Supplementary Material

Synthesis and Biological Evaluation of 1,4-Naphthoquinones and Quinoline-5,8-diones as Antimalarial and Schistosomicidal Agent

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Enzymatic studies

Enzyme preparation. Recombinant *h*GR was purified as previously reported.[1] One unit of GR activity is defined as the consumption of 1 µmol NADPH per min under conditions of substrate saturation. The enzyme stock solution (266 µm) used for kinetic determinations was > 98% pure as judged from silver stained SDS-PAGE and had specific activities of 200 U/mg (*h*GR). A *h*GR stock II solution was prepared by dilution (1/10) of the enzyme stock solution with *h*GR buffer (pH 6.9).[2] The *h*GR buffer (pH 6.9) was prepared by dissolving KH_2PO_4 (2.79 g), K_2HPO_4, 3 H_2O (6.04 g), EDTA (0.372 g), and KCl (14.91 g) in 1 L water. The pH was adjusted by dropwise addition of 5 M KOH. Recombinant *Sm*TGR was produced in *Escherichia coli* as previously described.[3]

Pharmacokinetics

Solubility express. Shake-flask method allowed determination of the apparent thermodynamic solubilities from DMSO stock solutions of compounds. Compound dilutions were prepared to 200 µM in an aqueous 7.4 HEPES buffer. The mix was equilibrated at 20 °C during 24 hours. After centrifugation, the supernatant was injected in an HPLC column coupled to a LC-MS apparatus (with UV-Vis detection) in order to determine the compound concentration. A reference solution at 200 µM was made in CH_3CN/water and a dilution at 100 µM allowed analysis of the linearity of the UV response. These solutions were also injected in order to calibrate the concentration determination. Comparison of the responses of the injections of three dilutions obtained from a DMSO reference solution allowed determination of the solubility if lower than 200 µM. Measurements were done in duplicate.

Determination of logD values. The partition coefficient between octanol and water is the most widely used physicochemical determination of lipophilicity. The "shake flask" method was used to determine the partition coefficients. A solution of 100 µM tested compound was prepared from a stock DMSO solution in a “mix” aqueous buffer / octanol. Three octanol / buffer volume ratios were used to cover partition coefficients ranging from -1.5 to +3.2. The partition experience with the best ratio was repeated twice. The mix was equilibrated at 20°C for one hour. Then, the aqueous phase and a reference solution at 100 µM were injected in an HPLC column coupled to a LC-MS apparatus (with UV-Vis detection) to determine compound concentration. The partition coefficient was calculated from the peak areas obtained in the chromatograms. Measurements were done in duplicate. For optimal oral absorption, logD values should be between 0.5 and 2.

Determination of CHI values. Compound lipophilicity influences permeability and propensity to nonspecific binding to plasma proteins. Although precise, the classical « shake flask » method is not always appropriate for determination of high hydrophobicity, which can be alternatively measured by the Chromatographic Hydrophobicity Index method. This HPLC-based technique leads to rapid and cheap estimates of the partition coefficients. The lipophilicity is determined by partition of the compound between a hydro-organic mobile phase and a reverse stationary phase, typically a C18 column, using a fast gradient. Compound solution samples (200 µM) were prepared in a 50/50 v/v mixture of water and acetonitrile. Five µL were injected onto the HPLC (with UV-Vis detection). CHI values were derived from the retention time and its comparison with 10 reference compounds of known CHI. Measurements were done in duplicate. In general, CHI values correlate satisfactorily with $logD_{7.4}$ values. The CHI is approximately equal to the proportion of acetonitrile inthe mobile phase when the compound is eluted from the column.

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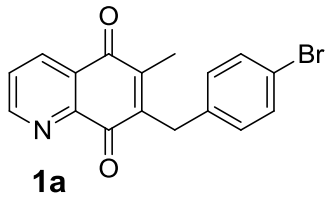
[1] A. Nordhoff, U. S. Bucheler, D. Werner, R. H. Schirmer, *Biochemistry,* 1993, **32**, 4060.

[2] a) T. Müller, L. Johann, B. Jannack, M. Brückner, D. A. Lanfranchi, H. Bauer, C. Sanchez, V. Yardley, C. Deregnaucourt, J. Schrevel, M. Lanzer, R. H. Schirmer, E. Davioud-Charvet, *J. Am. Chem. Soc.,* 2011, **133**, 11557. b) P. M. Färber, L. D. Arscott, C. H. Williams Jr, K. Becker, R. H. Schirmer, *FEBS Lett.,* 1998,**422**, 311

[3] A. N. Kuntz, E. Davioud-Charvet, J. Dessolin, A. A. Sayed, L. L. Califf, E. S. J. Arnér, D. L. Williams, *PLoS Med.,* 2007, **4**, e206, 1. Erratum in *PLoS Med.,* 2007, **4**, e264



1a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DW                       74.400 us
DE                       10.00 us
TE                       298.2 K
D1                    2.00000000 se
TD0                           1

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PL1                      -3.00 dB
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F2 - Processing parameters
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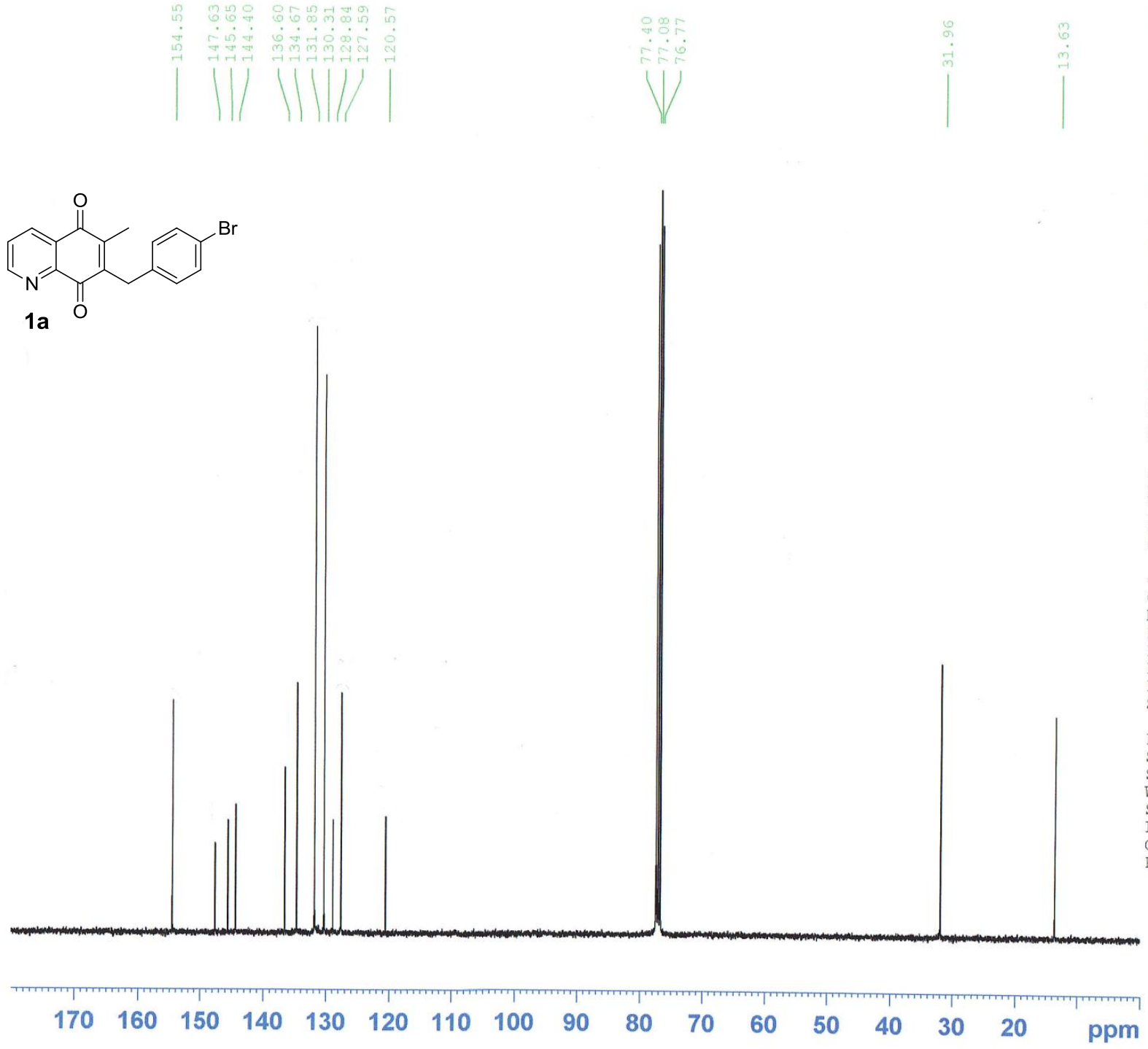


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RG                      1448.2
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TE                      299.2 K
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d11                 0.03000000 se
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PL1                    -6.00 dB
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======== CHANNEL f2 ======
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NUC2                       1H
PCPD2                  80.00 us
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PL13                   18.00 dB
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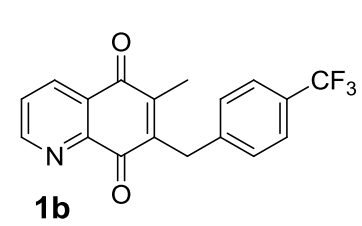

1b

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TE	295.9 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========

