

Supplementary Material

Novel Thiazolones for the Simultaneous Modulation of PPAR γ , COX-2 and 15-LOX to Address Metabolic Disease-associated Portal Inflammation

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Table S1. *In silico* prediction of physicochemical properties and drug likeness of compound **2a**: (<http://www.swissadme.ch/>)

Physicochemical Properties	
Formula	C17H16N2O2S
Molecular weight	312.39 g/mol
Num. heavy atoms	22
Num. arom. heavy atoms	6
Num. rotatable bonds	4
Num. H-bond acceptors	3
Num. H-bond donors	0
Molar Refractivity	97.03
TPSA	67.20 Å ²
Consensus Log <i>P</i>_{o/w}	3.07
Water Solubility	
Log <i>S</i> (ESOL)	-3.62
Solubility	7.43e-02 mg/ml ; 2.38e-04 mol/l
Class	Soluble
Log <i>S</i> (Ali)	-4.11
Solubility	2.44e-02 mg/ml ; 7.82e-05 mol/l
Class	Moderately soluble
Log <i>S</i> (SILICOS-IT)	-3.95
Solubility	3.53e-02 mg/ml ; 1.13e-04 mol/l
Class	Soluble
Pharmacokinetics	
GI absorption	High
P-gp substrate	No
Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailability Score	0.55

Table S2. *In silico* prediction of pharmacokinetic properties of compound **2a**:
(<https://preadmet.webservice.bmdrc.org/adme/>)

BBB	0.0170815
Buffer_solubility_mg_L	2264.34
Caco2	27.4134
HIA	98.532408
Plasma_Protein_Binding	96.228228

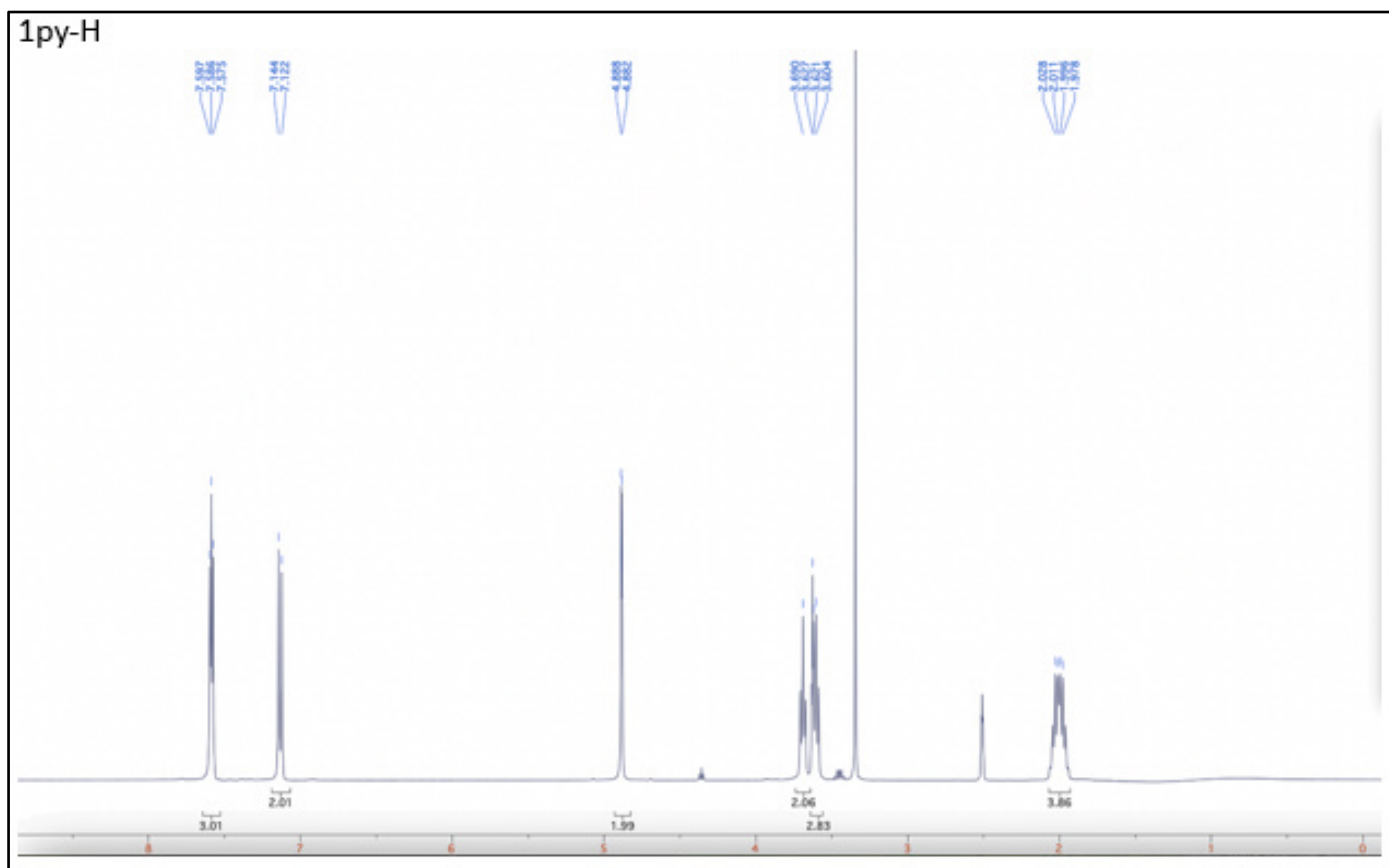
Table S3. Prediction of toxicological profile of compound **2a**:
(<https://tox.charite.de/protox3/index.php?site=home>)

Classification	Target	Prediction	Probability
Organ toxicity	Hepatotoxicity	Inactive	0.69
Organ toxicity	Nephrotoxicity	Inactive	0.56
Organ toxicity	Cardiotoxicity	Inactive	0.66
Toxicity end points	Carcinogenicity	Inactive	0.53
Toxicity end points	Immunotoxicity	Inactive	0.90
Toxicity end points	Mutagenicity	Inactive	0.62
Toxicity end points	Cytotoxicity	Inactive	0.68
Metabolism	Cytochrome CYP1A2	Inactive	0.80
Metabolism	Cytochrome CYP2C19	Inactive	0.70
Metabolism	Cytochrome CYP2C9	Inactive	0.58
Metabolism	Cytochrome CYP2D6	Active	0.50
Metabolism	Cytochrome CYP3A4	Inactive	0.77
Metabolism	Cytochrome CYP2E1	Inactive	0.99

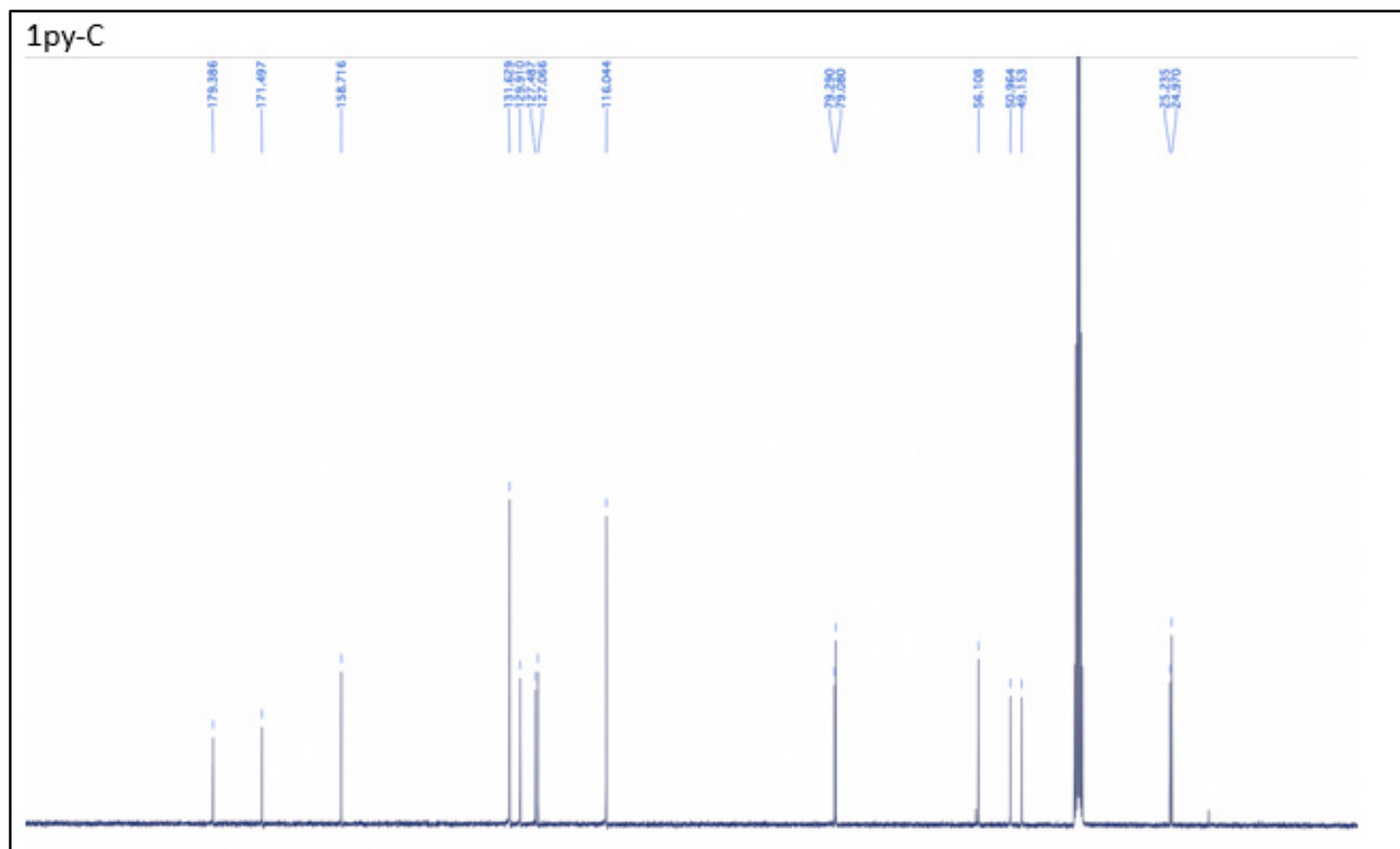
Table S4. Ligand efficiency metrics of compound **2a**:
(http://www.vulpinescience.co.uk/uploads/MedChem%20Calculators_Ver3.2/MedChem%20Calculators.htm)

LE (COX-2)	0.43
LLE	3.6
LELP	7.1
LE (15-LOX)	0.33
LLE	2.1
LELP	9.3

¹H-NMR Spectrum of compound 2a



¹³C-NMR Spectrum of compound 2a



¹H-NMR Spectrum of compound 2b

PEREHAN-1Pd
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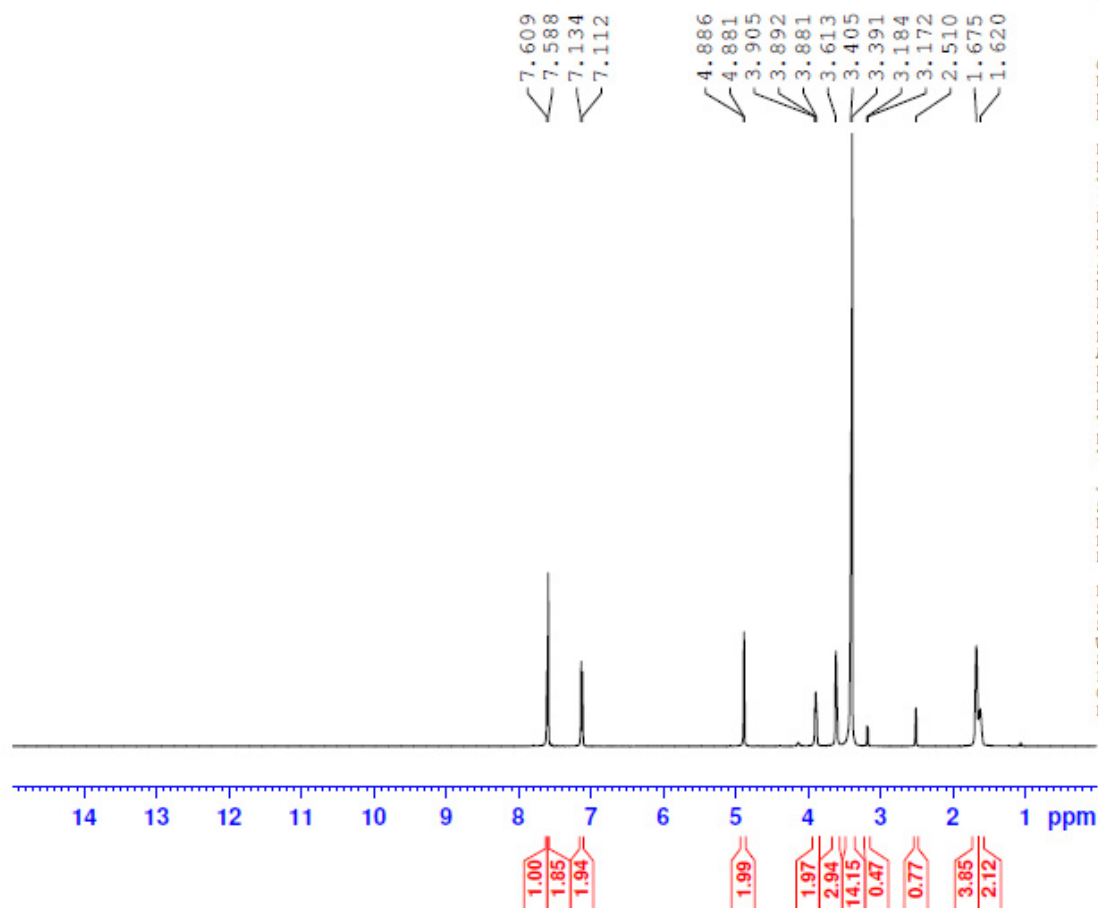


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TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 116.51
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

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NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

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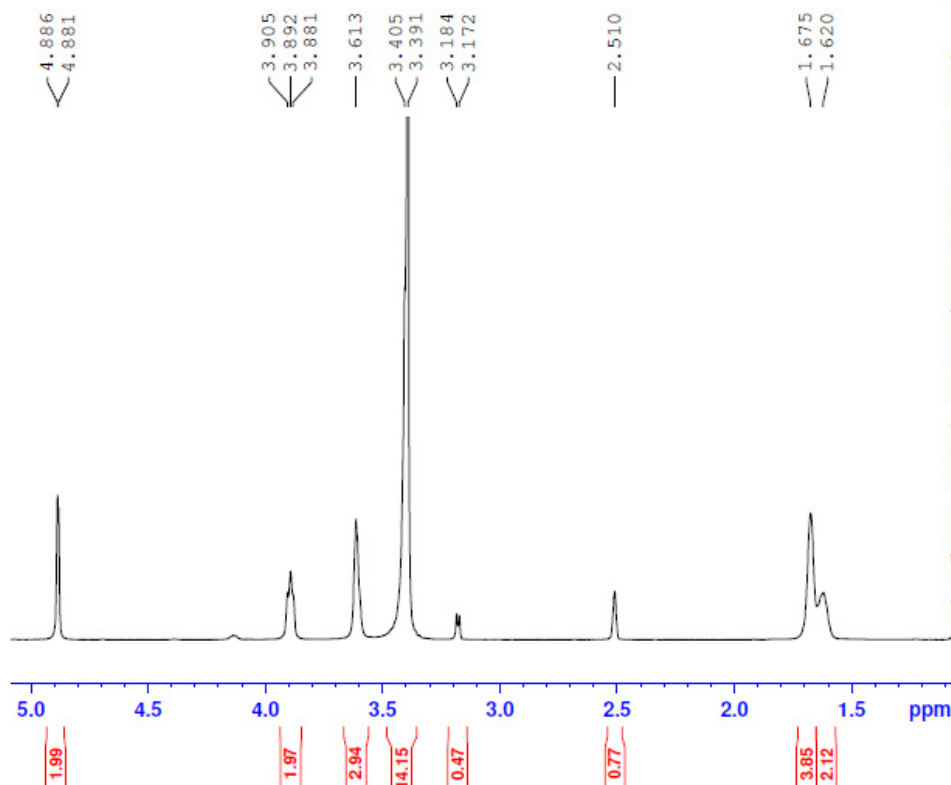


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NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 116.51
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
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NUC1 1H
P1 10.00 usec
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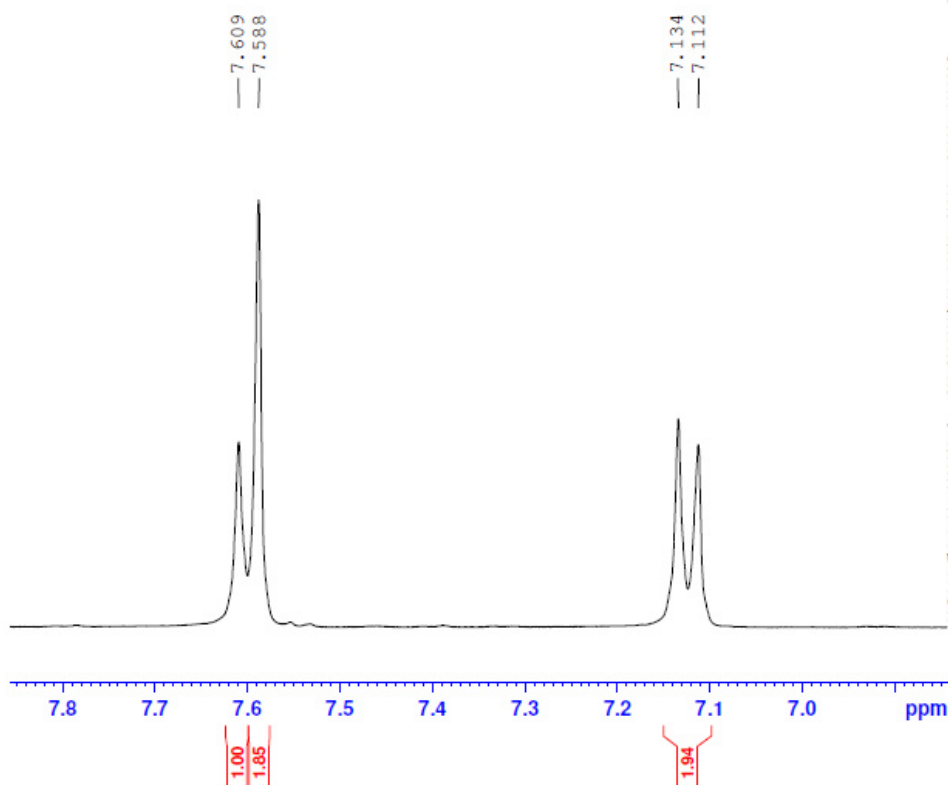


