

SUPPLEMENTAL SECTION

Does ortho substitution enhance cytotoxic potencies in a series of 3,5-bis(benzylidene)-4-piperidones?

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Contents:

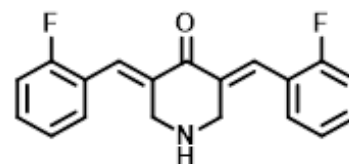
¹ H NMR spectra of the compounds 1a-1n	2 - 15
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128C

3,5-bis(2-Fluorobenzylidene)-4-piperidone (1a)

7.491
7.474
7.458
7.355
7.332
7.316
7.299

— 3.917
— 3.352
— 2.879
— 2.511

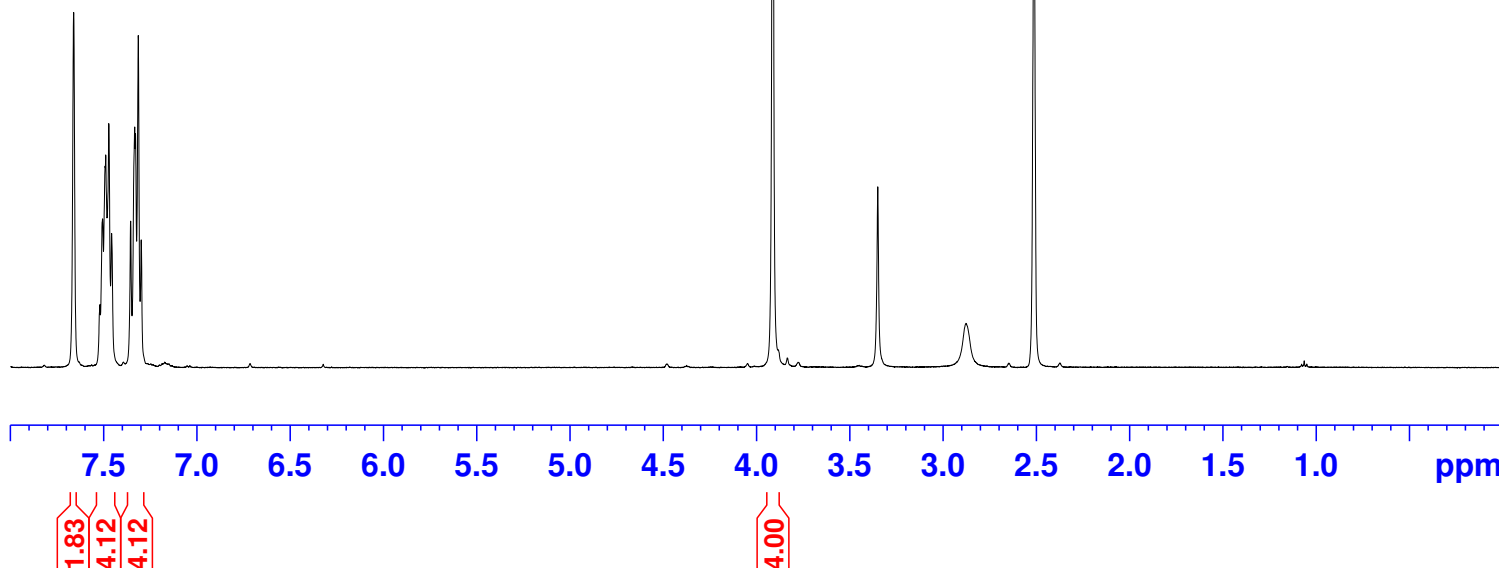


Current Data Parameters
NAME SK-01-128C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
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Time 3.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 203.2
DW 48.400 usec
DE 6.00 usec
TE 0 K
D1 1.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec

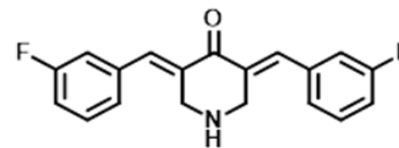
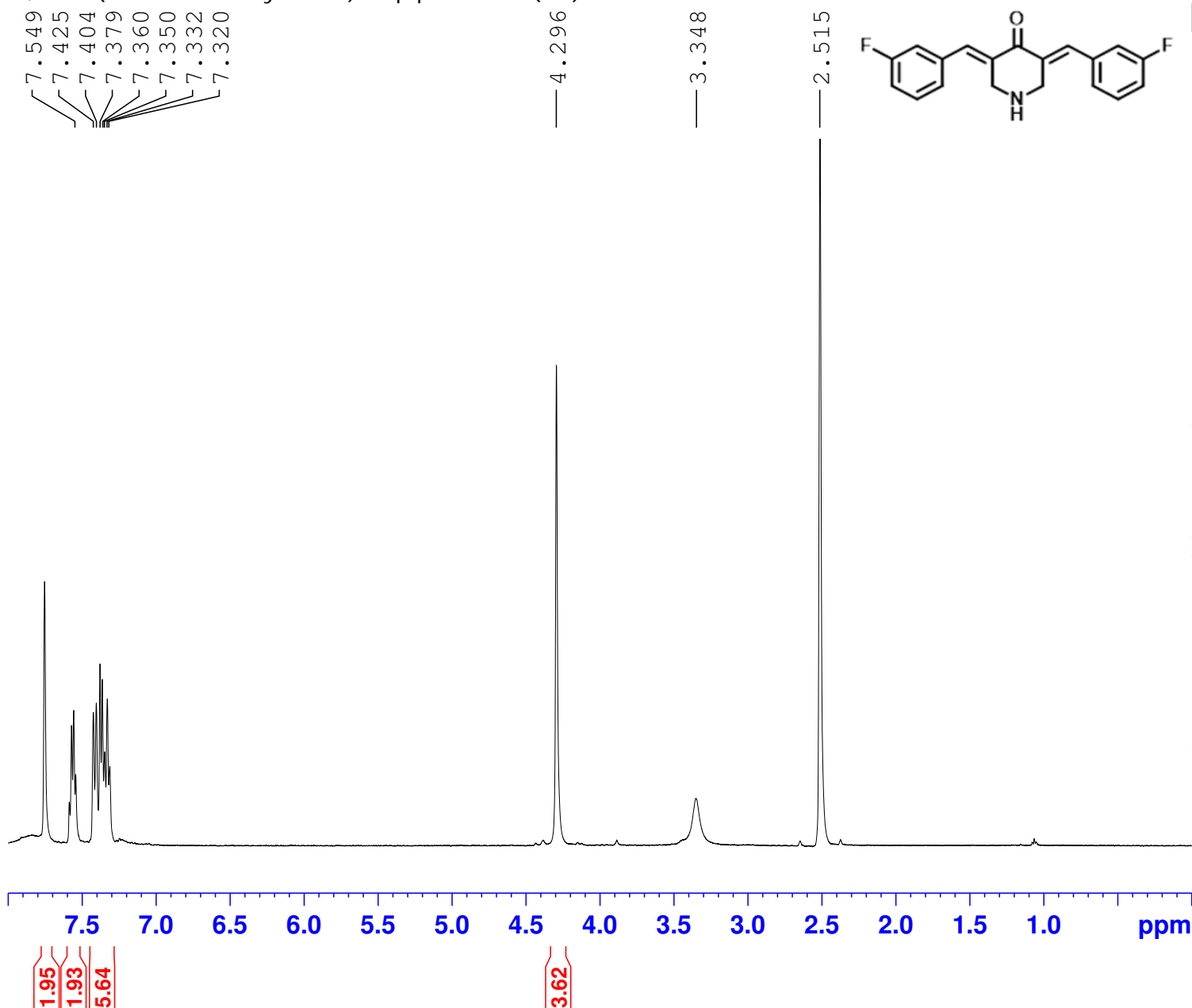
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P1 12.00 usec
PL1 -2.00 dB
SFO1 500.2830894 MHz

