Supporting Information

PREPARATION OF *meso*-SILYLPORPHYRINS VIA NICKEL-CATALYZED COUPLING OF *meso*-BROMINATED Ni(II) PORPHYRINS WITH SILYLZINC REAGENTS

Satoshi Hayashi,* Taiga Endo, and Toshikatsu Takanami*

Meiji Pharmaceutical University, 2-522-1 Noshio, Kiyose, Tokyo 204-8588,
e-mail: shayashi@my-pharm.ac.jp; and takanami@my-pharm.ac.jp

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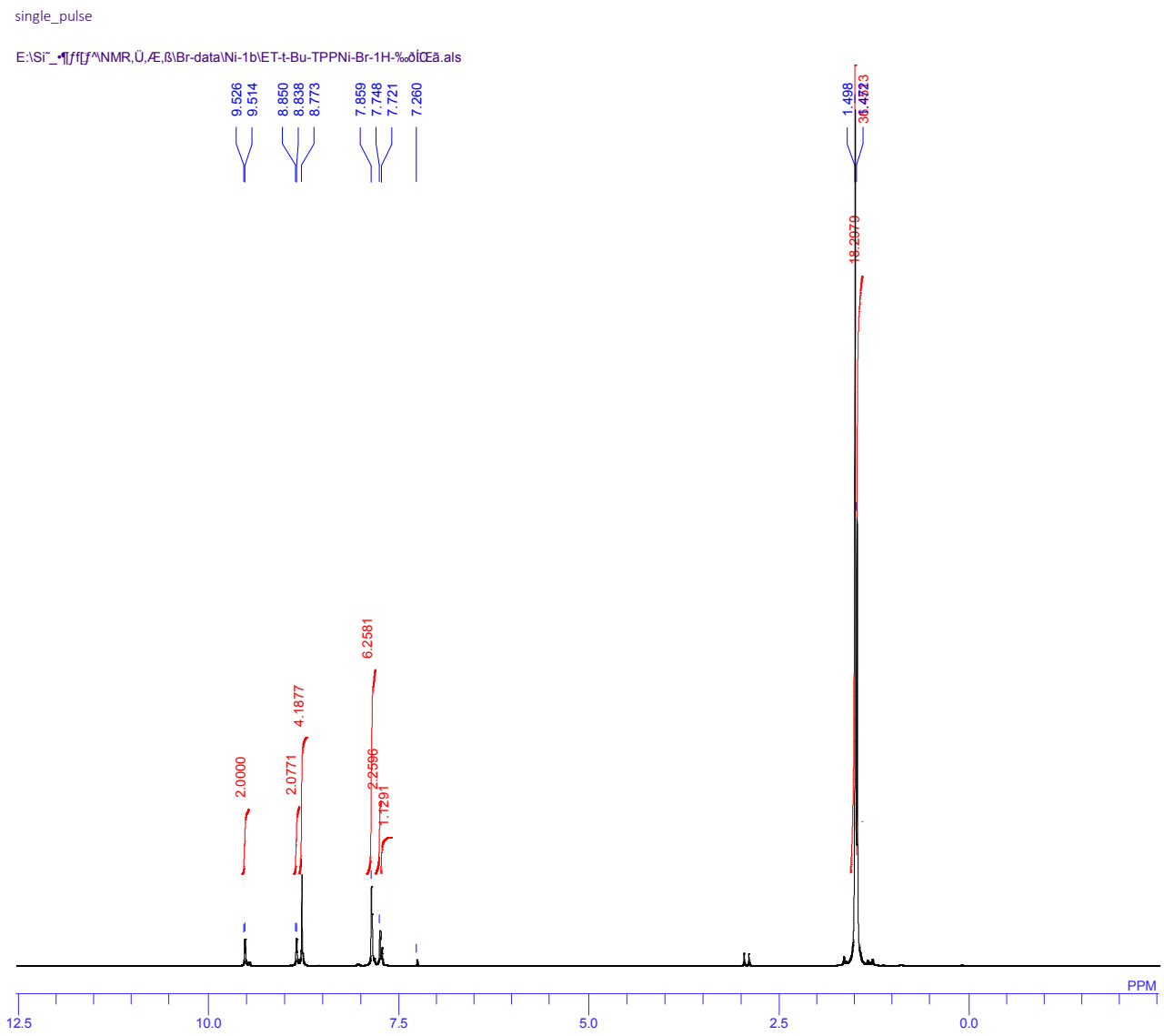
^{1}H NMR spectrum of 1b



DATIM 2018-01-25 19:47:57
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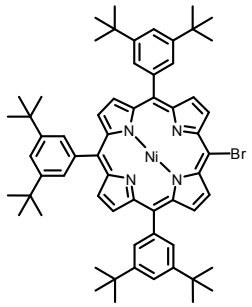
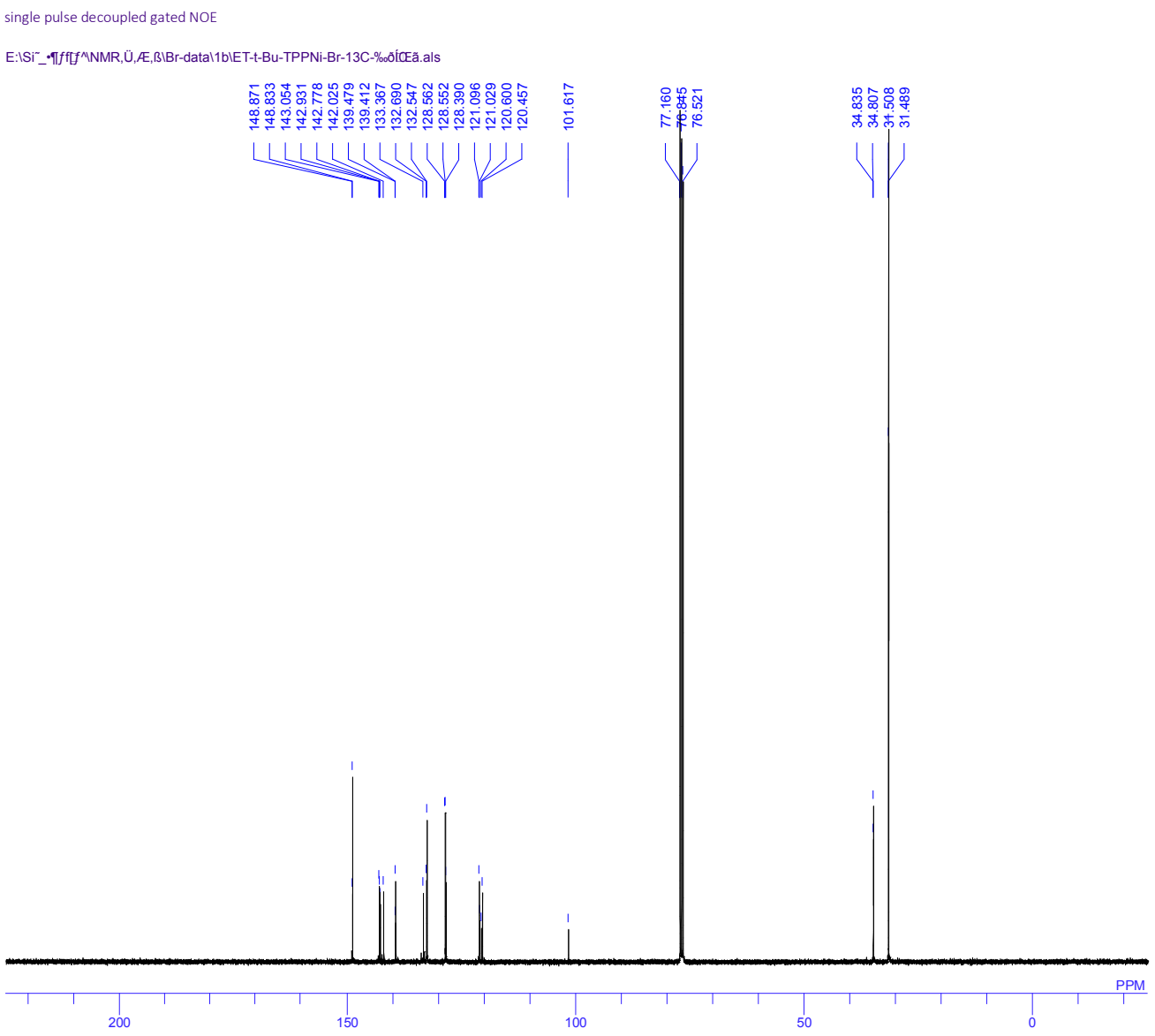
OBNUC 1H
EXMOD single_pulse.jxp
OFR 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 26214
FREQU 6002.40 Hz
SCANS 16
ACQTM 4.3673 sec
PD 2.0000 sec
PW1 3.05 usec
IRN
CTEMP 22.6 c
SLVNT CDCL3
EXREF 7.26 ppm
BF 0.01 Hz
RGAIN 36

1H-NMR (CDCl3) δ :
9.50 (2H, d, J = 4.81 Hz),
8.82 (2H, d, J = 4.81 Hz),
8.75 (4H, s),
7.84 (6H, s),
7.73 (2H, s),
7.70 (1H, s),
1.48 (36H, s),
1.45 (18H, s).



1b

^{13}C NMR spectrum of 1b



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EXMOD single_pulse_dec
OFR 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25125.63 Hz
SCANS 17500
ACQTM 1.0433 sec
PD 1.7000 sec
PW1 3.53 usec
IRN
CTEMP 21.7 c
SLVNT CDCL3
EXREF 77.16 ppm
BF 0.01 Hz
RGAIN 60

13C-NMR (CDCl3) δ :
148.87 (0H, s),
148.83 (0H, s),
143.05 (0H, s),
142.93 (0H, s),
142.78 (0H, s),
142.02 (0H, s),
139.48 (0H, s),
139.41 (0H, s),
133.37 (0H, s),
132.69 (0H, s),
132.55 (0H, s),
128.56 (0H, s),
128.55 (0H, s),
128.39 (0H, s),
121.10 (0H, s),
121.03 (0H, s),
120.60 (0H, s),
120.46 (0H, s),
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34.84 (0H, s),
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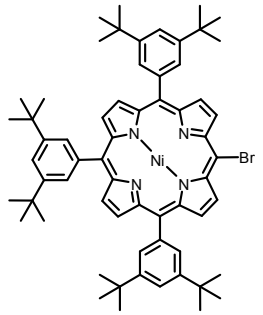
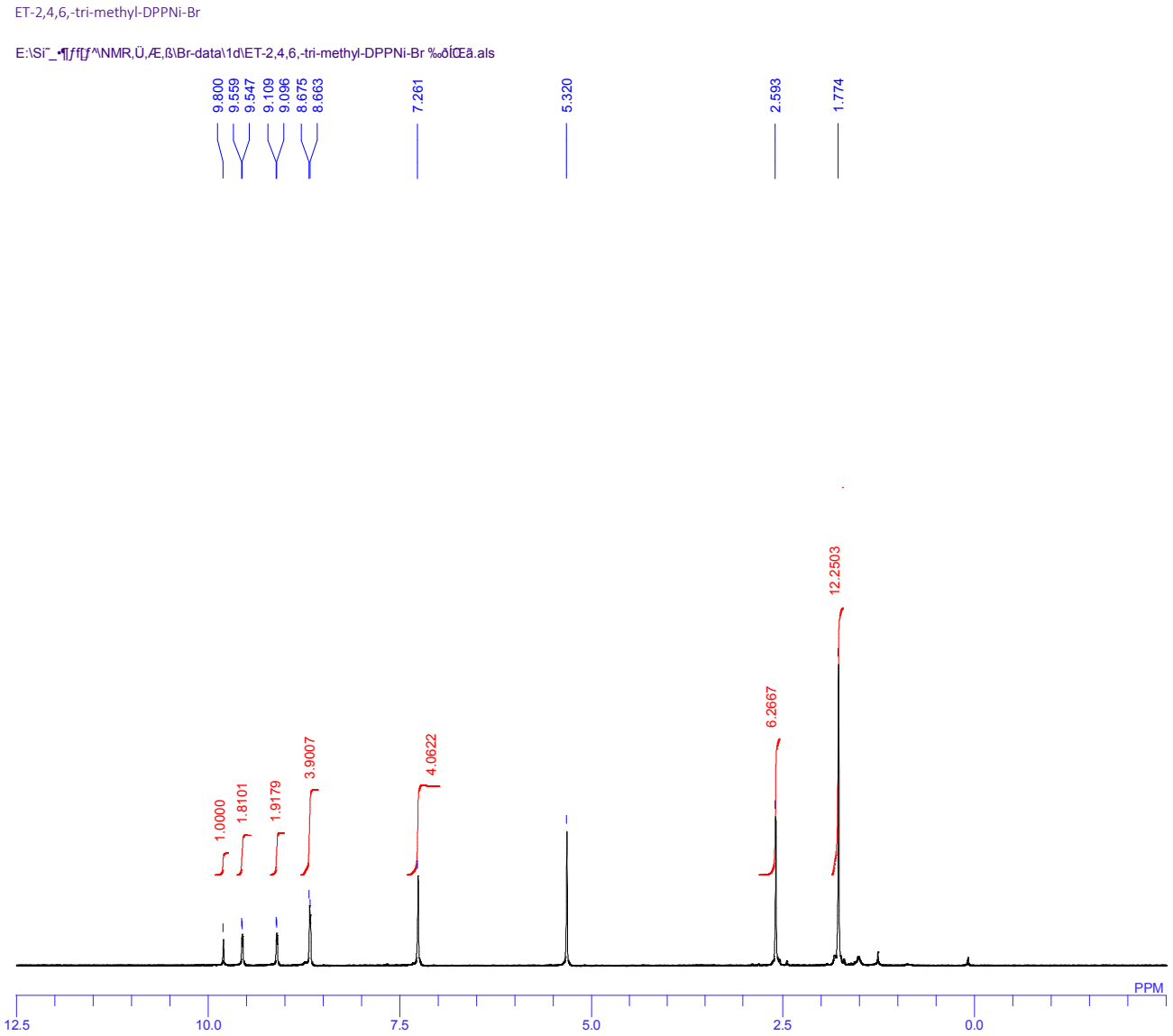
31.51 (0H, s),
31.49 (0H, s).



1b

^{1}H NMR spectrum of 1d



DATIM Fri Jan 26 21:20:31 2018
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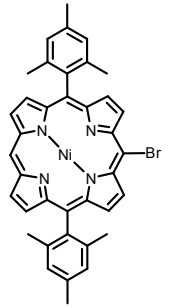
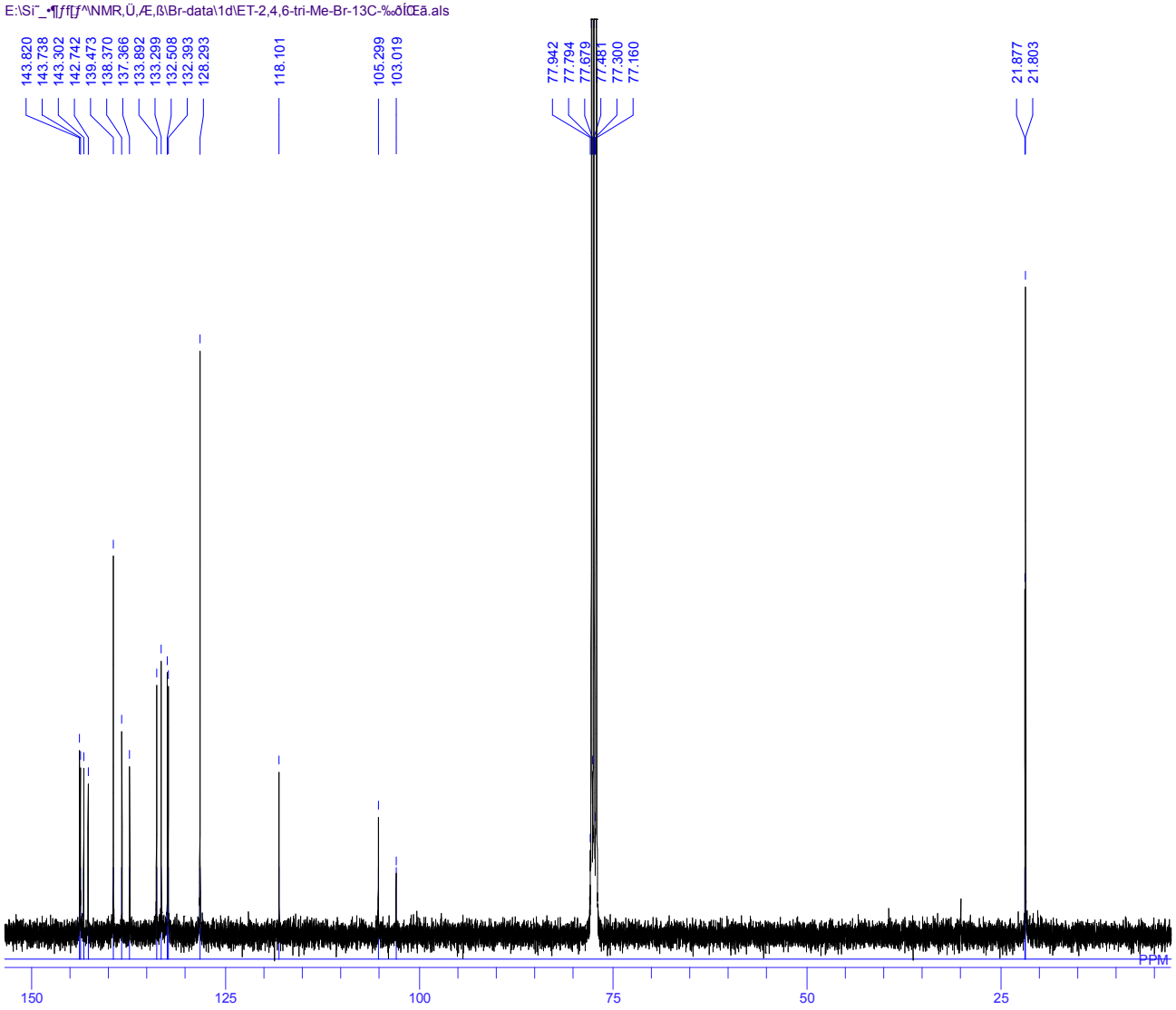
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
SCANS 16
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 5.80 usec
IRN
CTEMP 22.7 c
SLVNT CD2CL
EXREF 5.32 ppm
BF 0.12 Hz
RGAIN 22

1H-NMR (CD2Cl2) δ :
9.80 (1H, s),
9.55 (2H, d, J = 4.88 Hz),
9.10 (2H, d, J = 4.88 Hz),
8.67 (4H, d, J = 4.88 Hz),
7.26 (4H, s),
2.59 (6H, s),
1.77 (12H, s).



1d

^{13}C NMR spectrum of 1d



DATIM Tue Jun 13 08:47:15 2017
DFILE ET-2,4,6-tri-Me-Br-13C-‰ðÍŒÈã.als
OBNUC 13C
EXMOD BCM
OFR 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 27118.64 Hz
SCANS 15500
ACQTM 1.2083 sec
PD 1.7920 sec
PW1 5.80 usec
IRN
CTEMP 24.6 c
SLVNT CDCL3
EXREF 77.16 ppm
BF 0.09 Hz
RGAIN 25

13C-NMR (CDCl3) δ :
143.82 (0H, s),
143.74 (0H, s),
143.30 (0H, s),
142.74 (0H, s),
139.47 (0H, s),
138.37 (0H, s),
137.37 (0H, s),
133.89 (0H, s),
133.30 (0H, s),
132.51 (0H, s),
132.39 (0H, s),
128.29 (0H, s),
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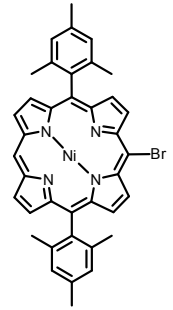
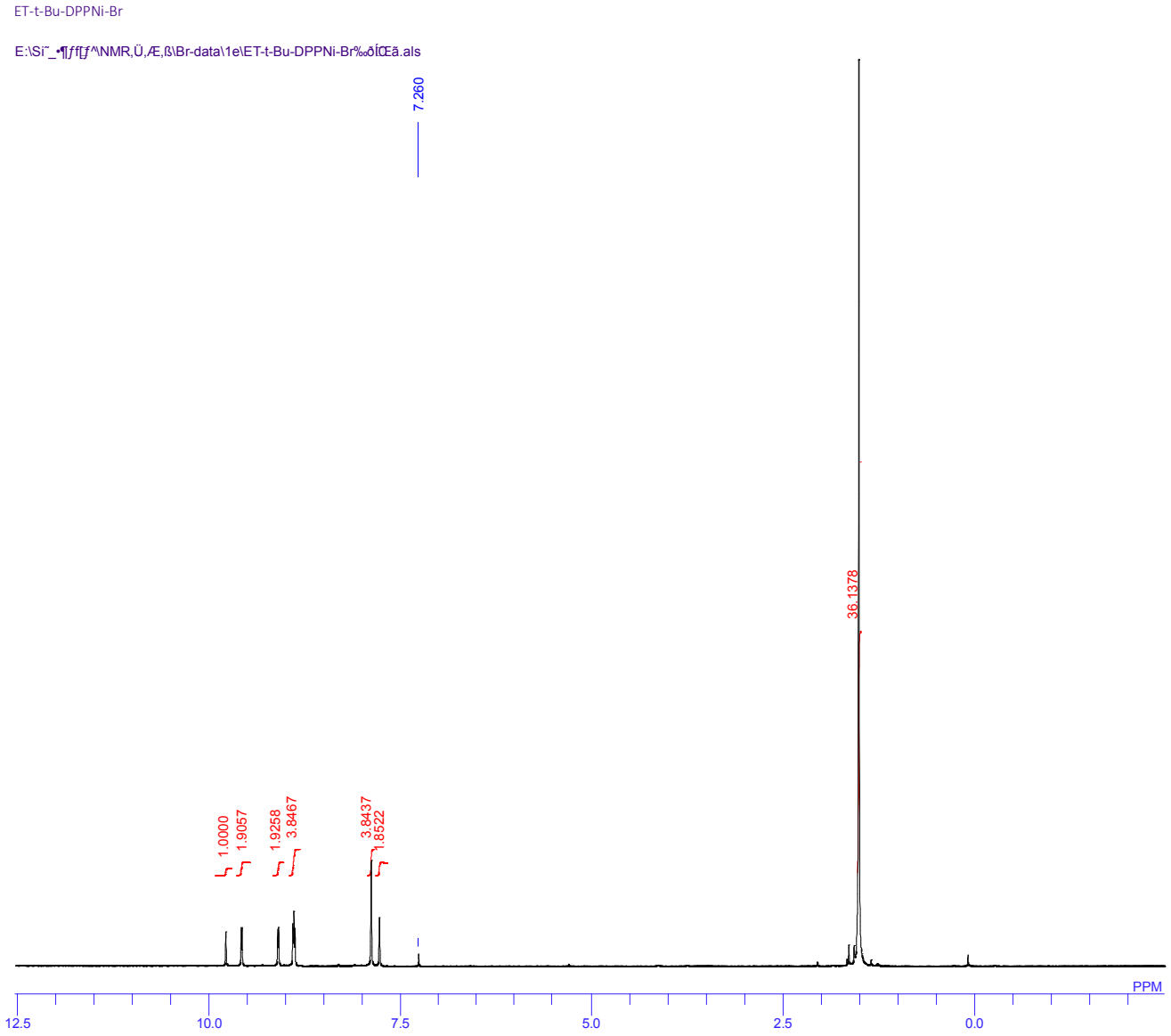
105.30 (0H, s),
103.02 (0H, s),
21.88 (0H, s),
21.80 (0H, s).



1d

^{1}H NMR spectrum of 1e



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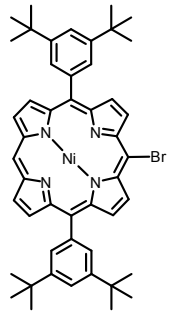
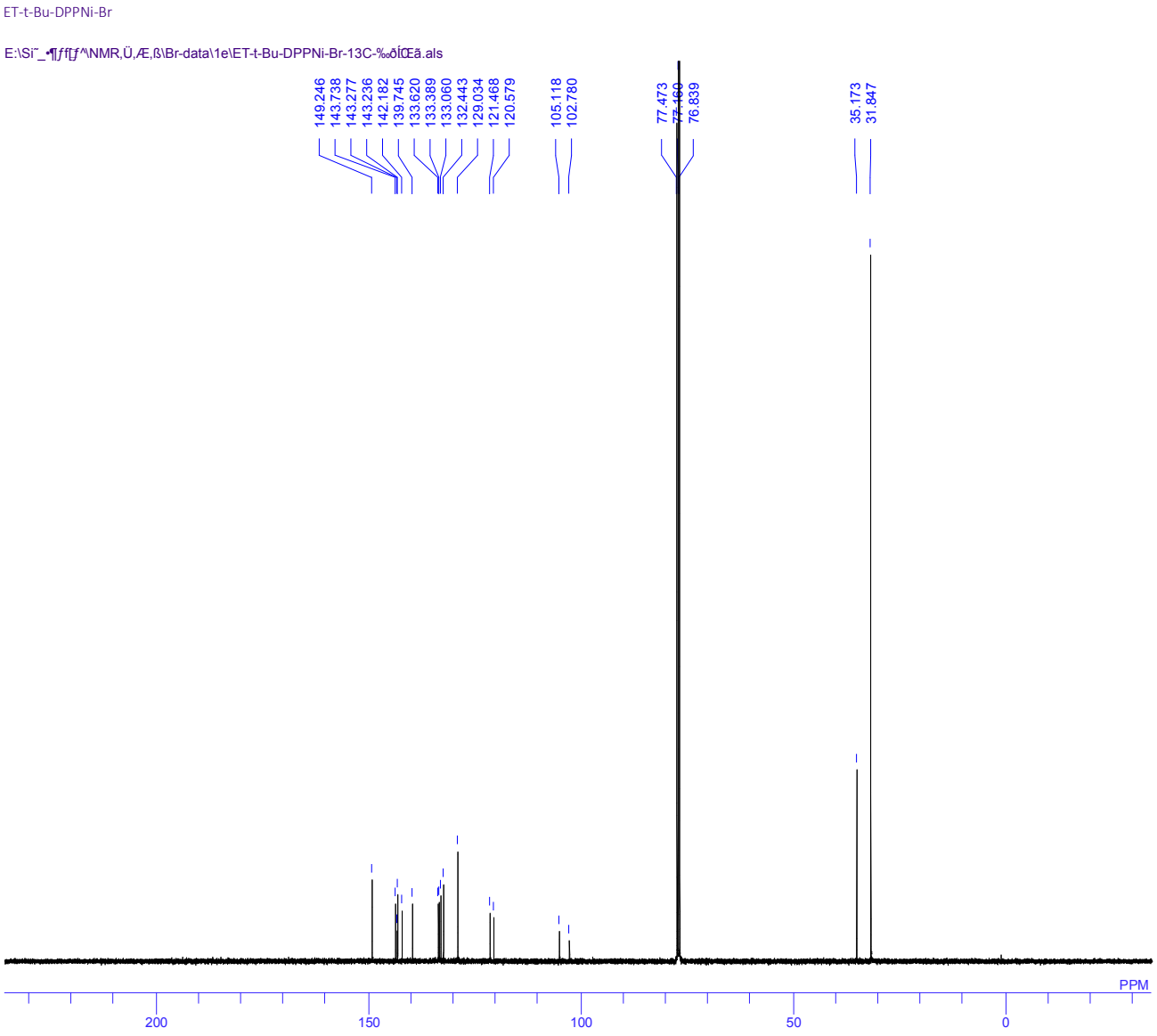
DFILE ET-t-Bu-DPPNi-Br‰ôÍŒã.als
OBNUC 1H
EXMOD NON
OFR 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
SCANS 16
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 5.80 usec
IRN
CTEMP 22.7 c
SLVNT CDCL3
EXREF 7.26 ppm
BF 0.12 Hz
RGAIN 19

1H-NMR (CDCl3) δ :
9.76 (1H, s),
9.55 (2H, d, J = 4.88 Hz),
9.07 (2H, d, J = 4.88 Hz),
8.87 (2H, d, J = 4.88 Hz),
8.86 (2H, d, J = 4.88 Hz),
7.86 (4H, s),
7.75 (2H, s),
1.49 (36H, s).