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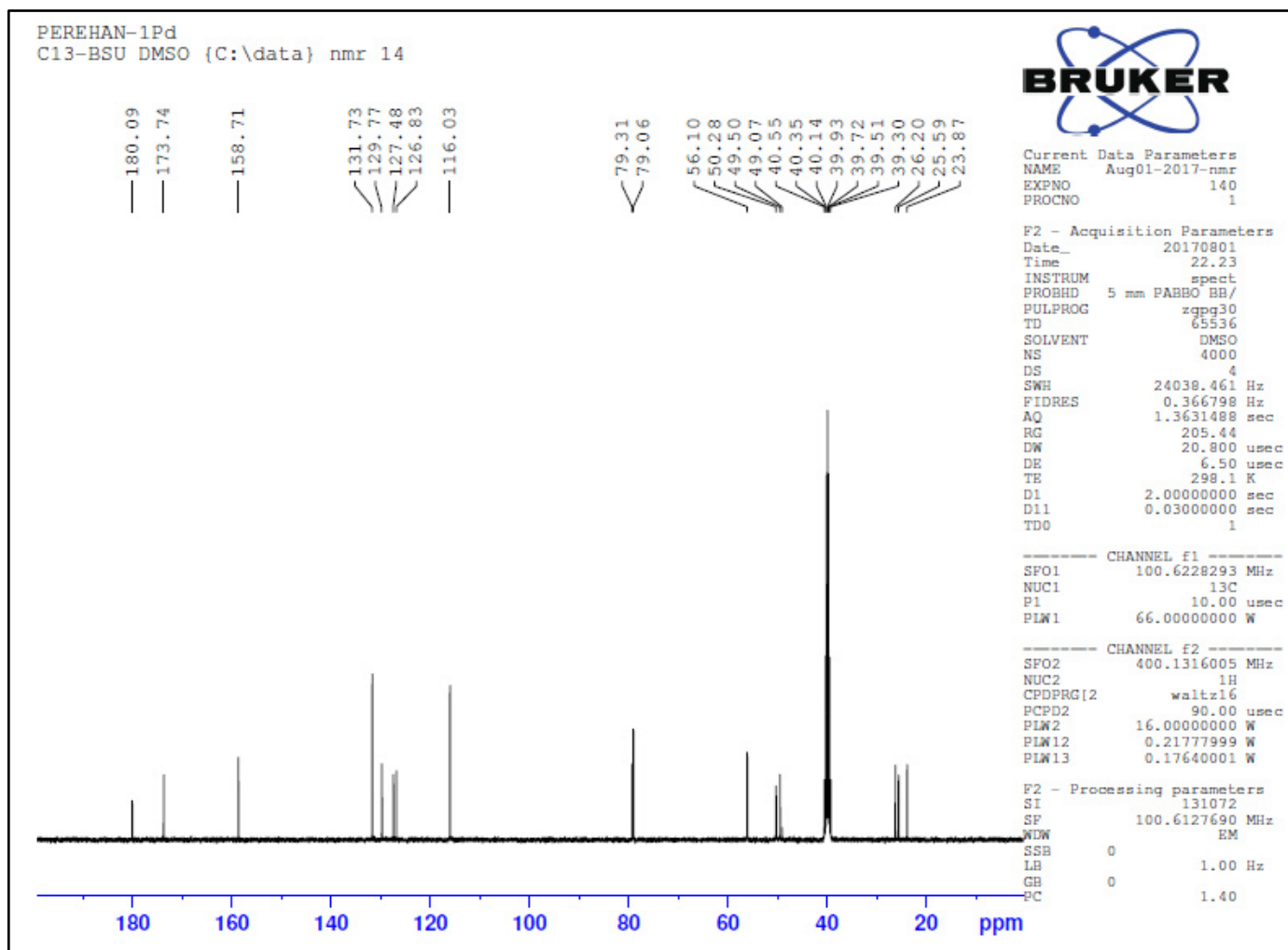
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SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 116.51
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
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¹³C-NMR Spectrum of compound 2b



PEREHAN-1Pd
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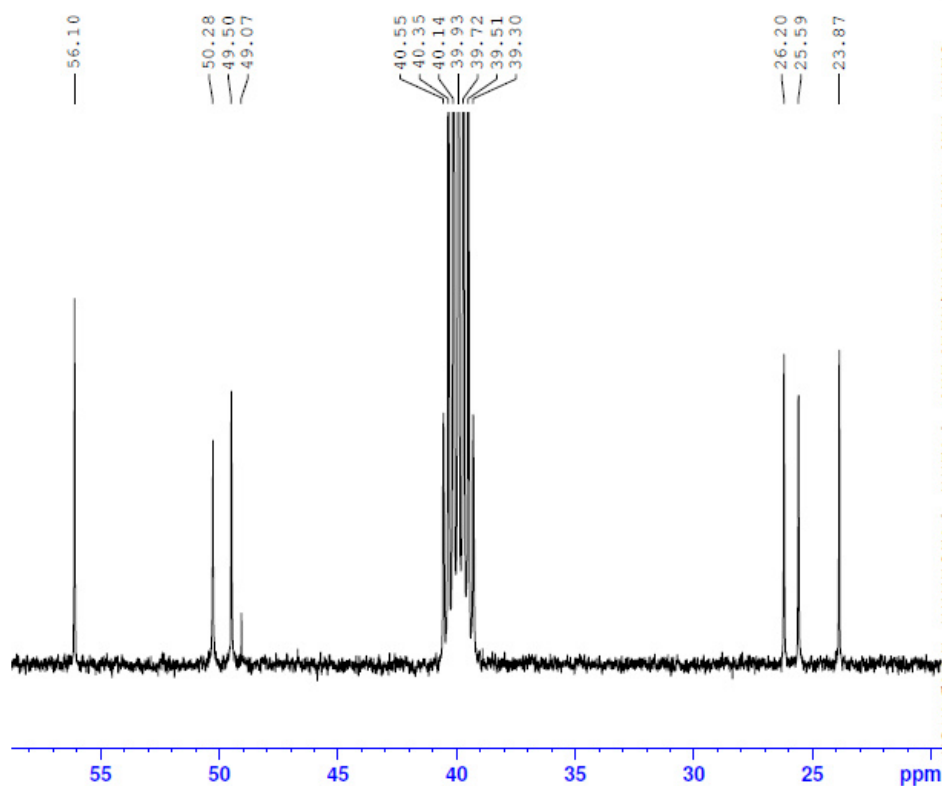
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NS 4000
DS 4
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FIDRES 0.366798 Hz
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DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

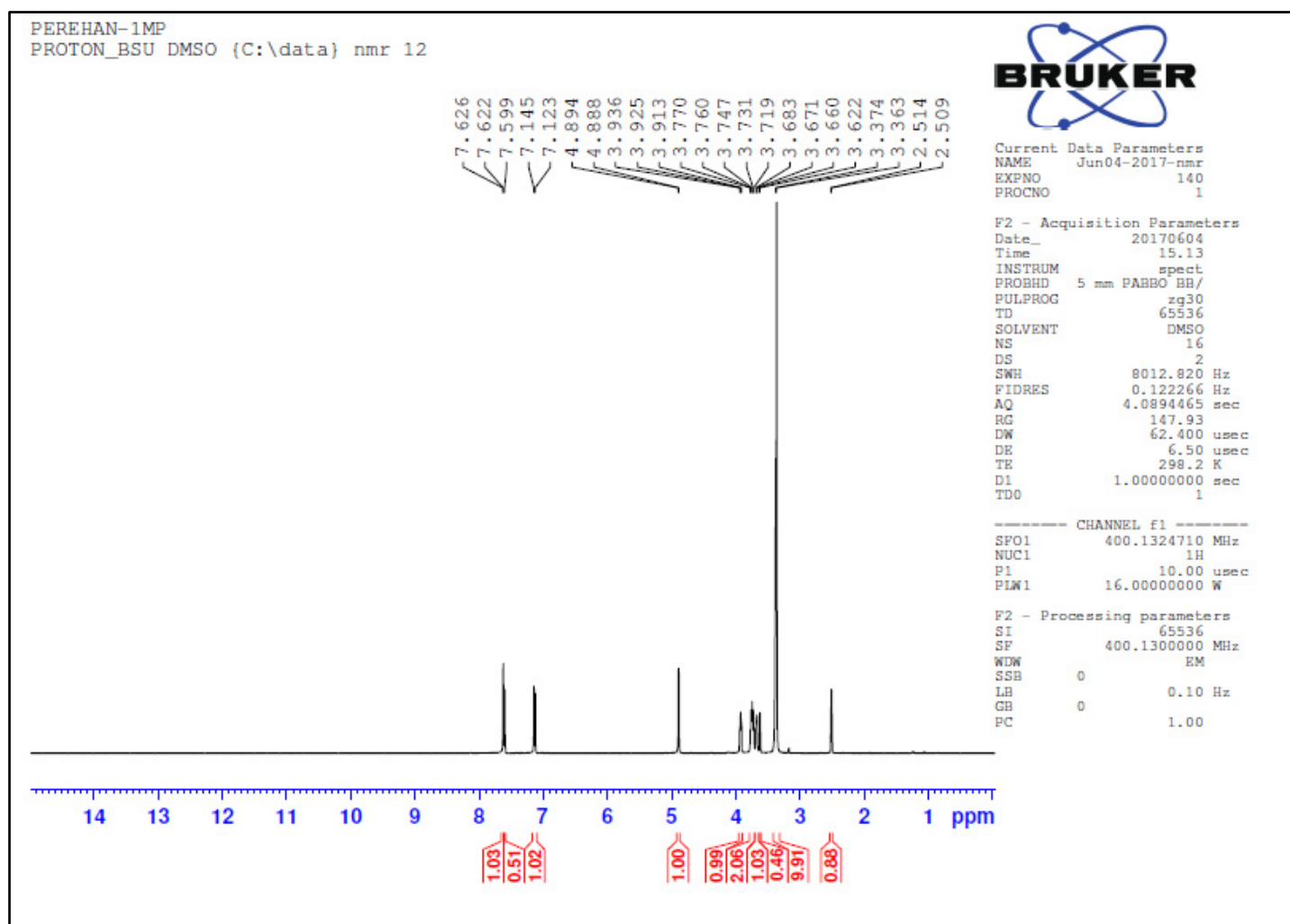
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PLW12 0.21777999 W
PLW13 0.17640001 W

F2 - Processing parameters
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PC 1.40



¹H-NMR Spectrum of compound 2c



PEREHAN-1MP
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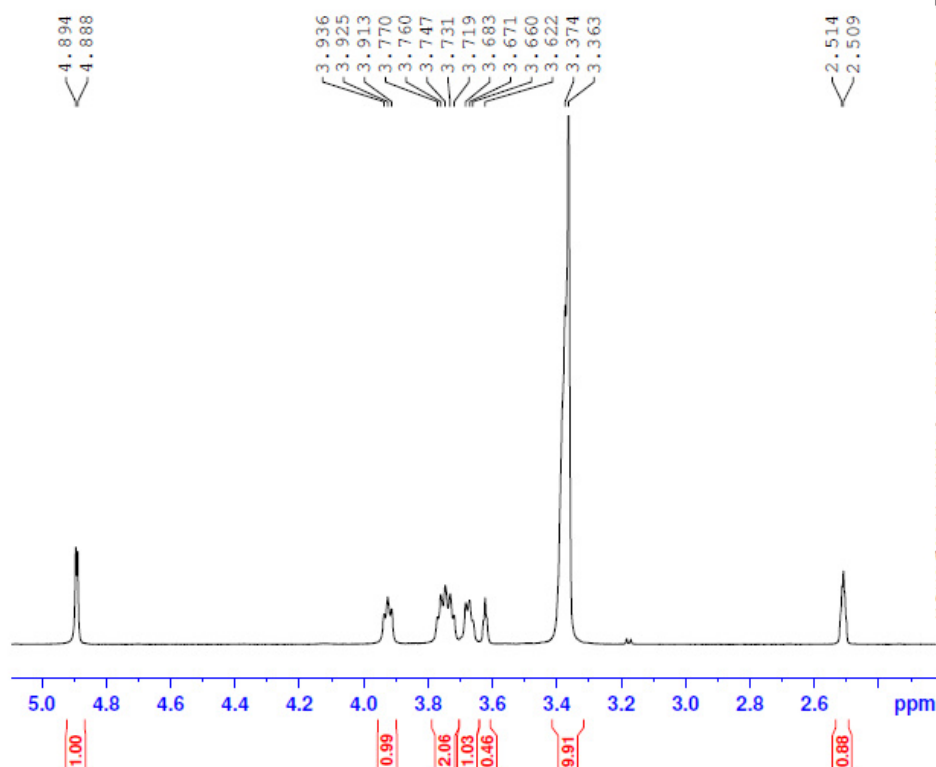


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FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 147.93
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
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NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
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PEREHAN-1MP
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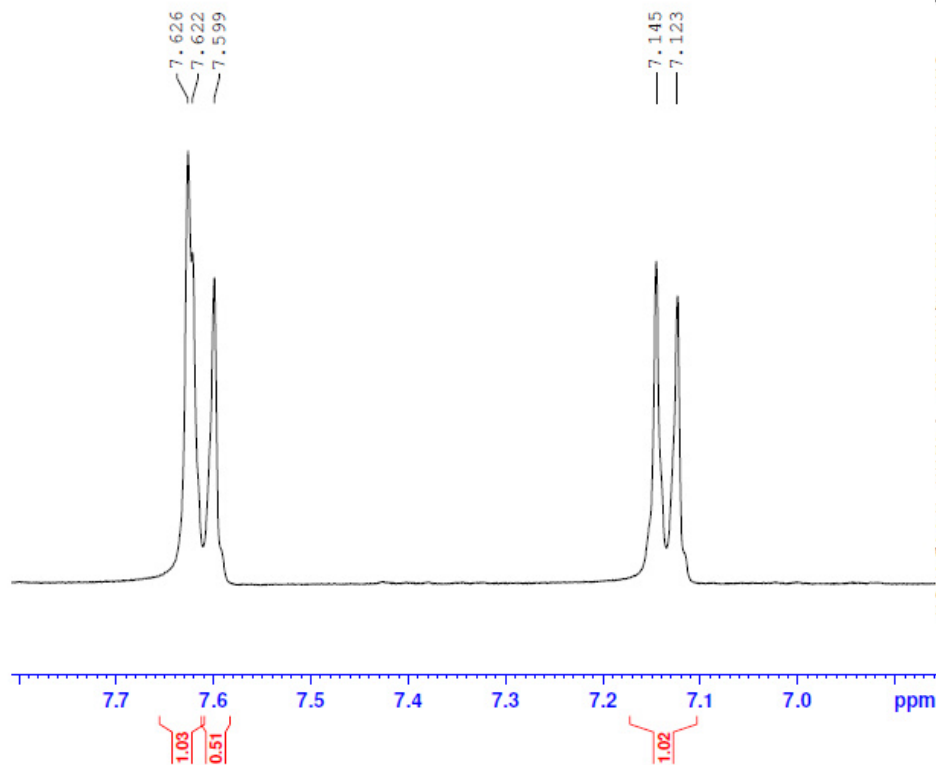


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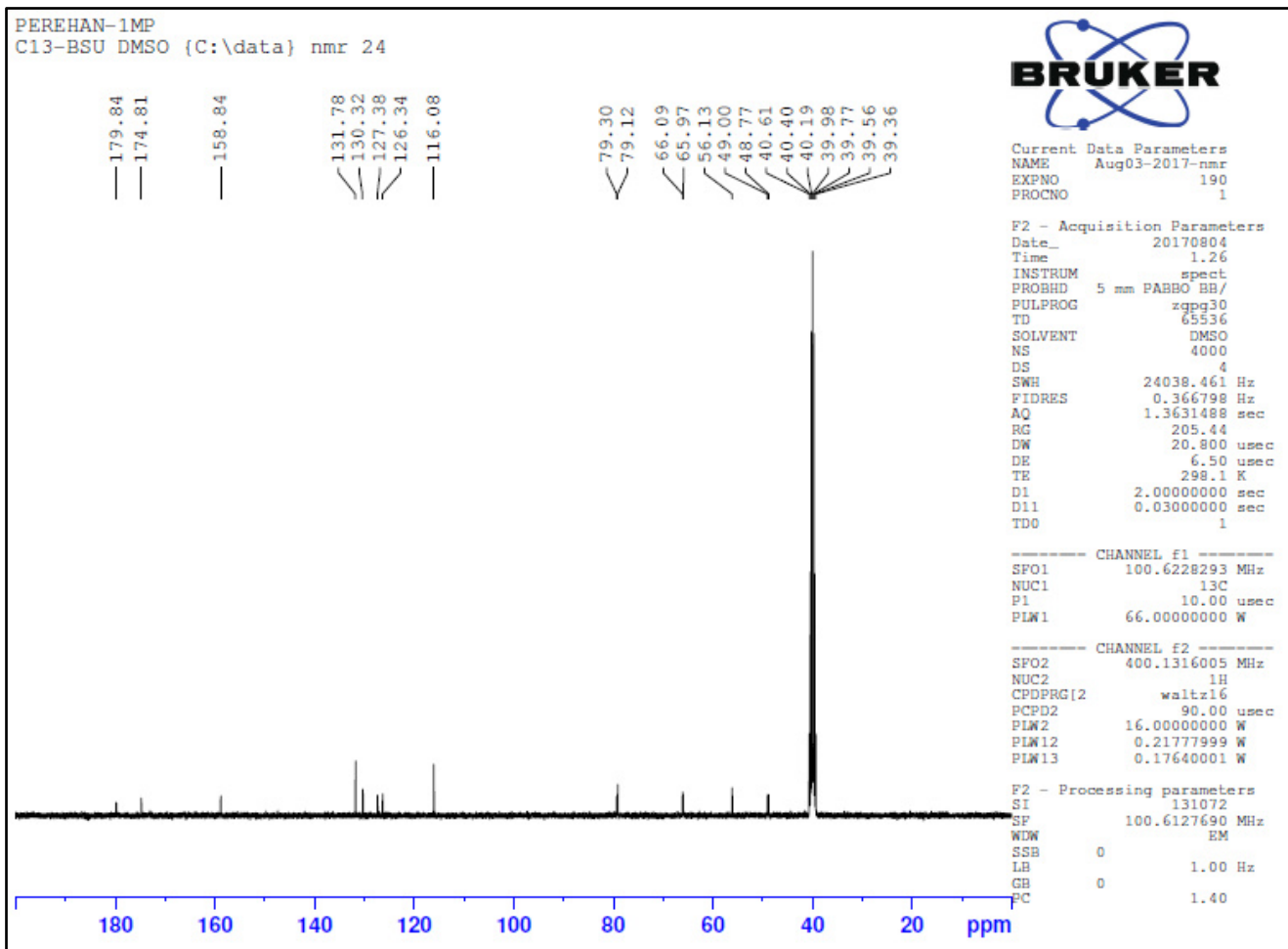
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SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 147.93
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
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TD0 1

