

RSC Advances

Electronic Supplementary Information

Three-Component Microwave-Assisted Synthesis of 3,5-Disubstituted Pyrazolo[3,4-*d*]pyrimidin-4-ones

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Molecular packing in 5-benzyl-3-(4-methylphenylamino)-1,5-dihydro-4H-pyrazolo[3,4-*d*]pyrimidin-4-one (4d)

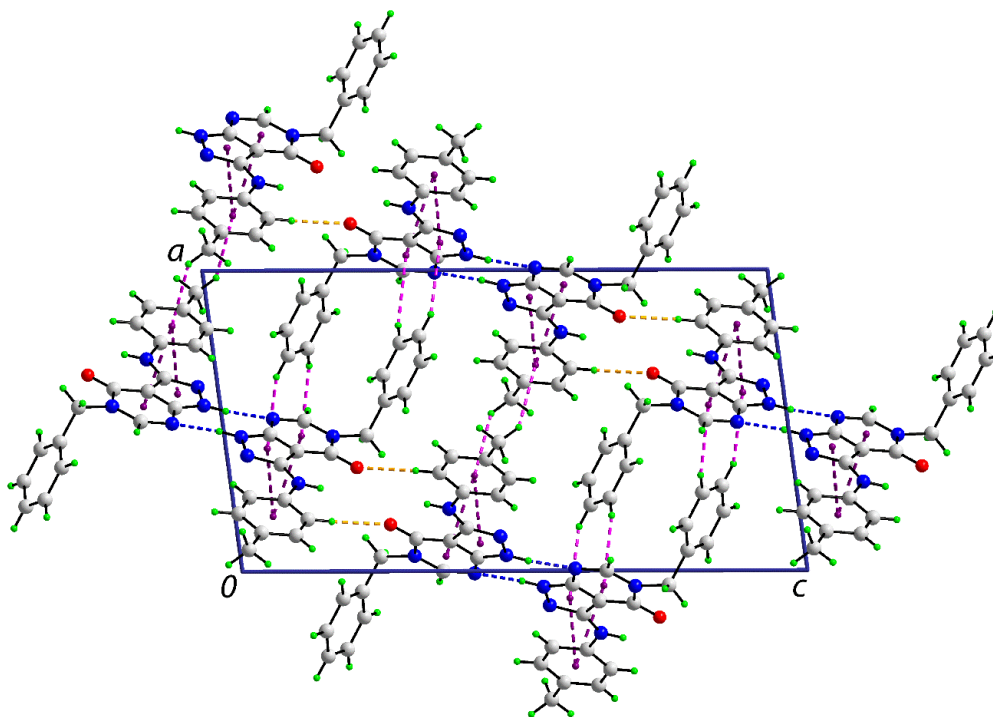


Figure S1. Molecular packing in **4d**: a view in projection down the *b*-axis of the unit cell contents. The N–H···N, C–H···O, C–H···π and π···π interactions are shown as blue, orange, pink and purple dashed lines, respectively.

Geometric parameters (Å, °) characterizing the identified intermolecular interactions

Interaction (A–H···B)	H···B	A···B	A–H···B	Symmetry operation
N31–H31···O1	2.589(12)	3.2035(12)	128.0(11)	x, y, z
N1–H1n···N7	2.061(12)	2.9215(12)	164.4(12)	$1-x, 1-y, -z$
C32–H32···O1	2.33	3.2751(14)	178	$\frac{1}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z$
C37–H37b···Cg3	2.71	3.5213(13)	141	$-x, 3-y, -z$
C54–H54···Cg(N5,N7,C3a,C4,C6,C7a)	2.76	3.5913(18)	146	$1\frac{1}{2}-x, -\frac{1}{2}+y, \frac{1}{2}-z$
C55–H55···Cg(N1,N2,C3,C3a,C7a)	2.91	3.7465(15)	147	$1\frac{1}{2}-x, -\frac{1}{2}+y, \frac{1}{2}-z$
Cg(N1,N2,C3,C3a,C7a)···Cg(C31-C36)		3.5566(6)	3.46(6)	$x, -1+y, z$
Cg(N5,N7,C3a,C4,C6,C7a)···Cg(C31-C36)		3.3616(6)	5.03(5)	$x, -1+y, z$

Molecular packing in 3-(4-bromophenylamino)-5-(4-methoxyphenyl)-1,5-dihydro-4*H*-pyrazolo[3,4-*d*]pyrimidin-4-one (4p)

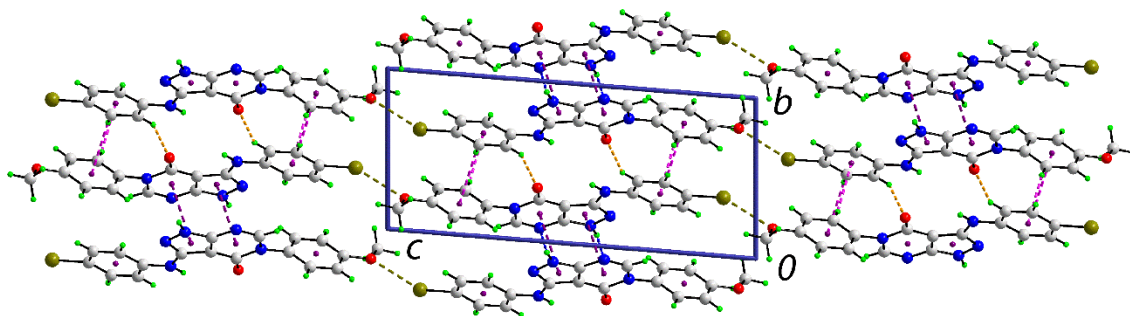


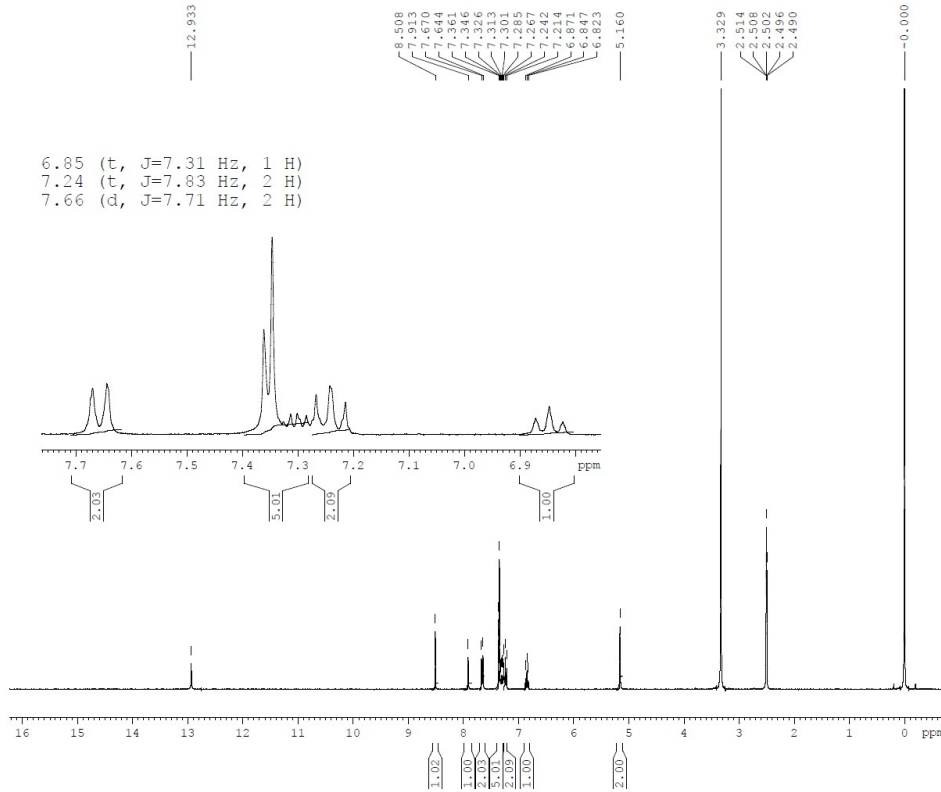
Figure S2. Molecular packing in **4p**: a view in projection down the *a*-axis of the unit-cell contents. The N–H···N, C–H···O, C–H··· π , π ··· π and Br···O interactions are shown as blue, orange, pink, purple and olive dashed lines, respectively.

Geometric parameters (\AA , $^\circ$) characterizing the identified intermolecular interactions:

Interaction (A–H···B)	H···B	A···B	A–H···B	Symmetry operation
N1–H1n···N7	2.039(18)	2.9005(18)	170.3(19)	3- <i>x</i> , 2- <i>y</i> , 1- <i>z</i>
C32–H32···O1	2.37	3.2264(18)	150	1- <i>x</i> , 1- <i>y</i> , 1- <i>z</i>
C33–H33···Cg(C51-C56)	2.86	3.6487(16)	142	1- <i>x</i> , 1- <i>y</i> , 1- <i>z</i>
C52–H52···Cg(C31-C36)	2.51	3.2868(16)	139	2- <i>x</i> , 1- <i>y</i> , 1- <i>z</i>
Cg(N1,N2,C3,C3a,C7a)···Cg(N5,N7,C3a,C4,C6,C7a)		3.4144(8)	4.52(8)	2- <i>x</i> , 2- <i>y</i> , 1- <i>z</i>
C34–Br31···O51		3.1620(11)	154.75(6)	-1+ <i>x</i> , <i>y</i> , 1+ <i>z</i>

**Copies of ^1H and ^{13}C NMR spectra for prepared
3,5-disubstituted pyrazolo[3,4-*d*]pyrimidin-4-ones (4a-t)**

5-Benzyl-3-(phenylamino)-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one (4a)

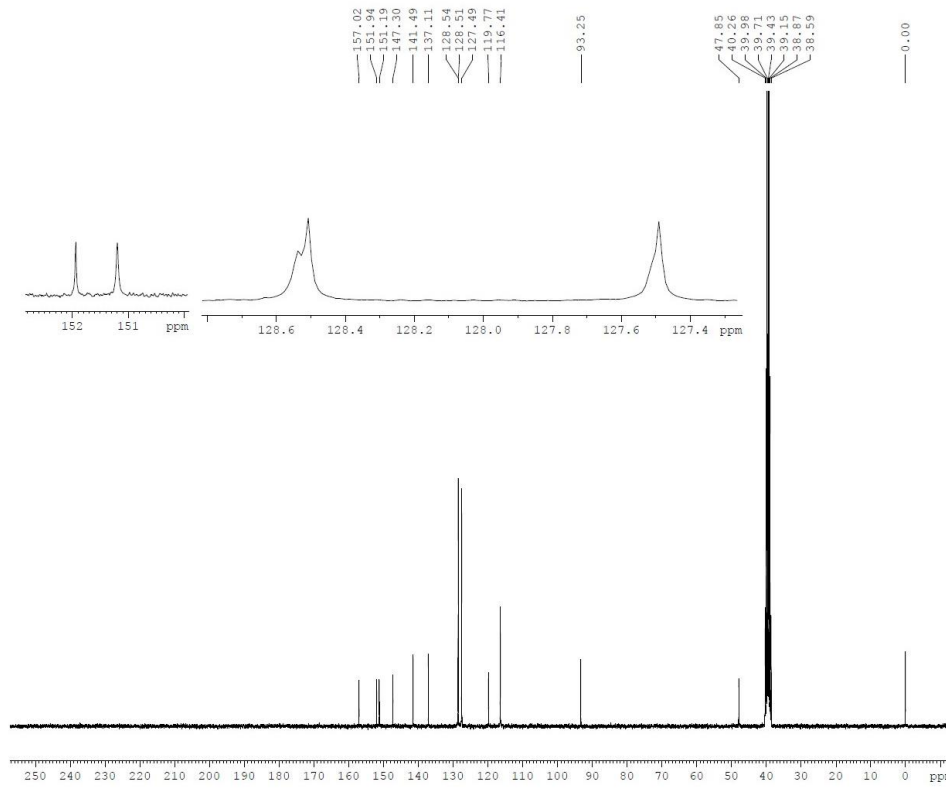


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RG 148.371
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TE 298.3 K
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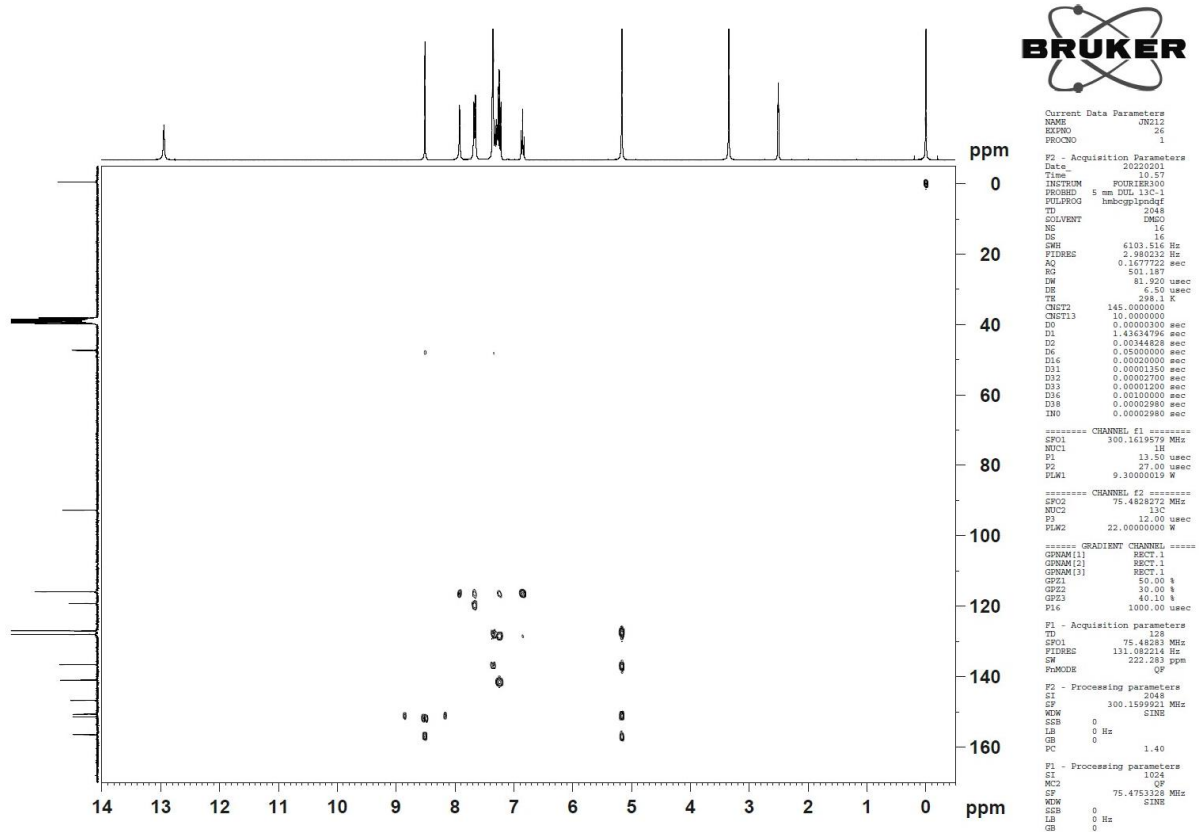
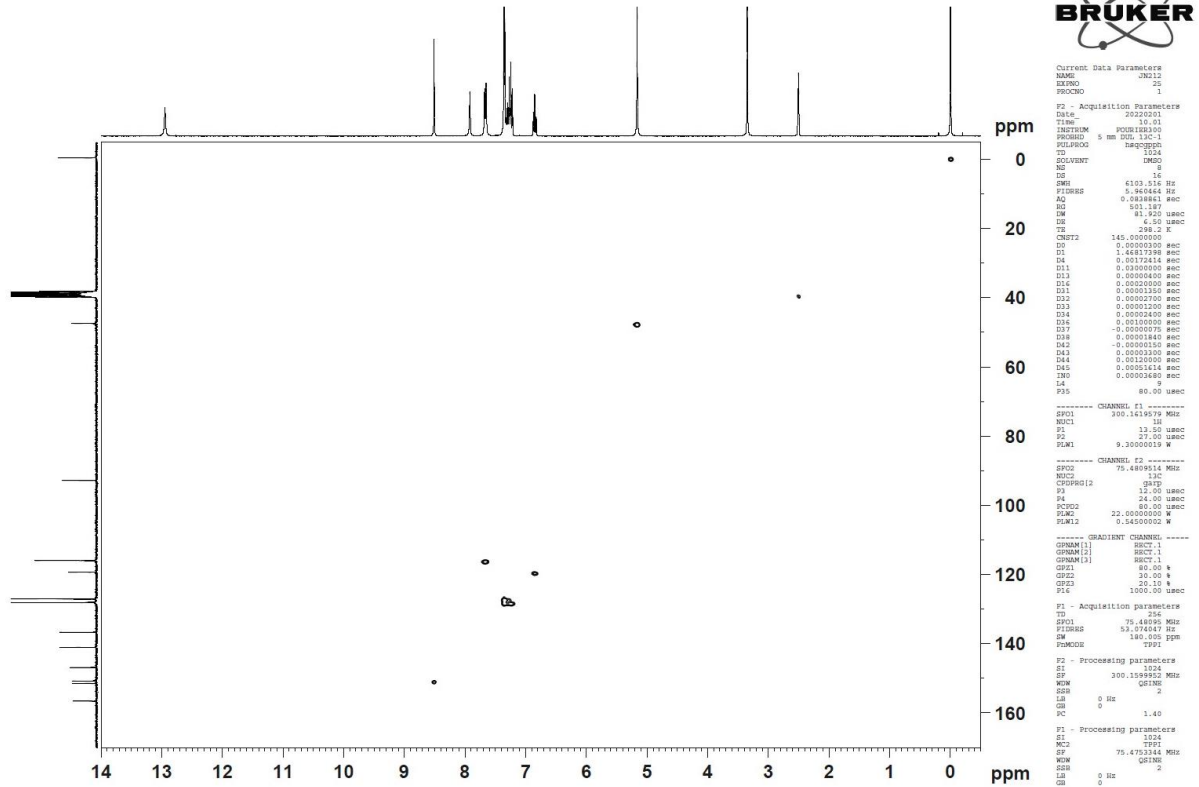
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FIDRES 0.372529 Hz
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RG 501.187
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DE 6.50 usec
TE 298.3 K
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D11 0.03000000 sec
D31 0.00001300 sec
D40 0.02898005 sec
L4 40
L5 57
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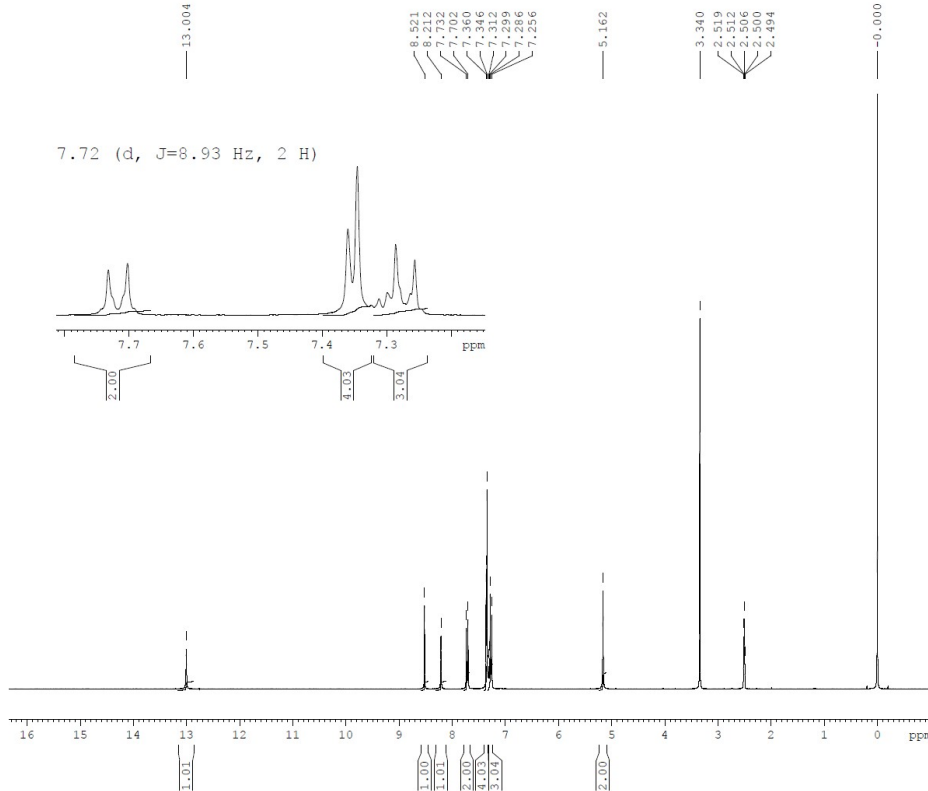
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PLW13 0.12650000 W

