Supporting Information

Repetitive Two-Step Method for *o,o,p*- and *o,p*-Oligophenylene Synthesis through Pd-Catalyzed Cross-Coupling of Hydroxyterphenylboronic Acid

Miyuki Yamaguchi, Takeshi Kimura, Naomi Shinohara, and Kei Manabe *

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HPLC Charts

For compounds that showed complicated NMR spectra due to the presence of rotamers, HPLC analysis was performed to confirm their purity.

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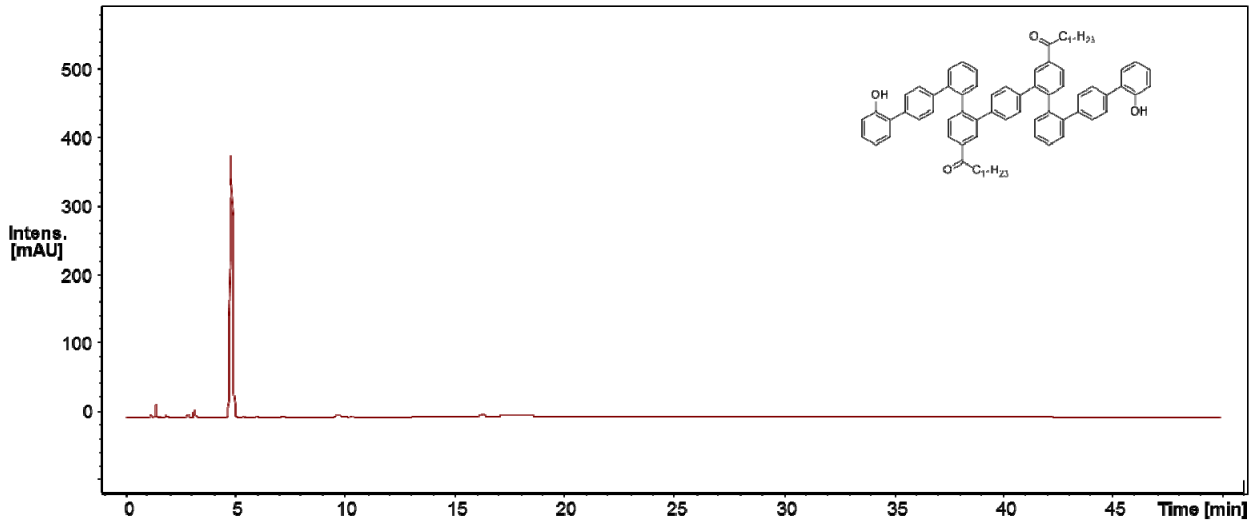
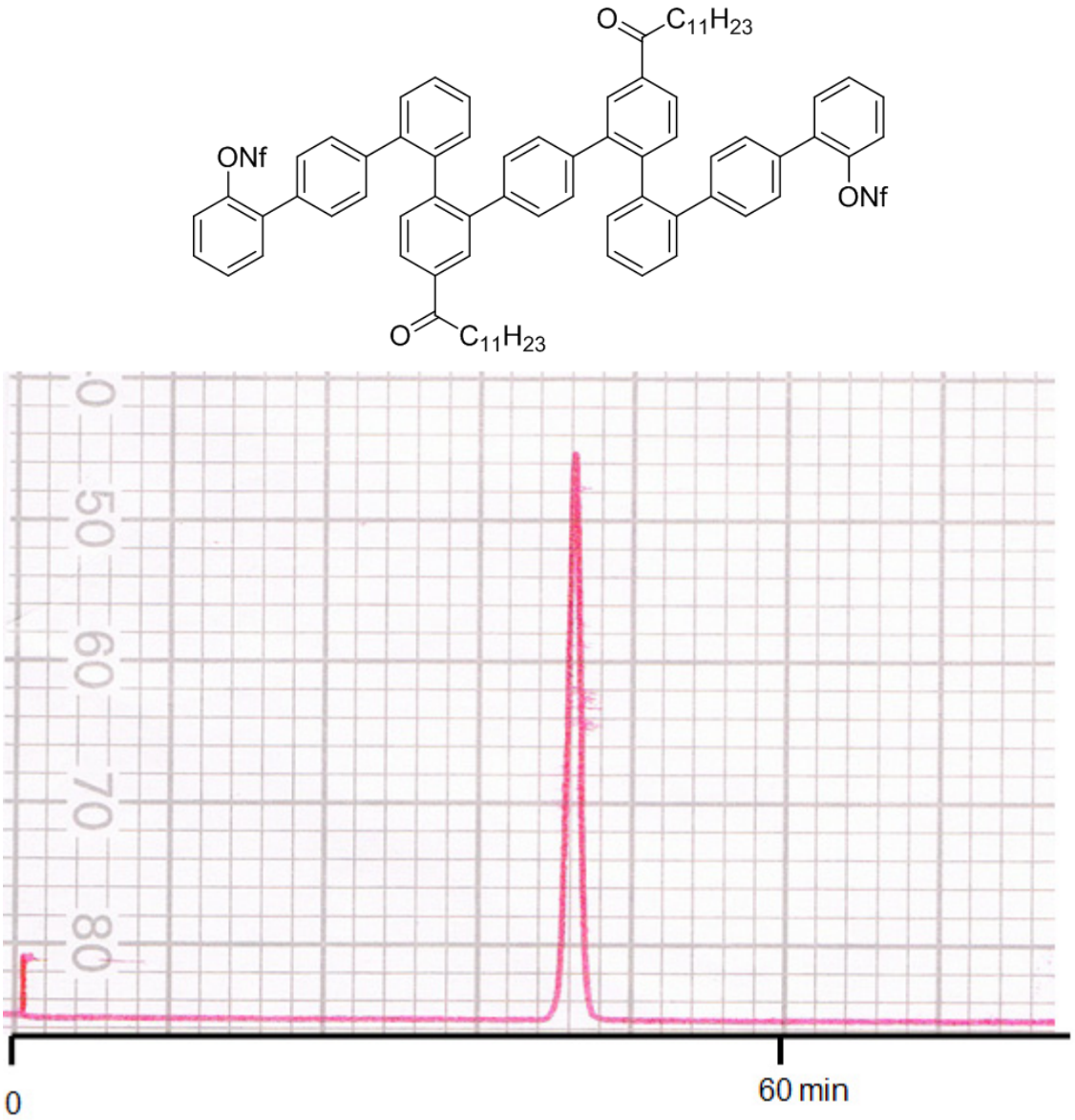


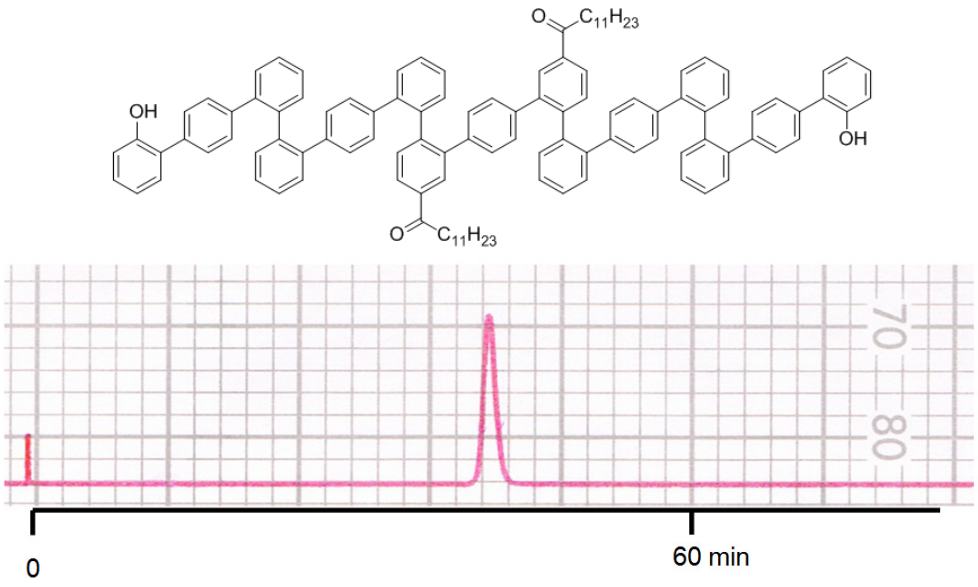
【HPLC method】
Analysis equipment: Agilent Technologies 1200 series
Column: Eclipse XDB-C18 (4.6 × 150mm)
Solvent A: 10% CH_3COONH_3aq, Solvent B : CH_3CN
Gradient (B): 0-15 min, 20 %, 15-40 min, 20-5 %, 40-40.1min, 5-20%
Oven column: 40℃
Injection: 10μl
Flow rate: 0.8mL/min
Detection: 254nm

6



[HPLC method] (gel permeation chromatography)
Analysis equipment: LC-9201 (Japan Analytical Industry)
Column: JALGEL-1H, 2H
Solvent: $CHCl_3$
Flow rate: 3.5 mL/min
Detection: 254 nm

7



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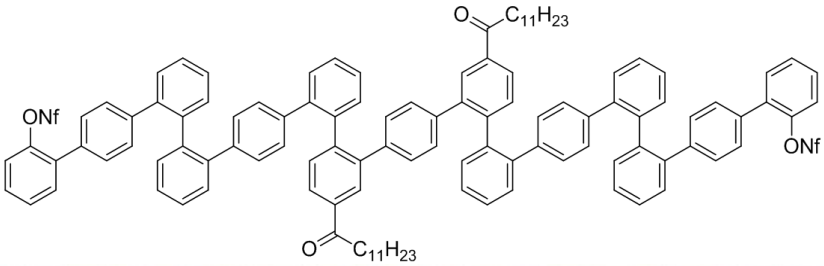

