

Supporting Information
for
**Quinolines from the cyclocondensation of isatoic
anhydride with ethyl acetoacetate: preparation of ethyl
4-hydroxy-2-methylquinoline-3-carboxylate and
derivatives**

Nicholas G. Jentsch, Jared D. Hume, Emily B. Crull, Samer M. Beauti, Amy H. Pham,
Julie A. Pigza, Jacques J. Kessl and Matthew G. Donahue*

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Mississippi, 118 College Drive #5043, Hattiesburg, MS 39406

Email: Matthew G. Donahue – matthew.donahue@usm.edu

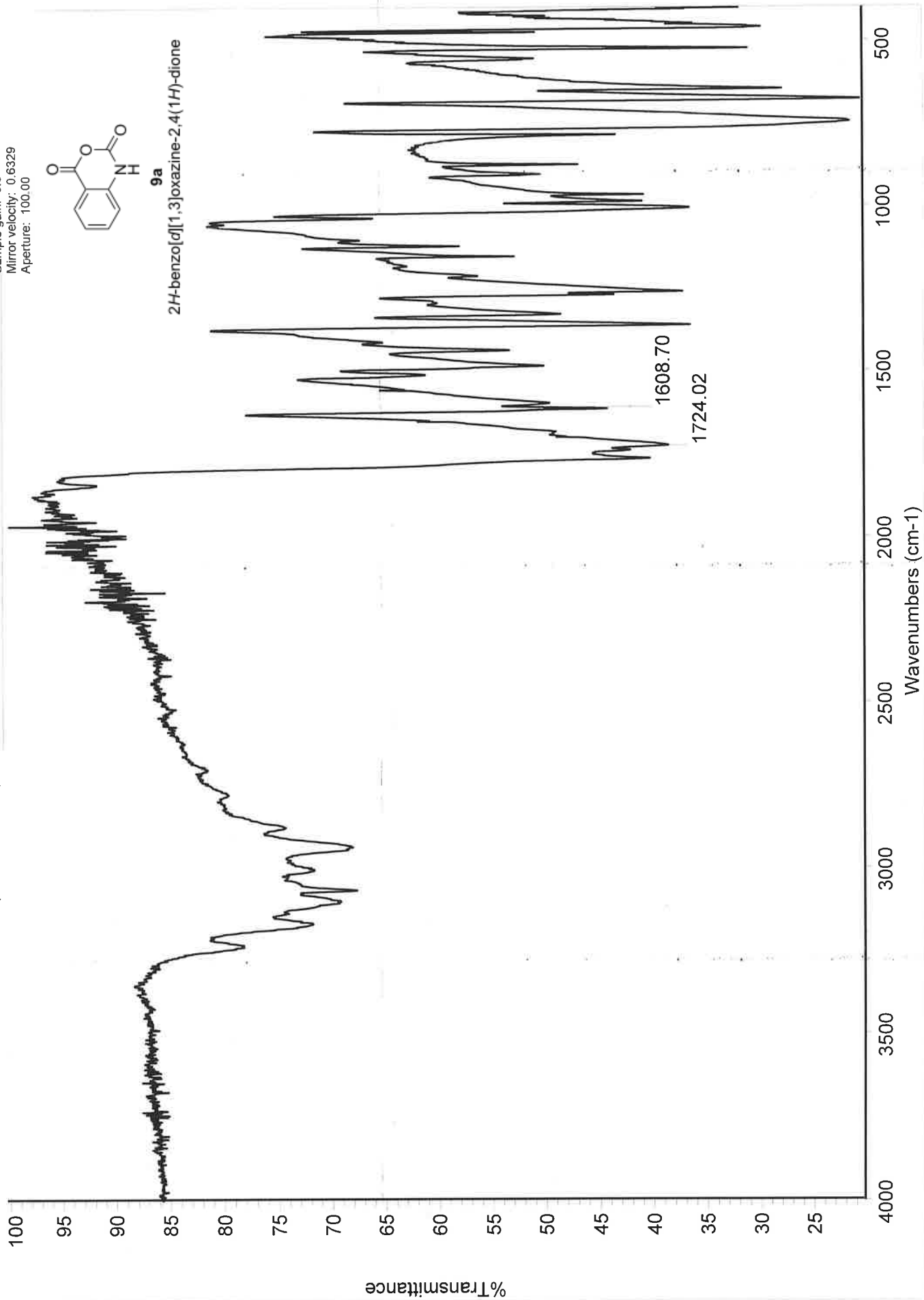
* Corresponding author

IR, NMR and mass spectra, as well as elemental analyses

AHP-1-017

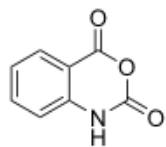
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Sample gain: 8.0
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Aperture: 100.00



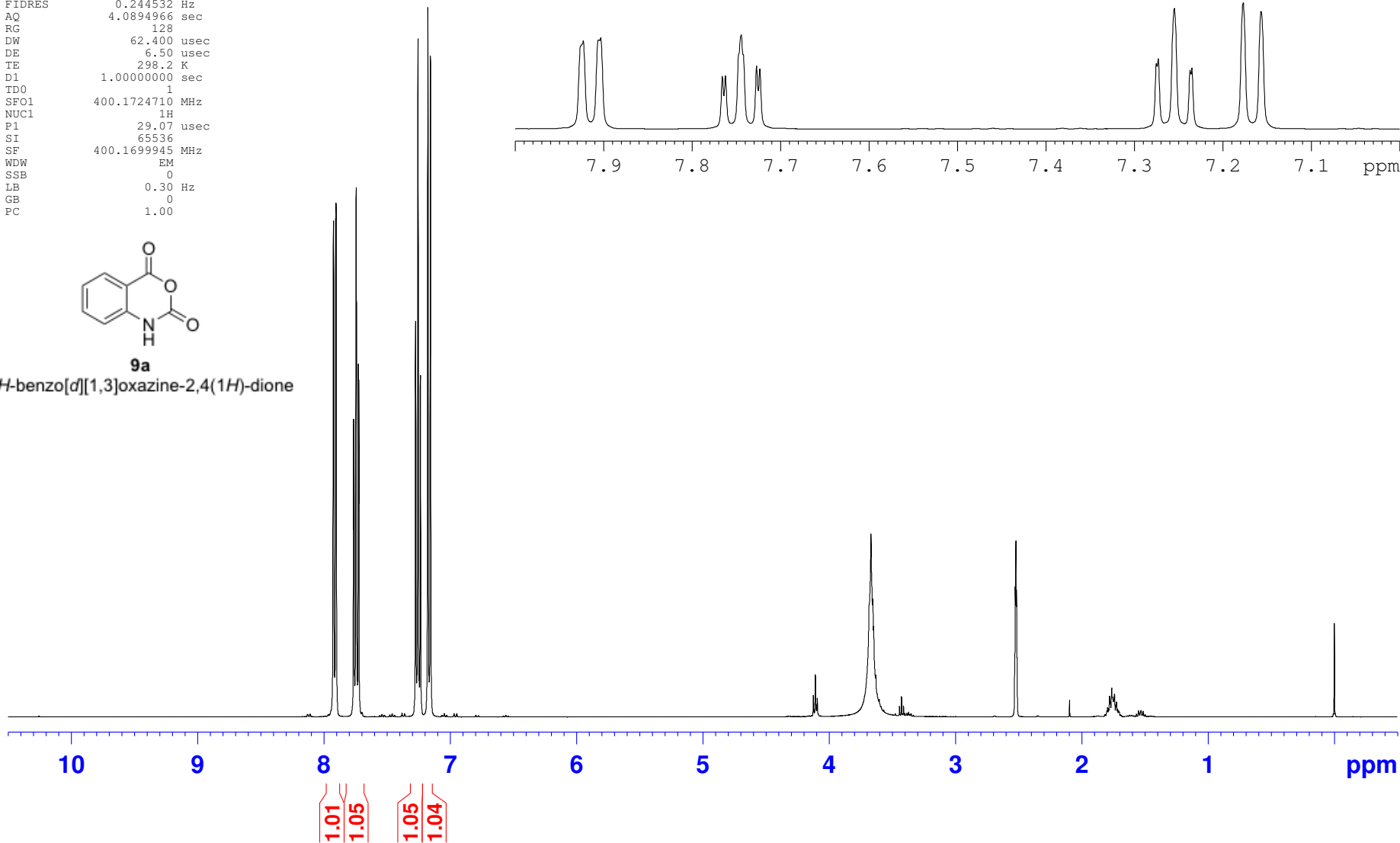
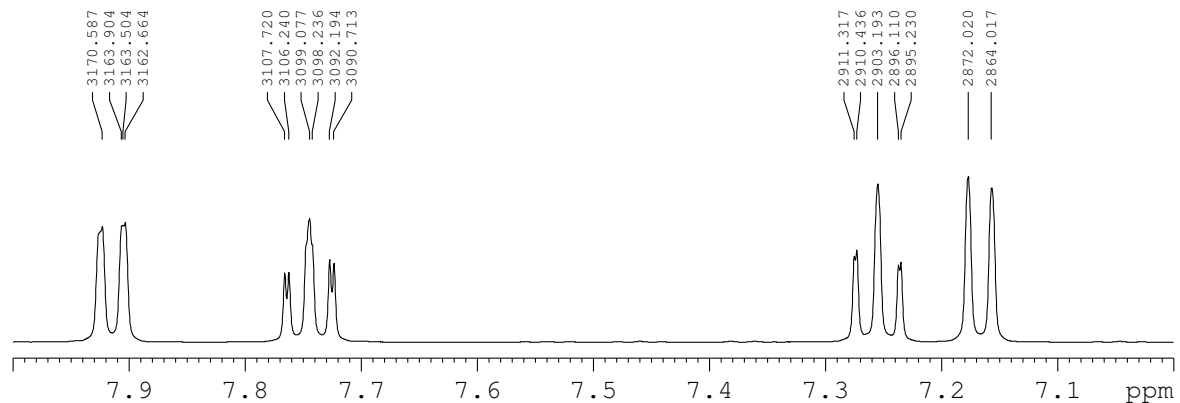
AHP-1-017 (DMSO, 400 MHz) Pure White Solid- Isatoic anhydride synthesis

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 PROCNO 1
 Date_ 20161202
 Time 19.50 h
 INSTRUM spect
 PROBHD Z108618_0161 (
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894966 sec
 RG 128
 DW 62.400 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.1724710 MHz
 NUC1 1H
 P1 29.07 usec
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 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

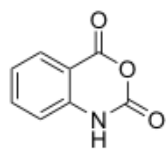


9a

2H-benzo[d][1,3]oxazine-2,4(1H)-dione

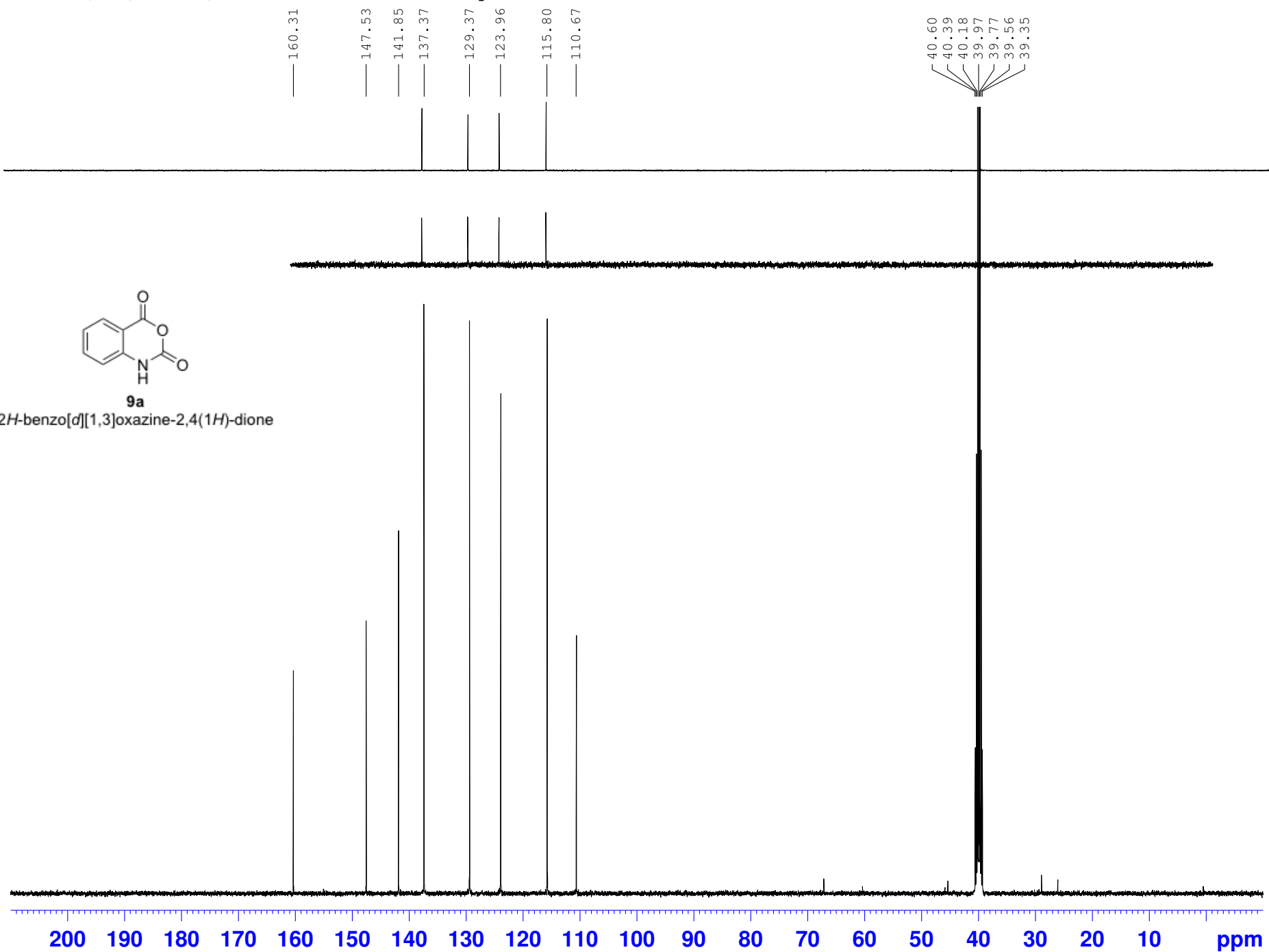


AHP-1-017 (DMSO, 400 MHz) Pure White Solid- Isatoic anhydride

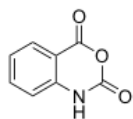


9a

2*H*-benzo[d][1,3]oxazine-2,4(1*H*)-dione

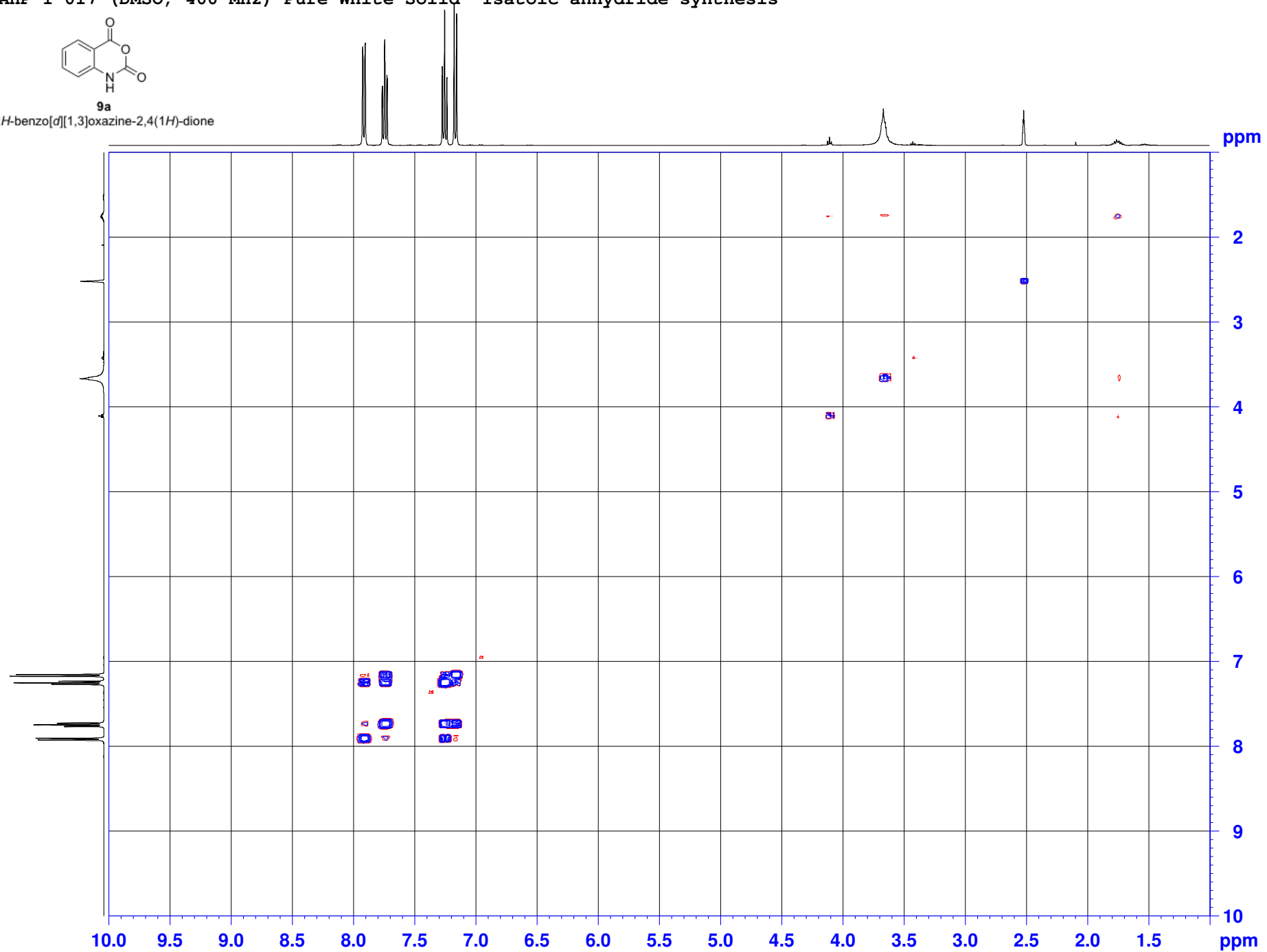


AHP-1-017 (DMSO, 400 MHz) Pure White Solid- Isatoic anhydride synthesis

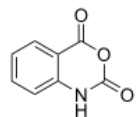


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2H-benzo[d][1,3]oxazine-2,4(1H)-dione

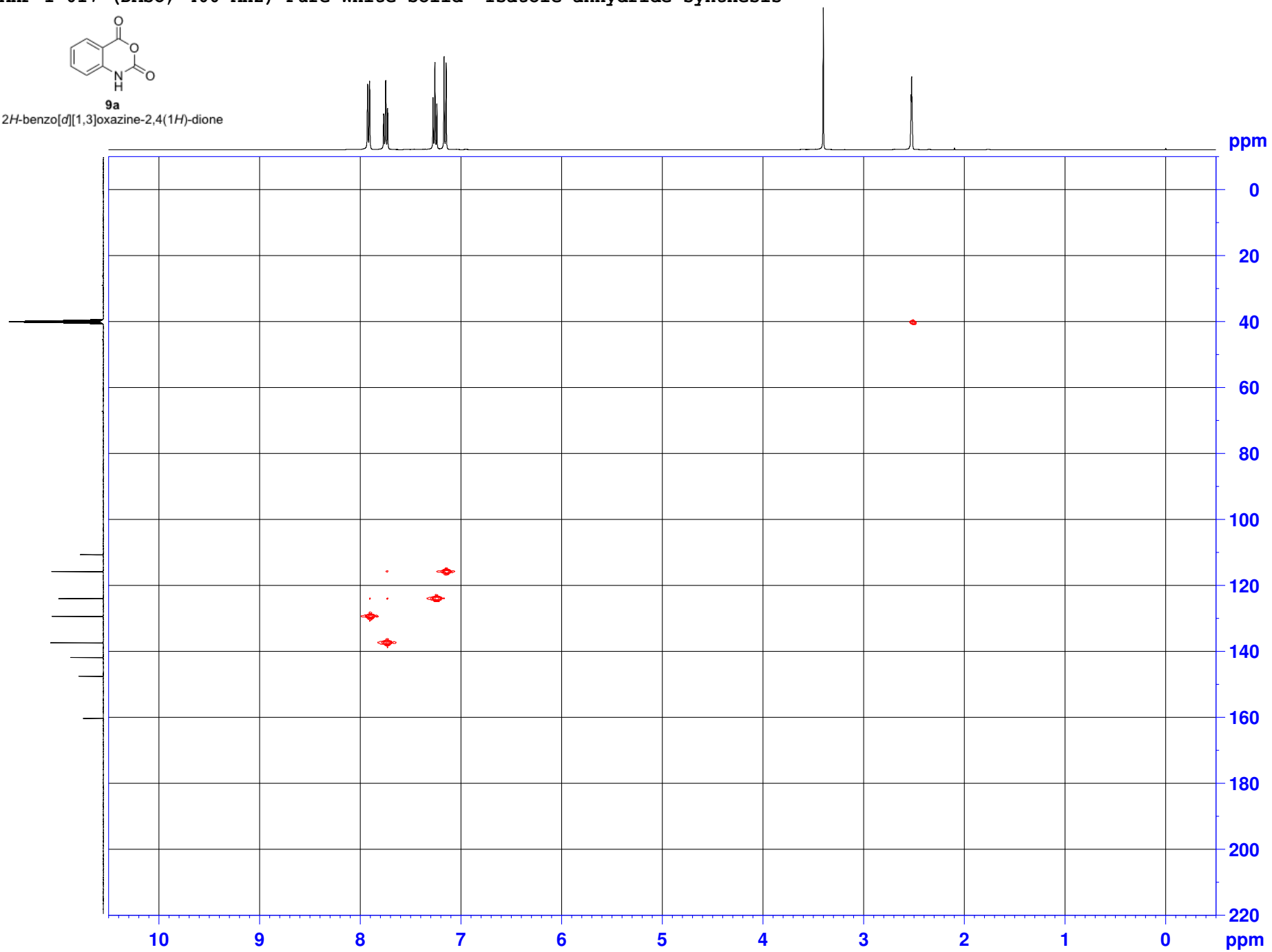


AHP-1-017 (DMSO, 400 MHz) Pure White Solid- Isatoic anhydride synthesis

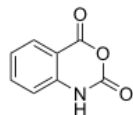


9a

2*H*-benzo[d][1,3]oxazine-2,4(1*H*)-dione

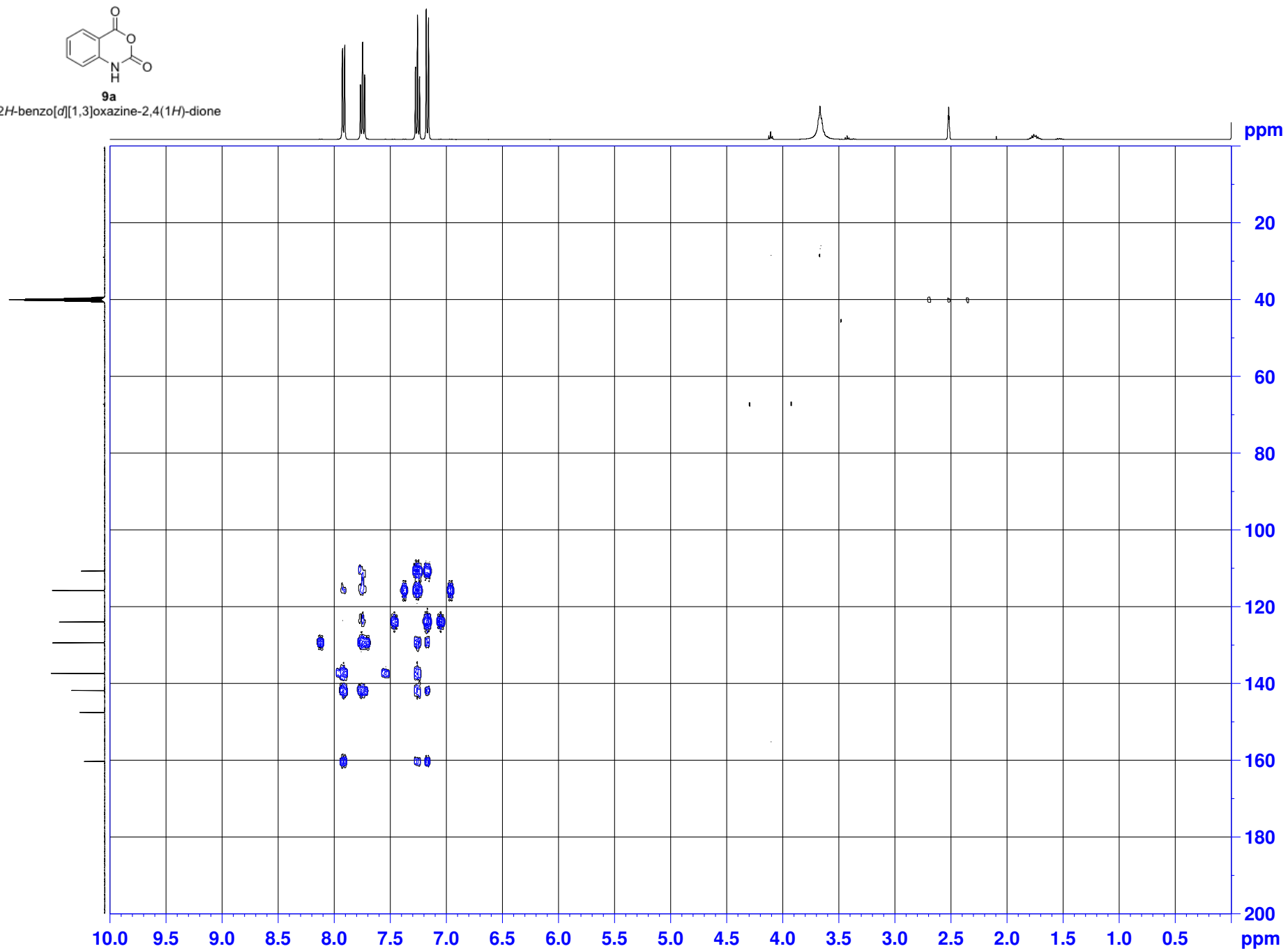


AHP-1-017 (DMSO, 400 MHz) Pure White Solid- Isatoic anhydride synthesis



9a

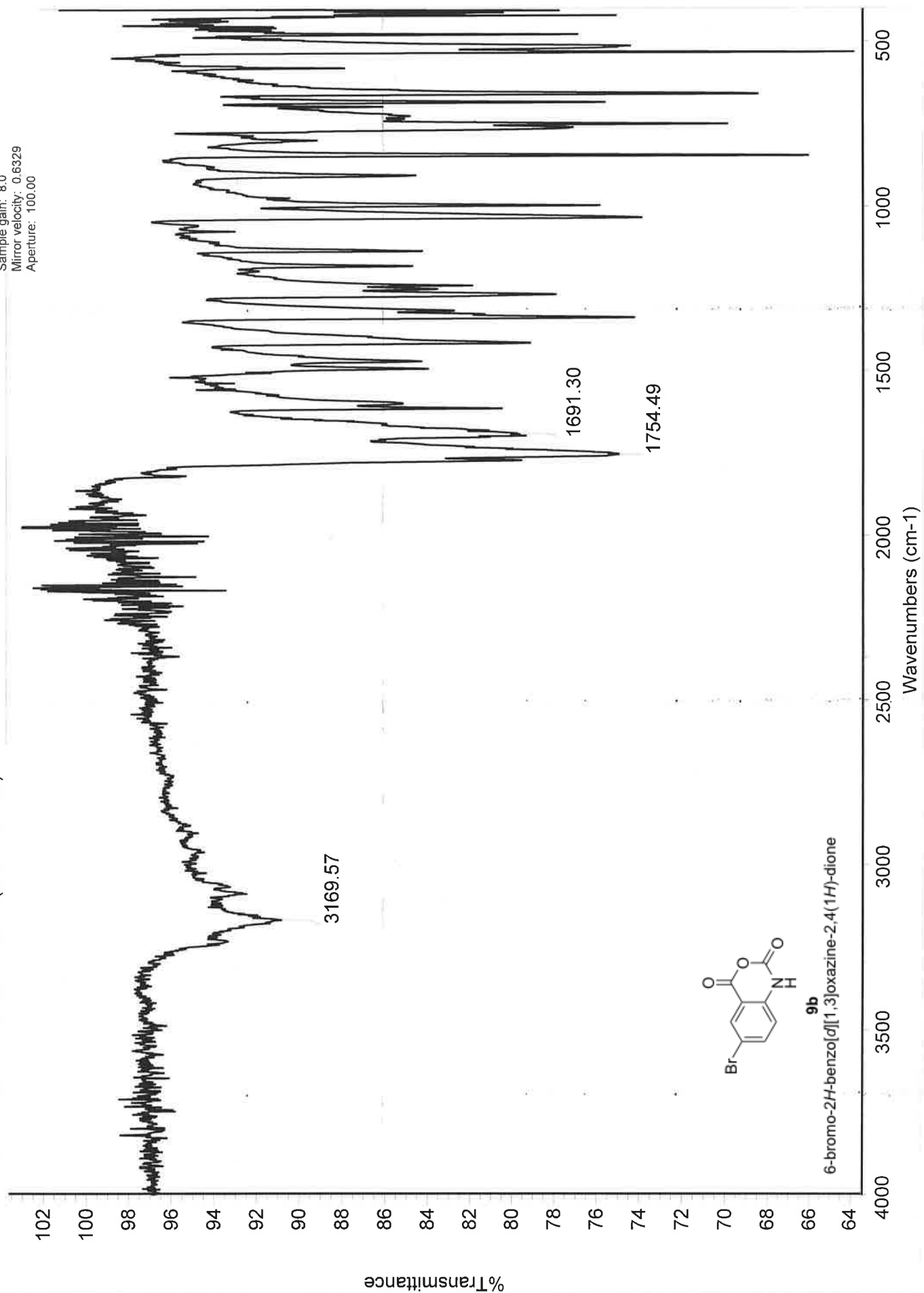
2H-benzo[d][1,3]oxazine-2,4(1H)-dione



SMB-1-012

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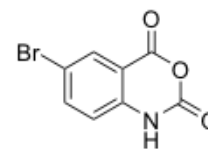
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Number of background scans: 8
Resolution: 2.000
Sample gain: 8.0
Mirror velocity: 0.6329
Aperture: 100.00



SMB-1-012 (DMSO, 400 MHz) Isotoic anhydride
PROTON DMSO {C:\Bruker\TOPSPIN} Donahue 1

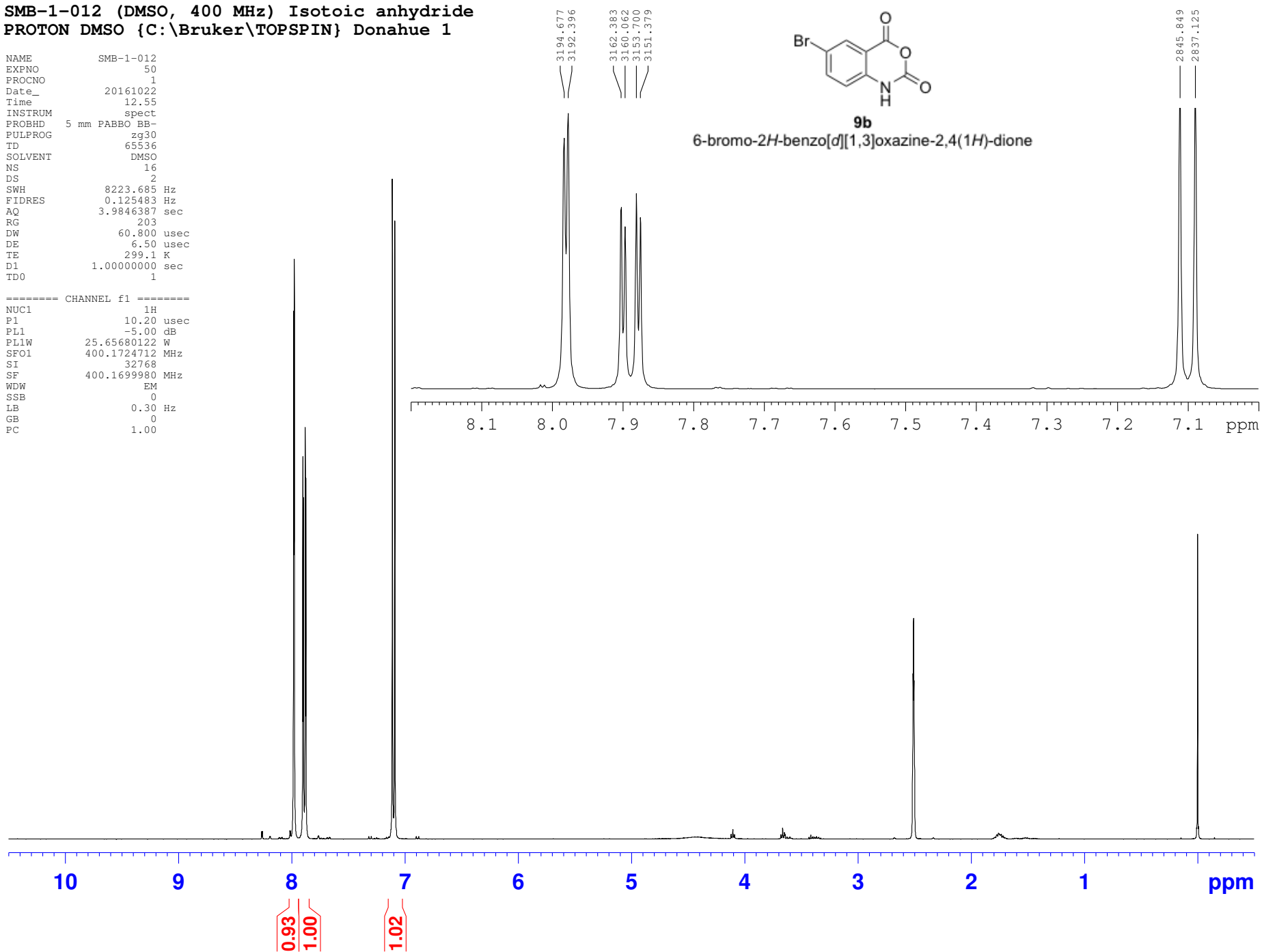
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Time 12.55
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PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 299.1 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.20 usec
PL1 -5.00 dB
PL1W 25.65680122 W
SFO1 400.1724712 MHz
SI 32768
SF 400.1699980 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

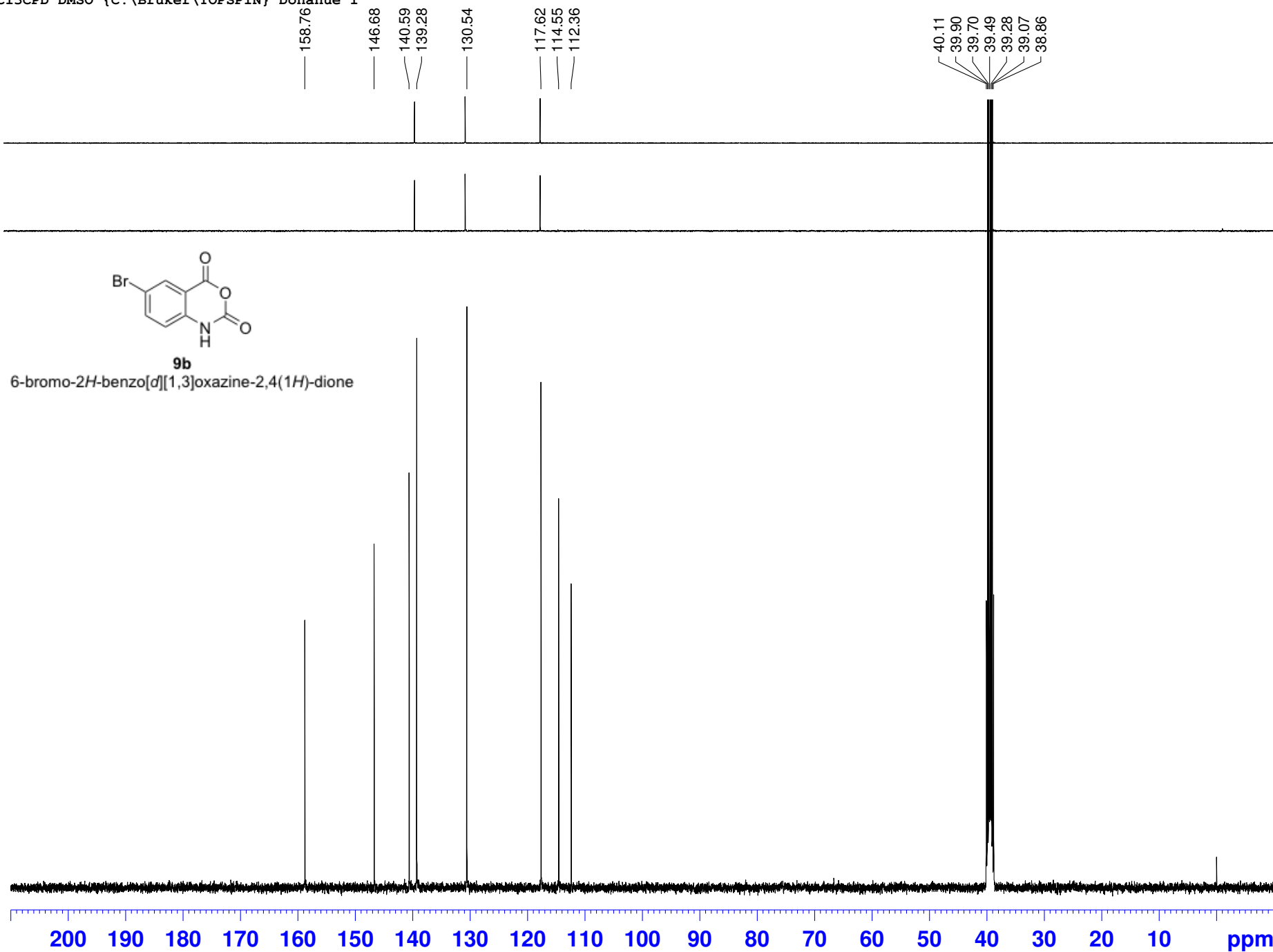


9b

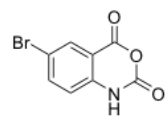
6-bromo-2H-benzo[d][1,3]oxazine-2,4(1H)-dione



SMB-1-012 (DMSO, 400 MHz) Isotoic anhydride
C13CPD DMSO {C:\Bruker\TOPSPIN} Donahue 1

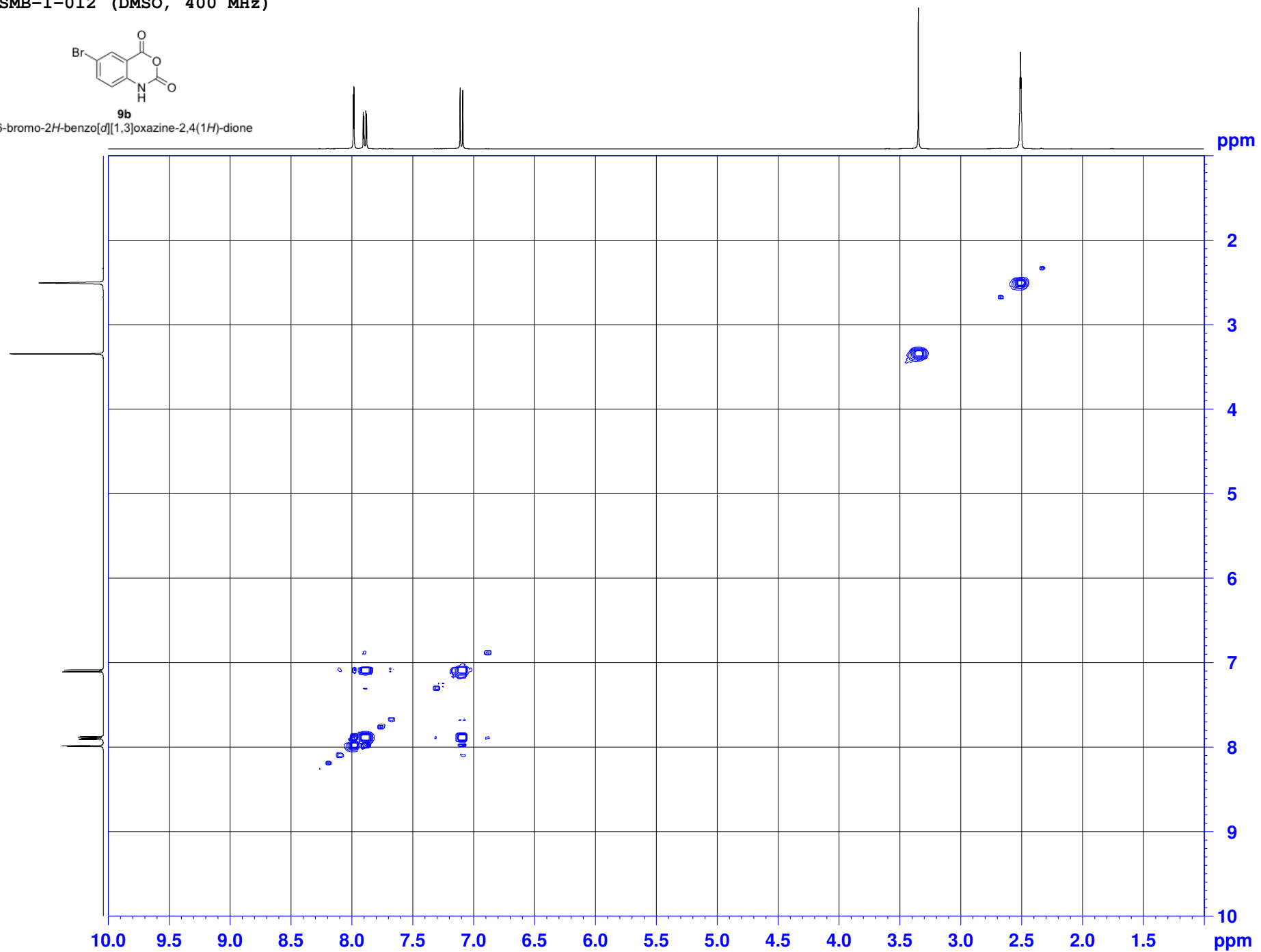


SMB-1-012 (DMSO, 400 MHz)

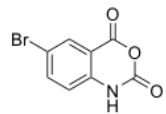


9b

6-bromo-2H-benzo[d][1,3]oxazine-2,4(1H)-dione

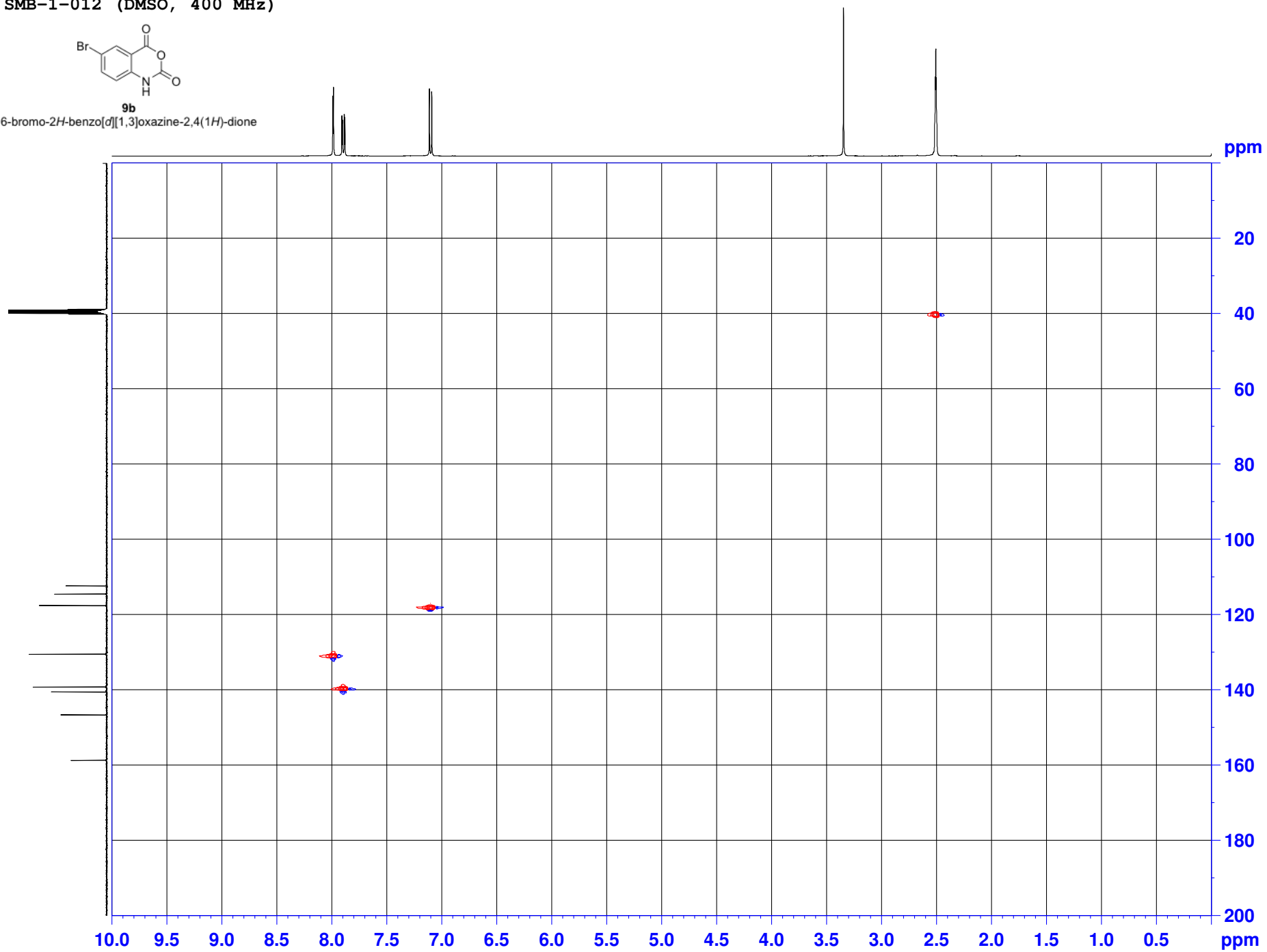


SMB-1-012 (DMSO, 400 MHz)

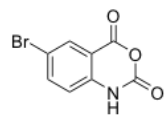


9b

6-bromo-2*H*-benzo[d][1,3]oxazine-2,4(1*H*)-dione

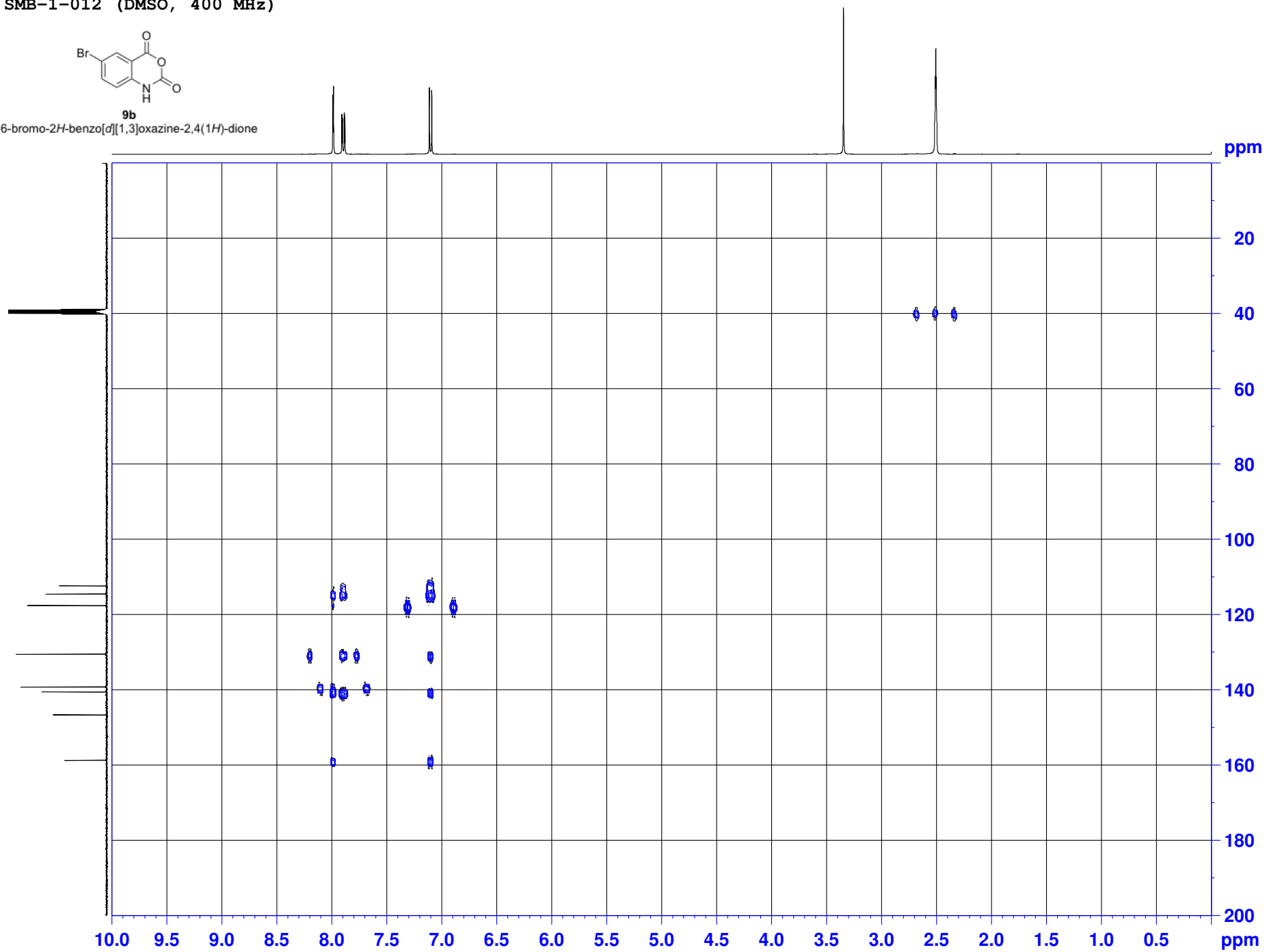


SMB-1-012 (DMSO, 400 MHz)



9b

6-bromo-2H-benzo[d][1,3]oxazine-2,4(1H)-dione



Mass Spectrum List Report

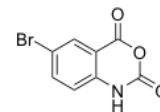
Analysis Info

Analysis Name G:\Data\apexdata111116\SMB-1-012_pos_000006.d
Method Neg_DOM_032112
Sample Name SMB-1-012
Comment SMB-1-012 in MeOH:H2O with NaCl added

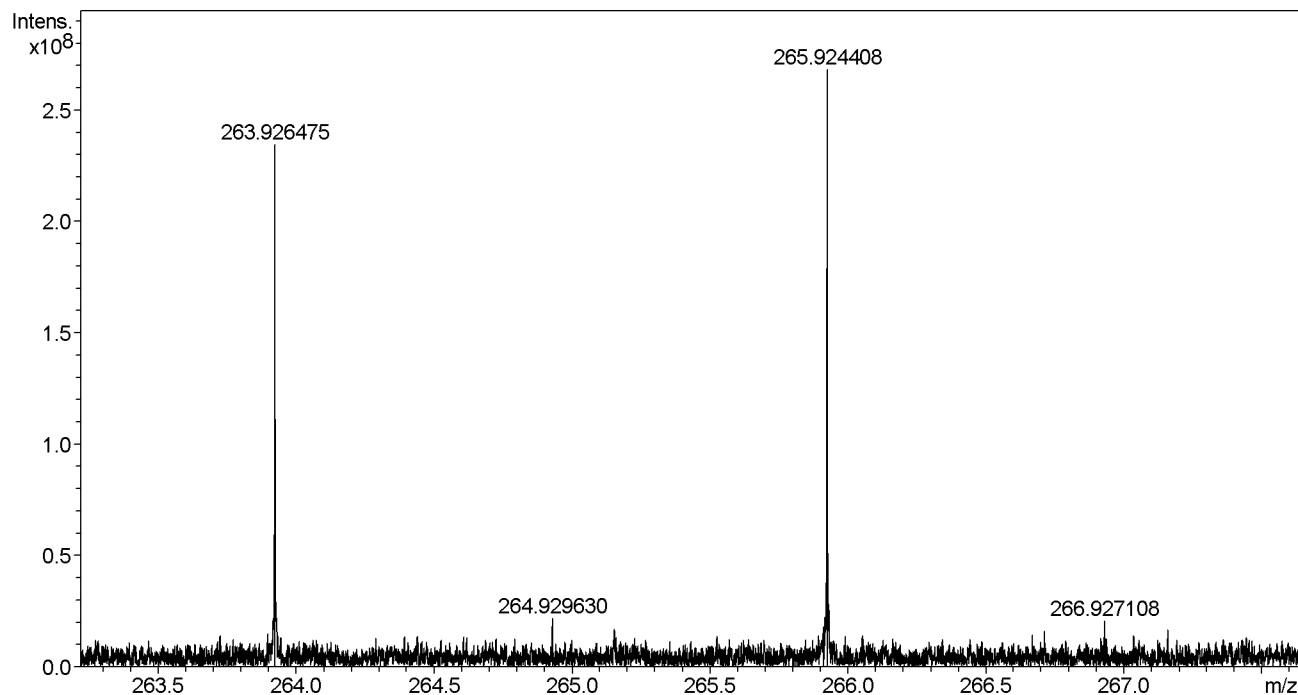
Acquisition Date 11/11/2016 3:45:13 PM

Operator FTMS_USER
Instrument apex-Qe

Sample Name SMB-1-012
Exact Mass of C₈H₄BrNO₃Na⁺ = 263.926677 m/z
Mass Observed with signature = 263.926475 m/z
Difference < -1.0 ppm



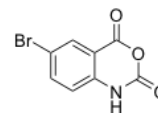
9b
6-bromo-2H-benzo[d][1,3]oxazine-2,4(1H)-dione



#	m/z	I
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2	184.318093	42775166
3	184.319018	39766398
4	209.440134	27024405
5	223.933903	27067184
6	241.944033	33785451
7	263.926475	234262671
8	265.924408	267869301
9	281.172242	25188311
10	296.955403	37178465
11	297.954288	59439899
12	298.952932	26643926
13	301.140721	34136216
14	304.961966	41642600
15	305.961179	27247913
16	309.203187	39712525
17	313.967500	36685598
18	317.910440	33984901
19	317.945622	27168194
20	321.956222	34530426

Mass Spectrum List Report

#	m/z	I
21	322.271327	41936530
22	323.182675	26556575
23	333.987027	32572363
24	339.177670	32285085
25	350.302566	26442052
26	351.214016	27704086
27	351.250310	25128785
28	351.966230	83996642
29	353.265909	52176936
30	353.964224	73075865
31	365.135518	34454264
32	365.229512	32318350
33	367.943724	34958455
34	368.804750	45575632
35	368.812119	28999644
36	368.819573	57075176
37	368.823127	50369005
38	368.826517	48318963
39	368.834408	184769024
40	368.837952	199592453
41	368.841638	82524683
42	368.845408	104487441
43	368.856624	44488227
44	368.867210	38727731
45	369.413982	36109720
46	369.941703	25207005
47	369.976812	67948821
48	371.974779	92032369
49	379.245097	29819410
50	381.297204	86464145
51	383.402055	43903831
52	384.401102	40925539
53	393.260560	26089097
54	393.297105	233443009
55	394.300451	51389624
56	395.240082	36698700
57	398.241098	68809740
58	407.276348	29357280
59	413.265844	81097572
60	422.008061	29705479
61	425.286961	32267113
62	494.865483	103637377
63	494.885708	56770967
64	495.367255	39707545
65	495.864406	170575274
66	496.366617	58460094
67	496.863385	92670411
68	497.365017	34173915
69	497.862464	29160933
70	498.880227	36538891
71	500.878633	28109338
72	502.854185	50151924
73	503.853222	84403680
74	504.354939	38408150
75	504.852157	51472837
76	506.861490	32530819
77	512.896085	65742849
78	514.894159	34371377
79	520.828697	62702532
80	522.826694	112134765
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83	524.824427	58081522
84	524.859833	304681232

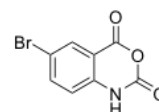


9b

6-bromo-2H-benzo[d][1,3]oxazine-2,4(1H)-dione

Mass Spectrum List Report

#	m/z	I
85	525.287556	25661040
86	525.862437	49669191
87	526.857636	152803184
88	527.860661	32619158
89	540.872291	70995998
90	542.870335	161711445
91	543.872967	35436517
92	544.868162	90540647
93	569.313656	27266344
94	594.901605	25363706
95	609.308266	26271211
96	655.351381	26094454
97	718.384106	26188354
98	747.786383	57826085
99	749.783764	61325943
100	1675.785499	34323639



9b

6-bromo-2H-benzo[d][1,3]oxazine-2,4(1H)-dione

Atlantic Microlab, Inc.

Sample No. SMB-1-012

6180 Atlantic Blvd. Suite M
Norcross, GA 30071
www.atlanticmicrolab.com

Company/School University of Southern Mississippi

Dept. Chemistry and Biochemistry

Address 118 College Dr. #5043

City, State, Zip Hattiesburg, MS 39406

Professor/Supervisor: Matthew G. Donahue

Name Matthew Donahue

Date 10/25/16

PO# / CC# Mastercard 9359 (On file)

Phone 614-203-1123

Element	Theory	Found	
C	39.70	39.51	
H	1.67	1.74	

Single ☒ Duplicate ☐

Elements Present:

Analyze for: C, H

Hygroscopic ☐ Explosive ☐

M.P. _____ B.P. _____

To be dried: Yes ☐ No ☒

Temp. _____ Vac. _____ Time _____

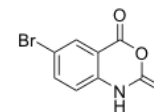
Rush Service ☐ Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.