F2 - Processing parameters
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WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

5-Benzyl-3-(phenylamino)-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one (4a)



5-Benzyl-3-(4-chlorophenylamino)-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one (4b)

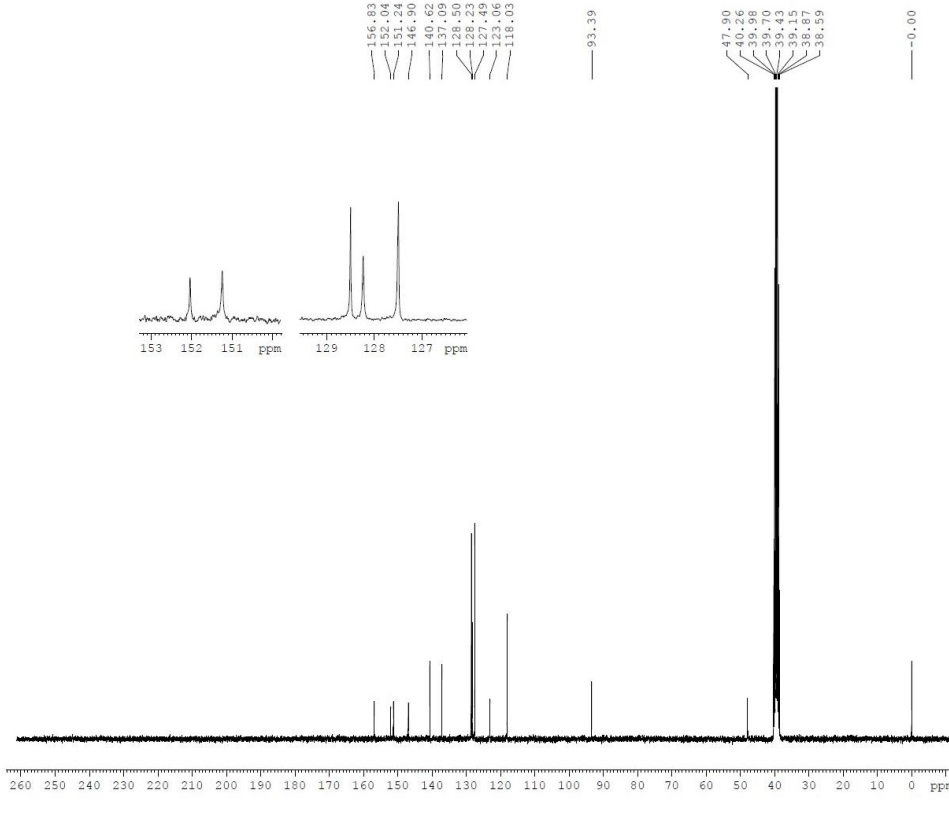


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 RG 101.537
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 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
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 NUC1 1H
 P1 13.50 usec
 PLW1 9.30000019 W

F2 - Processing parameters
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Current Data Parameters
 NAME JN218
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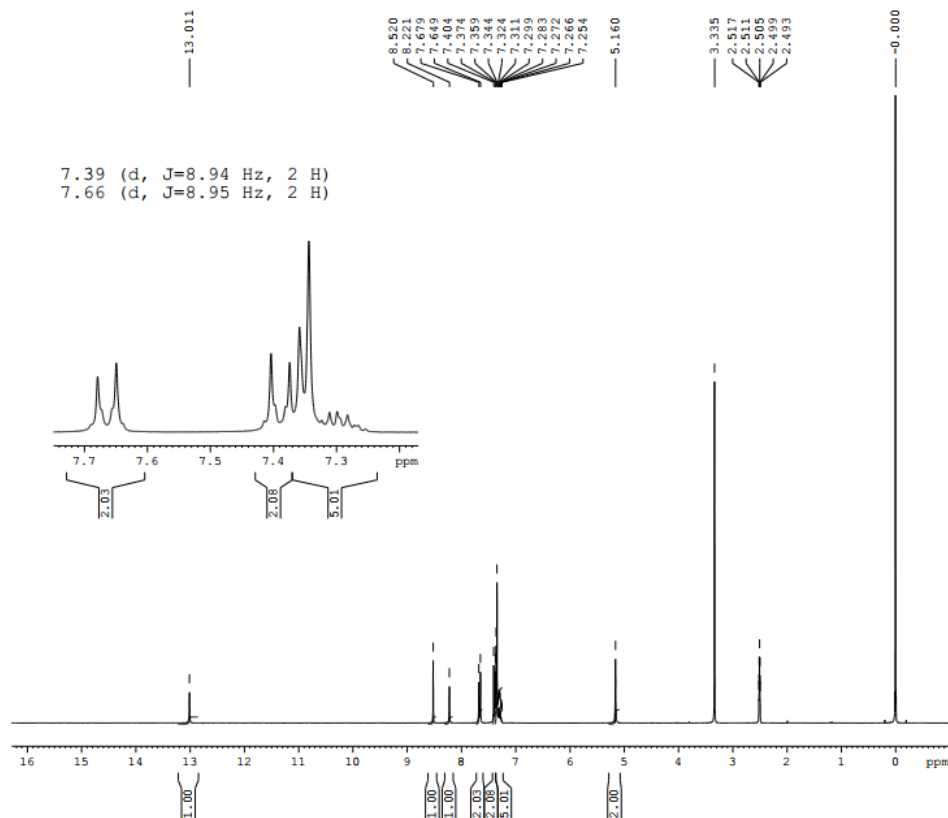
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 RG 501.187
 DW 20.480 usec
 DE 6.50 usec
 TE 298.3 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D31 0.00001300 sec
 D40 0.02898005 sec
 L4 40
 L5 57
 P32 90.00 usec
 TDO 3

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 NUC1 13C
 P1 13.00 usec
 PLW1 22.00000000 W

===== CHANNEL f2 =====
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 NUC2 1H
 CPDPRG2 waltz16
 PCDP2 90.00 usec
 PLW2 9.30000019 W
 PLW12 0.25149000 W
 PLW13 0.12650000 W

F2 - Processing parameters
 SI 32763
 SF 75.4753339 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

5-Benzyl-3-(4-bromophenylamino)-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one (4c)

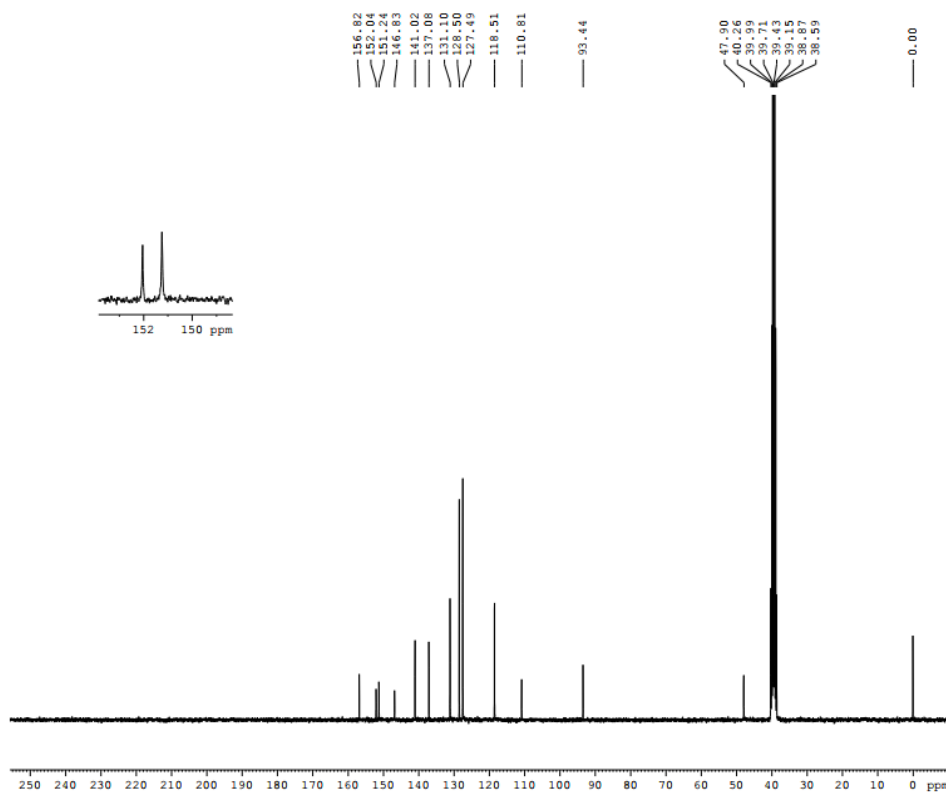


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FIDRES 0.093132 Hz
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RG 120.379
DW 81.920 usec
DE 6.50 usec
TE 298.2 K
D1 1.0000000 sec
TDO 1

----- CHANNEL f1 -----
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NUC1 1H
P1 13.50 usec
PLW1 9.30000019 W

F2 - Processing parameters
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LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME JN208
EXPNO 6
PROCNO 1

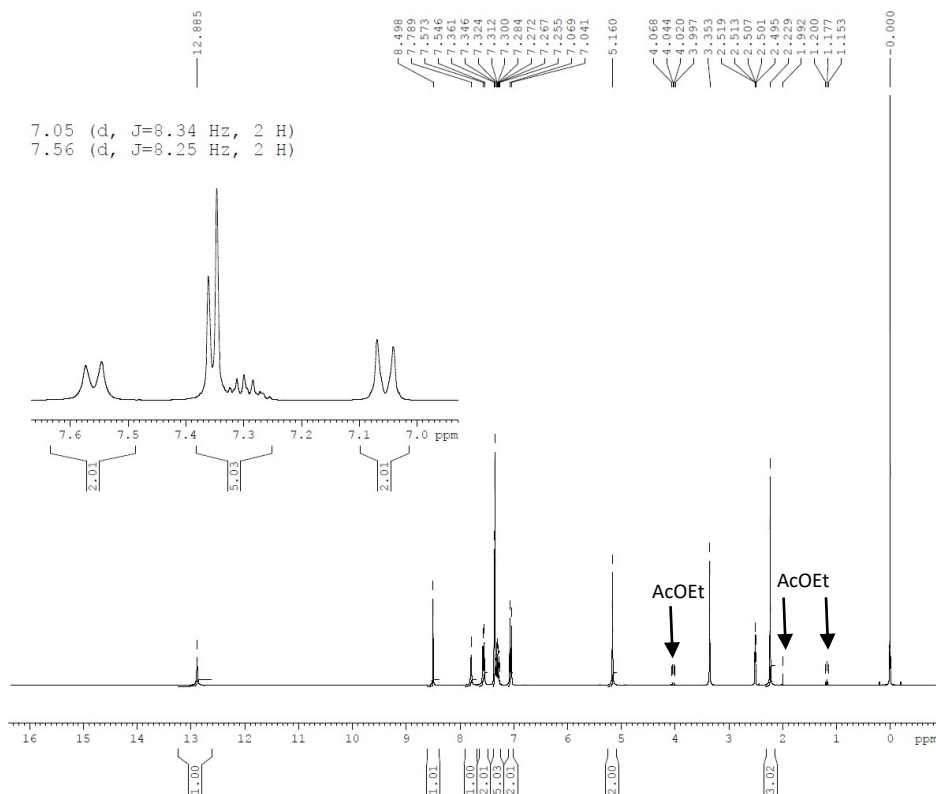
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FIDRES 0.372529 Hz
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RG 501.187
DW 20.480 usec
DE 6.50 usec
TE 298.3 K
D1 2.0000000 sec
D11 0.0300000 sec
D31 0.00001300 sec
D40 0.02898005 sec
L4 40
L5 57
P32 90.00 usec
TDO 4

----- CHANNEL f1 -----
SFO1 75.4828392 MHz
NUC1 13C
P1 13.00 usec
PLW1 22.00000000 W

----- CHANNEL f2 -----
SFO2 300.1612006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
FLW2 9.30000019 W
FLW12 0.25149000 W
FLW13 0.12650000 W

F2 - Processing parameters
SI 32768
SF 75.4753339 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

5-Benzyl-3-(4-methylphenylamino)-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one (4d)

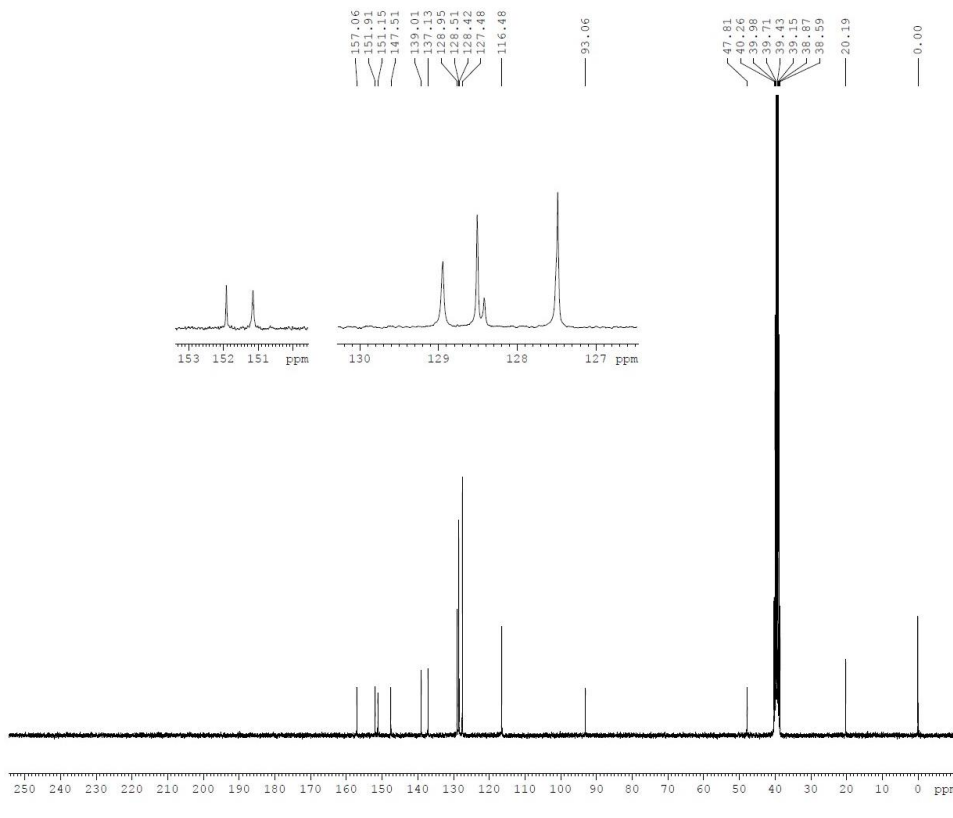


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 NS 16
 DS 2
 SWH 6103.516 Hz
 FIDRES 0.093132 Hz
 AQ 5.3687091 sec
 RG 52.7107
 DW 81.920 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TDO 1