CHANNEL f1
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P1 10.00 usec
PLW1 16.00000000 W

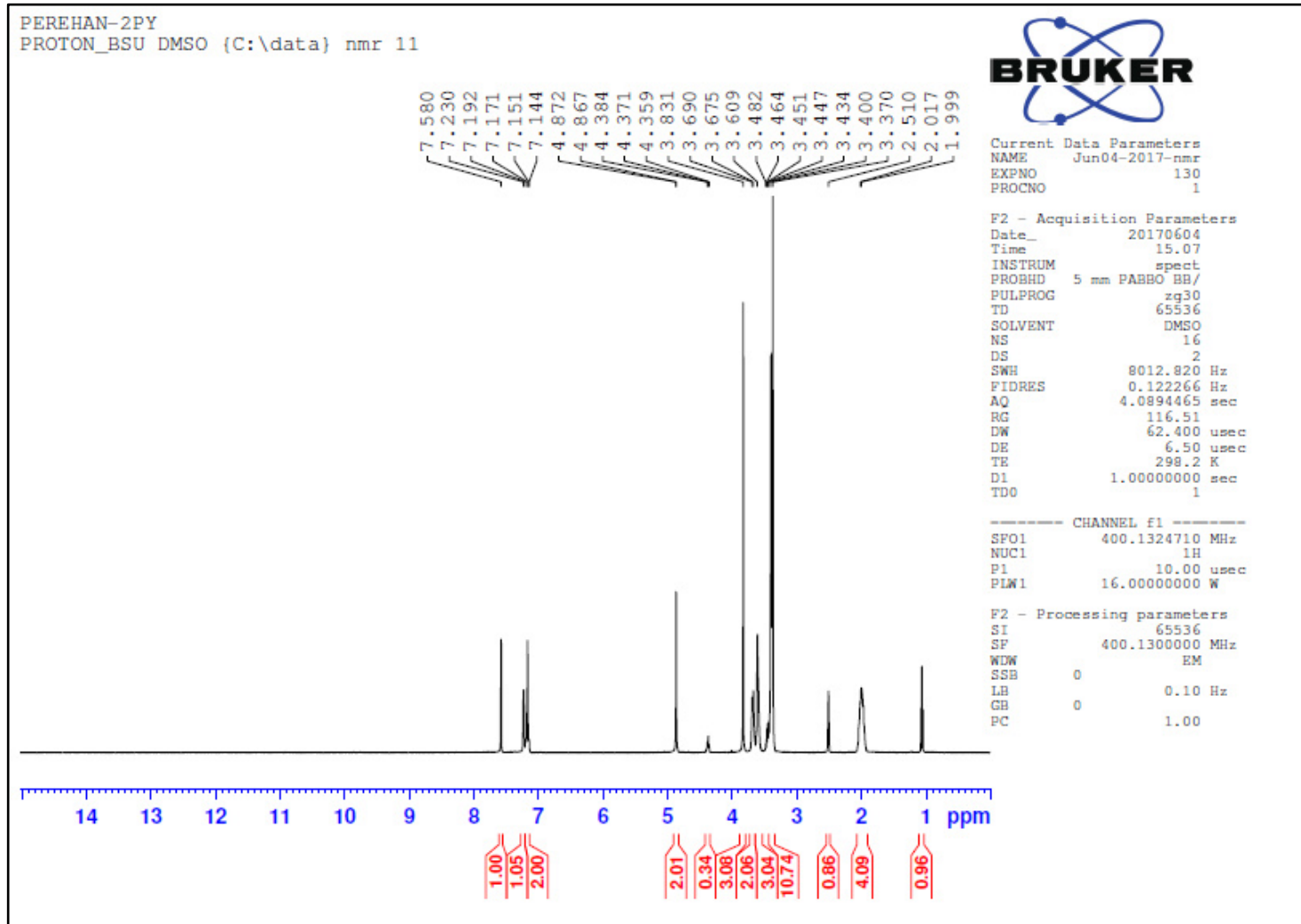
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¹³C-NMR Spectrum of compound 2c



¹H-NMR Spectrum of compound 2d



PEREHAN-2PY
PROTON_BSU DMSO {C:\data} nmr 11

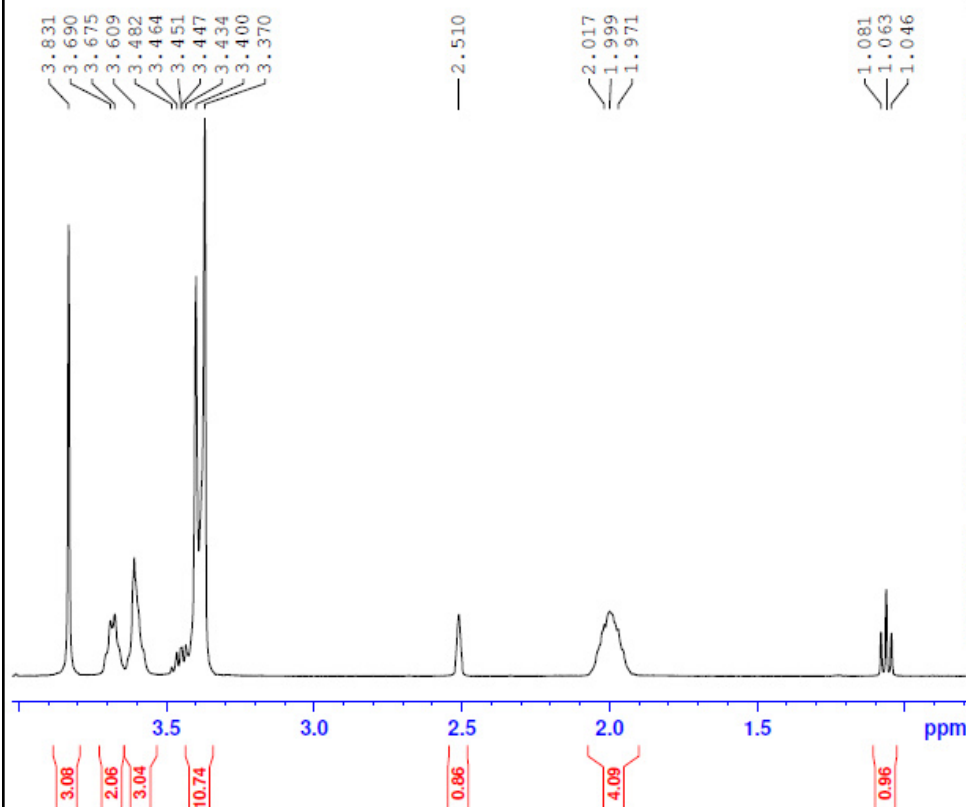


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EXPNO 130
PROCNO 1

F2 - Acquisition Parameters
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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 116.51
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
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WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00



PEREHAN-2PY
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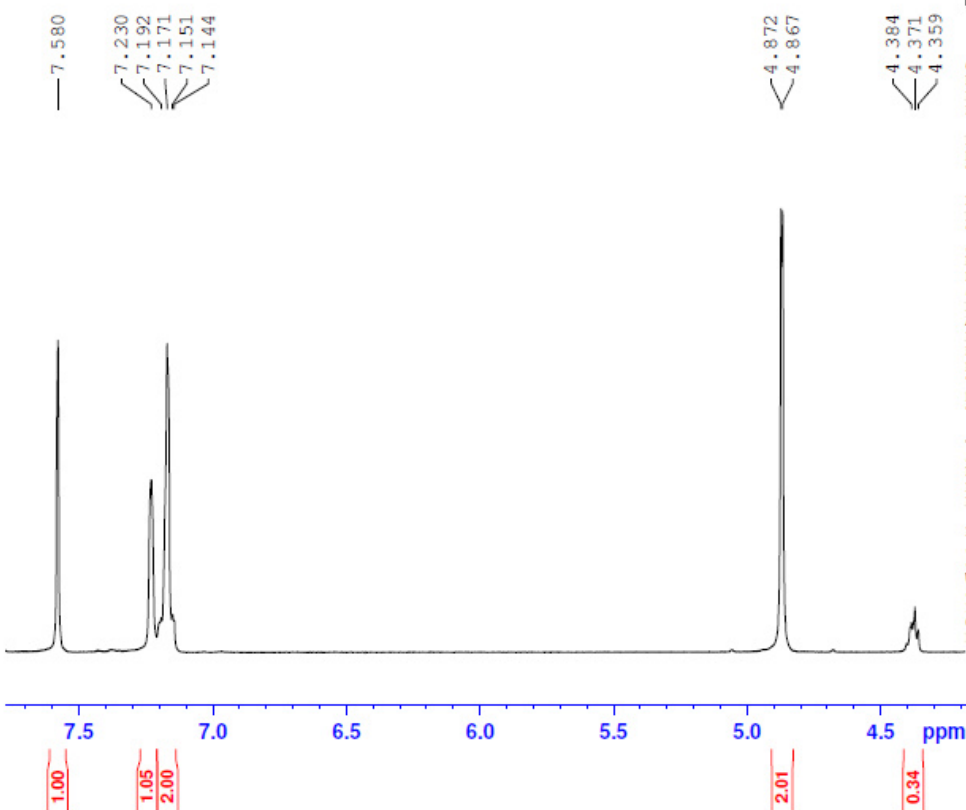


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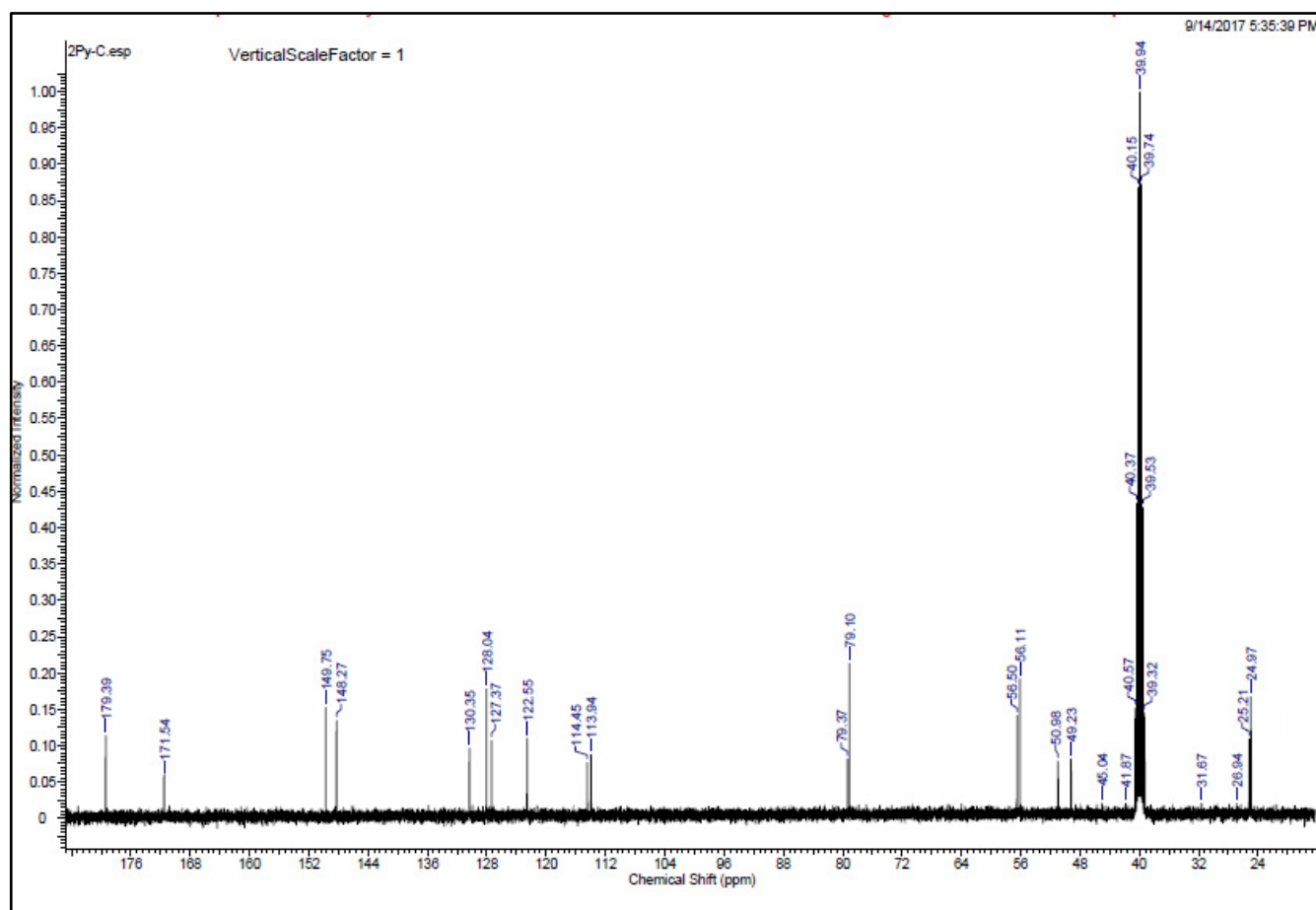
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NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 116.51
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
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SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00



¹³C-NMR Spectrum of compound 2d



¹H-NMR Spectrum of compound 2e

PEREHAN-2Pd
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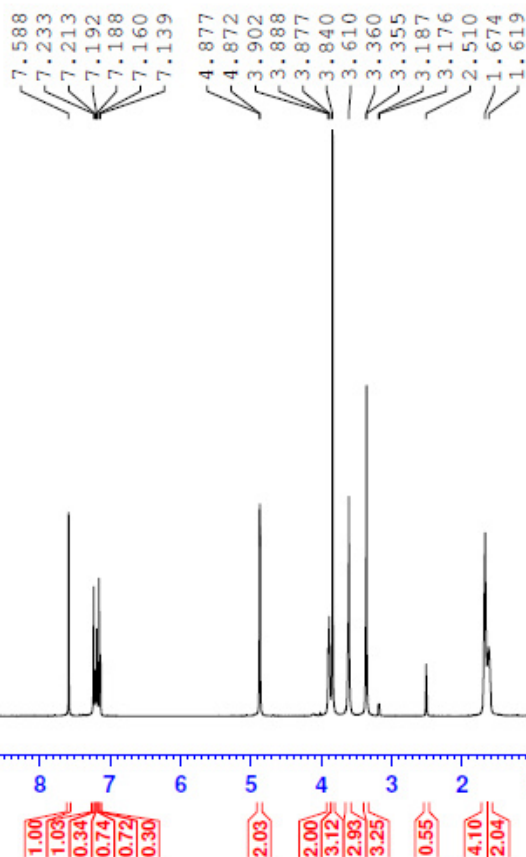


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SOLVENT DMSO
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FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 102.37
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00



PEREHAN-2Pd
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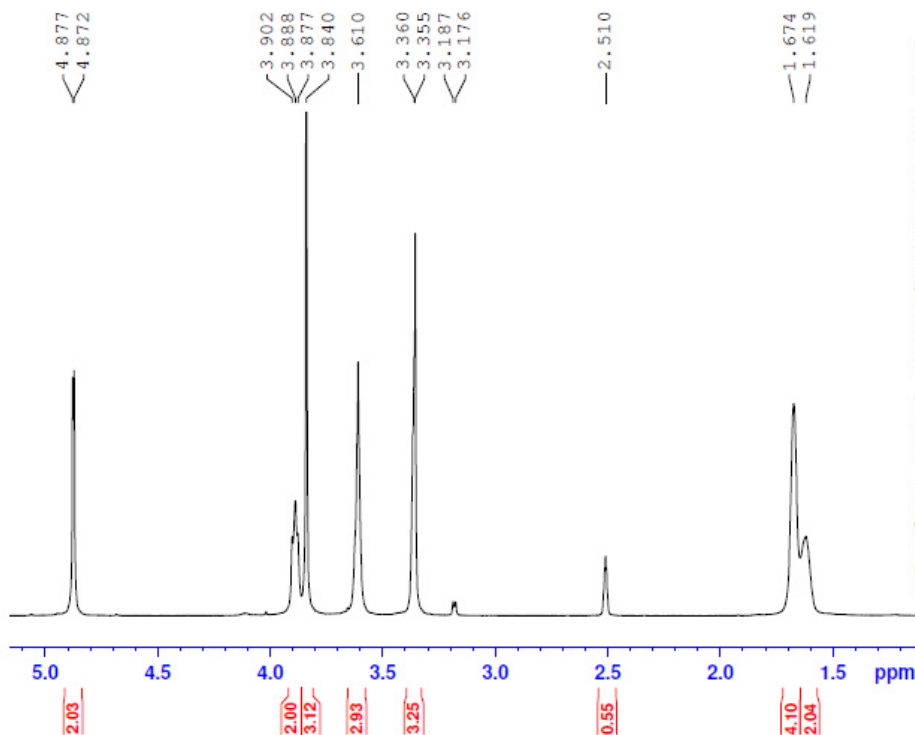


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SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 102.37
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TDO 1

CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
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PC 1.00



PEREHAN-2Pd
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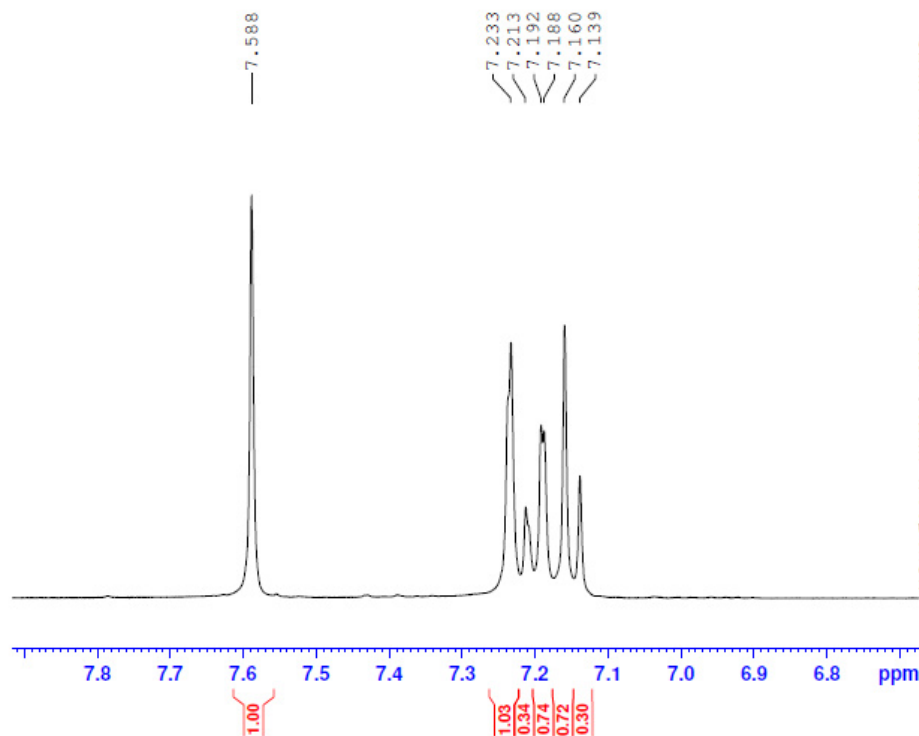


