

Supplementary Information to:

The oxime ethers with heterocyclic, alicyclic and aromatic moiety as potential anti-cancer agents

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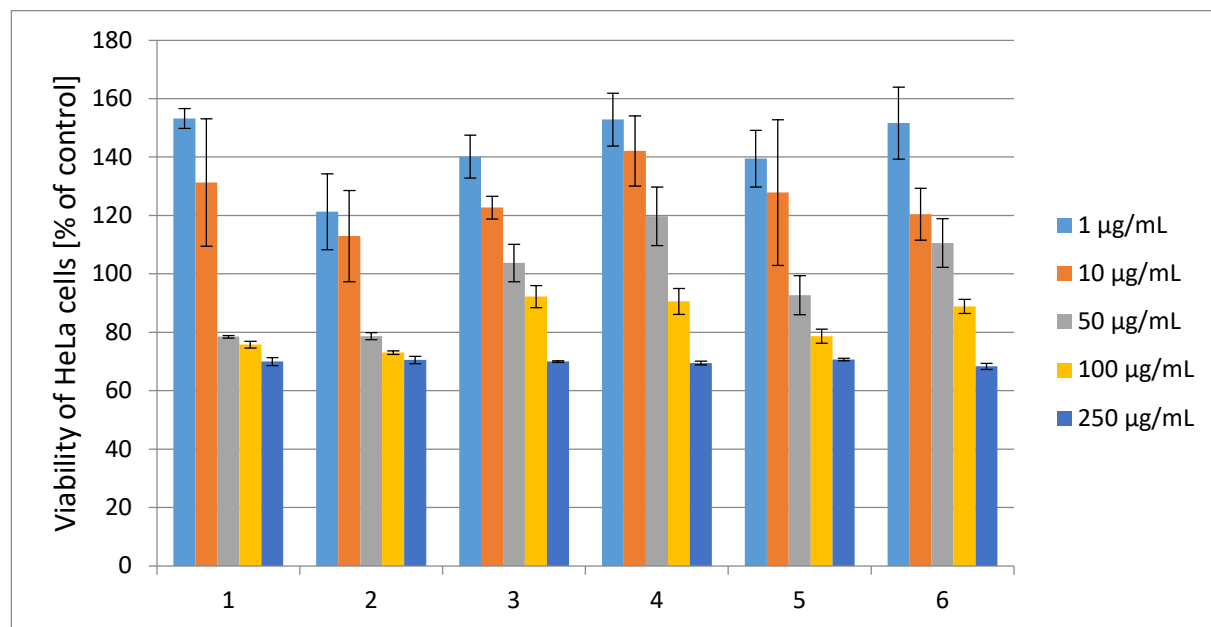
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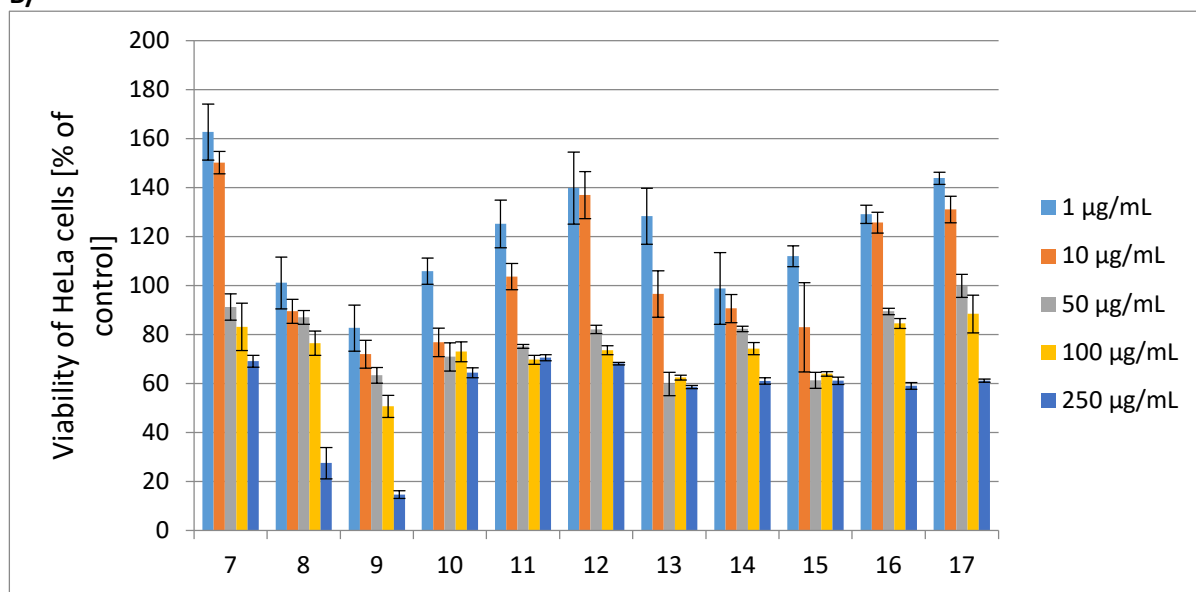
³ Nicolaus Copernicus University in Toruń, Collegium Medicum in Bydgoszcz, Faculty of Medicine, Department of Medical Biology and Biochemistry, Karłowicza 24, 85–092 Bydgoszcz, Poland; dariak@cm.umk.pl

S1. The cytotoxicity evaluation on HeLa cell culture after 24h of exposure to the compounds 1-27.

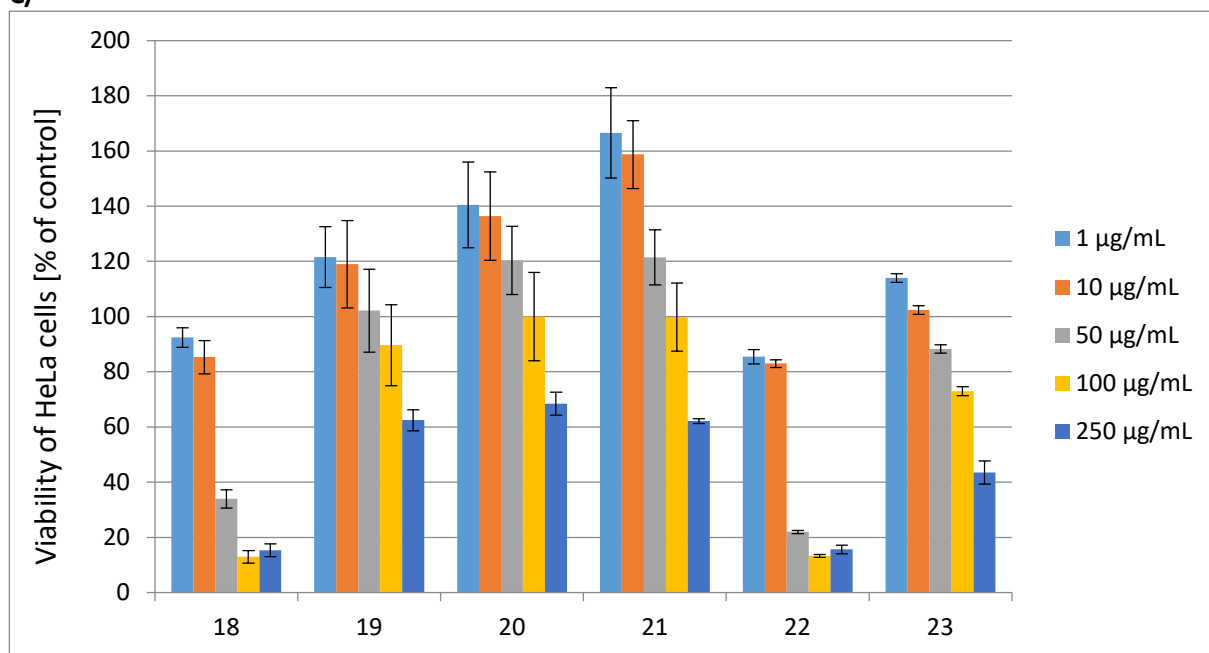
A/



B/



c/



D/

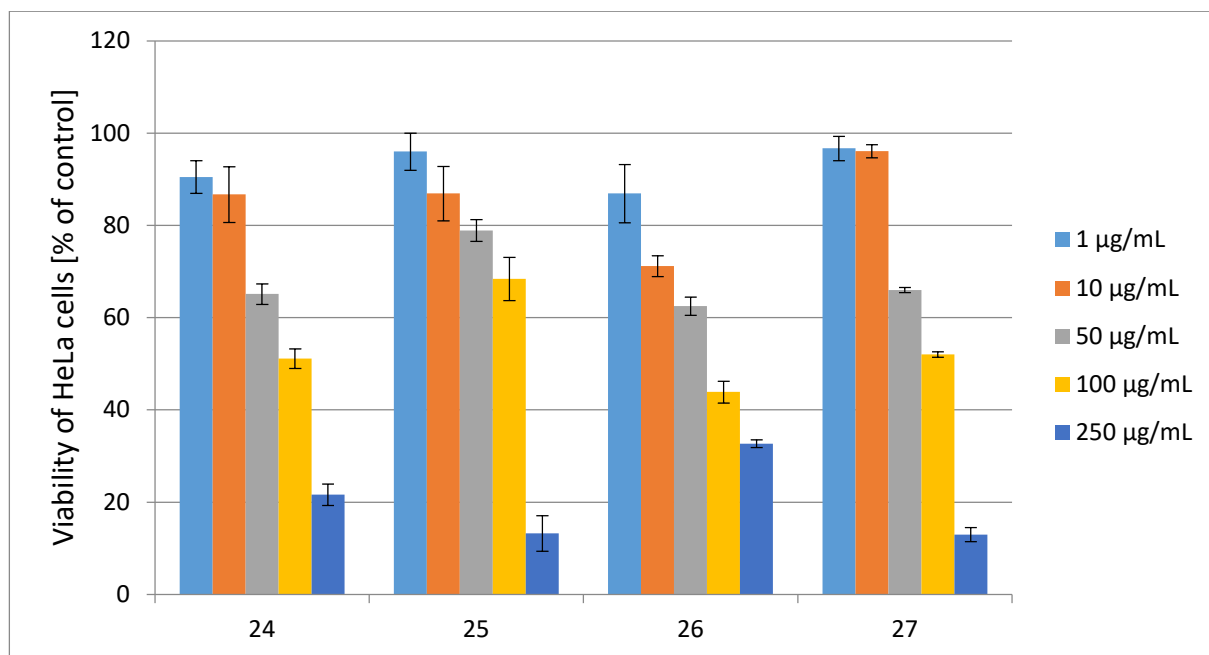
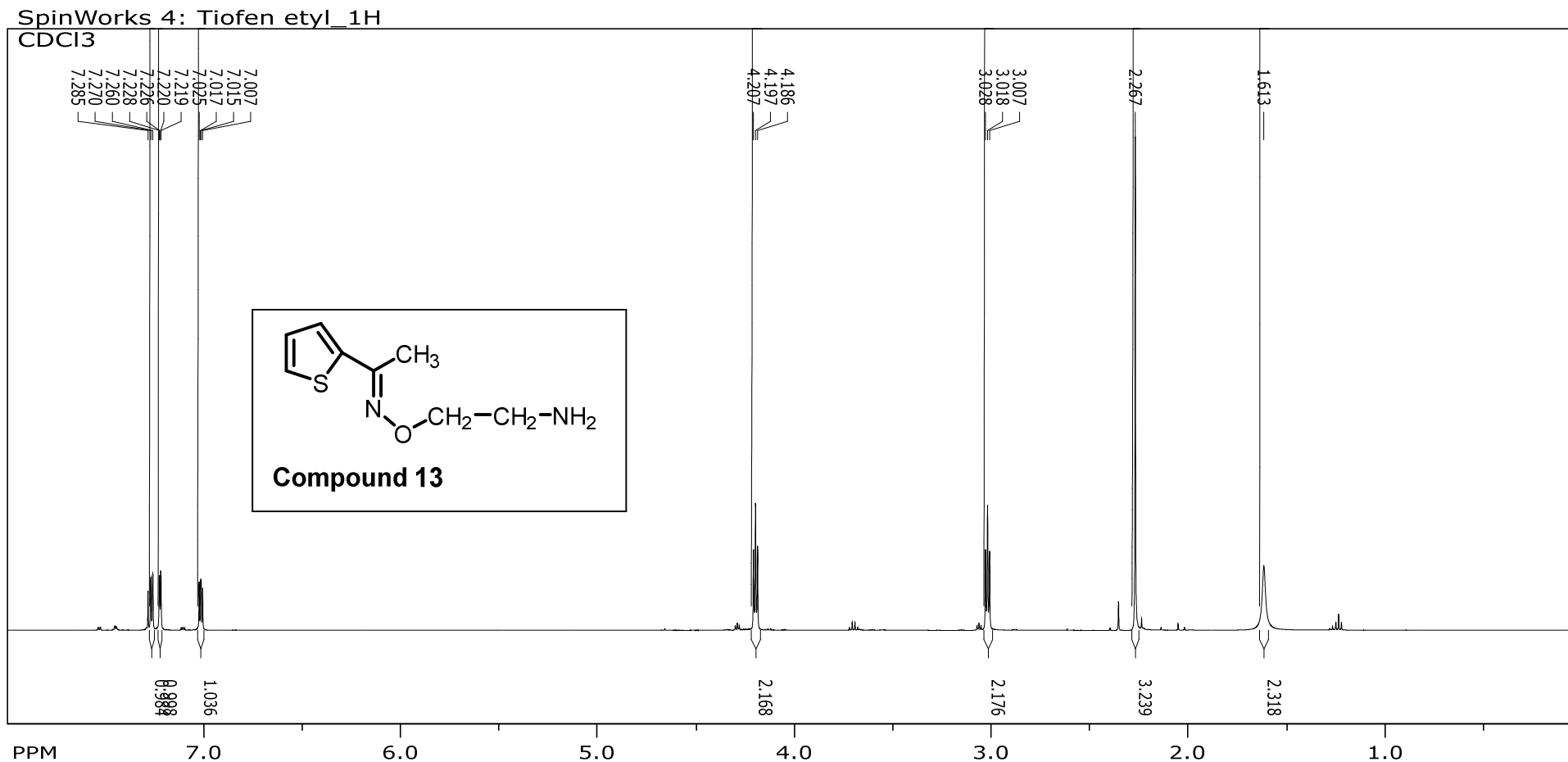


Figure S1. The cytotoxicity evaluation on HeLa cell culture after 24h of exposure to: A/ benzofuran oxime ethers (**1-5**) and 2-acetylbenzofuran oxime (**6**), B/ thiophene oxime ethers (**7-17**), C/ cyclohexanone and acetophenone oxime ethers (**18-23**), D/ thiazole and benzothiophene oxime ethers (**24-27**).

S2. Spectral data of the new synthesized compounds **13-15** and **24-27**.

Spectral data of the compound **13**.

^1H NMR spectrum of the compound **13**

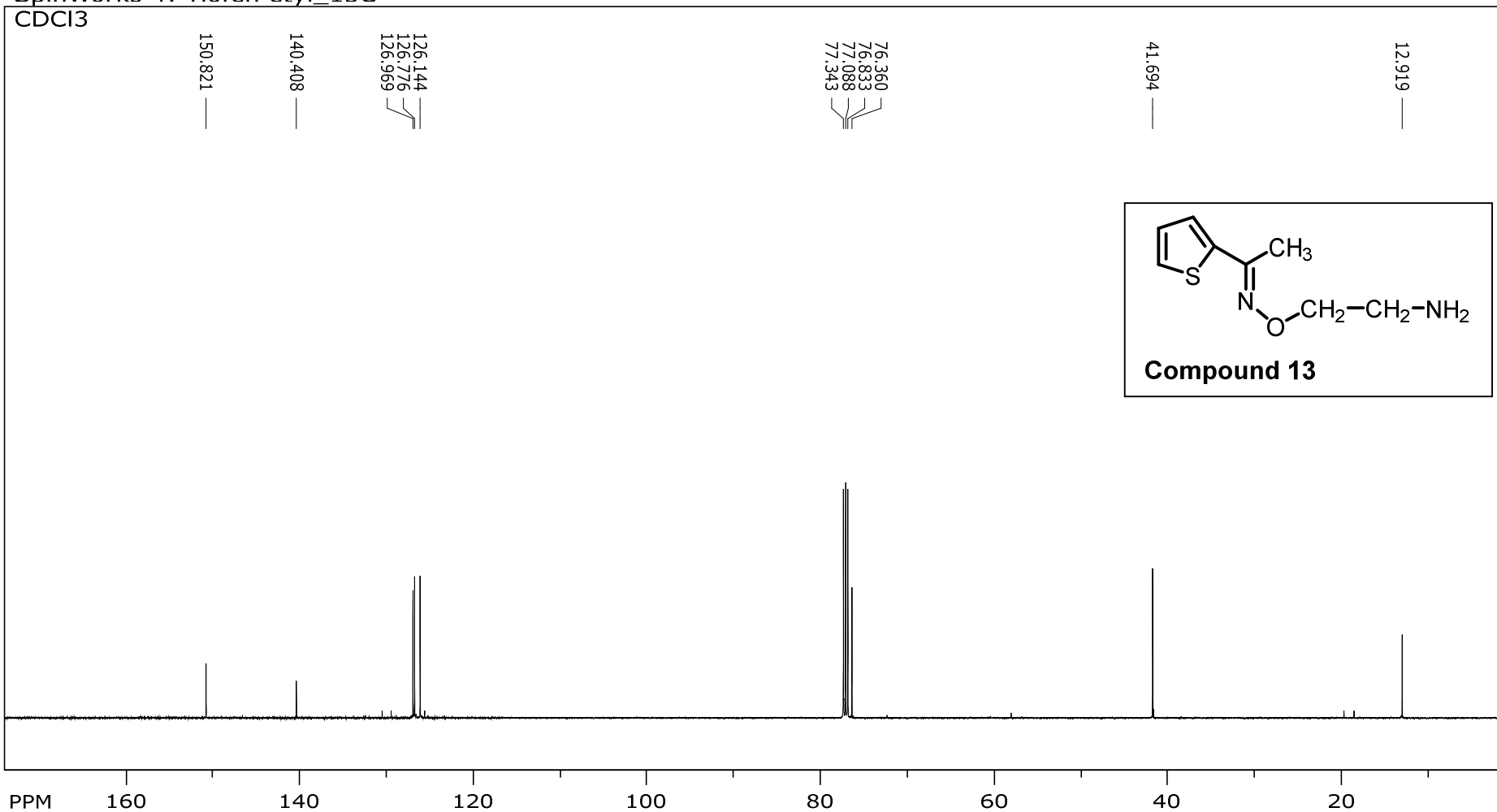


file: ...rs\user\Desktop\Widma 2022\3\3\fid expt: <zg30>
transmitter freq.: 500.255503 MHz
time domain size: 65536 points
width: 11520.74 Hz = 23.0297 ppm = 0.175793 Hz/pt
number of scans: 128

freq. of 0 ppm: 500.250000 MHz
processed size: 65536 complex points
LB: 0.300 GF: 0.0000

¹³C NMR spectrum of the compound **13**

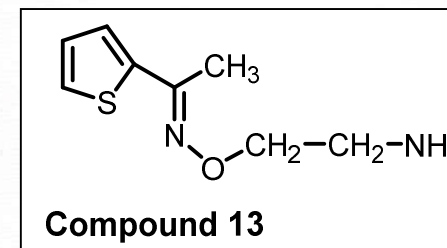
SpinWorks 4: Tiofen etyl_13C



file: ...rs\user\Desktop\Widma 2022\4\4\fid expt: <zgpg30>
transmitter freq.: 125.803057 MHz
time domain size: 65536 points
width: 32894.74 Hz = 261.4780 ppm = 0.501934 Hz/pt
number of scans: 1024

freq. of 0 ppm: 125.787963 MHz
processed size: 32768 complex points
LB: 1.000 GF: 0.0000

Mass spectrum of the compound 13



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 70.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions

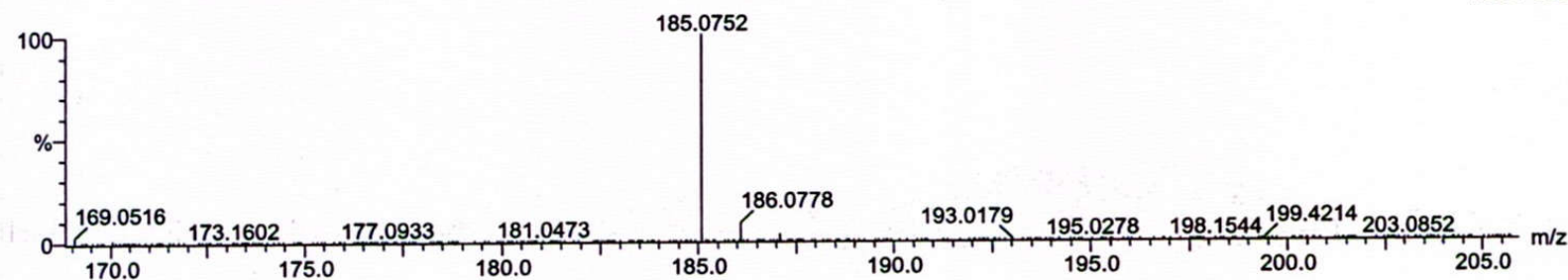
302 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 3-15 H: 0-25 N: 0-10 O: 0-10 S: 0-2

201009_Tiofen_etyl_NH2_A 42 (0.445) Cm (42:45)

TOF MS ES+
1.39e+006

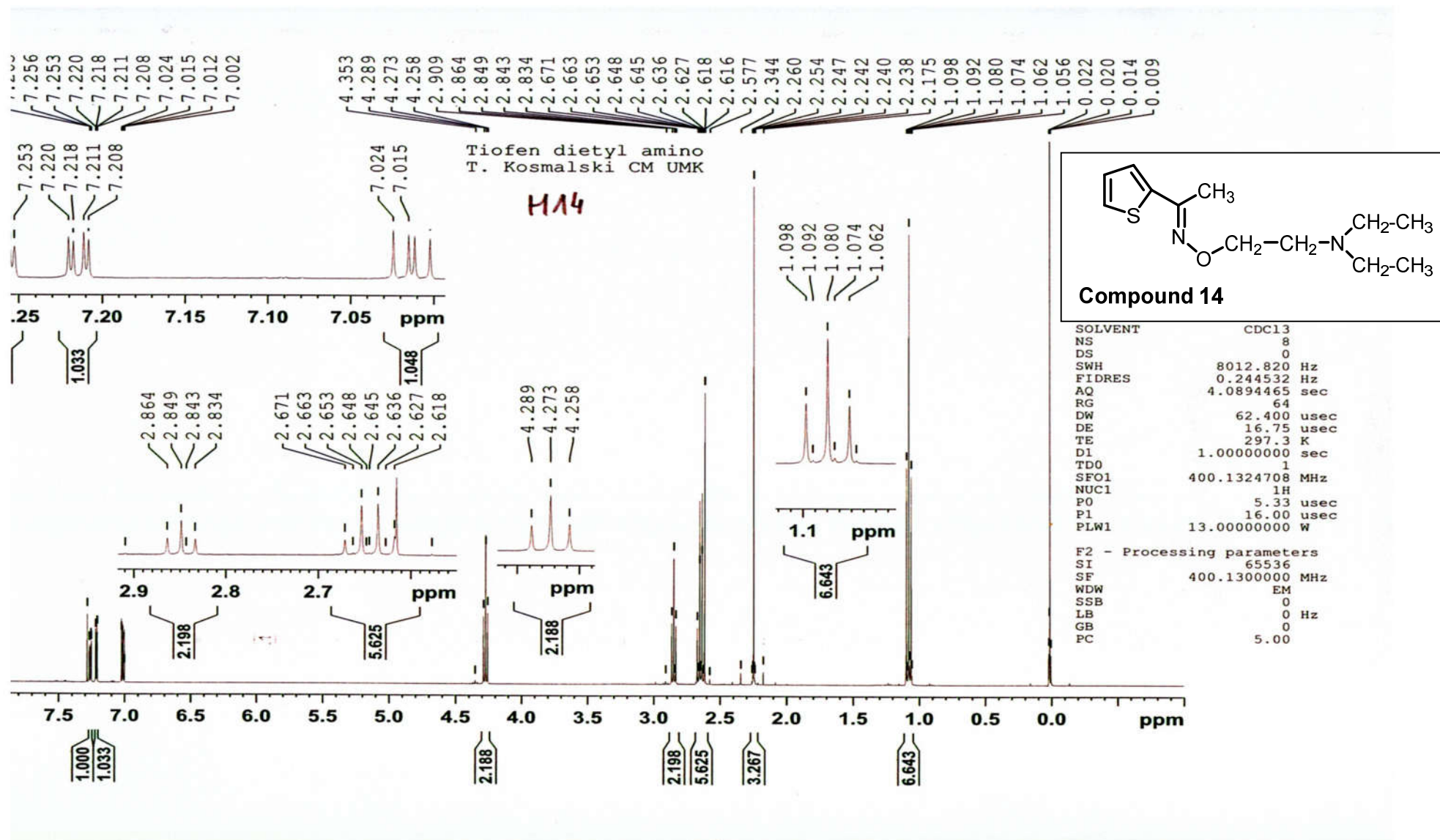


Minimum: -1.5
Maximum: 5.0 5.0 70.0

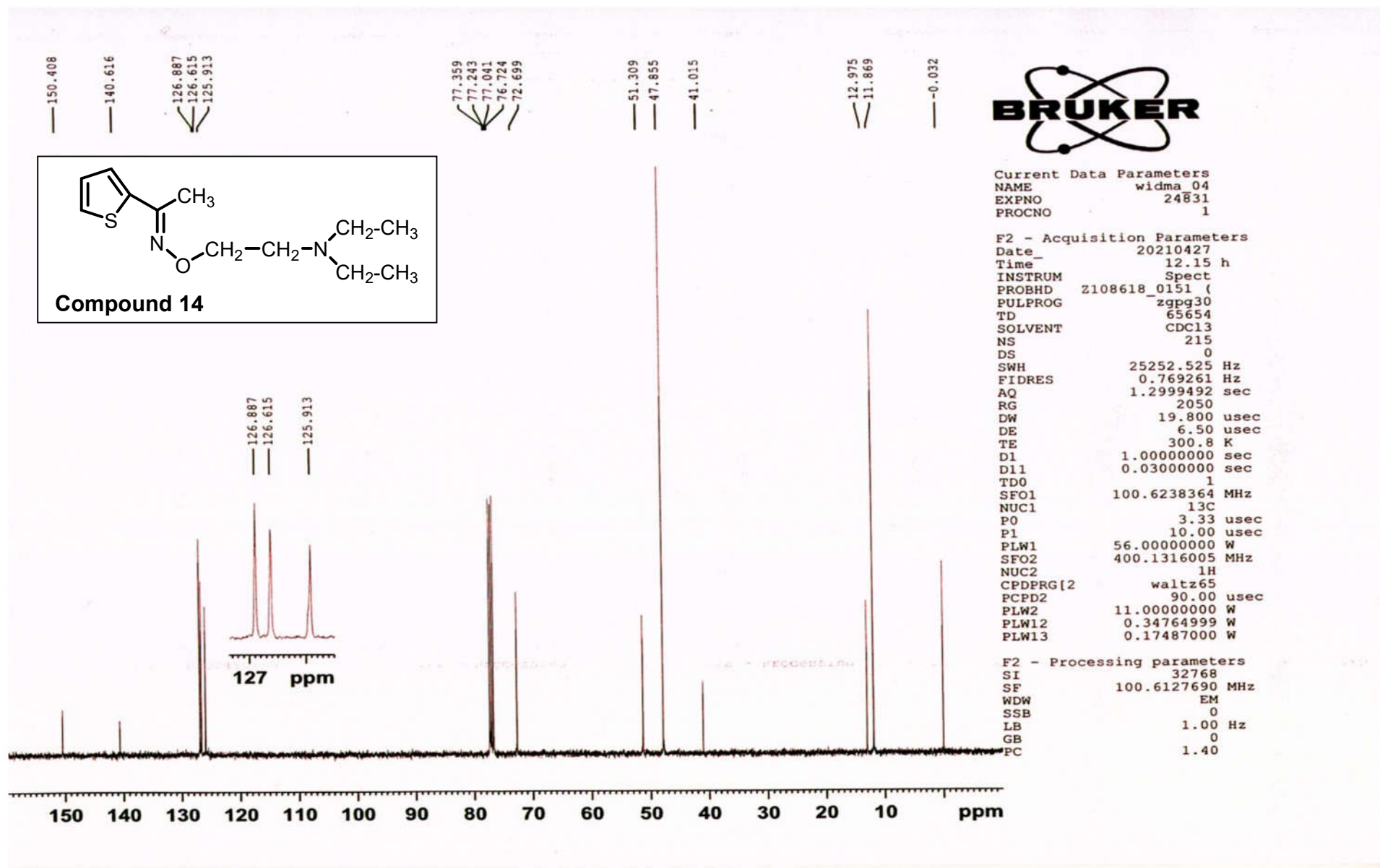
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
185.0752	185.0749	0.3	1.6	3.5	618.4	n/a	n/a	C8 H13 N2 O S

Spectral data of the compound **14**.