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 NUC1 1H
 P1 13.50 usec
 PLW1 9.30000019 W

F2 - Processing parameters
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 GB 0
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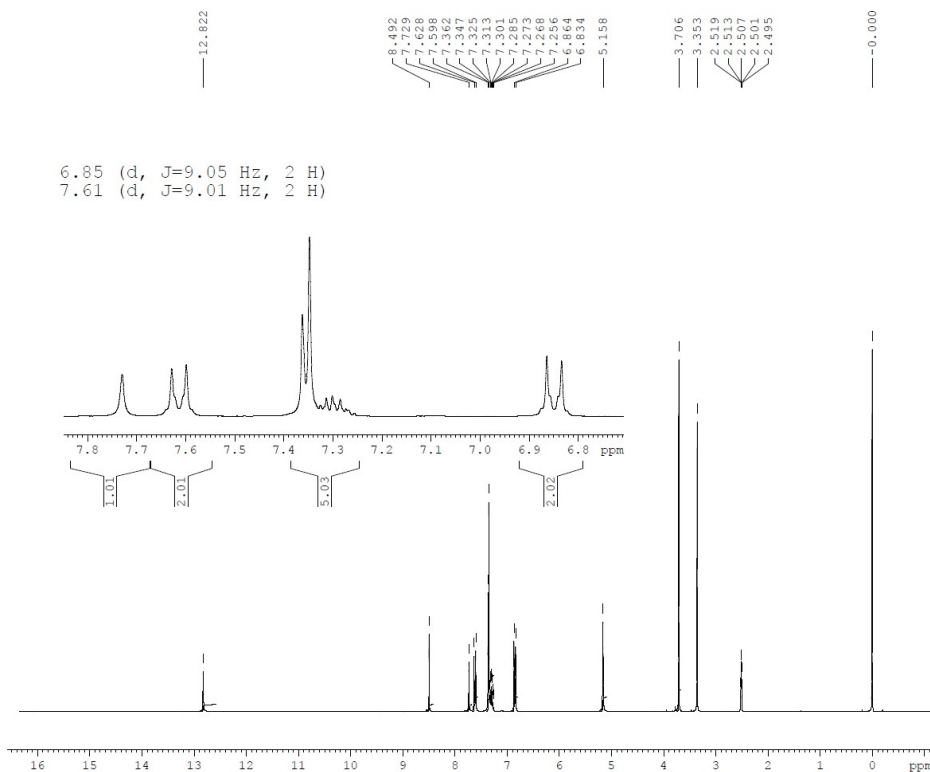
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 DW 20.480 usec
 DE 6.50 usec
 TE 298.3 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D31 0.00001300 sec
 D40 0.02898005 sec
 I4 40
 L5 57
 P32 90.00 usec
 TDO 4

==== CHANNEL f1 =====
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 NUC1 13C
 P1 13.00 usec
 PLW1 22.00000000 W

==== CHANNEL f2 =====
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 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 9.30000019 W
 PLW12 0.25149000 W
 PLW13 0.12650000 W

F2 - Processing parameters
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 SF 75.4753337 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
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5-Benzyl-3-(4-methoxyphenylamino)-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one (4e)

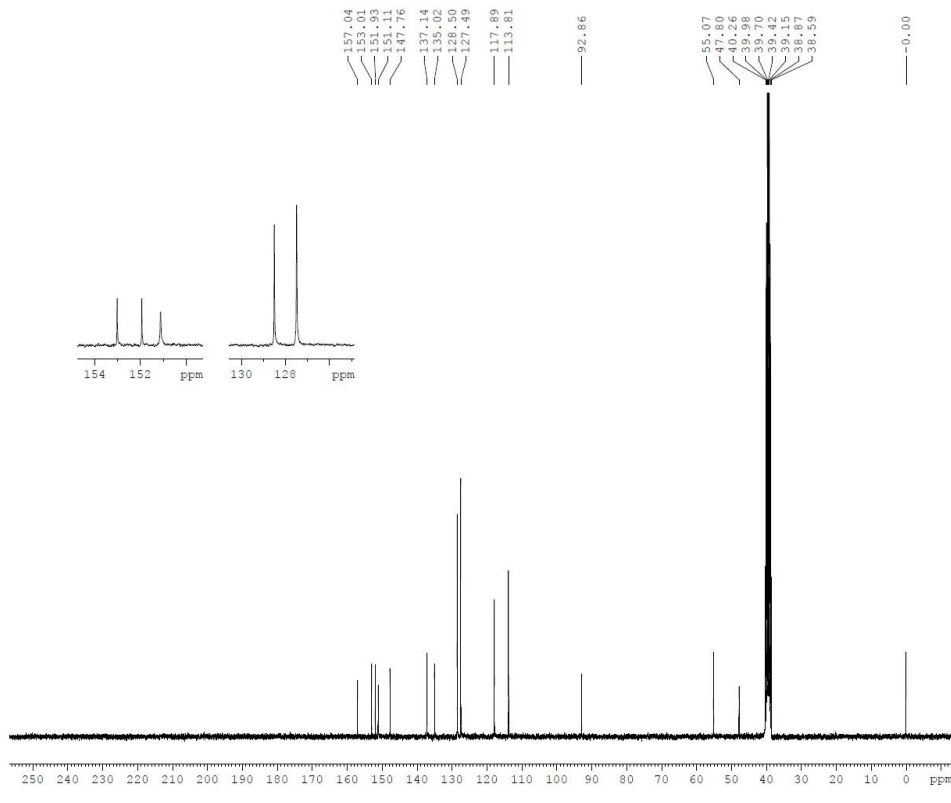


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RG 66.5041
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DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TDO 1

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NUC1 1H
P1 13.50 usec
PLW1 9.30000019 W

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EXPNO 6
PROCNO 1

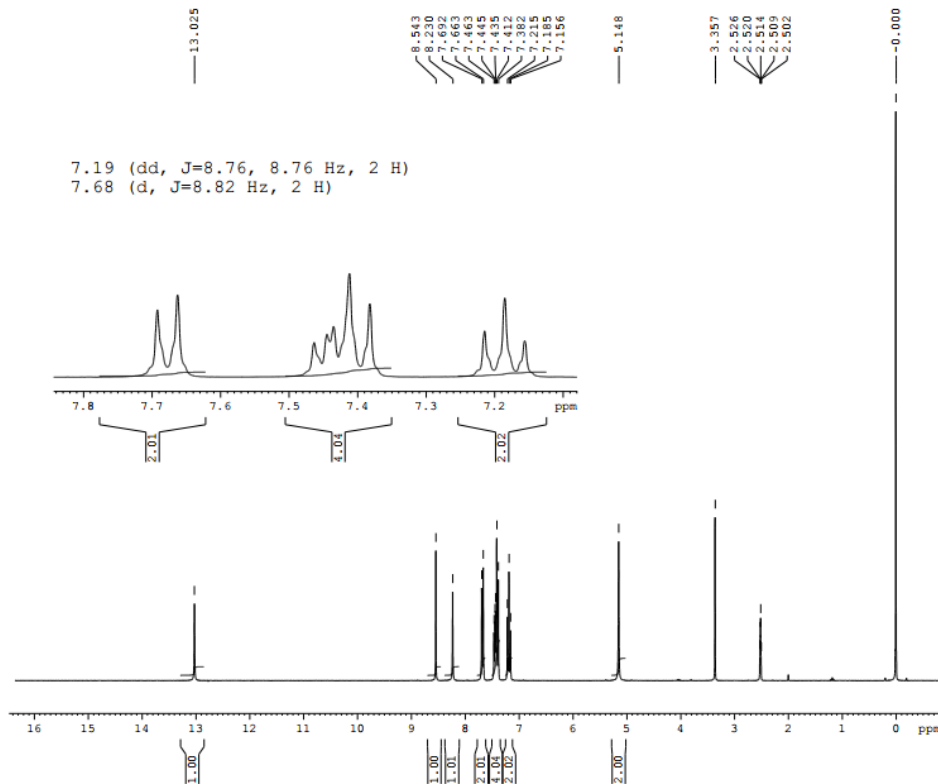
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FIDRES 0.372529 Hz
AQ 1.3421773 sec
RG 501.137
DW 20.480 usec
DE 6.50 usec
TE 298.3 K
D1 2.00000000 sec
D11 0.03000000 sec
D31 0.00001300 sec
D40 0.02898005 sec
L4 40
L5 57
P32 90.00 usec
TDO 4

==== CHANNEL f1 =====
SF01 75.4828392 MHz
NUC1 13C
P1 13.00 usec
PLW1 22.00000000 W

==== CHANNEL f2 =====
SF02 300.1612006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 9.30000019 W
PLW12 0.25149000 W
PLW13 0.12650000 W

F2 - Processing parameters
SI 32768
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WDW EM
SSB 0
LB 1.00 Hz
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PC 1.40

3-(4-Bromophenylamino)-5-(4-fluorobenzyl)-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one (4f)

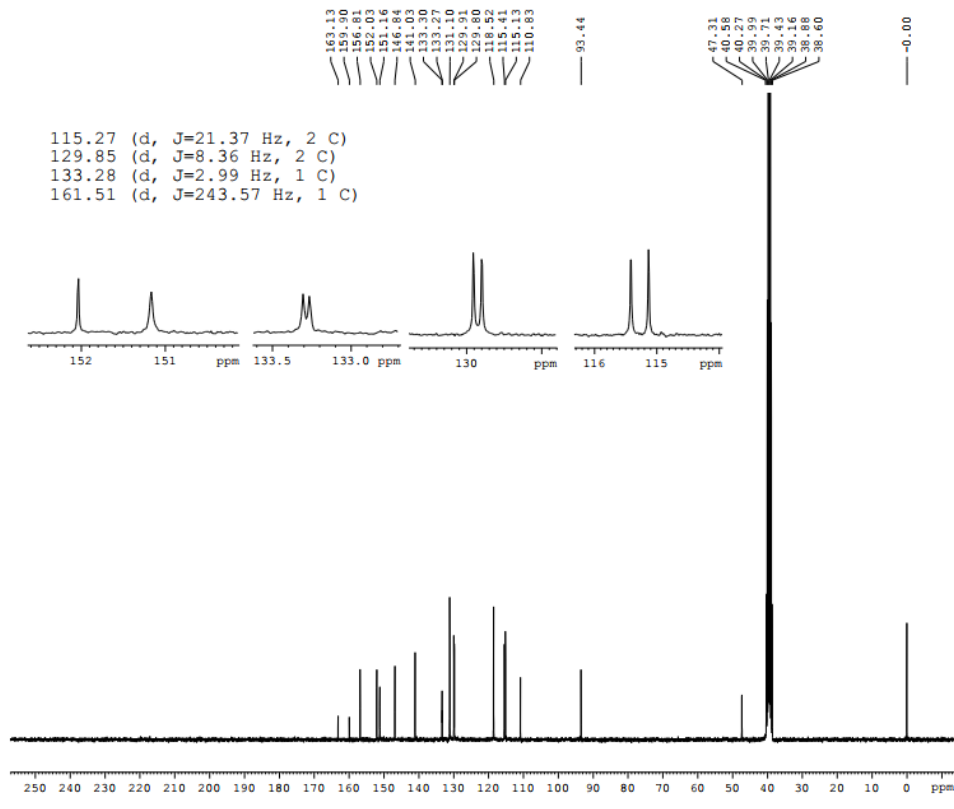


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SOLVENT DMSO
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DS 2
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FIDRES 0.093132 Hz
AQ 5.3687091 sec
RG 73.8752
DW 81.920 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 300.1618536 MHz
NUC1 1H
P1 13.50 usec
PLW1 9.30000019 W

F2 - Processing parameters
SI 65536
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WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
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EXPNO 4
PROCNO 1

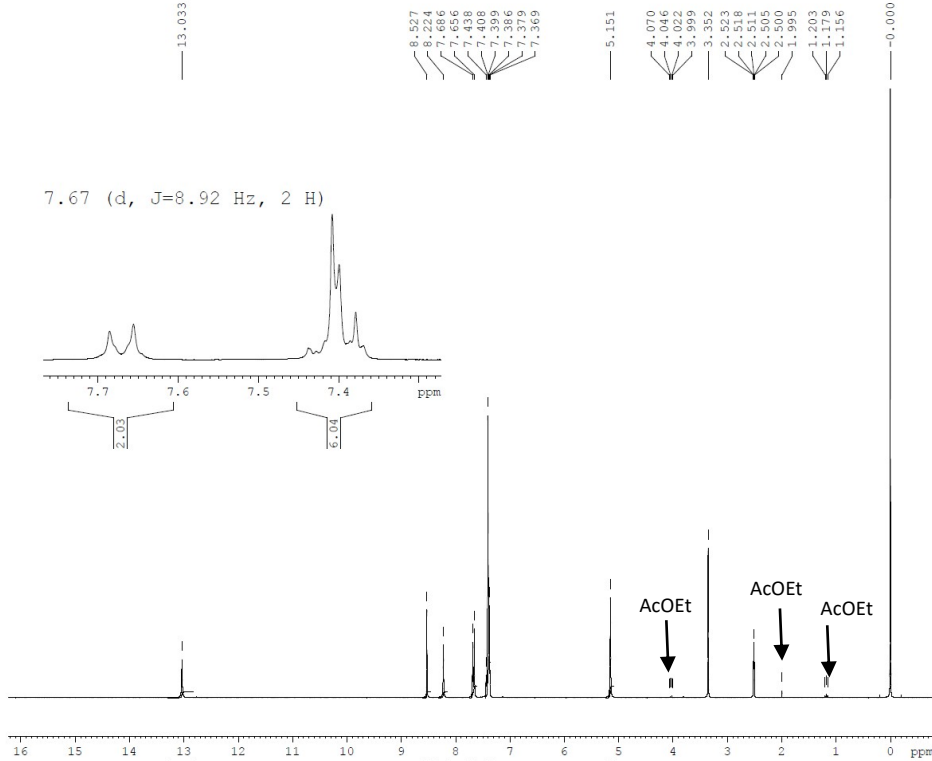
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SOLVENT DMSO
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DS 4
SWH 24414.063 Hz
FIDRES 0.372529 Hz
AQ 1.3421773 sec
RG 501.187
DW 20.480 usec
DE 6.50 usec
TE 298.3 K
D1 2.00000000 sec
D11 0.03000000 sec
D31 0.00001300 sec
D40 0.02898005 sec
L4 40
L5 57
P32 90.00 usec
TD0 5

----- CHANNEL f1 -----
SFO1 75.4828392 MHz
NUC1 13C
P1 13.00 usec
PLW1 22.00000000 W

----- CHANNEL f2 -----
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NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 9.30000019 W
PLW12 0.25149000 W
PLW13 0.12650000 W

F2 - Processing parameters
SI 32768
SF 75.4753331 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3-(4-Bromophenylamino)-5-(4-chlorobenzyl)-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one (4g)

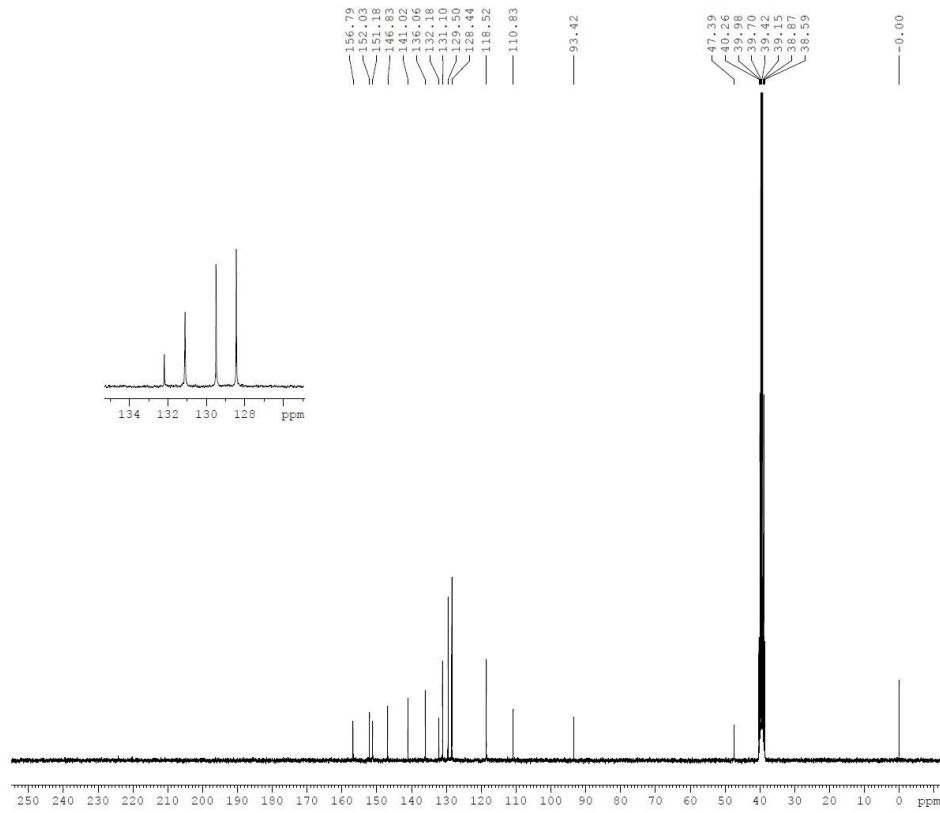


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 PULPROG zg30
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 SOLVENT DMSO
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 DS 2
 SWH 6103.516 Hz
 FIDRES 0.093132 Hz
 AQ 5.3687091 sec
 RG 73.1933
 DW 81.920 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.0000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 300.1618536 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 9.30000019 W

