

Electronic Supplementary Information

Application of Suzuki Arylation, Sonogashira Ethynylation, and Rosenmund-von Braun Cyanation in the Exploration of Substitution Effect on Anticancer Activity of 2-Aroylquinolines.

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HPLC purity determination:

The percentage purity of compounds were determined by an Agilent 1100 series HPLC system using C18 column.

Elution conditions: Mobile phase A-Acetonitrile; Mobile phase B-Water containing 0.1% formic acid + 10 mmol NH₄OAc. The flow-rate was 0.2 ml/min and the injection volume was 5 µl. The system operated at 25 °C. Peaks were detected at 210 nm.

Table 1. Elution condition

Time (min)	Mobile Phase A (ratio)	Mobile Phase B (ratio)
0	10	90
45	90	10
50	10	90
60	10	90

Table 2. Purity of compounds **6-12**

C18 column: Agilent ZORBAX Eclipse XDB-C18 5µm. 4.6 mm × 150 mm column

Compounds	Retention time (min)	% Purity
6	34.94	99.82
7	36.37	100.00
8	21.43	95.42
9	33.16	99.87
10	30.61	100.00
11	33.77	92.67
12	43.40	98.50
13	39.96	98.72
14	44.51	100.00
15	45.18	99.85
16	42.80	100.00

HRMS data for compound 6

[Elemental Composition]

Data : 200906649 Date : 15-Oct-2009 10:58
Sample: 8-723
Note : -
Inlet : Direct Ion Mode : EI+
RT : 0.74 min Scan#: 33
Elements : C 21/0, H 19/0, O 6/0, N 2/0, S 1/0
Mass Tolerance : 1000ppm, 3mmu if m/z < 3, 5mmu if m/z > 5
Unsaturation (U.S.) : -0.5 - 30.0

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Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
378.1216	100.0	+0.0 / +0.0	14.0	C 21 H 18 O 5 N 2

HRMS data for compound 7

[Elemental Composition]

Data : 201010173 Date : 24-Aug-2010 17:09
Sample: 8-996-2
Note : -
Inlet : Direct Ion Mode : EI+
RT : 1.62 min Scan#: 66
Elements : C 23/0, H 22/0, O 7/0, N 1/0
Mass Tolerance : 1000ppm, 3mmu if m/z < 3, 5mmu if m/z > 5
Unsaturation (U.S.) : -1.0 - 25.0

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Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
377.1263	16.3	-0.2 / -0.1	14.0	C 22 H 19 O 5 N

HRMS data for compound 8

[Elemental Composition]

Data : 201010165 Date : 21-Aug-2010 20:38
Sample: 8-983
Note : -
Inlet : Direct Ion Mode : EI+
RT : 0.21 min Scan#: 12
Elements : C 21/0, H 34/0, O 6/0, N 3/0
Mass Tolerance : 1000ppm, 3mmu if m/z < 3, 5mmu if m/z > 5
Unsaturation (U.S.) : -1.0 - 25.0

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Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
396.1323	62.9	+0.3 / +0.1	13.0	C 21 H 20 O 6 N 2

HRMS data for compound 9

[Elemental Composition]

Data : 200906581 Date : 25-Sep-2009 17:27
Sample: 8-823
Note : -
Inlet : Direct Ion Mode : EI+
RT : 0.79 min Scan#: 38
Elements : C 26/0, H 25/0, O 6/0, N 2/0, I 1/0
Mass Tolerance : 1000ppm, 3mmu if m/z < 3, 5mmu if m/z > 5
Unsaturation (U.S.) : -0.5 - 30.0

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Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
435.1681	100.0	-0.2 / -0.1	14.0	C 25 H 25 O 6 N

HRMS data for compound 10

[Theoretical Ion Distribution] Page: 1
Molecular Formula : C₂₅ H₂₂ O₅ N₂
(m/z 430.1529, MW 430.4601, U.S. 16.0)
Base Peak : 430.1529, Averaged MW : 430.4614(a), 430.4621(w)

m/z	INT.	
430.1529	100.0000	*****
431.1561	29.0611	*****
432.1589	5.0691	***
433.1616	0.6558	
434.1642	0.0682	
435.1668	0.0060	
436.1694	0.0005	

HRMS data for compound 11

[Elemental Composition] Page: 1
Data : 200906578 Date : 25-Sep-2009 17:11
Sample: 8-863
Note : -
Inlet : Direct Ion Mode : EI+
RT : 0.73 min Scan#: 35
Elements : C 26/0, H 24/0, O 6/0, N 1/0, I 1/0
Mass Tolerance : 1000ppm, 3mmu if m/z < 3, 5mmu if m/z > 5
Unsaturation (U.S.) : -0.5 - 30.0

Observed m/z	Int%	Err[ppm / mmu]	U.S. Composition
445.1526	22.0	+0.2 / +0.1	16.0 C 26 H 23 O 6 N

HRMS data for compound 12

[Elemental Composition] Page: 1
Data : 201010168 Date : 24-Aug-2010 16:07
Sample: 8-1024
Note : -
Inlet : Direct Ion Mode : EI+
RT : 0.23 min Scan#: 12
Elements : C 27/0, H 25/0, O 7/0, N 3/0
Mass Tolerance : 1000ppm, 3mmu if m/z < 3, 5mmu if m/z > 5
Unsaturation (U.S.) : -1.0 - 25.0

Observed m/z	Int%	Err[ppm / mmu]	U.S. Composition
459.1681	82.1	-0.3 / -0.1	16.0 C 27 H 25 O 6 N

HRMS data for compound 13

[Elemental Composition] Page: 1
Data : 201010171 Date : 24-Aug-2010 16:33
Sample: 8-1035
Note : -
Inlet : Direct Ion Mode : EI+
RT : 0.79 min Scan#: 44
Elements : C 27/0, H 22/0, O 7/0, N 3/0
Mass Tolerance : 1000ppm, 3mmu if m/z < 3, 5mmu if m/z > 5
Unsaturation (U.S.) : -1.0 - 25.0

Observed m/z	Int%	Err[ppm / mmu]	U.S. Composition
454.1527	4.4	-0.4 / -0.2	18.0 C 27 H 22 O 5 N 2

HRMS data for compound 14

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[Elemental Composition]
Data : 201010169 Date : 24-Aug-2010 16:12
Sample: 8-1034
Note : -
Inlet : Direct Ion Mode : EI+
RT : 1.12 min Scan#: 62
Elements : C 26/0, H 22/0, O 5/0, N 3/0, F 1/0
Mass Tolerance : 1000ppm, 3mmu if m/z < 3, 5mmu if m/z > 5
Unsaturation (U.S.) : -1.0 - 25.0

Observed m/z	Int%	Err [ppm / mmu]	U.S.	Composition
447.1484	100.0	+0.5 / +0.2	16.0	C 26 H 22 O 5 N F

HRMS data for compound 15

Page: 1

[Elemental Composition]
Data : 201010166 Date : 24-Aug-2010 15:44
Sample: 8-1006
Note : -
Inlet : Direct Ion Mode : EI+
RT : 0.99 min Scan#: 50
Elements : C 26/0, H 21/0, O 6/0, N 1/0, F 3/0
Mass Tolerance : 1000ppm, 3mmu if m/z < 3, 5mmu if m/z > 5
Unsaturation (U.S.) : -1.0 - 25.0

Observed m/z	Int%	Err [ppm / mmu]	U.S.	Composition
465.1390	60.0	+0.4 / +0.2	16.0	C 26 H 21 O 5 N F 2

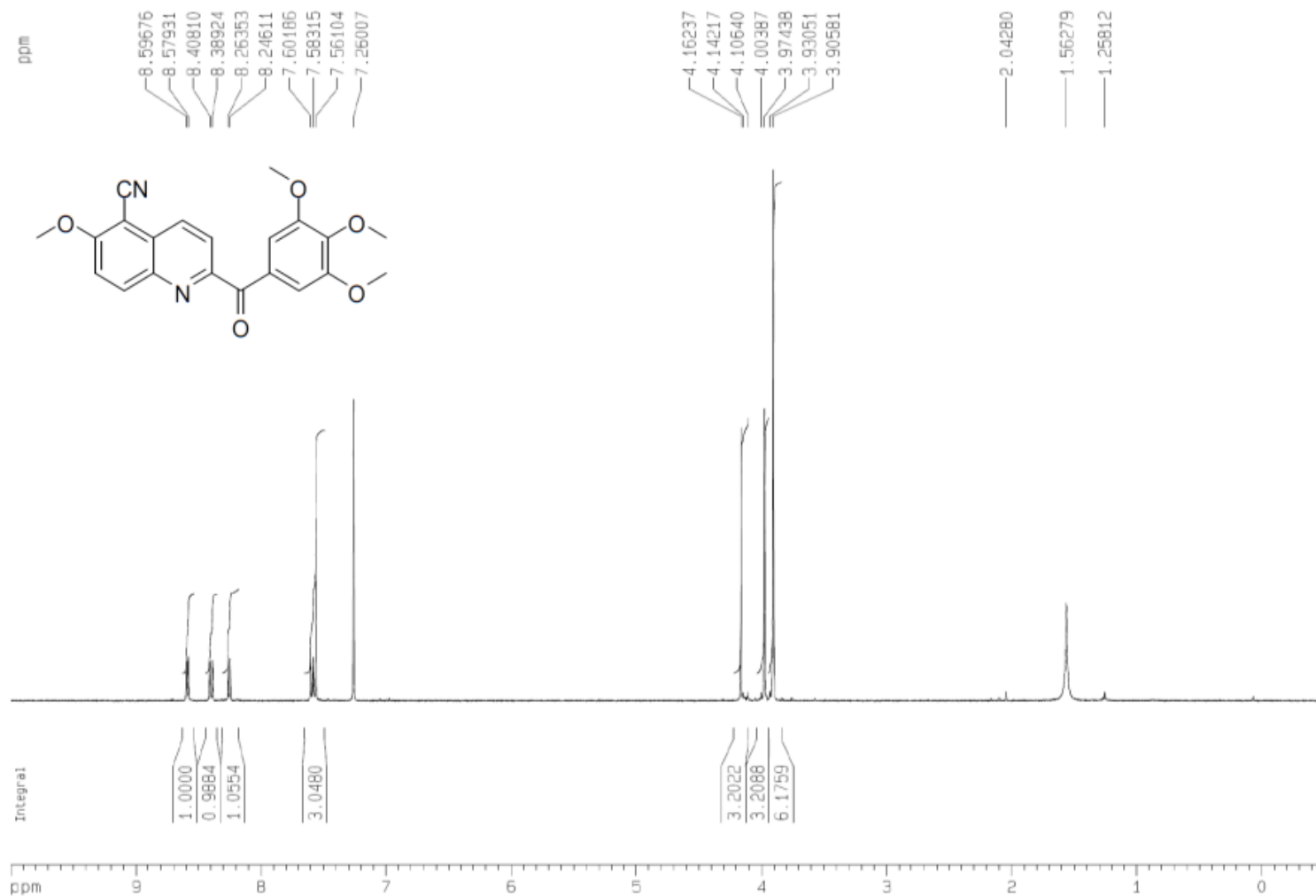
HRMS data for compound 16

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[Elemental Composition]
Data : 201010167 Date : 24-Aug-2010 15:59
Sample: 8-1022
Note : -
Inlet : Direct Ion Mode : EI+
RT : 0.32 min Scan#: 17
Elements : C 26/0, H 22/0, O 7/0, N 3/0
Mass Tolerance : 1000ppm, 3mmu if m/z < 3, 5mmu if m/z > 5
Unsaturation (U.S.) : -1.0 - 25.0

Observed m/z	Int%	Err [ppm / mmu]	U.S.	Composition
474.1426	100.0	-0.3 / -0.1	17.0	C 26 H 22 O 7 N 2