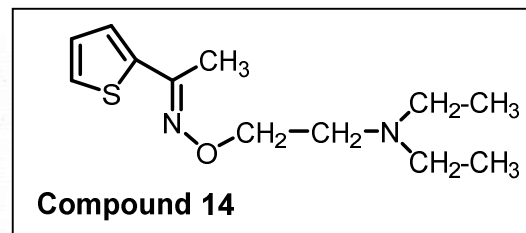
¹H NMR spectrum of the compound **14**



^{13}C NMR spectrum of the compound **14**



MS spectrum of the compound 14



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions

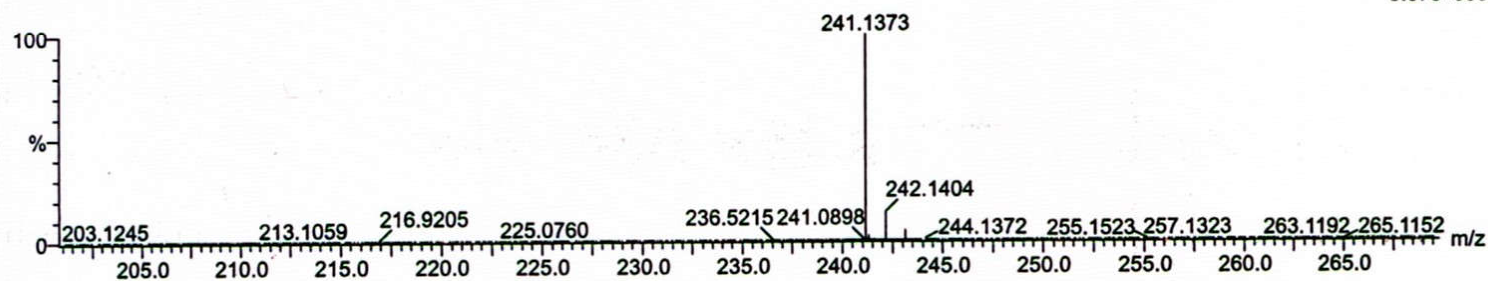
316 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-30 H: 0-50 N: 0-3 O: 0-10 S: 0-2

210427_Tiofen_dietylA 27 (0.294) Cm (27:30)

TOF MS ES+
9.07e+006

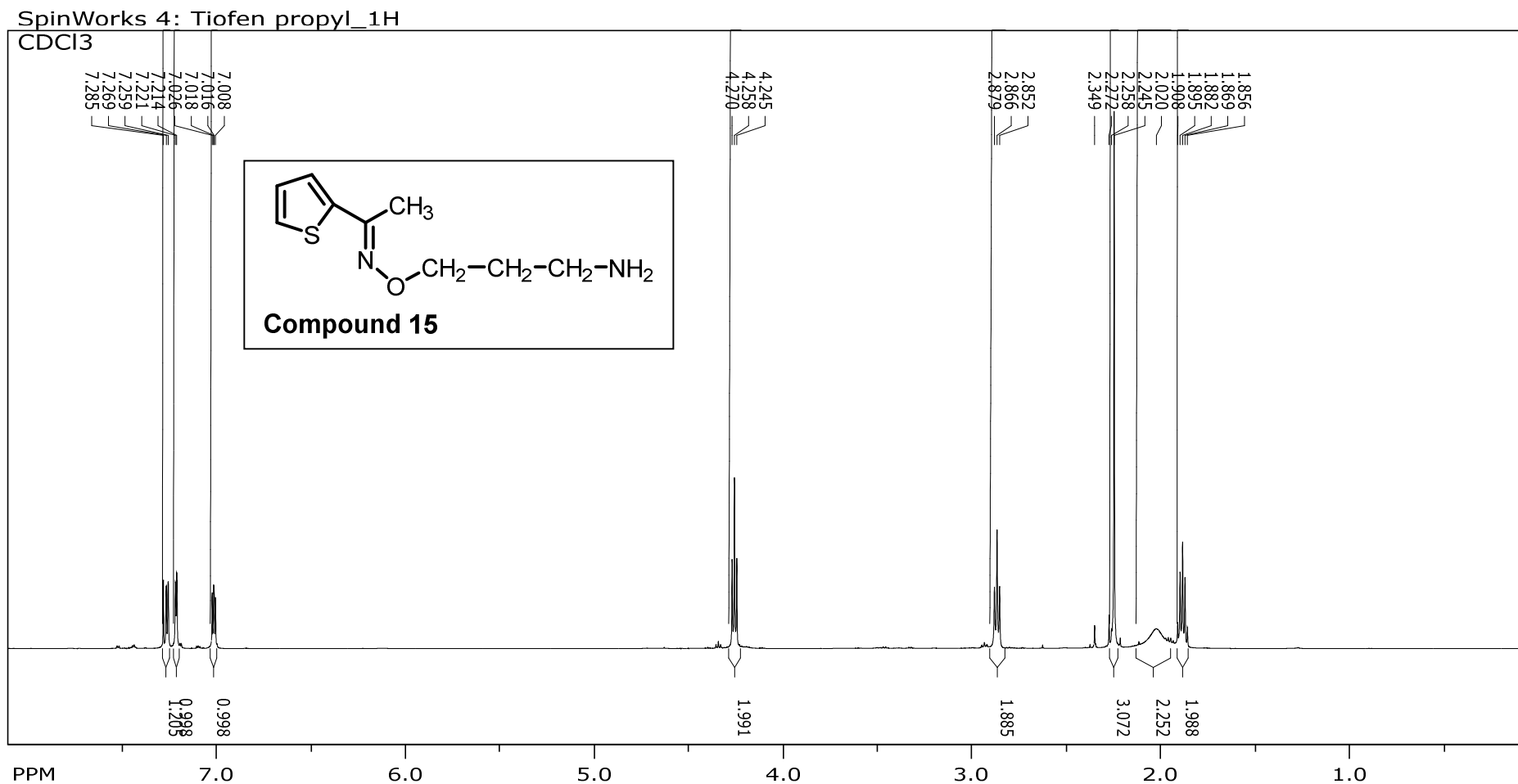


Minimum: -1.5
Maximum: 5.0 5.0 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
241.1373	241.1375	-0.2	-0.8	3.5	1254.5	n/a	n/a	C12 H21 N2 O S

Spectral data of the compound **15**.

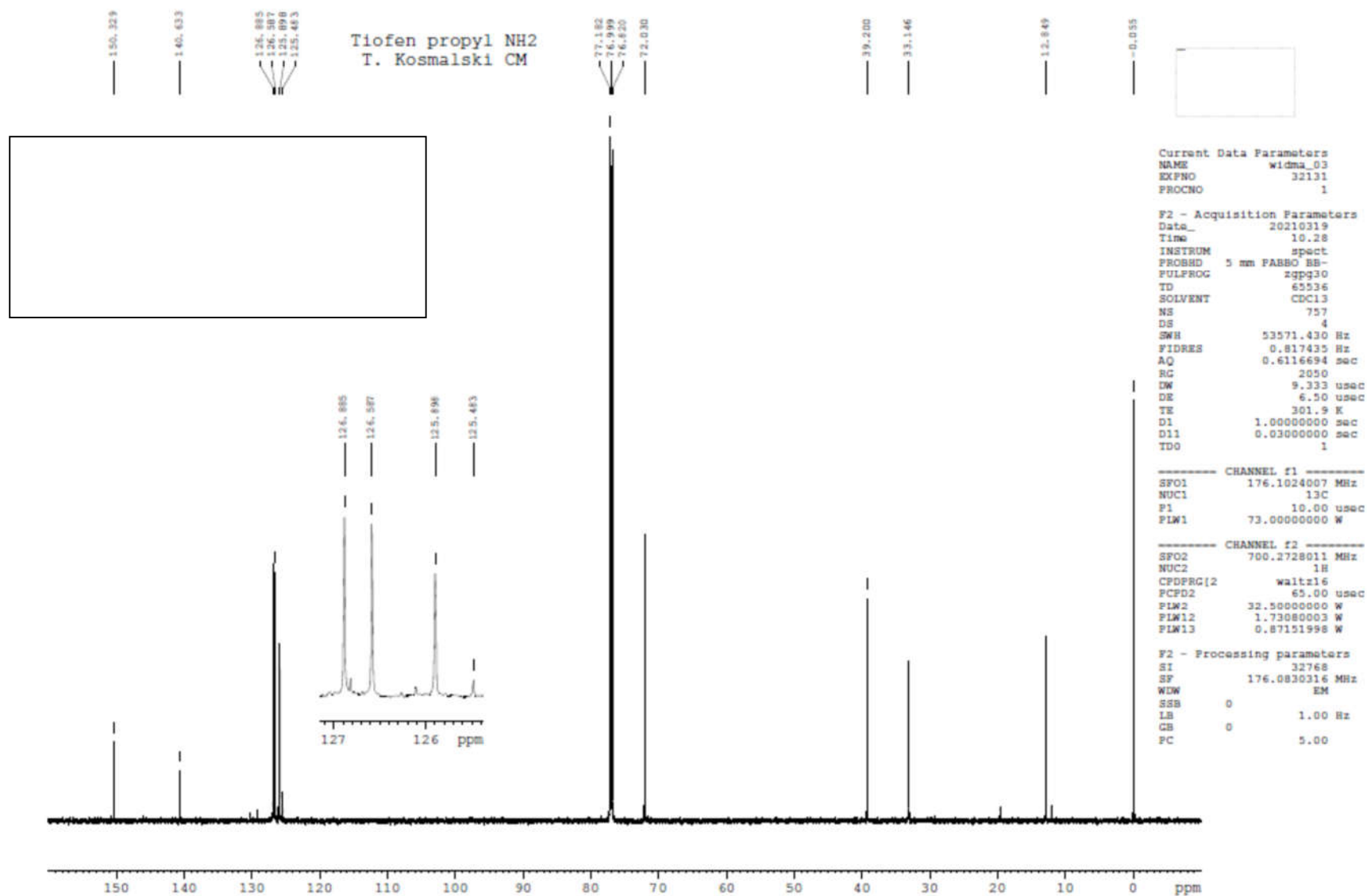
^1H NMR spectrum of the compound **15**



file: ...rs\user\Desktop\Widma 2022\5\5\fid expt: <zg30>
transmitter freq.: 500.255503 MHz
time domain size: 65536 points
width: 11520.74 Hz = 23.0297 ppm = 0.175793 Hz/pt
number of scans: 128

freq. of 0 ppm: 500.250000 MHz
processed size: 65536 complex points
LB: 0.300 GF: 0.0000

^{13}C NMR spectrum of the compound **15**



MS spectrum of the compound 15

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 70.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 9

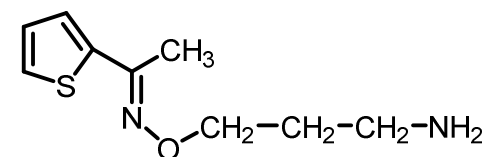
Monoisotopic Mass, Even Electron Ions

384 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

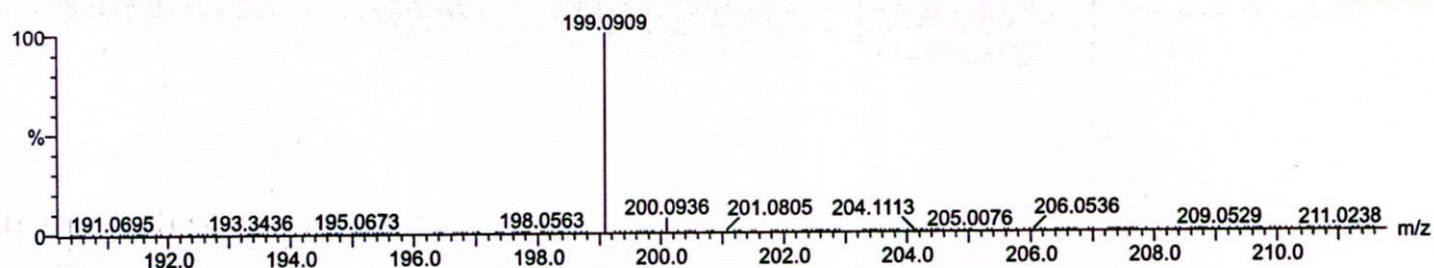
C: 3-40 H: 0-40 N: 0-10 O: 0-10 S: 0-2

201009_Tiofen_propyl_NH2_A 31 (0.328) Cm (31:39-4:8)



Compound 15

TOF MS ES+
6.80e+005

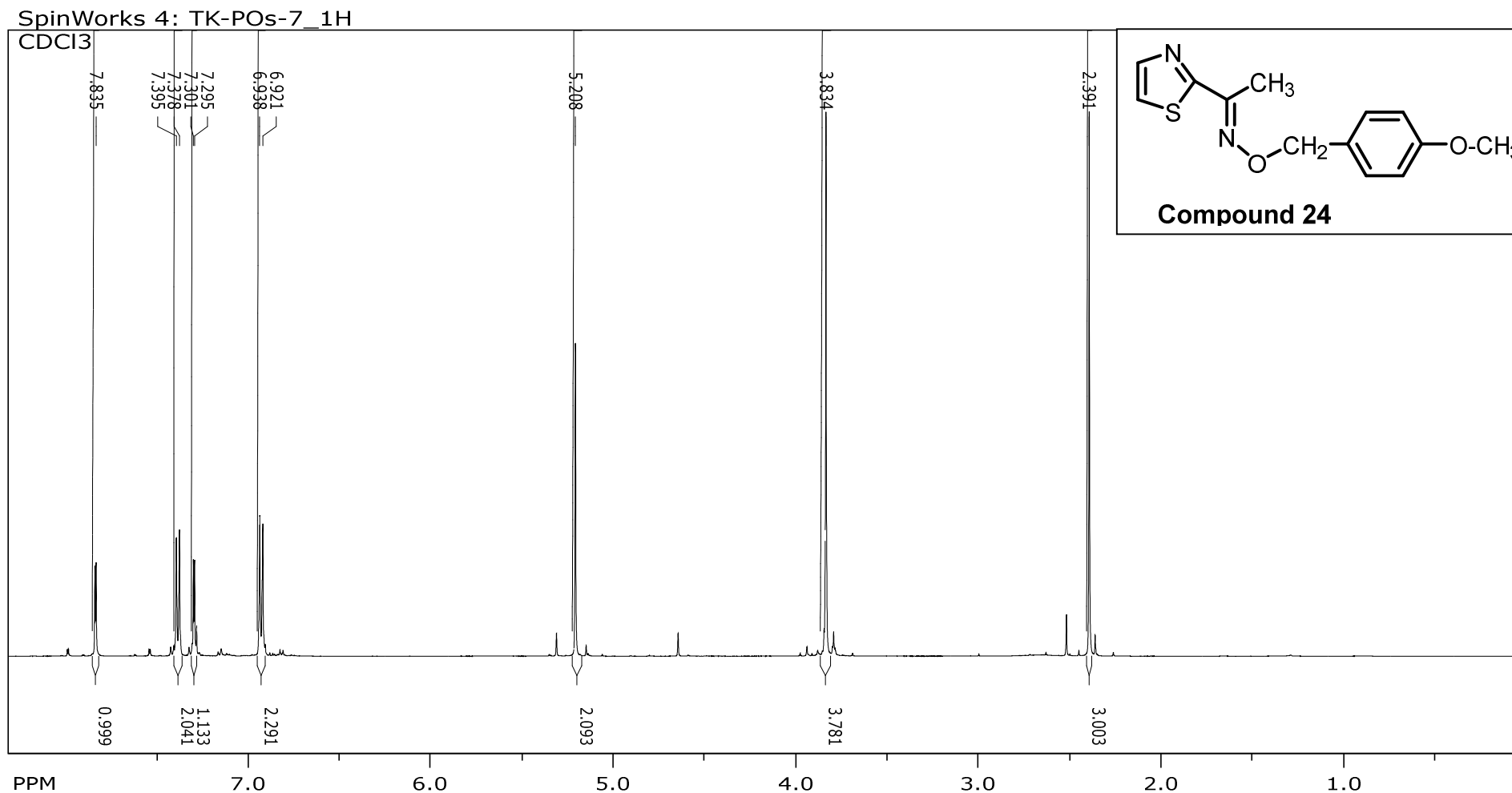


Minimum: -1.5
Maximum: 5.0 5.0 70.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
199.0909	199.0905	0.4	2.0	3.5	841.4	n/a	n/a	C9 H15 N2 O S

Spectral data of the compound **24**.

^1H NMR spectrum of the compound **24**

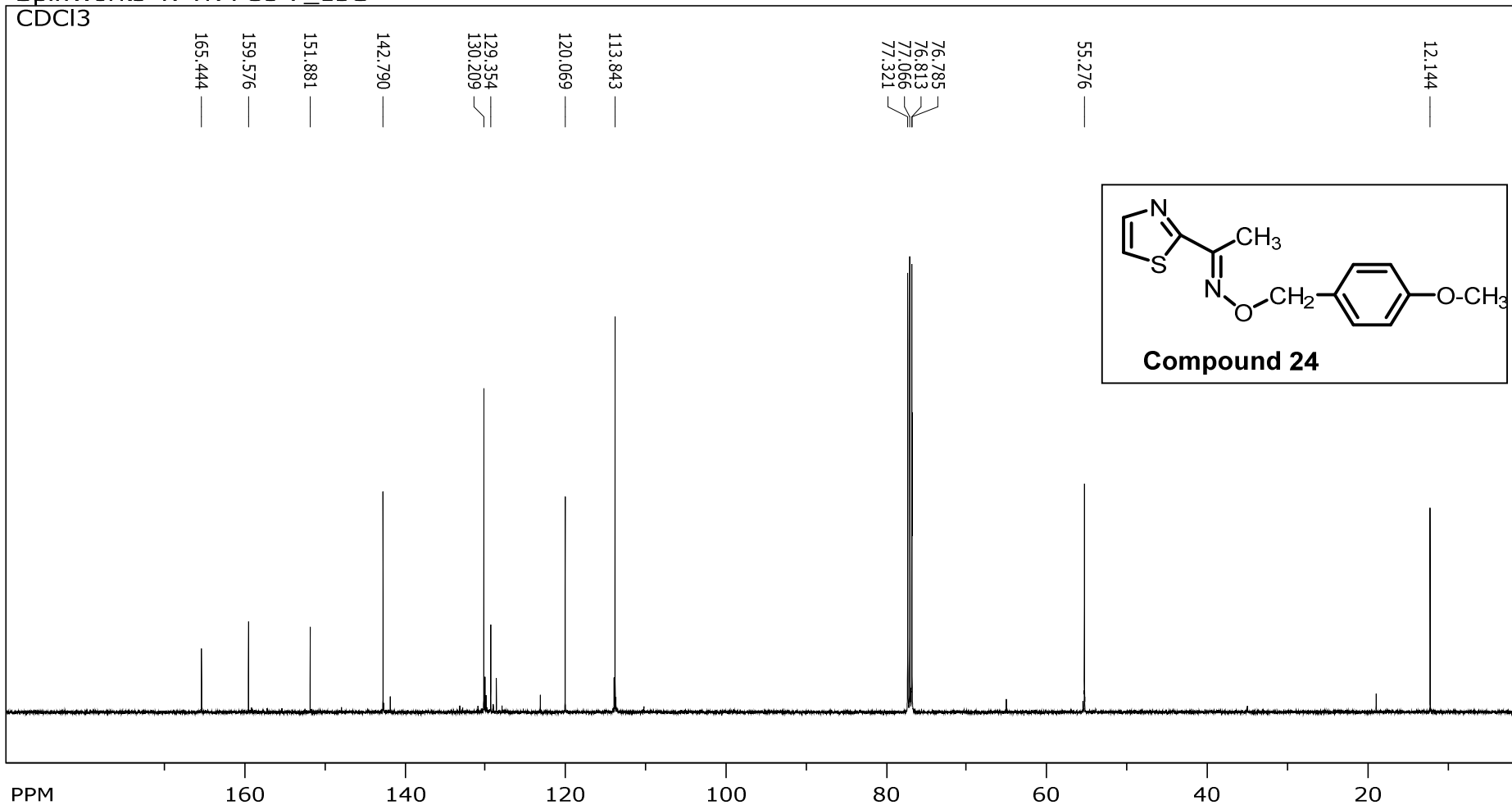


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transmitter freq.: 500.255003 MHz
time domain size: 65536 points
width: 11029.41 Hz = 22.0476 ppm = 0.168295 Hz/pt
number of scans: 128

freq. of 0 ppm: 500.250000 MHz
processed size: 65536 complex points
LB: 0.300 GF: 0.0000

¹³C NMR spectrum of the compound **24**

SpinWorks 4: TK-POs-7_13C



file: ...ers\user\Desktop\Widma 2021\36\fid expt: <zpgg30>
transmitter freq.: 125.803057 MHz
time domain size: 65536 points
width: 31250.00 Hz = 248.4041 ppm = 0.476837 Hz/pt
number of scans: 1024

freq. of 0 ppm: 125.787963 MHz
processed size: 32768 complex points
LB: 1.000 GF: 0.0000

MS spectrum of the compound **24**

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 9

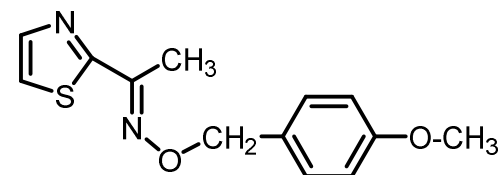
Monoisotopic Mass, Even Electron Ions

96 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

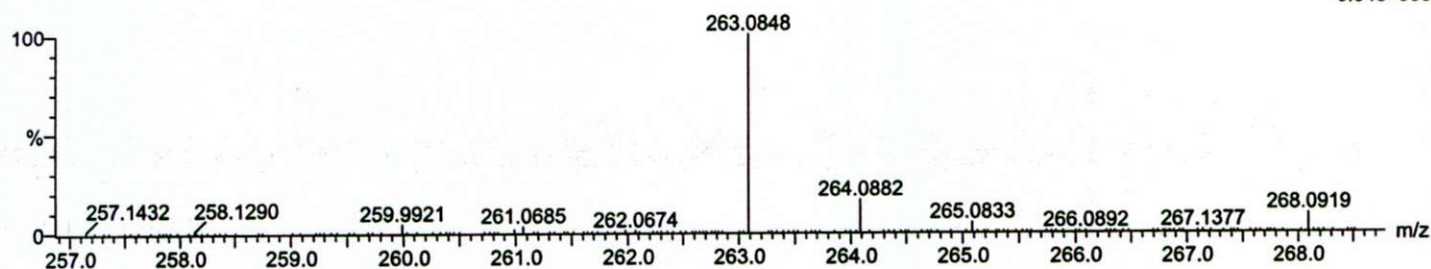
C: 0-30 H: 0-30 N: 0-2 O: 0-5 S: 1-2

210901_Tiazol_4_OMeA 20 (0.223) Cm (20:25-4:8)



Compound 24

TOF MS ES+
6.54e+005

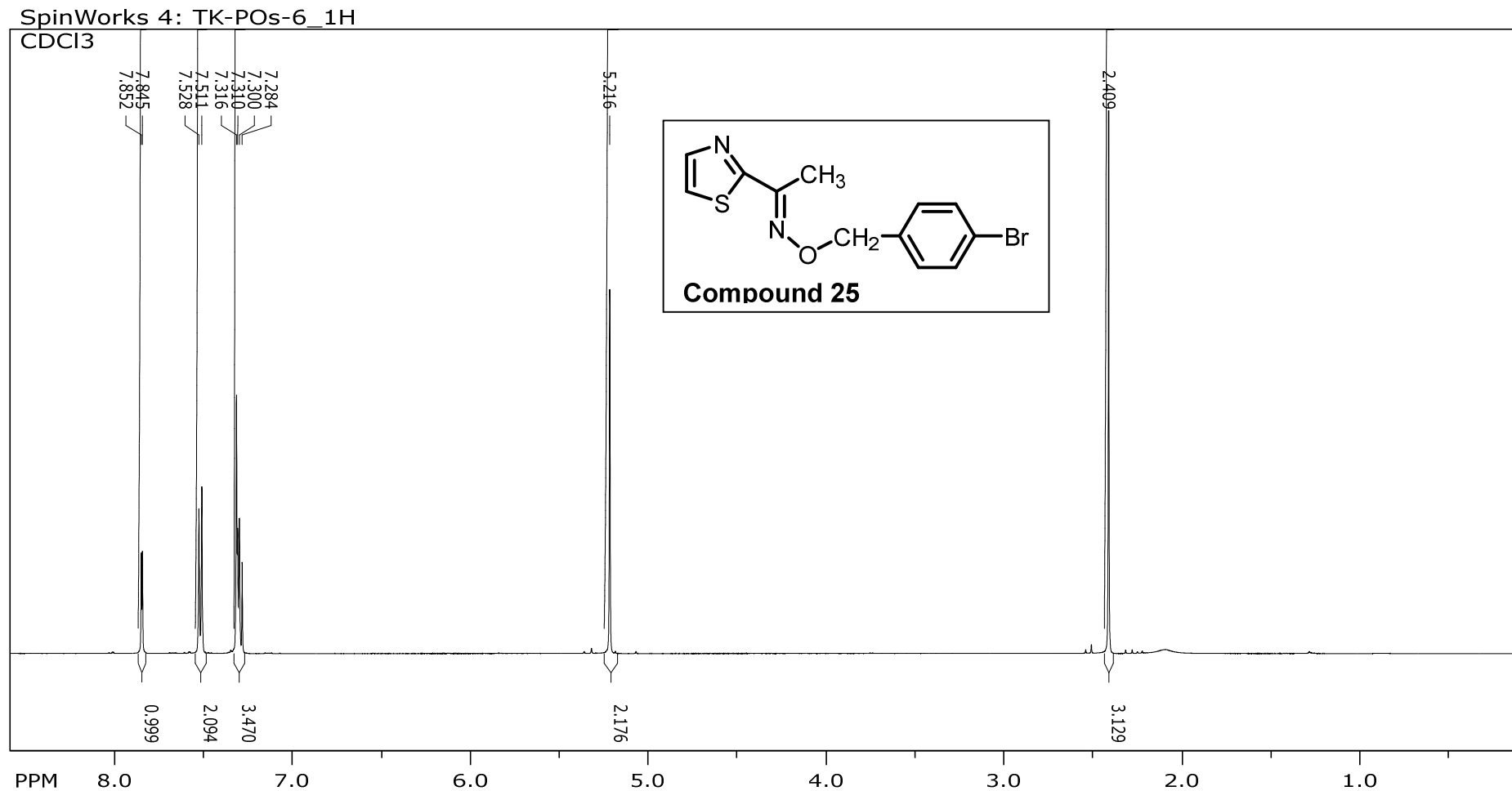


Minimum: -1.5
Maximum: 5.0 5.0 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
263.0848	263.0854	-0.6	-2.3	7.5	787.9	n/a	n/a	C13 H15 N2 O2 S

Spectral data of the compound **25**.

