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Communication

Synthesis and Spectral Characterization of 4,7-dichloro-6-nitroquinazoline

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Supporting Information

Spectral data of starting material **I**, intermediates **II**, **III** and title compound **IV**

Figure S1: FT-IR spectrum of compound 2-amino-4-chlorobenzoic acid (**I**)

Figure S2: ^{1}H-NMR spectrum of compound 2-amino-4-chlorobenzoic acid (**I**)

Figure S3: ^{13}C-NMR spectrum of compound 2-amino-4-chlorobenzoic acid (**I**)

Figure S4: MS spectrum of compound 7-chloroquinazolin-4(3*H*)-one (**II**)

Figure S5: FT-IR spectrum of compound 7-chloroquinazolin-4(3*H*)-one (**II**)

Figure S6: ^{1}H-NMR spectrum of compound 7-chloroquinazolin-4(3*H*)-one (**II**)

Figure S7: ^{13}C-NMR spectrum of compound 7-chloroquinazolin-4(3*H*)-one (**II**)

Figure S8: MS spectrum of compound 7-chloro-6-nitroquinazolin-4(3*H*)-one (**III**)

Figure S9: FT-IR spectrum of compound 7-chloro-6-nitroquinazolin-4(3*H*)-one (**III**)

Figure S10: ^{1}H-NMR spectrum of compound 7-chloro-6-nitroquinazolin-4(3*H*)-one (**III**)

Figure S11: ^{13}C-NMR spectrum of compound 7-chloro-6-nitroquinazolin-4(3*H*)-one (**III**)

Figure S12: MS spectrum of compound 4,7-dichloro-6-nitroquinazoline (**IV**)

Figure S13: FT-IR spectrum of compound 4,7-dichloro-6-nitroquinazoline (**IV**)

Figure S14: ^{1}H-NMR spectrum of compound 4,7-dichloro-6-nitroquinazoline (**IV**)

Figure S15: ^{13}C-NMR spectrum of compound 4,7-dichloro-6-nitroquinazoline (**IV**)

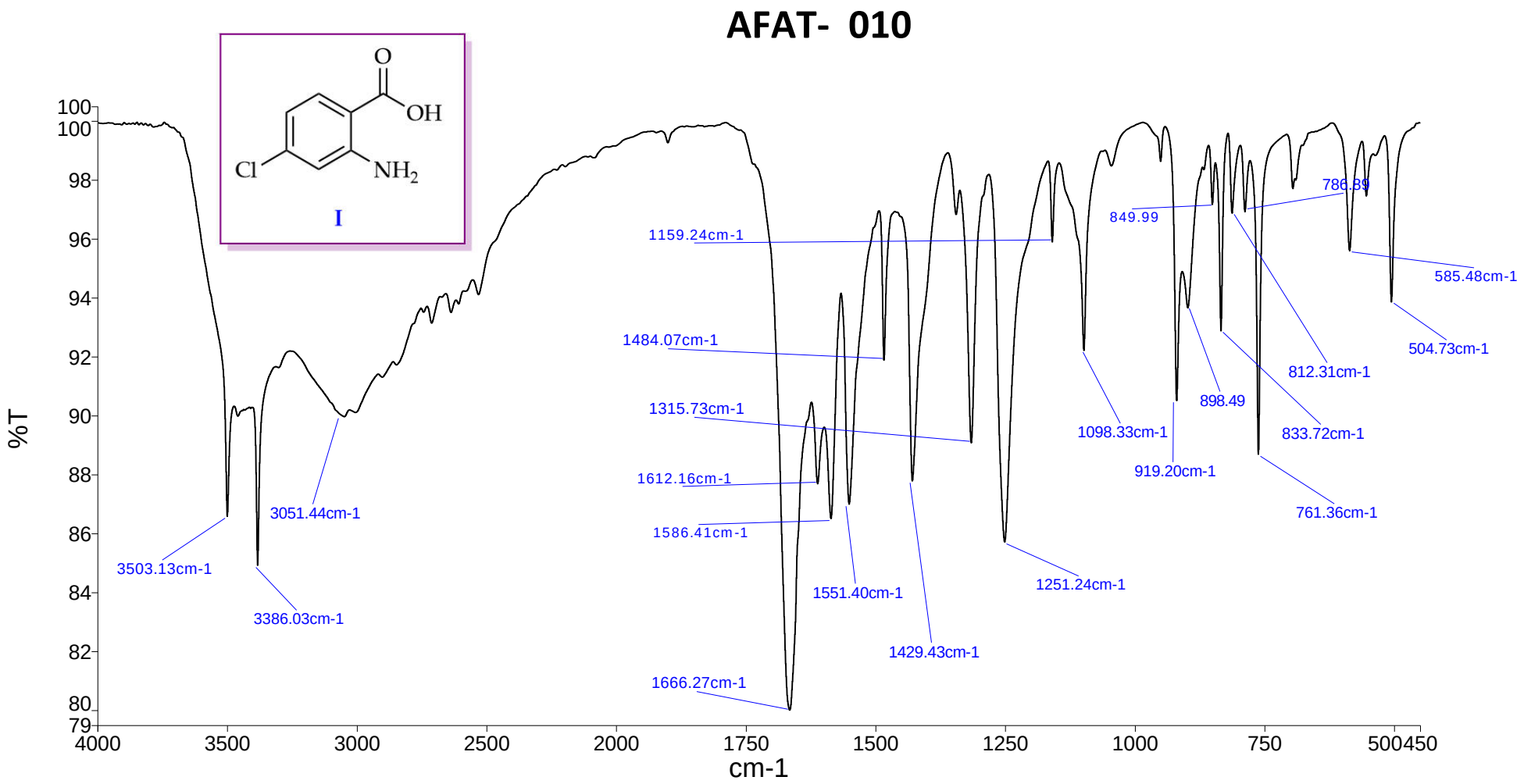

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Figure S1: FT-IR spectrum of compound 2-amino-4-chlorobenzoic acid (**I**)

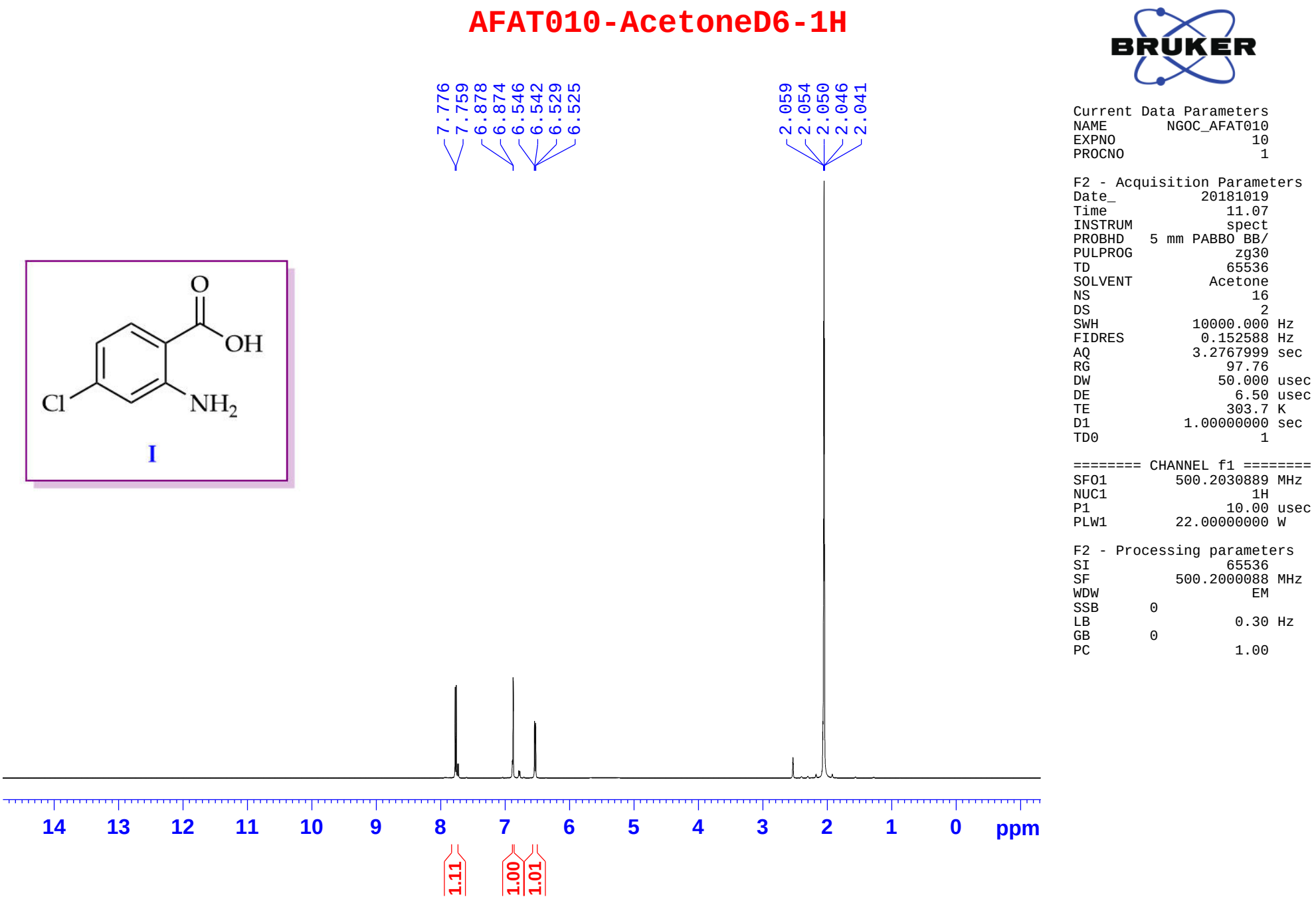


Figure S2: ^{1}H-NMR spectrum of compound 2-amino-4-chlorobenzoic acid (**I**)