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SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 102.37
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TDO 1

CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
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GB 0
PC 1.00



¹³C-NMR Spectrum of compound 2e

PEREHAN-2Pd
C13-BSU DMSO {C:\data} nmr 16



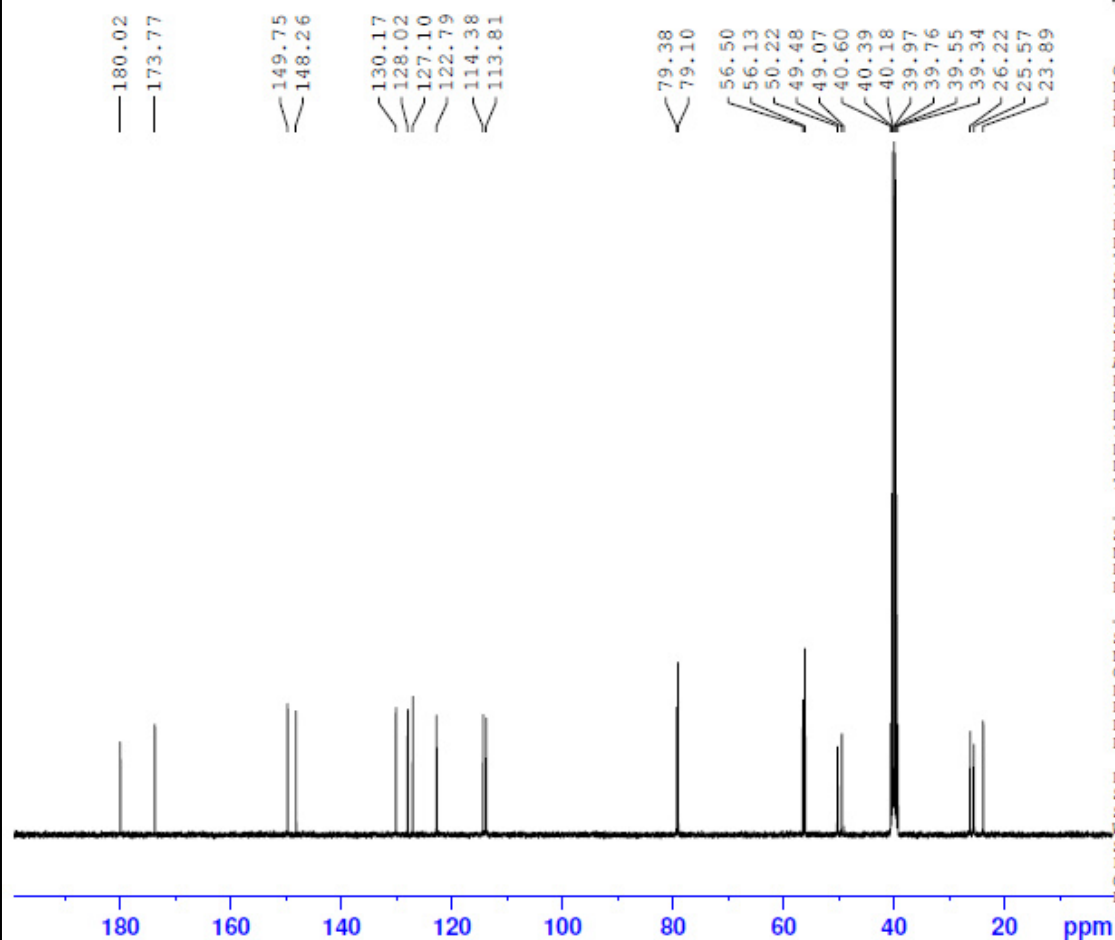
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EXPNO 160
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FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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NUC1 13C
P1 10.00 usec
PLW1 66.00000000 W

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NUC2 1H
CPDPRG12 waltz16
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21777999 W
PLW13 0.17640001 W

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PEREHAN-2Pd
C13-BSU DMSO {C:\data} nmr 16



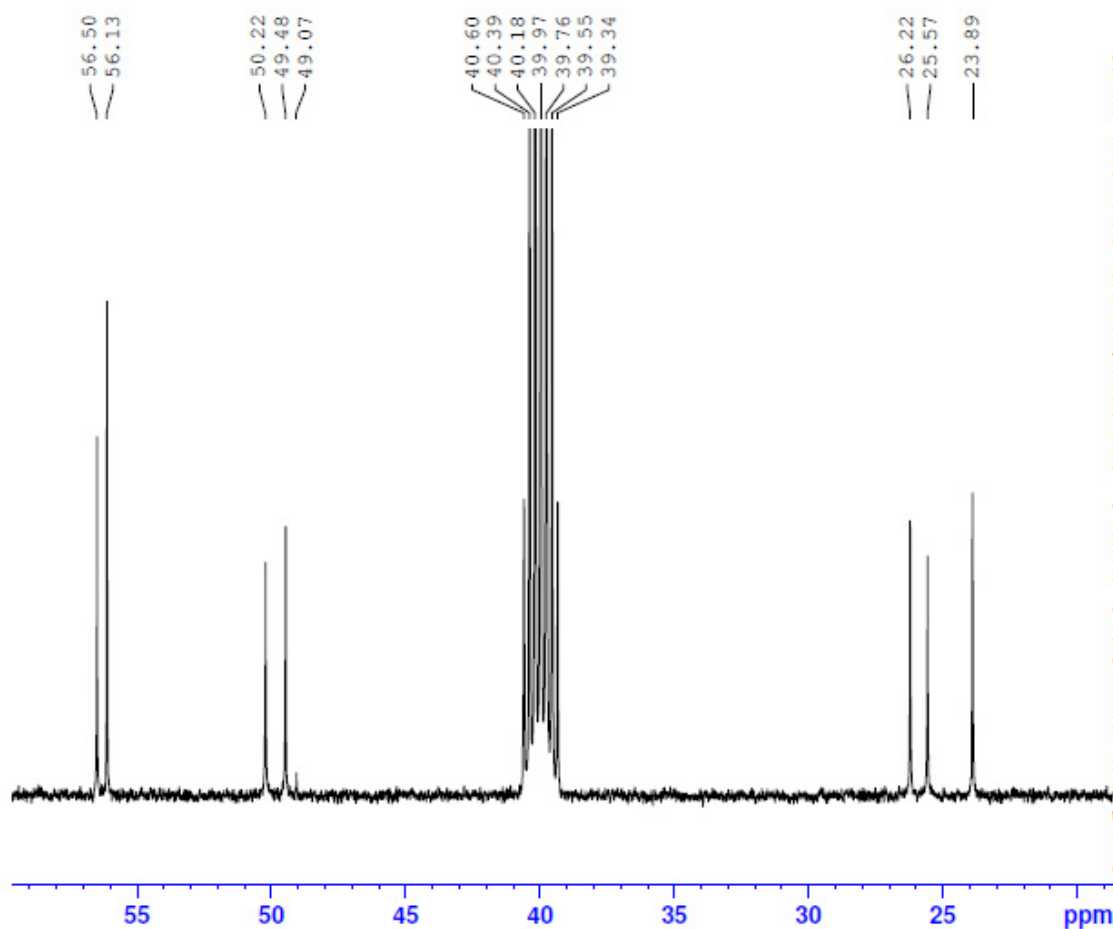
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PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

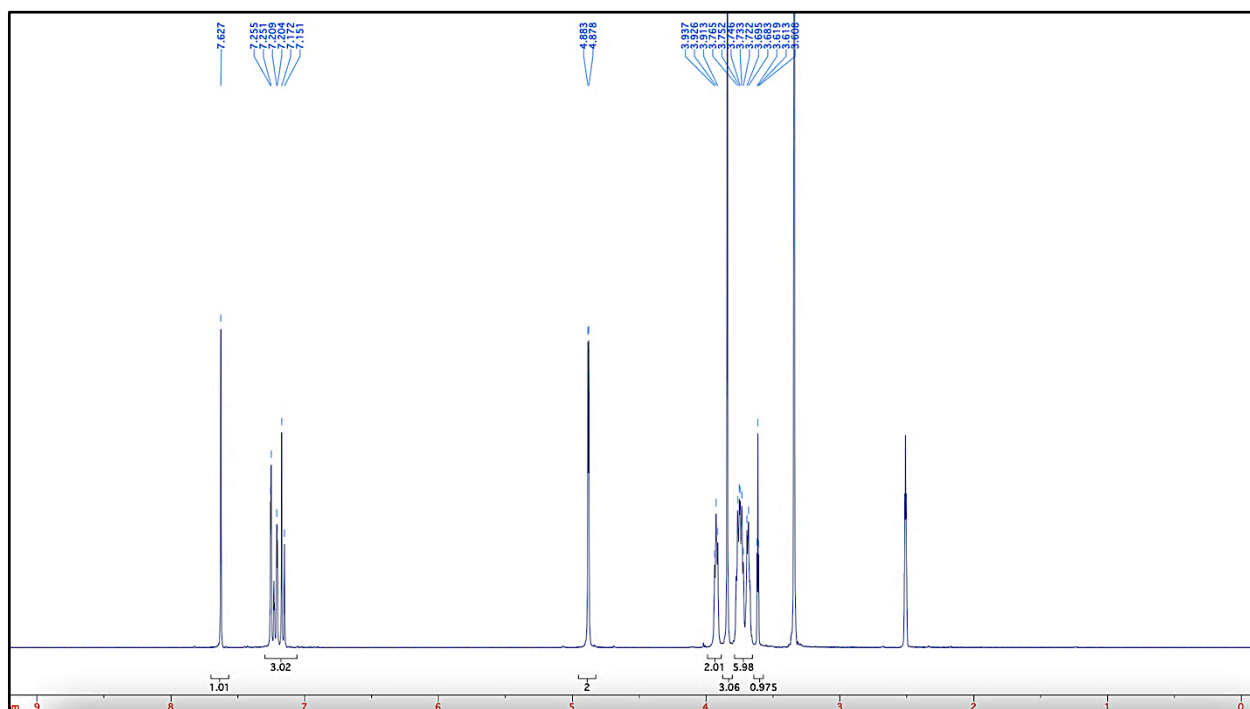
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PCPD2 90.00 usec
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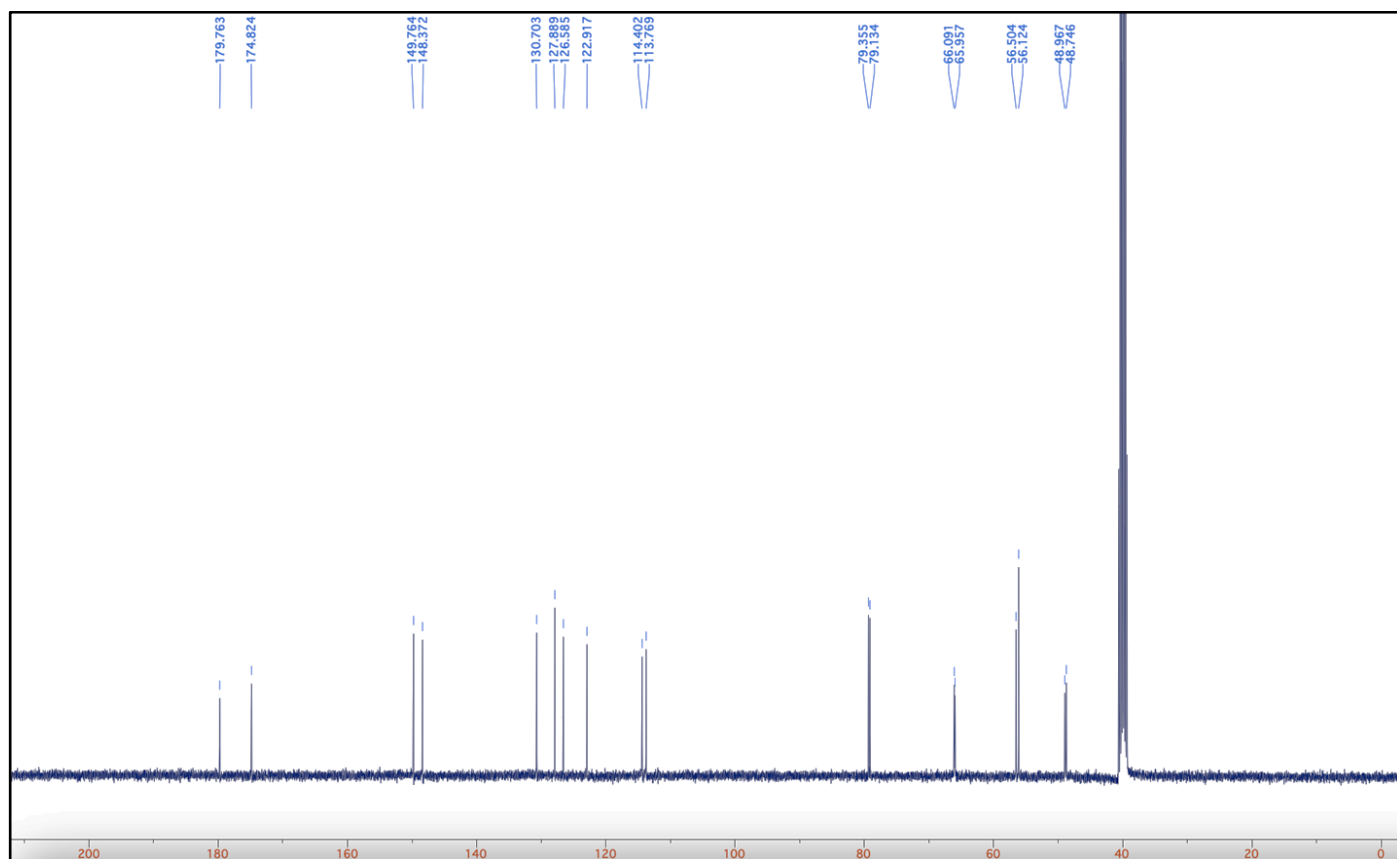
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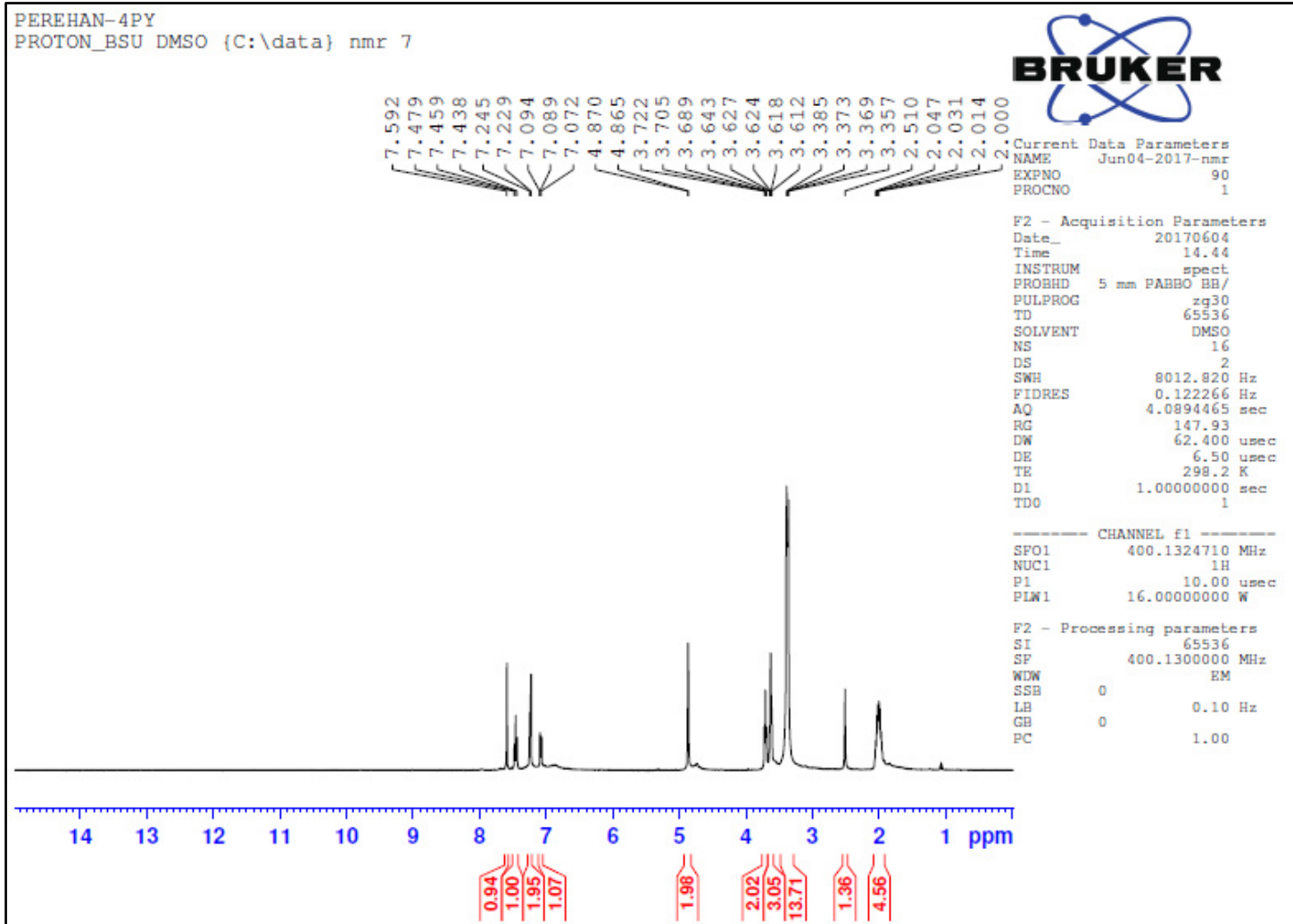
¹H-NMR Spectrum of compound 2f