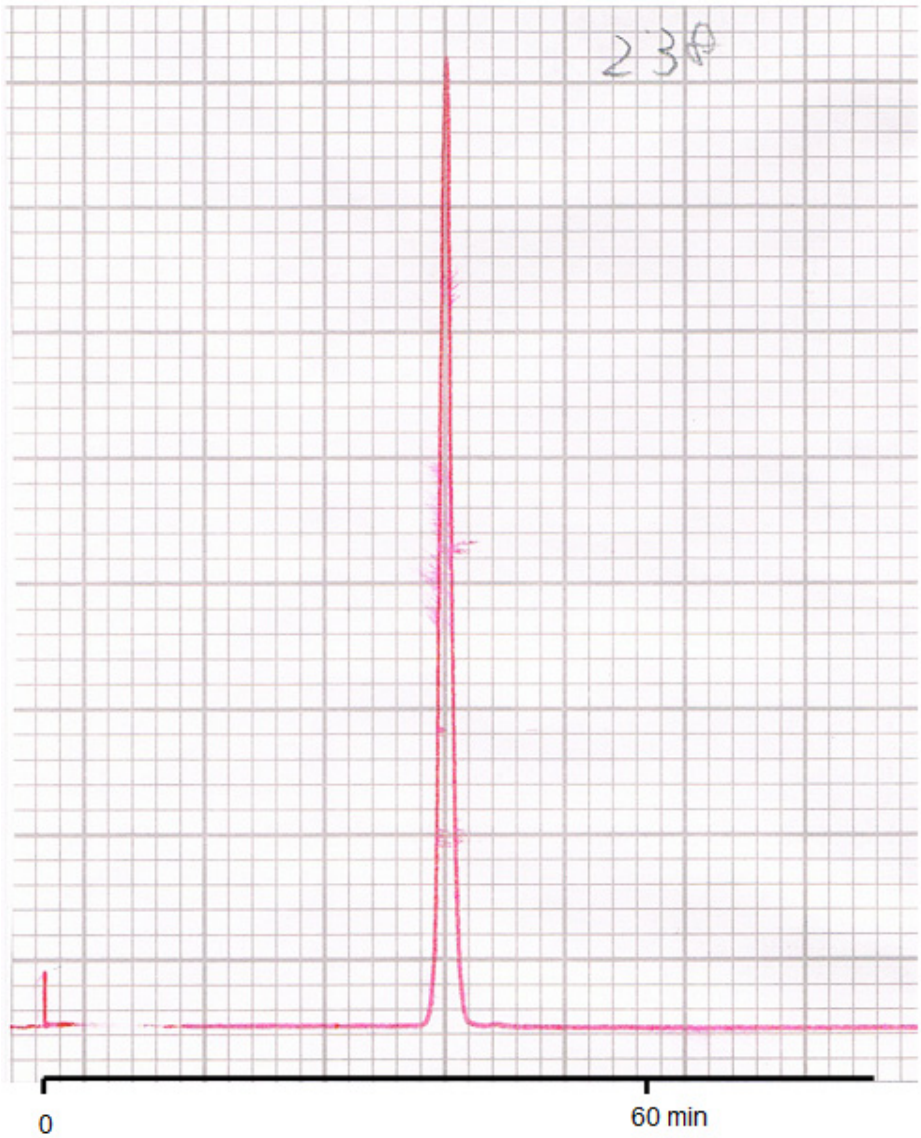

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Column: JALGEL-1H, 2H
Solvent: $CHCl_3$
Flow rate: 3.5 mL/min
Detection: 254 nm

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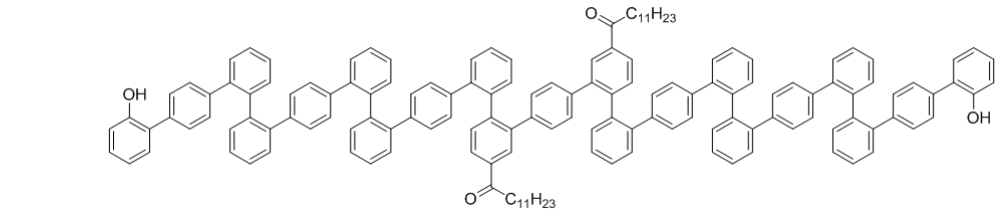

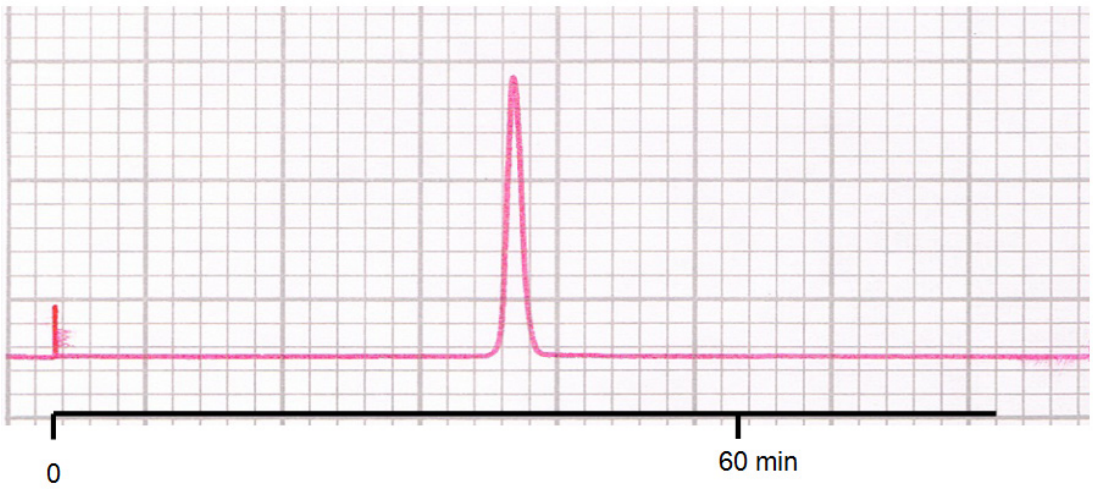

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Solvent: $CHCl_3$
Flow rate: 3.5 mL/min
Detection: 254 nm

NMR Spectra

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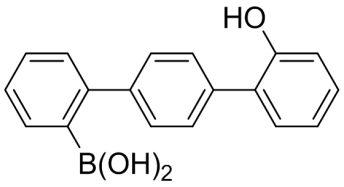