Include Email Address or FAX # Below

matthew.donahue@usm.edu

Date Received NOV 03 P.M. Date Completed NOV 08 2016

Remarks:

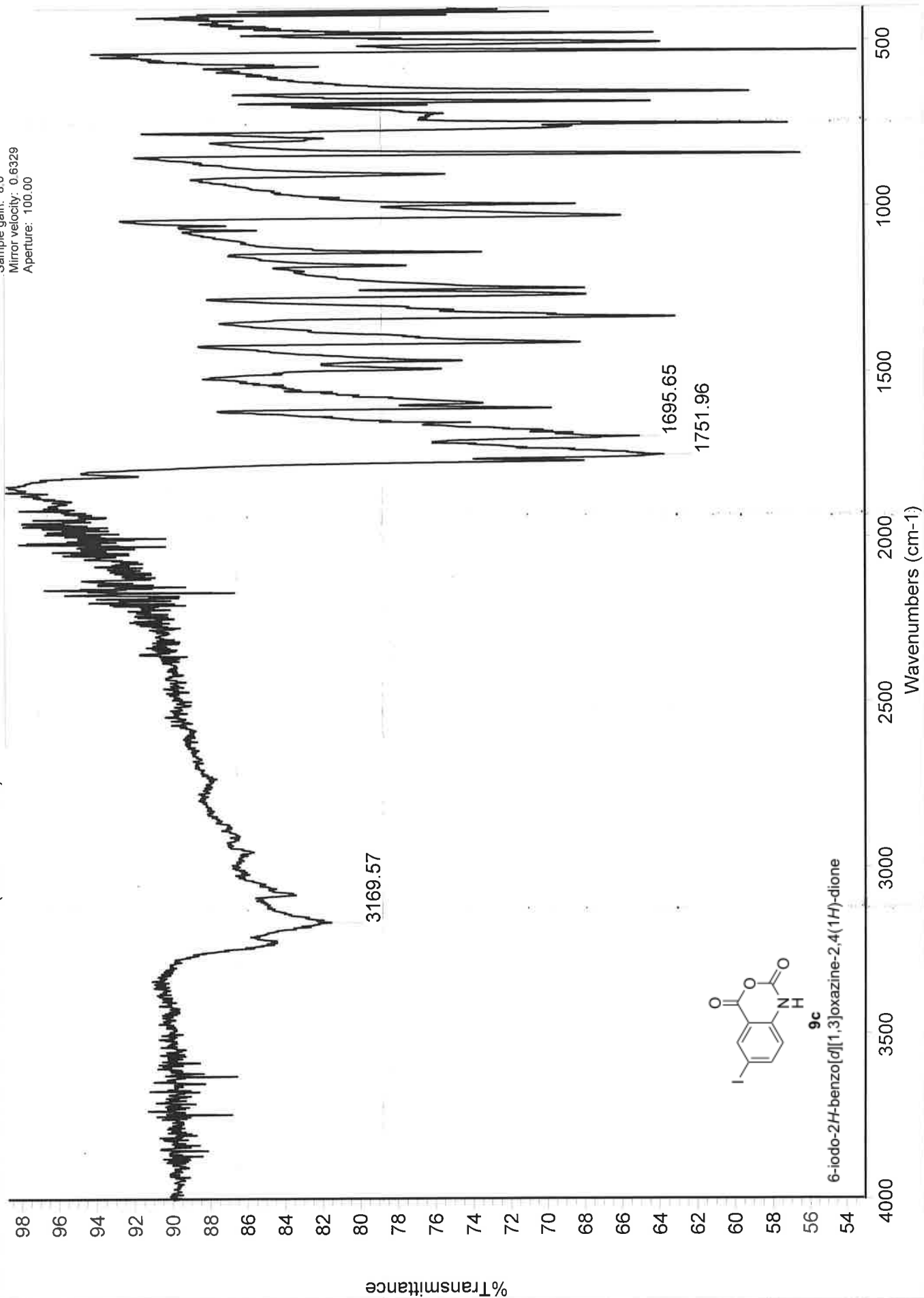


9b
6-bromo-2H-benzo[d][1,3]oxazine-2,4(1H)-dione

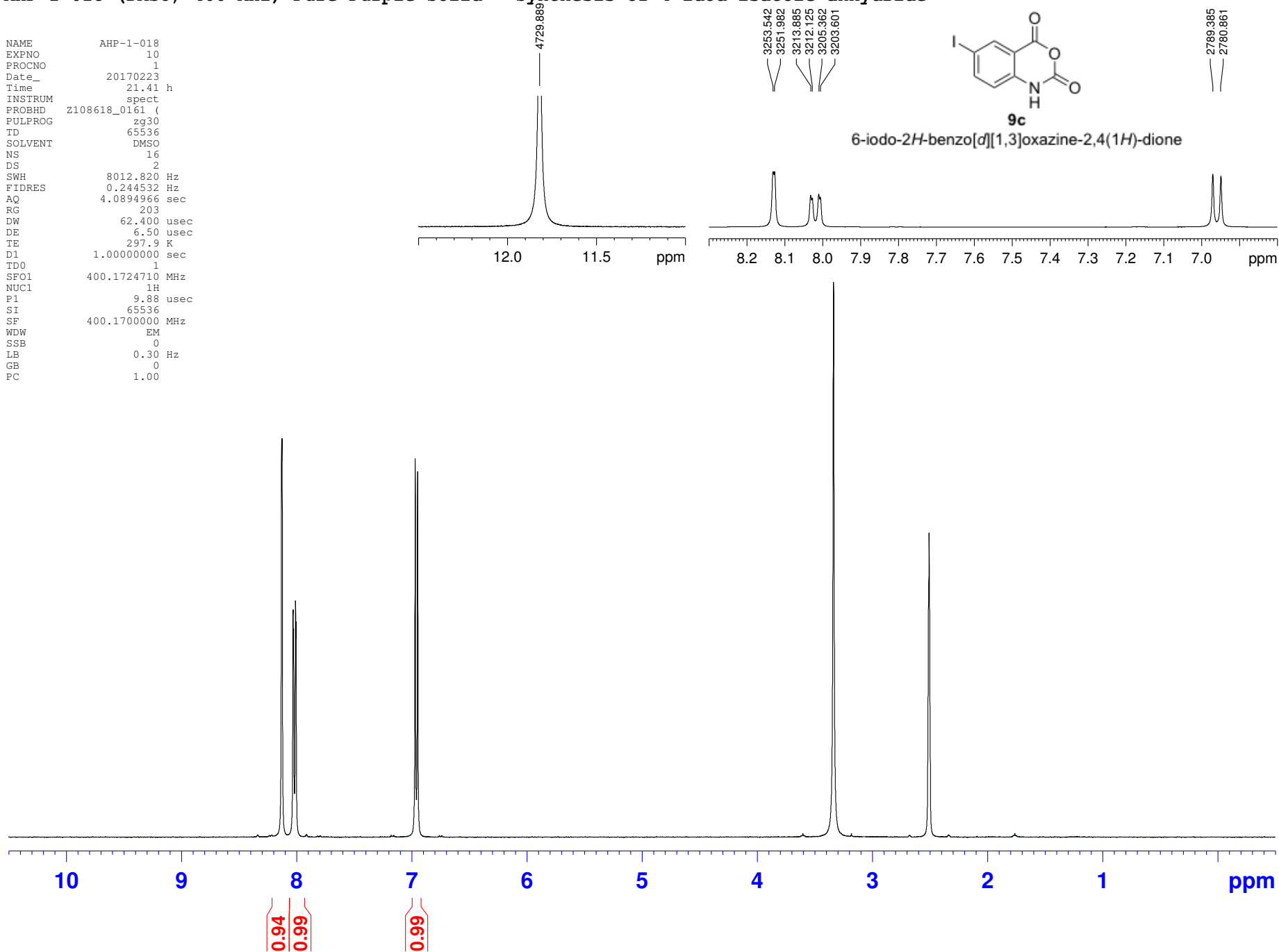
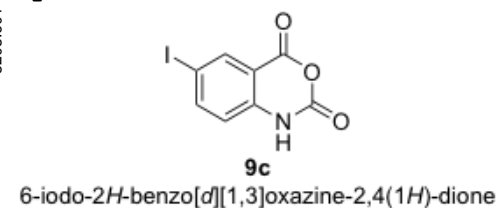
AHP-1-018

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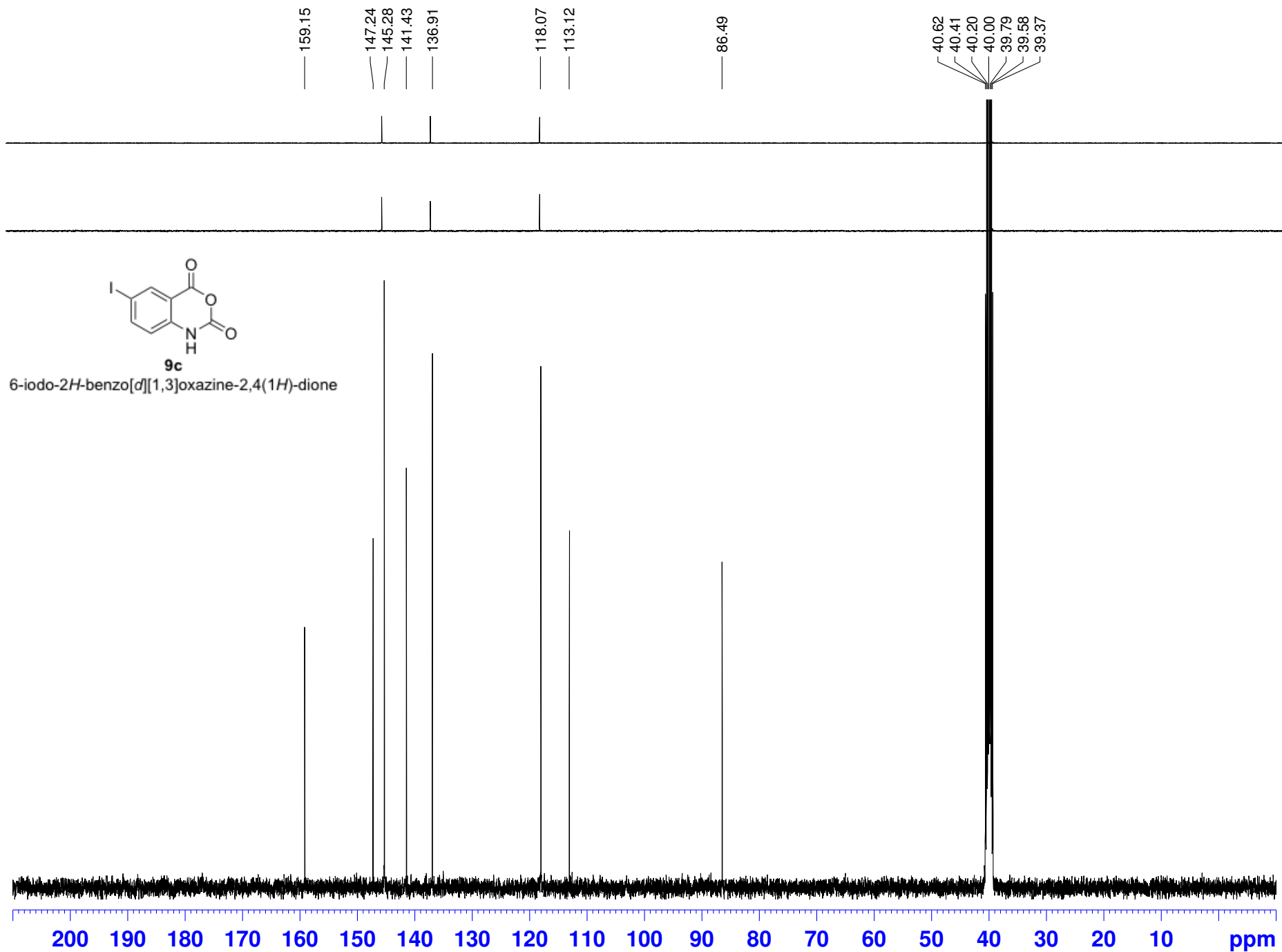
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Resolution: 2.000
Sample gain: 8.0
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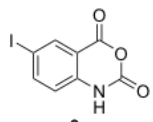
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PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
DS	2
SWH	8012.820 Hz
FIDRES	0.244532 Hz
AQ	4.0894966 sec
RG	203
DW	62.400 usec
DE	6.50 usec
TE	297.9 K
D1	1.00000000 sec
TD0	1
SFO1	400.1724710 MHz
NUC1	1H
P1	9.88 usec
SI	65536
SF	400.1700000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



AHP-1-018 (DMSO, 400 MHz) Pure Purple Solid - Synthesis of 4-i

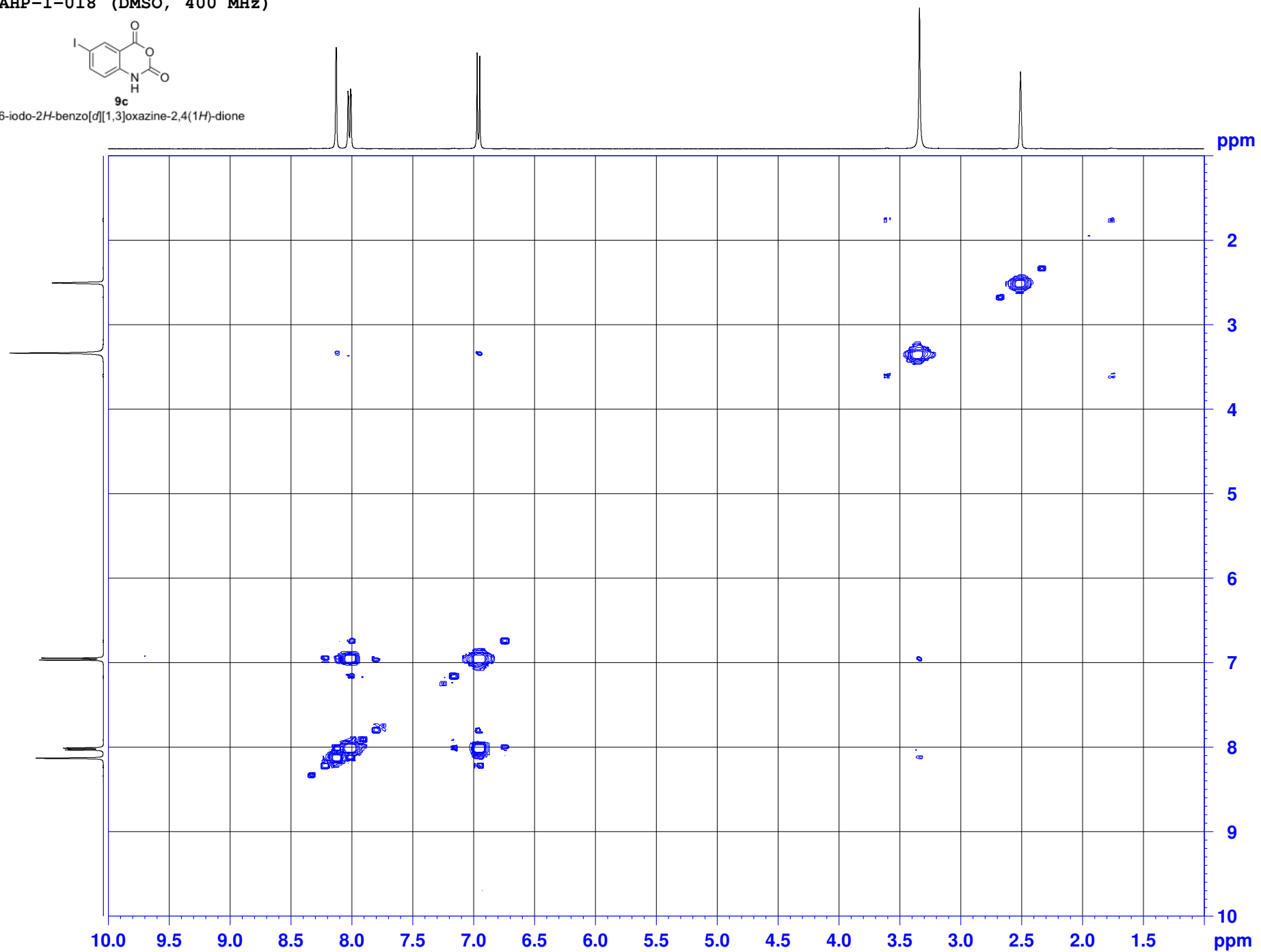


AHP-1-018 (DMSO, 400 MHz)

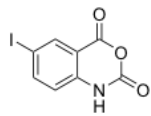


9c

6-iodo-2*H*-benzo[d][1,3]oxazine-2,4(1*H*)-dione

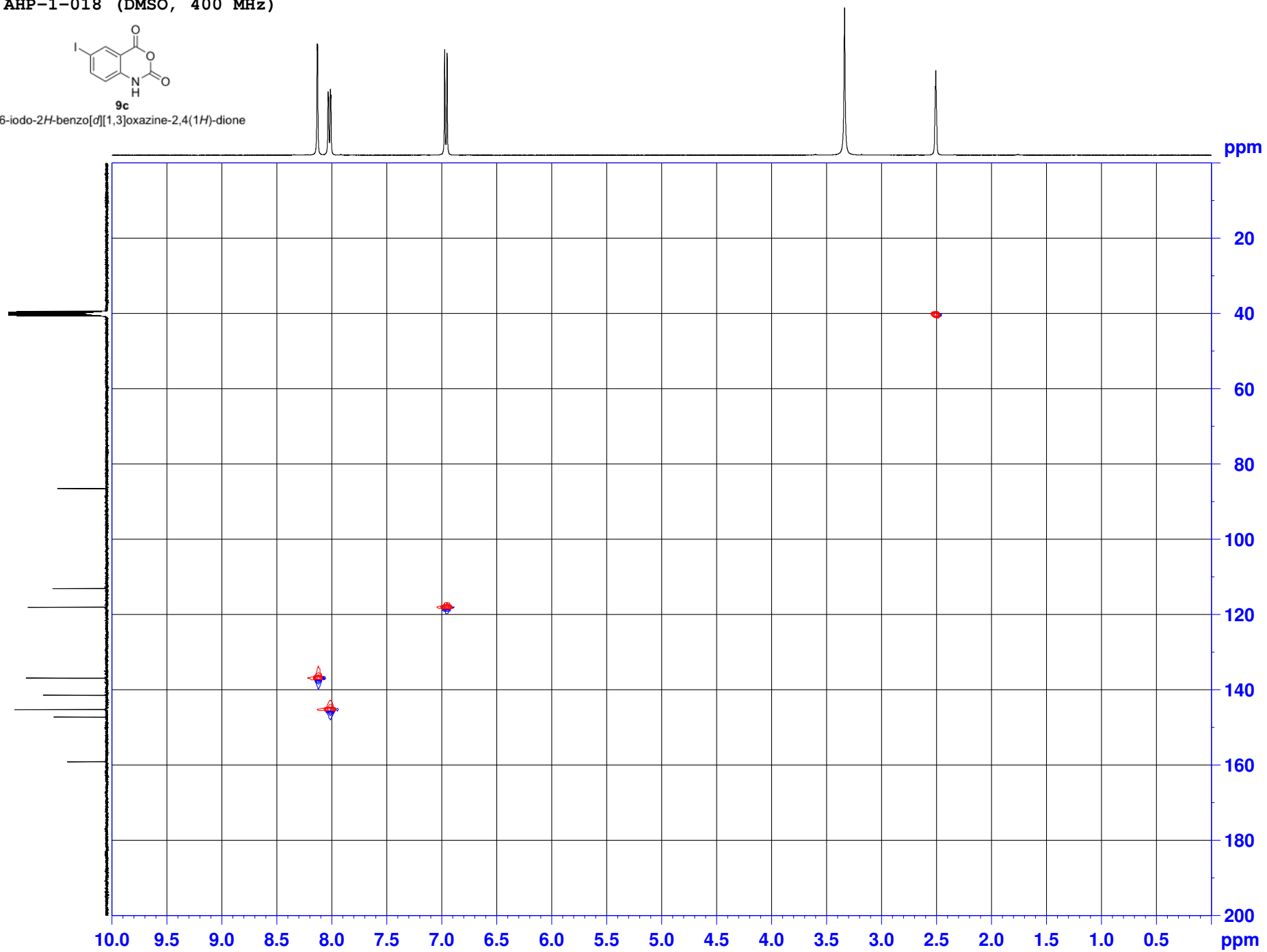


AHP-1-018 (DMSO, 400 MHz)

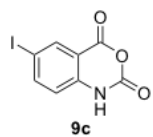


9c

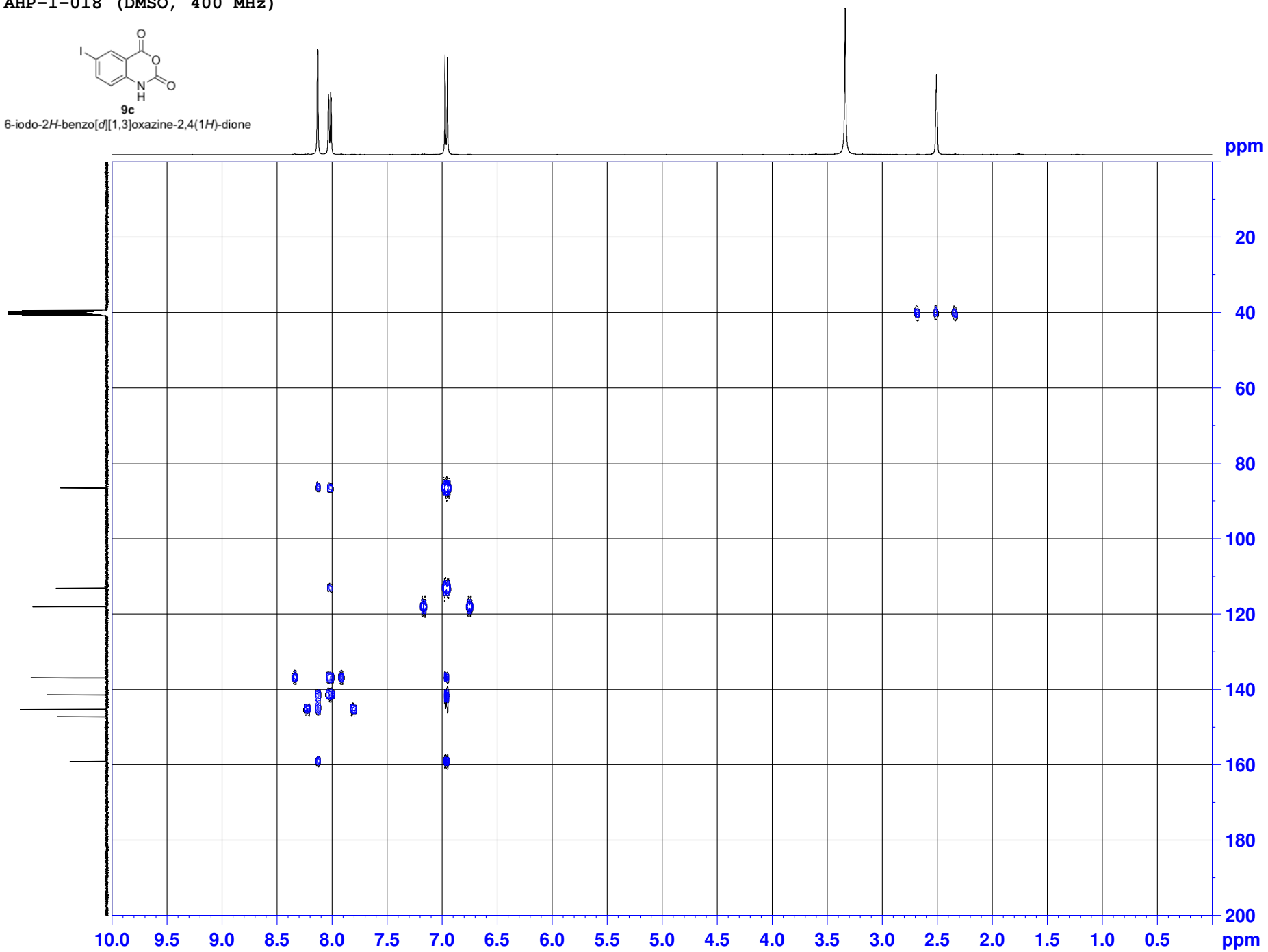
6-iodo-2*H*-benzo[d][1,3]oxazine-2,4(1*H*)-dione



AHP-1-018 (DMSO, 400 MHz)



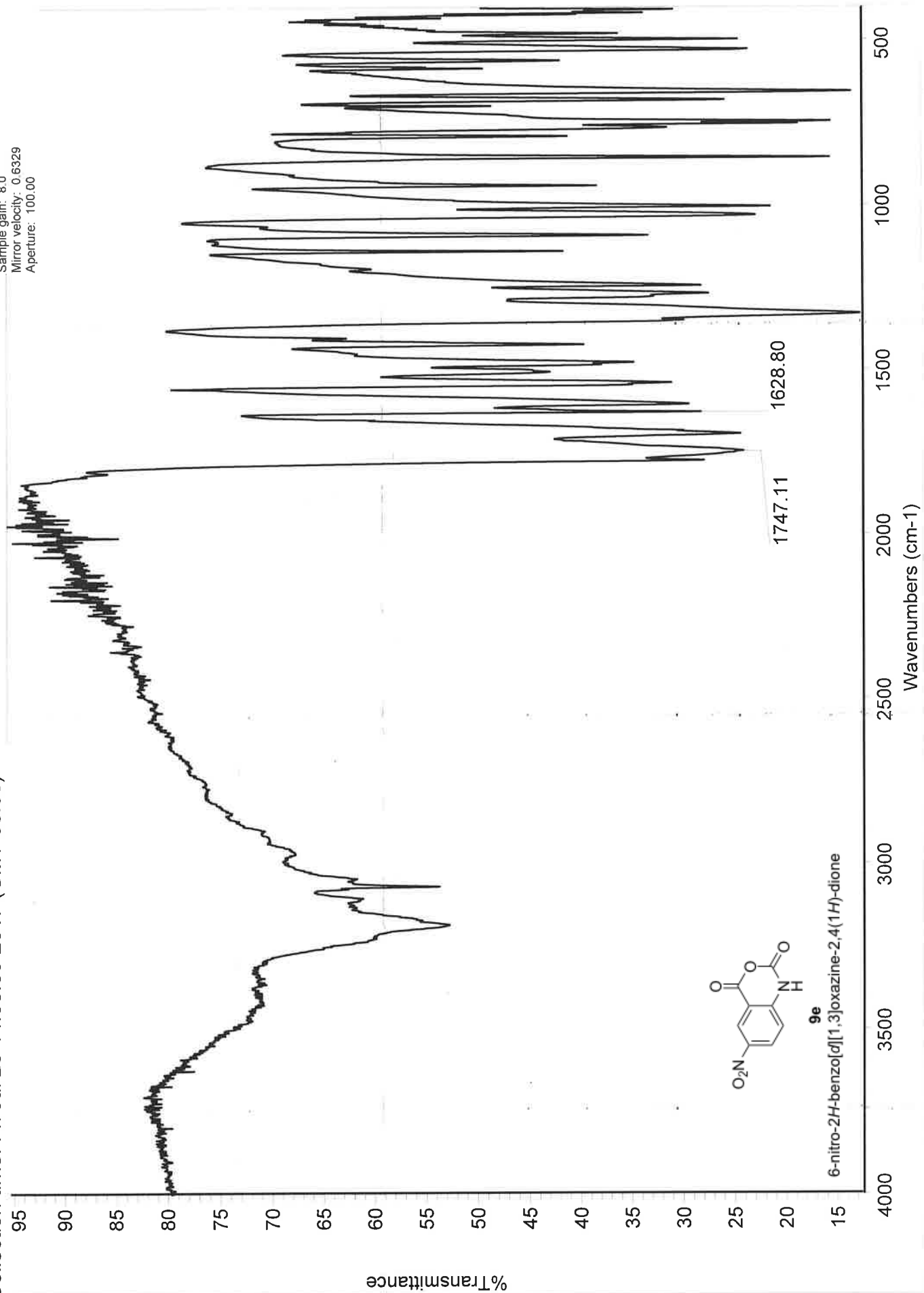
9c
6-iodo-2H-benzo[d][1,3]oxazine-2,4(1H)-dione



SMB-1-027

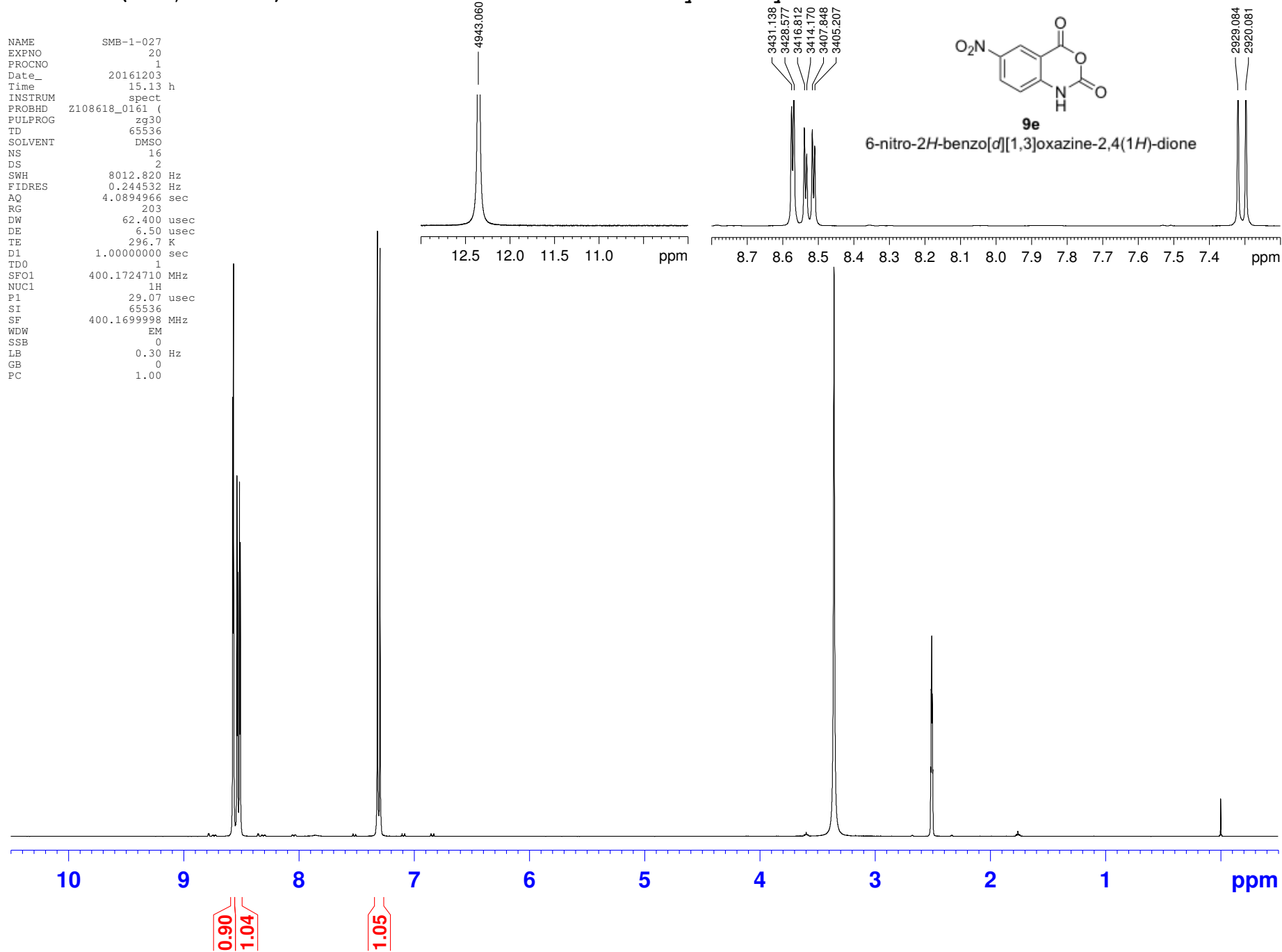
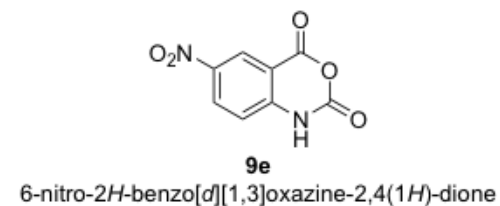
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Number of sample scans: 8
Number of background scans: 8
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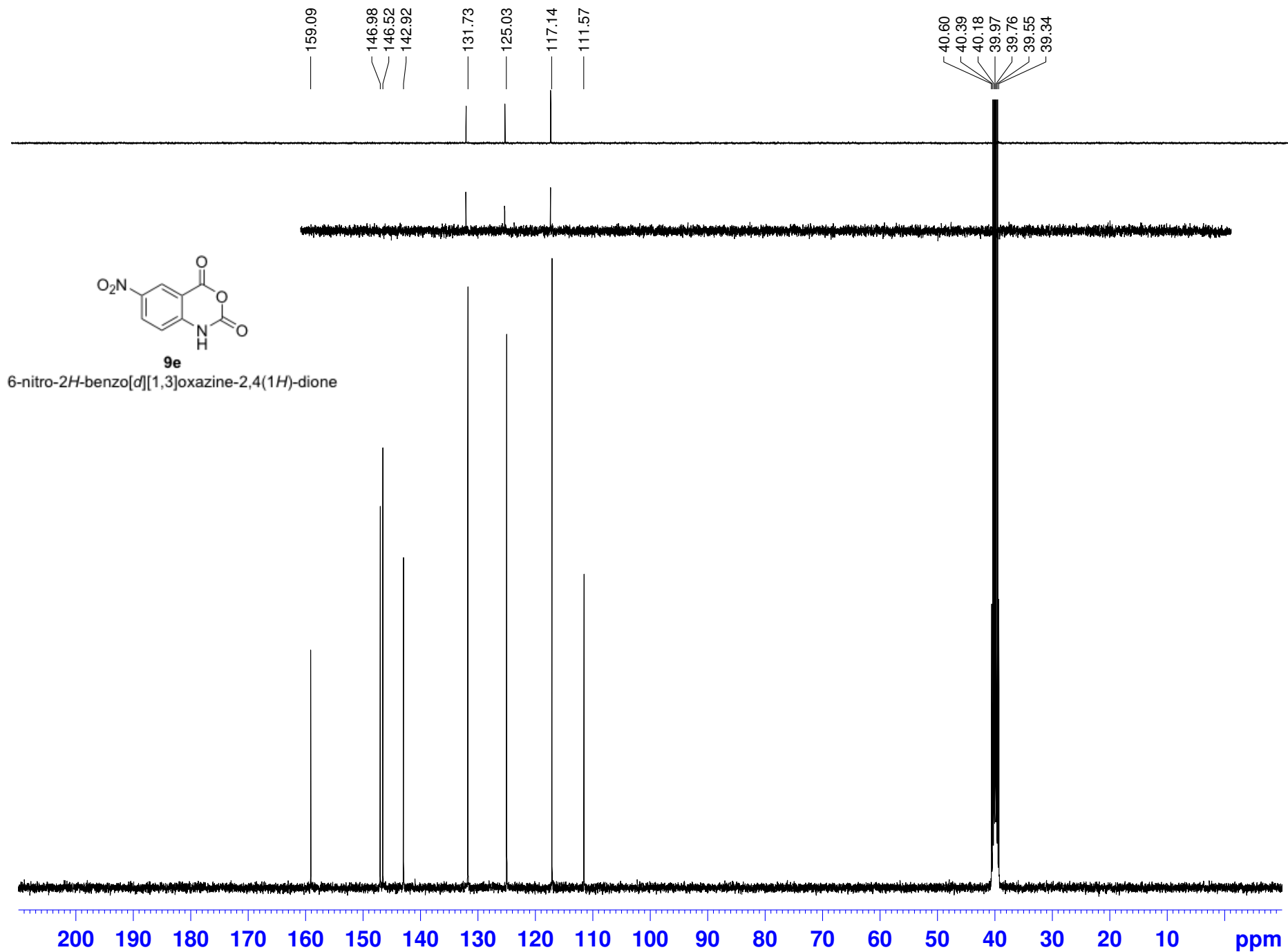


SMB-1-027 (DMSO, 400 MHz) Pure Tan Solid- 4-nitro isatoic anhydride synthesis

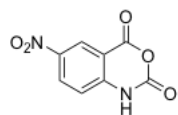
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 SOLVENT DMSO
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 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894966 sec
 RG 203
 DW 62.400 usec
 DE 6.50 usec
 TE 296.7 K
 D1 1.0000000 sec
 TD0 1
 SFO1 400.1724710 MHz
 NUC1 1H
 P1 29.07 usec
 SI 65536
 SF 400.1699998 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



SMB-1-027 (DMSO, 400 MHz) Pure Tan Solid- 4-nitro isatoic anhy

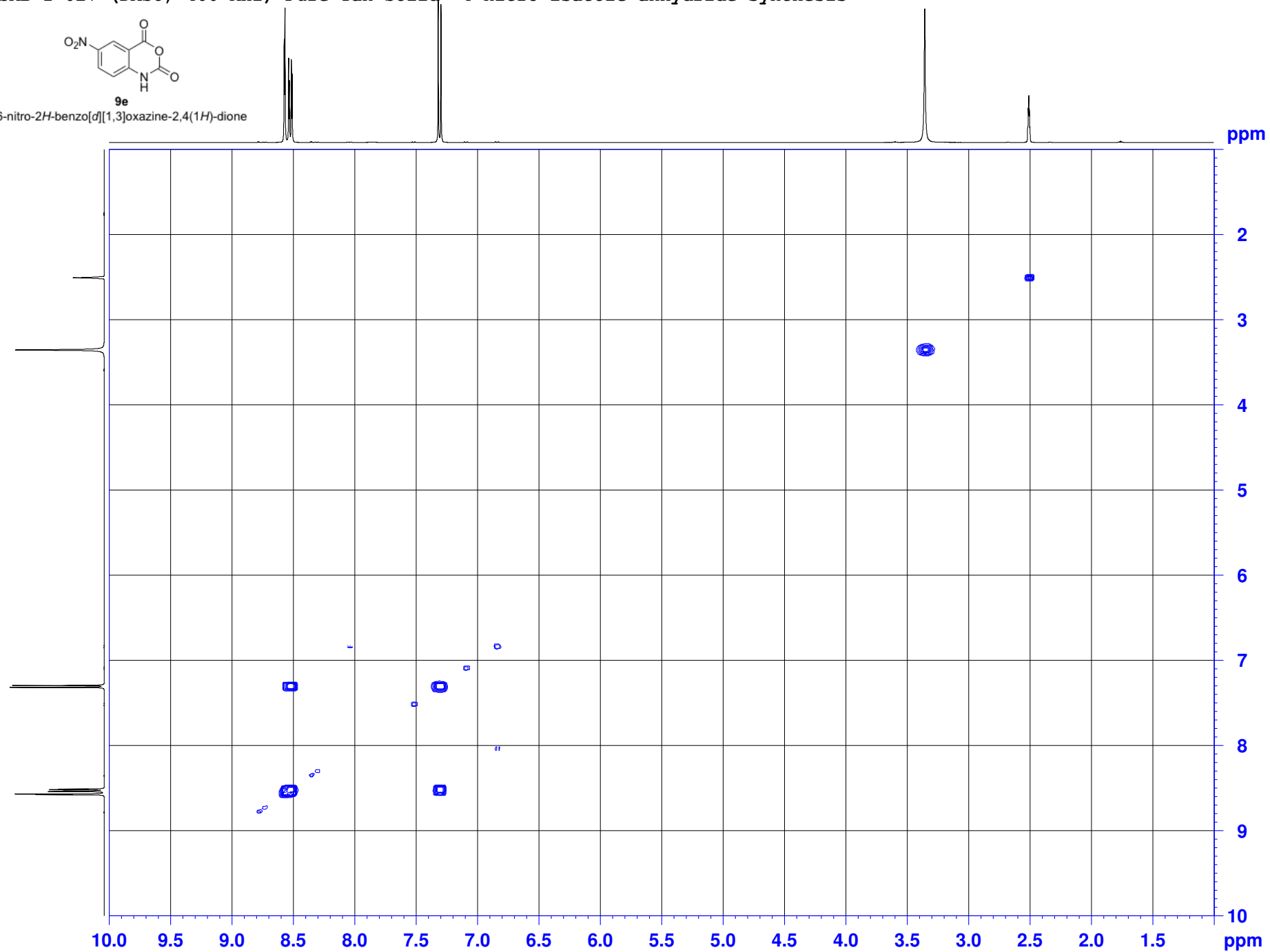


SMB-1-027 (DMSO, 400 MHz) Pure Tan Solid- 4-nitro isatoic anhydride synthesis

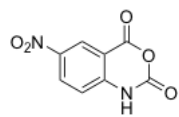


9e

6-nitro-2H-benzo[d][1,3]oxazine-2,4(1H)-dione

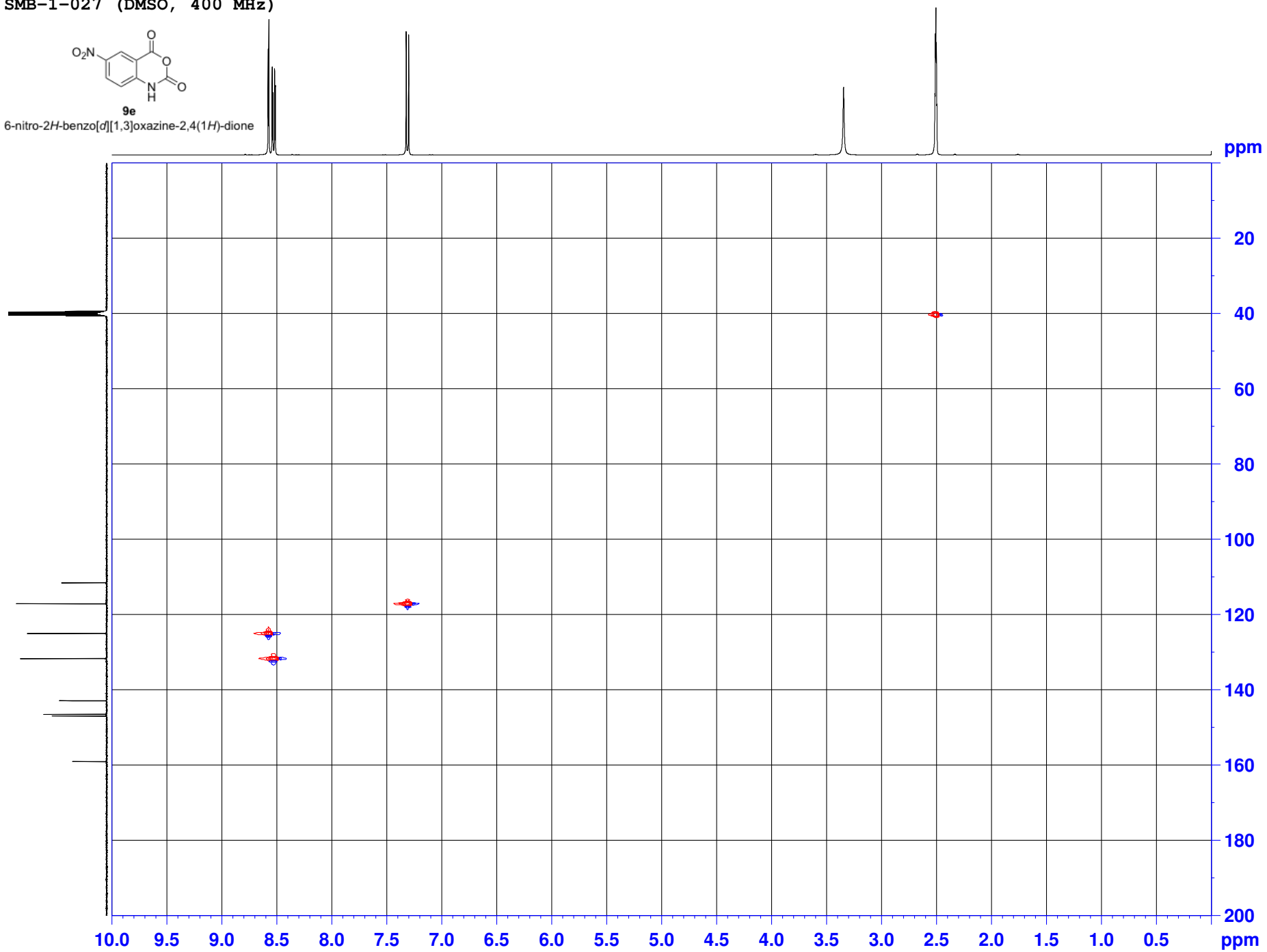


SMB-1-027 (DMSO, 400 MHz)

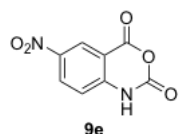


9e

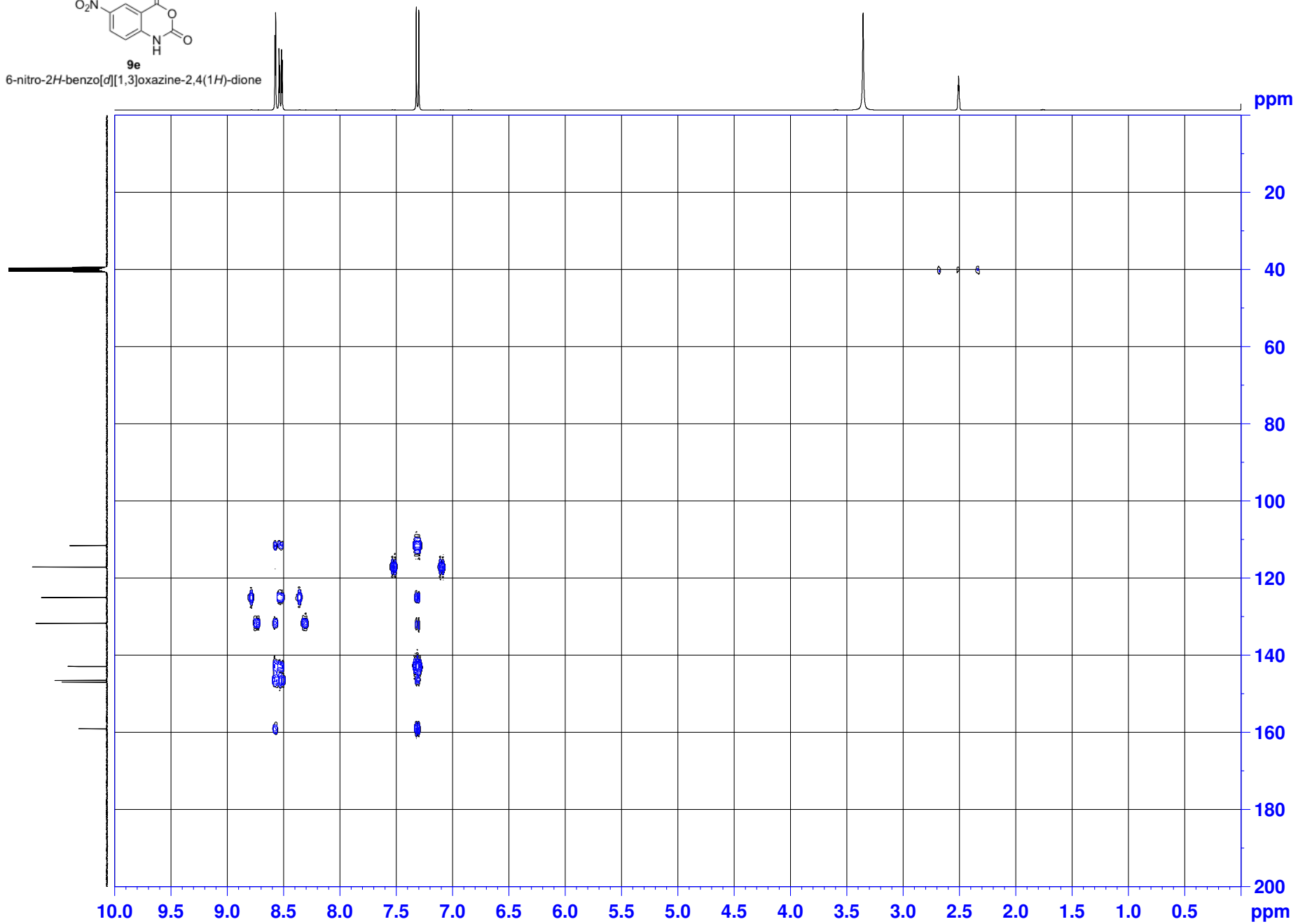
6-nitro-2H-benzo[d][1,3]oxazine-2,4(1H)-dione



SMB-1-027 (DMSO, 400 MHz) Pure Tan Solid- 4-nitro isatoic anhydride synthesis



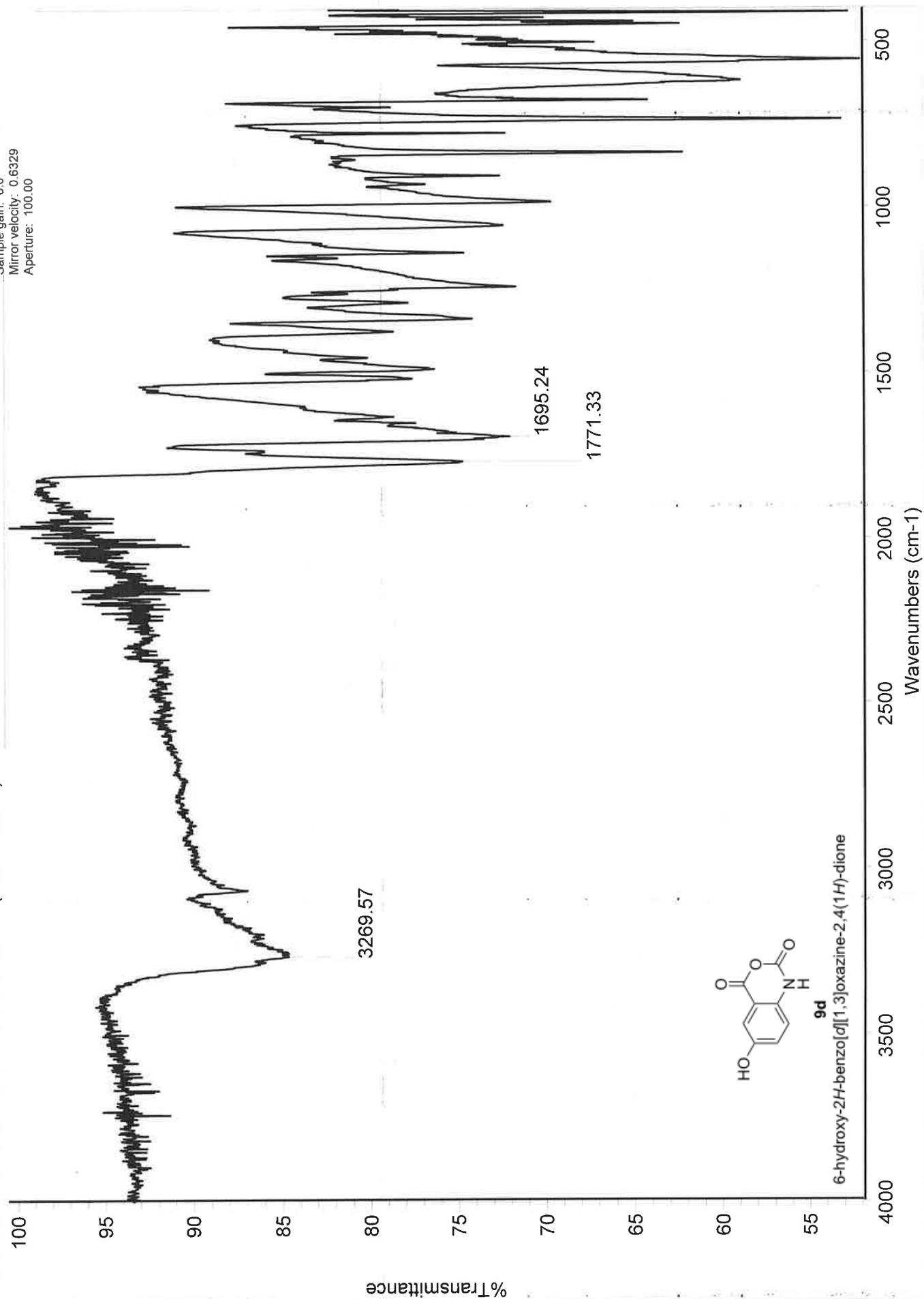
6-nitro-2H-benzo[d][1,3]oxazine-2,4(1H)-dione



SMB-1-029

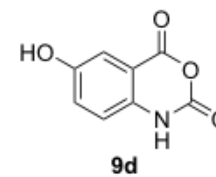
Collection time: Fri Jul 28 14:41:33 2017 (GMT-06:00)

Number of sample scans: 8
Number of background scans: 8
Resolution: 2.000
Sample gain: 8.0
Mirror velocity: 0.6329
Aperture: 100.00

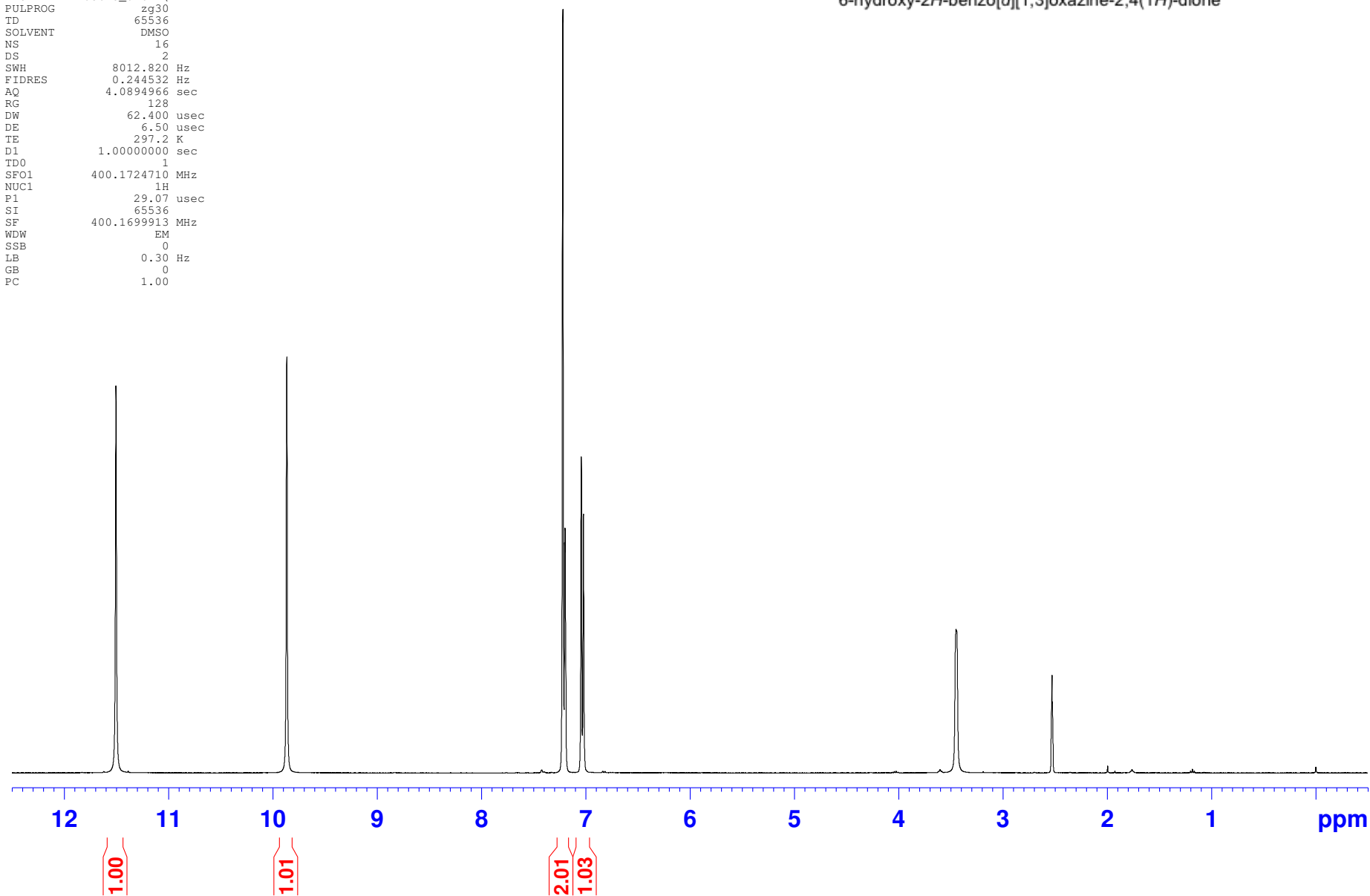


SMB-1-029 (DMSO, 400 MHz) Pure Brown Solid- hydroxy isatoic anhydride

NAME SMB-1-029
 EXPNO 20
 PROCNO 1
 Date_ 20161130
 Time_ 20.42 h
 INSTRUM spect
 PROBHD Z108618_0161 (
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894966 sec
 RG 128
 DW 62.400 usec
 DE 6.50 usec
 TE 297.2 K
 D1 1.00000000 sec
 TD0 1
 SF01 400.1724710 MHz
 NUC1 1H
 P1 29.07 usec
 SI 65536
 SF 400.1699913 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

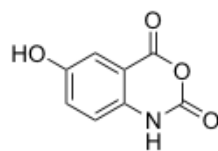


6-hydroxy-2H-benzo[d][1,3]oxazine-2,4(1H)-dione



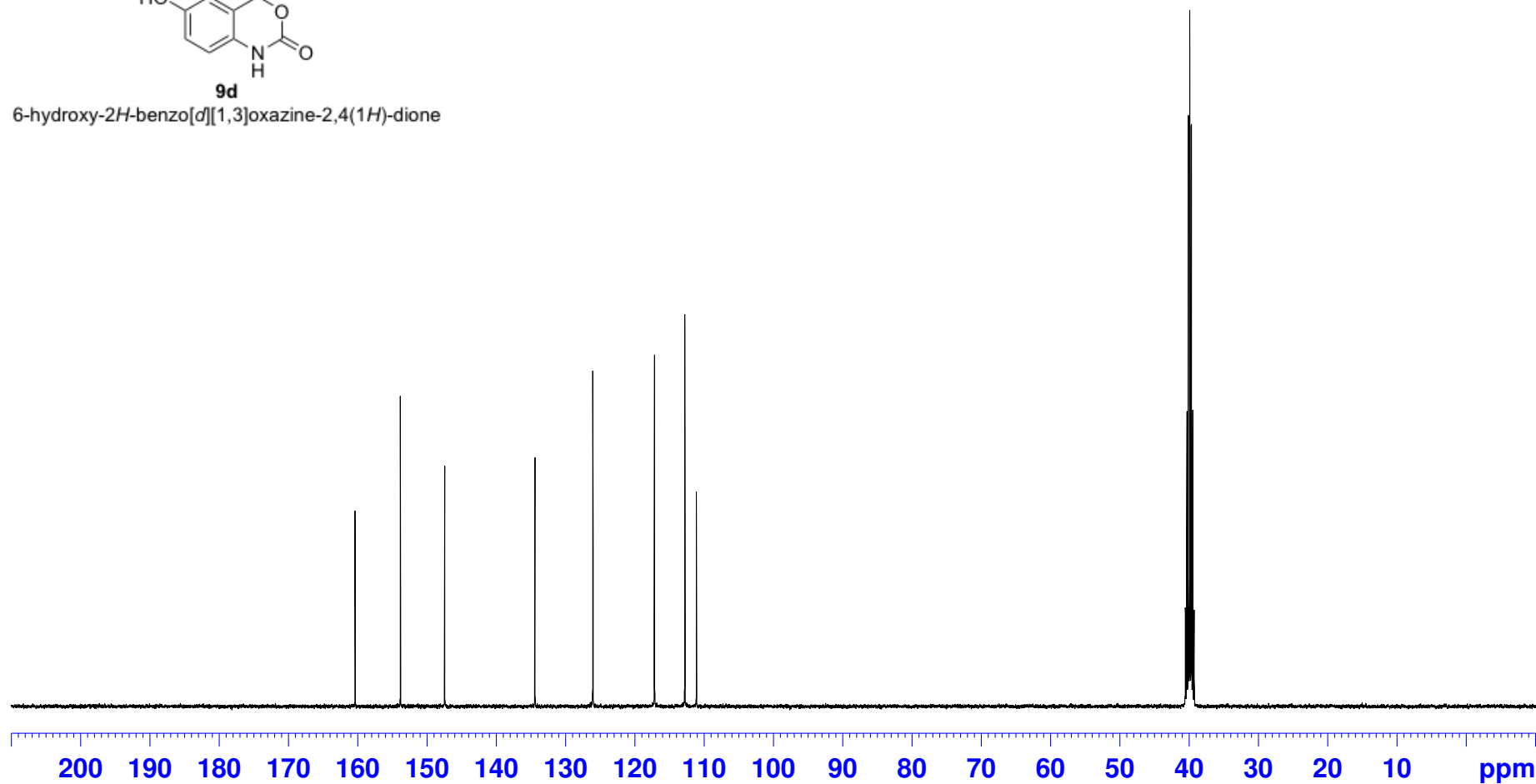
SMB-1-029 (DMSO, 400 MHz) Pure Brown Solid- hydroxy isatoic ar