¹³C-NMR Spectrum of compound 2f



¹H-NMR Spectrum of compound 4a



PEREHAN-4PY
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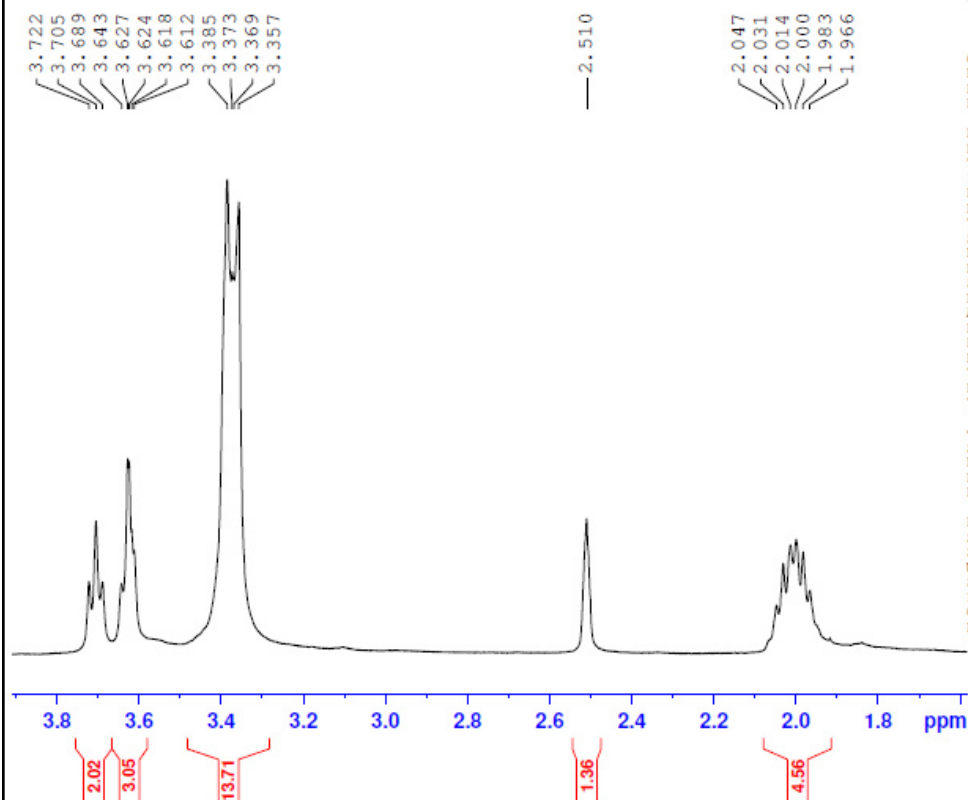


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PROCNO 1

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FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 147.93
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00



PEREHAN-4PY
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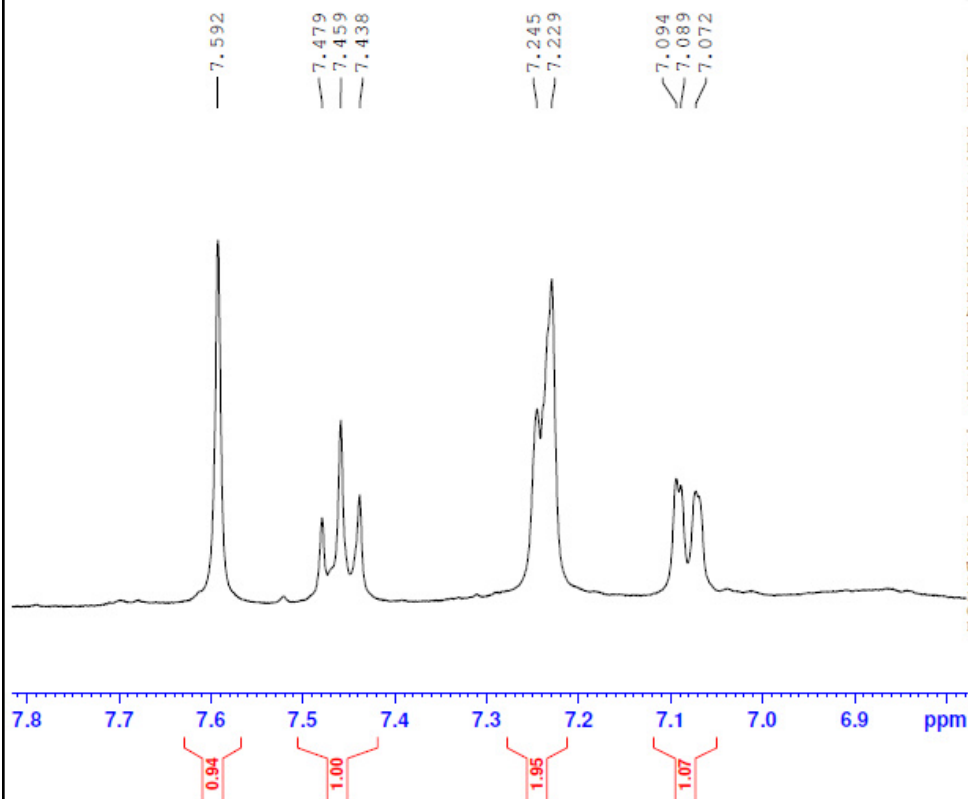


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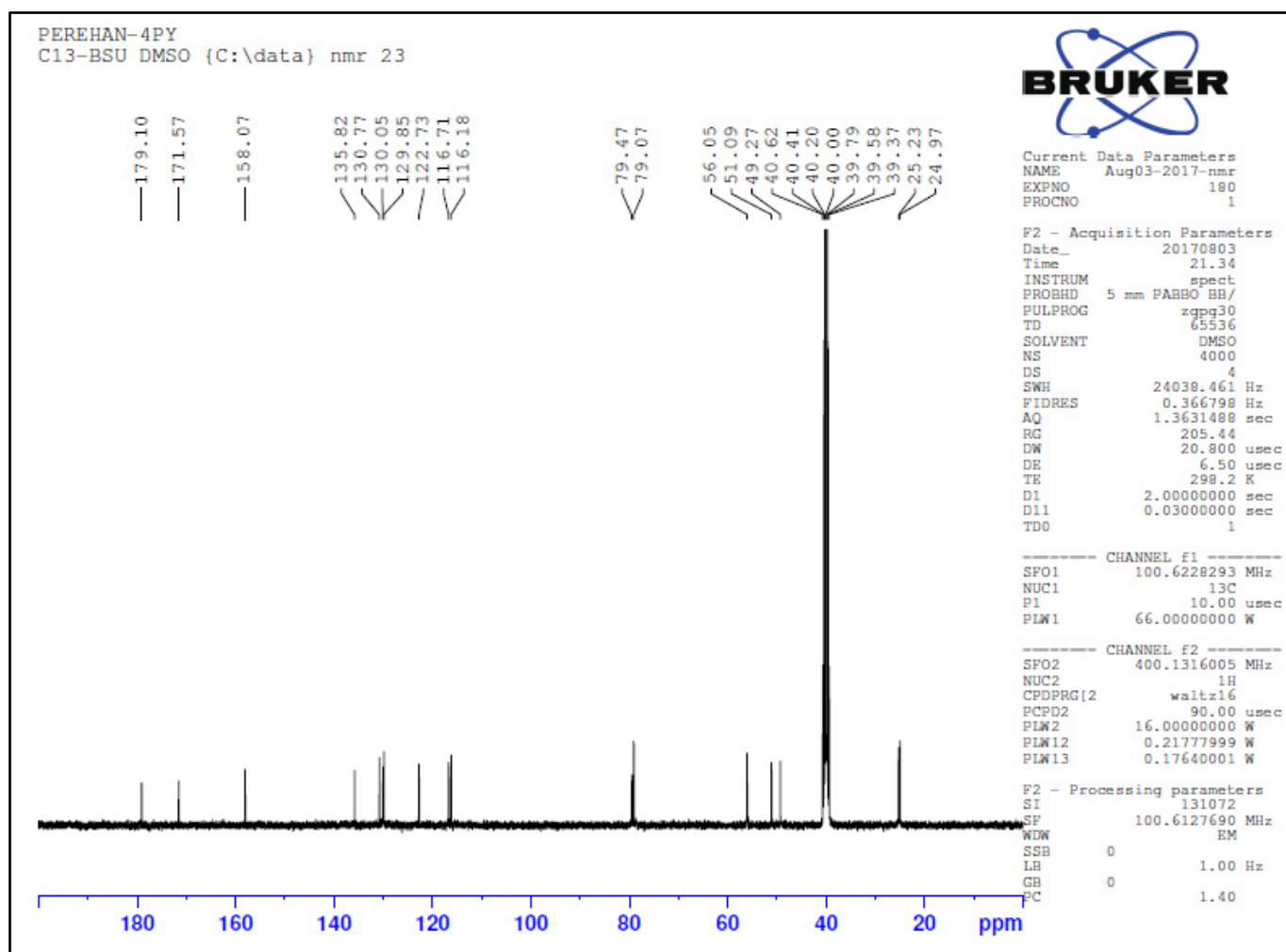
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PULPROG zg30
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SOLVENT DMSO
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DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 147.93
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

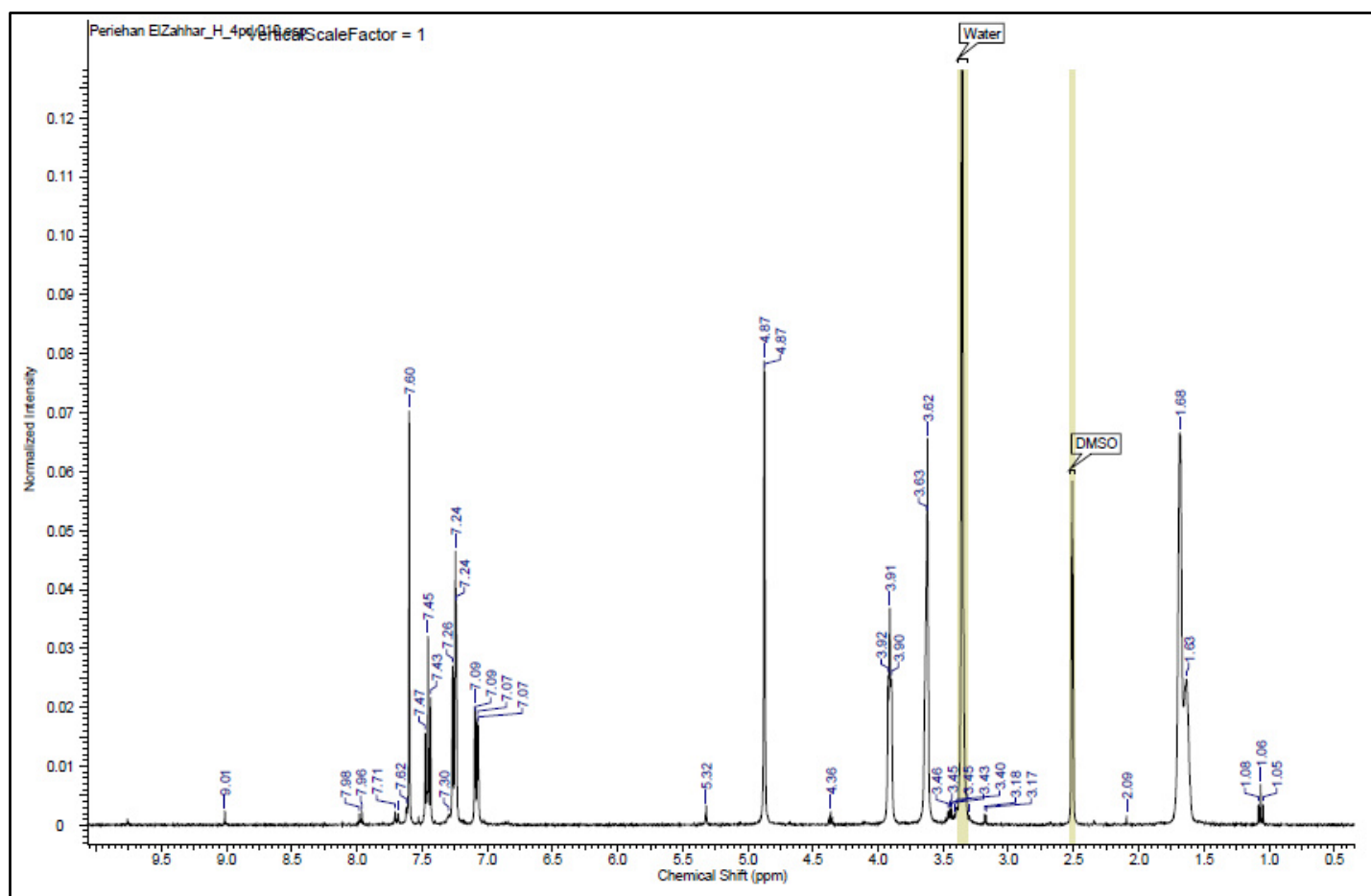
F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

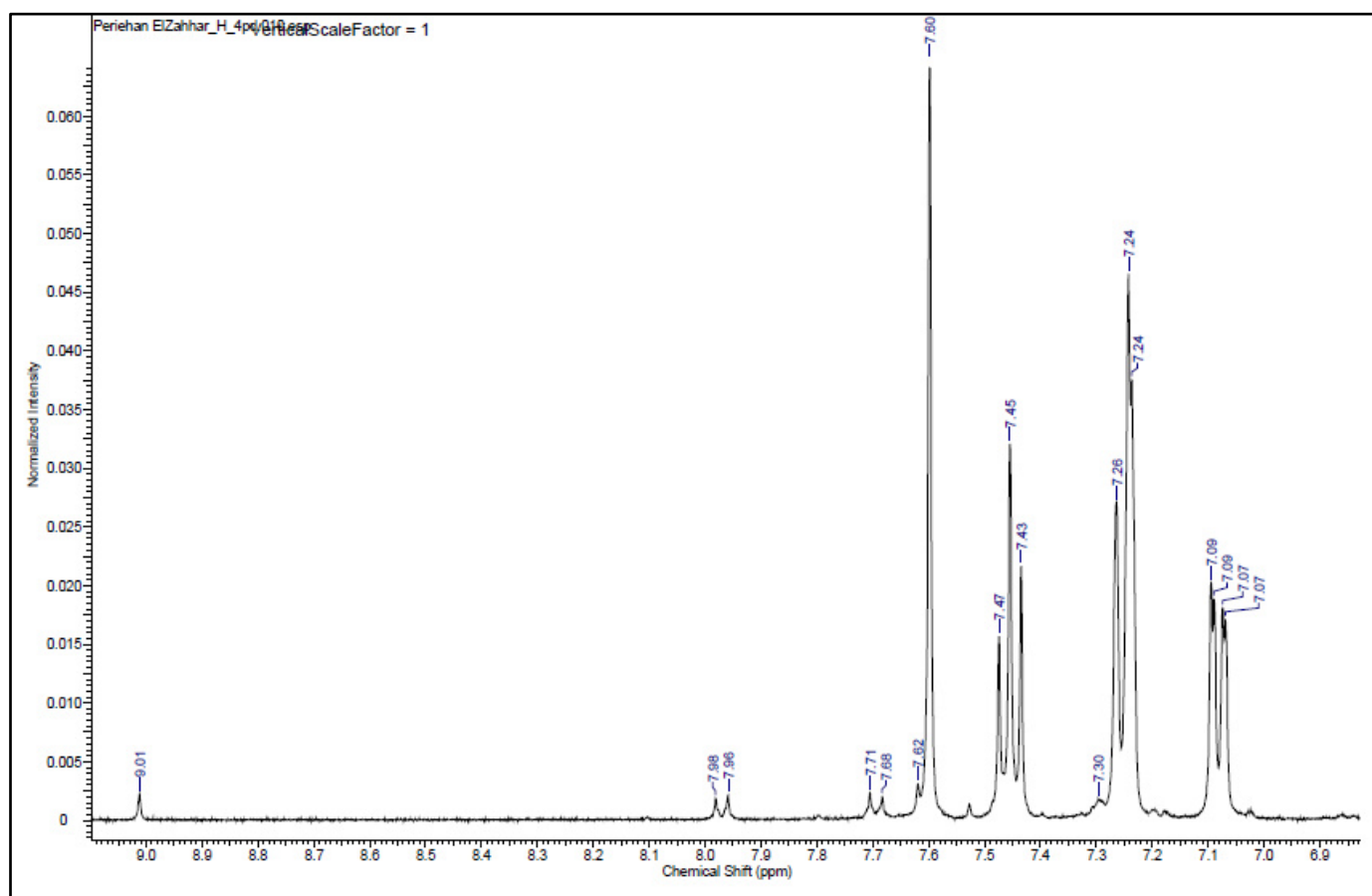
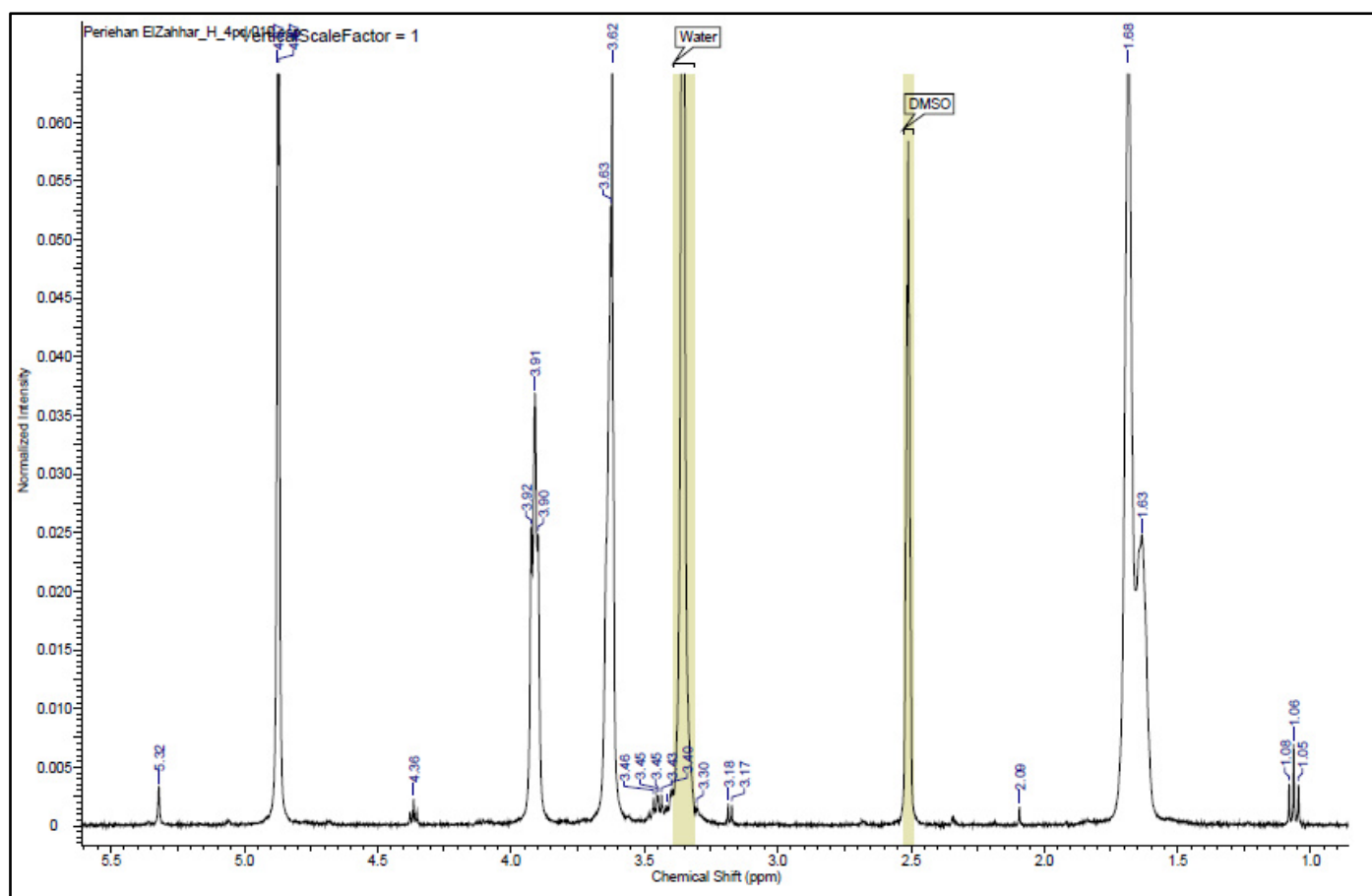