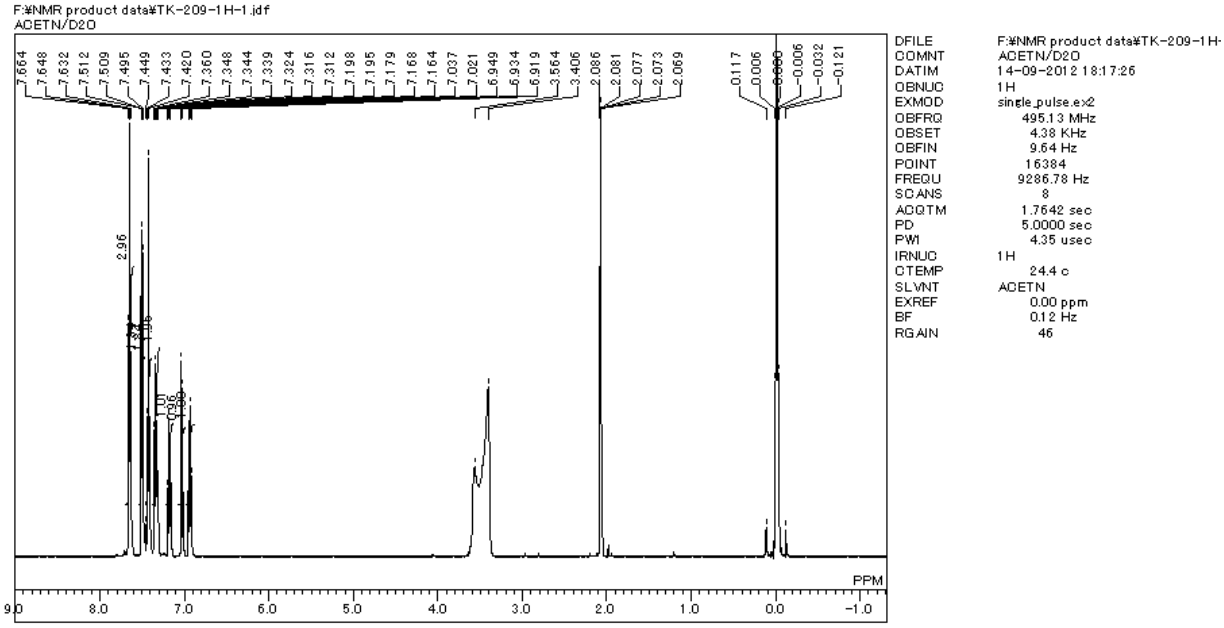

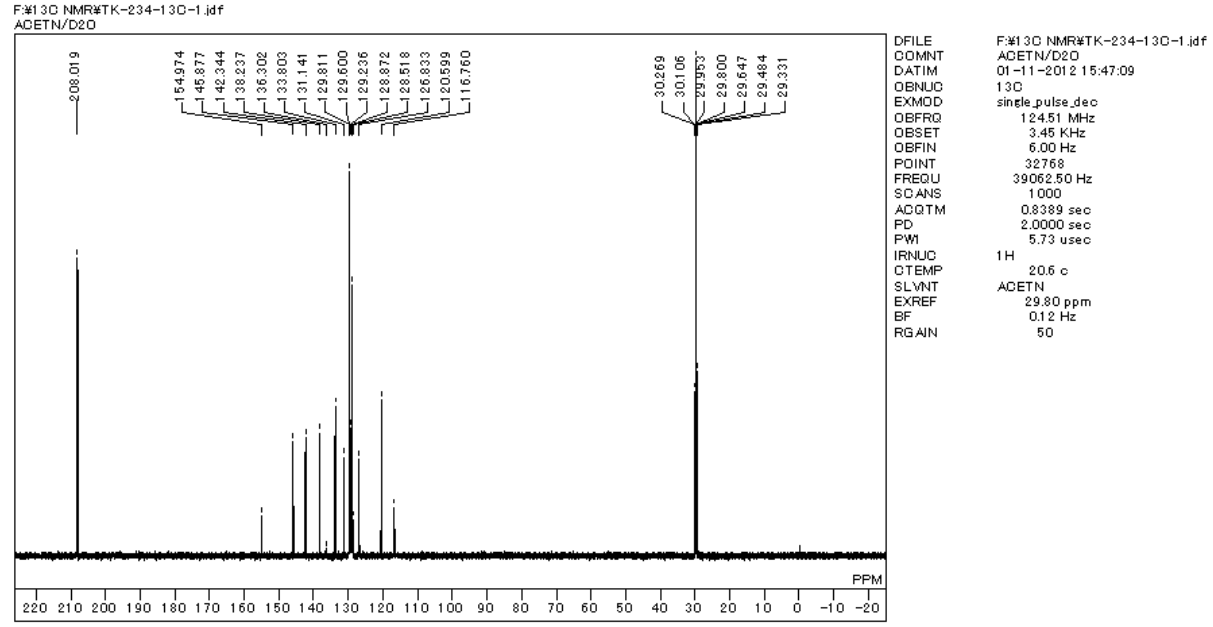

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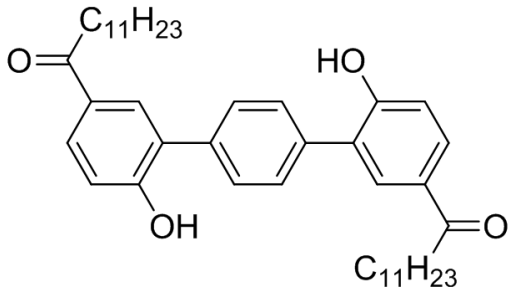
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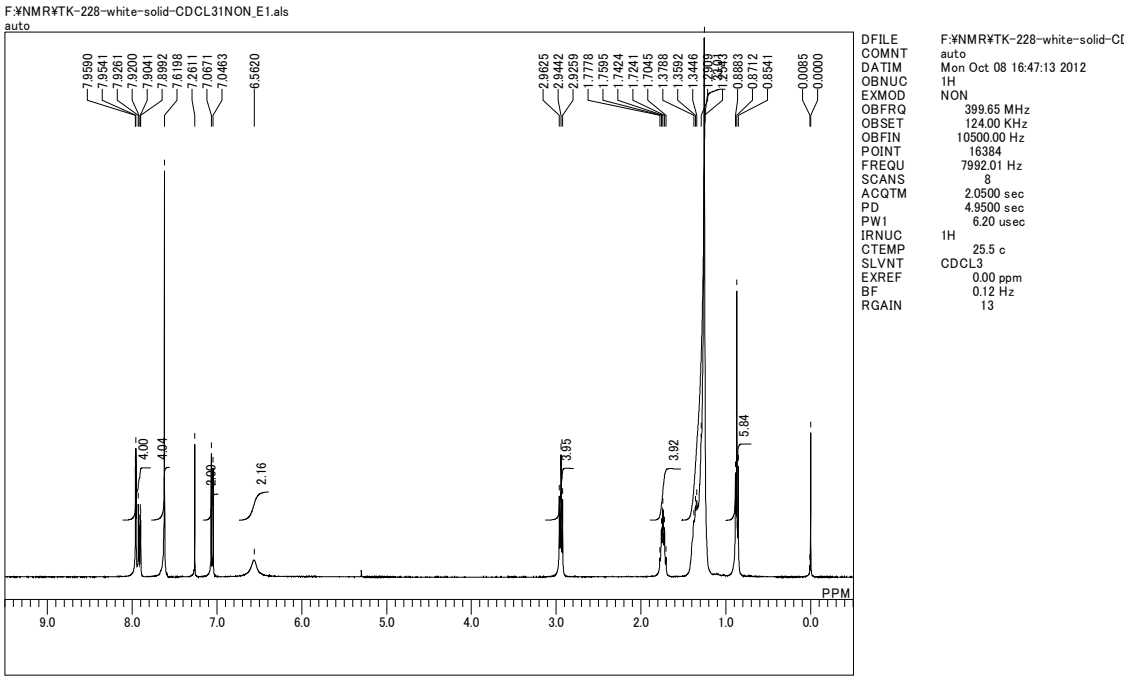
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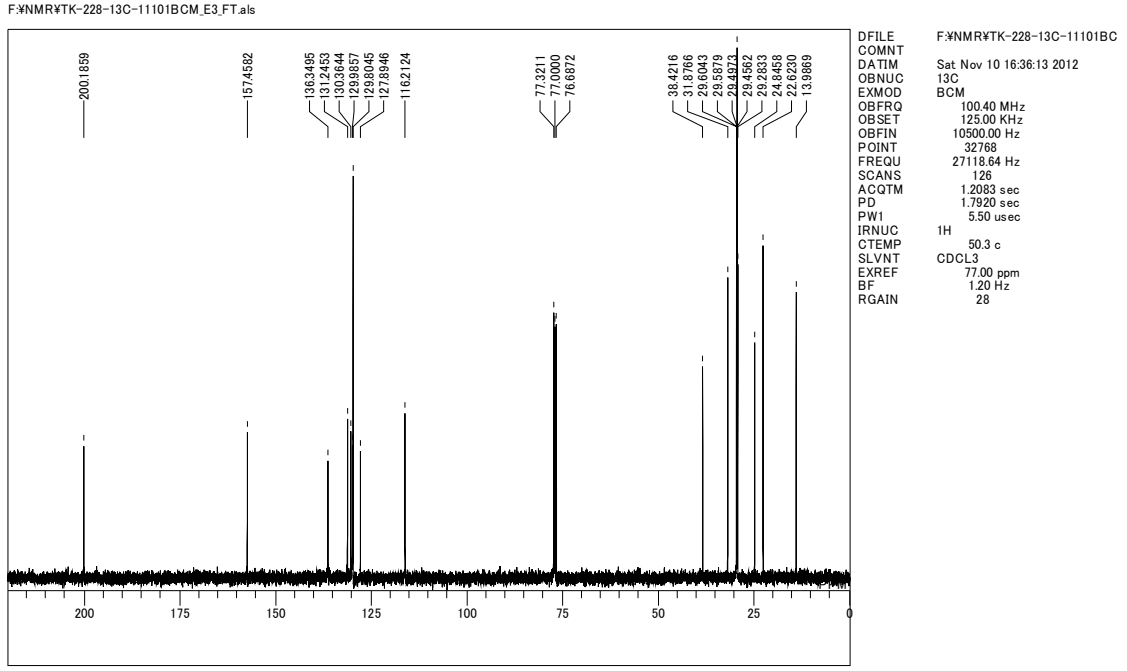
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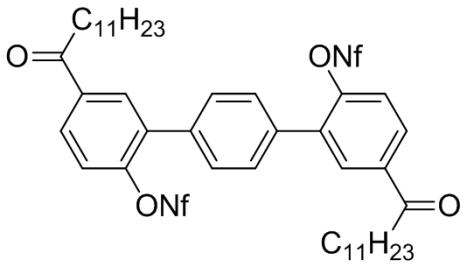
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O
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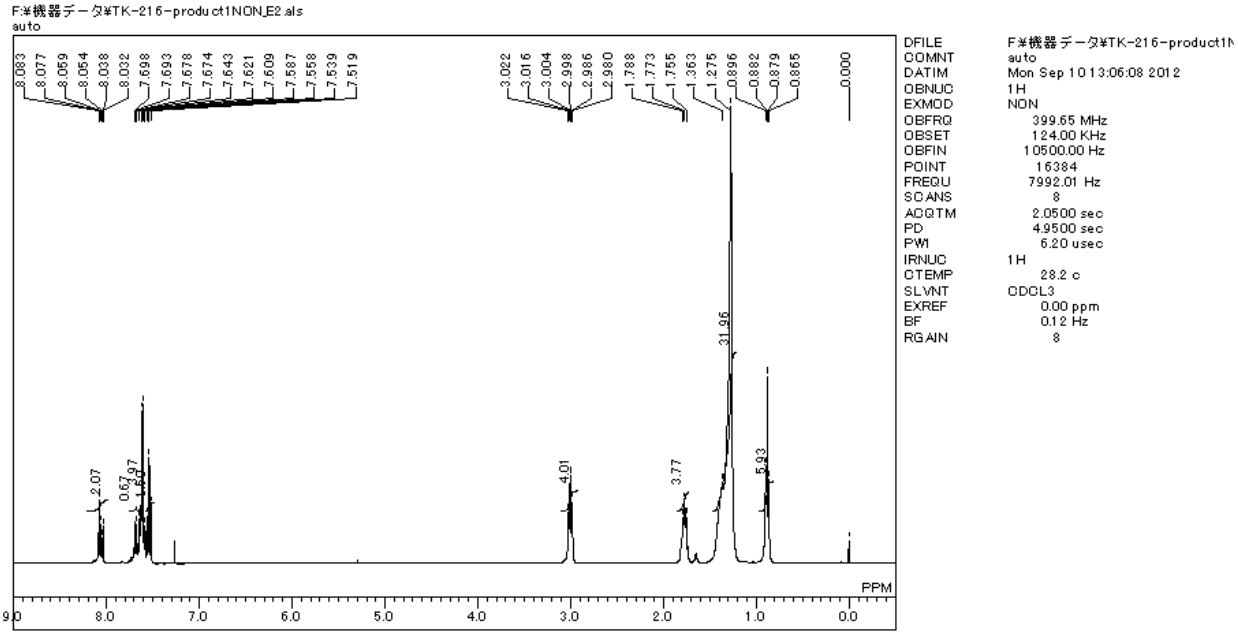
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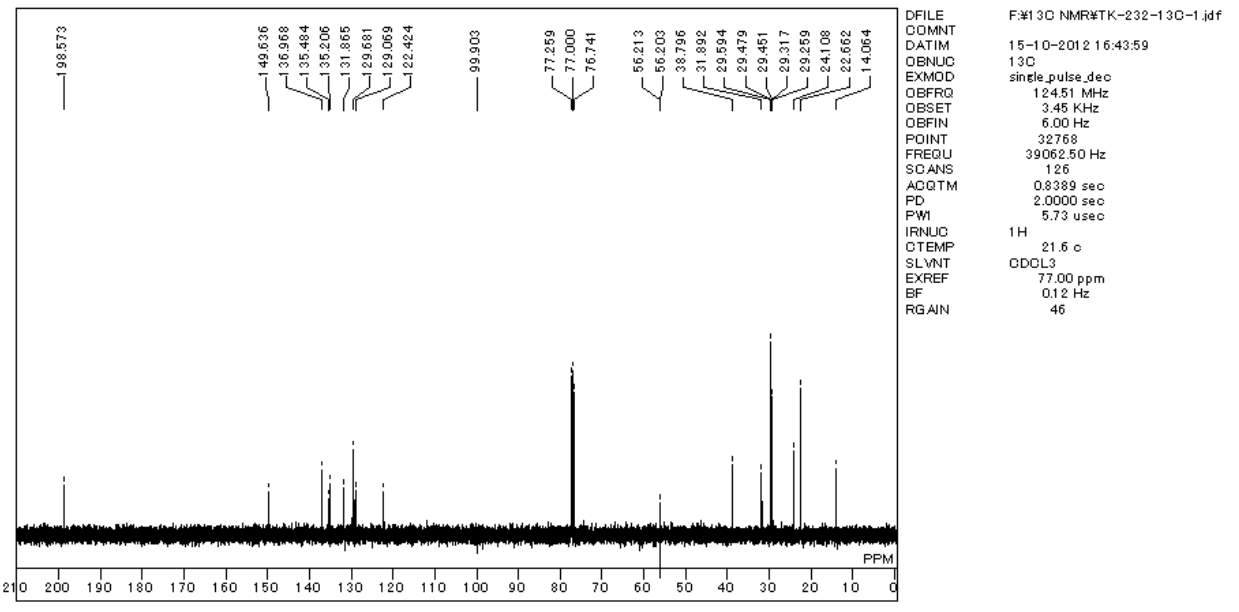
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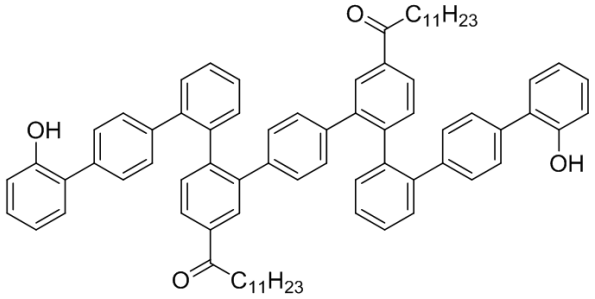

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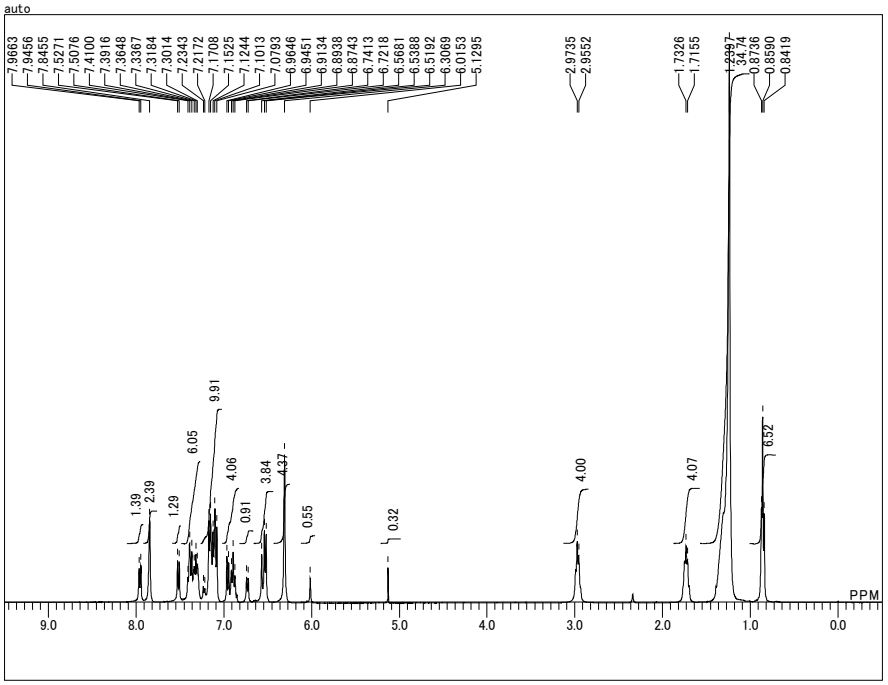