F2 - Processing parameters
 SI 65536
 SF 300.1599965 MHz
 WDW EM
 SSB 0
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 PROCNO 1

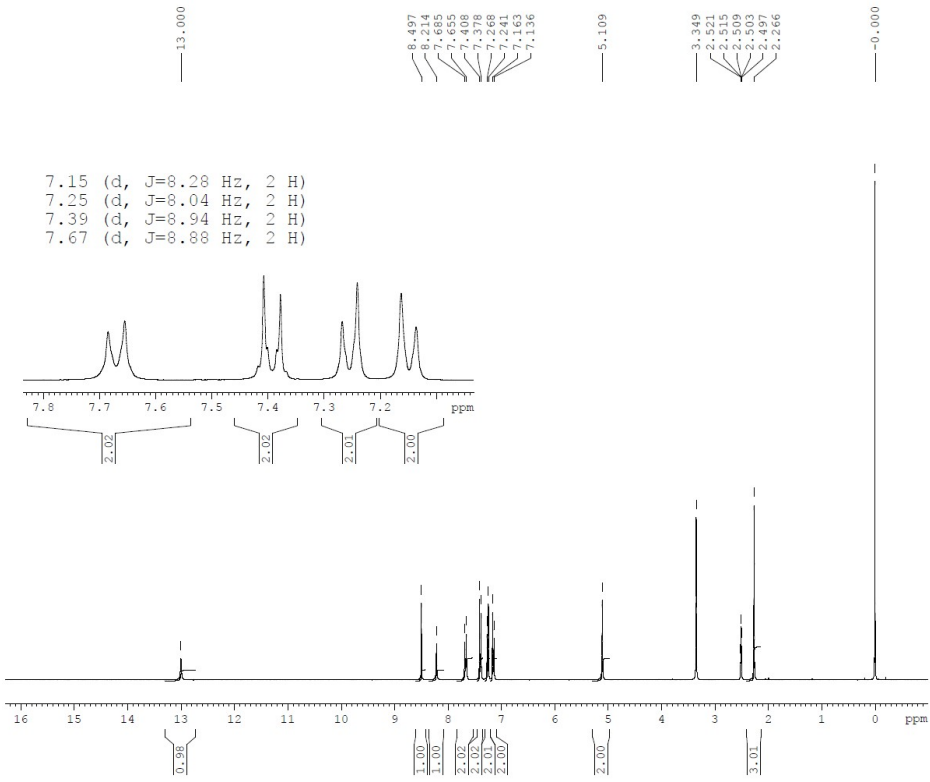
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 SOLVENT DMSO
 NS 4096
 DS 4
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 FIDRES 0.372529 Hz
 AQ 1.3421773 sec
 RG 501.187
 DW 20.480 usec
 DE 6.50 usec
 TE 298.3 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 D31 0.00001300 sec
 D40 0.02898005 sec
 L4 40
 L5 57
 P32 90.0 usec
 TDO 4

===== CHANNEL f1 =====
 SFO1 75.4828392 MHz
 NUC1 13C
 P1 13.00 usec
 PLW1 22.00000000 W

===== CHANNEL f2 =====
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 NUC2 1H
 CPDPRG2 waltz16
 PCPFD2 90.00 usec
 PLW2 9.30000019 W
 PLW12 0.25149000 W
 PLW13 0.12650000 W

F2 - Processing parameters
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 SF 75.4753336 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

3-(4-Bromophenylamino)-5-(4-methylbenzyl)-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one (4h)

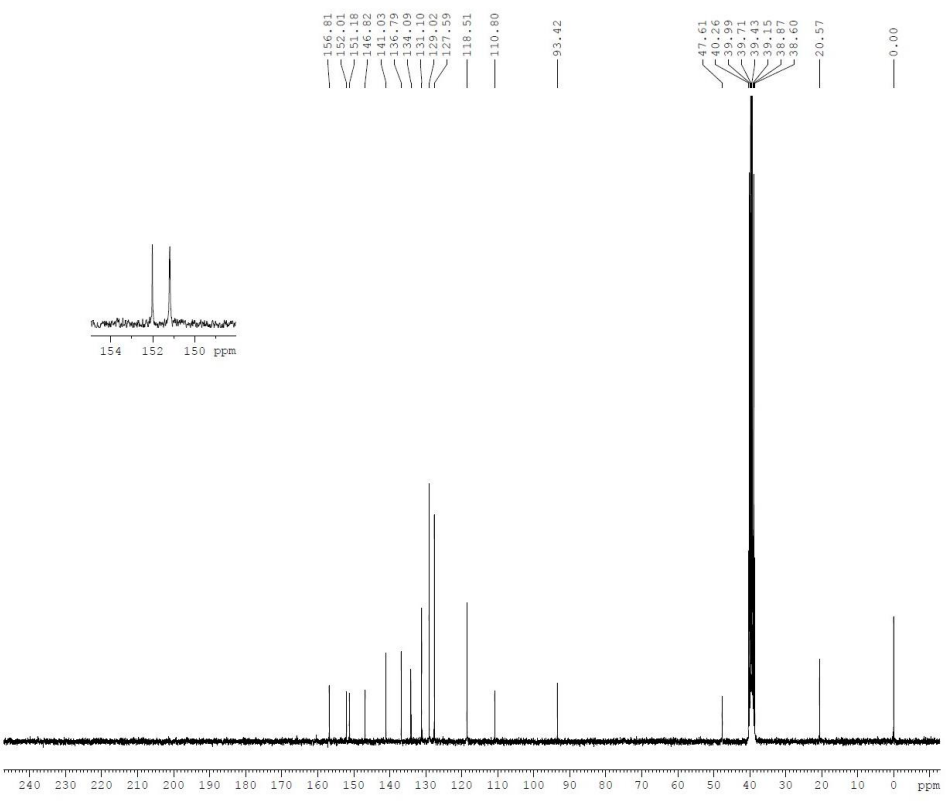


Current Data Parameters
 NAME JN214
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210317
 Time_ 13.42
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 6103.516 Hz
 FIDRES 0.093132 Hz
 AQ 5.3687091 sec
 RG 80.8202
 DW 81.920 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 300.1618536 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 9.30000019 W

F2 - Processing parameters
 SI 65536
 SF 300.1599973 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME JN214
 EXPNO 6
 PROCNO 1

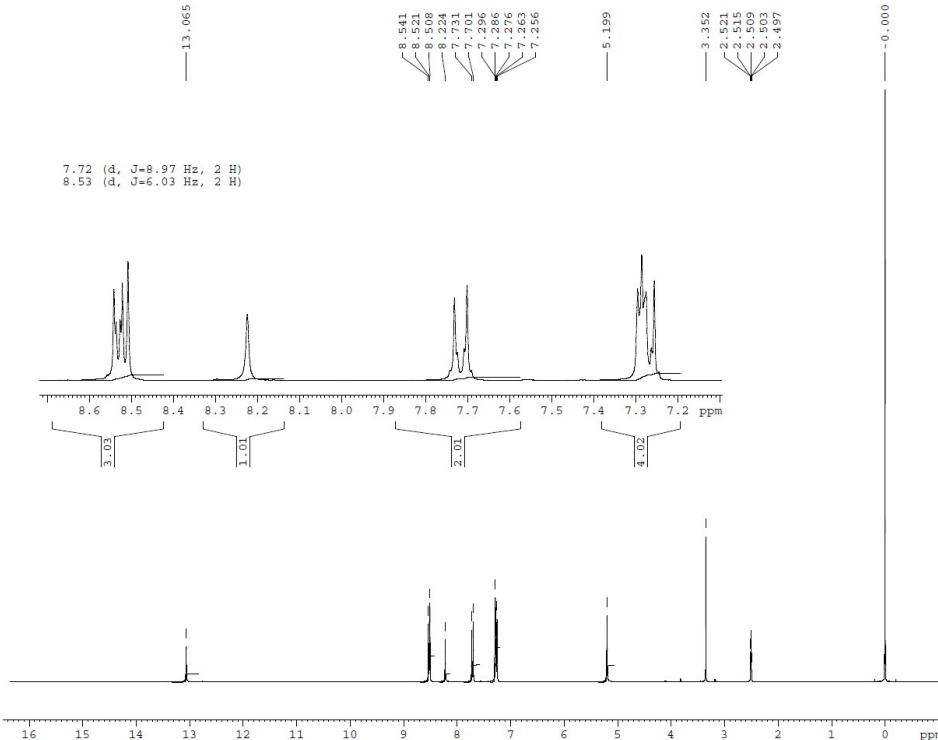
F2 - Acquisition Parameters
 Date_ 20210313
 Time_ 9.36
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 4096
 DS 4
 SWH 24414.063 Hz
 FIDRES 0.1372529 Hz
 AQ 1.3421773 sec
 RG 501.187
 DW 20.480 usec
 DE 6.50 usec
 TE 298.3 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D31 0.00001300 sec
 D40 0.02898005 sec
 L4 40
 L5 57
 P32 90.00 usec
 TD0 4

==== CHANNEL f1 =====
 SFO1 75.4828392 MHz
 NUC1 13C
 P1 13.00 usec
 PLW1 22.00000000 W

==== CHANNEL f2 =====
 SFO2 300.1612006 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 9.30000019 W
 PLW12 0.25149000 W
 PLW13 0.12650000 W

F2 - Processing parameters
 SI 32768
 SF 75.4753339 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

3-(4-Chlorophenylamino)-5-(4-picoyl)-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one (4i)

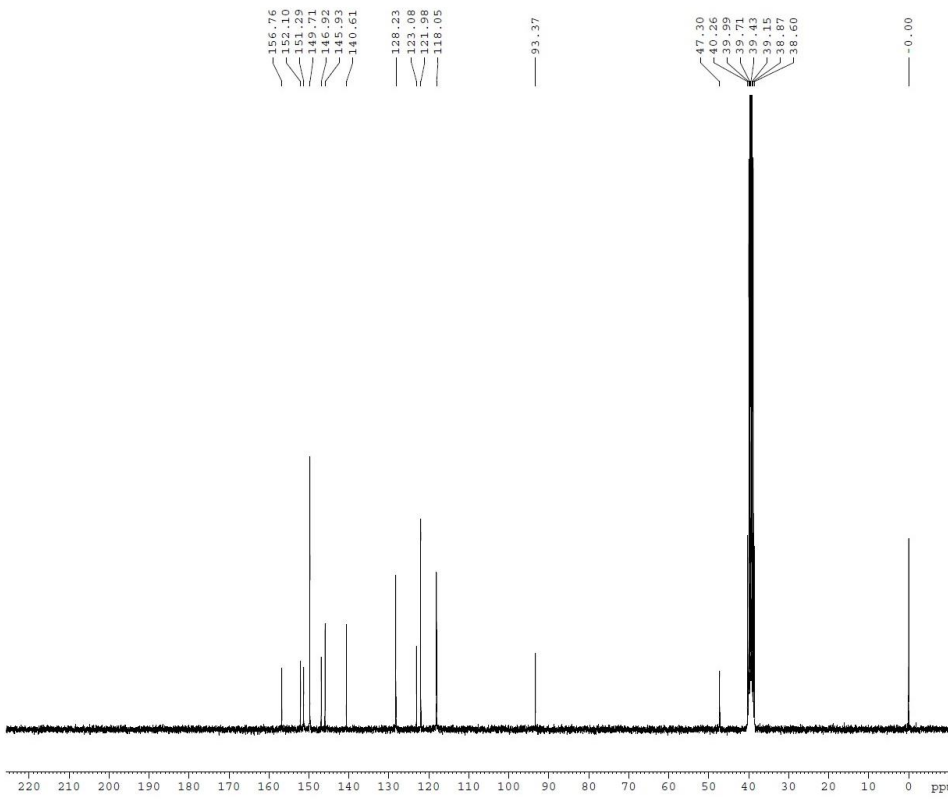


Current Data Parameters
 NAME JN221
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210921
 Time 12.10
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 6103.516 Hz
 FIDRES 0.093132 Hz
 AQ 5.3687091 sec
 RG 67.4741
 DW 81.920 usec
 DE 6.50 usec
 TE 298.3 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 300.1618536 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 9.30000019 W

F2 - Processing parameters
 SI 65536
 SF 300.1599972 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME JN221
 EXPNO 4
 PROCNO 1

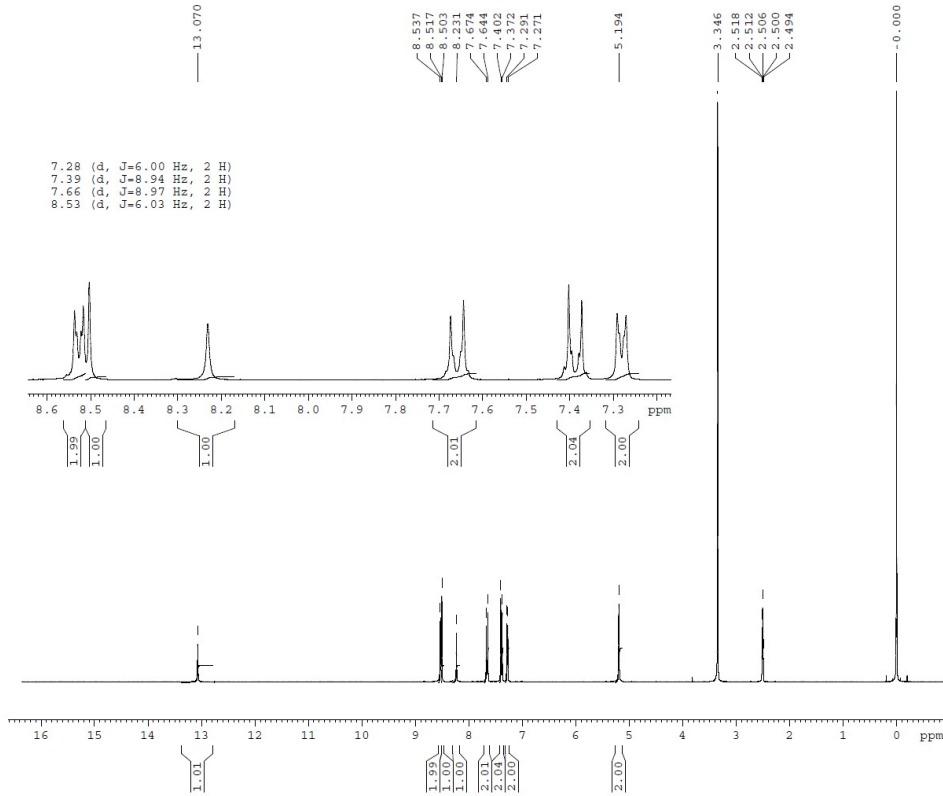
F2 - Acquisition Parameters
 Date_ 20210922
 Time 5.04
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 3072
 DS 4
 SWH 24414.063 Hz
 FIDRES 0.372529 Hz
 AQ 1.3421773 sec
 RG 501.187
 DW 20.480 usec
 DE 6.50 usec
 TE 298.3 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D31 0.00001300 sec
 D40 0.02898005 sec
 L4 40
 L5 57
 P32 90.00 usec
 TDO 3

===== CHANNEL f1 =====
 SFO1 75.4828992 MHz
 NUC1 13C
 P1 13.00 usec
 PLW1 22.00000000 W

===== CHANNEL f2 =====
 SFO2 300.1612006 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 9.30000019 W
 PLW12 0.25149000 W
 PLW13 0.12650000 W

F2 - Processing parameters
 SI 32768
 SF 75.4753337 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

3-(4-Bromophenylamino)-5-(4-picoly)-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one (4j)

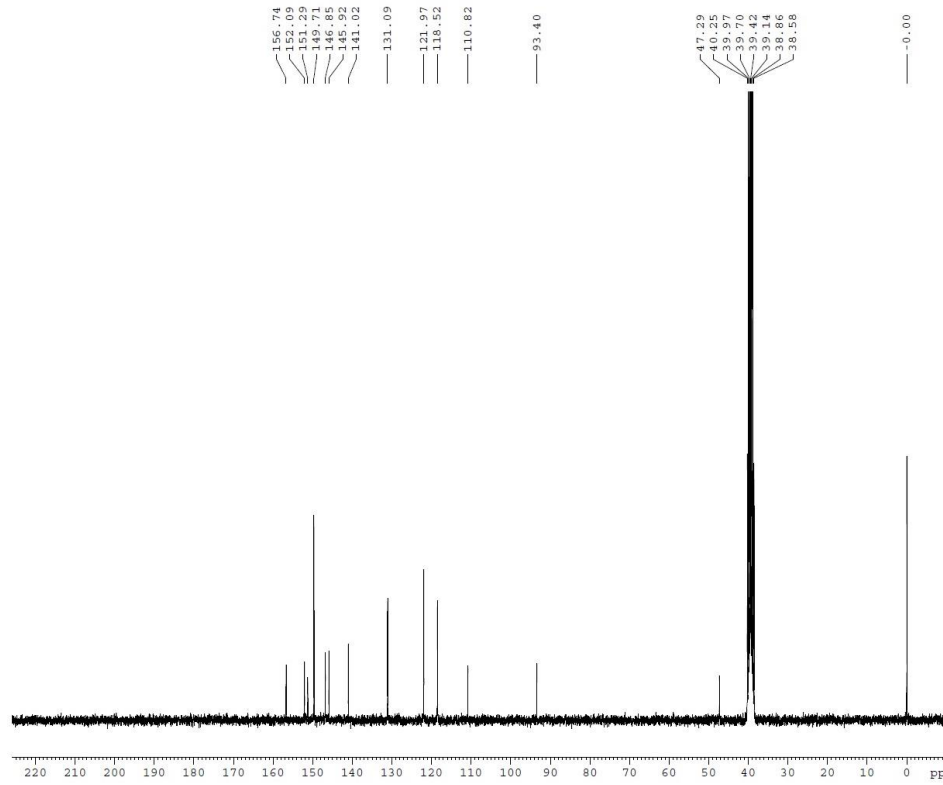


Current Data Parameters
NAME JN222
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210921
Time_ 12.14
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6103.516 Hz
FIDRES 0.093132 Hz
AQ 5.3687091 sec
RG 79.1896
DW 81.920 usec
DE 6.50 usec
TE 298.2 K
D1 1.0000000 sec
TDO 1