NUC1	1H
P1	8.60 usec
PL1	0.00 dB
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SI	16384
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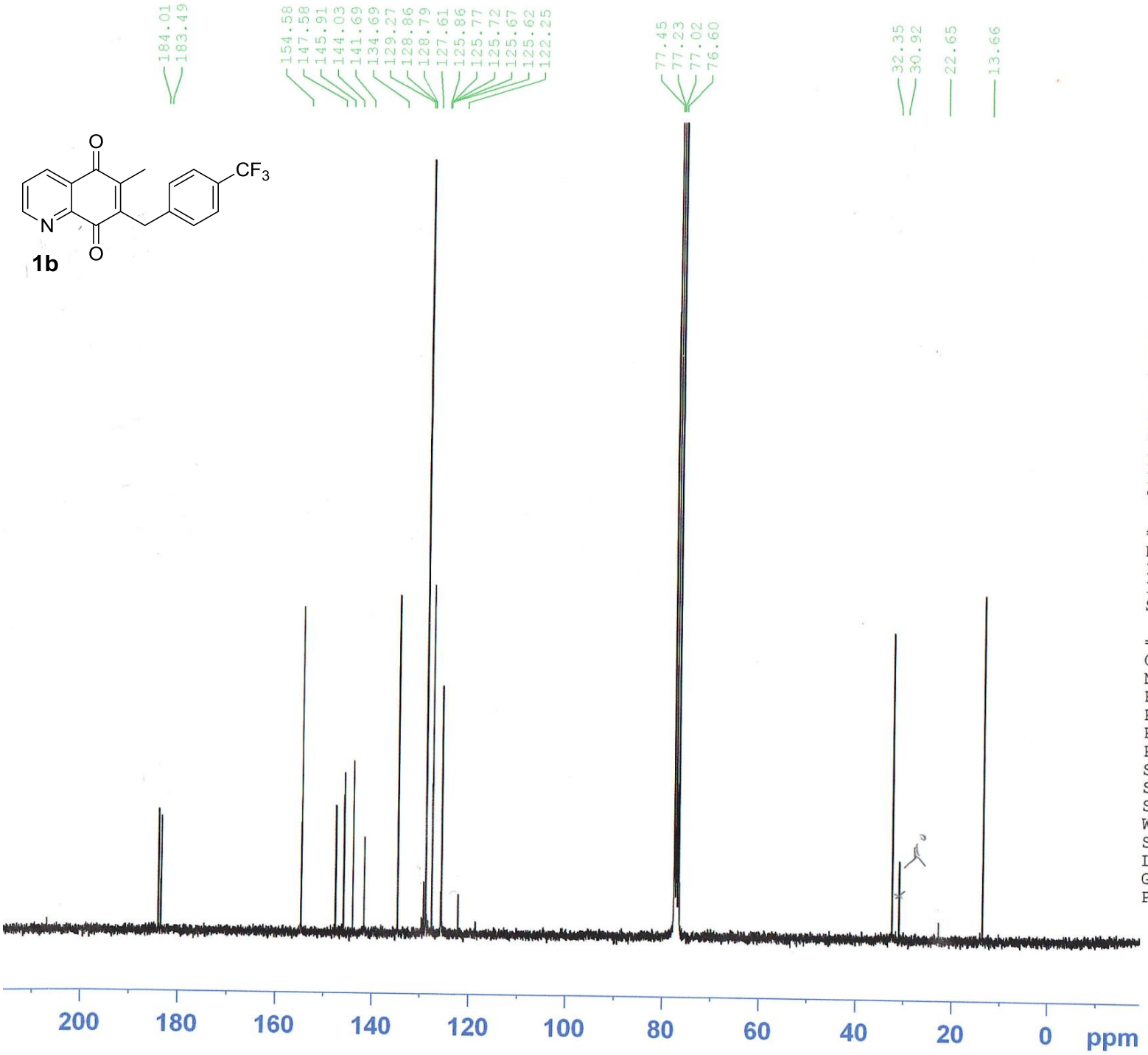
PC	1.00



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AQ	1.8219508 sec
RG	2580.3
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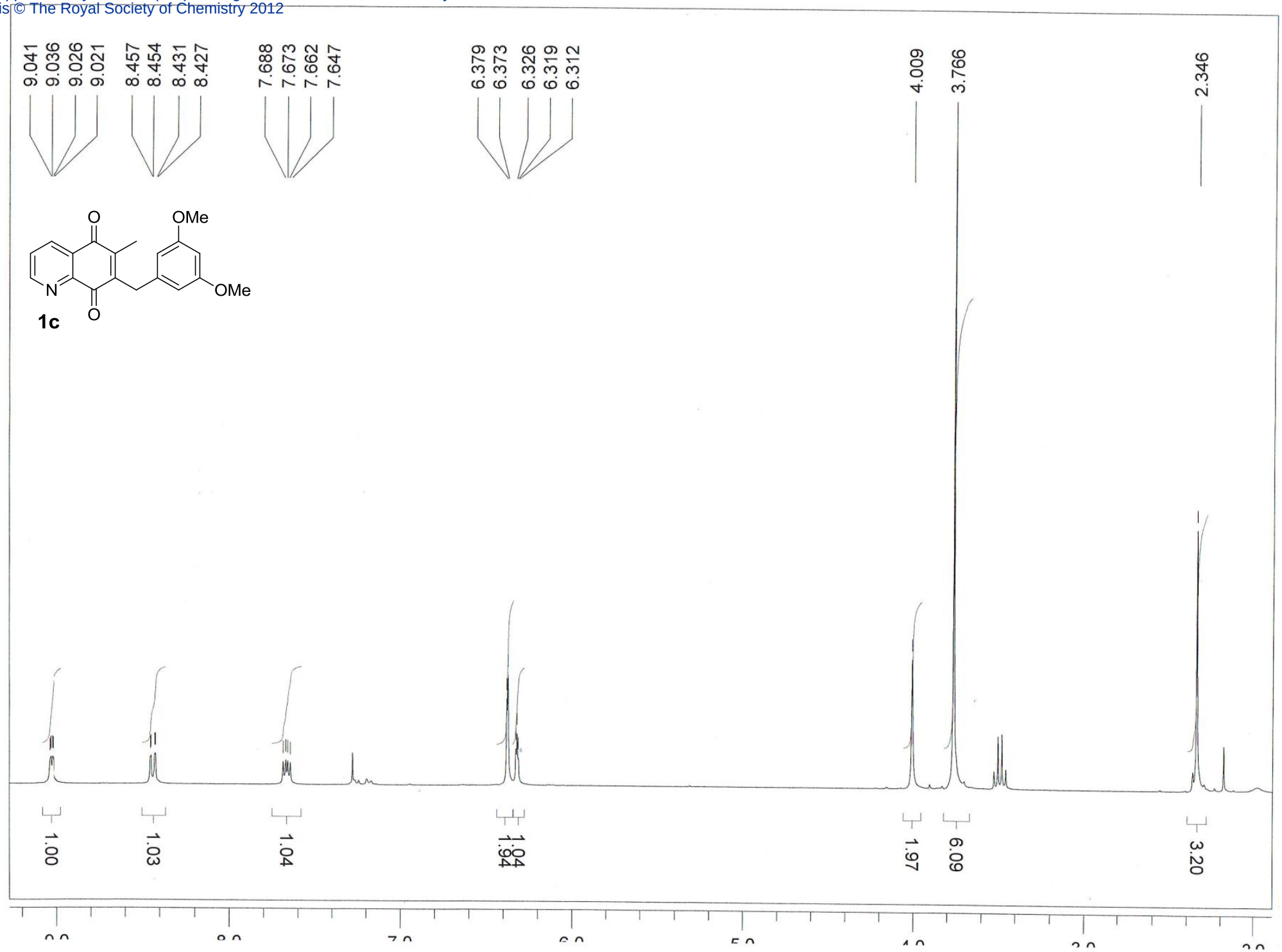
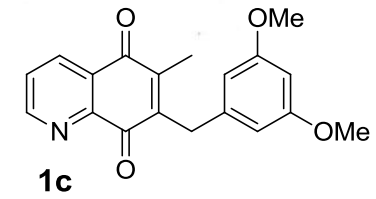
DE	6.50 usec
TE	296.3 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	5.50 usec
PL1	-6.00 dB
SFO1	75.4752953 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	18.06 dB
PL13	20.50 dB
SFO2	300.1312005 MHz
SI	32768
SF	75.4677490 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry





1c

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TD	65536
SOLVENT	CDCl3
NS	800
DS	4
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	4597.6
DW	27.800 usec
DE	6.50 usec
TE	297.3 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
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NUC1	13C
P1	5.50 usec
PL1	-6.00 dB
SFO1	75.4752953 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
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PL12	18.06 dB
PL13	20.50 dB
SFO2	300.1312005 MHz
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SF	75.4677490 MHz
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SSB	0
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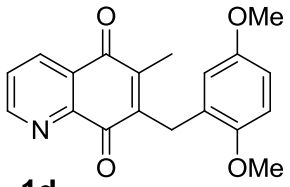

1d

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NS	16
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FIDRES	0.165138 Hz
AQ	3.0278132 sec
RG	456.1
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DE	6.50 usec
TE	297.1 K
D1	1.00000000 sec
TD0	1

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PL1	0.00 dB
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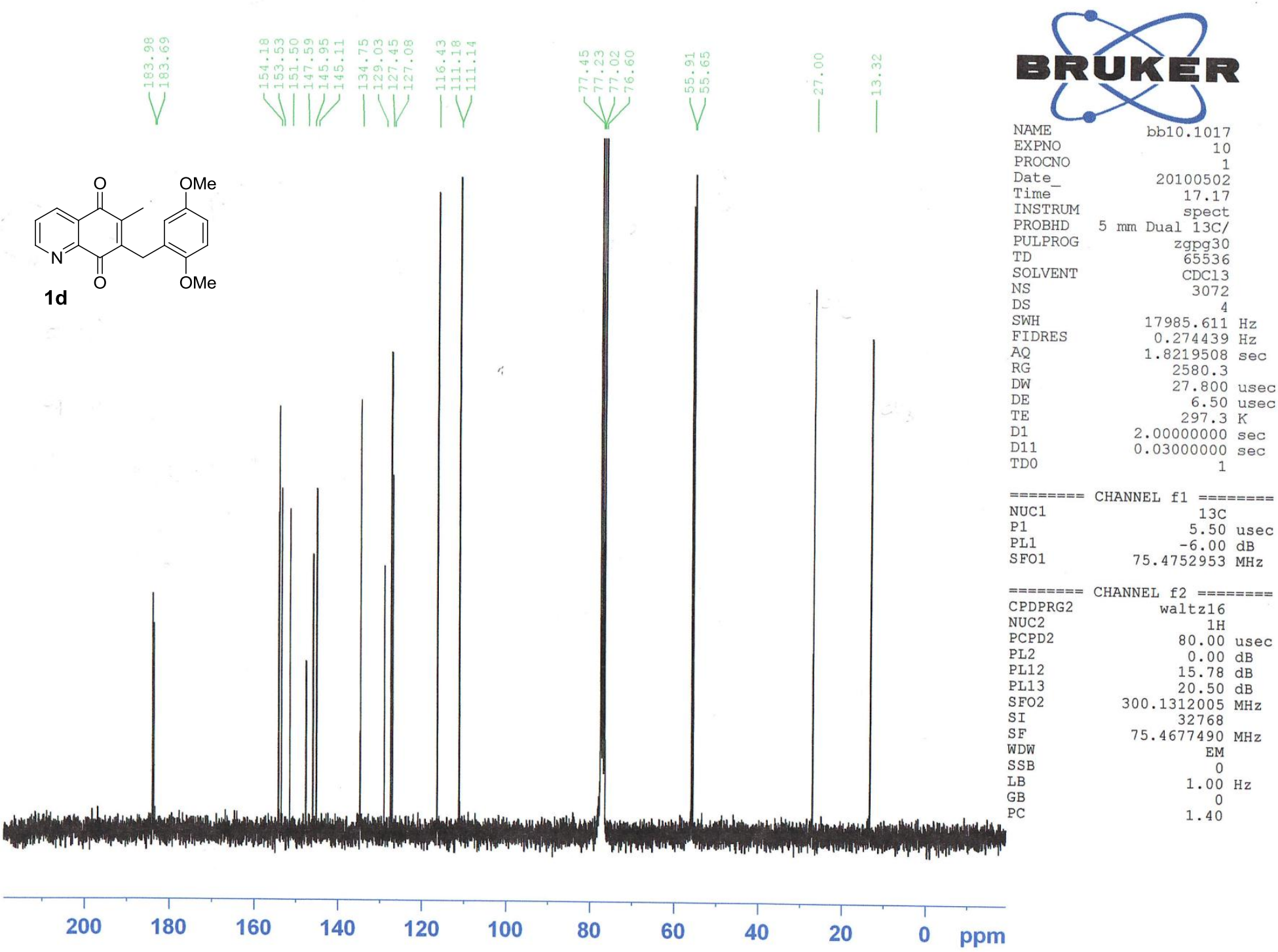
PC	1.00



