Supporting Information for

Push-Pull Tetraene Chromphores Derived From Dialkylamino-phenyl, Tetrahydroquinolinyl and Julolidinyl Moieties: Optimization of Second-Order Optical Nonlinearity by Fine-Tuning the Strength of Electron Donating Groups

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1. Quantum mechanical calculations.
2. ^{1}H and ^{13}C NMR spectra.

1. Quantum mechanical calculations.

DFT[1,2] calculations were performed using Gaussian 09(A.02)[3] employing the hybrid B3LYP[4,5] exchange-correlation functional with a split valence 6-31G*[6] basis set. All calculations converged to a RMS error in the density matrix of $< 10^{-11}$ au. Zero-frequency (static) hyperpolarizabilities [$\beta(0)$] were obtained using analytical derivatives.[7] Chromophores were rotated into frame such that the z axis was aligned with the dipole axis and $\beta_{zzz} = \beta_{\mu}$. Solvent-dependant data was acquired using the default PCM method included in the Gaussian09 program suite. Only a single conformer (all-E) was used for each hyperpolarizability calculation.
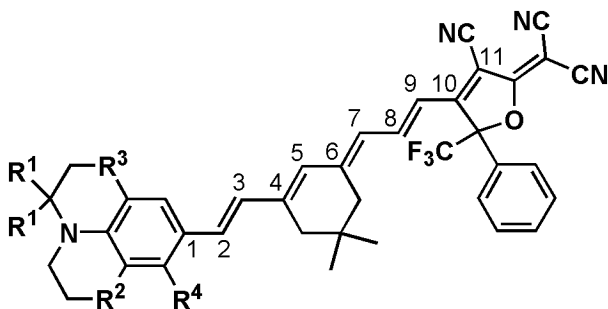

Fig. S1 Numbering of the carbon atoms in the conjugated bridge for chromophores **1**–**3**.

Table S1. Bond Lengths of the conjugated chain of Chromophores **1**–**3** Obtained by Full Geometry Optimizations using 6-31G* Basis set as a Function of Solvent (Atom numbering in Fig. S1).
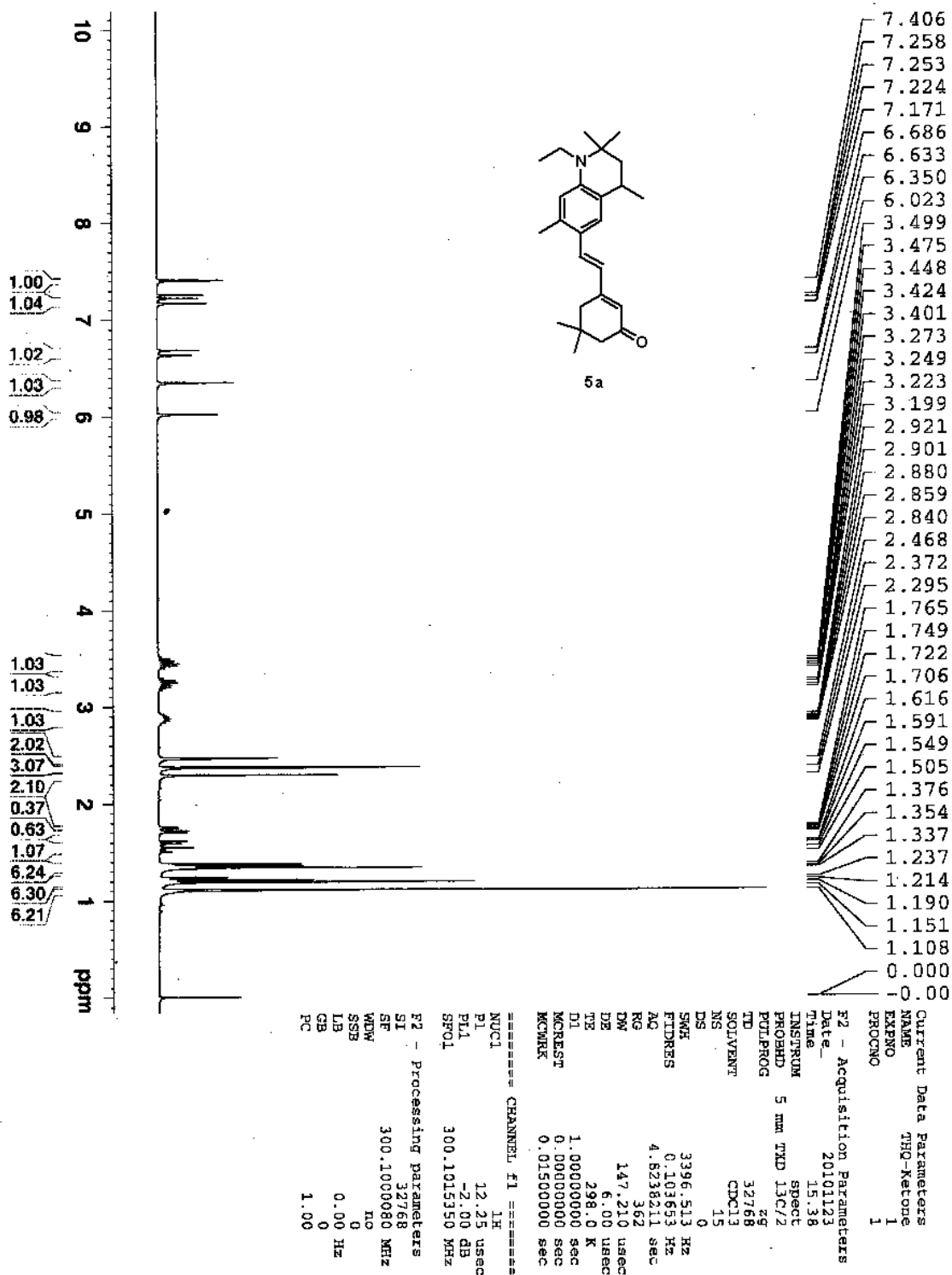
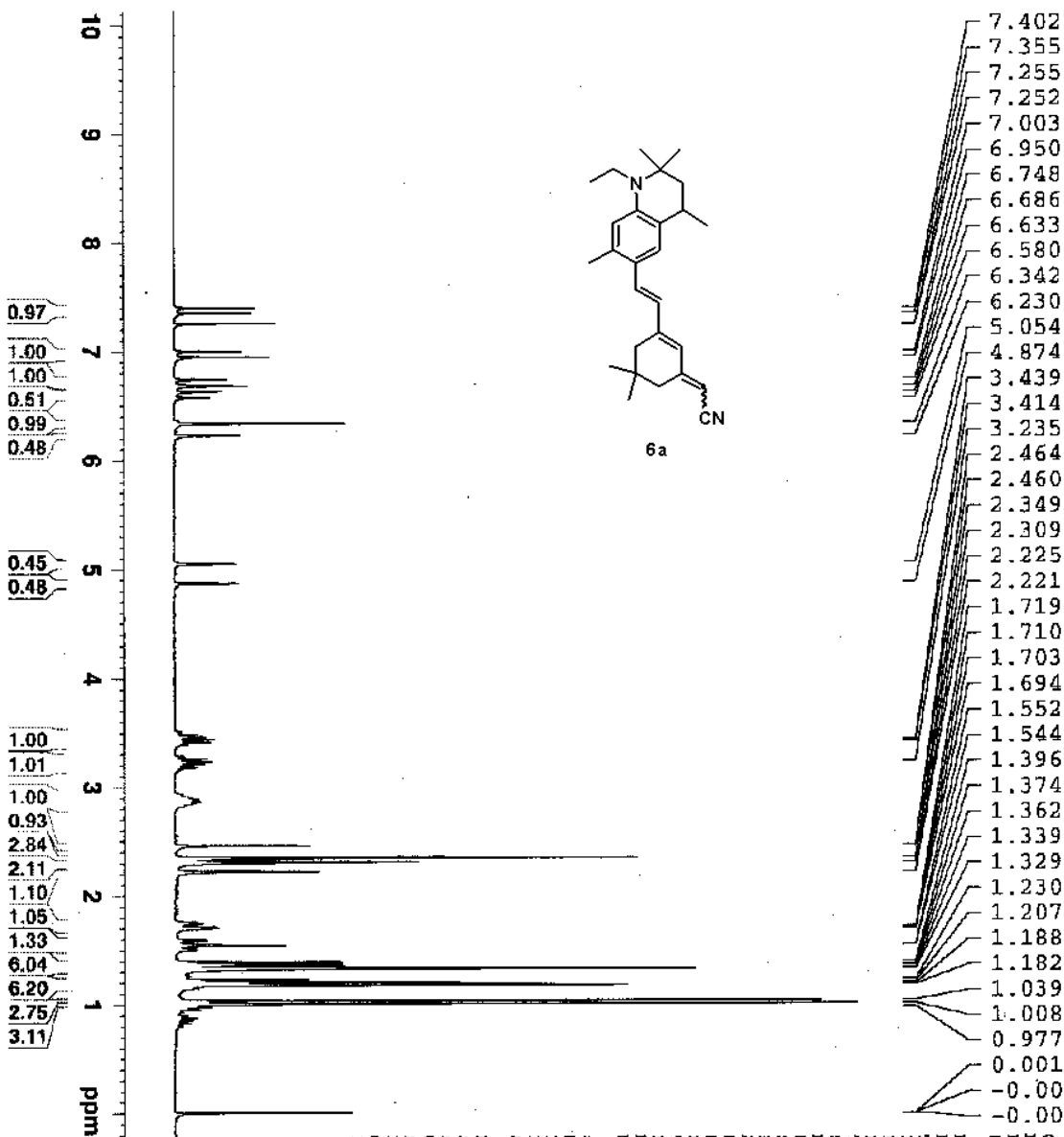| Compd.	Solvent	C_1–C_2	C_2–C_3	C_3–C_4	C_4–C_5	C_5–C_6	C_6–C_7	C_7–C_8	C_8–C_9	C_9–C_{10}	C_{10}–C_{11}
1	Vacuum	1.4467	1.3642	1.4368	1.3773	1.4261	1.3849	1.4126	1.3803	1.4114	1.3909
	Dioxane	1.4421	1.3680	1.4321	1.3825	1.4199	1.3918	1.4052	1.3875	1.4032	1.3985
	CHCl$_3$	1.4380	1.3714	1.4277	1.3873	1.4143	1.3979	1.3991	1.3938	1.3965	1.4055
	CH$_2$Cl$_2$	1.4354	1.374	1.4249	1.3905	1.4108	1.4019	1.3954	1.3979	1.3925	1.4101
	CH$_3$CN	1.4323	1.3763	1.4216	1.3941	1.4068	1.4063	1.3914	1.4024	1.3881	1.4152
2	Vacuum	1.4468	1.3664	1.4356	1.3785	1.4249	1.3858	1.4118	1.3811	1.4106	1.3915
	Dioxane	1.4413	1.3709	1.4301	1.3843	1.4180	1.3932	1.4039	1.3888	1.4019	1.3997
	CHCl$_3$	1.4364	1.3749	1.4251	1.3896	1.4119	1.3998	1.3974	1.3957	1.3948	1.4072
	CH$_2$Cl$_2$	1.4332	1.3775	1.4219	1.3932	1.4080	1.4041	1.3934	1.4001	1.3905	1.4121
	CH$_3$CN	1.4296	1.3806	1.4181	1.3973	1.4038	1.4090	1.3891	1.4050	1.3860	1.4176
3	Vacuum	1.4504	1.3666	1.4360	1.3785	1.4249	1.3859	1.4117	1.3810	1.4106	1.3917
	Dioxane	1.4425	1.3728	1.4286	1.3857	1.4165	1.3944	1.4027	1.3900	1.4008	1.4007
	CHCl$_3$	1.4365	1.3776	1.4229	1.3919	1.4097	1.4018	1.3956	1.3975	1.3932	1.4089
	CH$_2$Cl$_2$	1.4327	1.3808	1.4190	1.3960	1.4054	1.4066	1.3913	1.4024	1.3885	1.4144
	CH$_3$CN	1.4283	1.3845	1.4147	1.4008	1.4006	1.4120	1.3866	1.4078	1.3837	1.4205