==== CHANNEL f1 =====
SFO1 300.1618536 MHz
NUC1 1H
P1 13.50 usec
PLW1 9.30000019 W

F2 - Processing parameters
SI 65536
SF 300.1599982 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME JN222
EXPNO 4
PROCNO 1

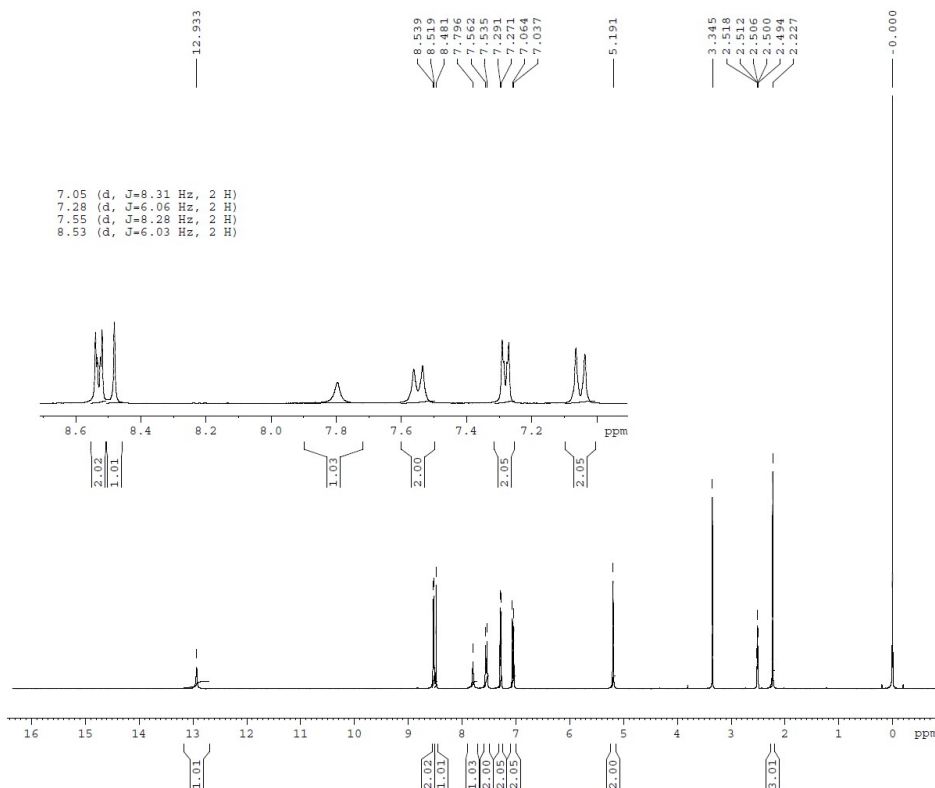
F2 - Acquisition Parameters
Date_ 20210922
Time_ 11.21
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 3072
DS 4
SWH 24414.063 Hz
FIDRES 0.372529 Hz
AQ 1.3421773 sec
RG 501.187
DW 20.480 usec
DE 6.50 usec
TE 298.3 K
D1 2.0000000 sec
D11 0.0300000 sec
D31 0.00001300 sec
D40 0.02898005 sec
L4 40
L5 57
P32 90.00 usec
TDO 3

==== CHANNEL f1 =====
SFO1 75.4828992 MHz
NUC1 13C
P1 13.00 usec
PLW1 22.00000000 W

==== CHANNEL f2 =====
SFO2 300.1612006 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 9.30000019 W
PLW12 0.25149000 W
PLW13 0.12650000 W

F2 - Processing parameters
SI 32768
SF 75.4753343 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3-(4-Methylphenylamino)-5-(4-picolyl)-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one (4k)

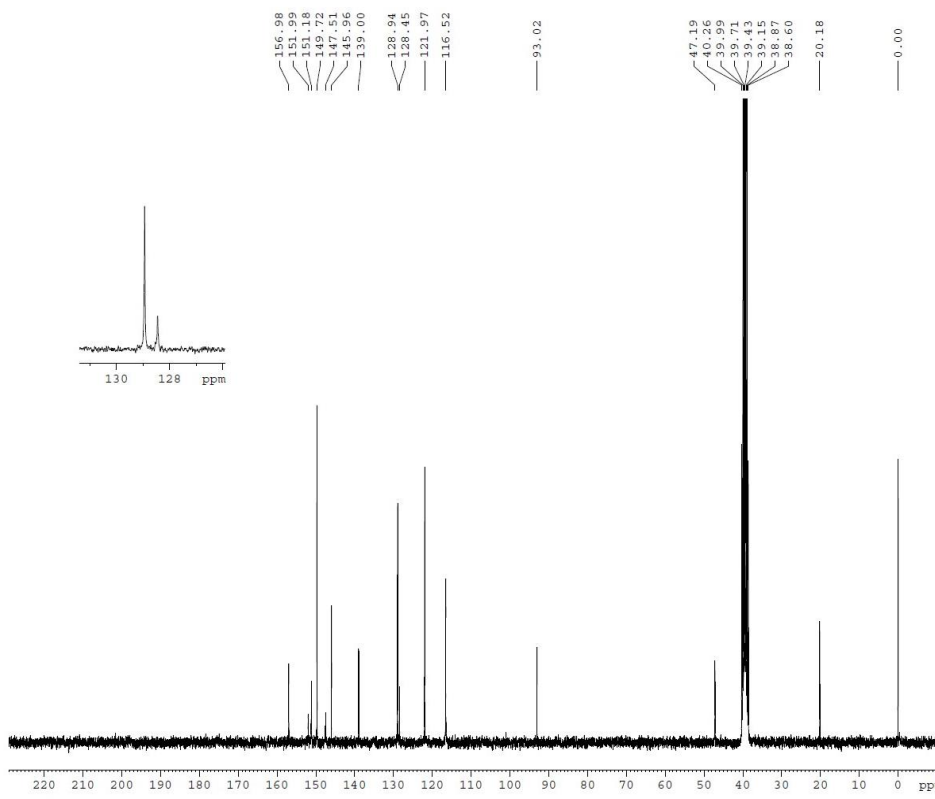


Current Data Parameters
 NAME JN130
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210921
 Time 12.05
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 6103.516 Hz
 FIDRES 0.093132 Hz
 AQ 5.3687091 sec
 RG 75.762
 DW 81.920 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.0000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 300.1618536 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 9.3000019 W

F2 - Processing parameters
 SI 65536
 SF 300.1599981 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME JN130
 EXPNO 5
 PROCNO 1

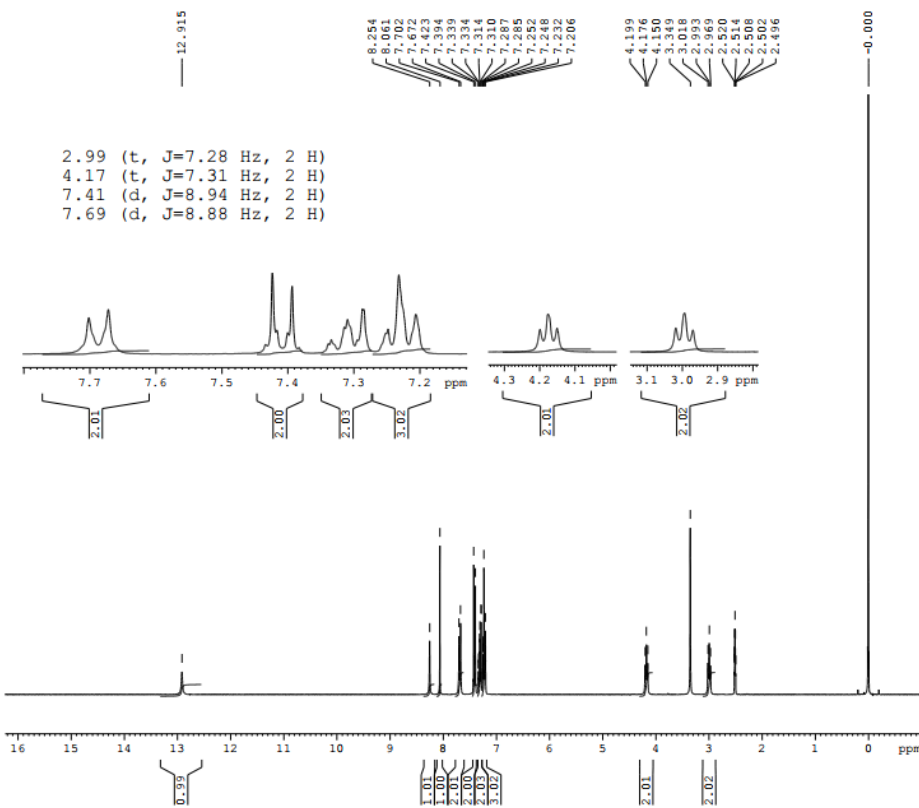
F2 - Acquisition Parameters
 Date_ 20210922
 Time 2.04
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 4
 DS 4
 SWH 24414.063 Hz
 FIDRES 0.372529 Hz
 AQ 1.3421773 sec
 RG 501.187
 DW 20.480 usec
 DE 6.50 usec
 TE 298.3 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 D31 0.00001300 sec
 D40 0.02898005 sec
 L4 40
 L5 57
 P32 90.00 usec
 TDO 3

===== CHANNEL f1 =====
 SFO1 75.4828392 MHz
 NUC1 13C
 P1 13.00 usec
 PLW1 22.0000000 W

===== CHANNEL f2 =====
 SFO2 300.1612006 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 9.3000019 W
 PLW12 0.25149000 W
 PLW13 0.12650000 W

F2 - Processing parameters
 SI 32768
 SF 75.4753339 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

3-(4-Bromophenylamino)-5-(4-phenethyl)-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one (4I)

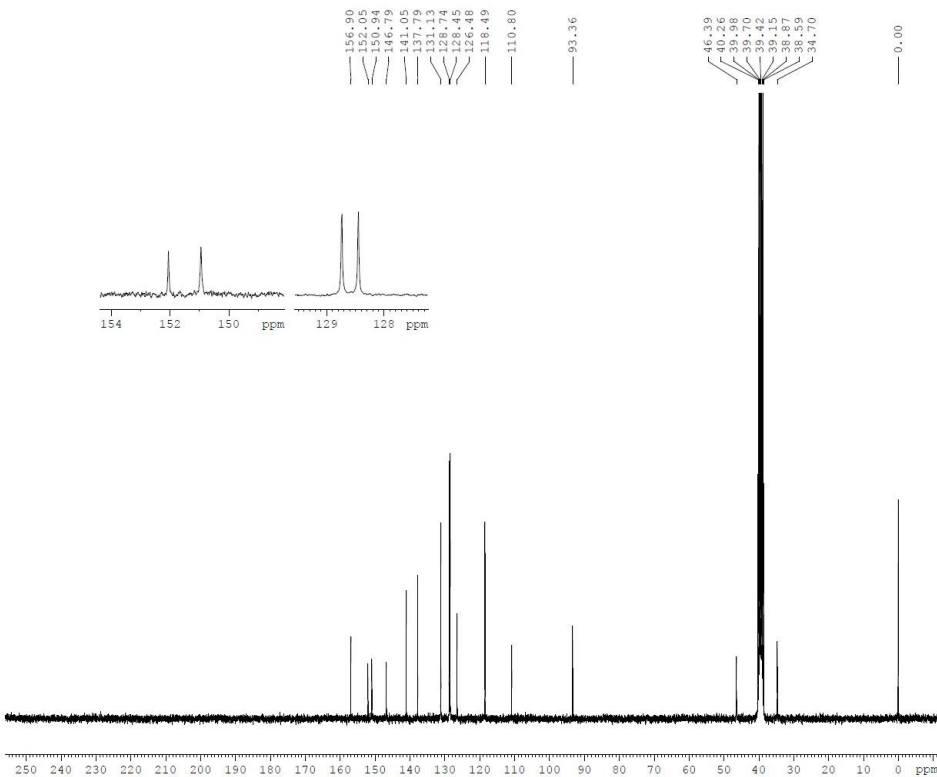


Current Data Parameters
 NAME JN220
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210319
 Time 14.54
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 6103.516 Hz
 FIDRES 0.093132 Hz
 AQ 5.3687091 sec
 RG 56.008
 DW 81.920 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.0000000 sec
 TD0 1

----- CHANNEL f1 -----
 SFO1 300.1618536 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 9.3000019 W

F2 - Processing parameters
 SI 65536
 SF 300.1599976 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME JN220
 EXPNO 6
 PROCNO 1

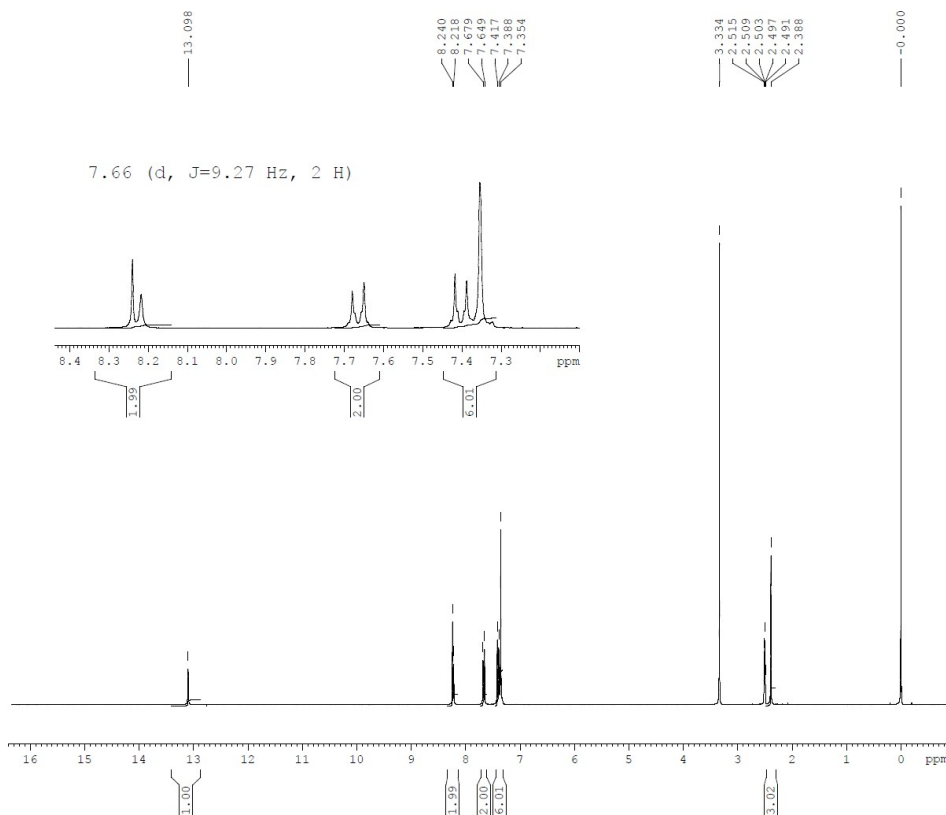
F2 - Acquisition Parameters
 Date_ 20210321
 Time 22.04
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 4096
 DS 4
 SWH 24414.063 Hz
 FIDRES 0.372529 Hz
 AQ 1.3421773 sec
 RG 501.187
 DW 20.480 usec
 DE 6.50 usec
 TE 298.3 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 D12 0.0000130 sec
 D40 0.0288005 sec
 L4 40
 L5 57
 P32 90.00 usec
 TD0 4

===== CHANNEL f1 =====
 SFO1 75.4828392 MHz
 NUC1 13C
 P1 13.00 usec
 PLW1 22.0000000 W

===== CHANNEL f2 =====
 SFO2 300.1612006 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 9.3000019 W
 PLW12 0.25149000 W
 PLW13 0.12650000 W

F2 - Processing parameters
 SI 32768
 SF 75.4753339 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

3-(4-Bromophenylamino)-5-(4-methylphenyl)-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one (4m)