F2 - Processing parameters
SI 32768
SF 500.2800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



128B

3,5-bis(3-Fluorobenzylidene)-4-piperidone (1b)



Current Data Parameters
NAME SK-01-128B
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20071228
Time 21.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 228.1
DW 48.400 usec
DE 6.00 usec
TE 0 K
D1 1.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 12.00 usec
PL1 -2.00 dB
SFO1 500.2830894 MHz

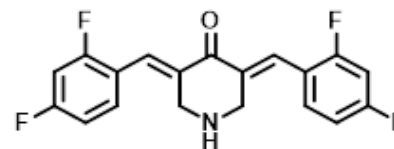
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SI 32768
SF 500.2800000 MHz
WDW EM
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LB 0.30 Hz
GB 0
PC 1.00

131C

3,5-bis(2,4-Difluorobenzylidene)-4-piperidone (1c)

7.528
7.514
7.437
7.418
7.397
7.232
7.213
7.199

— 3.896
— 3.352
— 3.036
— 2.513

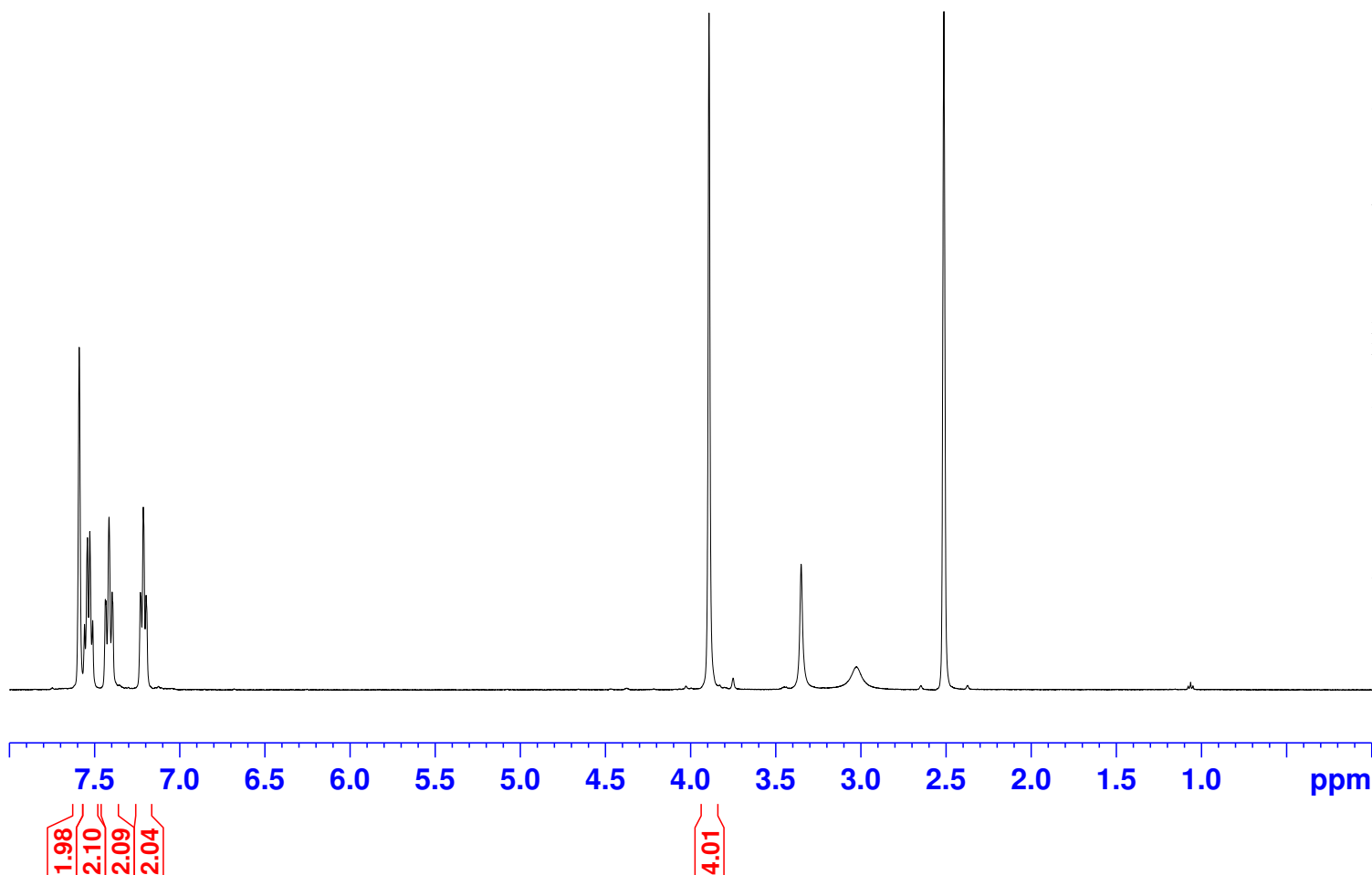


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EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080104
Time 22.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 203.2
DW 48.400 usec
DE 6.00 usec
TE 0 K
D1 1.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec