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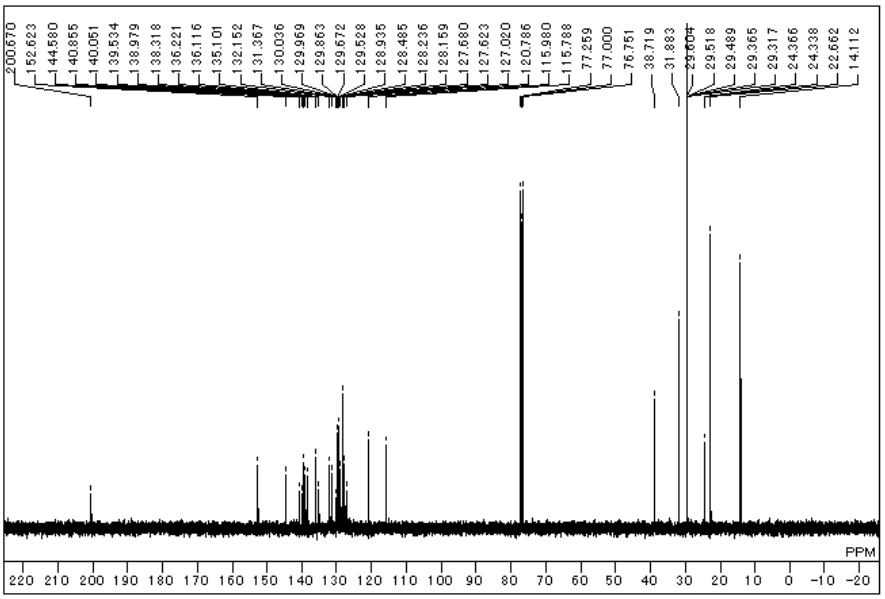

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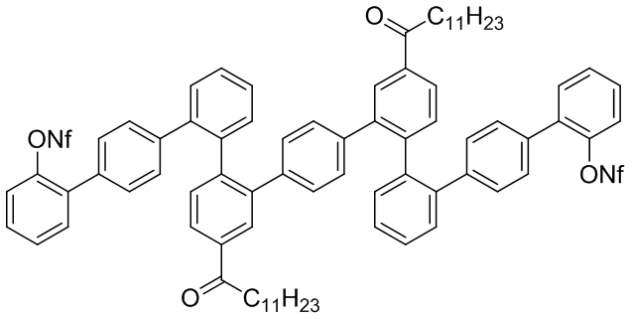

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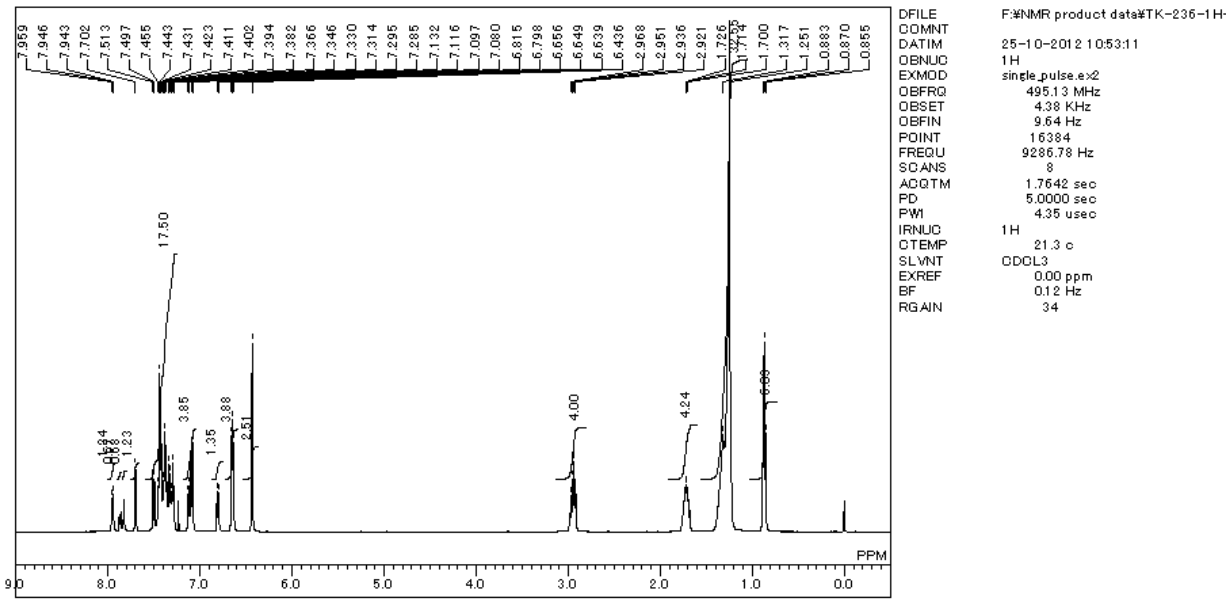

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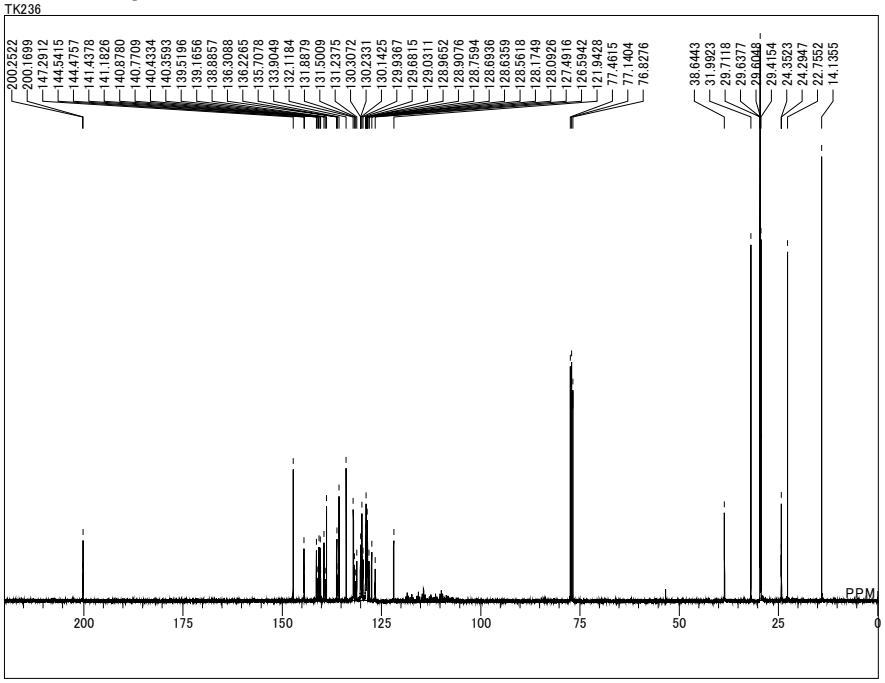

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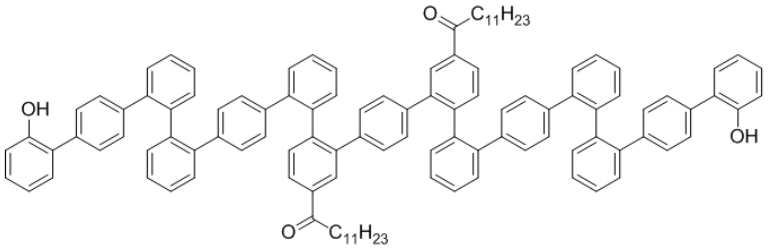
7



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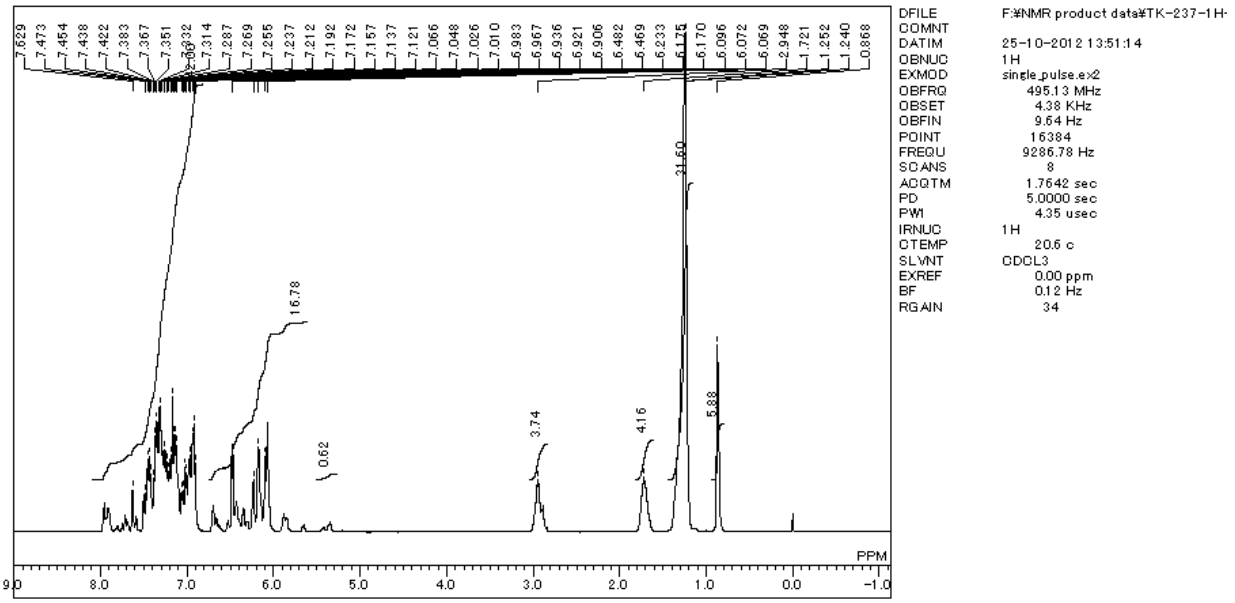