References

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3. Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, Jr., J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, N. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.
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2. ^{1}H and ^{13}C NMR spectra

5a

6a

Peak list (ppm):
7.402, 7.355, 7.255, 7.252, 7.003, 6.950, 6.748, 6.686, 6.633, 6.580, 6.342, 6.230, 5.054, 4.874, 3.439, 3.414, 3.235, 2.464, 2.460, 2.349, 2.309, 2.225, 2.221, 1.719, 1.710, 1.703, 1.694, 1.552, 1.544, 1.396, 1.374, 1.362, 1.339, 1.329, 1.230, 1.207, 1.188, 1.182, 1.039, 1.008, 0.977, 0.001, -0.00, -0.00

Integrations:
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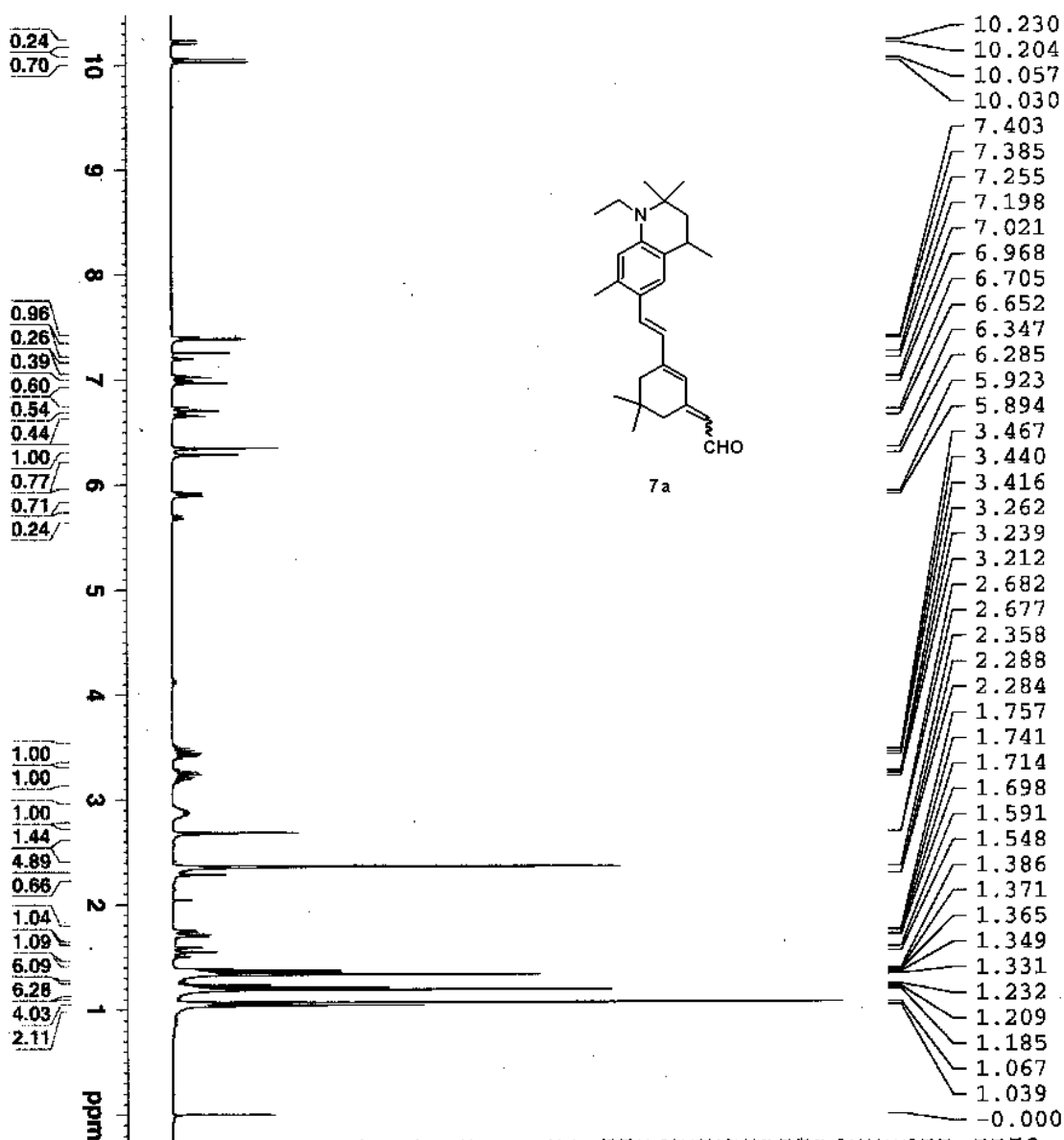MCREST   0.00000000 sec
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7a