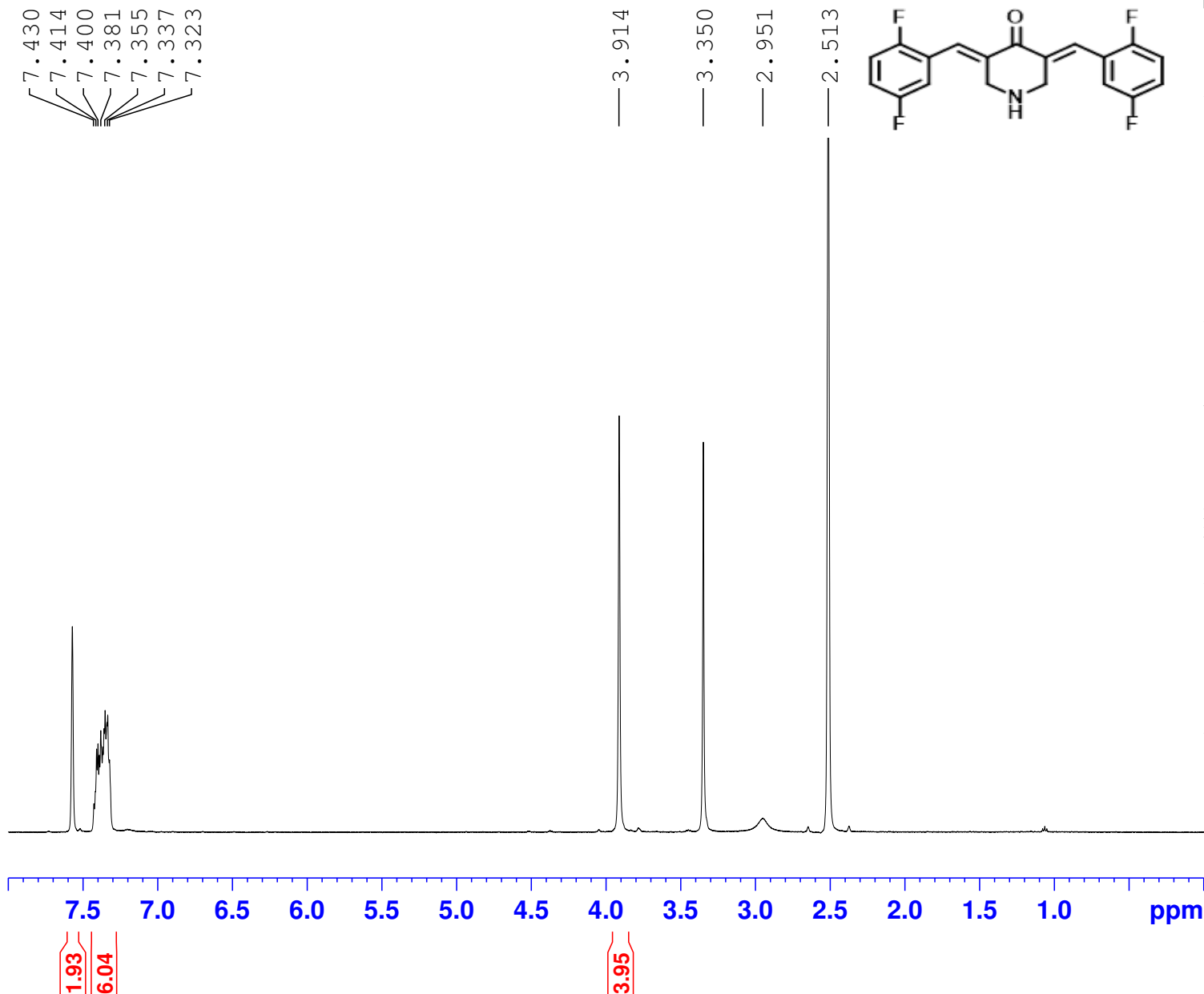
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NUC1 1H
P1 12.00 usec
PL1 -2.00 dB
SFO1 500.2830894 MHz

F2 - Processing parameters
SI 32768
SF 500.2800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



132C

3,5-bis(2,5-Difluorobenzylidene)-4-piperidone (1d)



Current Data Parameters
 NAME SK-01-132C
 EXPNO 1
 PROCNO 1

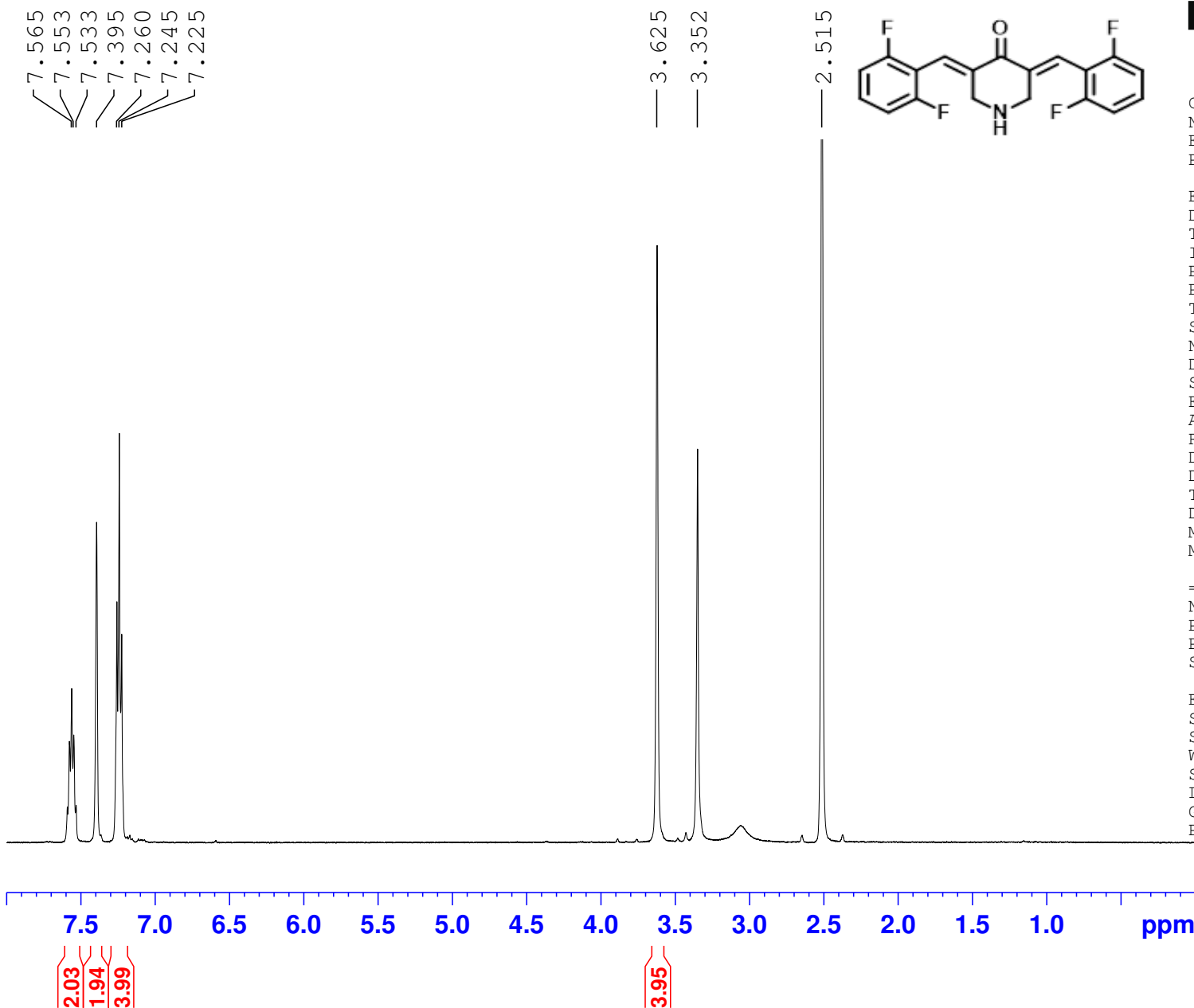
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 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719425 sec
 RG 228.1
 DW 48.400 usec
 DE 6.00 usec
 TE 0 K
 D1 1.00000000 sec
 MCREST 0 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 12.00 usec
 PL1 -2.00 dB
 SFO1 500.2830894 MHz