1e

^{13}C NMR spectrum of 1e



DATIM Sat Jan 27 09:08:15 2018
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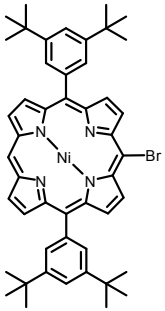
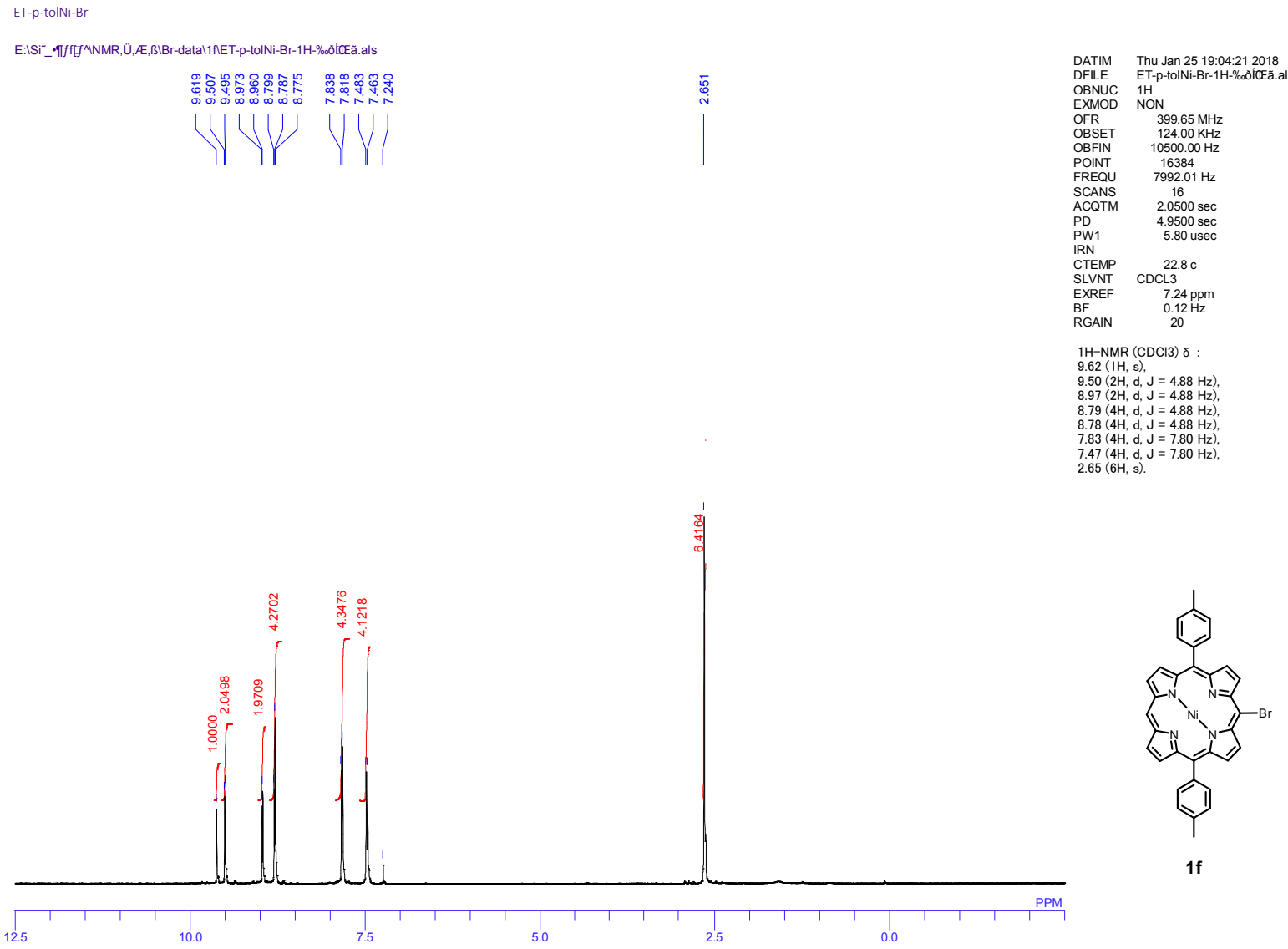
OBNUC 13C
EXMOD BCM
OFR 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 27118.64 Hz
SCANS 14000
ACQTM 1.2083 sec
PD 1.7920 sec
PW1 5.80 usec
IRN
CTEMP 23.0 c
SLVNT CDCL3
EXREF 77.16 ppm
BF 0.12 Hz
RGAIN 25

13C-NMR (CDCl3) δ :
149.25 (0H, s),
143.74 (0H, s),
143.28 (0H, s),
143.24 (0H, s),
142.18 (0H, s),
139.74 (0H, s),
133.62 (0H, s),
133.39 (0H, s),
133.06 (0H, s),
132.44 (0H, s),
129.03 (0H, s),
121.47 (0H, s),
120.58 (0H, s),
105.12 (0H, s),
102.78 (0H, s),
35.17 (0H, s),
31.85 (0H, s).

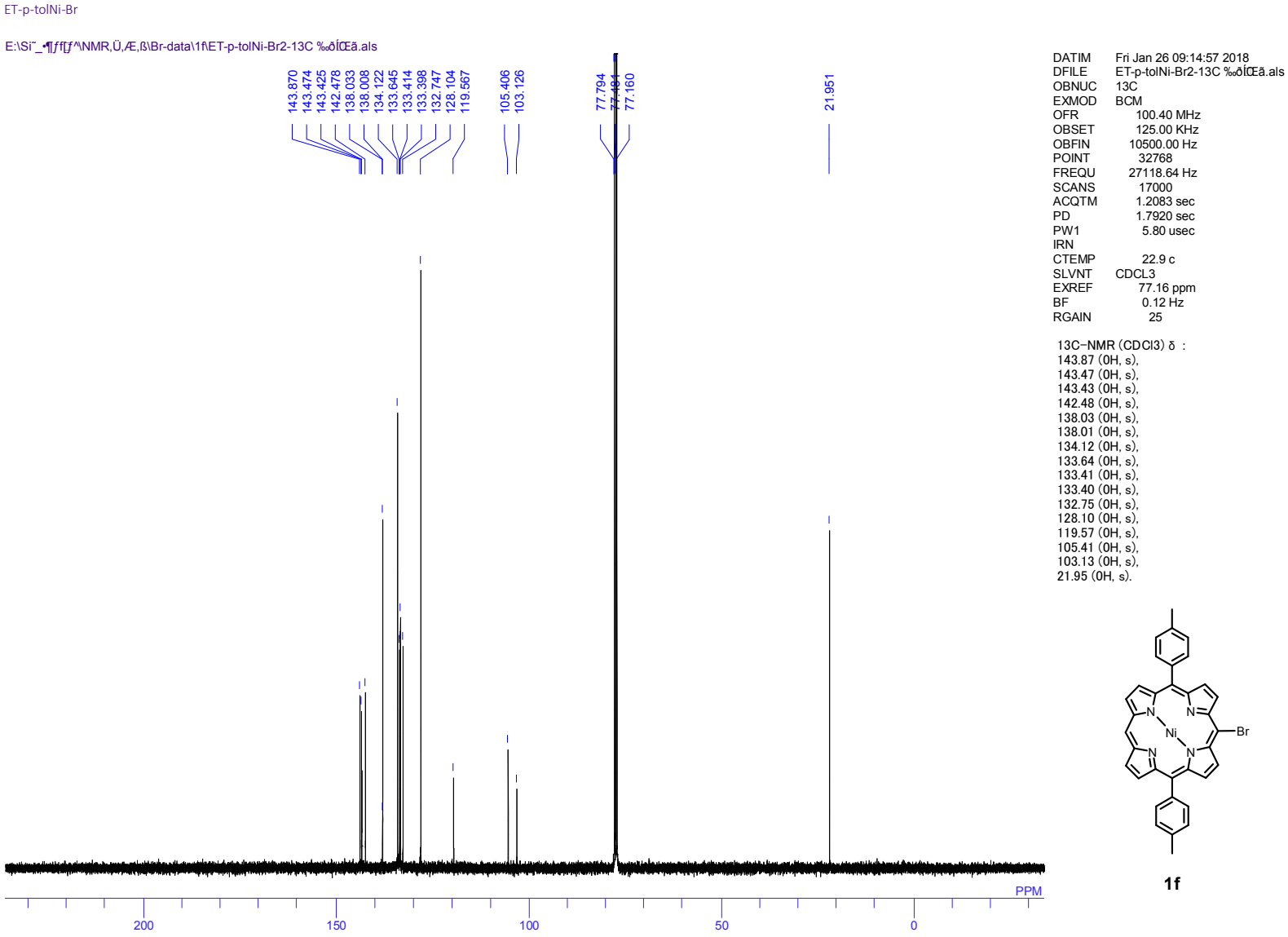


1e

^{1}H NMR spectrum of 1f



^{13}C NMR spectrum of 1f



DATIM Fri Jan 26 09:14:57 2018
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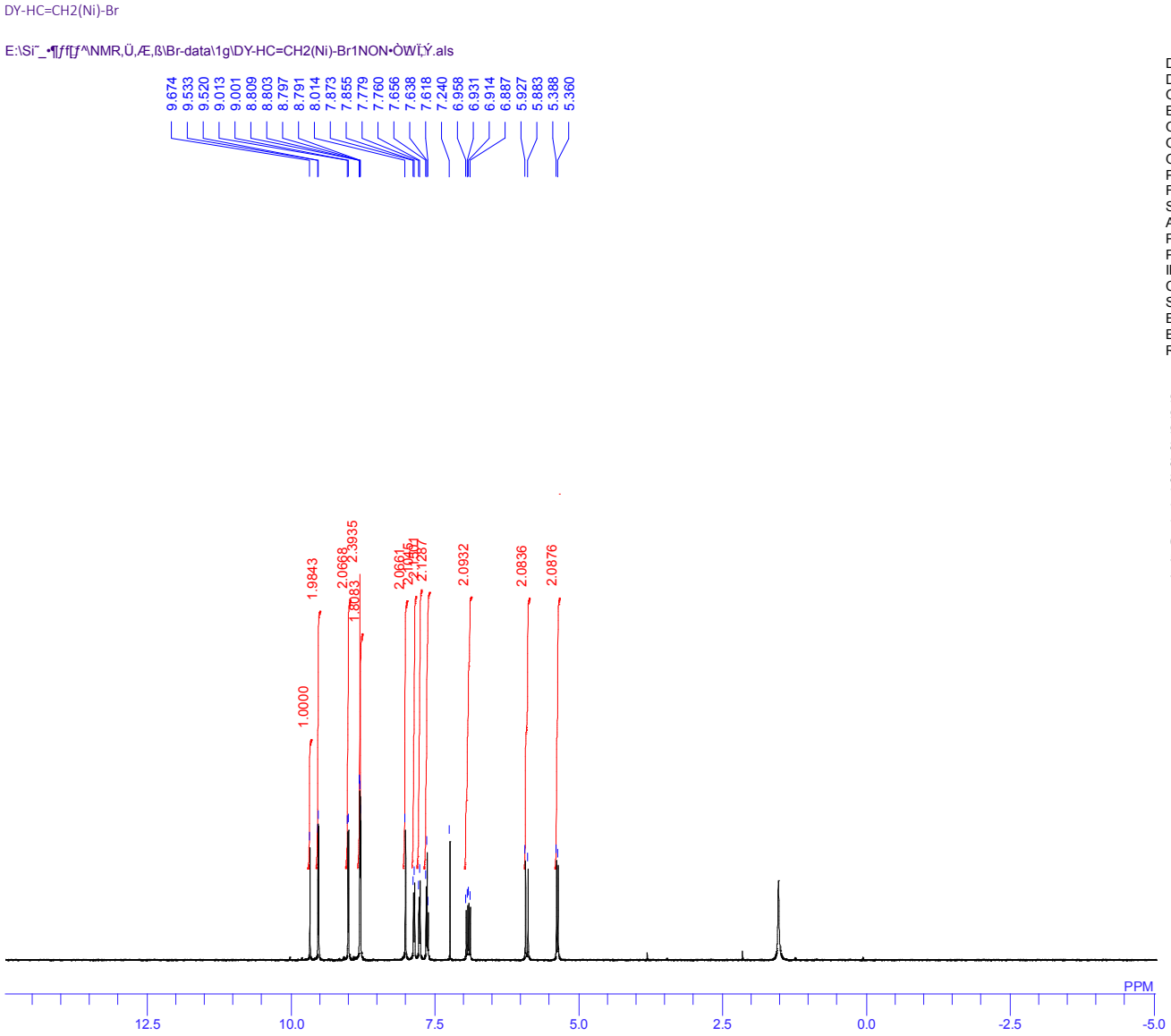
OBNUC 13C
EXMOD BCM
OFR 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 27118.64 Hz
SCANS 17000
ACQTM 1.2083 sec
PD 1.7920 sec
PW1 5.80 usec
IRN
CTEMP 22.9 c
SLVNT CDCL3
EXREF 77.16 ppm
BF 0.12 Hz
RGAIN 25

13C-NMR (CDCl3) δ :
143.87 (0H, s),
143.47 (0H, s),
143.43 (0H, s),
142.48 (0H, s),
138.03 (0H, s),
138.01 (0H, s),
134.12 (0H, s),
133.64 (0H, s),
133.41 (0H, s),
133.40 (0H, s),
132.75 (0H, s),
128.10 (0H, s),
119.57 (0H, s),
105.41 (0H, s),
103.13 (0H, s),
21.95 (0H, s).

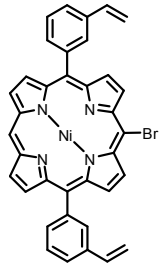
1f

^{1}H NMR spectrum of 1g



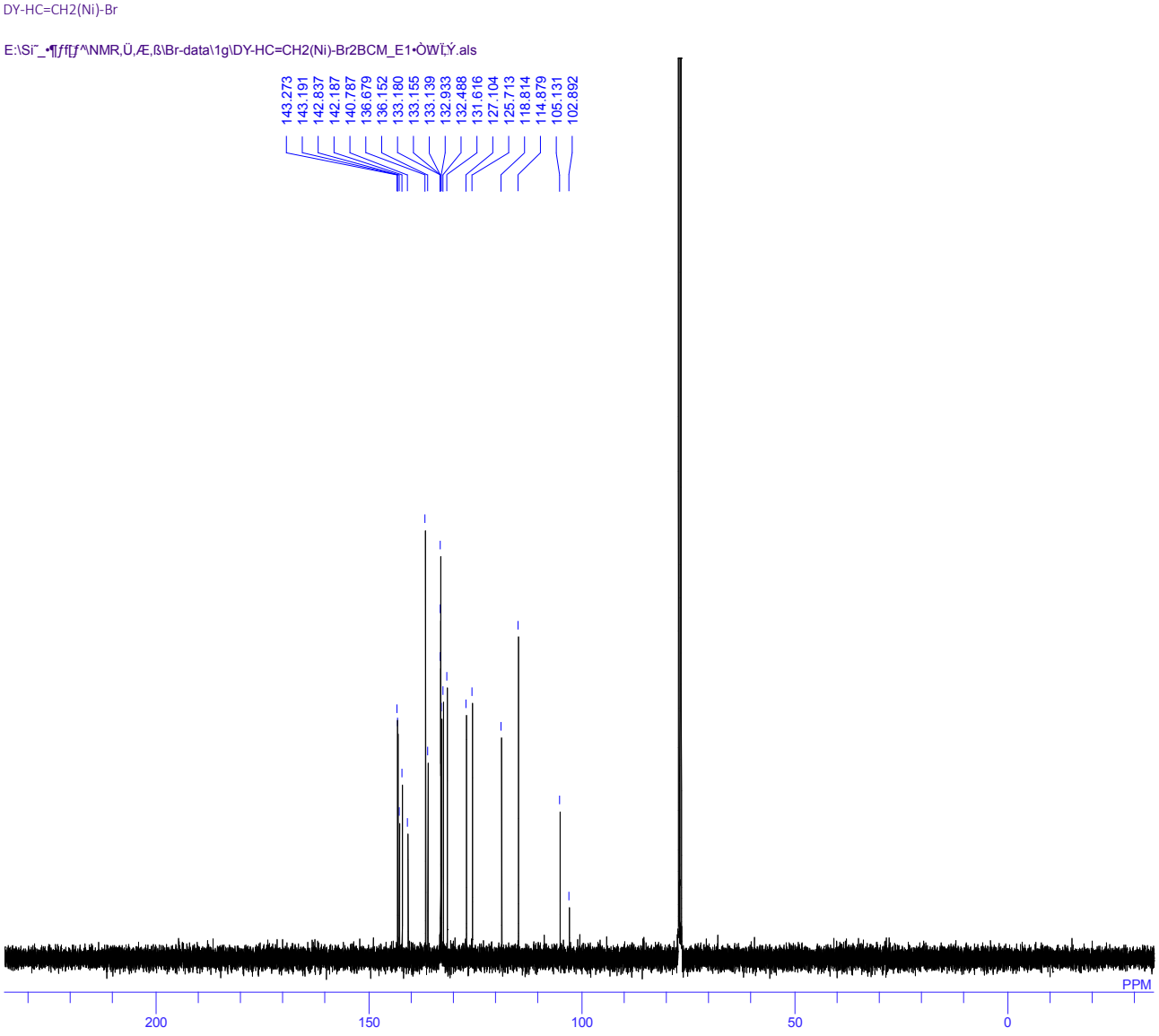
DATIM Mon May 13 17:17:48 2013
DFILE DY-HC=CH2(Ni)-Br1NON•ÒŴÏ¸Ý.als
OBNUC 1H
EXMOD NON
OFR 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
SCANS 8
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 5.80 usec
IRN
CTEMP 24.3 c
SLVNT CDCL3
EXREF 7.24 ppm
BF 0.12 Hz
RGAIN 22

1H-NMR (CDCl3) δ :
9.67 (1H, s),
9.53 (2H, d, J = 4.88 Hz),
9.01 (2H, d, J = 4.88 Hz),
8.80 (2H, d, J = 4.88 Hz),
8.80 (2H, d, J = 4.88 Hz),
8.01 (2H, s),
7.86 (2H, d, J = 7.32 Hz),
7.77 (2H, d, J = 7.80 Hz),
7.64 (2H, dd, J = 7.80, 7.30 Hz),
6.92 (2H, dd, J = 17.56, 10.73 Hz),
5.91 (2H, d, J = 17.56 Hz),
5.37 (2H, d, J = 10.70 Hz).



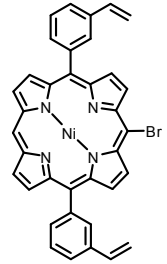
1g

^{13}C NMR spectrum of 1g



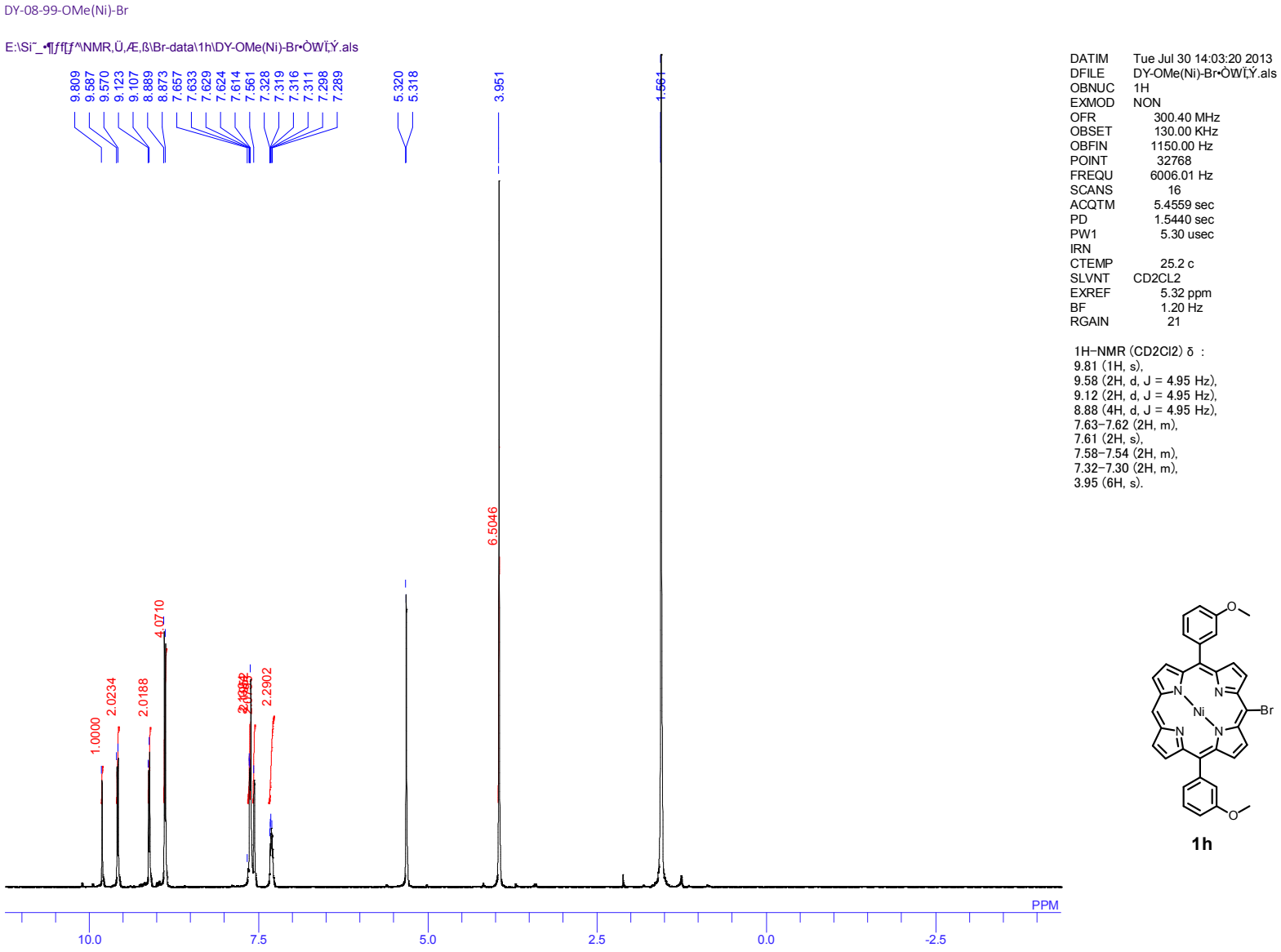
DATIM Mon May 13 22:20:32 2013
DFILE DY-HC=CH2(Ni)-Br2BCM_E1•ÒŴĬ,Ý.als
OBNUC 13C
EXMOD BCM
OFR 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 27118.64 Hz
SCANS 6000
ACQTM 1.2083 sec
PD 1.7920 sec
PW1 6.00 usec
IRN
CTEMP 24.8 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 25

13C-NMR (CDCl3) δ :
143.27 (0H, s),
143.19 (0H, s),
142.84 (0H, s),
142.19 (0H, s),
140.79 (0H, s),
136.68 (0H, s),
136.15 (0H, s),
133.18 (0H, s),
133.16 (0H, s),
133.14 (0H, s),
132.93 (0H, s),
132.49 (0H, s),
131.62 (0H, s),
127.10 (0H, s),
125.71 (0H, s),
118.81 (0H, s),
114.88 (0H, s),
105.13 (0H, s),
102.89 (0H, s).



1g

^{1}H NMR spectrum of 1h

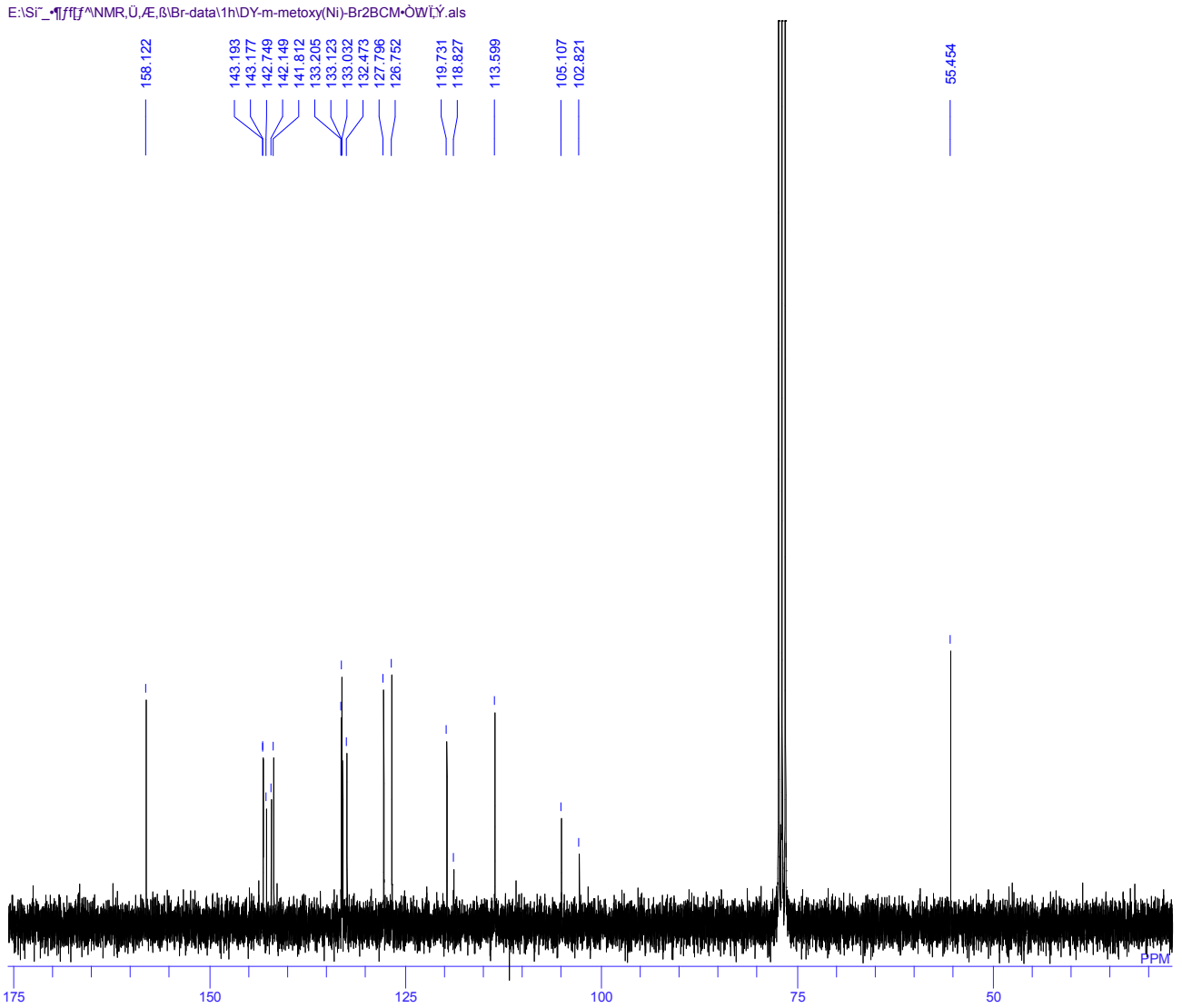


DATIM Tue Jul 30 14:03:20 2013
DFILE DY-OMe(Ni)-Br•ÒẄĪ¸Ý.als
OBNUC 1H
EXMOD NON
OFR 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.00 Hz
POINT 32768
FREQU 6006.01 Hz
SCANS 16
ACQTM 5.4559 sec
PD 1.5440 sec
PW1 5.30 usec
IRN
CTEMP 25.2 c
SLVNT CD2CL2
EXREF 5.32 ppm
BF 1.20 Hz
RGAIN 21

1H-NMR (CD2Cl2) δ :
9.81 (1H, s),
9.58 (2H, d, J = 4.95 Hz),
9.12 (2H, d, J = 4.95 Hz),
8.88 (4H, d, J = 4.95 Hz),
7.63−7.62 (2H, m),
7.61 (2H, s),
7.58−7.54 (2H, m),
7.32−7.30 (2H, m),
3.95 (6H, s).

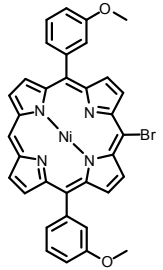
1h

^{13}C NMR spectrum of 1h



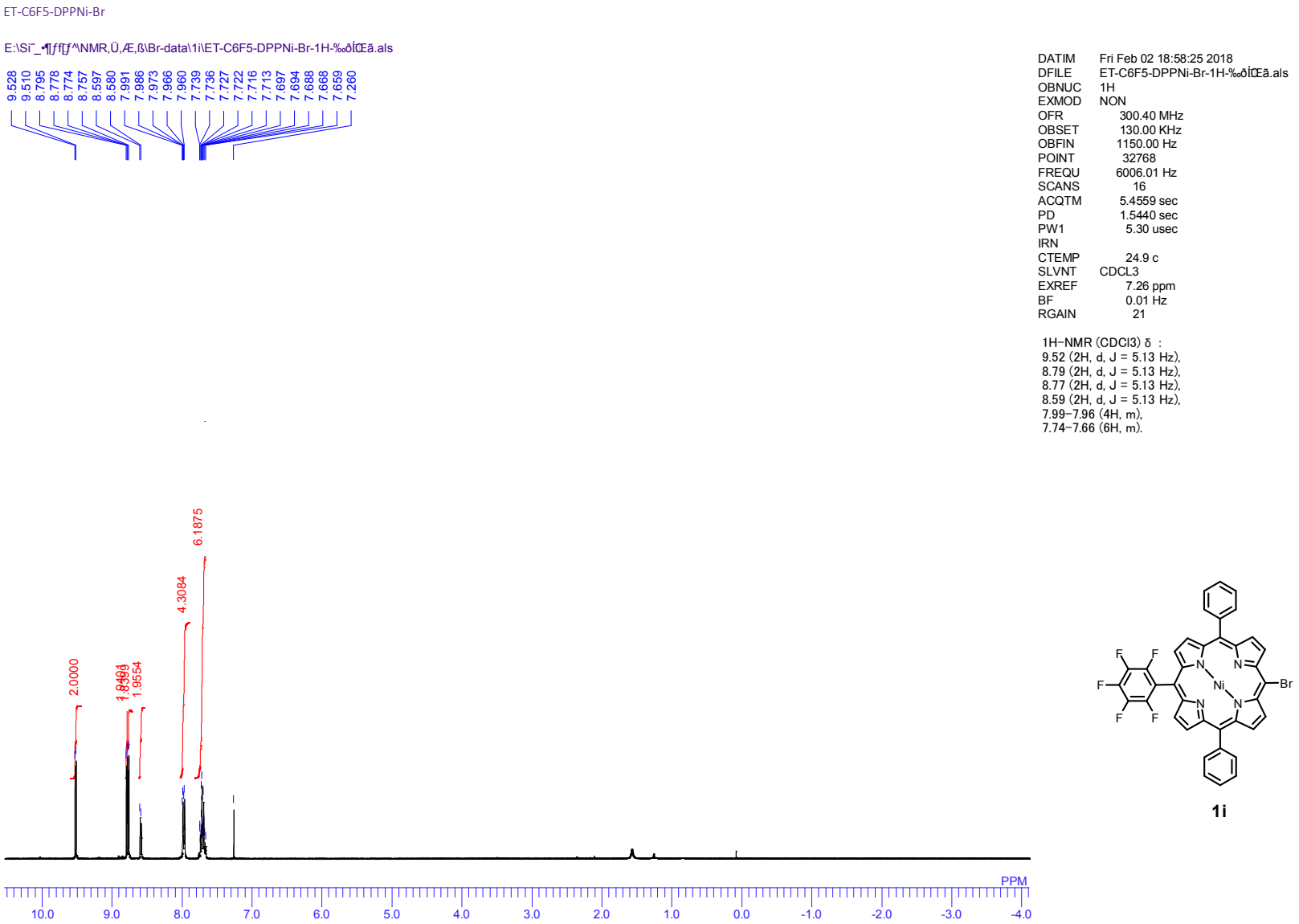
DATIM Tue Aug 27 07:06:11 2013
DFILE DY-m-metoxy(Ni)-Br2BCM•ÒŴĪ,Ý.als
OBNUC 13C
EXMOD BCM
OFR 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.00 Hz
POINT 32768
FREQU 20356.23 Hz
SCANS 10000
ACQTM 1.6097 sec
PD 1.3900 sec
PW1 4.30 usec
IRN
CTEMP 25.2 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 25

13C-NMR (CDCl3) δ :
158.12 (0H, s),
143.19 (0H, s),
143.18 (0H, s),
142.75 (0H, s),
142.15 (0H, s),
141.81 (0H, s),
133.20 (0H, s),
133.12 (0H, s),
133.03 (0H, s),
132.47 (0H, s),
127.80 (0H, s),
126.75 (0H, s),
119.73 (0H, s),
118.83 (0H, s),
113.60 (0H, s),
105.11 (0H, s),
102.82 (0H, s),
55.45 (0H, s).