¹H Spectra for compound 6



Current Data Parameters
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EXPNO 1
PROCNO 1

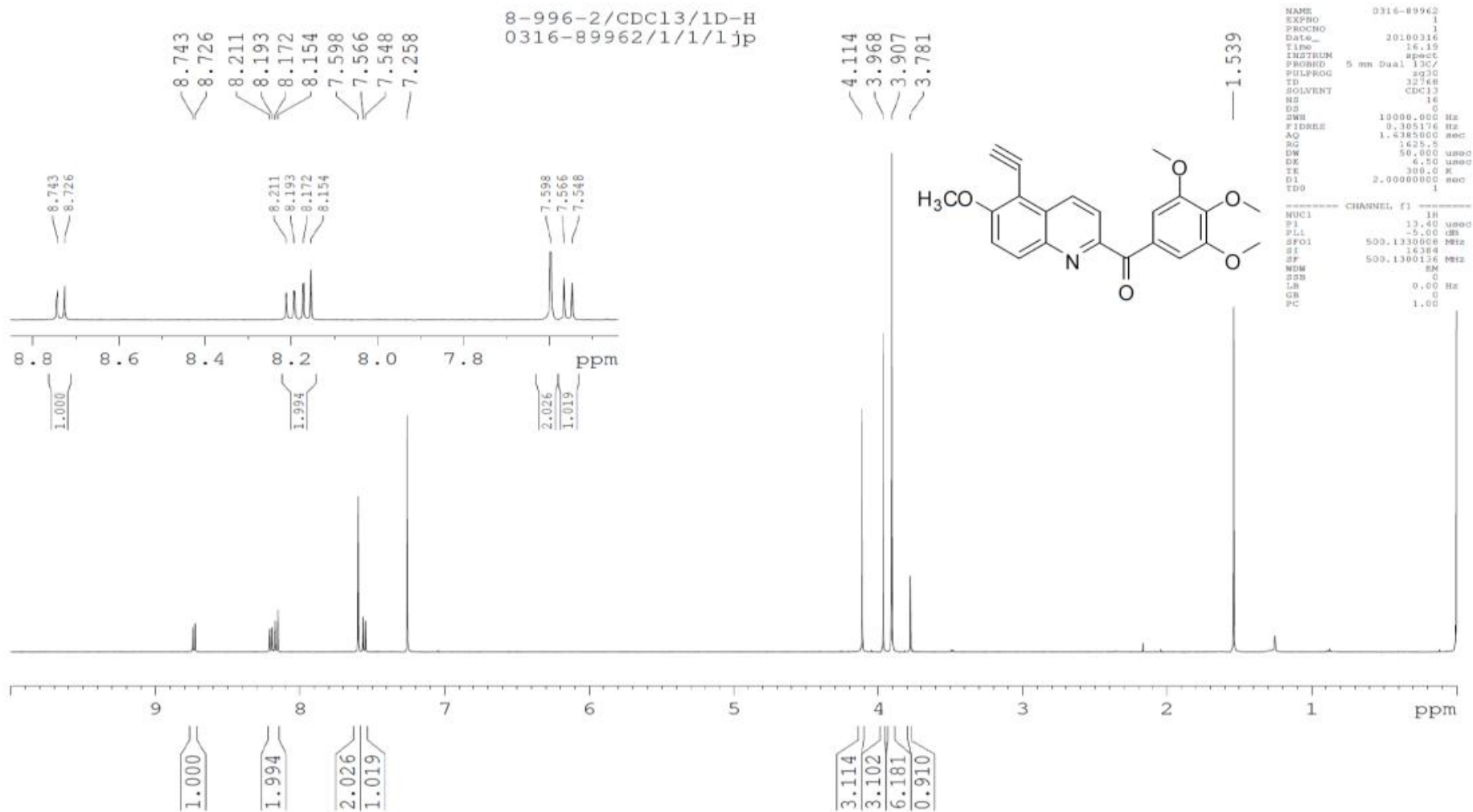
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PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 1.6384500 sec
RG 5792.6
DW 50.000 usec
DE 6.50 usec
TE 300.1 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.70 usec
PL1 -2.00 dB
SF01 500.1330685 MHz

F2 - Processing parameters
SI 16384
SF 500.1300136 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 22.00 cm
CY 10.00 cm
F1P 10.000 ppm
F1 5001.30 Hz
F2P -0.500 ppm
F2 -250.06 Hz
PPMCM 0.47727 ppm/cm
HZCM 238.59839 Hz/cm