F2 - Processing parameters
 SI 32768
 SF 500.2800000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

131A

3,5-bis(2,6-Difluorobenzylidene)-4-piperidone (1e)



Current Data Parameters
NAME SK-01-131A
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080103
Time 21.14
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 228.1
DW 48.400 usec
DE 6.00 usec
TE 0 K
D1 1.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 12.00 usec
PL1 -2.00 dB
SFO1 500.2830894 MHz

F2 - Processing parameters
SI 32768
SF 500.2800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

133B

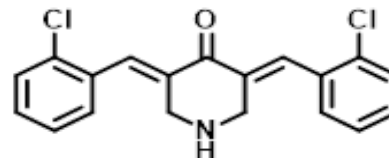
3,5-bis(2-Chlorobenzylidene)-4-piperidone (1f)

7.609
7.598
7.480
7.473
7.451

— 3.891

— 3.353

— 2.515

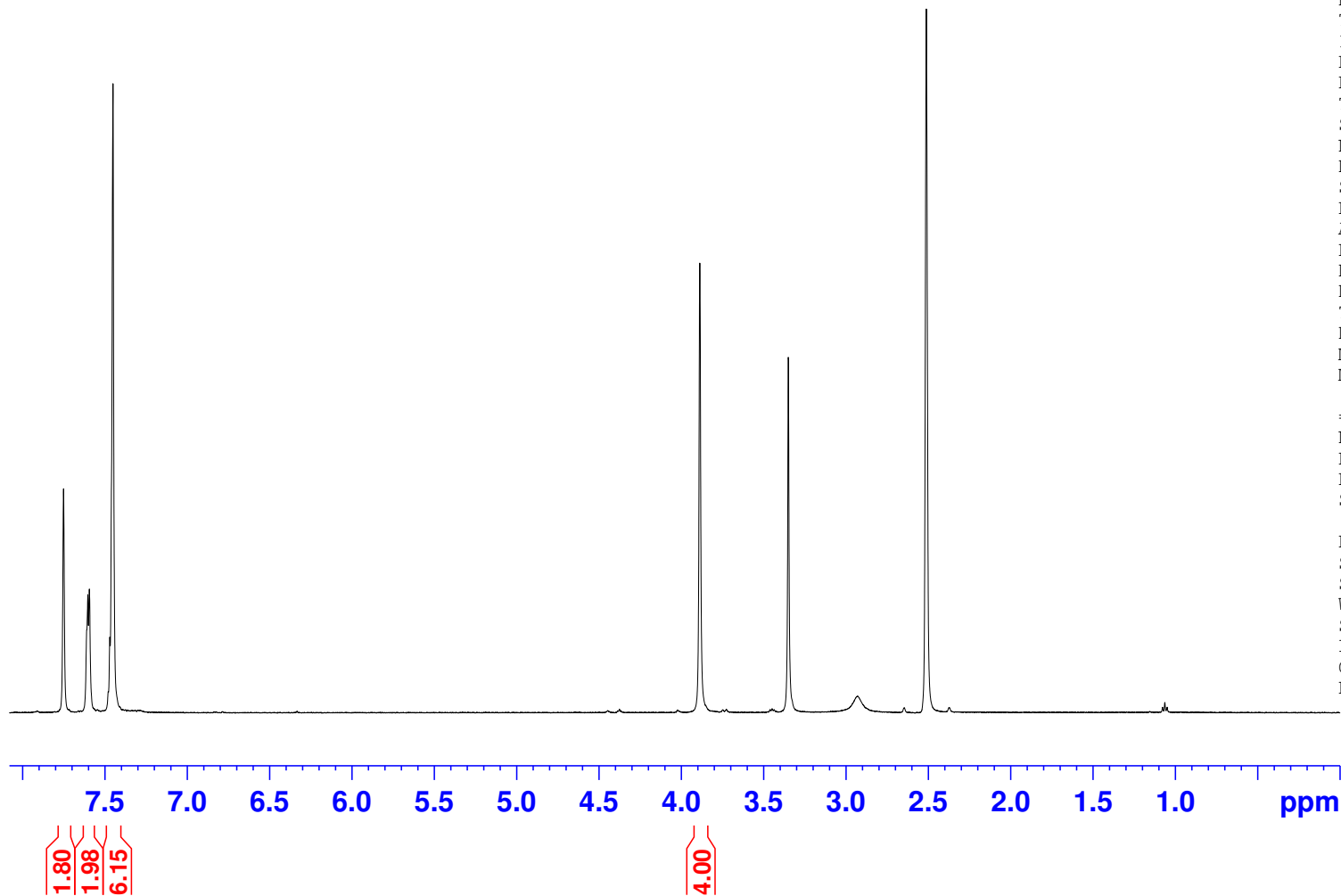


Current Data Parameters
NAME SK-01-133B
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080110
Time 22.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 228.1
DW 48.400 usec
DE 6.00 usec
TE 0 K
D1 1.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 12.00 usec
PL1 -2.00 dB
SFO1 500.2830894 MHz

F2 - Processing parameters
SI 32768
SF 500.2800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



132A

3,5-bis(2,4-Dichlorobenzylidene)-4-piperidone (1g)