160.36
153.81
147.43
134.40
126.10
117.21
112.82
111.16

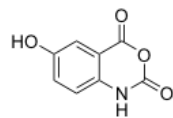


9d

6-hydroxy-2*H*-benzo[d][1,3]oxazine-2,4(1*H*)-dione

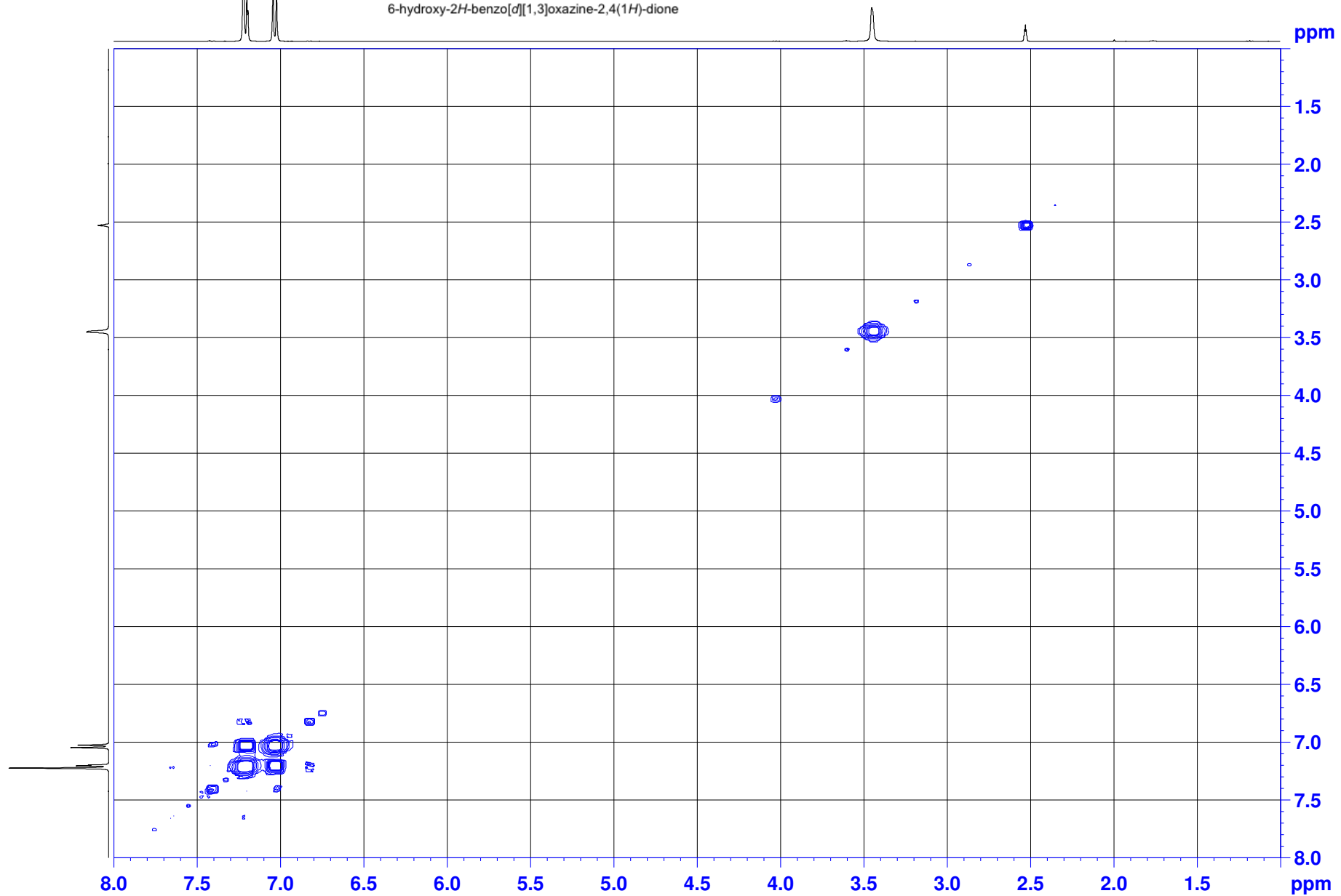


SMB-1-029 (DMSO, 400 MHz) Pure Brown Solid- hydroxy isatoic anhydride

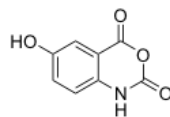


9d

6-hydroxy-2*H*-benzo[*d*][1,3]oxazine-2,4(1*H*)-dione

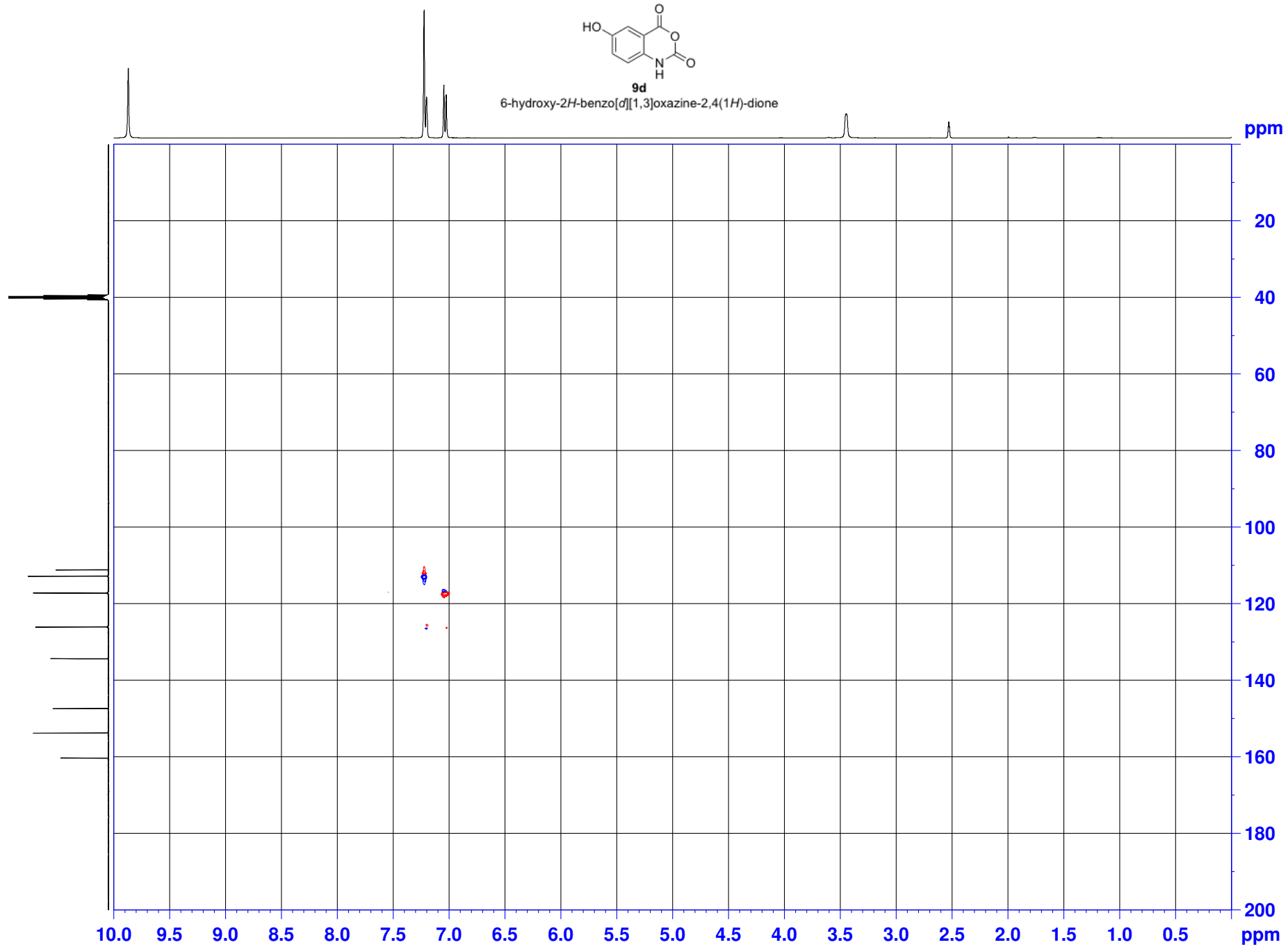


SMB-1-029 (DMSO, 400 MHz) Pure Brown Solid- hydroxy isatoic anhydride

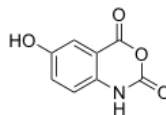


9d

6-hydroxy-2H-benzo[d][1,3]oxazine-2,4(1H)-dione

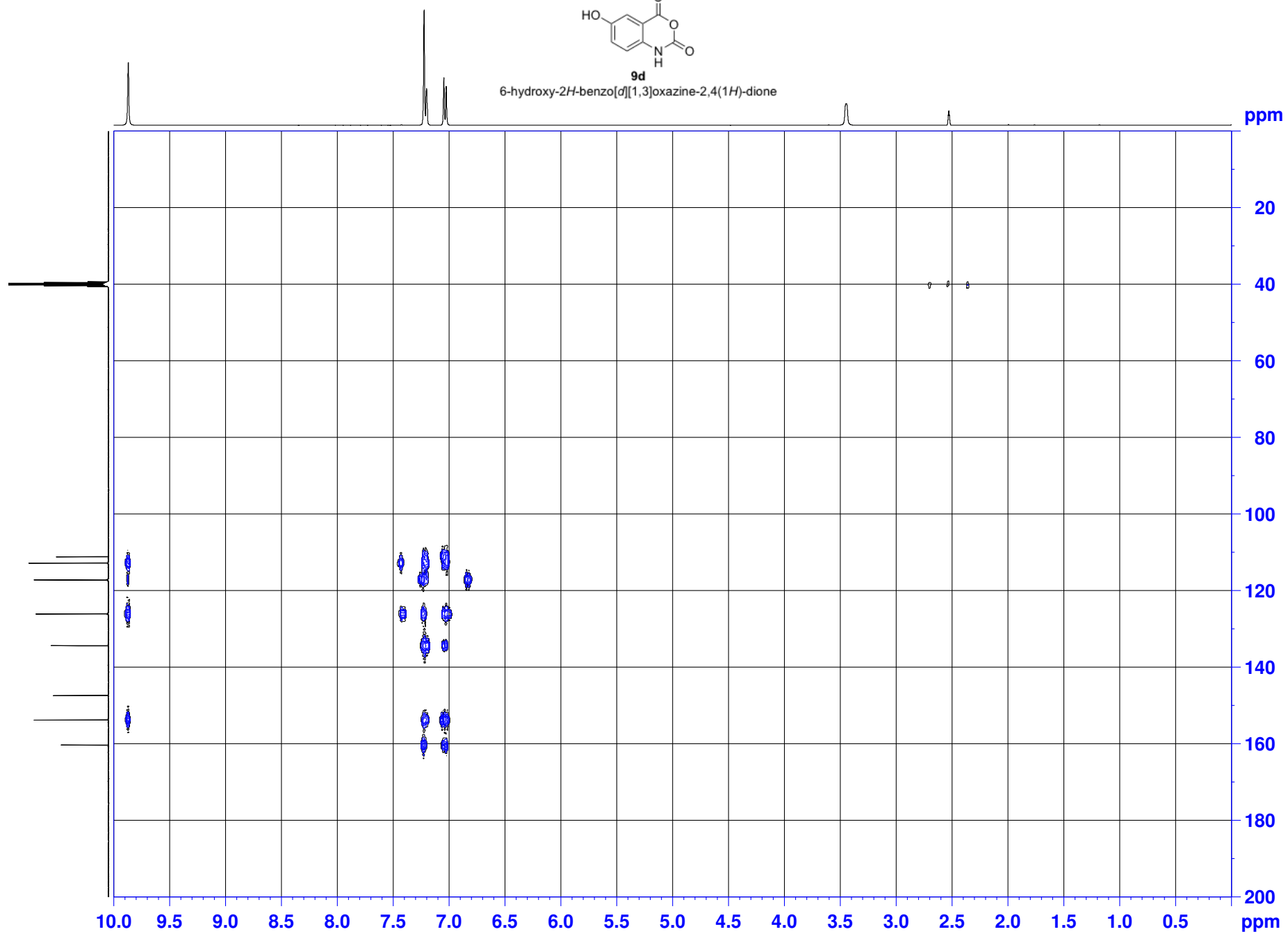


SMB-1-029 (DMSO, 400 MHz) Pure Brown Solid- hydroxy isatoic anhydride



9d

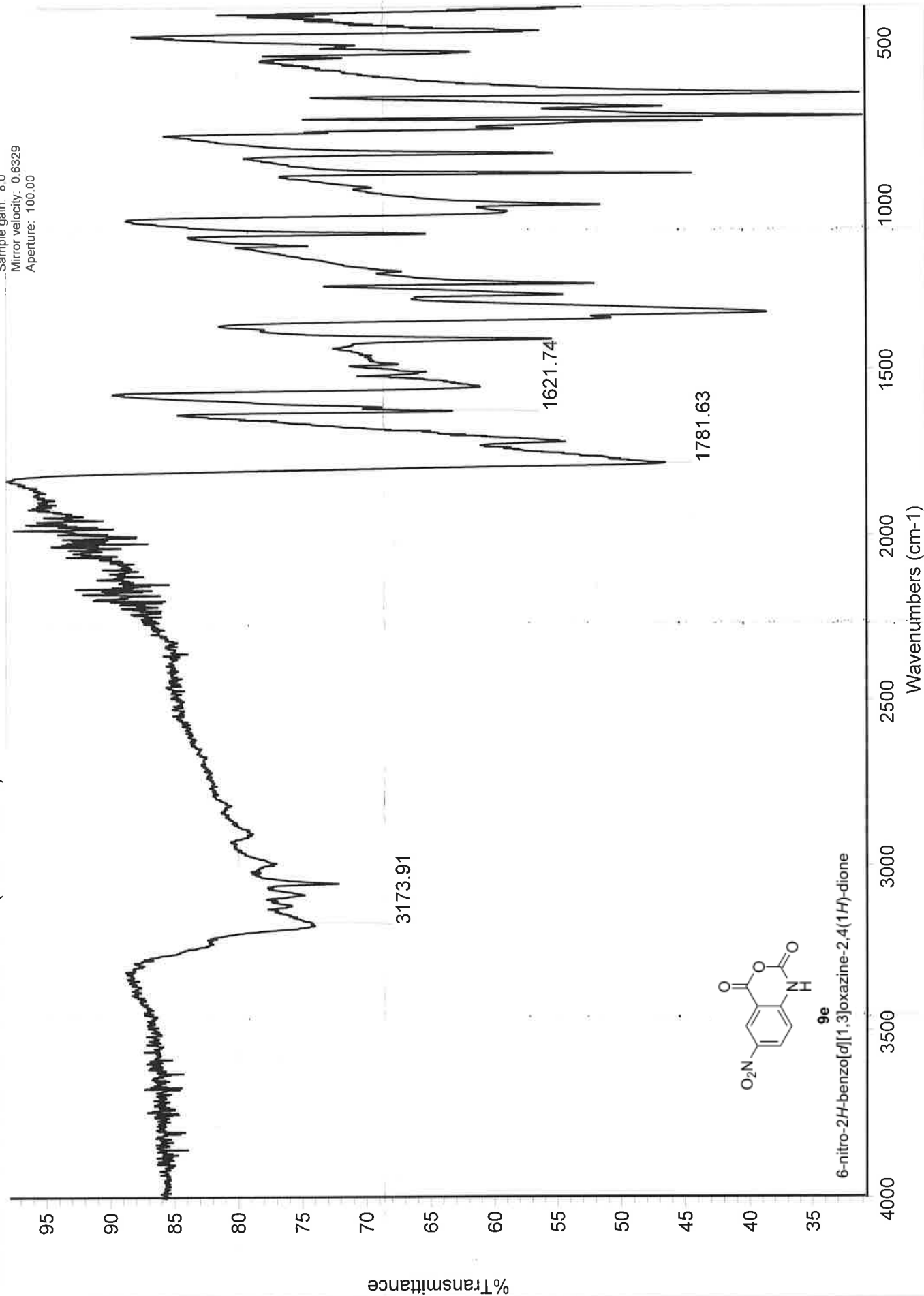
6-hydroxy-2H-benzo[d][1,3]oxazine-2,4(1H)-dione



smb-1-028

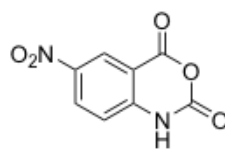
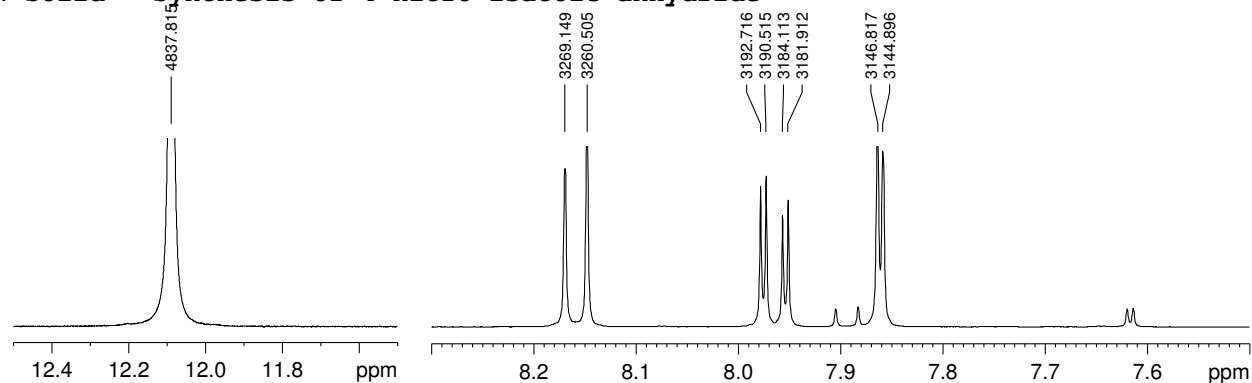
Collection time: Fri Jul 28 14:44:38 2017 (GMT-06:00)

Number of sample scans: 8
Number of background scans: 8
Resolution: 2.000
Sample gain: 8.0
Mirror velocity: 0.6329
Aperture: 100.00

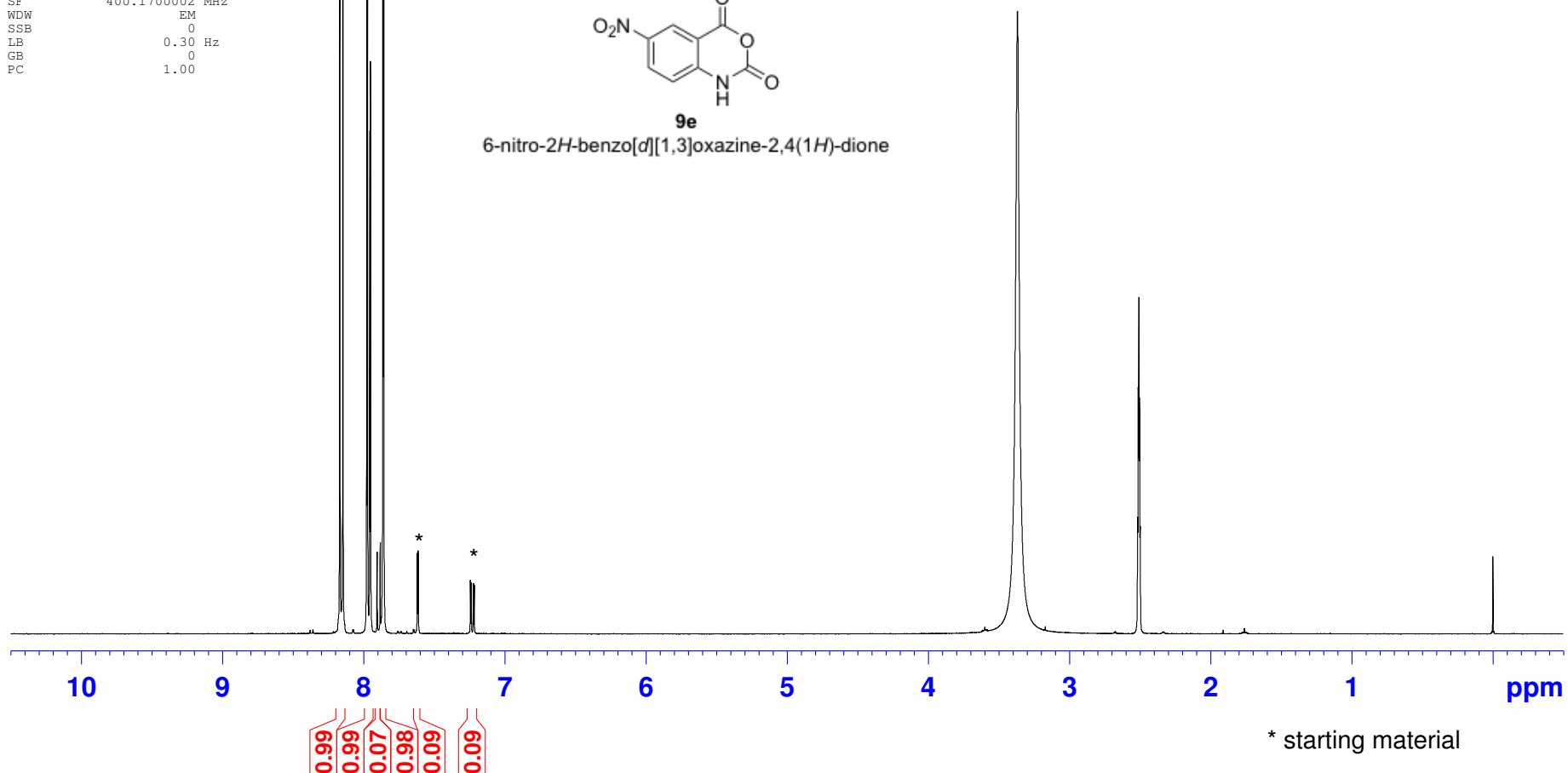


SMB-1-028 (DMSO, 400 MHz) Pure Yellow Solid - Synthesis of 4-nitro isatoic anhydride

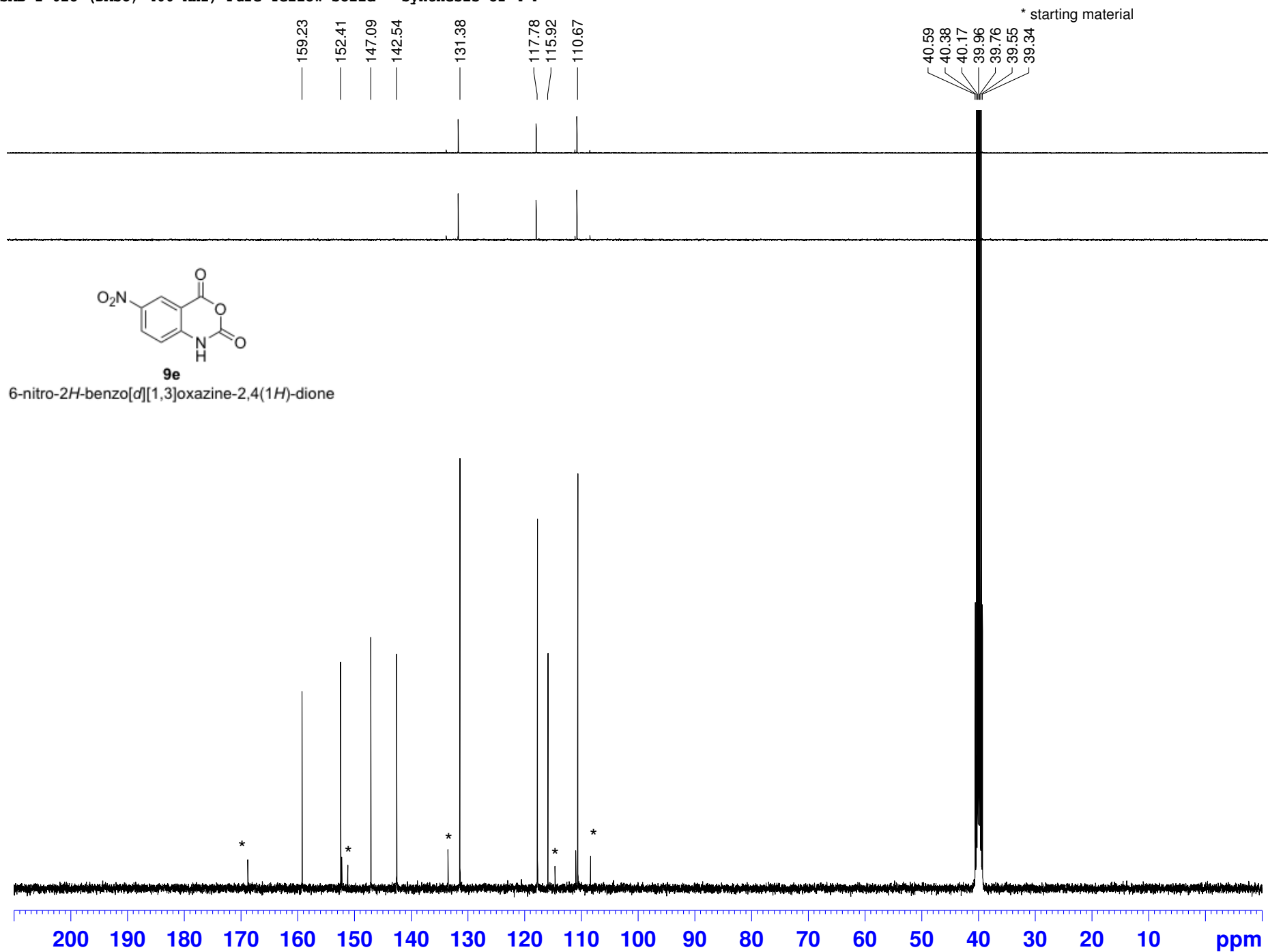
NAME SMB-1-028
 EXPNO 20
 PROCNO 1
 Date_ 20170223
 Time 20.06 h
 INSTRUM spect
 PROBHD Z108618_0161
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894966 sec
 RG 203
 DW 62.400 usec
 DE 6.50 usec
 TE 297.8 K
 D1 1.0000000 sec
 TD0 1
 SFO1 400.1724710 MHz
 NUC1 1H
 P1 9.88 usec
 SI 65536
 SF 400.1700002 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



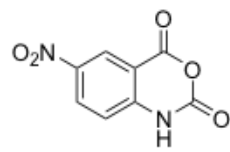
6-nitro-2H-benzo[d][1,3]oxazine-2,4(1H)-dione



SMB-1-028 (DMSO, 400 MHz) Pure Yellow Solid - Synthesis of 4-r

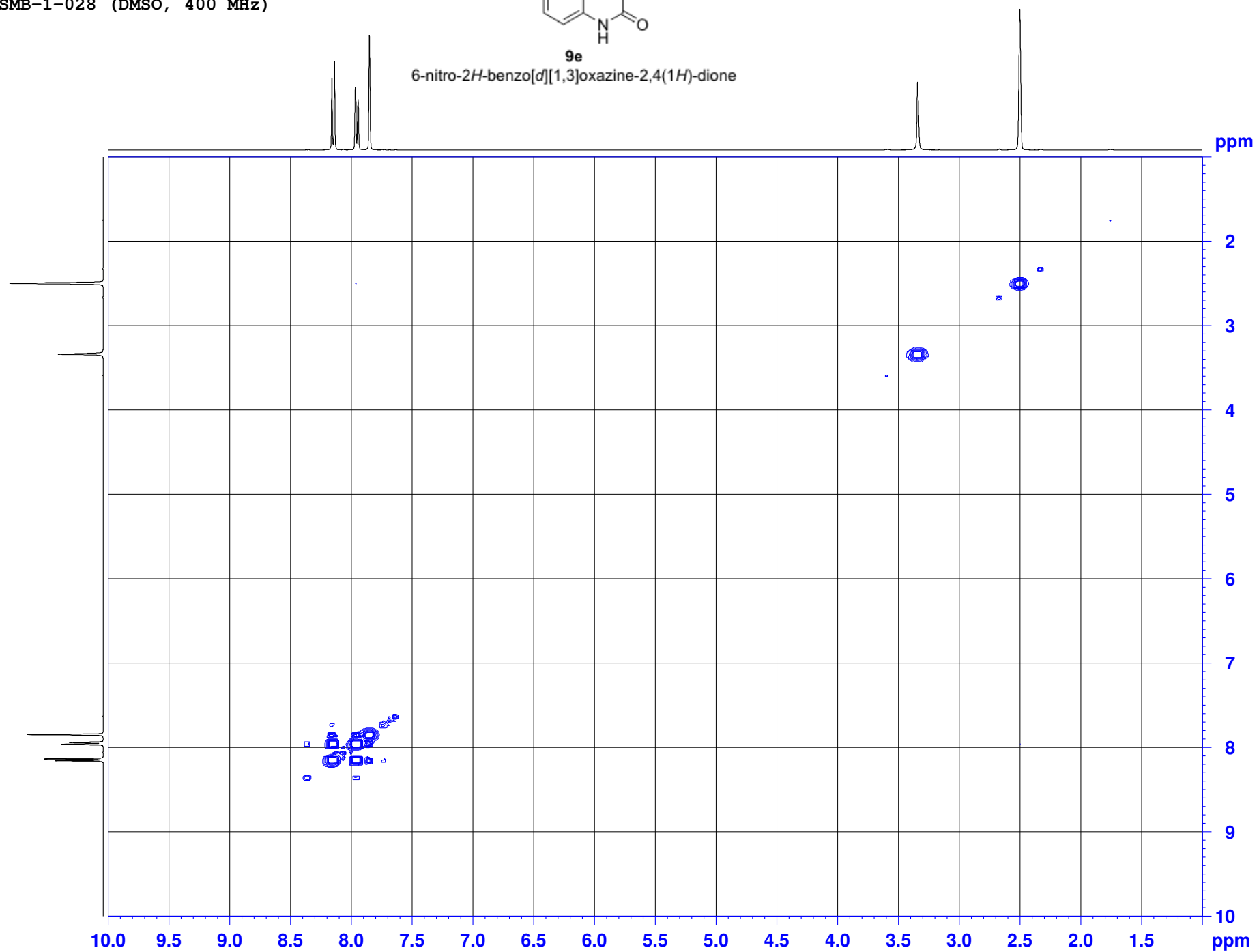


SMB-1-028 (DMSO, 400 MHz)

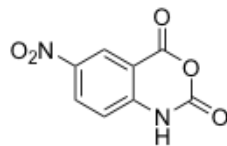


9e

6-nitro-2H-benzo[d][1,3]oxazine-2,4(1H)-dione

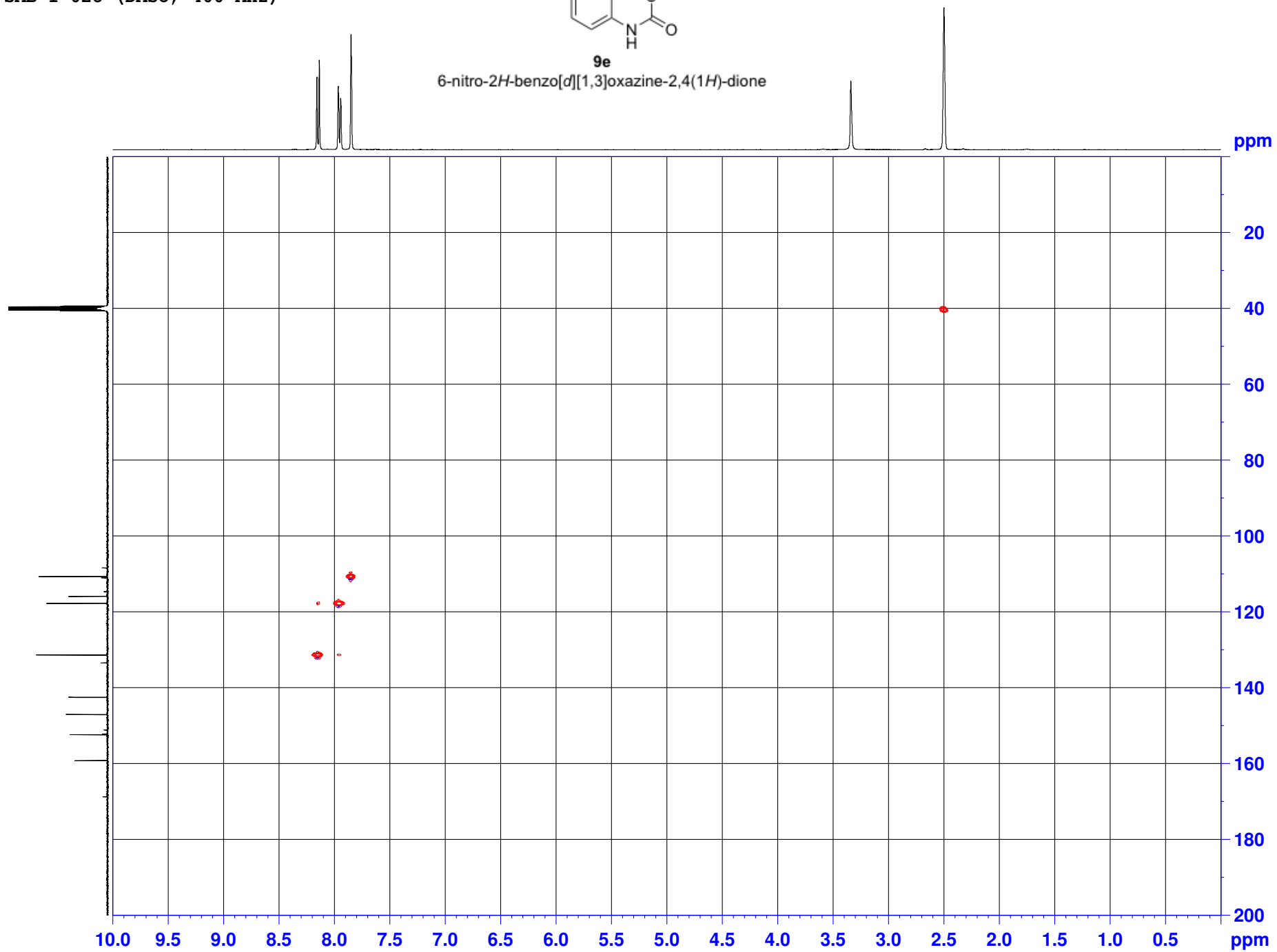


SMB-1-028 (DMSO, 400 MHz)

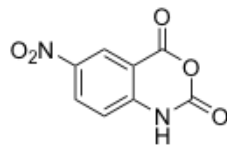


9e

6-nitro-2*H*-benzo[d][1,3]oxazine-2,4(1*H*)-dione

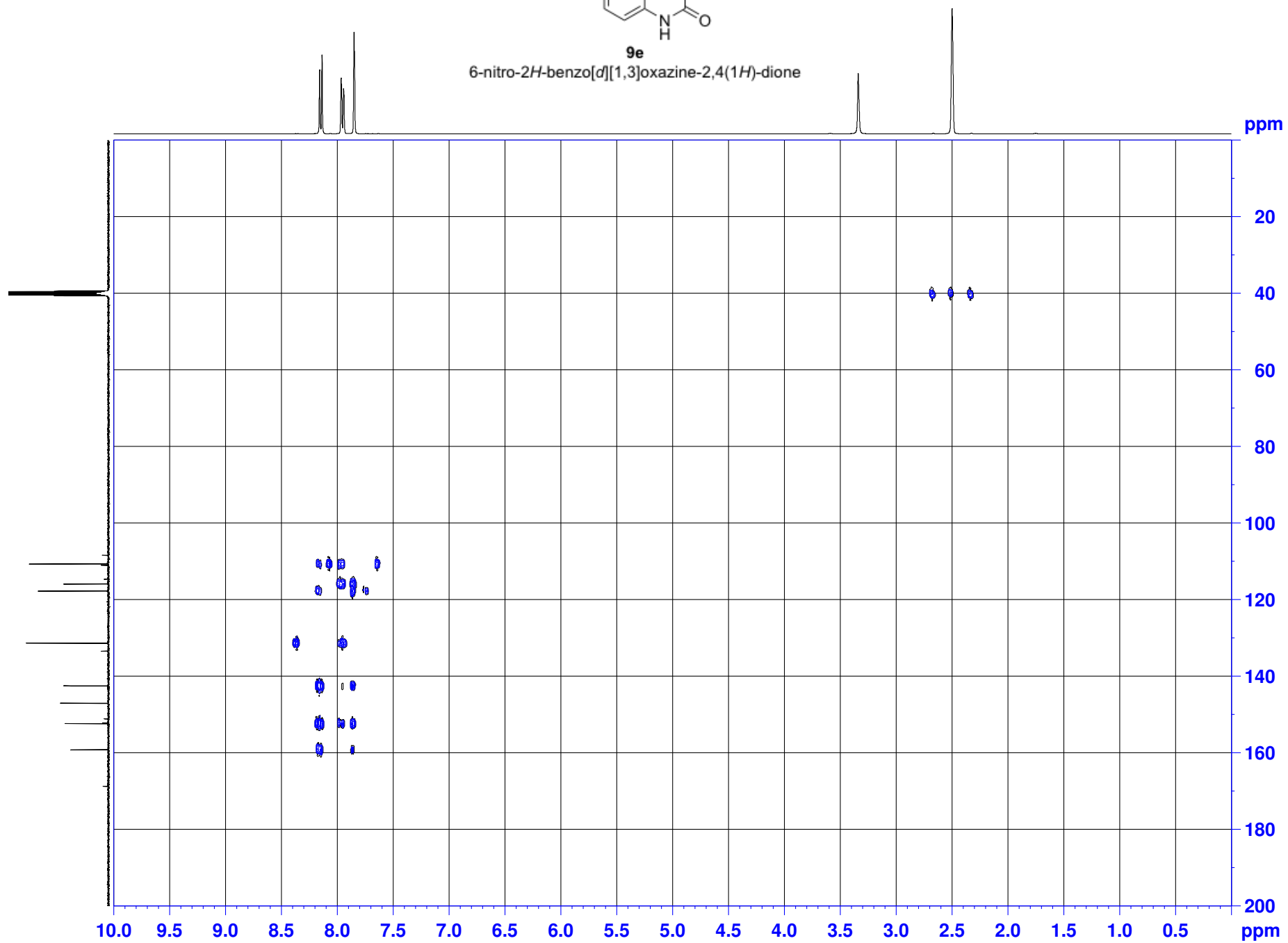


SMB-1-028 (DMSO, 400 MHz)



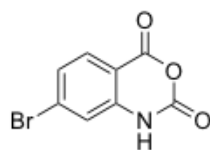
9e

6-nitro-2H-benzo[d][1,3]oxazine-2,4(1H)-dione



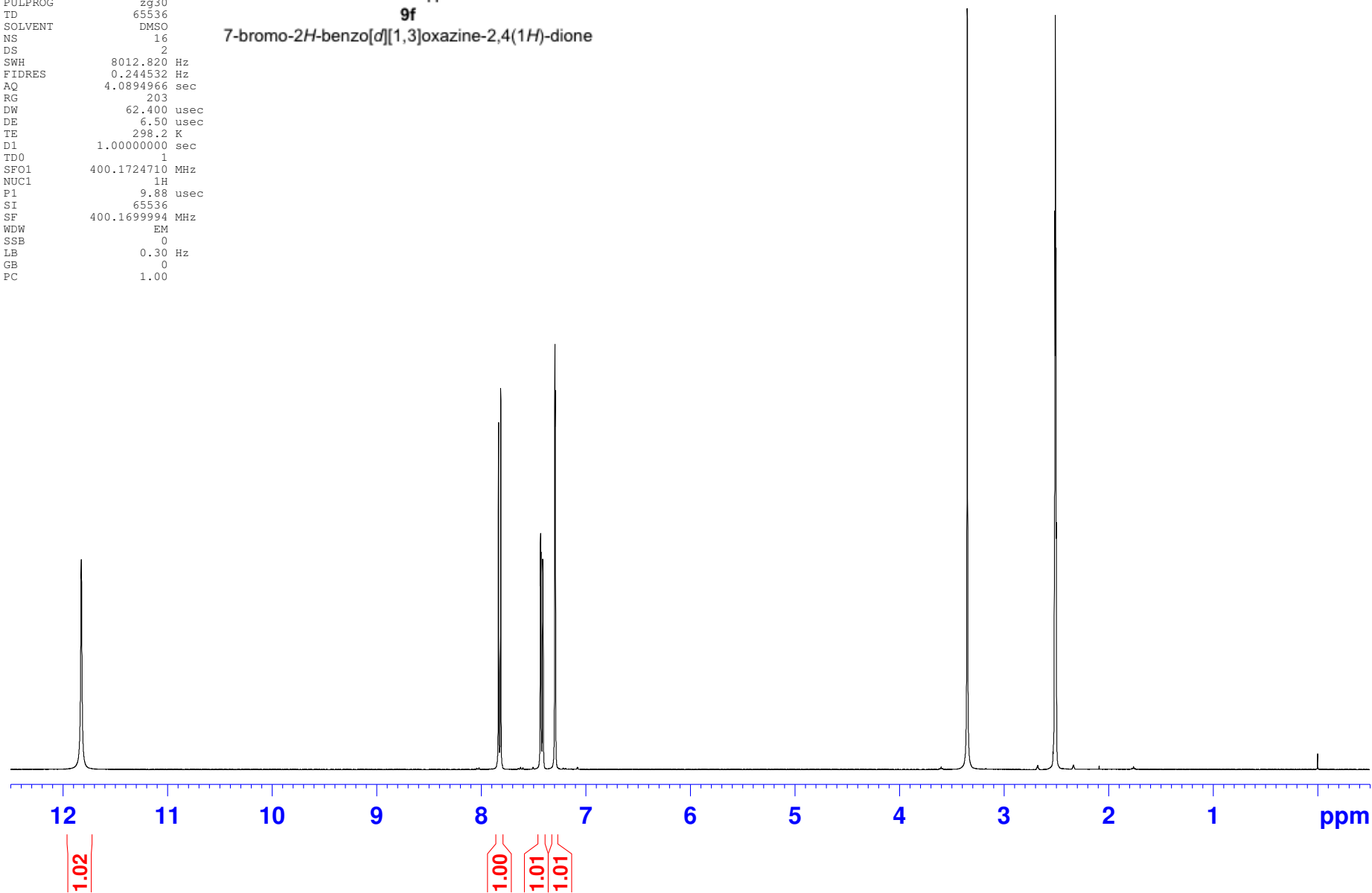
NGJ-8-029 (DMSO, 400 MHz) Crude White Solid - 7-bromoisatoic anhydride

NAME NGJ-8-029
 EXPNO 20
 PROCNO 1
 Date_ 20170816
 Time_ 18.00 h
 INSTRUM spect
 PROBHD Z108618_0161 (
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894966 sec
 RG 203
 DW 62.400 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.1724710 MHz
 NUC1 1H
 P1 9.88 usec
 SI 65536
 SF 400.1699994 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



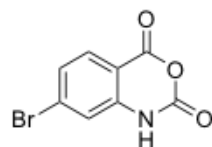
9f

7-bromo-2H-benzo[d][1,3]oxazine-2,4(1H)-dione



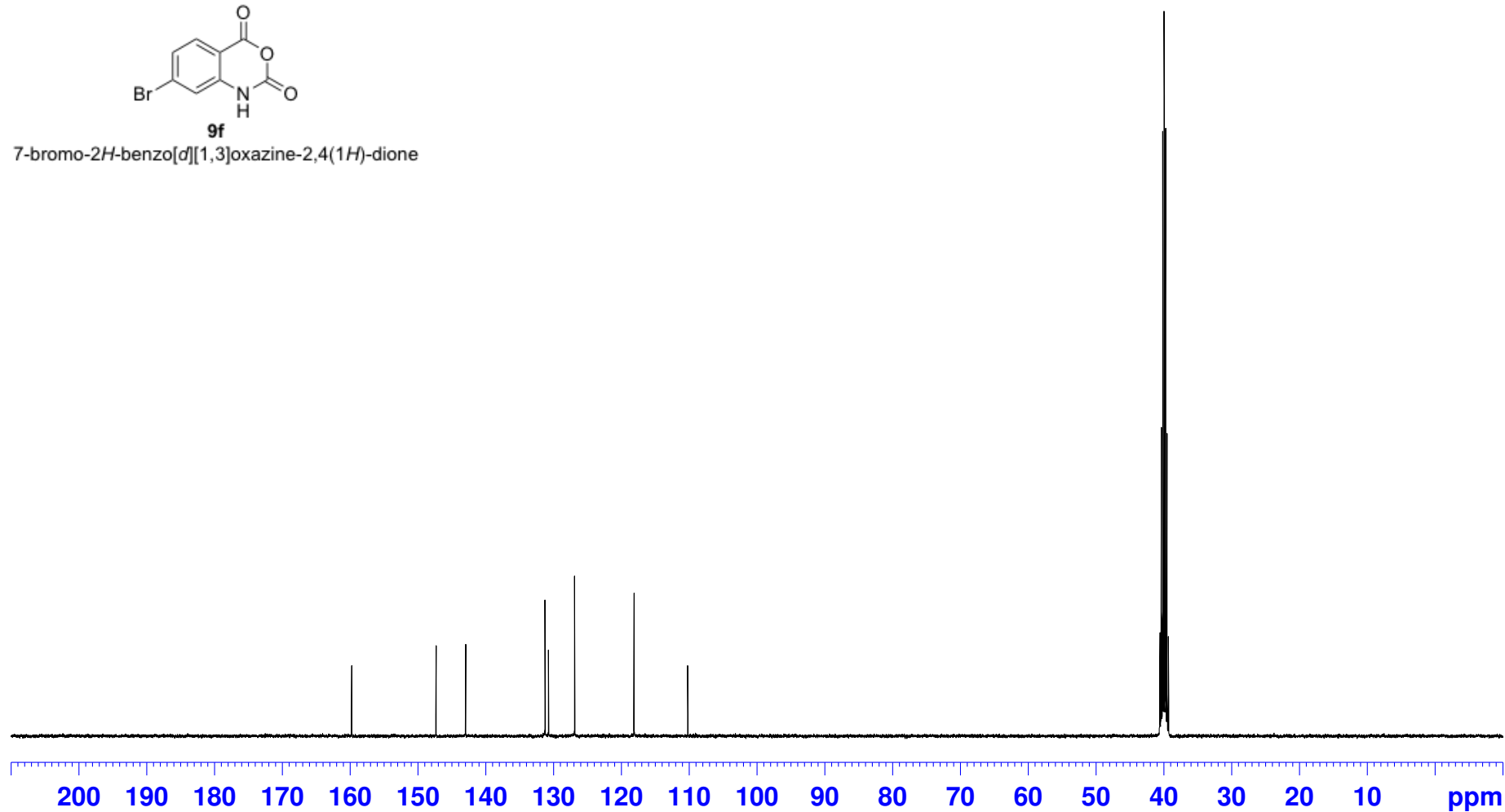
NGJ-8-029 (DMSO, 400 MHz) Crude White Solid - 7-bromoisatoic acid

159.76
147.31
142.93
131.23
130.73
126.93
118.17
110.24

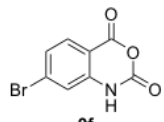


9f

7-bromo-2H-benzo[d][1,3]oxazine-2,4(1H)-dione

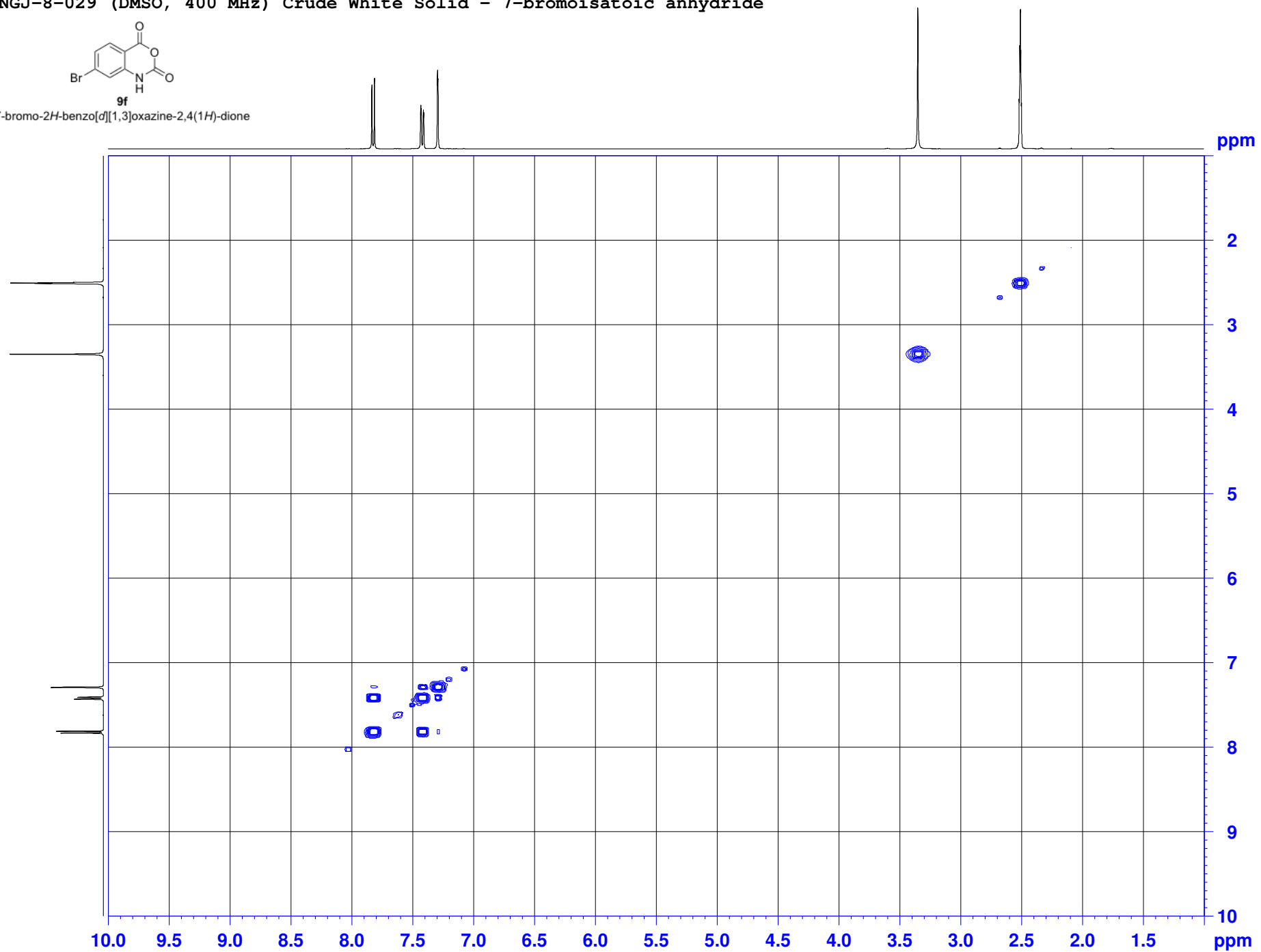


NGJ-8-029 (DMSO, 400 MHz) Crude White Solid - 7-bromoisatoic anhydride

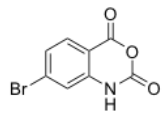


9f

7-bromo-2H-benzo[d][1,3]oxazine-2,4(1H)-dione

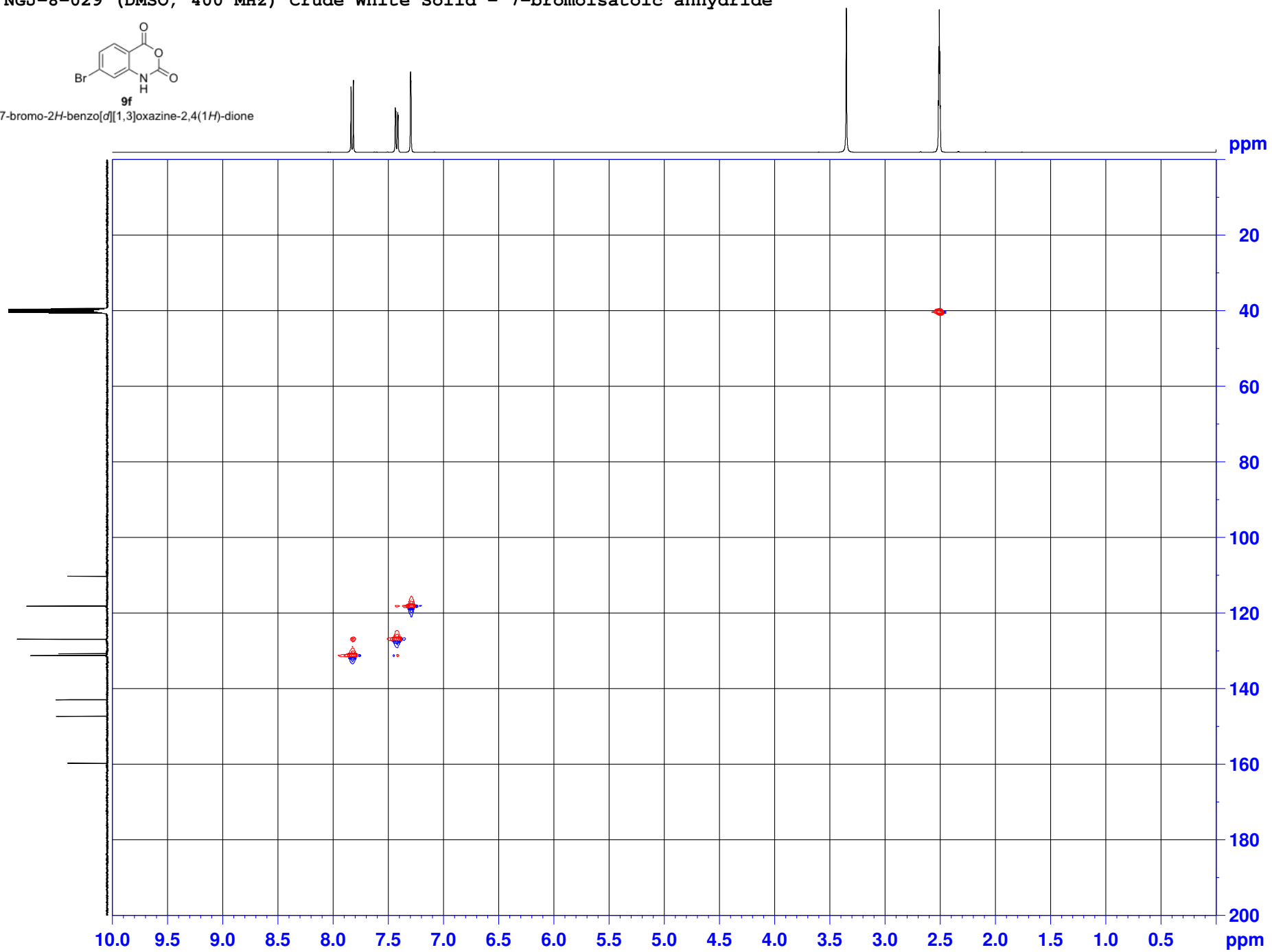


NGJ-8-029 (DMSO, 400 MHz) Crude White Solid - 7-bromoisatoic anhydride

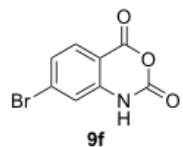


9f

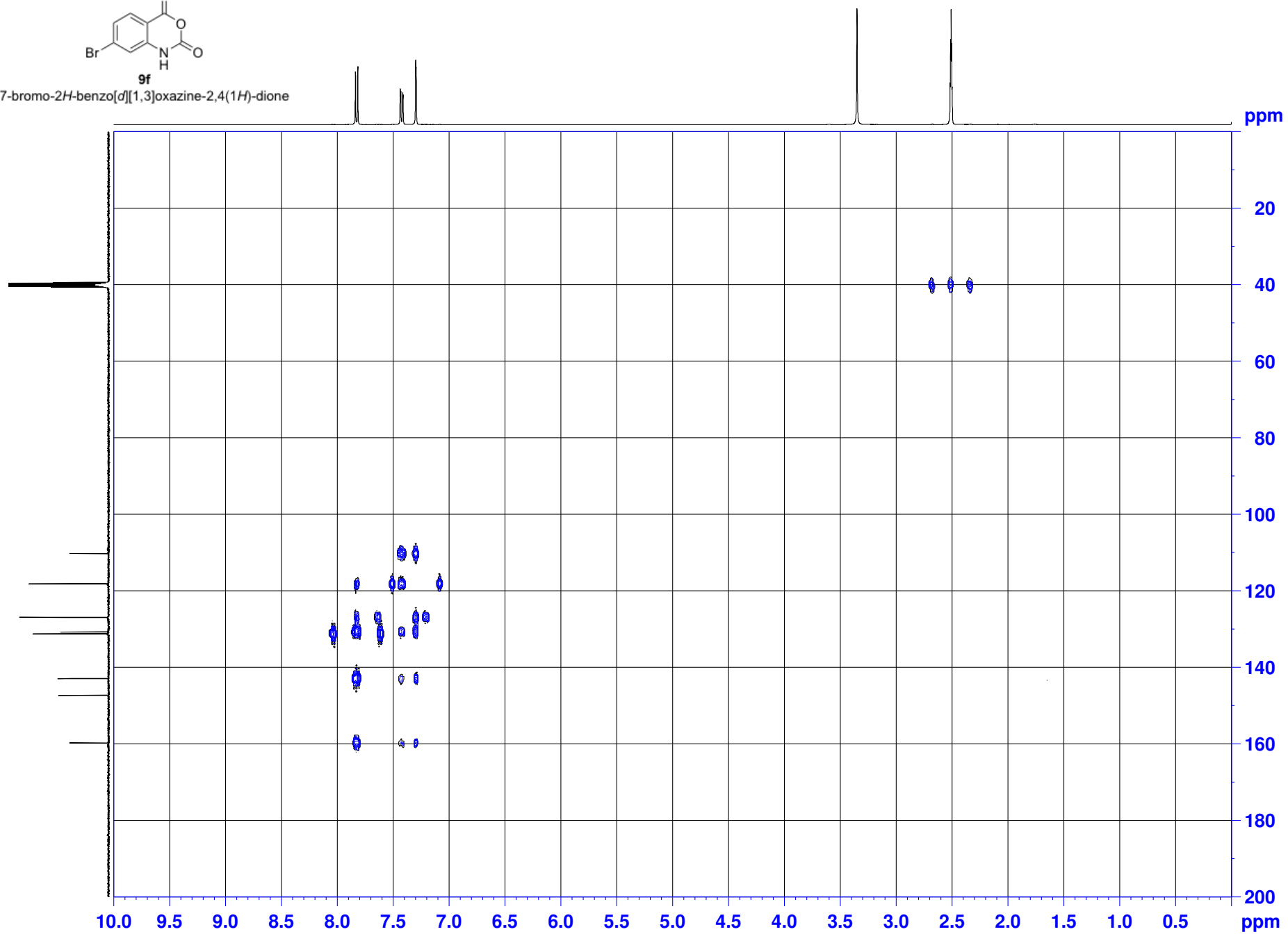
7-bromo-2*H*-benzo[*d*][1,3]oxazine-2,4(1*H*)-dione



NGJ-8-029 (DMSO, 400 MHz) Crude White Solid - 7-bromoisatoic anhydride

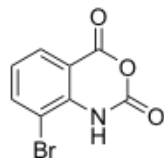


7-bromo-2H-benzo[d][1,3]oxazine-2,4(1H)-dione



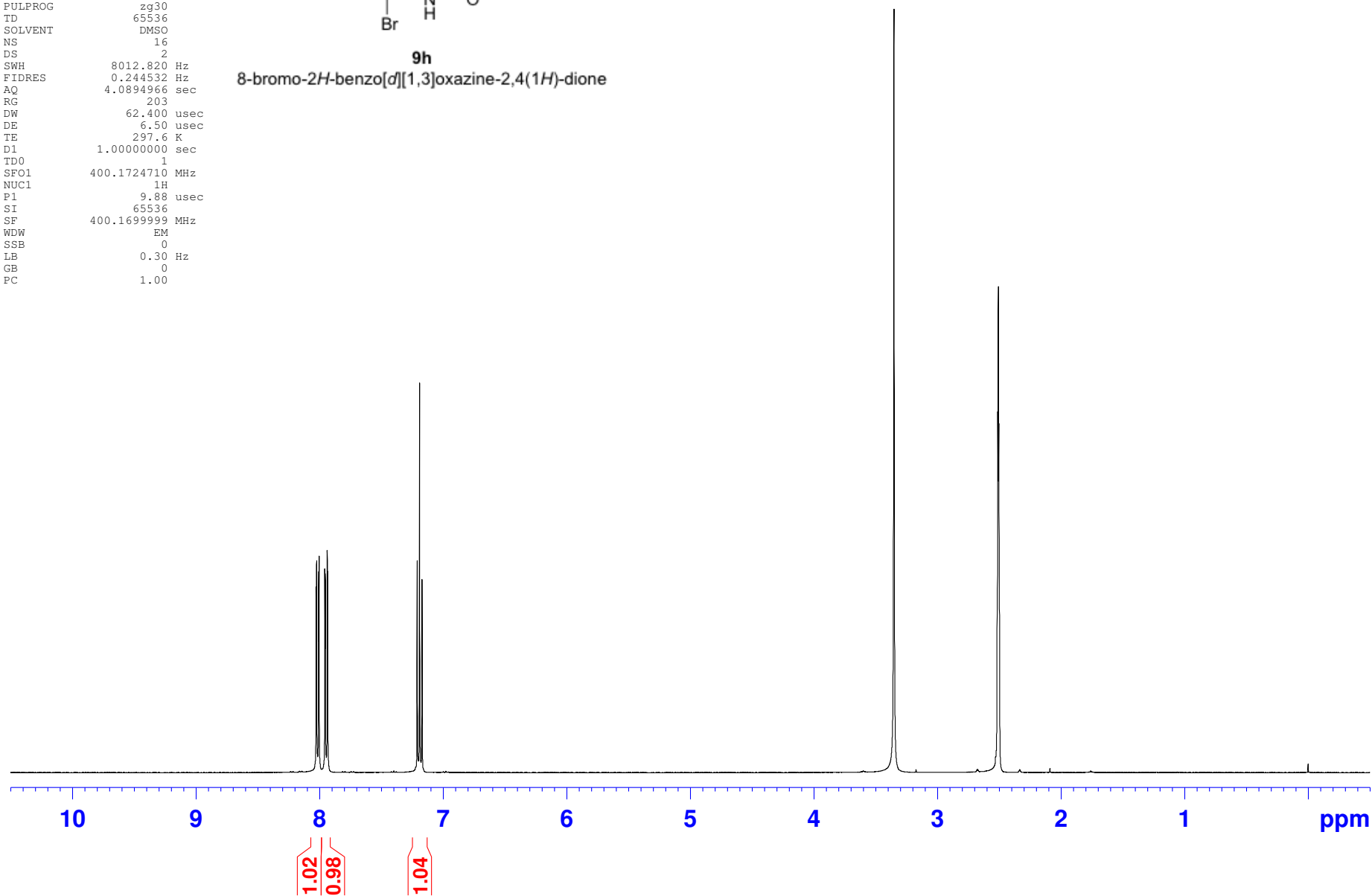
NGJ-8-034 (DMSO, 400 MHz) Pure Tan Solid - synthesis of 8-bromo isatoic anhydride

NAME NGJ-8-034
EXPNO 20
PROCNO 1
Date_ 20170823
Time_ 21.16 h
INSTRUM spect
PROBHD Z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 297.6 K
D1 1.00000000 sec
TD0 1
SF01 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1699999 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



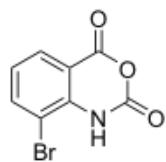
9h

8-bromo-2H-benzo[d][1,3]oxazine-2,4(1H)-dione



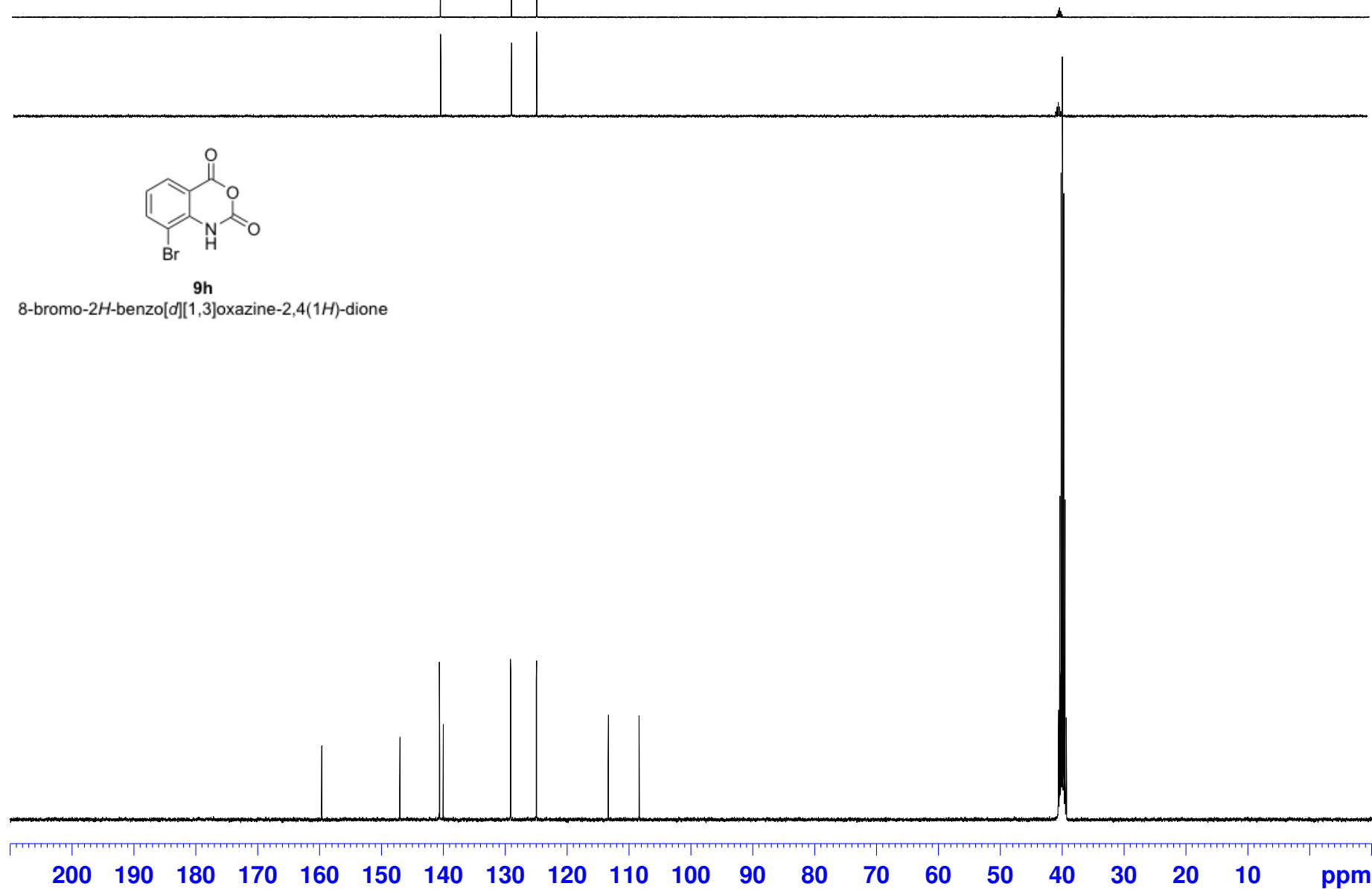
NGJ-8-034 (DMSO, 400 MHz) Pure Tan Solid - synthesis of 8-brom

159.60
147.00
140.59
139.98
129.10
124.99
113.38
108.40

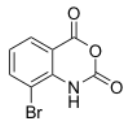


9h

8-bromo-2H-benzo[d][1,3]oxazine-2,4(1H)-dione

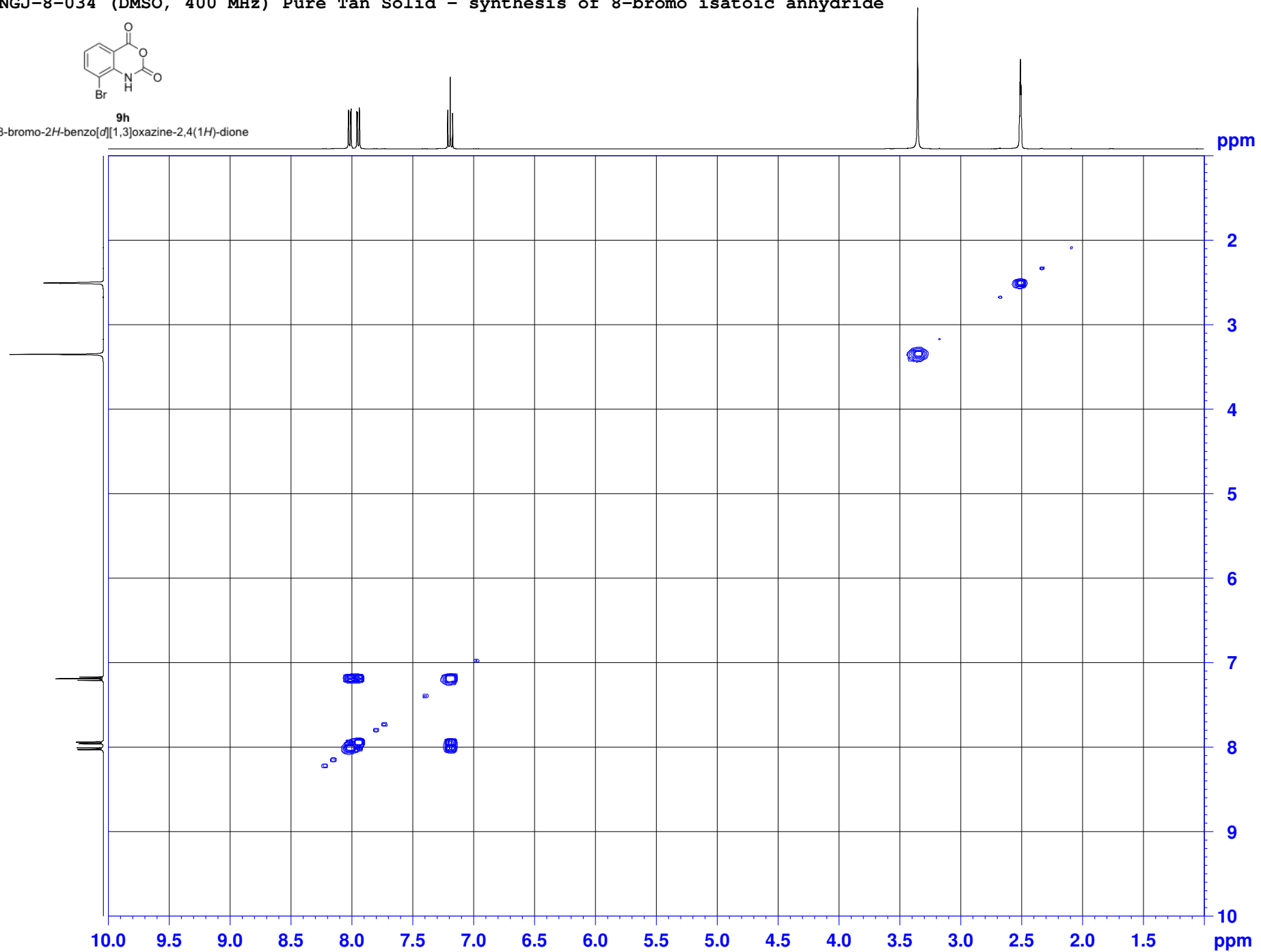


NGJ-8-034 (DMSO, 400 MHz) Pure Tan Solid - synthesis of 8-bromo isatoic anhydride