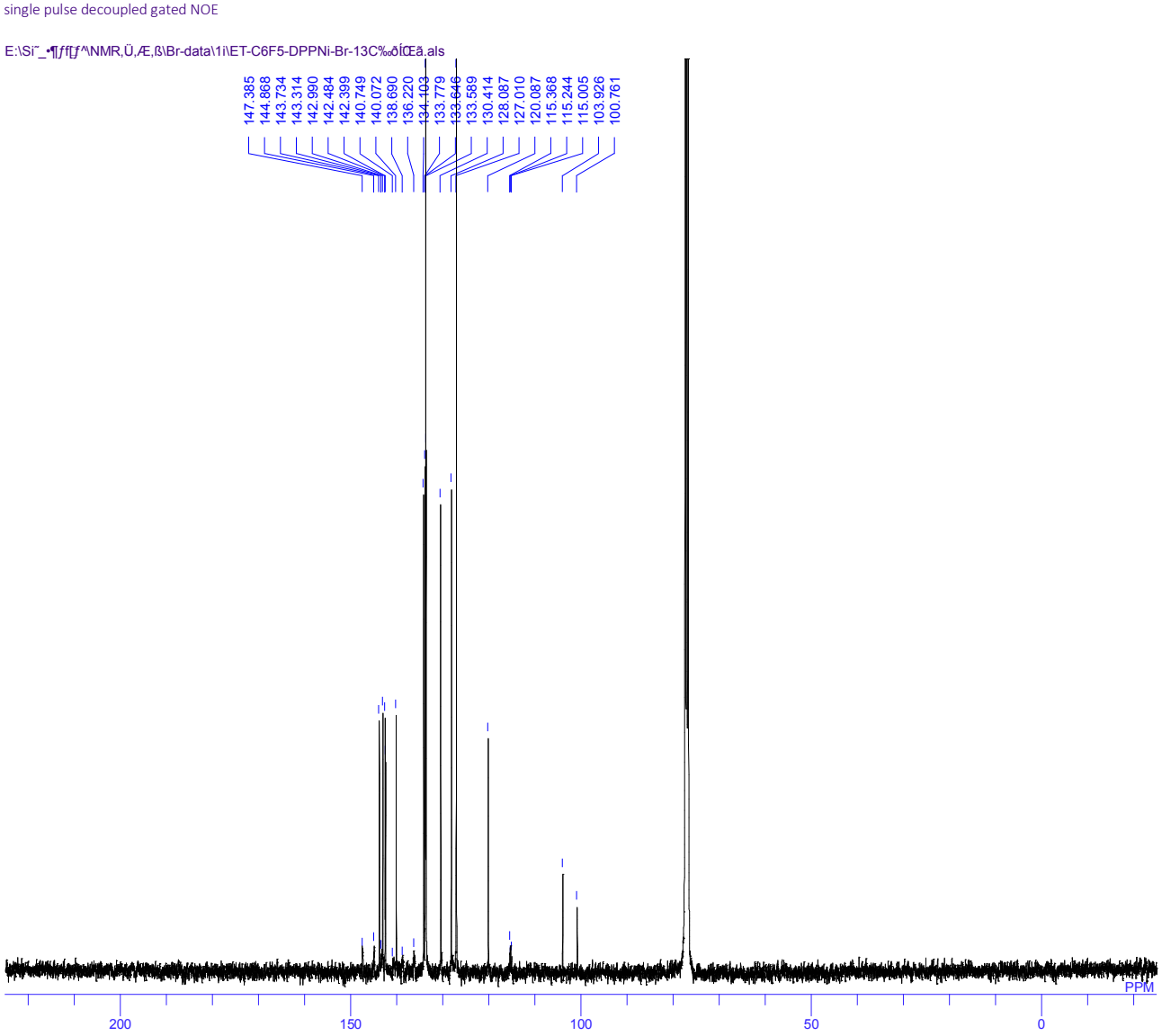
1h

^{1}H NMR spectrum of 1i



1i

^{13}C NMR spectrum of 1i



DATIM 2018-02-03 18:43:13
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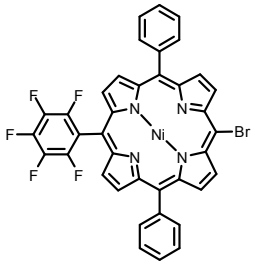
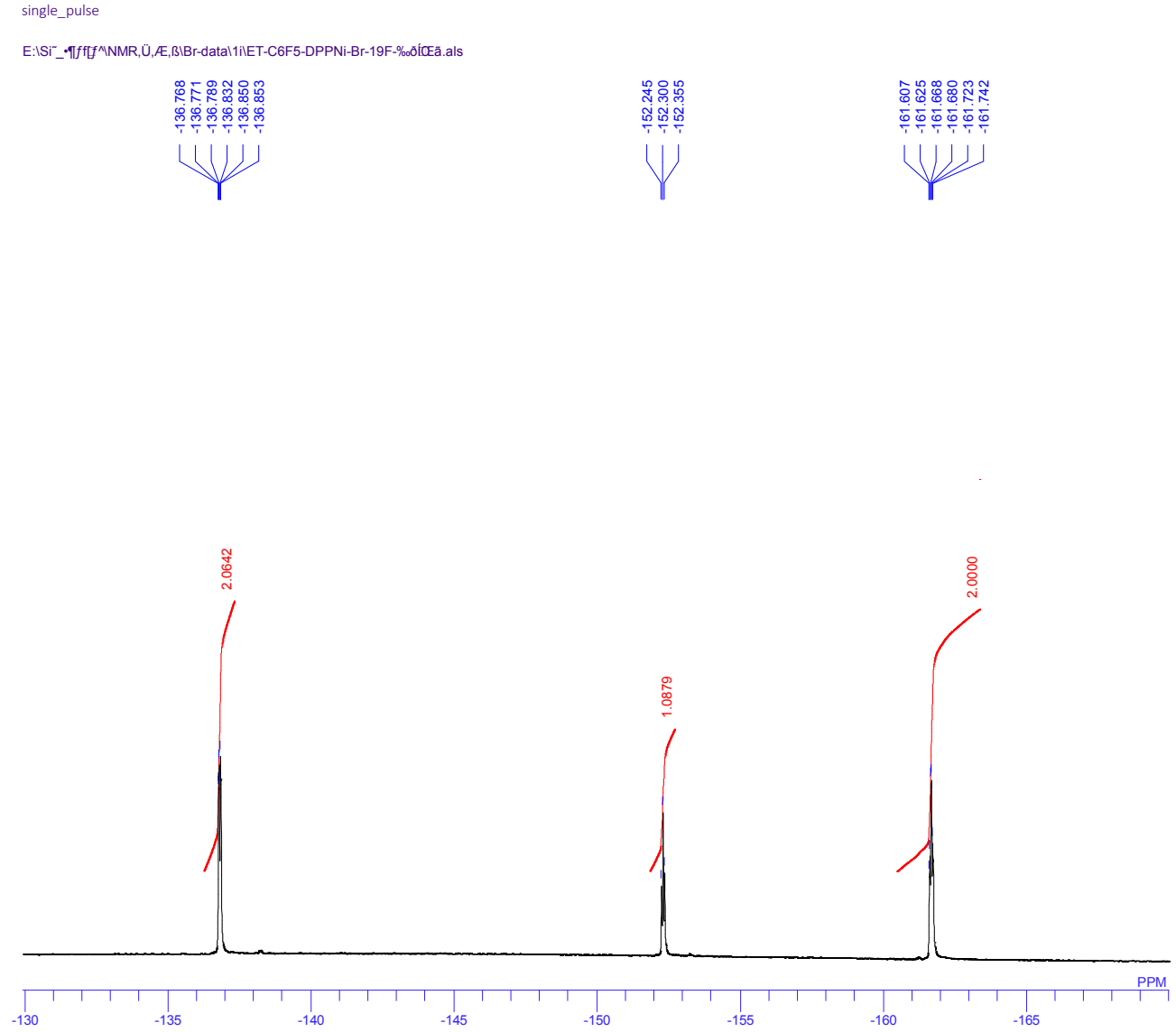
OBNUC 13C
EXMOD single_pulse_dec
OFR 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25125.63 Hz
SCANS 40000
ACQTM 1.0433 sec
PD 1.7000 sec
PW1 3.53 usec
IRN
CTEMP 23.6 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 2.32 Hz
RGAIN 60

13C-NMR (CDCl3) δ :
146.13 (0H, d, J = 253.04 Hz),
143.73 (0H, s),
142.99 (0H, s),
142.48 (0H, s),
142.40 (0H, s),
142.03 (0H, d, J = 257.83 Hz),
140.07 (0H, s),
137.45 (0H, d, J = 248.24 Hz),
134.10 (0H, s),
133.78 (0H, s),
133.64 (0H, s),
133.59 (0H, s),
130.41 (0H, s),
128.09 (0H, s),
127.01 (0H, s),
120.09 (0H, s),
115.19 (0H, t, J = 18.21 Hz),
103.93 (0H, s),
100.76 (0H, s).



1i

^{19}F NMR spectrum 1i



DATIM 2018-02-03 18:15:57
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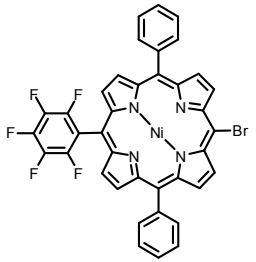
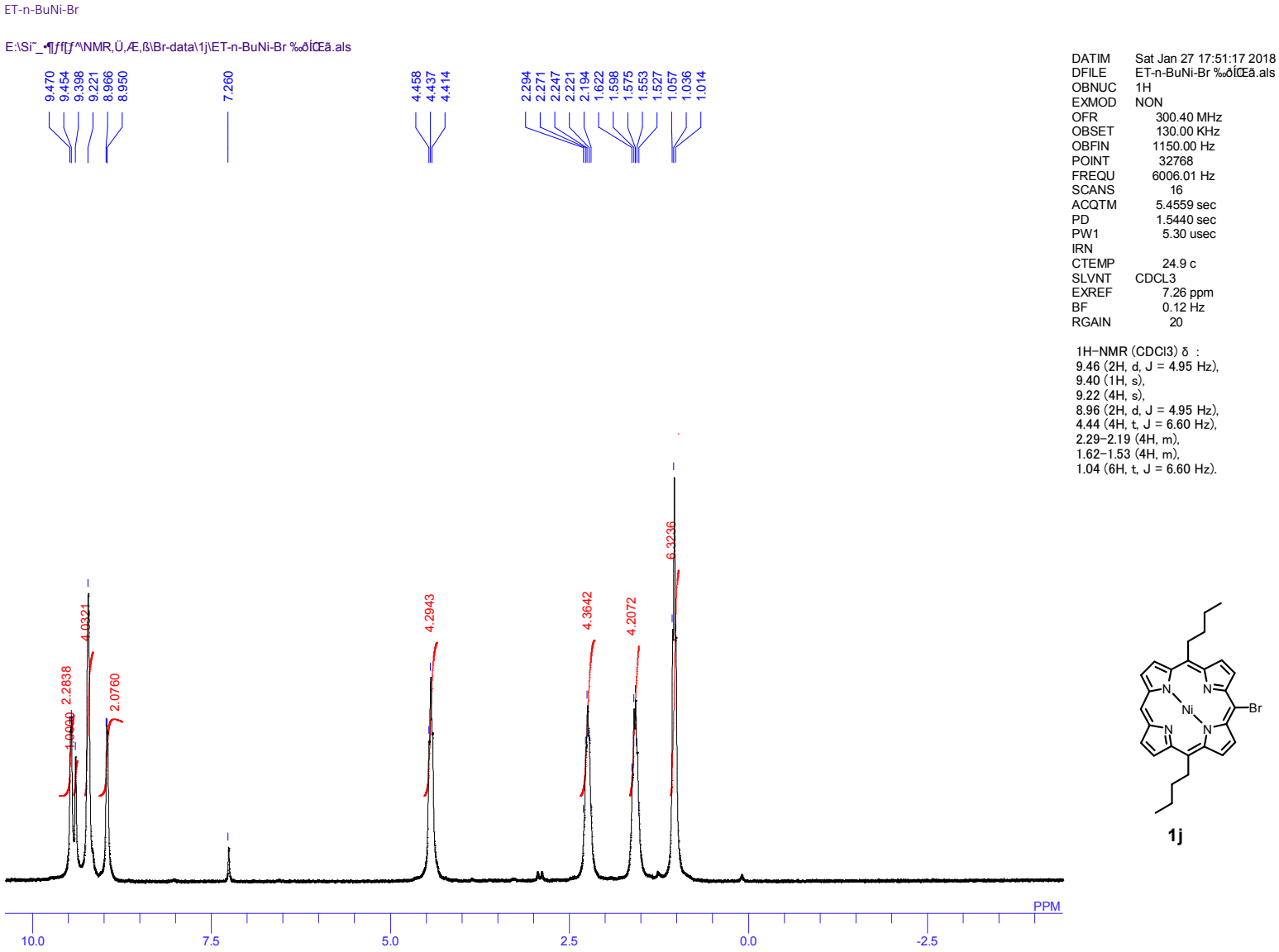
OBNUC 19F
EXMOD single_pulse.jxp
OFR 376.11 MHz
OBSET 4.62 KHz
OBFIN 8.27 Hz
POINT 13107
FREQU 15060.24 Hz
SCANS 16
ACQTM 0.8703 sec
PD 5.0000 sec
PW1 3.76 usec
IRN
CTEMP 21.2 c
SLVNT CDCL3
EXREF -152.30 ppm
BF 6.32 Hz
RGAIN 44

19F−NMR (CDCl3) δ :
−136.81 (2H, ddd, J = 26.04, 4.02, 2.01 Hz),
−152.30 (1H, t, J = 20.68 Hz),
−161.67 (2H, ddd, J = 21.83, 6.13, 3.06 Hz).

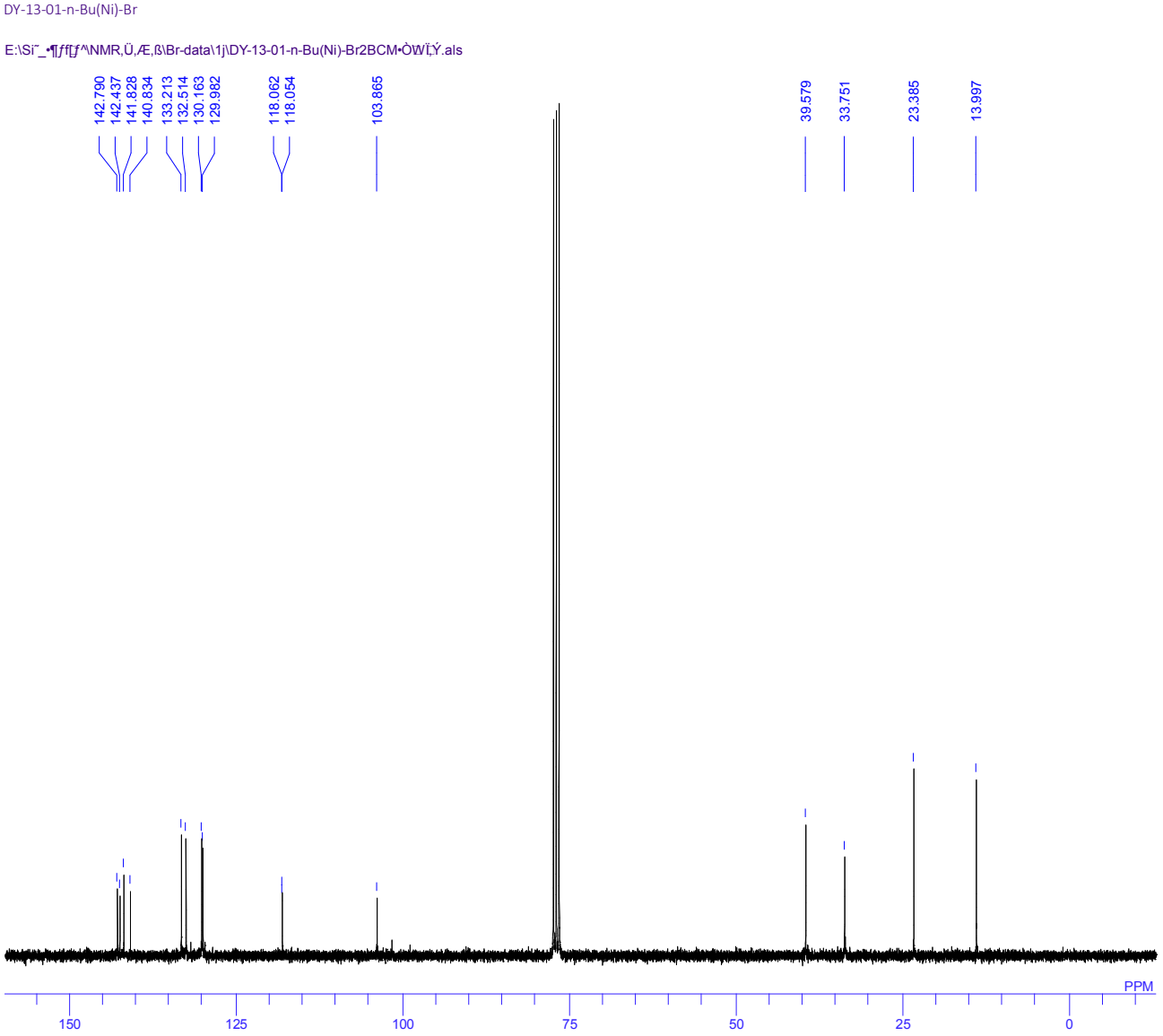


1i

^{1}H NMR spectrum of 1j

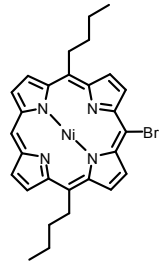


^{13}C NMR spectrum of 1j



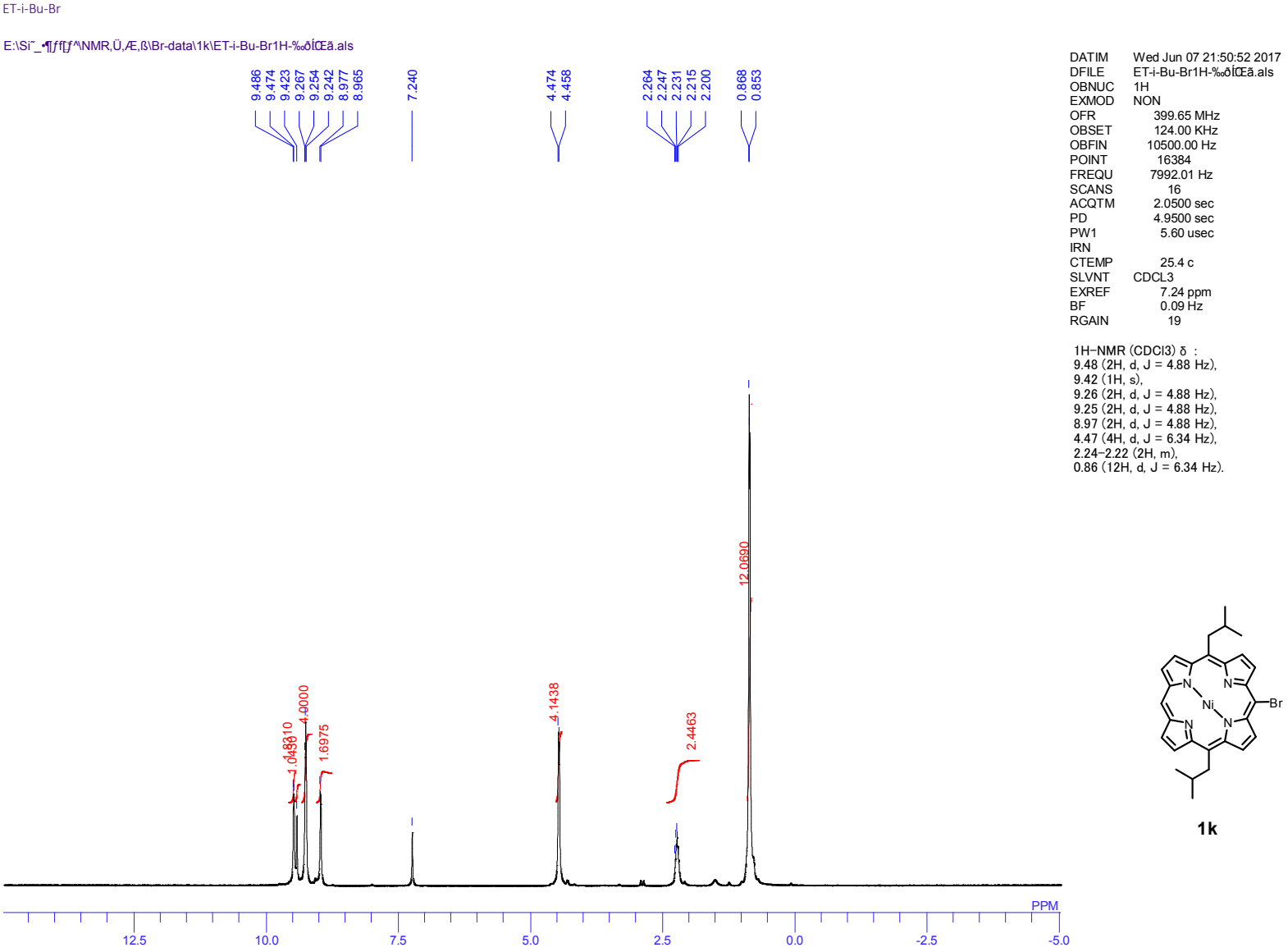
DATIM Thu Oct 16 08:31:16 2014
DFILE DY-13-01-n-Bu(Ni)-Br2BCM•ÒŴÏ¸Ý.als
OBNUC 13C
EXMOD BCM
OFR 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.00 Hz
POINT 32768
FREQU 20356.23 Hz
SCANS 11000
ACQTM 1.6097 sec
PD 1.3900 sec
PW1 4.30 usec
IRN
CTEMP 25.3 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 24

13C-NMR (CDCl3) δ :
142.79 (0H, s),
142.44 (0H, s),
141.83 (0H, s),
140.83 (0H, s),
133.21 (0H, s),
132.51 (0H, s),
130.16 (0H, s),
129.98 (0H, s),
118.06 (0H, s),
118.05 (0H, s),
103.87 (0H, s),
39.58 (0H, s),
33.75 (0H, s),
23.38 (0H, s),
14.00 (0H, s).



1j

^{1}H NMR spectrum of 1k

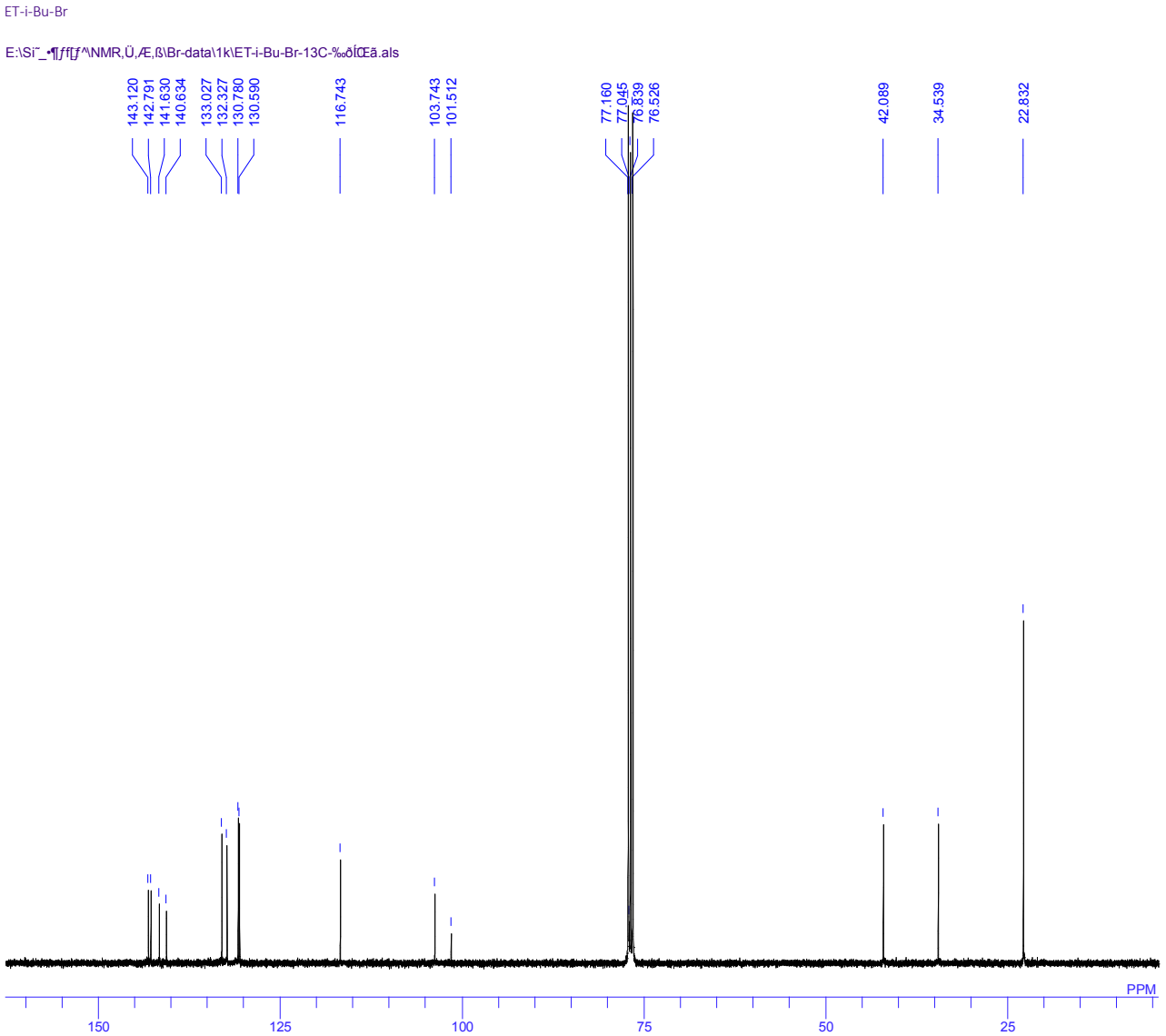


DATIM	Wed Jun 07 21:50:52 2017
DFILE	ET-i-Bu-Br1H-‰ôÍŒÈä.als
OBNUC	1H
EXMOD	NON
OFR	399.65 MHz
OBSET	124.00 KHz
OBFIN	10500.00 Hz
POINT	16384
FREQU	7992.01 Hz
SCANS	16
ACQTM	2.0500 sec
PD	4.9500 sec
PW1	5.60 usec
IRN	
CTEMP	25.4 c
SLVNT	CDCL3
EXREF	7.24 ppm
BF	0.09 Hz
RGAIN	19

1H–NMR (CDCl3) δ :
9.48 (2H, d, J = 4.88 Hz),
9.42 (1H, s),
9.26 (2H, d, J = 4.88 Hz),
9.25 (2H, d, J = 4.88 Hz),
8.97 (2H, d, J = 4.88 Hz),
4.47 (4H, d, J = 6.34 Hz),
2.24–2.22 (2H, m),
0.86 (12H, d, J = 6.34 Hz).