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SOLVENT	CDCl3
NS	3072
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FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	2580.3
DW	27.800 usec
DE	6.50 usec
TE	297.3 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	5.50 usec
PL1	-6.00 dB
SFO1	75.4752953 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	15.78 dB
PL13	20.50 dB
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SI	32768
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SSB	0
LB	1.00 Hz
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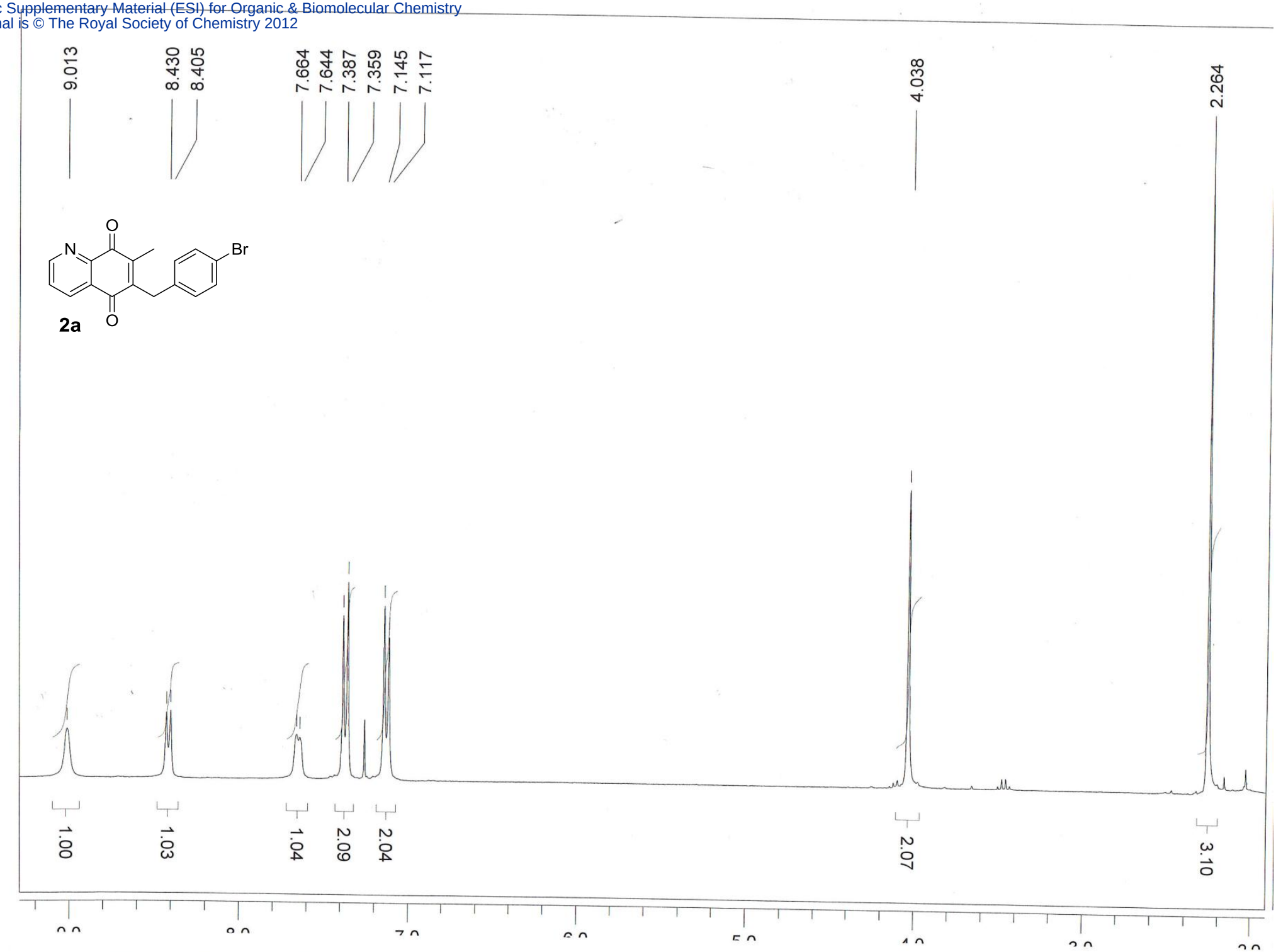
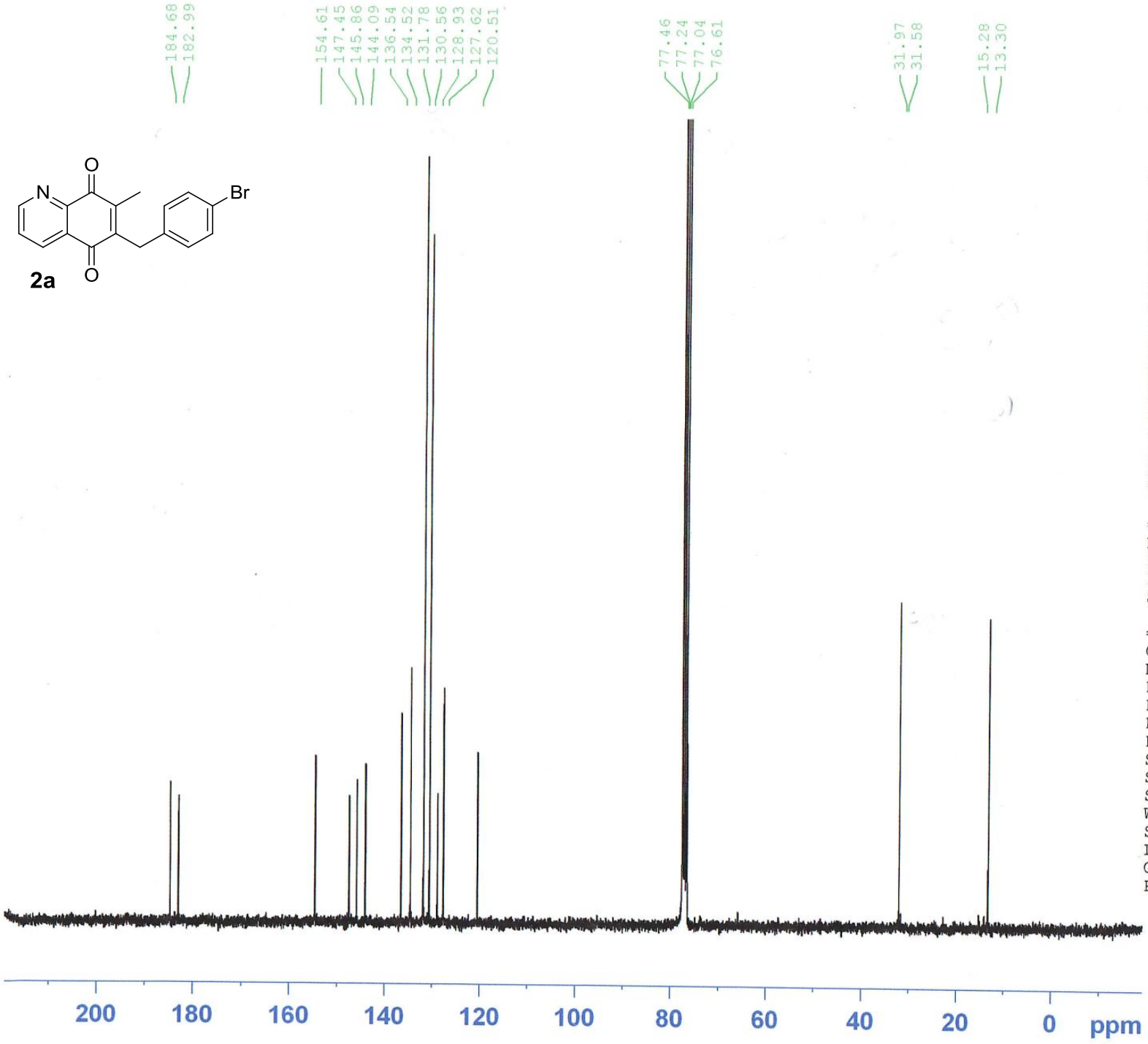
PC	1.40





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FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	4597.6
DW	27.800 usec
DE	6.50 usec
TE	296.7 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	5.50 usec
PL1	-6.00 dB
SFO1	75.4752953 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	18.06 dB
PL13	20.50 dB
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SSB	0
LB	1.00 Hz
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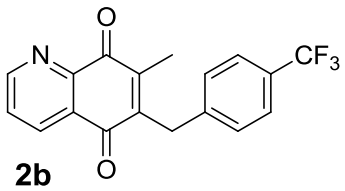
PC	1.40