¹³C-NMR Spectrum of compound 4a

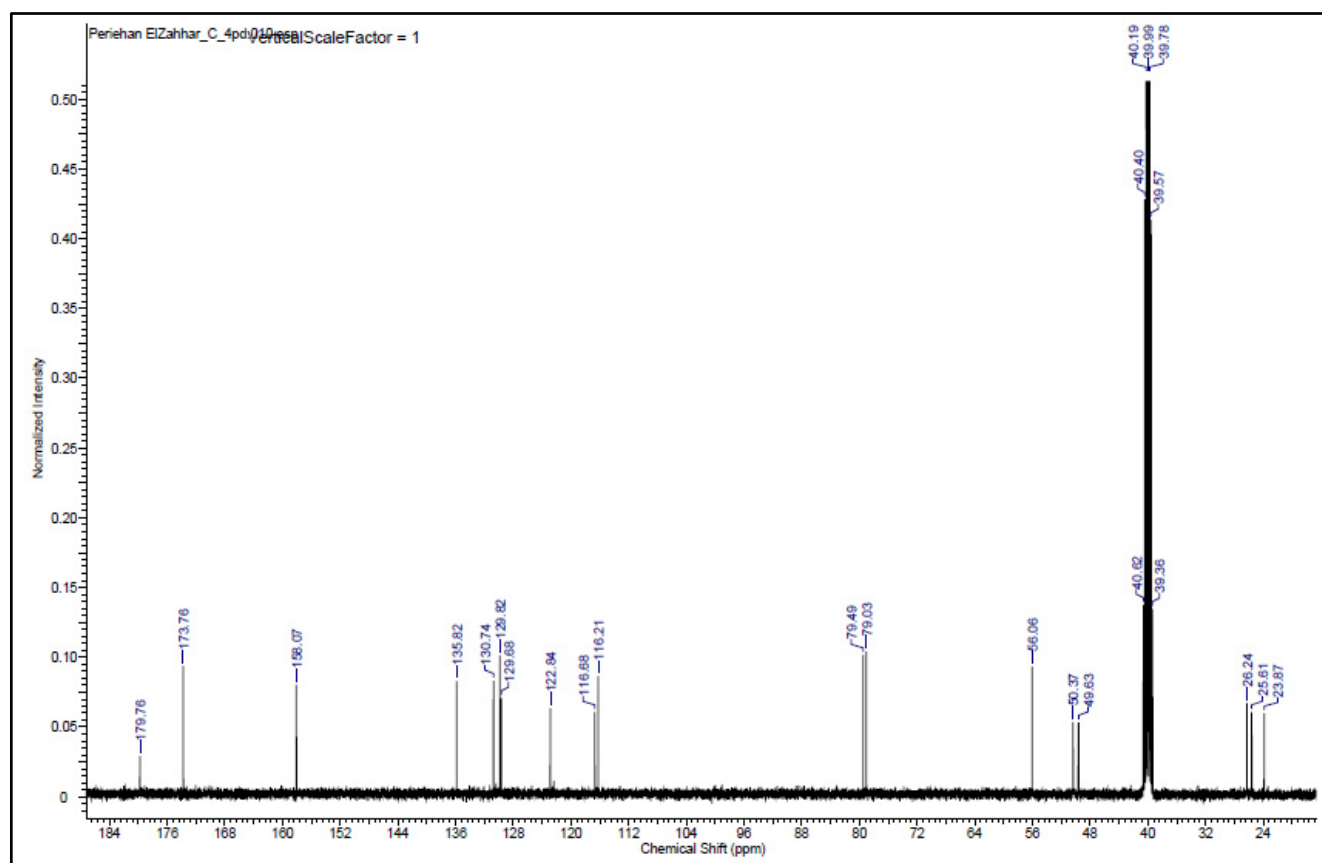


¹H-NMR Spectrum of compound 4b





¹³C-NMR Spectrum of compound 4b



¹H-NMR Spectrum of compound 4c

PEREHAN-4MP
PROTON_BSU DMSO {C:\data} nmr 1

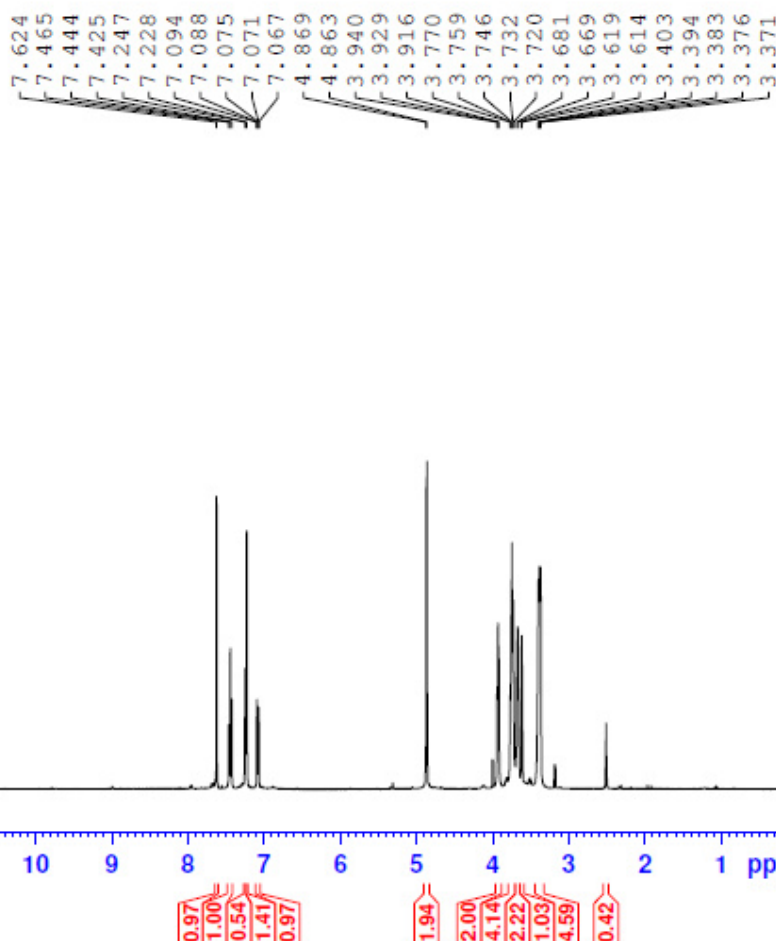


Current Data Parameters
NAME Jul30-2017-nmr
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170730
Time 14.08
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 91.28
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TDO 1

----- CHANNEL f1 -----
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00



PEREHAN-4MP
PROTON_BSU DMSO {C:\data} nmr 1

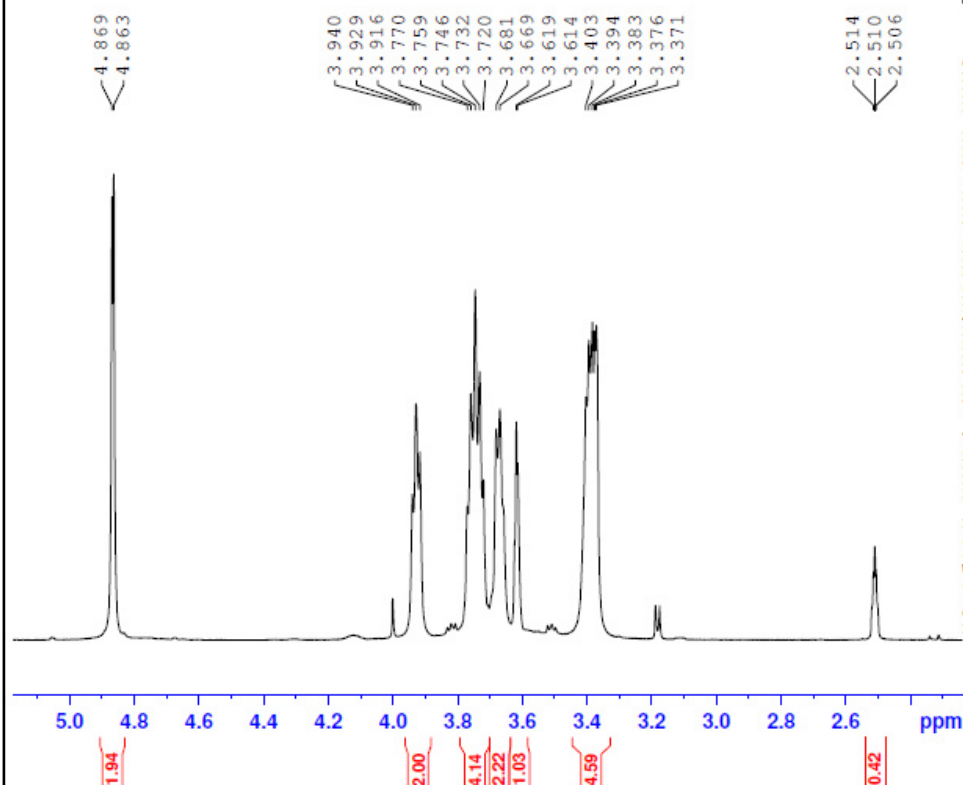


Current Data Parameters
NAME Jul30-2017-nmr
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170730
Time 14.08
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 91.28
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00



PEREHAN-4MP
PROTON_BSU DMSO {C:\data} nmr 1

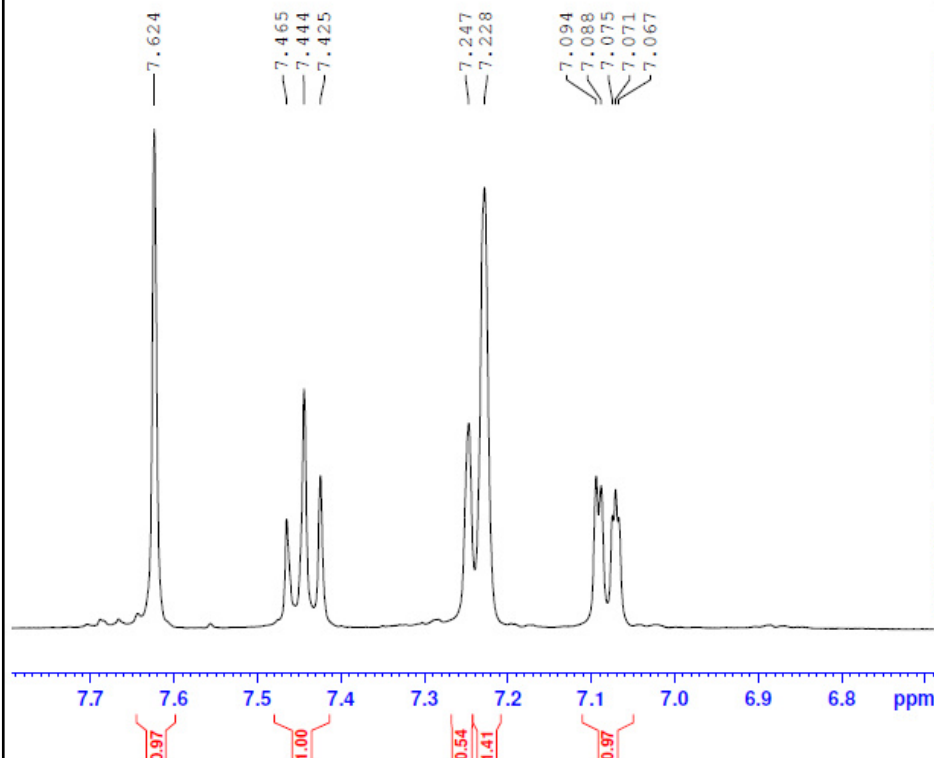


Current Data Parameters
NAME Jul30-2017-nmr
EXPNO 10
PROCNO 1

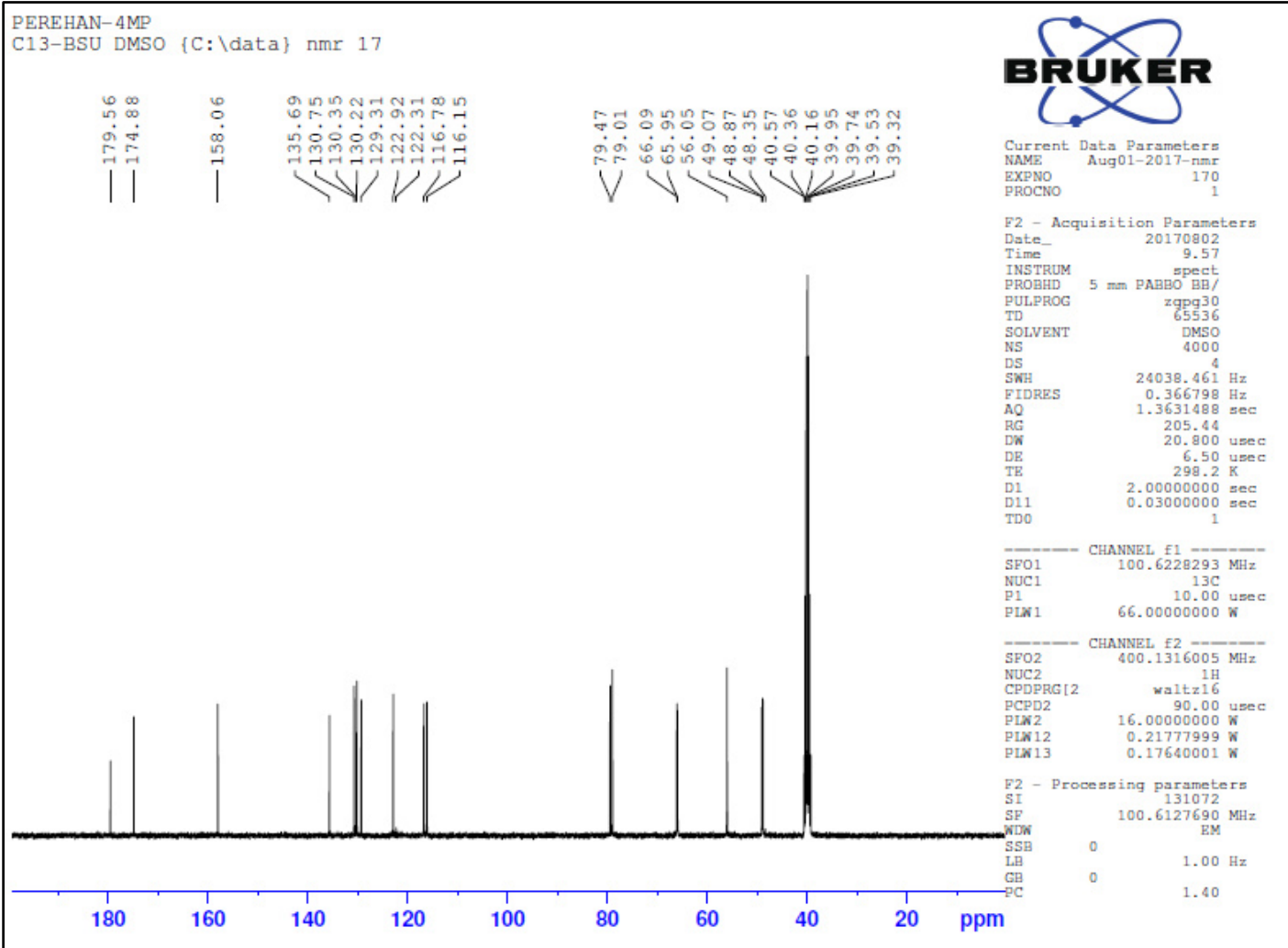
F2 - Acquisition Parameters
Date_ 20170730
Time 14.08
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 91.28
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