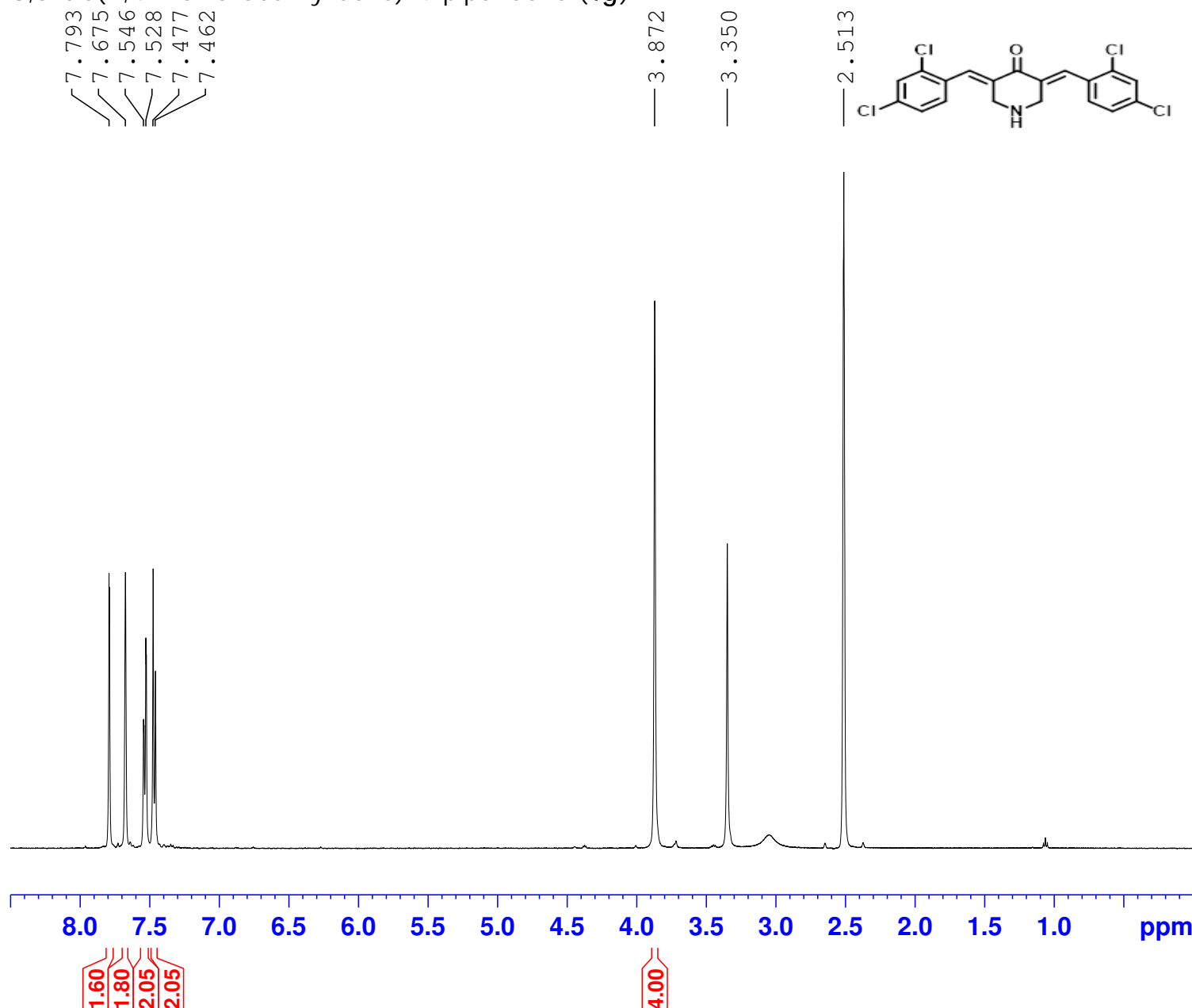


Current Data Parameters
 NAME SK-01-132A
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080103
 Time 21.21
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719425 sec
 RG 228.1
 DW 48.400 usec
 DE 6.00 usec
 TE 0 K
 D1 1.00000000 sec
 MCREST 0 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 12.00 usec
 PL1 -2.00 dB
 SFO1 500.2830894 MHz

F2 - Processing parameters
 SI 32768
 SF 500.2800000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



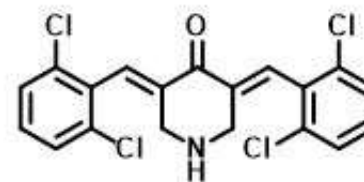
131B

3,5-bis(2,6-Dichlorobenzylidene)-4-piperidone (1h)

7.604
7.588
7.479
7.461
7.447

3.498
3.349

2.513

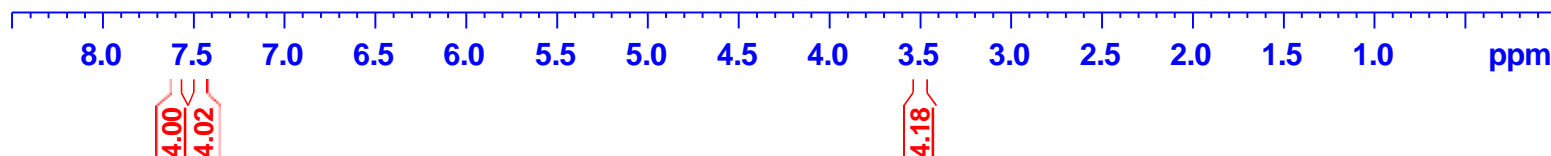


Current Data Parameters
NAME SK-01-131B_test
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080128
Time 10.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT D2O
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 203.2
DW 48.400 usec
DE 6.00 usec
TE 0 K
D1 1.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec