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5b
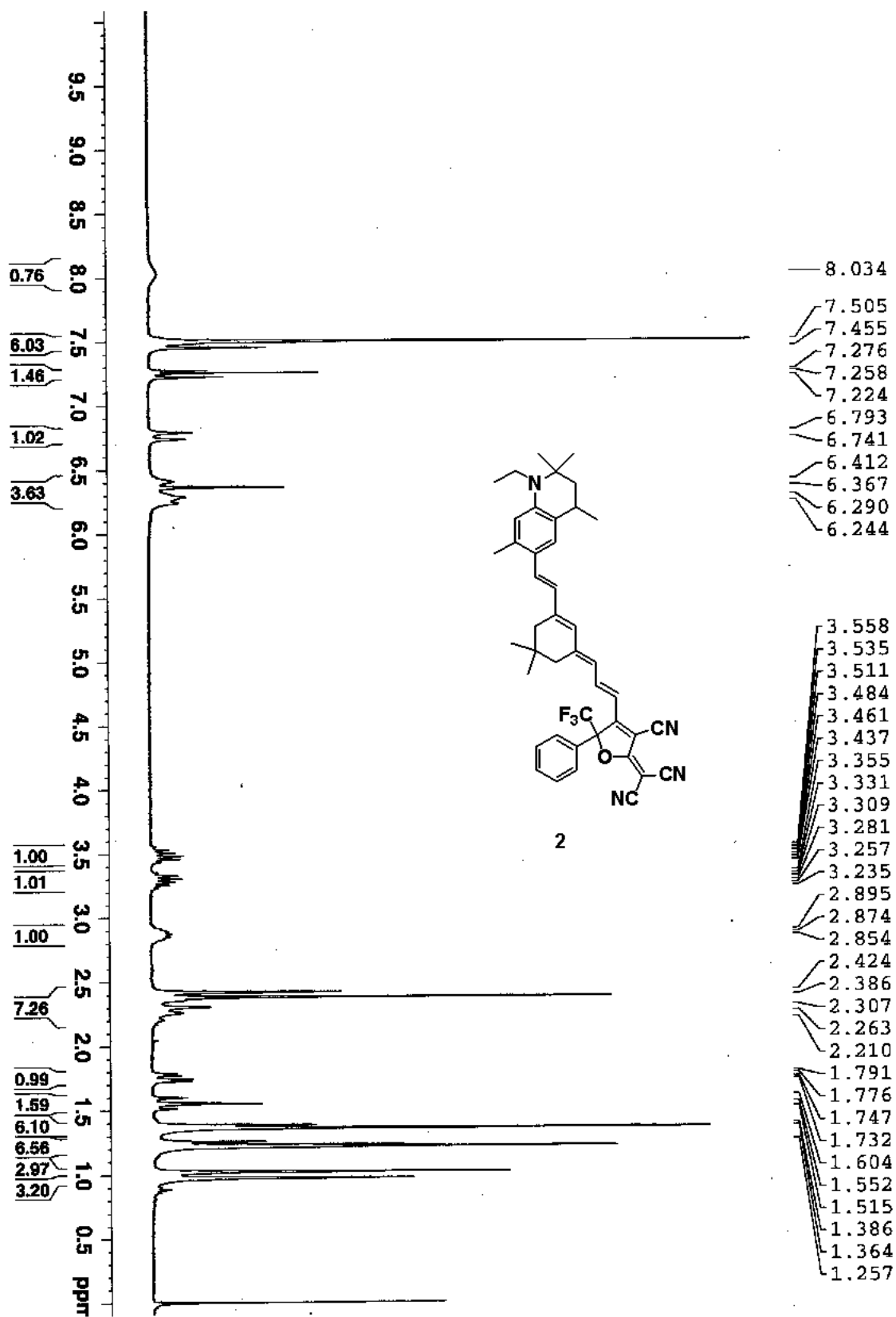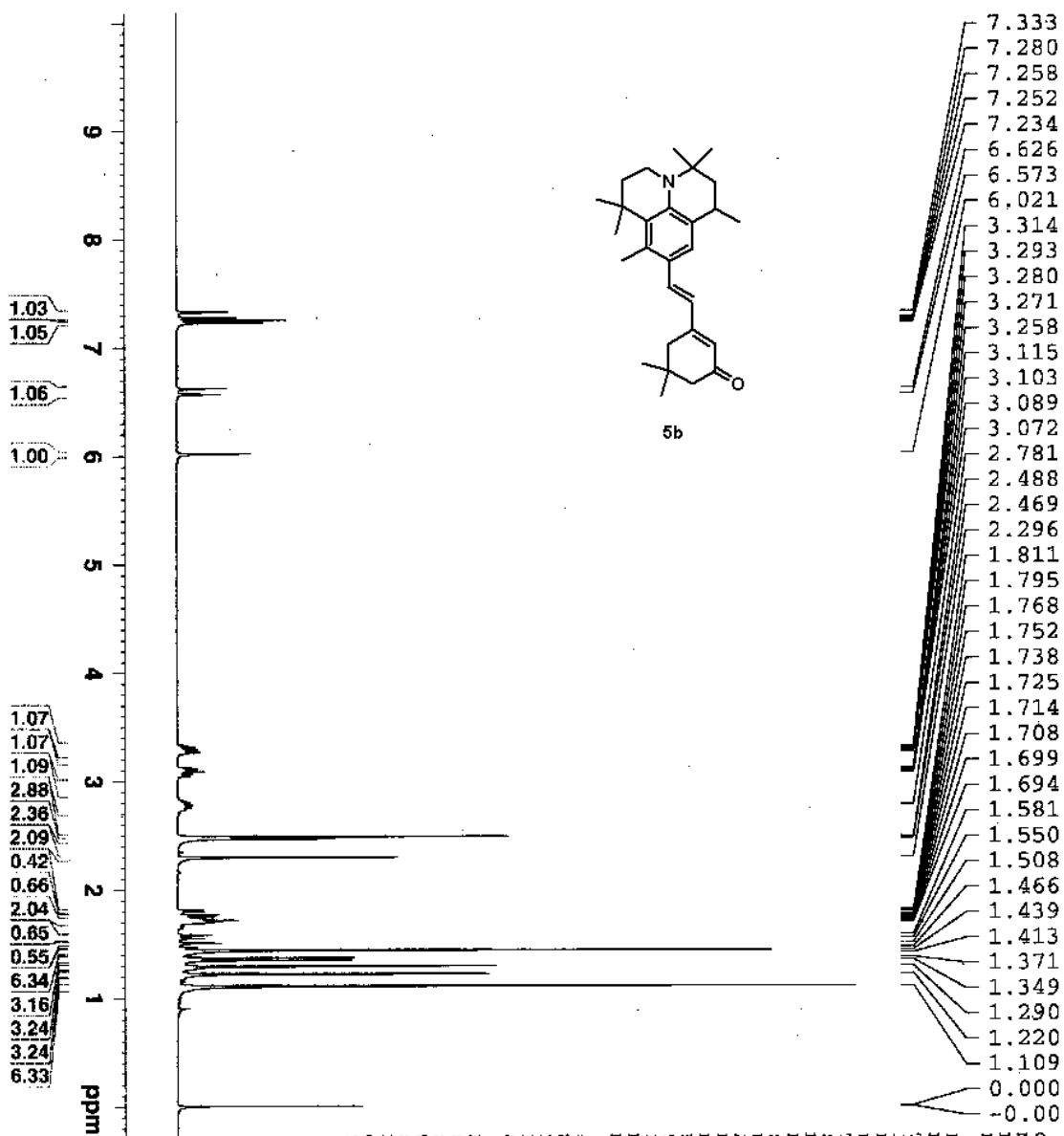
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3.103
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1.581
1.550
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1.413
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1.290
1.220
1.109
0.000
-0.00

1.03
1.05
1.06
1.00
1.07
1.07
1.09
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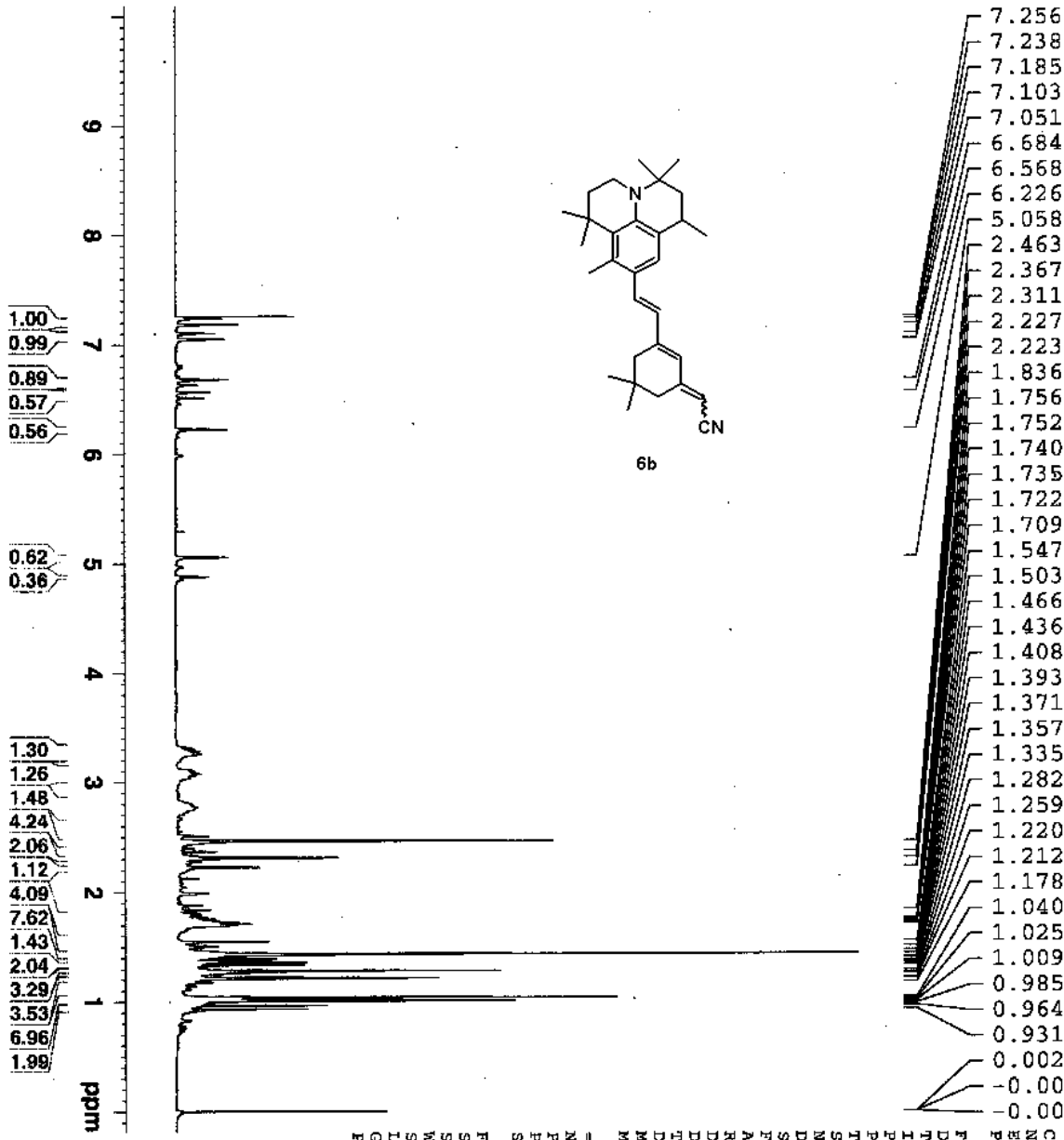Current Data Parameters
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6b

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Integrations:
1.00, 0.99, 0.89, 0.57, 0.56, 0.62, 0.36, 1.30, 1.26, 1.48, 4.24, 2.06, 1.12, 4.09, 7.62, 1.43, 2.04, 3.29, 3.53, 6.96, 1.99

Current Data Parameters
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PROCNO   1