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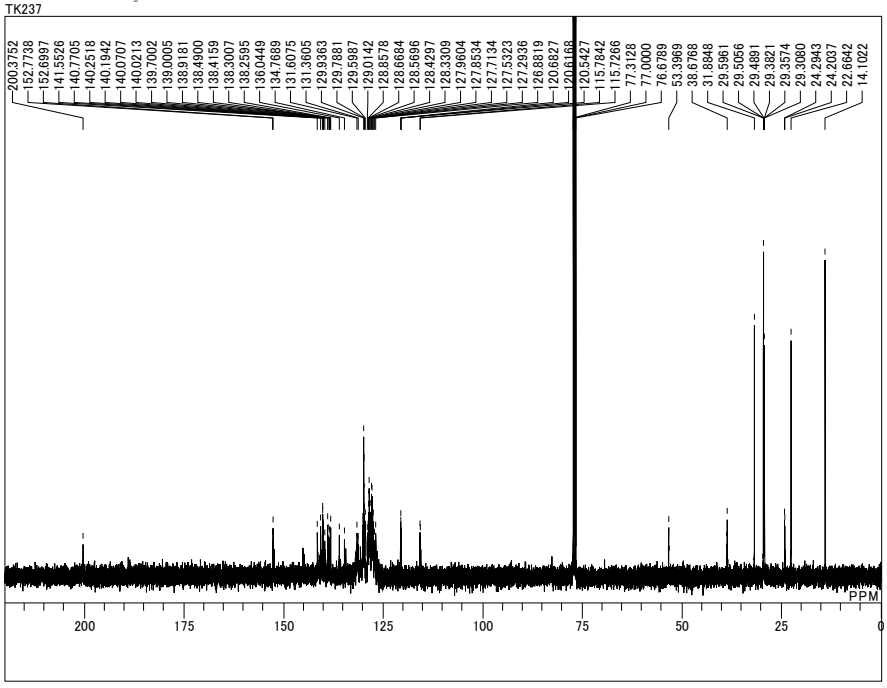

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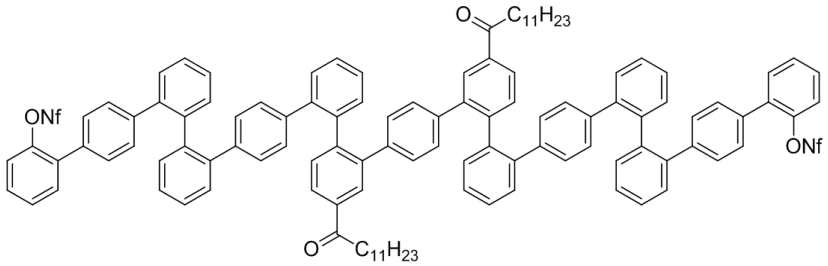
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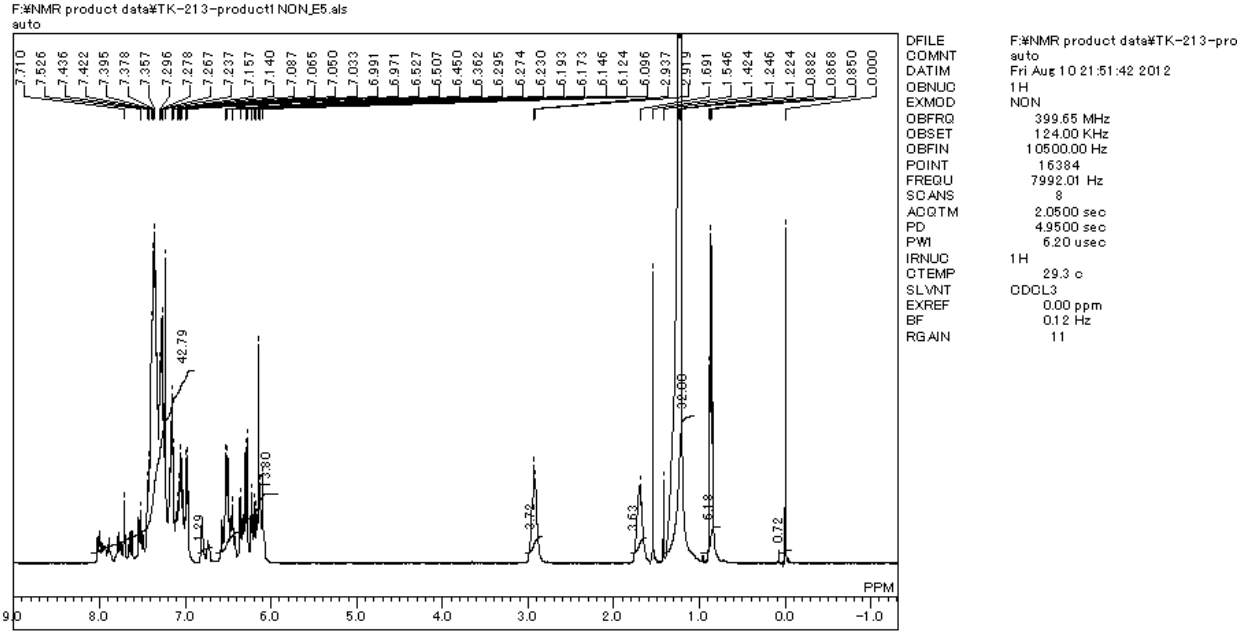
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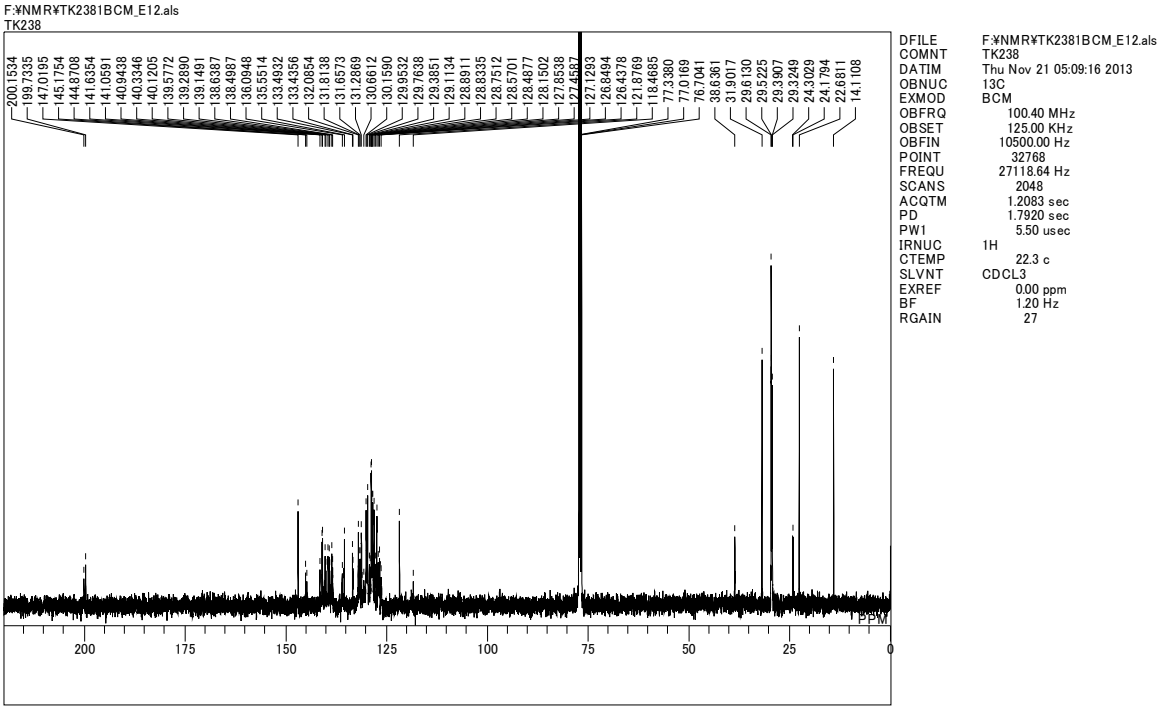
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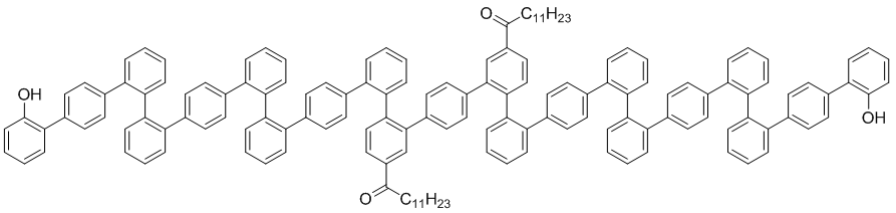
PPM

9



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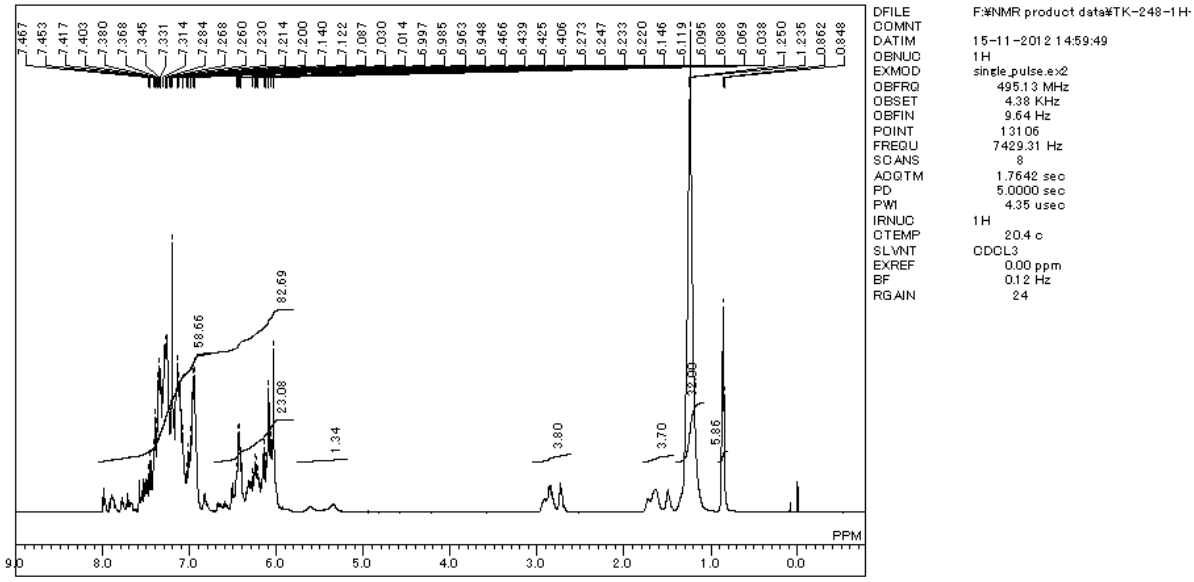

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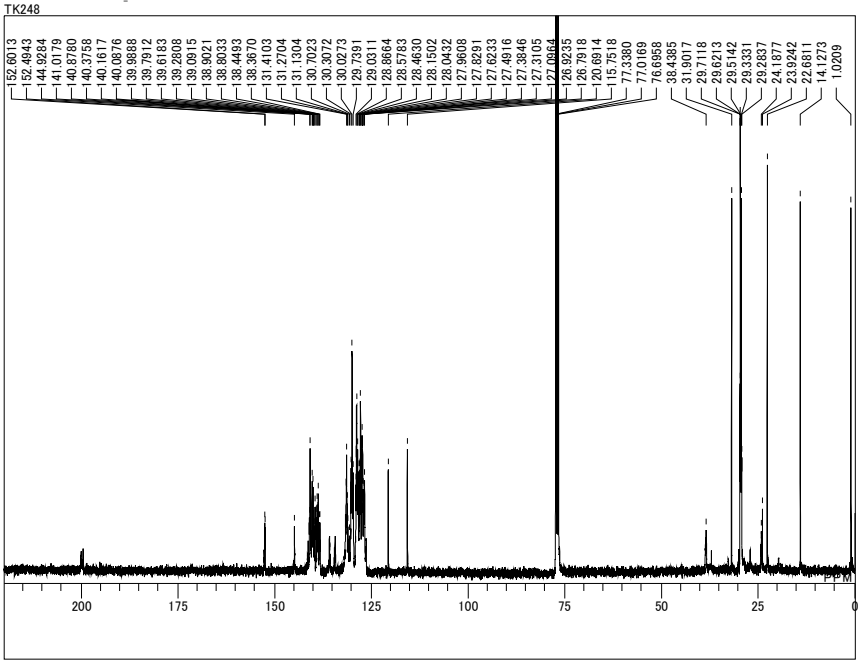