^1H NMR spectrum of the compound **25**



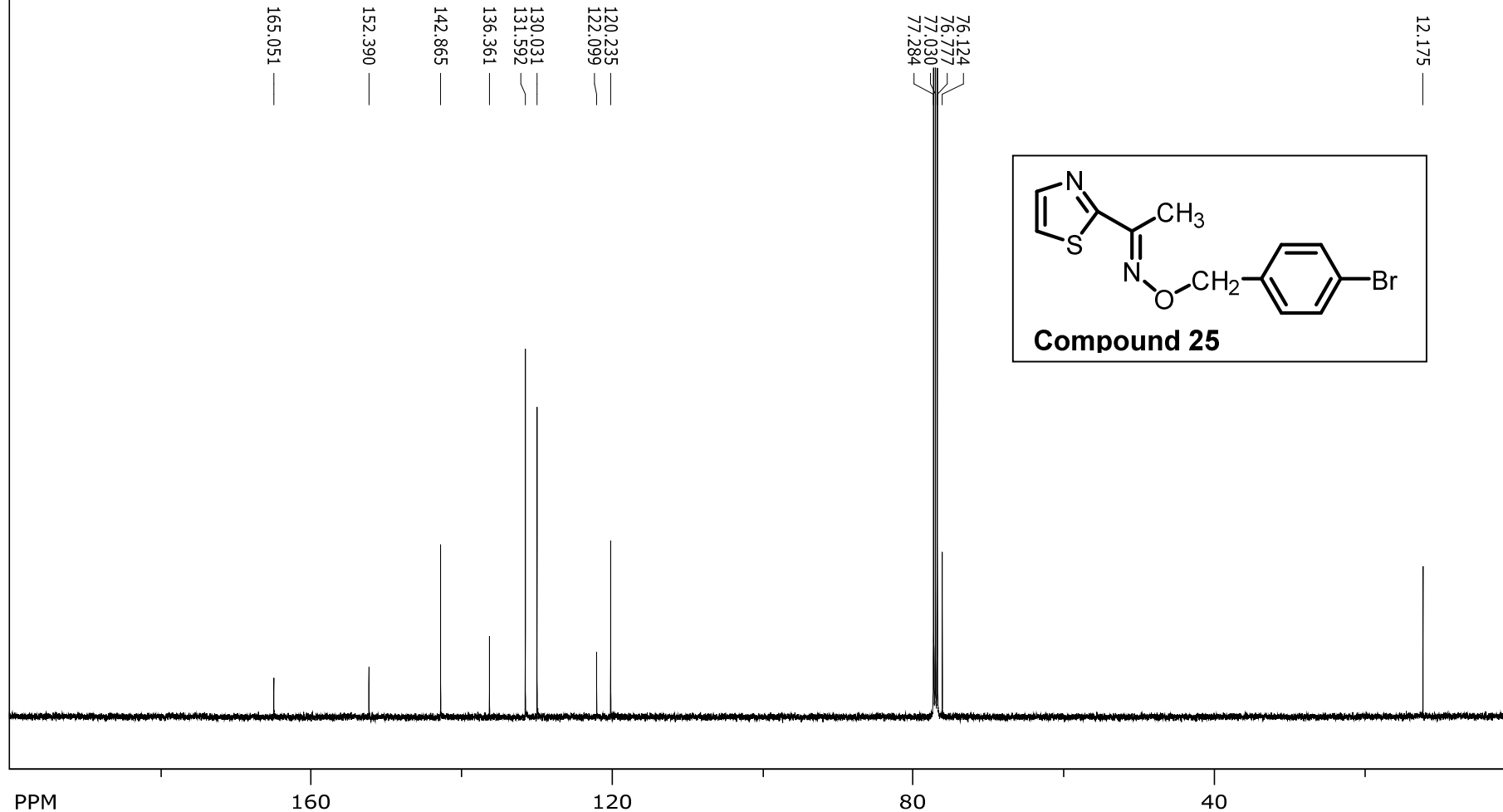
file: ...ers\user\Desktop\Widma 2021\33\fid expt: <zg30>
transmitter freq.: 500.255003 MHz
time domain size: 65536 points
width: 11029.41 Hz = 22.0476 ppm = 0.168295 Hz/pt
number of scans: 128

freq. of 0 ppm: 500.250000 MHz
processed size: 65536 complex points
LB: 0.300 GF: 0.0000

¹³C NMR spectrum of the compound **25**

SpinWorks 4: TK-POs-6_13C

CDCl₃



file: ...ers\user\Desktop\Widma 2021\34\fid expt: <zpgp30>
transmitter freq.: 125.803057 MHz
time domain size: 65536 points
width: 31250.00 Hz = 248.4041 ppm = 0.476837 Hz/pt
number of scans: 1024

freq. of 0 ppm: 125.787963 MHz
processed size: 32768 complex points
LB: 1.000 GF: 0.0000

MS spectrum of the compound 25

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 9

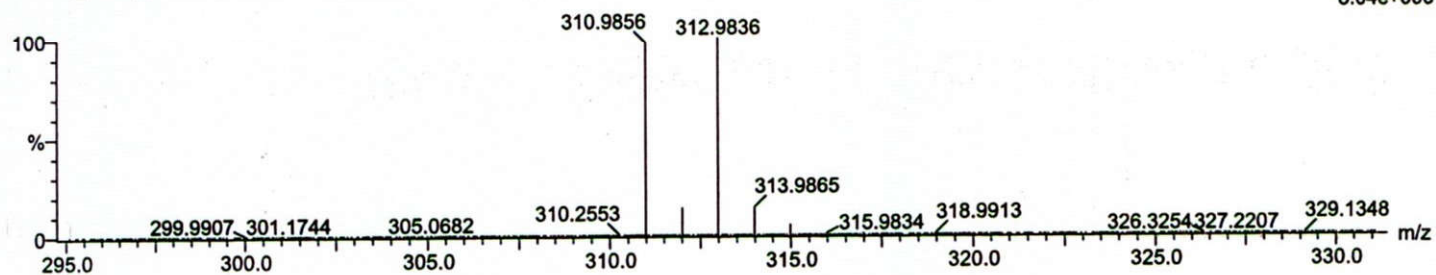
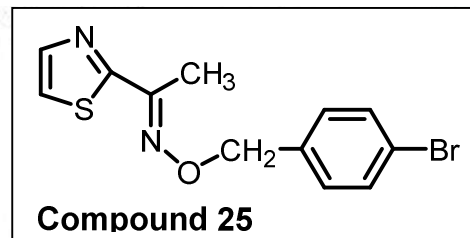
Monoisotopic Mass, Even Electron Ions

187 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-30 H: 0-30 N: 0-2 O: 0-5 S: 1-2 Br: 0-1

210901_Tiazol_BrA 43 (0.454) Cm (34:46-3:8)

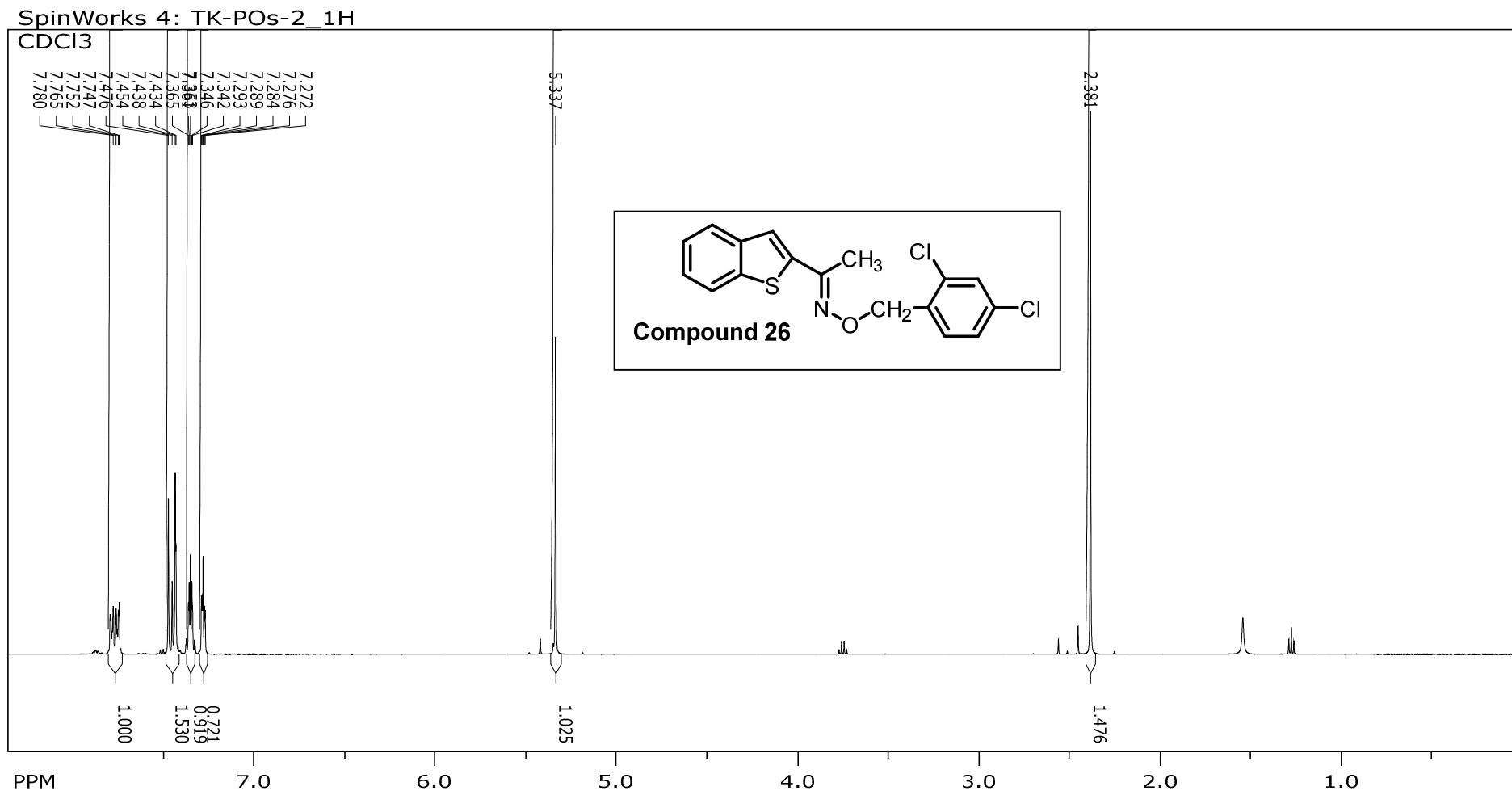


Minimum: -1.5
Maximum: 5.0 5.0 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
310.9856	310.9854	0.2	0.6	7.5	1966.8	n/a	n/a	C12 H12 N2 O S Br

Spectral data of the compound **26**.

¹H NMR spectrum of the compound **26**

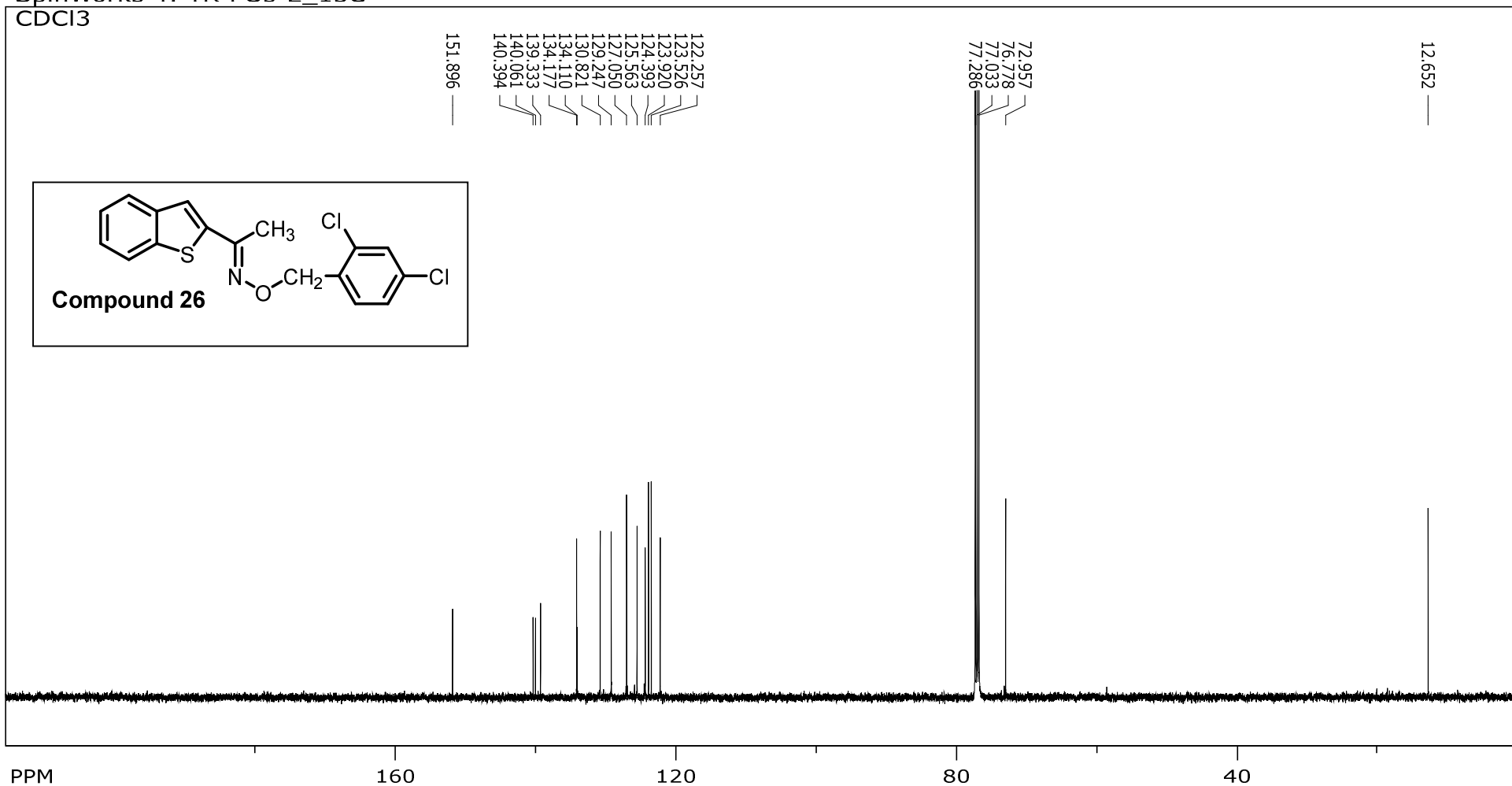


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time domain size: 65536 points
width: 11029.41 Hz = 22.0476 ppm = 0.168295 Hz/pt
number of scans: 128

freq. of 0 ppm: 500.250000 MHz
processed size: 65536 complex points
LB: 0.300 GF: 0.0000

¹³C NMR spectrum of the compound **26**

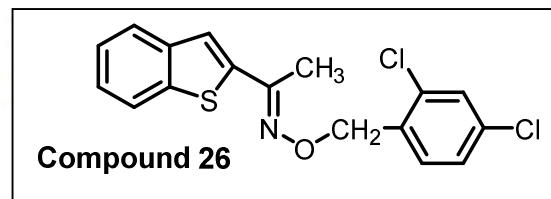
SpinWorks 4: TK-POs-2_13C
CDCl₃



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transmitter freq.: 125.803057 MHz
time domain size: 65536 points
width: 31250.00 Hz = 248.4041 ppm = 0.476837 Hz/pt
number of scans: 1024

freq. of 0 ppm: 125.787963 MHz
processed size: 32768 complex points
LB: 1.000 GF: 0.0000

MS spectrum of the compound **26**



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions

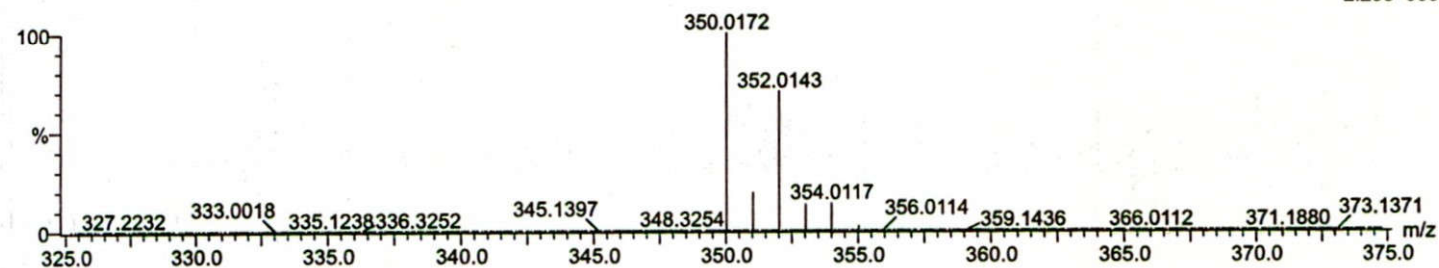
287 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-30 H: 0-30 N: 0-2 O: 0-5 S: 1-2 Cl: 0-2

210901_Benzotiof_DiCl_A 17 (0.197) Cm (14:27-3:8)

TOF MS ES+
2.23e+006

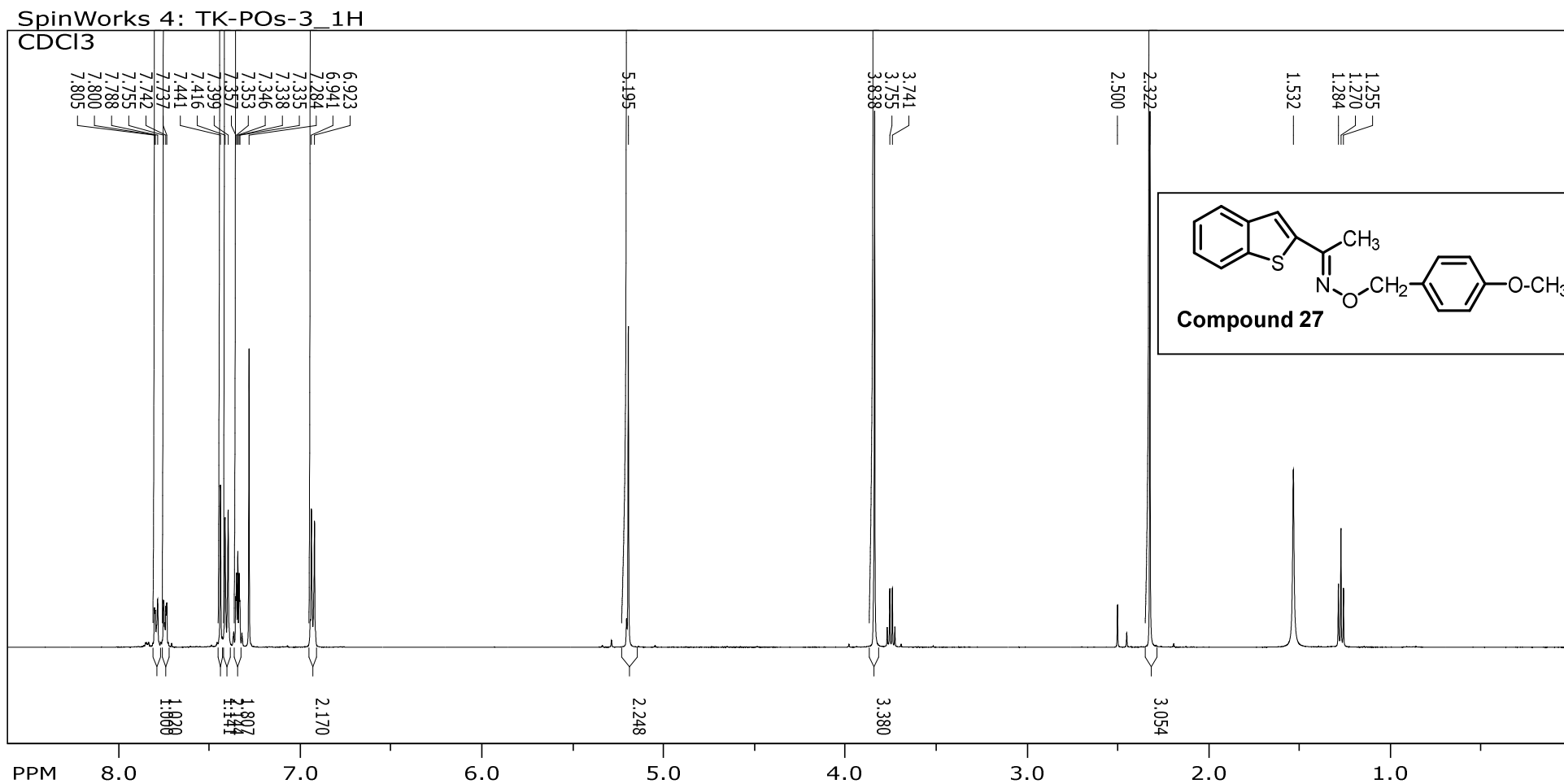


Minimum: -1.5
Maximum: 5.0 5.0 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
350.0172	350.0173	-0.1	-0.3	10.5	1616.9	0.000	100.00	C17 H14 N O S Cl2
	350.0157	1.5	4.3	10.5	1632.8	15.837	0.00	C15 H12 N O5 S2

Spectral data of the compound **27**.

^1H NMR spectrum of the compound **27**

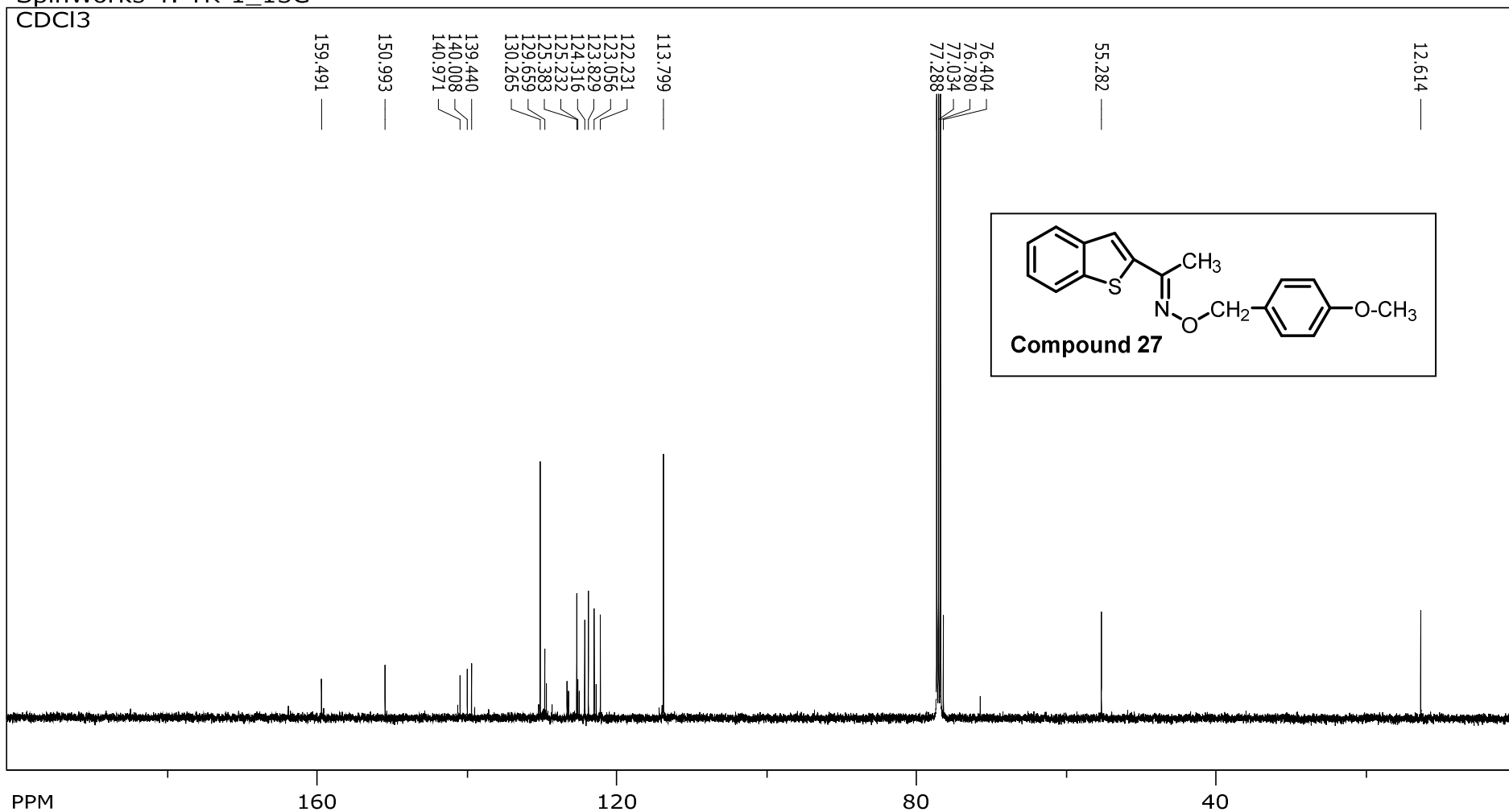


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time domain size: 65536 points
width: 11029.41 Hz = 22.0476 ppm = 0.168295 Hz/pt
number of scans: 128

freq. of 0 ppm: 500.250000 MHz
processed size: 65536 complex points
LB: 0.300 GF: 0.0000

¹³C NMR spectrum of the compound **27**

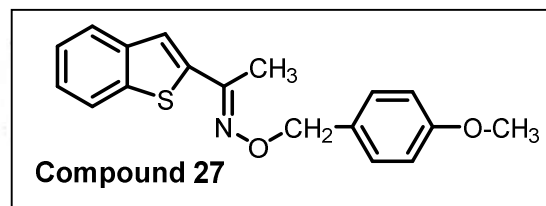
SpinWorks 4: TK-1_13C
CDCl₃



file: ...op\Widma 2021\Widma 09.2021\54\fid expt: <zgpg30>
transmitter freq.: 125.803057 MHz
time domain size: 65536 points
width: 31250.00 Hz = 248.4041 ppm = 0.476837 Hz/pt
number of scans: 1024

freq. of 0 ppm: 125.787963 MHz
processed size: 32768 complex points
LB: 1.000 GF: 0.0000

MS spectrum of the compound 27



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions

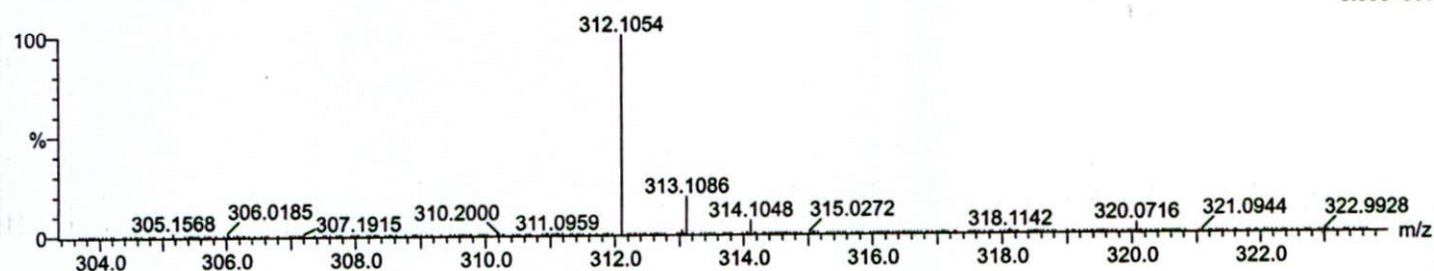
96 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-30 H: 0-30 N: 0-2 O: 0-5 S: 1-2

210901_BenzotiofOMe_4_B 18 (0.205) Cm (17:24-3:8)

TOF MS ES+
5.56e+005



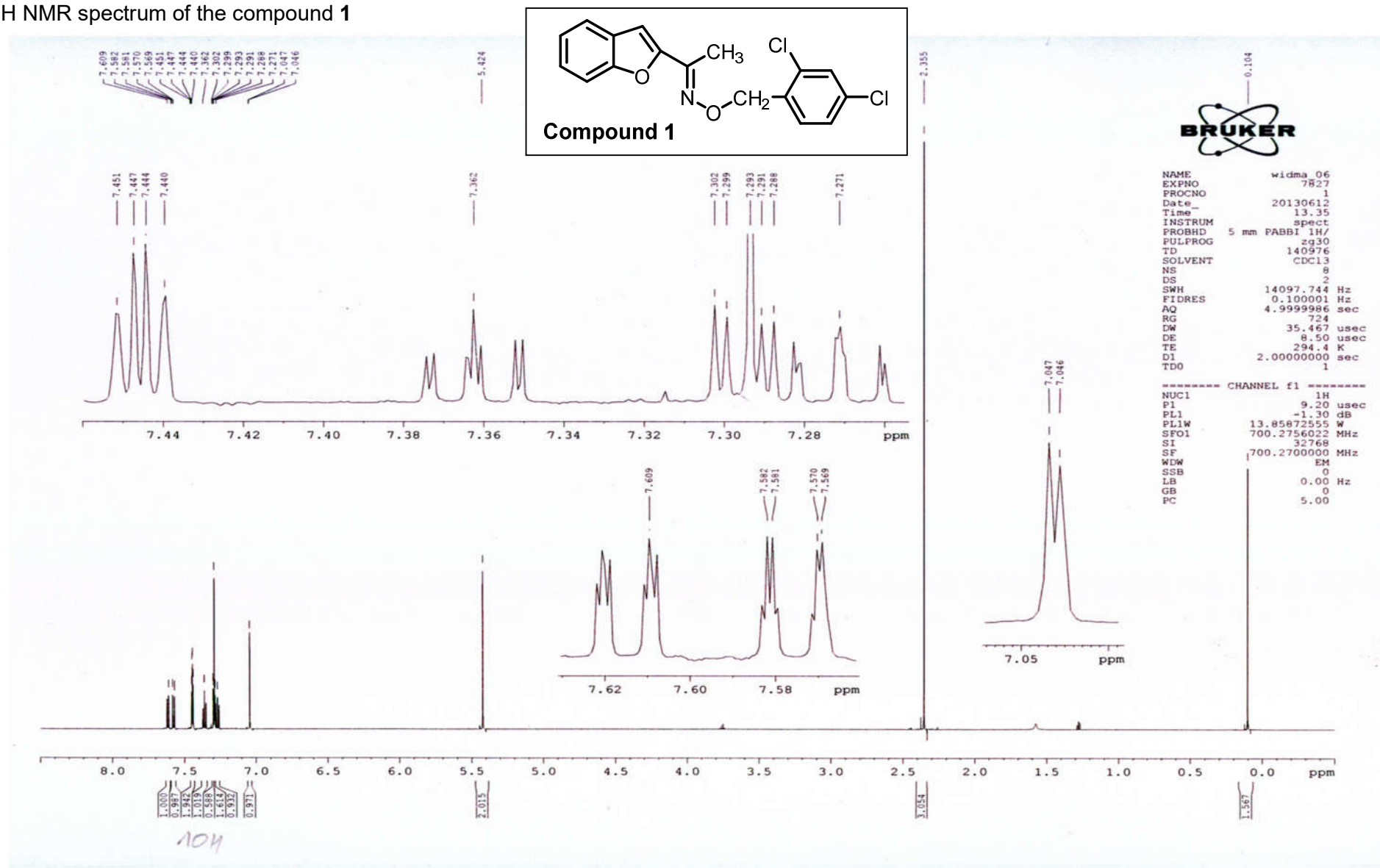
Minimum: -1.5
Maximum: 5.0 5.0 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
312.1054	312.1058	-0.4	-1.3	10.5	1426.6	n/a	n/a	C18 H18 N O2 S

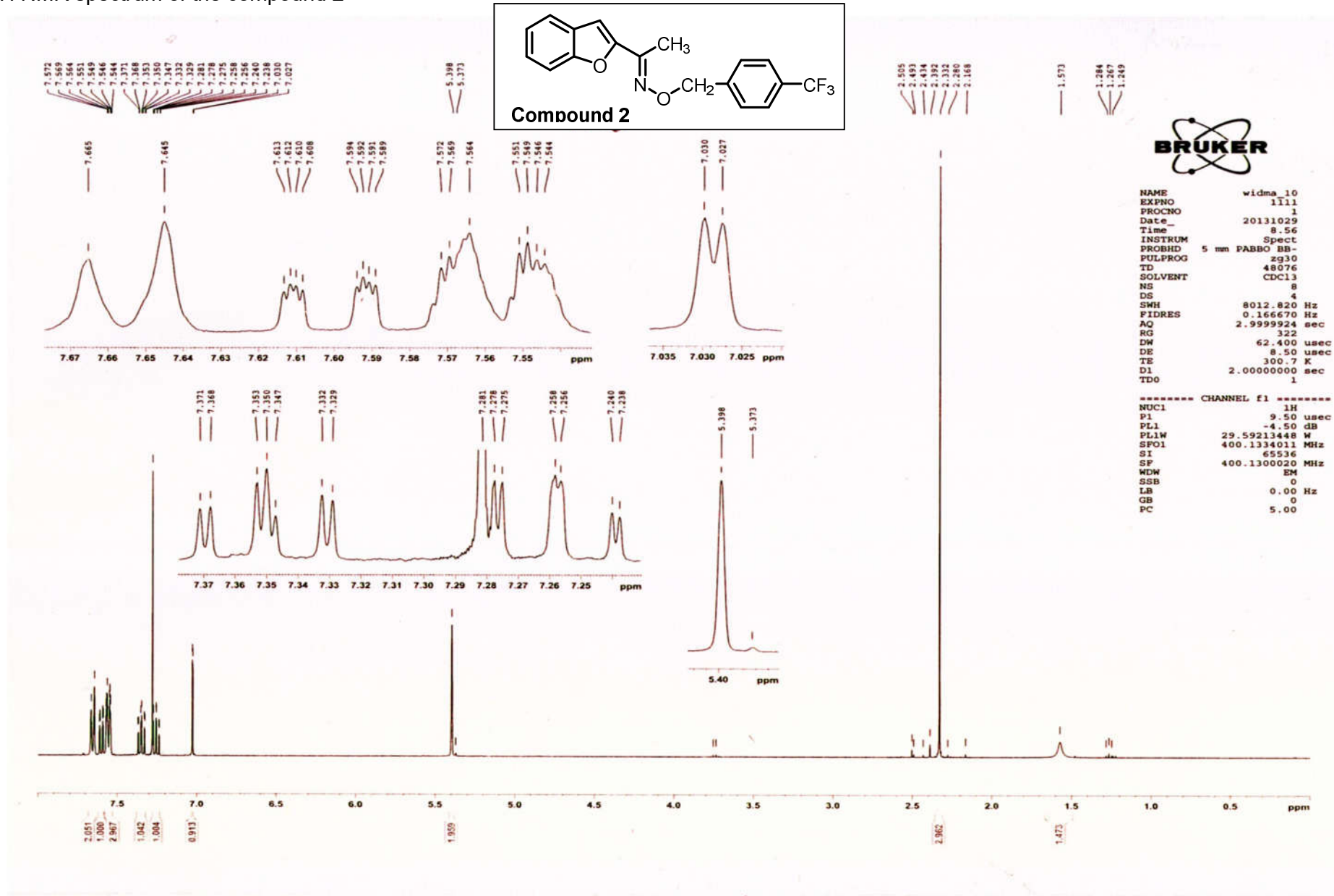
S3. NMR Spectra of the other compounds.