2b

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PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	2
SWH	5411.255 Hz
FIDRES	0.165138 Hz
AQ	3.0278132 sec
RG	645.1
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DE	6.50 usec
TE	297.3 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	28.00 usec
PL1	-3.00 dB
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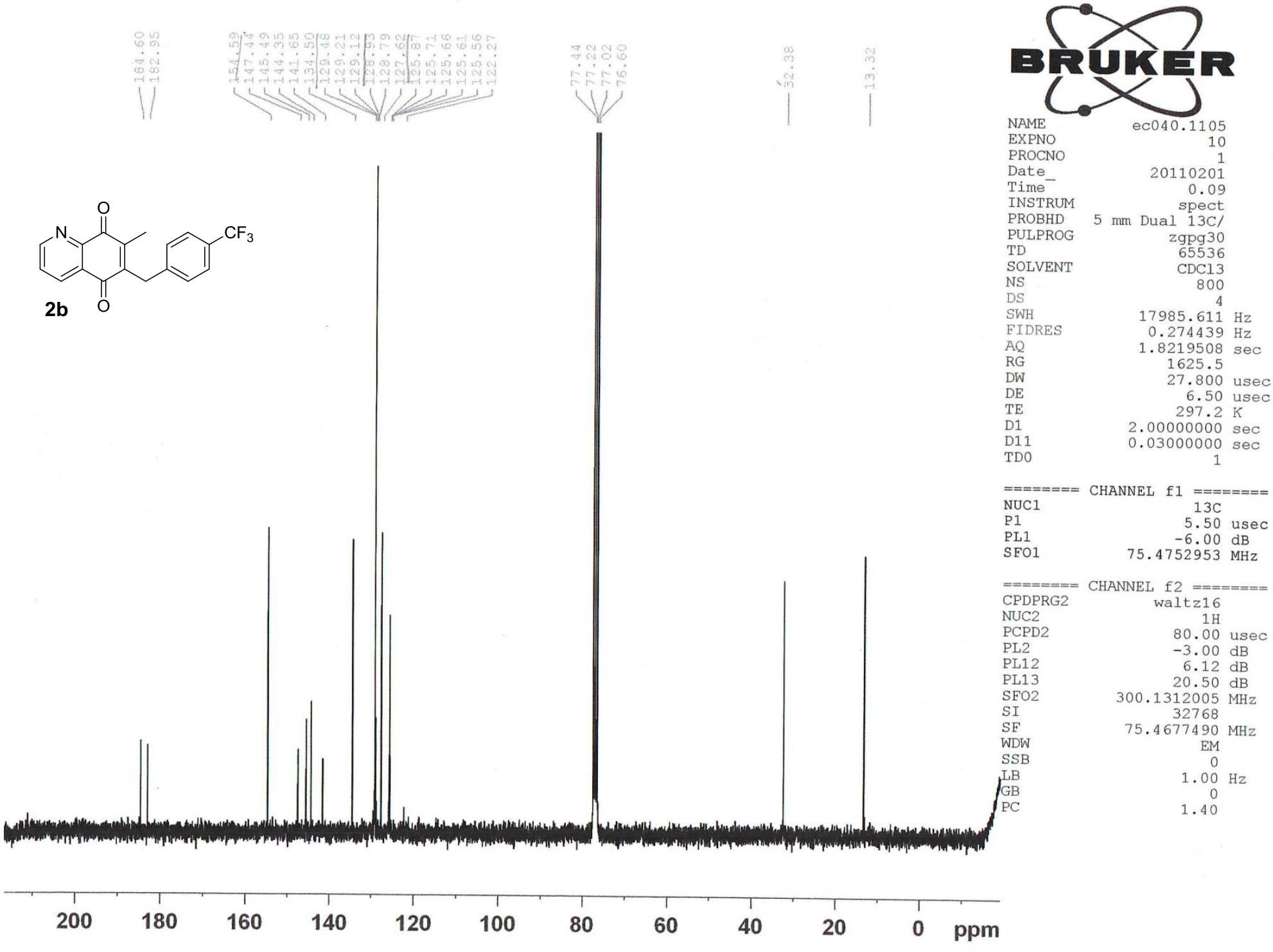

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SOLVENT	CDCl3
NS	800
DS	4
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	1625.5
DW	27.800 usec
DE	6.50 usec
TE	297.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	5.50 usec
PL1	-6.00 dB
SFO1	75.4752953 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-3.00 dB
PL12	6.12 dB
PL13	20.50 dB
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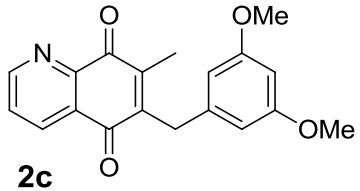
PC	1.40



2c

BRUKER

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NS	16
DS	2
SWH	5411.255 Hz
FIDRES	0.165138 Hz
AQ	3.0278132 sec
RG	362
DW	92.400 usec
DE	6.50 usec
TE	296.8 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========

NUC1	1H
P1	28.00 usec
PL1	-3.00 dB
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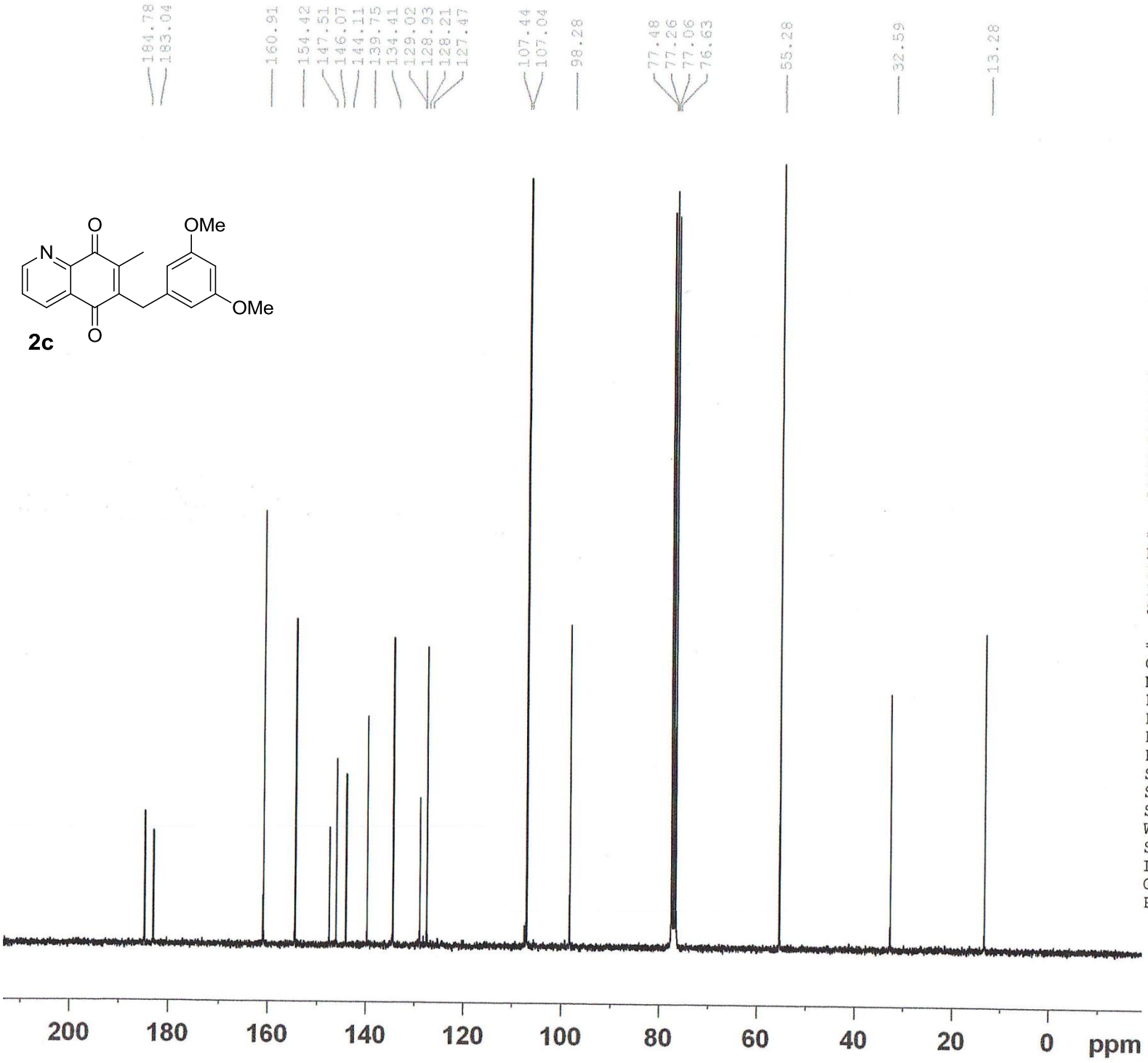

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NS	2048
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FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	574.7
DW	27.800 usec
DE	6.50 usec
TE	297.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	5.50 usec
PL1	-6.00 dB
SFO1	75.4752953 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-3.00 dB
PL12	6.12 dB
PL13	20.50 dB
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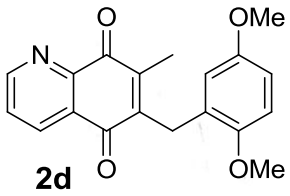
PC	1.40



2d

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DS	2
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FIDRES	0.165138 Hz
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RG	1149.4
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DE	6.50 usec
TE	297.4 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========