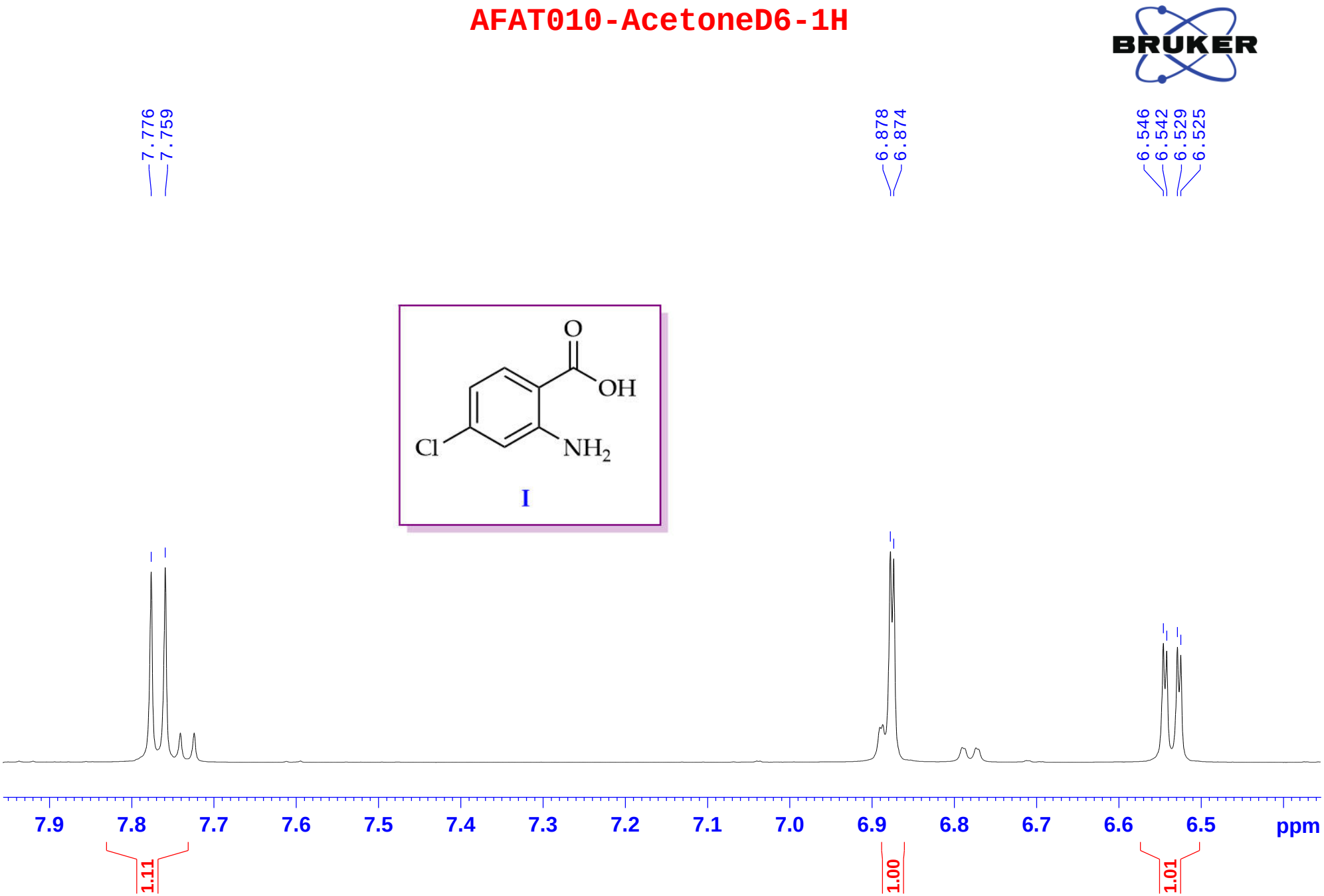
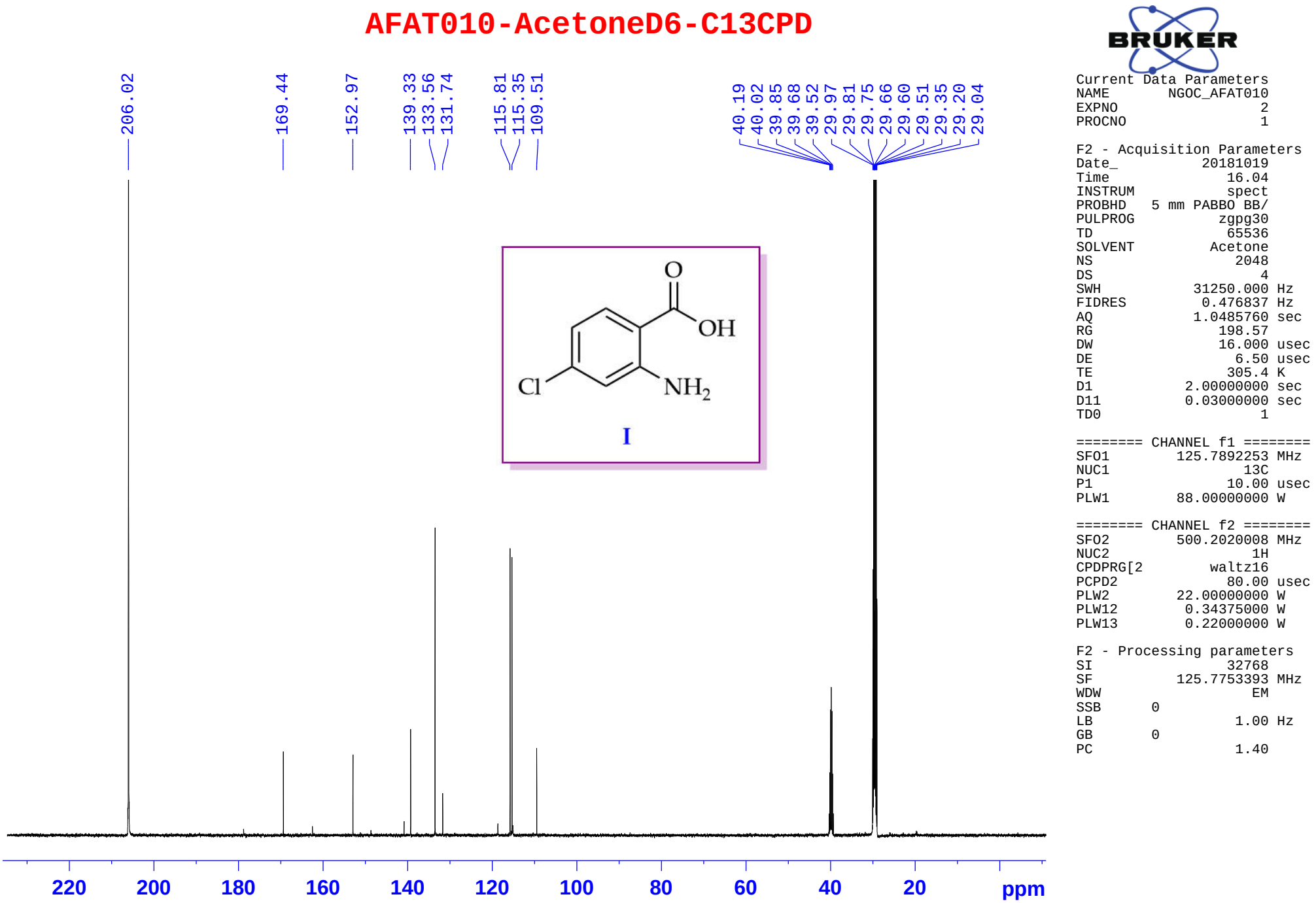


Figure S2: ^{1}H-NMR spectrum of compound 2-amino-4-chlorobenzoic acid (**I**)

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FIDRES         0.476837 Hz
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DE                6.50 usec
TE               305.4 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

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Figure S3: ^{13}C-NMR spectrum of compound 2-amino-4-chlorobenzoic acid (**I**)

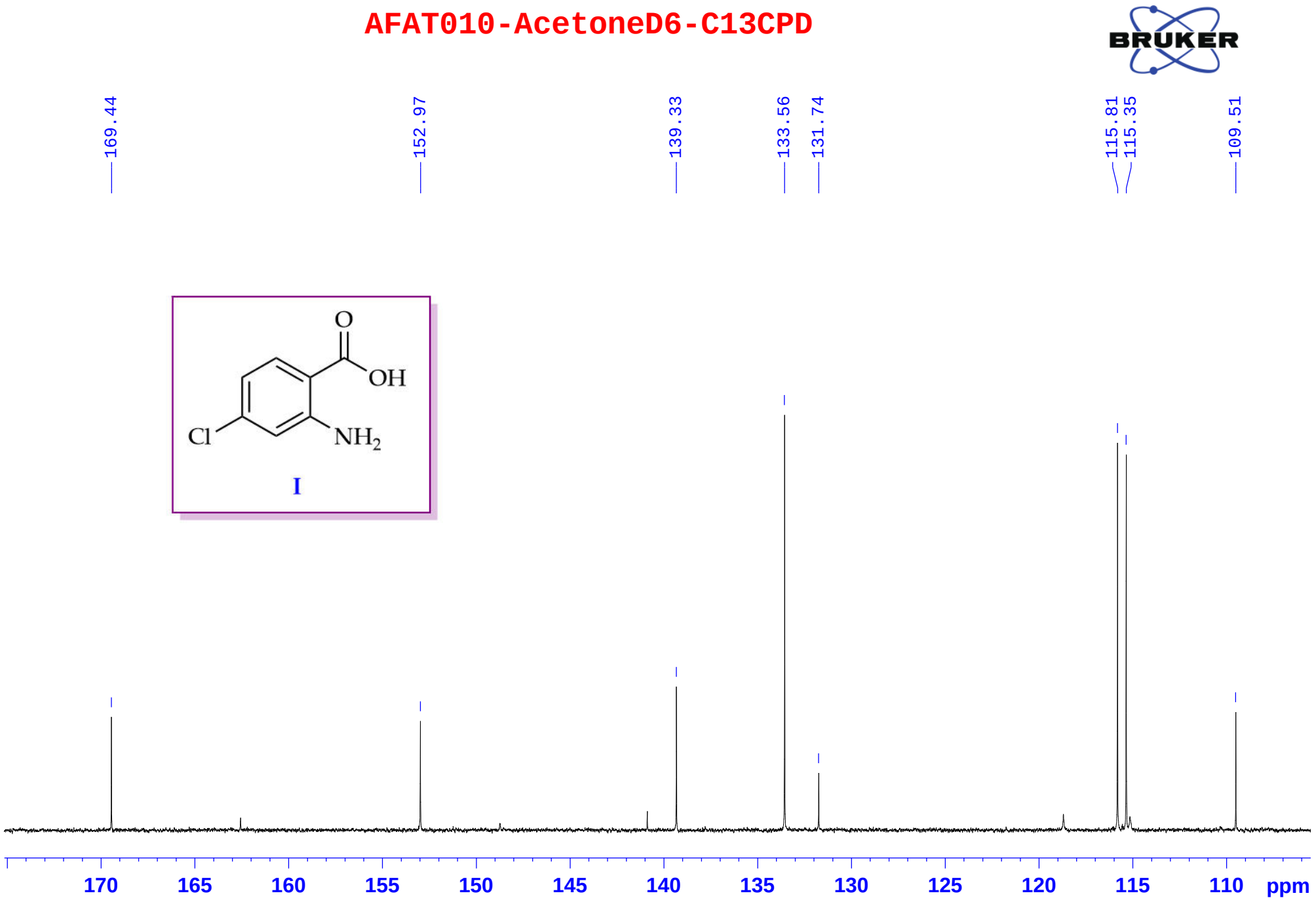
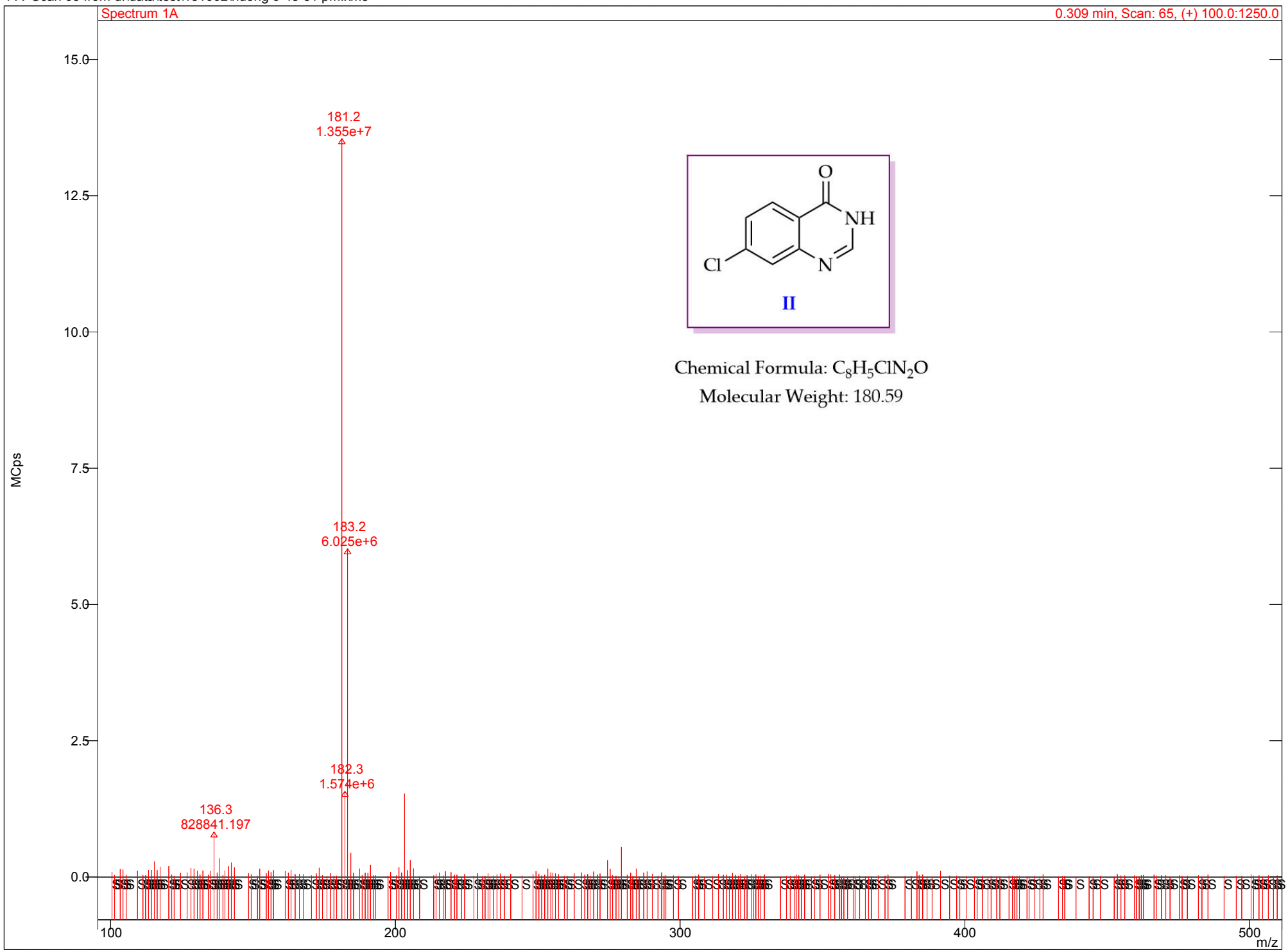


Figure S3: ^{13}C-NMR spectrum of compound 2-amino-4-chlorobenzoic acid (**I**)