¹H NMR Spectra of the compounds **1-5**, **7-12** and **16-23**.

¹H NMR spectrum of the compound **1**

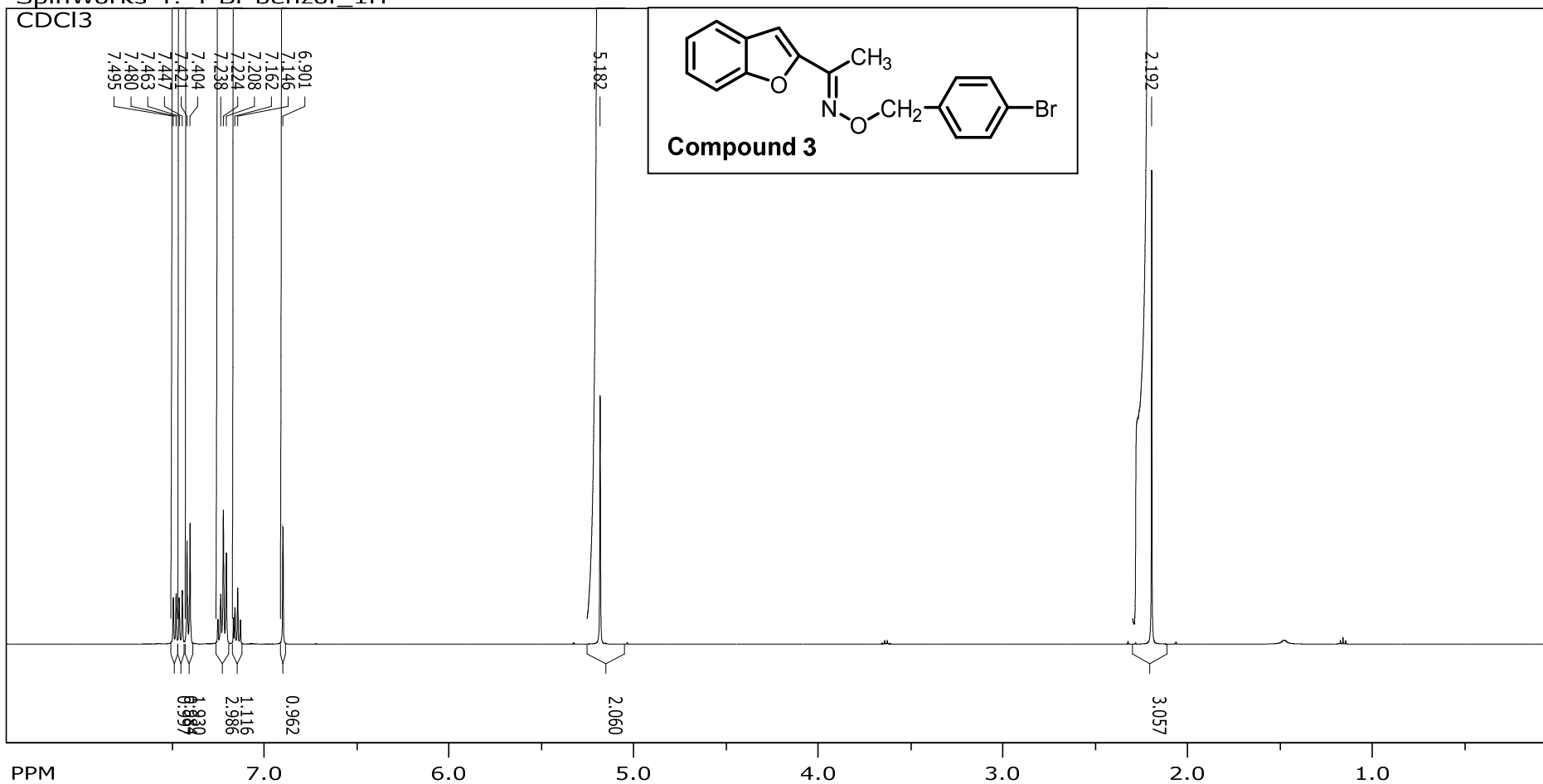


¹H NMR spectrum of the compound **2**



¹H NMR spectrum of the compound **3**

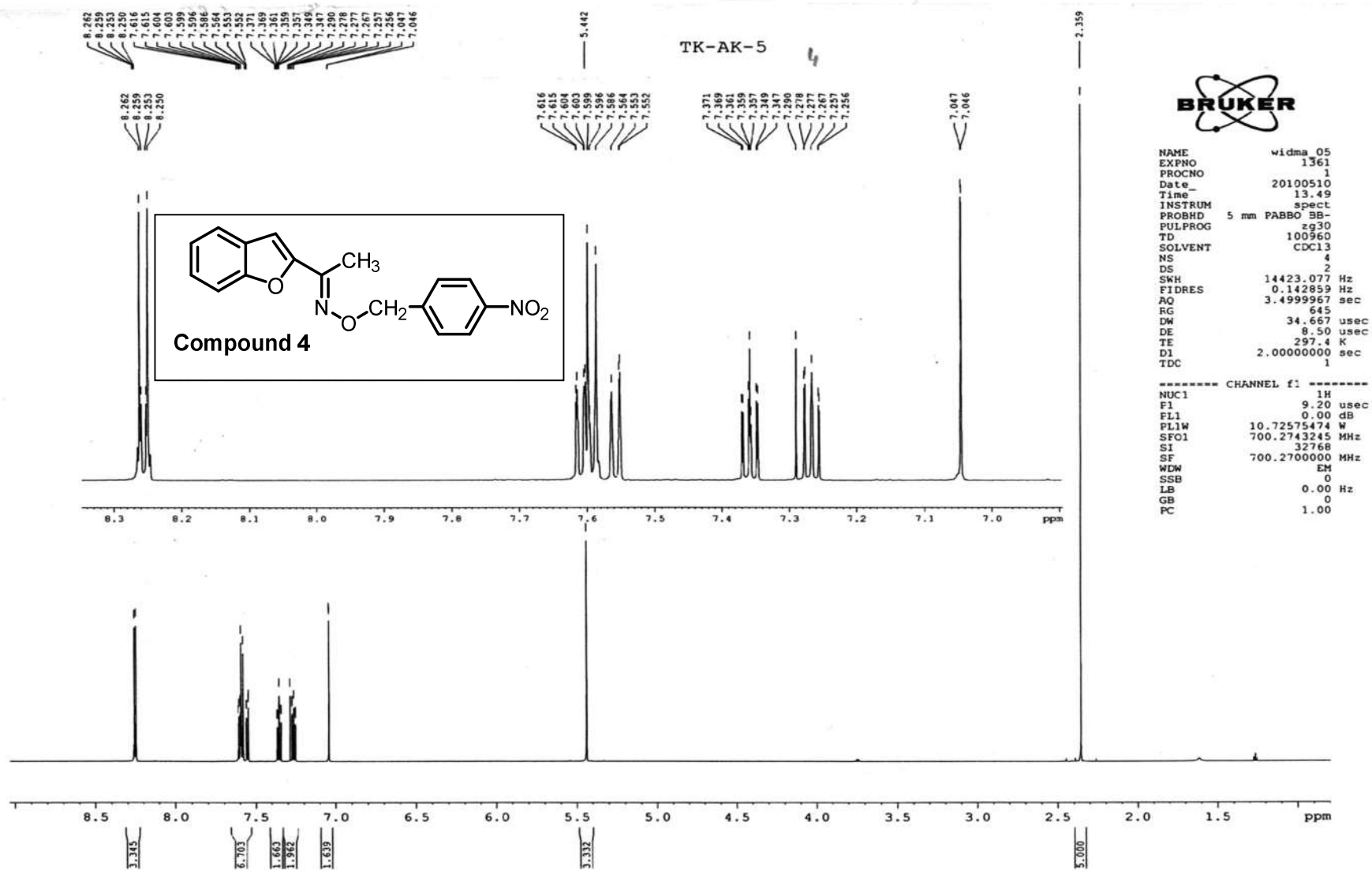
SpinWorks 4: 4-Br benzof_1H
CDCl₃



file: ...rs\user\Desktop\Widma 2022\1\1\fid expt: <zg30>
transmitter freq.: 500.255503 MHz
time domain size: 65536 points
width: 11520.74 Hz = 23.0297 ppm = 0.175793 Hz/pt
number of scans: 128

freq. of 0 ppm: 500.250057 MHz
processed size: 65536 complex points
LB: 0.300 GF: 0.0000

¹H NMR spectrum of the compound **4**



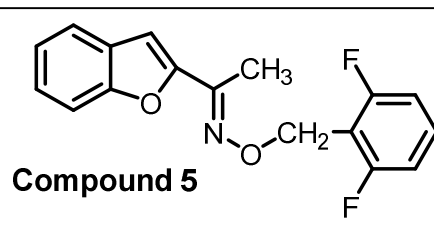
Compound 5

Cc1ccc(cc1)C(F)(F)F

Chemical Structure: 2-(2,4-difluorbenzyloxy)-1-benzofuran-3-ylideneacetone derivative.

¹H NMR Spectrum (CDCl₃):

Peak List (ppm): 7.600, 7.598, 7.582, 7.579, 7.561, 7.558, 7.554, 7.552, 7.550, 7.548, 7.546, 7.544, 7.542, 7.540, 7.538, 7.536, 7.534, 7.532, 7.530, 7.528, 7.526, 7.524, 7.522, 7.520, 7.518, 7.516, 7.514, 7.512, 7.510, 7.508, 7.506, 7.504, 7.502, 7.500, 7.498, 7.496, 7.494, 7.492, 7.490, 7.488, 7.486, 7.484, 7.482, 7.480, 7.478, 7.476, 7.474, 7.472, 7.470, 7.468, 7.466, 7.464, 7.462, 7.460, 7.458, 7.456, 7.454, 7.452, 7.450, 7.448, 7.446, 7.444, 7.442, 7.440, 7.438, 7.436, 7.434, 7.432, 7.430, 7.428, 7.426, 7.424, 7.422, 7.420, 7.418, 7.416, 7.414, 7.412, 7.410, 7.408, 7.406, 7.404, 7.402, 7.400, 7.398, 7.396, 7.394, 7.392, 7.390, 7.388, 7.386, 7.384, 7.382, 7.380, 7.378, 7.376, 7.374, 7.372, 7.370, 7.368, 7.366, 7.364, 7.362, 7.360, 7.358, 7.356, 7.354, 7.352, 7.350, 7.348, 7.346, 7.344, 7.342, 7.340, 7.338, 7.336, 7.334, 7.332, 7.330, 7.328, 7.326, 7.324, 7.322, 7.320, 7.318, 7.316, 7.314, 7.312, 7.310, 7.308, 7.306, 7.304, 7.302, 7.300, 7.298, 7.296, 7.294, 7.292, 7.290, 7.288, 7.286, 7.284, 7.282, 7.280, 7.278, 7.276, 7.274, 7.272, 7.270, 7.268, 7.266, 7.264, 7.262, 7.260, 7.258, 7.256, 7.254, 7.252, 7.250, 7.248, 7.246, 7.244, 7.242, 7.240, 7.238, 7.236, 7.234, 7.232, 7.230, 7.228, 7.226, 7.224, 7.222, 7.220, 7.218, 7.216, 7.214, 7.212, 7.210, 7.208, 7.206, 7.204, 7.202, 7.200, 7.198, 7.196, 7.194, 7.192, 7.190, 7.188, 7.186, 7.184, 7.182, 7.180, 7.178, 7.176, 7.174, 7.172, 7.170, 7.168, 7.166, 7.164, 7.162, 7.160, 7.158, 7.156, 7.154, 7.152, 7.150, 7.148, 7.146, 7.144, 7.142, 7.140, 7.138, 7.136, 7.134, 7.132, 7.130, 7.128, 7.126, 7.124, 7.122, 7.120, 7.118, 7.116, 7.114, 7.112, 7.110, 7.108, 7.106, 7.104, 7.102, 7.100, 7.098, 7.096, 7.094, 7.092, 7.090, 7.088, 7.086, 7.084, 7.082, 7.080, 7.078, 7.076, 7.074, 7.072, 7.070, 7.068, 7.066, 7.064, 7.062, 7.060, 7.058, 7.056, 7.054, 7.052, 7.050, 7.048, 7.046, 7.044, 7.042, 7.040, 7.038, 7.036, 7.034, 7.032, 7.030, 7.028, 7.026, 7.024, 7.022, 7.020, 7.018, 7.016, 7.014, 7.012, 7.010, 7.008, 7.006, 7.004, 7.002, 7.000, 6.998, 6.996, 6.994, 6.992, 6.990, 6.988, 6.986, 6.984, 6.982, 6.980, 6.978, 6.976, 6.974, 6.972, 6.970, 6.968, 6.966, 6.964, 6.962, 6.960, 6.958, 6.956, 6.954, 6.952, 6.950, 6.948, 6.946, 6.944, 6.942, 6.940, 6.938, 6.936, 6.934, 6.932, 6.930, 6.928, 6.926, 6.924, 6.922, 6.920, 6.918, 6.916, 6.914, 6.912, 6.910, 6.908, 6.906, 6.904, 6.902, 6.900, 6.898, 6.896, 6.894, 6.892, 6.890, 6.888, 6.886, 6.884, 6.882, 6.880, 6.878, 6.876, 6.874, 6.872, 6.870, 6.868, 6.866, 6.864, 6.862, 6.860, 6.858, 6.856, 6.854, 6.852, 6.850, 6.848, 6.846, 6.844, 6.842, 6.840, 6.838, 6.836, 6.834, 6.832, 6.830, 6.828, 6.826, 6.824, 6.822, 6.820, 6.818, 6.816, 6.814, 6.812, 6.810, 6.808, 6.806, 6.804, 6.802, 6.800, 6.798, 6.796, 6.794, 6.792, 6.790, 6.788, 6.786, 6.784, 6.782, 6.780, 6.778, 6.776, 6.774, 6.772, 6.770, 6.768, 6.766, 6.764, 6.762, 6.760, 6.758, 6.756, 6.754, 6.752, 6.750, 6.748, 6.746, 6.744, 6.742, 6.740, 6.738, 6.736, 6.734, 6.732, 6.730, 6.728, 6.726, 6.724, 6.722, 6.720, 6.718, 6.716, 6.714, 6.712, 6.710, 6.708, 6.706, 6.704, 6.702, 6.700, 6.698, 6.696, 6.694, 6.692, 6.690, 6.688, 6.686, 6.684, 6.682, 6.680, 6.678, 6.676, 6.674, 6.672, 6.670, 6.668, 6.666, 6.664, 6.662, 6.660, 6.658, 6.656, 6.654, 6.652, 6.650, 6.648, 6.646, 6.644, 6.642, 6.640, 6.638, 6.636, 6.634, 6.632, 6.630, 6.628, 6.626, 6.624, 6.622, 6.620, 6.618, 6.616, 6.614, 6.612, 6.610, 6.608, 6.606, 6.604, 6.602, 6.600, 6.598, 6.596, 6.594, 6.592, 6.590, 6.588, 6.586, 6.584, 6.582, 6.580, 6.578, 6.576, 6.574, 6.572, 6.570, 6.568, 6.566, 6.564, 6.562, 6.560, 6.558, 6.556, 6.554, 6.552, 6.550, 6.548, 6.546, 6.544, 6.542, 6.540, 6.538, 6.536, 6.534, 6.532, 6.530, 6.528, 6.526, 6.524, 6.522, 6.520, 6.518, 6.516, 6.514, 6.512, 6.510, 6.508, 6.506, 6.504, 6.502, 6.500, 6.498, 6.496, 6.494, 6.492, 6.490, 6.488, 6.486, 6.484, 6.482, 6.480, 6.478, 6.476, 6.474, 6.472, 6.470, 6.468, 6.466, 6.464, 6.462, 6.460, 6.458, 6.456, 6.454, 6.452, 6.450, 6.448, 6.446, 6.444, 6.442, 6.440, 6.438, 6.43