NUC1	1H
P1	28.00 usec
PL1	-3.00 dB
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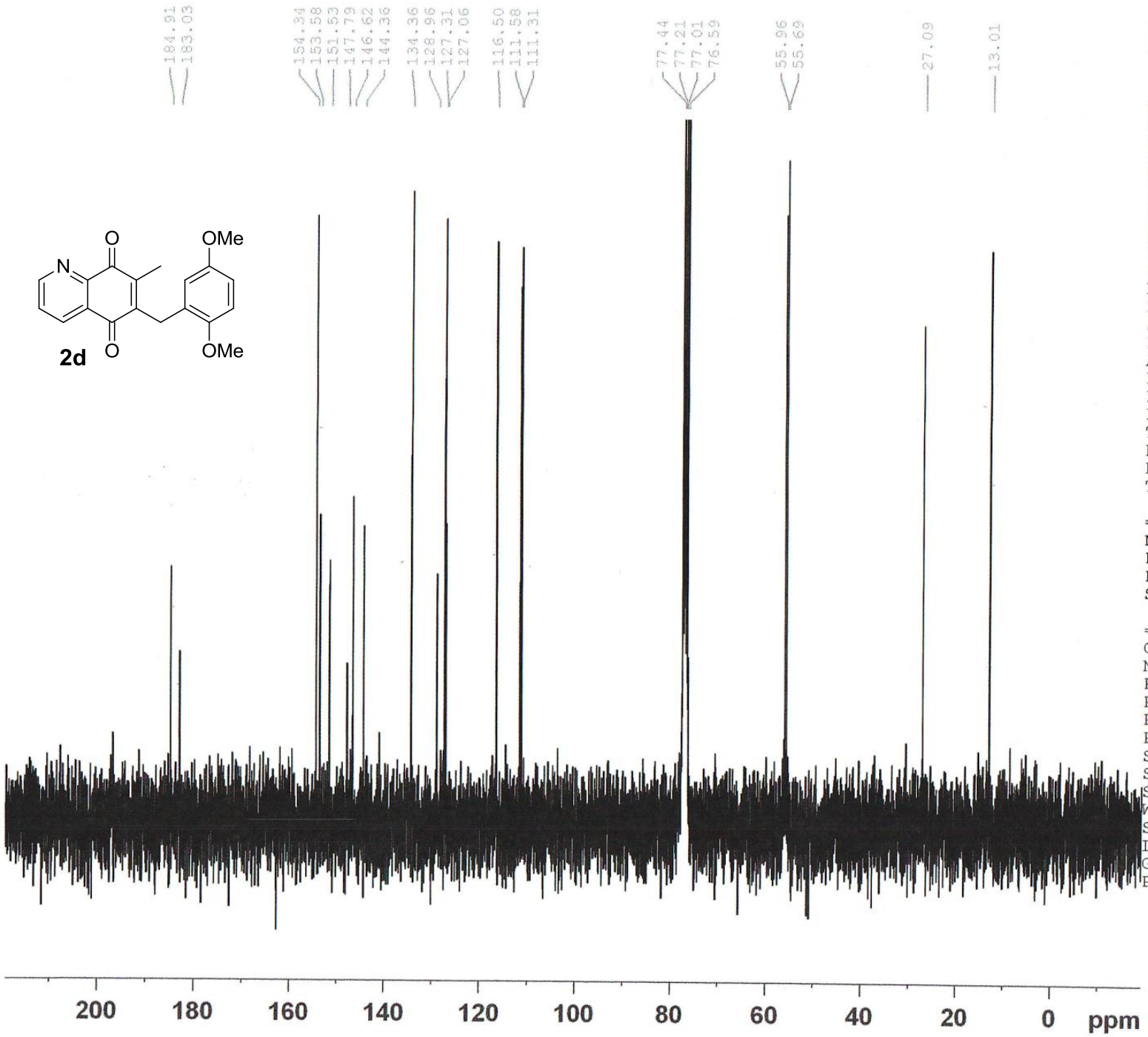

BRUKER

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DS	4
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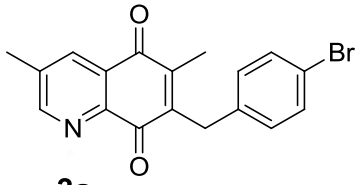
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	1625.5
DW	27.800 usec
DE	6.50 usec
TE	297.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	5.50 usec
PL1	-6.00 dB
SFO1	75.4752953 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-3.00 dB
PL12	6.12 dB
PL13	20.50 dB
SFO2	300.1312005 MHz
SI	32768
SF	75.4677490 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

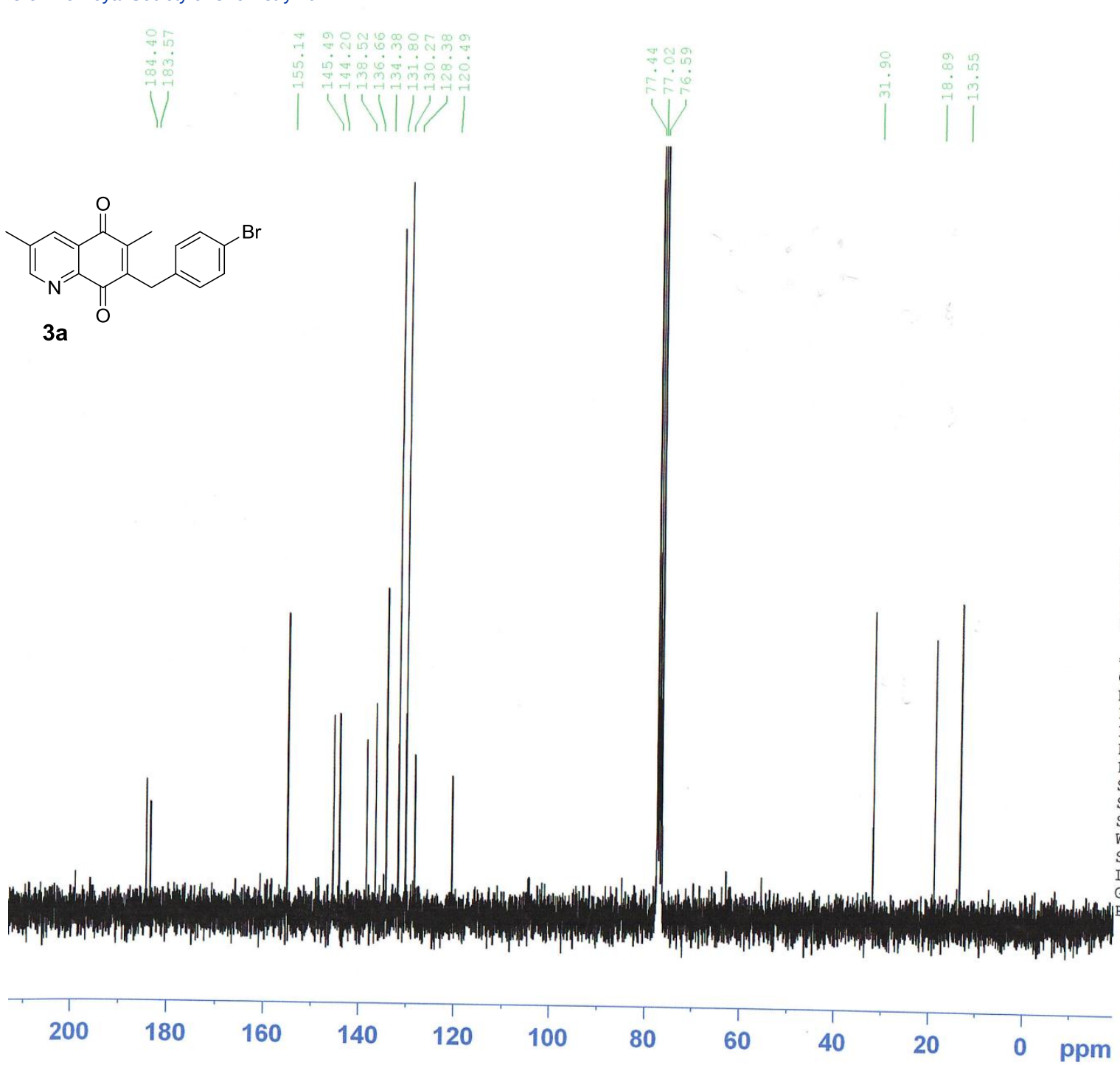


3a

NAME	bb8.1017
EXPNO	12
PROCNO	1
Date_	20100428
Time	1.49
INSTRUM	spect
PROBHD	5 mm Dual 13C/
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	2
SWH	5411.255 Hz
FIDRES	0.165138 Hz
AQ	3.0278132 sec
RG	574.7
DW	92.400 usec
DE	6.50 usec
TE	296.8 K
D1	1.00000000 sec
TD0	1

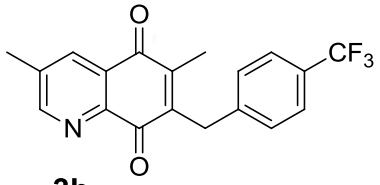
======== CHANNEL f1 ========

NUC1	1H
P1	13.00 usec
PL1	0.00 dB
SFO1	300.1314917 MHz
SI	16384
SF	300.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



BRUKER

NAME	bb8.1017
EXPNO	10
PROCNO	1
Date_	20100428
Time	1.29
INSTRUM	spect
PROBHD	5 mm Dual 13C/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	700
DS	4
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	2580.3
DW	27.800 usec
DE	6.50 usec
TE	297.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	5.50 usec
PL1	-6.00 dB
SFO1	75.4752953 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	15.78 dB
PL13	20.50 dB
SFO2	300.1312005 MHz
SI	32768
SF	75.4677490 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