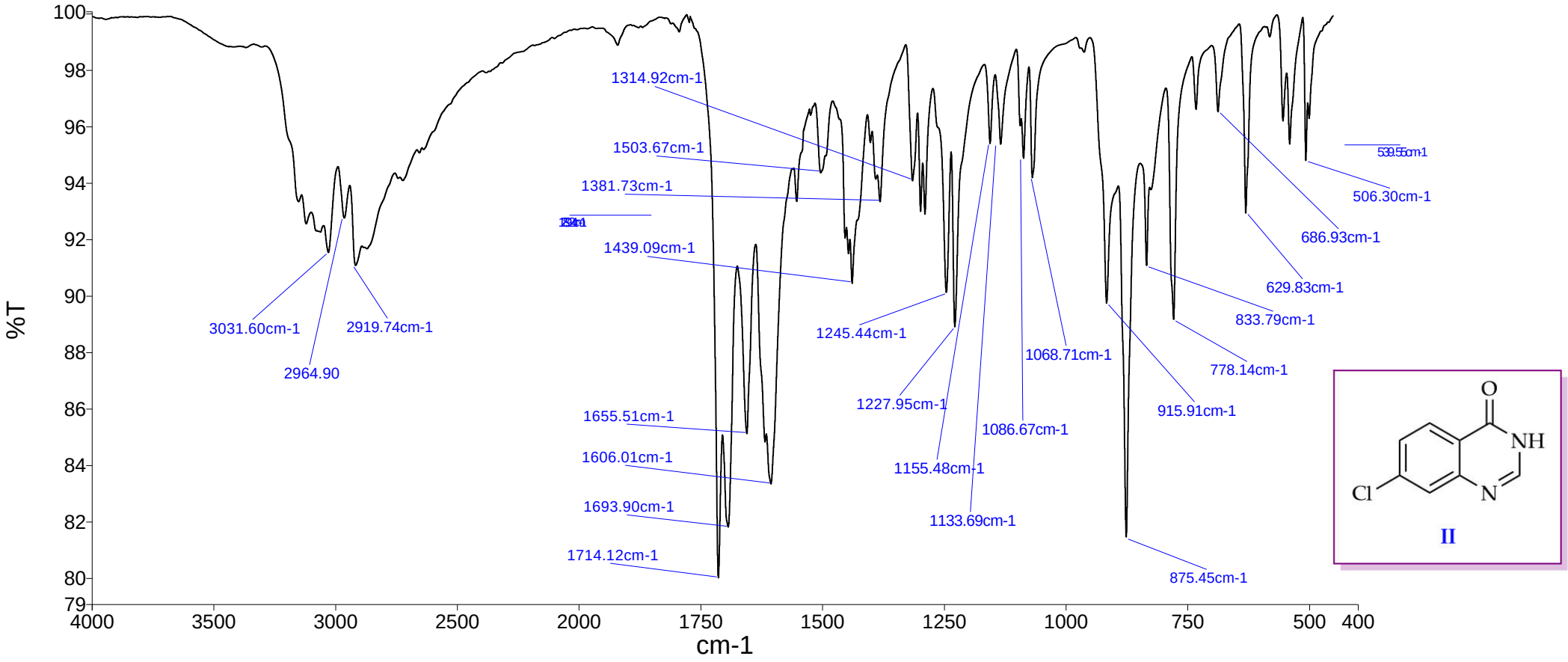
Print Date: 02 Oct 2018 18:55:42

Spectrum Plot - 10/2/2018 6:55 PM

Figure S4: MS spectrum of compound 7-chloroquinazolin-4(3*H*)-one (**II**)



AFAT-011



Sample Name	Description	Saved or unsaved State	Spectrum quality check summary	Pathlength (mm)
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Figure S5: FT-IR spectrum of compound 7-chloroquinazolin-4(3*H*)-one (**II**)

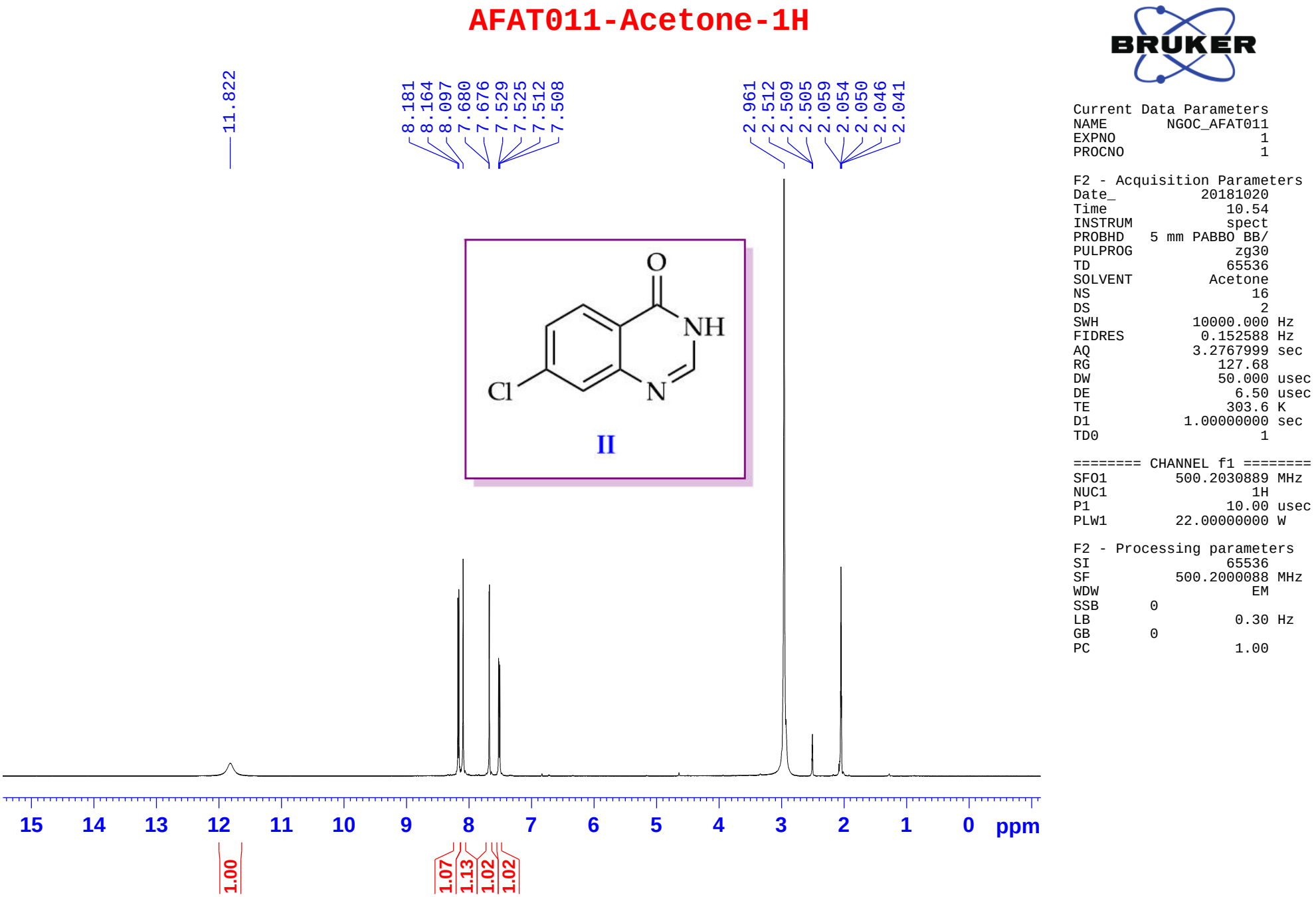


Figure S6: ^{1}H-NMR spectrum of compound 7-chloroquinazolin-4(3*H*)-one (**II**)

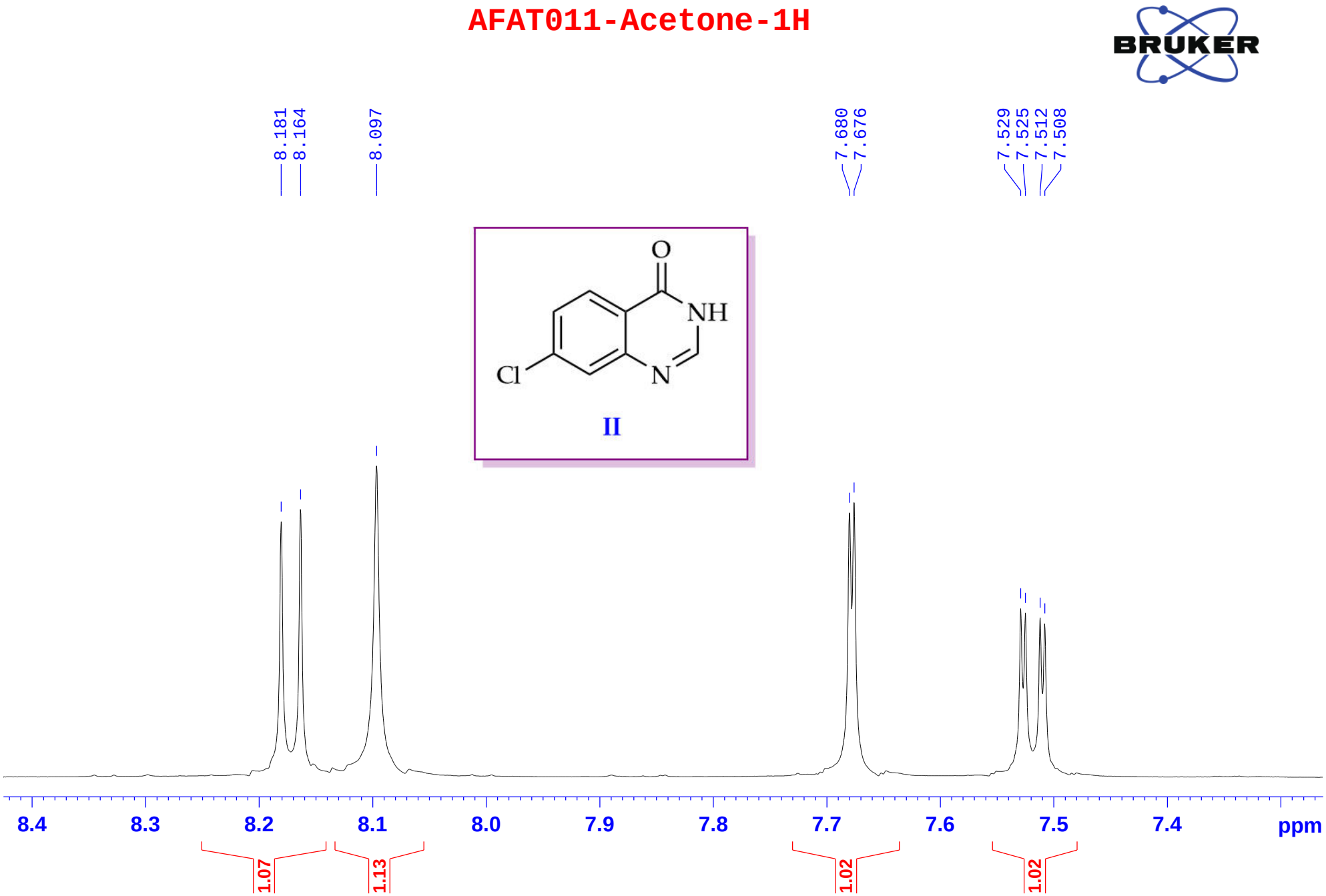
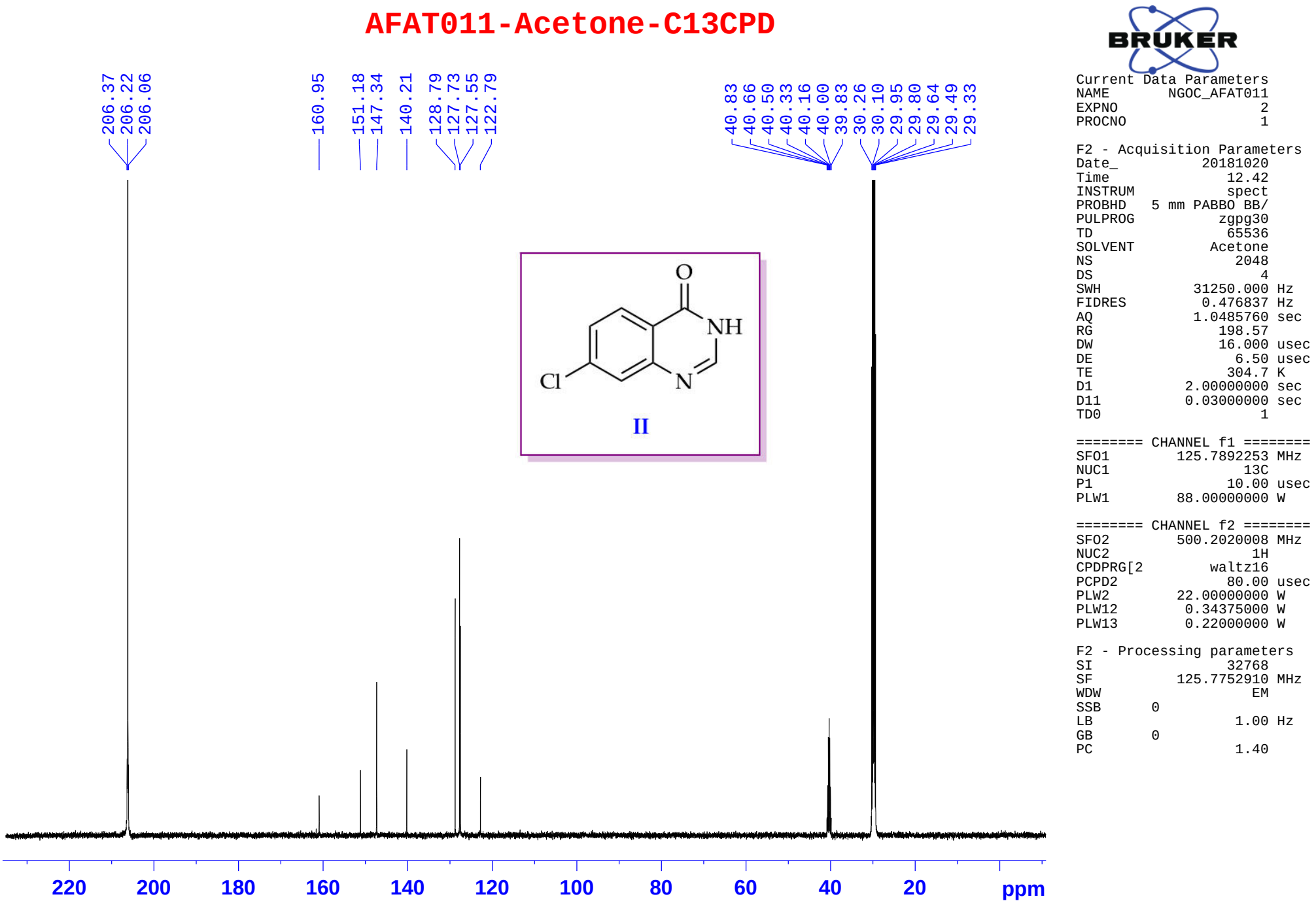