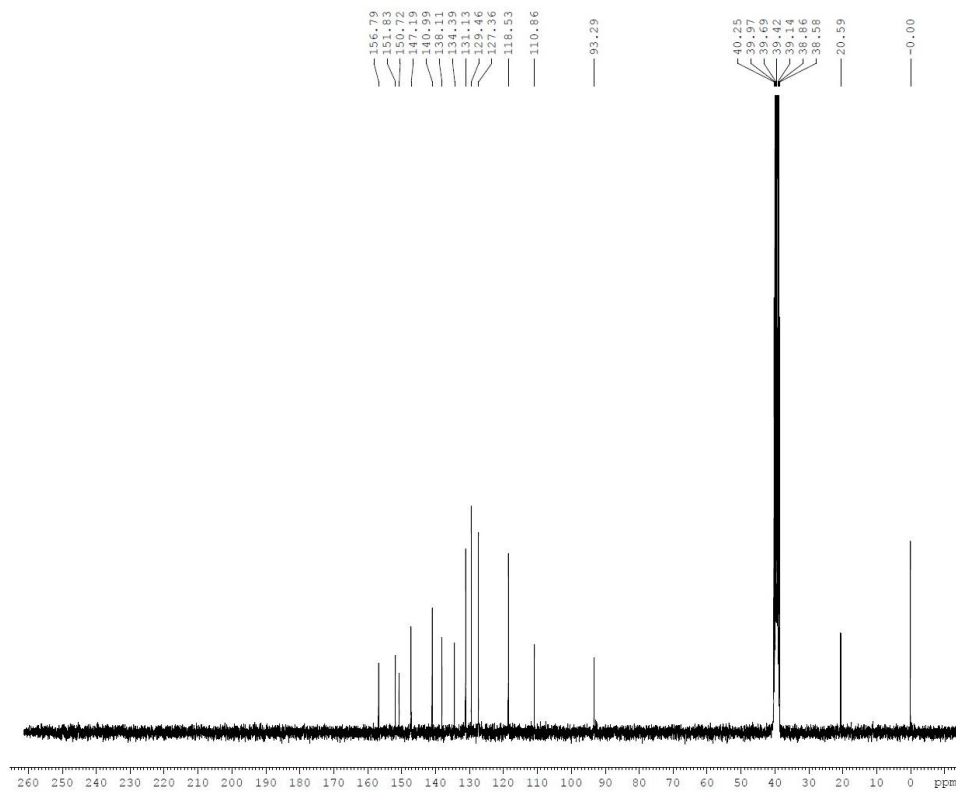


Current Data Parameters
 NAME JN216
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210318
 Time_ 13.31
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 6103.516 Hz
 FIDRES 0.093132 Hz
 AQ 5.3687091 sec
 RG 120.156
 DW 81.920 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 300.1618536 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 9.30000019 W

F2 - Processing parameters
 SI 65536
 SF 300.1599994 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME JN216
 EXPNO 4
 PROCNO 1

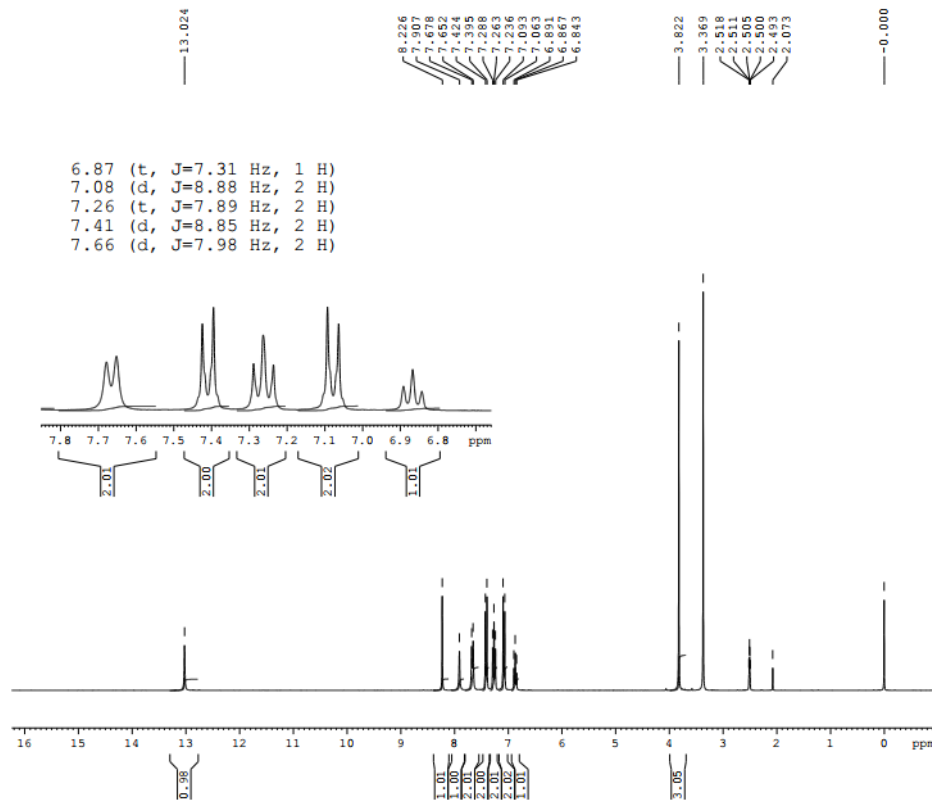
F2 - Acquisition Parameters
 Date_ 20210323
 Time_ 4.04
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 4096
 DS 4
 SWH 24414.063 Hz
 FIDRES 0.372529 Hz
 AQ 1.3421773 sec
 RG 501.187
 DW 20.480 usec
 DE 6.50 usec
 TE 298.3 K
 D1 2.00000000 sec
 D11 0.330000000 sec
 D31 0.00001300 sec
 D40 0.02898005 sec
 L4 40
 L5 57
 P32 90.00 usec
 TDO 4

===== CHANNEL f1 =====
 SFO1 75.4828392 MHz
 NUC1 13C
 P1 13.00 usec
 PLW1 22.00000000 W

===== CHANNEL f2 =====
 SFO2 300.1612006 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 9.30000019 W
 PLW12 0.25149000 W
 PLW13 0.12650000 W

F2 - Processing parameters
 SI 32768
 SF 75.4753347 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

5-(4-Methoxyphenyl)-3-phenylamino-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one (4n)

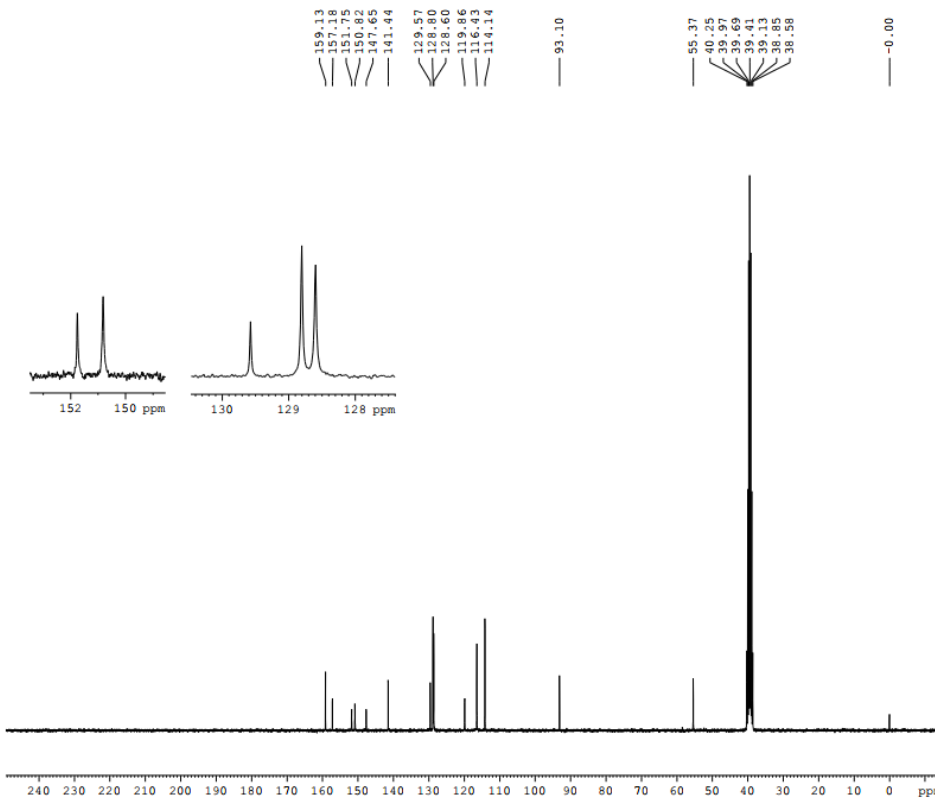


Current Data Parameters
 NAME JN123
 EXPNO 21
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20201016
 Time 10.16
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 6103.516 Hz
 FIDRES 0.093132 Hz
 AQ 5.3687091 sec
 RG 31.623
 DW 81.920 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

----- CHANNEL f1 -----
 SFO1 300.1618536 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 9.30000019 W

F2 - Processing parameters
 SI 65536
 SF 300.1599983 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME JN123
 EXPNO 22
 PROCNO 1

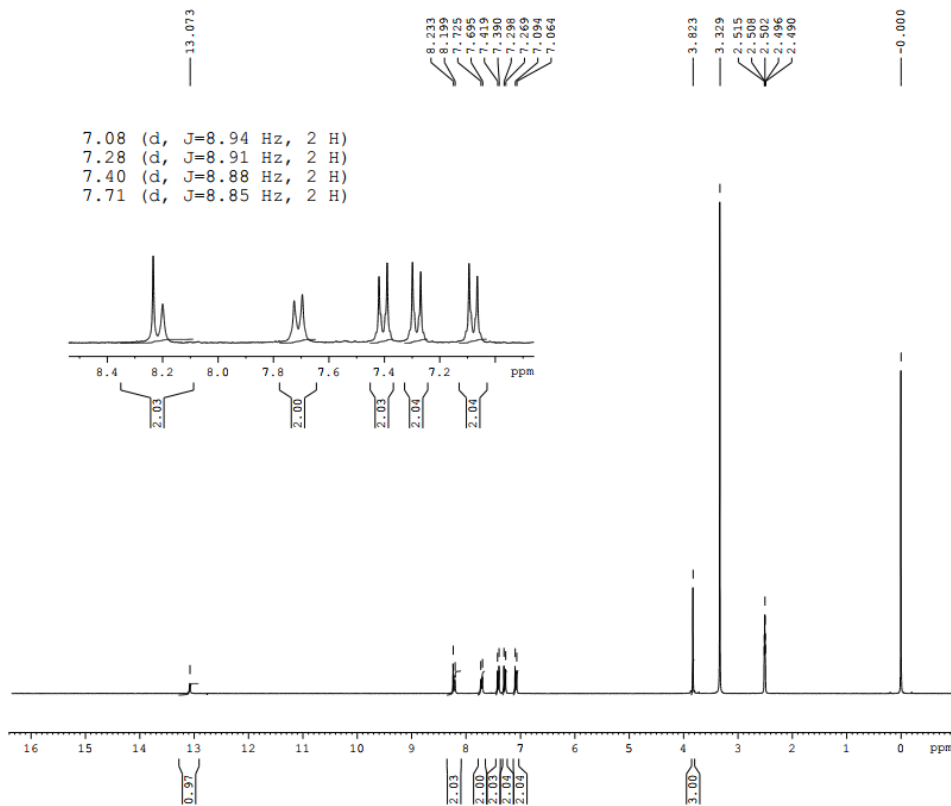
F2 - Acquisition Parameters
 Date_ 20201016
 Time 10.25
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 3072
 DS 4
 SWH 24414.063 Hz
 FIDRES 0.372529 Hz
 AQ 1.3421773 sec
 RG 501.187
 DW 20.480 usec
 DE 6.50 usec
 TE 298.3 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D31 0.00001300 sec
 D40 0.02898005 sec
 L4 40
 L5 57
 P32 90.00 usec
 TD0 3

----- CHANNEL f1 -----
 SFO1 75.4828392 MHz
 NUC1 13C
 P1 13.00 usec
 PLW1 22.00000000 W

----- CHANNEL f2 -----
 SFO2 300.1612006 MHz
 NUC2 1H
 CPDPRG2 waltz16
 FCF2 90.00 usec
 PLW2 9.30000019 W
 PLW12 0.25149000 W
 PLW13 0.12650000 W

F2 - Processing parameters
 SI 32768
 SF 75.4753338 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

3-(4-Chlorophenylamino)-5-(4-methoxyphenyl)-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one (4o)

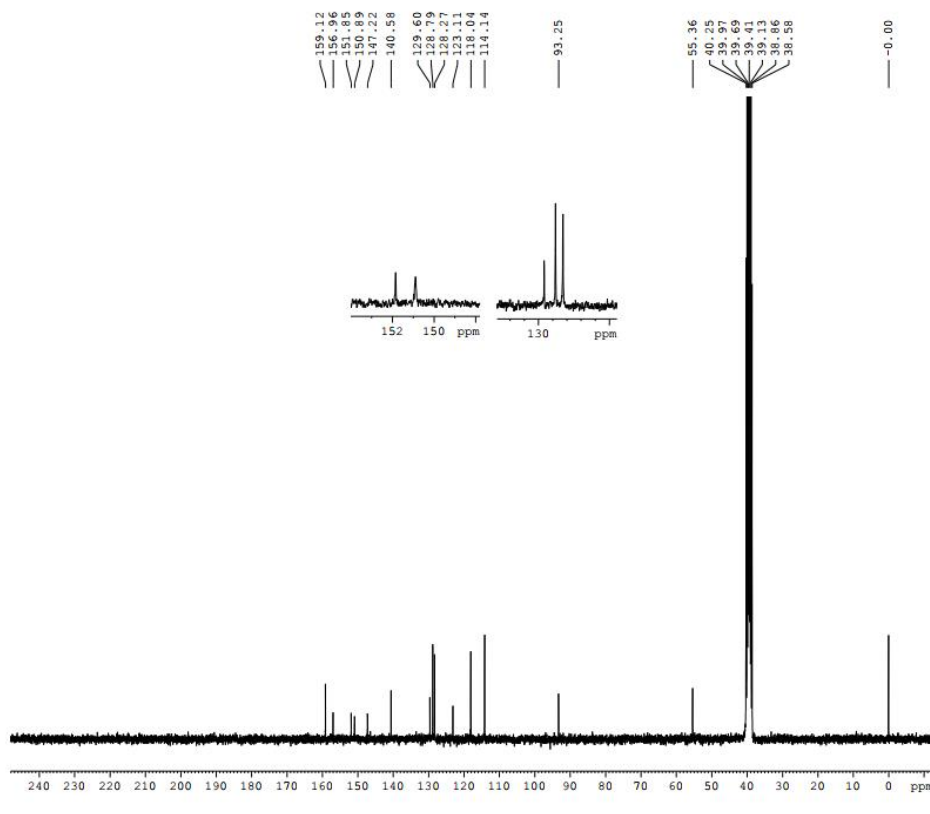


Current Data Parameters
 NAME JN122
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200915
 Time 10.08
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 6103.516 Hz
 FIDRES 0.093132 Hz
 AQ 5.3687091 sec
 RG 151.731
 DW 81.920 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 300.1618536 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 9.30000019 W

F2 - Processing parameters
 SI 65536
 SF 300.1599994 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME JN122
 EXPNO 6
 PROCNO 1

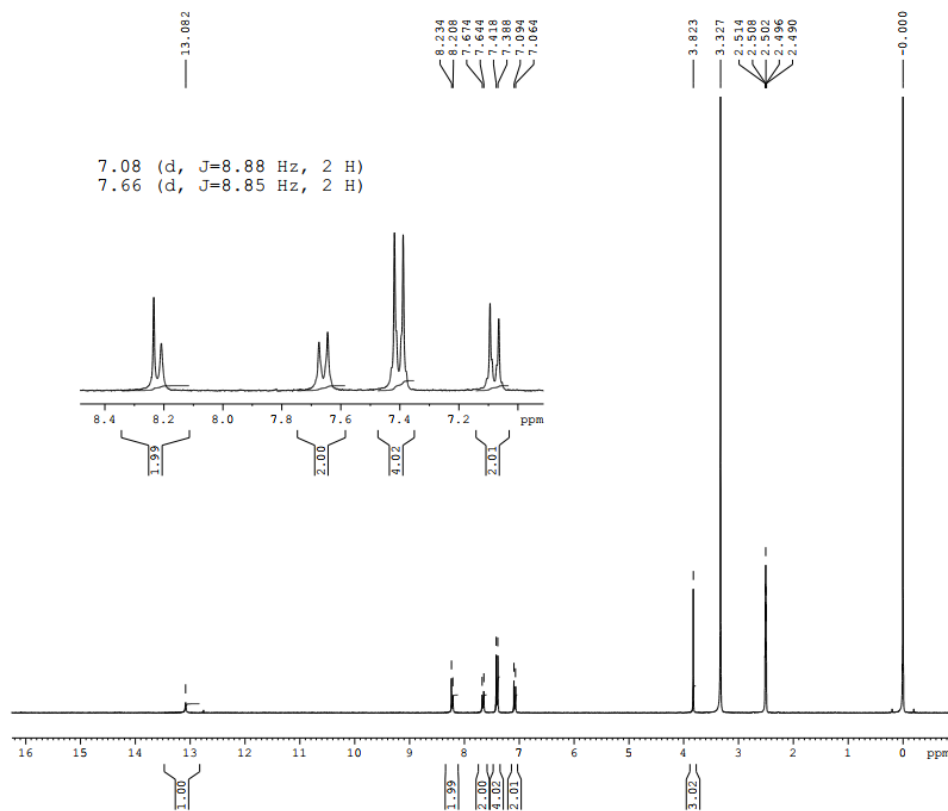
F2 - Acquisition Parameters
 Date_ 20200917
 Time 18.05
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 12288
 DS 4
 SWH 24414.063 Hz
 FIDRES 0.372529 Hz
 AQ 1.3421773 sec
 RG 501.187
 DW 20.480 usec
 DE 6.50 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D31 0.00001300 sec
 D40 0.02898005 sec
 L4 40
 L5 57
 P32 90.00 usec
 TD0 12