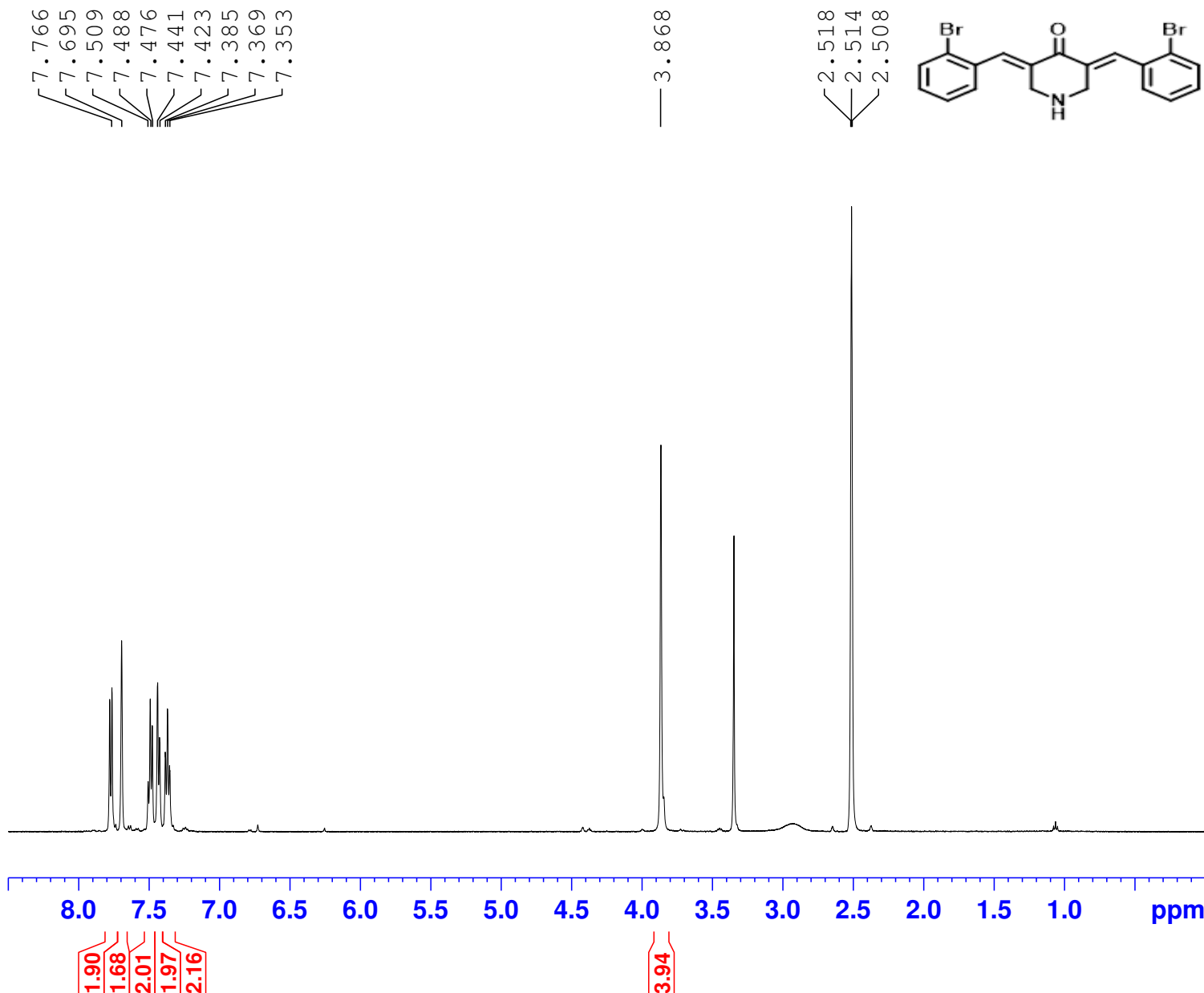
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NUC1 1H
P1 12.00 usec
PL1 -2.00 dB
SFO1 500.2830894 MHz

F2 - Processing parameters
SI 32768
SF 500.2800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



126A

3,5-bis(2-Bromobenzylidene)-4-piperidone (1i)



Current Data Parameters
 NAME SK-01-126A
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20071221
 Time 3.25
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719425 sec
 RG 228.1
 DW 48.400 usec
 DE 6.00 usec
 TE 0 K
 D1 1.00000000 sec
 MCREST 0 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 12.00 usec
 PL1 -2.00 dB
 SFO1 500.2830894 MHz

F2 - Processing parameters
 SI 32768
 SF 500.2800000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

132B

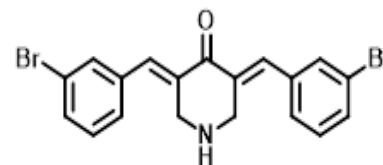
3,5-bis(3-Bromobenzylidene)-4-piperidone (1j)

7.565
7.509
7.493
7.456
7.439
7.427

3.996

3.348

2.511

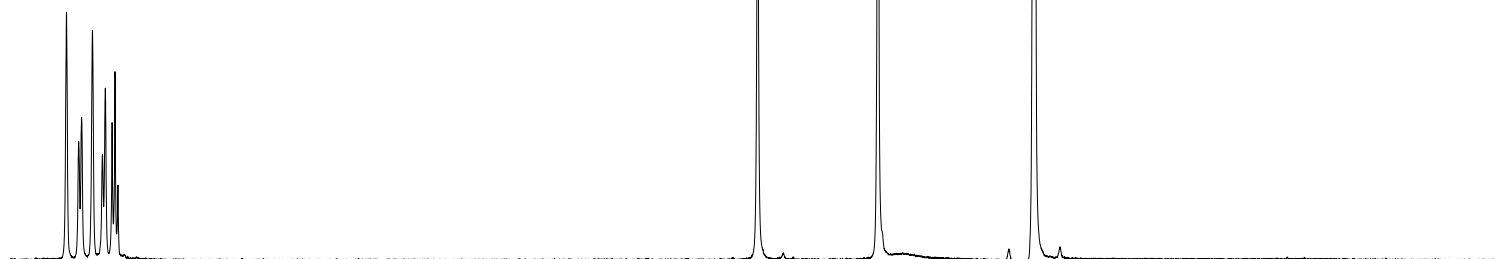


Current Data Parameters
NAME SK-01-132B
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080103
Time 21.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 228.1
DW 48.400 usec
DE 6.00 usec
TE 0 K
D1 1.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 12.00 usec
PL1 -2.00 dB
SFO1 500.2830894 MHz

F2 - Processing parameters
SI 32768
SF 500.2800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm

1.88
1.89
1.85
1.94
1.92

3.71

127B

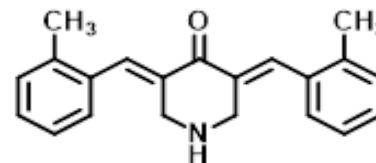
3,5-bis(2-Methylbenzylidene)-4-piperidone (1k)

7.758
7.311
7.290
7.281
7.266
7.241
7.224

3.851

3.348

2.515
2.329

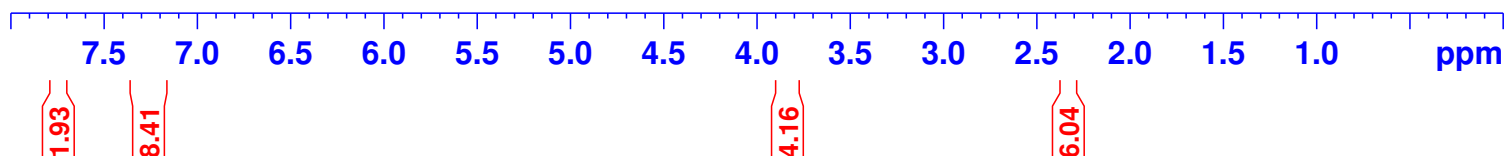


Current Data Parameters
NAME SK-01-127B
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20071221
Time 3.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 203.2
DW 48.400 usec
DE 6.00 usec
TE 0 K
D1 1.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec