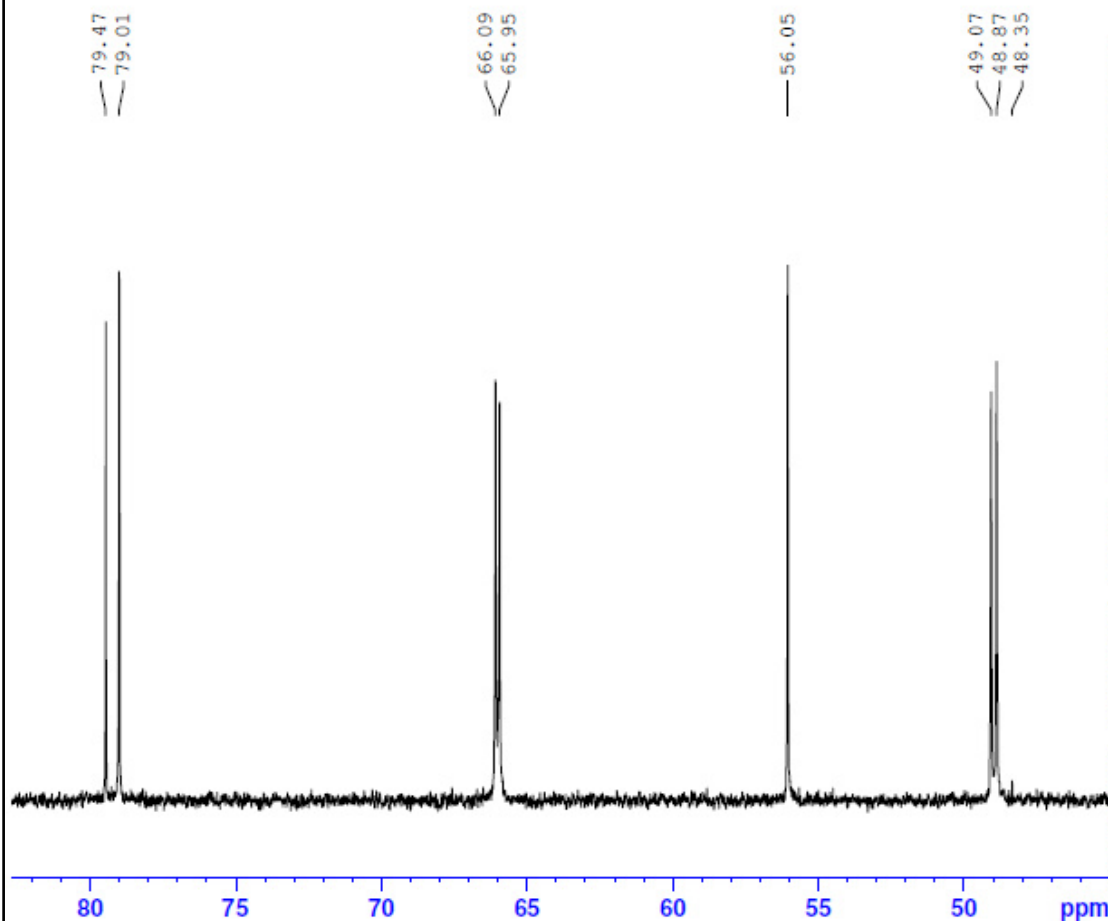
F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00



¹³C-NMR Spectrum of compound 4c



PEREHAN-4MP
C13-BSU DMSO {C:\data} nmr 17



Current Data Parameters
NAME Aug01-2017-nmr
EXPNO 170
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170802
Time 9.57
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

CHANNEL f1
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
PLW1 66.00000000 W

CHANNEL f2
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21777999 W
PLW13 0.17640001 W

F2 - Processing parameters
SI 131072
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

¹H-NMR Spectrum of compound 4d

PEREHAN-3PY
PROTON_BSU DMSO {C:\data} nmr 10

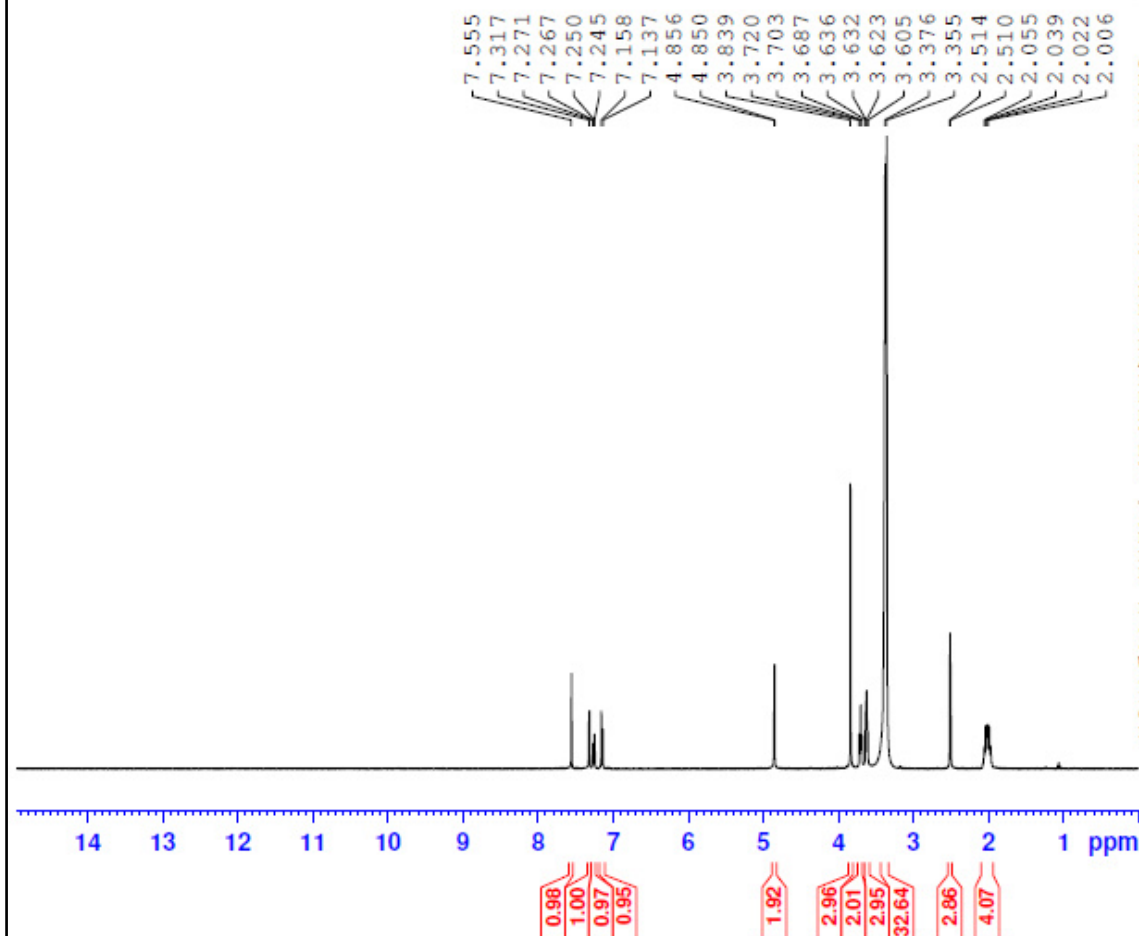


Current Data Parameters
NAME Jun04-2017-nmr
EXPNO 120
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170604
Time 15.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 147.93
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00



PEREHAN-3PY
PROTON_BSU DMSO {C:\data} nmr 10

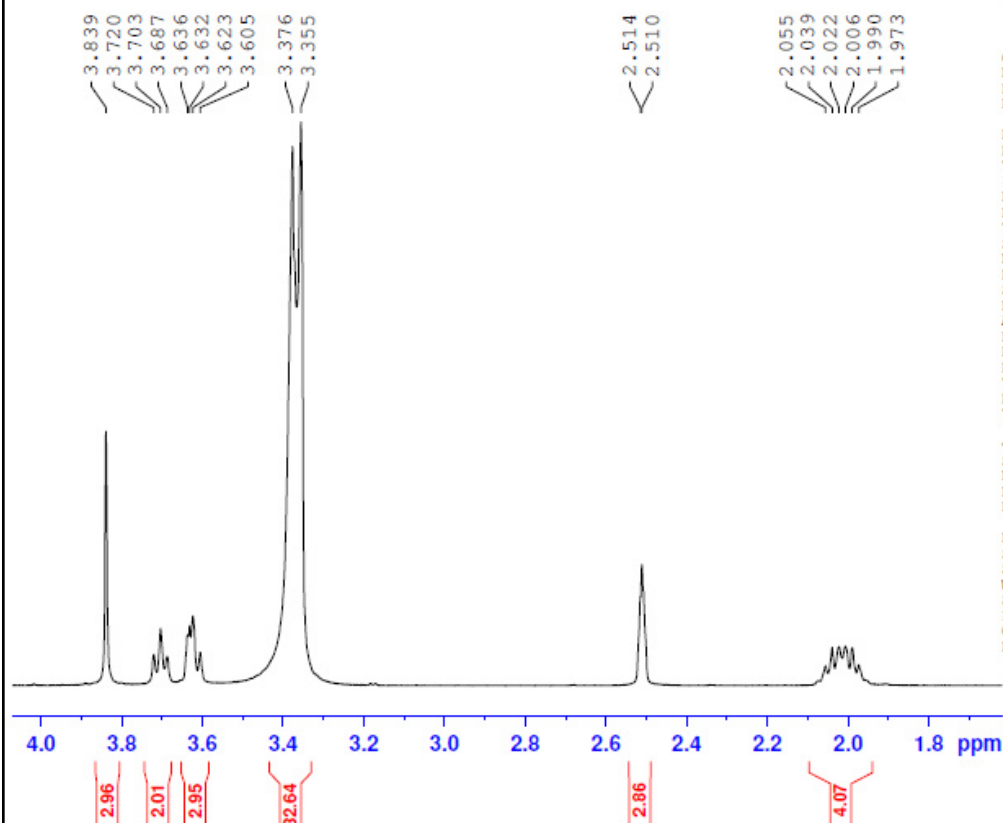


Current Data Parameters
NAME Jun04-2017-nmr
EXPNO 120
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170604
Time 15.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 147.93
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00



PEREHAN-3PY
PROTON_BSU DMSO {C:\data} nmr 10

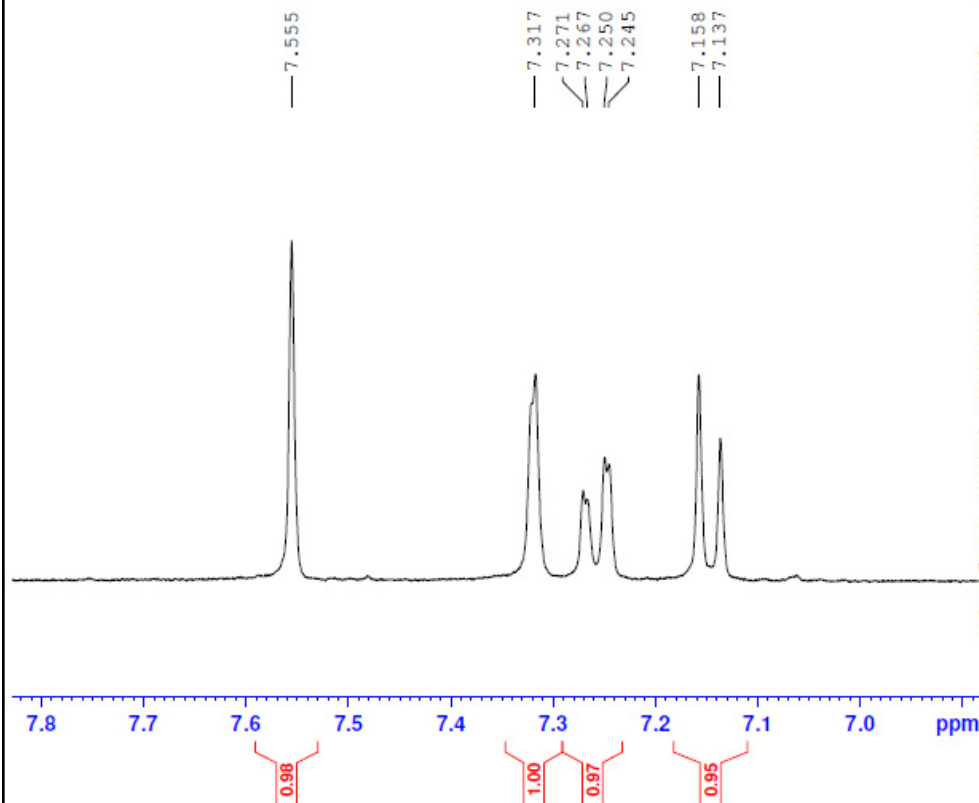


Current Data Parameters
NAME Jun04-2017-nmr
EXPNO 120
PROCNO 1

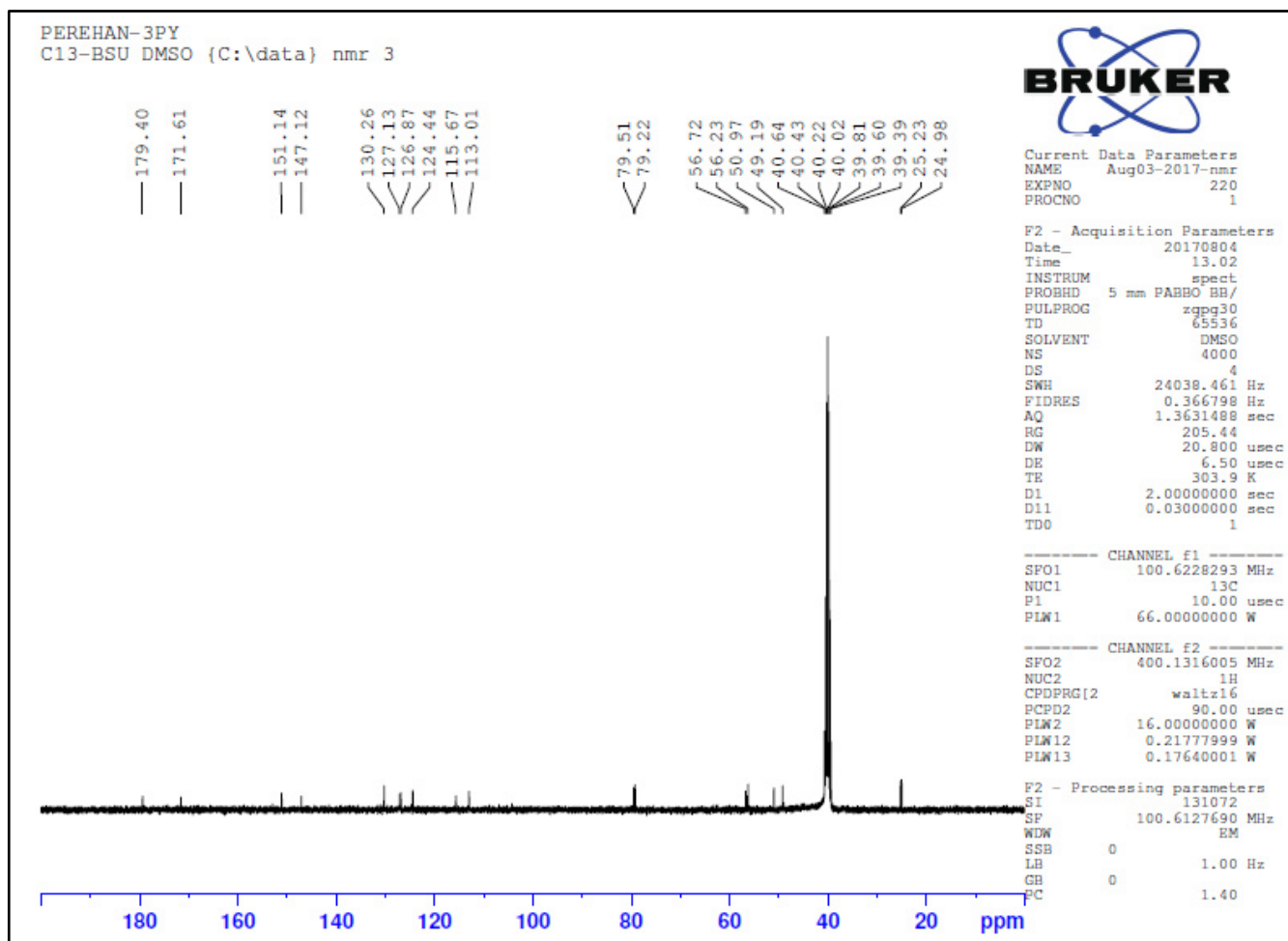
F2 - Acquisition Parameters
Date_ 20170604
Time 15.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 147.93
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

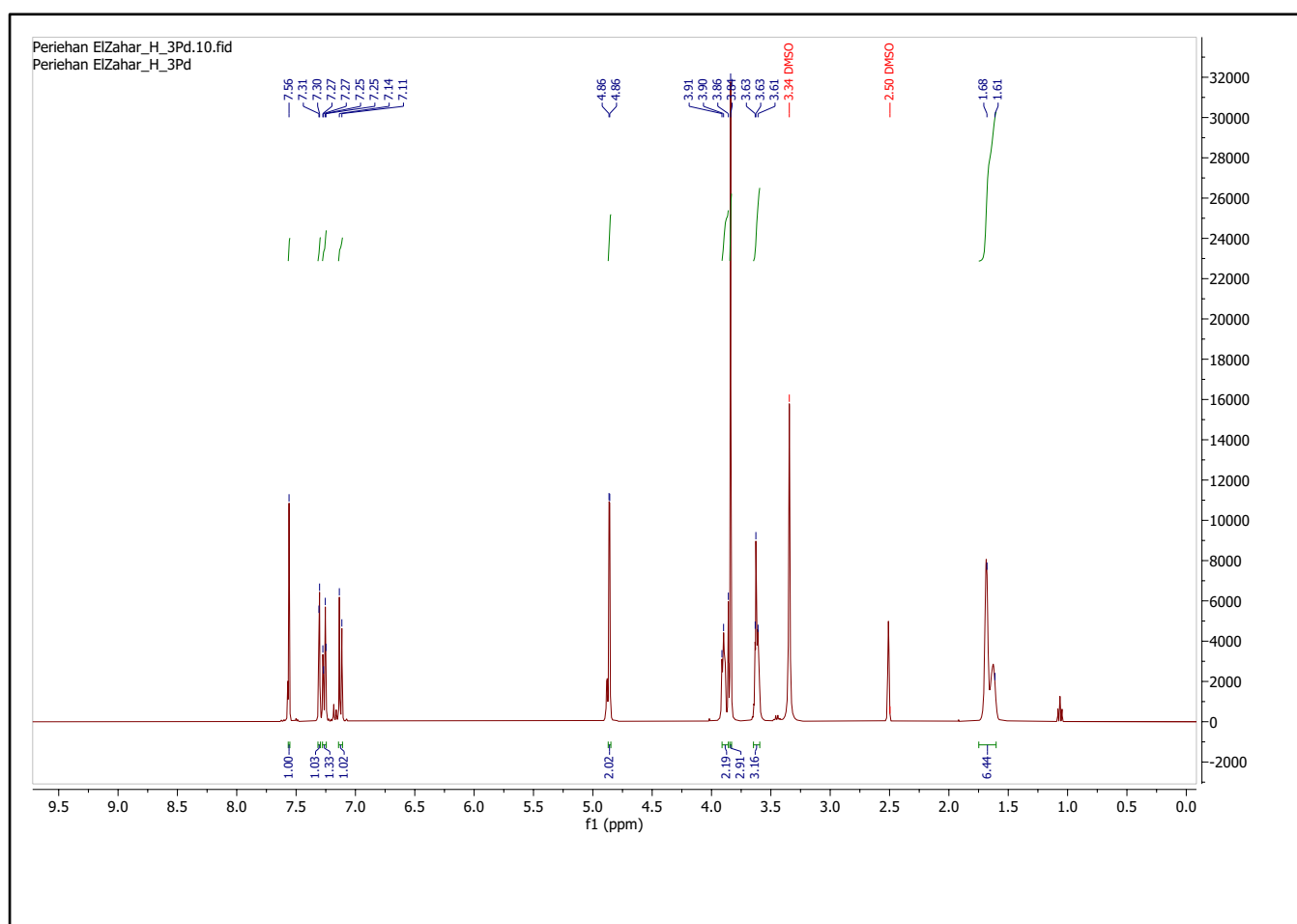
F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00