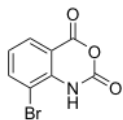


9h

8-bromo-2H-benzo[d][1,3]oxazine-2,4(1H)-dione

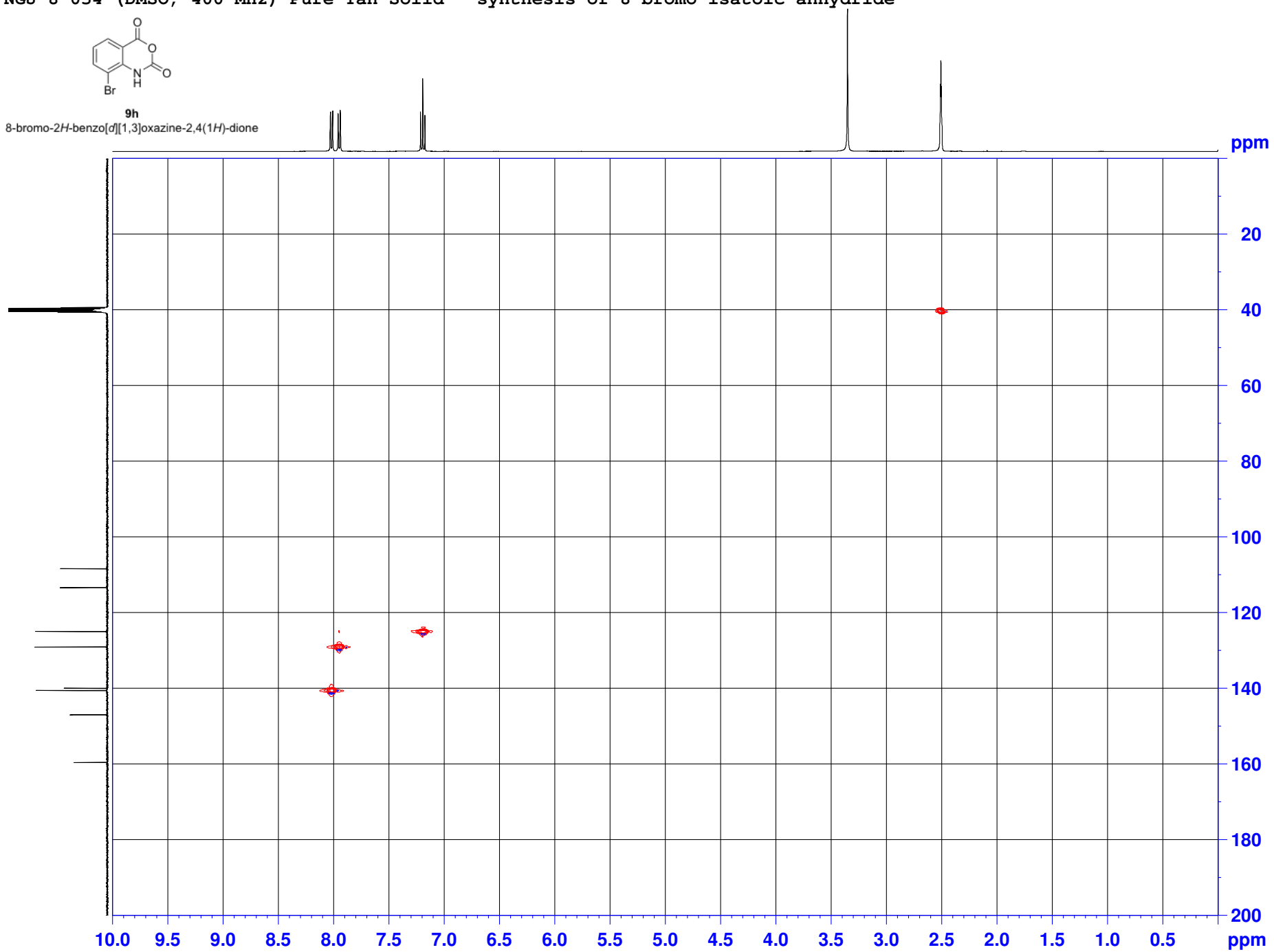


NGJ-8-034 (DMSO, 400 MHz) Pure Tan Solid - synthesis of 8-bromo isatoic anhydride

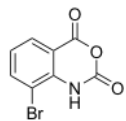


9h

8-bromo-2H-benzo[d][1,3]oxazine-2,4(1H)-dione

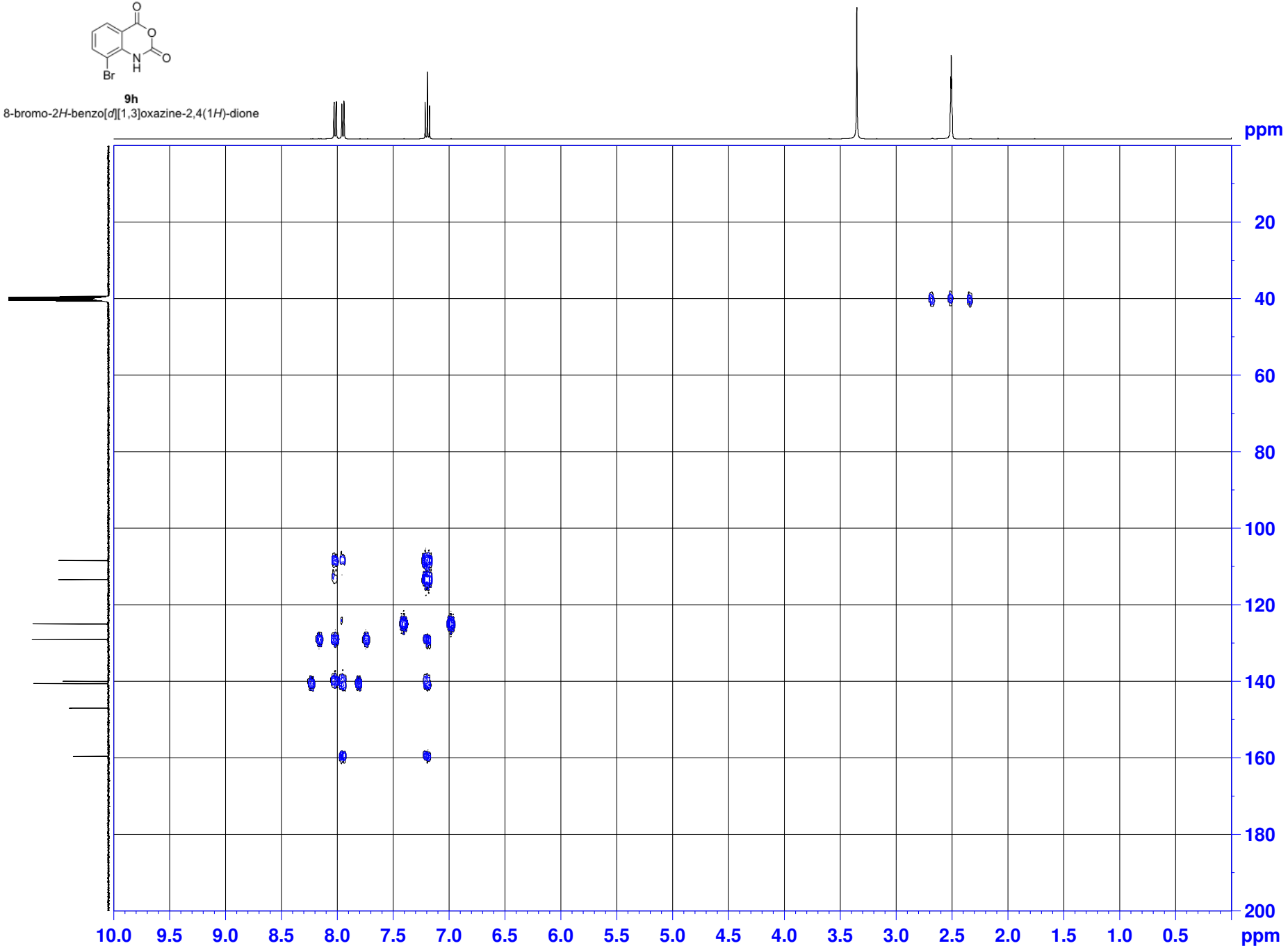


NGJ-8-034 (DMSO, 400 MHz) Pure Tan Solid - synthesis of 8-bromo isatoic anhydride



9h

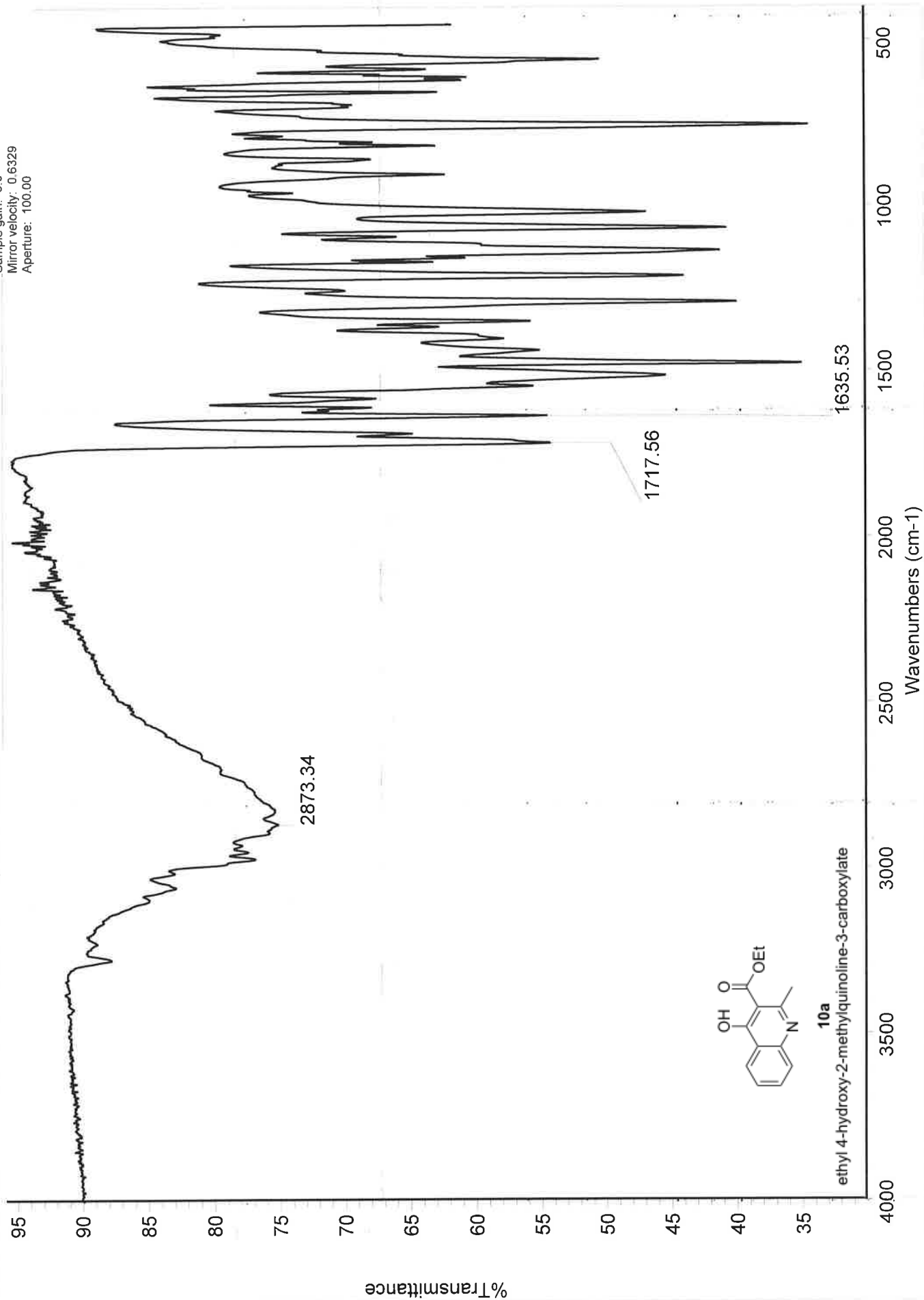
8-bromo-2H-benzo[d][1,3]oxazine-2,4(1H)-dione



AHP-1-020

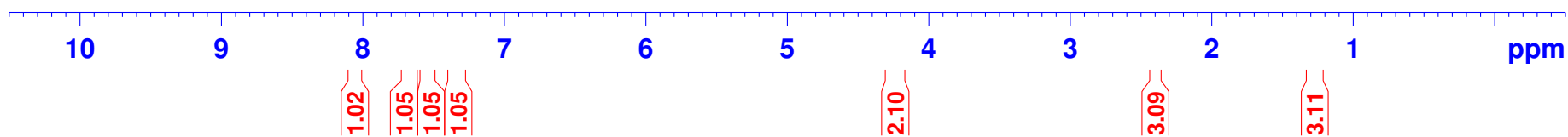
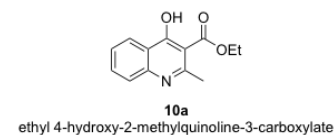
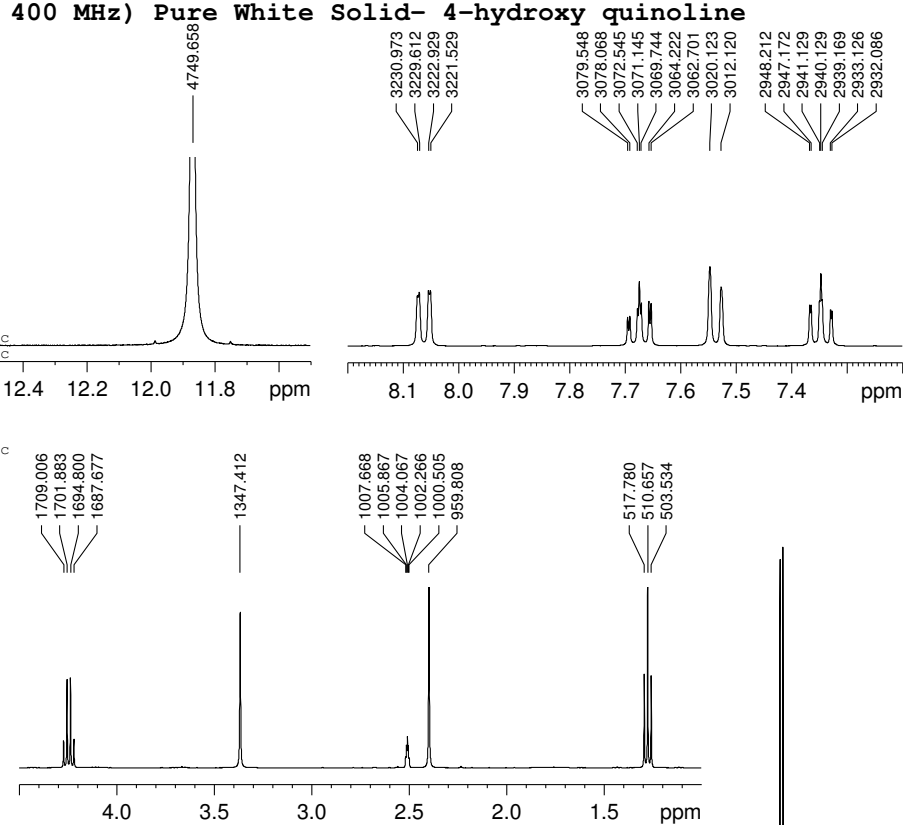
Collection time: Tue Dec 20 09:33:07 2016 (GMT-06:00)

Number of sample scans: 32
Number of background scans: 16
Resolution: 4.000
Sample gain: 8.0
Mirror velocity: 0.6329
Aperture: 100.00

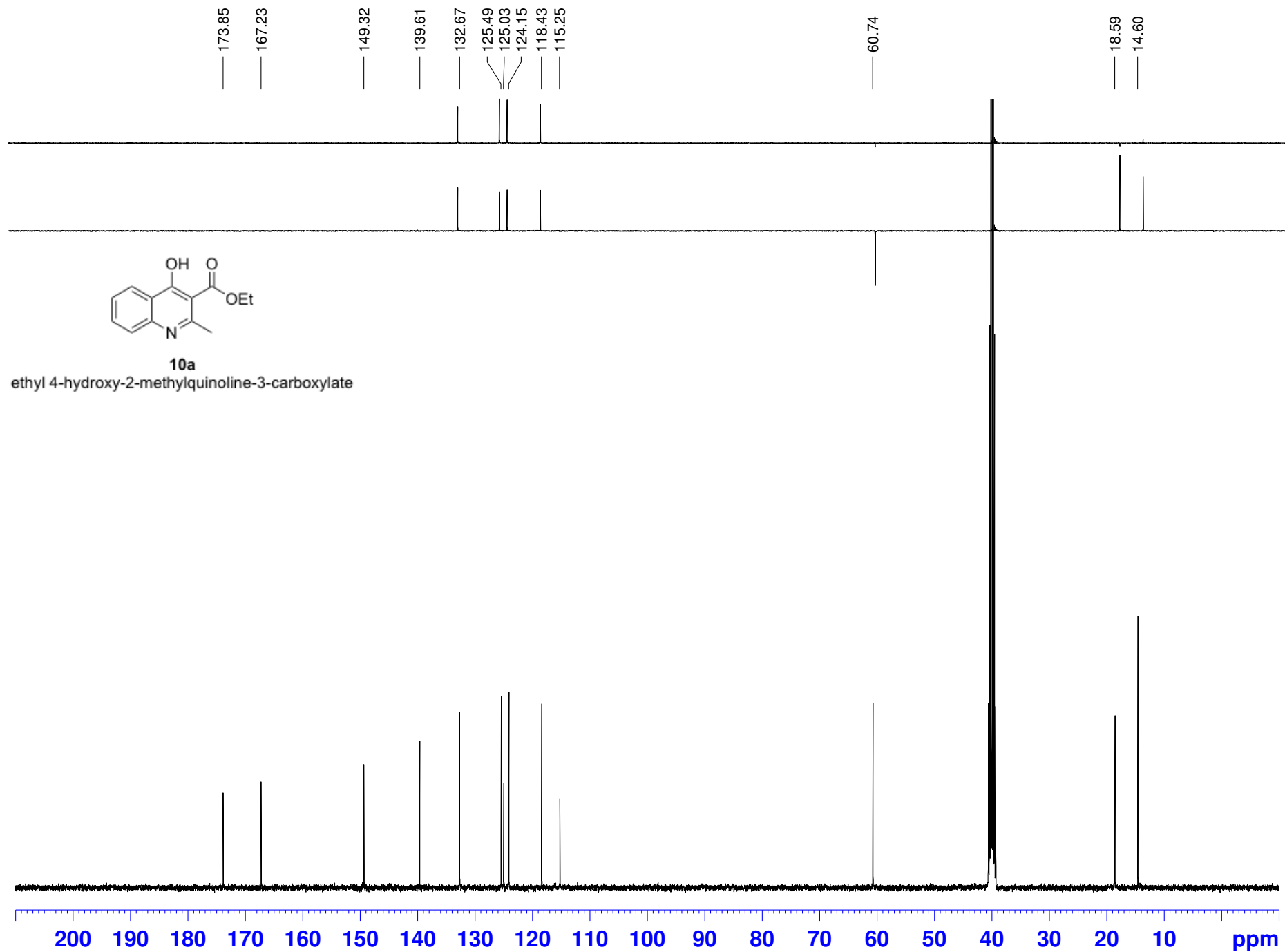


AHP-1-020 (DMSO, 400 MHz) Pure White Solid- 4-hydroxy quinoline

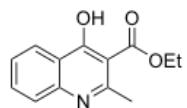
NAME AHP-1-020
 EXPNO 20
 PROCNO 1
 Date_ 20161203
 Time 17.45 h
 INSTRUM spect
 PROBHD Z108618_0161
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894966 sec
 RG 161
 DW 62.400 usec
 DE 6.50 usec
 TE 297.0 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.1724710 MHz
 NUC1 1H
 P1 29.07 usec
 SI 65536
 SF 400.1699992 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



AHP-1-020 (DMSO, 400 MHz)

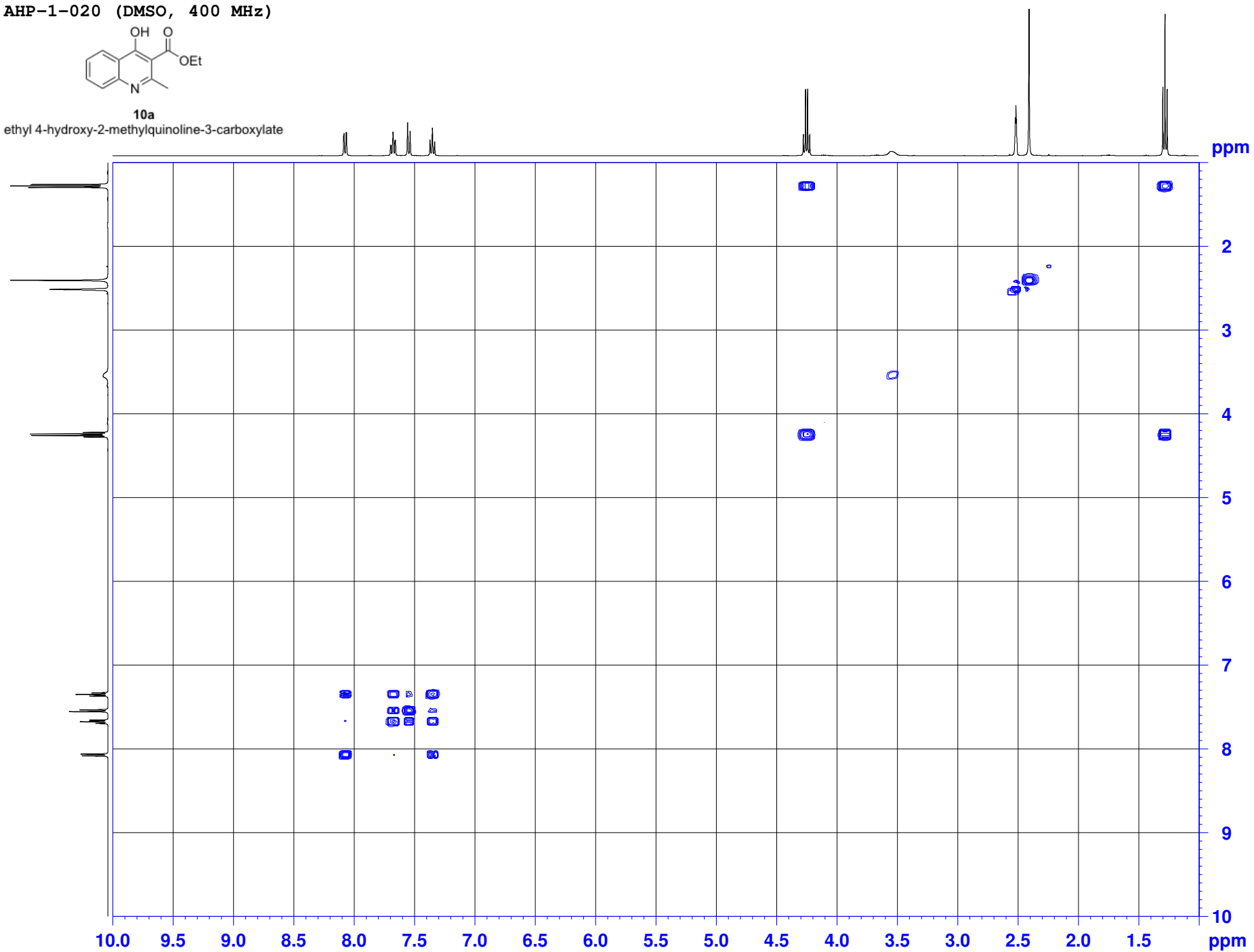


AHP-1-020 (DMSO, 400 MHz)

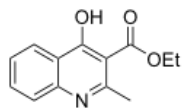


10a

ethyl 4-hydroxy-2-methylquinoline-3-carboxylate

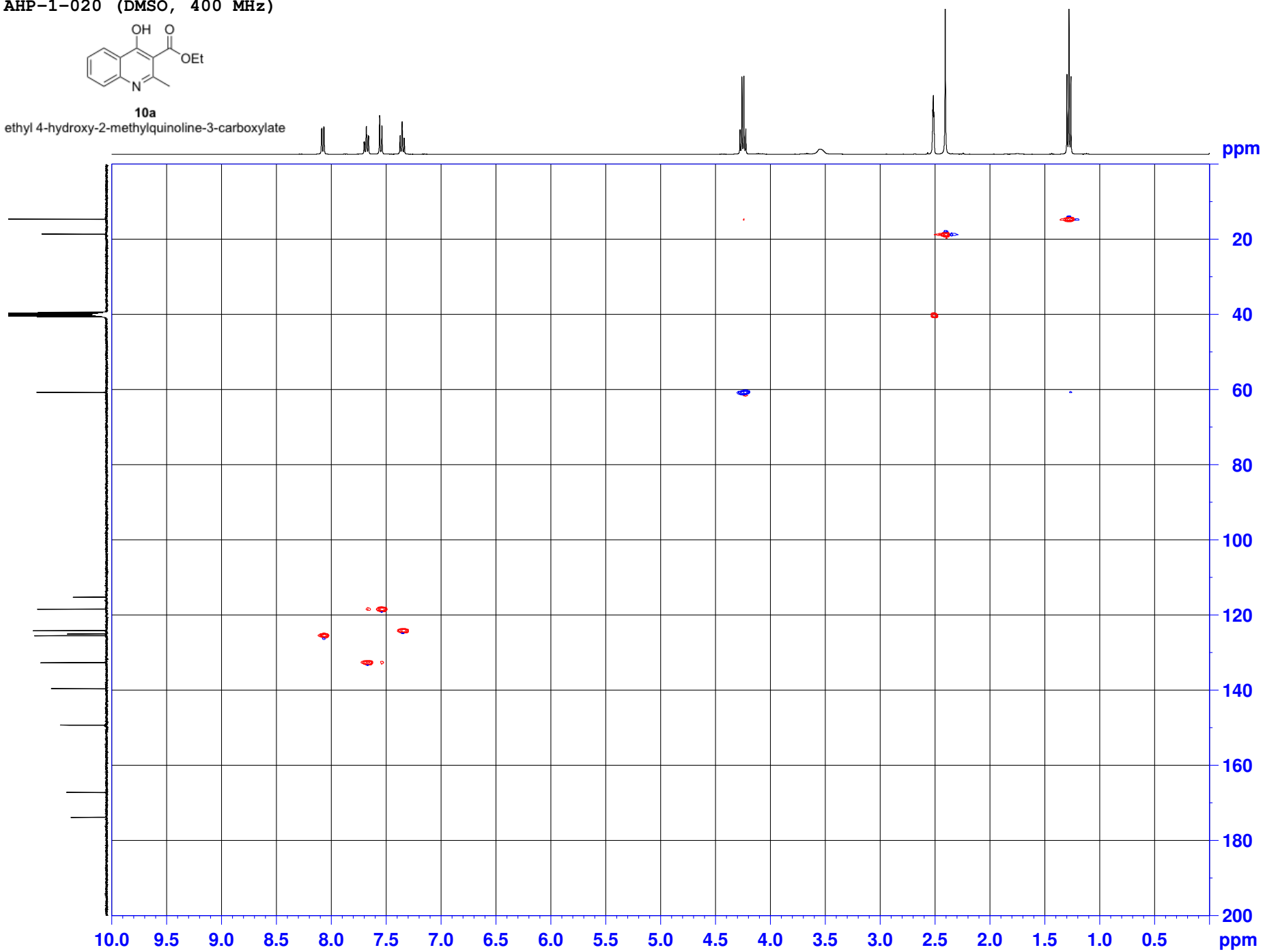


AHP-1-020 (DMSO, 400 MHz)

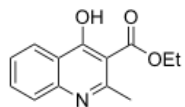


10a

ethyl 4-hydroxy-2-methylquinoline-3-carboxylate

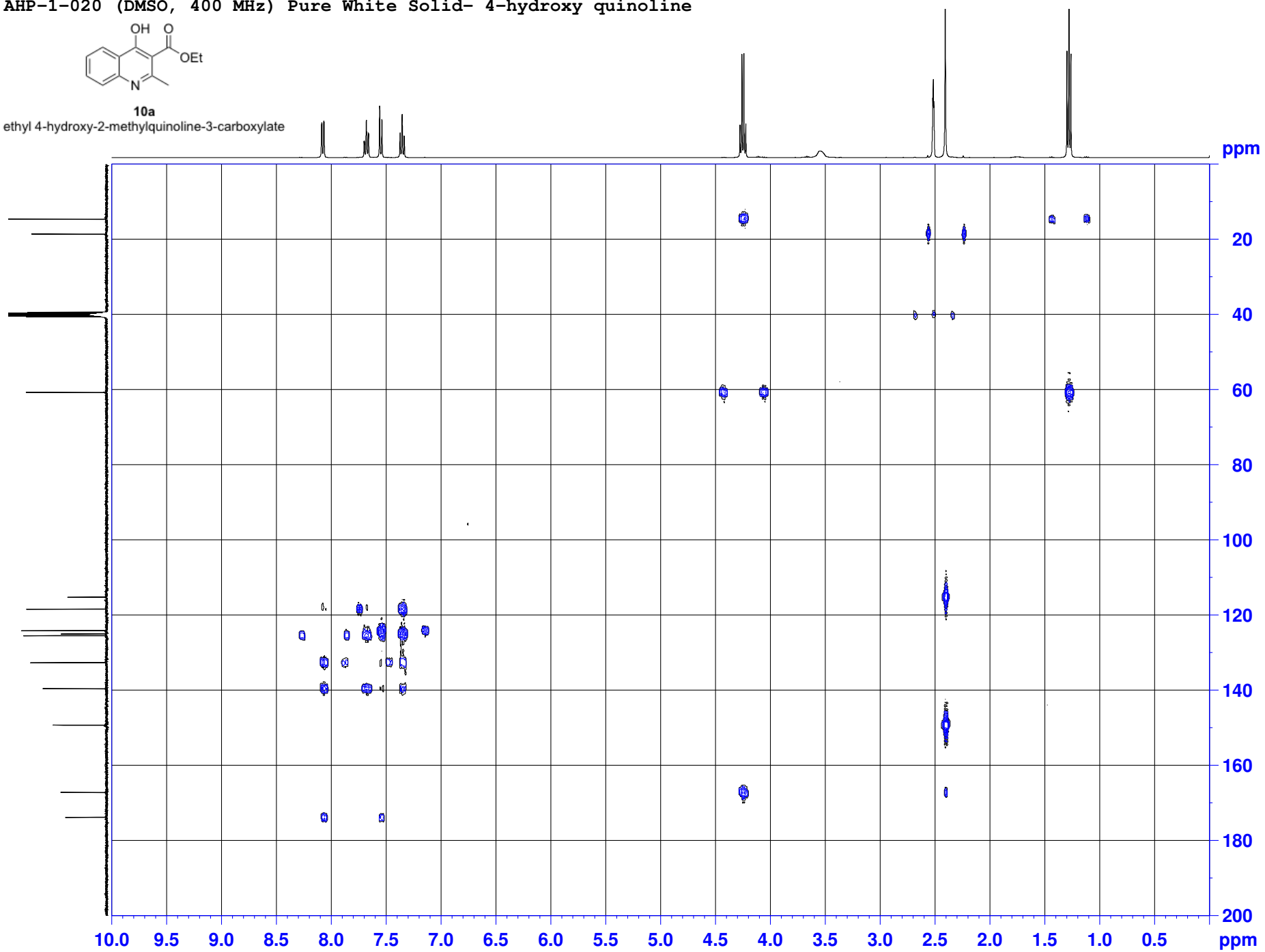


AHP-1-020 (DMSO, 400 MHz) Pure White Solid- 4-hydroxy quinoline



10a

ethyl 4-hydroxy-2-methylquinoline-3-carboxylate



Atlantic Microlab, Inc.

Sample No. AHP-1-020

6180 Atlantic Blvd. Suite M
Norcross, GA 30071
www.atlanticmicrolab.com

Professor/Supervisor: Matthew G. Donahue

PO# / CC# Visa 5794

Company/School University of Southern Mississippi

Dept. Chemistry and Biochemistry

Address 118 College Dr. #5043

City, State, Zip Hattiesburg, MS 39406

Name Matthew G. Donahue Date 2/25/12

Phone 614-203-1123

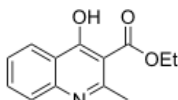
Element	Theory	Found	Single ☒	Duplicate ☐
C	67.52	66.52	Elements Present: C₁₃H₁₃NO₃	
H	5.67	5.76	Analyze for: C, H	
		5.73	Hygroscopic ☐ Explosive ☐	
			M.P. ☐ B.P. ☐	
			To be dried: Yes ☐ No ☒	
			Temp. ☐ Vac. ☐ Time ☐	
			Rush Service ☐ Rush service guarantees analysis will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.	
			Include Email Address or FAX # Below	
			matthew.donahue@usm.edu	

MAR 13 P.M.

Date Completed

MAR 14 2017

Date Received
Remarks:



10a

ethyl 4-hydroxy-2-methylquinoline-3-carboxylate

Mass Spectrum List Report

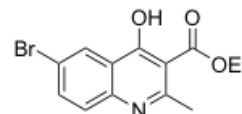
Analysis Info

Analysis Name G:\Data\apexdata111116\EBC-1-009_pos_000001.d
Method Neg_DOM_032112
Sample Name EBC-1-009
Comment EBC-1-009 in MeOH:THF with NaCl added

Acquisition Date 11/11/2016 3:33:29 PM

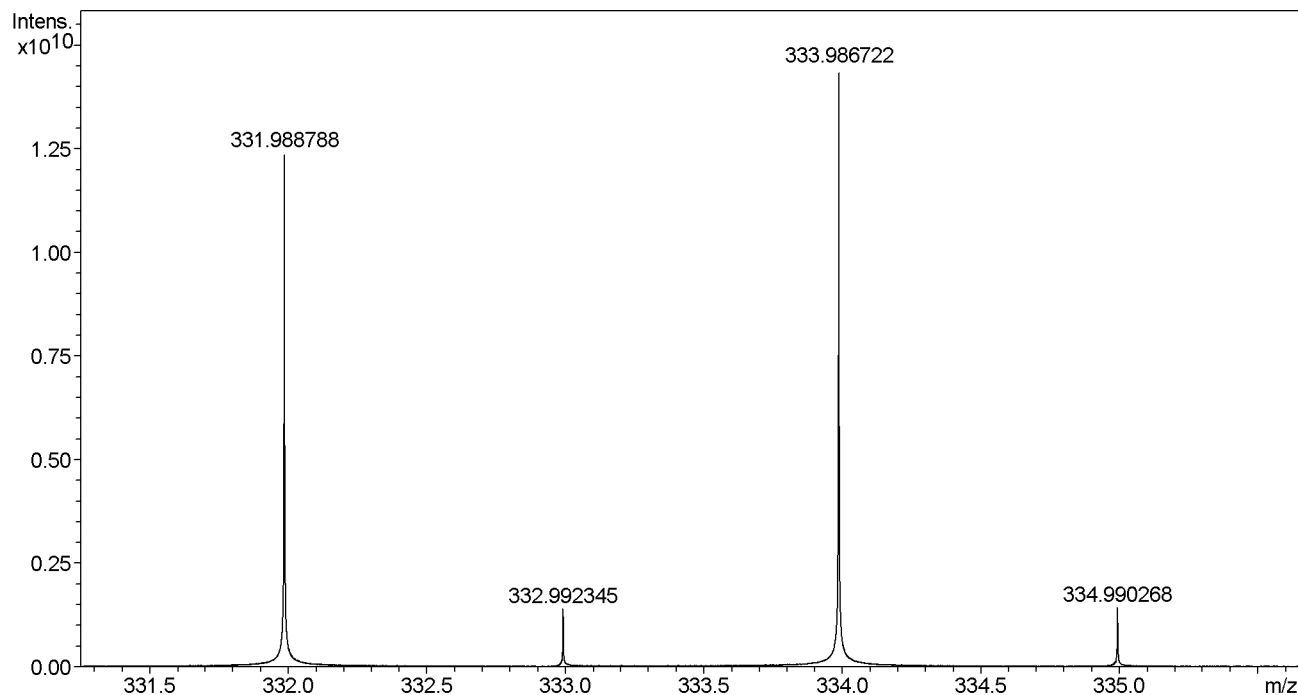
Operator FTMS_USER
Instrument apex-Qe

Sample Name EBC-1-009
Exact Mass of C₁₂H₁₂BrNO₃Na⁺ = 331.989277 m/z
Mass Observed with signature = 331.988788 m/z
Difference < -1.5 ppm



10b

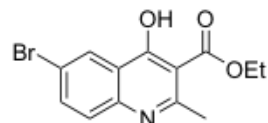
ethyl 6-bromo-4-hydroxy-2-methylquinoline-3-carboxylate



#	m/z	I
1	184.283963	24768120
2	184.318078	28267768
3	184.319972	28174904
4	215.088747	72876717
5	216.933685	53887112
6	218.207464	589511162
7	219.492165	49374700
8	220.812057	469930650
9	263.965289	65200142
10	265.963231	78783632
11	281.975883	59984049
12	283.973876	50207343
13	310.007021	204095469
14	312.004973	247188977
15	314.341485	40748245
16	331.988788	12405816634
17	332.989875	344055448
18	332.992345	1399439001
19	333.203861	27184092
20	333.597258	31554641

Mass Spectrum List Report

#	m/z	I
21	333.984417	3546070972
22	333.986722	14441103293
23	334.224004	38123002
24	334.987734	422723756
25	334.990268	1437450412
26	335.993673	65921381
27	337.965737	27704887
28	347.962923	103942939
29	349.182847	33175826
30	349.960911	125478823
31	351.213893	29969709
32	360.323427	110611657
33	367.208688	25808934
34	368.823514	53026242
35	368.834576	90639799
36	368.841783	77305264
37	370.404041	32155472
38	393.209189	27007712
39	393.260477	28799651
40	393.297140	167194231
41	394.300536	24820169
42	398.240992	121313202
43	399.244370	26374958
44	413.265883	81332931
45	425.287009	51091939
46	525.375814	53423870
47	550.628349	34942131
48	552.607372	41453689
49	567.386212	36247364
50	569.401918	138683102
51	570.405462	44318879
52	611.412388	63896188
53	612.415953	25293512
54	613.428127	203252495
55	614.431386	75319104
56	640.988804	254165193
57	641.992203	68068163
58	642.629037	52688075
59	642.986753	529171877
60	643.632136	26001190
61	643.989893	145917945
62	644.984851	249907766
63	645.987989	81747044
64	655.438894	64261521
65	656.441816	30328588
66	657.454308	221831290
67	658.457608	87695830
68	668.644704	29338704
69	672.926102	60968722
70	674.924044	132829198
71	675.927732	26824827
72	676.921573	64012507
73	685.435271	61993567
74	686.438601	27312733
75	699.464883	48537422
76	700.468086	29910751
77	701.480628	176123497
78	702.483870	66498031
79	711.506912	42365115
80	717.454283	27186339
81	722.265597	26638614
82	724.263715	29411219
83	743.491343	34842998
84	744.344042	106729704

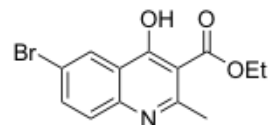


10b

ethyl 6-bromo-4-hydroxy-2-methylquinoline-3-carboxylate

Mass Spectrum List Report

#	m/z	I
85	745.347253	38457413
86	745.506598	111489068
87	746.341851	98832296
88	746.510448	42680205
89	747.345277	44797709
90	789.532665	42125751
91	877.534532	27960792
92	877.673538	30318135
93	919.683717	36163175
94	921.699388	34788645
95	963.710361	26770656
96	965.725532	28994480
97	994.434676	35133536
98	996.433484	27383399
99	997.436067	25610600
100	1009.752101	29787331

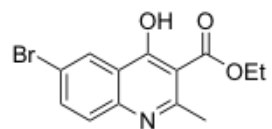


10b

ethyl 6-bromo-4-hydroxy-2-methylquinoline-3-carboxylate

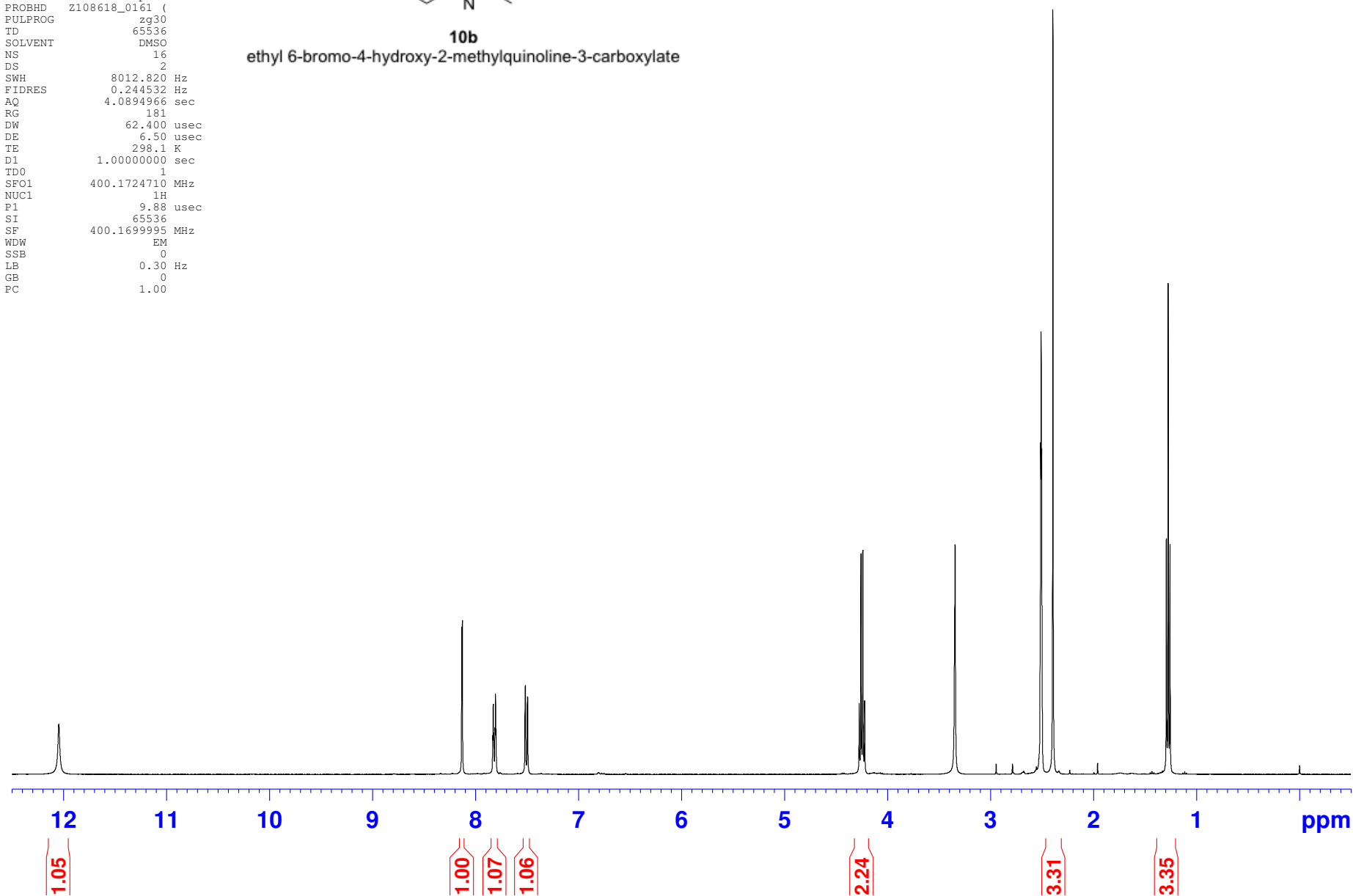
SMB-1-019 (DMSO, 400 MHz)

NAME SMB-1-019
EXPNO 60
PROCNO 1
Date_ 20170720
Time_ 20.24 h
INSTRUM spect
PROBHD Z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 181
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
SF01 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1699995 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

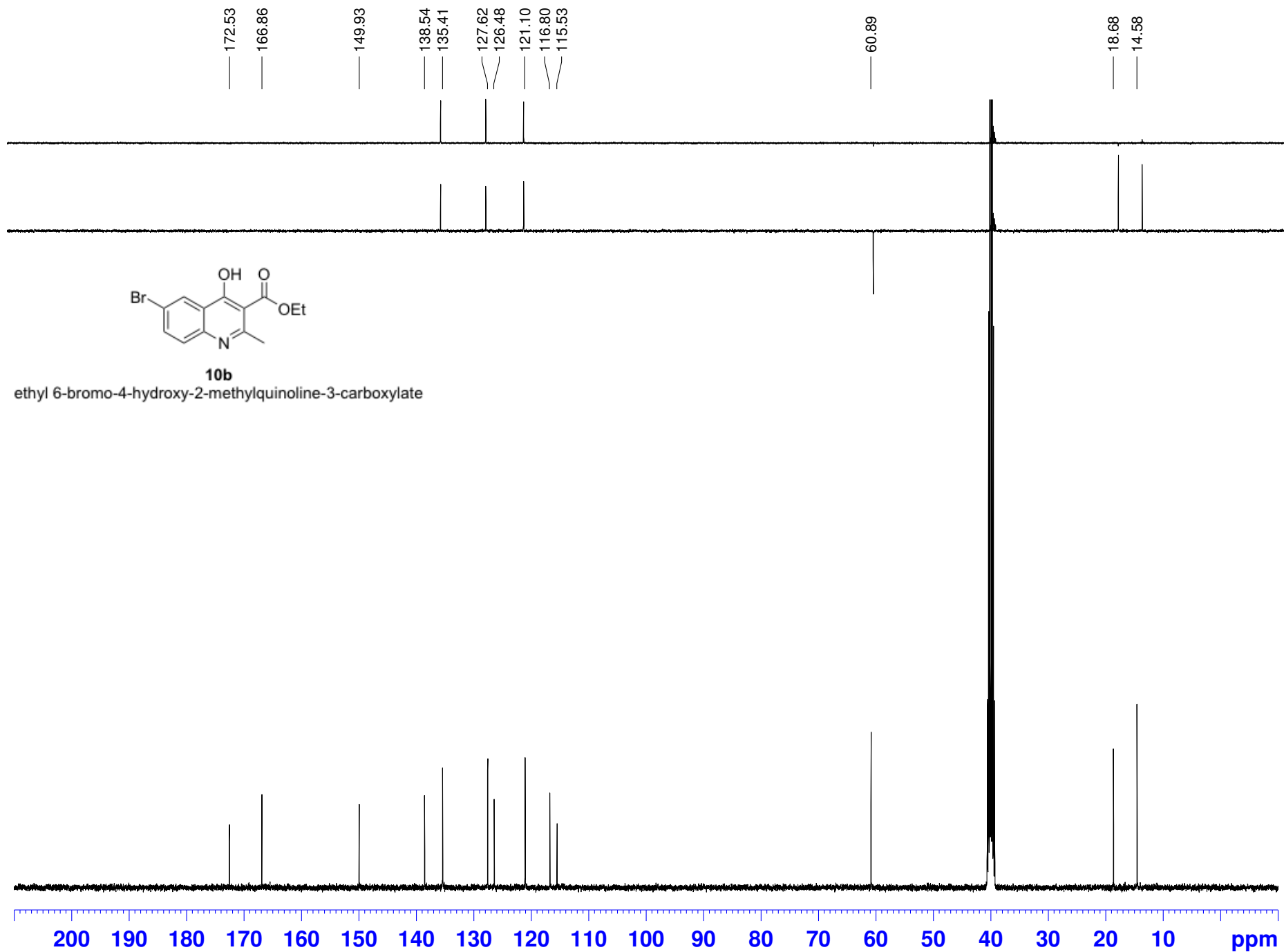


10b

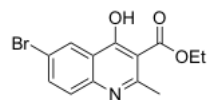
ethyl 6-bromo-4-hydroxy-2-methylquinoline-3-carboxylate



SMB-1-019 (DMSO, 400 MHz)

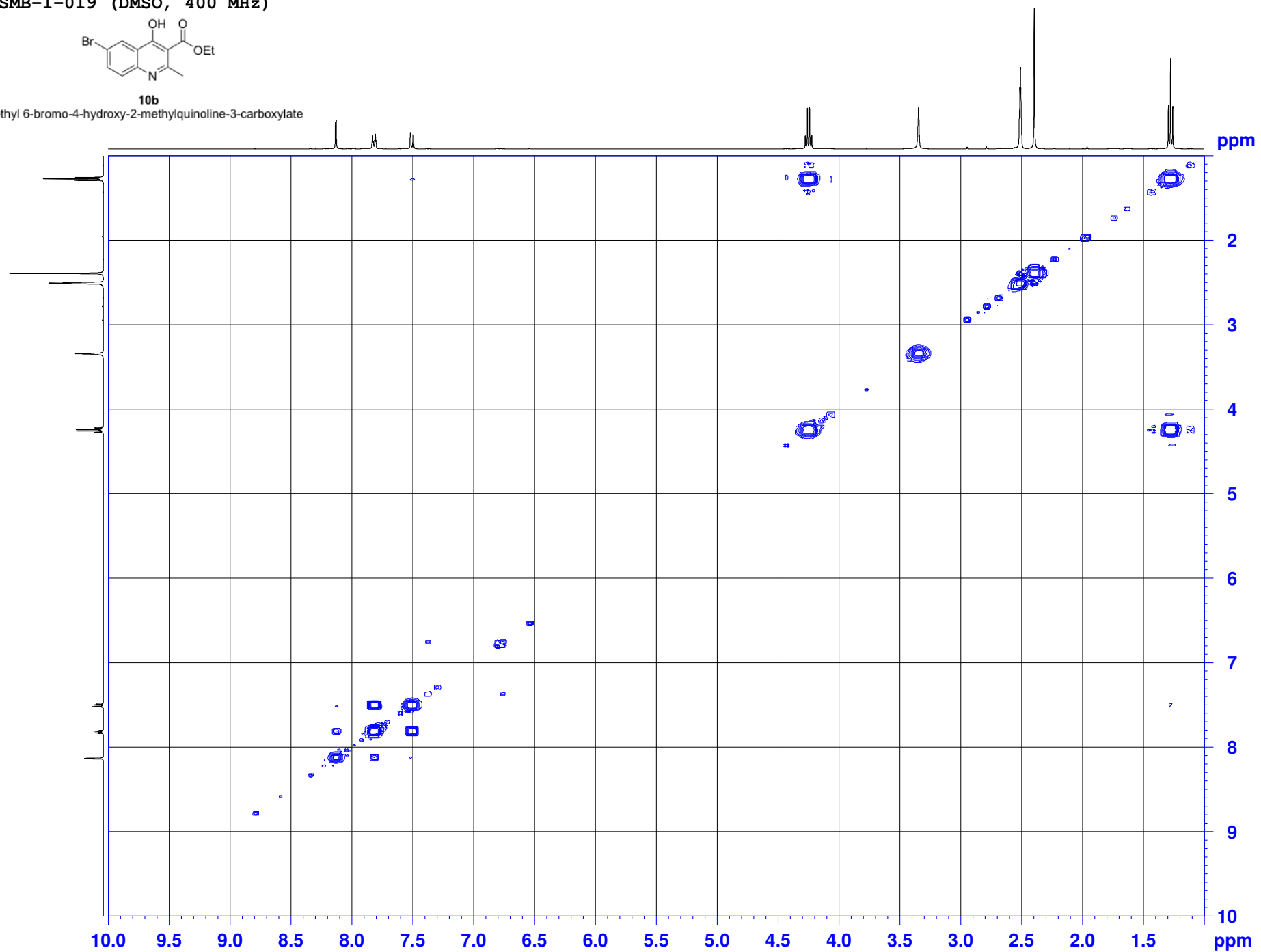


SMB-1-019 (DMSO, 400 MHz)

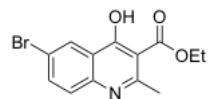


10b

ethyl 6-bromo-4-hydroxy-2-methylquinoline-3-carboxylate

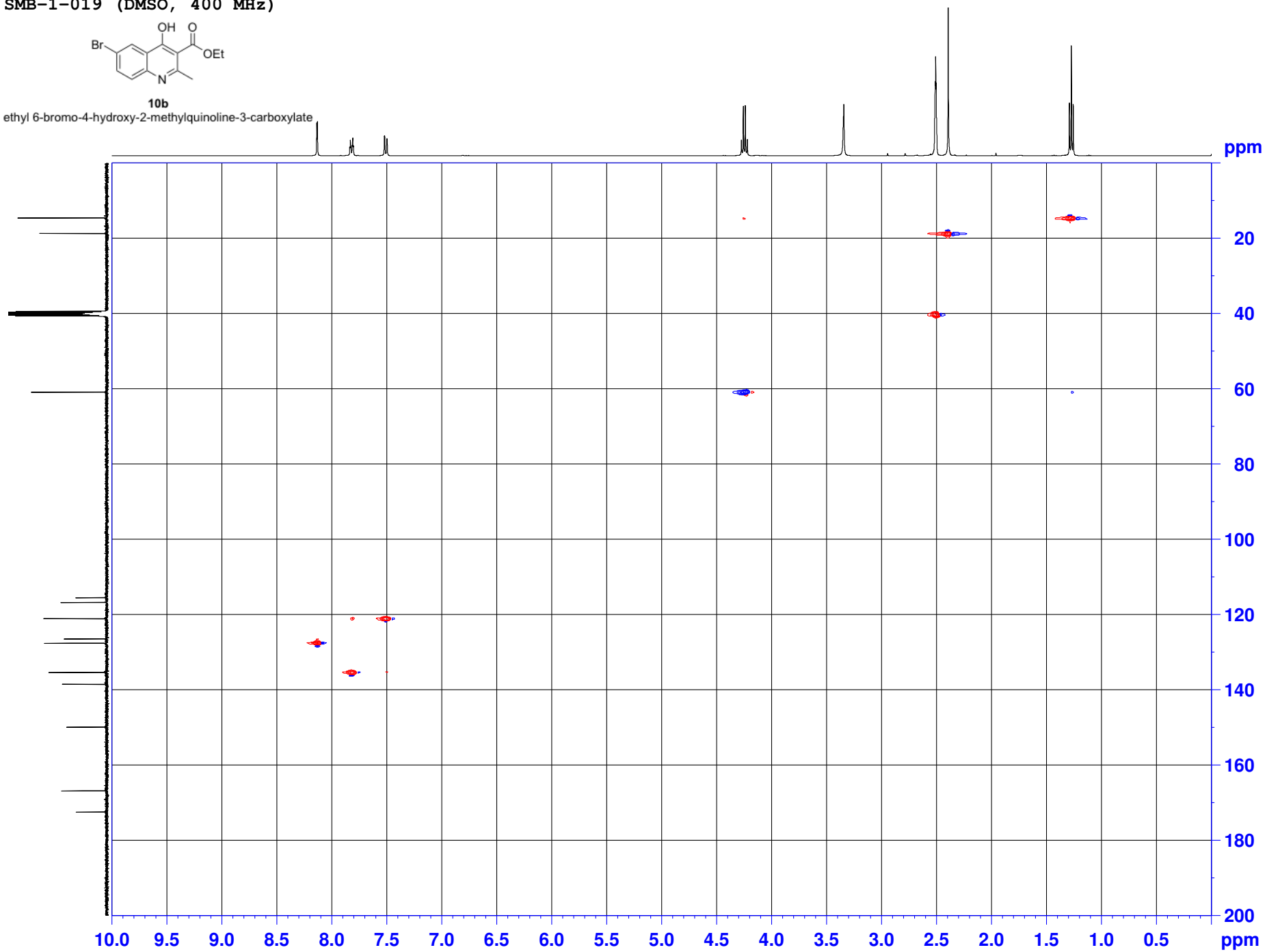


SMB-1-019 (DMSO, 400 MHz)

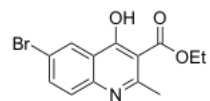


10b

ethyl 6-bromo-4-hydroxy-2-methylquinoline-3-carboxylate

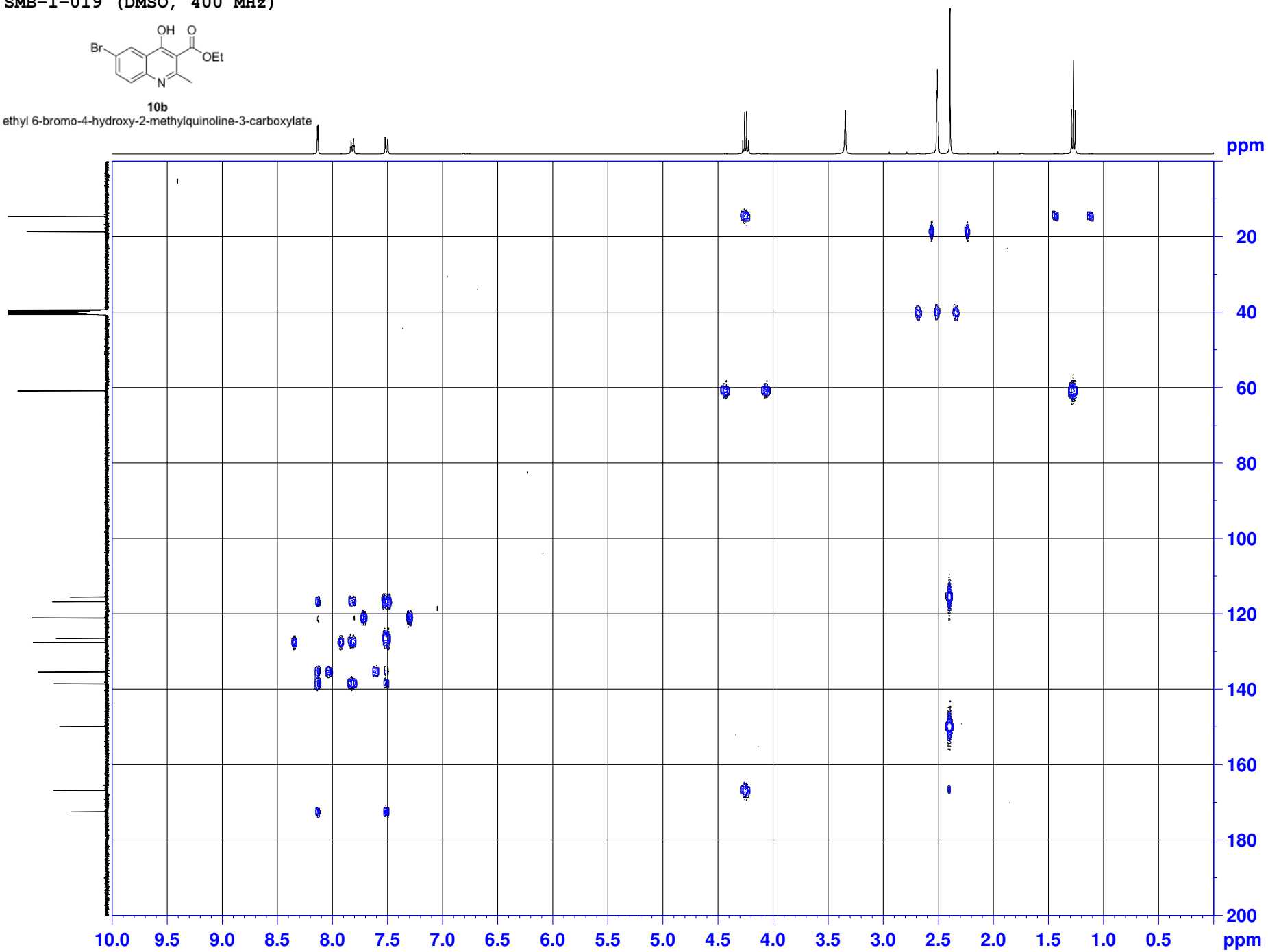


SMB-1-019 (DMSO, 400 MHz)



10b

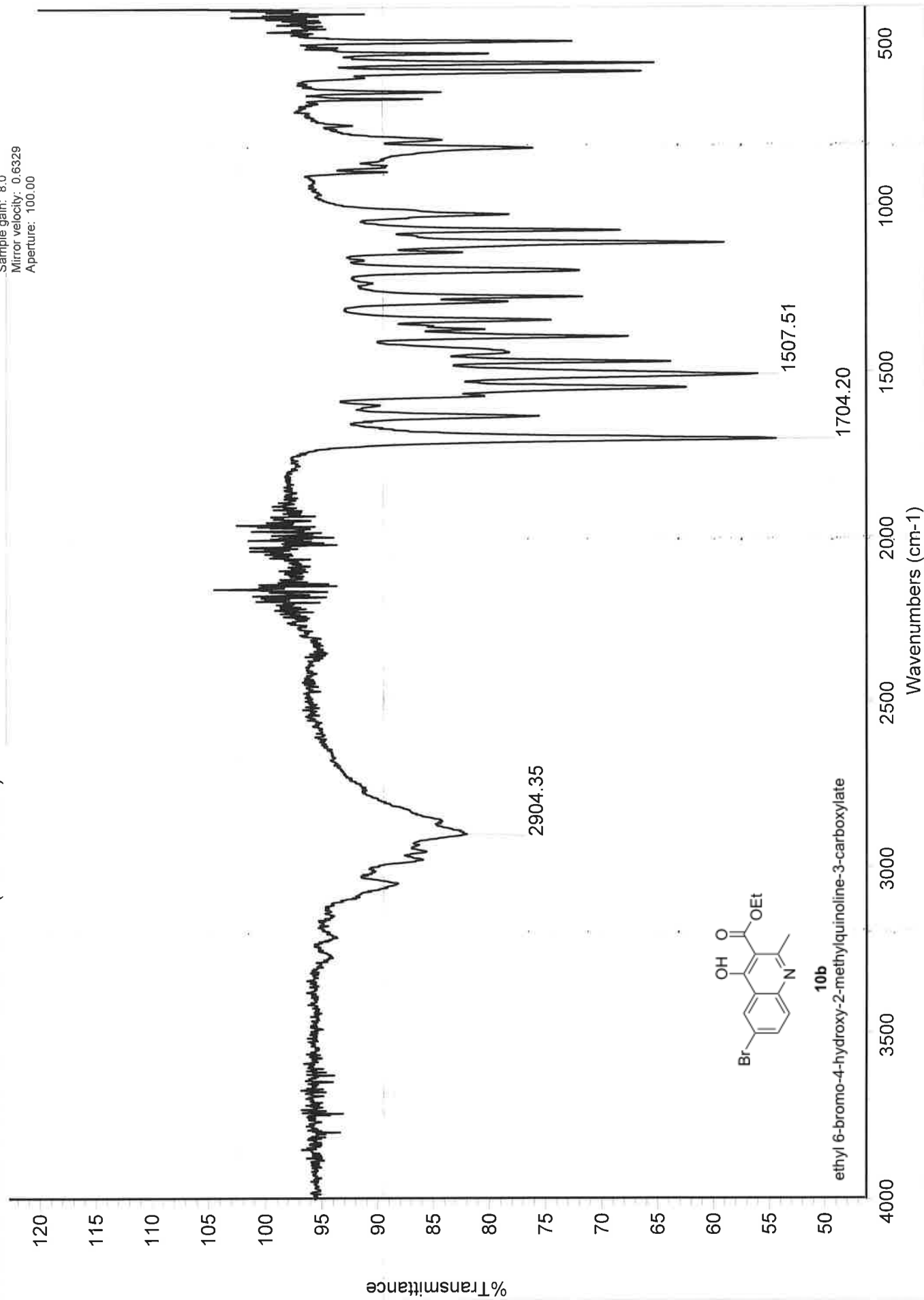
ethyl 6-bromo-4-hydroxy-2-methylquinoline-3-carboxylate



SMB-1-020

Collection time: Fri Jul 28 14:48:50 2017 (GMT-06:00)

Number of sample scans: 8
Number of background scans: 8
Resolution: 2.000
Sample gain: 8.0
Mirror velocity: 0.6329
Aperture: 100.00



Atlantic Microlab, Inc.