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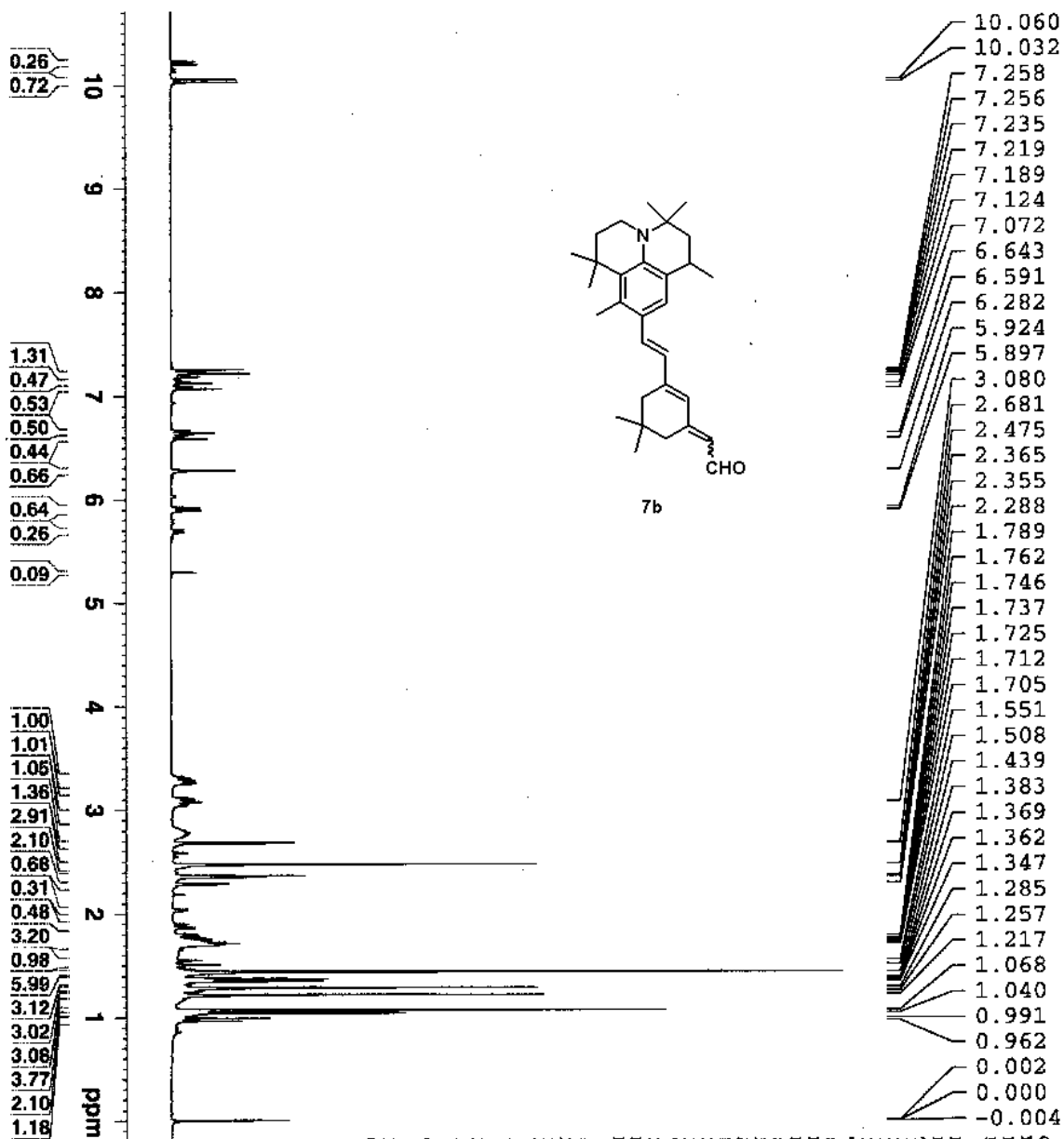MCREST   0.00000000 sec
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7b

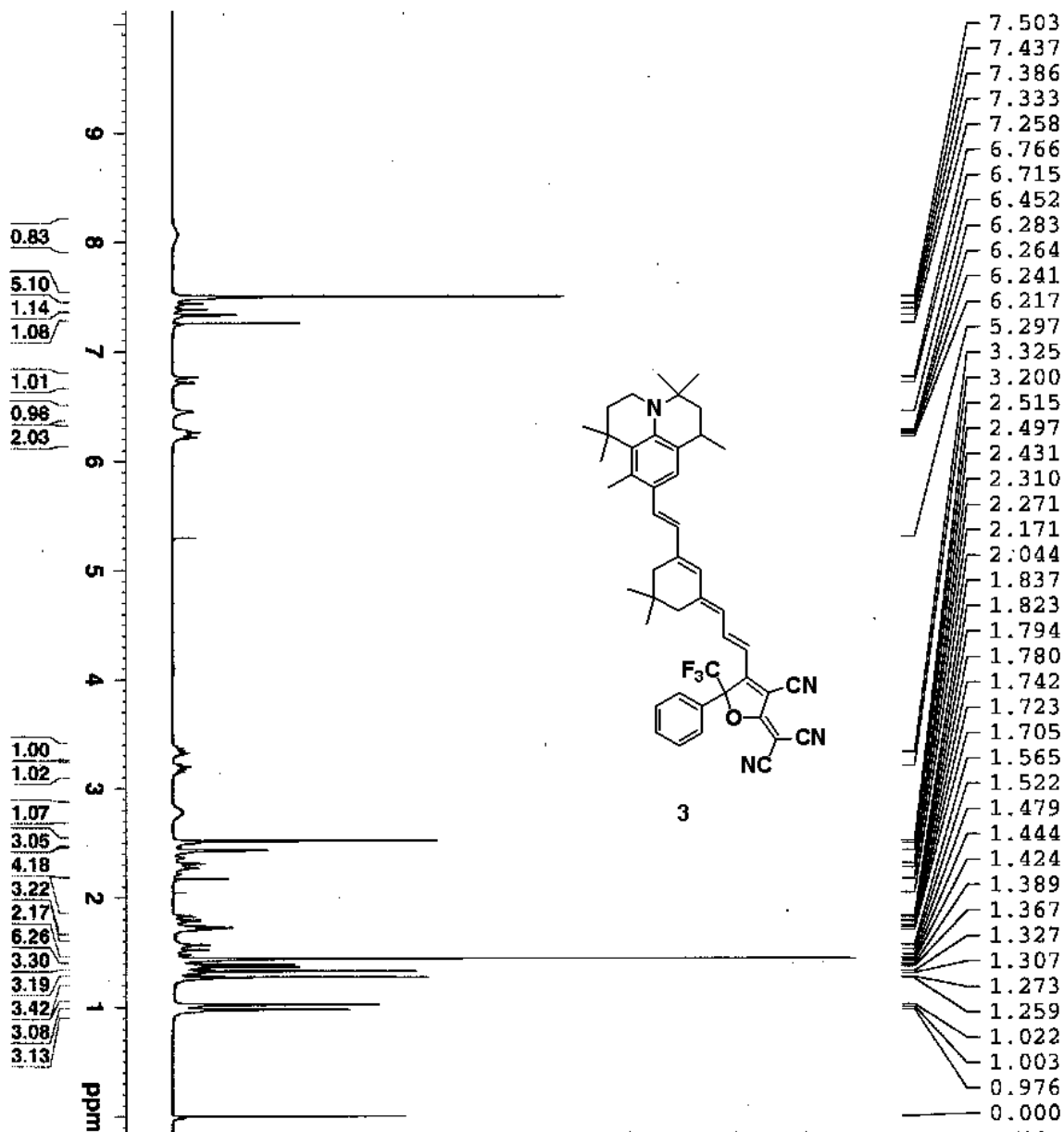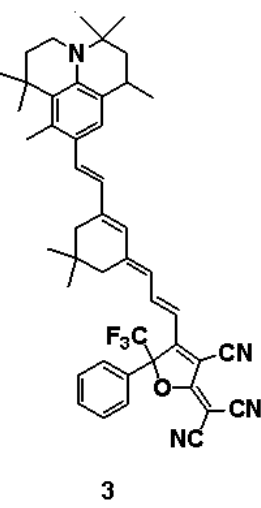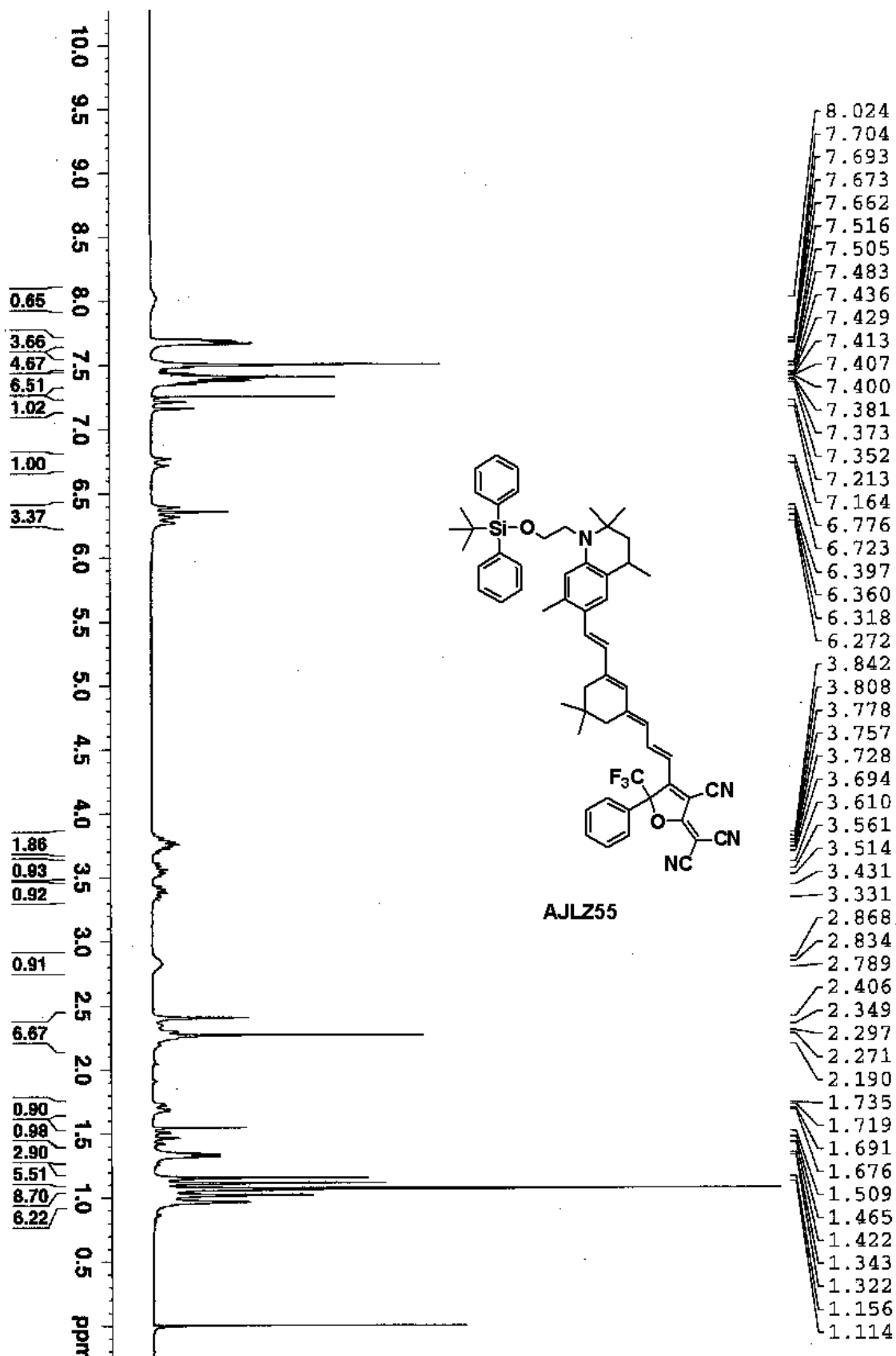Current Data Parameters
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DE   6.00 usec
TE   298.0 K
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======== CHANNEL f1 ========
NUC1   1H
P1   12.25 usec
PL1   -2.00 dB
SFO1   300.1015350 MHz