Figure S6: ^{1}H-NMR spectrum of compound 7-chloroquinazolin-4(3*H*)-one (**II**)

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DS                    4
SWH           31250.000 Hz
FIDRES         0.476837 Hz
AQ            1.0485760 sec
RG               198.57
DW               16.000 usec
DE                6.50 usec
TE               304.7 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

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NUC1               13C
P1               10.00 usec
PLW1         88.00000000 W

======== CHANNEL f2 ========
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NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2         22.00000000 W
PLW12         0.34375000 W
PLW13         0.22000000 W

F2 - Processing parameters
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SF           125.7752910 MHz
WDW                EM
SSB       0
LB                1.00 Hz
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PC                1.40
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Figure S7: ^{13}C-NMR spectrum of compound 7-chloroquinazolin-4(3*H*)-one (**II**)

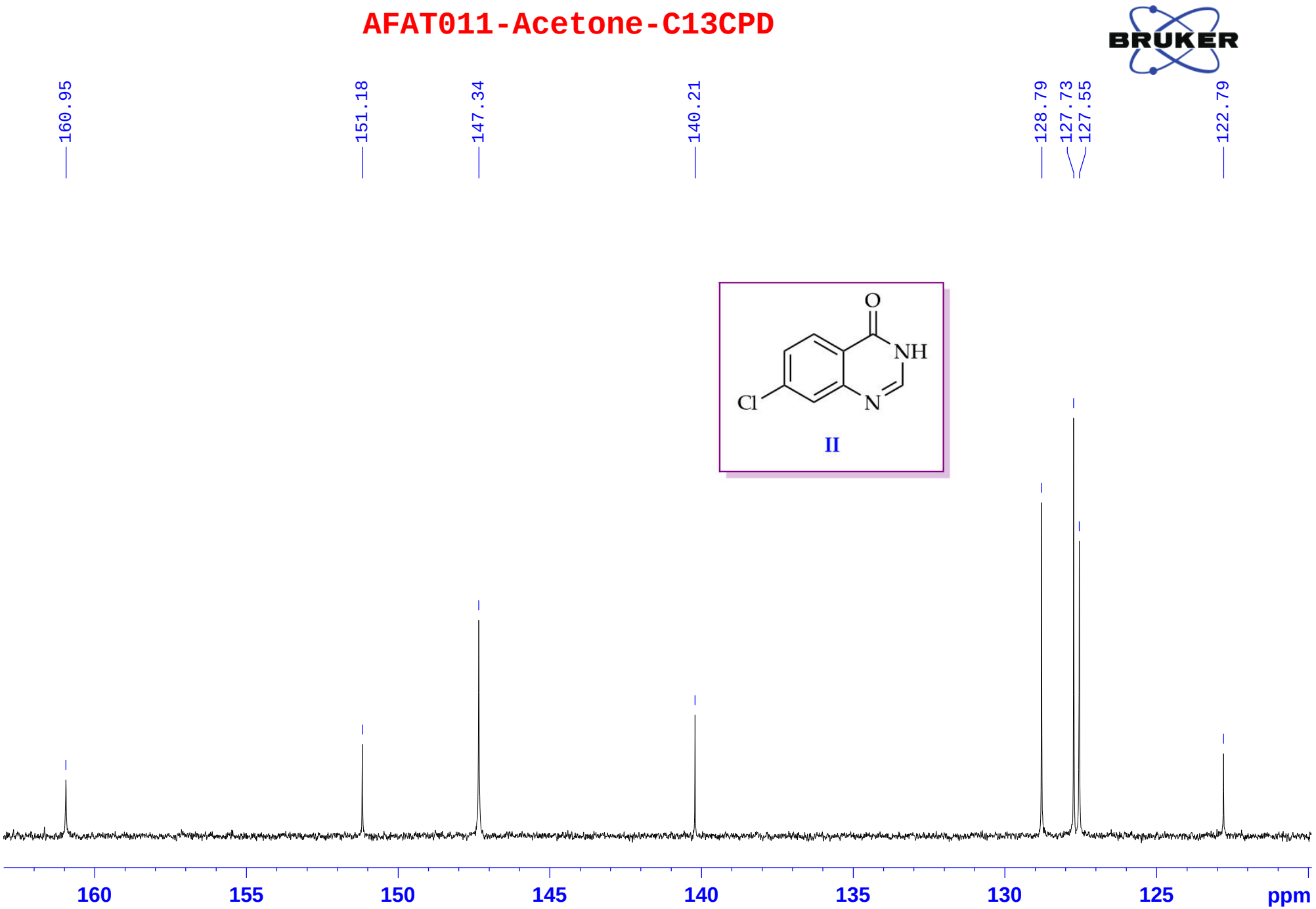


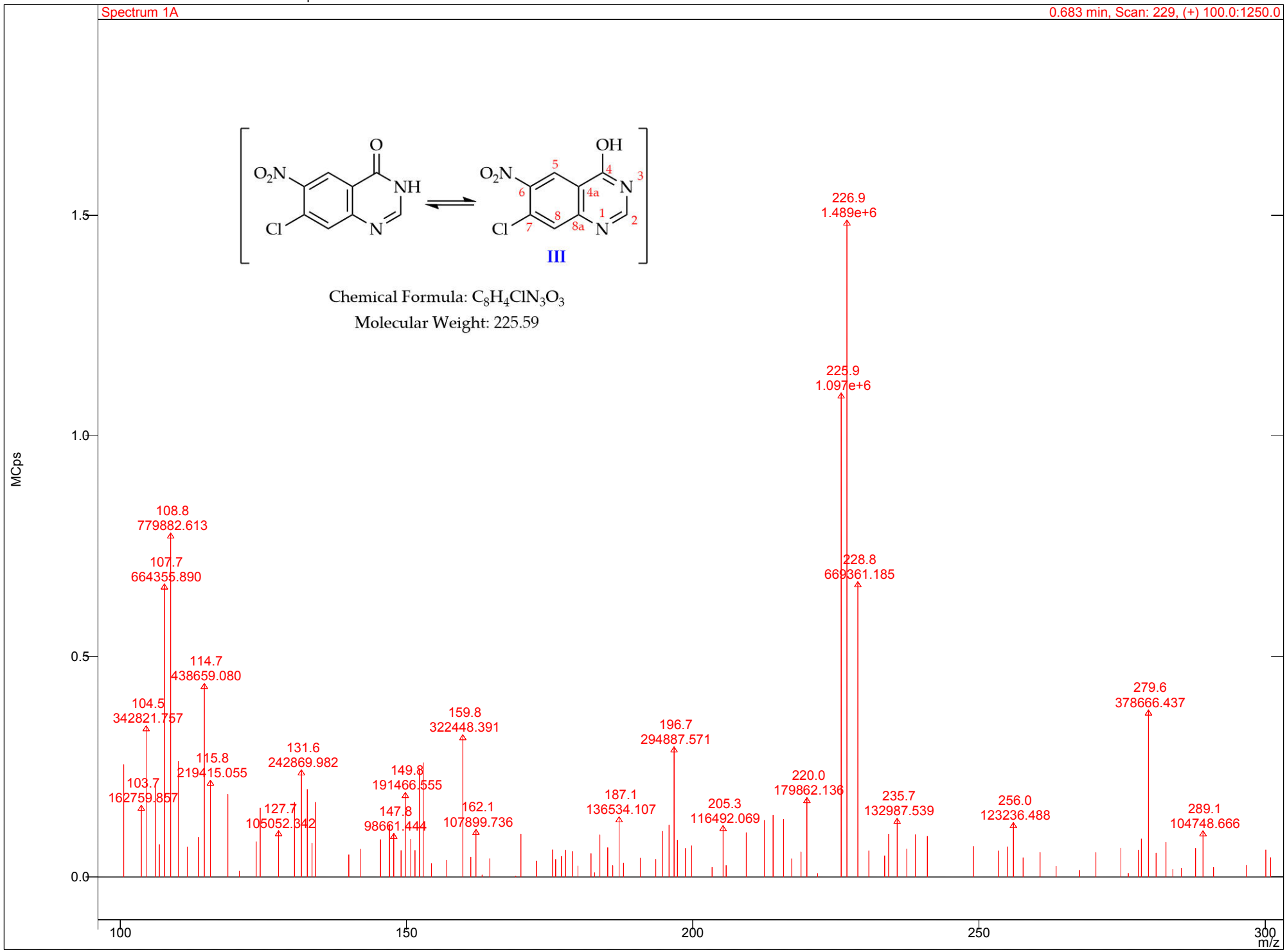
Figure S7: ^{13}C-NMR spectrum of compound 7-chloroquinazolin-4(3*H*)-one (**II**)

Print Date: 15 Nov 2018 07:54:53

Spectrum Plot - 11/15/2018 7:54 AM

Figure S8: MS spectrum of compound 7-chloro-6-nitroquinazolin-4(3*H*)-one (**III**)