Sample No. SM3-1-020

6180 Atlantic Blvd. Suite M
Norcross, GA 30071
www.atlanticmicrolab.com

Company/School University of Southern Mississippi

Dept. Chemistry and Biochemistry

Address 118 College Dr. #5043

City, State, Zip Hattiesburg, MS 39406

Professor/Supervisor: Matthew G. Donahue

PO# / CC# Visa 5794

Name Matthew G. Donahue

Phone 614-203-1123

Date 2/25/17

Element	Theory	Found	Single ☒	Duplicate ☐
C	50.34	50.10	Elements Present: <u>C₁₃H₁₂BrNO₃</u>	
H	3.90	3.88	Analyze for: <u>C, H</u>	
			Hygroscopic ☐ Explosive ☐	
			M.P. ☐ B.P. ☐	
			To be dried: Yes ☐ No ☒	
			Temp. ☐ Vac. ☒ Time ☐	
			Rush Service ☐ Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.	
			Include Email Address or FAX # Below	
			matthew.donahue@usm.edu	

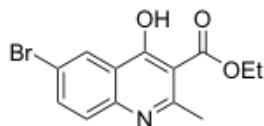
MAR 13 P.M.

Date Received

Remarks:

MAR 14 2017

Date Completed



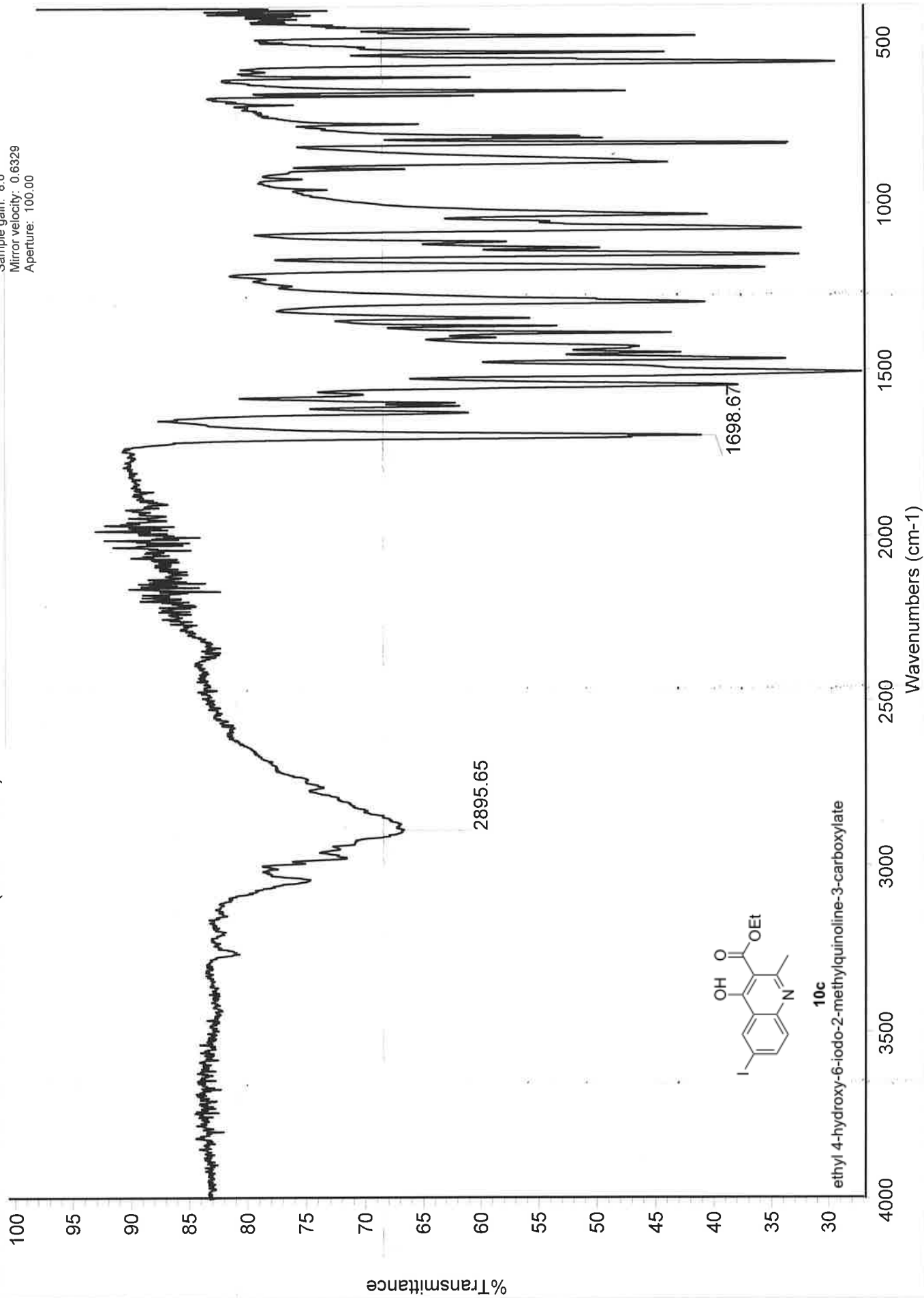
10b

ethyl 6-bromo-4-hydroxy-2-methylquinoline-3-carboxylate

AHP-1-019

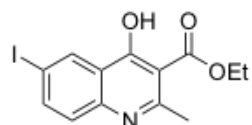
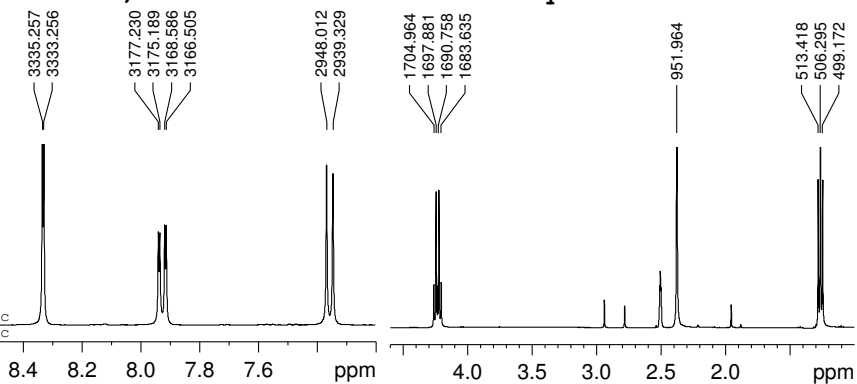
Collection time: Fri Jul 28 14:53:08 2017 (GMT-06:00)

Number of sample scans: 8
Number of background scans: 8
Resolution: 2.000
Sample gain: 8.0
Mirror velocity: 0.6329
Aperture: 100.00



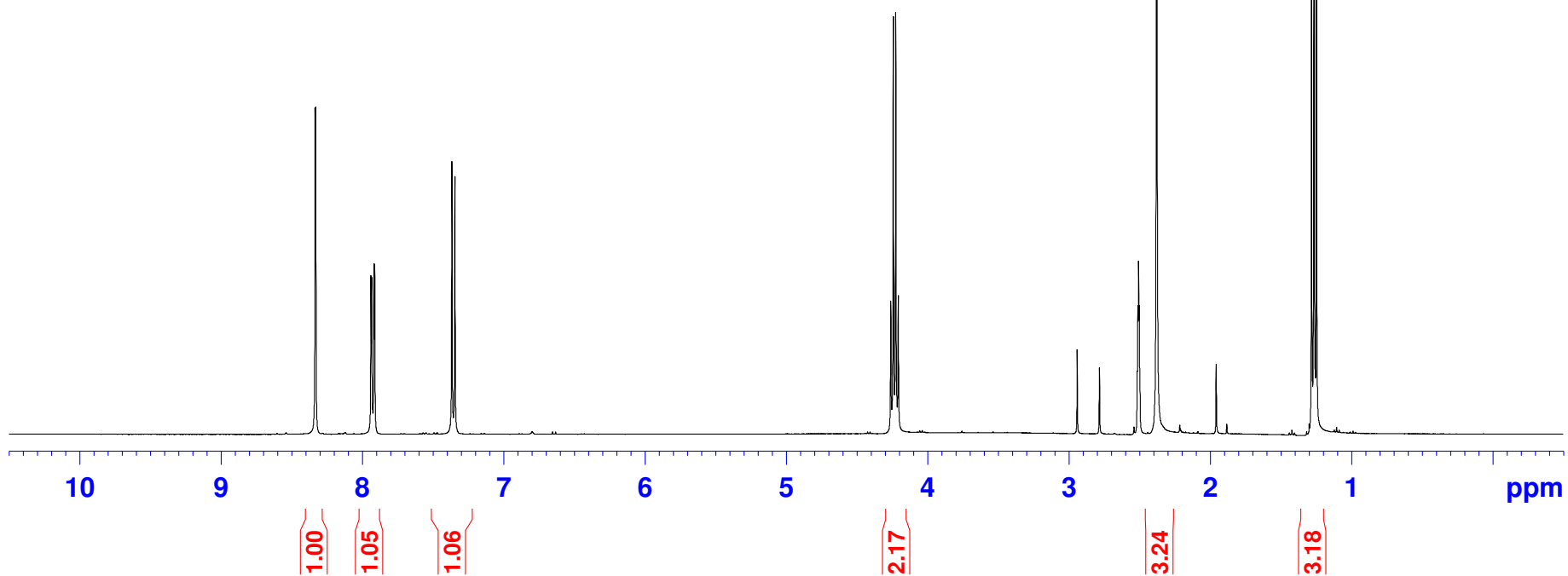
AHP-1-019 (DMSO, 400 MHz) Pure White Solid - Iodo quinoline

NAME AHP-1-019
EXPNO 20
PROCNO 1
Date_ 20170225
Time 13.06 h
INSTRUM spect
PROBHD Z108618_0161
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 161
DW 62.400 usec
DE 6.50 usec
TE 297.3 K
D1 1.00000000 sec
TD0 1
SF01 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

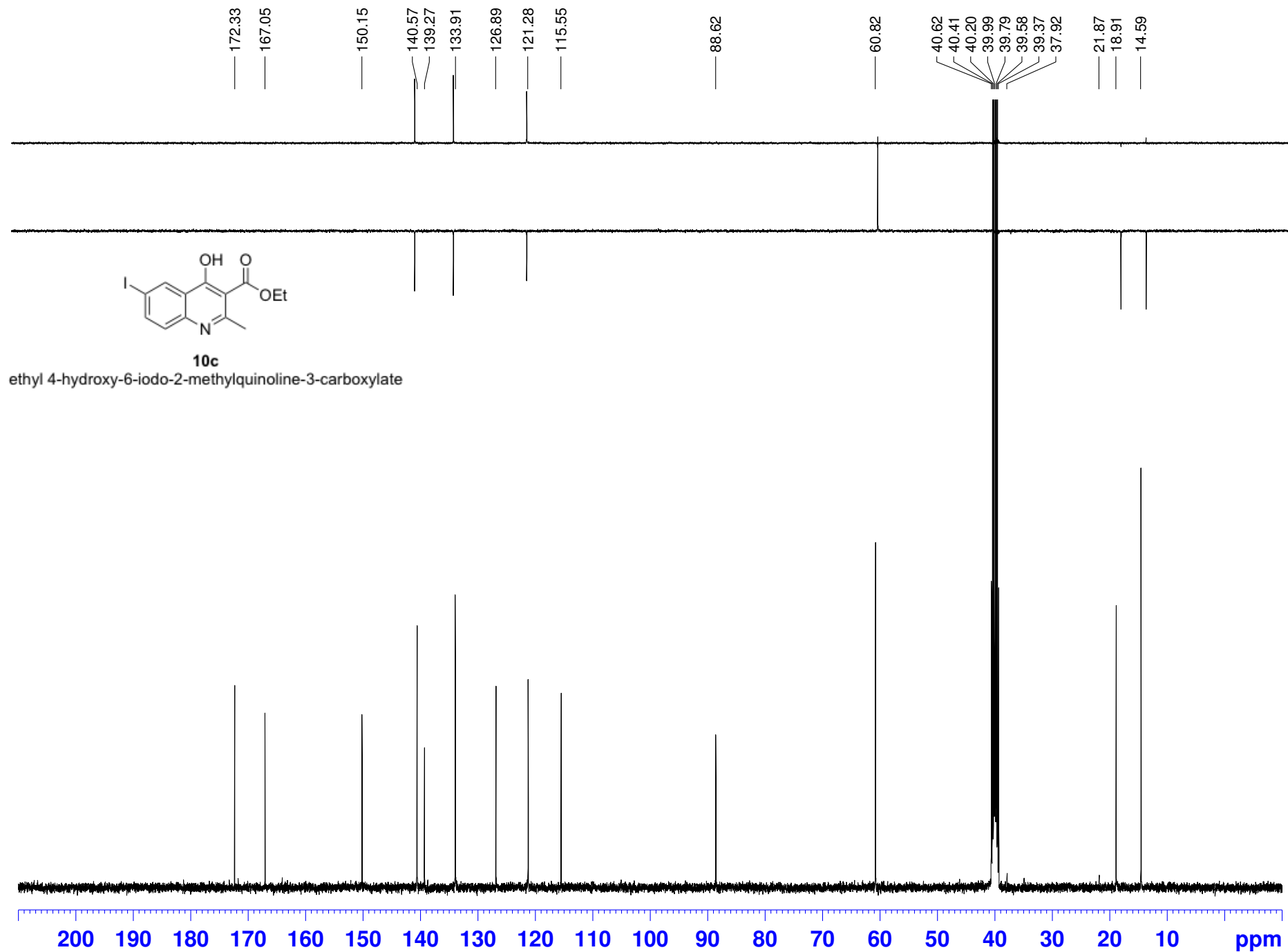


10c

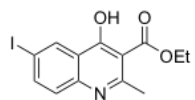
ethyl 4-hydroxy-6-iodo-2-methylquinoline-3-carboxylate



AHP-1-019 (DMSO, 400 MHz) Pure White Solid - Iodo quinoline

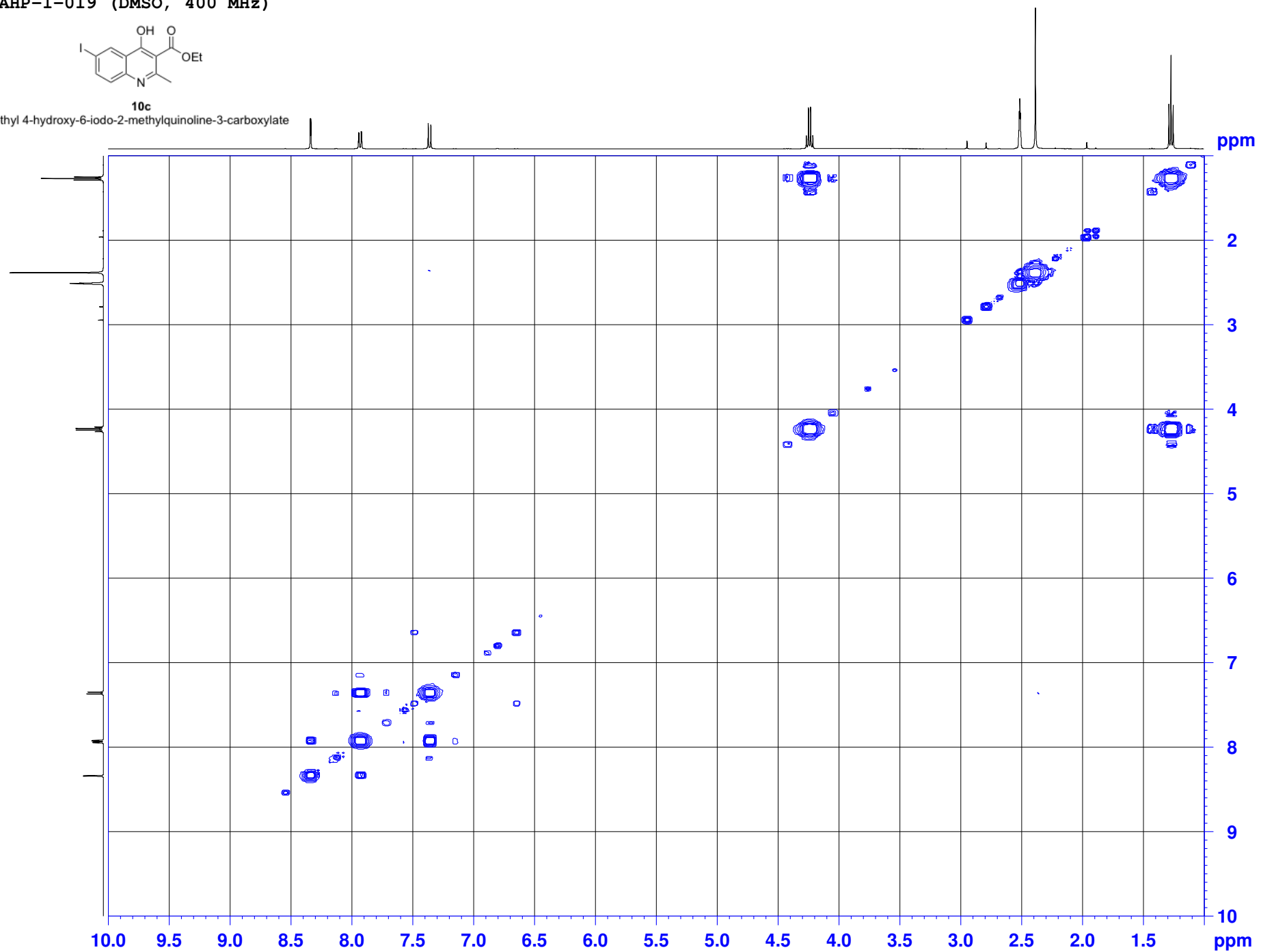


AHP-1-019 (DMSO, 400 MHz)

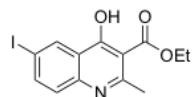


10c

ethyl 4-hydroxy-6-iodo-2-methylquinoline-3-carboxylate

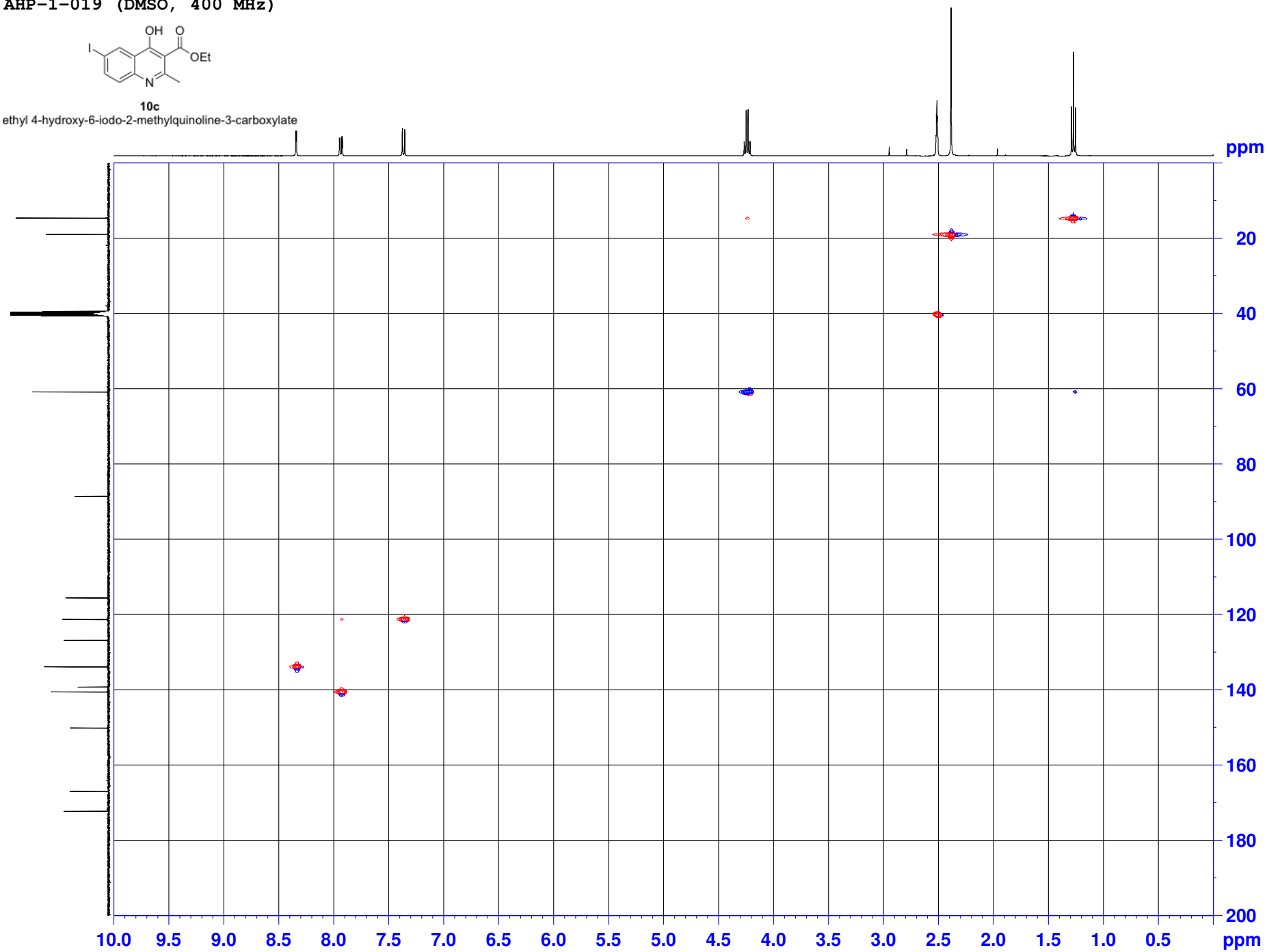


AHP-1-019 (DMSO, 400 MHz)

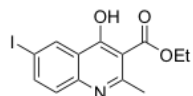


10c

ethyl 4-hydroxy-6-iodo-2-methylquinoline-3-carboxylate

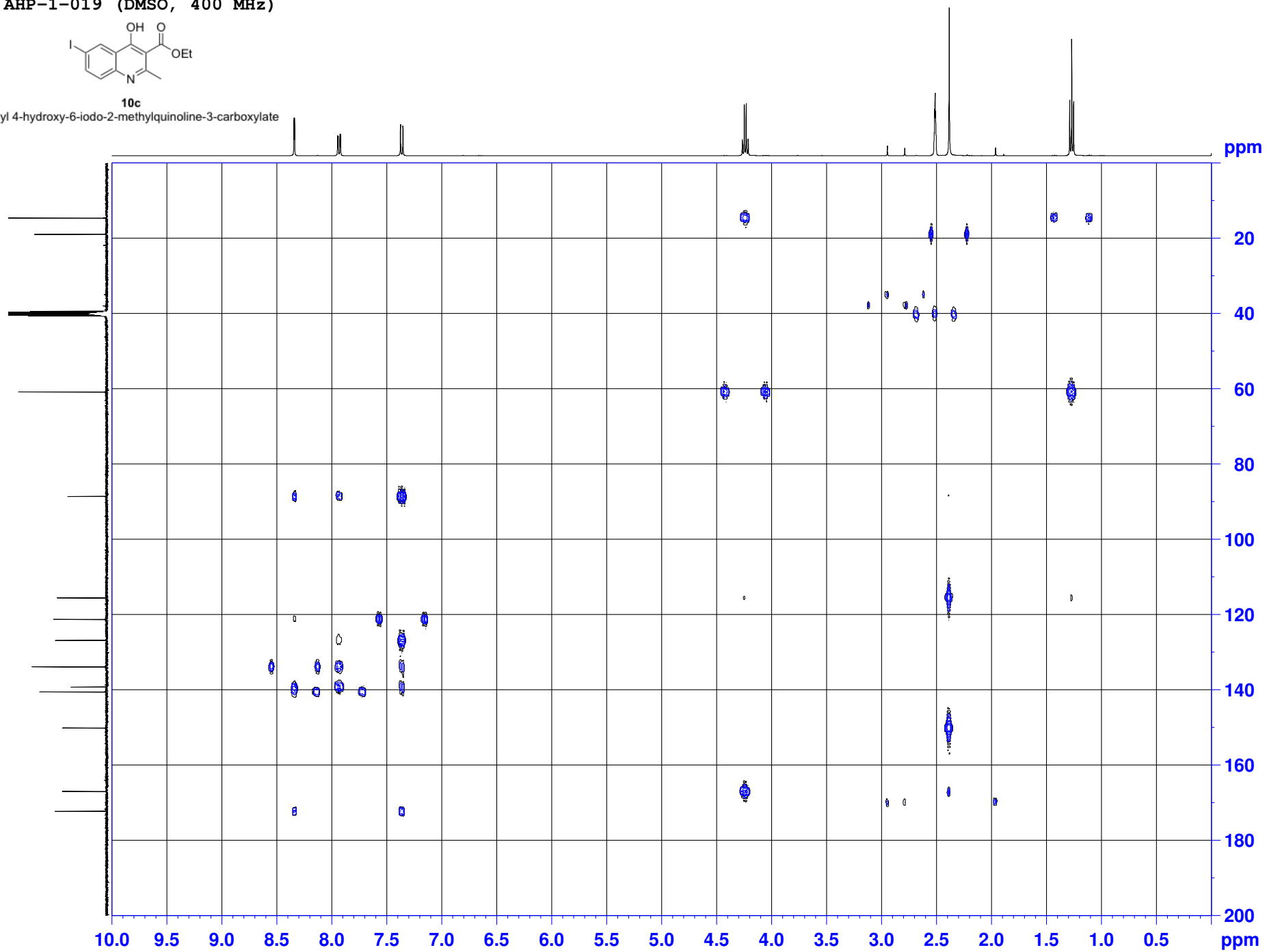


AHP-1-019 (DMSO, 400 MHz)



10c

ethyl 4-hydroxy-6-iodo-2-methylquinoline-3-carboxylate



Atlantic Microlab, Inc.

Sample No. AHP-1-019

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Dept. Chemistry and Biochemistry

Address 118 College Dr. #5043

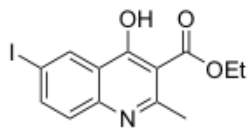
City, State, Zip Hattiesburg, MS 39406

Professor/Supervisor: Matthew G. Donahue

PO# / CC# Visa 5794

Name Matthew G. Donahue Date 2/25/17

Phone 614-203-1123



10c

ethyl 4-hydroxy-6-iodo-2-methylquinoline-3-carboxylate

Element	Theory	Found	Single ☒ Duplicate ☐
C	43.72	43.43	Elements Present: <u>C₁₃H₁₂INO₃</u>
H	3.39	3.29	Analyze for: <u>C, H</u>
			Hygroscopic ☐ Explosive ☐ M.P. <u>B.P.</u>
			To be dried: Yes ☐ No ☒ Time <u>1</u> hr
			Rush Service ☐ Rush service guarantees analysis will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.
			Include Email Address or FAX # Below <u>matthew.donahue@usm.edu</u>

MAR 13 P.M.

Date Received

MAR 14 2017

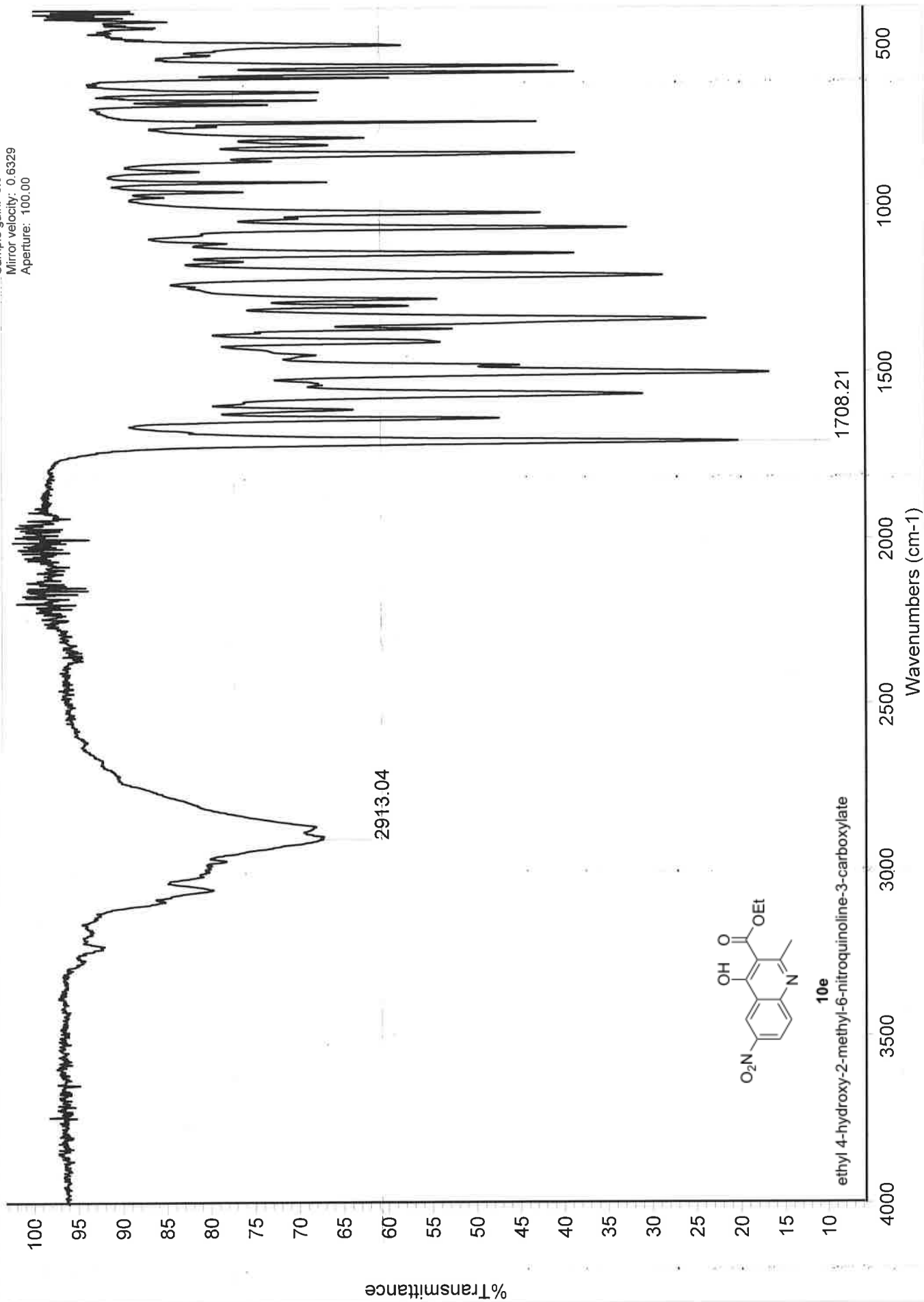
Date Completed

Remarks:

EBC-1-012

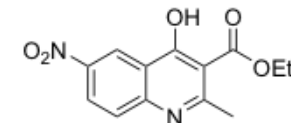
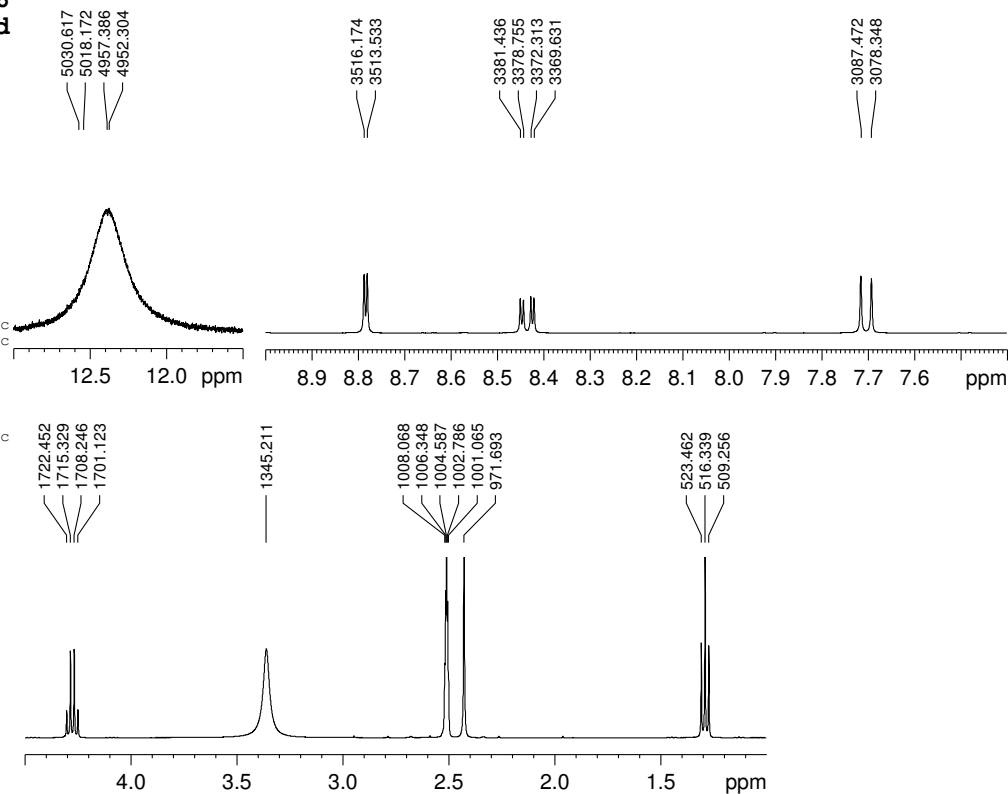
Collection time: Fri Jul 28 14:56:59 2017 (GMT-06:00)

Number of sample scans: 8
Number of background scans: 8
Resolution: 2.000
Sample gain: 8.0
Mirror velocity: 0.6329
Aperture: 100.00



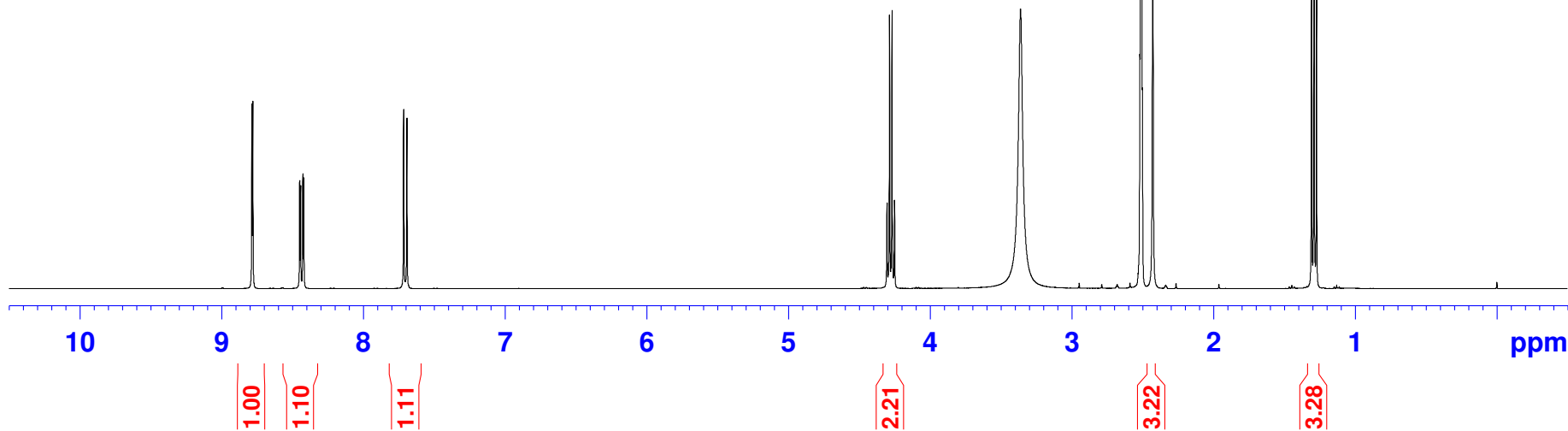
EBC-1-012 DMSO-d6
pale yellow solid

NAME EBC-1-012
EXPNO 20
PROCNO 1
Date_ 20161212
Time 16.58 h
INSTRUM spect
PROBHD Z108618_0161
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 144
DW 62.400 usec
DE 6.50 usec
TE 297.3 K
D1 1.00000000 sec
TD0 1
SFO1 400.1724710 MHz
NUC1 1H
P1 29.07 usec
SI 65536
SF 400.1699988 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

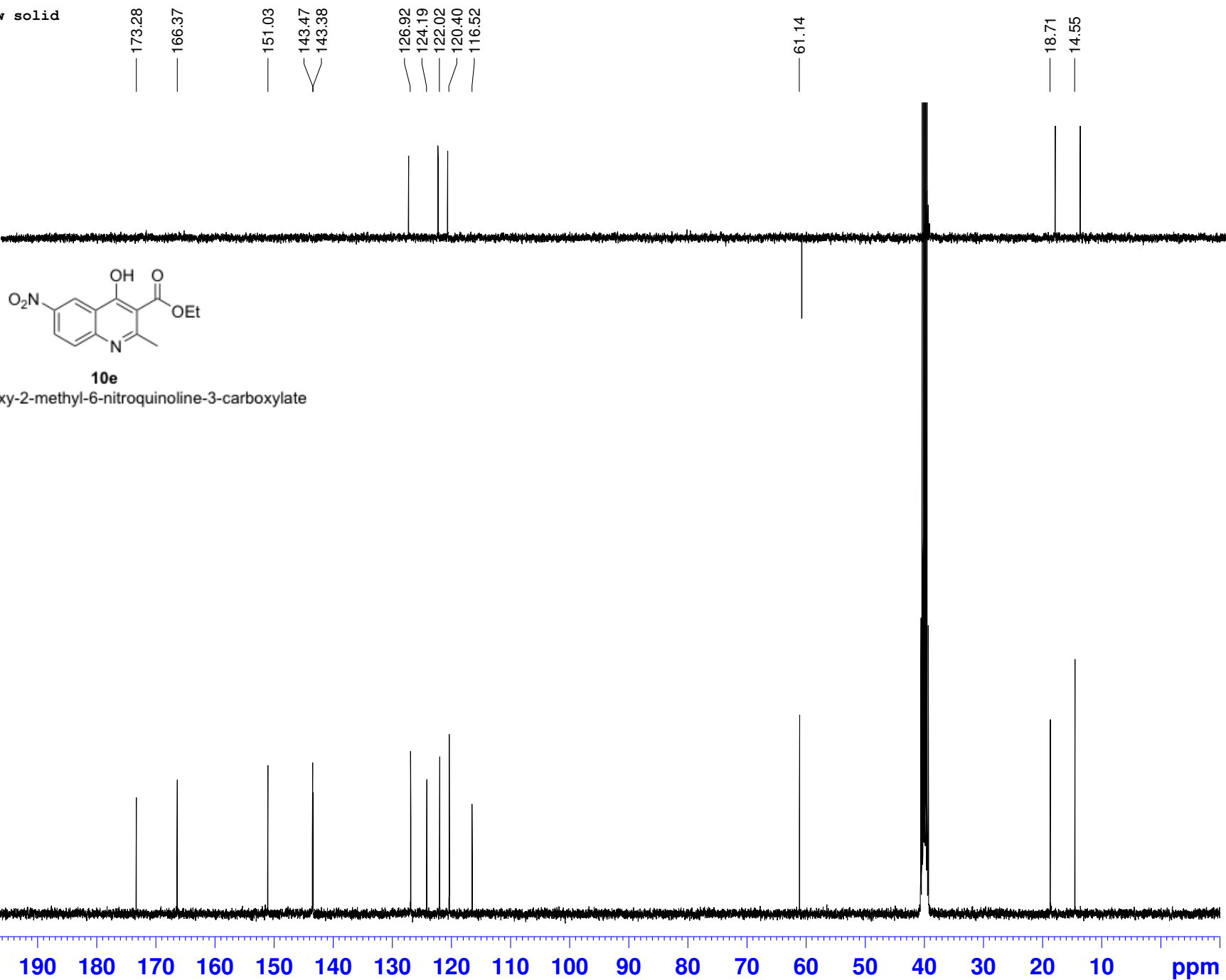


10e

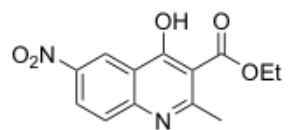
ethyl 4-hydroxy-2-methyl-6-nitroquinoline-3-carboxylate



EBC-1-012 DMSO-d6
old sample
pale yellow solid

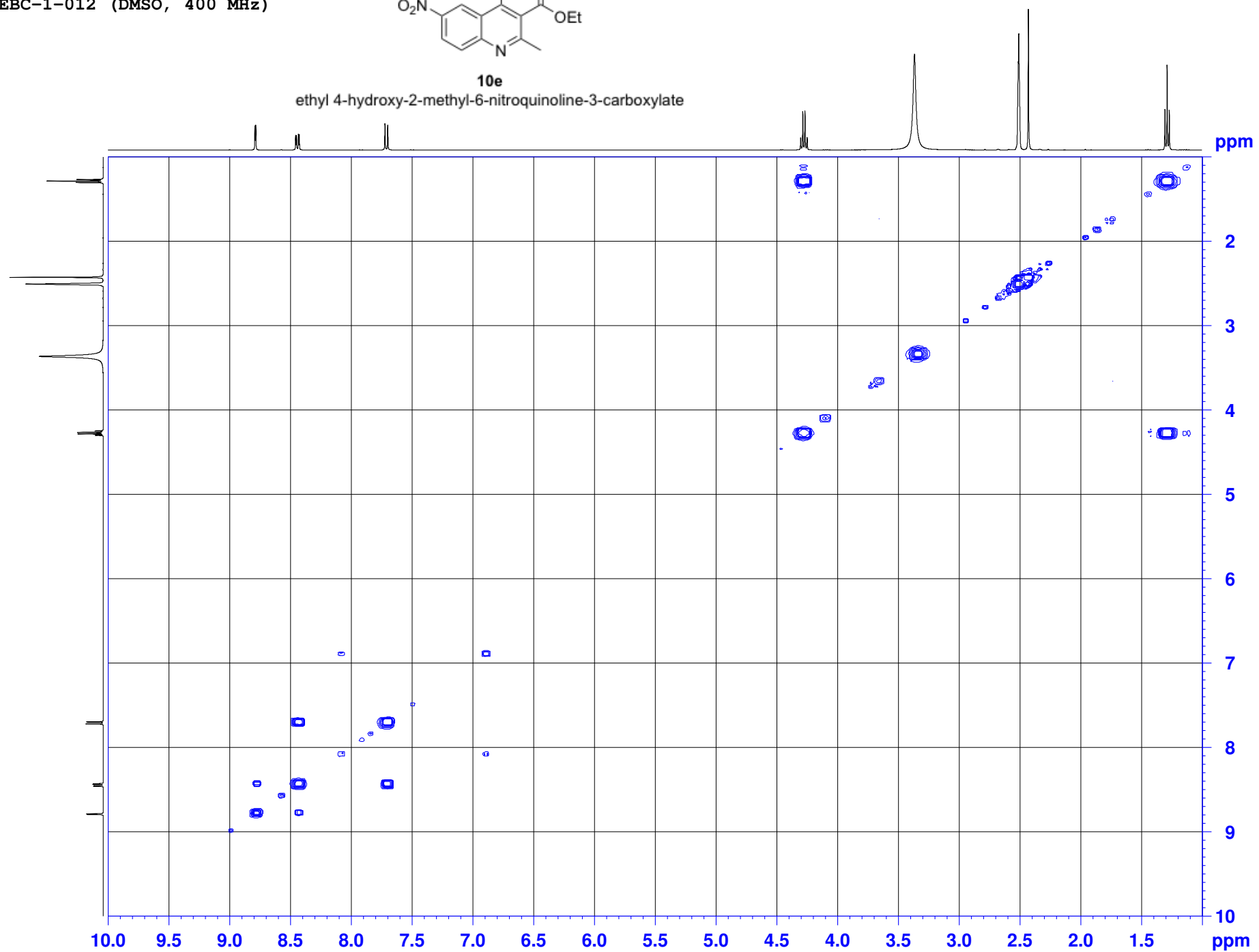


EBC-1-012 (DMSO, 400 MHz)

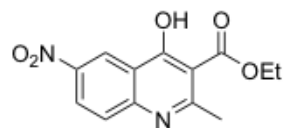


10e

ethyl 4-hydroxy-2-methyl-6-nitroquinoline-3-carboxylate

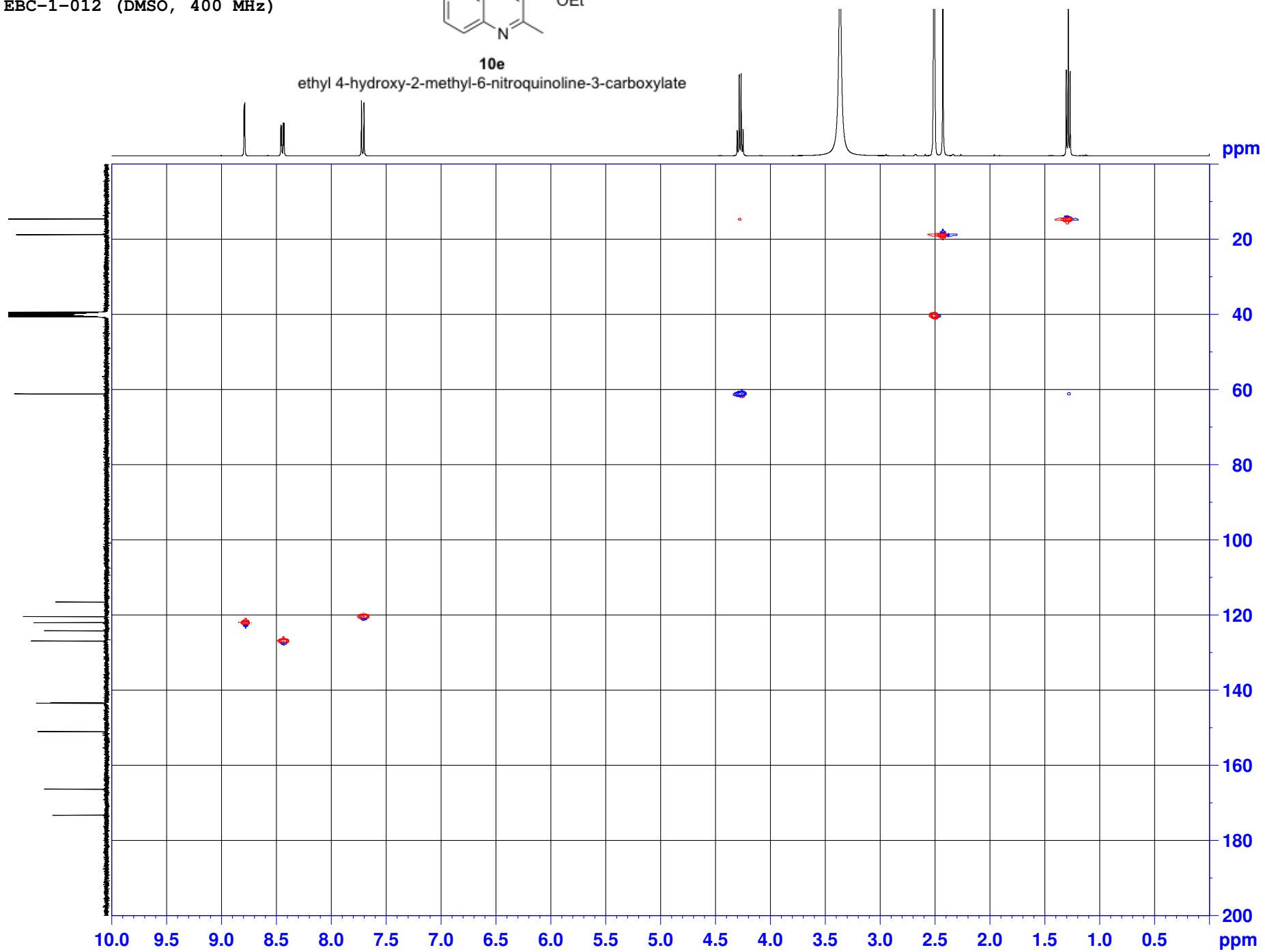


EBC-1-012 (DMSO, 400 MHz)

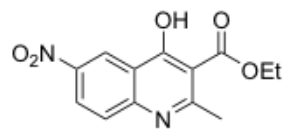


10e

ethyl 4-hydroxy-2-methyl-6-nitroquinoline-3-carboxylate

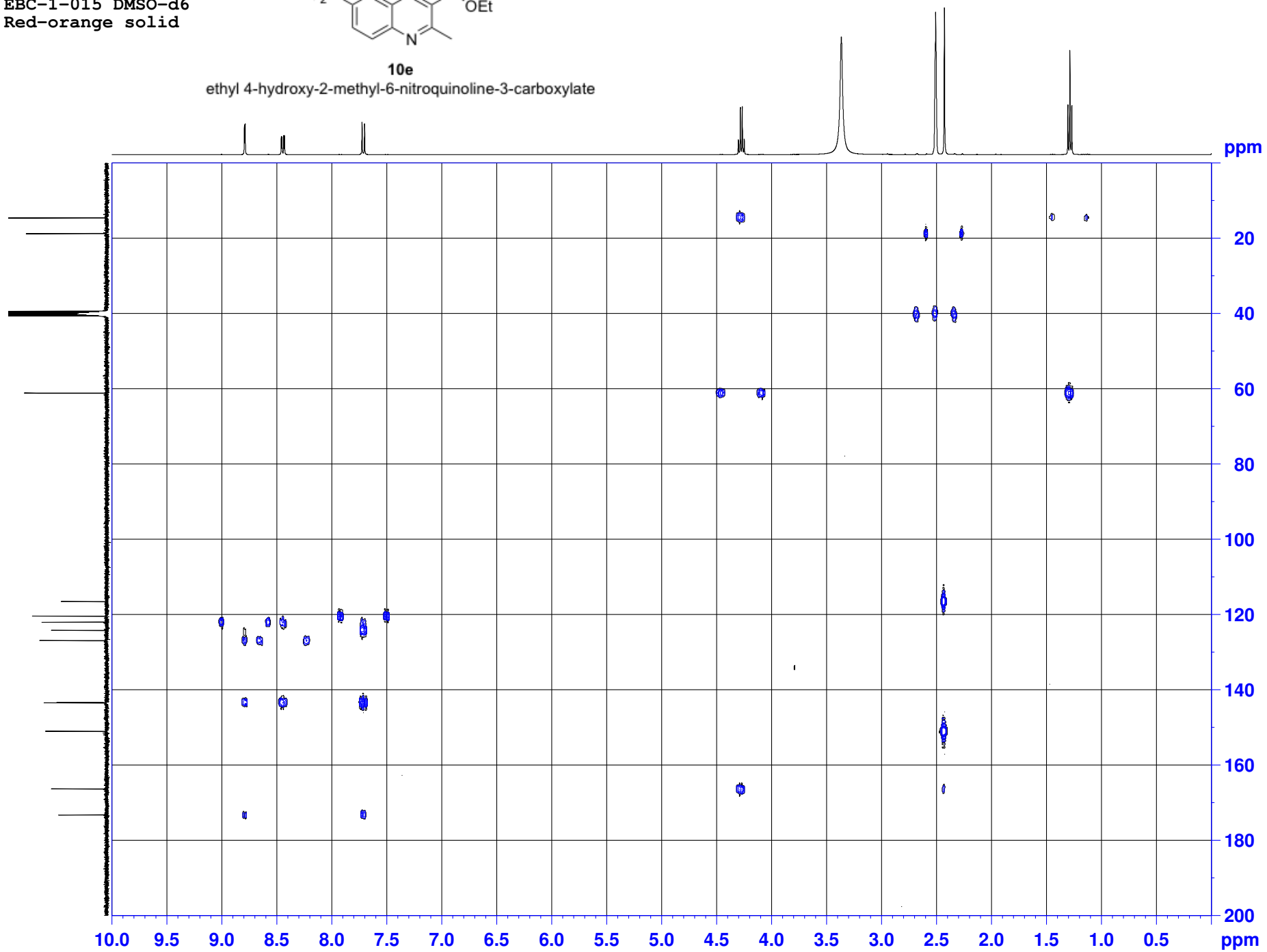


EBC-1-015 DMSO-d6
Red-orange solid



10e

ethyl 4-hydroxy-2-methyl-6-nitroquinoline-3-carboxylate



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Sample No. EBC-1-012

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Dept. Chemistry and Biochemistry

Address 118 College Dr. #5043

City, State, Zip Hattiesburg, MS 39406

Name Matthew G. Donahue Date 2/25/17

Phone 614-203-1123

Professor/Supervisor: Matthew G. Donahue

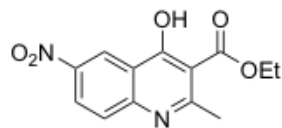
PO# / CC# Visa 5194

Element	Theory	Found	Single ☒	Duplicate ☐
C	56.52	56.26	Elements Present: <u>C₁₃H₁₂N₂O₅</u>	
H	4.38	4.43	Analyze for: <u>C, H</u>	
			Hygroscopic ☐ Explosive ☐	
			M.P. <u> </u> B.P. <u> </u>	
			To be dried: Yes ☐ No ☒	
			Temp. <u> </u> Vac. <u> </u> Inert <u> </u>	
			Rush Service ☐ Rush service guarantees analyses will be completed and results available by 6 PM EST on the day the sample is received by 11 AM.	
			Include Email Address or FAX # Below	
			matthew.donahue@usm.edu	

Date Received MAR 13 PM

Date Completed MAR 14 2017

Remarks:



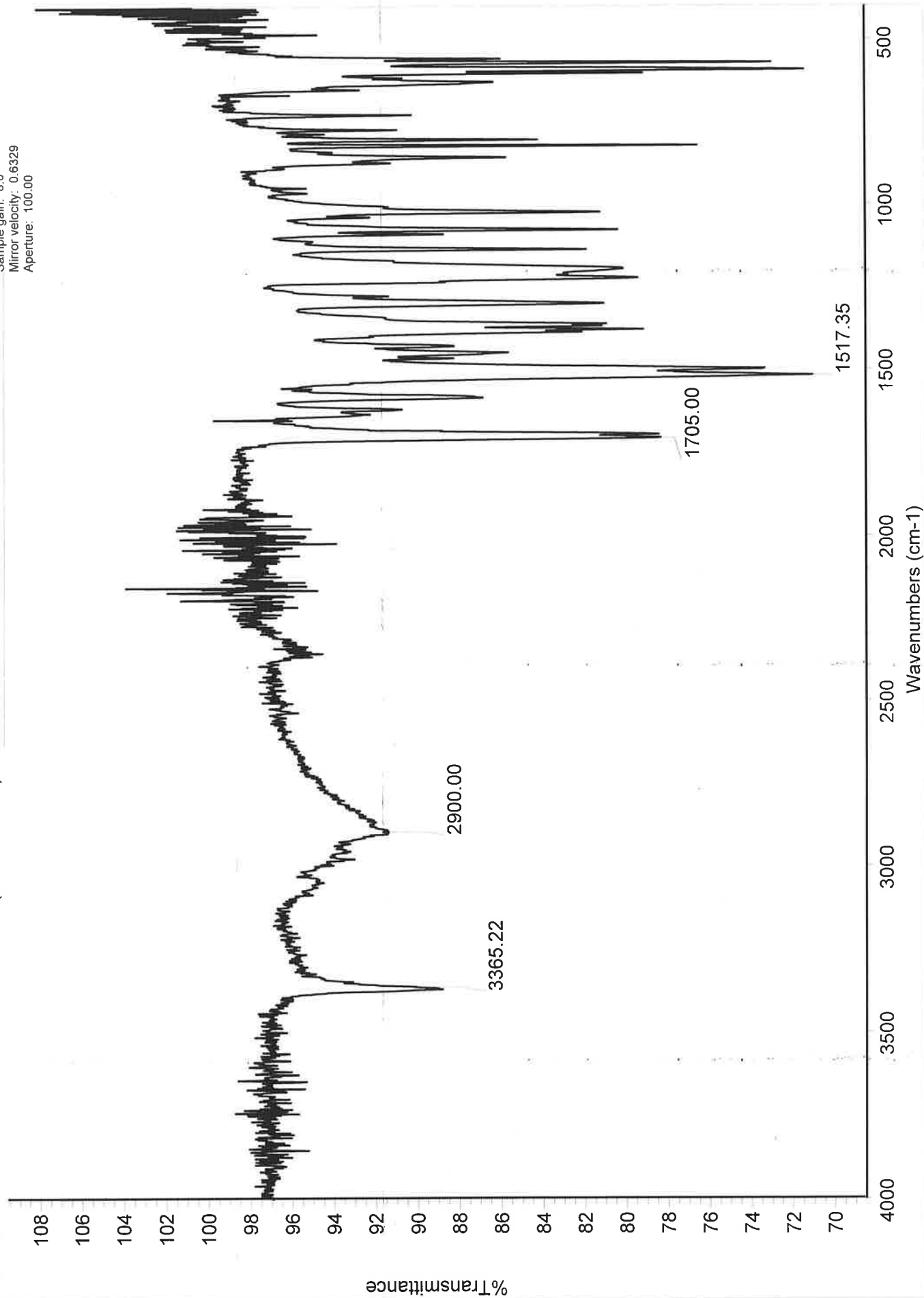
10e

ethyl 4-hydroxy-2-methyl-6-nitroquinoline-3-carboxylate

MEW-1-004

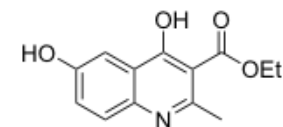
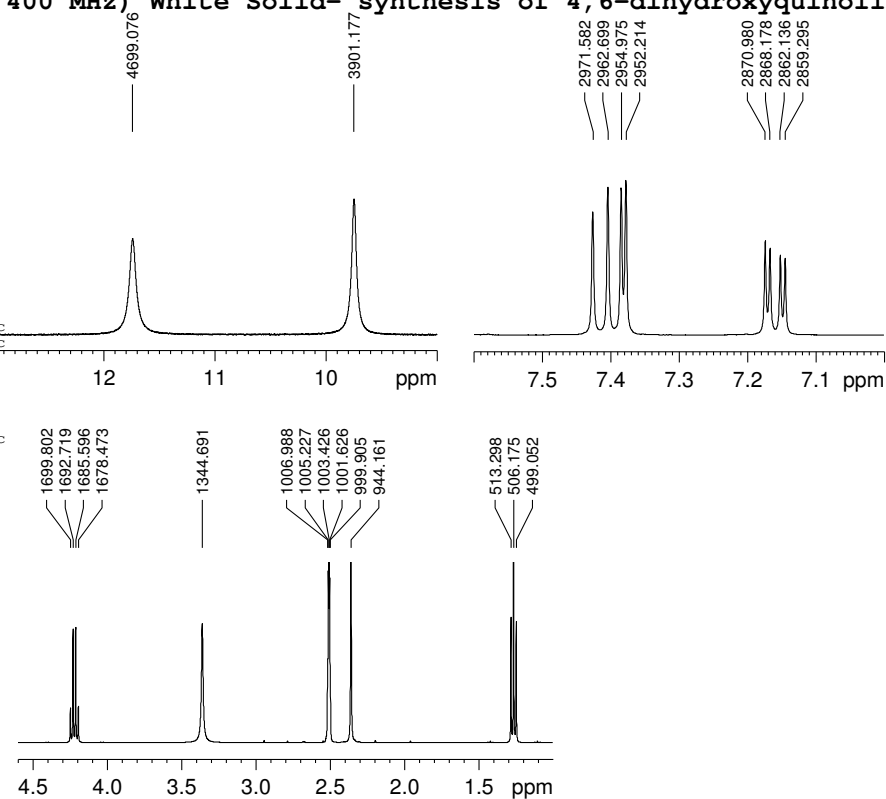
Collection time: Fri Jul 28 15:01:21 2017 (GMT-06:00)

Number of sample scans: 8
Number of background scans: 8
Resolution: 2.000
Sample gain: 8.0
Mirror velocity: 0.6329
Aperture: 100.00



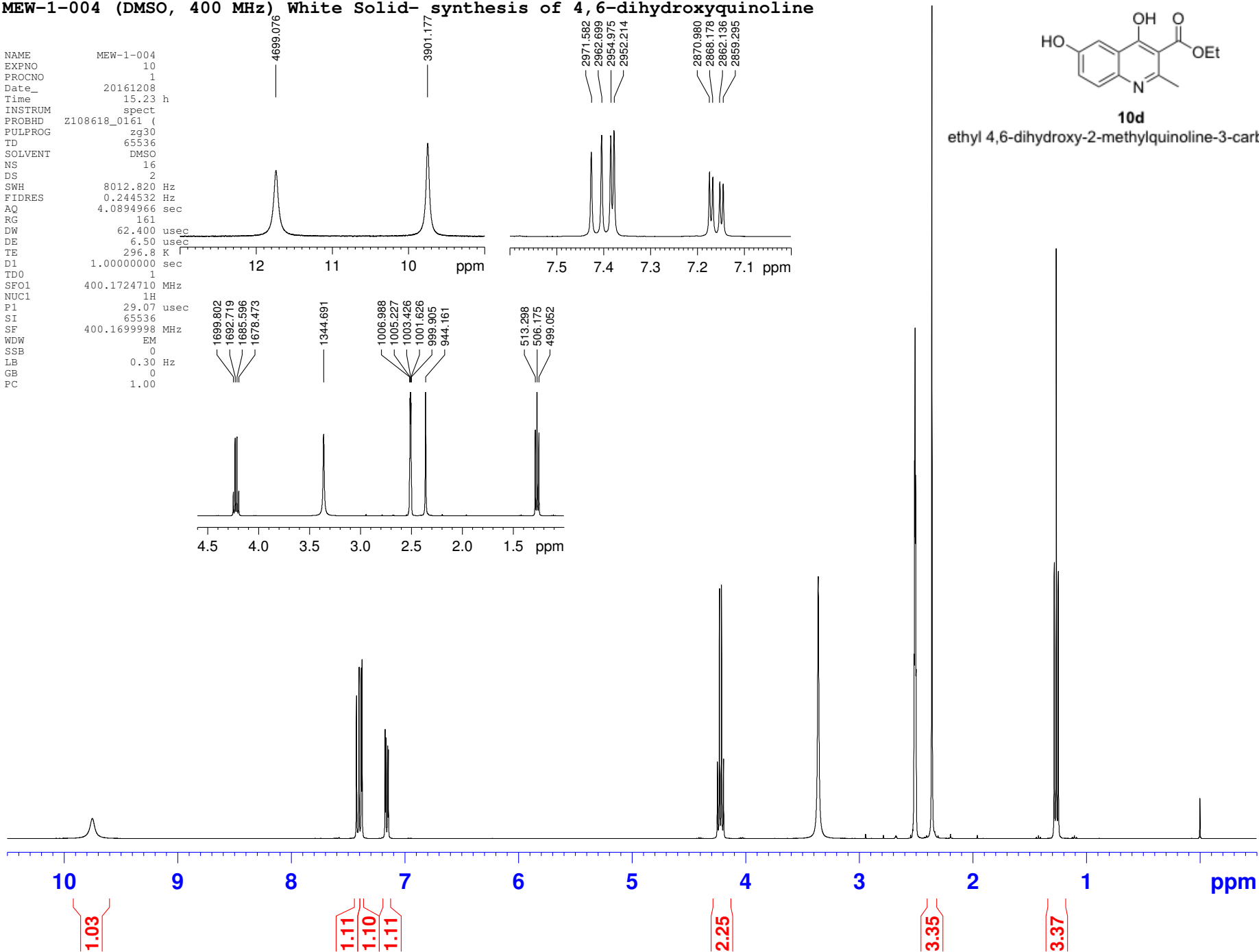
MEW-1-004 (DMSO, 400 MHz) White Solid- synthesis of 4,6-dihydroxyquinoline