F2 — Processing parameters
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WDW   no
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2.10
1.18

AJLZ55

5a

199.78

156.21

145.53

136.06
132.96
125.62
124.49
124.42
123.30
121.27

112.47

54.55
51.32

46.53
39.12
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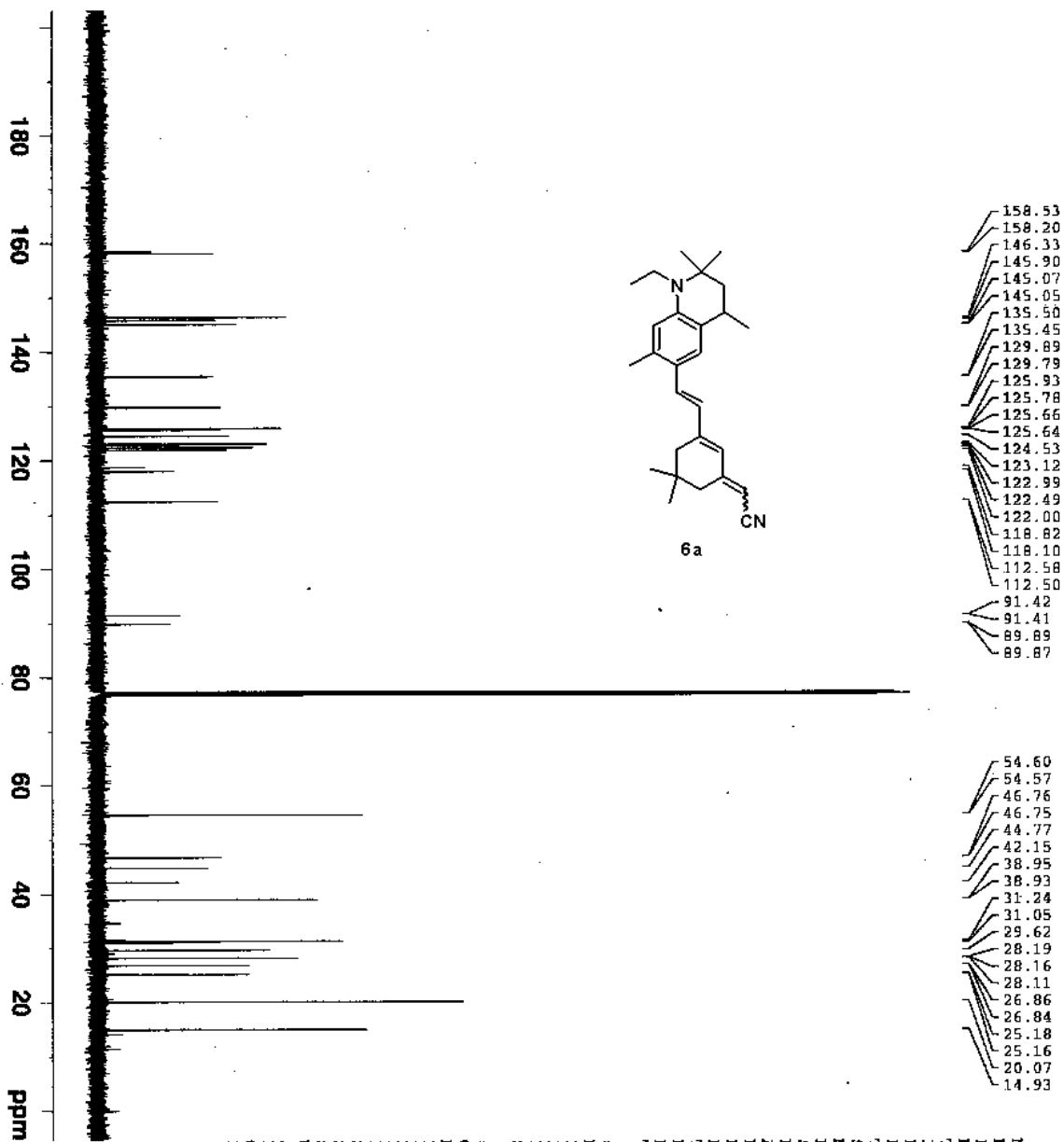NAME   THQ-Kto-C13
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RG   20642.5
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DE   6.50 usec
TE   298.0 K
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D11   0.03000000 sec
TDO   1

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NUC1   13C
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PL1   6.00 dB
PL1W   19.93825150 W
SFO1   125.7492404 MHz

======= CHANNEL f2 =======
CPDPRG2   waltz16
NUC2   1H
PCPD2   70.00 usec
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PL12   12.96 dB
PL13   20.00 dB
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SI   32768
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6a

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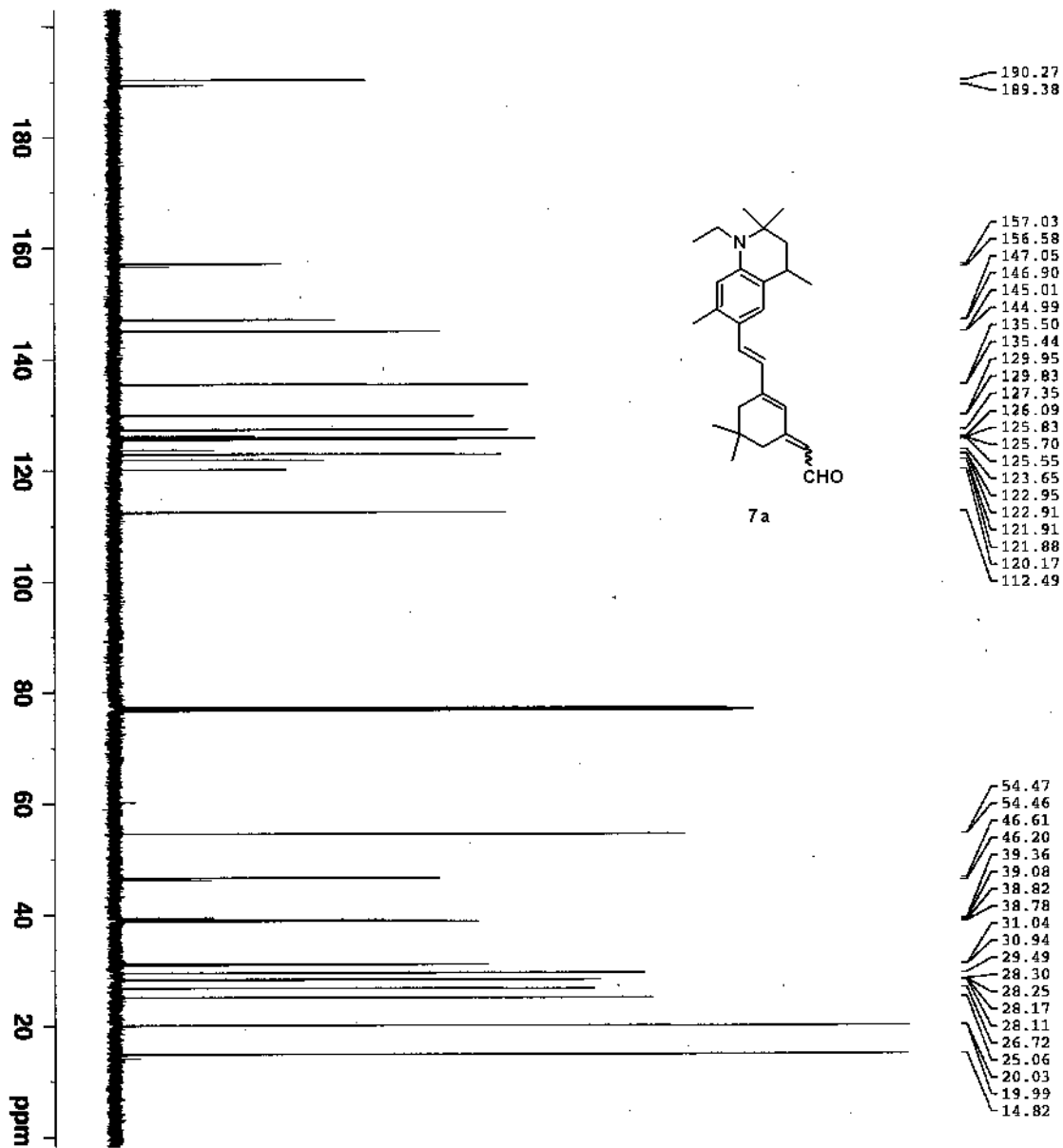122.00
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DW   16.650 usec
DE   6.50 usec
TE   298.0 K
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TD0   1

======== CHANNEL f1 ========
NUC1   13C
P1   15.00 usec
PL1   6.00 dB
PL1W   19.93825150 W
SFO1   125.7492404 MHz