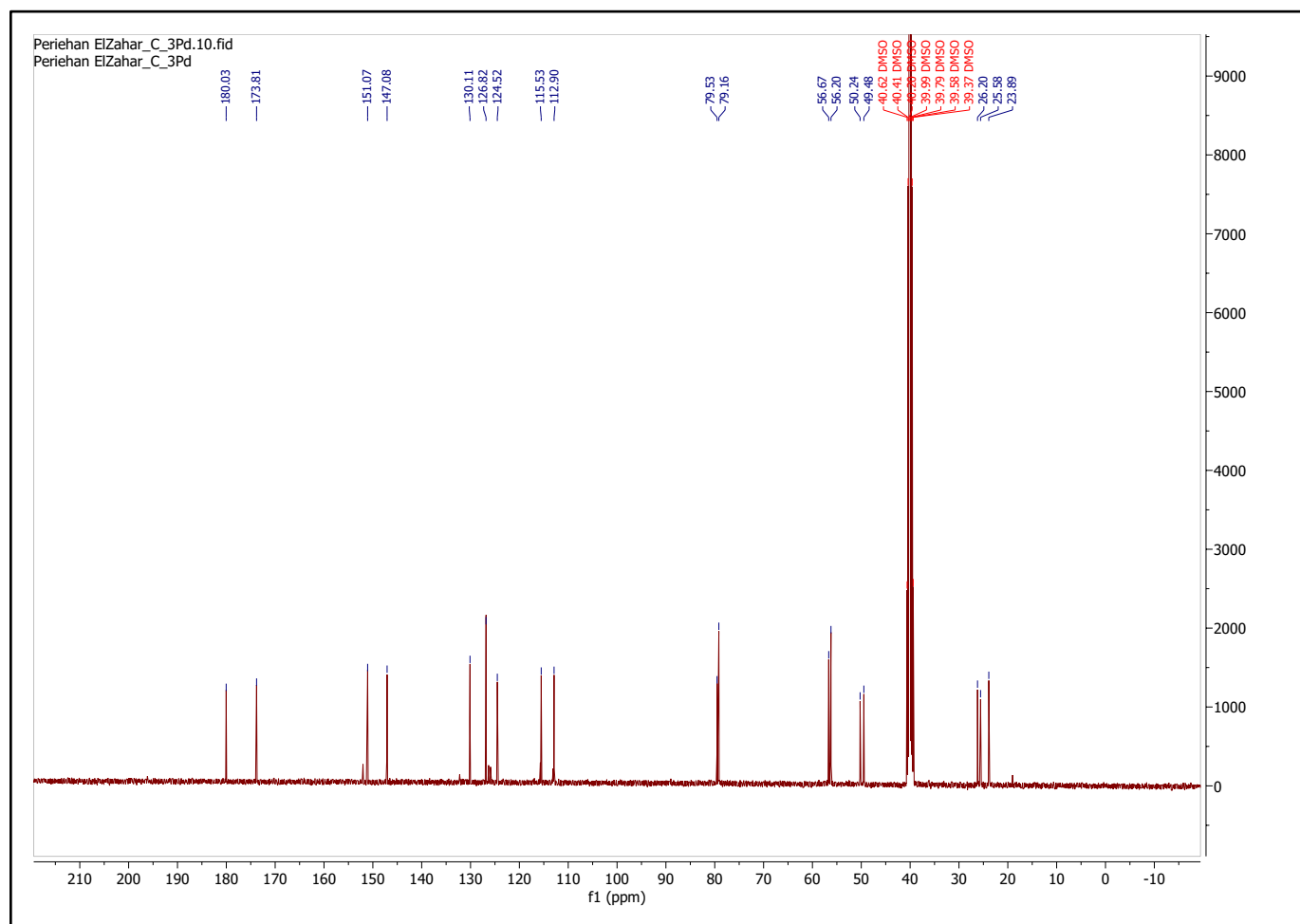
¹³C-NMR Spectrum of compound 4d



¹H-NMR Spectrum of compound 4e



¹³C-NMR Spectrum of compound 4e



¹H-NMR Spectrum of compound 4f

PEREHAN-3MP

PROTON_BSU DMSO {C:\data} nmr 5

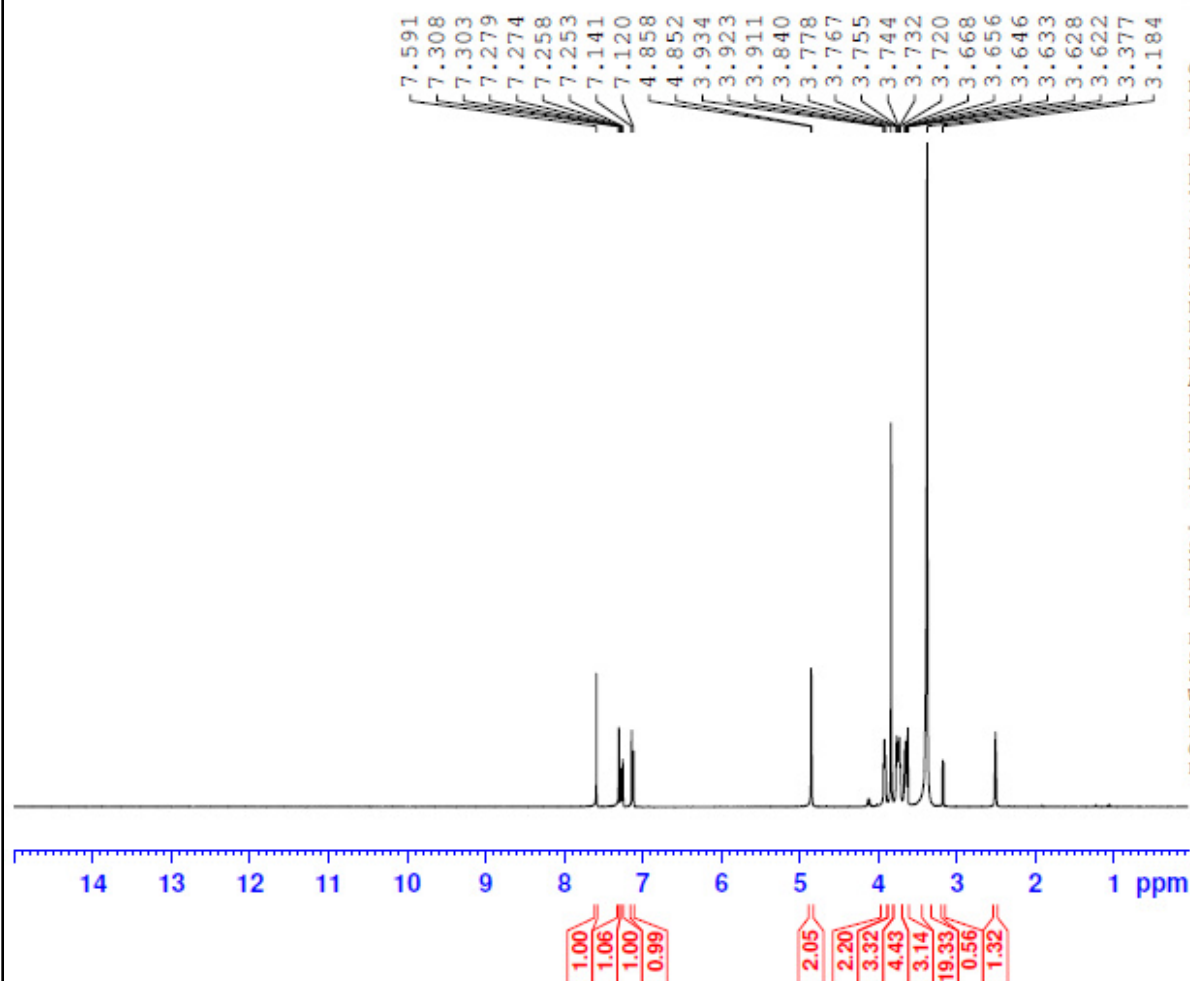


Current Data Parameters
NAME Jul30-2017-nmr
EXPNO 50
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170730
Time 14.28
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 147.93
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TDO 1

CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00



PEREHAN-3MP
PROTON_BSU DMSO {C:\data} nmr 5

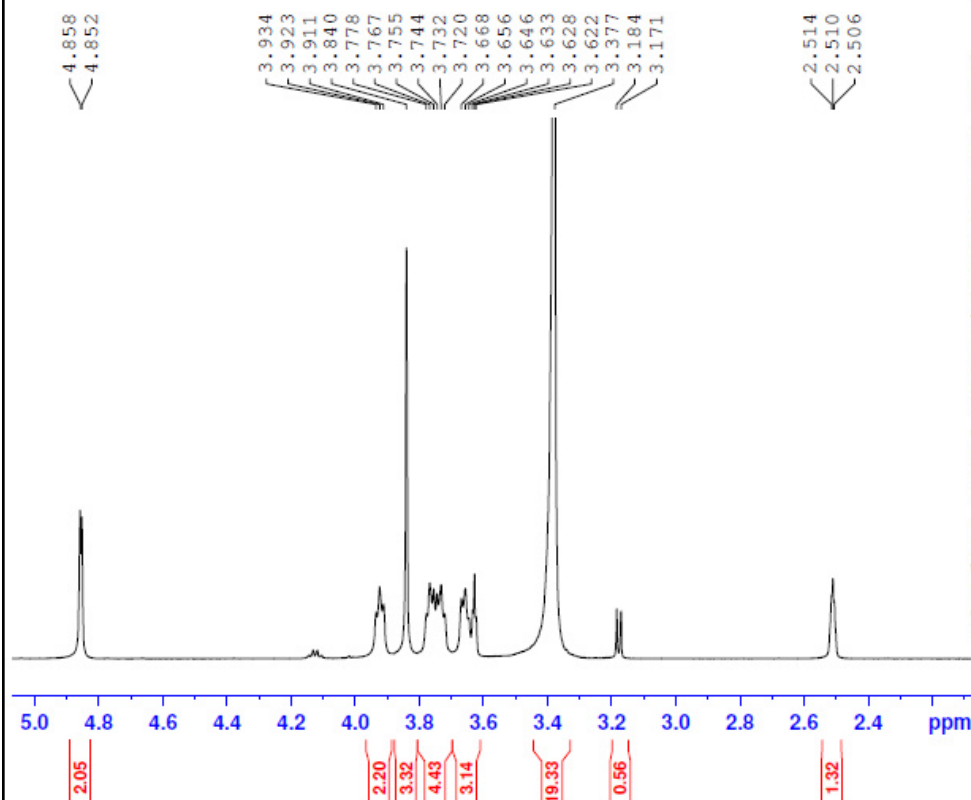


Current Data Parameters
NAME Jul30-2017-nmr
EXPNO 50
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170730
Time 14.28
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 147.93
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00



PEREHAN-3MP
PROTON_BSU DMSO {C:\data} nmr 5

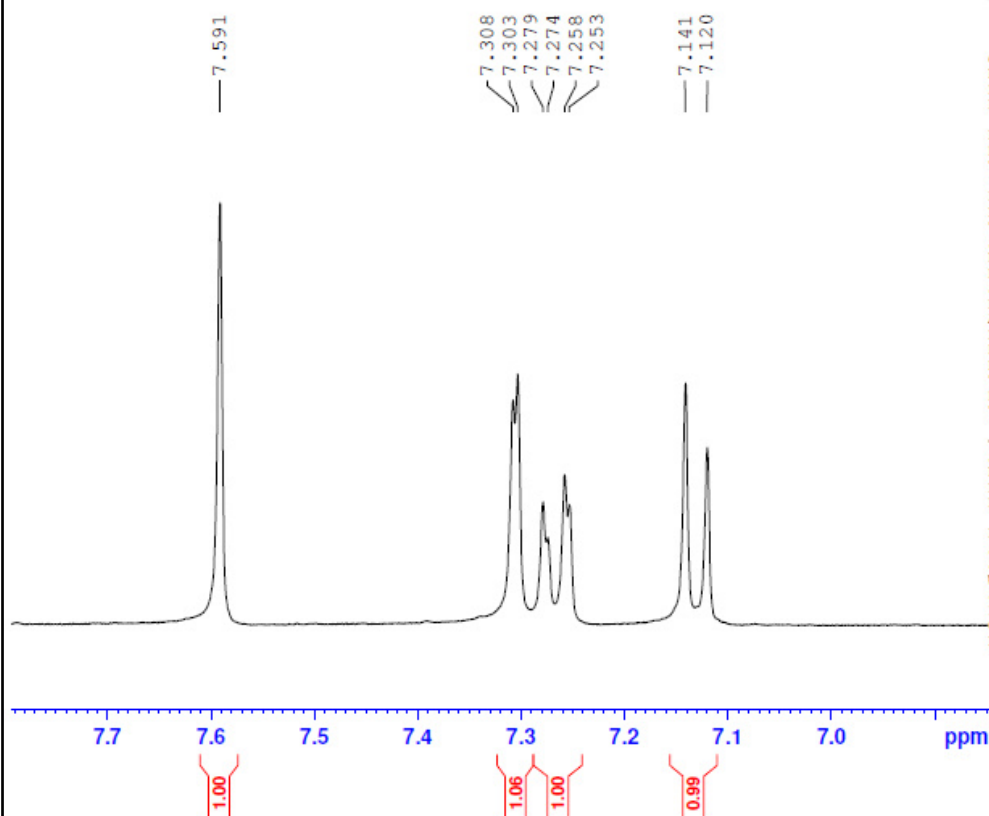


Current Data Parameters
NAME Jul30-2017-nmr
EXPNO 50
PROCNO 1

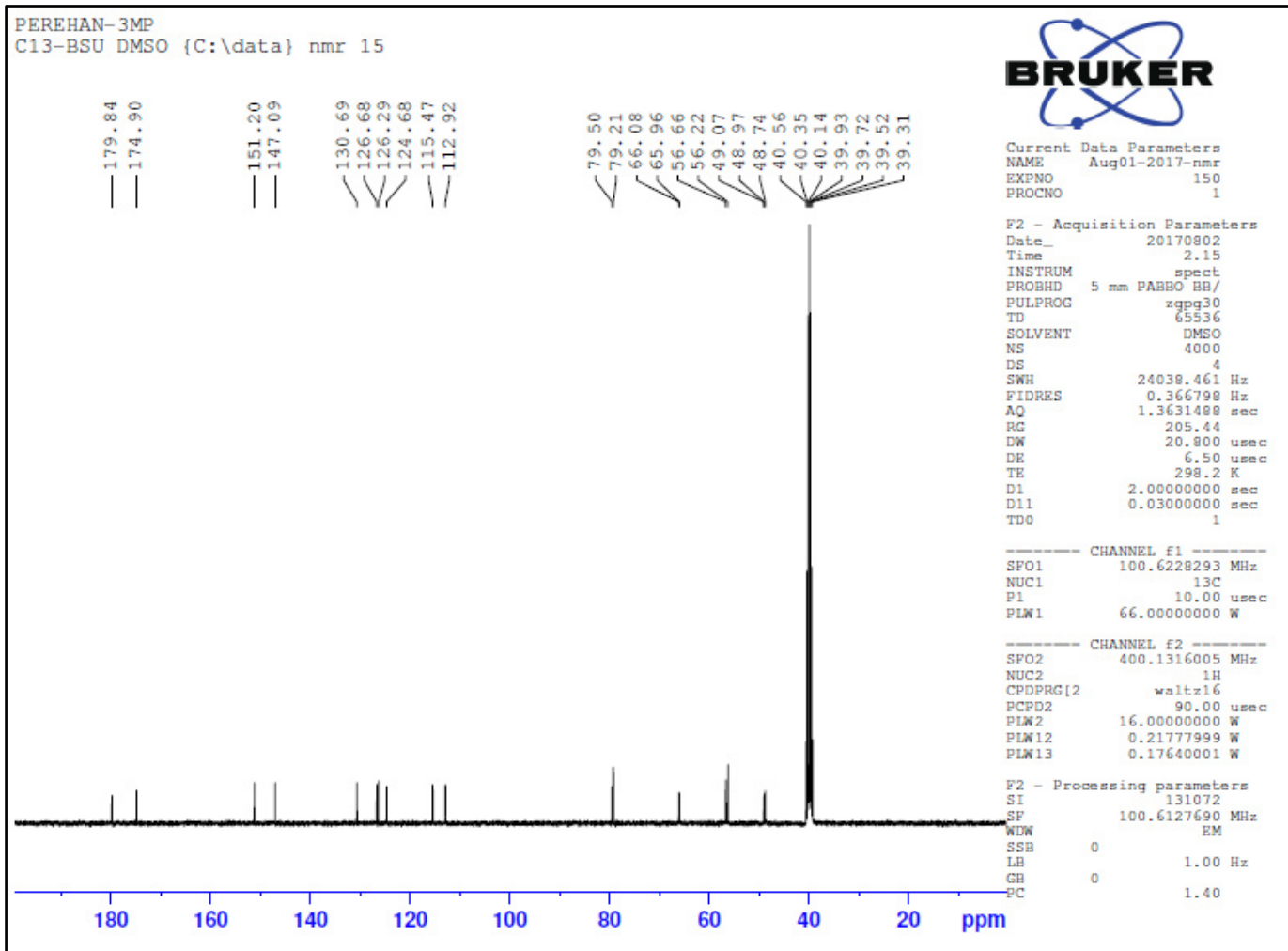
F2 - Acquisition Parameters
Date_ 20170730
Time 14.28
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 147.93
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00



¹³C-NMR Spectrum of compound 4f



PEREHAN-3MP
C13-BSU DMSO {C:\data} nmr 15



Current Data Parameters
NAME Aug01-2017-nmr
EXPNO 150
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170802
Time 2.15
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
PLW1 66.00000000 W

----- CHANNEL f2 -----
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21777999 W
PLW13 0.17640001 W

F2 - Processing parameters
SI 131072
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