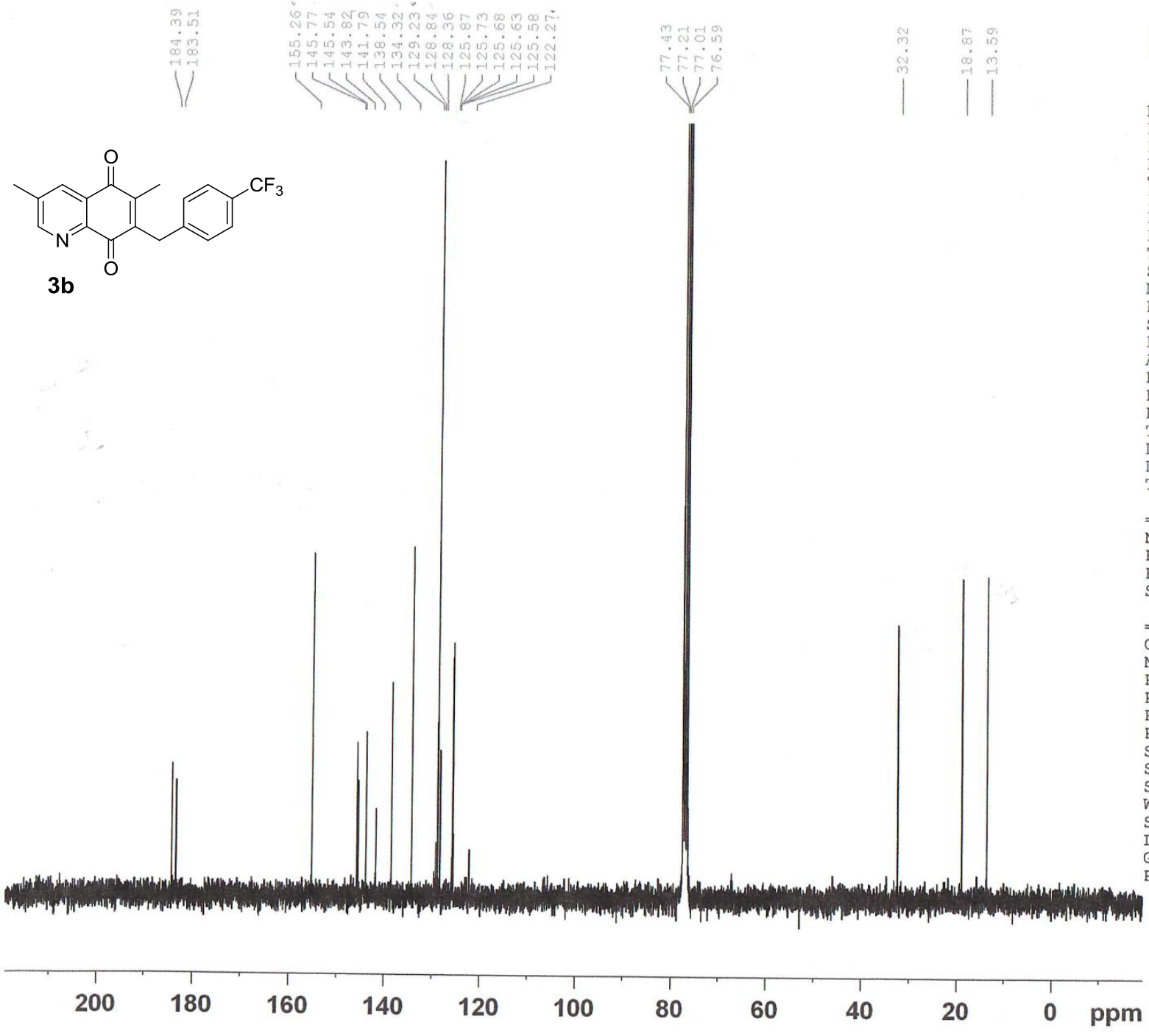
3b

BRUKER

NAME	bb19r.1023
EXPNO	12
PROCNO	1
Date_	20100610
Time	1.05
INSTRUM	spect
PROBHD	5 mm Dual 13C/
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	2
SWH	5411.255 Hz
FIDRES	0.165138 Hz
AQ	3.0278132 sec
RG	645.1
DW	92.400 usec
DE	6.50 usec
TE	297.8 K
D1	1.00000000 sec
TD0	1

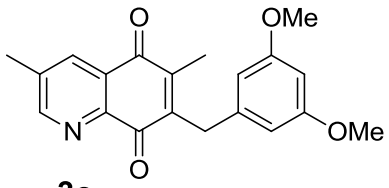
======== CHANNEL f1 ========

NUC1	1H
P1	13.00 usec
PL1	0.00 dB
SFO1	300.1314917 MHz
SI	16384
SF	300.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



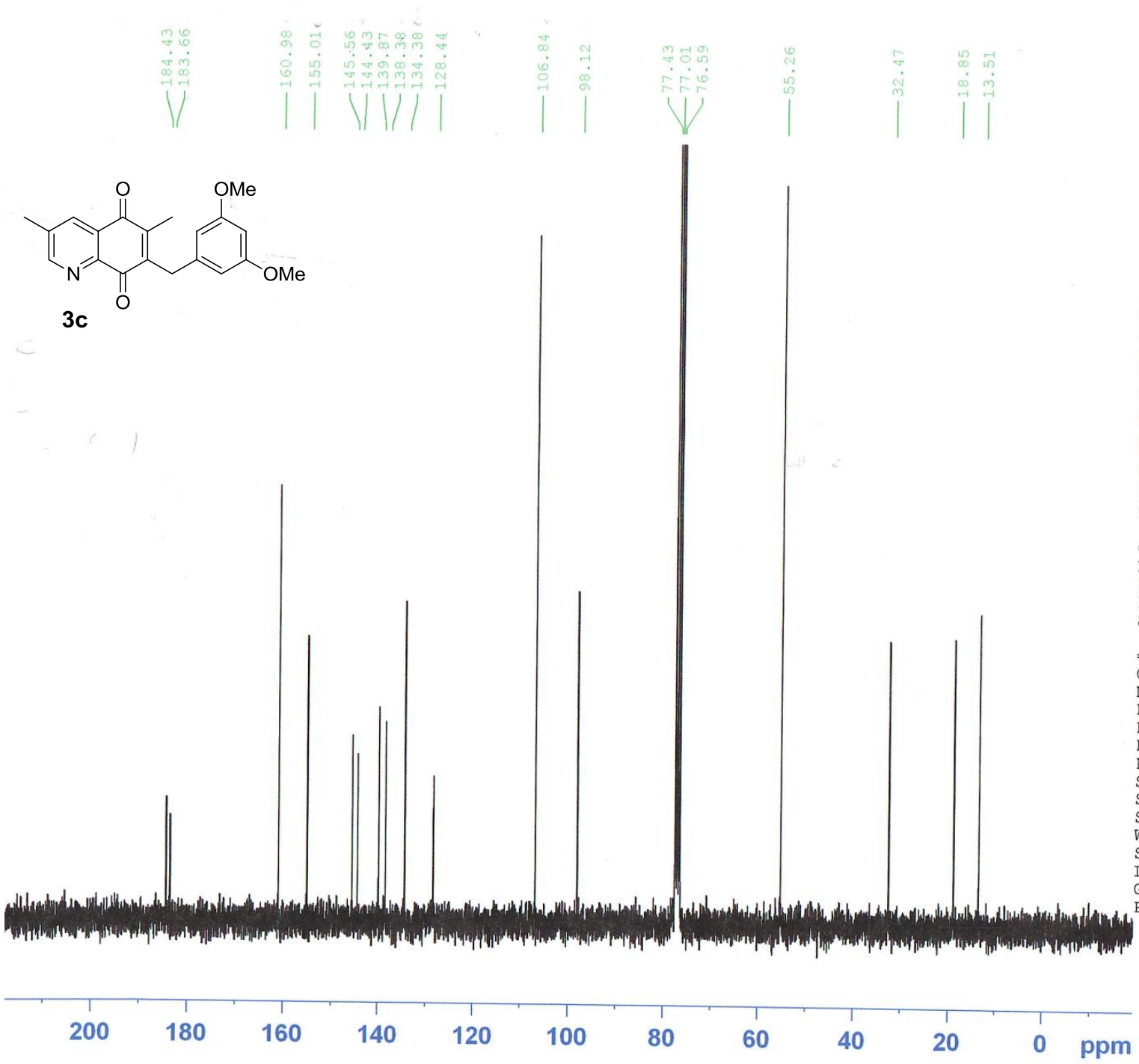
BRUKER

NAME	bb19r.1023
EXPNO	10
PROCNO	1
Date_	20100610
Time	0.24
INSTRUM	spect
PROBHD	5 mm Dual 13C/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	2048
DS	4
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	4597.6
DW	27.800 usec
DE	6.50 usec
TE	298.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	5.50 usec
PL1	-6.00 dB
SFO1	75.4752953 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	15.78 dB
PL13	20.50 dB
SFO2	300.1312005 MHz
SI	32768
SF	75.4677490 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



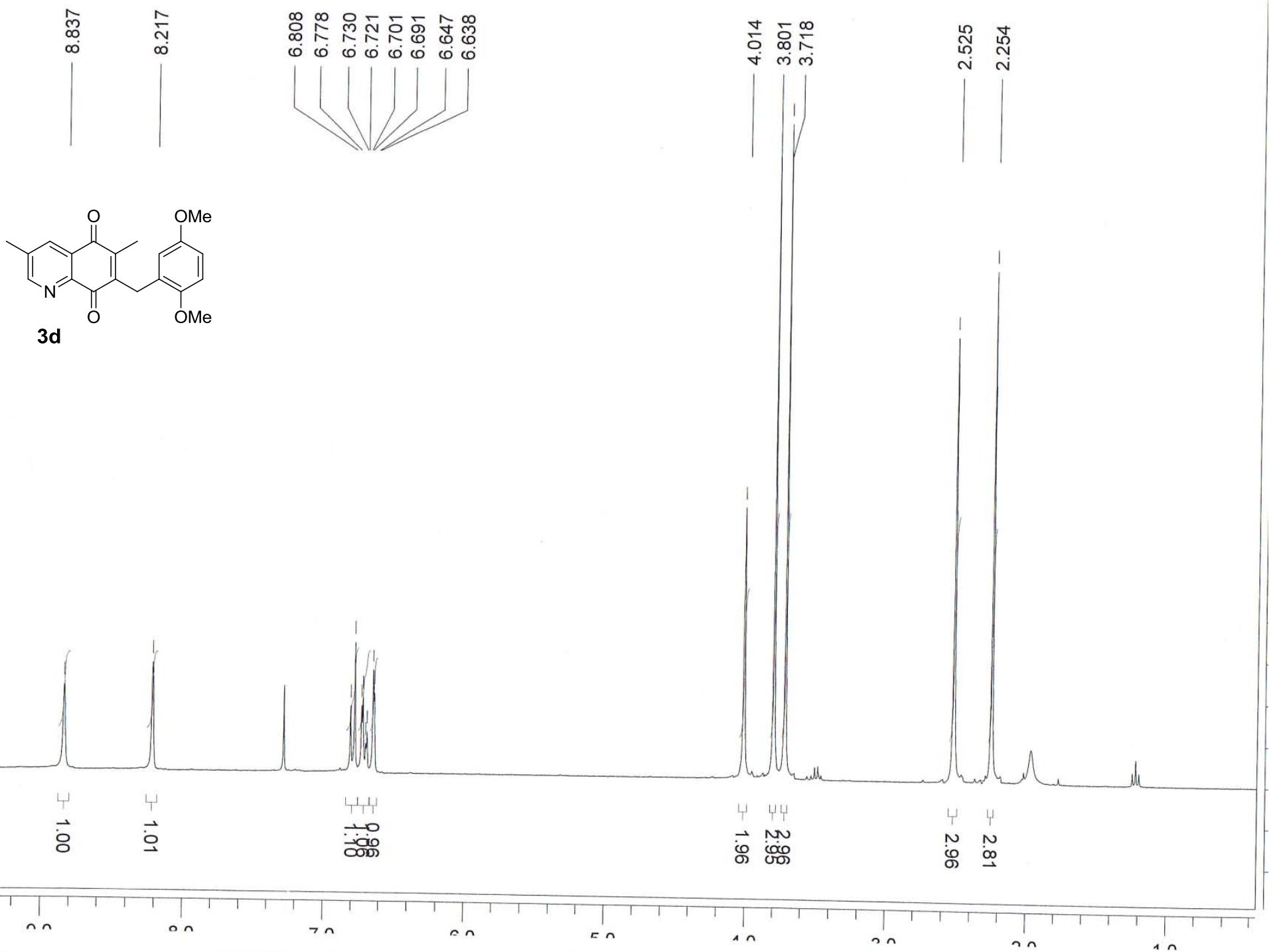
3c

NAME	bb16.1020
EXPNO	12
PROCNO	1
Date_	20100519
Time	19.27
INSTRUM	spect
PROBHD	5 mm Dual 13C/
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	2
SWH	5411.255 Hz
FIDRES	0.165138 Hz
AQ	3.0278132 sec
RG	512
DW	92.400 usec
DE	6.50 usec
TE	300.0 K
D1	1.00000000 sec
TD0	1
========	CHANNEL f1 ========
NUC1	1H
P1	13.00 usec
PL1	0.00 dB
SFO1	300.1314917 MHz
SI	16384
SF	300.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