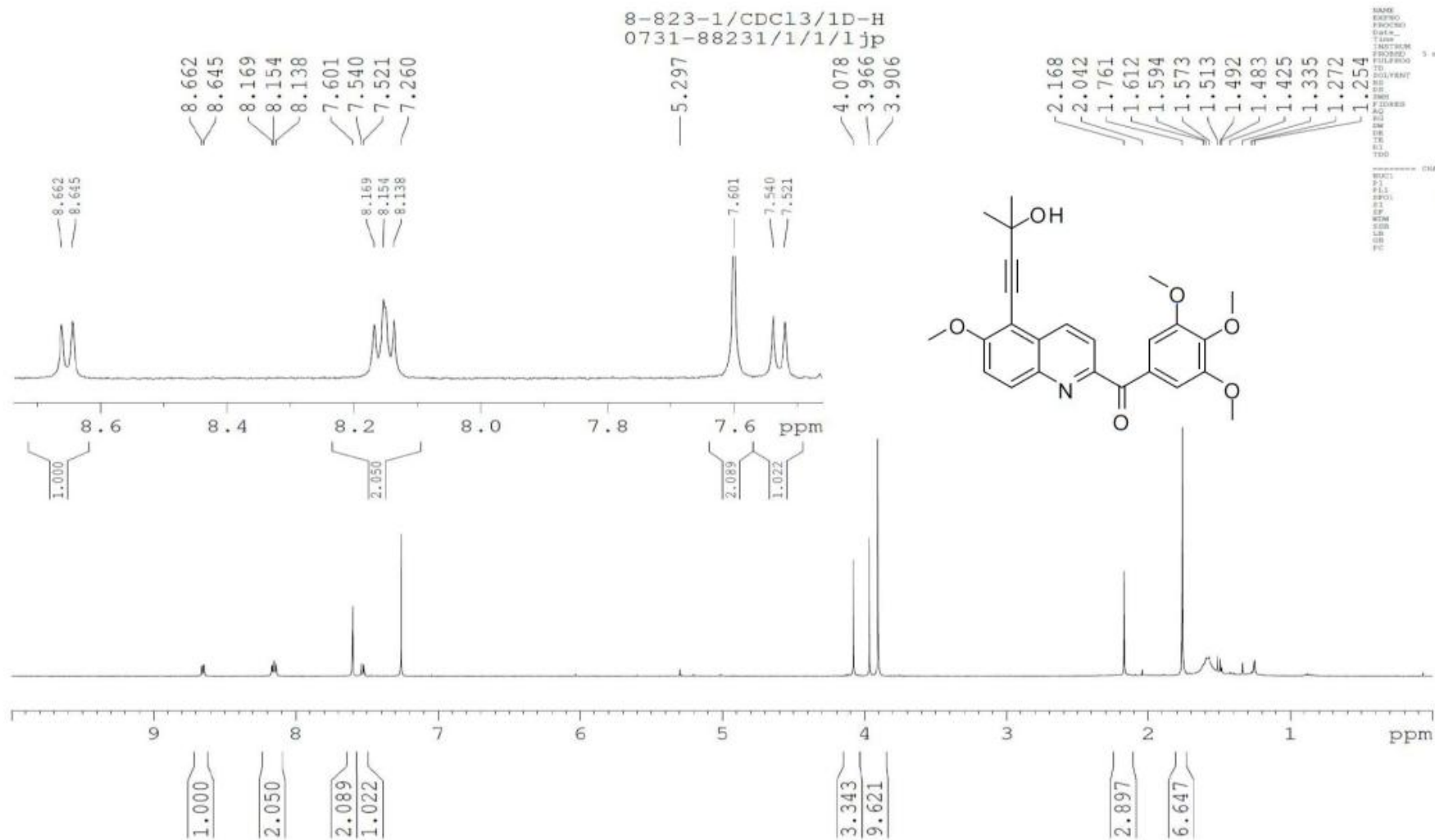
¹H Spectra for compound 7



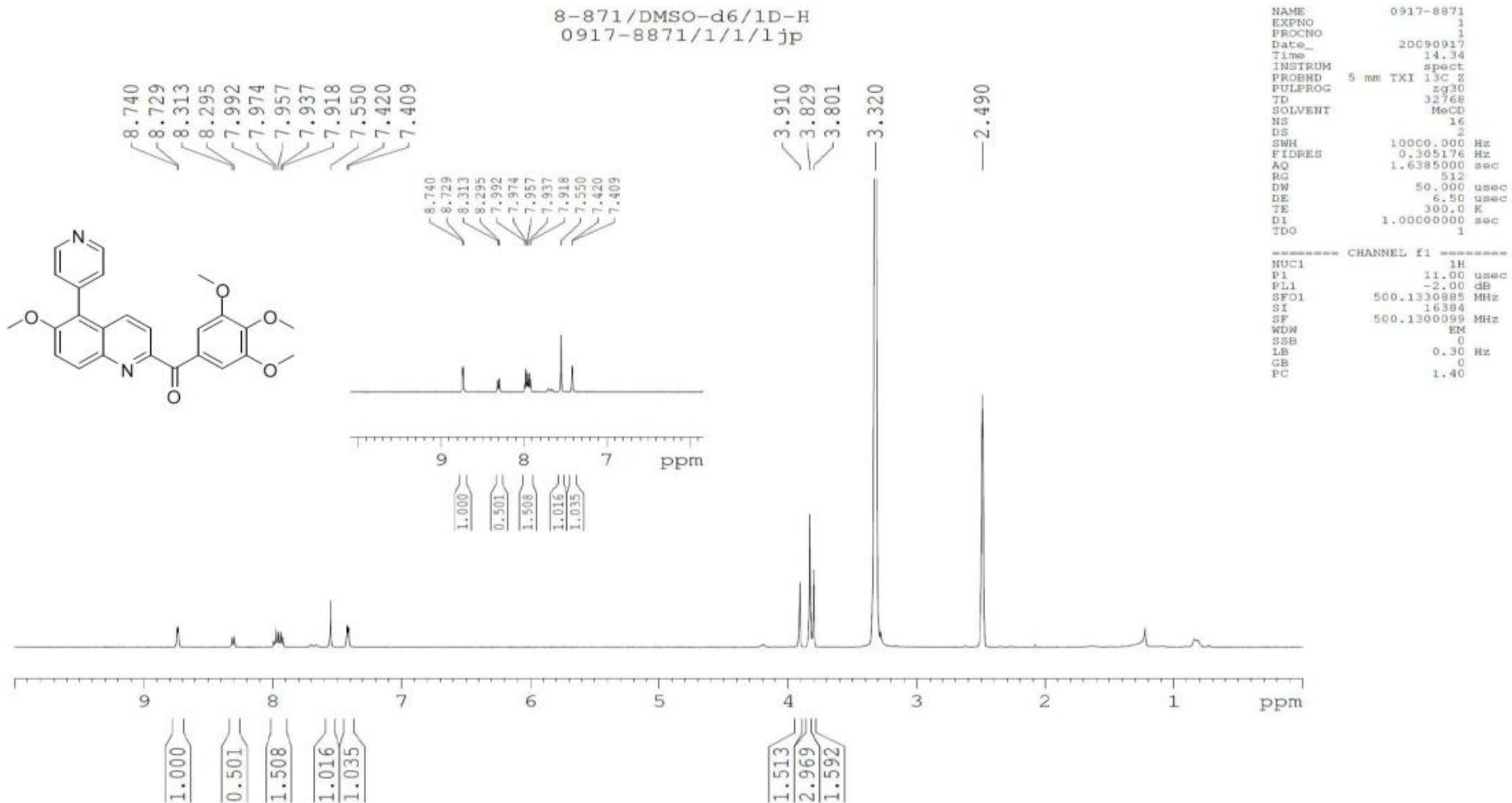
¹H Spectra for compound 8



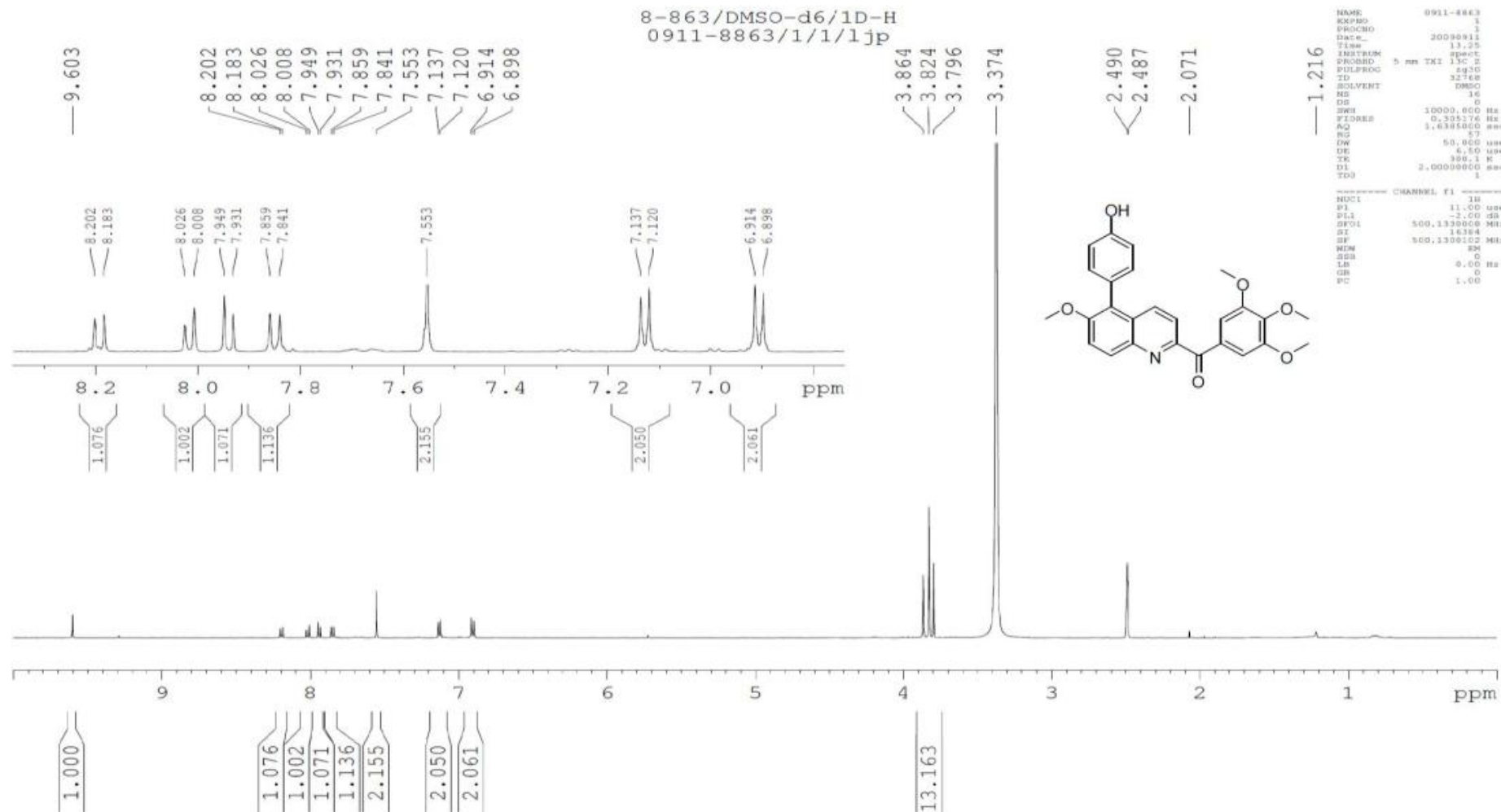
¹H Spectra for compound 9



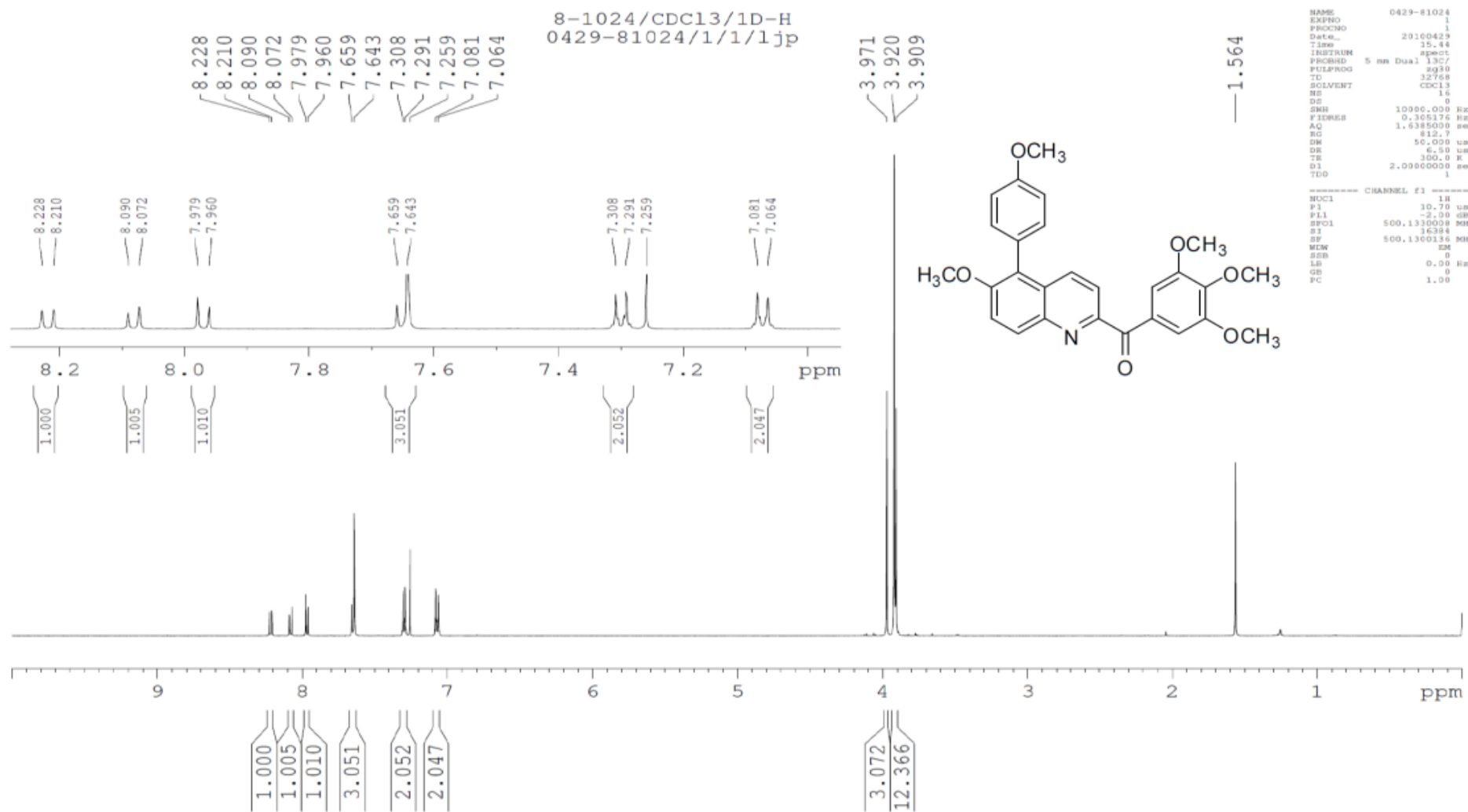
¹H Spectra for compound 10



