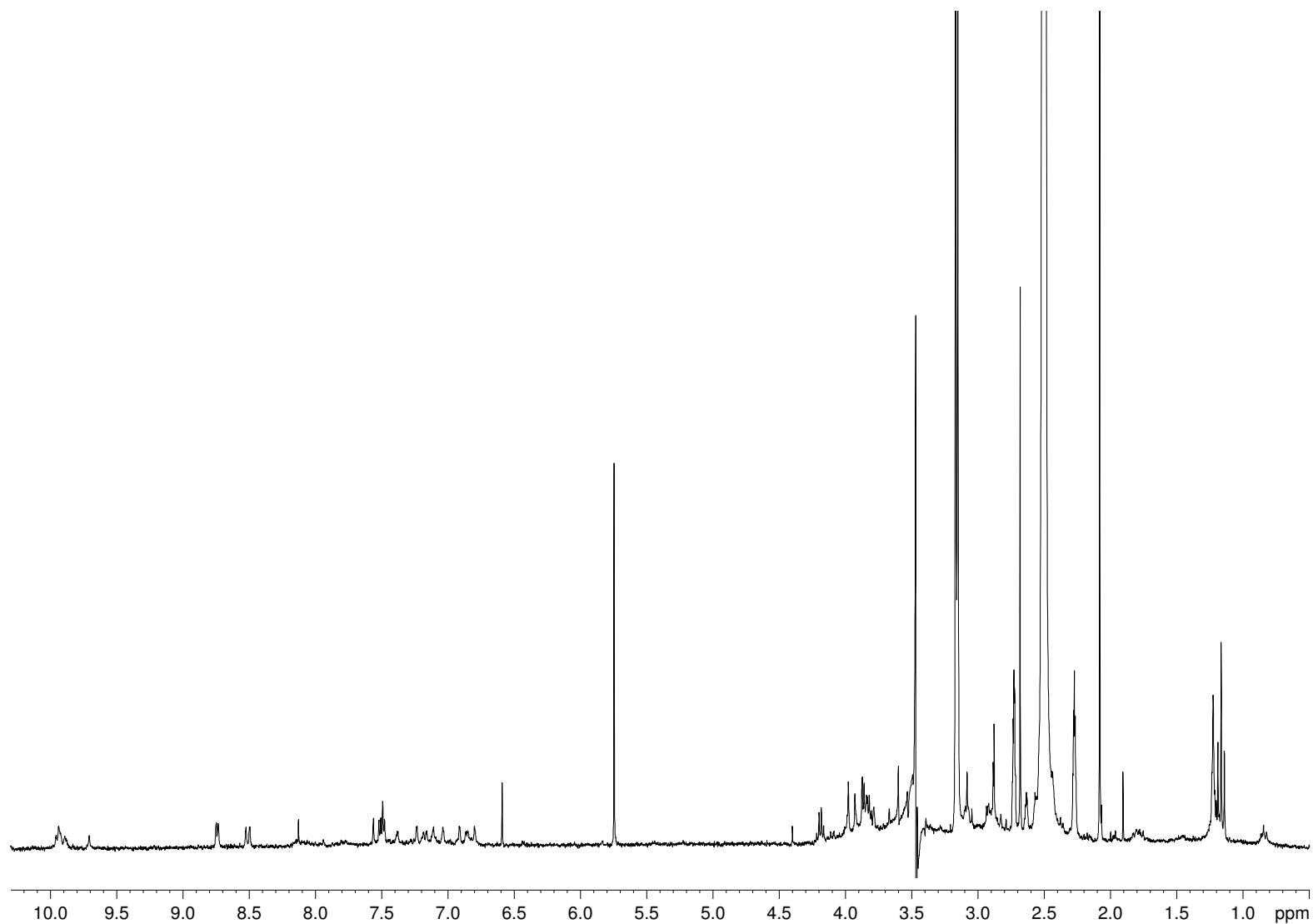


NAME	FH1028C
EXPNO	1
PROCNO	1
Date_	20120507
Time	16.10
INSTRUM	spect
PROBHD	5 mm Multinu
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	1509
DS	2
SWH	10416.667 Hz
FIDRES	0.158946 Hz
AQ	3.1457779 sec
RG	2048
DW	48.000 usec
DE	68.57 usec
TE	300.0 K
D1	1.00000000 sec
P1	12.50 usec
SFO1	500.1330885 MHz
NUCLEUS	1H
SI	32768
SF	500.1300084 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

# KJK6162

NAME kjk6162  
EXPNO 2  
PROCNO 1  
Date\_ 20170920  
Time 14.44  
INSTRUM spect  
PROBHD 5 mm QNP 1H/13  
PULPROG zgpgpr  
TD 32768  
SOLVENT DMSO  
NS 2048  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.188380 Hz  
AQ 2.6542580 sec  
RG 1149.4  
DW 81.000 usec  
DE 6.50 usec  
TE 290.4 K  
D1 2.00000000 sec  
D12 0.00002000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 14.00 usec  
PL1 4.30 dB  
PL9 53.16 dB  
PLIW 5.59952545 W  
PL9W 0.00007280 W  
SF01 300.1310402 MHz  
SI 16384  
SF 300.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



KJK6162