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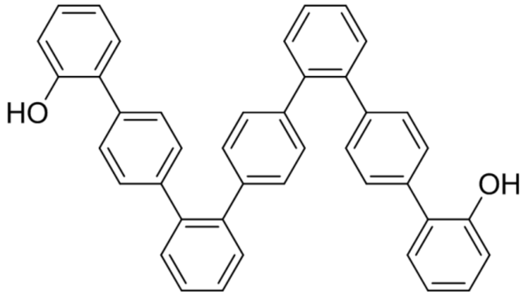
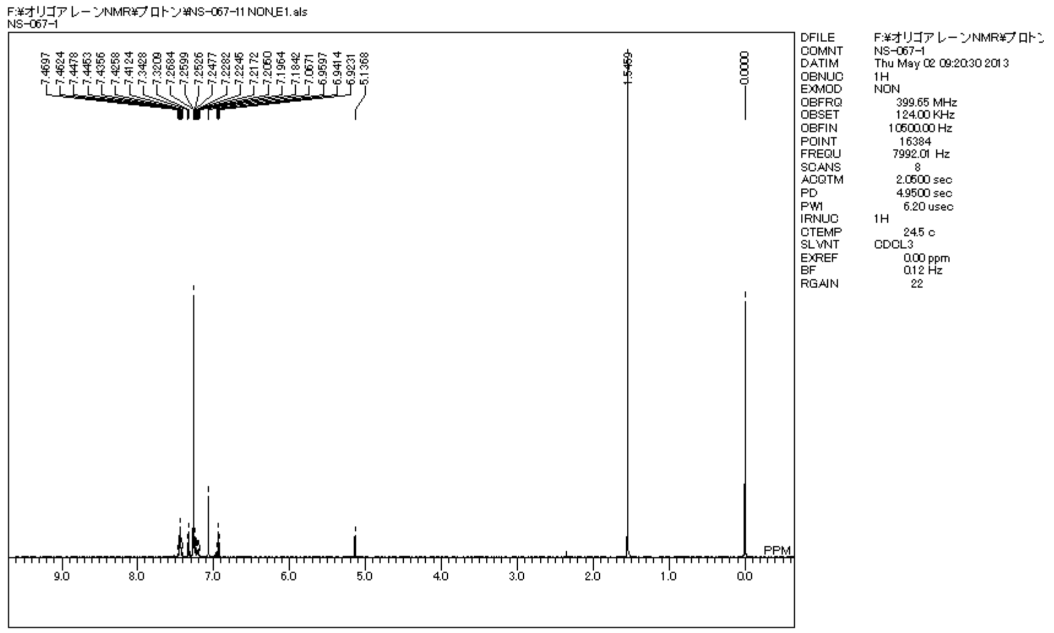
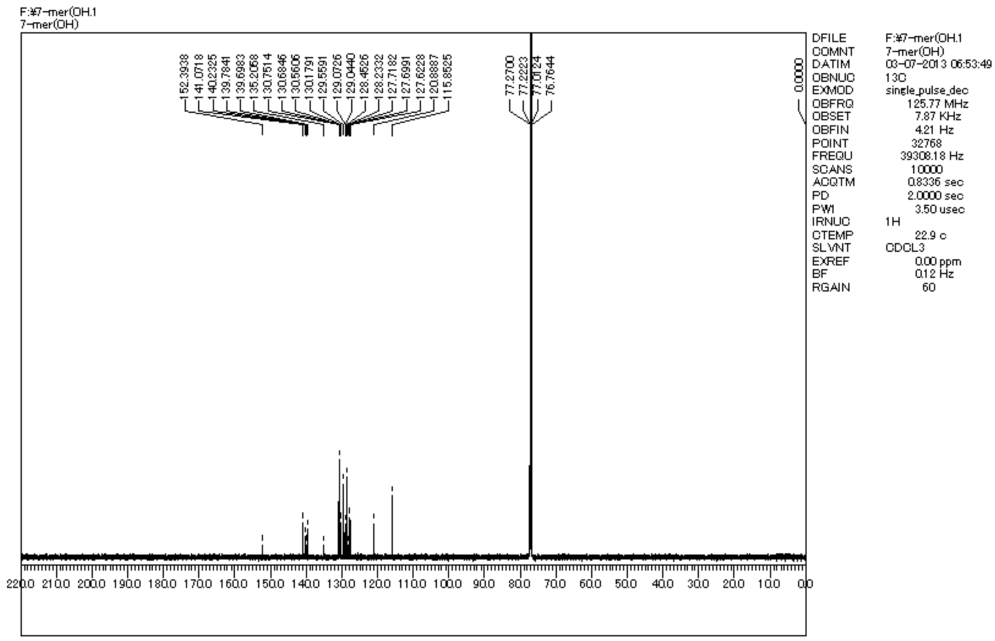
SCANS	10000
ACQTM	1.2083 sec
PD	1.7920 sec
PW1	5.50 usec
IRNUC	1H
CTEMP	22.4 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	1.20 Hz
RGAIN	27

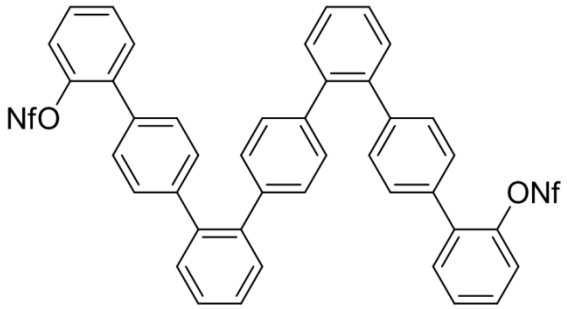
10

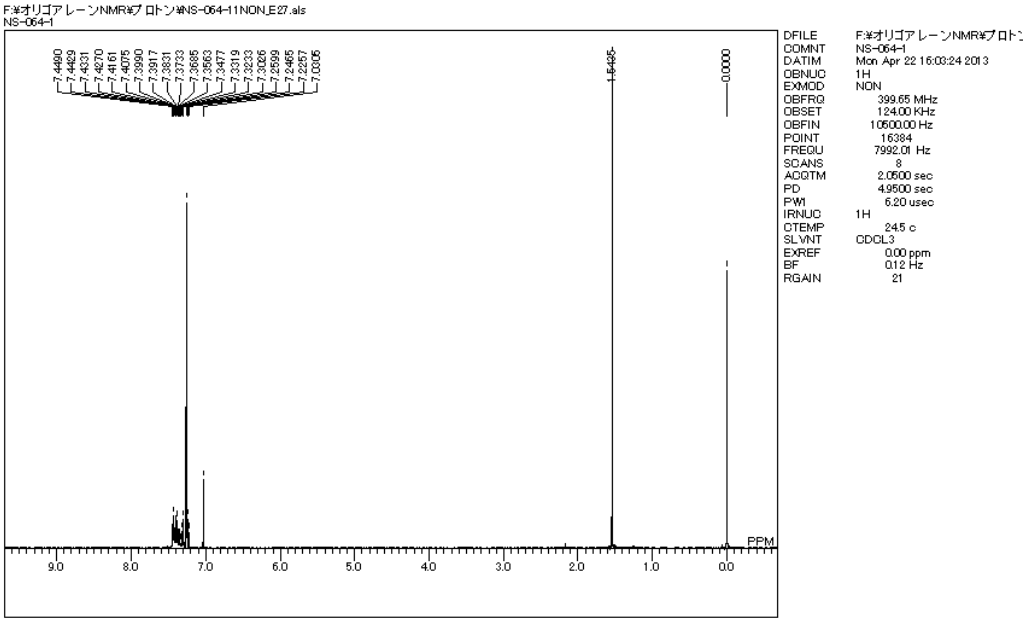

HO
OH

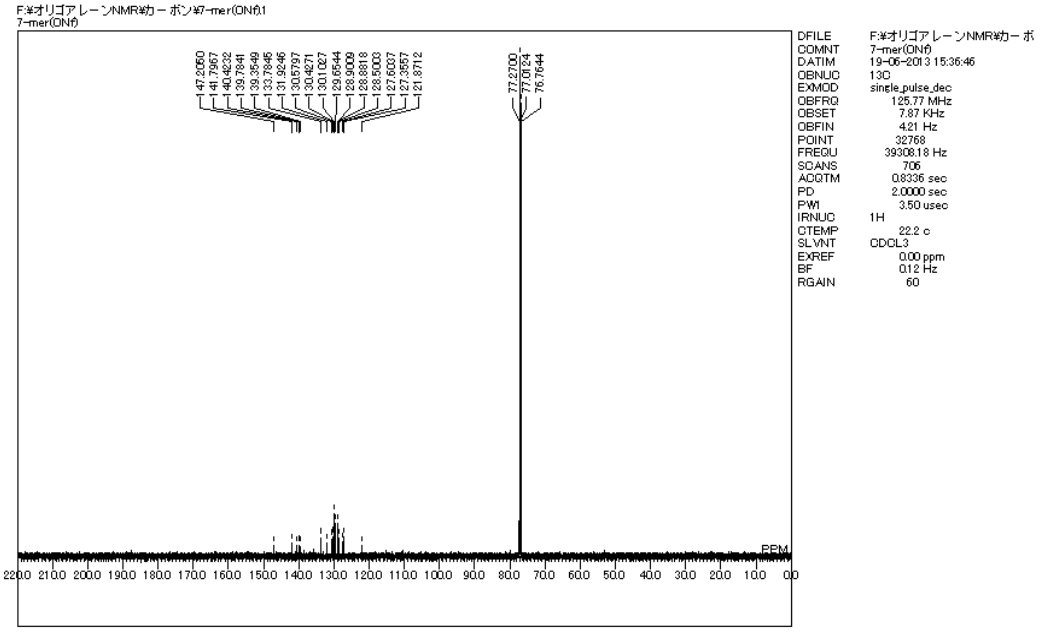

F:¥オリゴアレーンNMR¥プロトン¥NS-067-11 NON_E1.als
NS-067-1
7.4697 7.4624 7.4478 7.4453 7.4356 7.4258 7.4124 7.3428 7.3209 7.2684 7.2599 7.2526 7.2477 7.2282 7.2245 7.2172 7.2050 7.1964 7.1842 7.0671 6.9597 6.9414 6.9231 5.1368
1.5459
0.0000
PPM
9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
DFILE F:¥オリゴアレーンNMR¥プロトン
COMNT NS-067-1
DATIM Thu May 02 09:20:30 2013
OBNUC 1H
EXMOD NON
OBFRQ 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 6.20 usec
IRNUC 1H
CTEMP 24.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 22