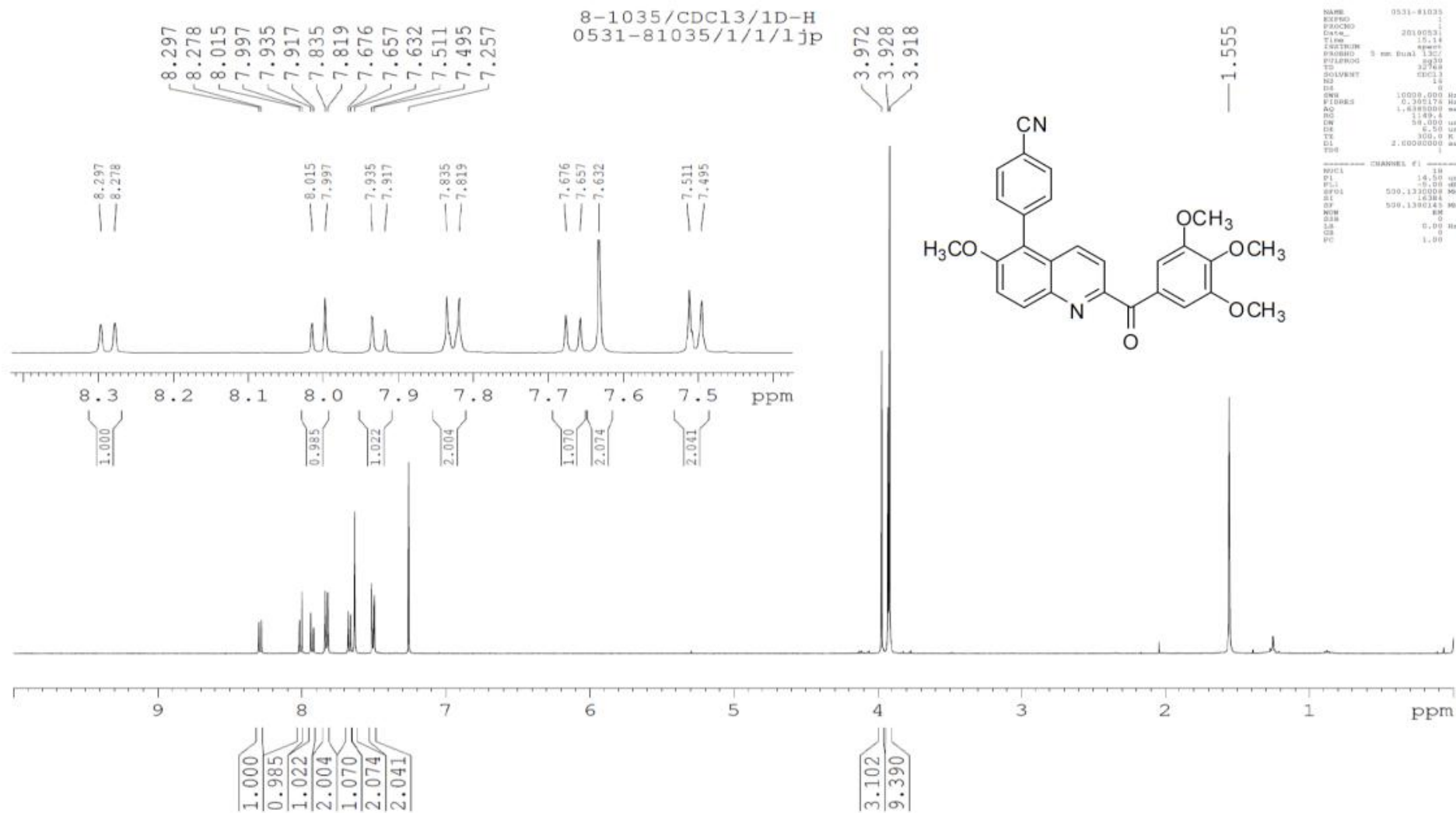
¹H Spectra for compound 11



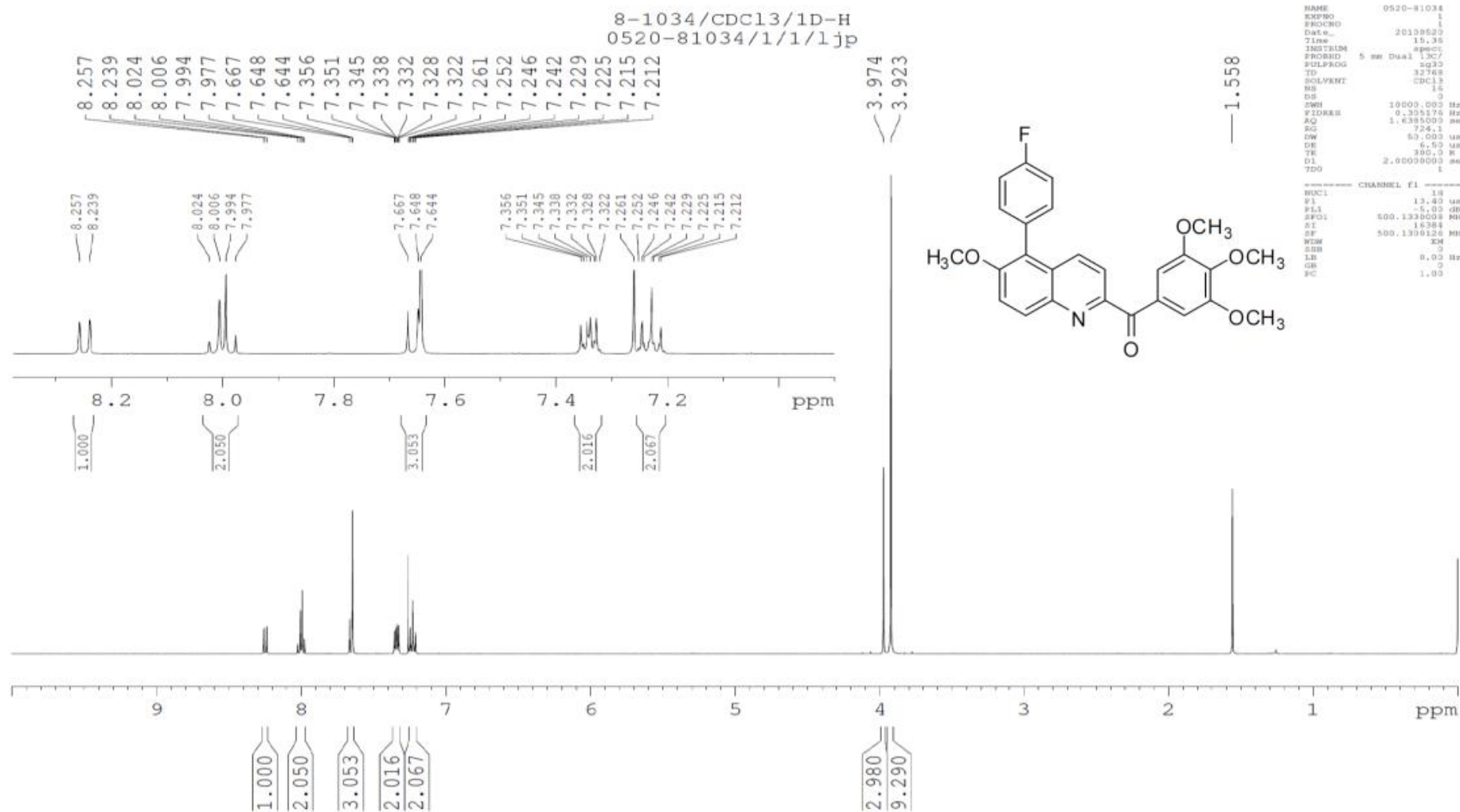
¹H Spectra for compound 12



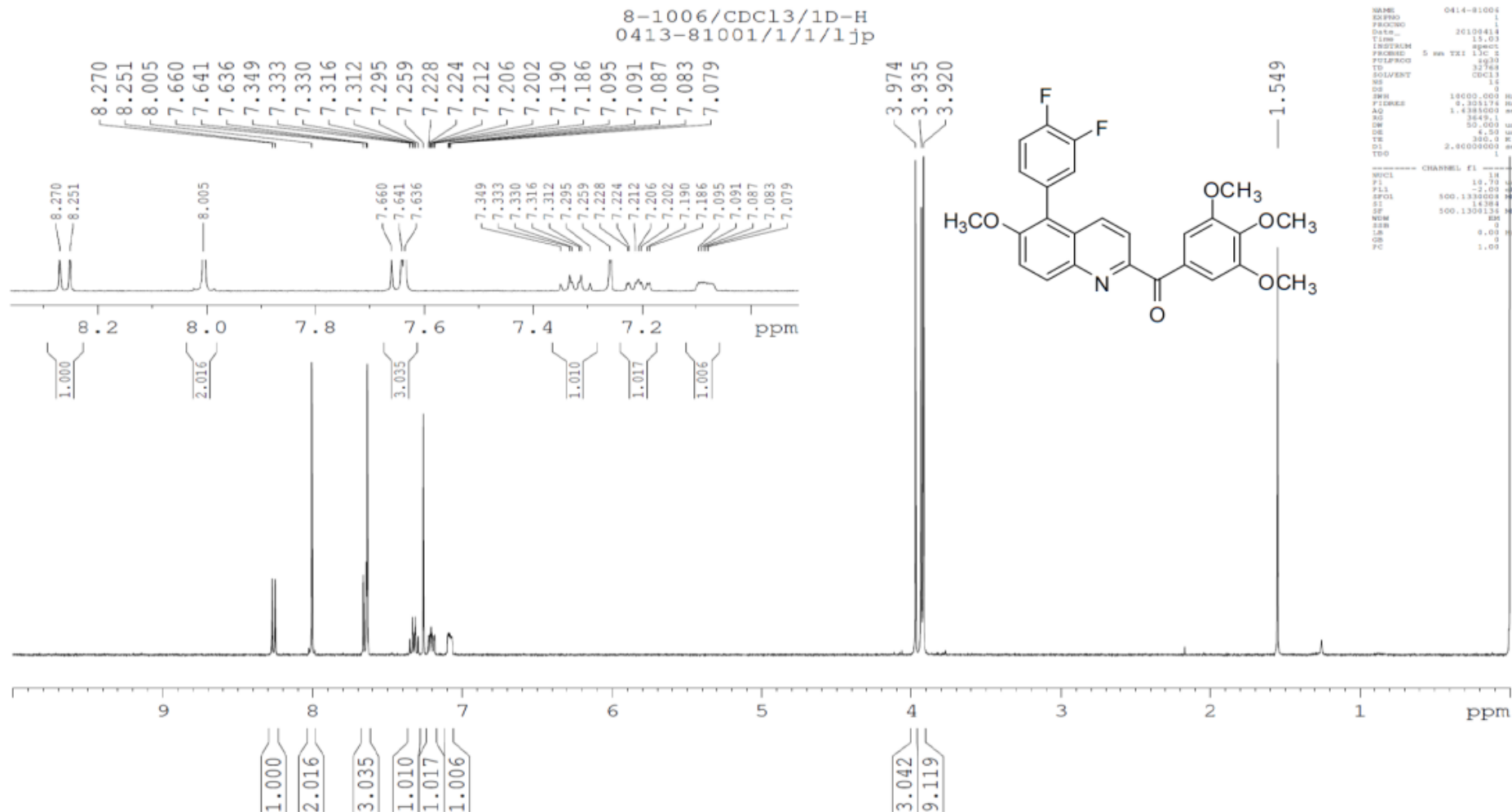
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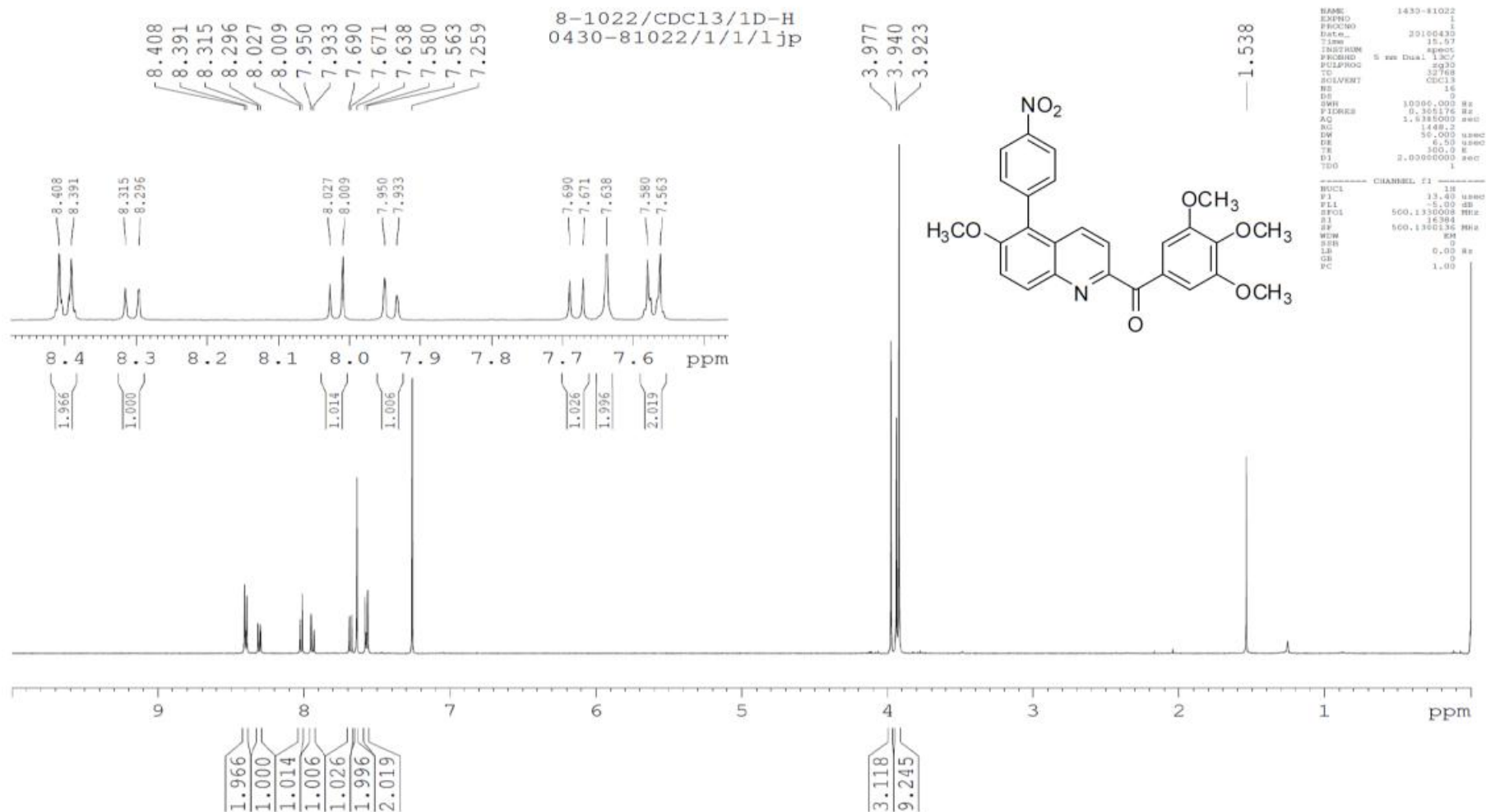
¹H Spectra for compound 14