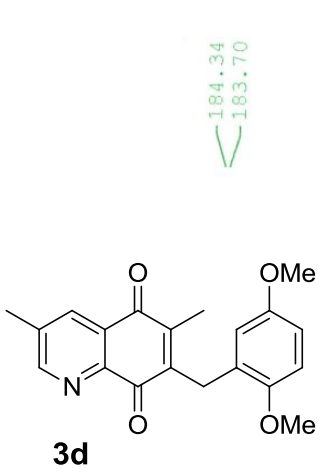


BRUKER

NAME	bb16.1020
EXPNO	10
PROCNO	1
Date_	20100519
Time	18.58
INSTRUM	spect
PROBHD	5 mm Dual 13C/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	7298.2
DW	27.800 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	5.50 usec
PL1	-6.00 dB
SFO1	75.4752953 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	15.78 dB
PL13	20.50 dB
SFO2	300.1312005 MHz
SI	32768
SF	75.4677490 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

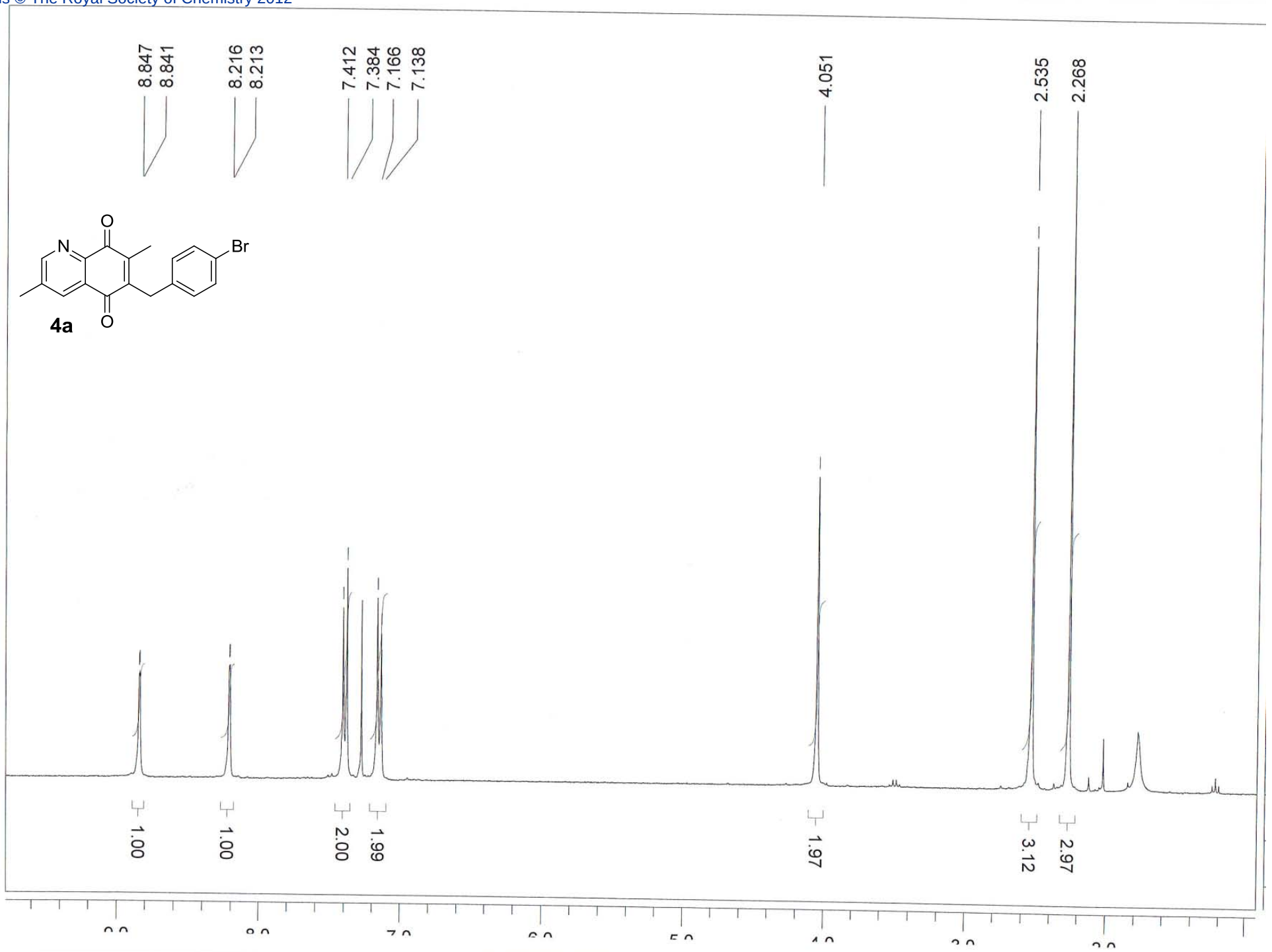


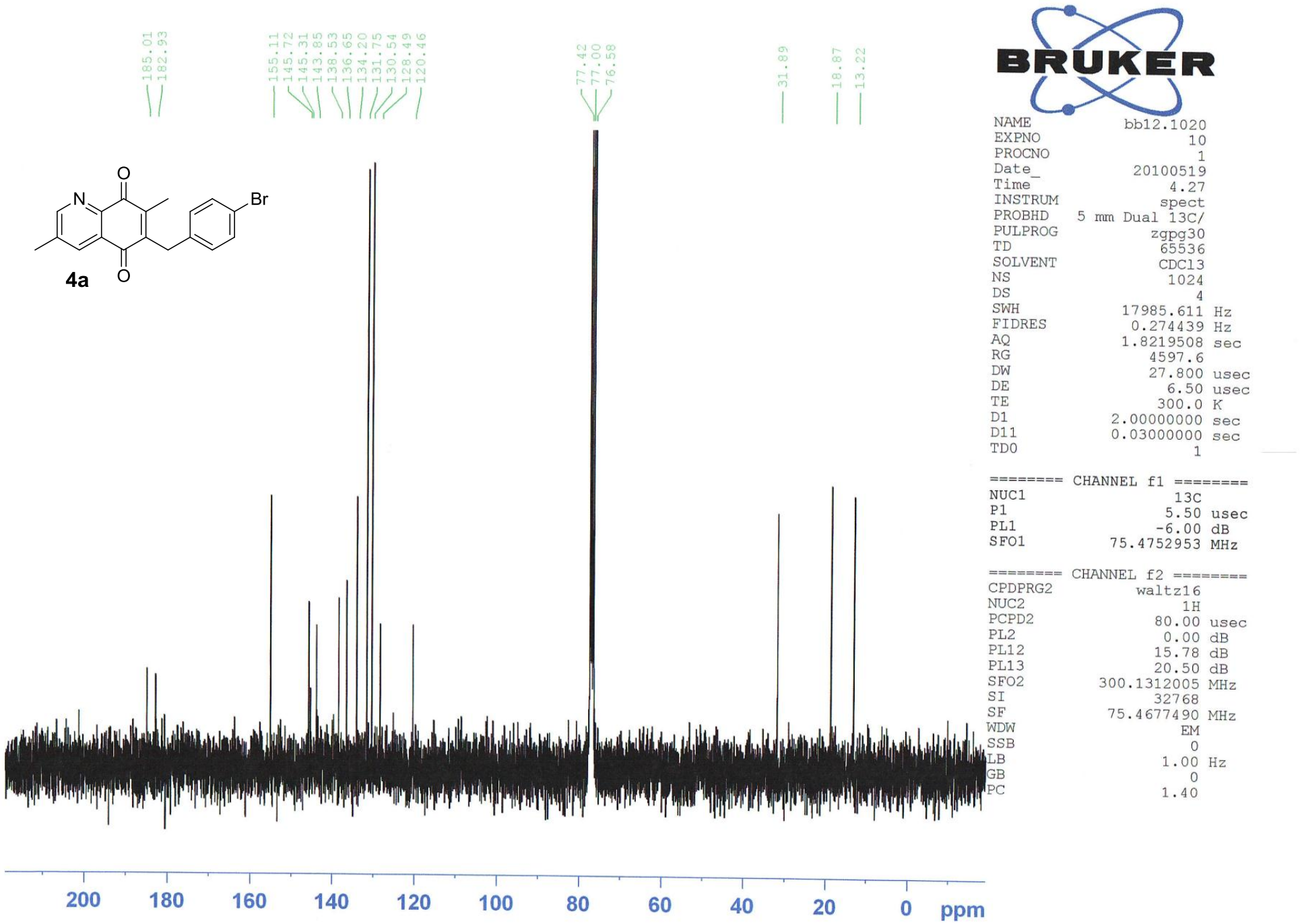
3d



3d

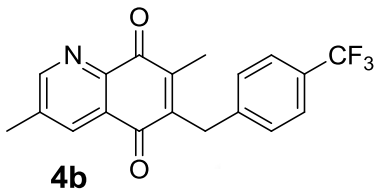
NAME	bb17.1021
EXPNO	10
PROCNO	1
Date_	20100525
Time	20.18
INSTRUM	spect
PROBHD	5 mm Dual 13C/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	900
DS	4
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	4096
DW	27.800 usec
DE	6.50 usec
TE	298.5 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	5.50 usec
PL1	-6.00 dB
SFO1	75.4752953 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	15.78 dB
PL13	20.50 dB
SFO2	300.1312005 MHz
SI	32768
SF	75.4677490 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40