NAME MEW-1-004
EXPNO 10
PROCNO 1
Date_ 20161208
Time 15.23 h
INSTRUM spect
PROBHD Z108618_0161
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 161
DW 62.400 usec
DE 6.50 usec
TE 296.8 K
D1 1.00000000 sec
TD0 1
SFO1 400.1724710 MHz
NUC1 1H
P1 29.07 usec
SI 65536
SF 400.1699998 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

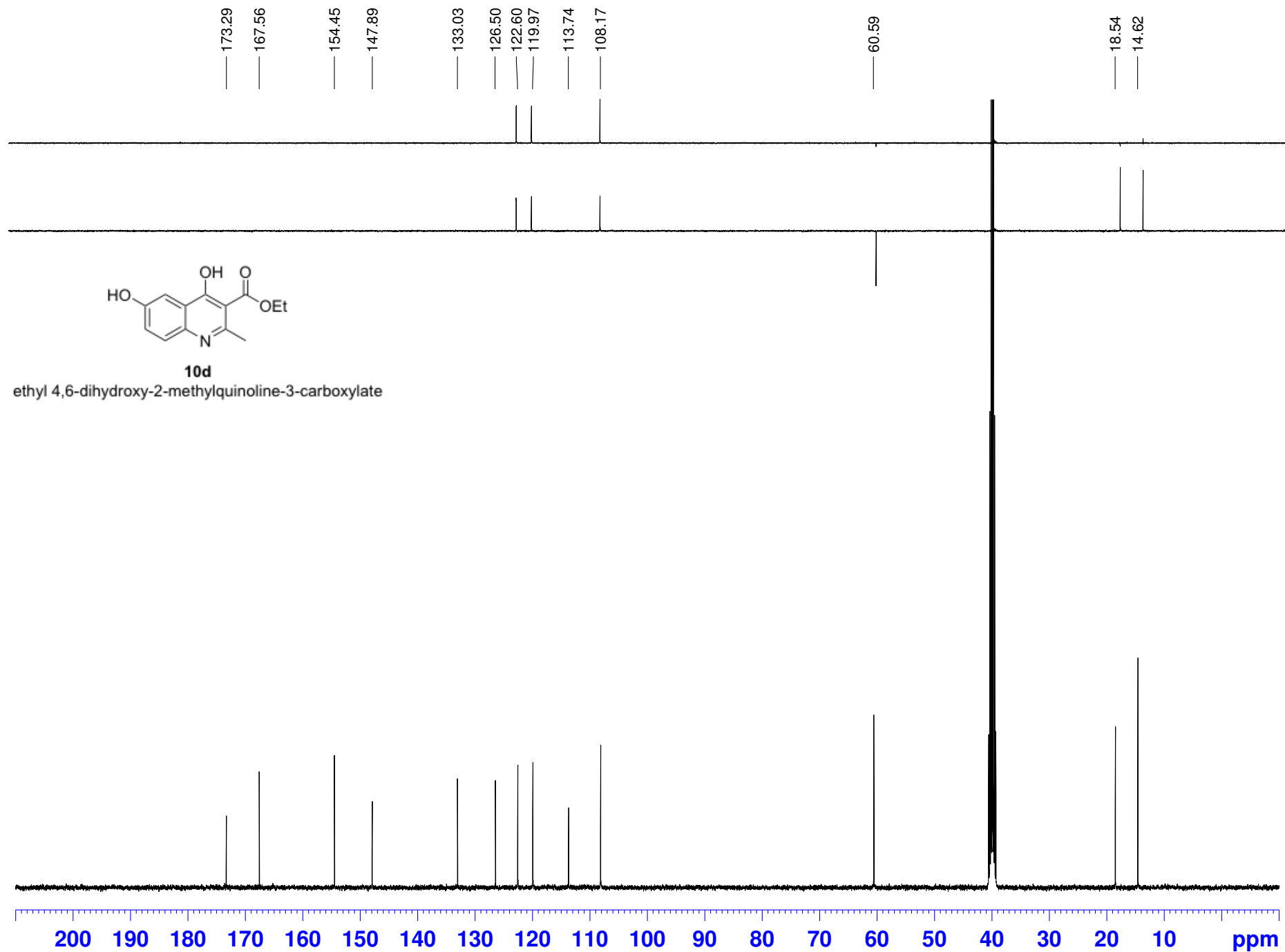


10d

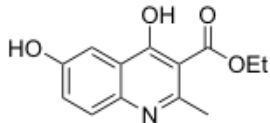
ethyl 4,6-dihydroxy-2-methylquinoline-3-carboxylate



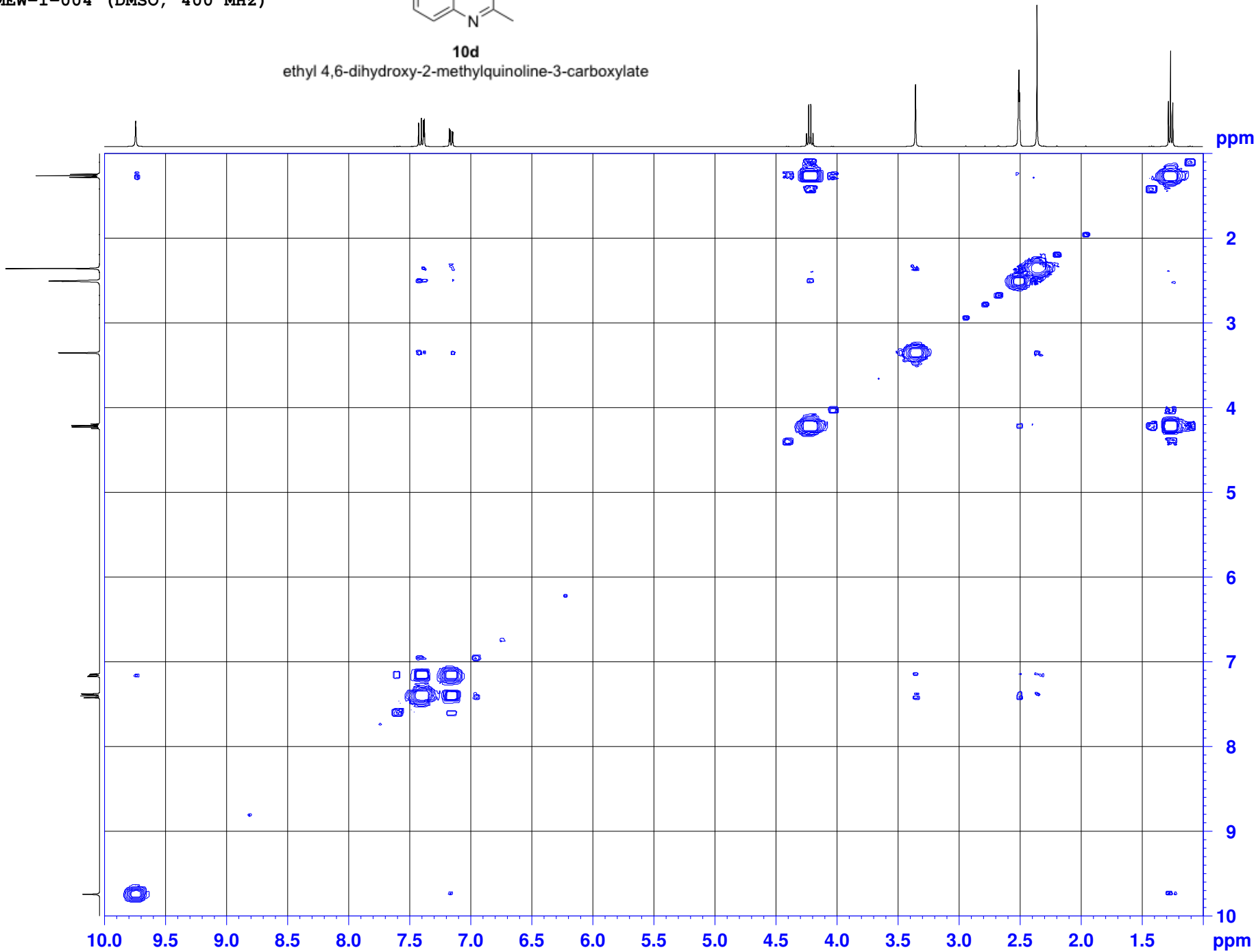
MEW-1-004 (DMSO, 400 MHz) Pure White Solid - dihydroxy quinoli



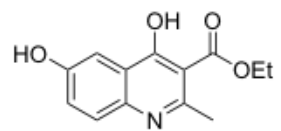
MEW-1-004 (DMSO, 400 MHz)



10d
ethyl 4,6-dihydroxy-2-methylquinoline-3-carboxylate

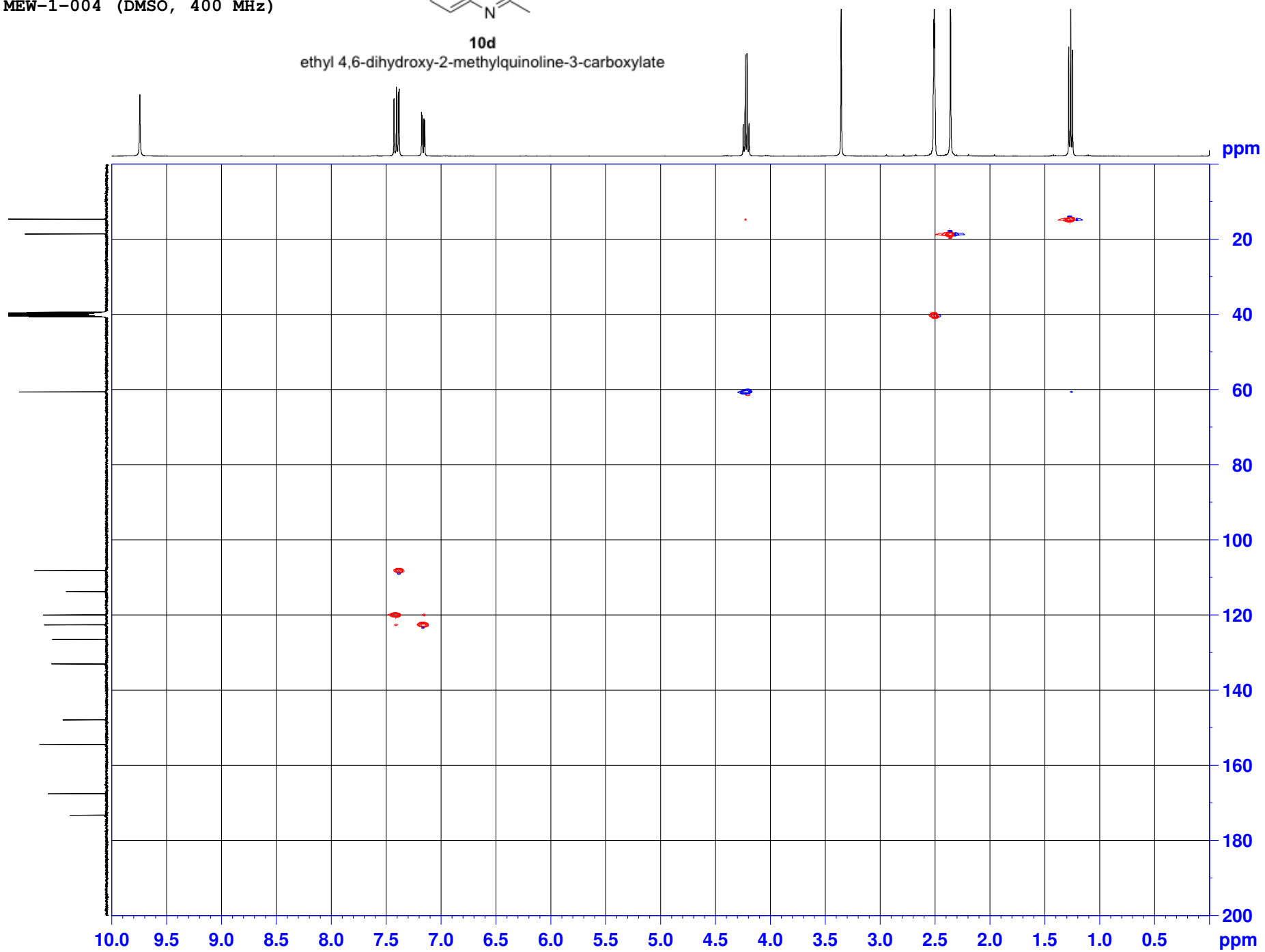


MEW-1-004 (DMSO, 400 MHz)

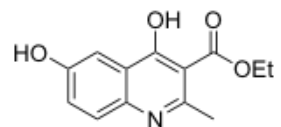


10d

ethyl 4,6-dihydroxy-2-methylquinoline-3-carboxylate

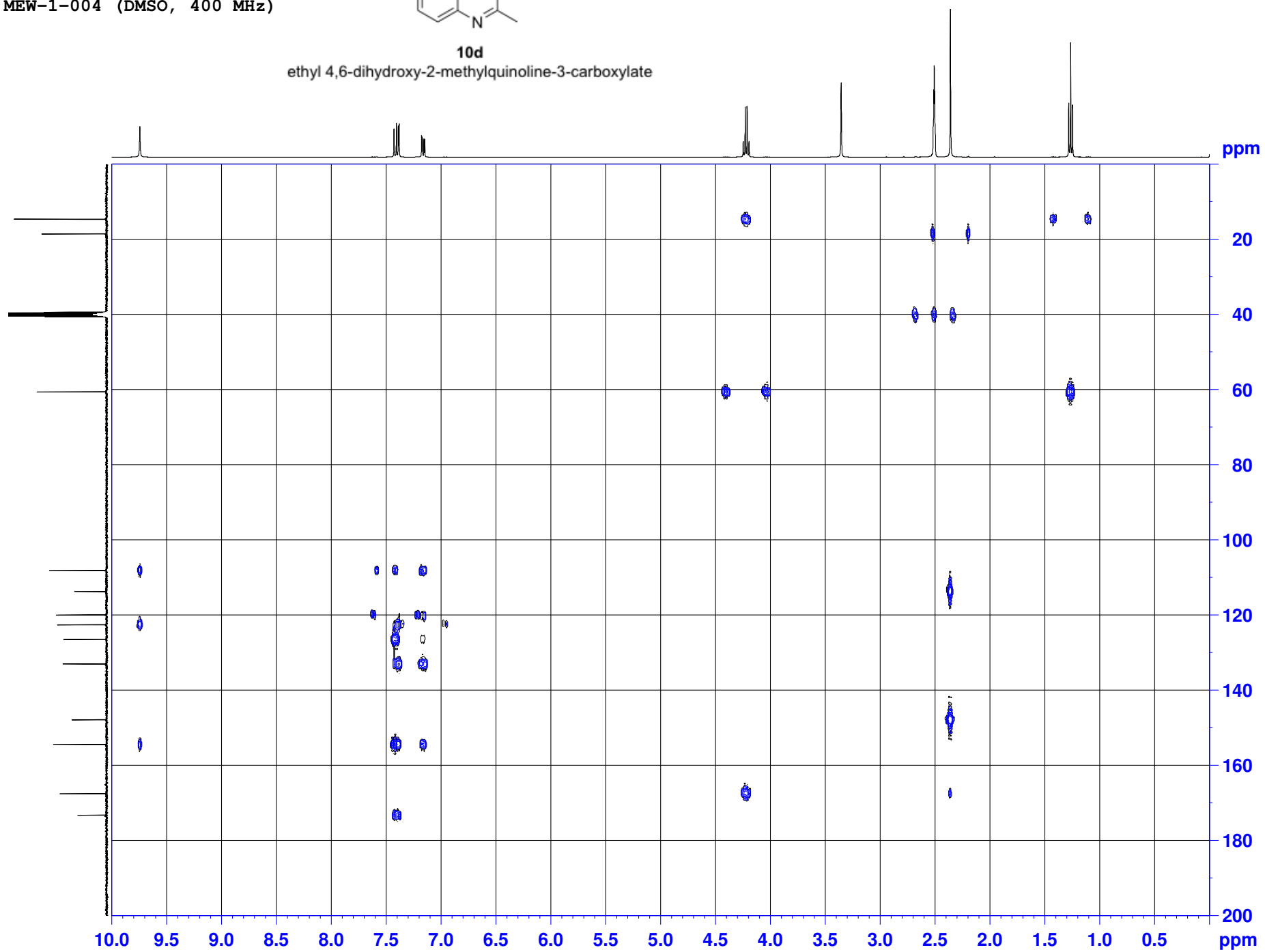


MEW-1-004 (DMSO, 400 MHz)



10d

ethyl 4,6-dihydroxy-2-methylquinoline-3-carboxylate



Atlantic Microlab, Inc.

Sample No. MEW-1-009
 6180 Atlantic Blvd. Suite M
 Norcross, GA 30071
 www.atlanticmicrolab.com

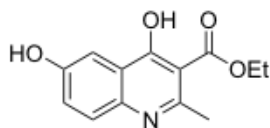
Company/School University of Southern Mississippi
 Dept. Chemistry and Biochemistry
 Address 118 College Dr. #5043
 City, State, Zip Hattiesburg, MS 39406

Professor/Supervisor: Matthew G. Donahue
 Name Matthew G. Donahue Date 3/25/17
 PO# / CC# Visa 5794 Phone 614-203-1123

Element	Theory	Found	Single ☒ Duplicate ☐
C	63.15	62.89	Elements Present: <u>C₁₃H₁₃NO₄</u>
H	5.30	5.44	Analyze for: <u>C, H</u>
			Hygroscopic ☐ Explosive ☐ M.P. <u> </u> B.P. <u> </u>
			To be dried: Yes ☐ No ☒ Time <u> </u>
			Temp. <u> </u> Vac. <u> </u>
			Rush Service ☐ Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.
			Include Email Address or FAX # Below <u>matthew.donahue@usm.edu</u>

Date Received MAR 13 P.M. Date Completed MAR 14 2017

Remarks:



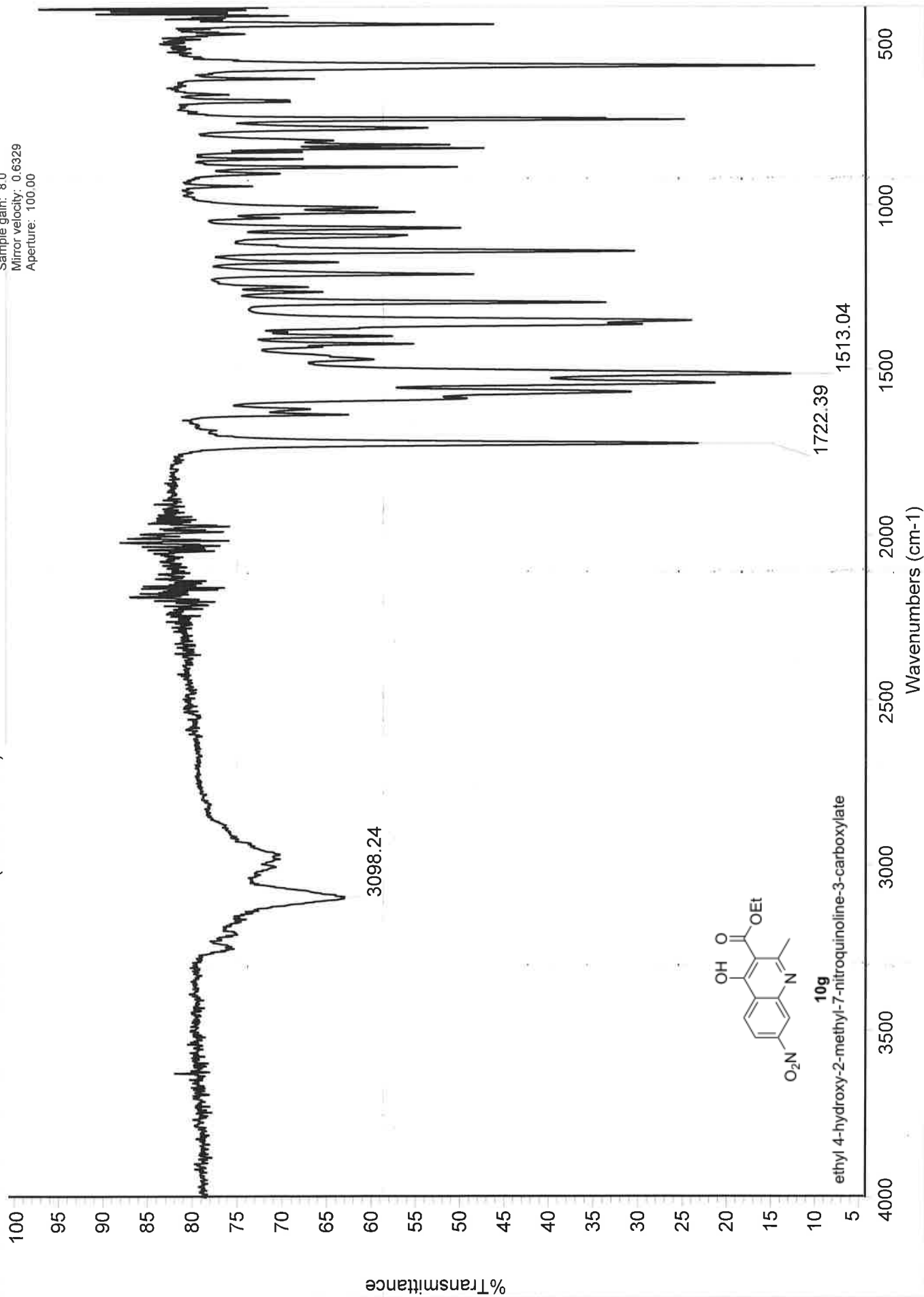
10d

ethyl 4,6-dihydroxy-2-methylquinoline-3-carboxylate

*EBC-1-013

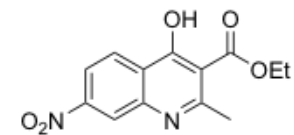
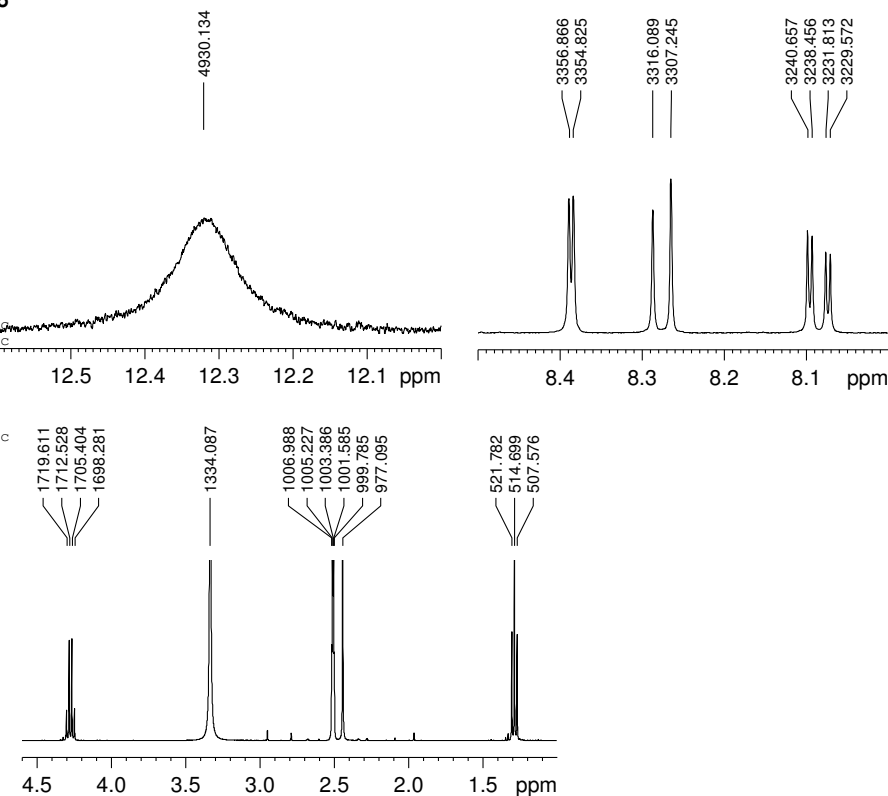
Collection time: Thu Mar 16 12:33:49 2017 (GMT-06:00)

Number of sample scans: 8
Number of background scans: 8
Resolution: 2.000
Sample gain: 8.0
Mirror velocity: 0.6329
Aperture: 100.00



EBC-1-013 DMSO-D6
yellow solid

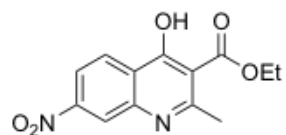
NAME EBC-1-013
EXPNO 20
PROCNO 1
Date_ 20170228
Time 17.03 h
INSTRUM spect
PROBHD Z108618_0161
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 297.6 K
D1 1.00000000 sec
TD0 1
SFO1 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



10g

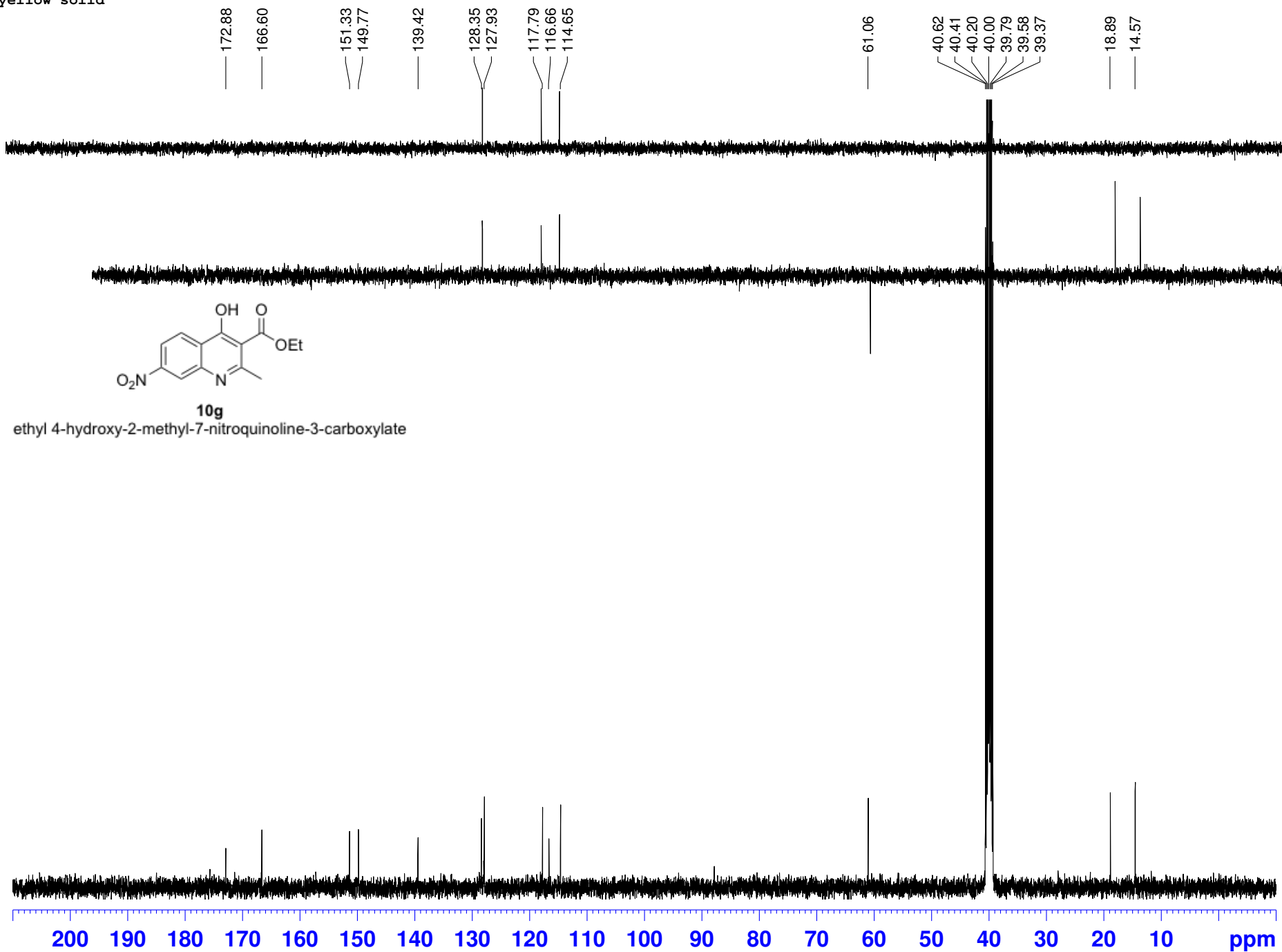
ethyl 4-hydroxy-2-methyl-7-nitroquinoline-3-carboxylate

EBC-1-013 DMSO-D6
yellow solid

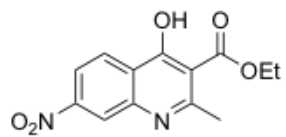


10g

ethyl 4-hydroxy-2-methyl-7-nitroquinoline-3-carboxylate

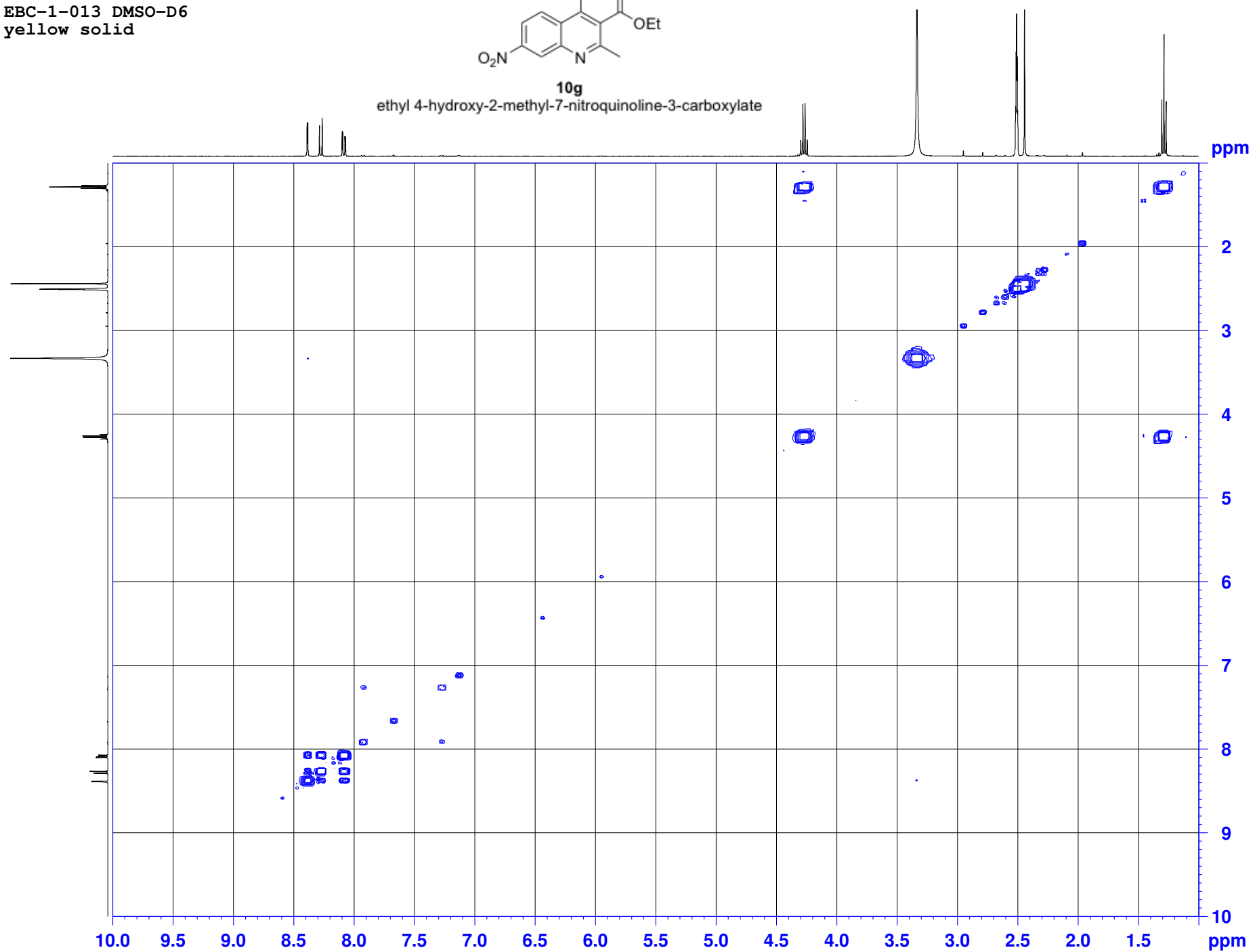


EBC-1-013 DMSO-D6
yellow solid

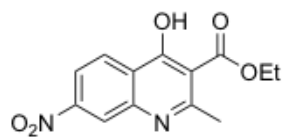


10g

ethyl 4-hydroxy-2-methyl-7-nitroquinoline-3-carboxylate

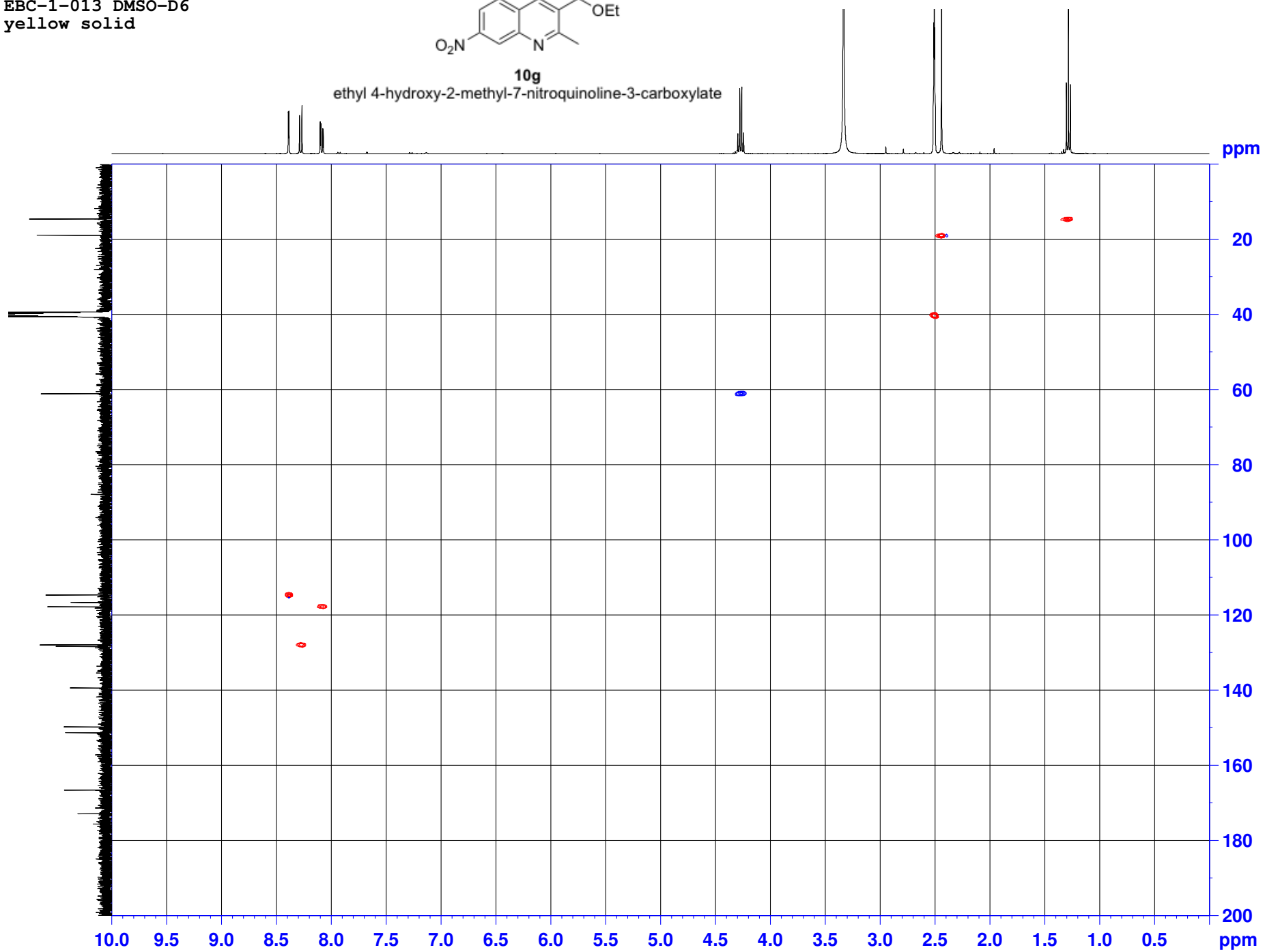


EBC-1-013 DMSO-D6
yellow solid

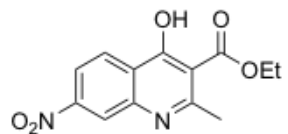


10g

ethyl 4-hydroxy-2-methyl-7-nitroquinoline-3-carboxylate

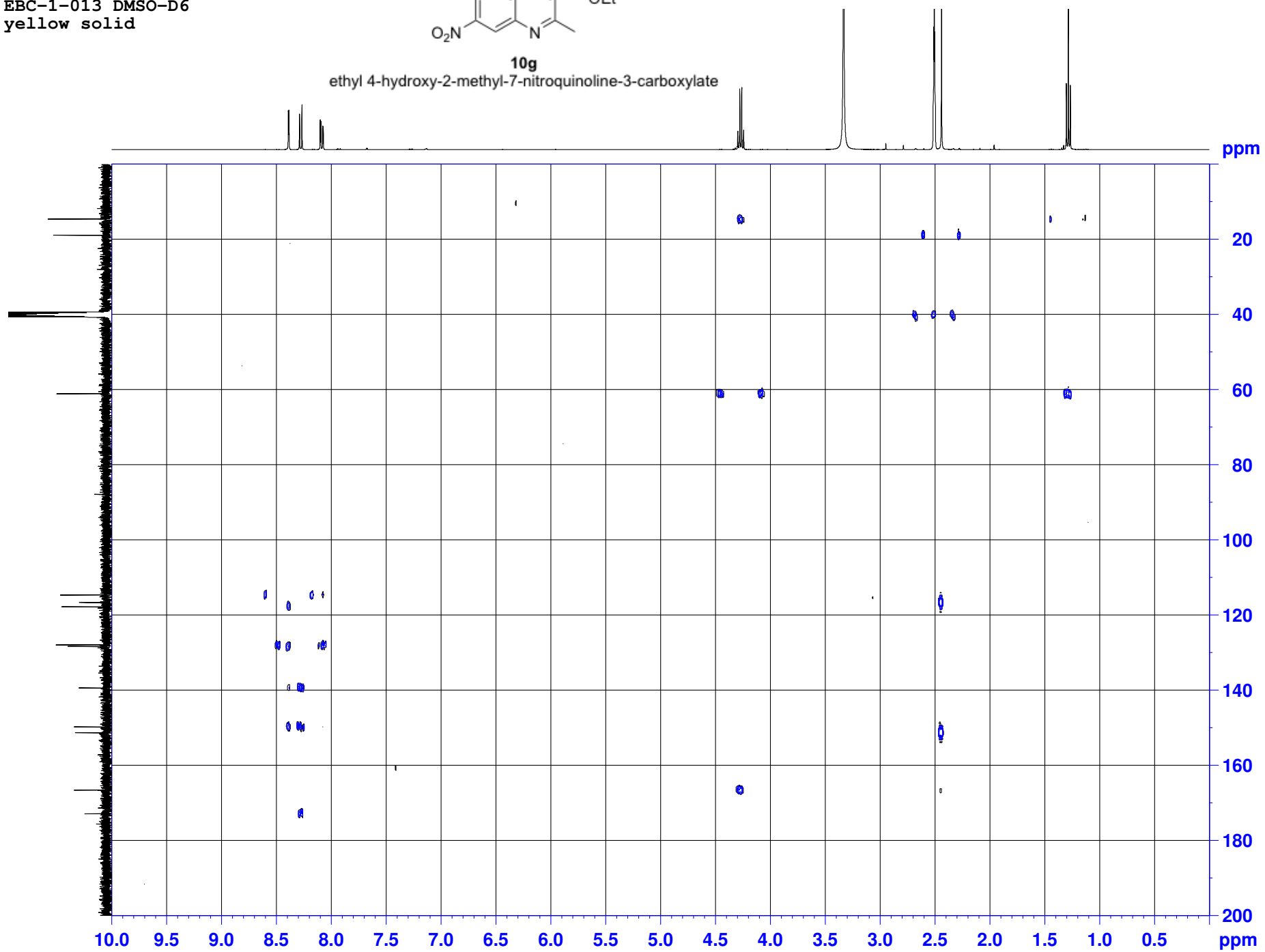


EBC-1-013 DMSO-D6
yellow solid



10g

ethyl 4-hydroxy-2-methyl-7-nitroquinoline-3-carboxylate



Atlantic Microlab, Inc.

Sample No. EBC-1-013

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Norcross, GA 30071
www.atlanticmicrolab.com

Company/School University of Southern Mississippi

Dept. Chemistry and Biochemistry

Address 118 College Dr. #5043

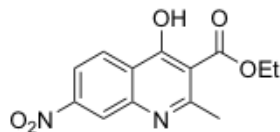
City, State, Zip Hattiesburg, MS 39406

Name Matthew G. Donahue Date 2/25/17

Professor/Supervisor: Matthew G. Donahue

PO# / CC# Visa 5794

Phone 614-203-1123



10g

ethyl 4-hydroxy-2-methyl-7-nitroquinoline-3-carboxylate

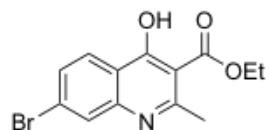
Element	Theory	Found	Single ☒ Duplicate ☐
C	56.52	56.23	Elements Present: <u>C₁₃H₁₂N₂O₅</u>
H	4.38	4.40	Analyze for: <u>C, H</u>
			Hygroscopic ☐ Explosive ☐
			M.P. <u> </u> B.P. <u> </u>
			To be dried: Yes ☐ No ☒ Time <u> </u>
			Rush Service ☐ Rush service guarantees analysis will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.
			Include Email Address or FAX # Below
			<u>matthew.donahue@usm.edu</u>

Date Received MAR 13 P.M. Date Completed MAR 14 2017

Remarks:

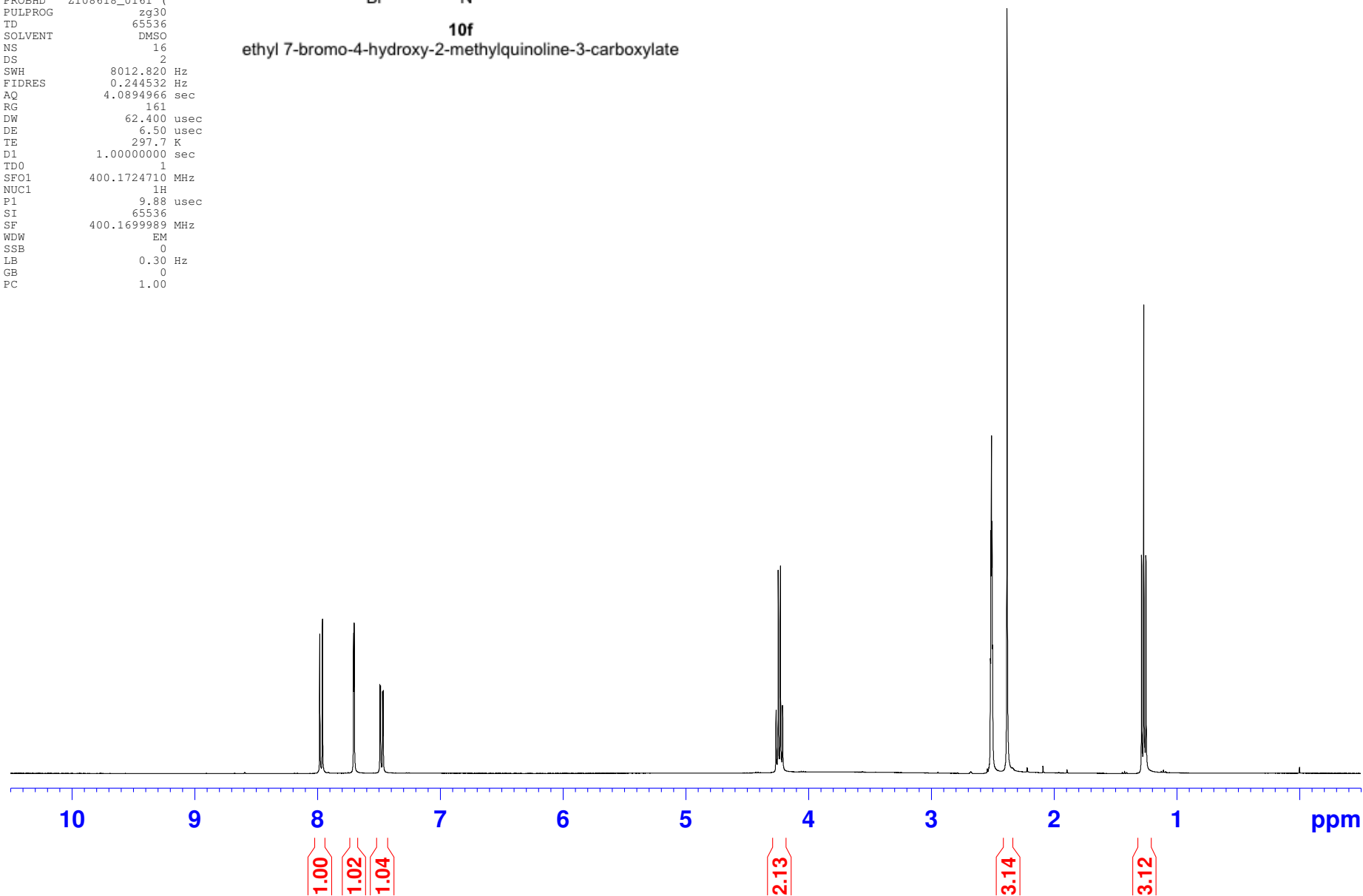
NGJ-8-030 (DMSO, 400 MHz) Pure White Solid - 7-bromoquinoline synthesis

NAME NGJ-8-030
 EXPNO 40
 PROCNO 1
 Date_ 20170823
 Time_ 17.45 h
 INSTRUM spect
 PROBHD Z108618_0161 (
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894966 sec
 RG 161
 DW 62.400 usec
 DE 6.50 usec
 TE 297.7 K
 D1 1.00000000 sec
 TD0 1
 SF01 400.1724710 MHz
 NUC1 1H
 P1 9.88 usec
 SI 65536
 SF 400.1699989 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

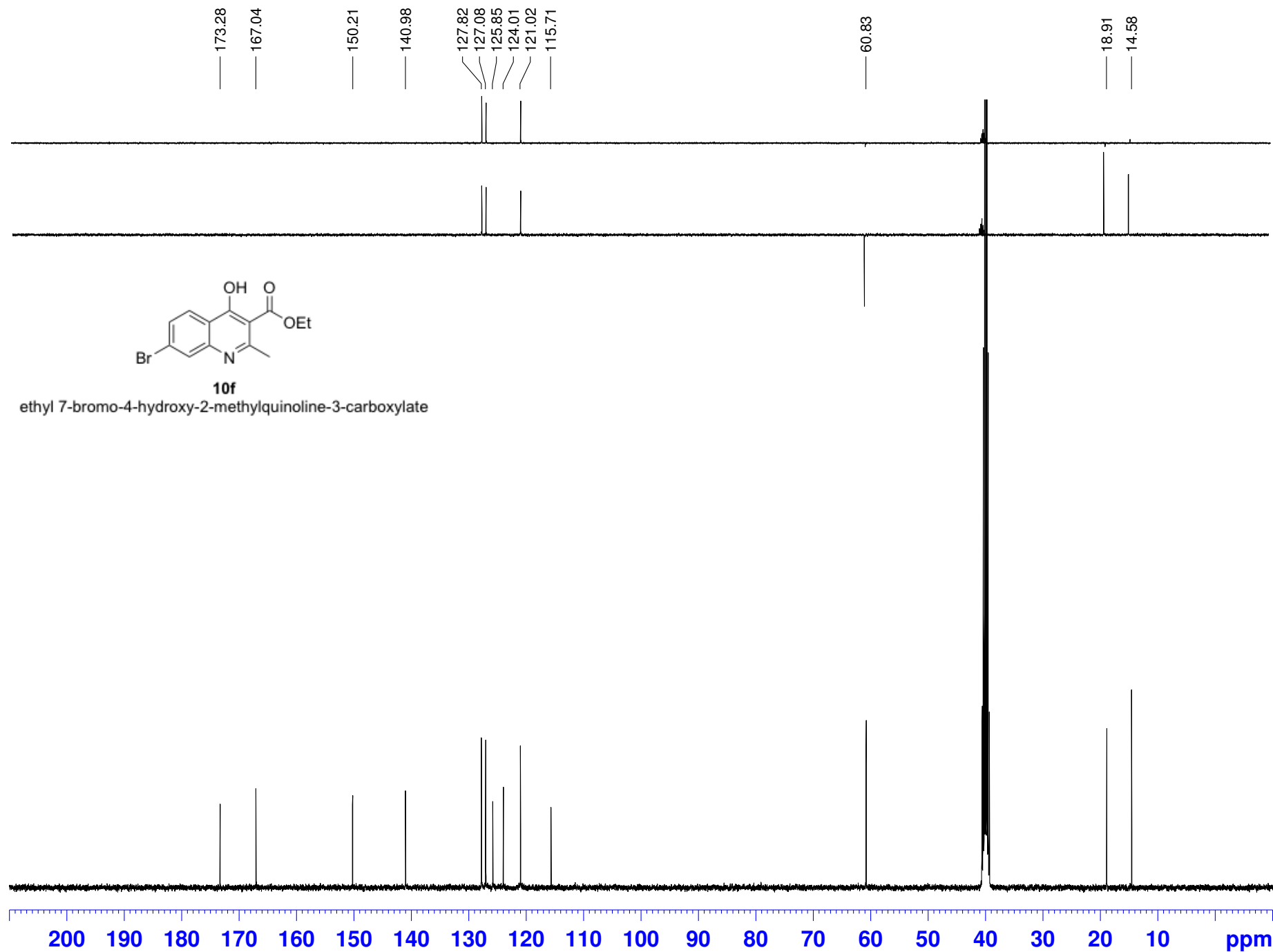


10f

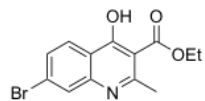
ethyl 7-bromo-4-hydroxy-2-methylquinoline-3-carboxylate



NGJ-8-030 (DMSO, 400 MHz) Pure White Solid - 7-bromoquinoline

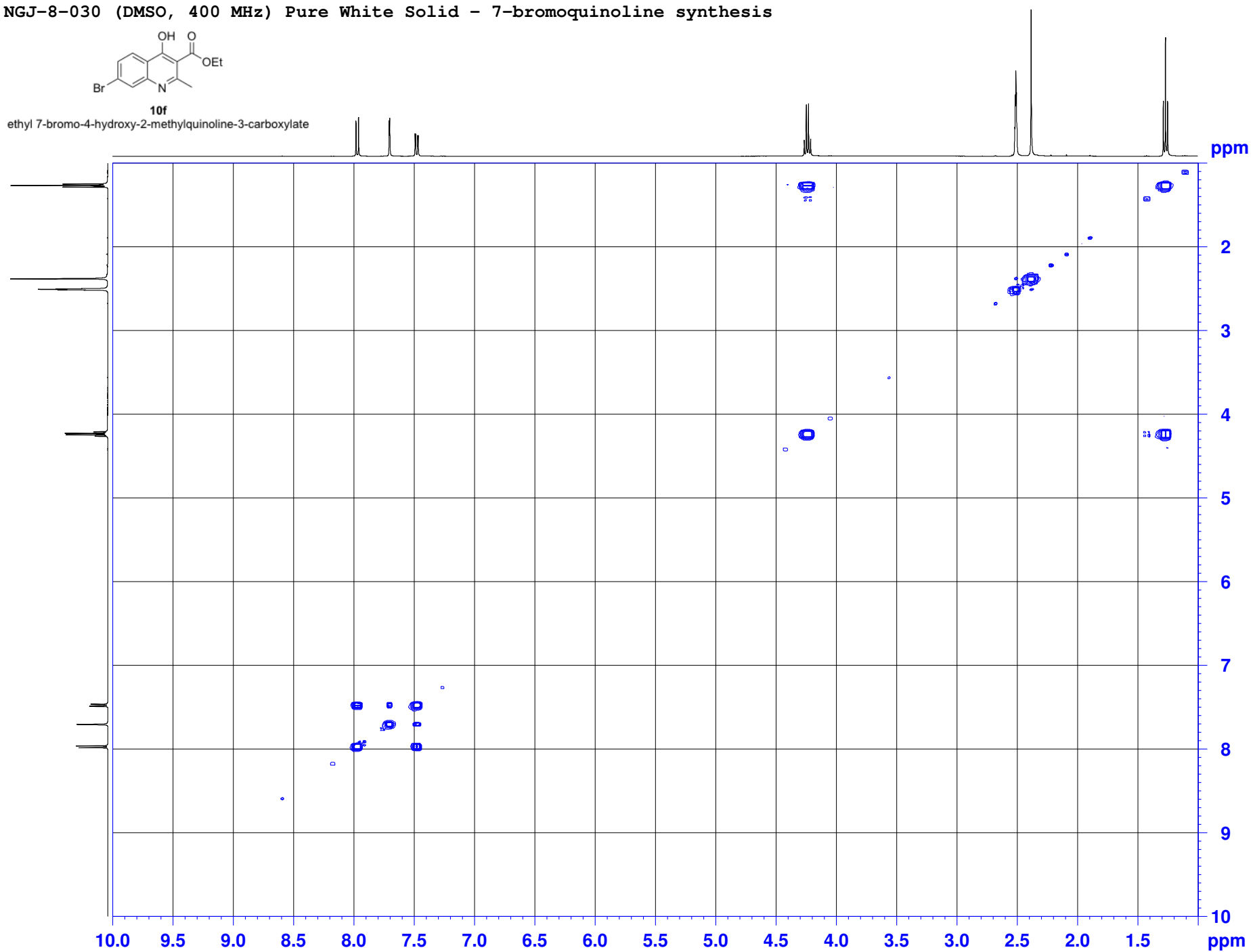


NGJ-8-030 (DMSO, 400 MHz) Pure White Solid - 7-bromoquinoline synthesis

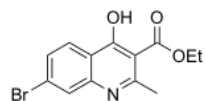


10f

ethyl 7-bromo-4-hydroxy-2-methylquinoline-3-carboxylate

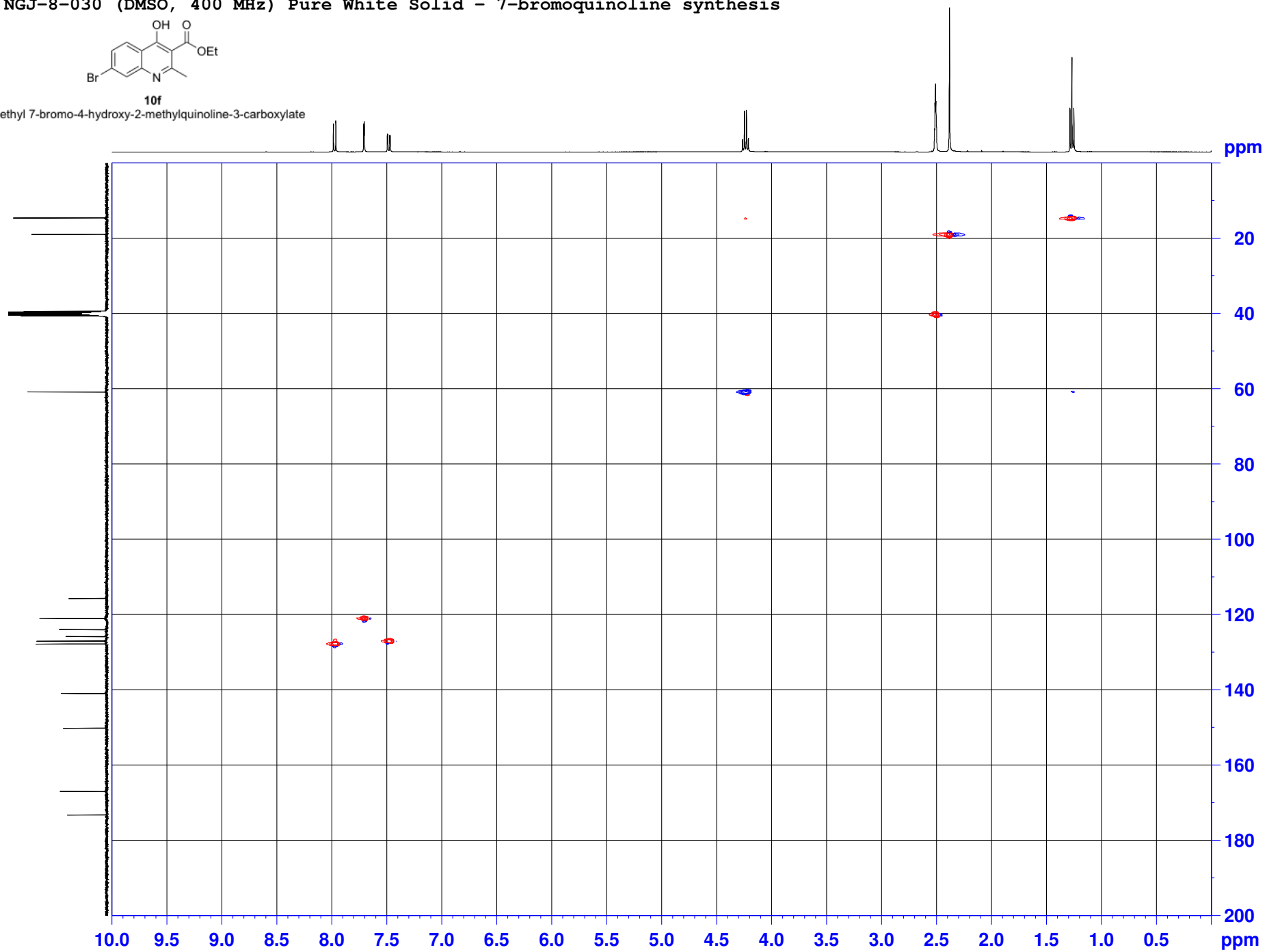


NGJ-8-030 (DMSO, 400 MHz) Pure White Solid - 7-bromoquinoline synthesis

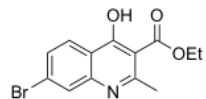


10f

ethyl 7-bromo-4-hydroxy-2-methylquinoline-3-carboxylate

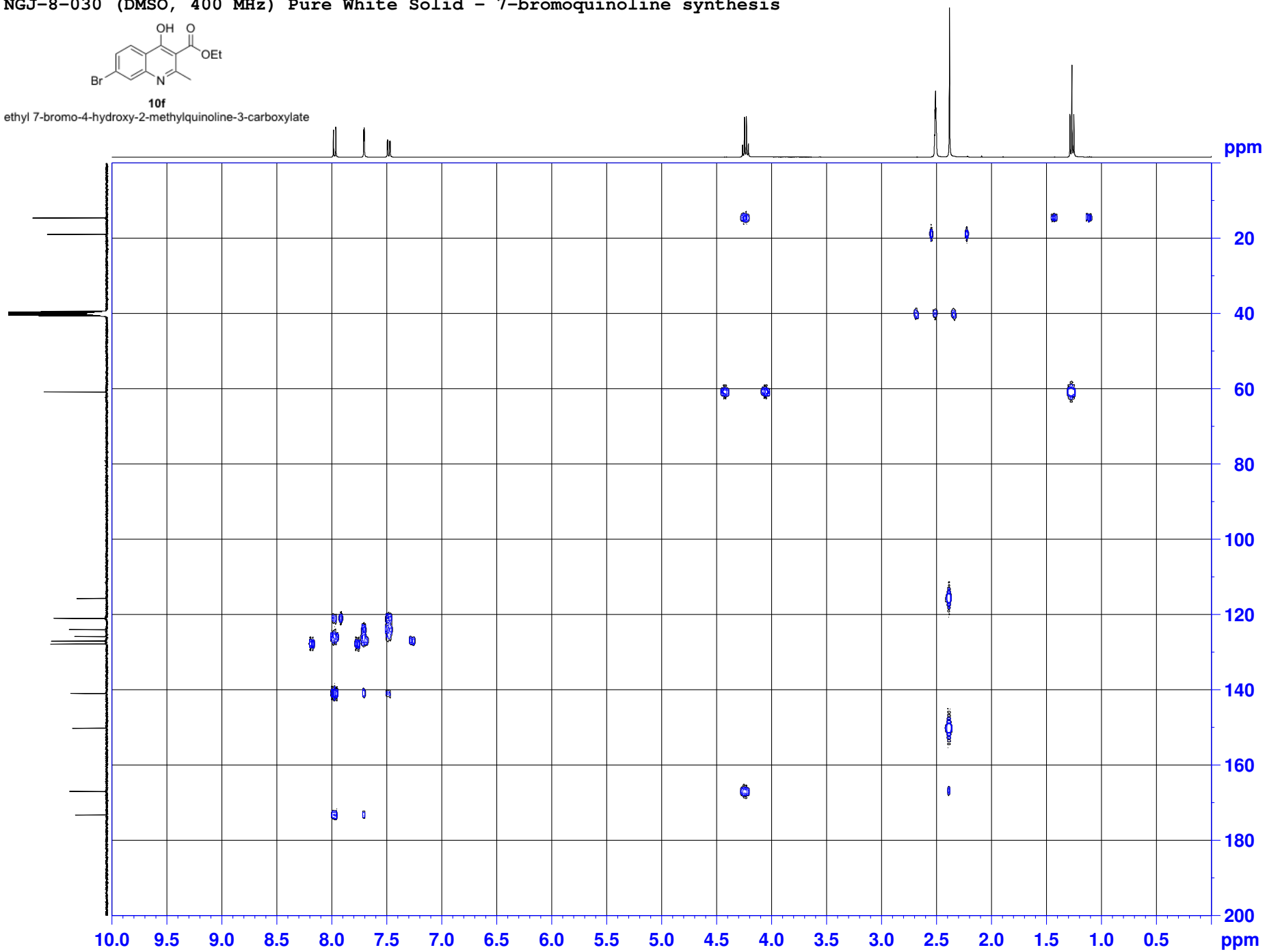


NGJ-8-030 (DMSO, 400 MHz) Pure White Solid - 7-bromoquinoline synthesis



10f

ethyl 7-bromo-4-hydroxy-2-methylquinoline-3-carboxylate



Atlantic Microlab, Inc.