¹H Spectra for compound 15

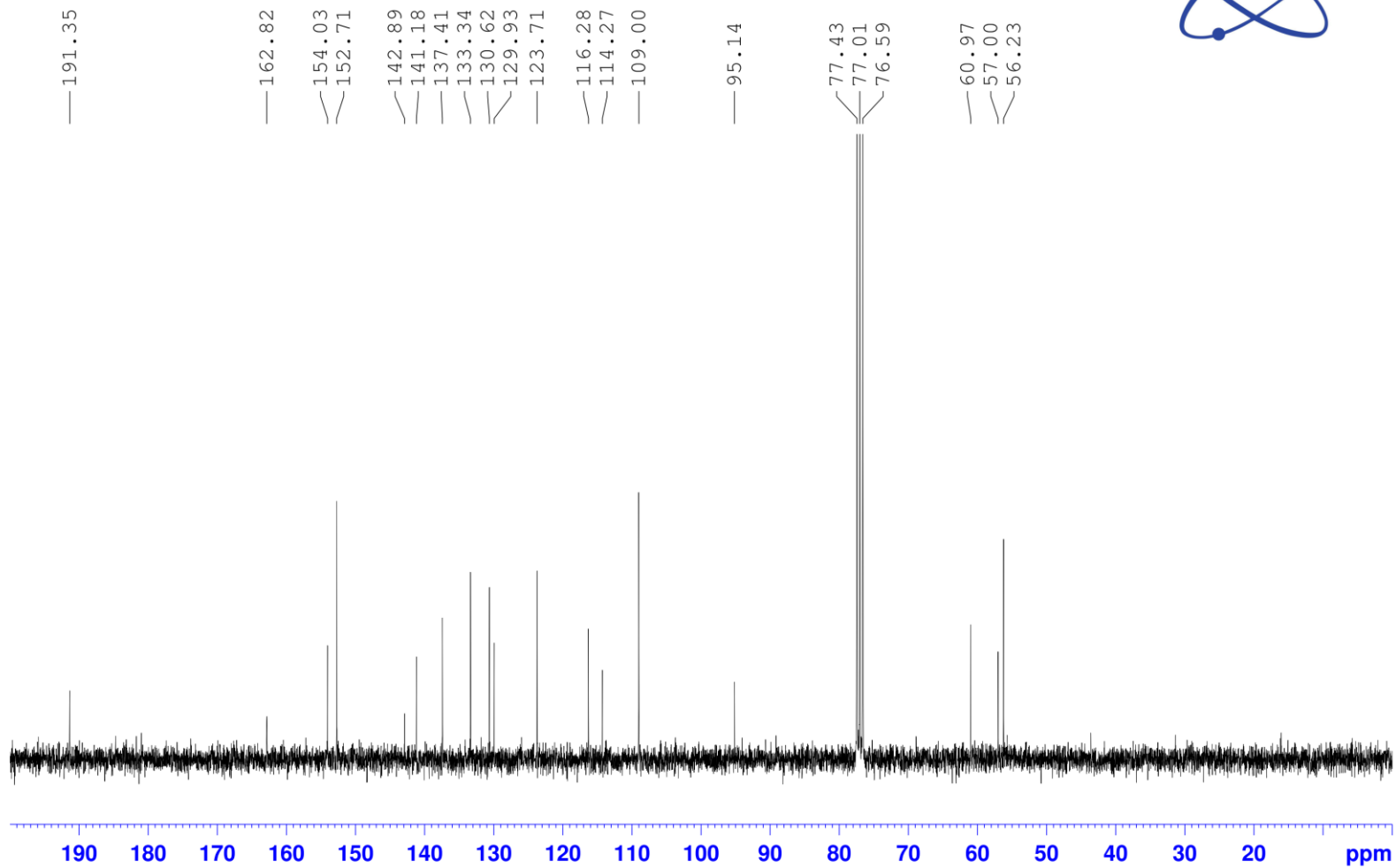


¹H Spectra for compound 16



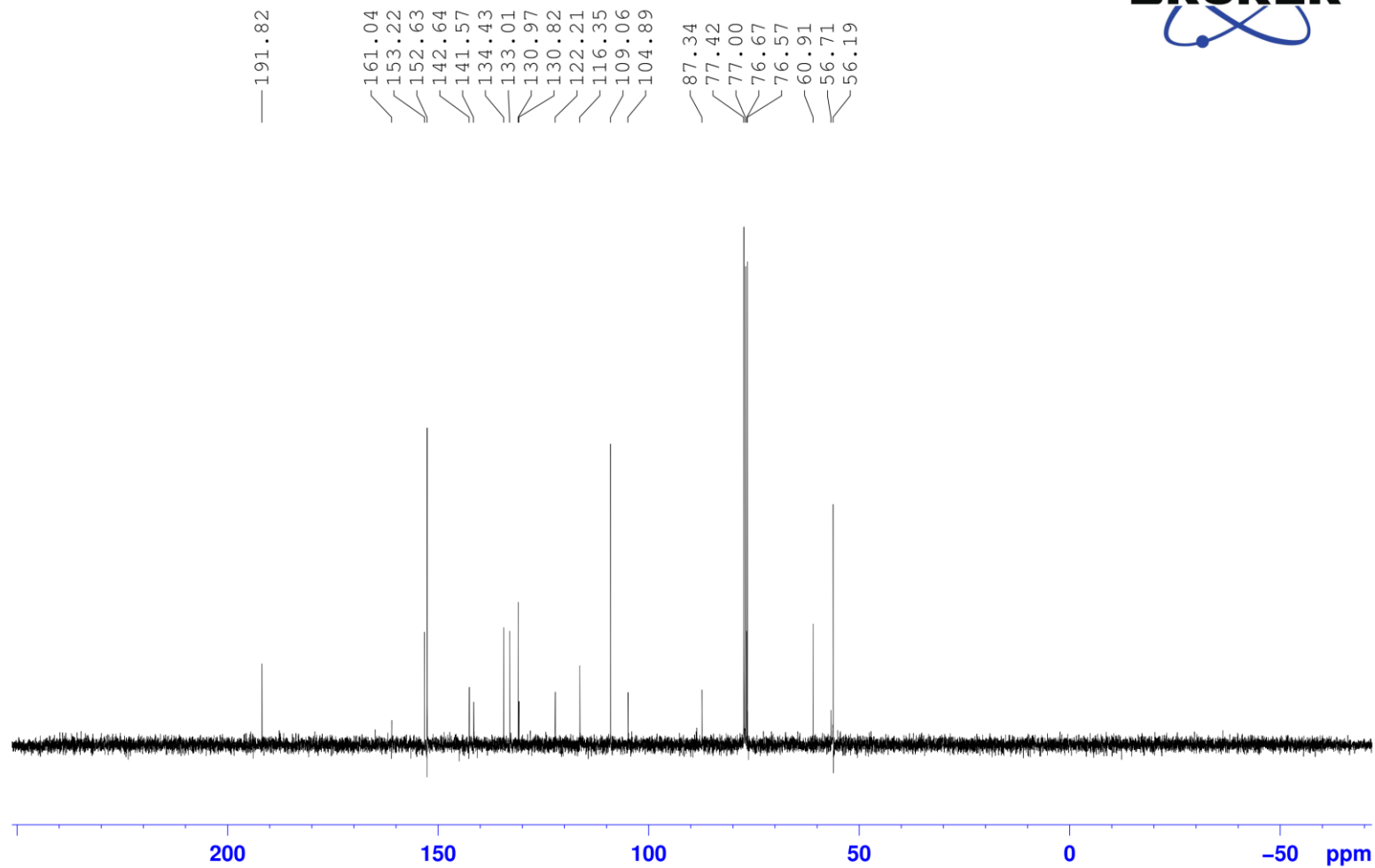
¹³C Spectra for compound 6

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1008-8-723/1/1/1jp



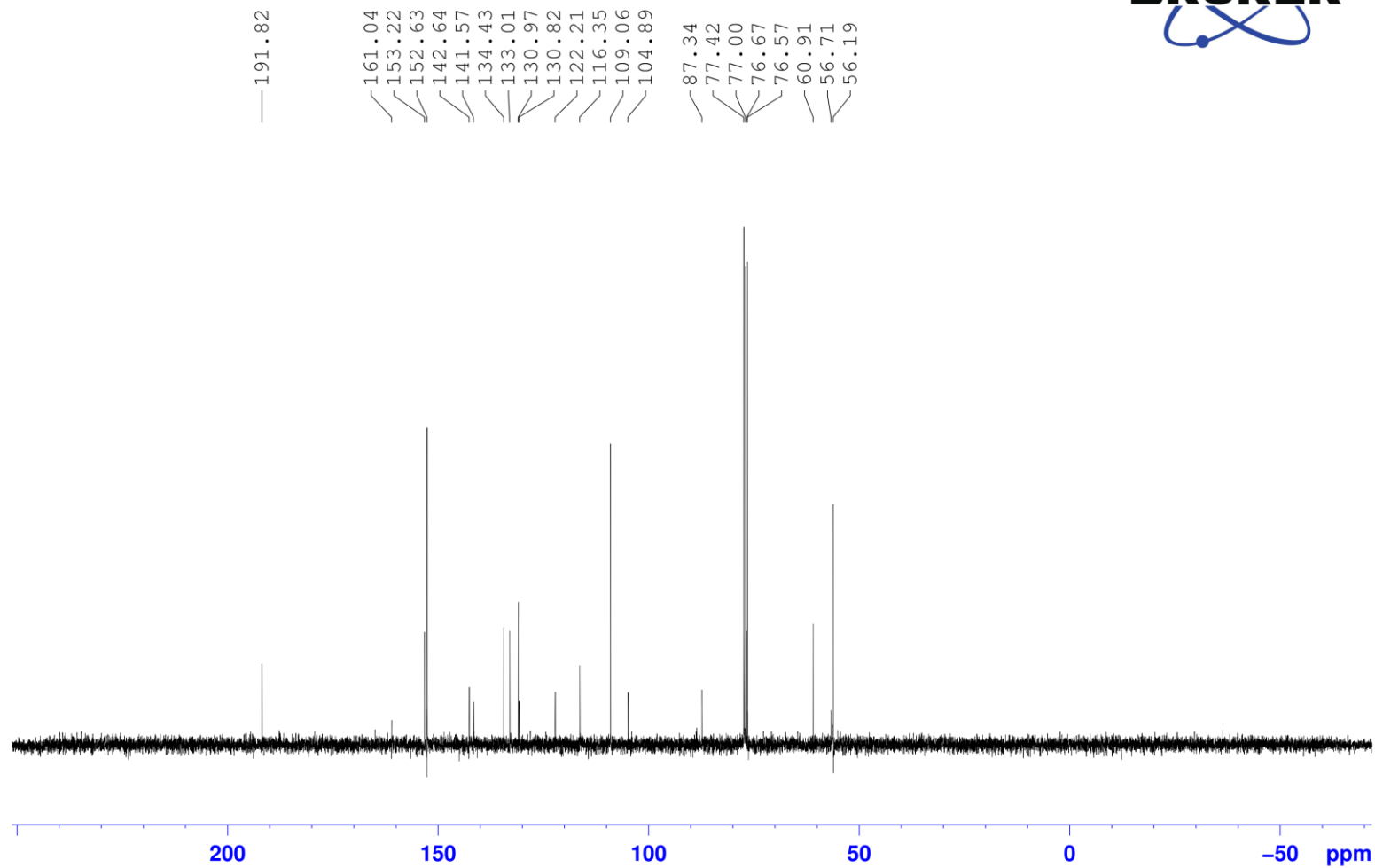
¹³C Spectra for compound 7

1008-8-996-2/CDC13/C13