===== CHANNEL f1 =====
 SFO1 75.4828392 MHz
 NUC1 13C
 P1 13.00 usec
 PLW1 22.00000000 W

===== CHANNEL f2 =====
 SFO2 300.1612006 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 9.30000019 W
 PLW12 0.25149000 W
 PLW13 0.12650000 W

F2 - Processing parameters
 SI 32768
 SF 75.4753350 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

3-(4-Bromophenylamino)-5-(4-methoxyphenyl)-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one (4p)

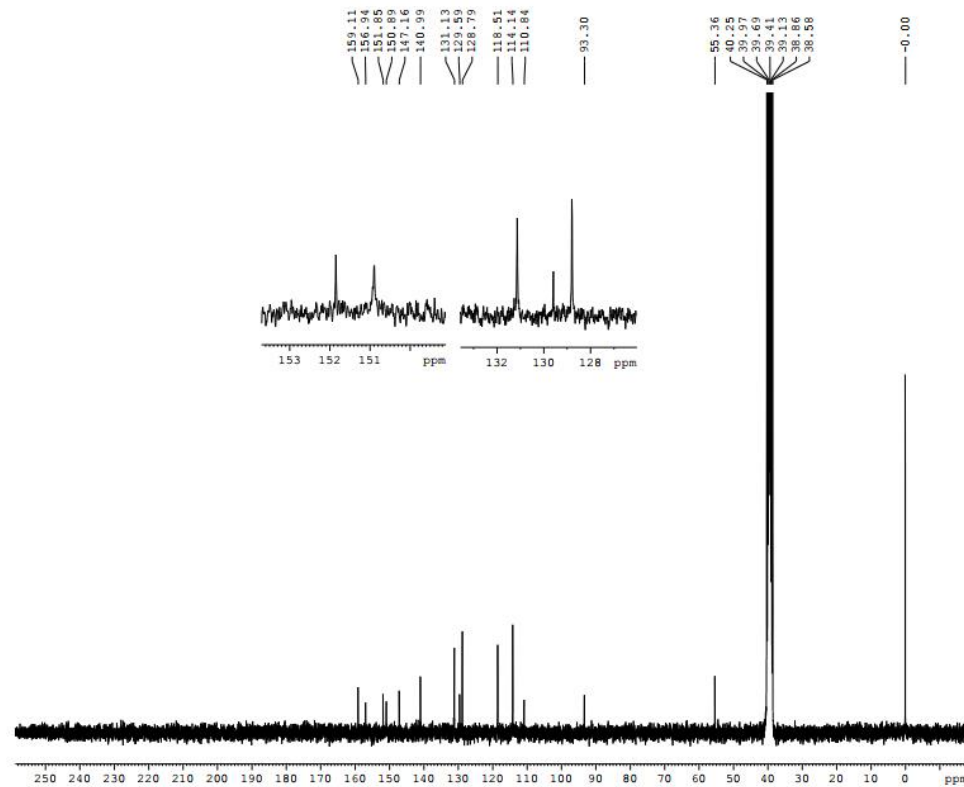


Current Data Parameters
 NAME JN204
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210323
 Time 11.41
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 6103.516 Hz
 FIDRES 0.093132 Hz
 AQ 5.3687091 sec
 RG 160.971
 DW 81.920 usec
 DE 6.50 usec
 TE 297.3 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SF01 300.1618536 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 9.30000019 W

F2 - Processing parameters
 SI 65536
 SF 300.1599994 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME JN204
 EXPNO 6
 PROCNO 1

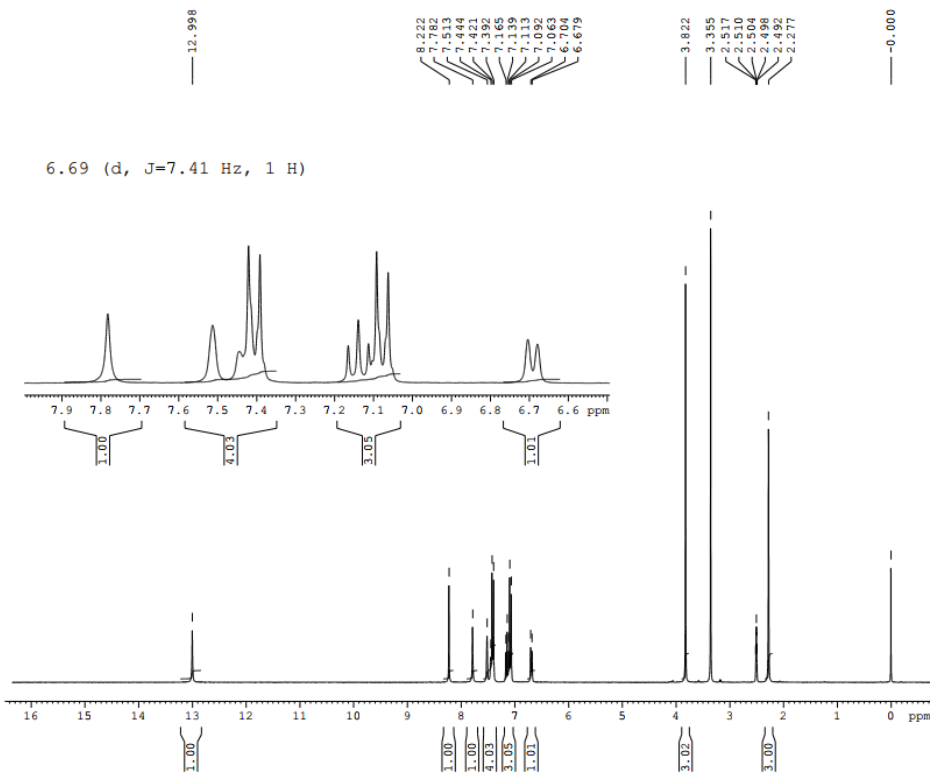
F2 - Acquisition Parameters
 Date_ 20210323
 Time 18.05
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 12288
 DS 4
 SWH 24414.063 Hz
 FIDRES 0.372529 Hz
 AQ 1.3421773 sec
 RG 501.187
 DW 20.480 usec
 DE 6.50 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D31 0.00001300 sec
 D40 0.02898005 sec
 L4 40
 L5 57
 F32 90.00 usec
 TD0 12

----- CHANNEL f1 -----
 SF01 75.4828392 MHz
 NUC1 13C
 P1 13.00 usec
 PLW1 22.00000000 W

----- CHANNEL f2 -----
 SF02 300.1612006 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLM2 9.30000019 W
 PLW12 0.25149000 W
 PLW13 0.12650000 W

F2 - Processing parameters
 SI 32768
 SF 75.4753352 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

5-(4-Methoxyphenyl)-3-(3-methylphenylamino)-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one (4q)

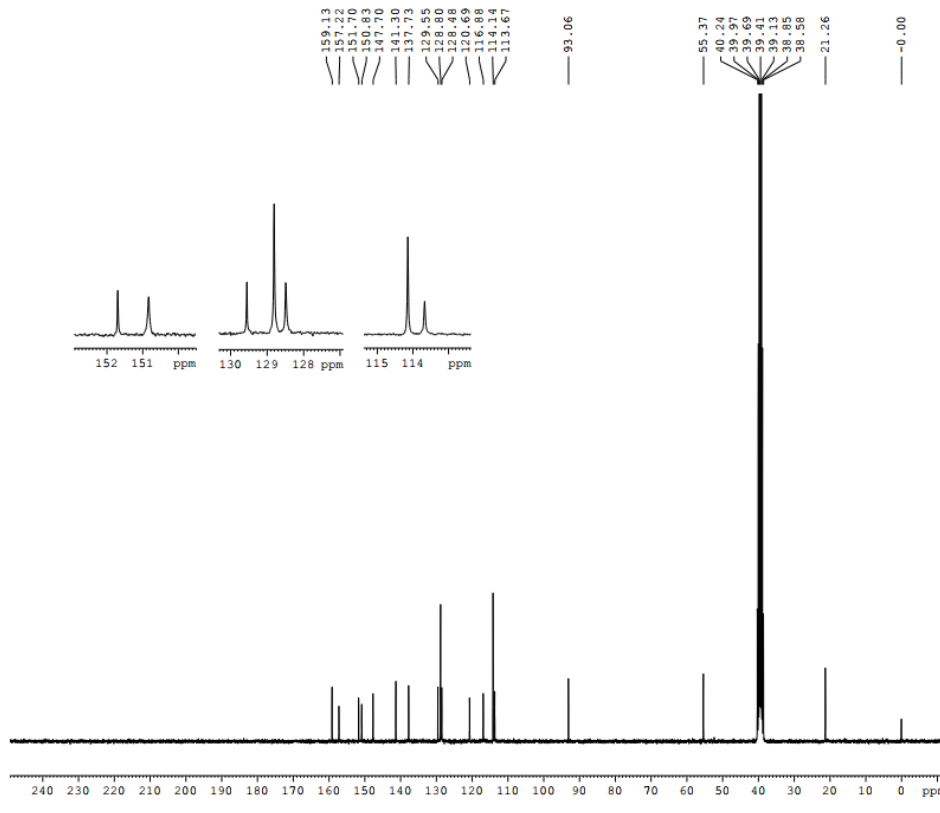


Current Data Parameters
 NAME JN203
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210304
 Time 14.38
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 6103.516 Hz
 FIDRES 0.093132 Hz
 AQ 5.3687091 sec
 RG 56.2431
 DW 81.920 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 300.1618536 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 9.30000019 W

F2 - Processing parameters
 SI 65536
 SF 300.1599988 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME JN203
 EXPNO 4
 PROCNO 1

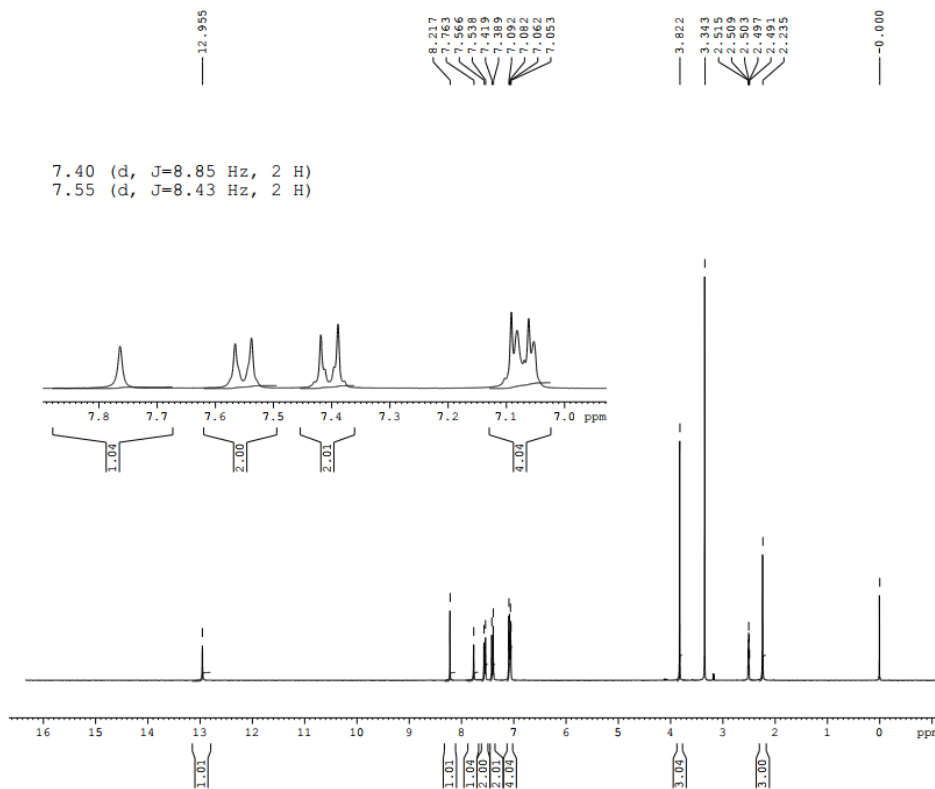
F2 - Acquisition Parameters
 Date_ 20210314
 Time 12.08
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 5120
 DS 4
 SWH 24414.063 Hz
 FIDRES 0.372529 Hz
 AQ 1.3421773 sec
 RG 501.187
 DW 20.480 usec
 DE 6.50 usec
 TE 298.3 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D31 0.00001300 sec
 D40 0.02898005 sec
 L4 40
 L5 57
 P32 90.00 usec
 TDO 5

===== CHANNEL f1 =====
 SFO1 75.4828392 MHz
 NUC1 13C
 P1 13.00 usec
 PLW1 22.00000000 W

===== CHANNEL f2 =====
 SFO2 300.1612006 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 9.30000019 W
 PLW12 0.25149000 W
 PLW13 0.12650000 W

F2 - Processing parameters
 SI 32768
 SF 75.4753339 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

5-(4-Methoxyphenyl)-3-(4-methylphenylamino)-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one (4r)

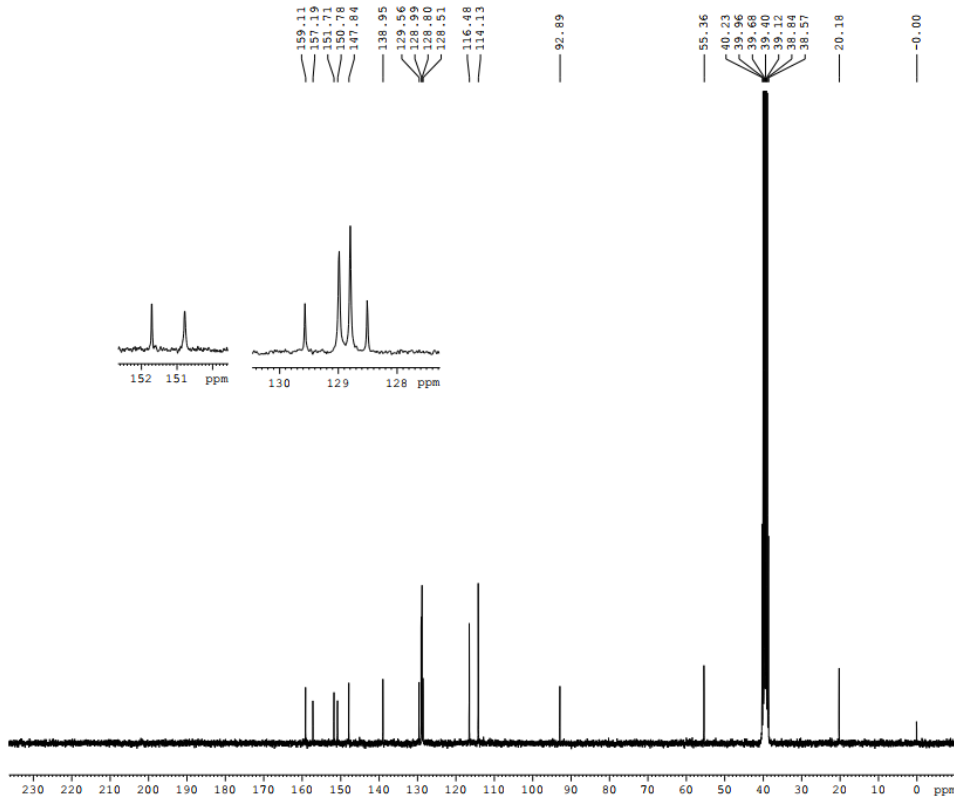


Current Data Parameters
 NAME JN205
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210227
 Time 14.09
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 6103.516 Hz
 FIDRES 0.093132 Hz
 AQ 5.3687091 sec
 RG 83.0129
 DW 81.920 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 300.1618536 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 9.30000019 W

F2 - Processing parameters
 SI 65536
 SF 300.1599992 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME JN205
 EXPNO 4
 PROCNO 1