1 A Scan 229 from d:\data\test\181114\hv 2-09-26 pm.xms



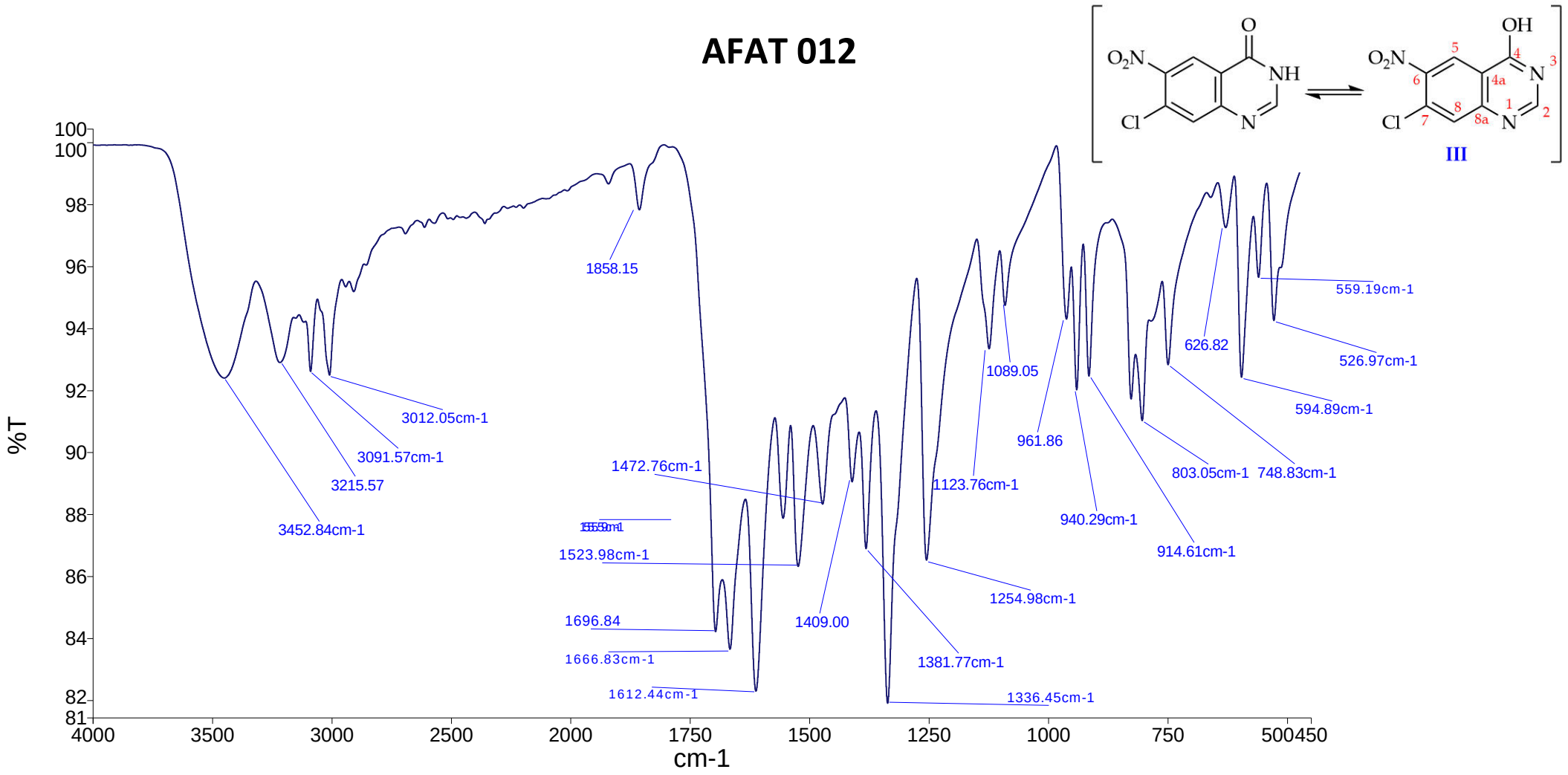


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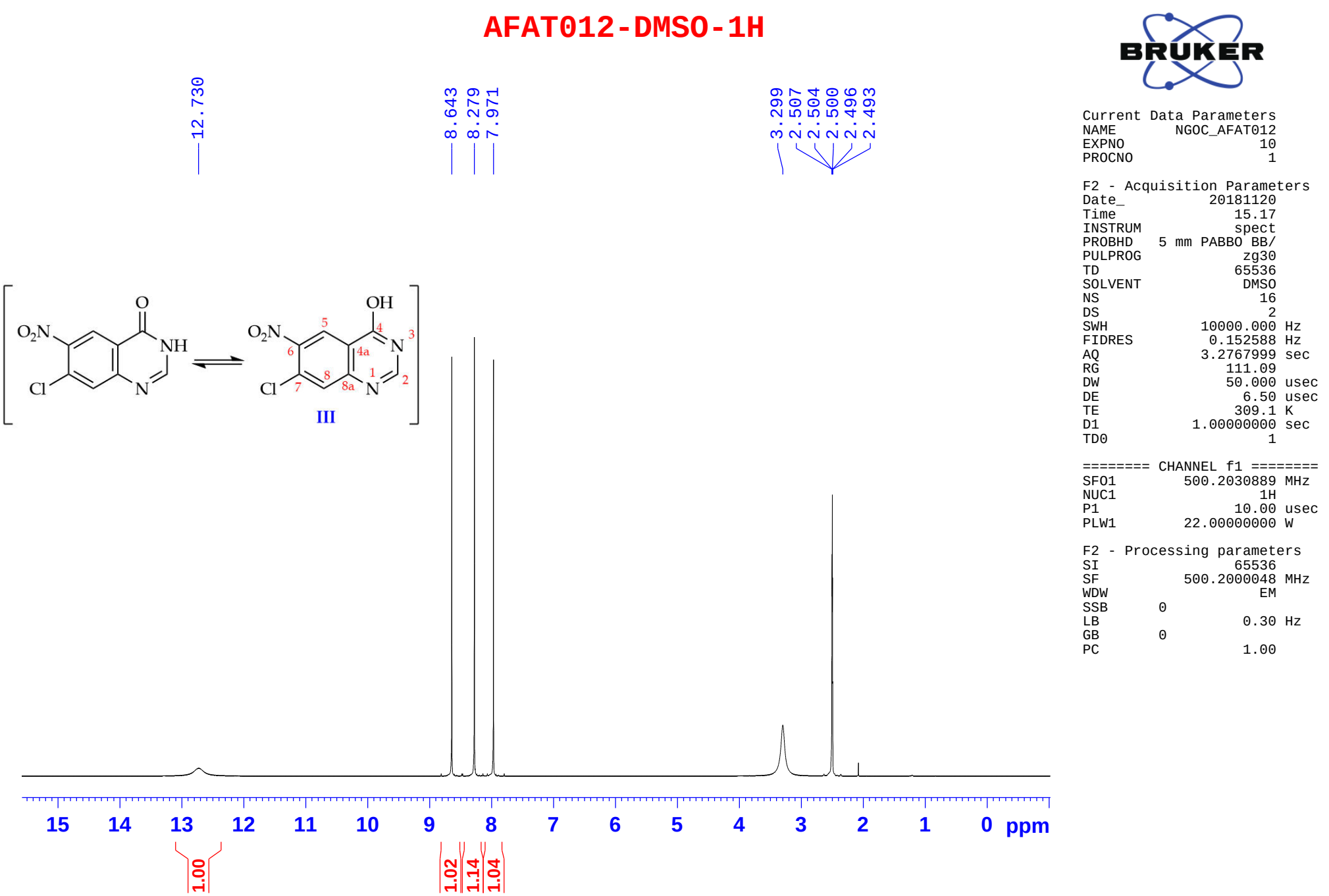
Figure S9: FT-IR spectrum of compound 7-chloro-6-nitroquinazolin-4(3*H*)-one (**III**)

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PROCNO                 1

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PULPROG             zg30
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SOLVENT             DMSO
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DS                     2
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D1           1.00000000 sec
TD0                    1

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P1                10.00 usec
PLW1         22.00000000 W

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WDW                  EM
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PC                1.00
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Figure S10: ^{1}H-NMR spectrum of compound 7-chloro-6-nitroquinazolin-4(3*H*)-one (**III**)

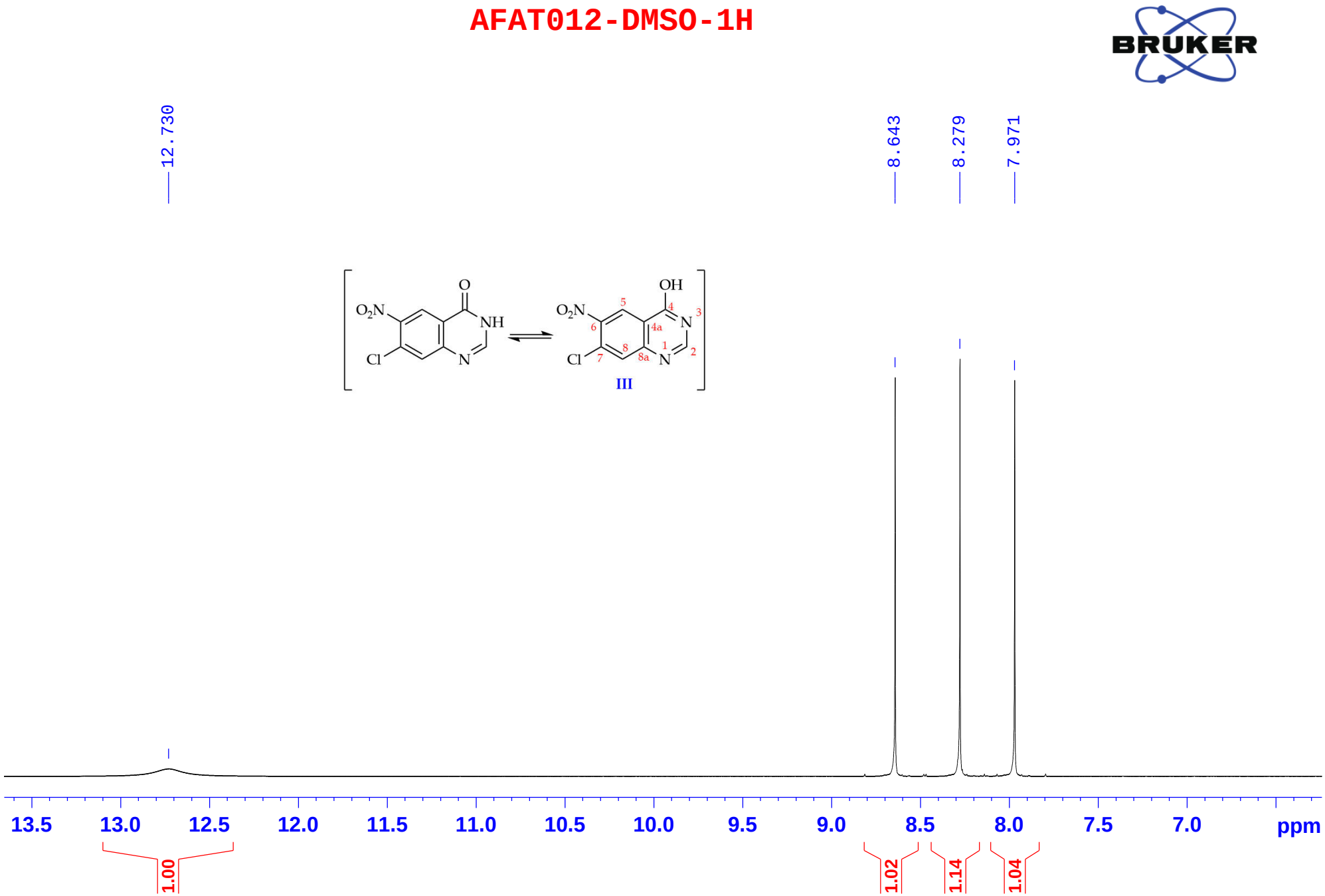
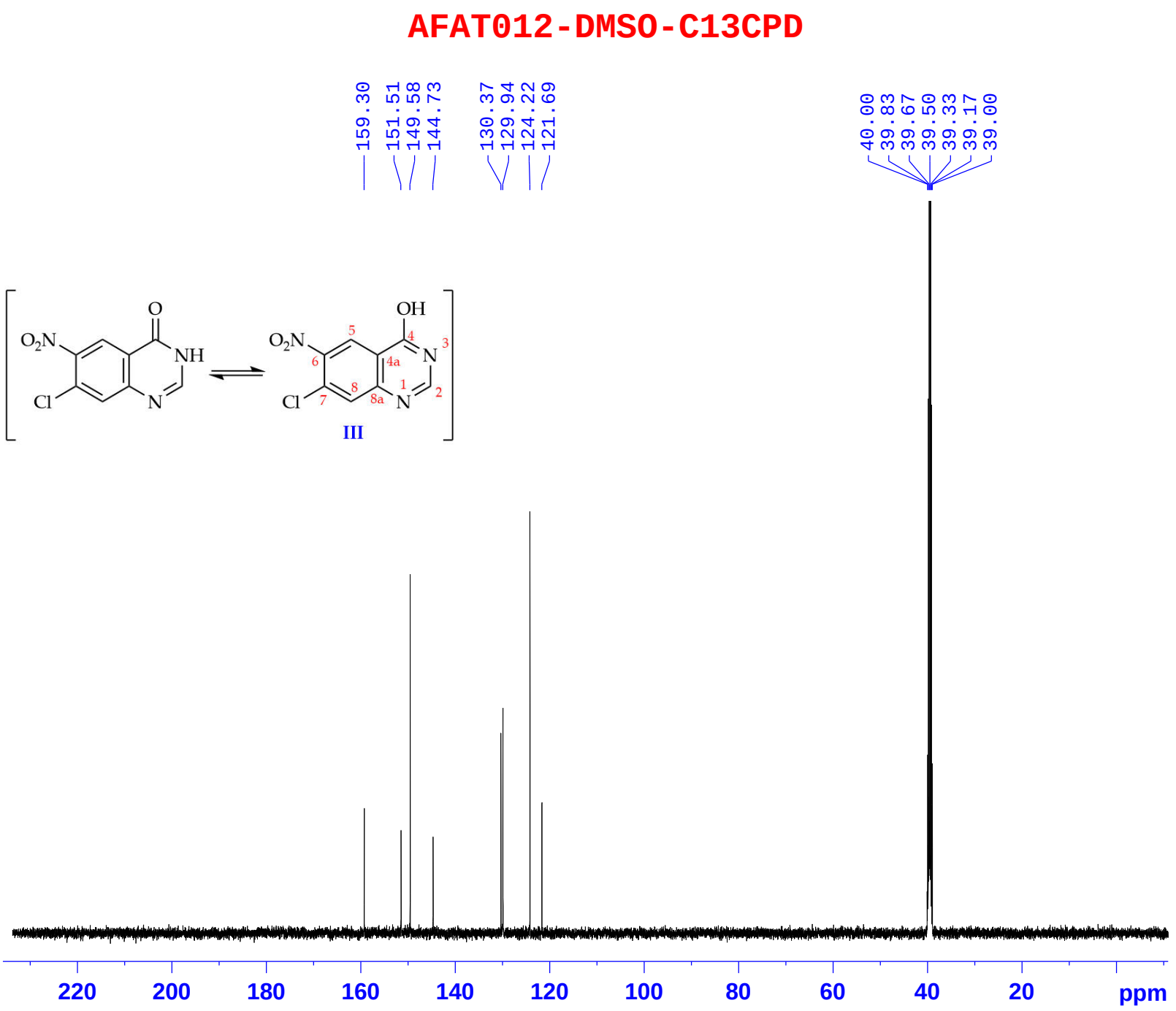