Sample No. N4T-08-030

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Norcross, GA 30071
www.atlanticmicrolab.com

Company/School University of Southern Mississippi

Dept. Chemistry and Biochemistry

Address 118 College Dr. #5043

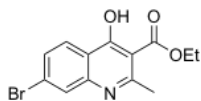
City, State, Zip Hattiesburg, MS 39406

Name Matthew G. Donahue Date 25 July 2018

Phone 614-203-1123

Professor/Supervisor: Matthew G. Donahue

PO# / CC# Mastercard 9359 (On file)



10f

ethyl 7-bromo-4-hydroxy-2-methylquinoline-3-carboxylate

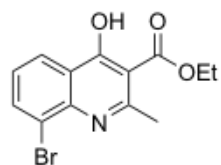
Element	Theory	Found	Single ☒ Duplicate ☐
C	50.34	49.75	Elements Present: <u>C₁₃H₁₂BrN₂O₃</u>
H	3.90	3.89	Analyze for: <u>C, H</u>
			Hygrosopic ☐ Explosive ☐
			M.P. <u> </u> B.P. <u> </u>
			To be dried: Yes ☐ No ☒
			Temp. <u> </u> Vac. <u> </u> Time <u> </u>
			Rush Service ☐ Rush service guarantees analysis will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.
			Include Email Address or FAX # Below
			<u>matthew.donahue@usm.edu</u>

Date Received JUL 30 2018 Date Completed JUL 31 2018

Remarks:

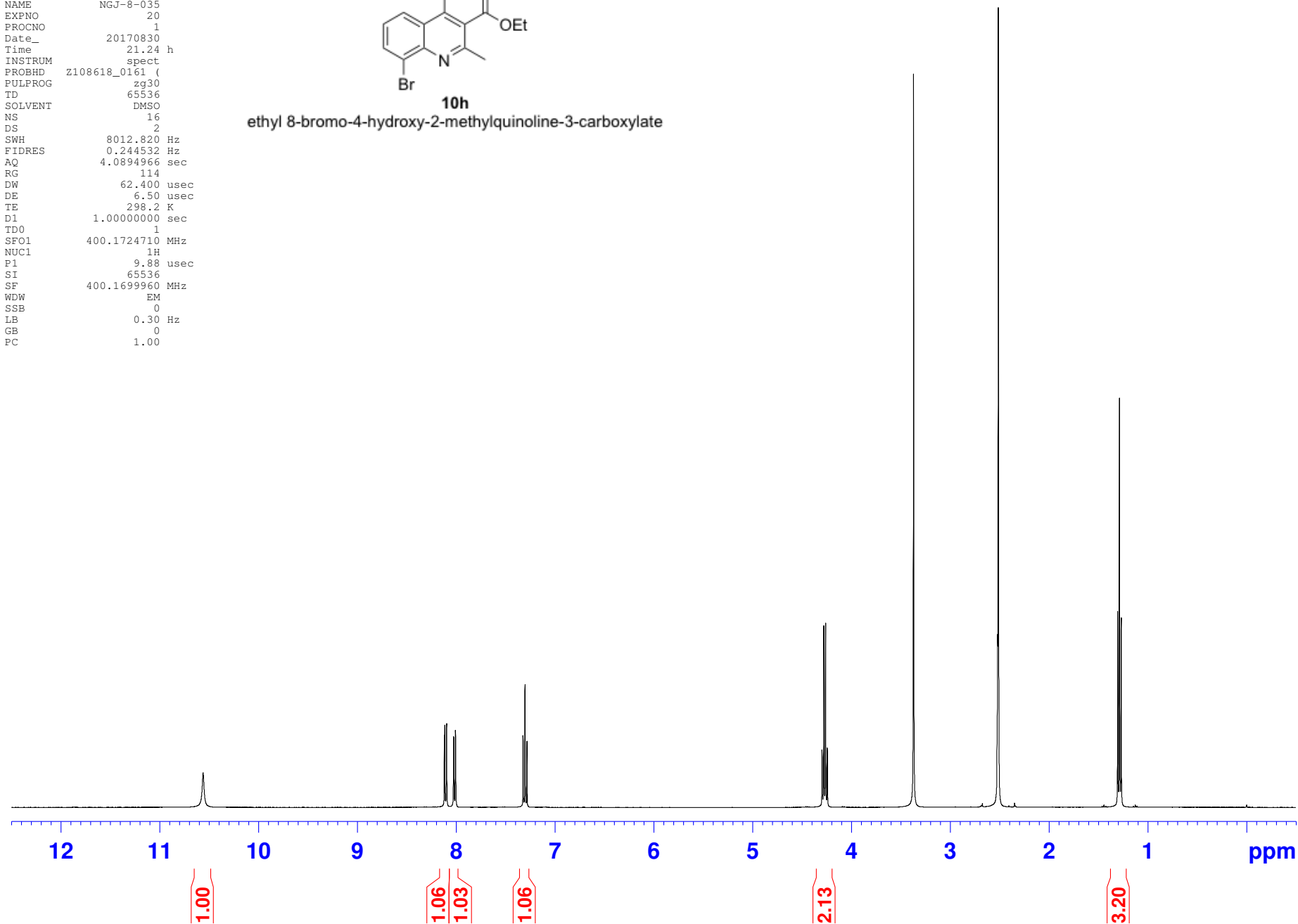
NGJ-8-035 (DMSO, 400 MHz) Pure White Solid - Synthesis of 8-bromoquinoline

NAME NGJ-8-035
EXPNO 20
PROCNO 1
Date_ 20170830
Time_ 21.24 h
INSTRUM spect
PROBHD Z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 114
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
SF01 400.1724710 MHz
NUC1 1H
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SF 400.1699960 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

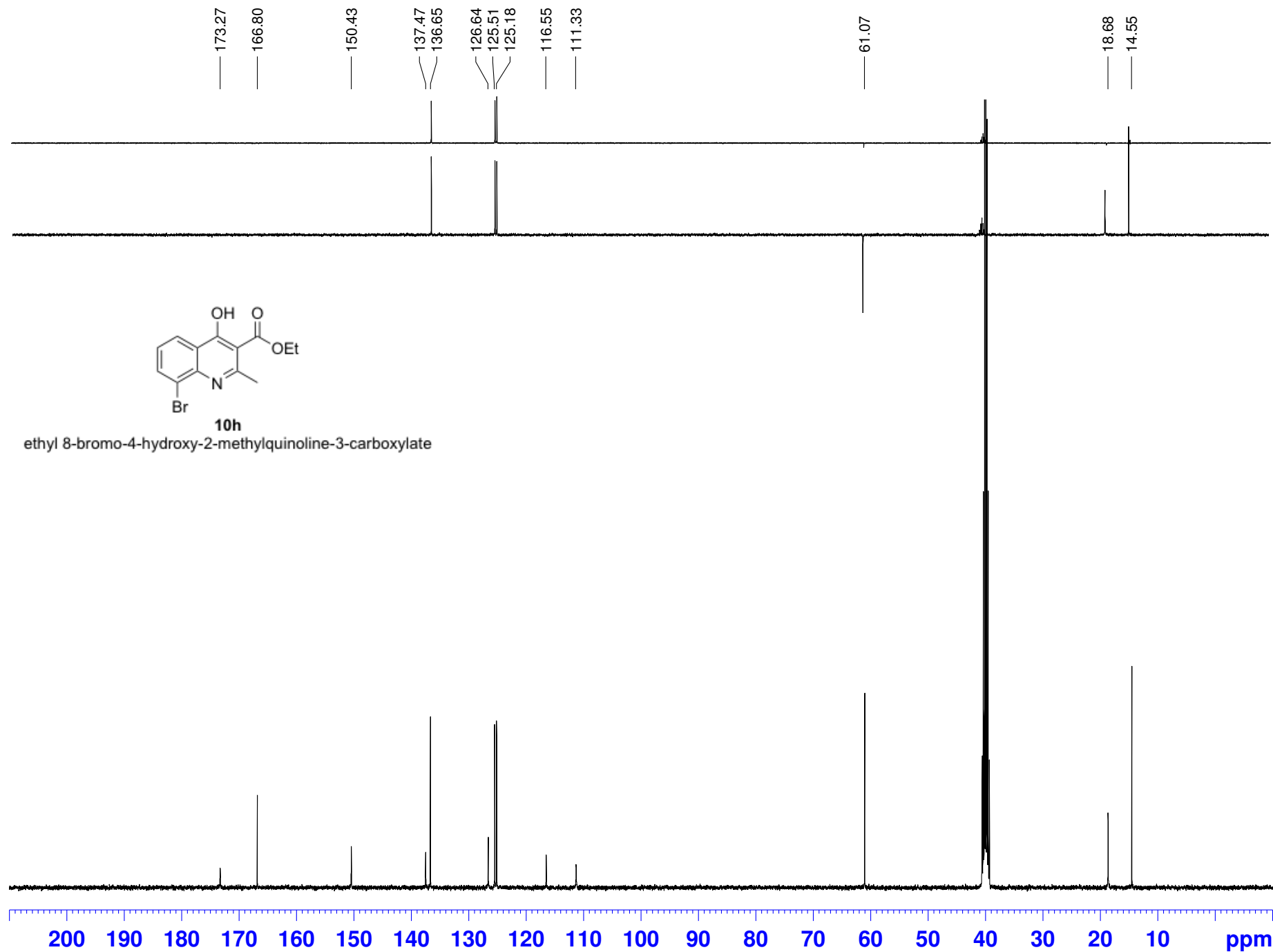


10h

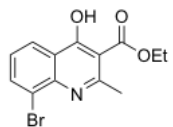
ethyl 8-bromo-4-hydroxy-2-methylquinoline-3-carboxylate



NGJ-8-035 (DMSO, 400 MHz) Pure White Solid - Synthesis of 8-b

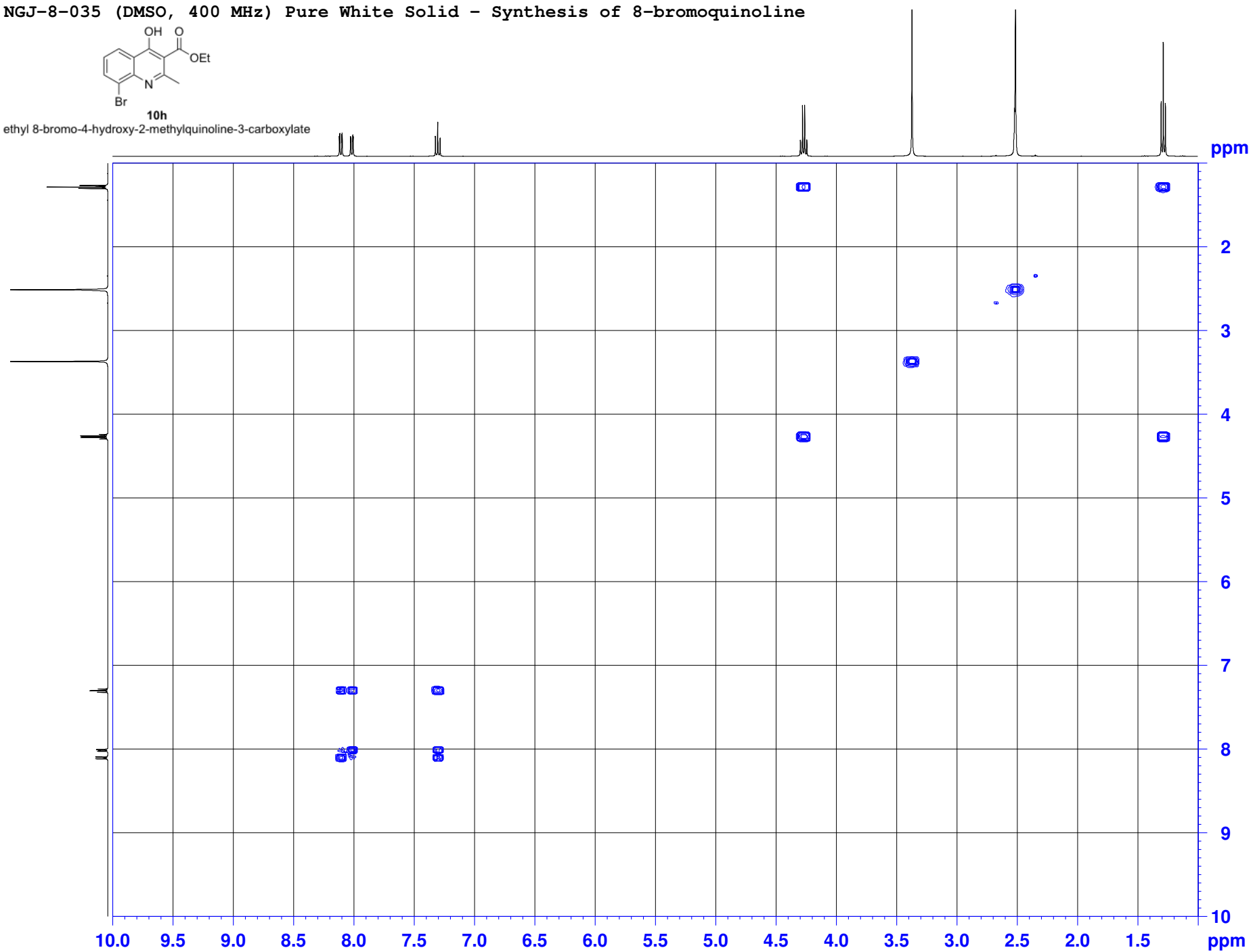


NGJ-8-035 (DMSO, 400 MHz) Pure White Solid - Synthesis of 8-bromoquinoline

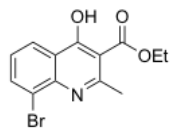


10h

ethyl 8-bromo-4-hydroxy-2-methylquinoline-3-carboxylate

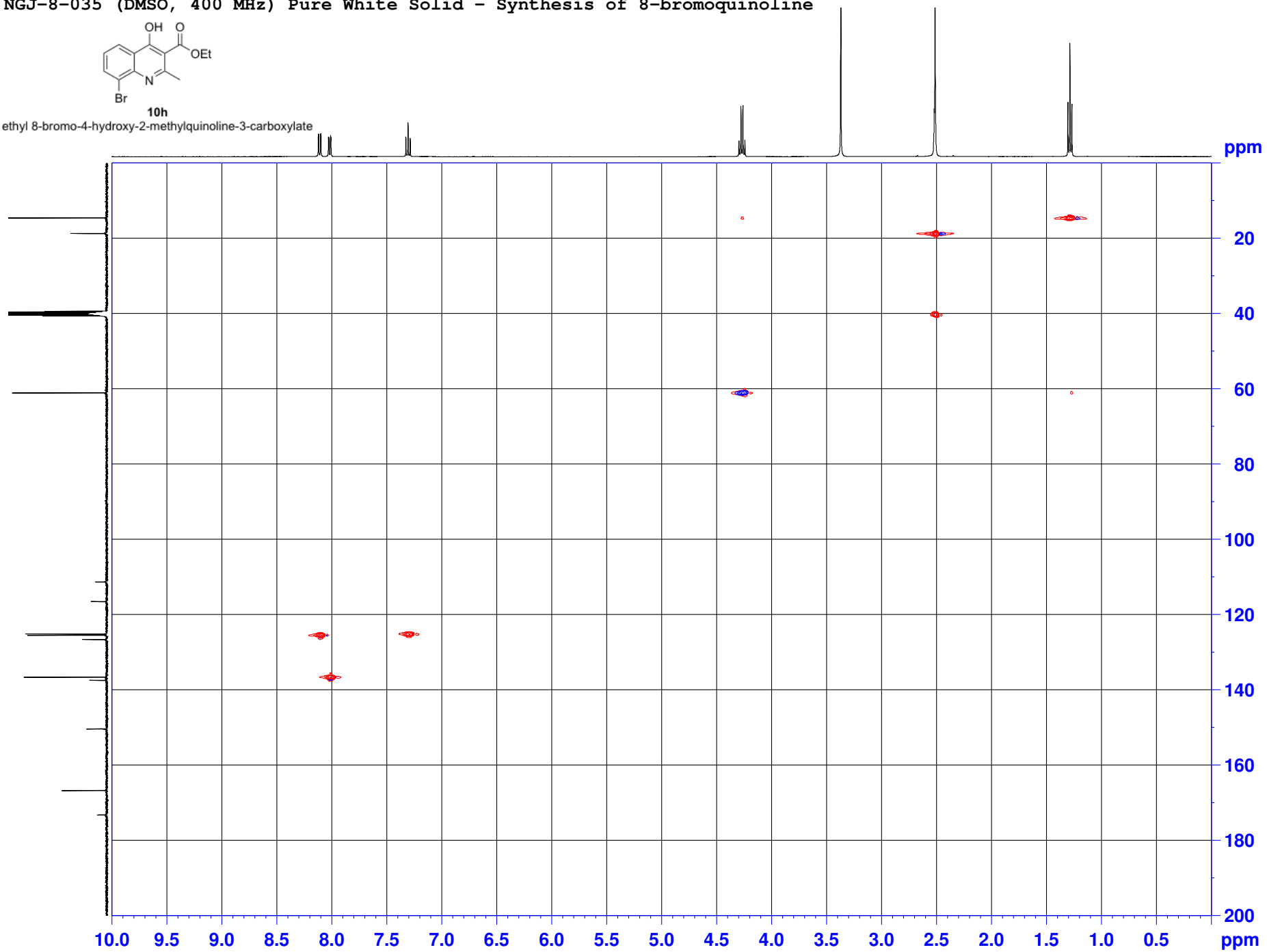


NGJ-8-035 (DMSO, 400 MHz) Pure White Solid - Synthesis of 8-bromoquinoline

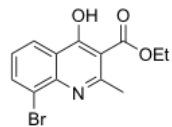


10h

ethyl 8-bromo-4-hydroxy-2-methylquinoline-3-carboxylate

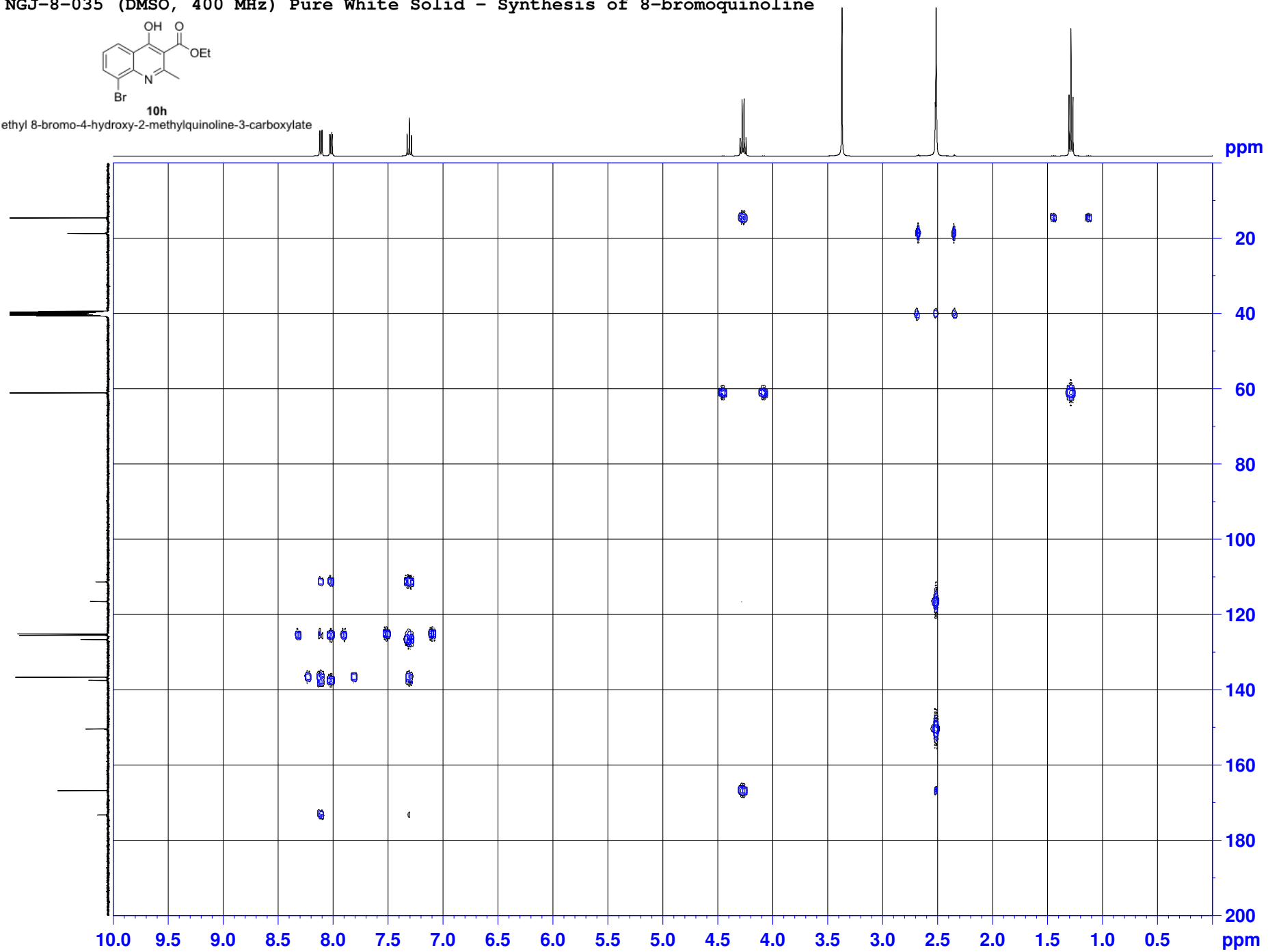


NGJ-8-035 (DMSO, 400 MHz) Pure White Solid - Synthesis of 8-bromoquinoline



10h

ethyl 8-bromo-4-hydroxy-2-methylquinoline-3-carboxylate

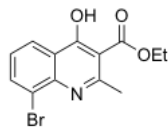


Atlantic Microlab, Inc.

Sample No. N6J-8-035
 6180 Atlantic Blvd. Suite M
 Norcross, GA 30071
 www.atlanticmicrolab.com

Professor/Supervisor: Matthew G. Donahue
 PO# / CC# Mastercard 9359 (On file)

Company/School University of Southern Mississippi
 Dept. Chemistry and Biochemistry
 Address 118 College Dr. #5043
Hattiesburg, MS 39406
 City, State, Zip
 Name Matthew Donahue Date 31 Aug
 Phone 614-203-1123 2017



10h

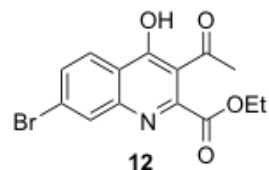
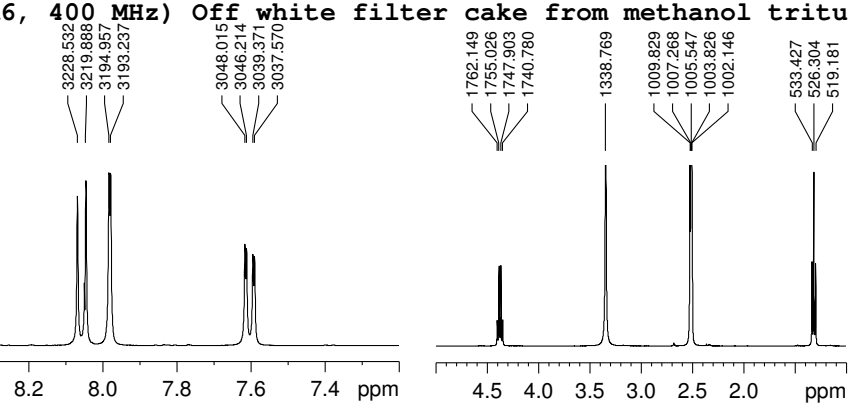
ethyl 8-bromo-4-hydroxy-2-methylquinoline-3-carboxylate

Element	Theory	Found	Single ☒ Duplicate ☐
C	50.34	47.63	Elements Present: <u>C₁₃H₁₂BrNO₃</u>
H	3.90	4.24	Analyze for: <u>C, H</u>
		NO CHARGE FOR DUPLICATES	Hygroscopic ☐ Explosive ☐ M.P. _____ B.P. _____
			To be dried: Yes ☐ No ☒ Time _____
			Temp. _____ Vac. _____
			Rush Service ☐ Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.
			Include Email Address or FAX # Below <u>matthew.donahue@usm.edu</u>

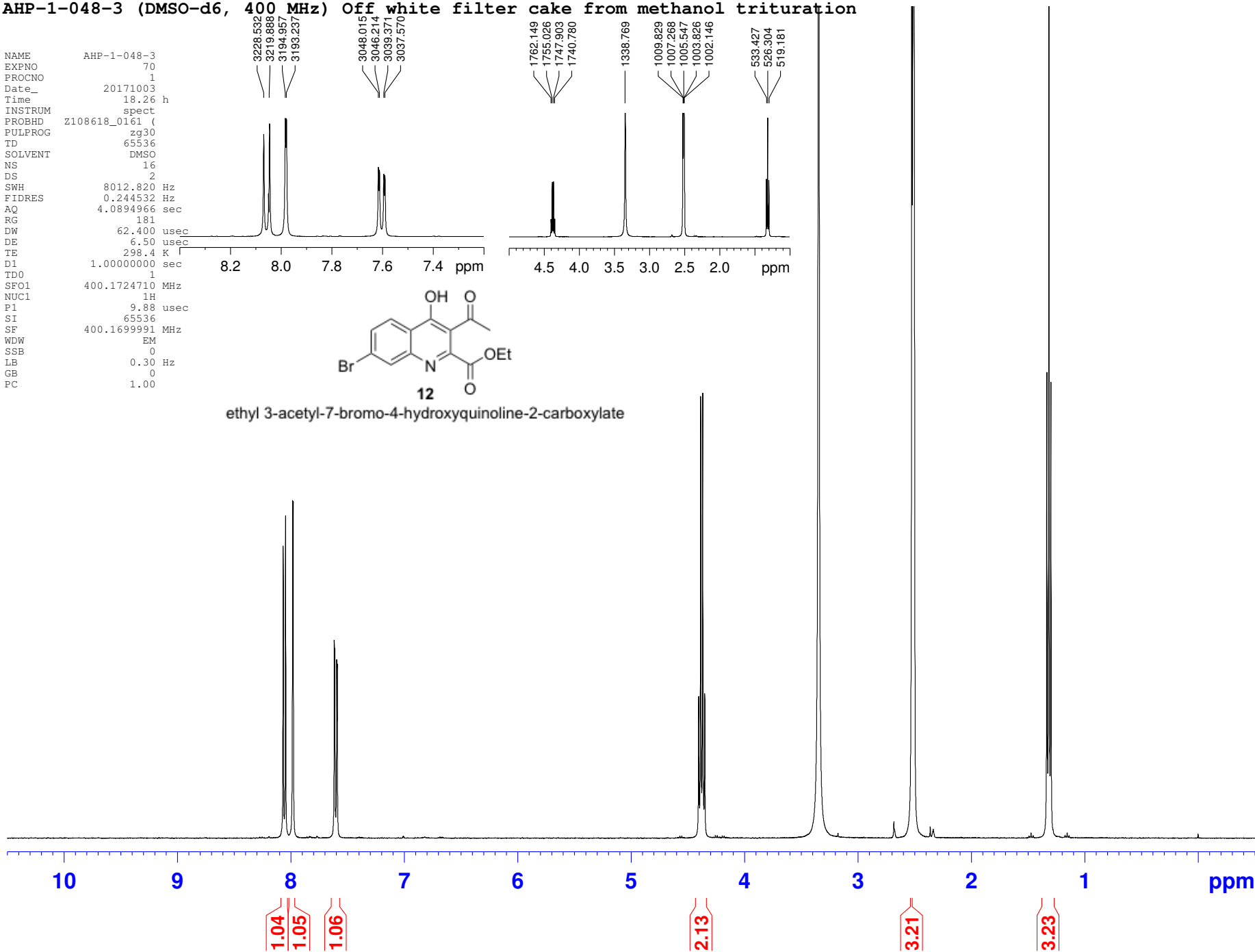
Date Received SEP 06 2017 Date Completed SEP 07 2017
 Remarks:

AHP-1-048-3 (DMSO-d₆, 400 MHz) Off white filter cake from methanol trituration

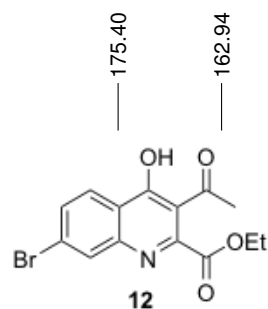
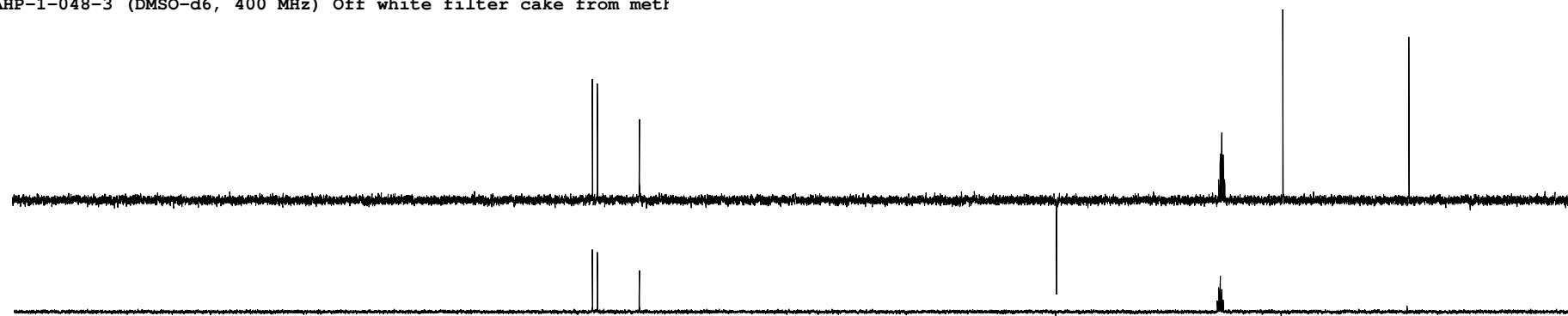
NAME AHP-1-048-3
 EXPNO 70
 PROCNO 1
 Date_ 20171003
 Time 18.26 h
 INSTRUM spect
 PROBHD Z108618_0161
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894966 sec
 RG 181
 DW 62.400 usec
 DE 6.50 usec
 TE 298.4 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.1724710 MHz
 NUC1 1H
 P1 9.88 usec
 SI 65536
 SF 400.1699991 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



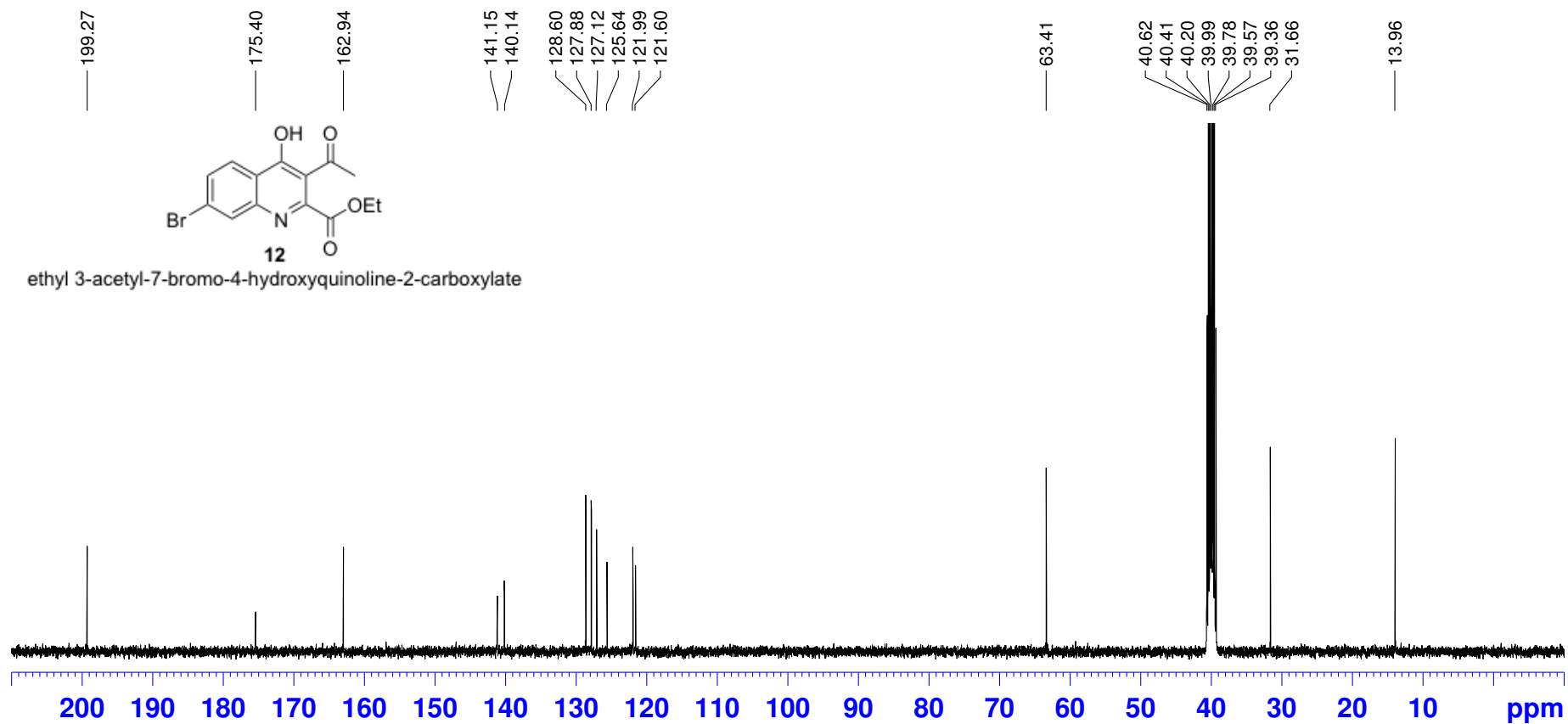
ethyl 3-acetyl-7-bromo-4-hydroxyquinoline-2-carboxylate



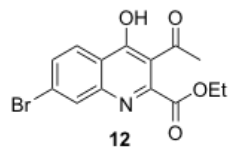
AHP-1-048-3 (DMSO-d6, 400 MHz) Off white filter cake from metl



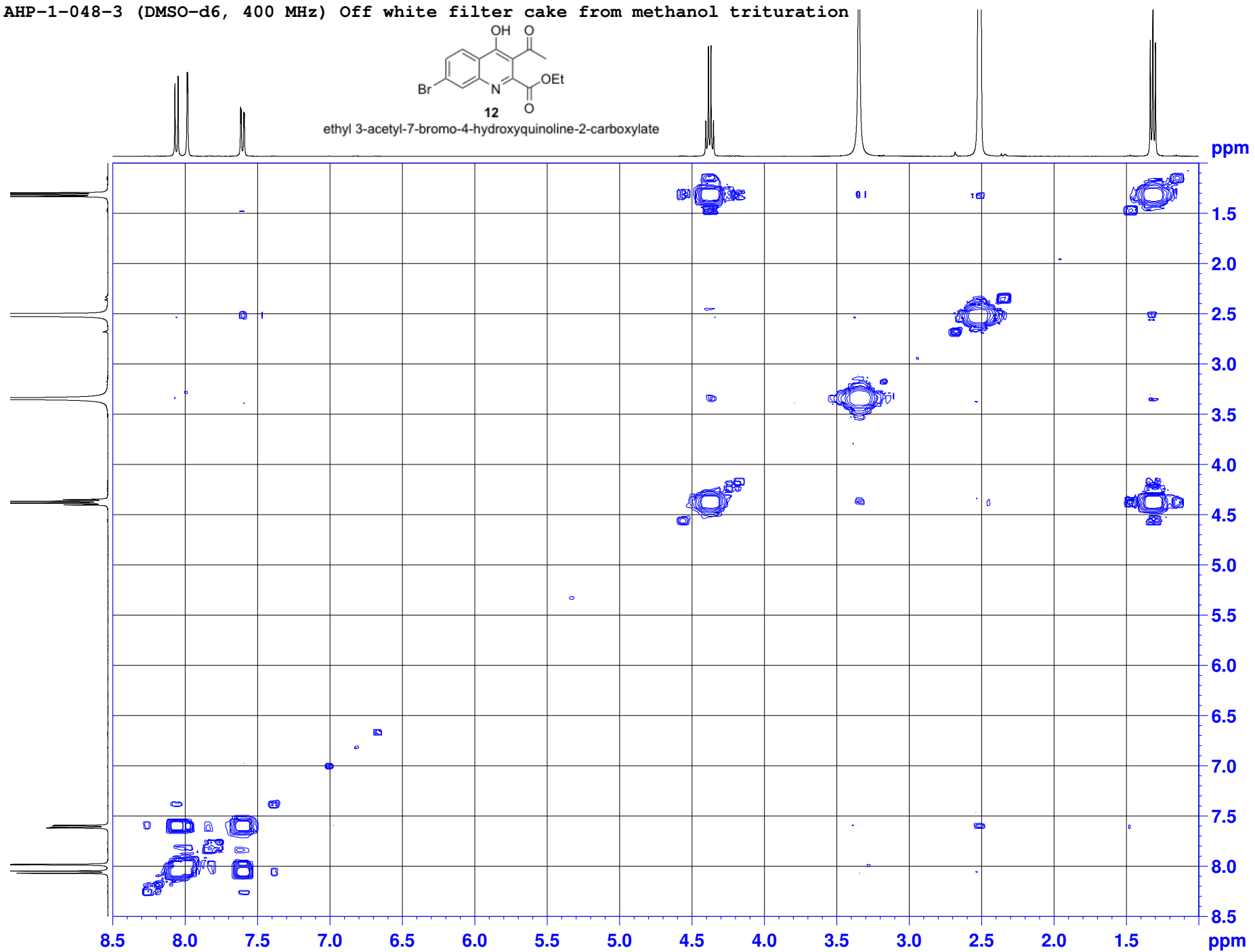
ethyl 3-acetyl-7-bromo-4-hydroxyquinoline-2-carboxylate



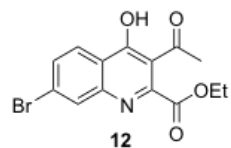
AHP-1-048-3 (DMSO-d₆, 400 MHz) Off white filter cake from methanol trituration



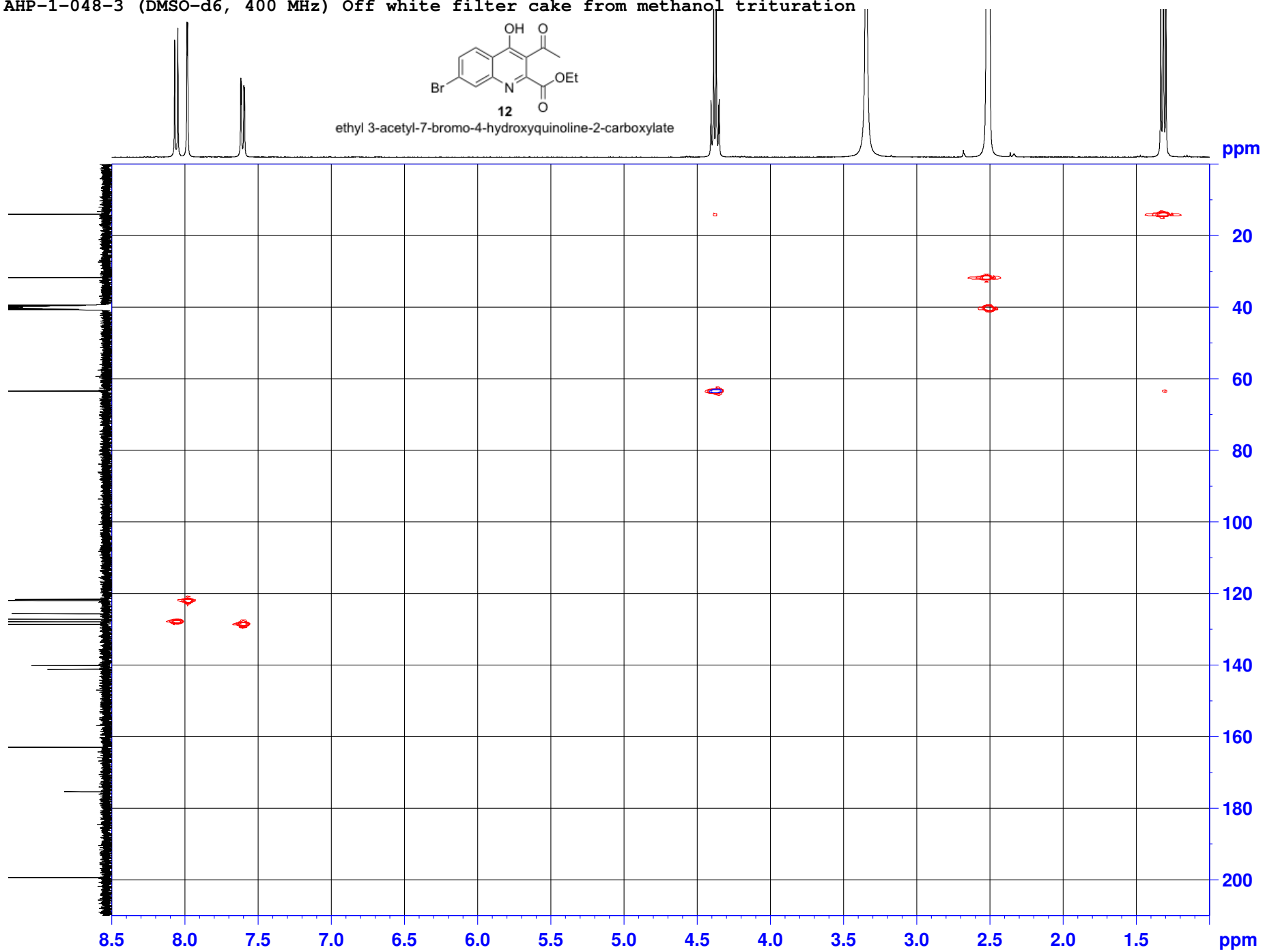
ethyl 3-acetyl-7-bromo-4-hydroxyquinoline-2-carboxylate



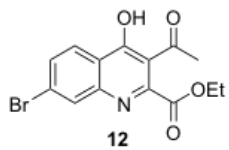
AHP-1-048-3 (DMSO-d₆, 400 MHz) Off white filter cake from methanol trituration



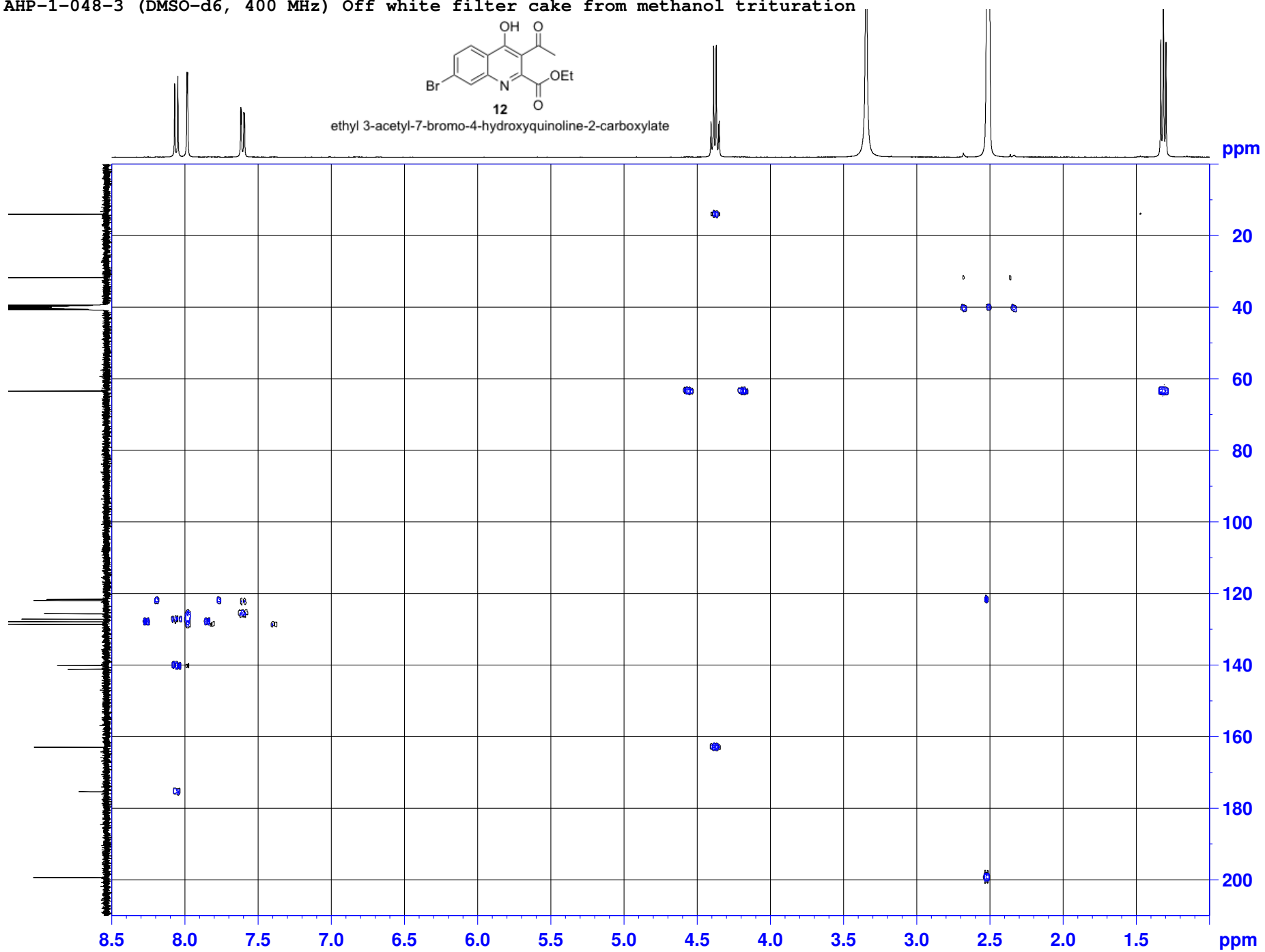
ethyl 3-acetyl-7-bromo-4-hydroxyquinoline-2-carboxylate



AHP-1-048-3 (DMSO-d₆, 400 MHz) Off white filter cake from methanol trituration



ethyl 3-acetyl-7-bromo-4-hydroxyquinoline-2-carboxylate



Atlantic Microlab, Inc.

Sample No. **ATP-1-048-3**

6180 Atlantic Blvd. Suite M
Norcross, GA 30071
www.atlanticmicrolab.com

Company/School **University of Southern Mississippi**
Dept. **Chemistry and Biochemistry**
Address **118 College Dr. #5043**
City, State, Zip **Hattiesburg, MS 39406**
Name **Matthew Donahue** Date **04/06/2017**
Phone **614-203-1123**

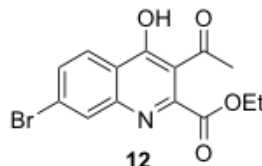
Professor/Supervisor: **Matthew G. Donahue**
PO# / CC# **1 Visa 5794**

Element	Theory	Found	Single ☒	Duplicate ☐
C	49.73	49.81	Elements Present: C₁₄H₁₂BrNO₄	
H	3.58	3.47	Analyze for: C, H	
			Hydroscopic ☐ Explosive ☐ M.P. 178-201°C B.P.	
			To be dried: Yes ☐ No ☒	
			Temp. Vac. Time	
			Rush Service ☐ Rush service guarantees analysis will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.	
			Include Email Address or FAX # Below matthew.donahue@usm.edu	

Date Received **JUL 30 2018**

Date Completed **JUL 31 2018**

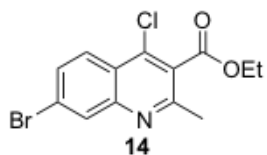
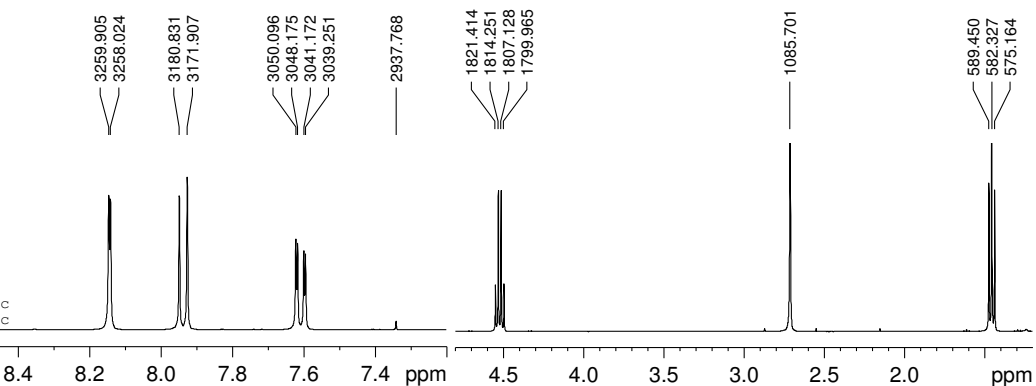
Remarks:



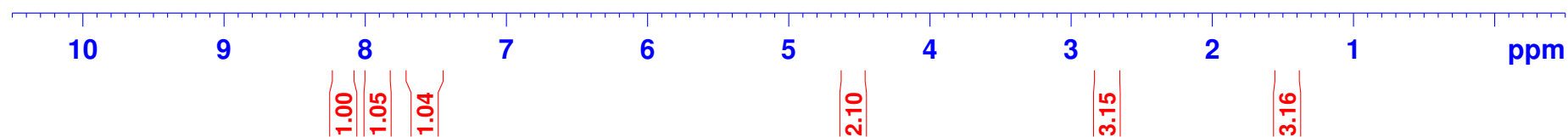
12
ethyl 3-acetyl-7-bromo-4-hydroxyquinoline-2-carboxylate

JDH-1-216 (400MHz, CDCl3) Chlorination of 4-Hydroxyquinoline

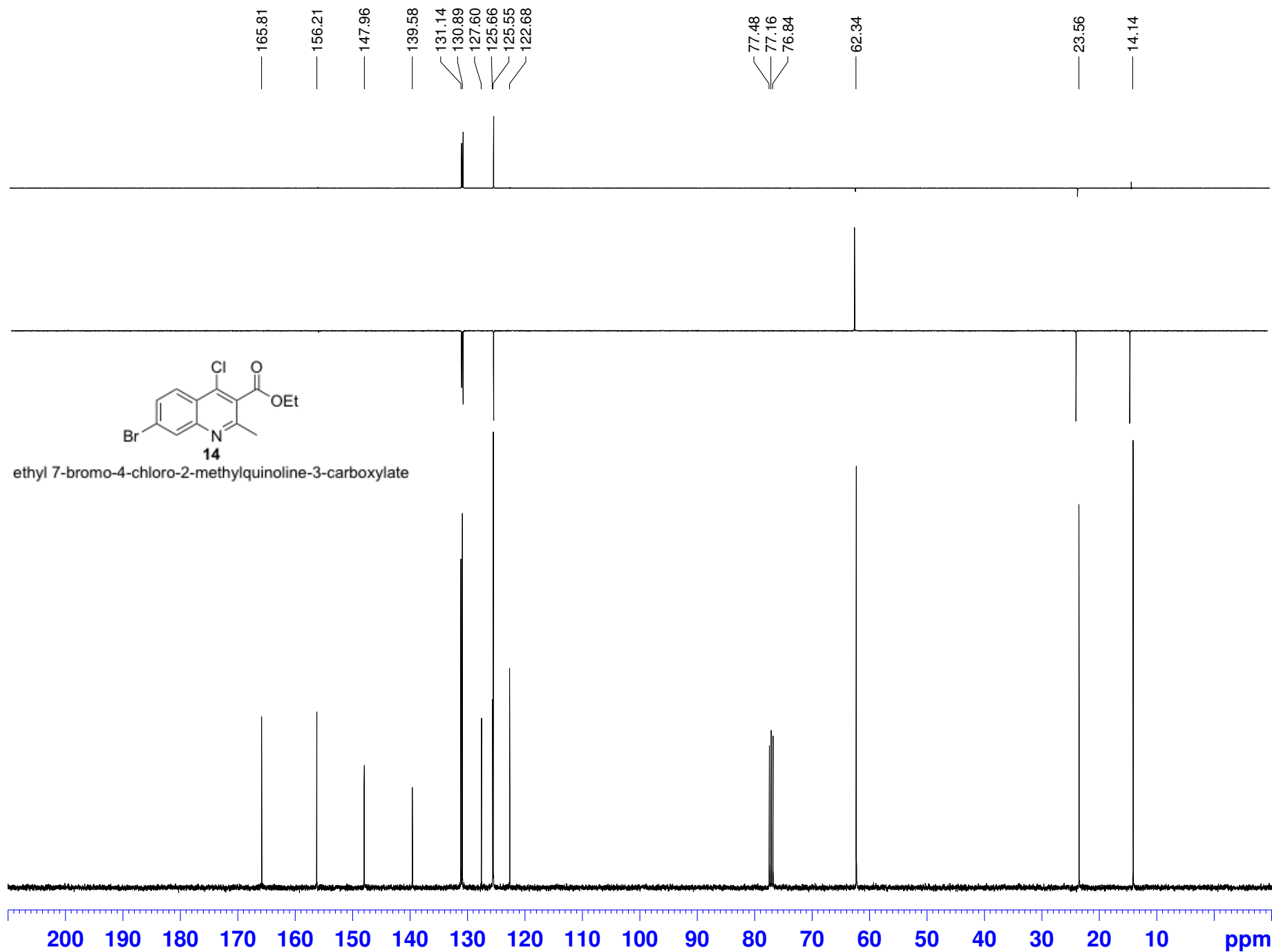
NAME JDH-1-216
 EXPNO 40
 PROCNO 1
 Date_ 20171027
 Time 10.29 h
 INSTRUM spect
 PROBHD Z108618_0161
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894966 sec
 RG 32
 DW 62.400 usec
 DE 6.50 usec
 TE 298.3 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.1724710 MHz
 NUC1 1H
 P1 9.88 usec
 SI 65536
 SF 400.1699764 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



ethyl 7-bromo-4-chloro-2-methylquinoline-3-carboxylate



JDH-1-216 (400MHz, CDCl3) Chlorination of 4-hydroxyquinoline



Atlantic Microlab, Inc.

Sample No. SKW-1-085

6180 Atlantic Blvd. Suite M
Norcross, GA 30071
www.atlanticmicrolab.com

Company/School University of Southern Mississippi

Dept. Chemistry and Biochemistry

Address 118 College Dr. #5043

City, State, Zip Hattiesburg, MS 39406

Professor/Supervisor: Matthew G. Donahue

PO# / CC# Mastercard 9359 (On file)

Name Matthew G. Donahue

Phone 614-203-1123

Date 25 July 2018

Element	Theory	Found	Single ☒	Duplicate ☐
C	47.52	44.86	Present: <u>C13H11BrClNO2</u>	
H	3.37	3.23	Analyze for: <u>C, H</u>	
			Hygroscopic ☐	Explosive ☐
			M.P. <u> </u>	B.P. <u> </u>
			To be dried: Yes ☐ No ☒	
			Temp. <u> </u>	
			Rush Service ☐	
			Include Email Address or FAX # Below	
			matthew.donahue@usm.edu	

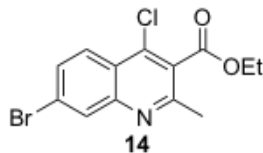
Date Received

JUL 30 2018

Date Completed

JUL 31 2018

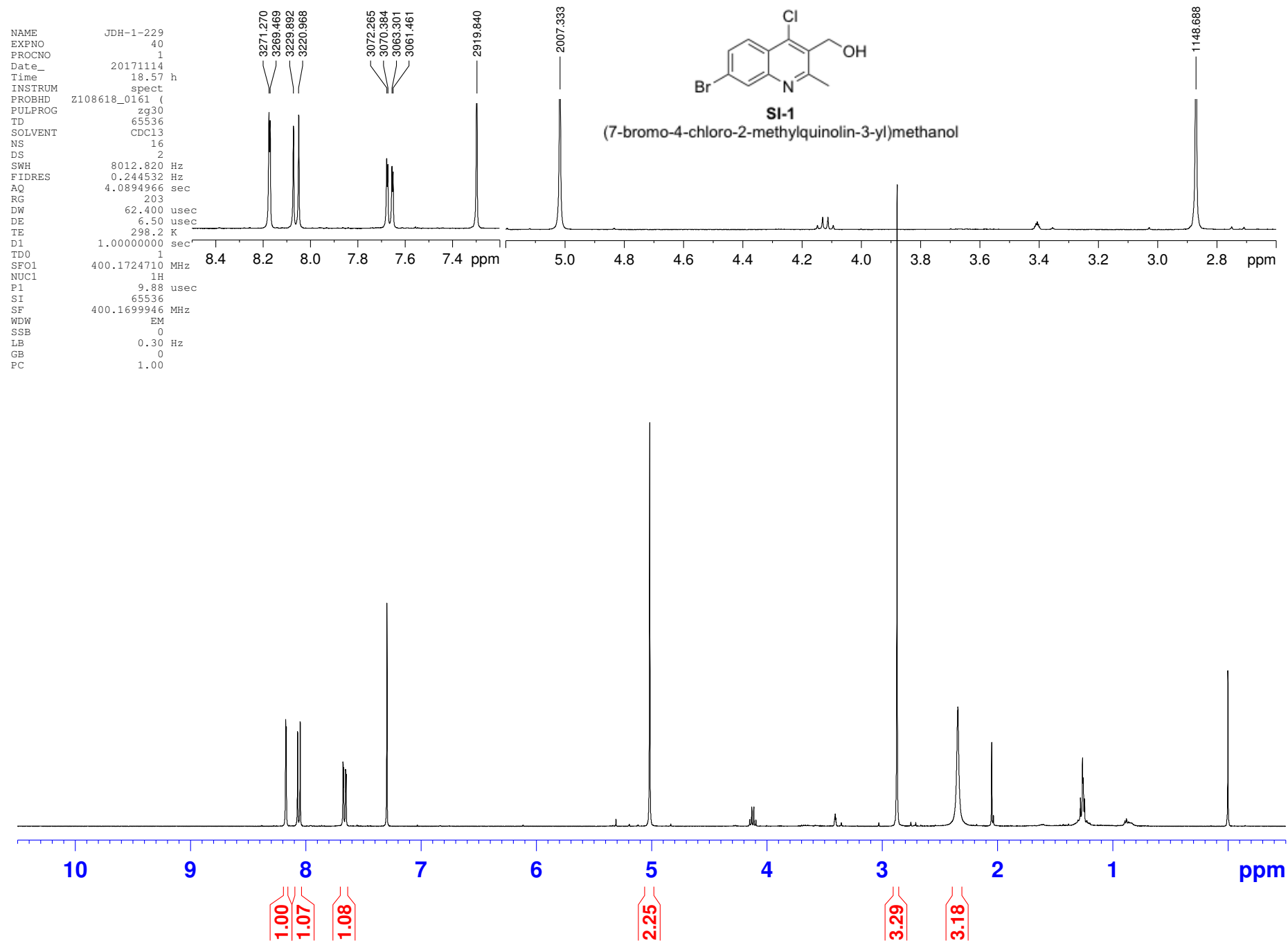
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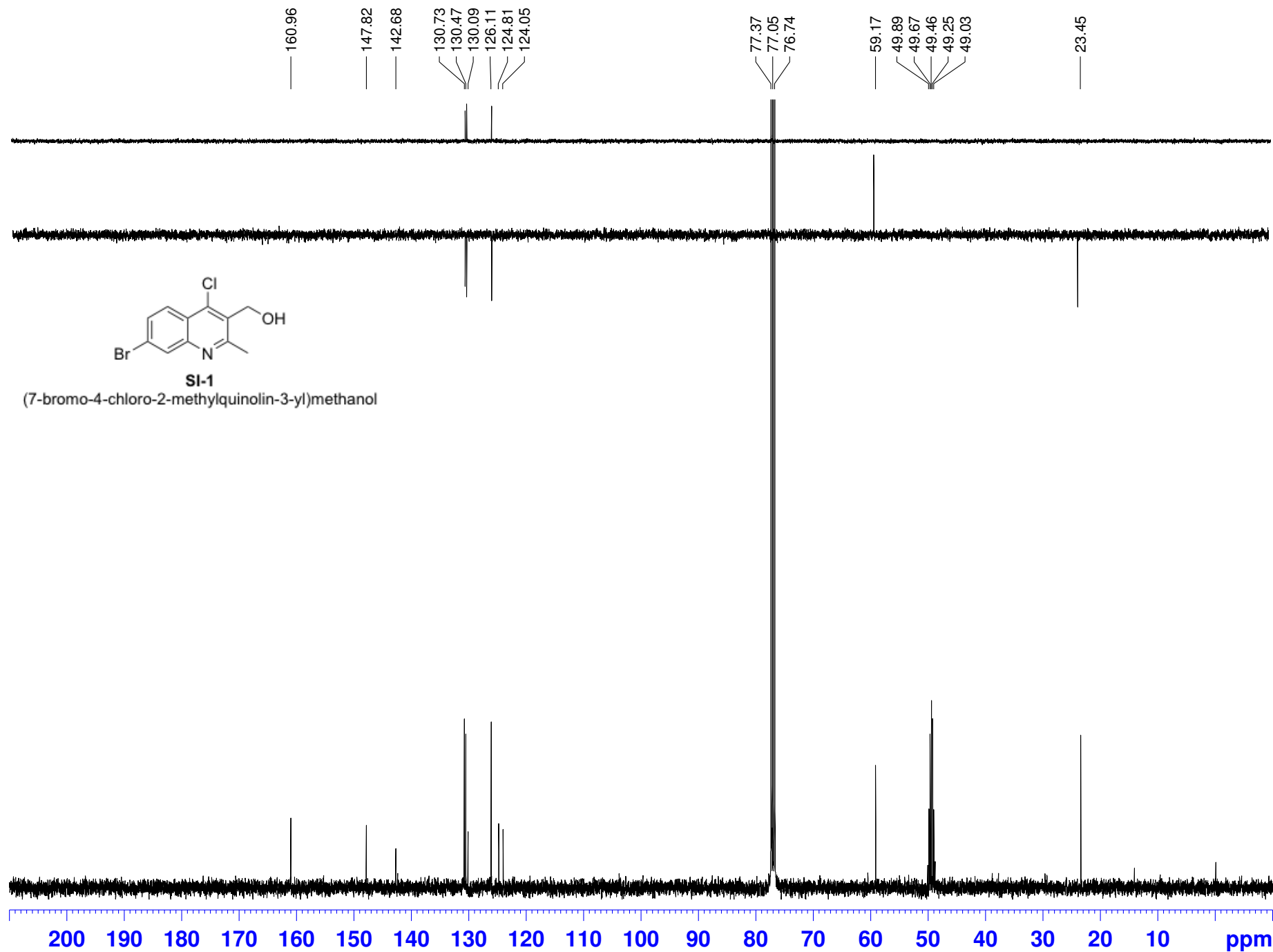
14

ethyl 7-bromo-4-chloro-2-methylquinoline-3-carboxylate

JDH-1-229B DIBAL-H reduction (400MHz, CDC13)

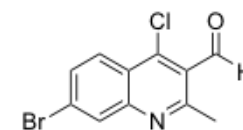
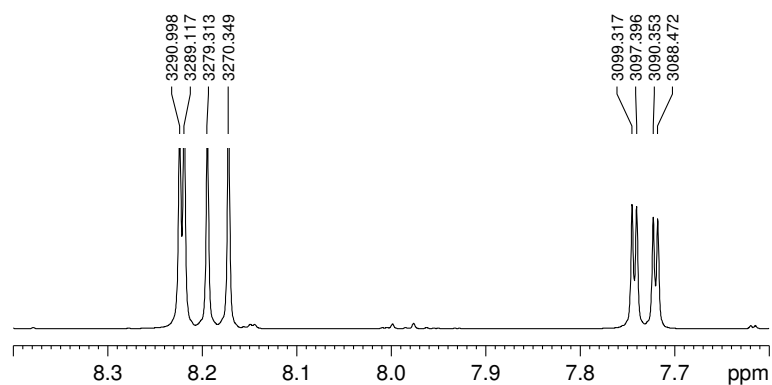


JDH-1-229B DIBAL-H reduction (400MHz, CDC13)



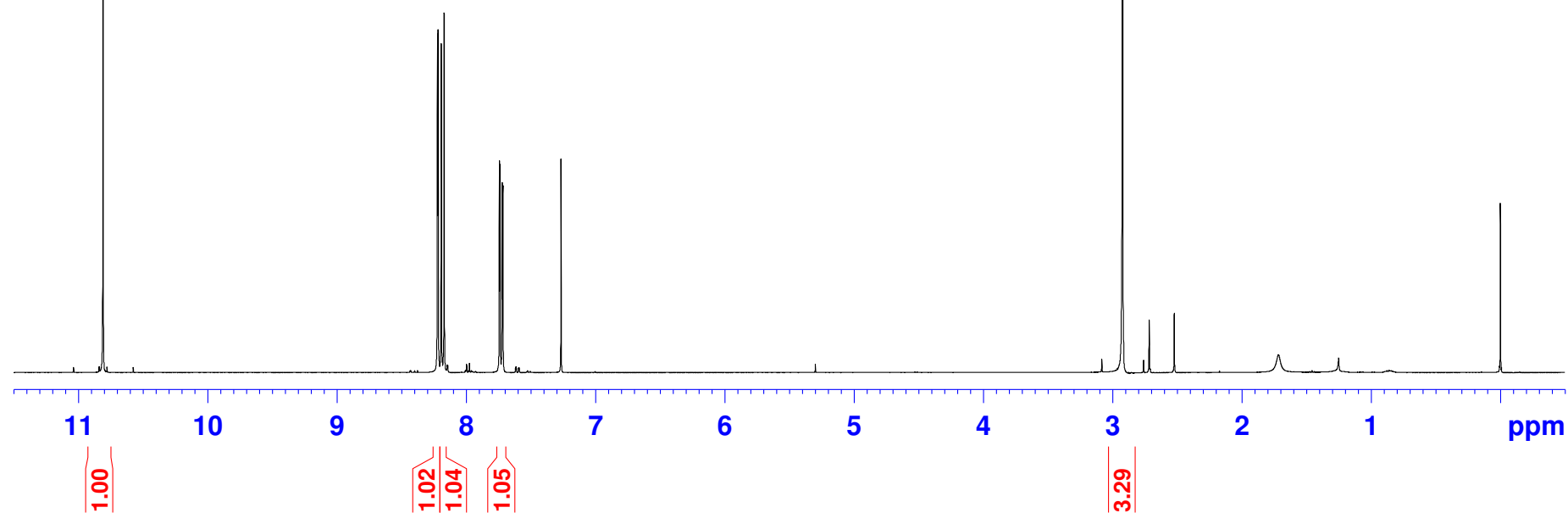
JDH-1-226 Parikh-Doering Oxidation (CDC13, 400MHz)

NAME JDH-1-226
 EXPNO 20
 PROCNO 1
 Date_ 20171113
 Time 17.50 h
 INSTRUM spect
 PROBHD Z108618_0161
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894966 sec
 RG 203
 DW 62.400 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.0000000 sec
 TD0 1
 SFO1 400.1724710 MHz
 NUC1 1H
 P1 9.88 usec
 SI 65536
 SF 400.1700063 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

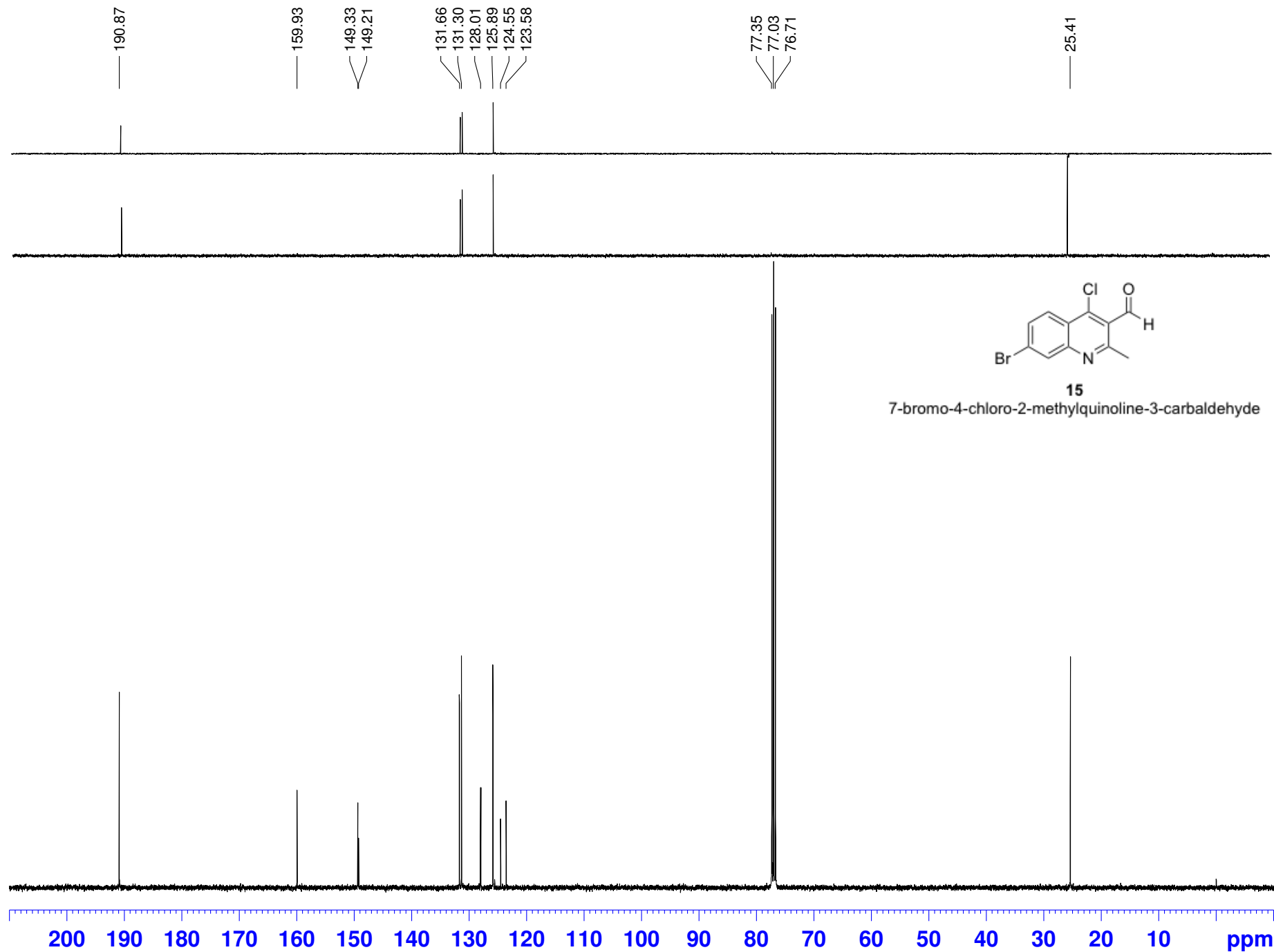


15

7-bromo-4-chloro-2-methylquinoline-3-carbaldehyde



JDH-1-226B Pyr*SO3 oxidation (400MHz, CDC13)



Atlantic Microlab, Inc.