1008-8-996-2/1/1/1jp



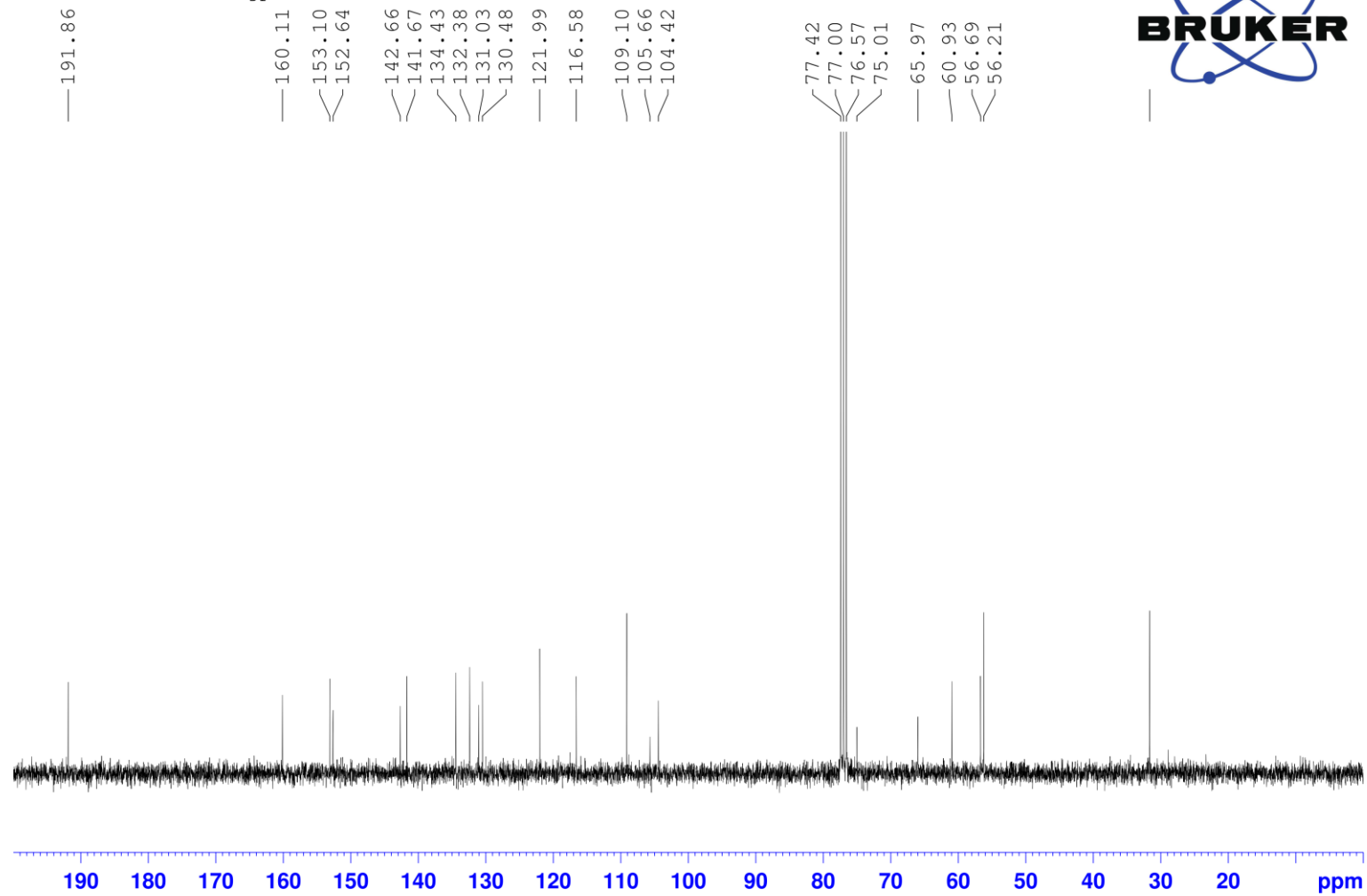
¹³C Spectra for compound 8

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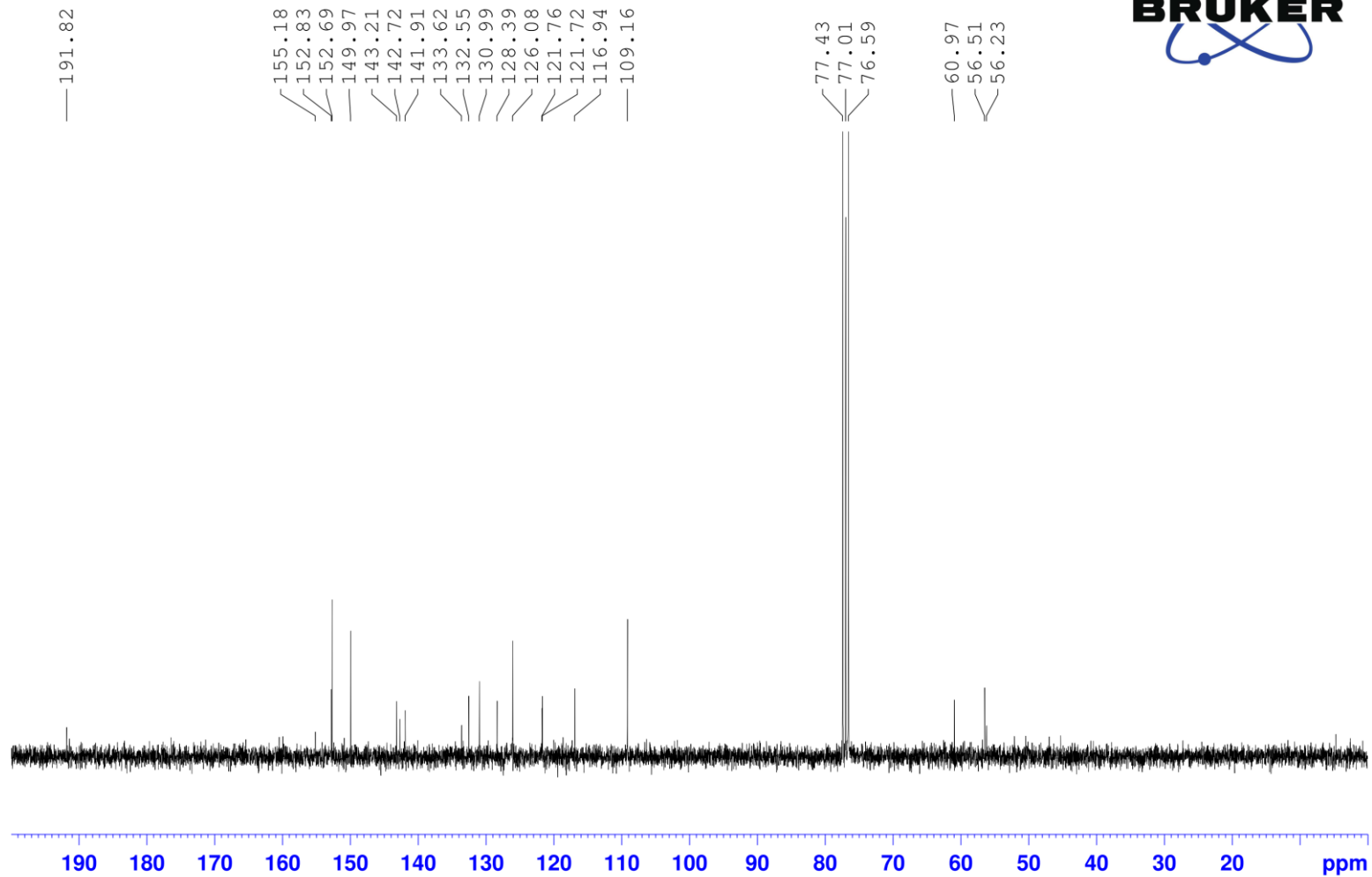
¹³C Spectra for compound 9

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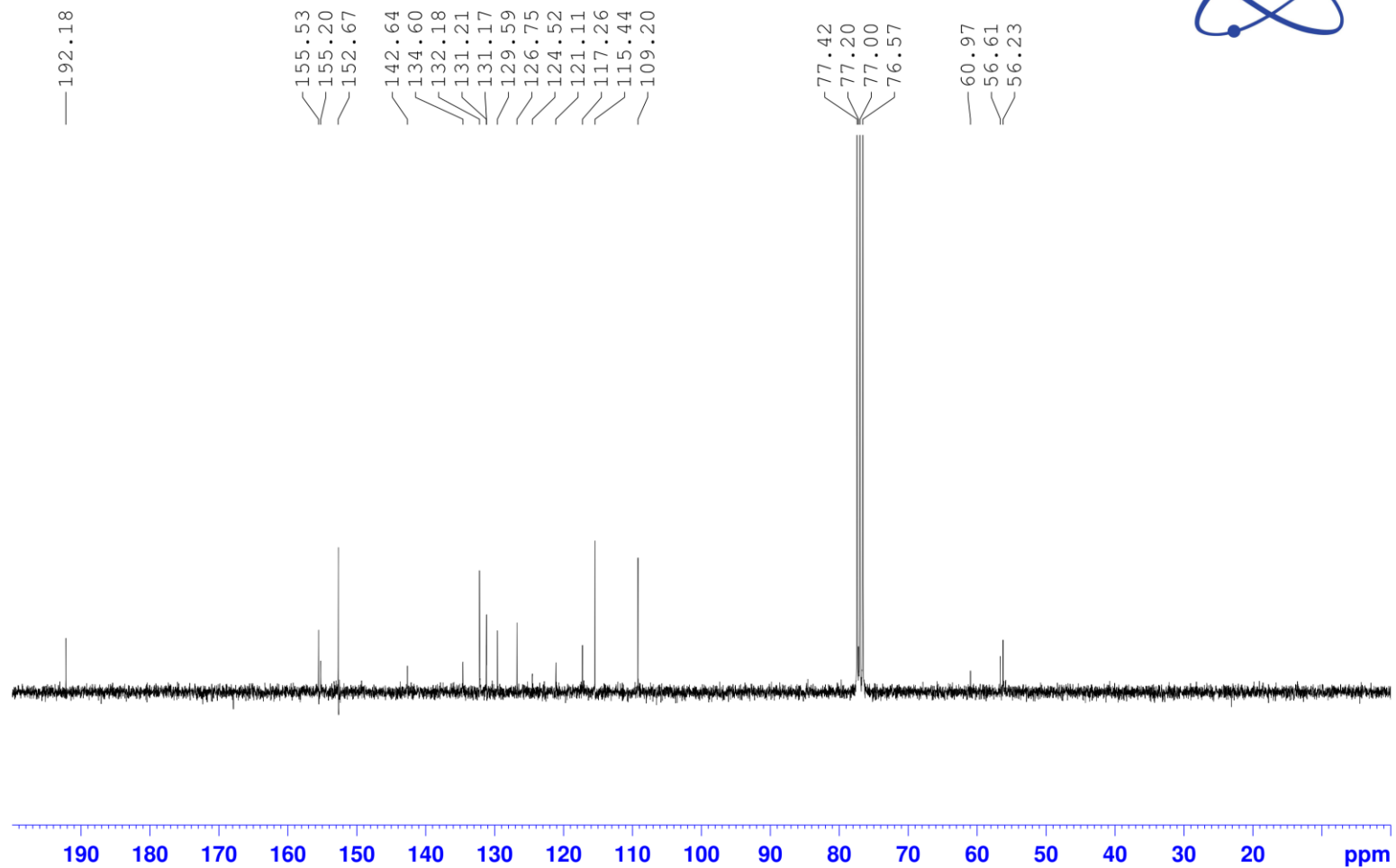
¹³C Spectra for compound 10