======== CHANNEL f2 ========
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PL12   12.96 dB
PL13   20.00 dB
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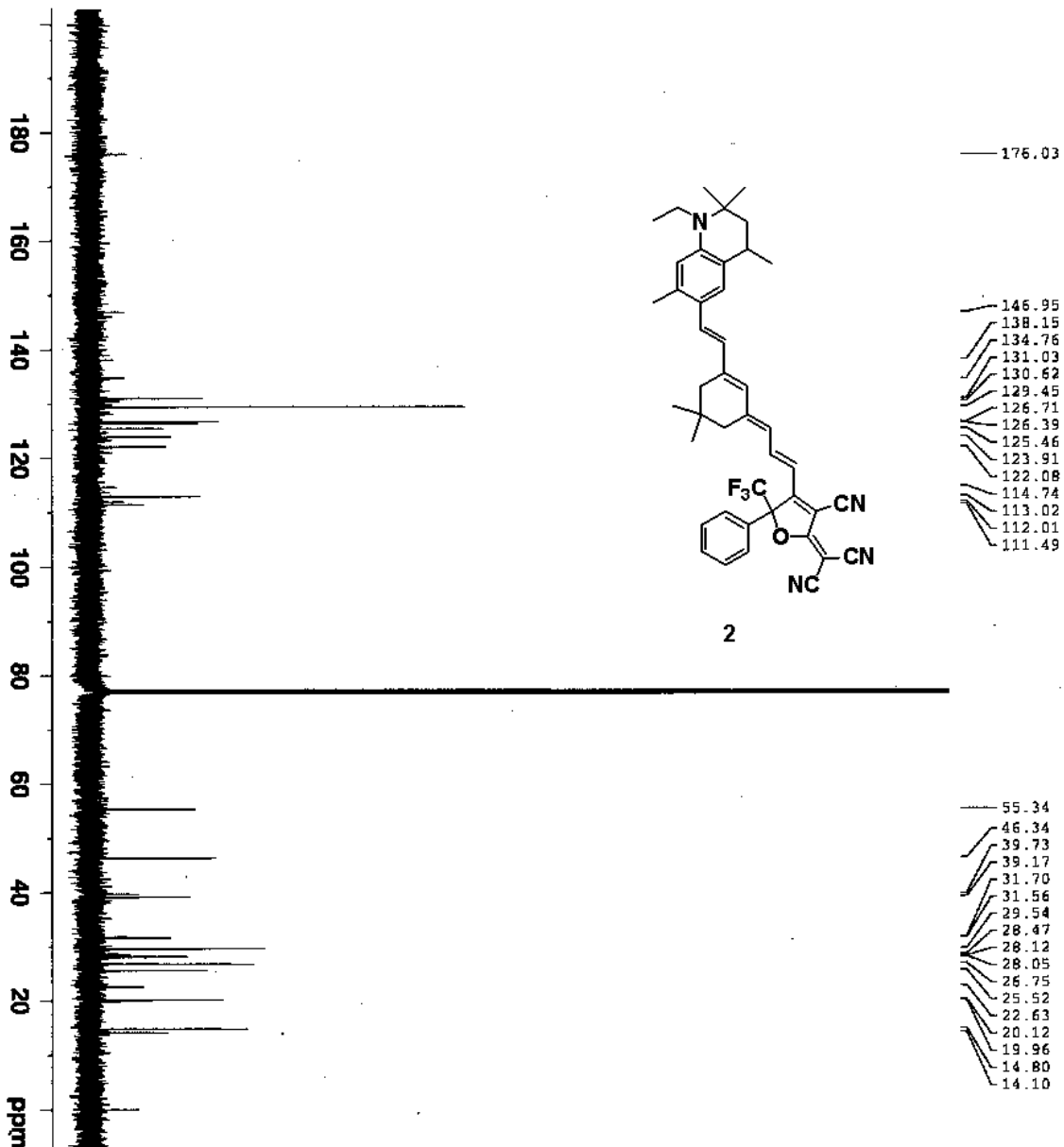SI   32768
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7a

Peak labels:
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189.38

157.03
156.58
147.05
146.90
145.01
144.99
135.50
135.44
129.95
129.83
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123.65
122.95
122.91
121.91
121.88
120.17
112.49

54.47
54.46
46.61
46.20
39.36
39.08
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38.78
31.04
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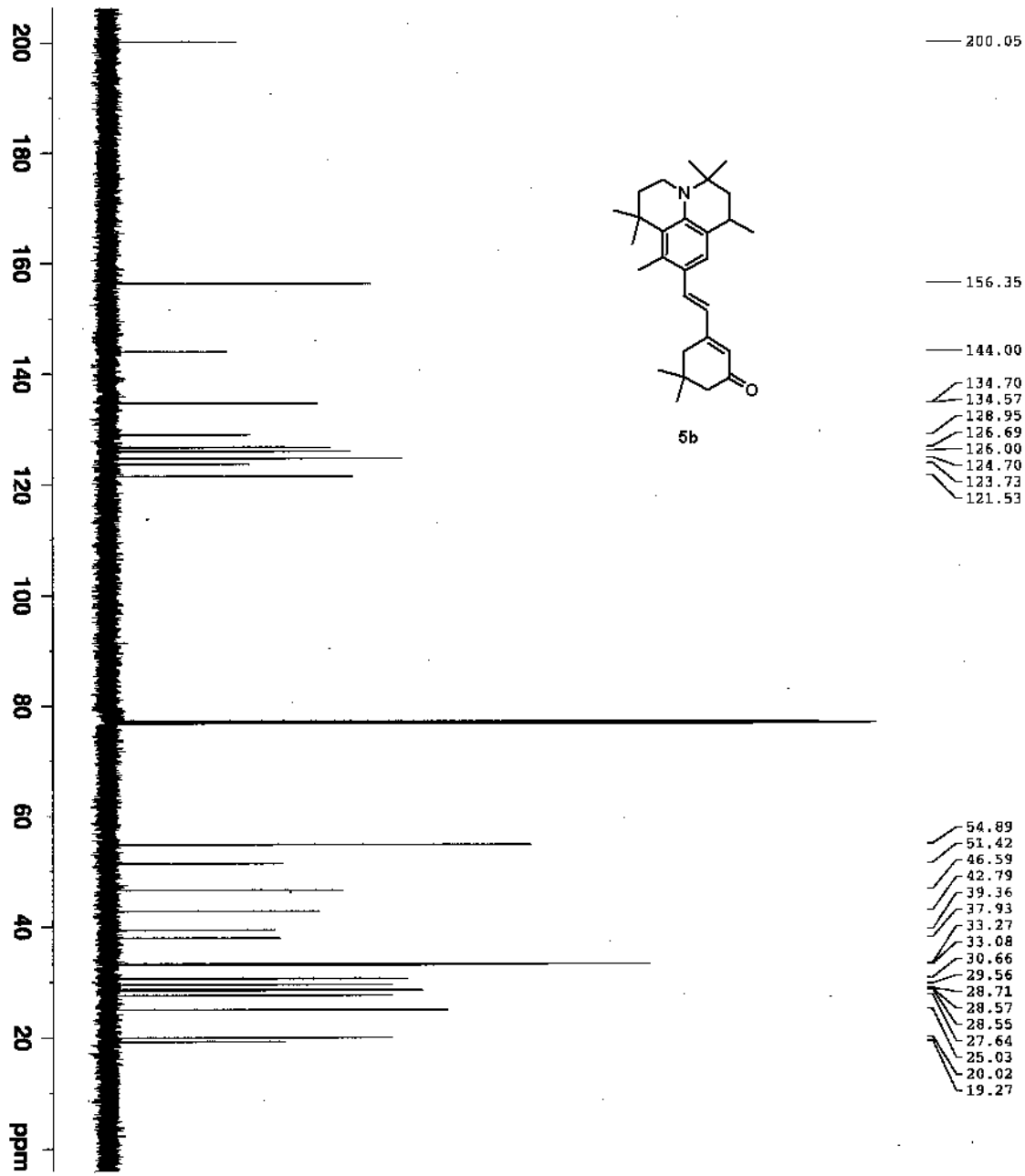PROCNO   1
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RG   18390.4
DW   16.650 usec
DE   6.50 usec
TE   298.0 K
D1   2.00000000 sec
D11   0.03000000 sec
TDO   1

======== CHANNEL f1 ========
NUC1   13C
P1   15.00 usec
PL1   6.00 dB
PL1W   19.93825150 W
SFO1   125.7492404 MHz

======== CHANNEL f2 ========
CPDPRG2   waltz16
NUC2   1H
PCPD2   70.00 usec
PL2   -2.00 dB
PL12   12.96 dB
PL13   20.00 dB
SFO2   500.0480002 MHz
SI   32768
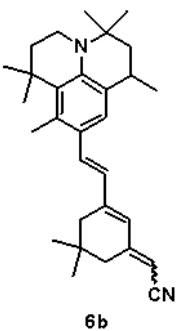SF   125.7366944 MHz
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— 146.95
— 138.15
— 134.76
— 131.03
— 130.62
— 129.45
— 126.71
— 126.39
— 125.46
— 123.91
— 122.08
— 114.74
— 113.02
— 112.01
— 111.49

2

— 55.34
— 46.34
— 39.73
— 39.17
— 31.70
— 31.56
— 29.54
— 28.47
— 28.12
— 28.05
— 26.75
— 25.52
— 22.63
— 20.12
— 19.96
— 14.80
— 14.10

NAME   THIQ-Chirp C13
EXPNO   1
PROCNO   1
Date_   20101130
Time_   14.12
INSTRUM   spect
PROBHD   5 mm BBO BB-1H
PULPROG   zgpg30
TD   65536
SOLVENT   CDCl3
NS   1368
DS   4
SWH   30030.029 Hz
FIDRES   0.458222 Hz
AQ   1.0912410 sec
RG   20642.5
DW   16.650 usec
DE   6.50 usec
TE   298.0 K
D1   2.00000000 sec
D11   0.03000000 sec
TD0   1

======== CHANNEL f1 ========
NUC1   13C
P1   15.00 usec
PL1   6.00 dB
PL1W   19.93825150 W
SFO1   125.7492404 MHz