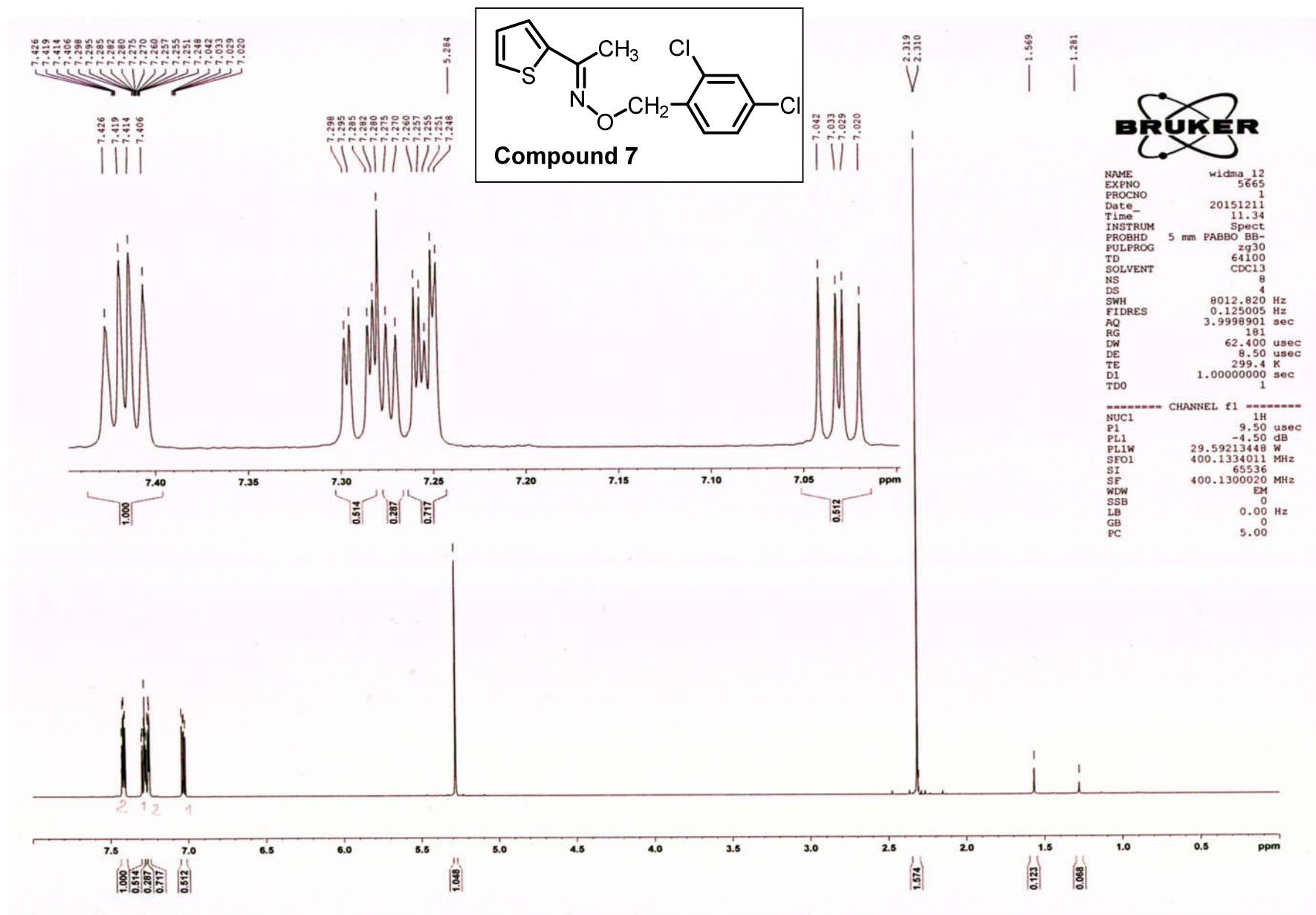
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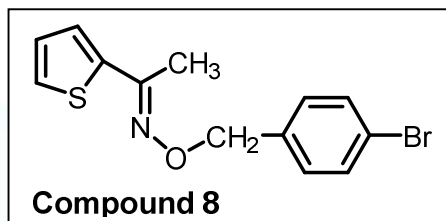
NAME          widma 10
EXPNO         I26
PROCNO        1
Date_         20131029
Time_         18.52
INSTRUM       Spect
PROBHD        5 mm PABBO BB-
PULPRG        zg30
TD            48076
SOLVENT       CDCl3
NS             8
DS            4
SWH           8012.820 Hz
FIDRES        0.166670 Hz
AQ            2.9999924 sec
RG            144
DW            62.400 usec
DE            8.50 usec
TE            300.5 K
D1            2.00000000 sec
TDO           1
===== CHANNEL f1 =====
NUC1          1H
P1            9.50 usec
PL1          -4.50 dB
PL1/FW       29.59213448 W
SF01         400.1334011 MHz
SI            65536
SF           400.1300020 MHz
WDW           EM
SSB           0
LB           0.00 Hz
GB            0
PC            5.00

```


¹H NMR spectrum of the compound 7

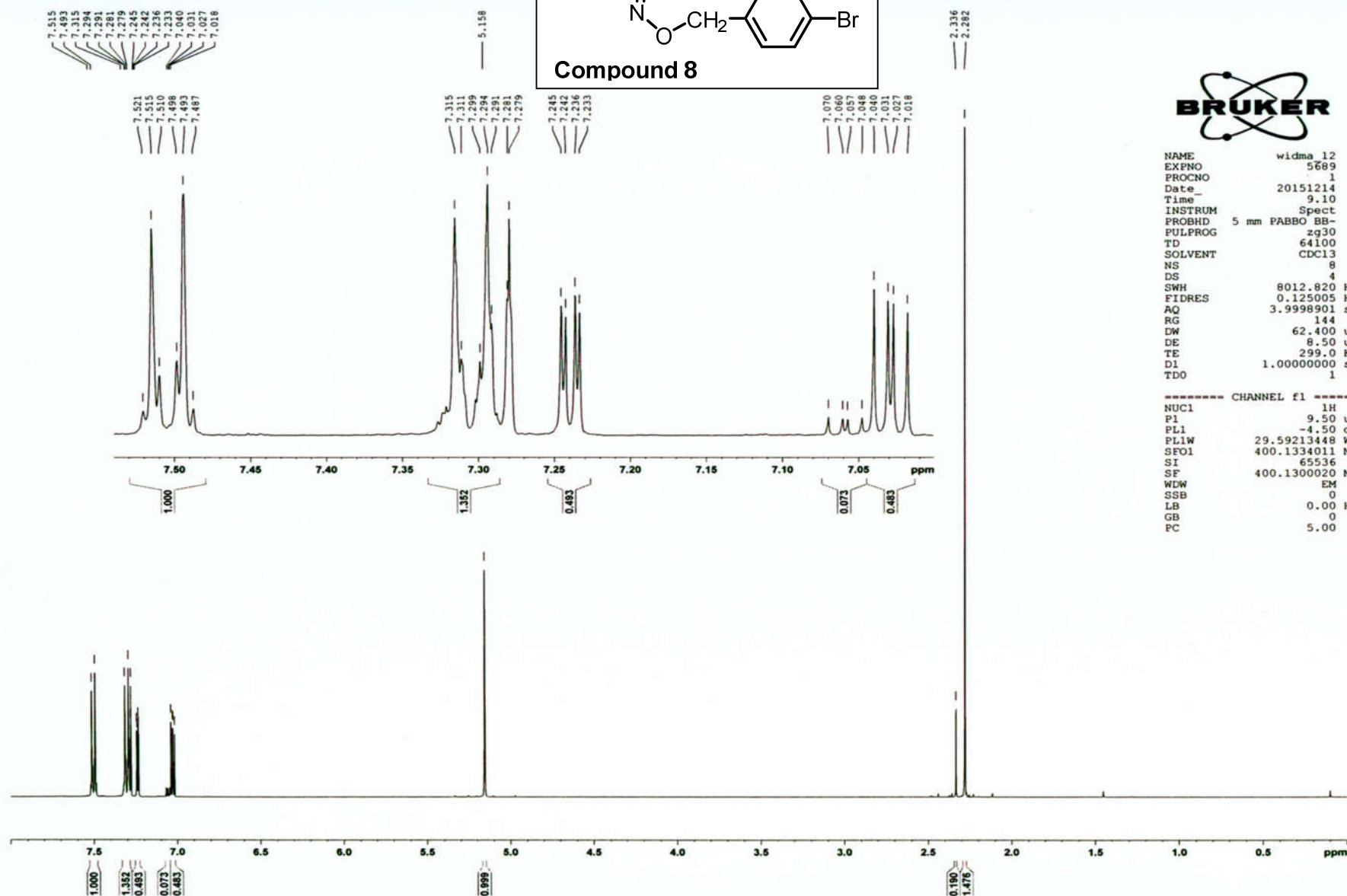


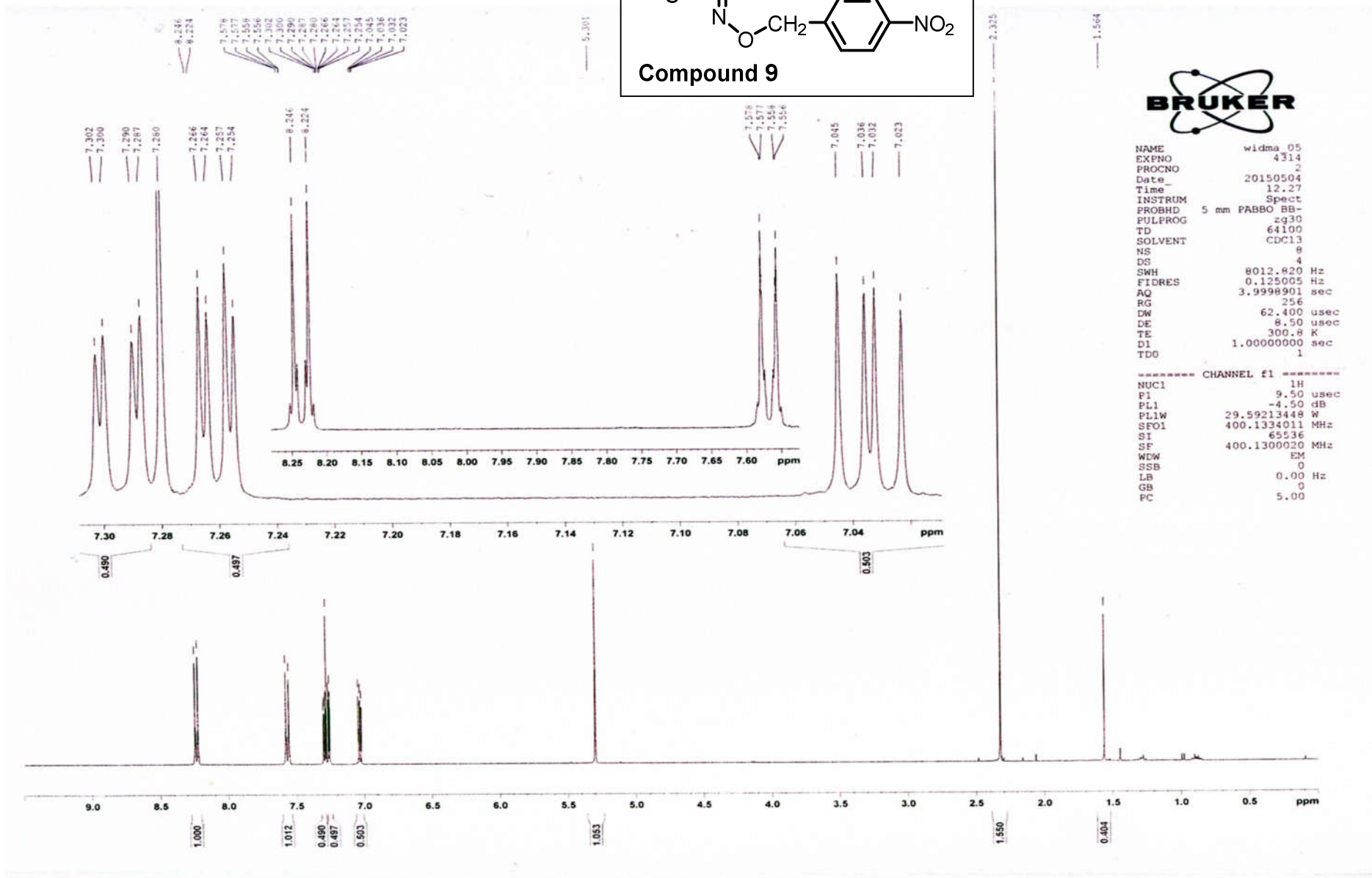
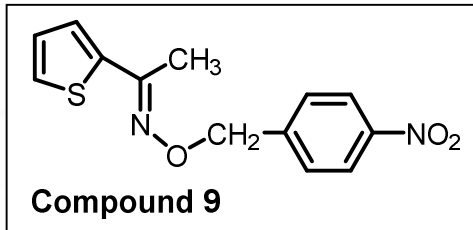
¹H NMR spectrum of the compound 8



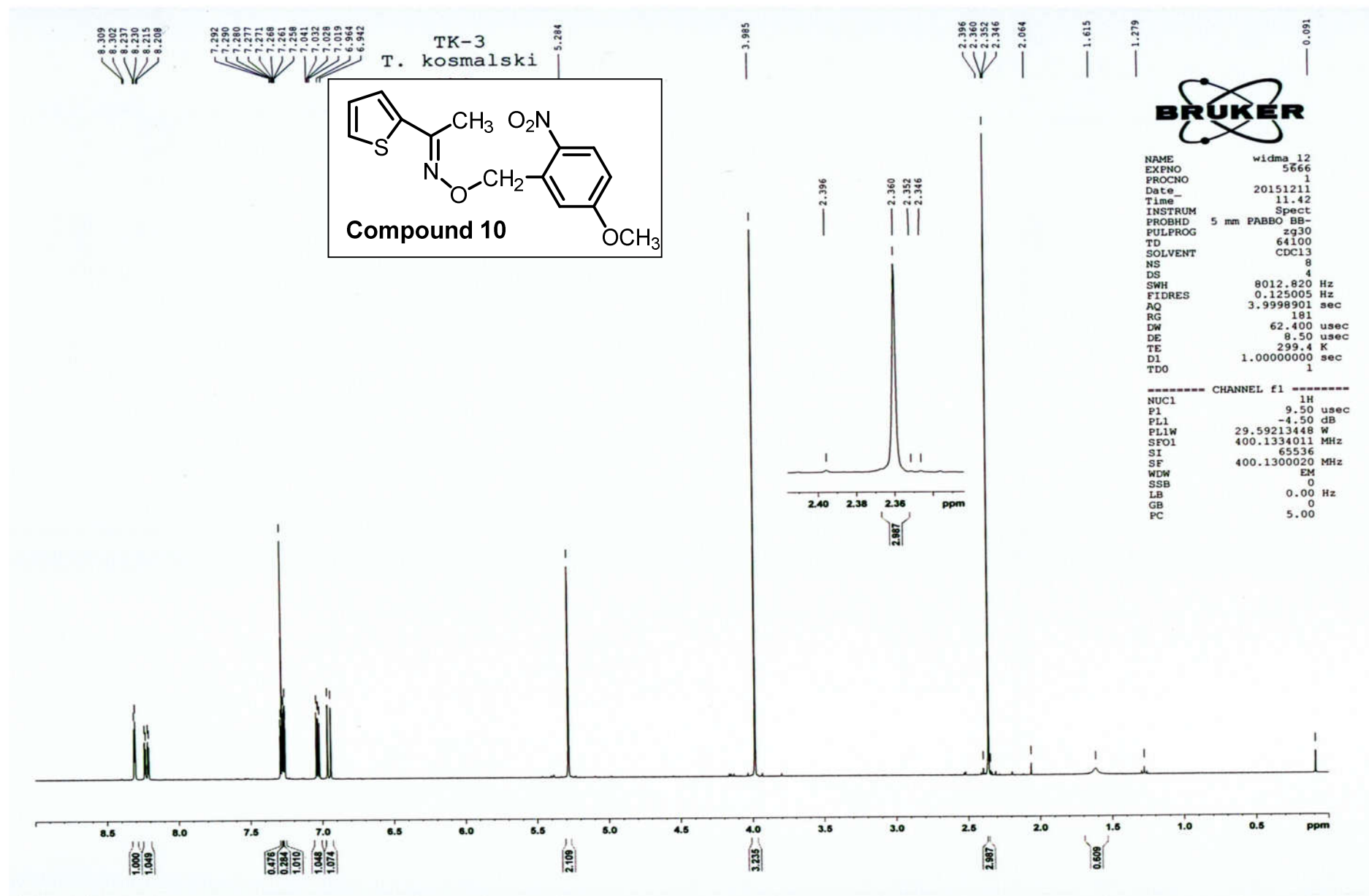
NAME widma 12
EXPNO 5689
PROCNO 1
Date_ 20151214
Time_ 9.10
INSTRUM Spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 64100
SOLVENT CDCl3
NS 8
DS 4
SWH 8012.820 Hz
FIDRES 0.125005 Hz
AQ 3.9998901 sec
RG 144
DW 62.400 usec
DE 8.50 usec
TE 299.0 K
D1 1.00000000 sec
TDO 1

----- CHANNEL f1 -----
NUC1 1H
P1 9.50 usec
PL1 -4.50 dB
PL1W 29.59213448 W
SFO1 400.1334011 MHz
SI 65536
SF 400.1300020 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 5.00

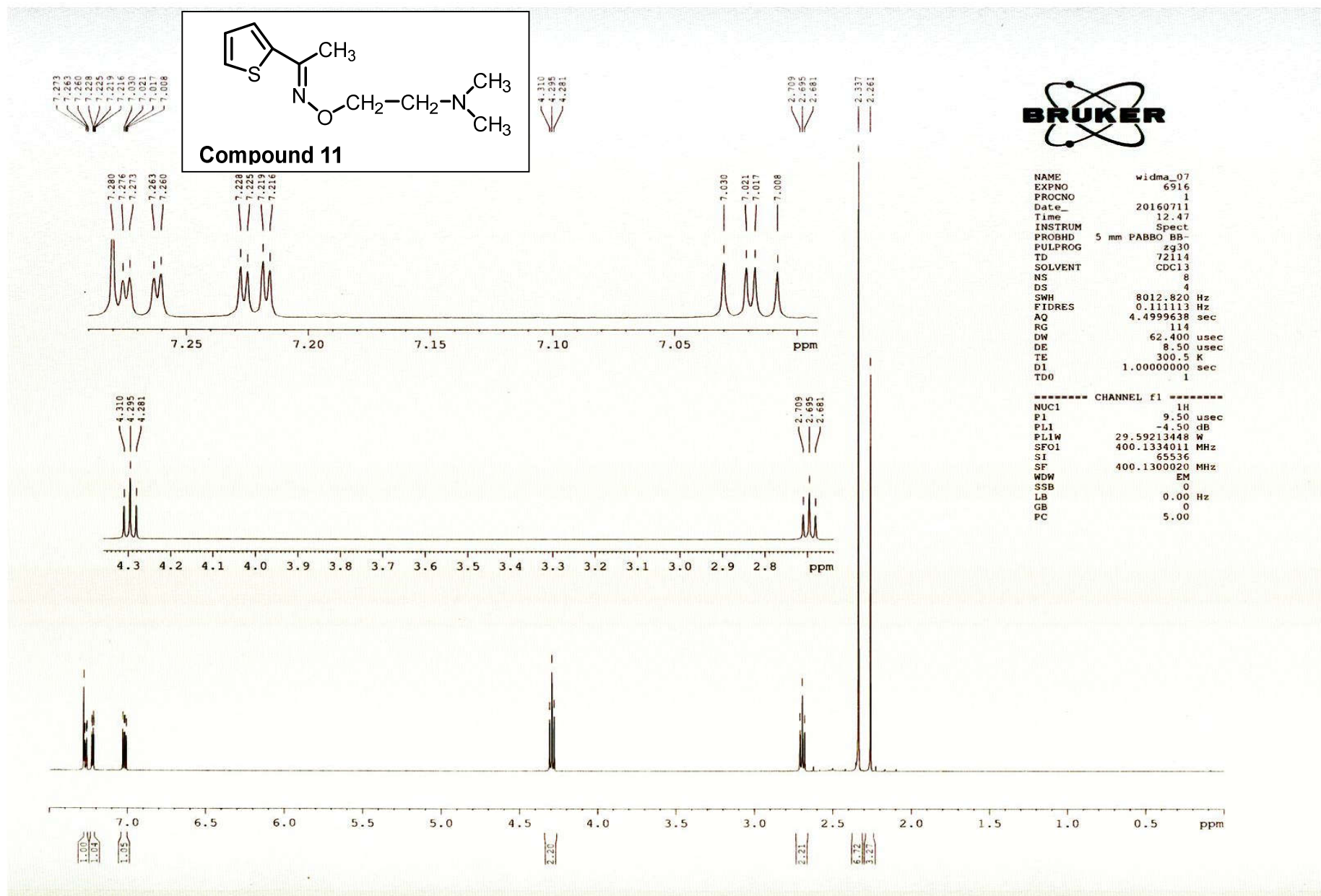


¹H NMR spectrum of the compound **9**

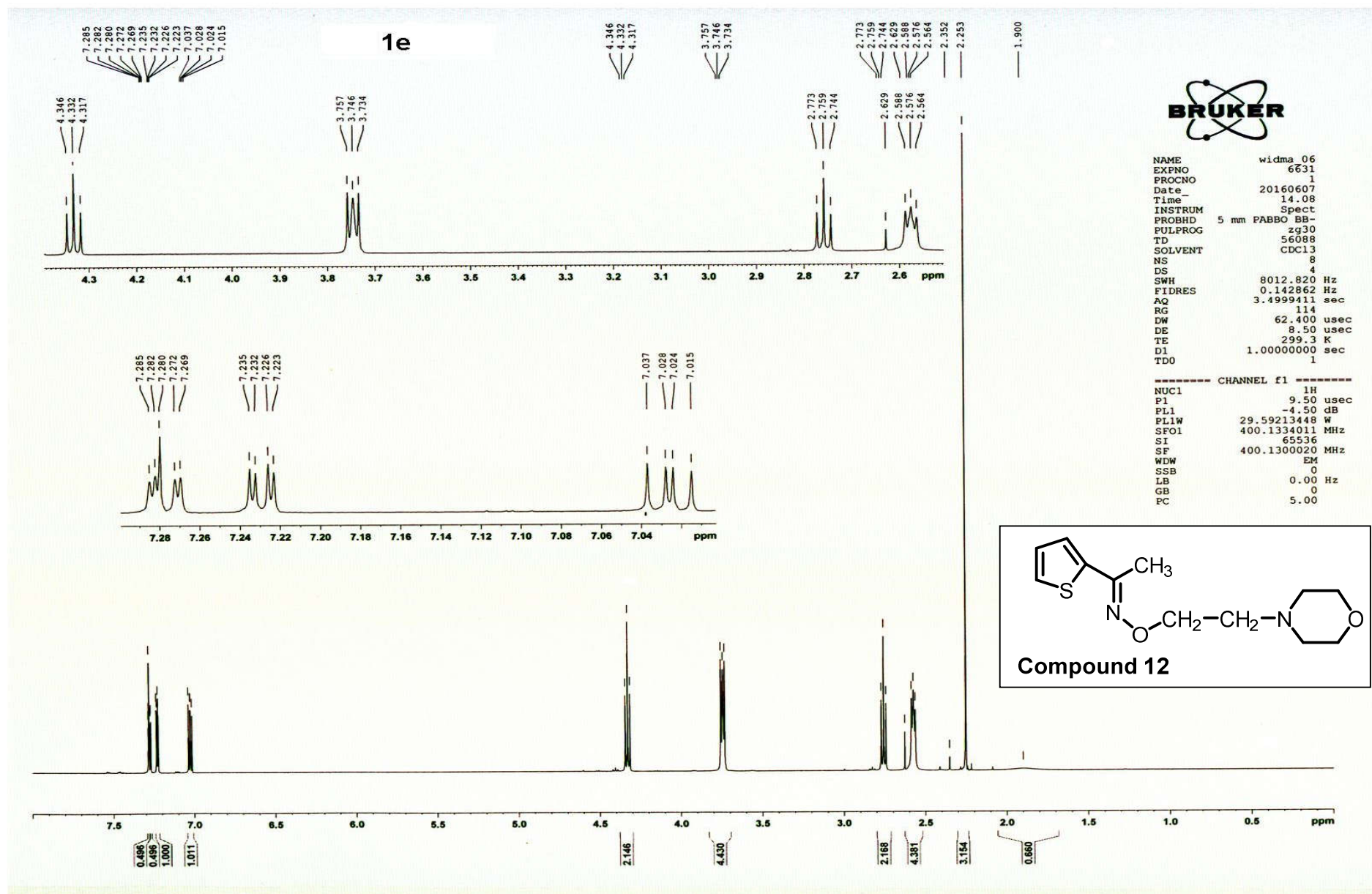
¹H NMR spectrum of the compound **10**