F:¥7-mer(OH.1
7-mer(OH)
152.3938 141.0718 140.2325 139.7841 139.6983 135.2058 130.7514 130.6846 130.5606 130.1791 129.5591 129.0726 129.0440 128.4626 128.2332 127.7182 127.6991 127.6228 120.8887 115.8525
77.2700 77.2223 77.0124 76.7644
0.0000
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0.0
DFILE F:¥7-mer(OH.1
COMNT 7-mer(OH)
DATIM 03-07-2013 06:53:49
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 125.77 MHz
OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 32768
FREQU 39308.18 Hz
SCANS 10000
ACQTM 0.8336 sec
PD 2.0000 sec
PW1 3.50 usec
IRNUC 1H
CTEMP 22.9 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 60

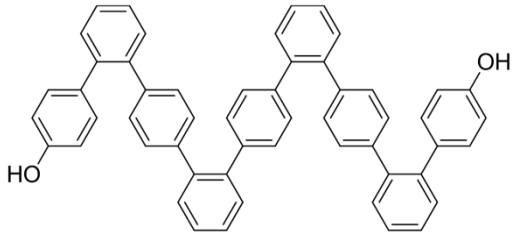
11

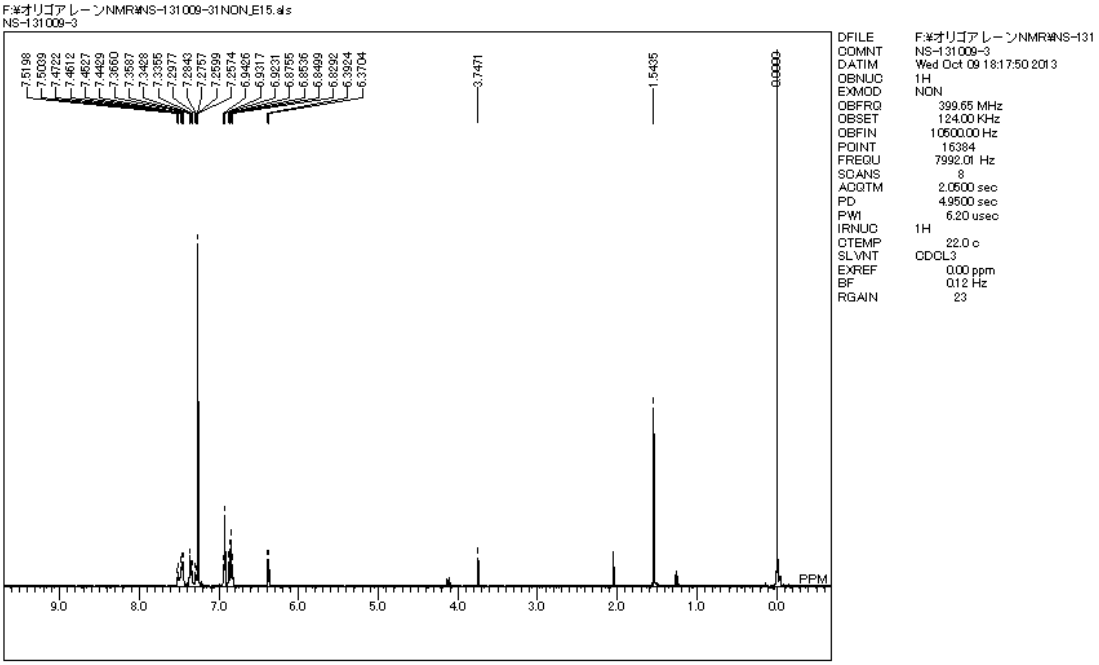

NfO
ONf

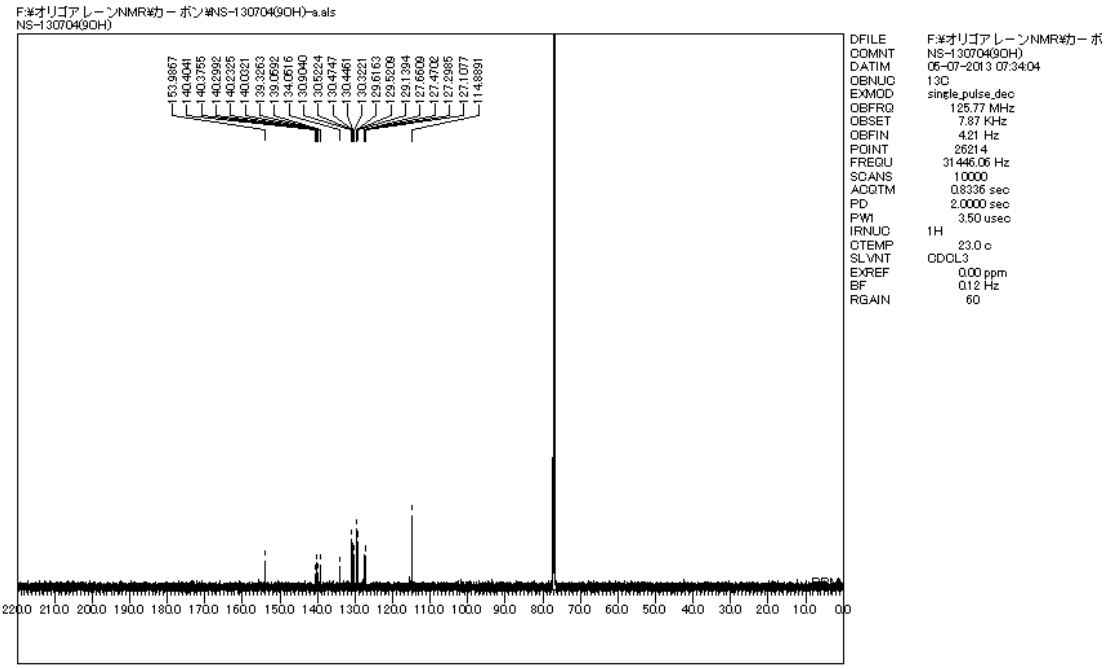

F:¥オリゴアレーンNMR¥プロトン¥NS-064-1 NON_E27.als
NS-064-1
7.4490
7.4429
7.4331
7.4270
7.4161
7.4075
7.3990
7.3917
7.3831
7.3733
7.3685
7.3563
7.3477
7.3319
7.3233
7.3026
7.2599
7.2465
7.2257
7.0306
1.5485
0.0000
PPM
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
DFILE F:¥オリゴアレーンNMR¥プロトン
COMNT NS-064-1
DATIM Mon Apr 22 16:03:24 2013
OBNUC 1H
EXMOD NON
OBFRQ 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 6.20 usec
IRNUC 1H
CTEMP 24.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 21


F:¥オリゴアレーンNMR¥カーボン¥7-mer(ONf).1
7-mer(ONf)
147.2050
141.7967
140.4232
139.7941
139.3549
138.7846
131.9246
130.5797
130.4471
130.1037
129.6544
129.3000
128.8818
128.5003
127.6037
127.3557
121.8712
77.2700
77.0124
76.7544
PPM
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0.0
DFILE F:¥オリゴアレーンNMR¥カーボ
COMNT 7-mer(ONf)
DATIM 19-06-2013 15:36:46
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 125.77 MHz
OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 32768
FREQU 39306.18 Hz
SCANS 706
ACQTM 0.8336 sec
PD 2.0000 sec
PW1 3.50 usec
IRNUC 1H
CTEMP 22.2 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 60