======== CHANNEL f2 ========
CPDPRG2   waltz16
NUC2   1H
PCPD2   70.00 usec
PL2   -2.00 dB
PL12   12.96 dB
PL13   20.00 dB
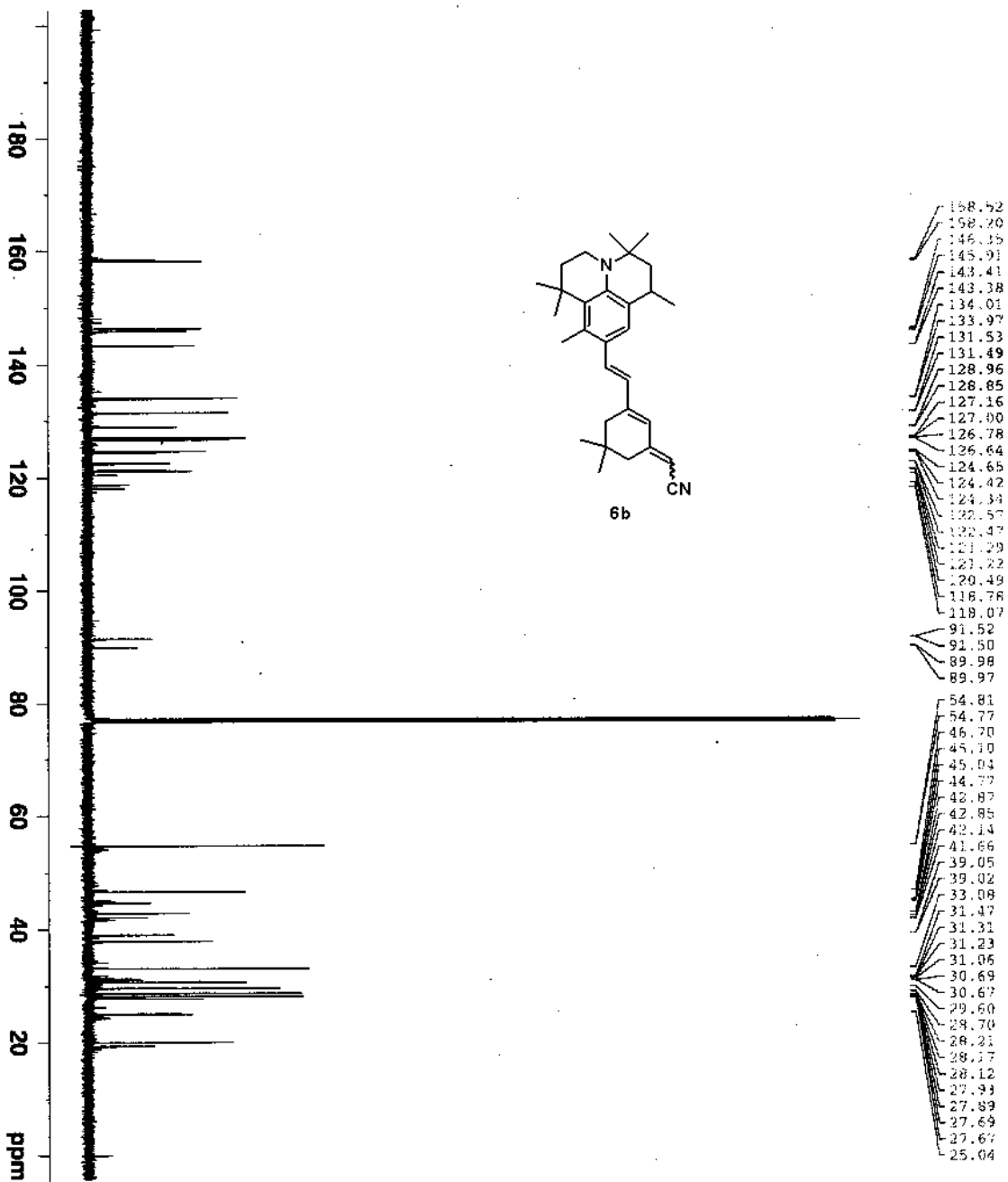SFO2   500.0480002 MHz
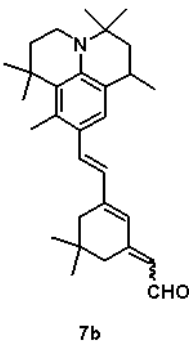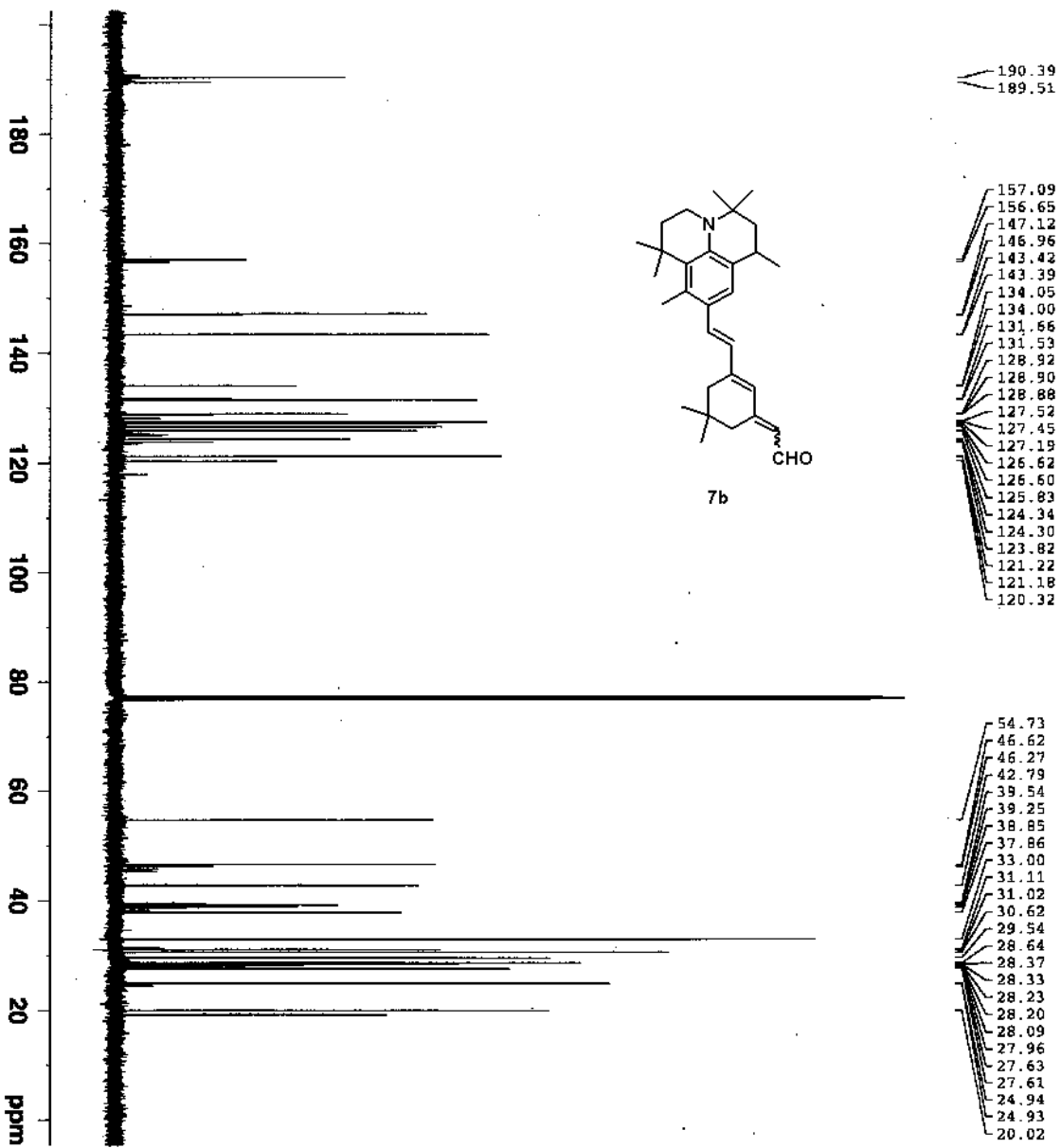SI   32768
SF   125.7366723 MHz
WDW   no
SSB   0
LB   0.00 Hz
GB   0
PC   1.40

5b

— 200.05

— 156.35

— 144.00

— 134.70
— 134.57
— 128.95
— 126.69
— 126.00
— 124.70
— 123.73
— 121.53

— 54.89
— 51.42
— 46.59
— 42.79
— 39.36
— 37.93
— 33.27
— 33.08
— 30.66
— 29.56
— 28.71
— 28.57
— 28.55
— 27.64
— 25.03
— 20.02
— 19.27

NAME   JLR-Rto-C13
EXPNO   1
PROCNO   1
Date_   20101123
Time   17.29
INSTRUM   spect
PROBHD   5 mm BBO BB-1H
PULPROG   zgpg30
TD   65536
SOLVENT   CDCl3
NS   268
DS   4
SWH   30030.029 Hz
FIDRES   0.458222 Hz
AQ   1.0912410 se
RG   20642.5
DW   16.650 us
DE   6.50 us
TE   298.0 K
D1   2.00000000 se
D11   0.03000000 se
TD0   1

======== CHANNEL f1 ========
NUC1   13C
P1   15.00 us
PL1   6.00 dB
PL1W   19.93825150 W
SFO1   125.7492404 MH

======== CHANNEL f2 ========
CPDPRG2   waltz16
NUC2   1H
PCPD2   70.00 us
PL2   -2.00 dB
PL12   12.96 dB
PL13   20.00 dB
SFO2   500.0480002 MH
SI   32768
SF   125.7365760 MH
WDW   no
SSB   0
LB   0.00 Hz
GB   0
PC   1.40

200   180   160   140   120   100   80   60   40   20   ppm

6b

Peak list (ppm):
158.52, 158.20, 146.05, 145.91, 143.41, 143.38, 134.01, 133.97, 131.53, 131.49, 128.96, 128.85, 127.16, 127.00, 126.78, 126.64, 124.65, 124.42, 124.34, 122.57, 122.47, 121.29, 121.22, 120.49, 118.76, 118.07, 91.52, 91.50, 89.98, 89.97, 54.81, 54.77, 46.70, 45.10, 45.04, 44.77, 42.87, 42.85, 42.14, 41.66, 39.05, 39.02, 33.08, 31.47, 31.31, 31.23, 31.06, 30.69, 30.67, 29.60, 28.70, 28.21, 28.17, 28.12, 27.93, 27.89, 27.69, 27.67, 25.04