Figure S10: ^{1}H-NMR spectrum of compound 7-chloro-6-nitroquinazolin-4(3*H*)-one (**III**)

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FIDRES          0.476837 Hz
AQ             1.0485760 sec
RG                198.57
DW                16.000 usec
DE                 6.50 usec
TE                306.3 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         125.7892253 MHz
NUC1                 13C
P1                10.00 usec
PLW1         88.00000000 W

======== CHANNEL f2 ========
SFO2         500.2020008 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         22.00000000 W
PLW12         0.34375000 W
PLW13         0.22000000 W

F2 - Processing parameters
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WDW                   EM
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LB                 1.00 Hz
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PC                 1.40
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Figure S11: ^{13}C-NMR spectrum of compound 7-chloro-6-nitroquinazolin-4(3*H*)-one (**III**)

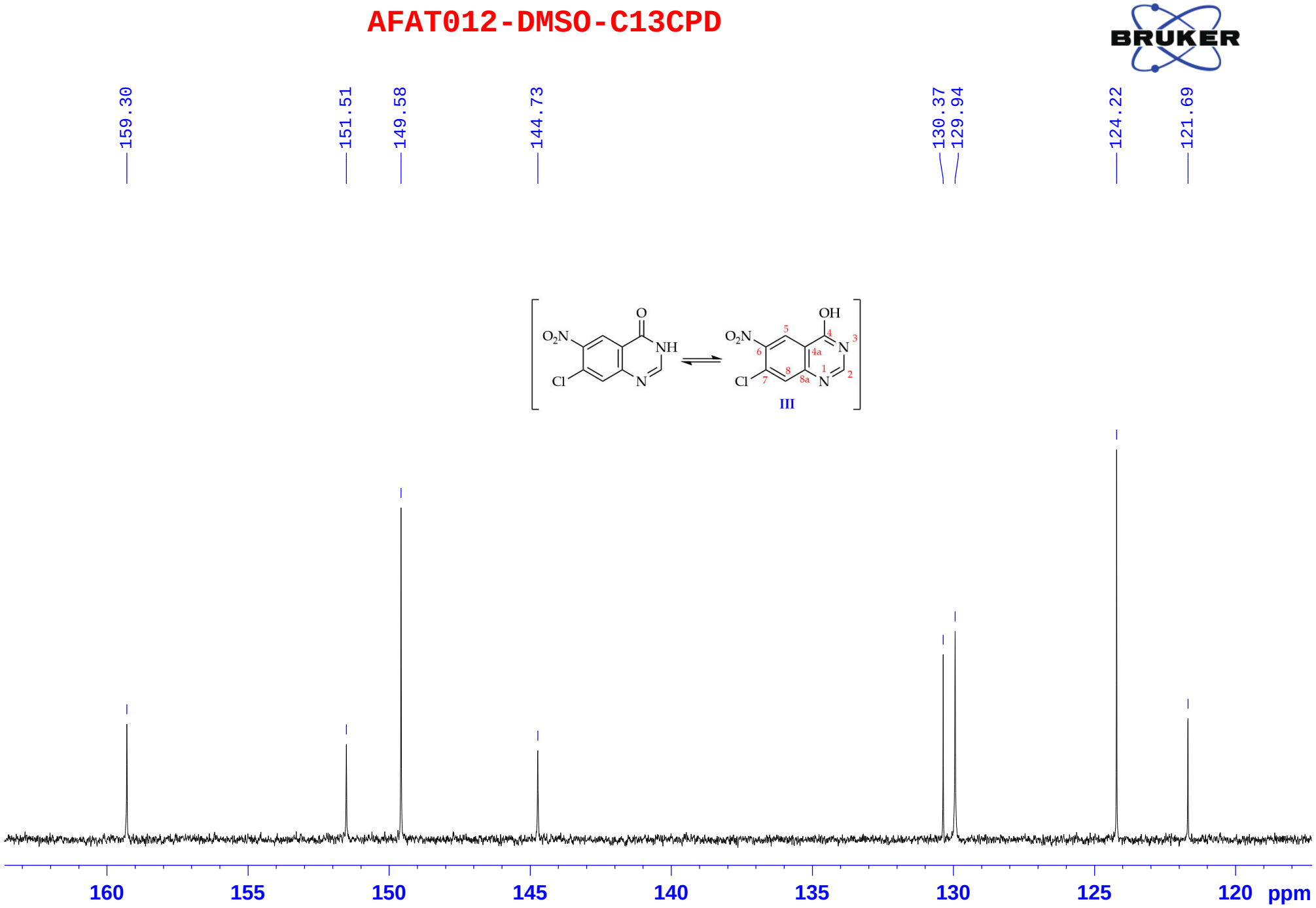

Figure S11: ^{13}C-NMR spectrum of compound 7-chloro-6-nitroquinazolin-4(3*H*)-one (**III**)

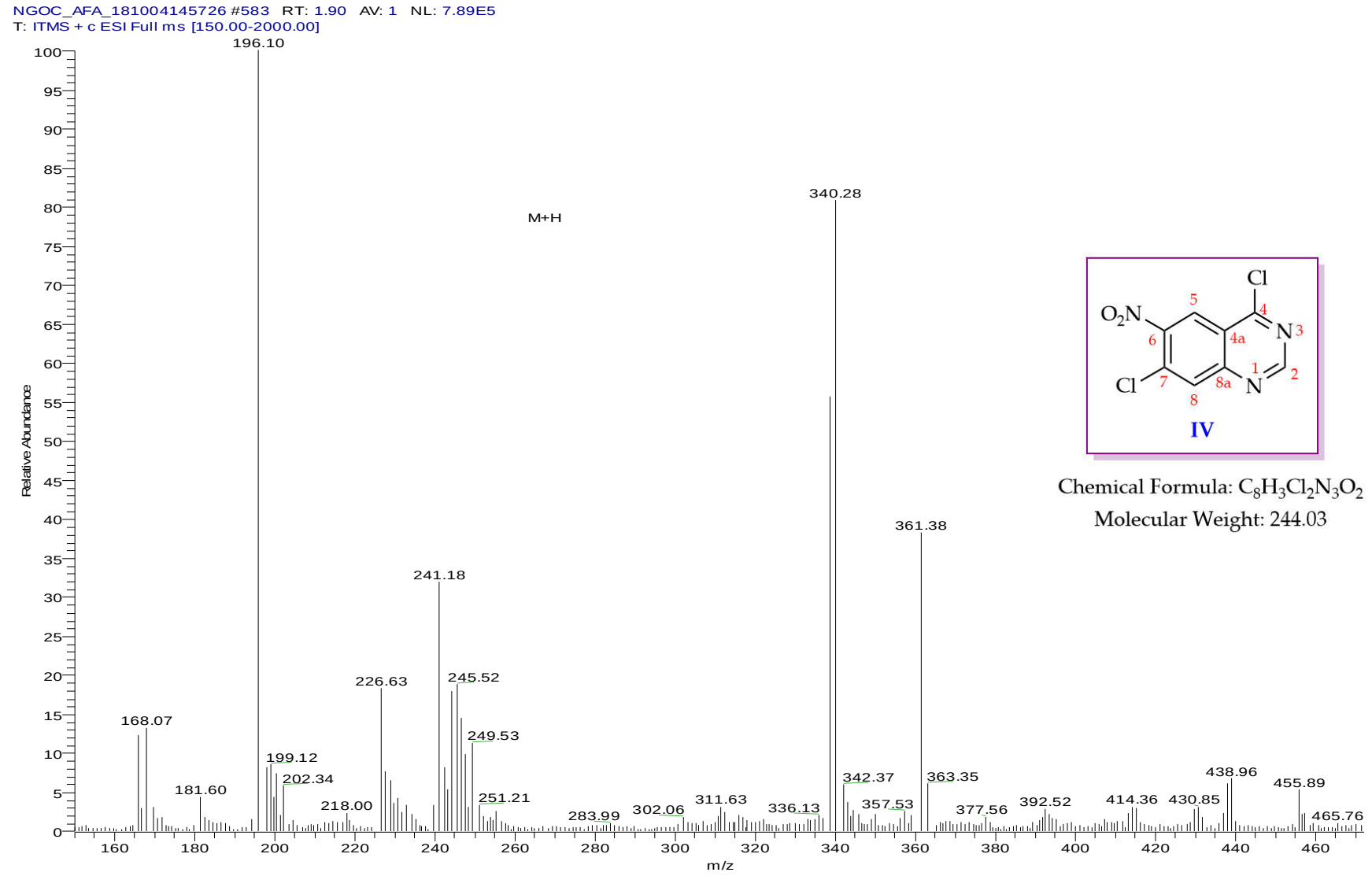

Figure S12: MS spectrum of compound 4,7-dichloro-6-nitroquinazoline (**IV**)

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m/z= 150.00-472.02

m/z	Intensity	Relative
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168.07	104157.2	13.21
196.10	788551.8	100.00
198.10	64517.8	8.18
199.12	66660.1	8.45
200.60	57614.8	7.31
226.63	143374.9	18.18
227.89	59958.9	7.60
228.98	50979.5	6.46
241.18	251771.6	31.93
242.71	63581.8	8.06
244.43	140837.2	17.86
245.52	148257.0	18.80
246.75	114508.2	14.52
247.73	77002.2	9.77
249.53	88592.3	11.23
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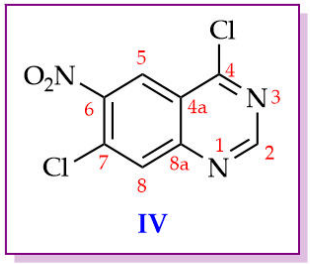

IV

Chemical Formula: $C_8H_3Cl_2N_3O_2$
Molecular Weight: 244.03

Figure S12: MS spectrum of compound 4,7-dichloro-6-nitroquinazoline (**IV**)

Lab: Materials chemistry, Faculty of Chemistry, HUS-VNU
19 Le Thanh Tong, Hoan Kiem, Ha Noi