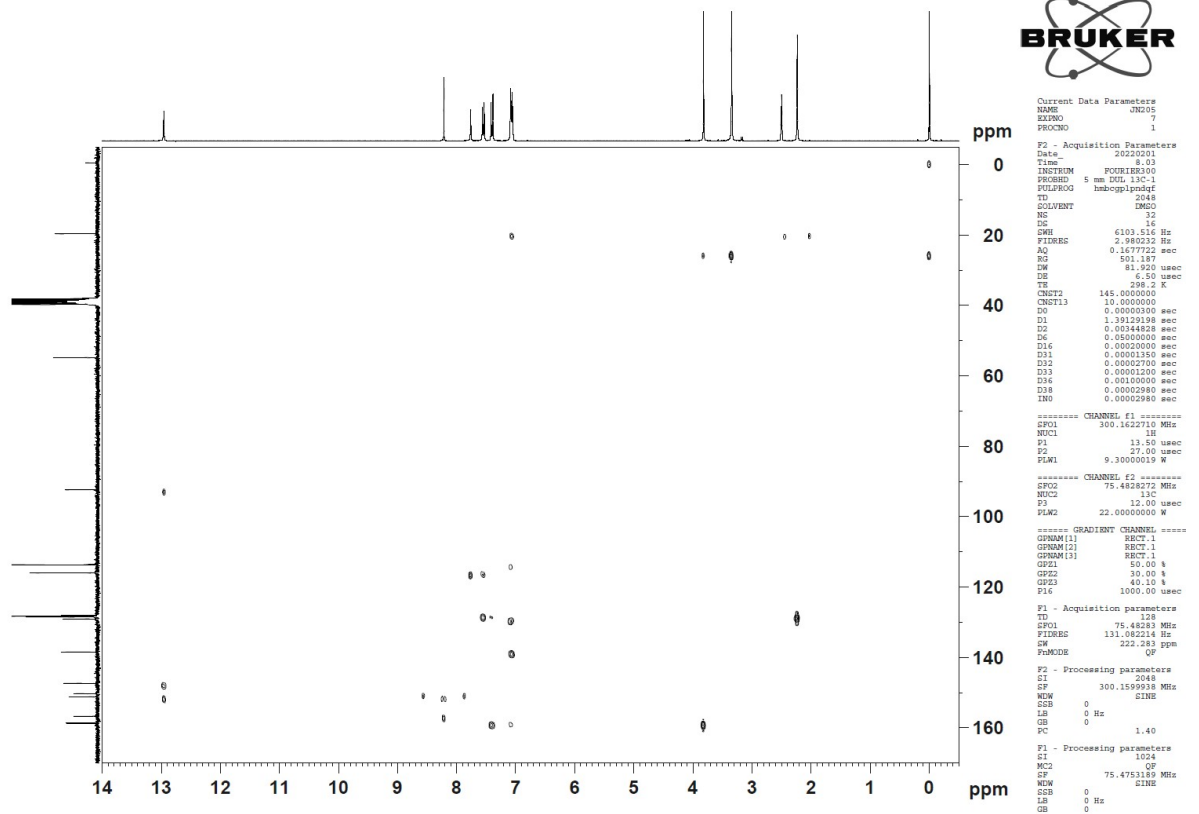
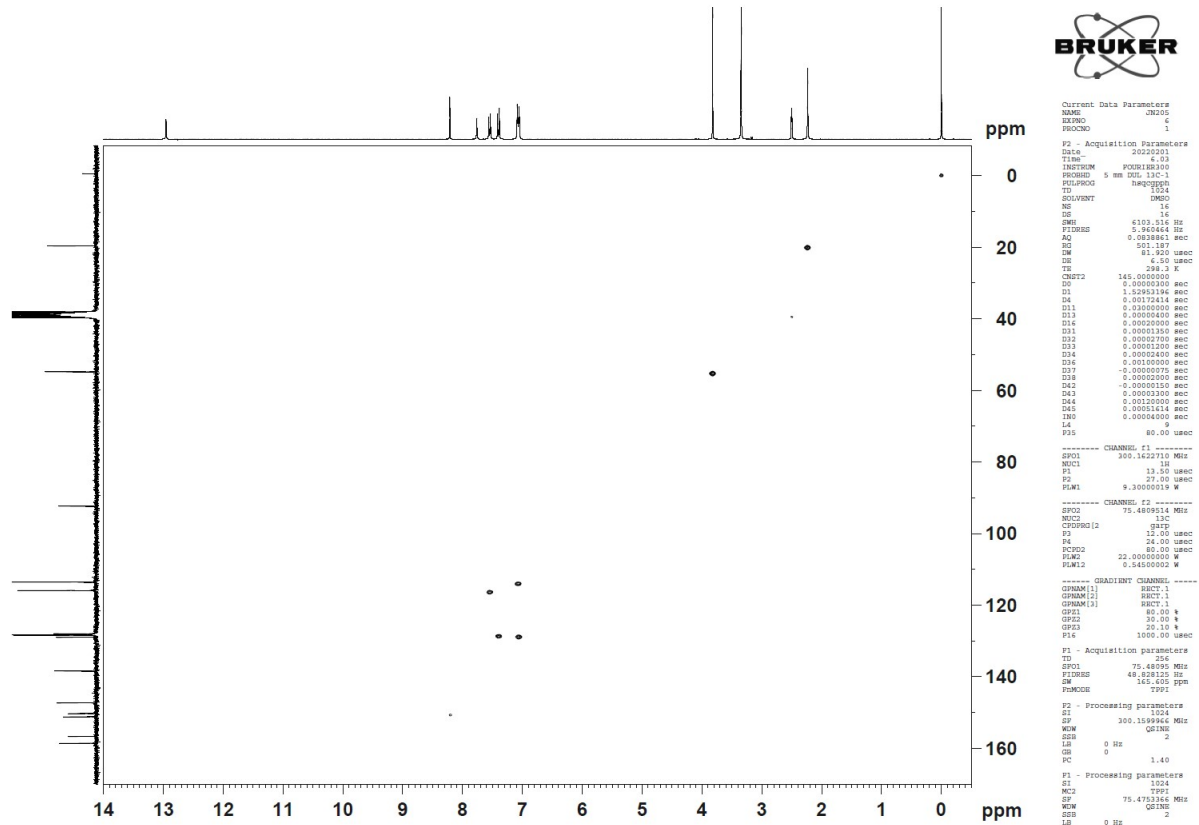
F2 - Acquisition Parameters
 Date_ 20210313
 Time 13.04
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 4096
 DS 4
 SWH 24414.063 Hz
 FIDRES 0.372529 Hz
 AQ 1.3421773 sec
 RG 501.187
 DW 20.480 usec
 DE 6.50 usec
 TE 298.3 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D31 0.00001300 sec
 D40 0.02898005 sec
 L4 40
 L5 57
 P32 90.00 usec
 TD0 4

===== CHANNEL f1 =====
 SFO1 75.4828392 MHz
 NUC1 13C
 P1 13.00 usec
 PLW1 22.00000000 W

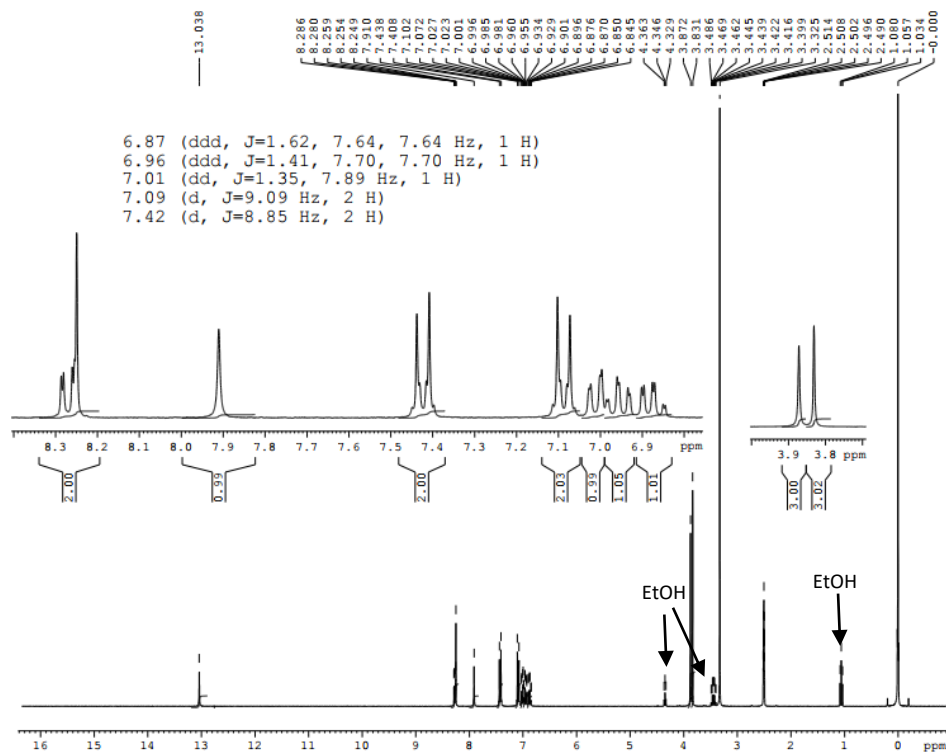
===== CHANNEL f2 =====
 SFO2 300.1612006 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 9.30000019 W
 PLW12 0.25149000 W
 PLW13 0.12650000 W

F2 - Processing parameters
 SI 32768
 SF 75.4753345 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

5-(4-Methoxyphenyl)-3-(4-methylphenylamino)-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one (4r)



3-(2-Methoxyphenylamino)-5-(4-methoxyphenyl)-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one (4s)

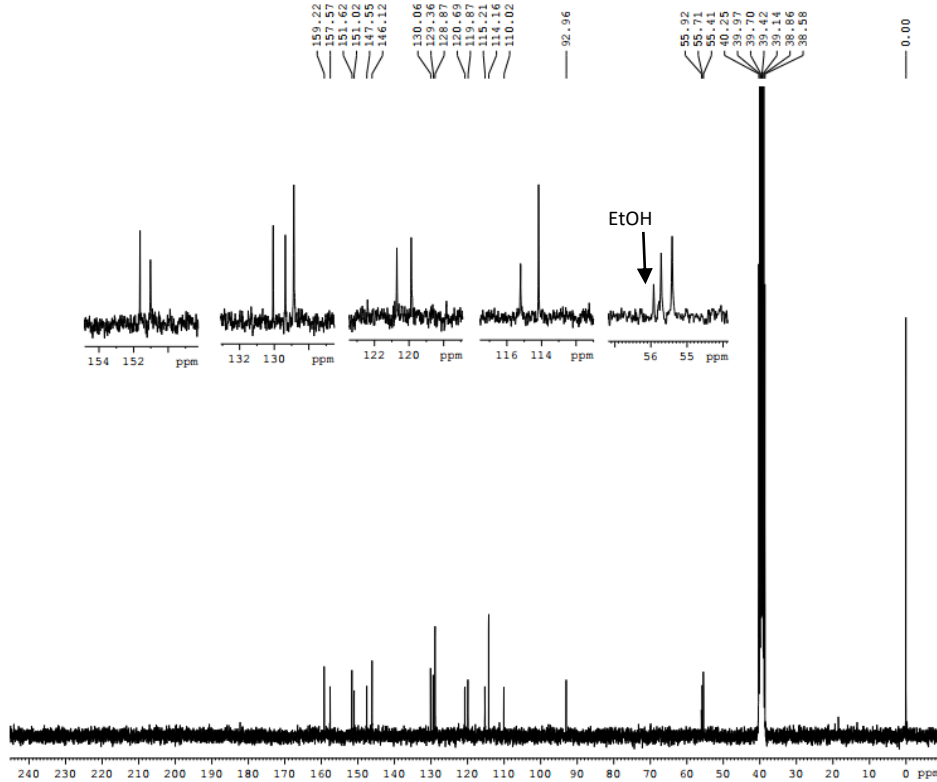


Current Data Parameters
 NAME JN202
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210319
 Time 14.45
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 6103.516 Hz
 FIDRES 0.093132 Hz
 AQ 5.3687091 sec
 RG 106.345
 DW 81.920 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.0000000 sec
 TDO 1

CHANNEL f1
 SFO1 300.1618536 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 9.30000019 W

F2 - Processing parameters
 SI 65536
 SF 300.1599994 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME JN202
 EXPNO 6
 PROCNO 1

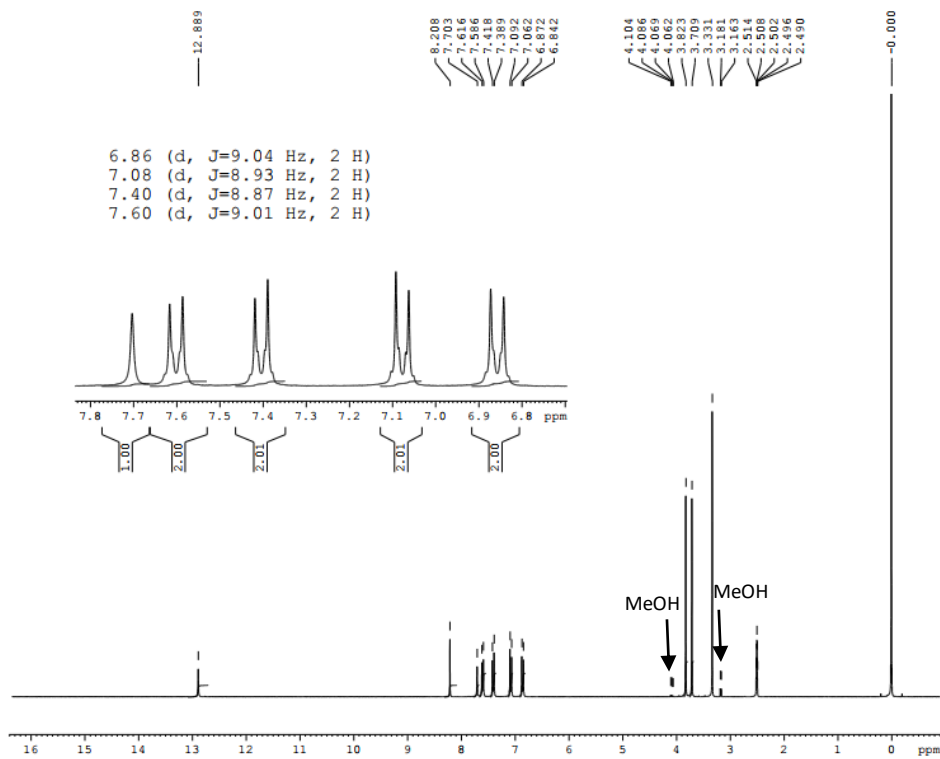
F2 - Acquisition Parameters
 Date_ 20210321
 Time 18.04
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 4096
 DS 4
 SWH 24414.063 Hz
 FIDRES 0.372529 Hz
 AQ 1.3421773 sec
 RG 501.187
 DW 20.480 usec
 DE 6.50 usec
 TE 298.3 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 D31 0.0001300 sec
 D40 0.02898005 sec
 I4 40
 L5 57
 F32 90.00 usec
 TDO 4

CHANNEL f1
 SFO1 75.4828392 MHz
 NUC1 13C
 P1 13.00 usec
 PLW1 22.00000000 W

CHANNEL f2
 SFO2 300.1612006 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 9.30000019 W
 PLW12 0.25149000 W
 PLW13 0.12650000 W

F2 - Processing parameters
 SI 32768
 SF 75.4753346 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

3-(4-Methoxyphenylamino)-5-(4-methoxyphenyl)-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one (4t)

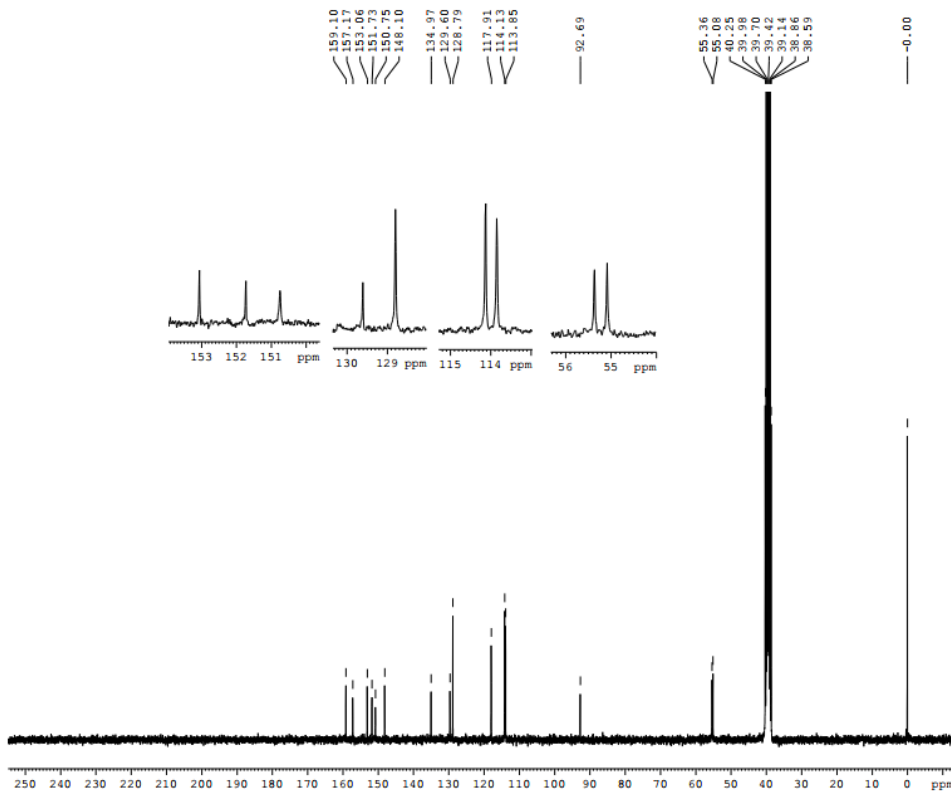


Current Data Parameters
 NAME JN206
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210319
 Time 14.49
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 6103.516 Hz
 FIDRES 0.093132 Hz
 AQ 5.3687091 sec
 RG 87.9148
 DW 81.920 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TDO 1

----- CHANNEL f1 -----
 SFO1 300.1618536 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 9.30000019 W

F2 - Processing parameters
 SI 65536
 SF 300.1599993 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME JN206
 EXPNO 6
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210321
 Time 5.42
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 6144
 DS 4
 SWH 24414.063 Hz
 FIDRES 0.372529 Hz
 AQ 1.3421773 sec
 RG 501.187
 DW 20.480 usec
 DE 6.50 usec
 TE 298.3 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D31 0.00001300 sec
 D40 0.02898005 sec
 L4 40
 L5 57
 P32 90.00 usec
 TDO 6

----- CHANNEL f1 -----
 SFO1 75.4828392 MHz
 NUC1 13C
 P1 13.00 usec
 PLW1 22.00000000 W

----- CHANNEL f2 -----
 SFO2 300.1612006 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLM2 9.30000019 W
 PLW12 0.25149000 W
 PLW13 0.12650000 W

F2 - Processing parameters
 SI 32768
 SF 75.4753346 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40