Sample No. N6T-10-007

6180 Atlantic Blvd. Suite M
Norcross, GA 30071
www.atlanticmicrolab.com

Company/School University of Southern Mississippi

Dept. Chemistry and Biochemistry

Address 118 College Dr. #5043

City, State, Zip Hattiesburg, MS 39406

Professor/Supervisor: Matthew G. Donahue

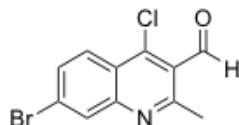
PO# / CC# Mastercard 9359 (On file)

Name Matthew G. Donahue

Phone 614-203-1123

Date 25 July

2018



15

7-bromo-4-chloro-2-methylquinoline-3-carbaldehyde

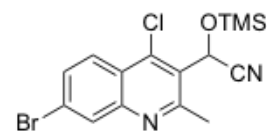
Element	Theory	Found	Single ☒ Duplicate ☐
C	46.43	45.72	Elements Present: <u>C, H, Br, Cl, N, O</u>
H	2.48	2.41	Analyze for: <u>C, H</u>
			Hydroscopic ☐ Explosive ☐
			M.P. <u>NO CHARGE FOR DUPLICATES</u> B.P.
			To be dried: Yes ☐ No ☒
			Temp. <u> </u> Vac. <u> </u> Time <u> </u>
			Rush Service ☐ Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.
			Include Email Address or FAX # Below
			<u>matthew.donahue@usm.edu</u>

Date Received JUL 30 2018 Date Completed JUL 31 2018

Remarks:

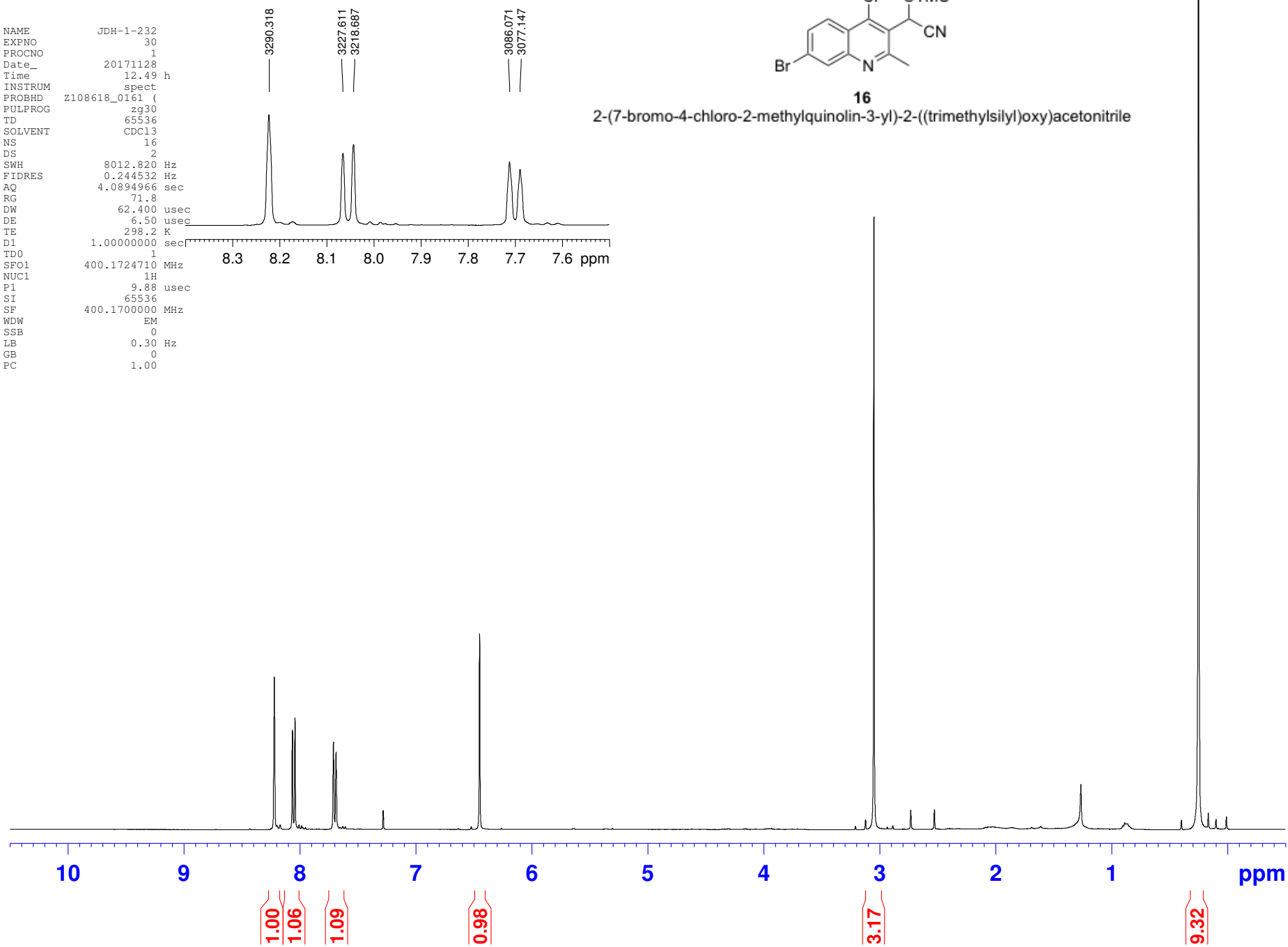
JDH-1-232 Cyanosilylation (400MHz, CDCl3)

NAME JDH-1-232
 EXPNO 30
 PROCNO 1
 Date_ 20171128
 Time 12.49 h
 INSTRUM spect
 PROBHD Z108618_0161
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894966 sec
 RG 71.8
 DW 62.400 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.1724710 MHz
 NUC1 1H
 P1 9.88 usec
 SI 65536
 SF 400.1700000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

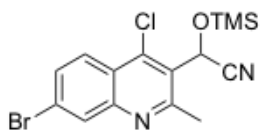
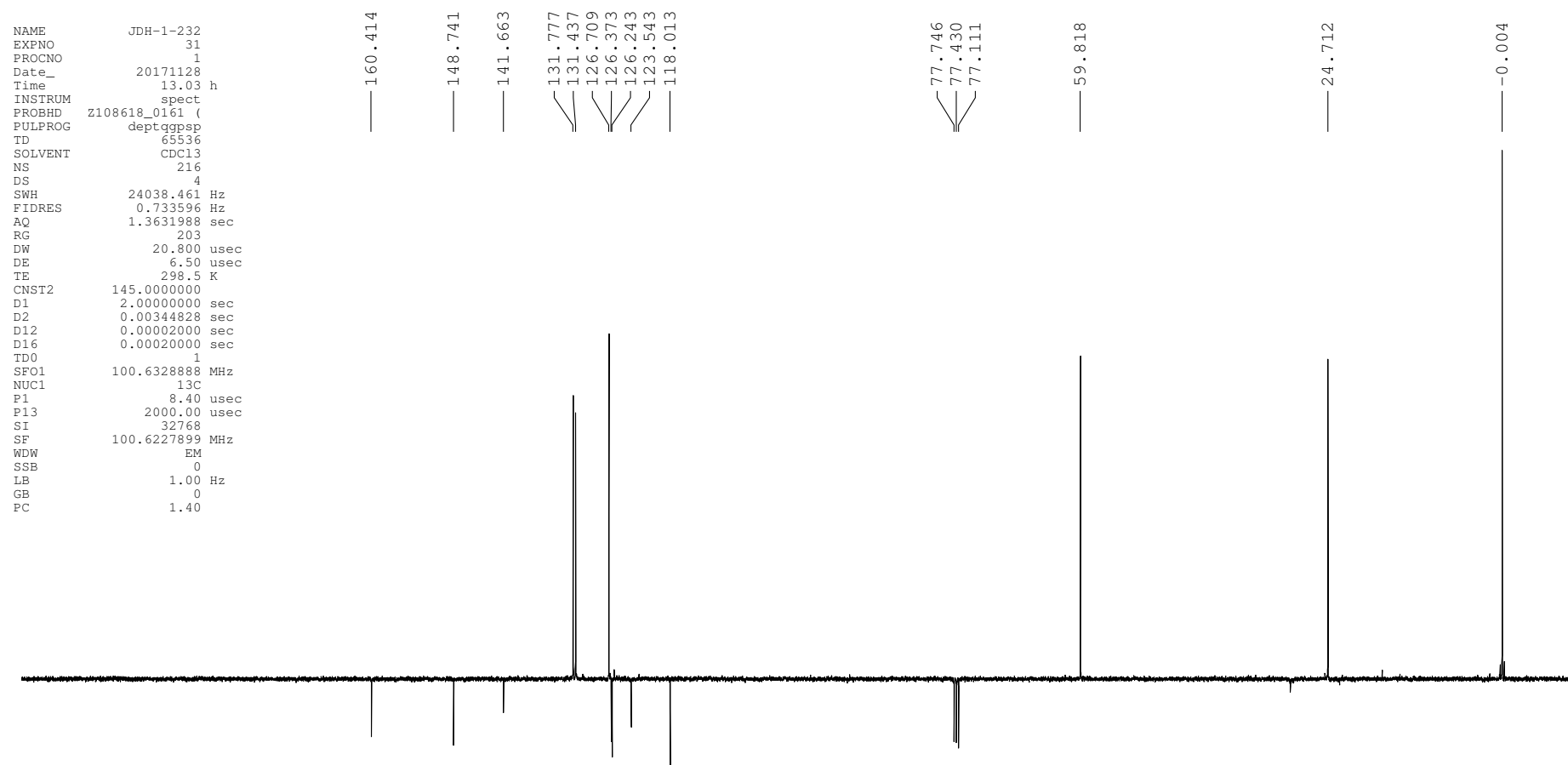


16

2-(7-bromo-4-chloro-2-methylquinolin-3-yl)-2-((trimethylsilyl)oxy)acetonitrile

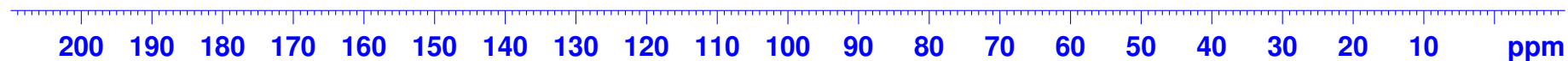


JDH-1-232 Cyanosilylation (400MHz, CDC13)

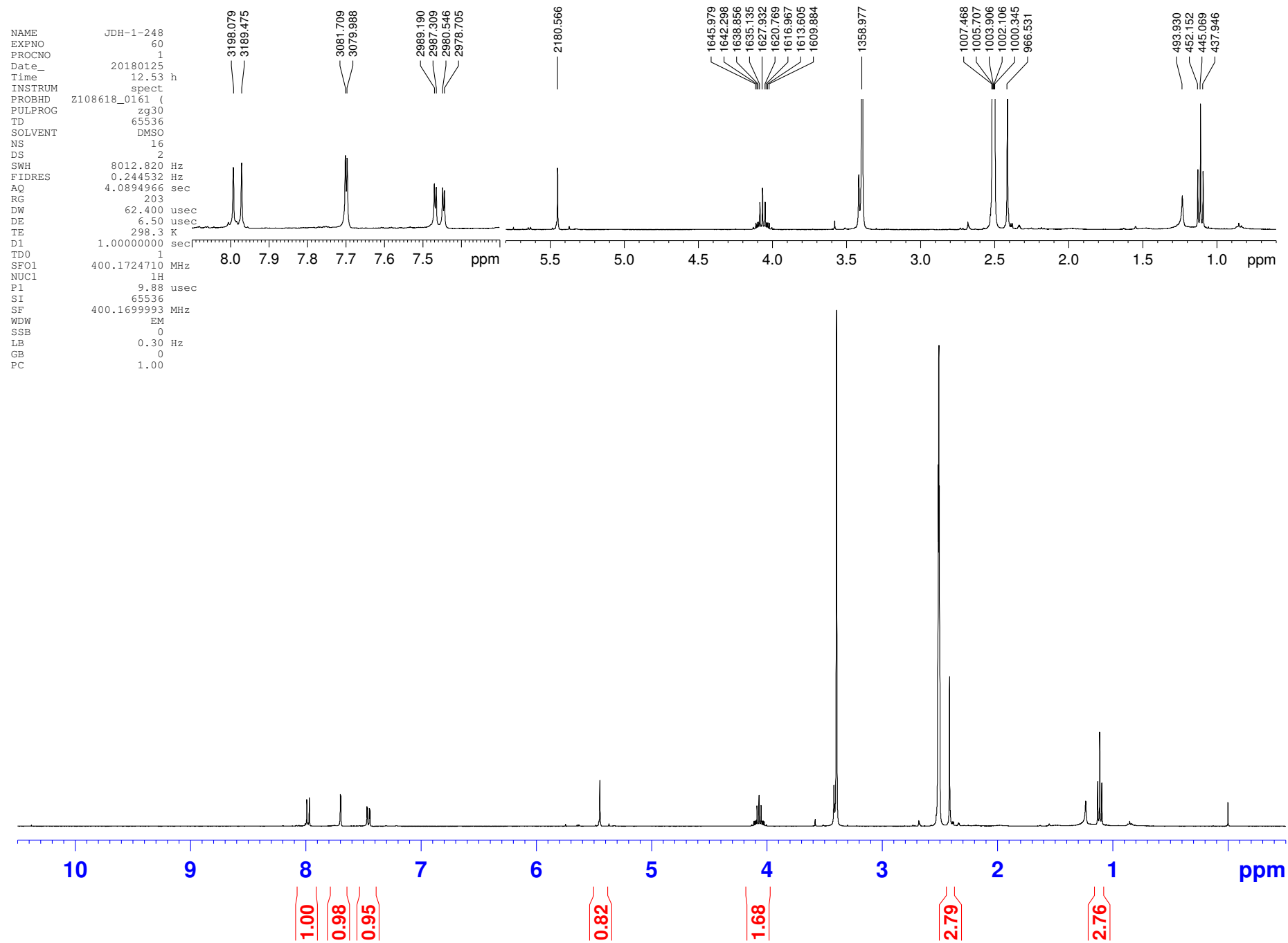


16

2-(7-bromo-4-chloro-2-methylquinolin-3-yl)-2-((trimethylsilyl)oxy)acetonitrile



JDH-1-251 (400MHz, DMSO) Cyanide Hydrolysis



JDH-1-248 (400Mhz, DMSO)
1 drop D2O

NAME JDH-1-248
EXPNO 71
PROCNO 1
Date_ 20180125
Time 21.50 h
INSTRUM spect
PROBHD Z108618_0161 (
PULPROG deptgpgsp
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
D16 0.00020000 sec
TD0 1
SF01 100.6328888 MHz
NUC1 13C
P1 8.40 usec
P13 2000.00 usec
SI 32768
SF 100.6228270 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

174.925
173.804

149.534

140.439

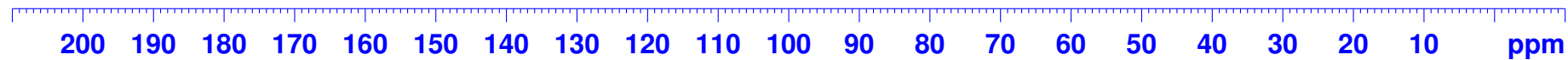
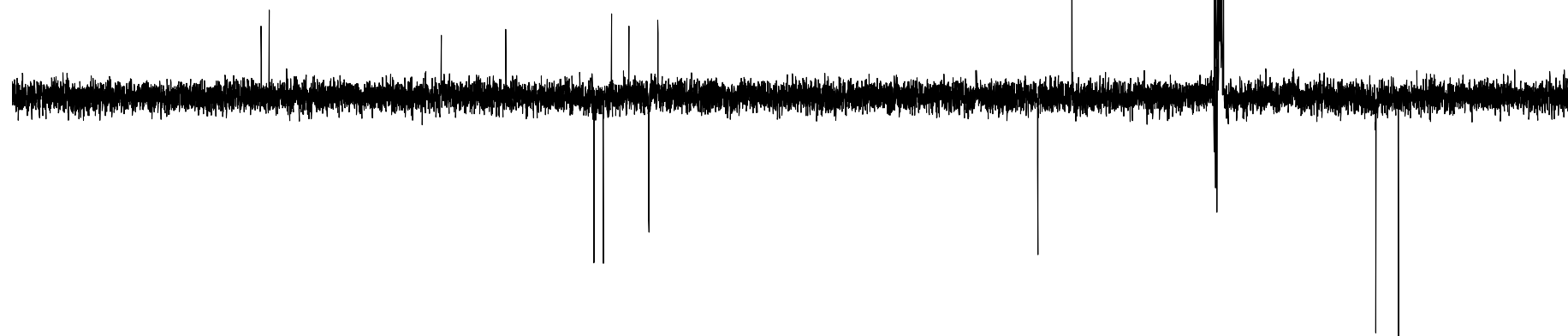
128.001
126.678
125.537
123.087
120.279
118.990

65.421

60.627

40.567
40.361
40.152

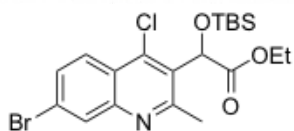
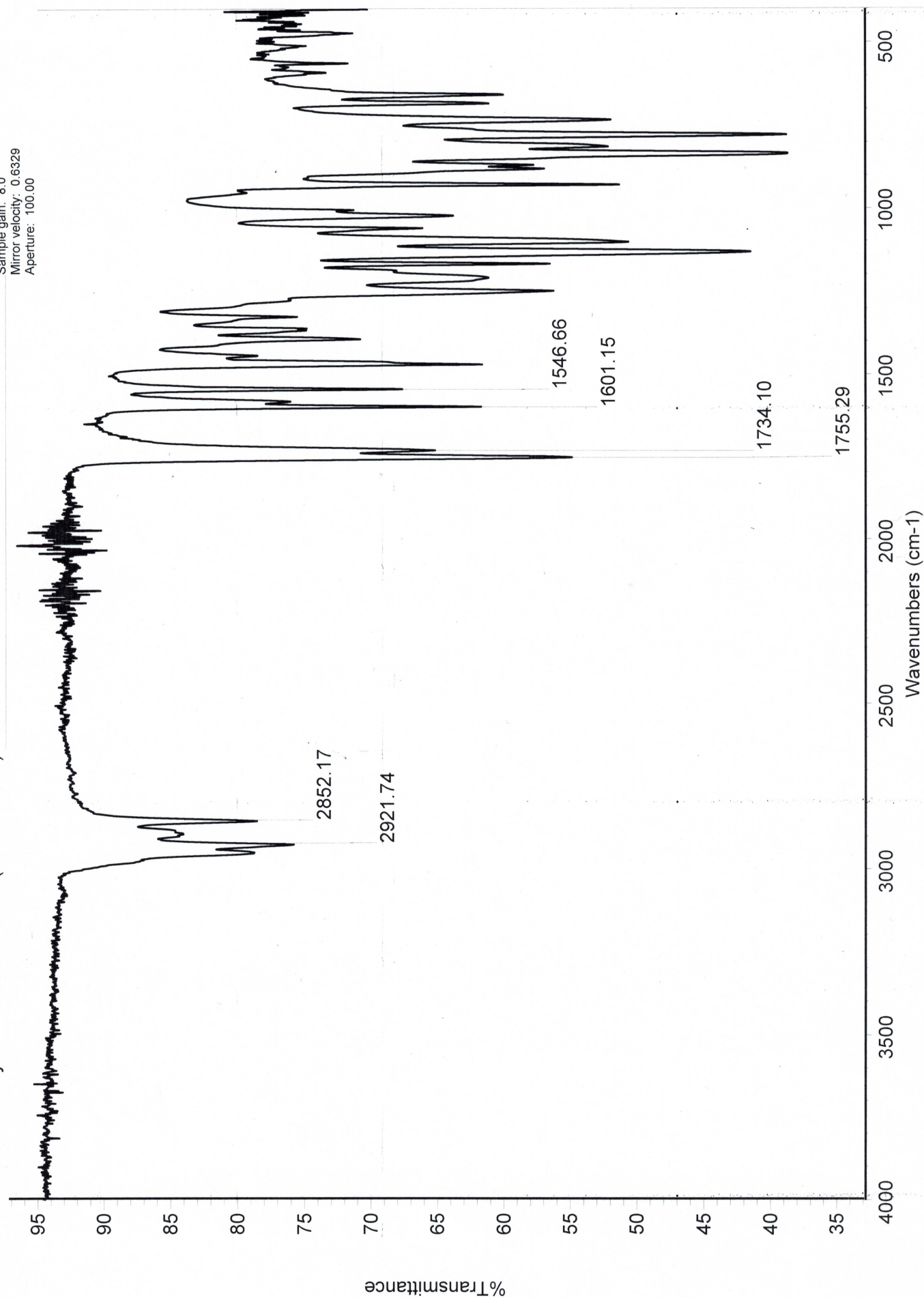
17.761
14.573



NGJ-9-057

Collection time: Thu May 31 10:55:49 2018 (GMT-06:00)

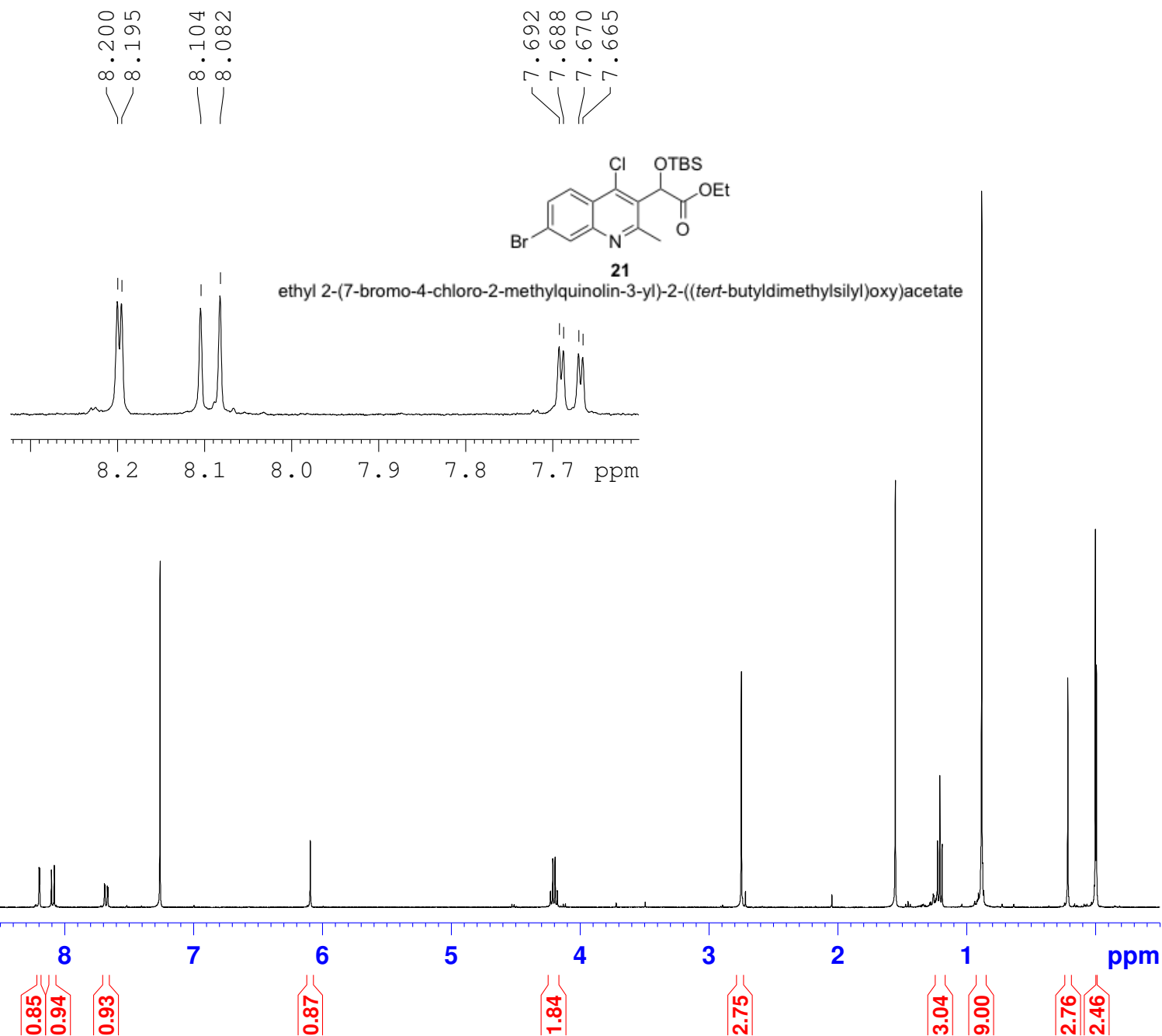
Number of sample scans: 32
Number of background scans: 8
Resolution: 2.000
Sample gain: 8.0
Mirror velocity: 0.6329
Aperture: 100.00



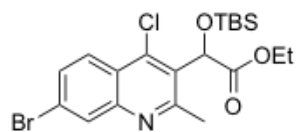
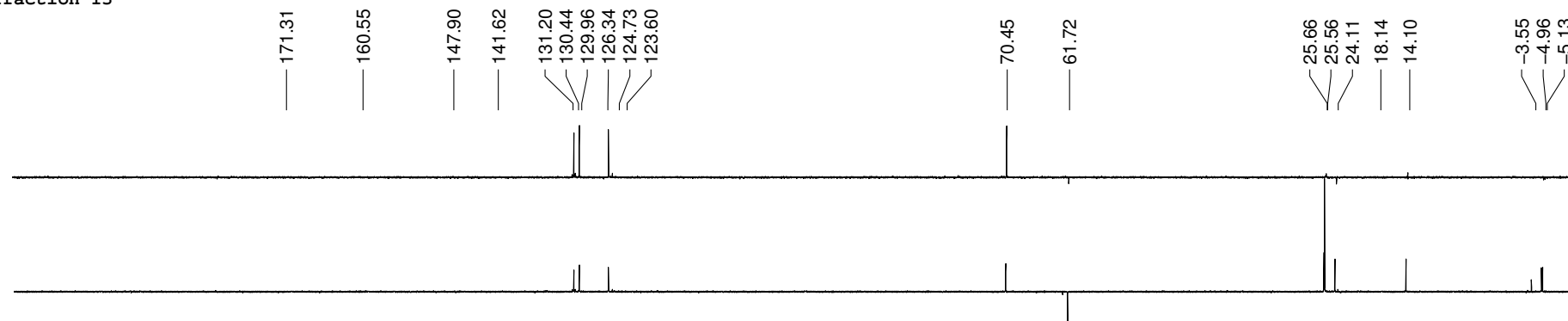
21

ethyl 2-(7-bromo-4-chloro-2-methylquinolin-3-yl)-2-((tert-butyldimethylsilyl)oxy)acetate

NAME	NGJ-9-057
EXPNO	40
PROCNO	1
Date_	20180417
Time	17.47 h
INSTRUM	spect
PROBHD	Z108618_0161 (
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8012.820 Hz
FIDRES	0.244532 Hz
AQ	4.0894966 sec
RG	203
DW	62.400 usec
DE	6.50 usec
TE	298.1 K
D1	1.00000000 sec
TD0	1
SFO1	400.1724710 MHz
NUC1	1H
P1	9.88 usec
SI	65536
SF	400.1700096 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

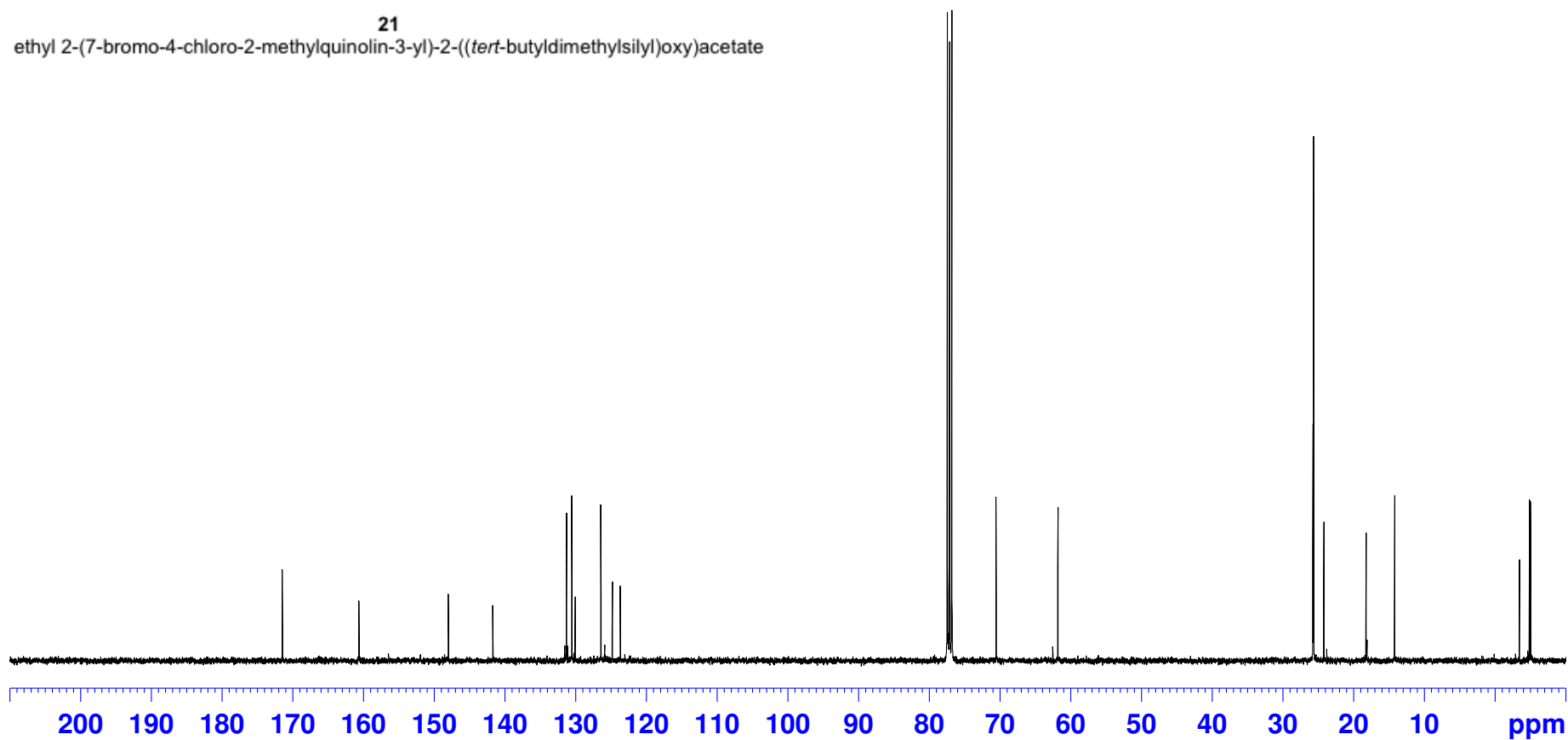


NGJ-9-057-2 (CDCl₃, 400 MHz) Crude Yellow Oil - MAC acylation
fraction 13

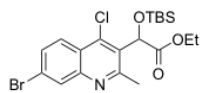


21

ethyl 2-(7-bromo-4-chloro-2-methylquinolin-3-yl)-2-((*tert*-butyldimethylsilyl)oxy)acetate

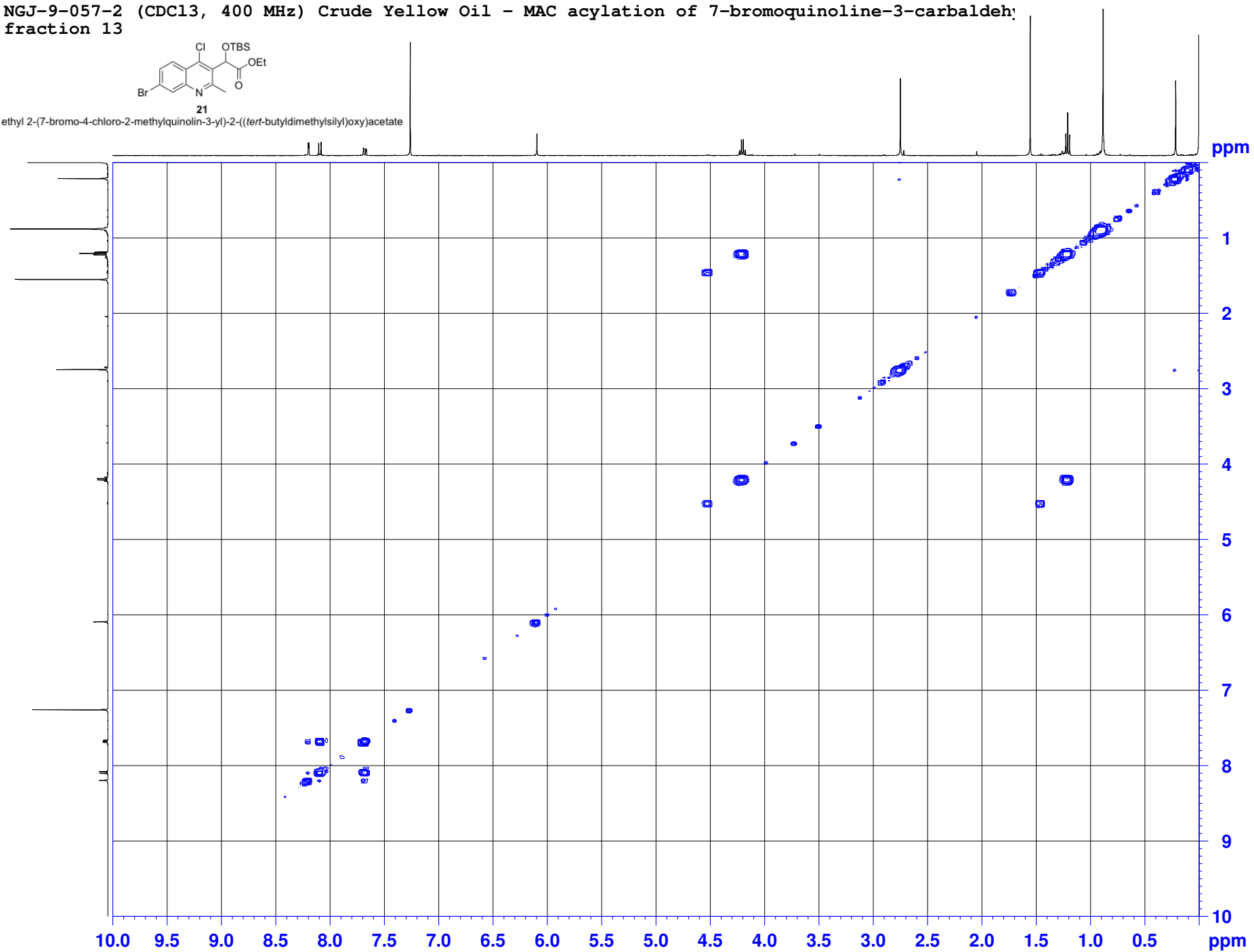


NGJ-9-057-2 (CDCl₃, 400 MHz) Crude Yellow Oil - MAC acylation of 7-bromoquinoline-3-carbaldehyde
fraction 13

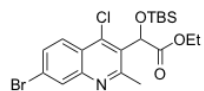


21

ethyl 2-(7-bromo-4-chloro-2-methylquinolin-3-yl)-2-((tert-butyldimethylsilyl)oxy)acetate

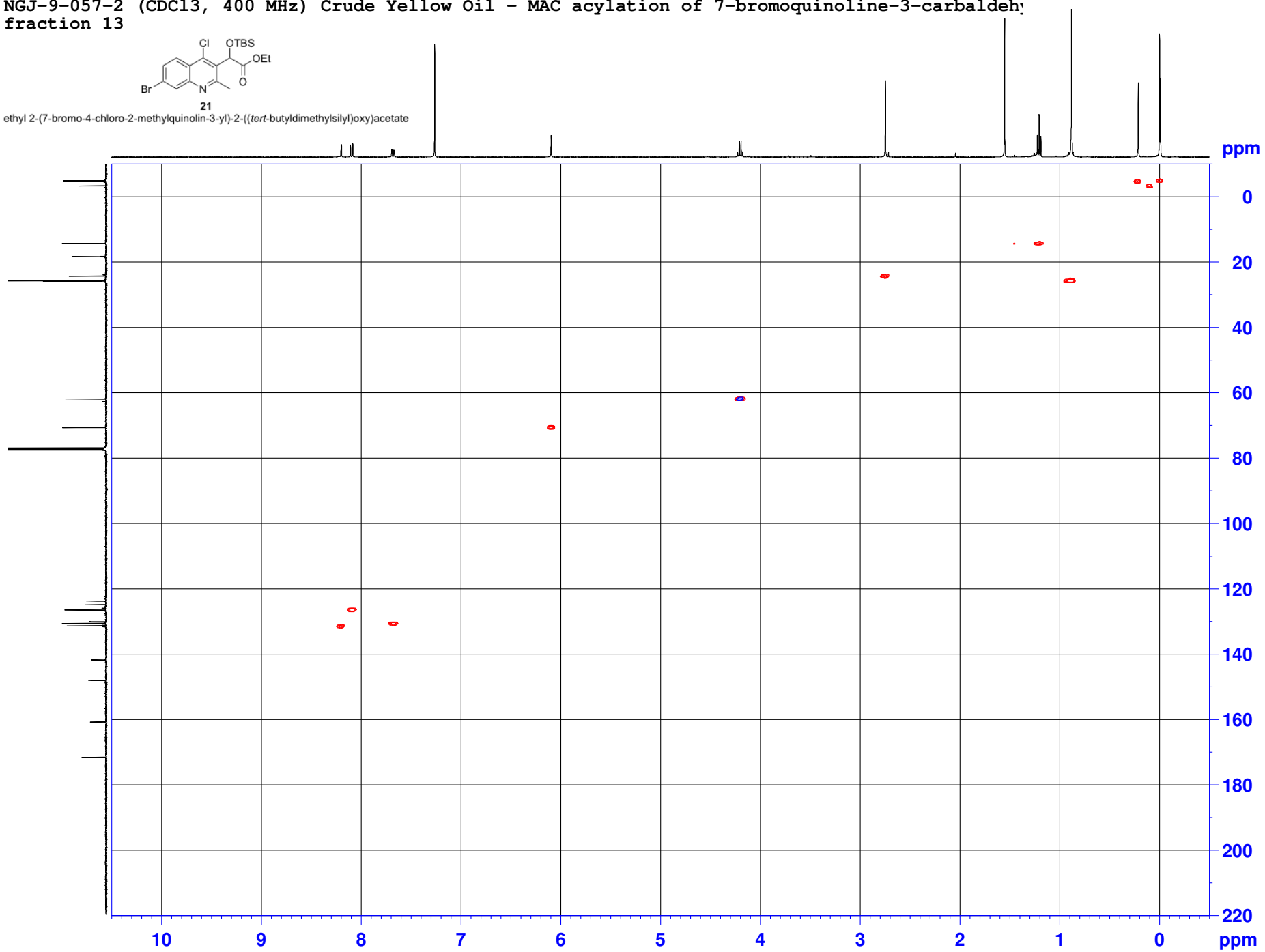


NGJ-9-057-2 (CDCl₃, 400 MHz) Crude Yellow Oil - MAC acylation of 7-bromoquinoline-3-carbaldehyde
fraction 13

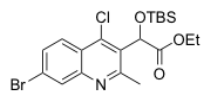


21

ethyl 2-(7-bromo-4-chloro-2-methylquinolin-3-yl)-2-((tert-butyldimethylsilyl)oxy)acetate

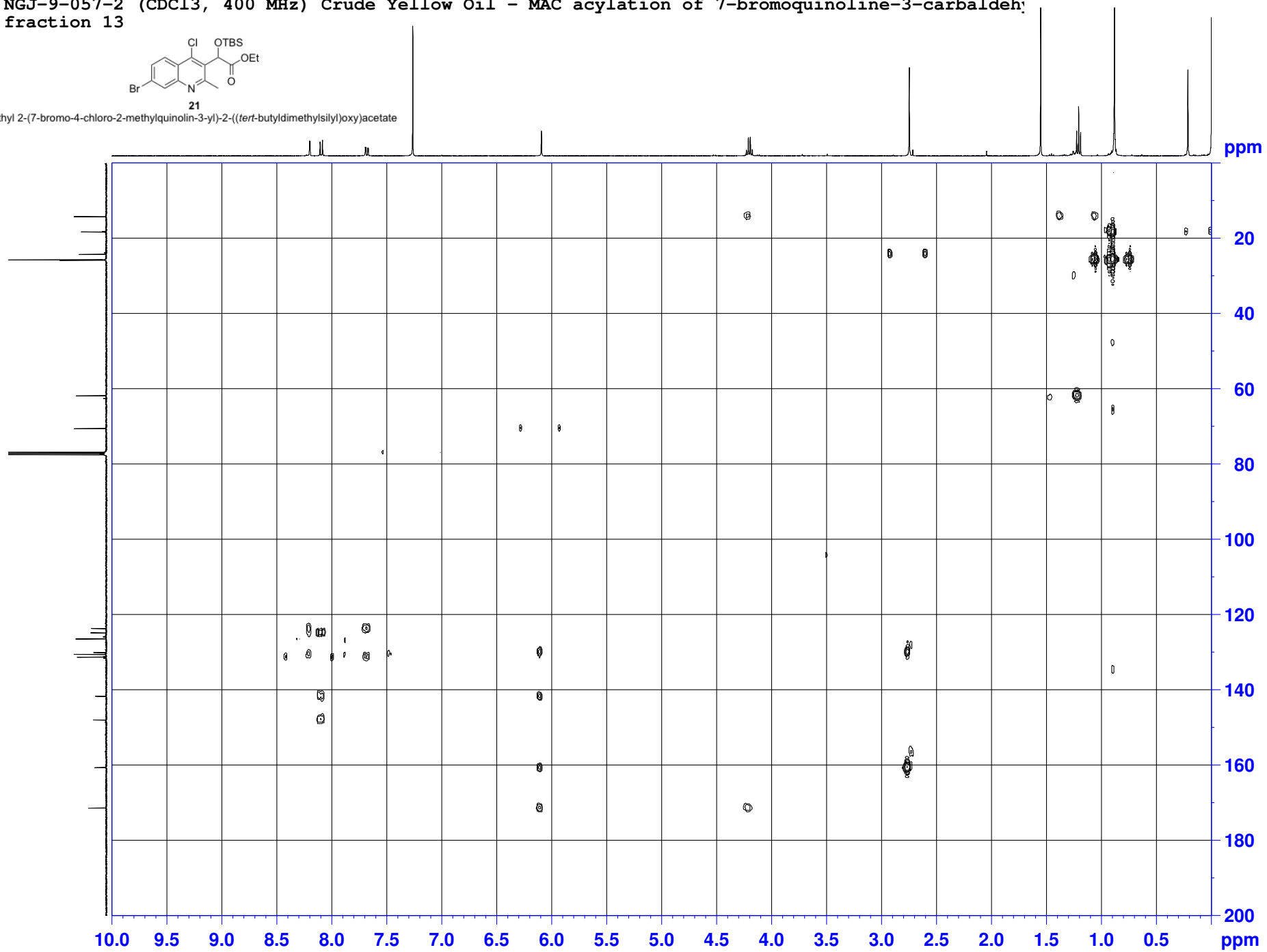


NGJ-9-057-2 (CDCl₃, 400 MHz) Crude Yellow Oil - MAC acylation of 7-bromoquinoline-3-carbaldehyde, fraction 13



21

ethyl 2-(7-bromo-4-chloro-2-methylquinolin-3-yl)-2-((tert-butyldimethylsilyl)oxy)acetate



Mass Spectrum List Report

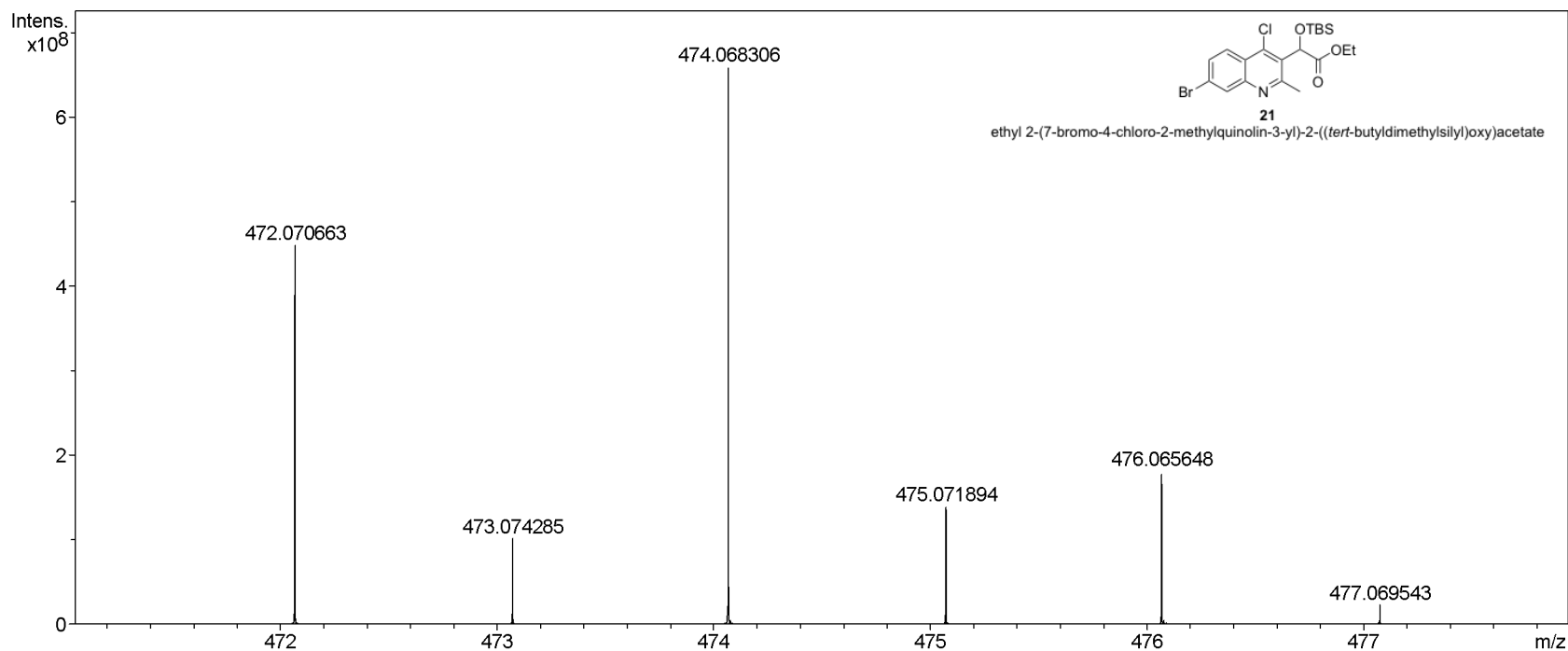
Analysis Info

Analysis Name Y:\FTICR-MS\MS-1\Data\apexdata080818\NGJ-9-057_pos_000001.d
Method
Sample Name NGJ-9-057_pos
Comment NGJ-9-057 in THF:MeOH C20H27BrClNO3Si H+

Acquisition Date 8/8/2018 3:00:04 PM

Operator FTMS_USER
Instrument apex-Qe

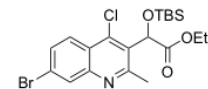
Sample Name NGJ-9-057 in THF:MeOH
Exact Mass of C20H27BrClNO3Si H+ = 472.070487 m/z
Mass Observed with signature = 472.070663 m/z
Difference < 1.0 ppm



#	m/z	I
1	190.060842	559930
2	199.093957	1361850

Mass Spectrum List Report

#	m/z	I
3	199.094212	3484556
4	201.201209	762026
5	208.146237	2155854
6	209.211102	1475350
7	209.441439	1005758
8	213.073487	477454
9	213.109836	3077182
10	214.113235	648390
11	215.089047	50210399
12	216.092507	1136879
13	219.759178	2820643
14	220.397648	2124596
15	221.048875	7251621
16	221.050375	481513
17	221.700567	1991494
18	222.365244	6137447
19	229.104807	803274
20	231.084096	419570
21	231.120410	8383106
22	232.123797	467182
23	236.039870	3146520
24	236.538299	435675
25	237.038775	3110174
26	237.540539	966848
27	238.037416	842051
28	239.125565	689625
29	245.099737	1460158
30	245.136147	2323790
31	247.031340	722875
32	269.136181	1520211
33	271.151875	472870
34	278.175336	468873
35	283.151873	428920
36	284.331432	588899
37	285.131206	479627
38	301.162448	1070012
39	323.019626	760351
40	326.136668	1061107
41	329.989509	638795
42	331.987481	568599
43	340.394218	908874
44	341.971794	587604
45	342.728085	464024
46	354.409874	453281
47	359.984598	1530053

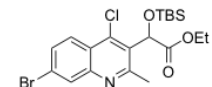


21

ethyl 2-((7-bromo-4-chloro-2-methylquinolin-3-yl)-2-((tert-butyldimethylsilyl)oxy)acetate

Mass Spectrum List Report

#	m/z	I
48	360.324155	1177032
49	361.982626	1422547
50	362.000289	544275
51	363.998262	649441
52	365.136403	1060073
53	365.266652	447018
54	371.163231	486934
55	381.152493	479018
56	383.205014	444477
57	384.181826	2376198
58	392.029701	446806
59	393.298018	1859939
60	394.301396	496430
61	398.241932	5926299
62	399.042148	1461412
63	399.245342	1205158
64	401.040083	1467323
65	403.037058	484499
66	413.212507	1172817
67	413.266908	897233
68	423.199586	704463
69	424.231606	17888989
70	425.231223	1375977
71	425.235006	3136745
72	425.288053	1975274
73	426.228444	1125366
74	428.121617	469070
75	435.345217	3290984
76	436.348501	742900
77	438.110137	539017
78	440.108106	545953
79	441.298184	735791
80	458.055551	2978402
81	459.059020	505067
82	460.053680	2303604
83	462.050630	702086
84	463.303924	1078160
85	472.068324	15427793
86	472.070663	448440529
87	472.071810	29419729
88	472.072365	14076114
89	472.072942	8612050
90	472.073507	5642450
91	472.074093	3969234
92	472.074683	3024082

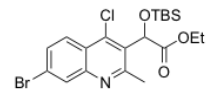


21

ethyl 2-((7-bromo-4-chloro-2-methylquinolin-3-yl)-2-((tert-butyldimethylsilyl)oxy)acetate

Mass Spectrum List Report

#	m/z	I
93	472.075262	2381010
94	472.076428	1576146
95	473.068077	1559512
96	473.071018	12174552
97	473.074285	101574872
98	473.075429	7198936
99	473.075987	3331288
100	473.077784	1314008
101	474.064775	15997150
102	474.066169	19015902
103	474.068306	658811102
104	474.069897	22878430
105	474.070523	13576414
106	474.071093	9314526
107	474.071671	6454494
108	474.072277	4903134
109	474.073999	3498206
110	474.075342	2494686
111	474.077713	4693214
112	475.064961	1516772
113	475.066063	2351332
114	475.067809	3633380
115	475.069252	10743524
116	475.071894	139733220
117	475.073022	9525476
118	475.075595	1458148
119	476.063477	10916074
120	476.065648	180889834
121	476.072556	1646442
122	476.074629	1400298
123	476.075935	4472042
124	476.083110	502890
125	476.087165	1318122
126	477.063076	620783
127	477.066617	3275503
128	477.069543	22653167
129	478.063289	1979124
130	478.073163	1268724
131	478.085223	1158900
132	480.551254	791169
133	481.253391	1180164
134	487.423976	587037
135	494.050312	9177393
136	494.052782	101443889
137	494.053901	8522033

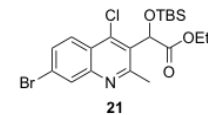


21

ethyl 2-(7-bromo-4-chloro-2-methylquinolin-3-yl)-2-((tert-butyldimethylsilyl)oxy)acetate

Mass Spectrum List Report

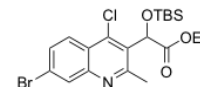
#	m/z	I
138	494.055185	2493745
139	494.566873	507954
140	495.049883	601651
141	495.053671	2520371
142	495.056642	11864371
143	496.047236	7064885
144	496.048232	11149621
145	496.050410	126200117
146	496.051633	10324277
147	496.052227	5118261
148	496.052856	3142965
149	496.056659	800565
150	496.060317	721845
151	497.050642	1680695
152	497.051710	2572087
153	497.053575	3496247
154	497.054654	10318135
155	498.045372	4625721
156	498.048217	21186873
157	498.058161	912697
158	499.048776	1106491
159	499.051774	2846523
160	508.152452	458054
161	508.579519	1792327
162	508.582629	4036935
163	509.582956	660423
164	509.586053	1250631
165	512.046366	448264
166	513.082743	572873
167	515.080551	654793
168	519.439393	1396553
169	520.442694	519881
170	522.598248	1467720
171	523.325163	5754183
172	523.601507	542151
173	524.060491	1121863
174	524.063883	20699463
175	524.328562	1574727
176	524.577632	1171271
177	525.067457	3069255
178	525.377154	778822
179	526.061700	18196806
180	527.065436	2342213
181	528.059063	4463941
182	529.062481	840900



ethyl 2-((7-bromo-4-chloro-2-methylquinolin-3-yl)-2-((tert-butyl(dimethylsilyl)oxy)acetate

Mass Spectrum List Report

#	m/z	I
183	533.455165	1561153
184	534.458586	589632
185	534.598326	860480
186	536.610934	3767102
187	536.613689	27150654
188	537.396008	584381
189	537.614656	1655805
190	537.617306	6846781
191	538.620697	1272380
192	542.488666	494520
193	542.491980	1251896
194	543.495203	478136
195	544.507616	603831
196	550.629599	1304882
197	551.632953	580529
198	552.605312	706992
199	552.608938	3200304
200	553.612311	1204015
201	564.645325	11942187
202	565.648687	4206891
203	566.652038	649643
204	568.109349	463404
205	569.403639	1946412
206	570.407105	570412
207	578.661166	841267
208	580.640377	1391925
209	581.643790	504759
210	590.661064	1014602
211	591.664603	452556
212	592.676665	20035919
213	593.680136	6785362
214	594.683452	1090390
215	599.549729	529639
216	604.630326	585342
217	608.671843	2534292
218	609.675231	993177
219	611.414454	911780
220	613.430033	3255729
221	614.433405	1094071
222	620.708318	1355494
223	621.711654	458095
224	642.631228	855247
225	645.359324	1992946
226	646.362830	504448
227	648.739761	758815

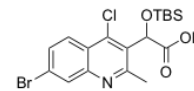


21

ethyl 2-(7-bromo-4-chloro-2-methylquinolin-3-yl)-2-((tert-butyl(dimethyl)silyl)oxy)acetate

Mass Spectrum List Report

#	m/z	I
228	655.441070	1293179
229	657.456549	4540310
230	658.459843	1618852
231	685.431008	1606904
232	685.436979	77376760
233	685.439376	4721912
234	686.440652	30280962
235	687.444219	4273420
236	688.448147	486806
237	699.467193	1097581
238	701.482851	3390840
239	702.486283	1196413
240	732.211387	474199
241	734.209248	566987
242	743.493609	762632
243	745.509300	1919225
244	746.512785	766961
245	789.535706	934728
246	790.539495	574412
247	804.989930	477763
248	806.987375	1088987
249	808.985156	690037
250	875.661084	507747
251	877.676876	655345
252	919.688181	963063
253	920.691435	489844
254	921.703072	1207026
255	963.713587	1094487
256	964.717620	673249
257	965.730236	1302891
258	966.733747	949622
259	1007.741254	1265104
260	1008.744665	772576
261	1009.756928	1146608
262	1010.759627	646911
263	1051.767502	711863
264	1052.771124	566204
265	1053.783609	1036480
266	1054.786882	569668



21
ethyl 2-(7-bromo-4-chloro-2-methylquinolin-3-yl)-2-((tert-butyldimethylsilyl)oxy)acetate