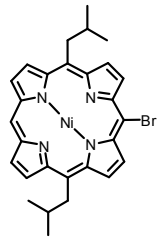
1k

^{13}C NMR spectrum of 1k



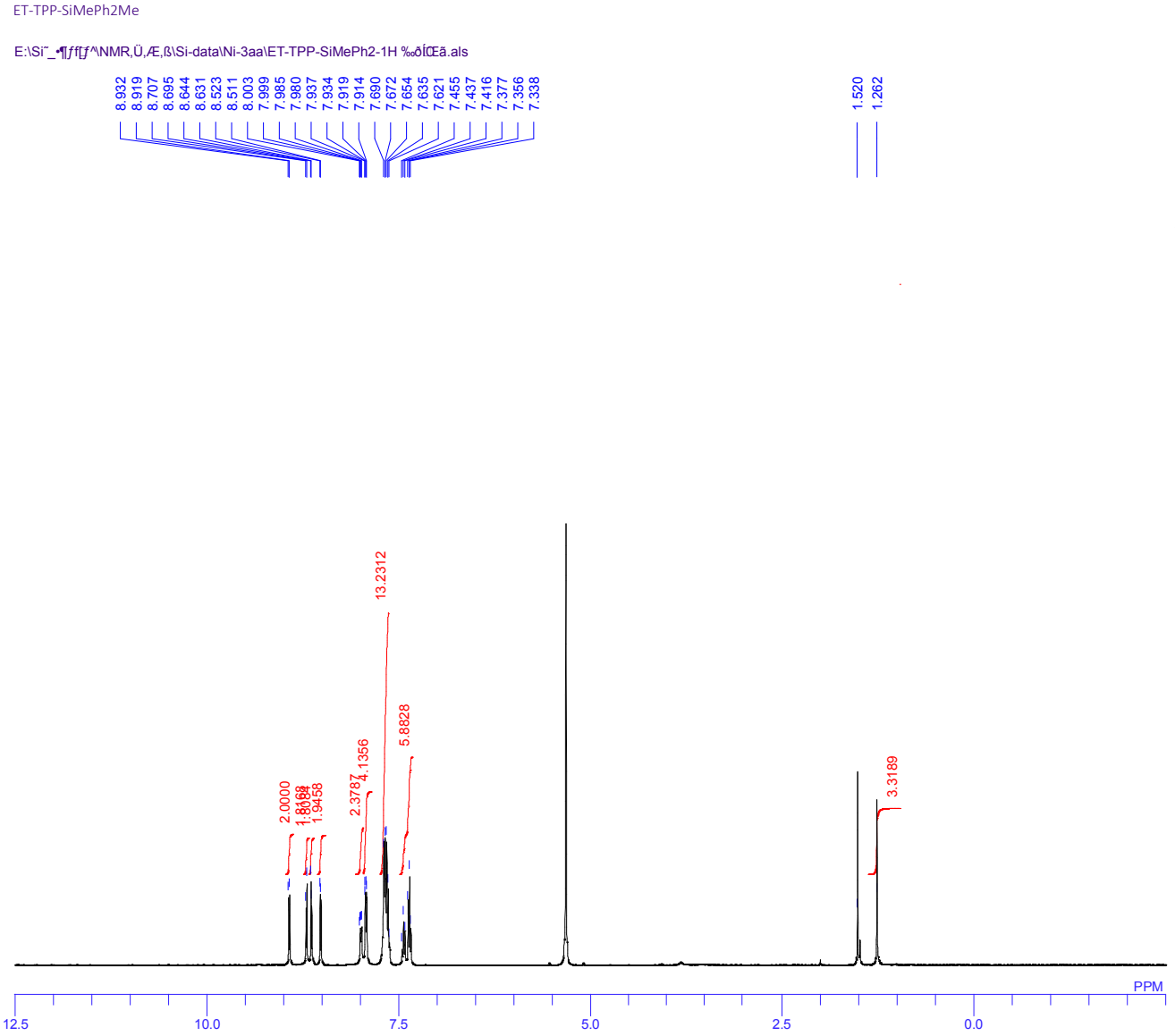
DATIM Thu Jun 08 09:56:25 2017
DFILE ET-i-Bu-Br-13C-‰ôÍŒã.als
OBNUC 13C
EXMOD BCM
OFR 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 27118.64 Hz
SCANS 14500
ACQTM 1.2083 sec
PD 1.7920 sec
PW1 5.80 usec
IRN
CTEMP 24.9 c
SLVNT CDCL3
EXREF 77.16 ppm
BF 0.09 Hz
RGAIN 25

13C-NMR (CDCl3) δ :
143.12 (0H, s),
142.79 (0H, s),
141.63 (0H, s),
140.63 (0H, s),
133.03 (0H, s),
132.33 (0H, s),
130.78 (0H, s),
130.59 (0H, s),
116.74 (0H, s),
103.74 (0H, s),
101.51 (0H, s),
42.09 (0H, s),
34.54 (0H, s),
22.83 (0H, s).



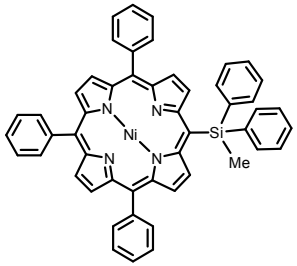
1k

^{1}H NMR spectrum of 3aa



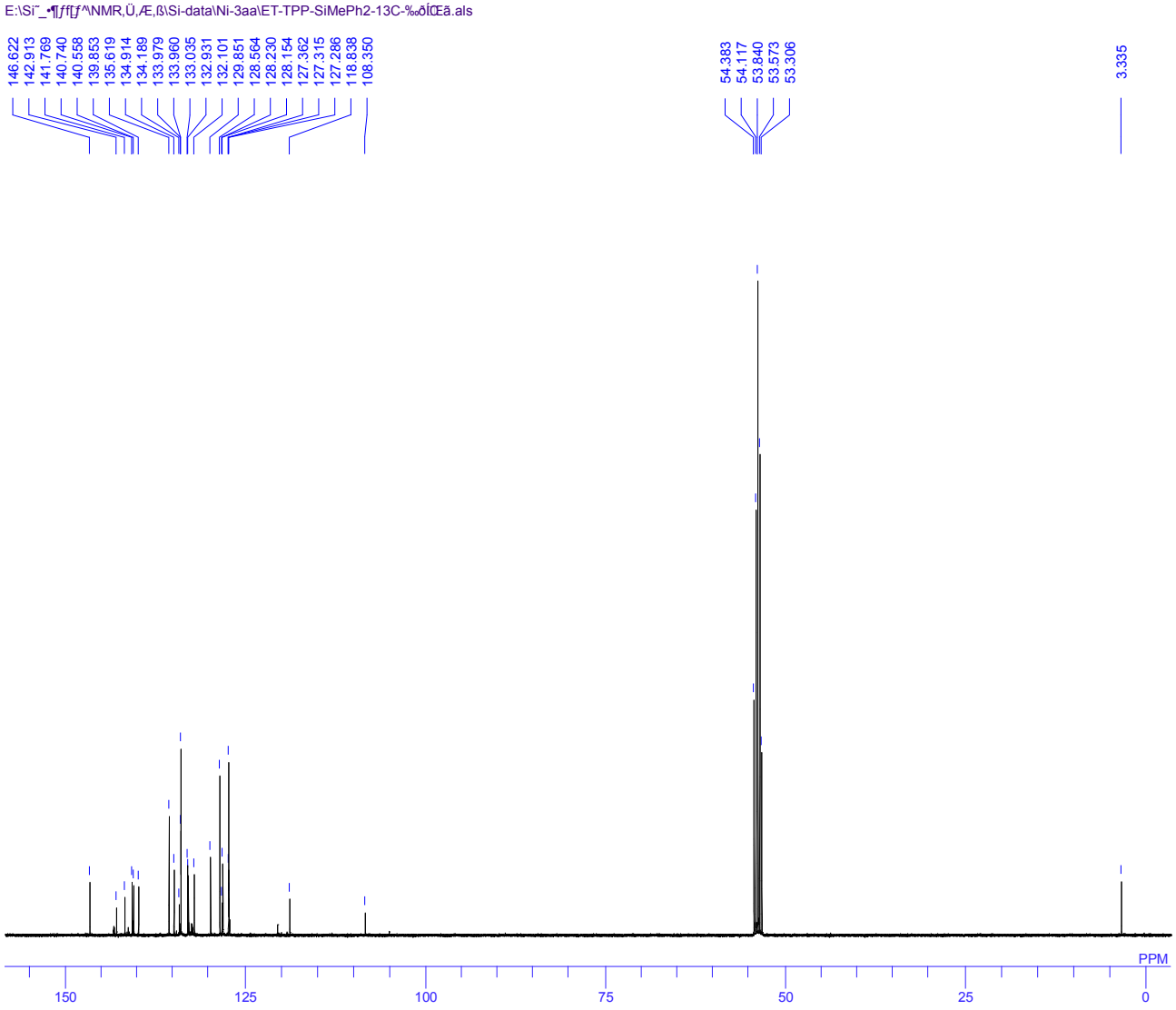
DATIM Thu May 25 17:21:42 2017
DFILE ET-TPP-SiMePh2-1H ‰ðÍŒã.als
OBNUC 1H
EXMOD NON
OFR 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
SCANS 16
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 5.60 usec
IRN
CTEMP 25.7 c
SLVNT CD2CL
EXREF 5.32 ppm
BF 1.20 Hz
RGAIN 23

1H–NMR (CD2Cl2) δ :
8.93 (2H, d, J = 4.88 Hz),
8.70 (2H, d, J = 4.88 Hz),
8.64 (2H, d, J = 4.88 Hz),
8.52 (2H, d, J = 4.88 Hz),
7.99 (2H, dd, J = 7.56, 1.71 Hz),
7.93 (4H, dd, J = 7.56, 1.71 Hz),
7.69–7.62 (13H, m),
7.44–7.36 (6H, m),
1.26 (3H, s).



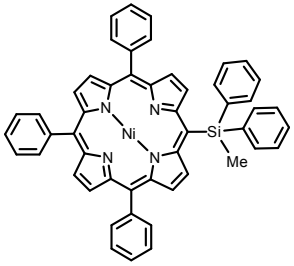
3aa

^{13}C NMR spectrum of 3aa



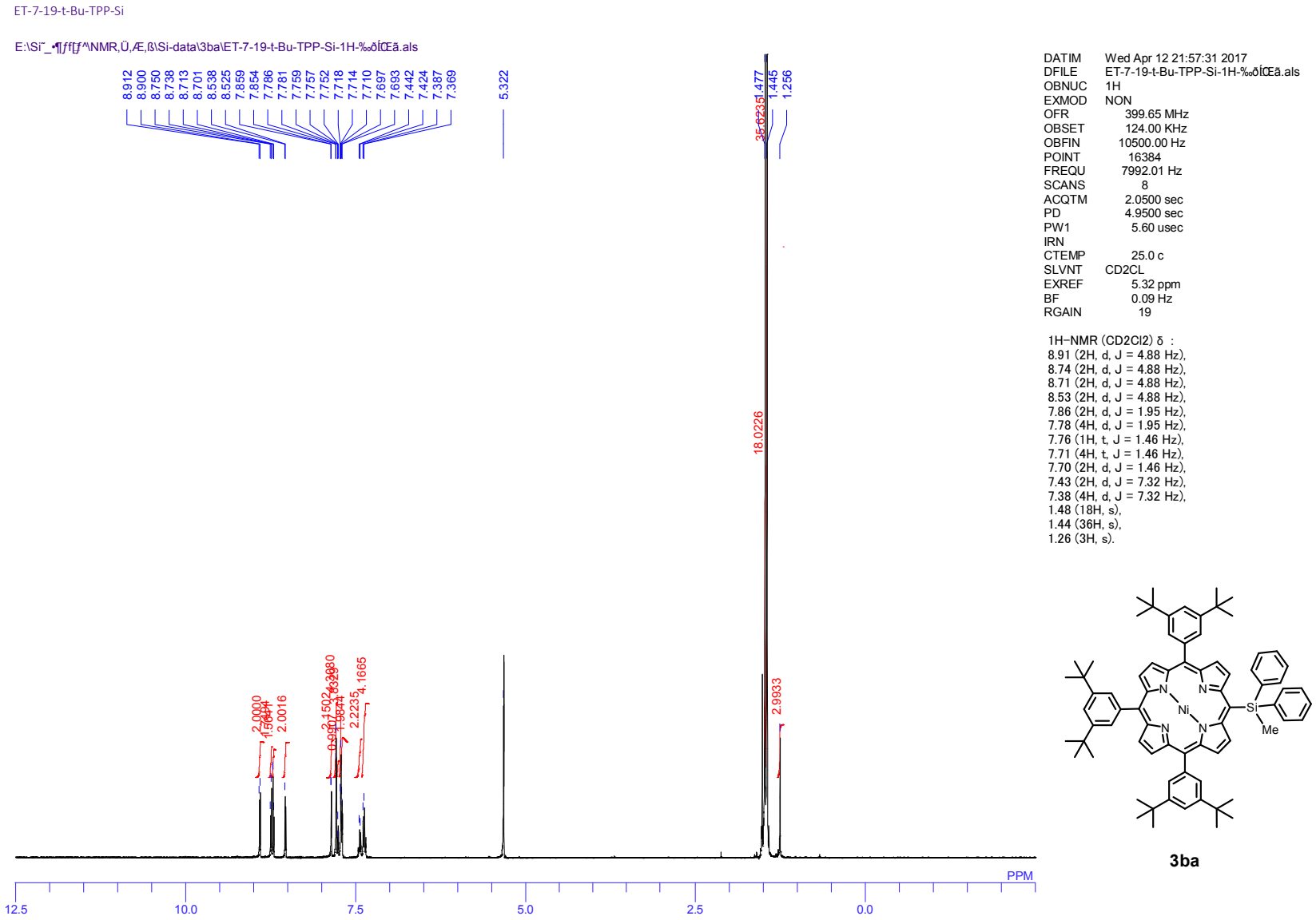
DATIM 2017-05-18 21:20:34
DFILE ET-TPP-SiMePh2-13C-‰ôÍŒEã.als
OBNUC 13C
EXMOD single_pulse_dec
OFR 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25125.63 Hz
SCANS 16000
ACQTM 1.0433 sec
PD 1.7000 sec
PW1 3.53 usec
IRN
CTEMP 20.7 c
SLVNT CD2CL2
EXREF 53.84 ppm
BF 0.09 Hz
RGAIN 60

13C-NMR (CD2Cl2) δ :
146.62 (0H, s),
142.91 (0H, s),
141.77 (0H, s),
140.74 (0H, s),
140.56 (0H, s),
139.85 (0H, s),
135.62 (0H, s),
134.91 (0H, s),
134.19 (0H, s),
133.98 (0H, s),
133.96 (0H, s),
133.04 (0H, s),
132.93 (0H, s),
132.10 (0H, s),
129.85 (0H, s),
128.56 (0H, s),
128.23 (0H, s),
128.15 (0H, s),
127.36 (0H, s),
127.31 (0H, s),
127.29 (0H, s),
118.84 (0H, s),
108.35 (0H, s),
3.33 (0H, s).



3aa

^{1}H NMR spectrum of 3ba

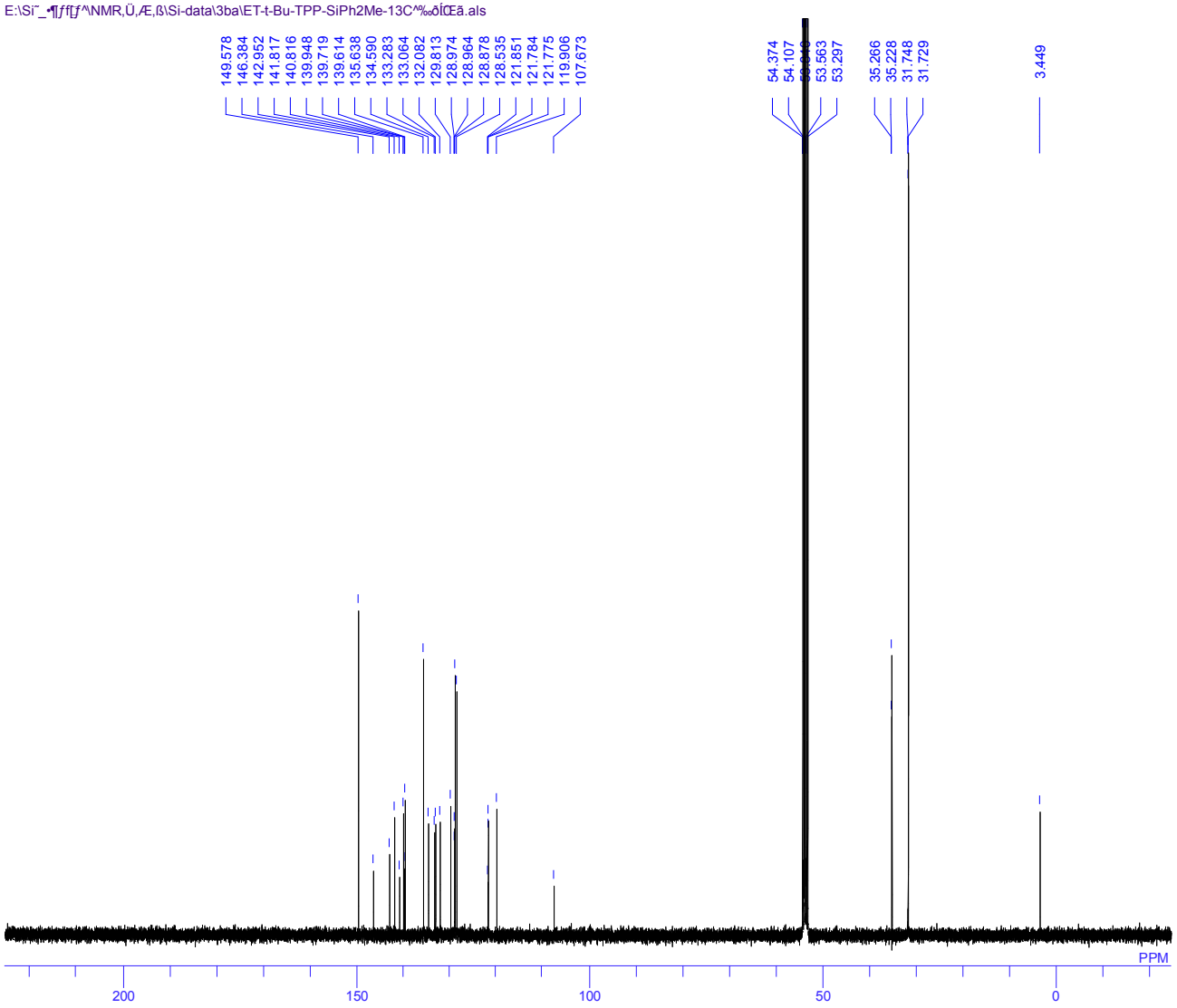


DATIM Wed Apr 12 21:57:31 2017
DFILE ET-7-19-t-Bu-TPP-Si-1H-‰ôÍŒã.als
OBNUC 1H
EXMOD NON
OFR 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
SCANS 8
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 5.60 usec
IRN
CTEMP 25.0 c
SLVNT CD2CL
EXREF 5.32 ppm
BF 0.09 Hz
RGAIN 19

1H−NMR (CD2Cl2) δ :
8.91 (2H, d, J = 4.88 Hz),
8.74 (2H, d, J = 4.88 Hz),
8.71 (2H, d, J = 4.88 Hz),
8.53 (2H, d, J = 4.88 Hz),
7.86 (2H, d, J = 1.95 Hz),
7.78 (4H, d, J = 1.95 Hz),
7.76 (1H, t, J = 1.46 Hz),
7.71 (4H, t, J = 1.46 Hz),
7.70 (2H, d, J = 1.46 Hz),
7.43 (2H, d, J = 7.32 Hz),
7.38 (4H, d, J = 7.32 Hz),
1.48 (18H, s),
1.44 (36H, s),
1.26 (3H, s).

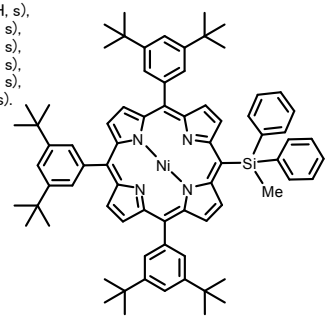
3ba

^{13}C NMR spectrum of 3ba



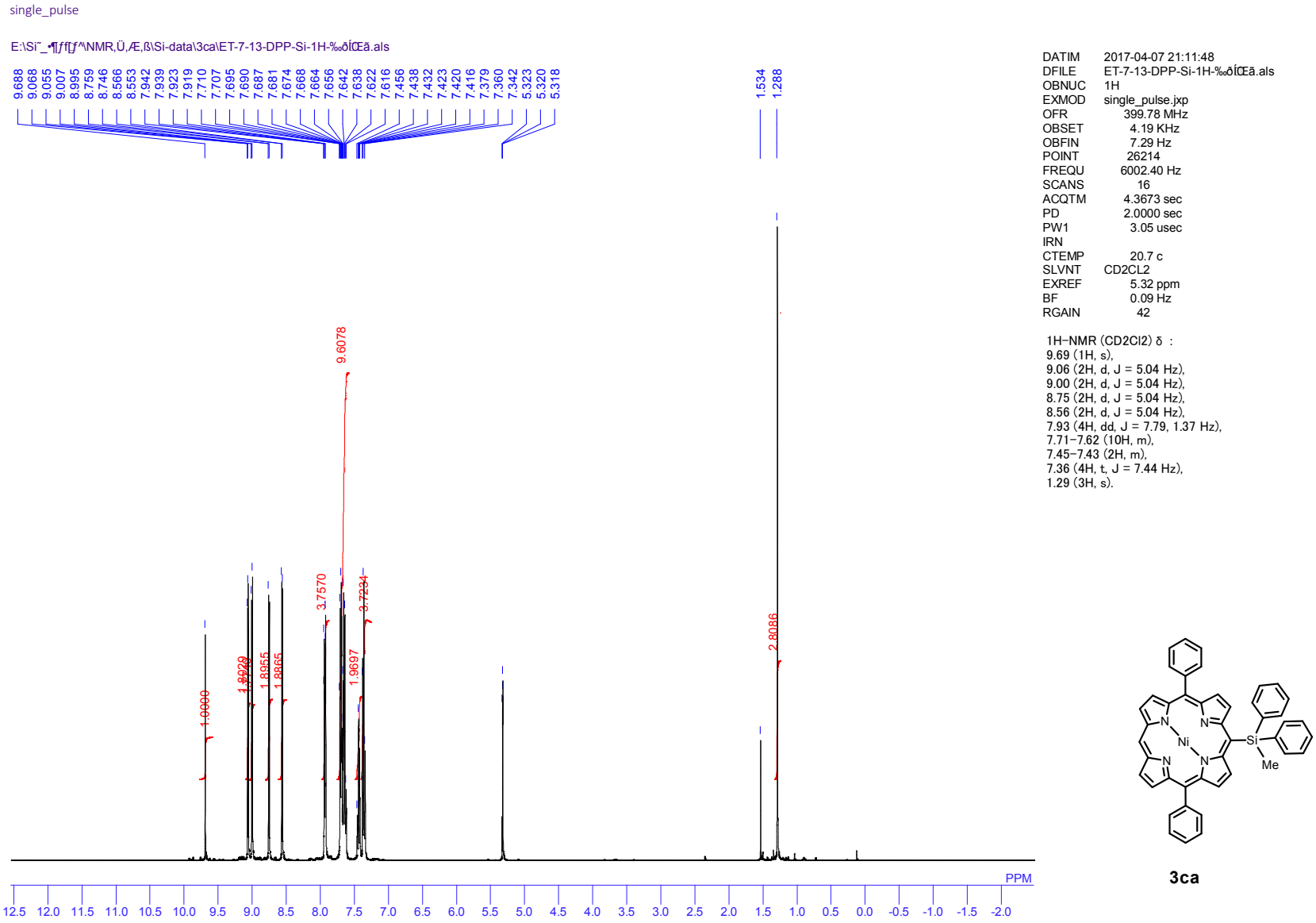
DATIM 2017-05-23 20:02:45
DFILE ET-t-Bu-TPP-SiPh2Me-13C^‰ðÍŒã.als
OBNUC 13C
EXMOD single_pulse_dec
OFR 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25125.63 Hz
SCANS 15000
ACQTM 1.0433 sec
PD 1.7000 sec
PW1 3.53 usec
IRN
CTEMP 20.4 c
SLVNT CD2CL2
EXREF 53.84 ppm
BF 0.09 Hz
RGAIN 60

13C-NMR (CD2Cl2) δ :
149.58 (0H, s),
146.38 (0H, s),
142.95 (0H, s),
141.82 (0H, s),
140.82 (0H, s),
139.95 (0H, s),
139.72 (0H, s),
139.61 (0H, s),
135.64 (0H, s),
134.59 (0H, s),
133.28 (0H, s),
133.06 (0H, s),
132.08 (0H, s),
129.81 (0H, s),
128.97 (0H, s),
128.96 (0H, s),
128.88 (0H, s),
128.54 (0H, s),
121.85 (0H, s),
121.78 (0H, s),
121.77 (0H, s),
119.91 (0H, s),
107.67 (0H, s),
35.27 (0H, s),
35.23 (0H, s),
31.75 (0H, s),
31.73 (0H, s),
3.45 (0H, s).



3ba

^{1}H NMR spectrum of 3ca

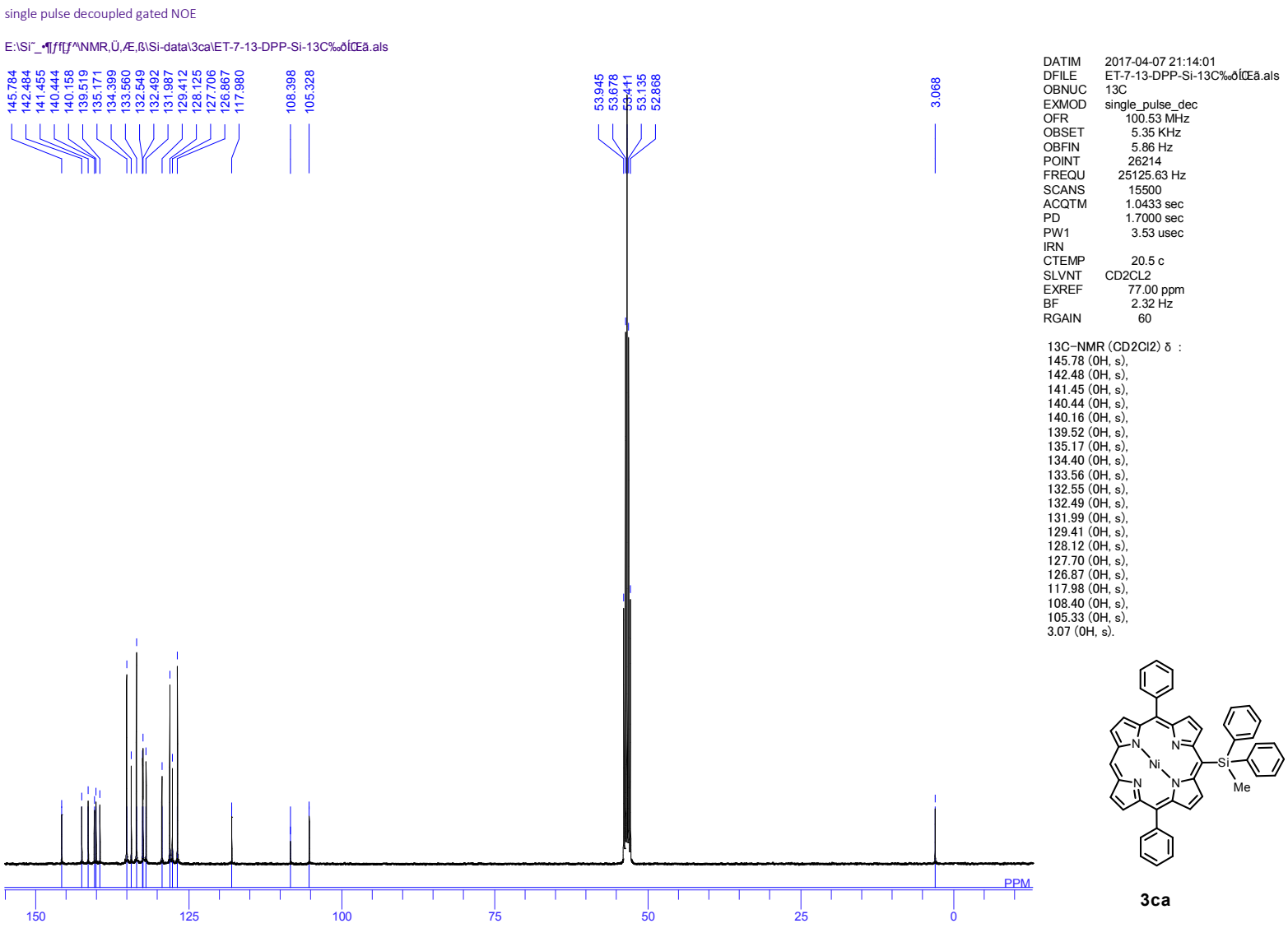


DATIM 2017-04-07 21:11:48
DFILE ET-7-13-DPP-Si-1H-‰ôÍŒĒā.als
OBNUC 1H
EXMOD single_pulse.jxp
OFR 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 26214
FREQU 6002.40 Hz
SCANS 16
ACQTM 4.3673 sec
PD 2.0000 sec
PW1 3.05 usec
IRN
CTEMP 20.7 c
SLVNT CD2CL2
EXREF 5.32 ppm
BF 0.09 Hz
RGAIN 42

1H-NMR (CD2Cl2) δ :
9.69 (1H, s),
9.06 (2H, d, J = 5.04 Hz),
9.00 (2H, d, J = 5.04 Hz),
8.75 (2H, d, J = 5.04 Hz),
8.56 (2H, d, J = 5.04 Hz),
7.93 (4H, dd, J = 7.79, 1.37 Hz),
7.71−7.62 (10H, m),
7.45−7.43 (2H, m),
7.36 (4H, t, J = 7.44 Hz),
1.29 (3H, s).