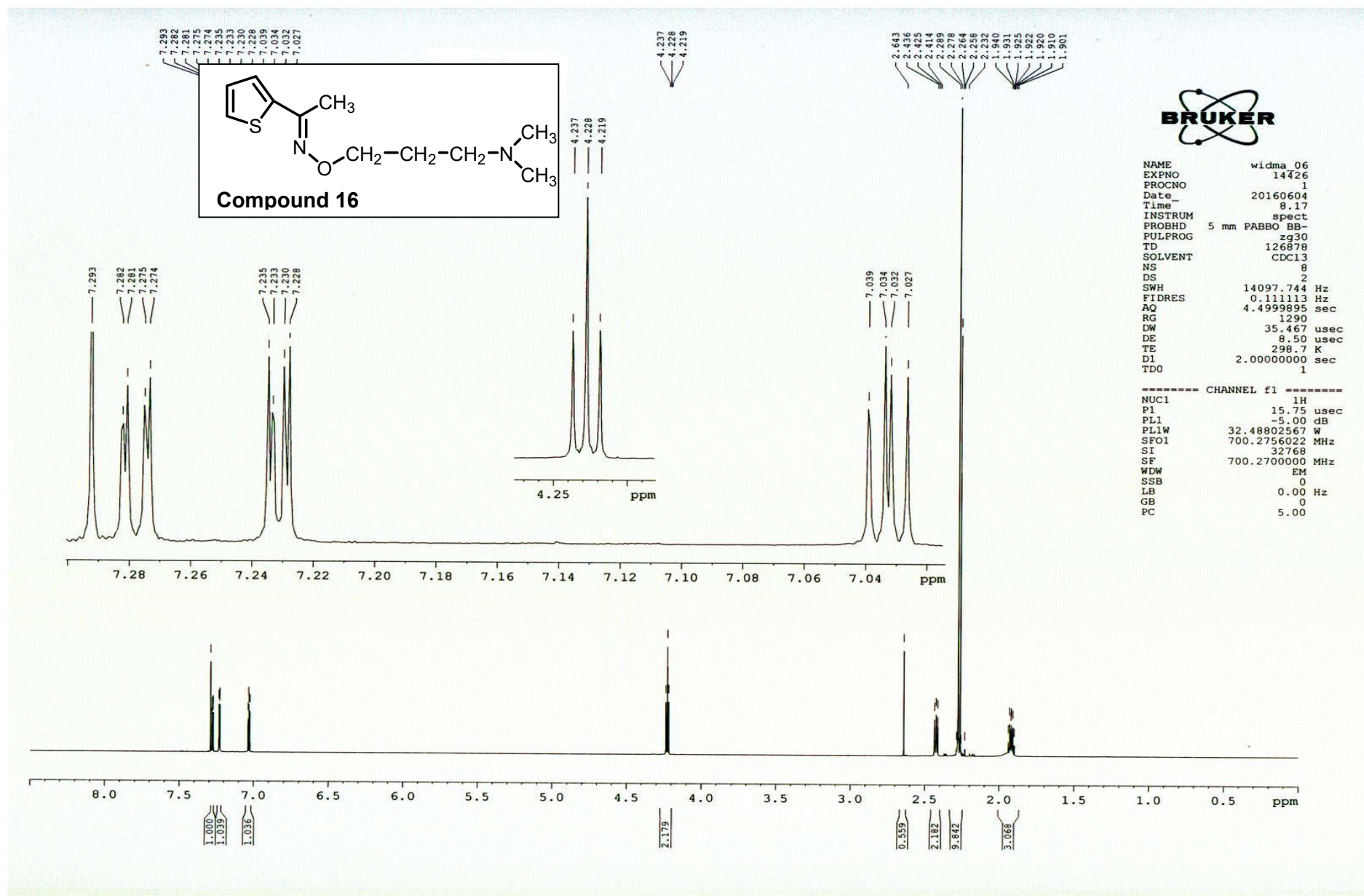
¹H NMR spectrum of the compound 11



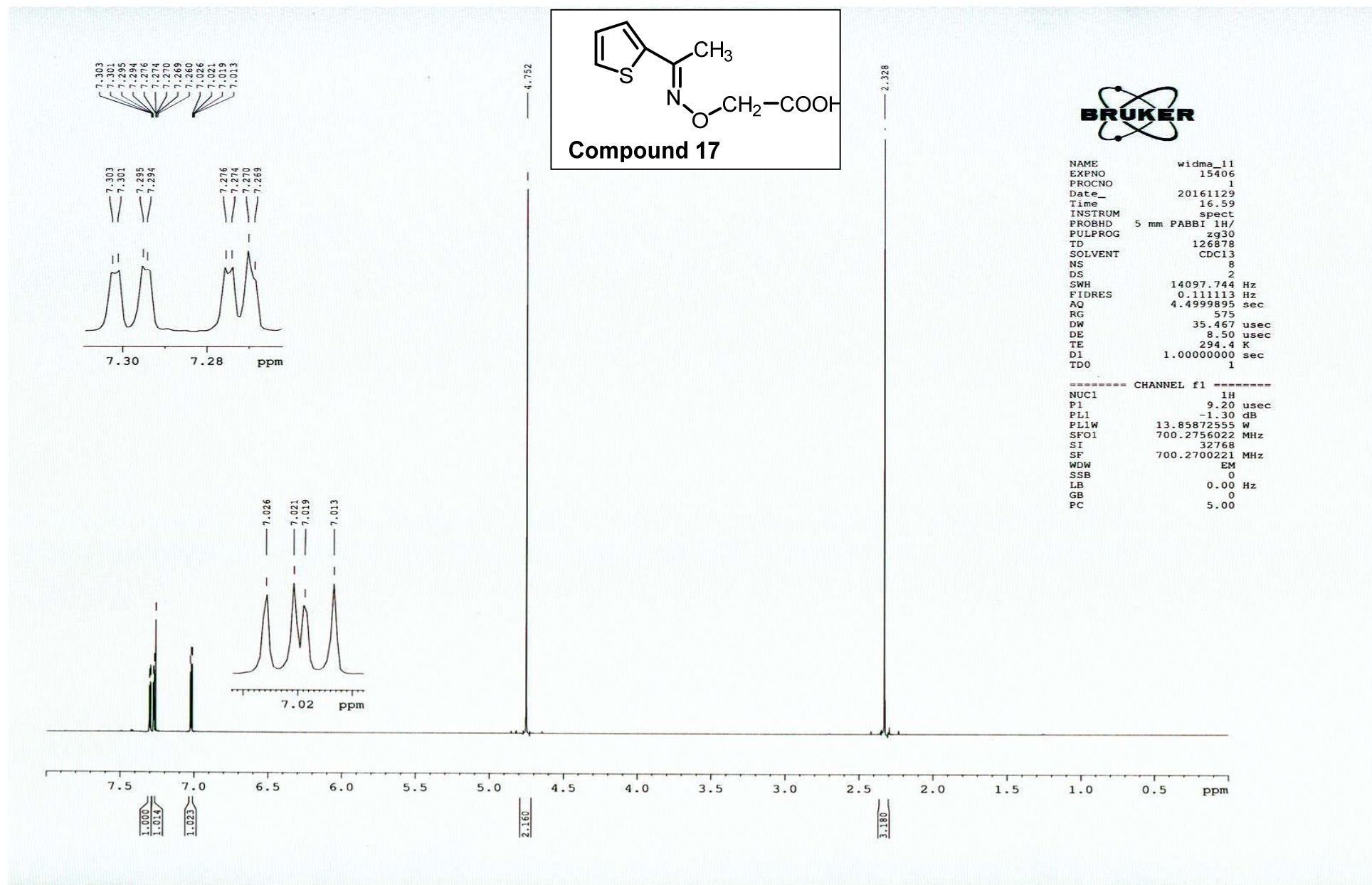
¹H NMR spectrum of the compound **12**



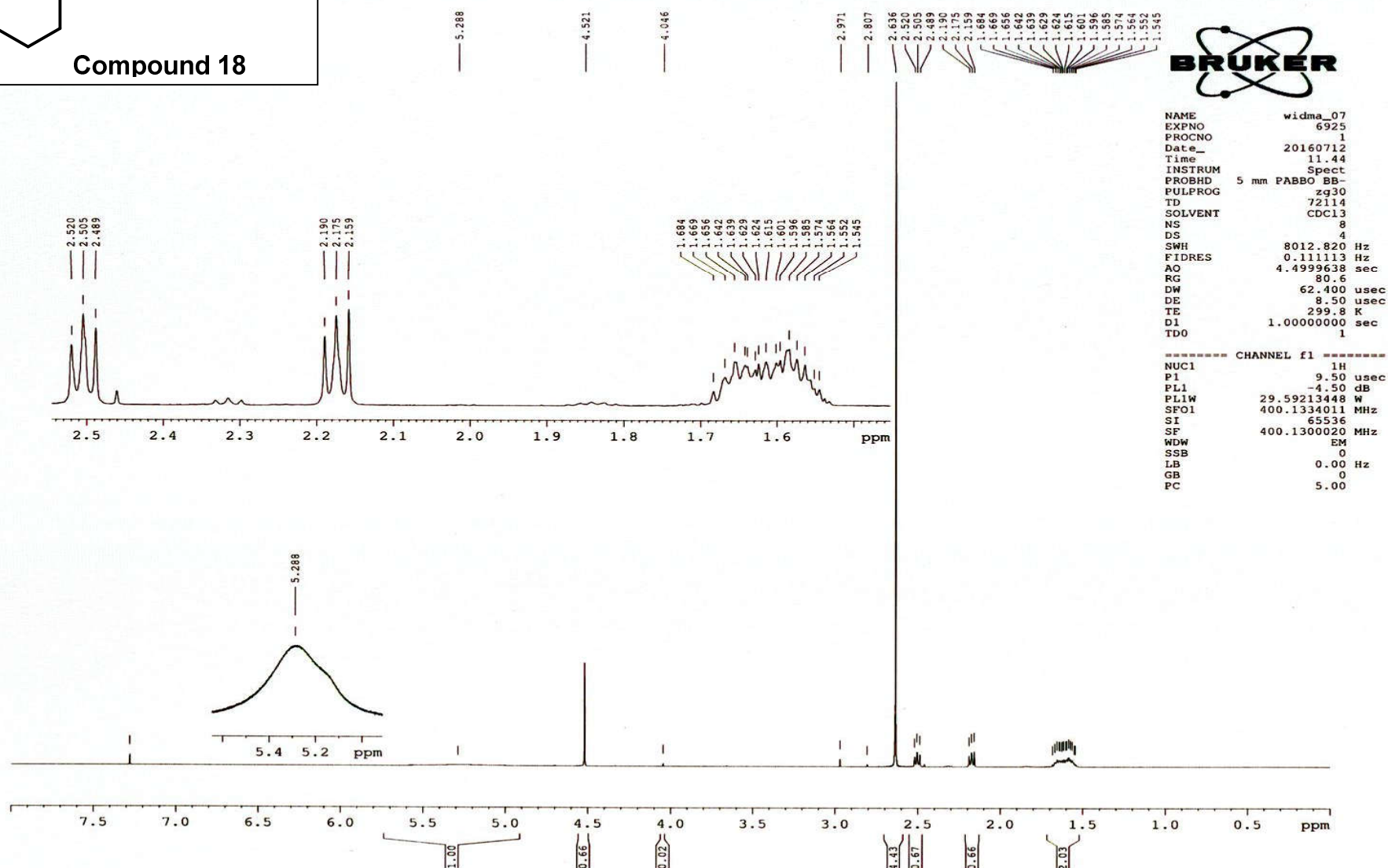
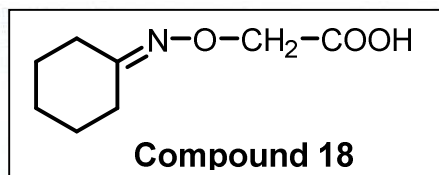
¹H NMR spectrum of the compound **16**



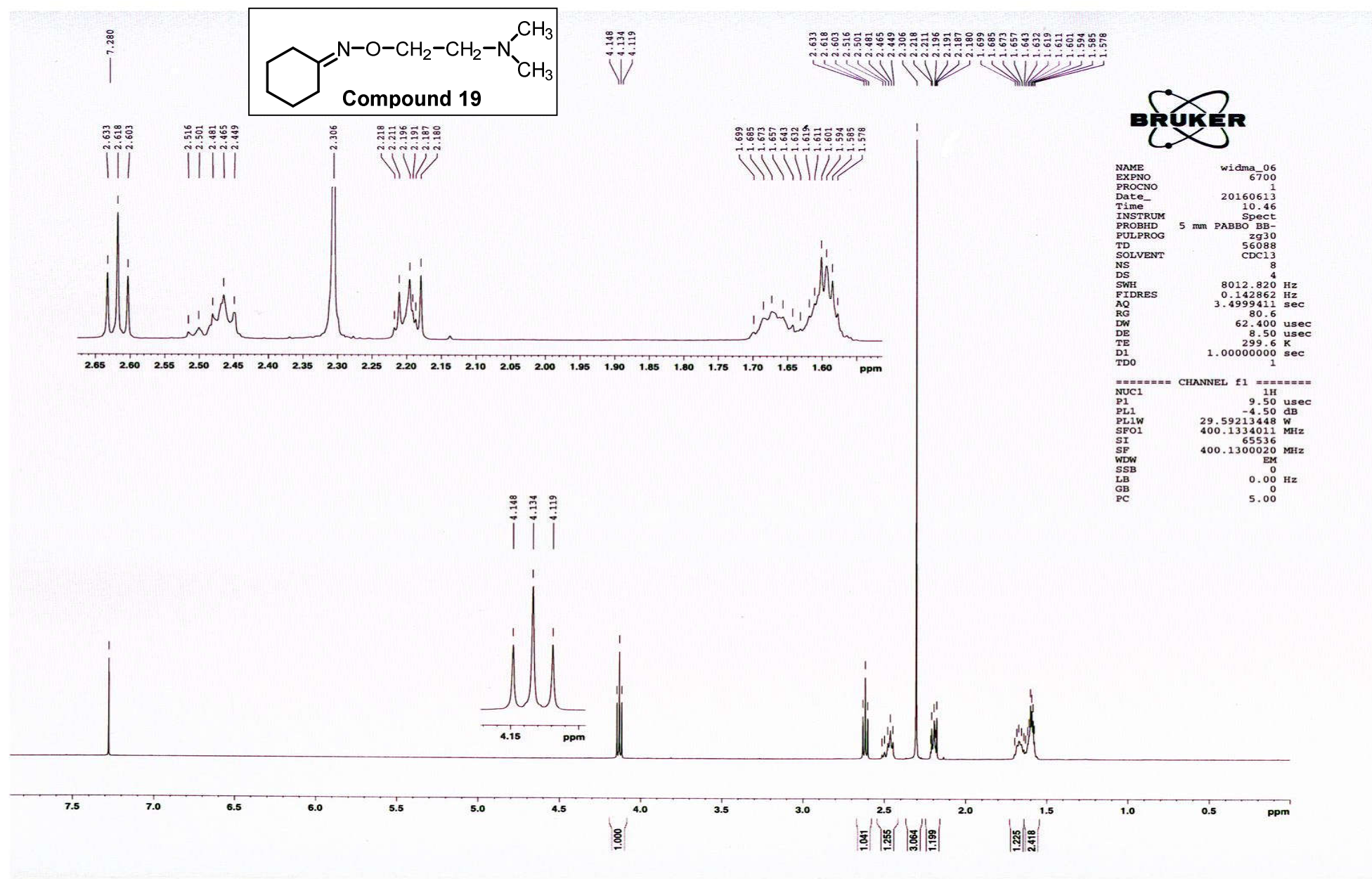
¹H NMR spectrum of the compound 17



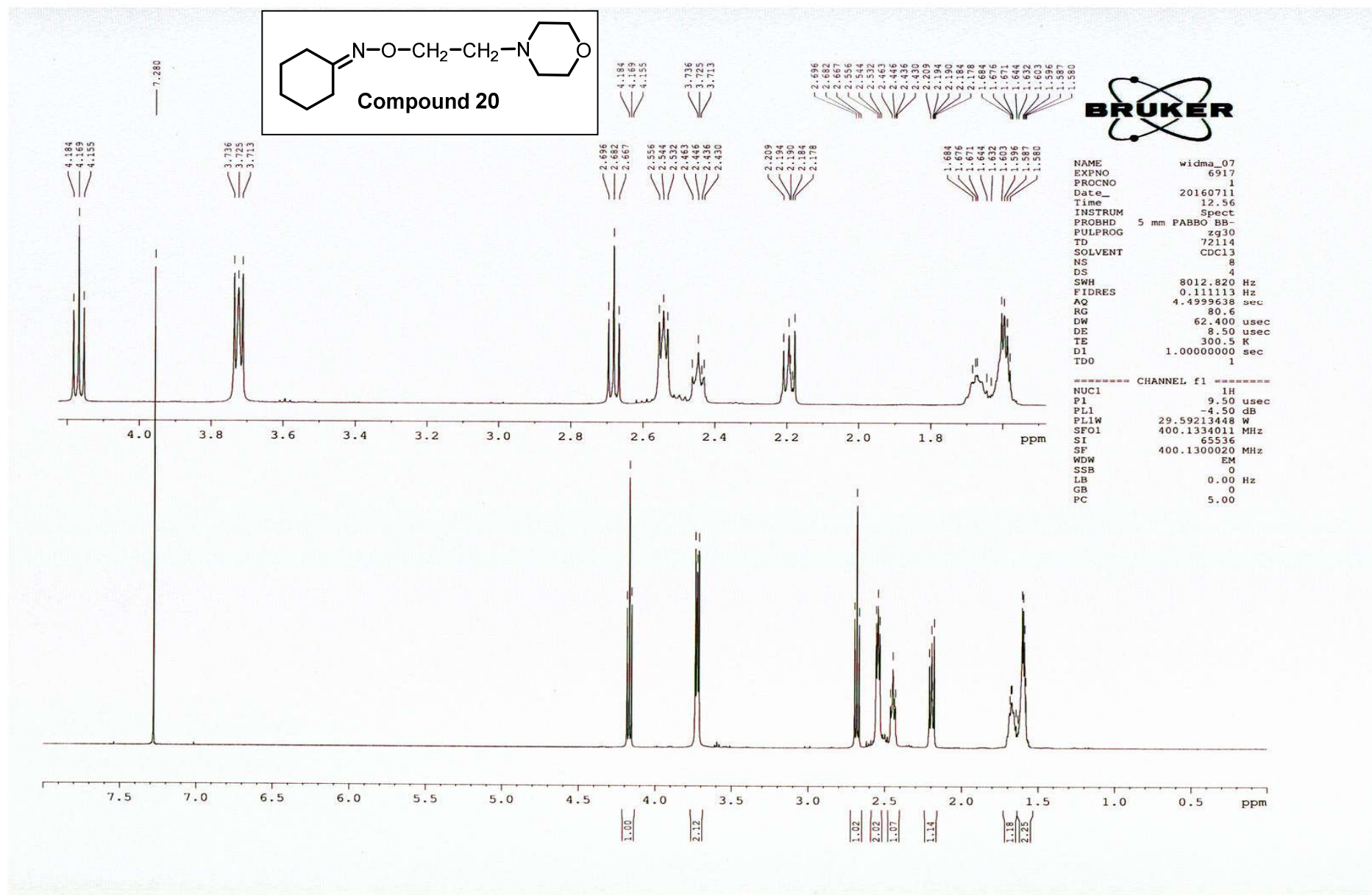
¹H NMR spectrum of the compound **18**



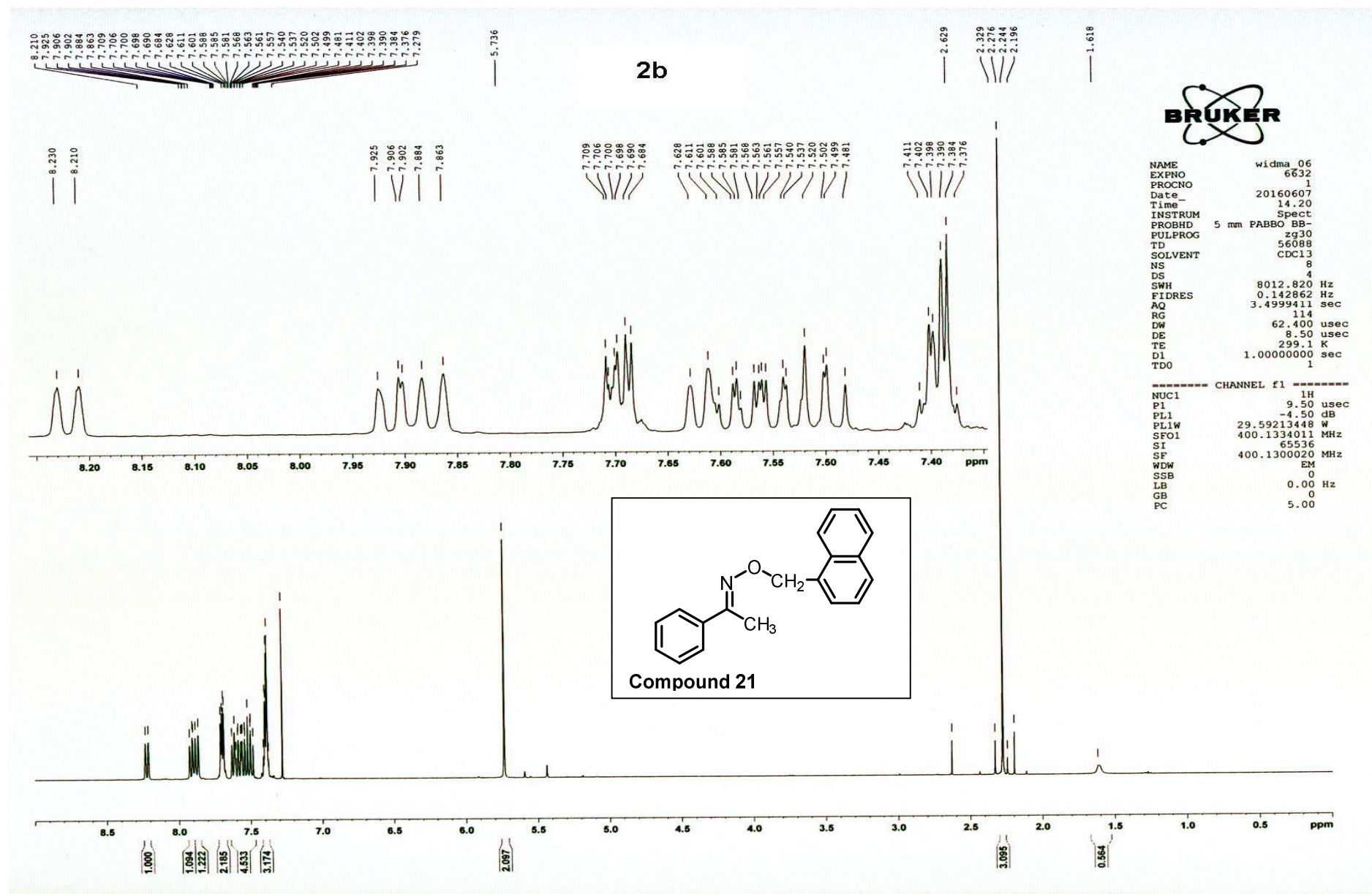
¹H NMR spectrum of the compound **19**



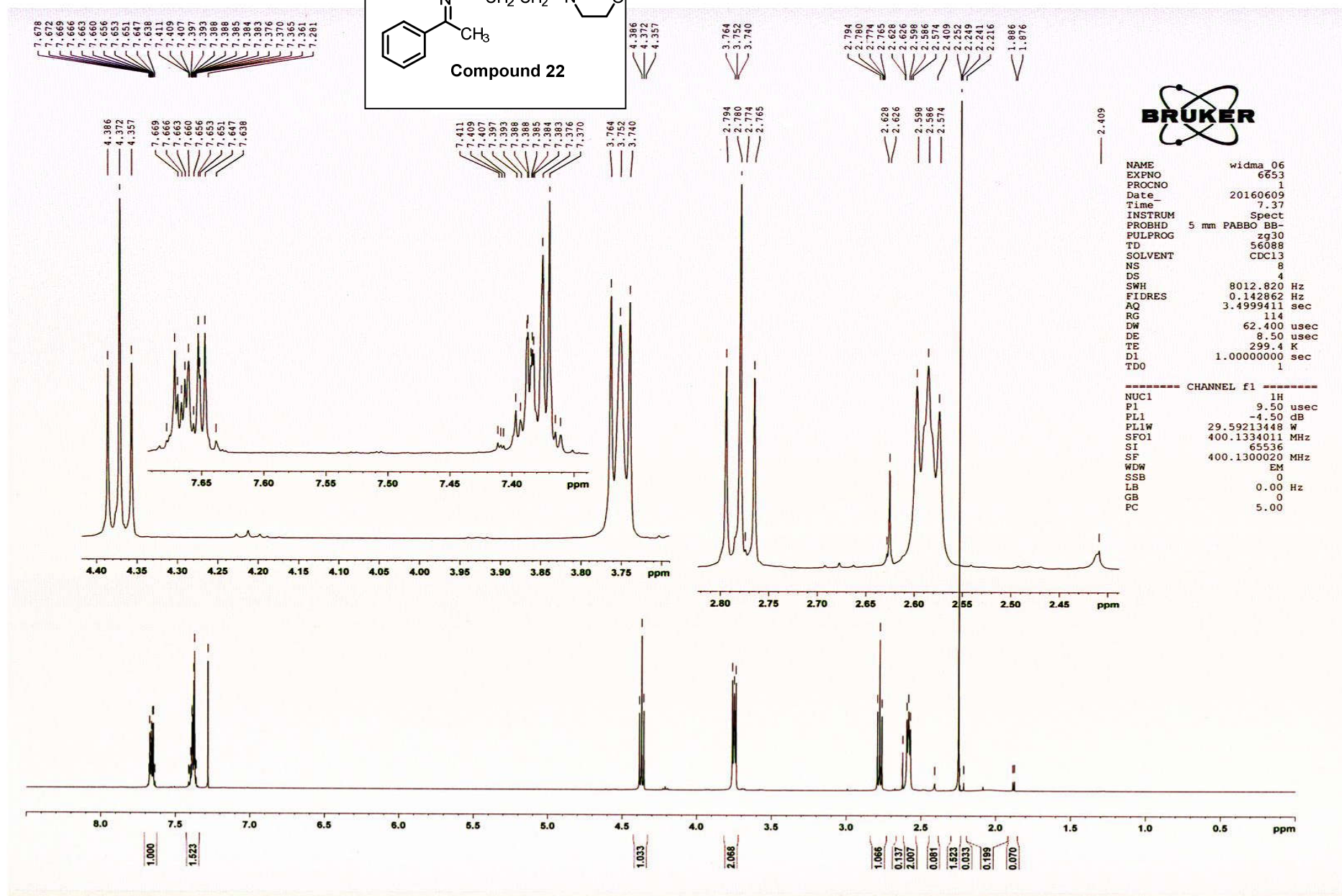
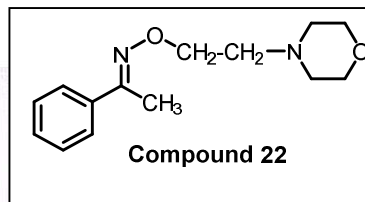
^1H NMR spectrum of the compound **20**



¹H NMR spectrum of the compound **21**

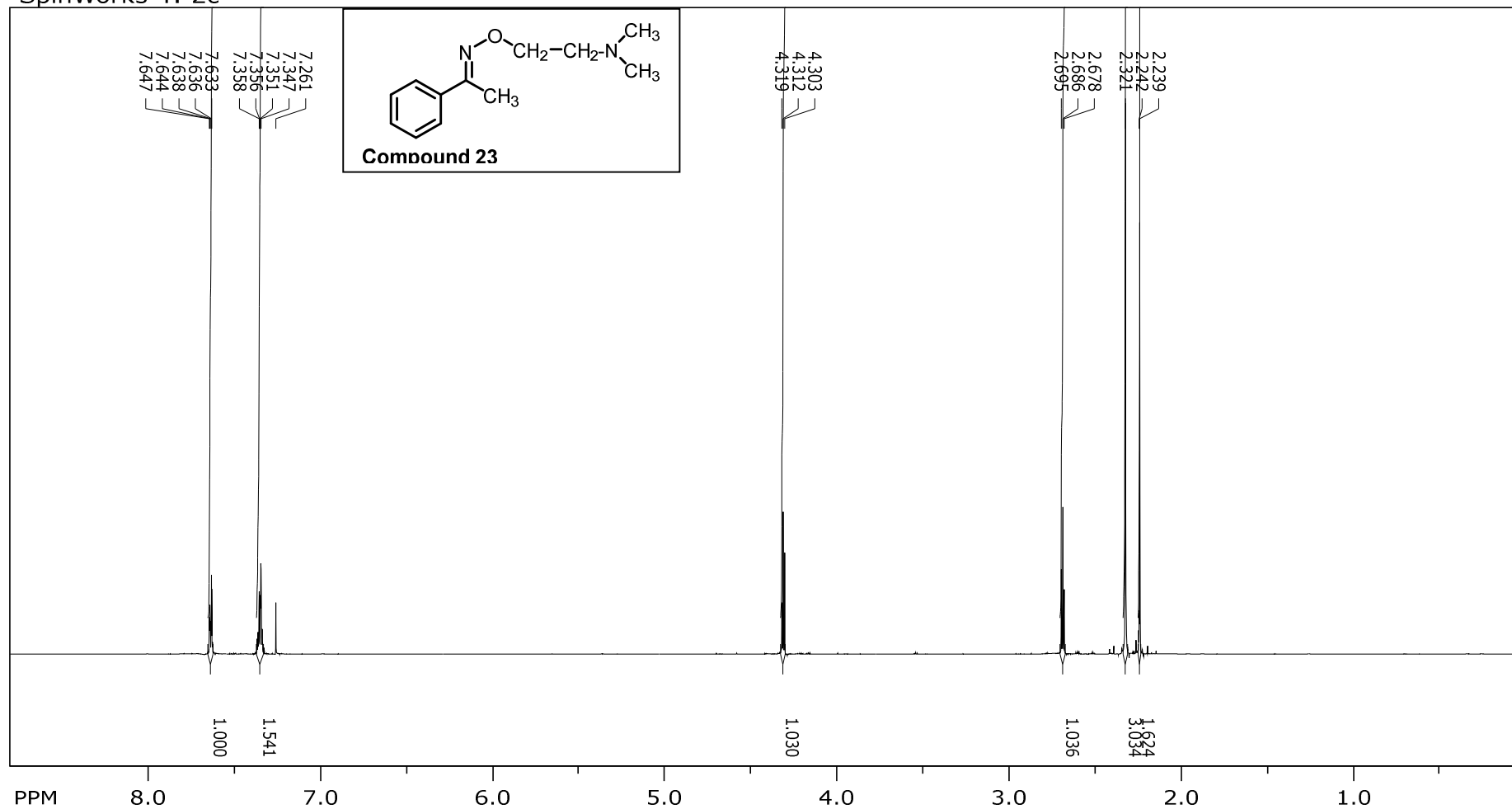


¹H NMR spectrum of the compound **22**



¹H NMR spectrum of the compound **23**

SpinWorks 4: 2c

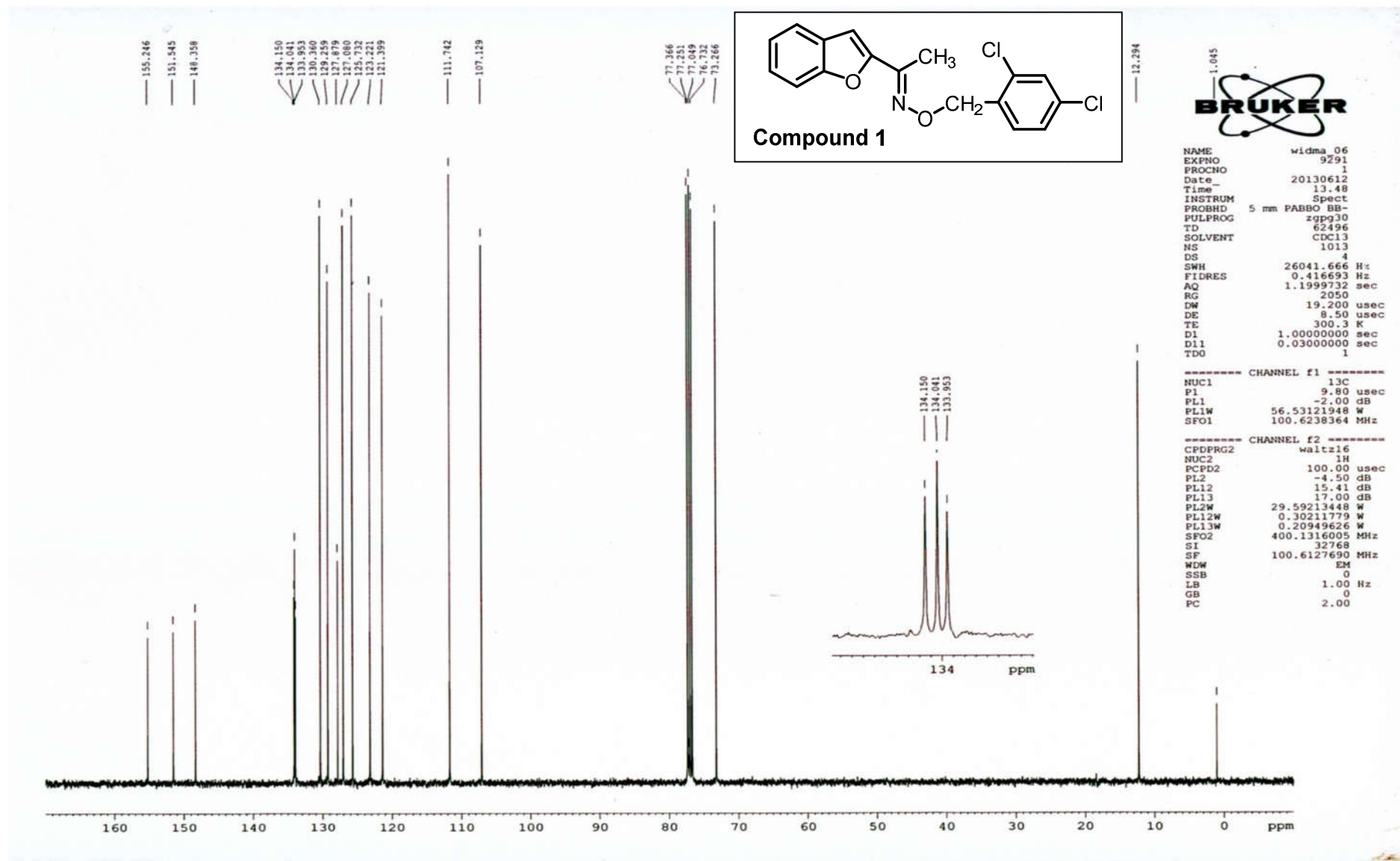


file: ...rs\Tomek\Desktop\NMR 700\15405\fid expt: <zg30>
transmitter freq.: 700.275602 MHz
time domain size: 126878 points
width: 14097.74 Hz = 20.1317 ppm = 0.111113 Hz/pt
number of scans: 8

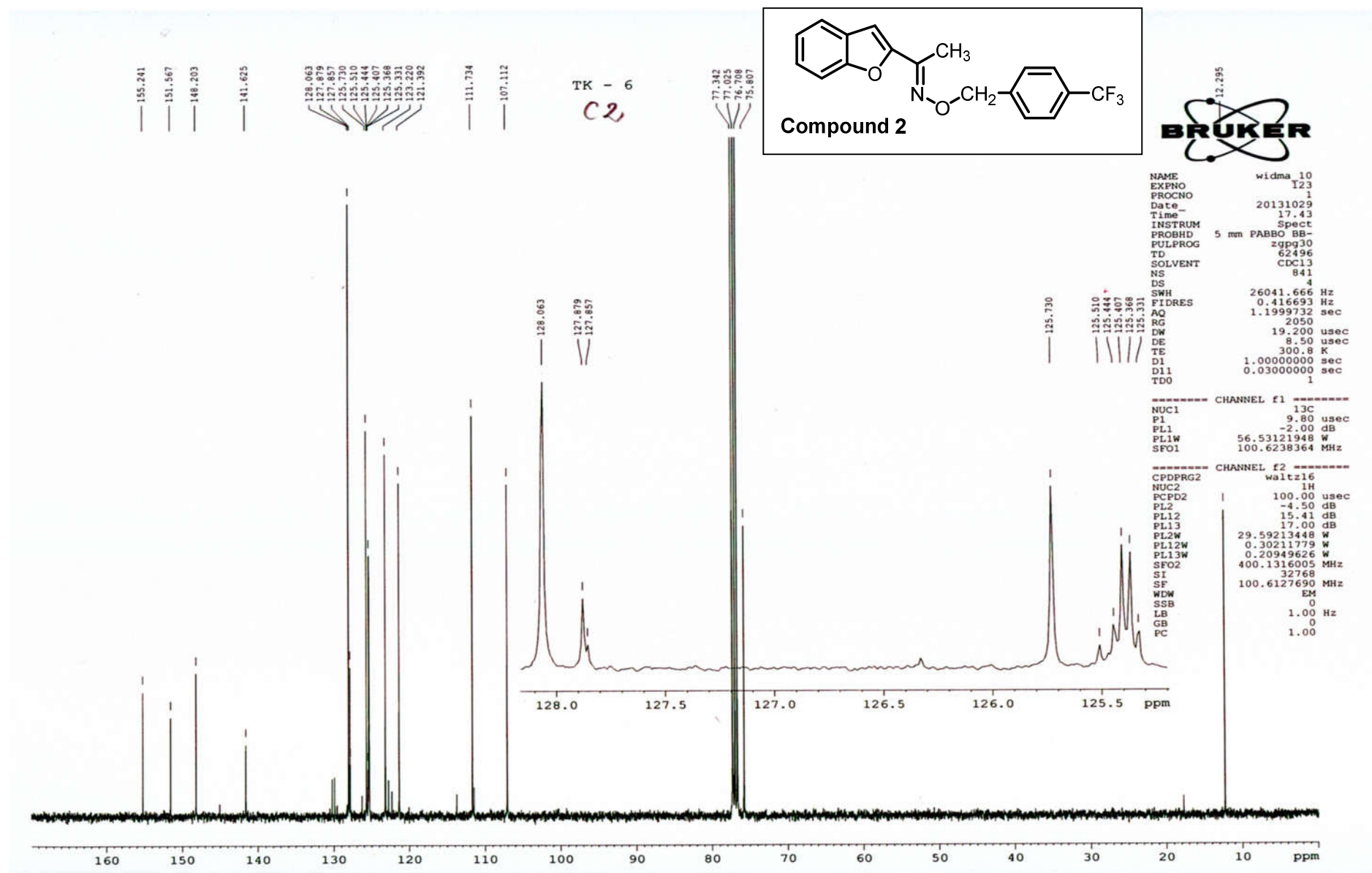
freq. of 0 ppm: 700.270022 MHz
processed size: 16384 complex points
LB: 0.000 GF: 0.0000

¹³C NMR Spectra of the compounds **1-5**, **7-12** and **16-23**.

¹³C NMR spectrum of the compound **1**

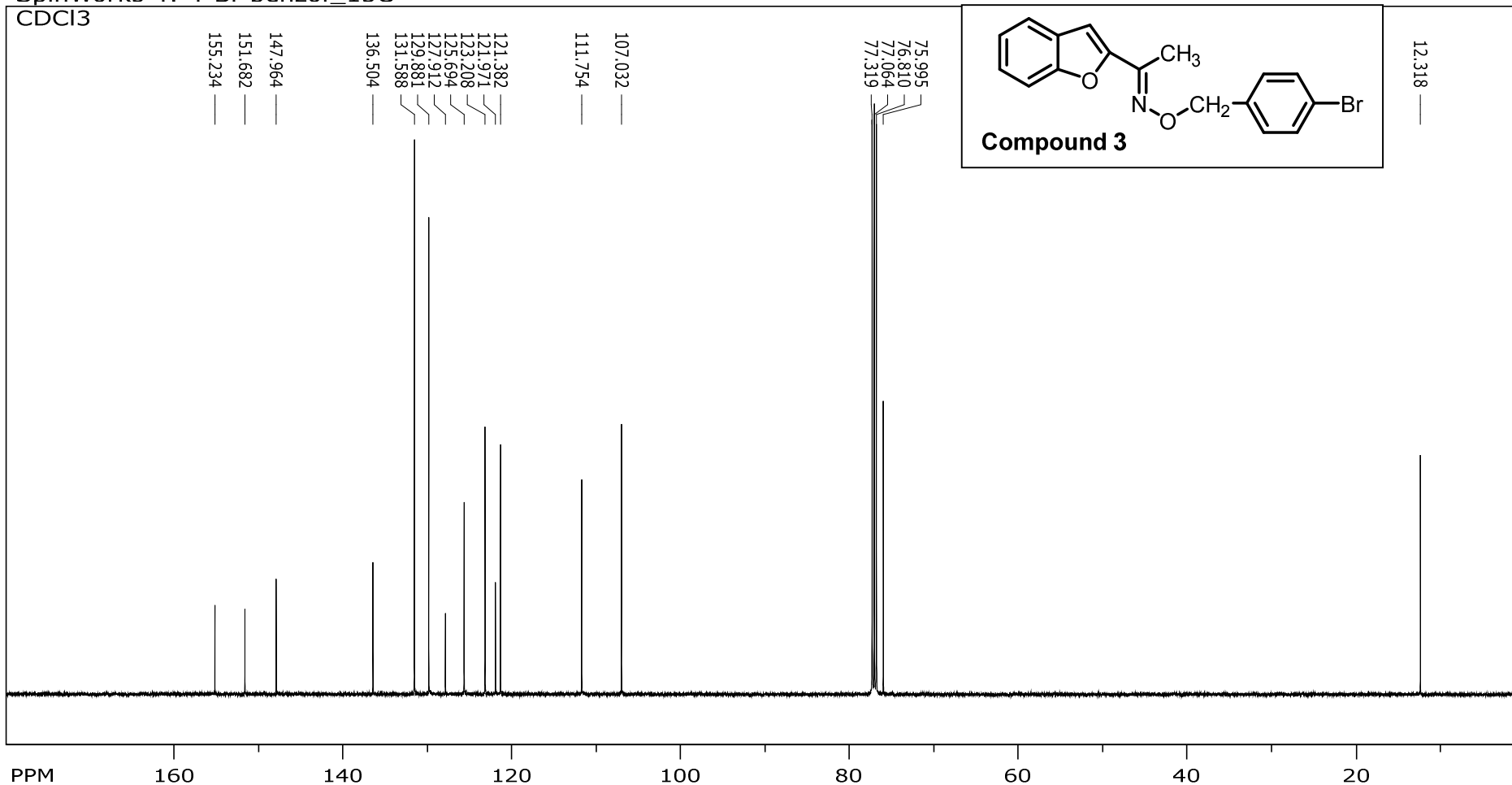


¹³C NMR spectrum of the compound 2



¹³C NMR spectrum of the compound **3**

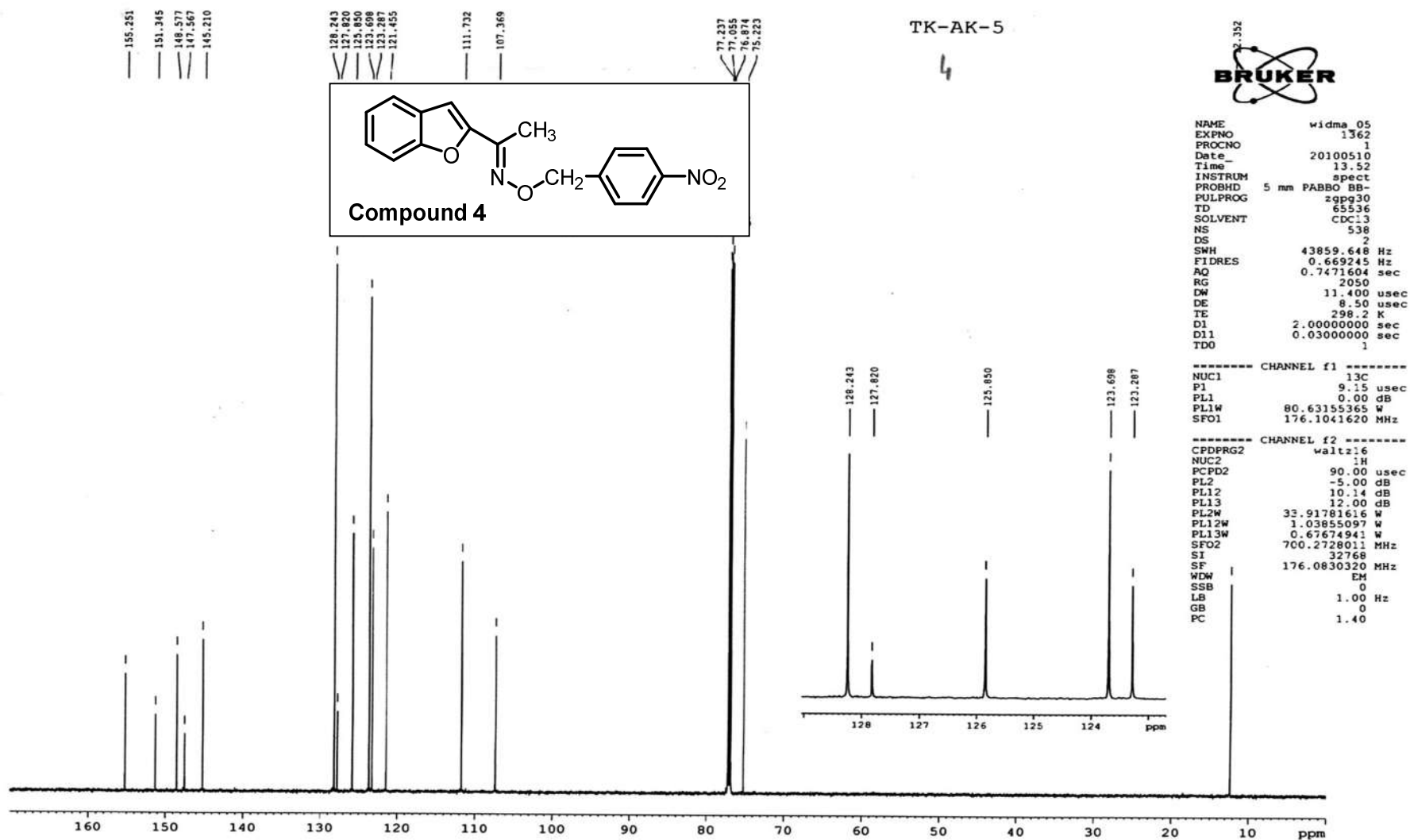
SpinWorks 4: 4-Br benzo_13C



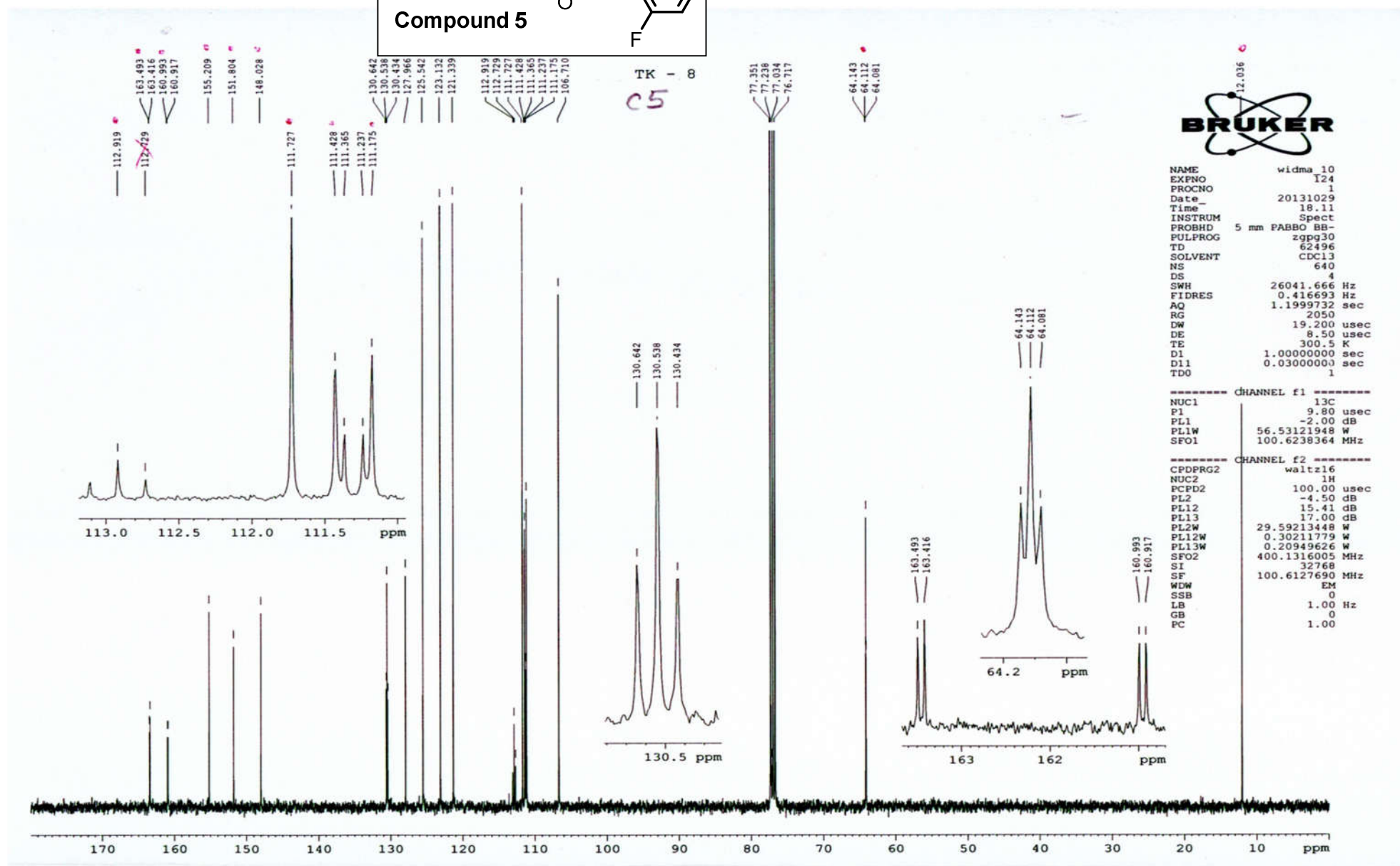
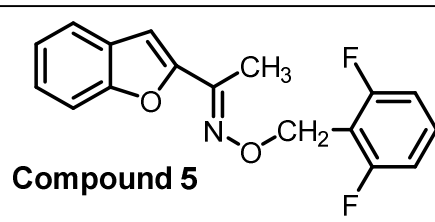
file: ...rs\user\Desktop\Widma 2022\2\2\fid expt: <zpgpg30>
transmitter freq.: 125.803057 MHz
time domain size: 65536 points