190.39
189.51

157.09
156.65
147.12
146.96
143.42
143.39
134.05
134.00
131.66
131.53
128.92
128.90
128.88
127.52
127.45
127.19
126.62
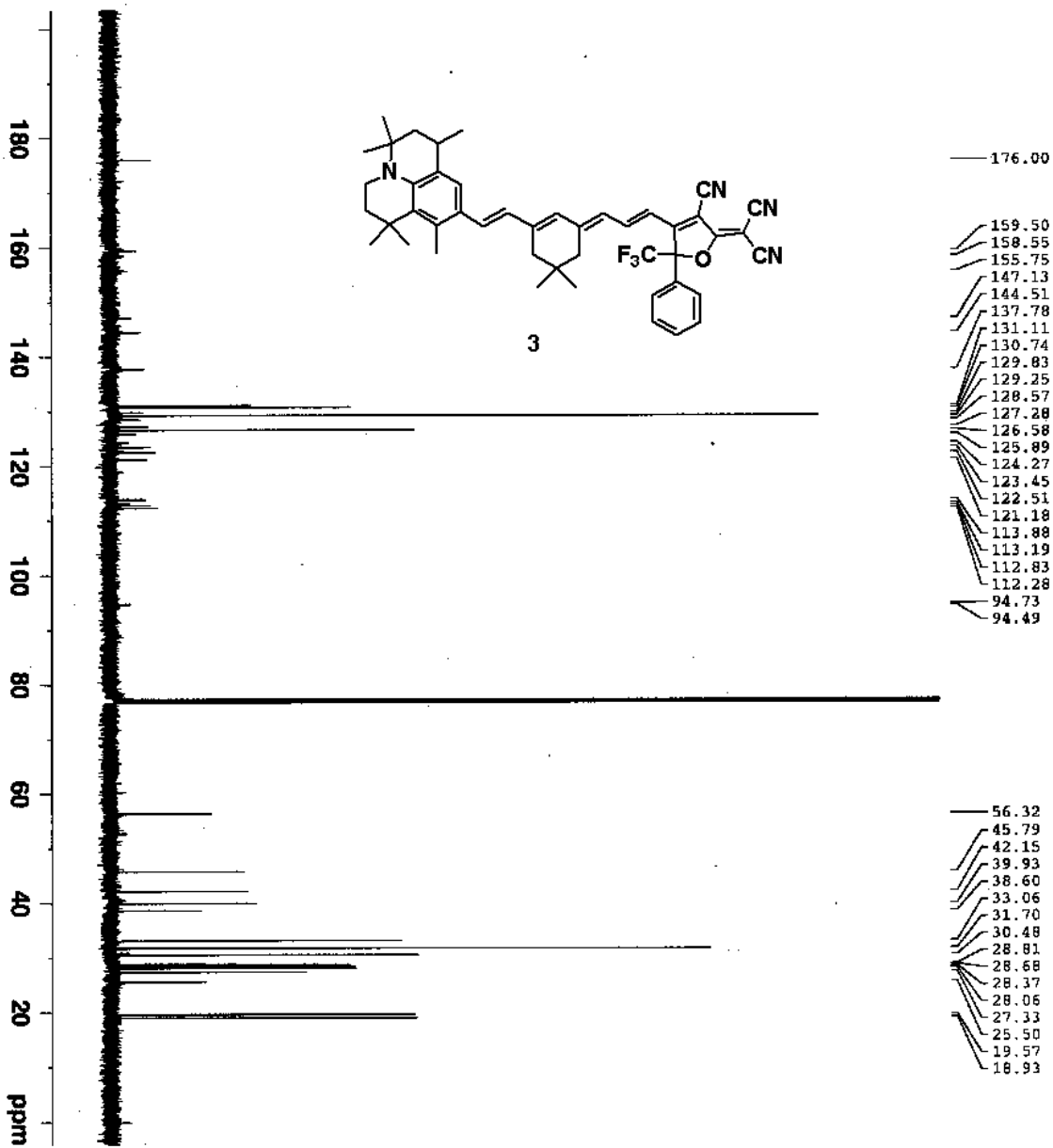126.60
125.83
124.34
124.30
123.82
121.22
121.18
120.32

7b

54.73
46.62
46.27
42.79
39.54
39.25
38.85
37.86
33.00
31.11
31.02
30.62
29.54
28.64
28.37
28.33
28.23
28.20
28.09
27.96
27.63
27.61
24.94
24.93
20.02

NAME   JLD-CHO C13
EXPNO   1
PROCNO   1
Date_   20101129
Time   15.23
INSTRUM   spect
PROBHD   5 mm BBO BB-1H
PULPROG   zgpg30
TD   65536
SOLVENT   CDCl3
NS   411
DS   4
SWH   30030.029 Hz
FIDRES   0.458222 Hz
AQ   1.0912410 sec
RG   18390.4
DW   16.650 usec
DE   6.50   usec
TE   298.0   K
D1   2.00000000 sec
D11   0.03000000 sec
TD0   1

======== CHANNEL f1 ========
NUC1   13C
P1   15.00 usec
PL1   6.00 dB
PL1W   19.93825150 W
SFO1   125.7492404 MHz

======== CHANNEL f2 ========
CPDPRG2   waltz16
NUC2   1H
PCPD2   70.00 usec
PL2   -2.00 dB
PL12   12.96 dB
PL13   20.00 dB
SFO2   500.0480002 MHz
SI   32768
SF   125.7366870 MHz
WDW   no
SSB   0
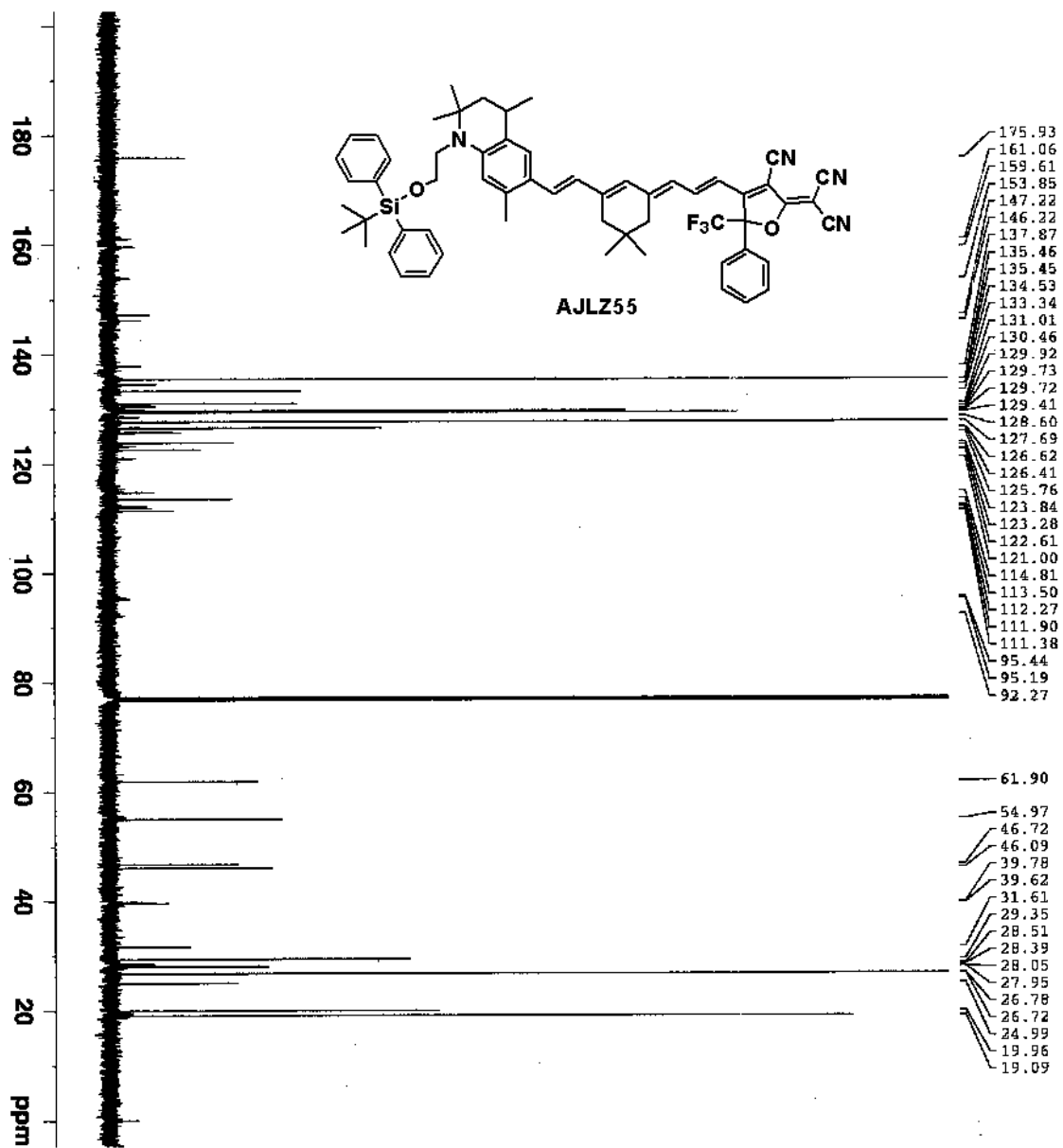LB   0.00 Hz
GB   0
PC   1.40

180   160   140   120   100   80   60   40   20   ppm

—176.00

159.50
158.55
155.75
147.13
144.51
137.78
131.11
130.74
129.83
129.25
128.57
127.28
126.58
125.89
124.27
123.45
122.51
121.18
113.88
113.19
112.83
112.28
94.73
94.49

56.32
45.79
42.15
39.93
38.60
33.06
31.70
30.48
28.81
28.68
28.37
28.06
27.33
25.50
19.57
18.93

3

NAME   JLD-Chrmp C13
EXPNO   1
PROCNO   1
Date_   20101201
Time   16.07
INSTRUM   spect
PROBHD   5 mm BBO BB-1H
PULPROG   zgpg30
TD   65536
SOLVENT   CDC13
NS   2049
DS   4
SWH   30030.029 Hz
FIDRES   0.458222 Hz
AQ   1.0912410 se
RG   20642.5
DW   16.650 us
DE   6.50 us
TE   298.0 K
D1   2.00000000 se
D11   0.03000000 se
TD0   1

======== CHANNEL f1 =======
NUC1   13C
P1   15.00 us
PL1   6.00 dB
PL1W   19.93825150 W
SFO1   125.7492404 MH

======== CHANNEL f2 =======
CPDPRG2   waltz16
NUC2   1H
PCPD2   70.00 us
PL2   -2.00 dB
PL12   12.96 dB
PL13   20.00 dB
SFO2   500.0480002 MH
SI   32768
SF   125.7366833 MH
WDW   no
SSB   0
LB   -0.00 Hz
GB   0
PC   1.40

AJLZ55