3ca

^{13}C NMR spectrum of 3ca

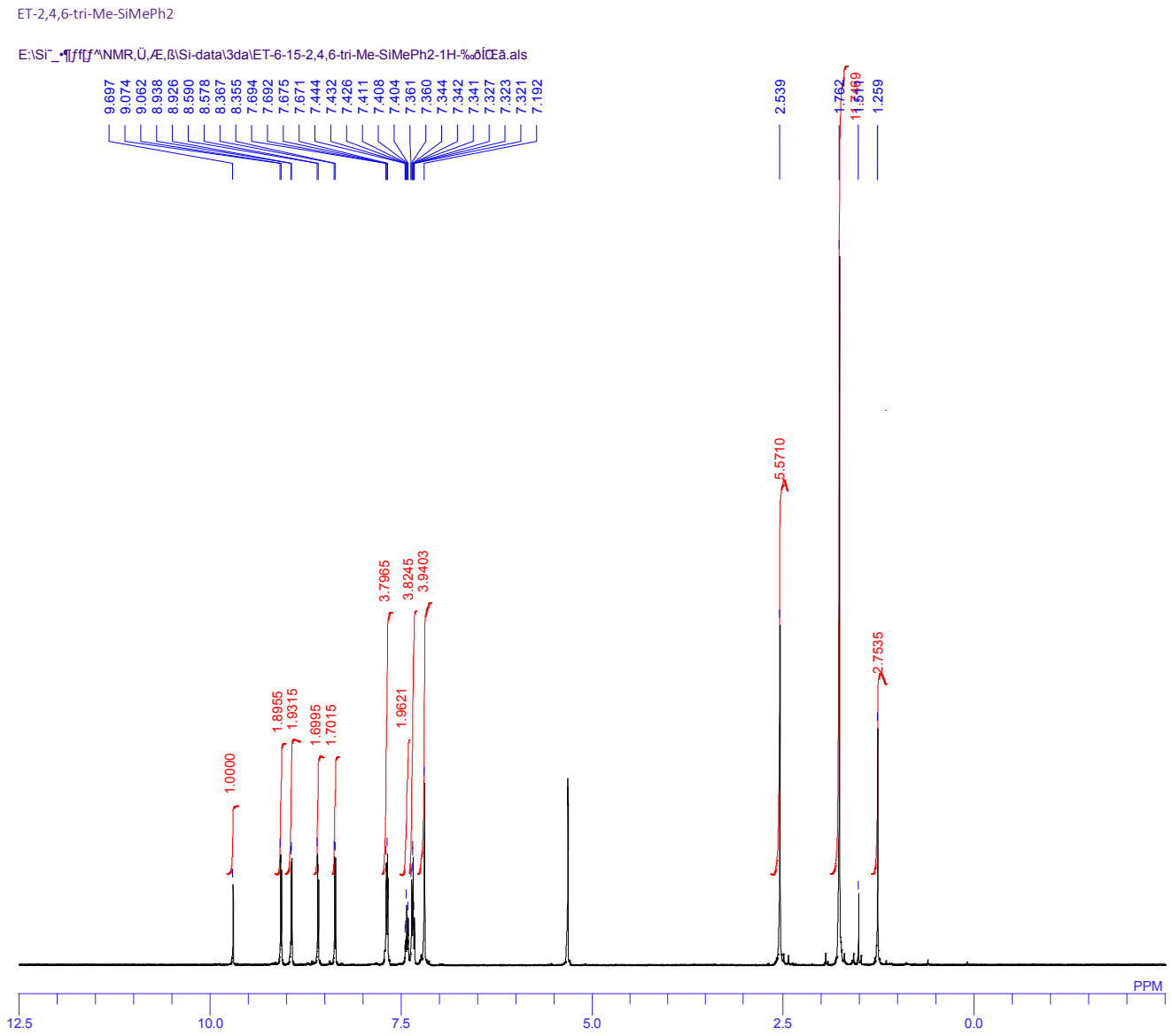


DATIM 2017-04-07 21:14:01
DFILE ET-7-13-DPP-Si-13C‰ðÍŒËã.als
OBNUC 13C
EXMOD single_pulse_dec
OFR 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25125.63 Hz
SCANS 15500
ACQTM 1.0433 sec
PD 1.7000 sec
PW1 3.53 usec
IRN
CTEMP 20.5 c
SLVNT CD2CL2
EXREF 77.00 ppm
BF 2.32 Hz
RGAIN 60

13C-NMR (CD2Cl2) δ :
145.78 (0H, s),
142.48 (0H, s),
141.45 (0H, s),
140.44 (0H, s),
140.16 (0H, s),
139.52 (0H, s),
135.17 (0H, s),
134.40 (0H, s),
133.56 (0H, s),
132.55 (0H, s),
132.49 (0H, s),
131.99 (0H, s),
129.41 (0H, s),
128.12 (0H, s),
127.70 (0H, s),
126.87 (0H, s),
117.98 (0H, s),
108.40 (0H, s),
105.33 (0H, s),
3.07 (0H, s).

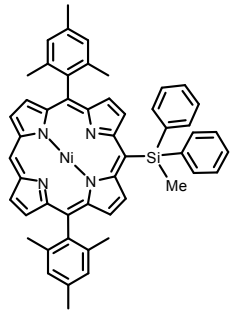
3ca

^{1}H NMR spectrum of 3da



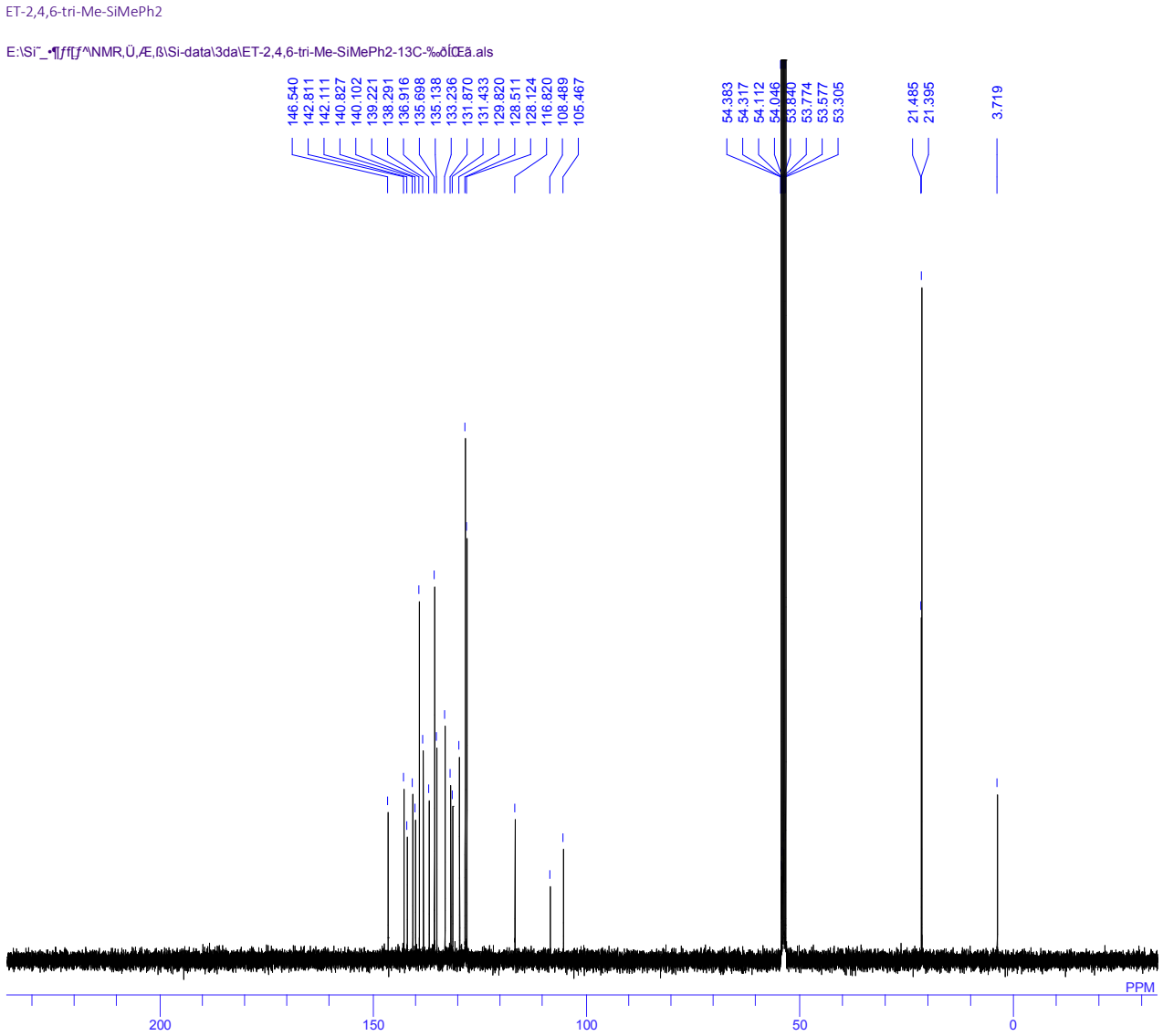
DATIM Mon Jun 05 21:42:04 2017
DFILE ET-6-15-2,4,6-tri-Me-SiMePh2-1H-‰ôÍŒã.als
OBNUC 1H
EXMOD NON
OFR 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
SCANS 16
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 5.60 usec
IRN
CTEMP 26.5 c
SLVNT CD2CL
EXREF 5.32 ppm
BF 0.09 Hz
RGAIN 21

1H-NMR (CD2Cl2) δ :
9.70 (1H, s),
9.07 (2H, d, J = 4.88 Hz),
8.93 (2H, d, J = 4.88 Hz),
8.58 (2H, d, J = 4.88 Hz),
8.36 (2H, d, J = 4.88 Hz),
7.68 (4H, dd, J = 8.05, 1.22 Hz),
7.43–7.42 (2H, m),
7.35–7.33 (4H, m),
7.19 (4H, s),
2.54 (6H, s),
1.76 (12H, s),
1.26 (3H, s).



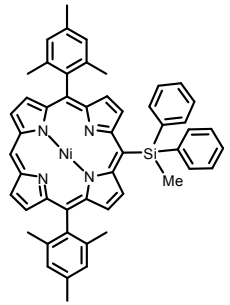
3da

^{13}C NMR spectrum of 3da



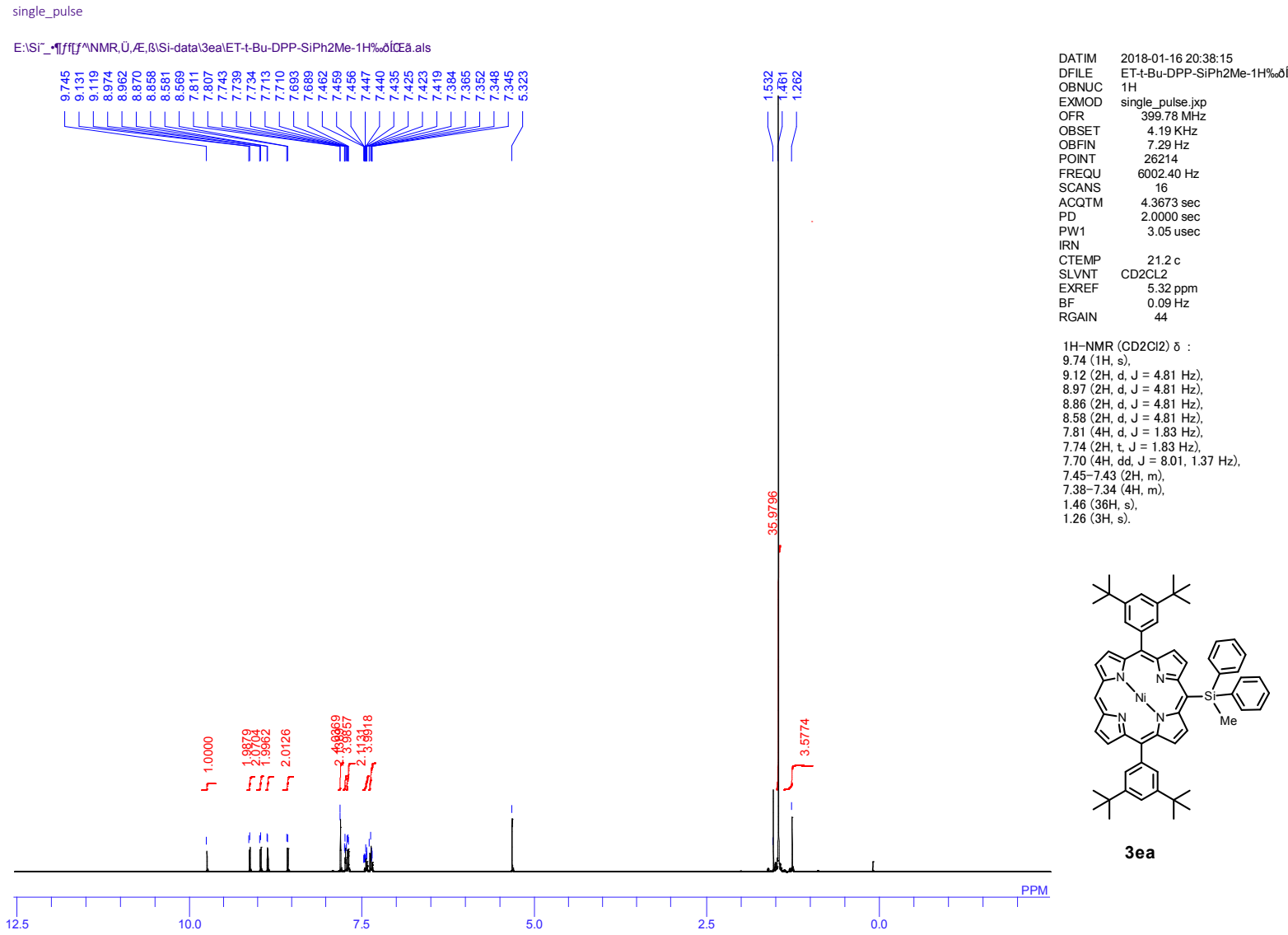
DATIM Tue Jun 06 10:12:38 2017
DFILE ET-2,4,6-tri-Me-SiMePh2-13C-‰ôÍŒã.als
OBNUC 13C
EXMOD BCM
OFR 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 27118.64 Hz
SCANS 15000
ACQTM 1.2083 sec
PD 1.7920 sec
PW1 5.80 usec
IRN
CTEMP 24.7 c
SLVNT CD2CL
EXREF 53.84 ppm
BF 0.09 Hz
RGAIN 25

13C-NMR (CD2Cl2) δ :
146.54 (0H, s),
142.81 (0H, s),
142.11 (0H, s),
140.83 (0H, s),
140.10 (0H, s),
139.22 (0H, s),
138.29 (0H, s),
136.92 (0H, s),
135.70 (0H, s),
135.14 (0H, s),
133.24 (0H, s),
131.87 (0H, s),
131.43 (0H, s),
129.82 (0H, s),
128.51 (0H, s),
128.12 (0H, s),
116.82 (0H, s),
108.49 (0H, s),
105.47 (0H, s),
21.49 (0H, s),
21.39 (0H, s),
3.72 (0H, s).



3da

^{1}H NMR spectrum of 3ea

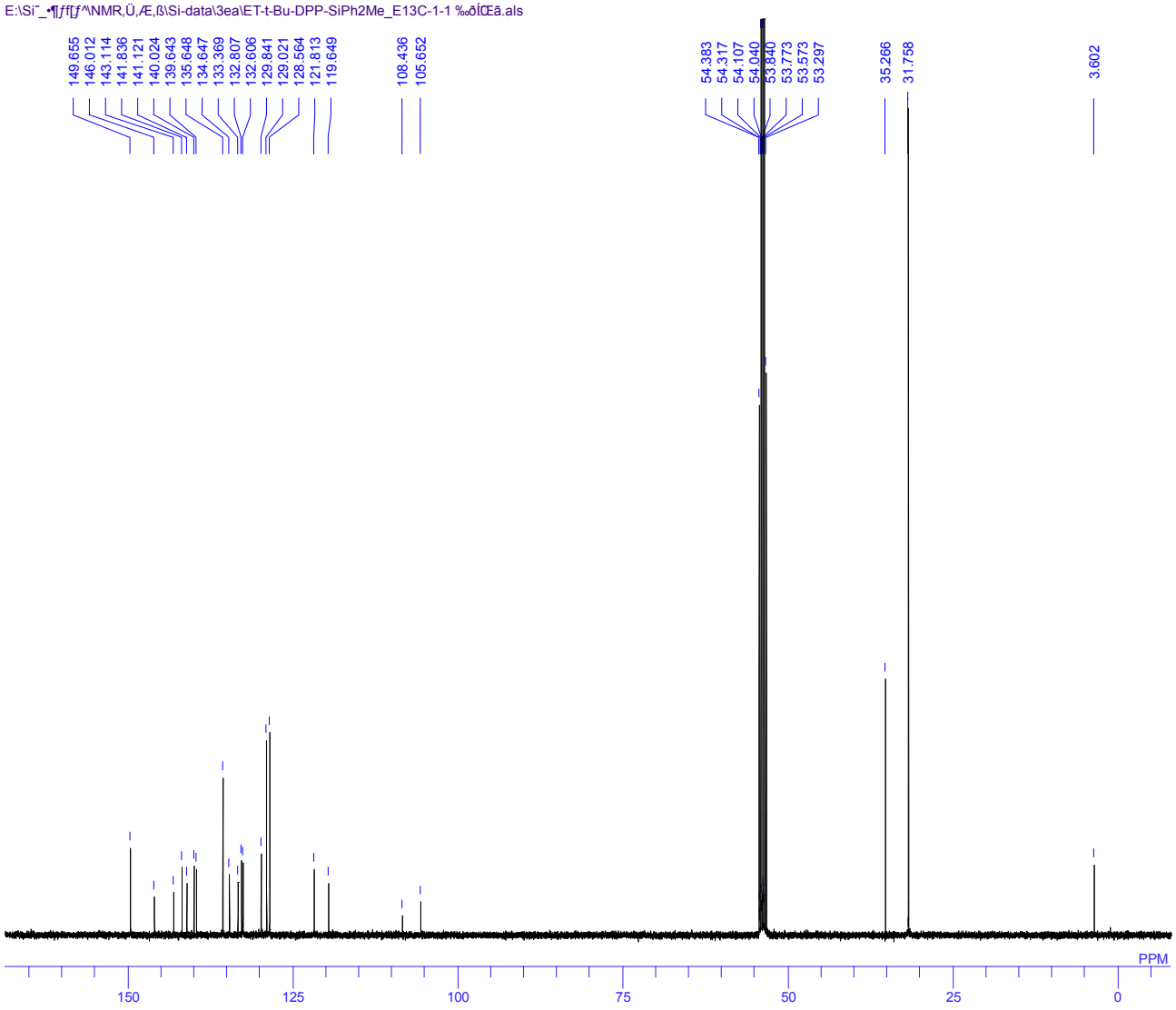


DATIM 2018-01-16 20:38:15
DFILE ET-t-Bu-DPP-SiPh2Me-1H‰ôÍŒã.als
OBNUC 1H
EXMOD single_pulse.jxp
OFR 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 26214
FREQU 6002.40 Hz
SCANS 16
ACQTM 4.3673 sec
PD 2.0000 sec
PW1 3.05 usec
IRN
CTEMP 21.2 c
SLVNT CD2CL2
EXREF 5.32 ppm
BF 0.09 Hz
RGAIN 44

1H-NMR (CD2Cl2) δ :
9.74 (1H, s),
9.12 (2H, d, J = 4.81 Hz),
8.97 (2H, d, J = 4.81 Hz),
8.86 (2H, d, J = 4.81 Hz),
8.58 (2H, d, J = 4.81 Hz),
7.81 (4H, d, J = 1.83 Hz),
7.74 (2H, t, J = 1.83 Hz),
7.70 (4H, dd, J = 8.01, 1.37 Hz),
7.45–7.43 (2H, m),
7.38–7.34 (4H, m),
1.46 (36H, s),
1.26 (3H, s).

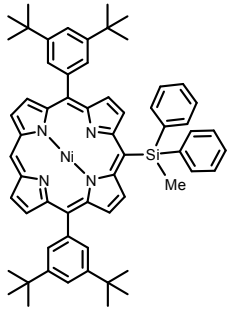
3ea

^{13}C NMR spectrum of 3ea



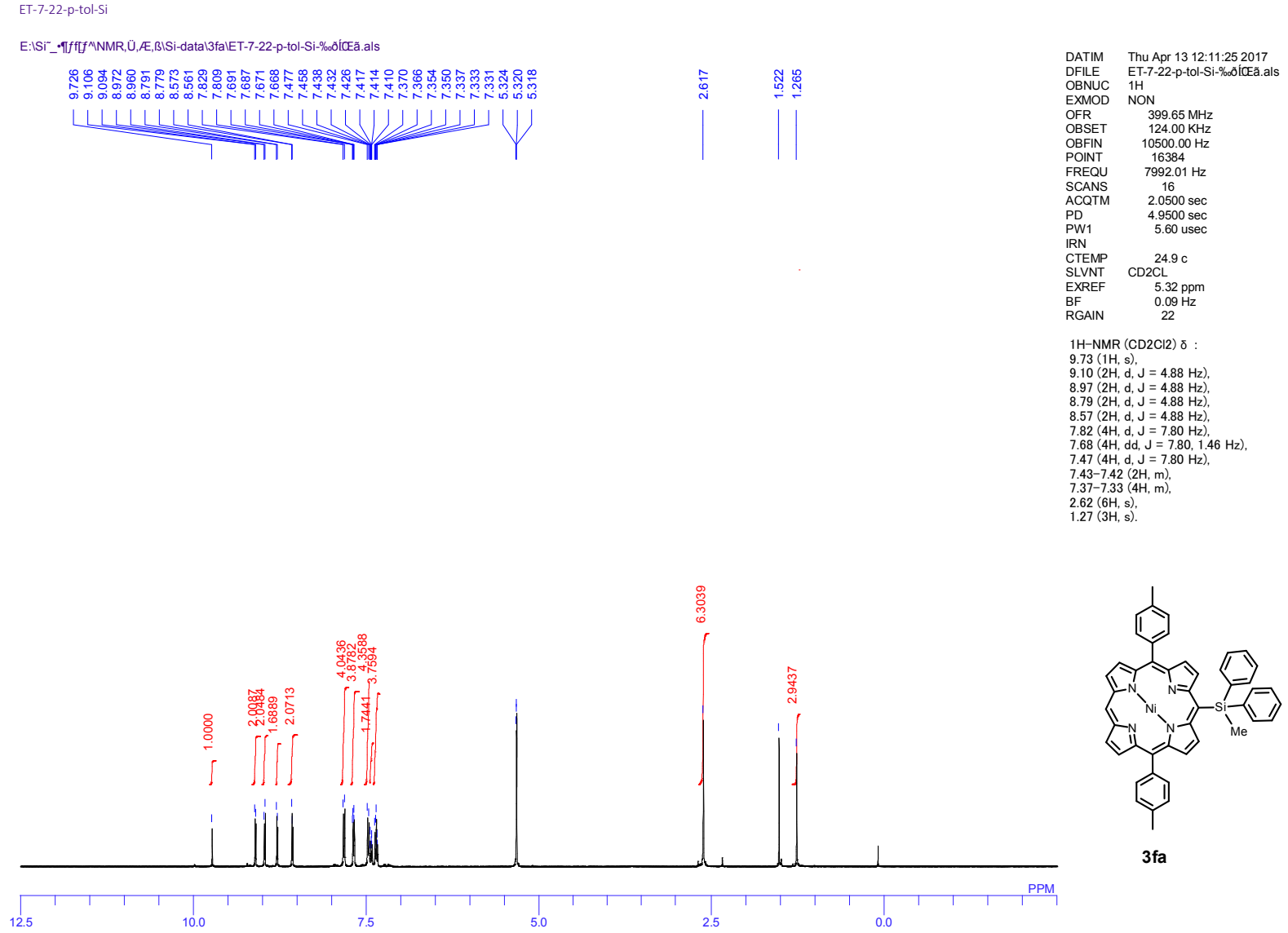
DATIM 2018-01-16 20:40:28
DFILE ET-t-Bu-DPP-SiPh2Me_E13C-1-1 ‰ðÍŒËã.als
OBNUC 13C
EXMOD single_pulse_dec
OFR 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25125.63 Hz
SCANS 16000
ACQTM 1.0433 sec
PD 1.7000 sec
PW1 3.53 usec
IRN
CTEMP 22.3 c
SLVNT CD2CL2
EXREF 53.84 ppm
BF 0.09 Hz
RGAIN 60

13C-NMR (CD2Cl2) δ :
149.65 (0H, s),
146.01 (0H, s),
143.11 (0H, s),
141.84 (0H, s),
141.12 (0H, s),
140.02 (0H, s),
139.64 (0H, s),
135.65 (0H, s),
134.65 (0H, s),
133.37 (0H, s),
132.81 (0H, s),
132.61 (0H, s),
129.84 (0H, s),
129.02 (0H, s),
128.56 (0H, s),
121.81 (0H, s),
119.65 (0H, s),
108.44 (0H, s),
105.65 (0H, s),
35.27 (0H, s),
31.76 (0H, s),
3.60 (0H, s).