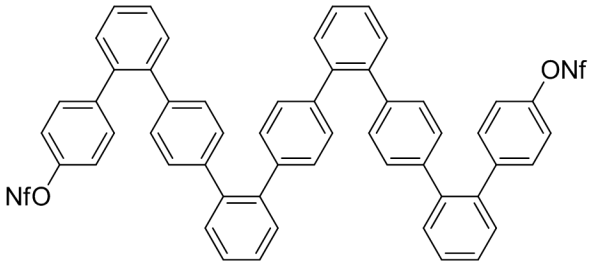
12

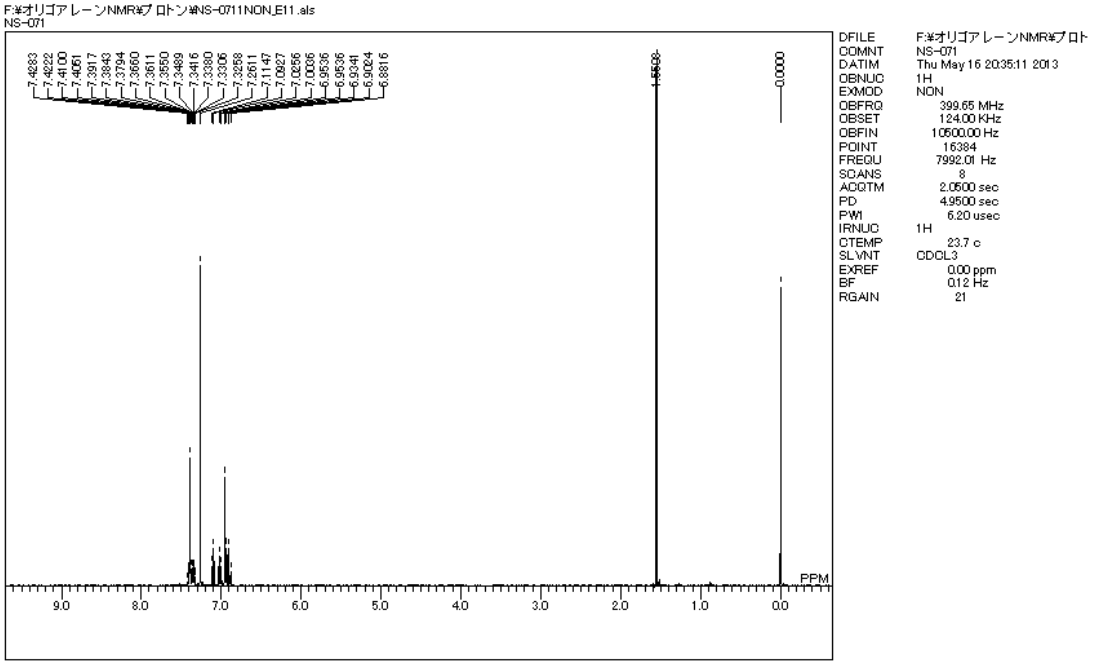

OH
HO

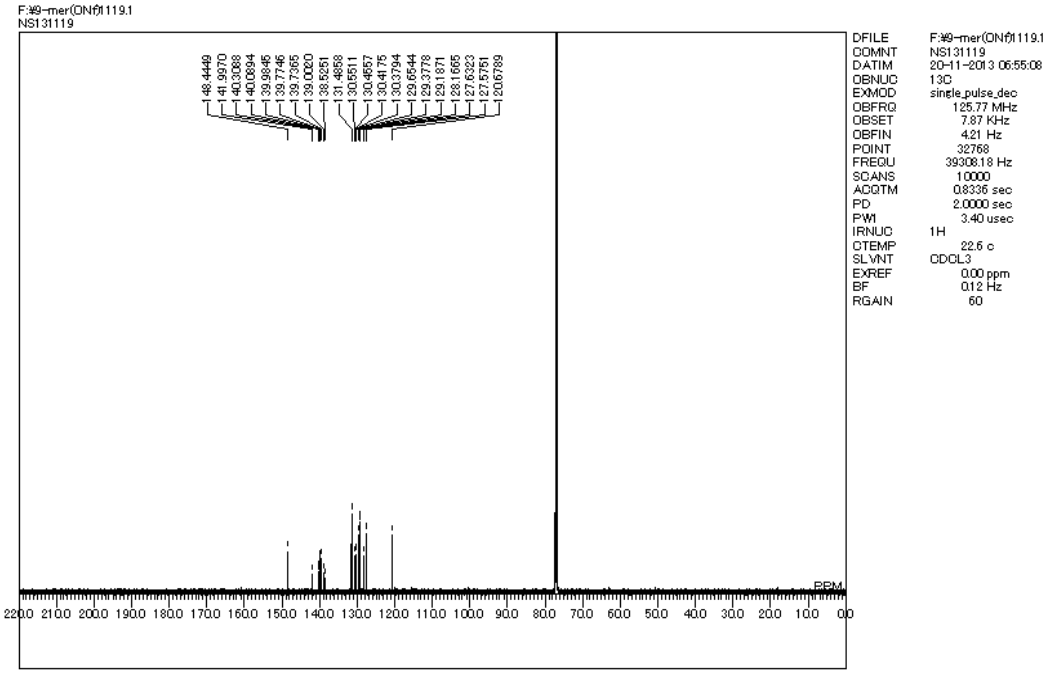

F:¥オリゴアレーンNMR¥NS-131009-31NON_E15.als
NS-131009-3
7.5198
7.5009
7.4722
7.4612
7.4627
7.4459
7.3660
7.3587
7.3428
7.3355
7.2977
7.2843
7.2757
7.2599
7.2574
6.9426
6.9317
6.9231
6.8755
6.8536
6.8499
6.8292
6.3924
6.3704
3.7471
1.5435
0.0000
PPM
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
DFILE F:¥オリゴアレーンNMR¥NS-131
COMNT NS-131009-3
DATIM Wed Oct 09 18:17:50 2013
OBNUC 1H
EXMOD NON
OBFRQ 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 6.20 usec
IRNUC 1H
CTEMP 22.0 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 23


F:¥オリゴアレーンNMR¥カーボン¥NS-130704(9OH)-a.als
NS-130704(9OH)
153.9867
140.4041
140.3755
140.2992
140.2325
140.0321
139.3263
139.0692
134.0616
130.9040
130.5224
130.4747
130.4461
130.3221
129.6163
129.5209
129.1394
127.6609
127.4702
127.2985
127.1077
114.8891
PPM
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0.0
DFILE F:¥オリゴアレーンNMR¥カーボ
COMNT NS-130704(9OH)
DATIM 05-07-2013 07:34:04
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 125.77 MHz
OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 26214
FREQU 31446.06 Hz
SCANS 10000
ACQTM 0.8336 sec
PD 2.0000 sec
PW1 3.50 usec
IRNUC 1H
CTEMP 23.0 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 60

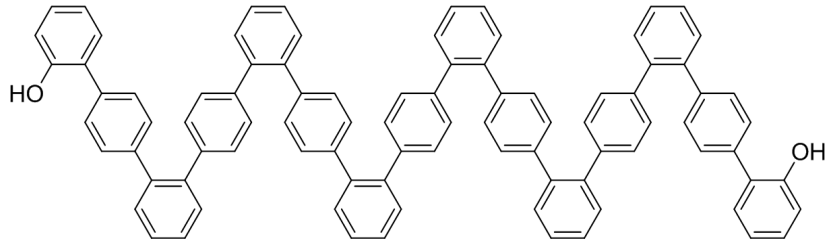
13

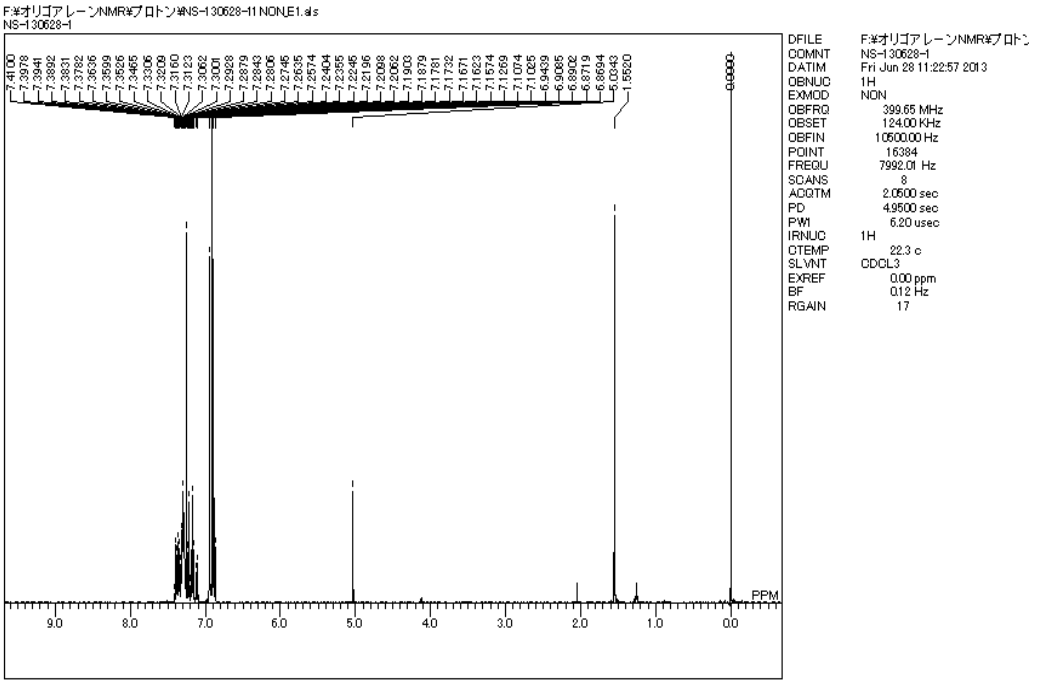

ONf
NfO

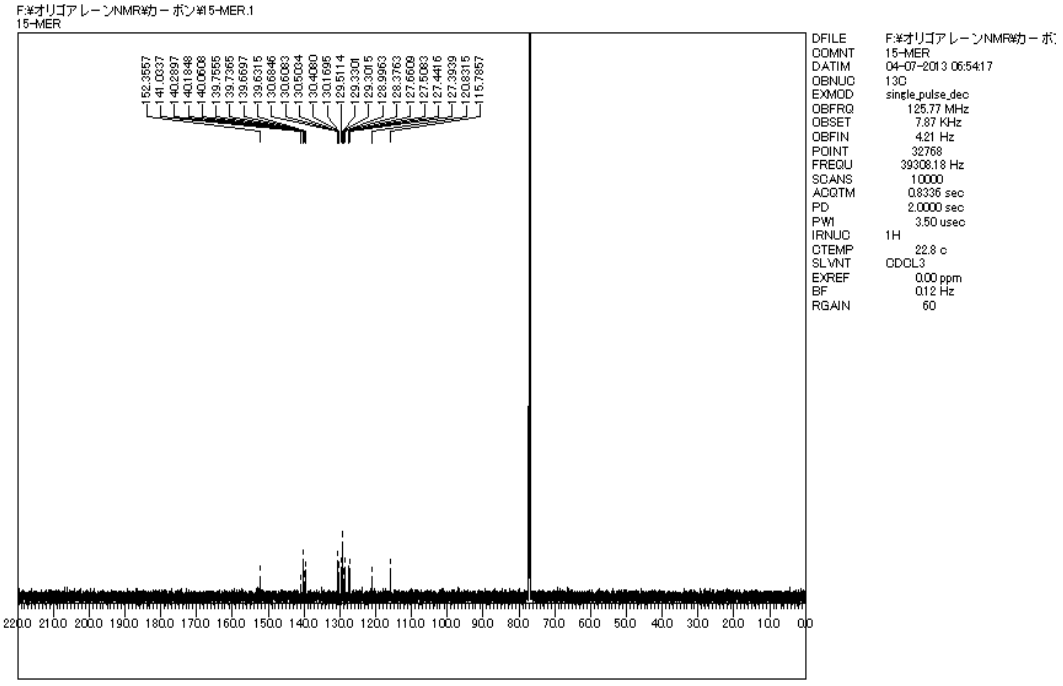

F:¥オリゴアレーンNMR¥プロトン¥NS-0711NON_E11.als
NS-071
7.4283
7.4222
7.4100
7.4051
7.3917
7.3843
7.3794
7.3660
7.3611
7.3550
7.3489
7.3416
7.3380
7.3306
7.3258
7.2611
7.1147
7.0927
7.0256
7.0036
6.9536
6.9341
6.9024
6.8816
1.5528
0.0000
PPM
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
DFILE F:¥オリゴアレーンNMR¥プロト
COMNT NS-071
DATIM Thu May 16 20:35:11 2013
OBNUC 1H
EXMOD NON
OBFRQ 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 6.20 usec
IRNUC 1H
CTEMP 23.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 21


F:¥9-mer(ONf)1119.1
NS131119
148.4449
141.9970
140.3088
140.0894
139.9845
139.7746
139.7365
139.0020
138.5251
131.4858
130.5511
130.4557
130.4173
130.3794
129.6544
129.3778
129.1871
128.1665
127.6323
127.5751
120.6789
PPM
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0.0
DFILE F:¥9-mer(ONf)1119.1
COMNT NS131119
DATIM 20-11-2013 06:55:08
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 125.77 MHz
OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 32768
FREQU 39308.18 Hz
SCANS 10000
ACQTM 0.8336 sec
PD 2.0000 sec
PW1 3.40 usec
IRNUC 1H
CTEMP 22.6 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 60

14


HO
OH


F:¥オリゴアレーンNMR¥プロトン¥NS-130628-1 NON_E1.als
NS-130628-1
7.4100
7.4078
7.3944
7.3892
7.3831
7.3782
7.3636
7.3599
7.3526
7.3465
7.3306
7.3209
7.3160
7.3123
7.3062
7.3001
7.2928
7.2879
7.2843
7.2806
7.2745
7.2635
7.2574
7.2404
7.2355
7.2245
7.2196
7.2088
7.2062
7.1903
7.1879
7.1781
7.1732
7.1671
7.1623
7.1574
7.1269
7.1074
7.1025
6.9439
6.9085
6.8902
6.8719
6.8694
6.8643
5.0343
1.5520
0.0000
PPM
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
DFILE F:¥オリゴアレーンNMR¥プロトン
COMNT NS-130628-1
DATIM Fri Jun 28 11:22:57 2013
OBNUC 1H
EXMOD NON
OBFRQ 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 6.20 usec
IRNUC 1H
CTEMP 22.3 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 17


F:¥オリゴアレーンNMR¥カーボン¥15-MER.1
15-MER
152.3557
141.0337
140.2897
140.1848
140.0608
139.7555
139.7365
139.6697
139.6315
130.6846
130.6083
130.5034
130.4080
130.1695
129.5114
129.3301
129.3015
128.9963
128.3763
127.6609
127.5083
127.4416
127.3939
120.8315
115.7857
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0.0
DFILE F:¥オリゴアレーンNMR¥カーボ
COMNT 15-MER
DATIM 04-07-2013 06:54:17
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 125.77 MHz
OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 32768
FREQU 39308.18 Hz
SCANS 10000
ACQTM 0.8336 sec
PD 2.0000 sec
PW1 3.50 usec
IRNUC 1H
CTEMP 22.8 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 60