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1008-8-871/1/1/1.jp



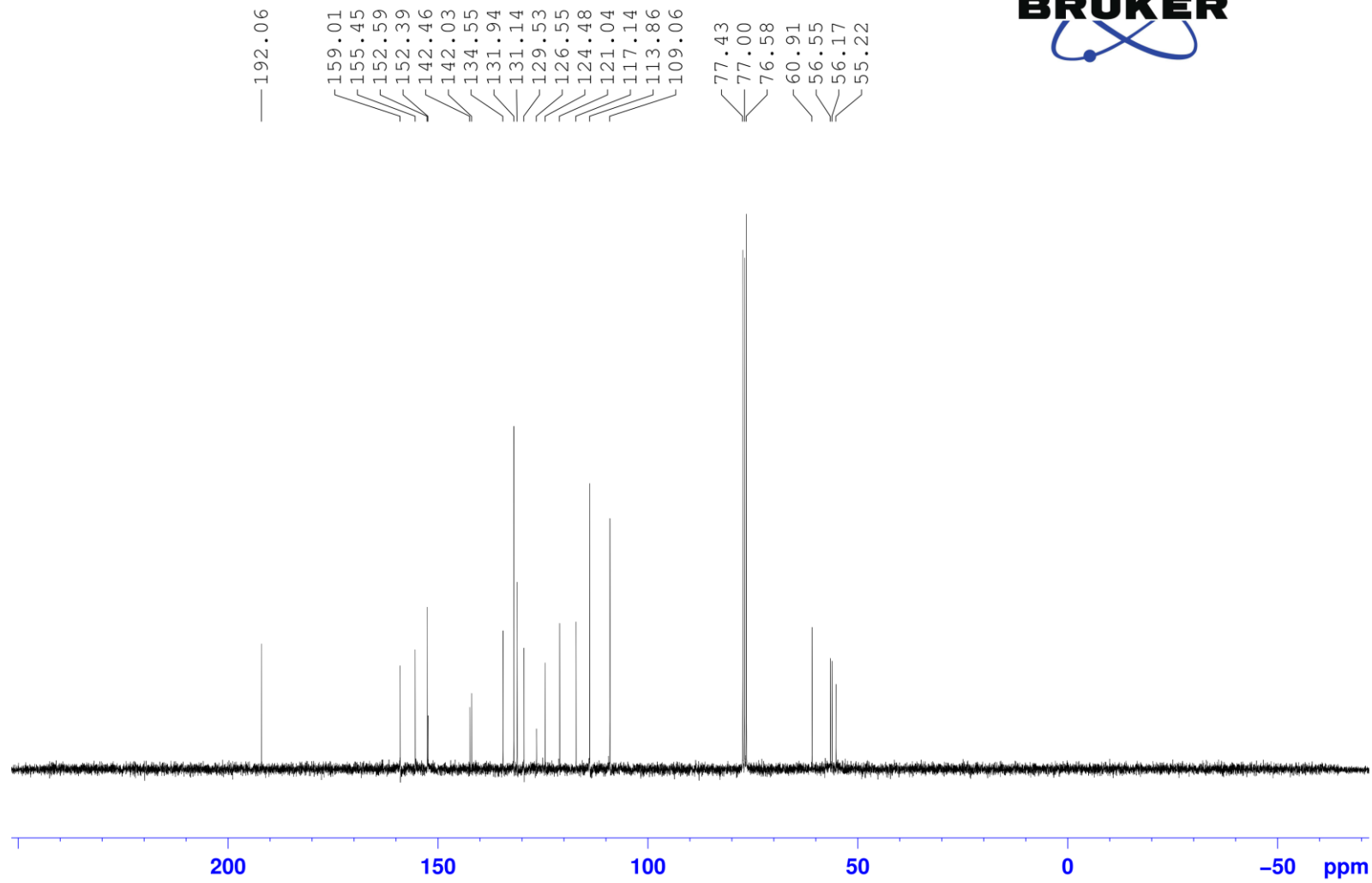
¹³C Spectra for compound 11

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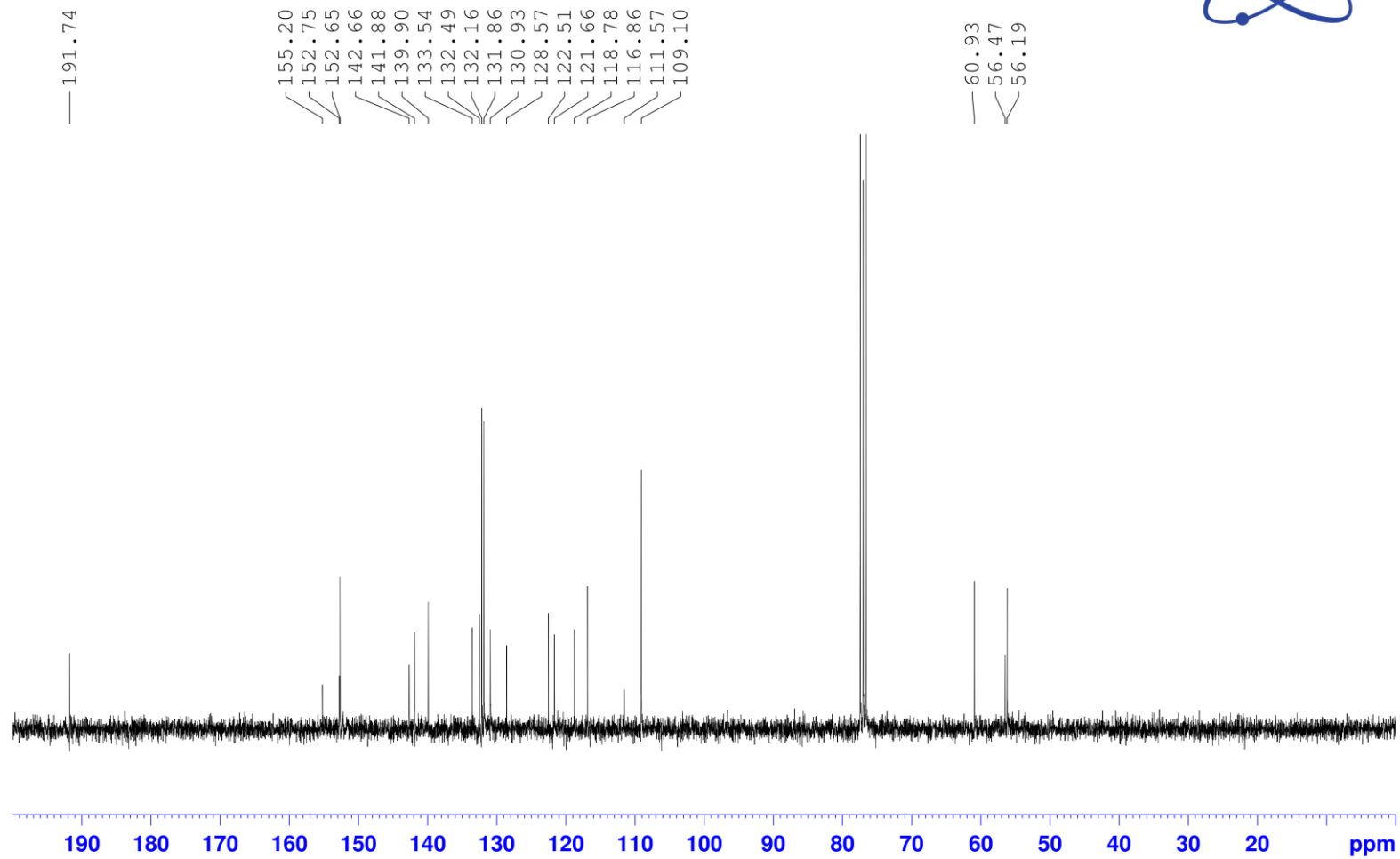
¹³C Spectra for compound 12

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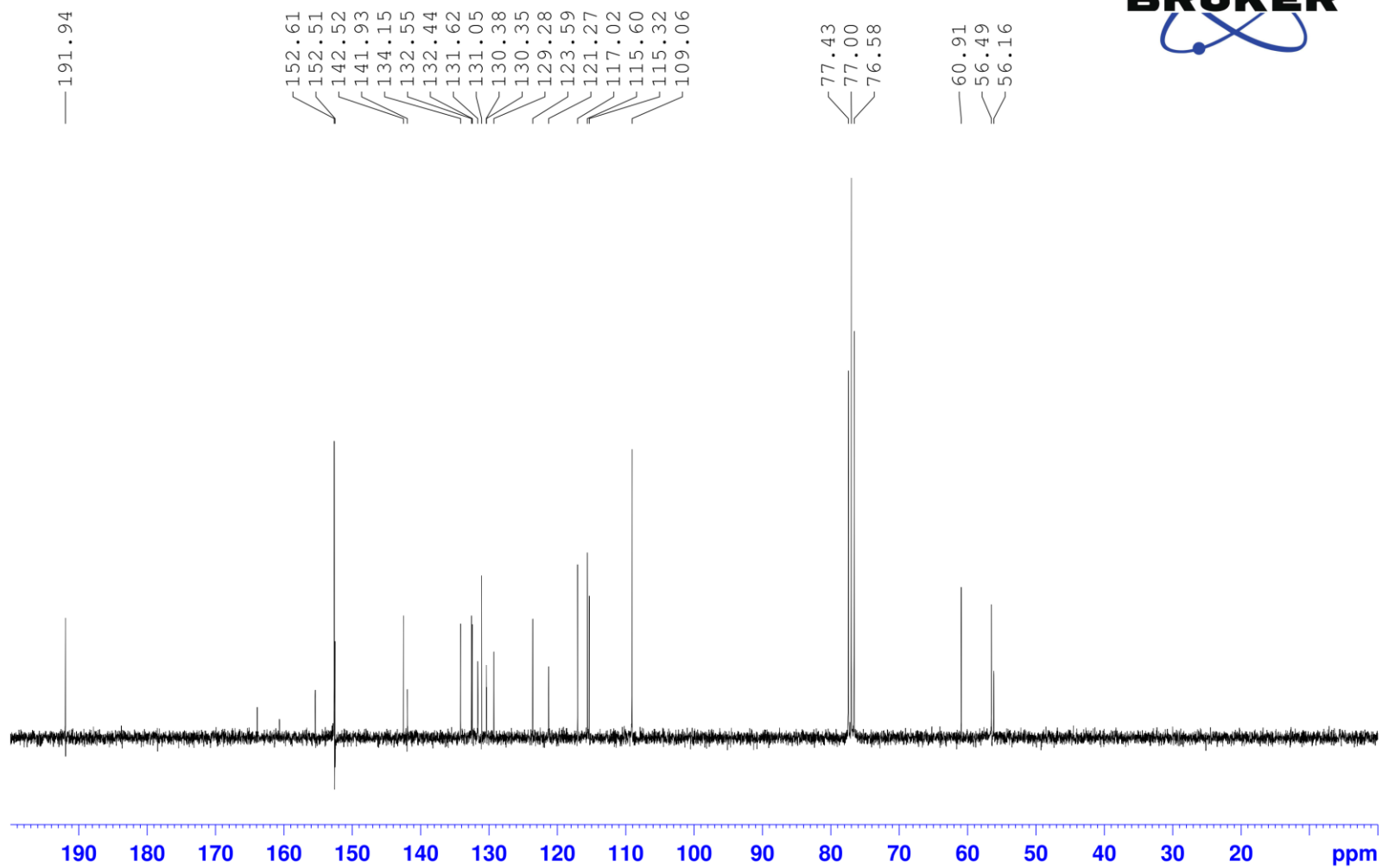
¹³C Spectra for compound 13