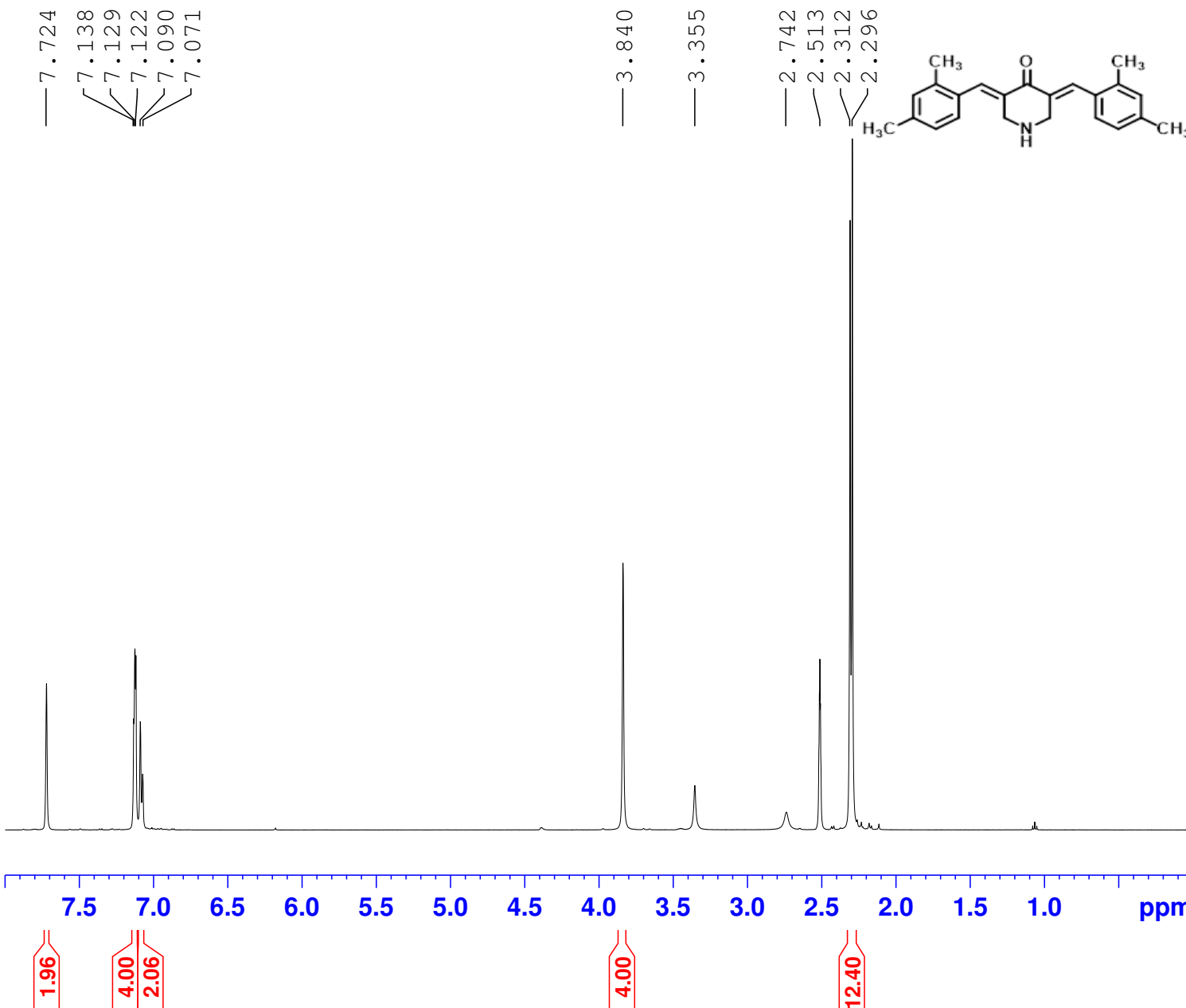
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NUC1 1H
P1 12.00 usec
PL1 -2.00 dB
SFO1 500.2830894 MHz

F2 - Processing parameters
SI 32768
SF 500.2800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



132D

3,5-bis(2,4-Dimethylbenzylidene)-4-piperidone (11)



Current Data Parameters
 NAME SK-01-132D
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080124
 Time 0.56
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719425 sec
 RG 143.7
 DW 48.400 usec
 DE 6.00 usec
 TE 0 K
 D1 1.00000000 sec
 MCREST 0 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
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 P1 12.00 usec
 PL1 -2.00 dB
 SFO1 500.2830894 MHz

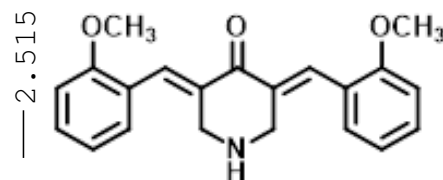
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 SF 500.2800000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

126B

3,5-bis(2-Methoxybenzylidene)-4-piperidone (1m)