Tel: 844.38.253.053; **Fax**: 844.38.241.140 **Mail**: Chem.vnu@.edu.vn

Operator: Ms. Dao Thi Nhung

Mobile: 0948 119 043; Email: daothinhungtn@yahoo.com

Mass Spectrometer
LTQ Orbitrap XL™

Sample name : IV
Mode: ESI, M+H

C:\LTQ Orbitrap\...\IV_200225144517 2/27/2020 11:37:48 AM

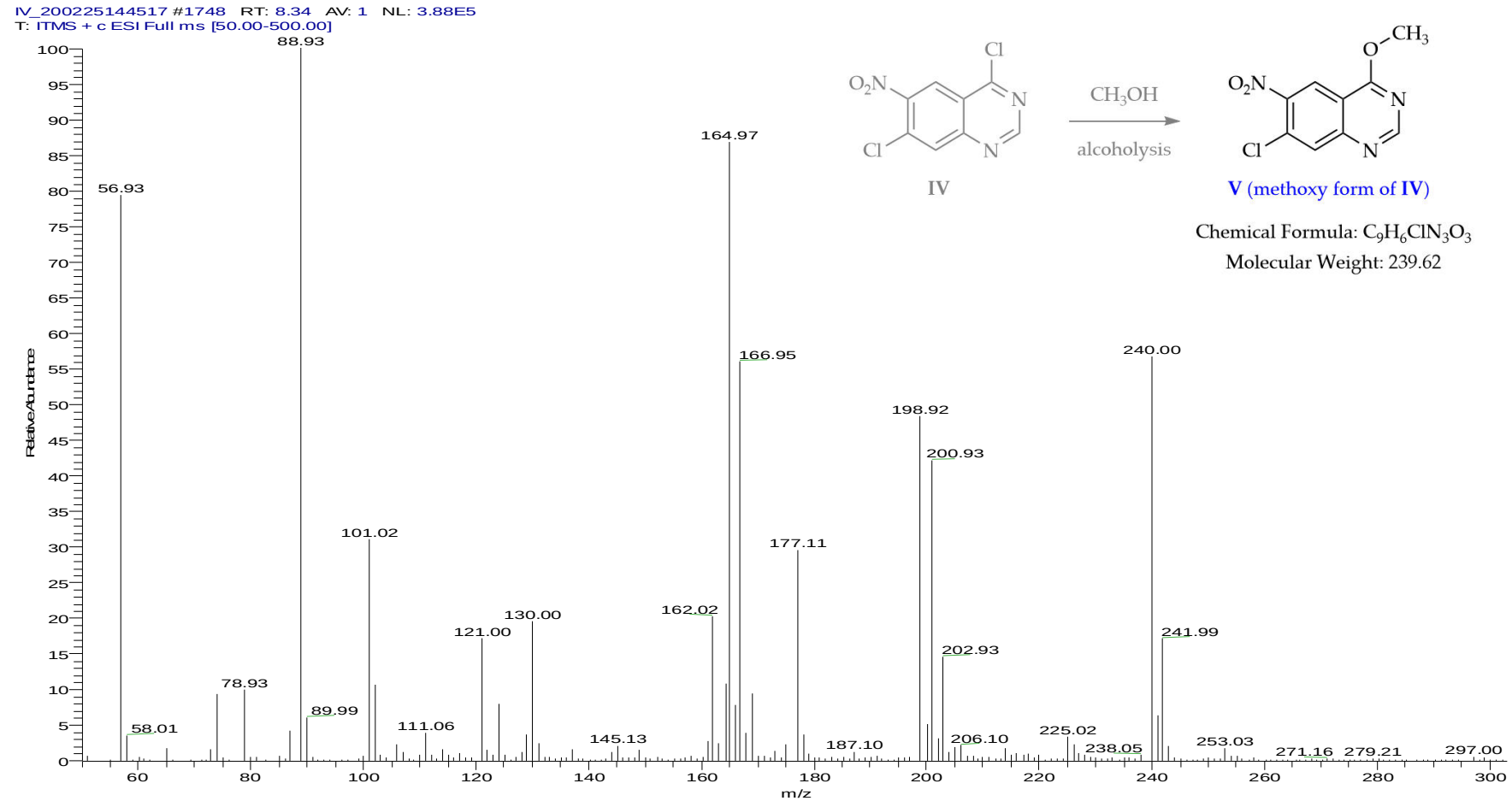

Figure S12: MS spectrum of compound 4,7-dichloro-6-nitroquinazoline (**IV**)

C:\LTQ Orbitrap\...\IV_200225144517 2/27/2020 11:37:48 AM

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m/z= 50.00-302.94

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106.04	8396.6	2.16
111.06	14913.6	3.84
114.01	6105.6	1.57
121.00	66231.7	17.06
122.03	5512.8	1.42
124.07	30870.1	7.95
129.07	13902.3	3.58
130.00	75993.3	19.58
131.06	9127.7	2.35
137.09	6124.6	1.58
145.13	7387.1	1.90
149.05	5487.4	1.41
161.09	10039.6	2.59
162.02	78349.6	20.18
163.10	9018.4	2.32
164.30	41534.2	10.70
164.97	336948.8	86.80
166.11	29994.5	7.73
166.95	217280.5	55.97
167.96	14732.6	3.80
168.95	36223.2	9.33
175.07	8801.7	2.27
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200.13	19600.2	5.05
200.93	163341.8	42.08
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202.93	56225.2	14.48
204.92	7011.2	1.81
206.10	7984.5	2.06
214.07	6630.9	1.71
225.02	12672.7	3.26
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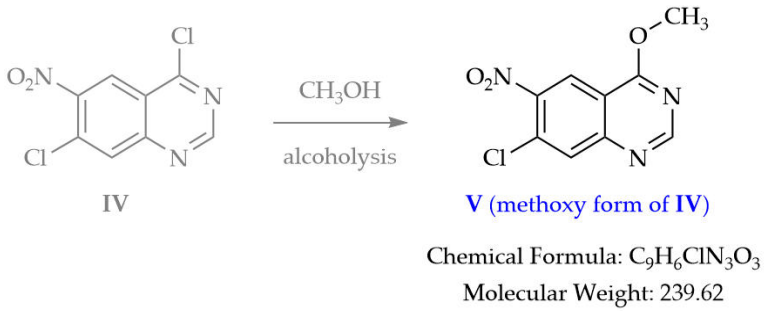
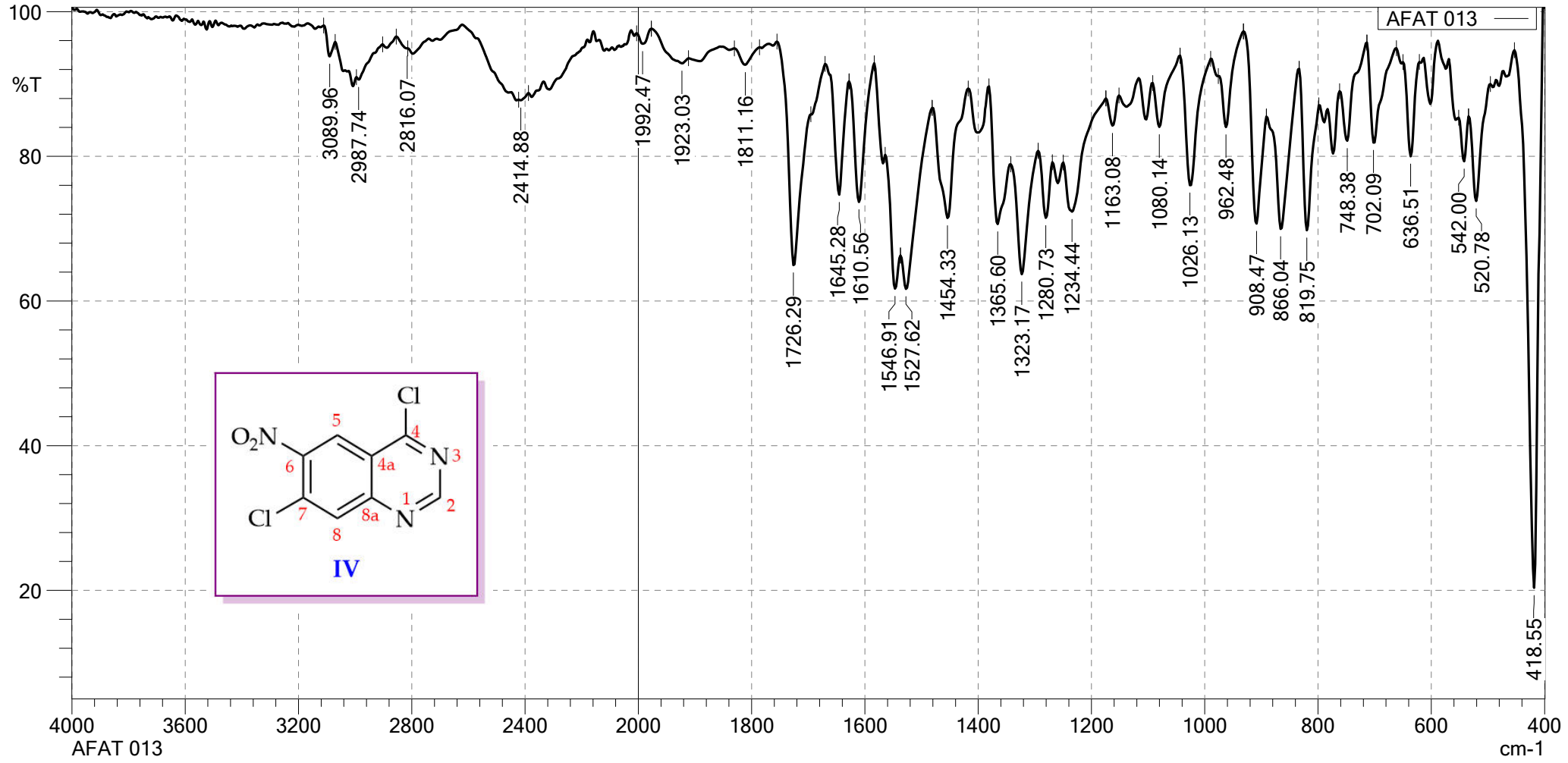


Figure S12: MS spectrum of compound 4,7-dichloro-6-nitroquinazoline (**IV**)



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Atmosphere Correction: OFF

Figure S13: FT-IR spectrum of compound 4,7-dichloro-6-nitroquinazoline (**IV**)

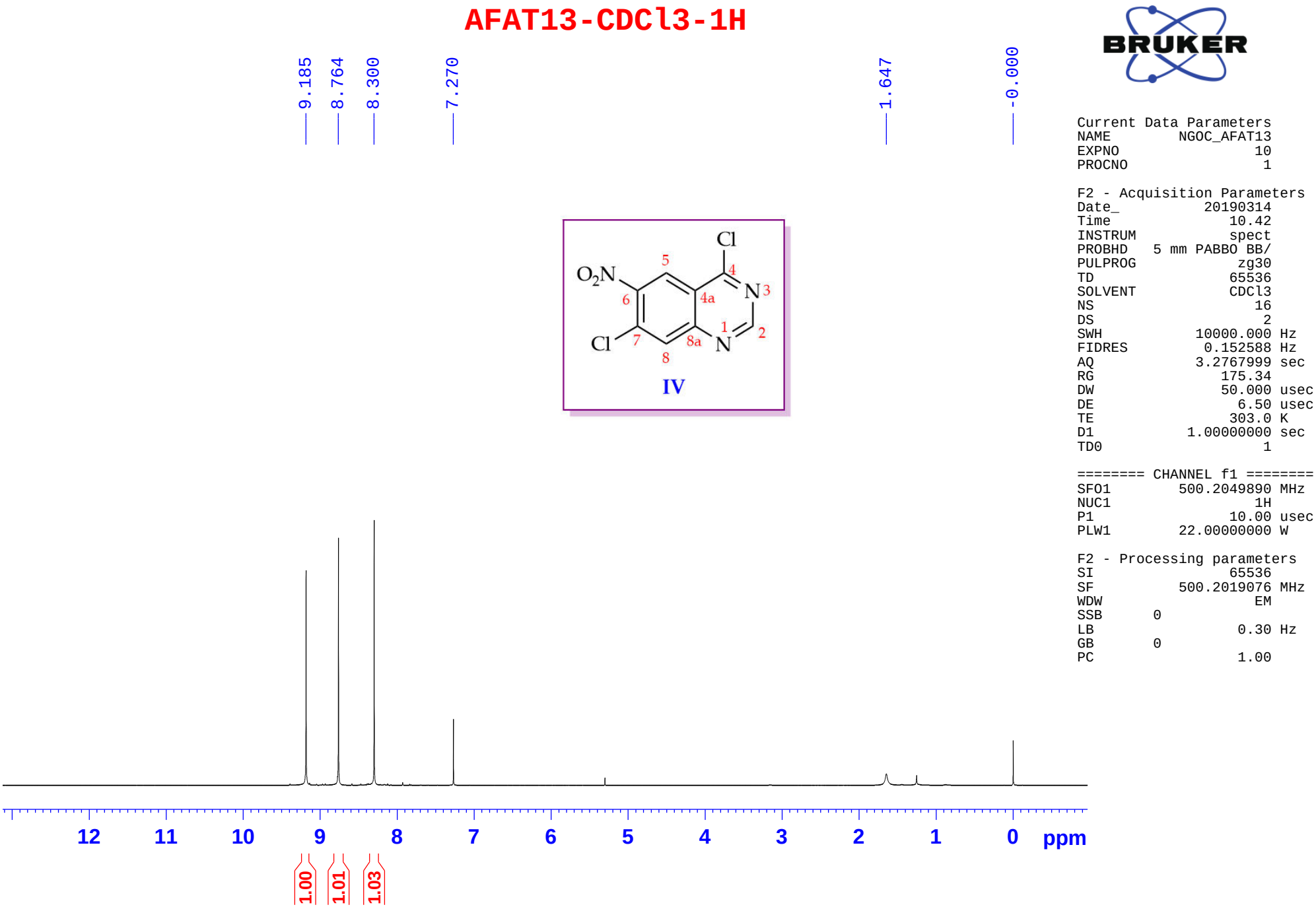


Figure S14: ^{1}H-NMR spectrum of compound 4,7-dichloro-6-nitroquinazoline (**IV**)