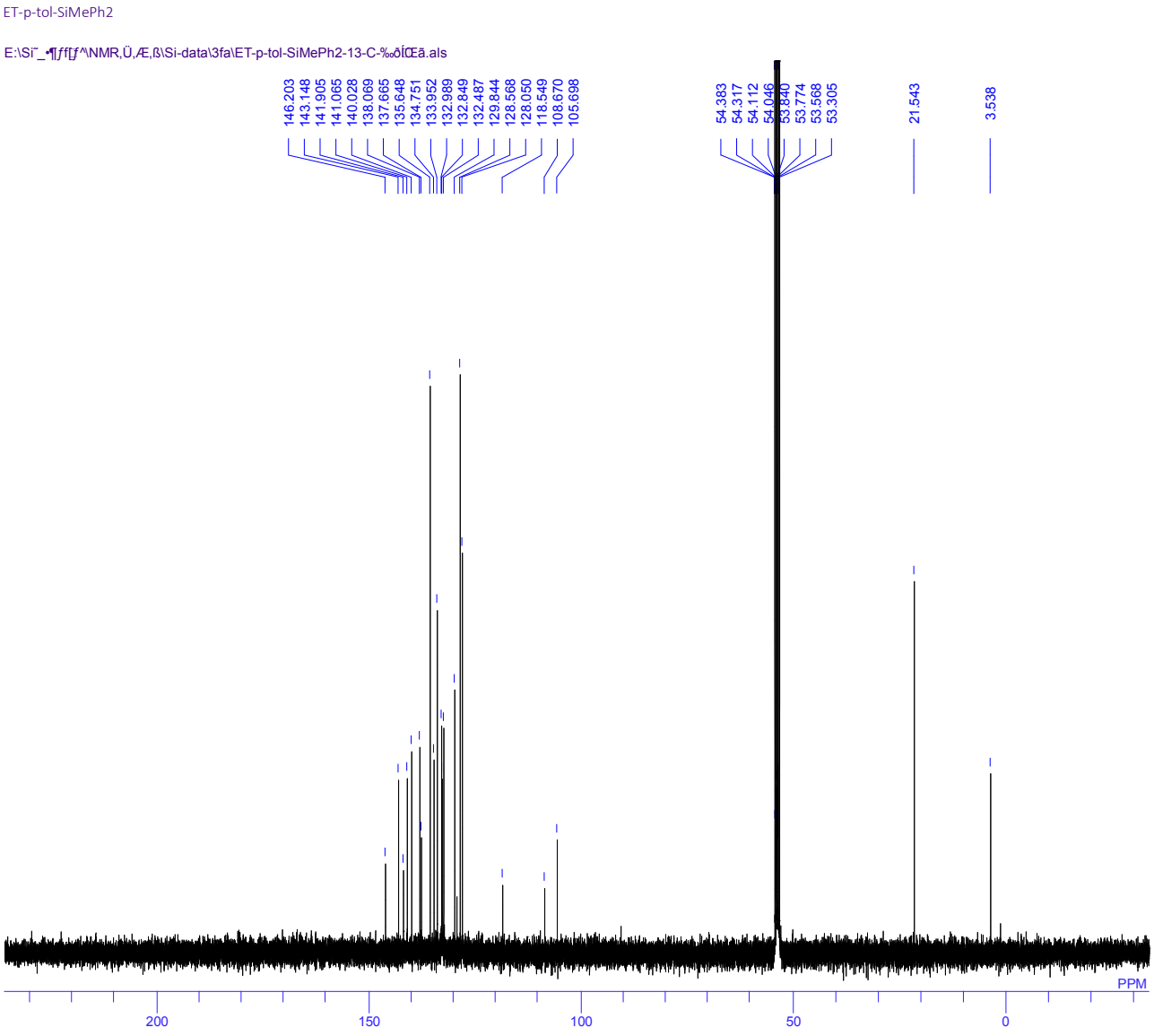


3ea

^{1}H NMR spectrum of 3fa

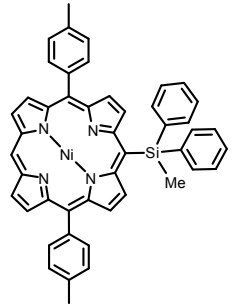


^{13}C NMR spectrum of 3fa



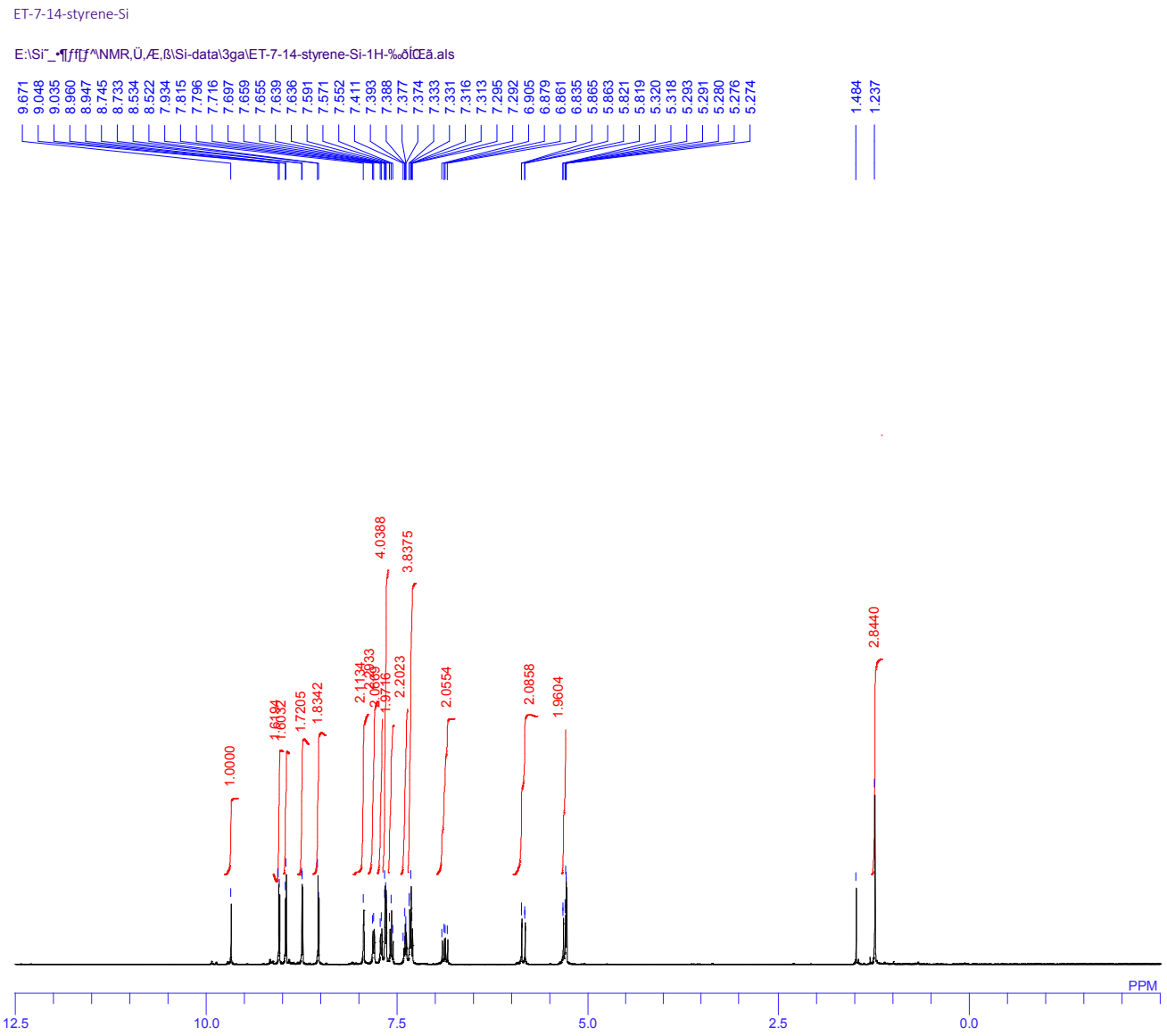
DATIM Thu Apr 20 10:09:20 2017
DFILE ET-p-tol-SiMePh2-13-C-‰ôÍŒĕã.als
OBNUC 13C
EXMOD BCM
OFR 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 27118.64 Hz
SCANS 15500
ACQTM 1.2083 sec
PD 1.7920 sec
PW1 5.80 usec
IRN
CTEMP 24.7 c
SLVNT CD2CL
EXREF 53.84 ppm
BF 0.09 Hz
RGAIN 24

13C-NMR (CD2Cl2) δ :
146.20 (0H, s),
143.15 (0H, s),
141.91 (0H, s),
141.07 (0H, s),
140.03 (0H, s),
138.07 (0H, s),
137.67 (0H, s),
135.65 (0H, s),
134.75 (0H, s),
133.95 (0H, s),
132.99 (0H, s),
132.85 (0H, s),
132.49 (0H, s),
129.84 (0H, s),
128.57 (0H, s),
128.05 (0H, s),
118.55 (0H, s),
108.67 (0H, s),
105.70 (0H, s),
21.54 (0H, s),
3.54 (0H, s).



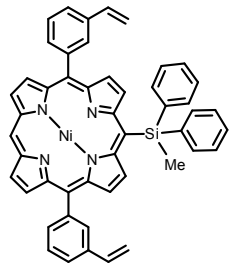
3fa

^{1}H NMR spectrum of 3ga



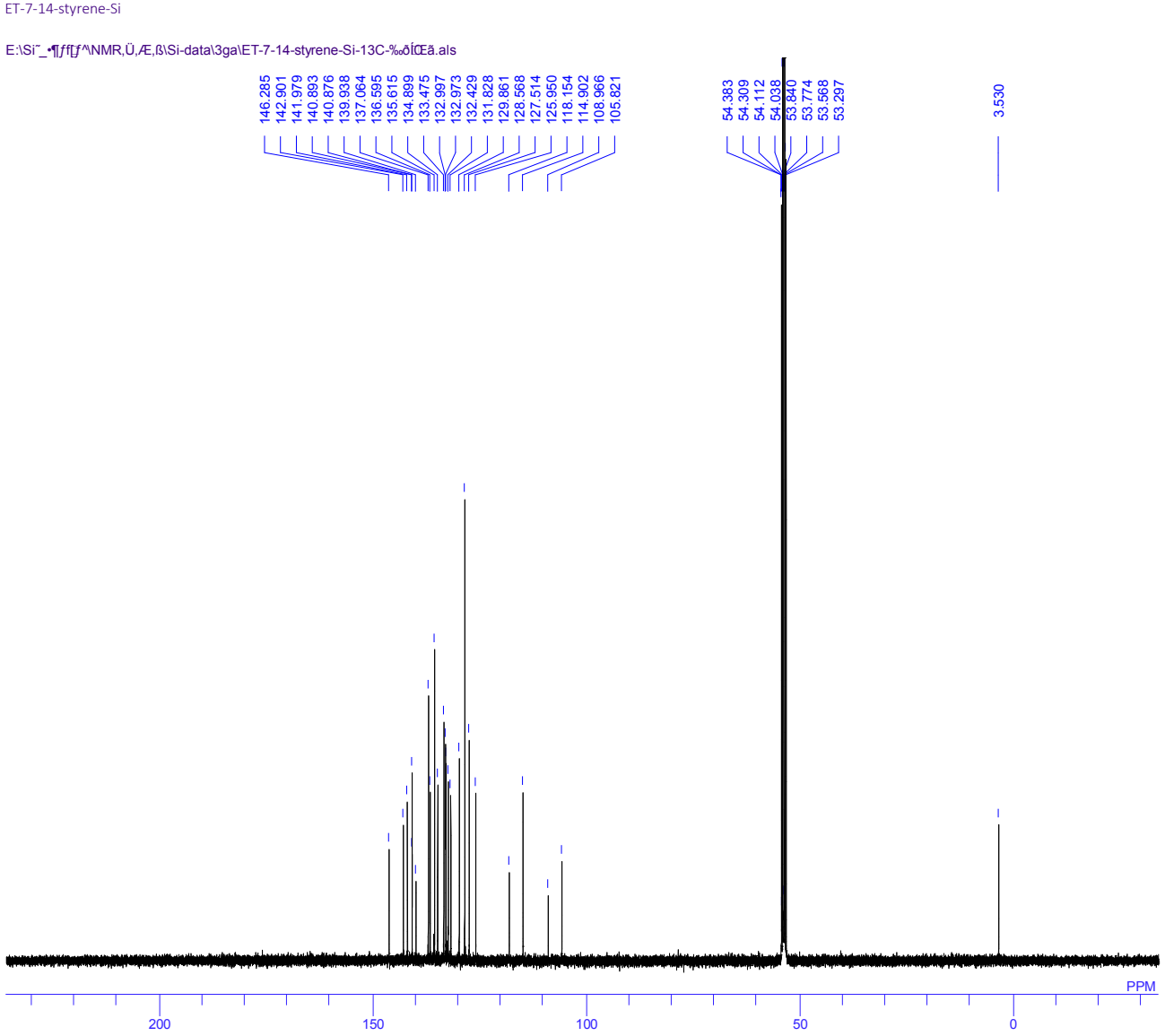
DATIM Thu Apr 06 22:21:56 2017
DFILE ET-7-14-styrene-Si-1H-‰ðÍŒËã.als
OBNUC 1H
EXMOD NON
OFR 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
SCANS 8
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 5.60 usec
IRN
CTEMP 22.7 c
SLVNT CD2CL
EXREF 5.32 ppm
BF 0.09 Hz
RGAIN 18

1H−NMR (CD2Cl2) δ :
9.67 (1H, s),
9.04 (2H, d, J = 4.88 Hz),
8.95 (2H, d, J = 4.88 Hz),
8.74 (2H, d, J = 4.88 Hz),
8.53 (2H, d, J = 4.88 Hz),
7.93 (2H, s),
7.81 (2H, d, J = 7.80 Hz),
7.71 (2H, d, J = 7.80 Hz),
7.65 (4H, dd, J = 7.80, 1.46 Hz),
7.57 (2H, t, J = 7.80 Hz),
7.41−7.37 (2H, m),
7.32−7.30 (4H, m),
6.87 (2H, dd, J = 17.56, 10.24 Hz),
5.84 (2H, dd, J = 17.56, 0.98 Hz),
5.31 (2H, dd, J = 10.73, 0.98 Hz),
1.24 (3H, s).



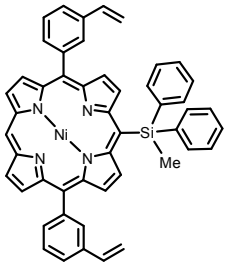
3ga

^{13}C NMR spectrum of 3ga



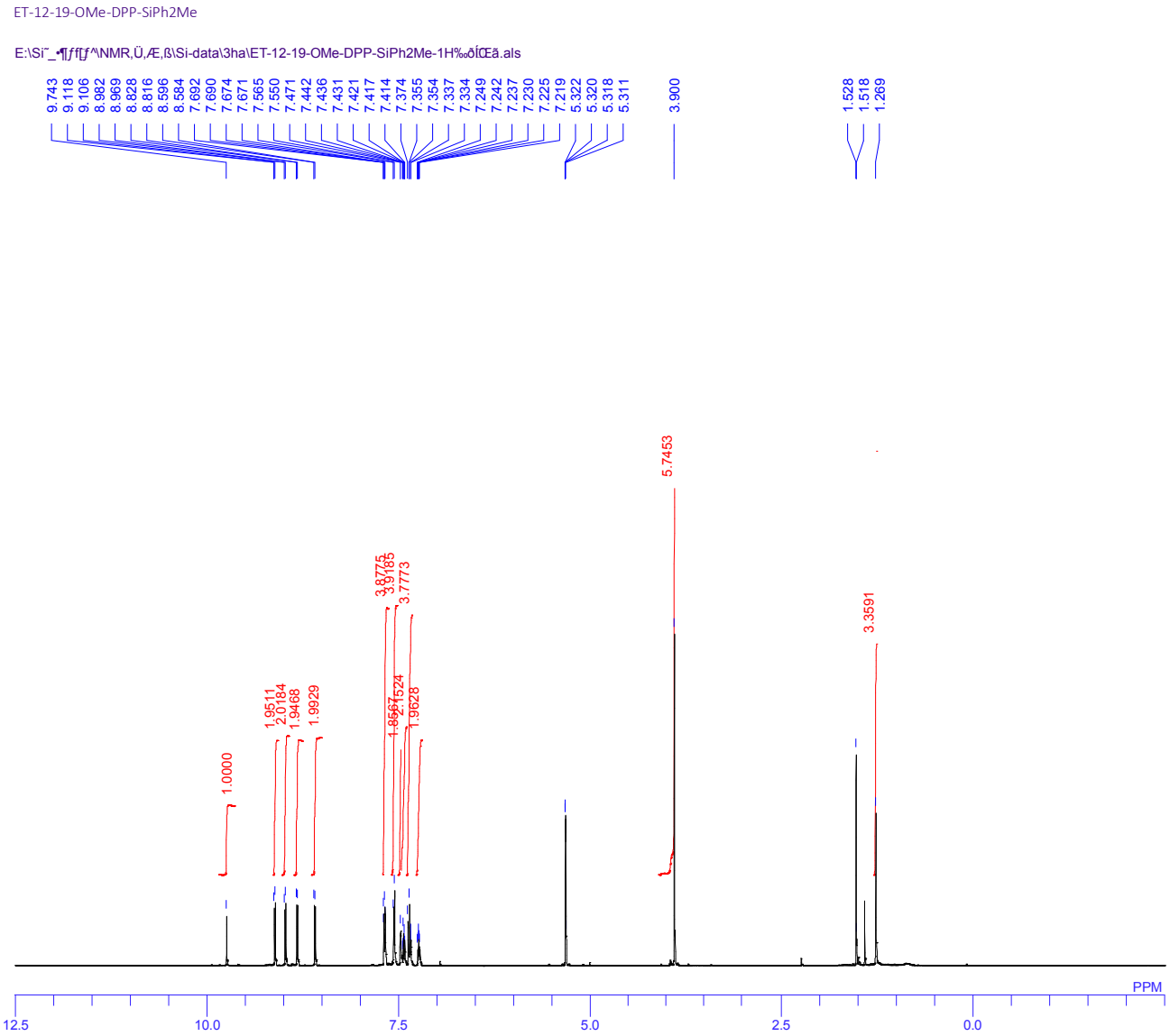
DATIM Fri Apr 07 11:17:31 2017
DFILE ET-7-14-styrene-Si-13C-‰ðÍŒĒã.als
OBNUC 13C
EXMOD BCM
OFR 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 27118.64 Hz
SCANS 15500
ACQTM 1.2083 sec
PD 1.7920 sec
PW1 5.80 usec
IRN
CTEMP 22.0 c
SLVNT CD2CL
EXREF 53.84 ppm
BF 0.09 Hz
RGAIN 25

13C-NMR (CD2Cl2) δ :
146.29 (0H, s),
142.90 (0H, s),
141.98 (0H, s),
140.89 (0H, s),
140.88 (0H, s),
139.94 (0H, s),
137.06 (0H, s),
136.60 (0H, s),
135.62 (0H, s),
134.90 (0H, s),
133.47 (0H, s),
133.00 (0H, s),
132.97 (0H, s),
132.43 (0H, s),
131.83 (0H, s),
129.86 (0H, s),
128.57 (0H, s),
127.51 (0H, s),
125.95 (0H, s),
118.15 (0H, s),
114.90 (0H, s),
108.97 (0H, s),
105.82 (0H, s),
3.53 (0H, s).



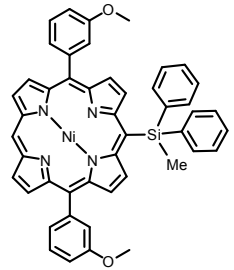
3ga

^{1}H NMR spectrum of 3ha



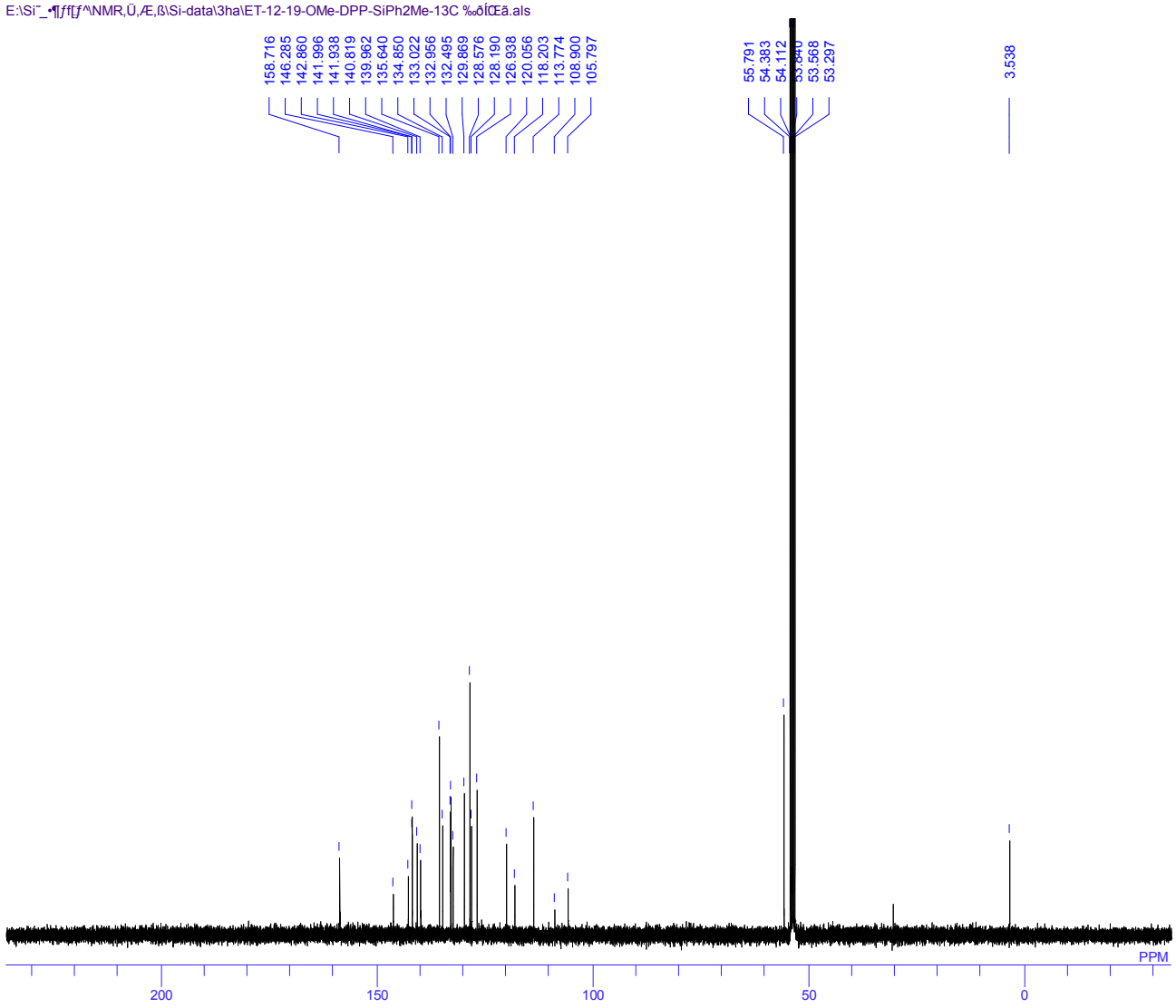
DATIM Thu Jan 18 20:33:02 2018
DFILE ET-12-19-OMe-DPP-SiPh2Me-1H‰ôÍŒÈã.als
OBNUC 1H
EXMOD NON
OFR 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
SCANS 16
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 5.80 usec
IRN
CTEMP 23.7 c
SLVNT CD2CL
EXREF 5.32 ppm
BF 0.09 Hz
RGAIN 22

1H-NMR (CD2Cl2) δ :
9.74 (1H, s),
9.11 (2H, d, J = 4.88 Hz),
8.98 (2H, d, J = 4.88 Hz),
8.82 (2H, d, J = 4.88 Hz),
8.59 (2H, d, J = 4.88 Hz),
7.68 (4H, dd, J = 7.32, 0.98 Hz),
7.56 (4H, d, J = 5.85 Hz),
7.47 (2H, s),
7.43-7.42 (2H, m),
7.37-7.33 (4H, m),
7.24-7.23 (2H, m),
3.90 (6H, s),
1.27 (3H, s).



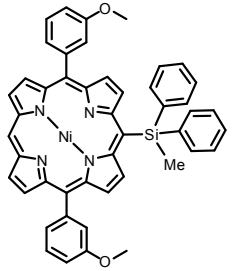
3ha

^{13}C NMR spectrum of 3ha



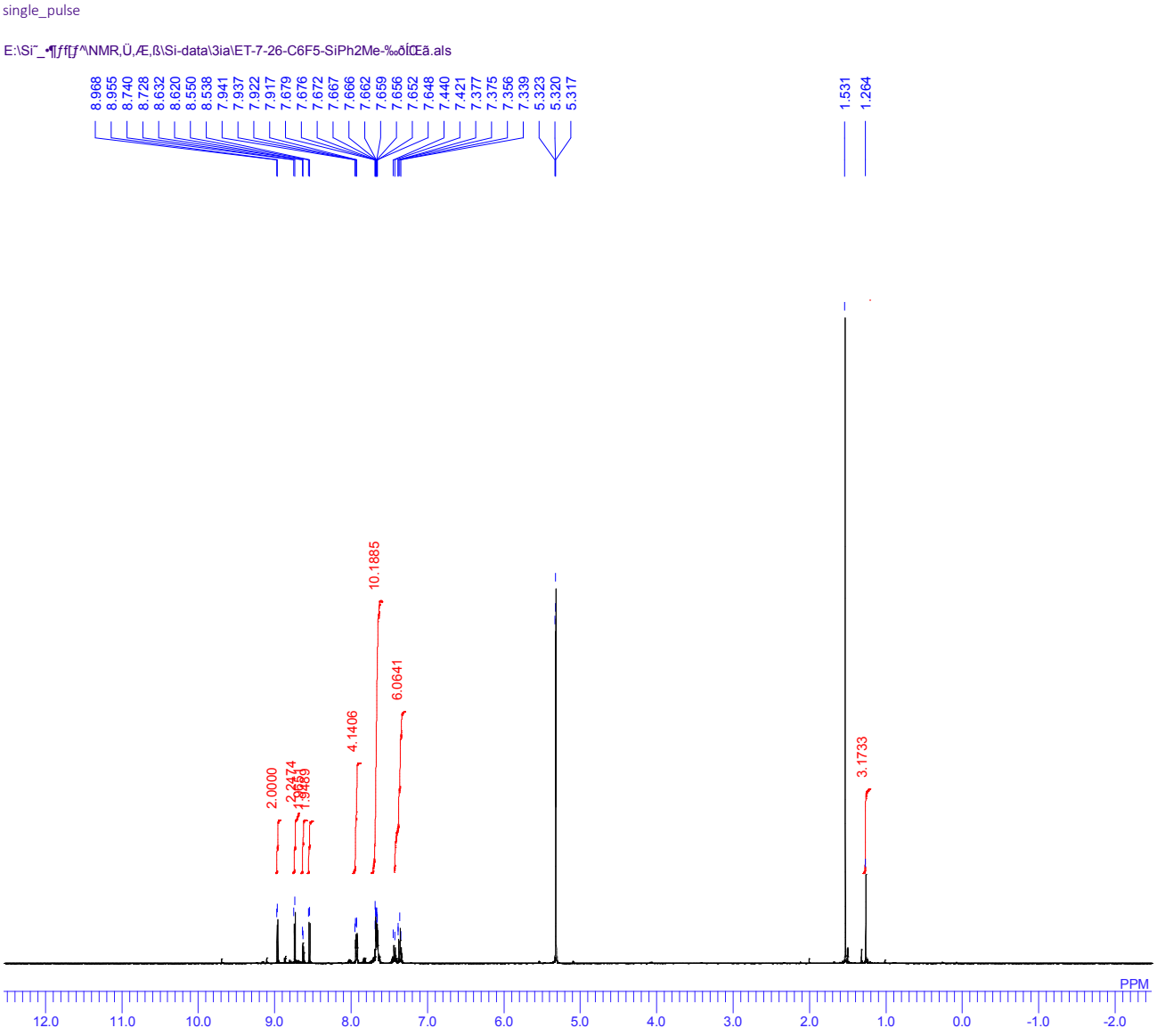
DATIM Fri Jan 19 09:03:36 2018
DFILE ET-12-19-OMe-DPP-SiPh2Me-13C ‰ôÍŒĕä.als
OBNUC 13C
EXMOD BCM
OFR 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 27118.64 Hz
SCANS 15000
ACQTM 1.2083 sec
PD 1.7920 sec
PW1 5.80 usec
IRN
CTEMP 23.1 c
SLVNT CD2CL
EXREF 53.84 ppm
BF 0.01 Hz
RGAIN 25

13C-NMR (CD2Cl2) δ :
158.72 (0H, s),
146.29 (0H, s),
142.86 (0H, s),
142.00 (0H, s),
141.94 (0H, s),
140.82 (0H, s),
139.96 (0H, s),
135.64 (0H, s),
134.85 (0H, s),
133.02 (0H, s),
132.96 (0H, s),
132.50 (0H, s),
129.87 (0H, s),
128.58 (0H, s),
128.19 (0H, s),
126.94 (0H, s),
120.06 (0H, s),
118.20 (0H, s),
113.77 (0H, s),
108.90 (0H, s),
105.80 (0H, s),
55.79 (0H, s),
3.54 (0H, s).



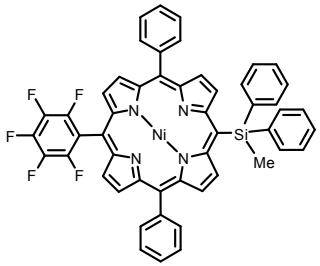
3ha

^{1}H NMR spectrum of 3ia



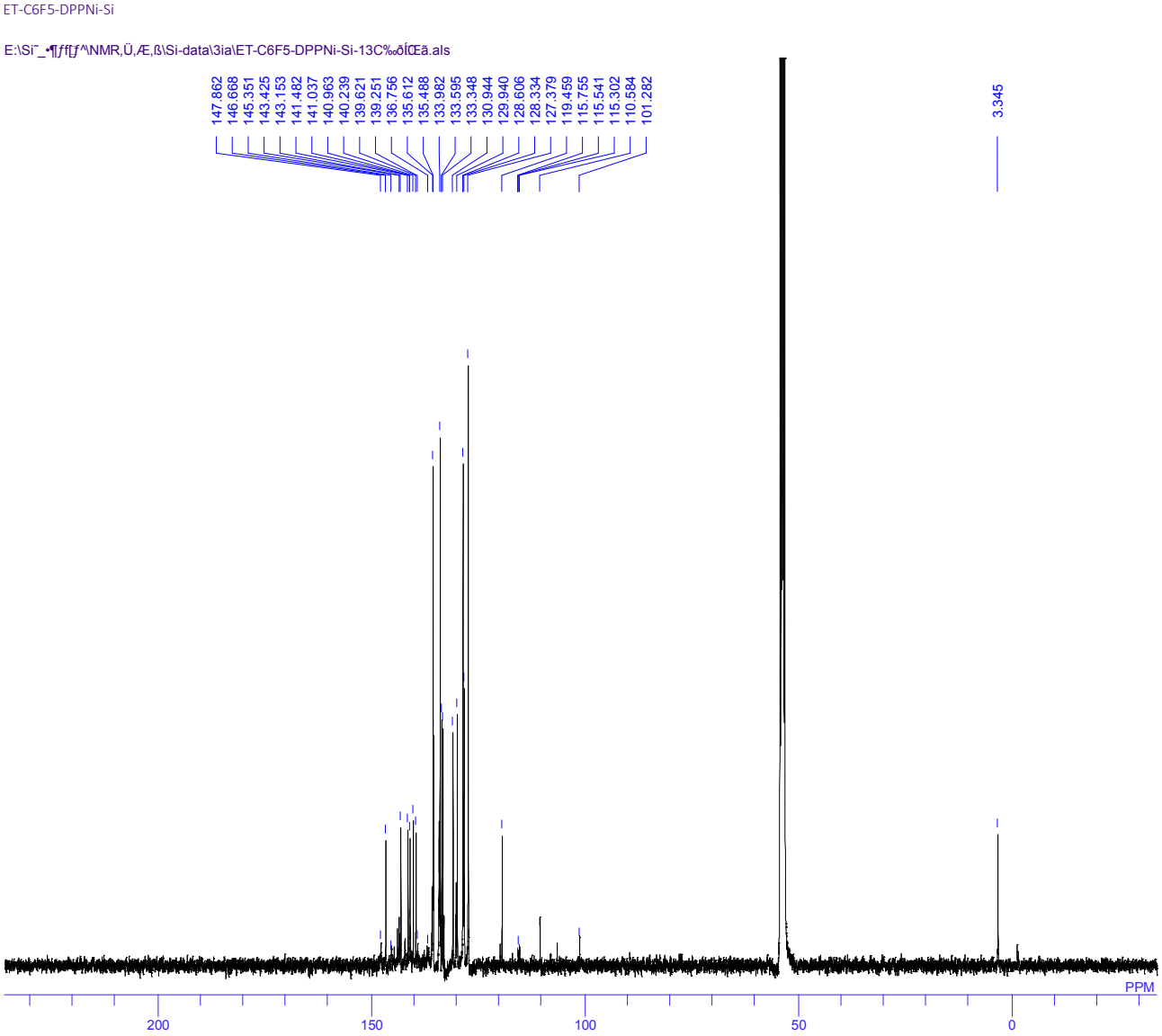
DATIM 2017-04-24 18:58:53
DFILE ET-7-26-C6F5-SiPh2Me-‰ôÍŒã.als
OBNUC 1H
EXMOD single_pulse.jxp
OFR 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 26214
FREQU 6002.40 Hz
SCANS 16
ACQTM 4.3673 sec
PD 2.0000 sec
PW1 3.05 usec
IRN
CTEMP 20.2 c
SLVNT CD2CL2
EXREF 5.32 ppm
BF 0.09 Hz
RGAIN 52

1H–NMR (CD2Cl2) δ :
8.96 (2H, d, J = 5.04 Hz),
8.73 (2H, d, J = 5.04 Hz),
8.63 (2H, d, J = 5.04 Hz),
8.54 (2H, d, J = 5.04 Hz),
7.93 (4H, dd, J = 7.79, 3.89 Hz),
7.68–7.65 (10H, m),
7.42–7.36 (6H, m),
1.26 (3H, s).