7.794
7.427
7.413
7.399
7.274
7.257
7.110
7.092
7.040
7.024
7.006

3.884
3.858

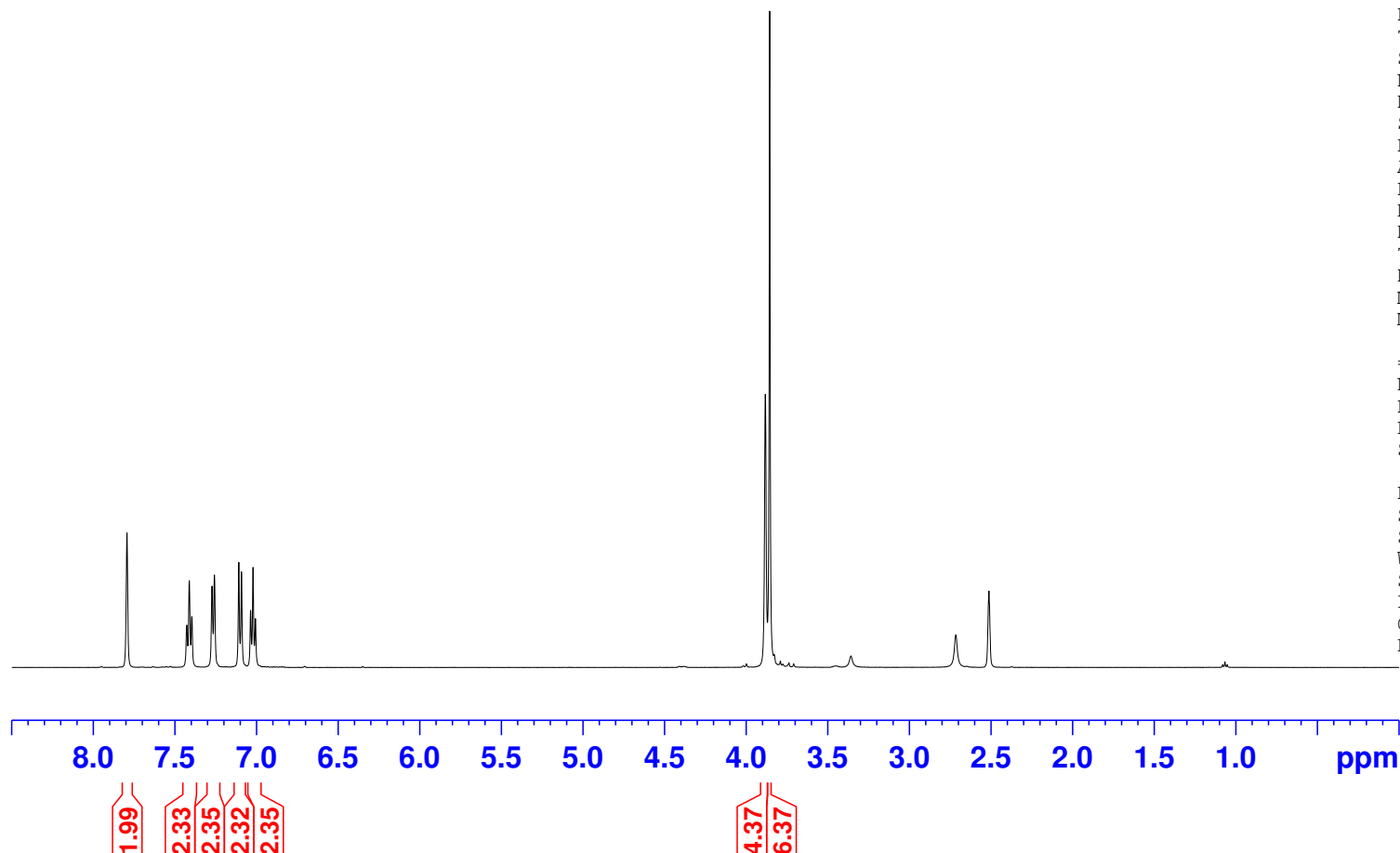


Current Data Parameters
NAME SK-01-126B
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20071221
Time 3.32
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 128
DW 48.400 usec
DE 6.00 usec
TE 0 K
D1 1.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec

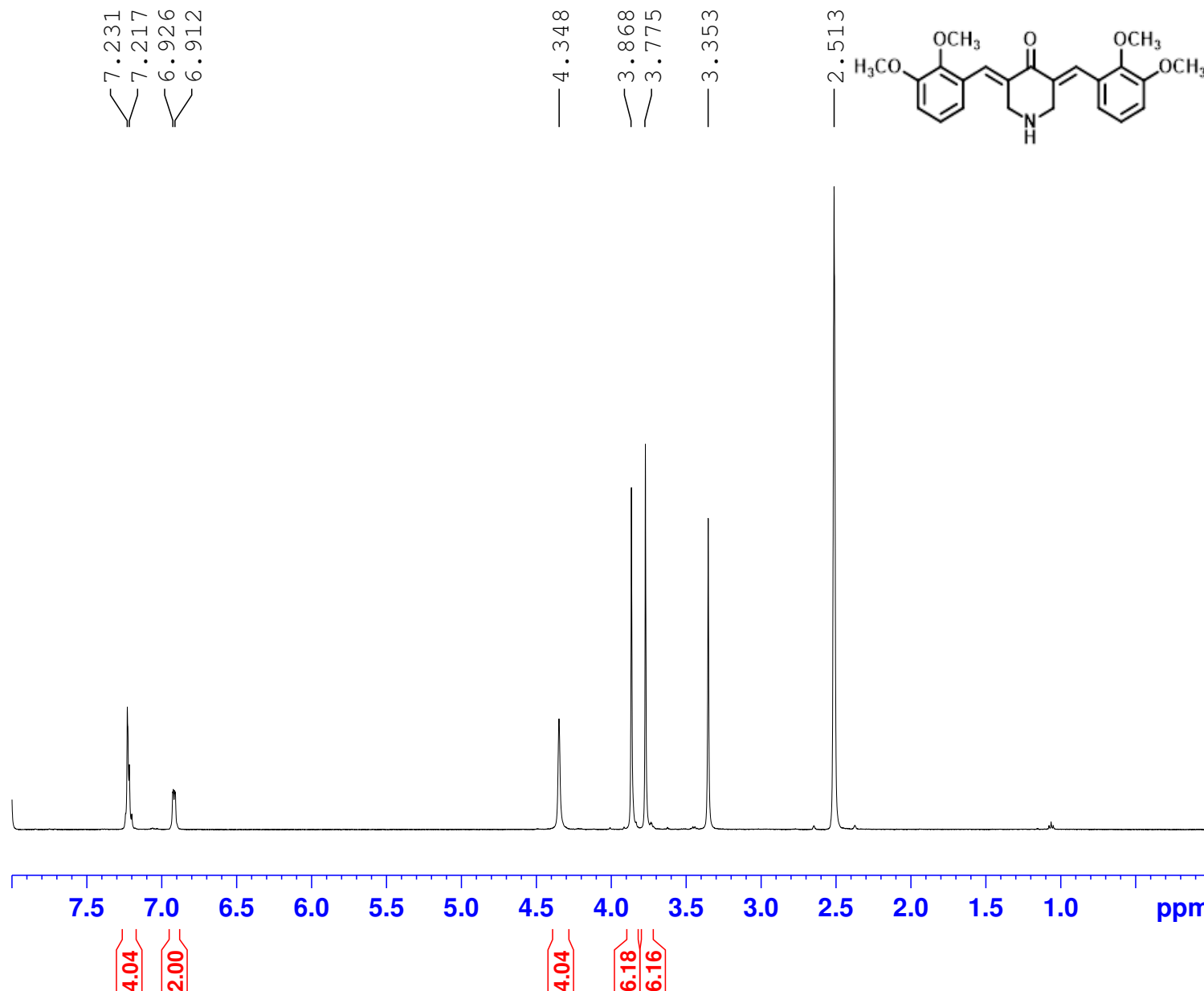
===== CHANNEL f1 =====
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P1 12.00 usec
PL1 -2.00 dB
SFO1 500.2830894 MHz

F2 - Processing parameters
SI 32768
SF 500.2800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



133A

3,5-bis(2, 3-Dimethoxybenzylidene)-4-piperidone (**1n**)



Current Data Parameters
 NAME SK-01-133A
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080110
 Time 22.28
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719425 sec
 RG 228.1
 DW 48.400 usec
 DE 6.00 usec
 TE 0 K
 D1 1.00000000 sec
 MCREST 0 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 12.00 usec
 PL1 -2.00 dB
 SFO1 500.2830894 MHz

F2 - Processing parameters
 SI 32768
 SF 500.2800000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00