width: 32894.74 Hz = 261.4780 ppm = 0.501934 Hz/pt
number of scans: 1024

freq. of 0 ppm: 125.787963 MHz
processed size: 32768 complex points
LB: 1.000 GF: 0.0000

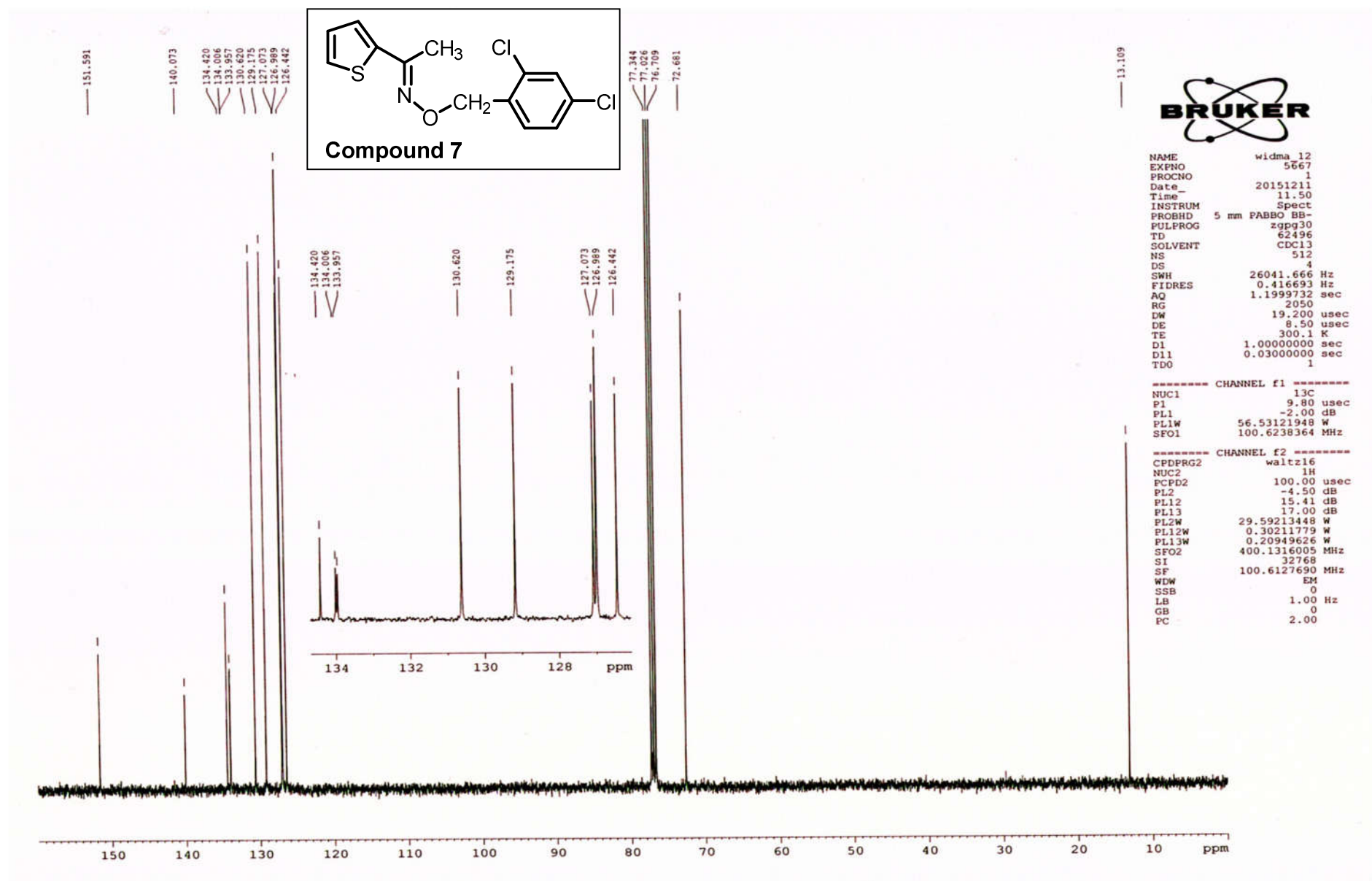
¹³C NMR spectrum of the compound 4



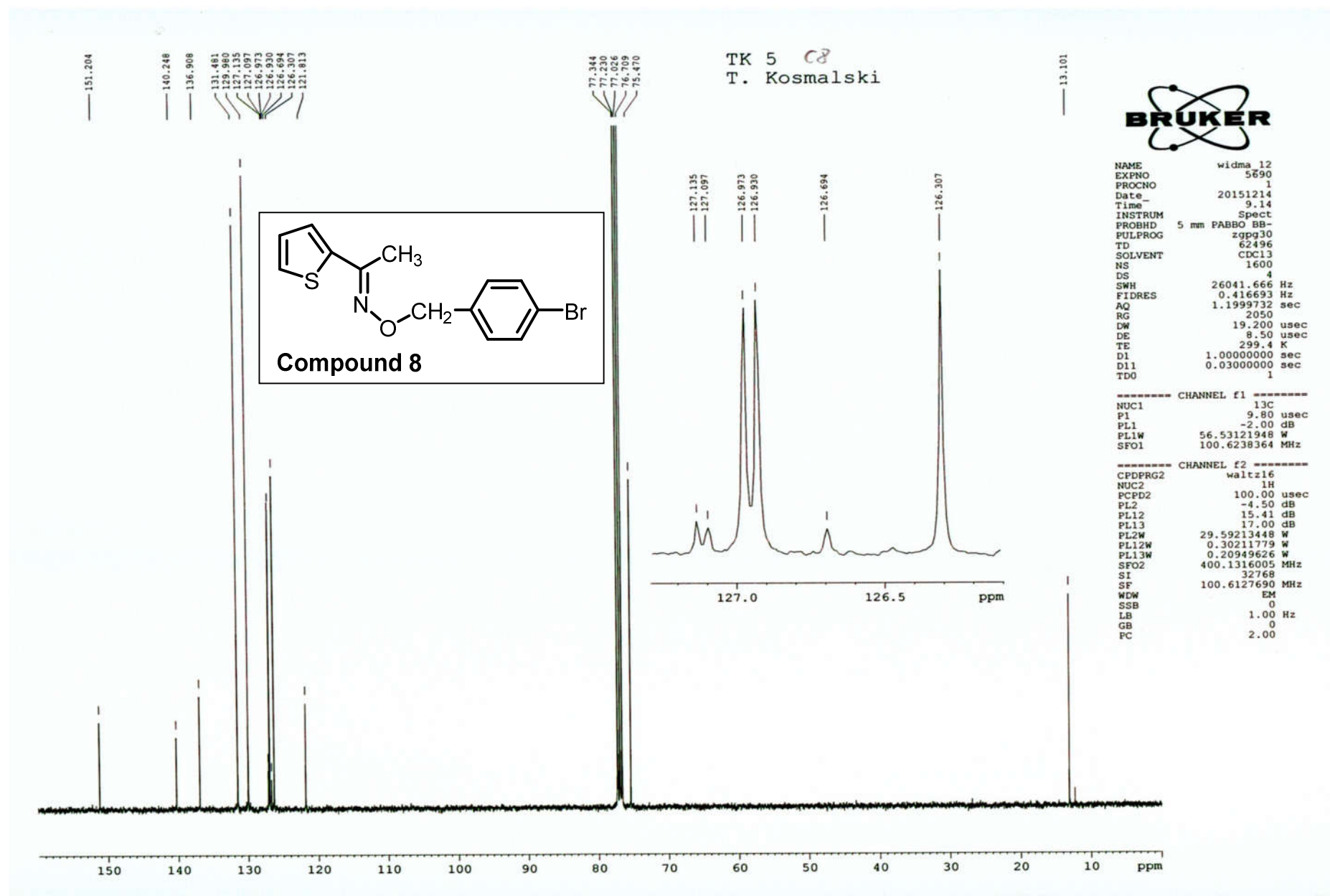
^{13}C NMR spectrum of the compound **5**



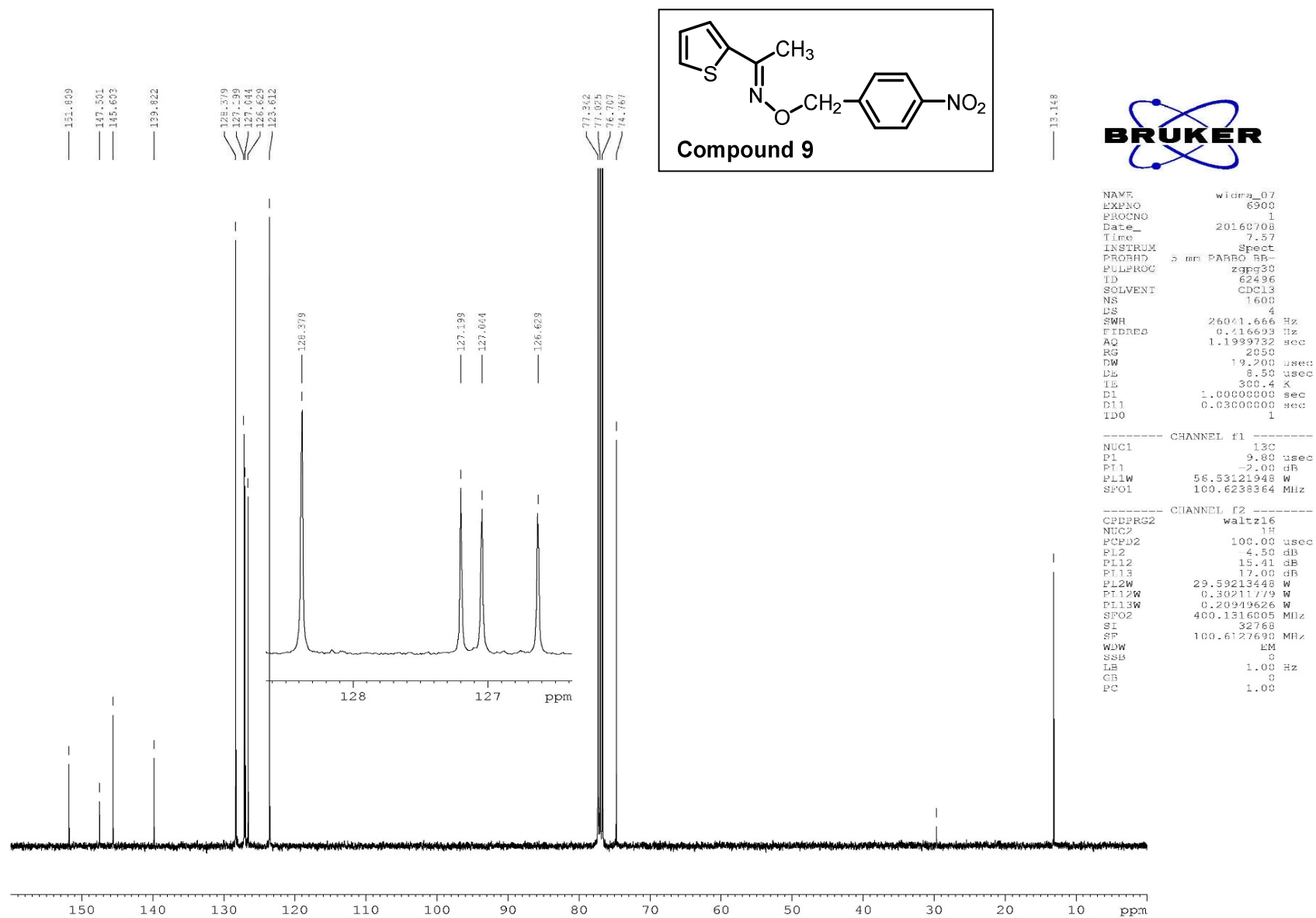
^{13}C NMR spectrum of the compound 7



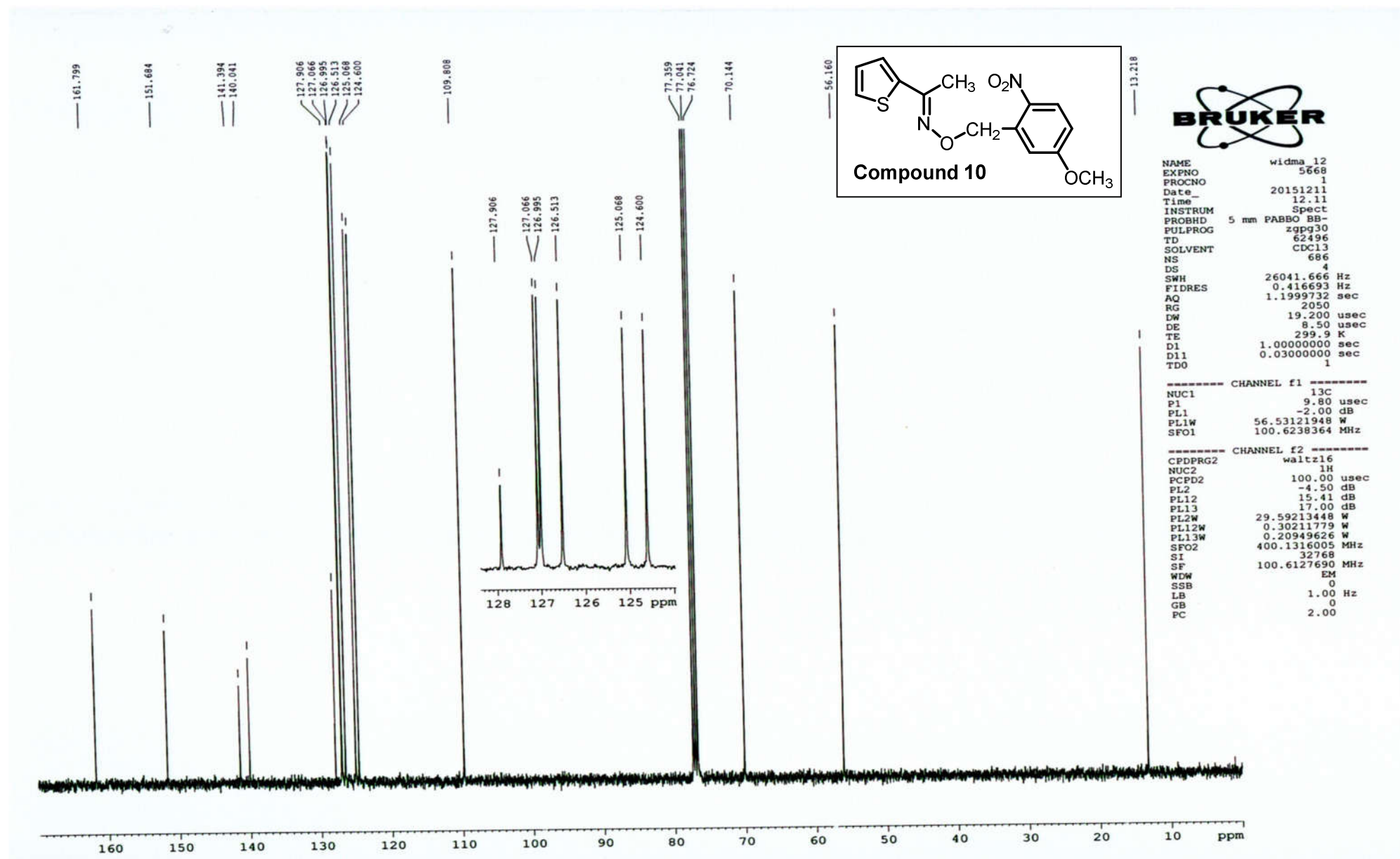
^{13}C NMR spectrum of the compound 8



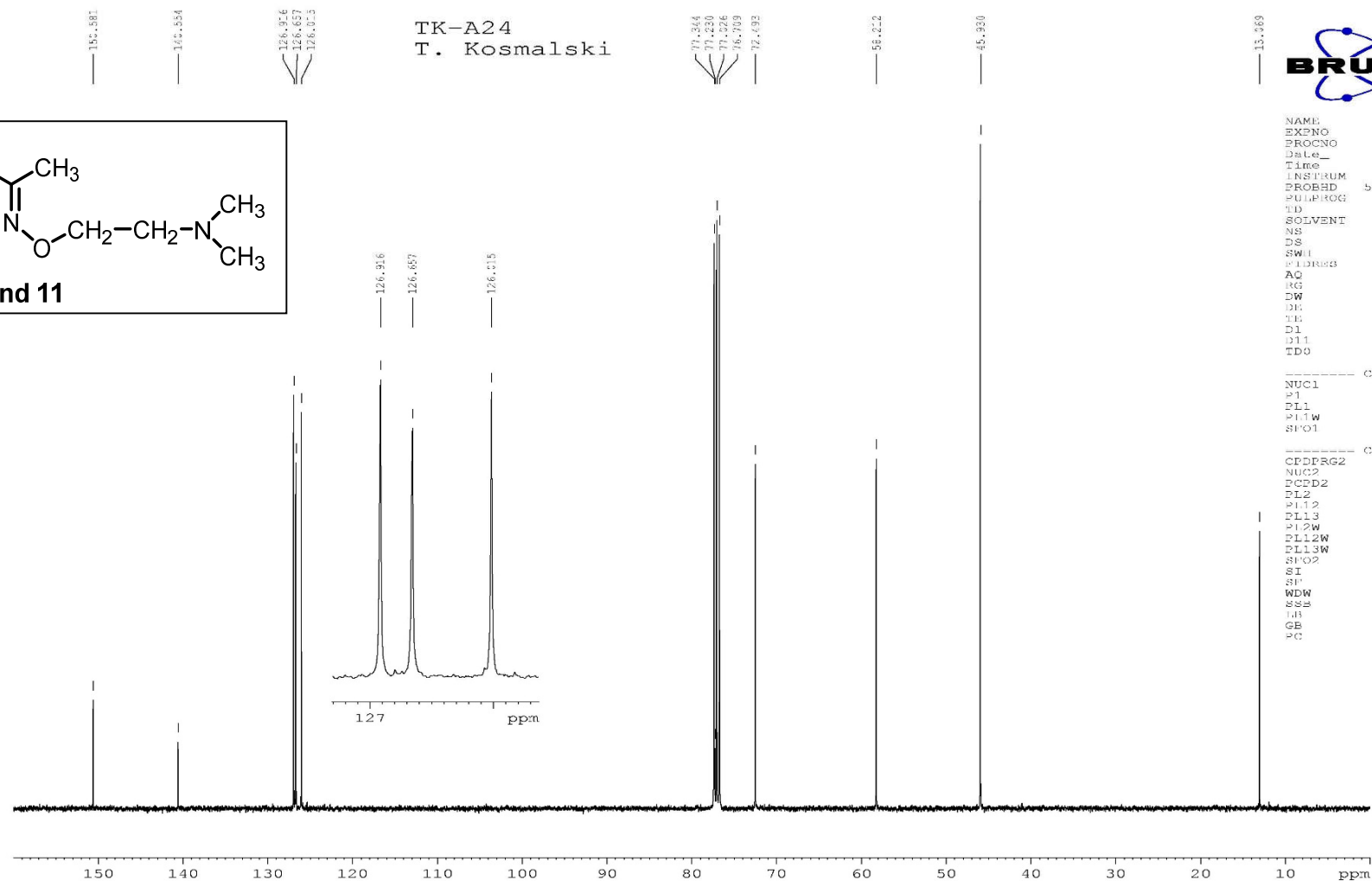
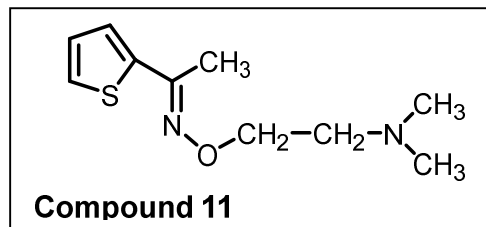
¹³C NMR spectrum of the compound 9



^{13}C NMR spectrum of the compound **10**



¹³C NMR spectrum of the compound **11**



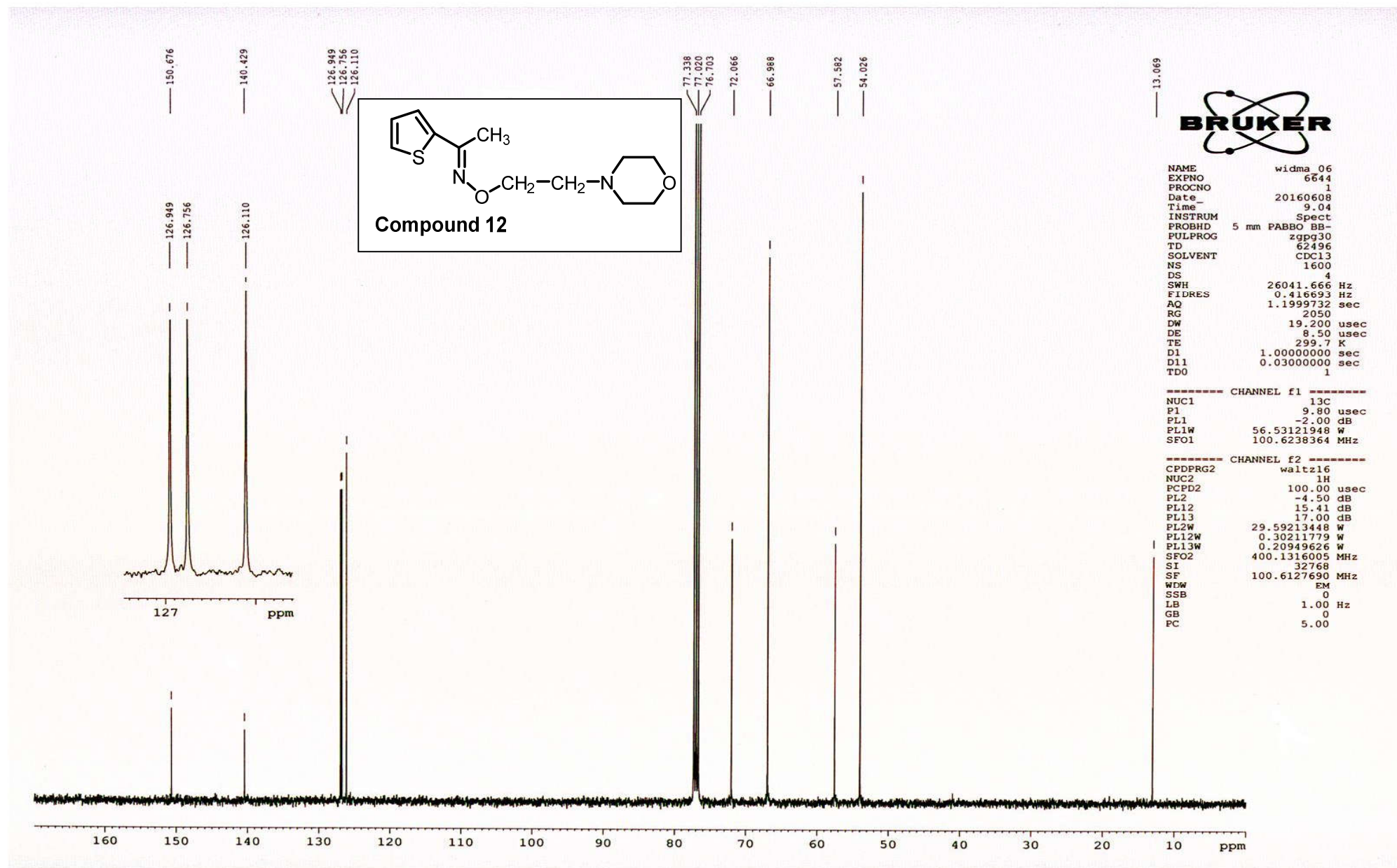
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NAME      widma_07
EXPNO     6921
PROCNO    1
Date_     20160712
Time      9.54
INSTRUM   Spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD        62496
SOLVENT   CDCl3
NS        1600
DS        4
SWH       26041.666 Hz
FIDRES    0.416693 Hz
AQ        1.1999732 sec
RG        2050
DW        19.200 usec
DE        8.50 usec
TE        301.0 K
D1        1.0000000 sec
D11       0.0300000 sec
TD0       1

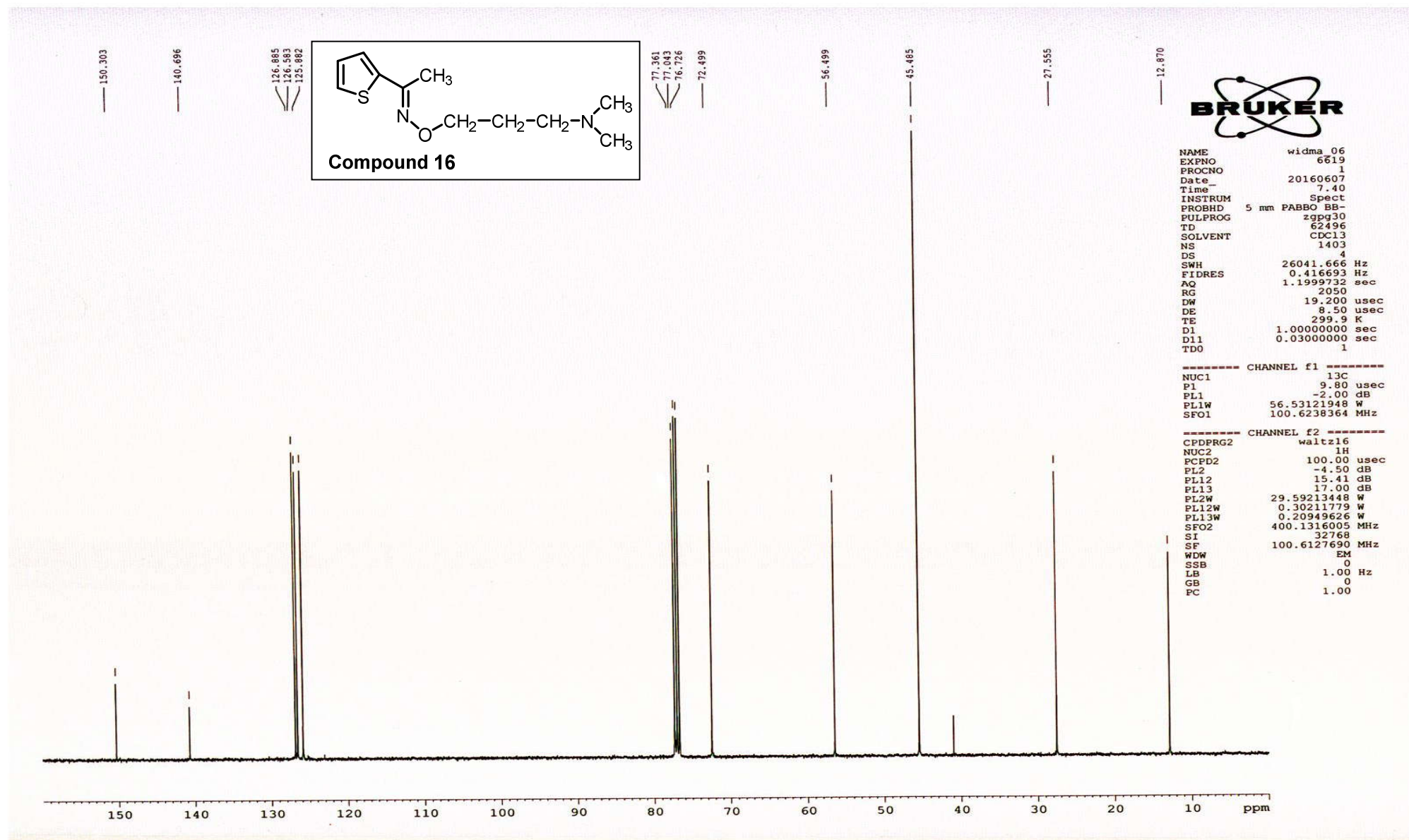
----- CHANNEL f1 -----
NUC1      13C
P1        9.80 usec
PL1       -2.00 dB
PL1W      56.53121948 W
SFO1      100.6238364 MHz

----- CHANNEL f2 -----
CPDPRG2   waltz16
NUC2      1H
PCPD2     100.00 usec
PL2       -4.50 dB
PL12      15.41 dB
PL13      17.00 dB
PL12W     29.59213448 W
PL12W     0.30211779 W
PL13W     0.20949626 W
SFO2      400.1316005 MHz
SI        32768
SF        100.6127690 MHz
WDW       EM
SSB       0
GB        1.00 Hz
PC        1.00
    
```