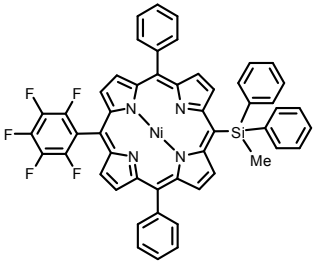
3ia

^{13}C NMR spectrum of 3ia



DATIM Mon Feb 05 04:21:22 2018
DFILE ET-C6F5-DPPNi-Si-13C‰ôÍŒã.als
OBNUC 13C
EXMOD BCM
OFR 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 27118.64 Hz
SCANS 40000
ACQTM 1.2083 sec
PD 1.7920 sec
PW1 5.80 usec
IRN
CTEMP 22.9 c
SLVNT CD2CL
EXREF 53.82 ppm
BF 2.32 Hz
RGAIN 25

13C-NMR (CD2Cl2) δ :
146.67 (0H, s),
146.61 (0H, d, J = 252.42 Hz),
143.15 (0H, s),
142.19 (0H, d, J = 247.45 Hz),
141.48 (0H, s),
141.04 (0H, s),
140.24 (0H, s),
139.62 (0H, s),
138.00 (0H, d, J = 250.76 Hz),
135.61 (0H, s),
135.49 (0H, s),
133.98 (0H, s),
133.59 (0H, s),
133.35 (0H, s),
130.94 (0H, s),
129.94 (0H, s),
128.61 (0H, s),
128.33 (0H, s),
127.38 (0H, s),
119.46 (0H, s),
115.53 (0H, t, J = 22.76 Hz),
110.58 (0H, s),
101.28 (0H, s),
3.35 (0H, s).

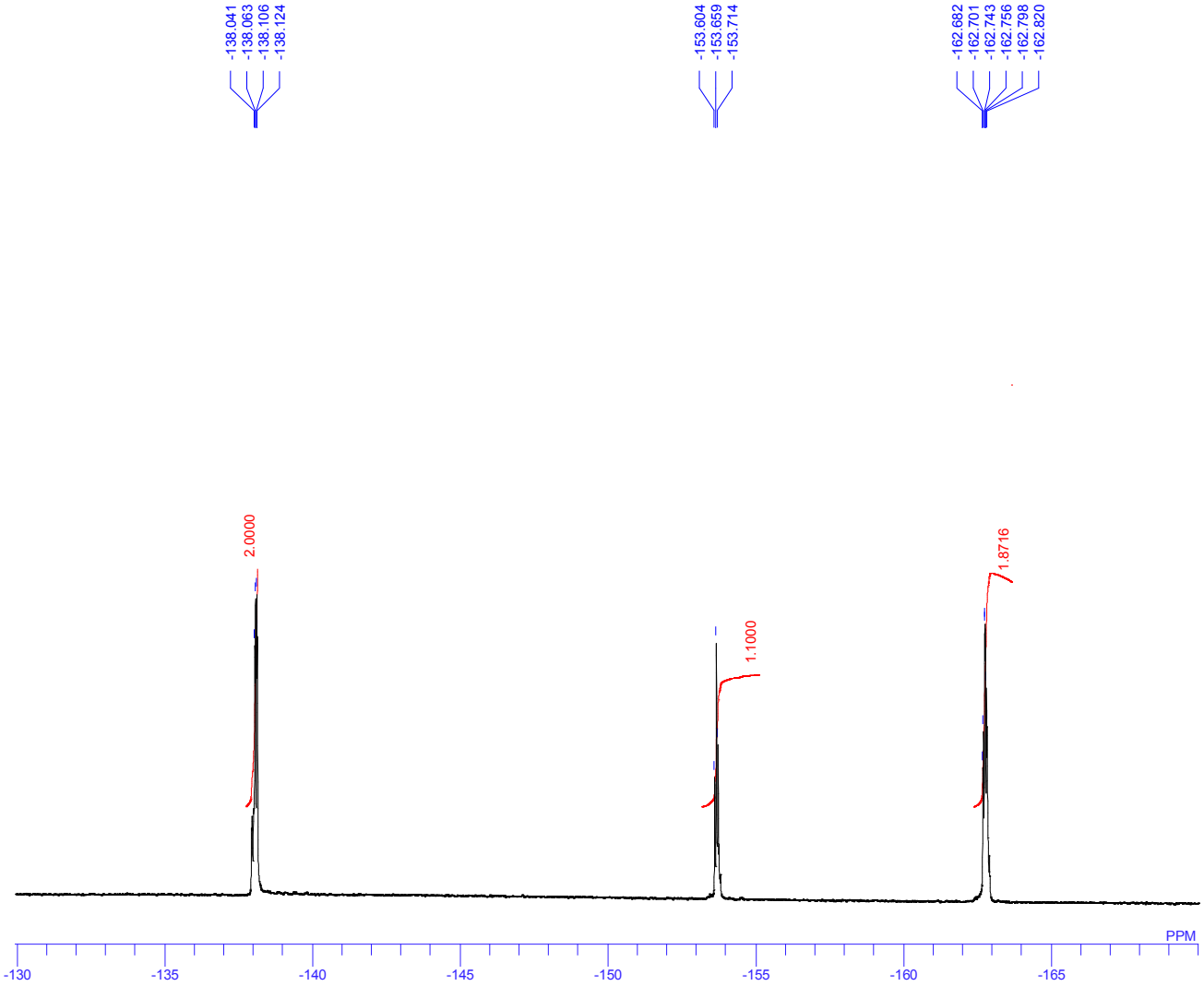


3ia

^{19}F NMR spectrum of 3ia

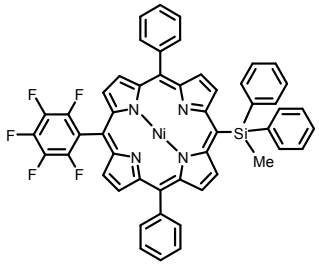
single_pulse

E:\Si¯_•¶ƒf[ƒ^\NMR,Ü,Æ,ß\Si-data\3ia\ET-C6F5-DPPNi-SiPh2Me-19F-‰ðÍŒã.als



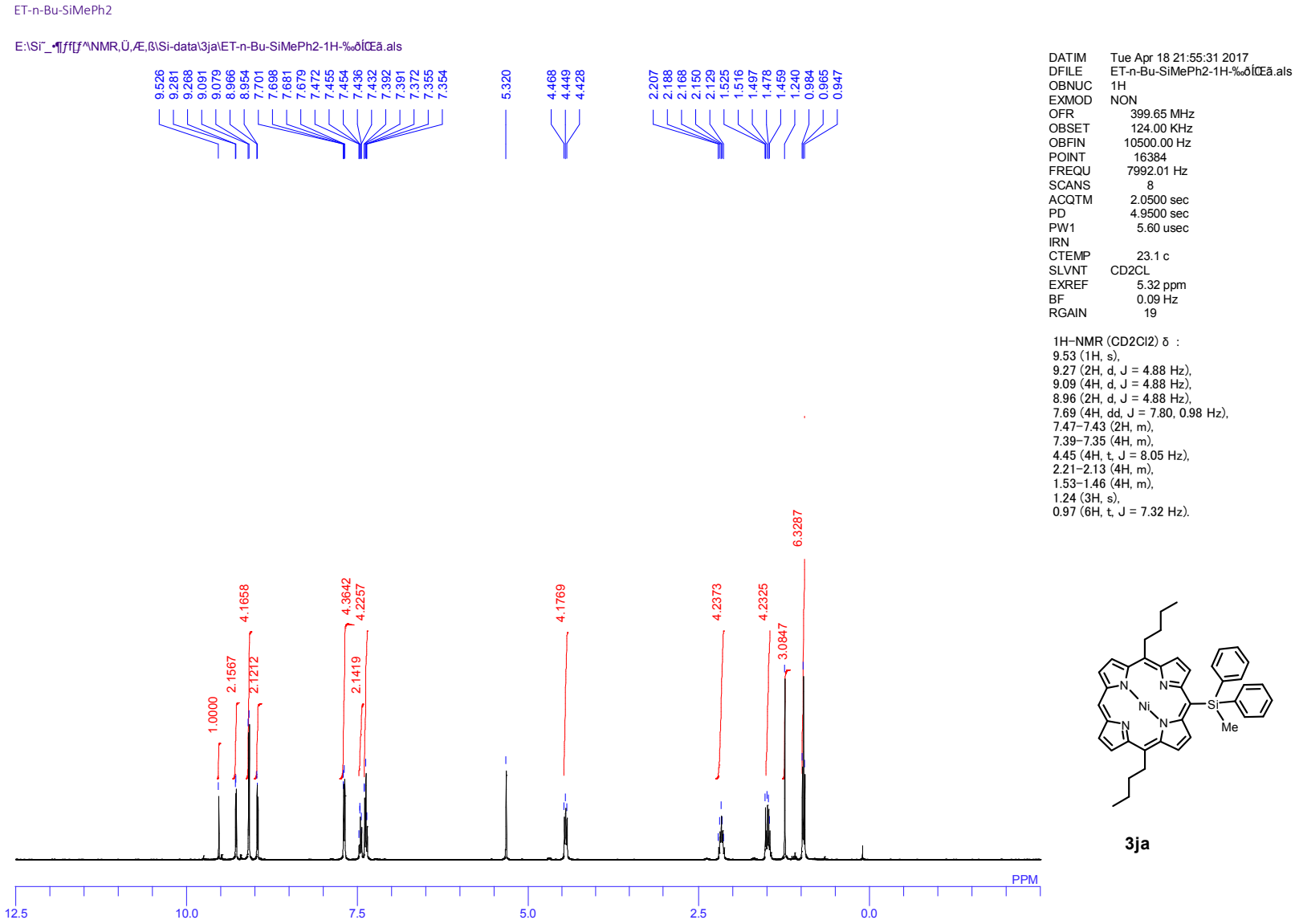
DATIM	2018-02-03 18:28:20
DFILE	ET-C6F5-DPPNi-SiPh2Me-19F-‰ðÍŒã.als
OBNUC	19F
EXMOD	single_pulse.jxp
OFR	376.11 MHz
OBSET	4.62 KHz
OBFIN	8.27 Hz
POINT	13107
FREQU	15060.24 Hz
SCANS	16
ACQTM	0.8703 sec
PD	5.0000 sec
PW1	3.76 usec
IRN	
CTEMP	22.7 c
SLVNT	CD2CL2
EXREF	-152.30 ppm
BF	3.72 Hz
RGAIN	46

19F-NMR (CD2Cl2) δ :
−138.08 (2H, dd, J = 23.55, 7.47 Hz),
−153.66 (1H, t, J = 20.68 Hz),
−162.75 (2H, ddd, J = 22.12, 6.51, 3.26 Hz).

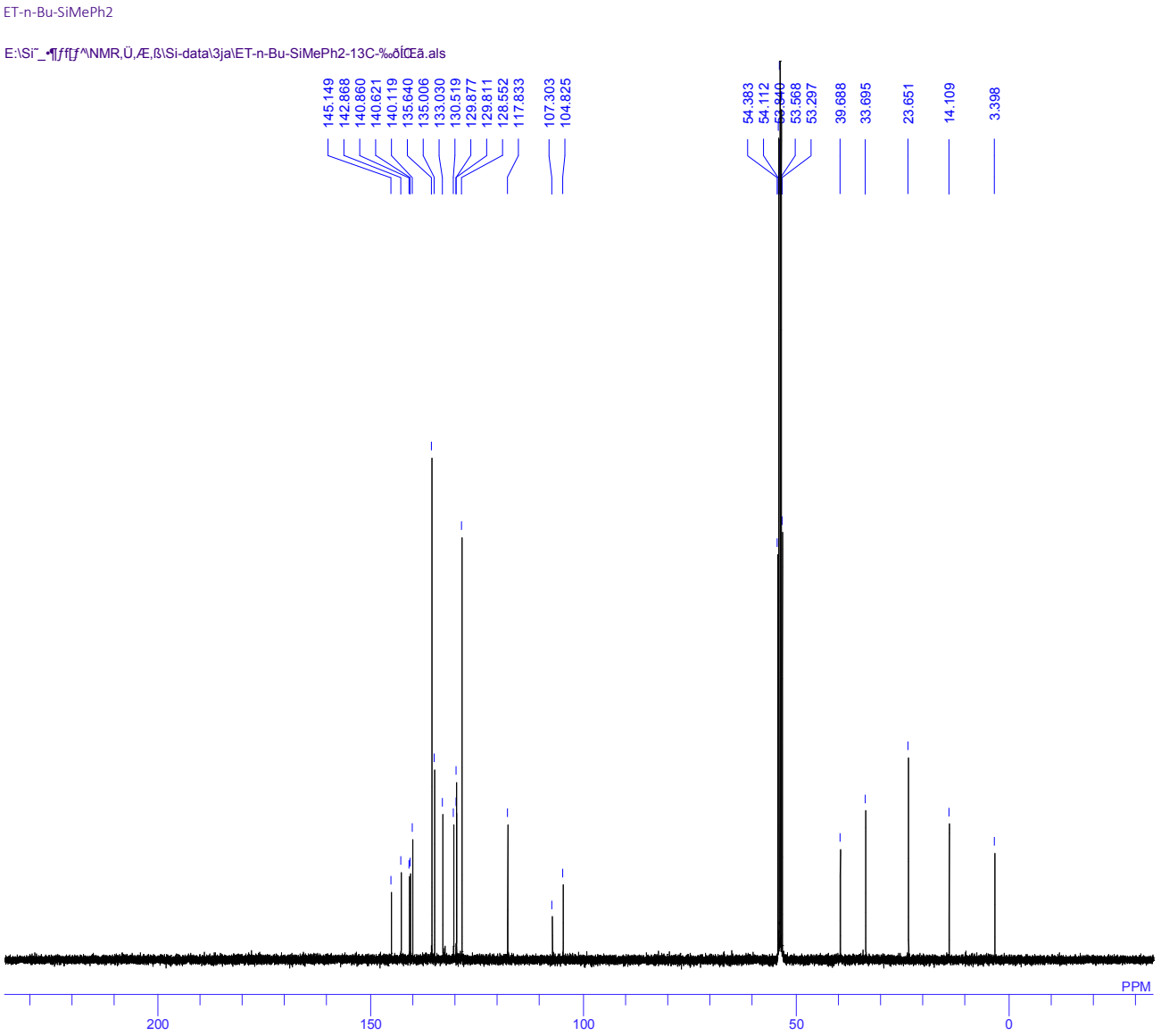


3ia

^{1}H NMR spectrum of 3ja

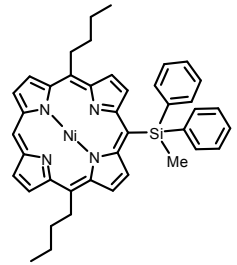


^{13}C NMR spectrum of 3ja



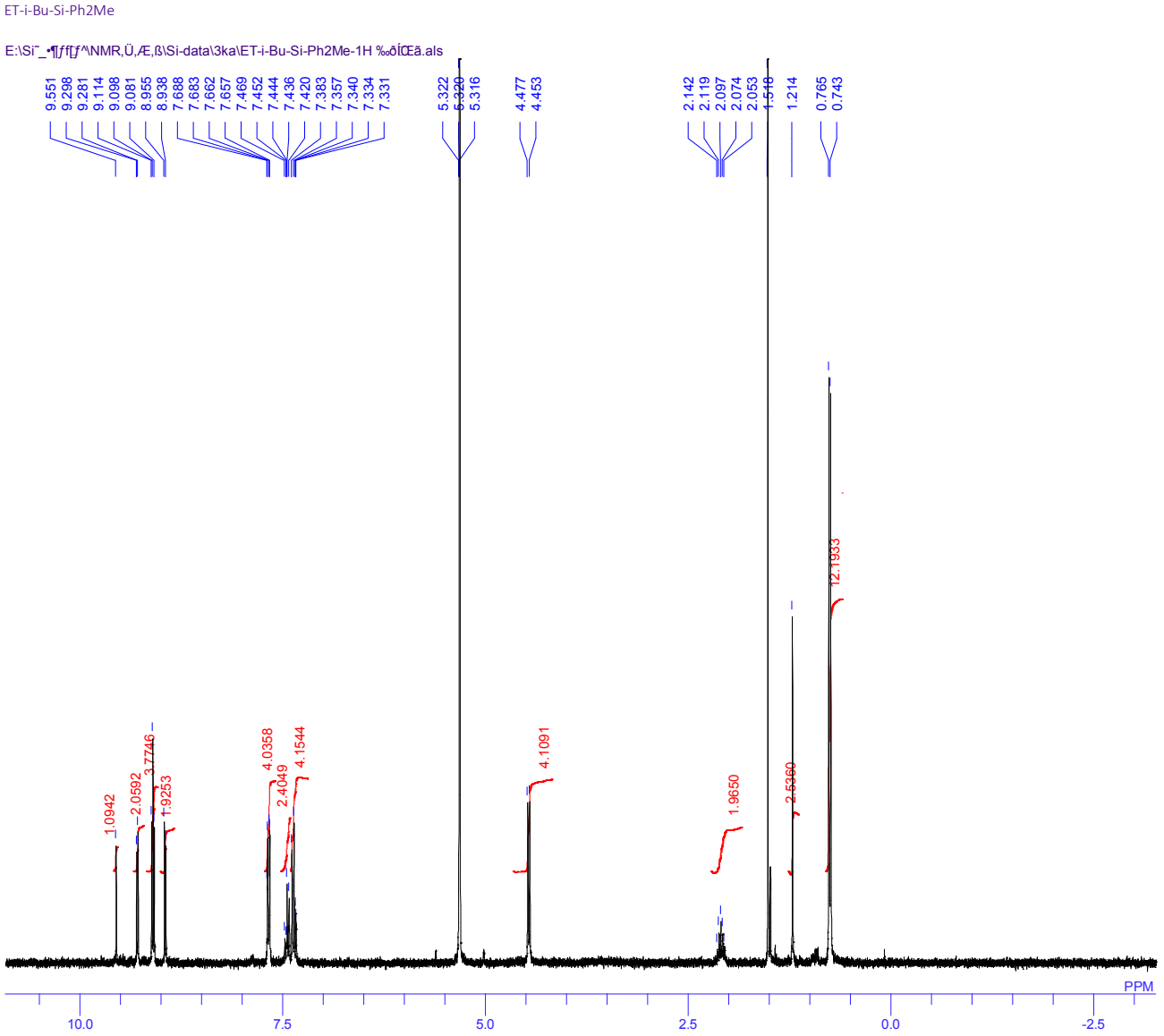
DATIM Wed Apr 19 11:16:13 2017
DFILE ET-n-Bu-SiMePh2-13C-‰ðÍŒã.als
OBNUC 13C
EXMOD BCM
OFR 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 27118.64 Hz
SCANS 16000
ACQTM 1.2083 sec
PD 1.7920 sec
PW1 5.80 usec
IRN
CTEMP 22.2 c
SLVNT CD2CL
EXREF 53.84 ppm
BF 0.09 Hz
RGAIN 25

13C-NMR (CD2CL2) δ :
145.15 (0H, s),
142.87 (0H, s),
140.86 (0H, s),
140.62 (0H, s),
140.12 (0H, s),
135.64 (0H, s),
135.01 (0H, s),
133.03 (0H, s),
130.52 (0H, s),
129.88 (0H, s),
129.81 (0H, s),
128.55 (0H, s),
117.83 (0H, s),
107.30 (0H, s),
104.83 (0H, s),
39.69 (0H, s),
33.69 (0H, s),
23.65 (0H, s),
14.11 (0H, s),
3.40 (0H, s).



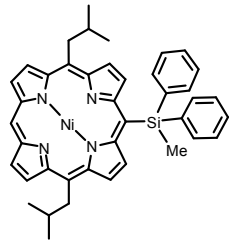
3ja

^{1}H NMR spectrum of 3ka



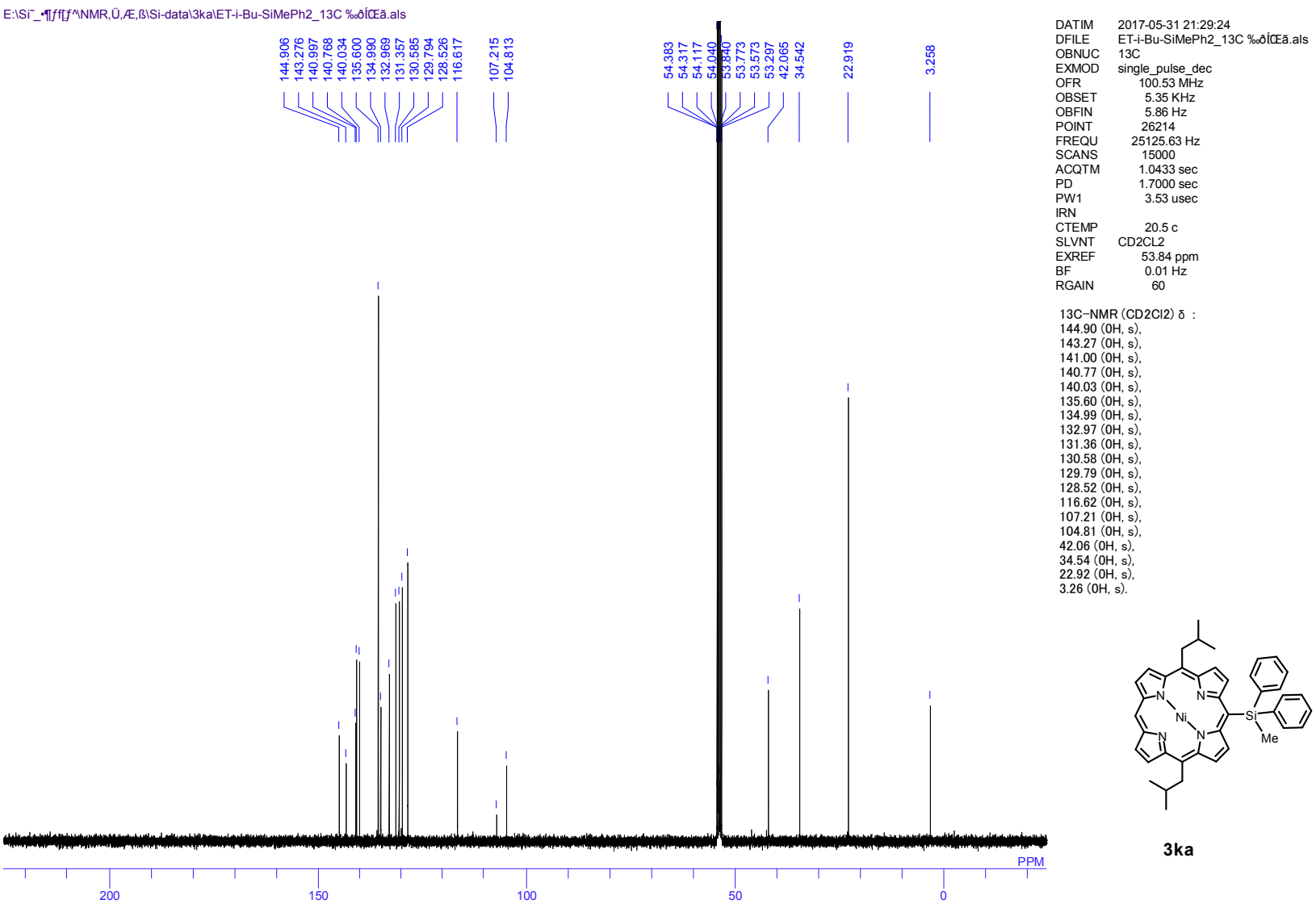
DATIM Tue May 02 12:10:11 2017
DFILE ET-i-Bu-Si-Ph2Me-1H ‰ðÍŒëã.als
OBNUC 1H
EXMOD NON
OFR 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.00 Hz
POINT 32768
FREQU 6006.01 Hz
SCANS 16
ACQTM 5.4559 sec
PD 1.5440 sec
PW1 5.60 usec
IRN
CTEMP 26.1 c
SLVNT CD2CL2
EXREF 5.32 ppm
BF 0.09 Hz
RGAIN 24

1H-NMR (CD2Cl2) δ :
9.55 (1H, s),
9.29 (2H, d, J = 4.95 Hz),
9.11 (2H, d, J = 4.95 Hz),
9.09 (2H, d, J = 4.95 Hz),
8.95 (2H, d, J = 4.95 Hz),
7.67 (4H, dd, J = 7.88, 1.47 Hz),
7.47−7.42 (2H, m),
7.38−7.33 (4H, m),
4.47 (4H, d, J = 7.15 Hz),
2.14−2.05 (2H, m),
1.21 (3H, s),
0.75 (12H, d, J = 6.60 Hz).



3ka

^{13}C NMR spectrum of 3ka

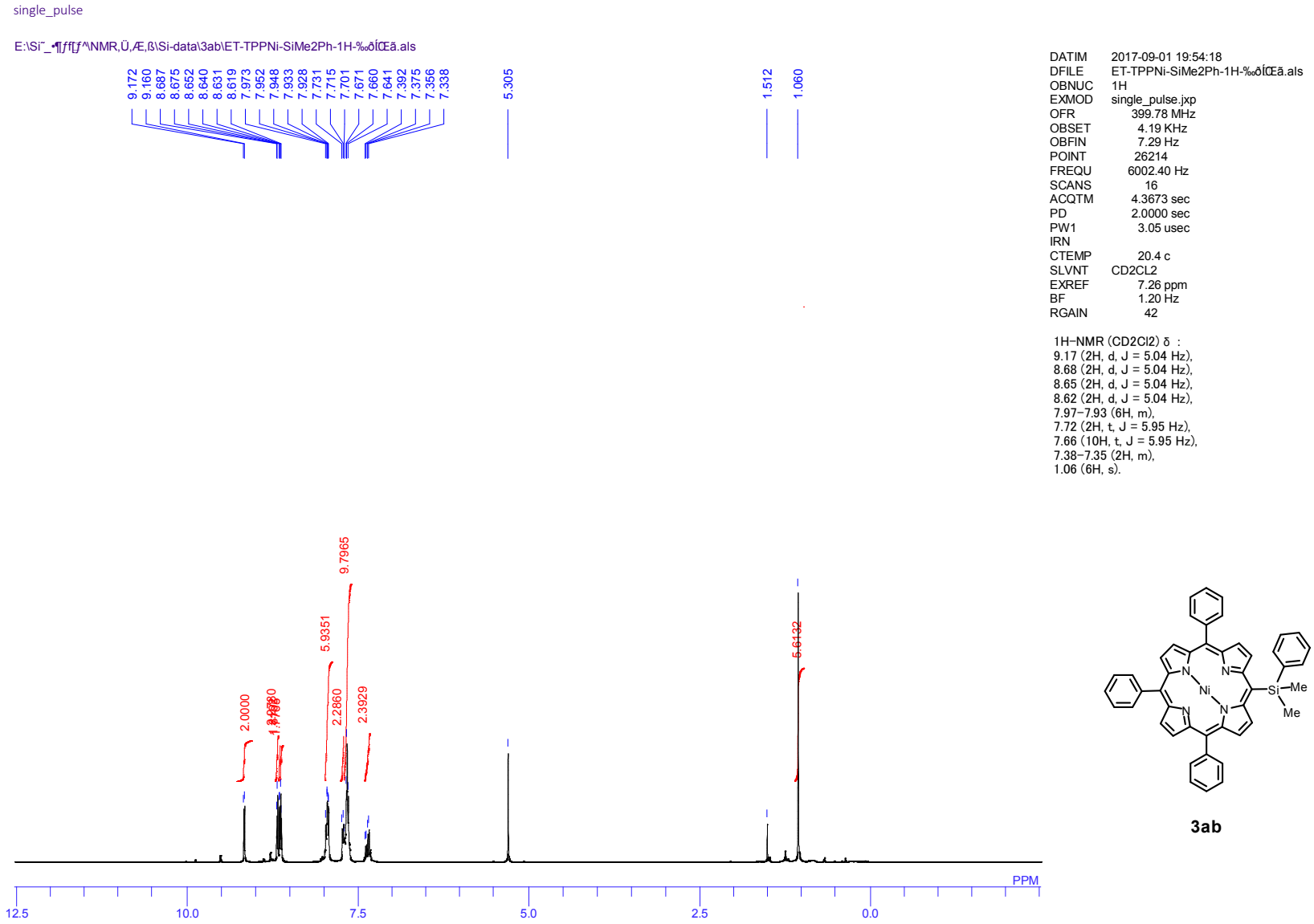


DATIM 2017-05-31 21:29:24
DFILE ET-i-Bu-SiMePh2_13C ‰ðÍŒËã.als
OBNUC 13C
EXMOD single_pulse_dec
OFR 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25125.63 Hz
SCANS 15000
ACQTM 1.0433 sec
PD 1.7000 sec
PW1 3.53 usec
IRN
CTEMP 20.5 c
SLVNT CD2CL2
EXREF 53.84 ppm
BF 0.01 Hz
RGAIN 60

13C-NMR (CD2Cl2) δ :
144.90 (0H, s),
143.27 (0H, s),
141.00 (0H, s),
140.77 (0H, s),
140.03 (0H, s),
135.60 (0H, s),
134.99 (0H, s),
132.97 (0H, s),
131.36 (0H, s),
130.58 (0H, s),
129.79 (0H, s),
128.52 (0H, s),
116.62 (0H, s),
107.21 (0H, s),
104.81 (0H, s),
42.06 (0H, s),
34.54 (0H, s),
22.92 (0H, s),
3.26 (0H, s).