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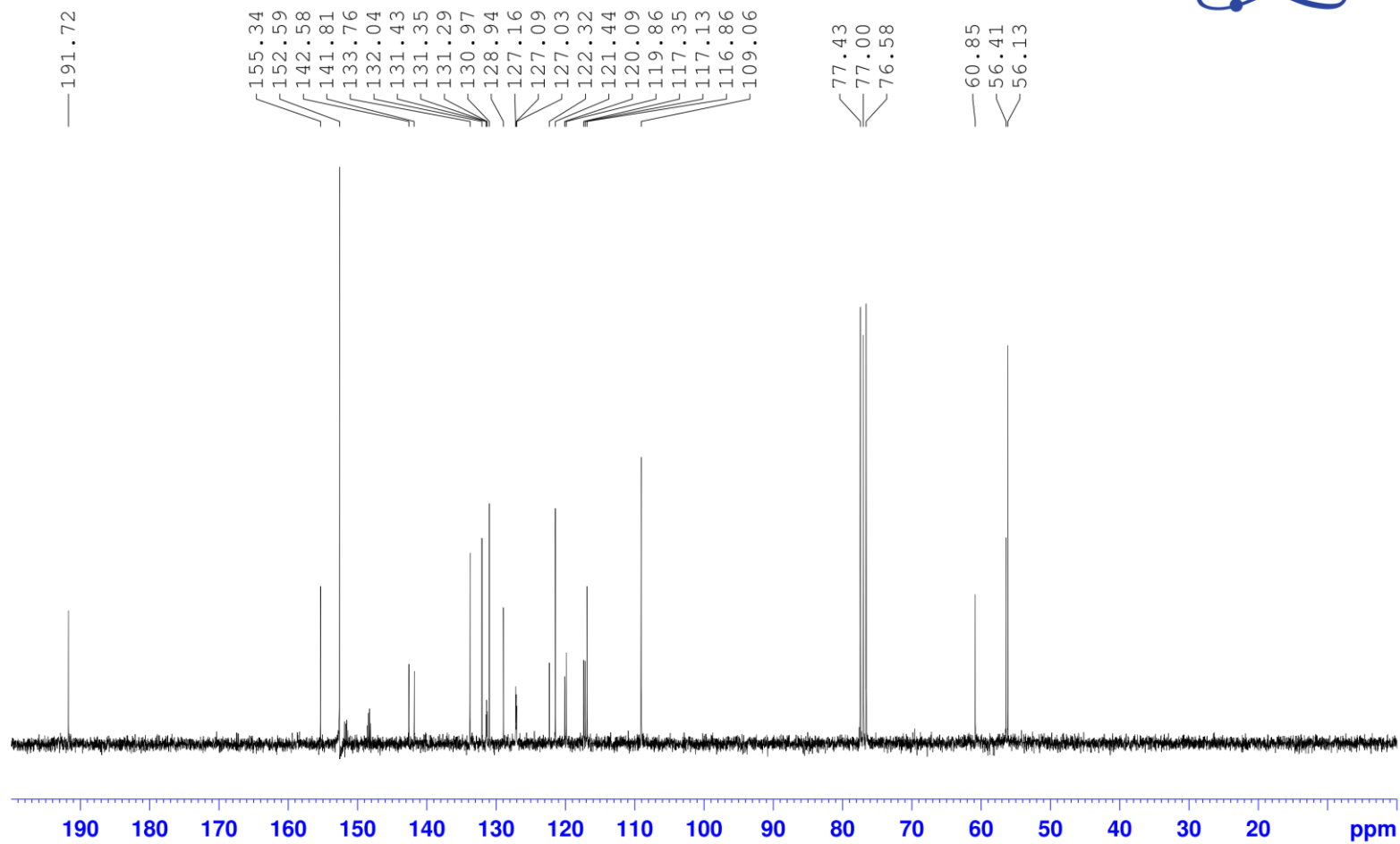
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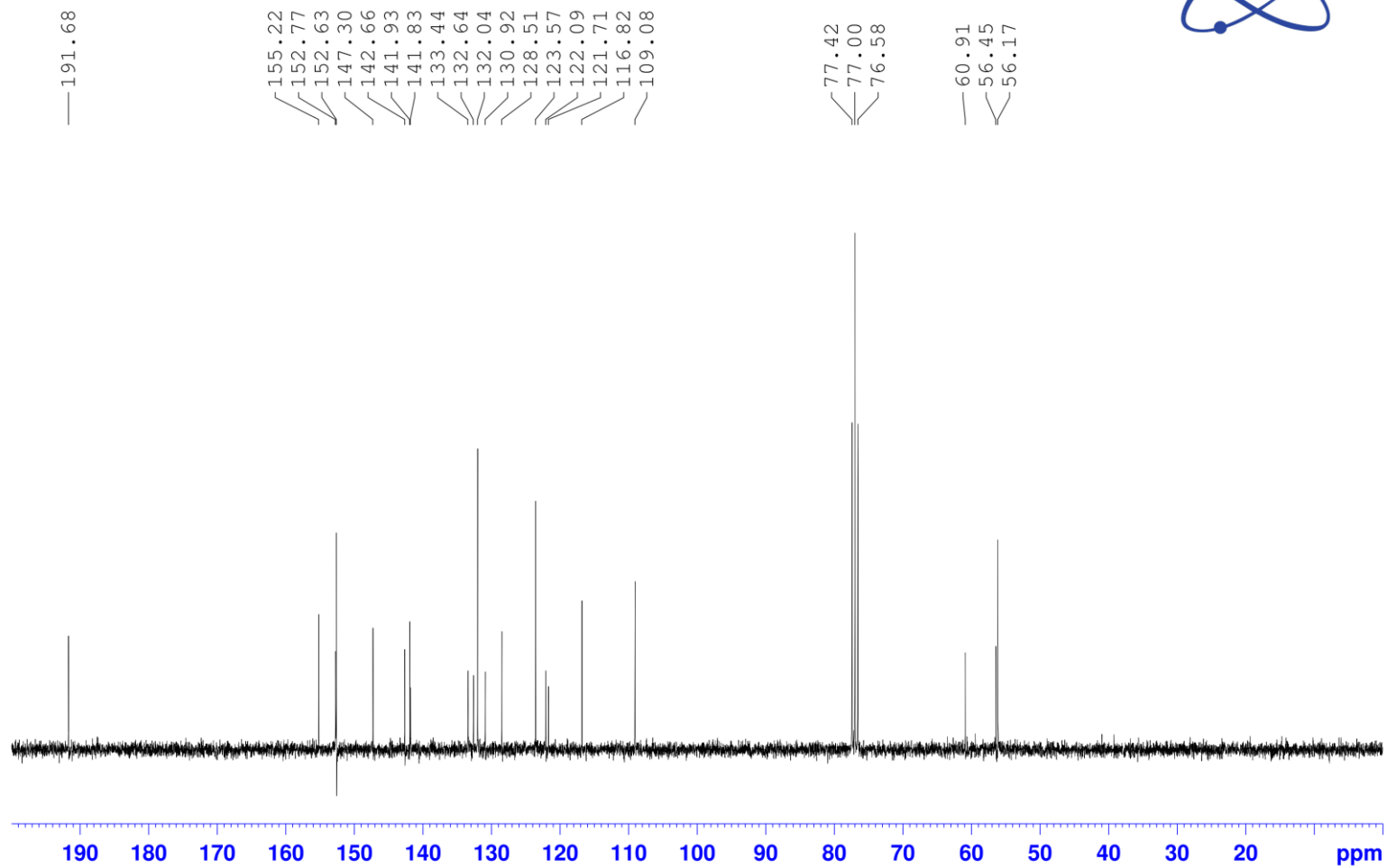
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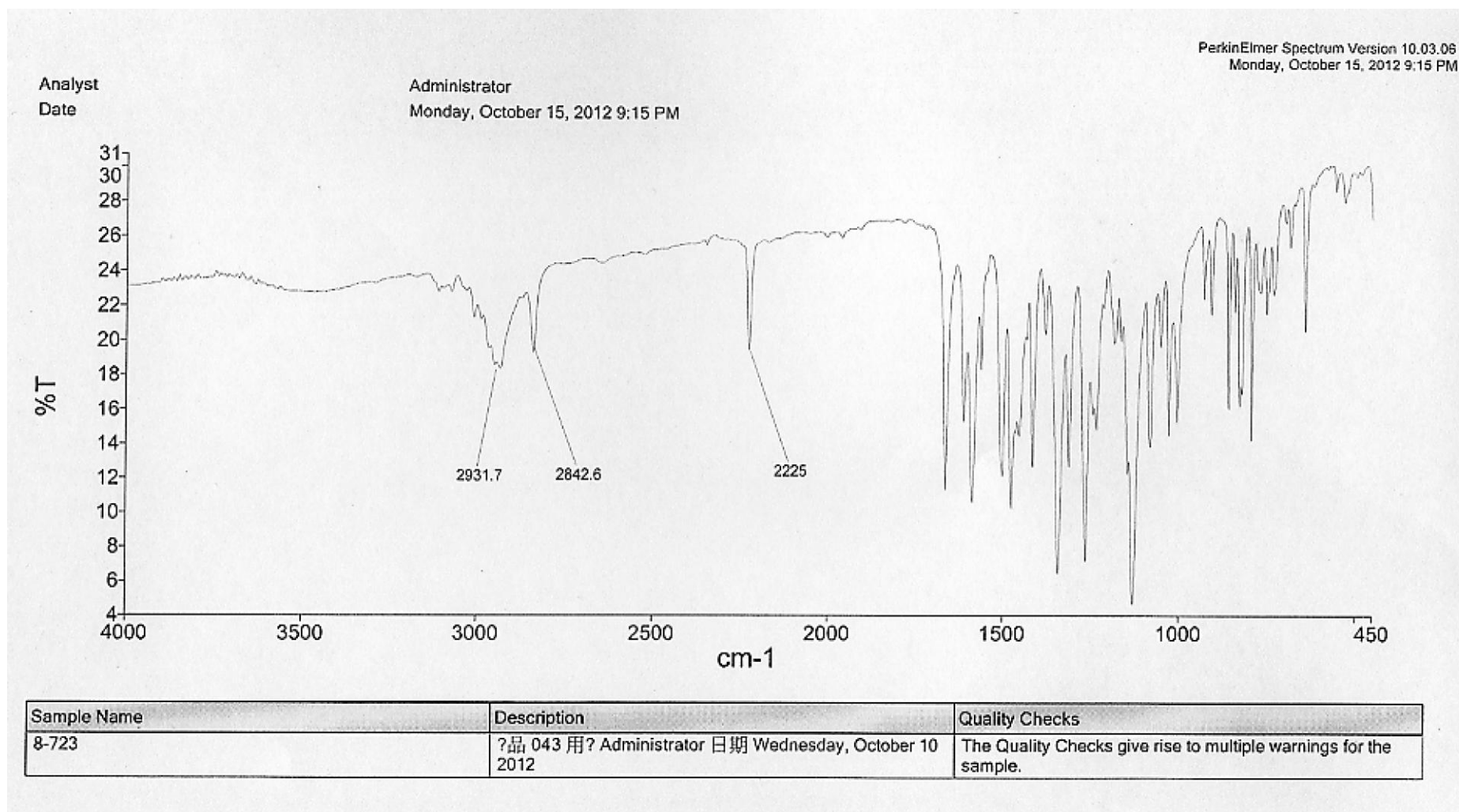


¹³C Spectra for compound 16

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IR Spectra for compound 6



IR Spectra for compound 7