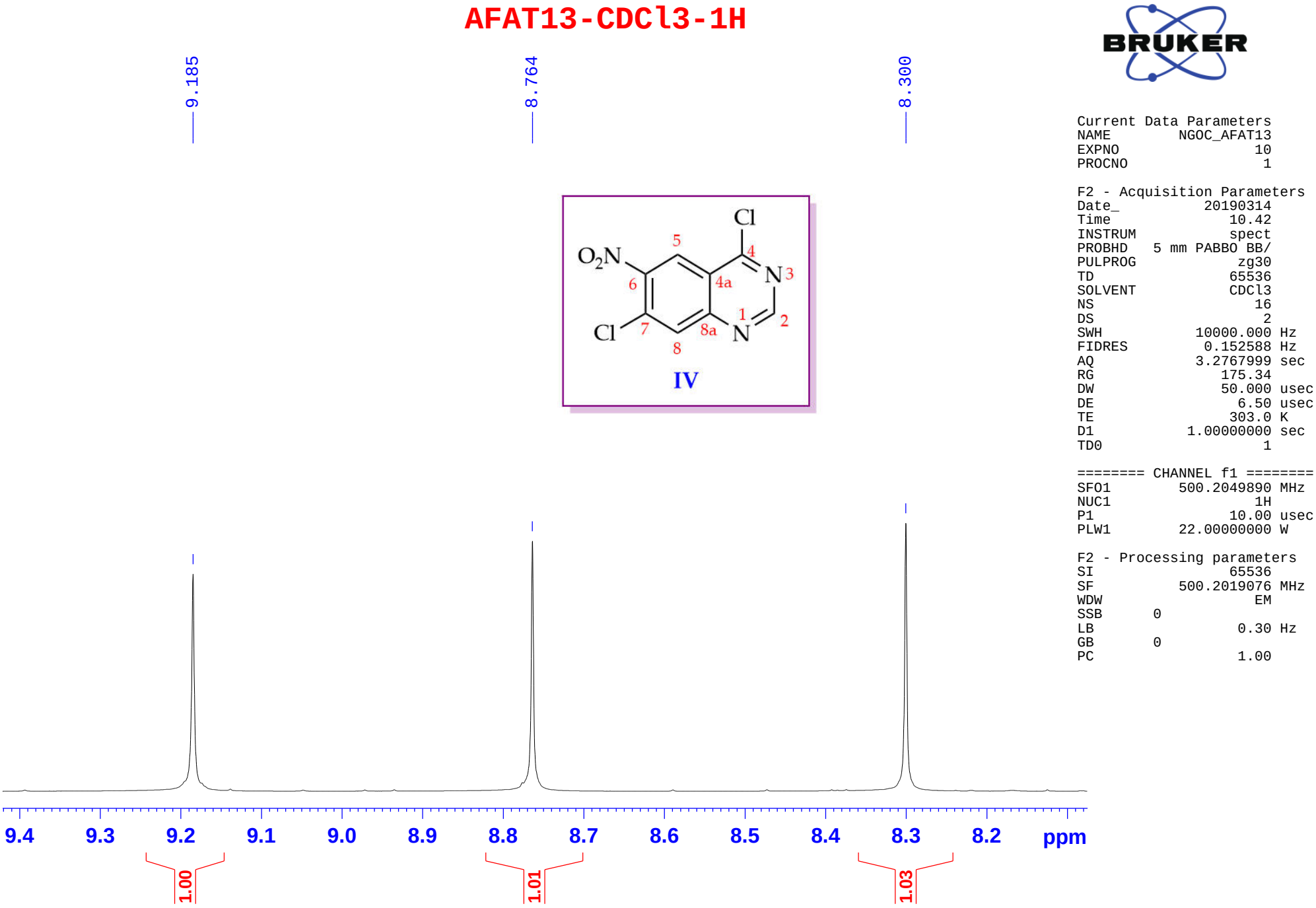
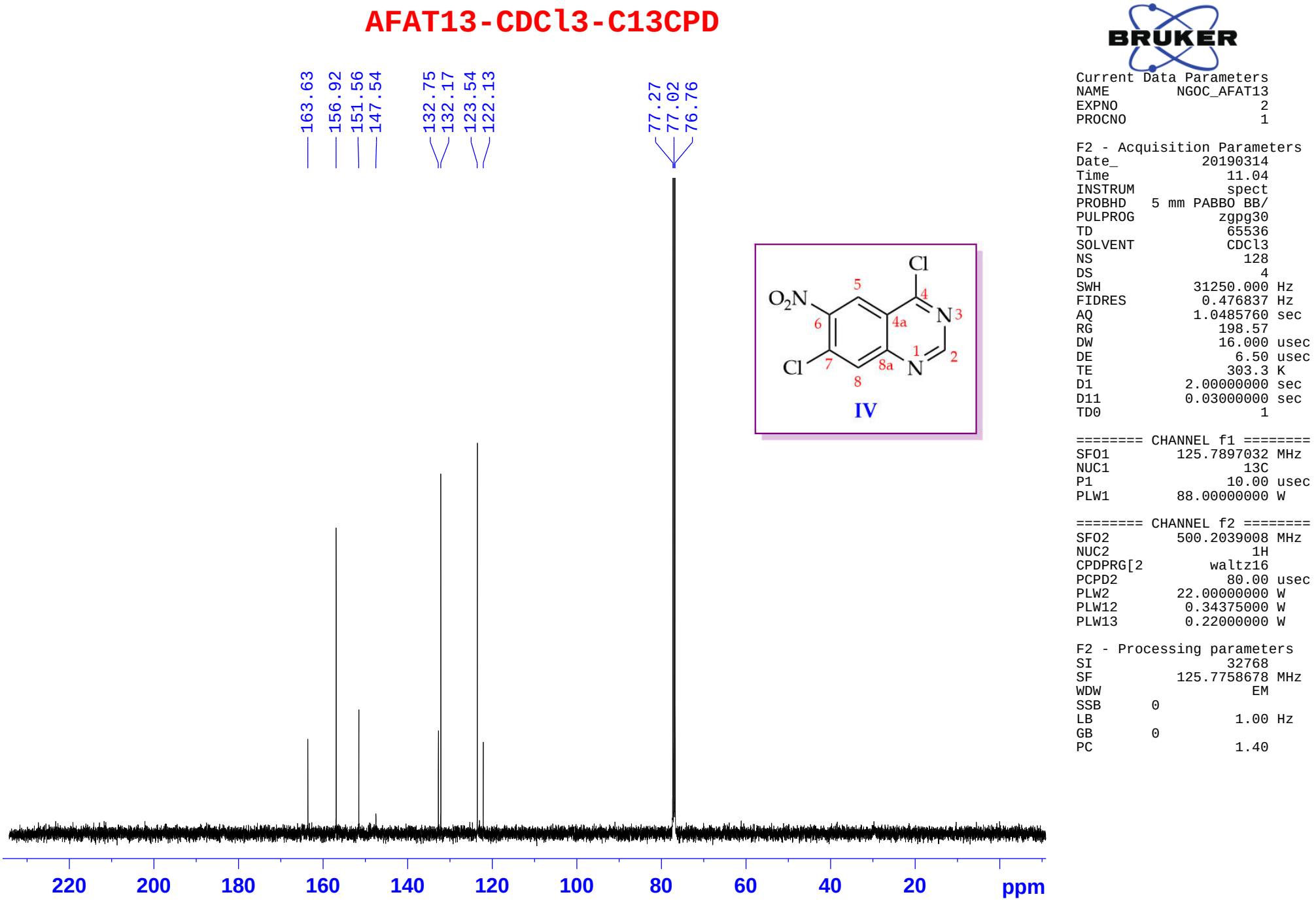


Figure S14: ^{1}H-NMR spectrum of compound 4,7-dichloro-6-nitroquinazoline (**IV**)

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NS                  128
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FIDRES         0.476837 Hz
AQ            1.0485760 sec
RG               198.57
DW               16.000 usec
DE                6.50 usec
TE               303.3 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

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NUC1               13C
P1               10.00 usec
PLW1        88.00000000 W

======== CHANNEL f2 ========
SFO2        500.2039008 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2        22.00000000 W
PLW12        0.34375000 W
PLW13        0.22000000 W

F2 - Processing parameters
SI                32768
SF          125.7758678 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```

Figure S15: ^{13}C-NMR spectrum of compound 4,7-dichloro-6-nitroquinazoline (**IV**)

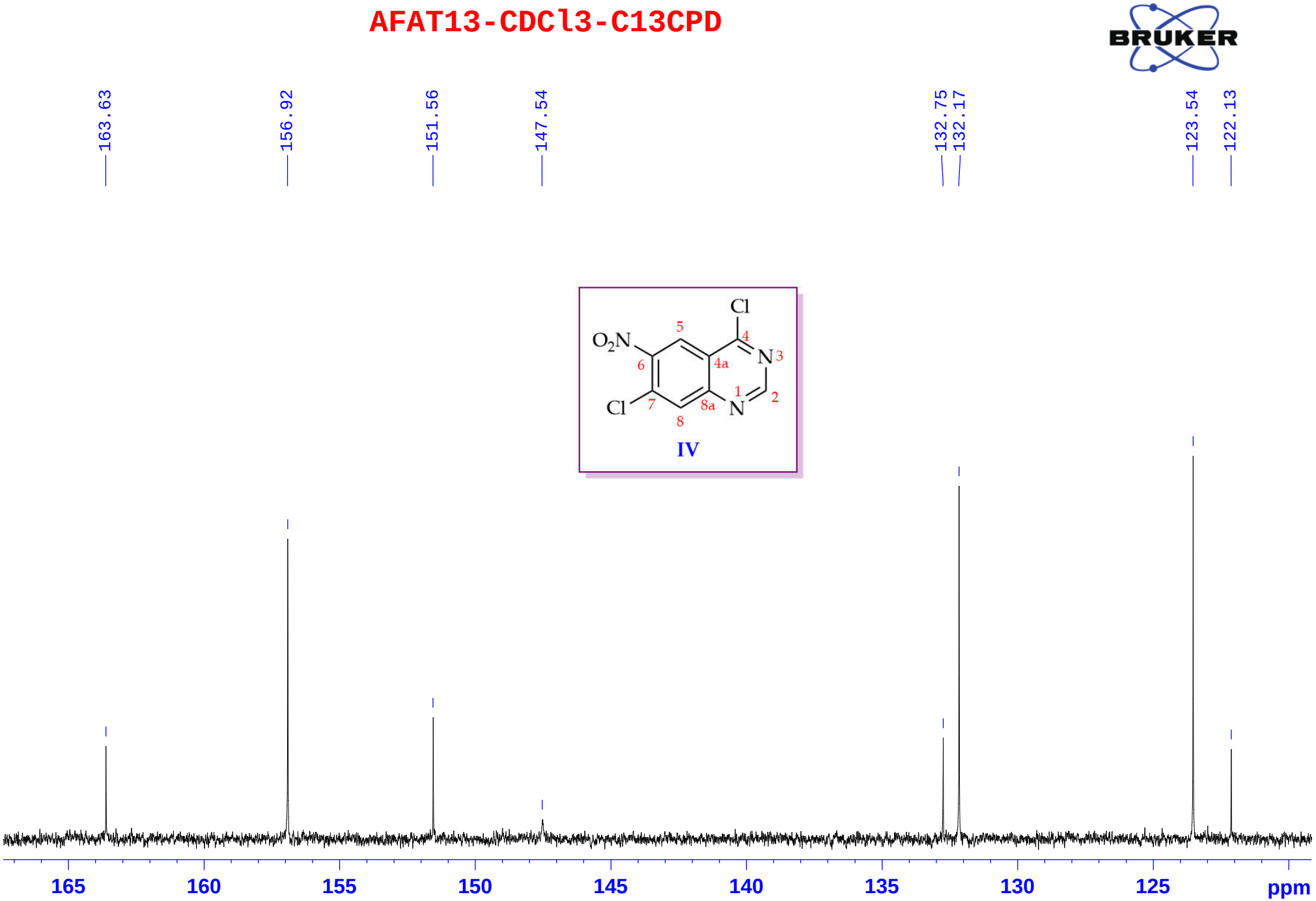

Figure S15: ^{13}C-NMR spectrum of compound 4,7-dichloro-6-nitroquinazoline (**IV**)