3ka

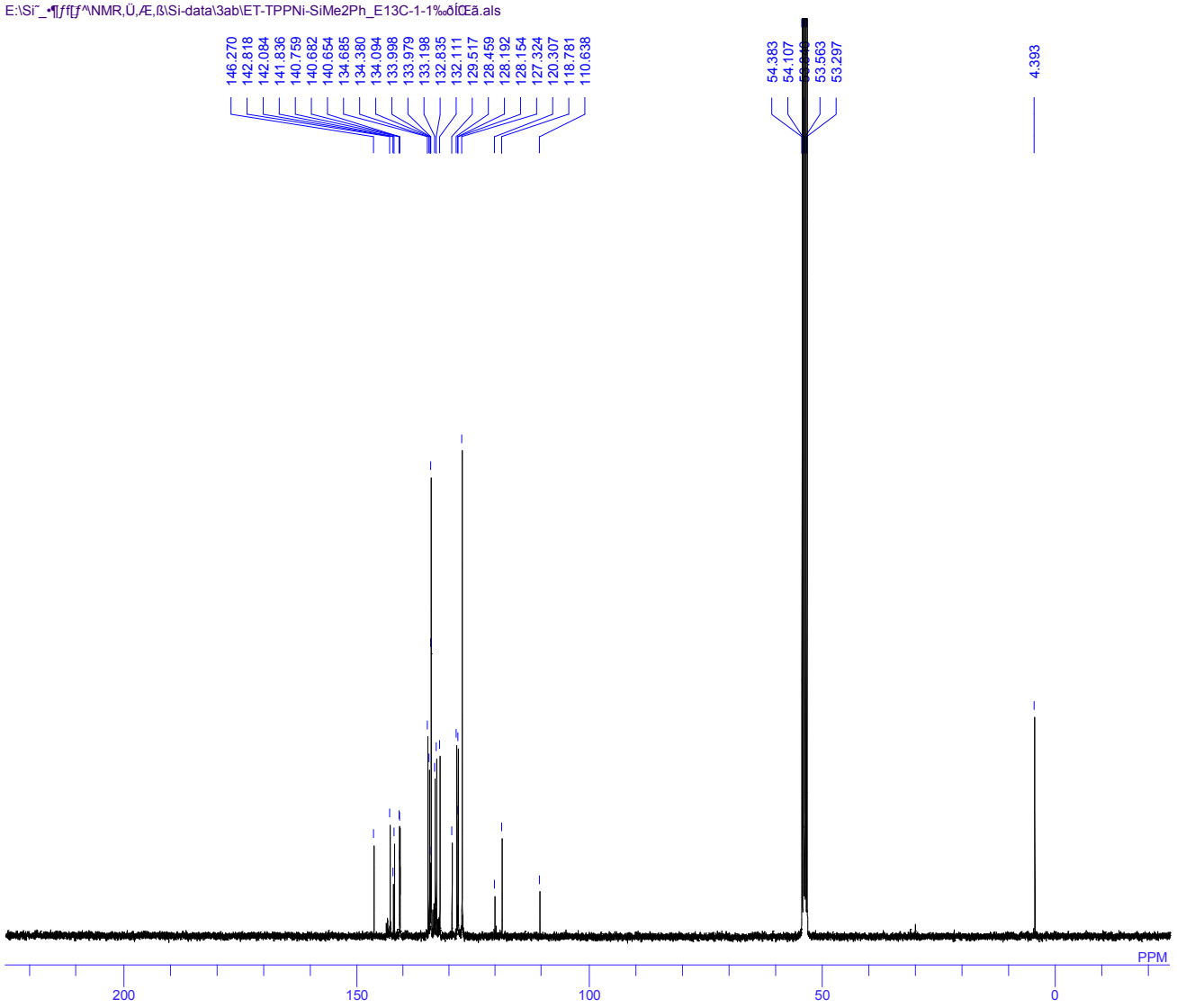
^{1}H NMR spectrum of 3ab



^{13}C NMR spectrum of 3ab

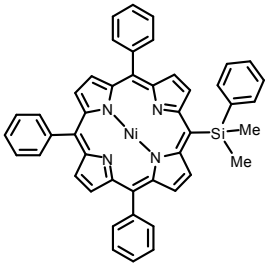
single pulse decoupled gated NOE

E:\Si¯_•¶ƒf[ƒ^\NMR,Ü,Æ,ß\Si-data\3ab\ET-TPPNi-SiMe2Ph_E13C-1-1‰ðÍŒÈã.als



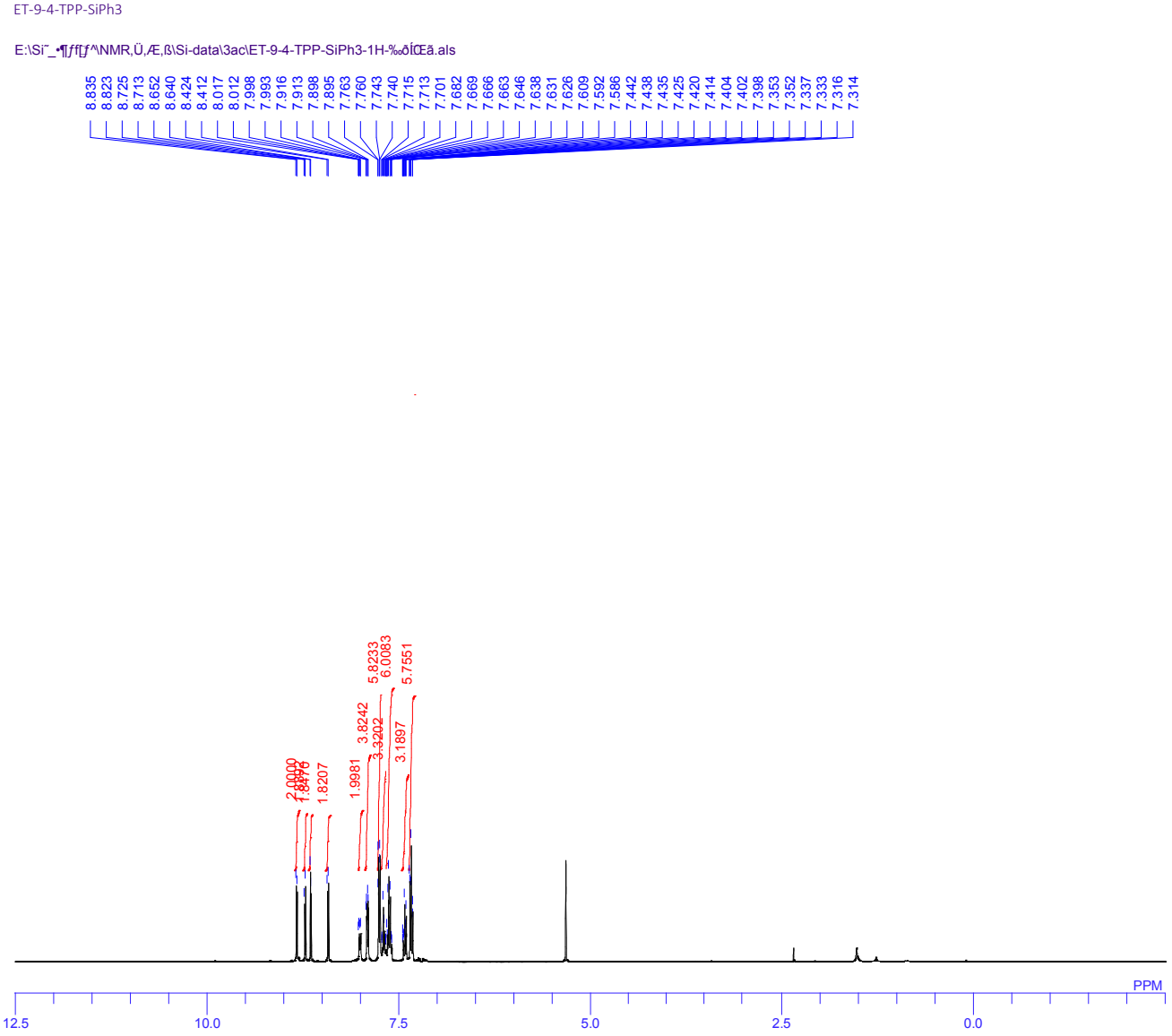
DATIM 2017-09-01 19:56:26
DFILE ET-TPPNi-SiMe2Ph_E13C-1-1‰ðÍŒÈã.als
OBNUC 13C
EXMOD single_pulse_dec
OFR 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25125.63 Hz
SCANS 17000
ACQTM 1.0433 sec
PD 1.7000 sec
PW1 3.53 usec
IRN
CTEMP 20.7 c
SLVNT CD2CL2
EXREF 53.84 ppm
BF 1.20 Hz
RGAIN 60

13C-NMR (CD2Cl2) δ :
146.27 (0H, s),
142.82 (0H, s),
142.08 (0H, s),
141.83 (0H, s),
140.76 (0H, s),
140.68 (0H, s),
140.65 (0H, s),
134.68 (0H, s),
134.38 (0H, s),
134.09 (0H, s),
134.00 (0H, s),
133.98 (0H, s),
133.20 (0H, s),
132.83 (0H, s),
132.11 (0H, s),
129.52 (0H, s),
128.46 (0H, s),
128.19 (0H, s),
128.15 (0H, s),
127.32 (0H, s),
120.31 (0H, s),
118.78 (0H, s),
110.64 (0H, s),
4.39 (0H, s).



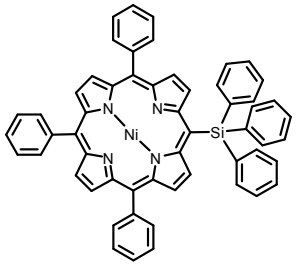
3ab

^{1}H NMR spectrum of 3ac



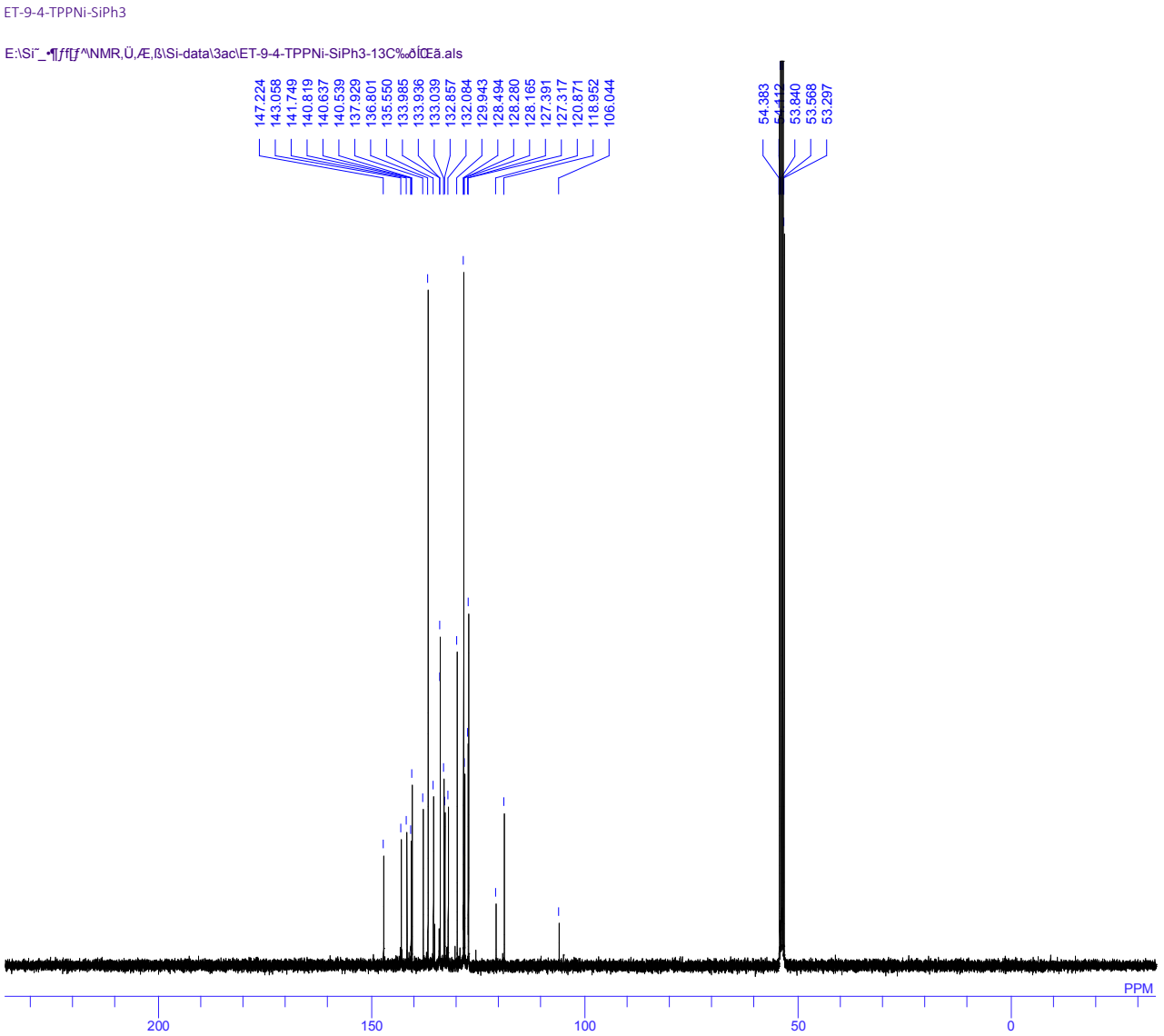
DATIM Wed Jul 12 20:34:12 2017
DFILE ET-9-4-TPP-SiPh3-1H-‰ðÍŒËã.als
OBNUC 1H
EXMOD NON
OFR 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
SCANS 16
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 5.60 usec
IRN
CTEMP 23.4 c
SLVNT CD2CL
EXREF 5.32 ppm
BF 0.09 Hz
RGAIN 18

1H-NMR (CD2Cl2) δ :
8.83 (2H, d, J = 4.88 Hz),
8.72 (2H, d, J = 4.88 Hz),
8.65 (2H, d, J = 4.88 Hz),
8.42 (2H, d, J = 4.88 Hz),
8.00 (2H, dd, J = 7.32, 1.95 Hz),
7.91 (4H, dd, J = 7.32, 1.46 Hz),
7.75 (6H, dd, J = 8.05, 1.22 Hz),
7.72−7.66 (3H, m),
7.65−7.59 (6H, m),
7.43−7.41 (3H, m),
7.35−7.32 (6H, m).



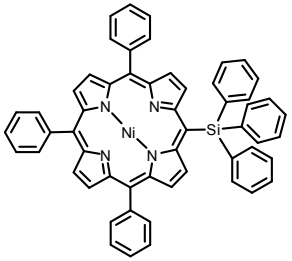
3ac

^{13}C NMR spectrum of 3ac



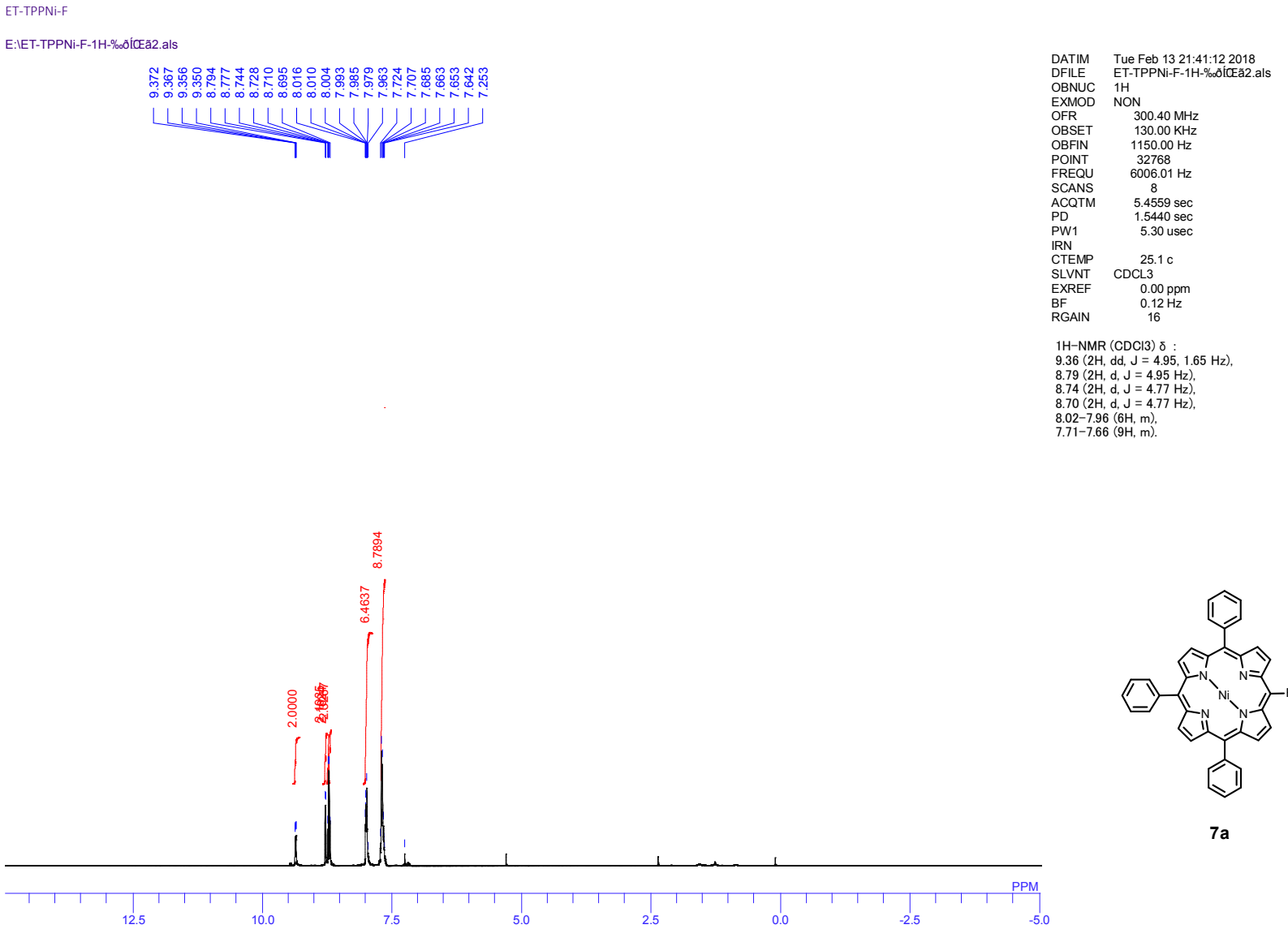
DATIM Wed Jul 26 09:26:31 2017
DFILE ET-9-4-TPPNi-SiPh3-13C‰ðÍŒÈã.als
OBNUC 13C
EXMOD BCM
OFR 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 27118.64 Hz
SCANS 14500
ACQTM 1.2083 sec
PD 1.7920 sec
PW1 5.80 usec
IRN
CTEMP 24.4 c
SLVNT CD2CL
EXREF 53.84 ppm
BF 0.09 Hz
RGAIN 25

13C-NMR (CD2Cl2) δ :
147.22 (0H, s),
143.06 (0H, s),
141.75 (0H, s),
140.82 (0H, s),
140.64 (0H, s),
140.54 (0H, s),
137.93 (0H, s),
136.80 (0H, s),
135.55 (0H, s),
133.99 (0H, s),
133.94 (0H, s),
133.04 (0H, s),
132.86 (0H, s),
132.08 (0H, s),
129.94 (0H, s),
128.49 (0H, s),
128.28 (0H, s),
128.16 (0H, s),
127.39 (0H, s),
127.32 (0H, s),
120.86 (0H, s),
118.95 (0H, s),
106.04 (0H, s).

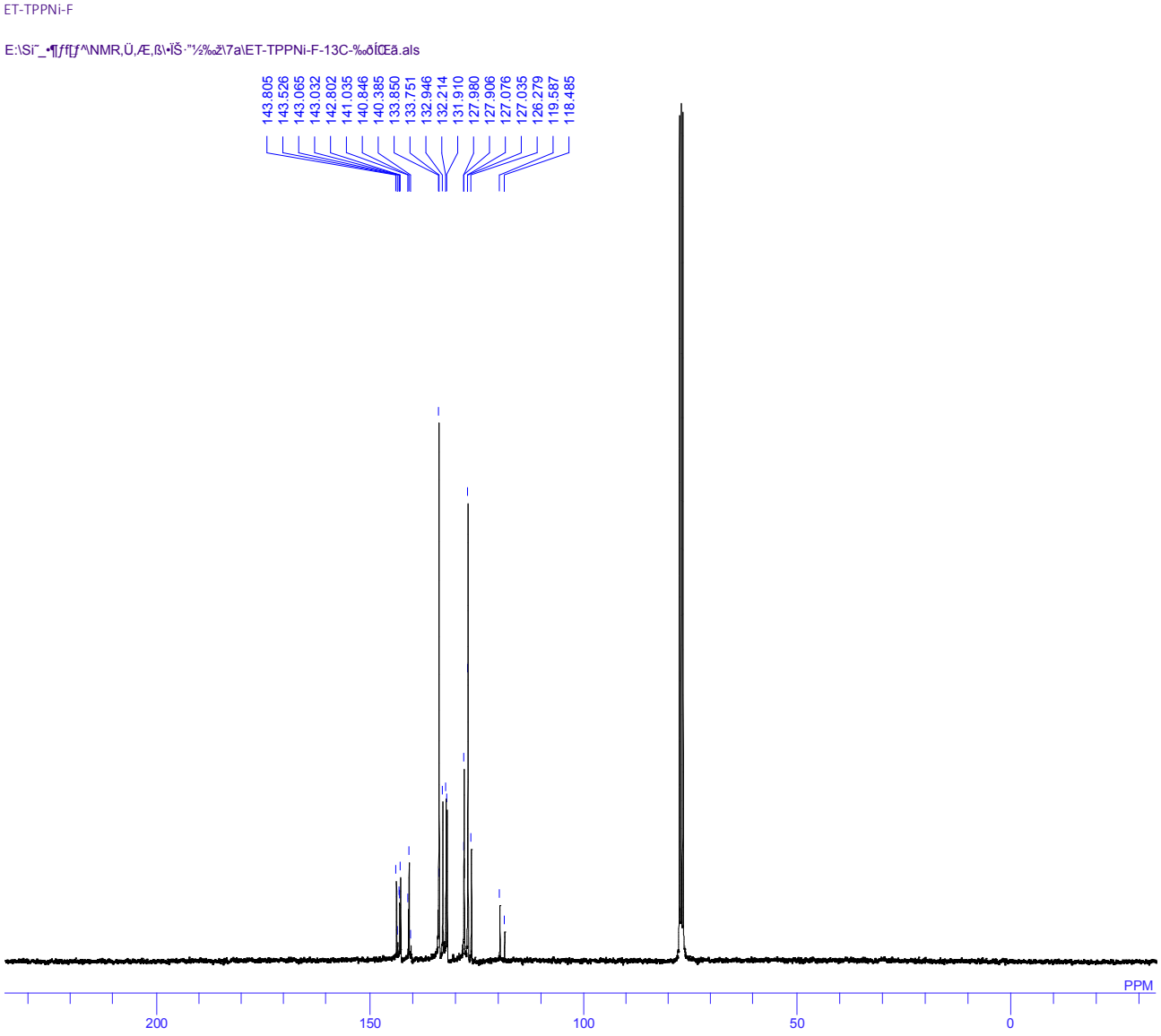


3ac

^{1}H NMR spectrum of 7a

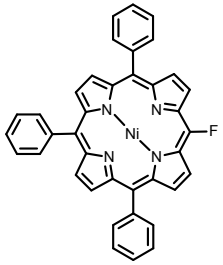


^{13}C NMR spectrum of 7a



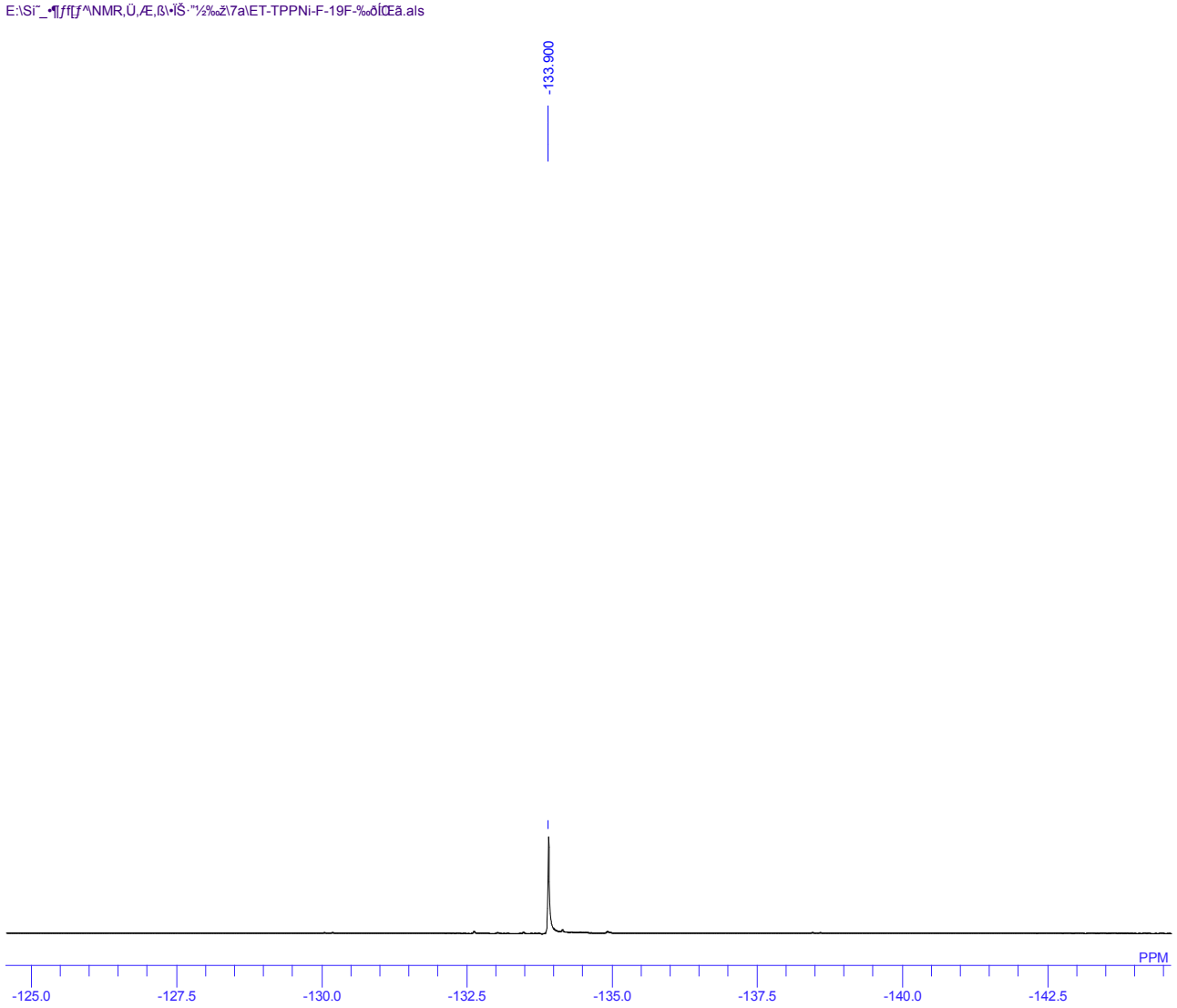
DATIM Wed Feb 14 08:28:13 2018
DFILE ET-TPPNi-F-13C-‰ðÍŒã.als
OBNUC 13C
EXMOD BCM
OFR 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.00 Hz
POINT 32768
FREQU 20356.23 Hz
SCANS 12928
ACQTM 1.6097 sec
PD 1.3900 sec
PW1 4.30 usec
IRN
CTEMP 23.5 c
SLVNT CDCL3
EXREF 77.16 ppm
BF 3.00 Hz
RGAIN 25

13C-NMR (CDCl3) δ :
143.81 (0H, s),
143.07 (0H, s),
143.03 (0H, s),
142.80 (0H, s),
141.96 (0H, d, J = 237.31 Hz),
141.03 (0H, s),
140.85 (0H, s),
133.85 (0H, s),
133.75 (0H, s),
132.95 (0H, s),
132.21 (0H, s),
131.91 (0H, s),
127.98 (0H, s),
127.91 (0H, s),
127.08 (0H, s),
127.03 (0H, s),
126.28 (0H, s),
119.59 (0H, s),
118.49 (0H, s).



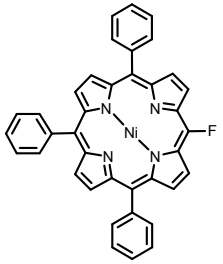
7a

^{19}F NMR spectrum of 7a



DATIM 2018-02-14 19:25:31
DFILE ET-TPPNi-F-19F-‰ôÍŒÈã.als
OBNUC 19F
EXMOD single_pulse.jxp
OFR 376.13 MHz
OBSET 3.43 KHz
OBFIN 6.82 Hz
POINT 13107
FREQU 37878.79 Hz
SCANS 16
ACQTM 0.3460 sec
PD 5.0000 sec
PW1 3.76 usec
IRN
CTEMP 21.0 c
SLVNT CDCL3
EXREF -133.90 ppm
BF 3.72 Hz
RGAIN 46

19F-NMR (CDCl3) δ :
−133.90 (0H, s).



7a