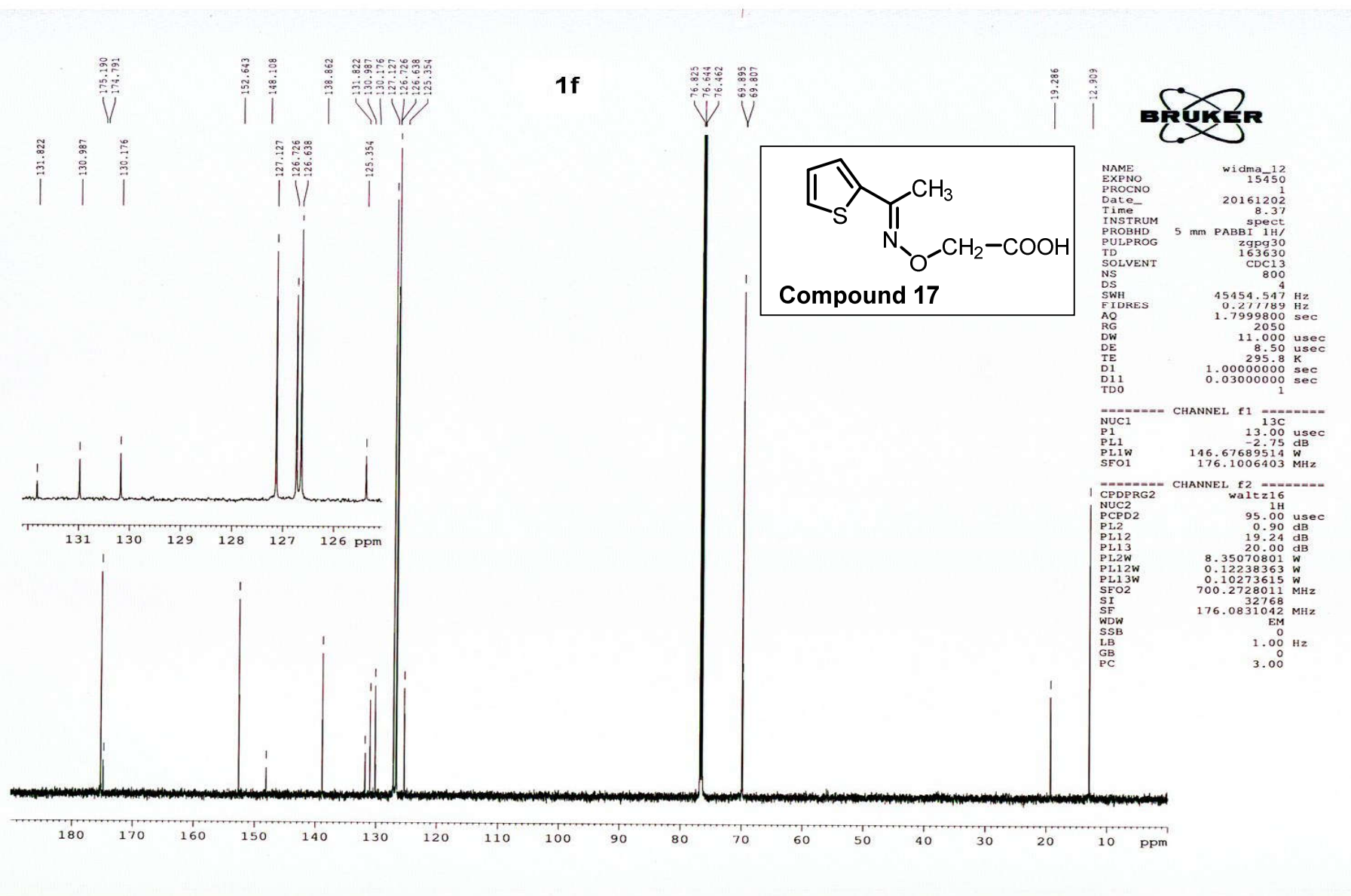

^{13}C NMR spectrum of the compound **12**



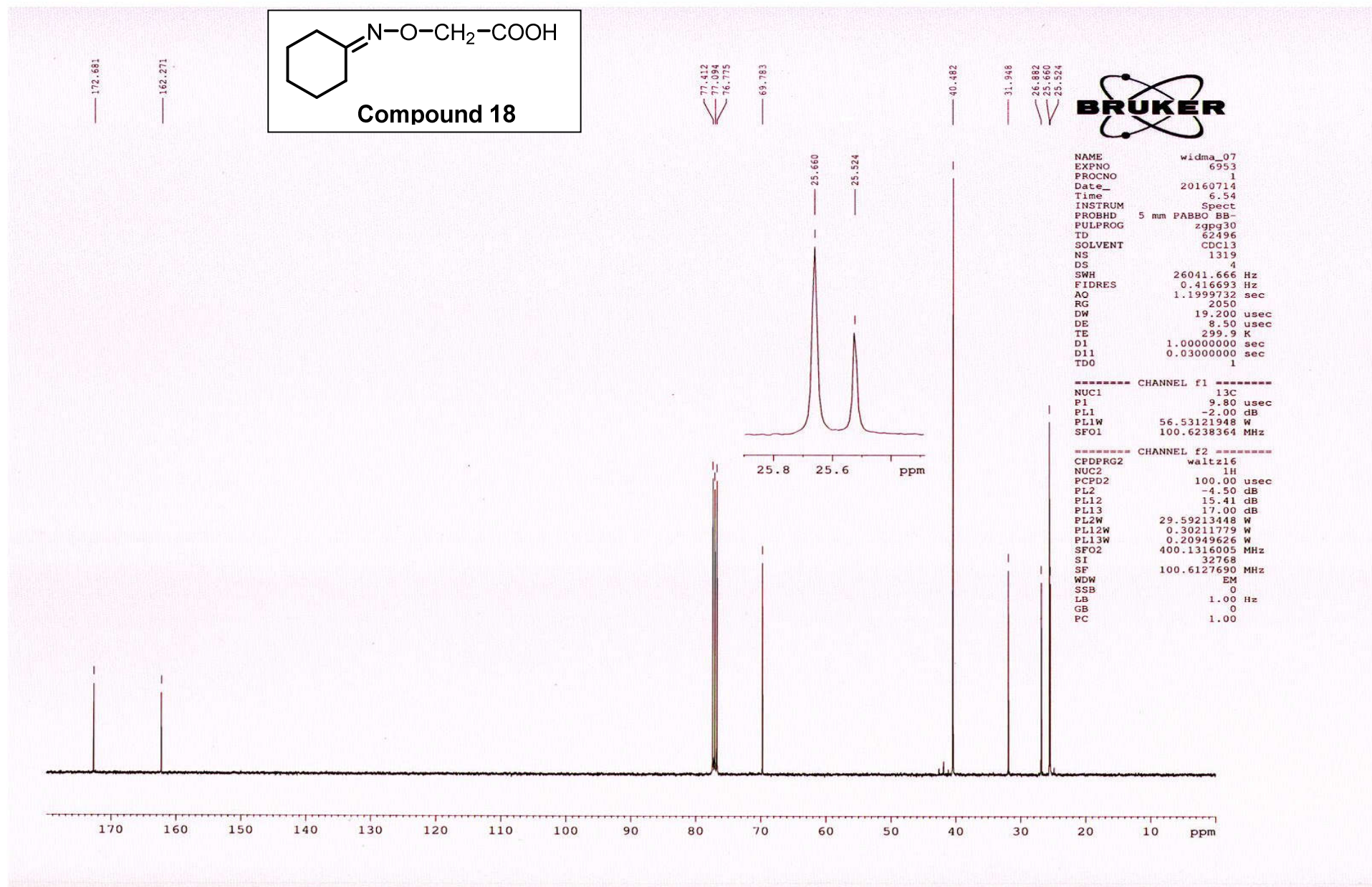
¹³C NMR spectrum of the compound **16**



^{13}C NMR spectrum of the compound **17**



¹³C NMR spectrum of the compound **18**



Compound 19

¹³C NMR Spectrum (ppm)

The spectrum shows peaks at the following chemical shifts (ppm): 160.281, 77.341, 77.226, 77.023, 76.704, 71.370, 58.094, 45.913, 32.223, 32.188, 32.153, 27.019, 26.947, 25.881, 25.819, 25.730, 25.643, 25.422, 24.284.

Acquisition Parameters:

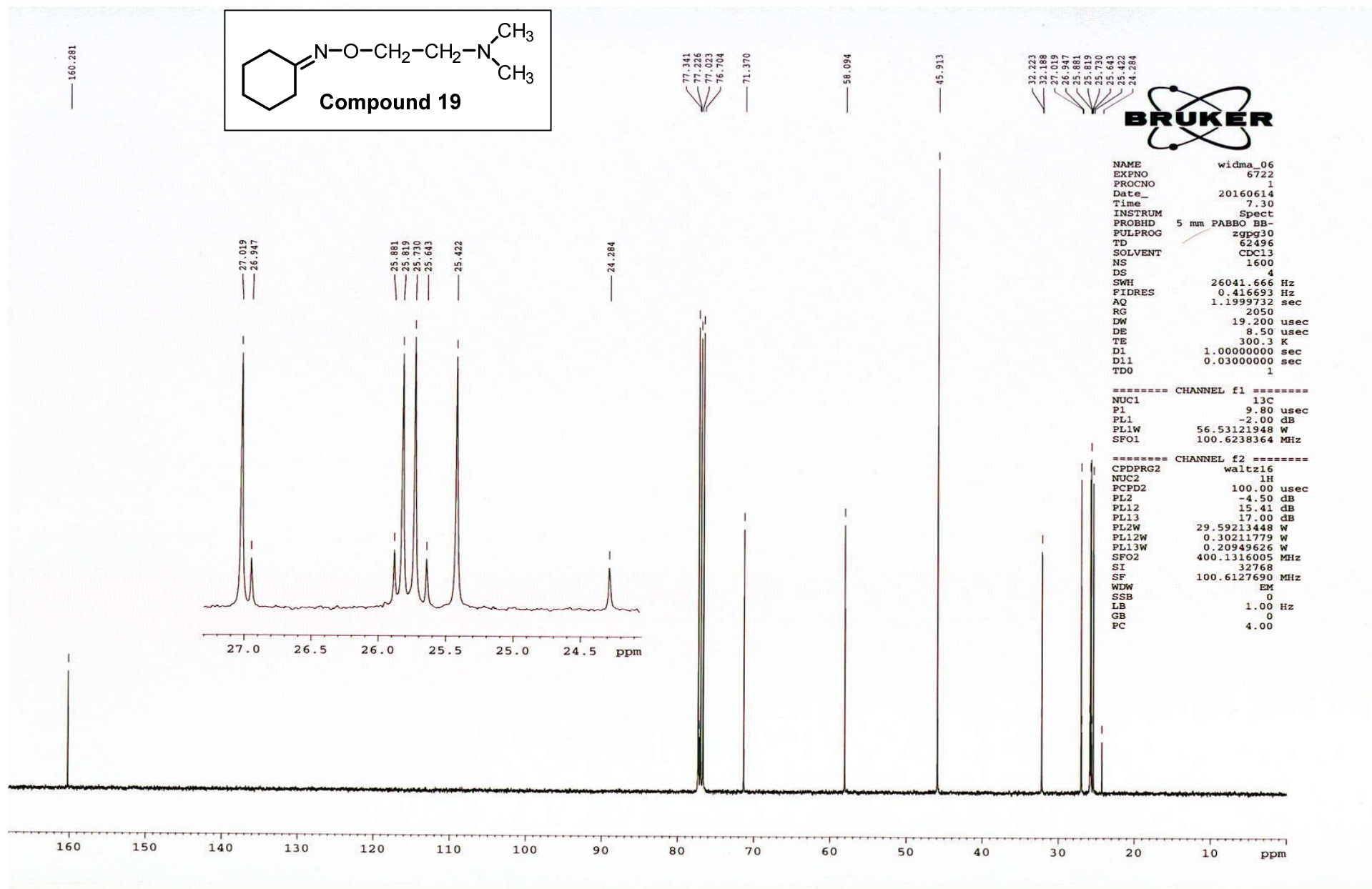
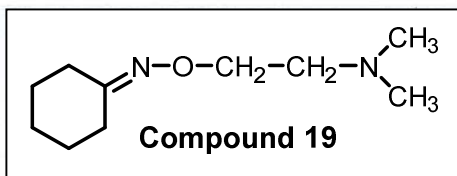
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NAME	widma_06
EXPNO	6722
PROCNO	1
Date_	20160614
Time	7.30
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PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	62496
SOLVENT	CDC13
NS	1600
DS	4
SWH	26041.666 Hz
FIDRES	0.416693 Hz
AQ	1.1999732 sec
RG	2050
DW	19.200 usec
DE	8.50 usec
TE	300.3 K
D1	1.00000000 sec
D11	0.03000000 sec
TDO	1

Channel f1 Parameters:

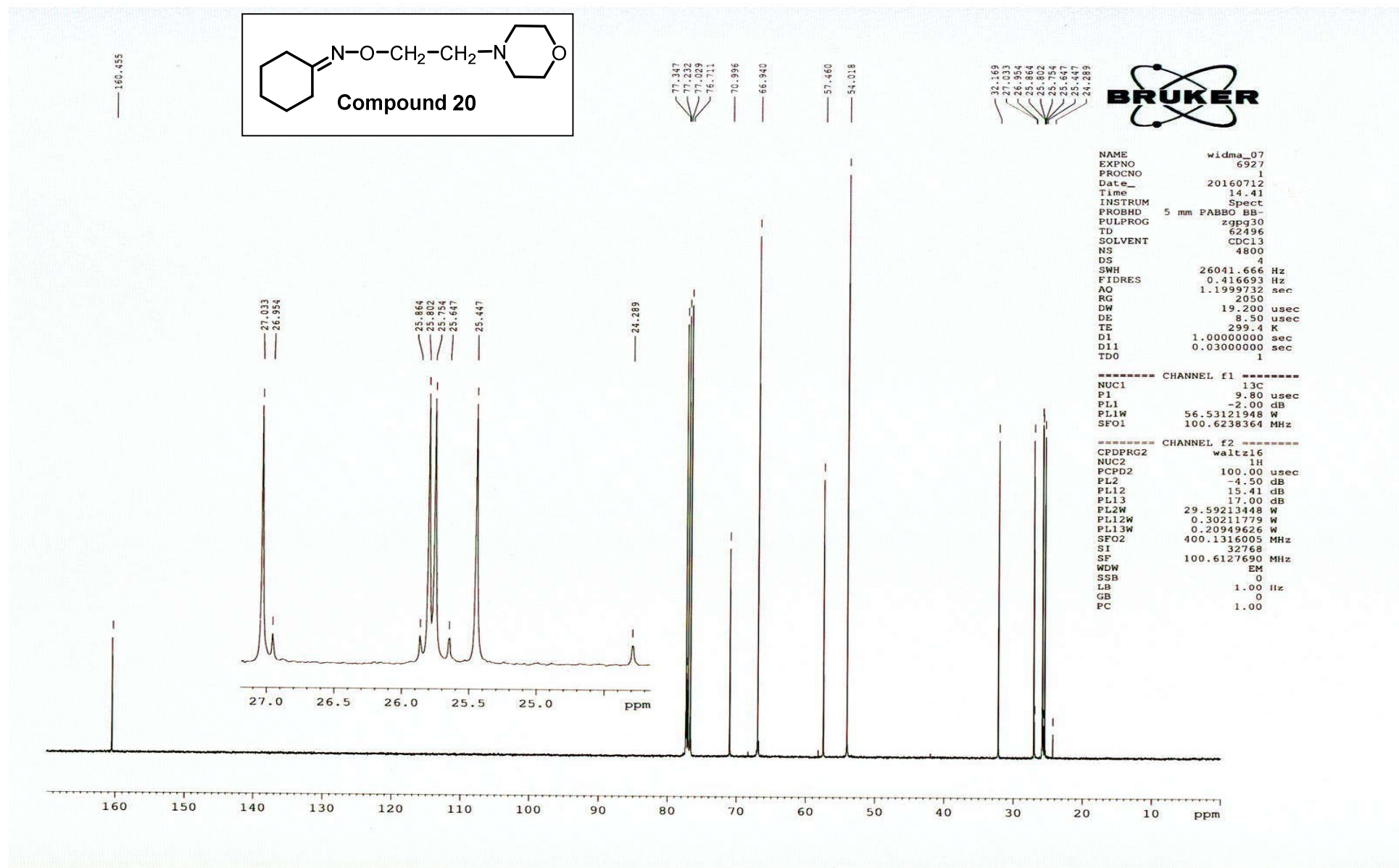
Parameter	Value
NUC1	13C
P1	9.80 usec
PL1	-2.00 dB
PL1W	56.53121948 W
SFO1	100.6238364 MHz

Channel f2 Parameters:

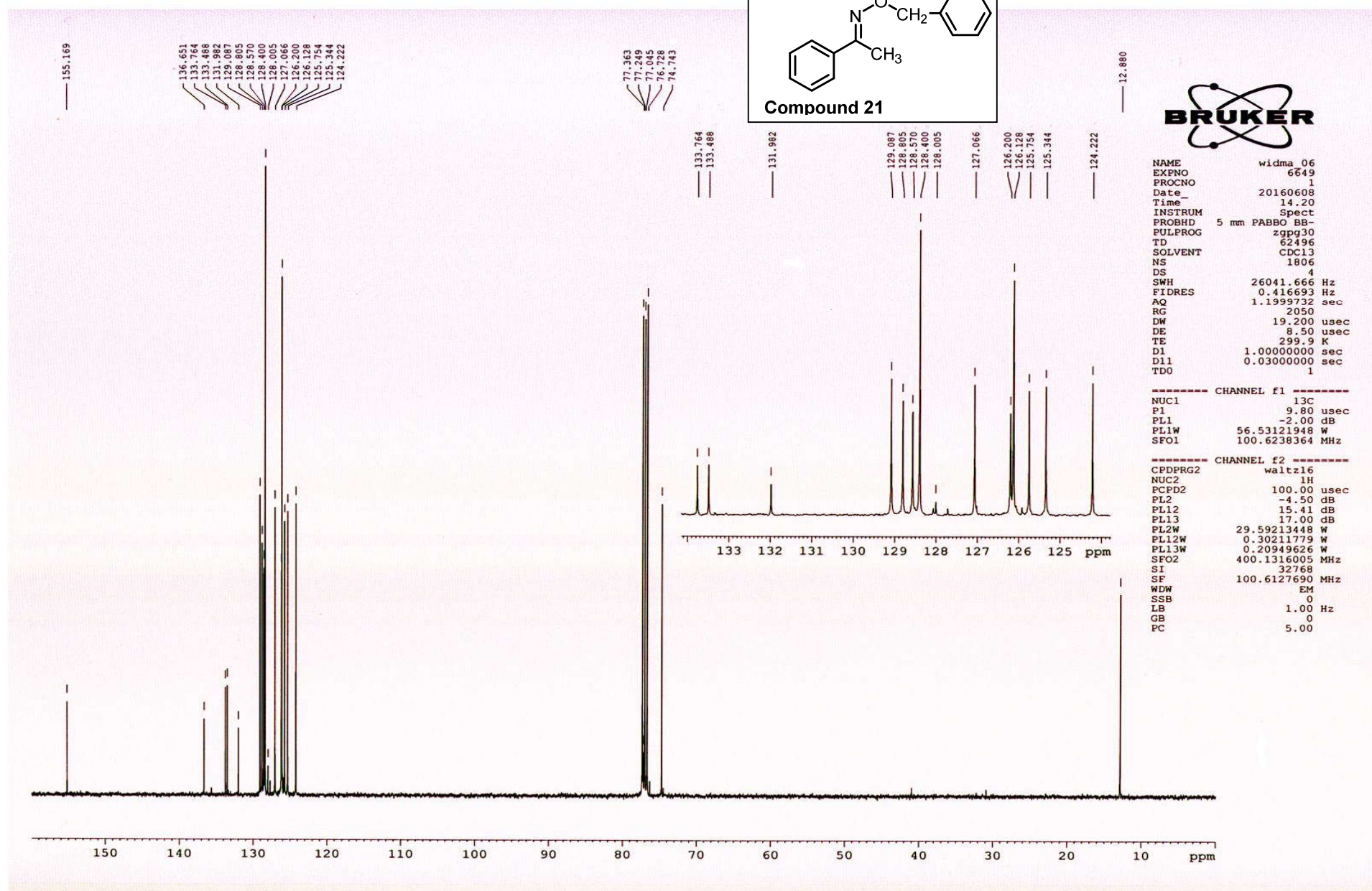
Parameter	Value
CPDPRG2	waltz16
NUC2	1H
PCPD2	100.00 usec
PL2	-4.50 dB
PL12	15.41 dB
PL13	17.00 dB
PL2W	29.59213448 W
PL12W	0.30211779 W
PL13W	0.20949626 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	4.00



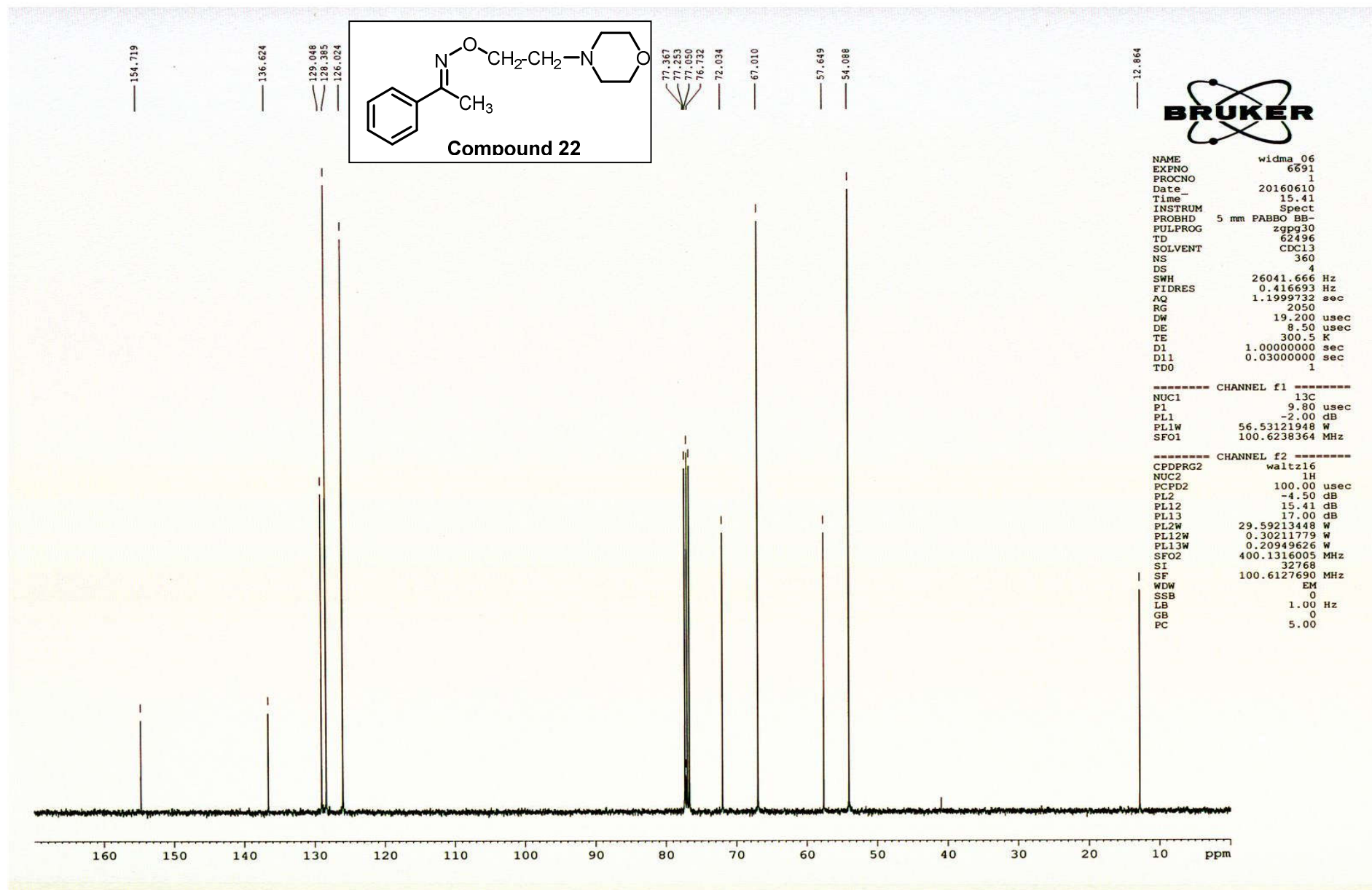
¹³C NMR spectrum of the compound **20**



¹³C NMR spectrum of the compound **21**

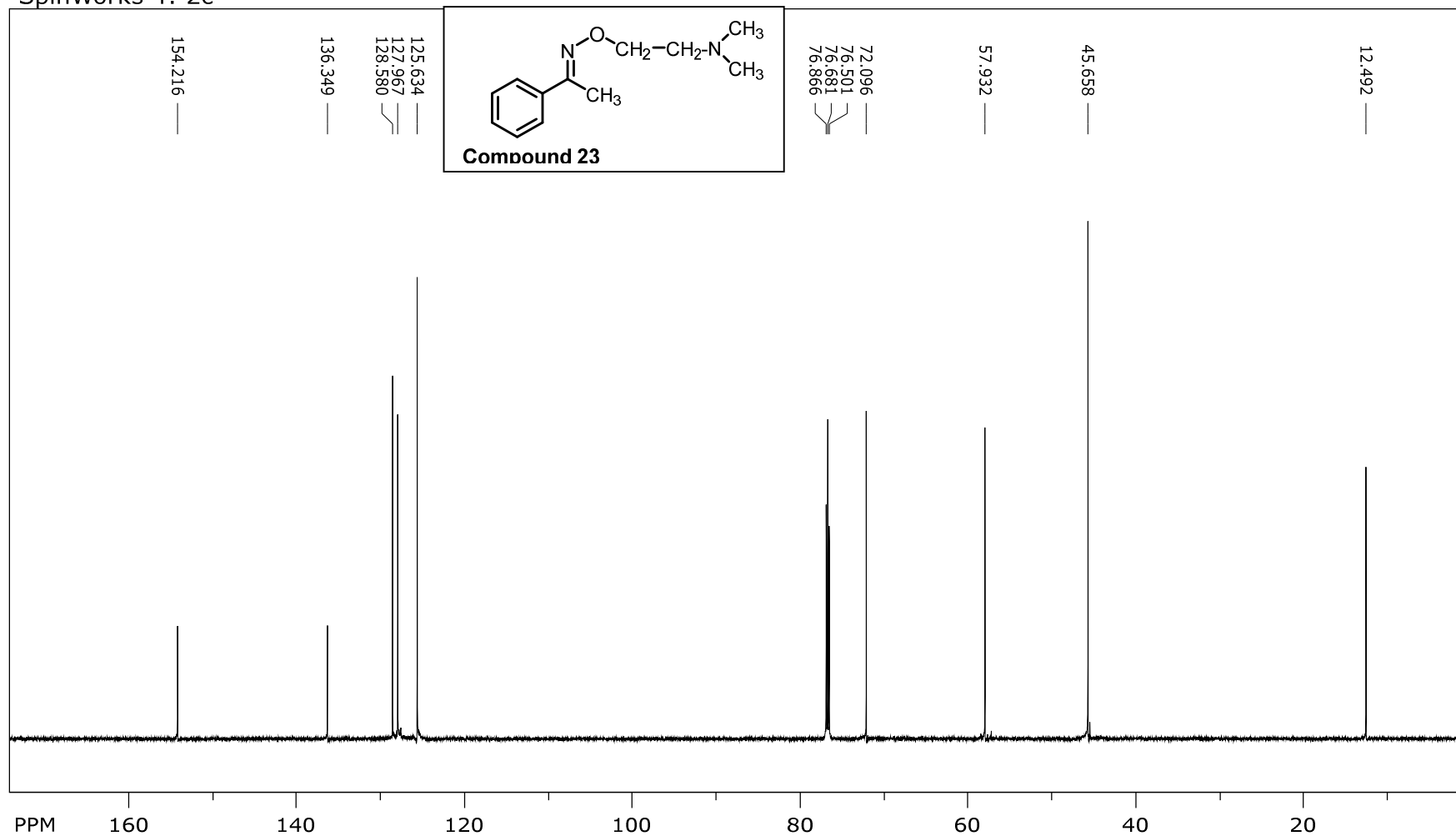


¹³C NMR spectrum of the compound **22**



¹³C NMR spectrum of the compound **23**

SpinWorks 4: 2c



file: ...rs\Tomek\Desktop\NMR 700\15448\fid exp: <zpgp30>
transmitter freq.: 176.100640 MHz
time domain size: 163630 points
width: 45454.55 Hz = 258.1169 ppm = 0.277789 Hz/pt
number of scans: 601

freq. of 0 ppm: 176.083104 MHz
processed size: 16384 complex points
LB: 1.000 GF: 0.0000