BRUKER

NAME	bb12.1020
EXPNO	10
PROCNO	1
Date_	20100519
Time	4.27
INSTRUM	spect
PROBHD	5 mm Dual 13C/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	4597.6
DW	27.800 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	5.50 usec
PL1	-6.00 dB
SFO1	75.4752953 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	15.78 dB
PL13	20.50 dB
SFO2	300.1312005 MHz
SI	32768
SF	75.4677490 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



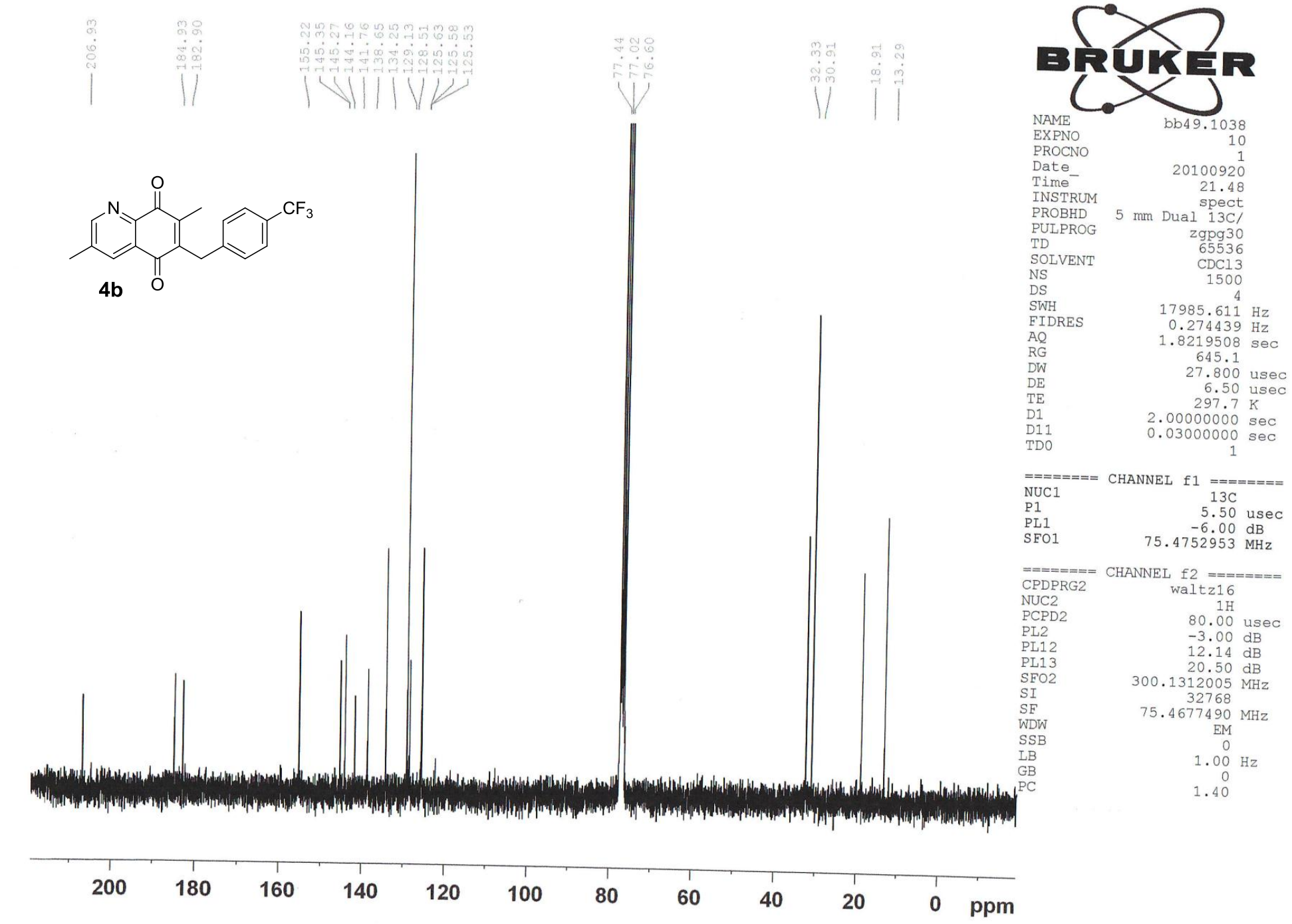
4b

BRUKER

NAME	bb49.1038
EXPNO	12
PROCNO	1
Date_	20100920
Time	22.24
INSTRUM	spect
PROBHD	5 mm Dual 13C/
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	2
SWH	5411.255 Hz
FIDRES	0.165138 Hz
AQ	3.0278132 sec
RG	574.7
DW	92.400 usec
DE	6.50 usec
TE	297.3 K
D1	1.00000000 sec
TD0	1

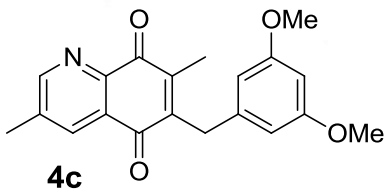
======== CHANNEL f1 ========

NUC1	1H
P1	14.00 usec
PL1	-3.00 dB
SFO1	300.1314917 MHz
SI	16384
SF	300.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



BRUKER

NAME	bb49.1038
EXPNO	10
PROCNO	1
Date_	20100920
Time_	21.48
INSTRUM	spect
PROBHD	5 mm Dual 13C/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1500
DS	4
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	645.1
DW	27.800 usec
DE	6.50 usec
TE	297.7 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	5.50 usec
PL1	-6.00 dB
SFO1	75.4752953 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-3.00 dB
PL12	12.14 dB
PL13	20.50 dB
SFO2	300.1312005 MHz
SI	32768
SF	75.4677490 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



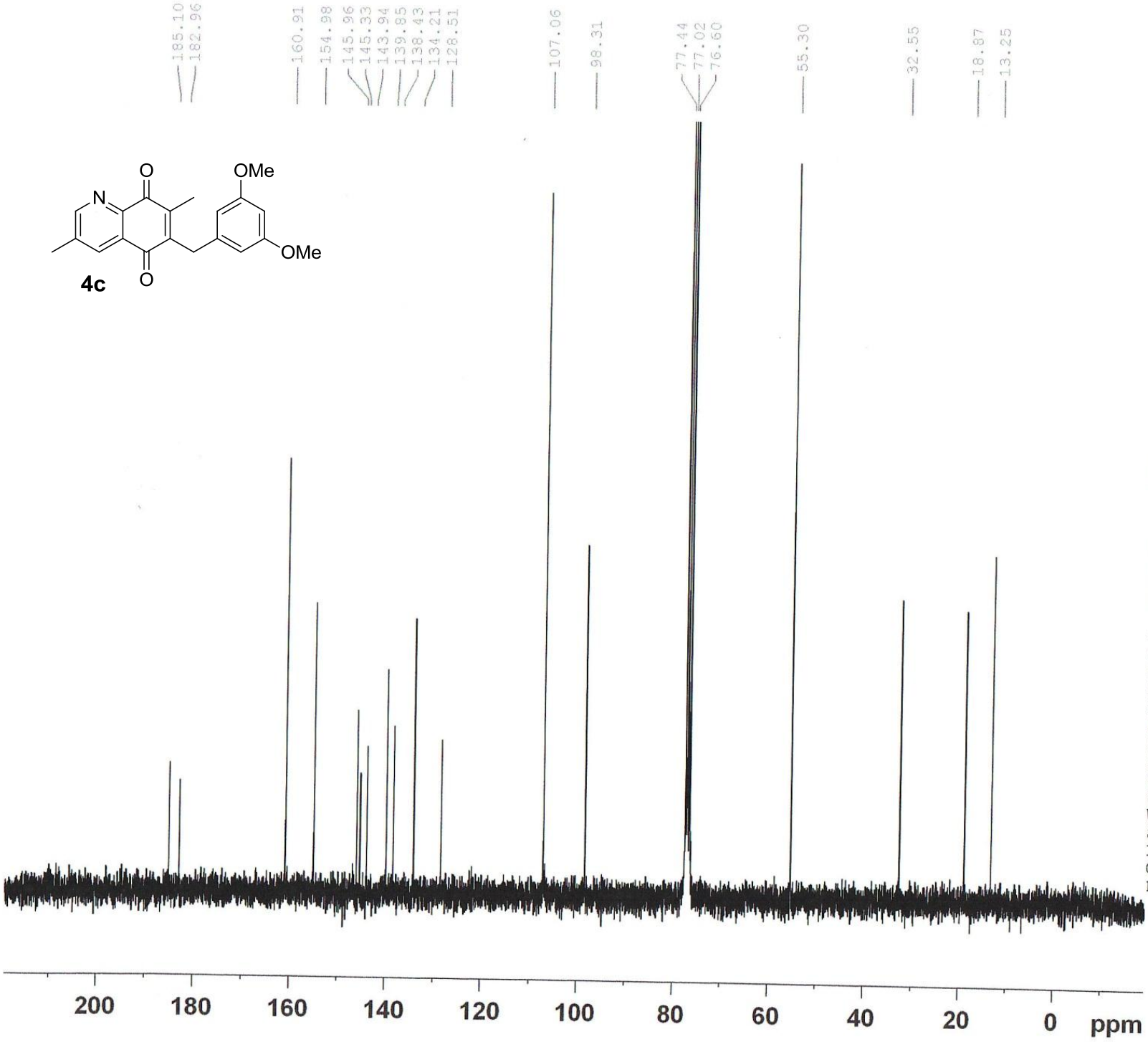
4c

BRUKER

NAME	bb48.1038
EXPNO	12
PROCNO	1
Date_	20100920
Time	19.23
INSTRUM	spect
PROBHD	5 mm Dual 13C/
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	2
SWH	5411.255 Hz
FIDRES	0.165138 Hz
AQ	3.0278132 sec
RG	574.7
DW	92.400 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1

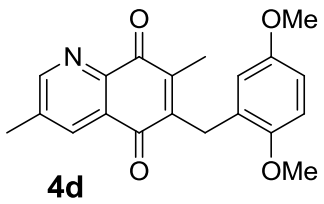
======== CHANNEL f1 ========

NUC1	1H
P1	14.00 usec
PL1	-3.00 dB
SFO1	300.1314917 MHz
SI	16384
SF	300.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



BRUKER

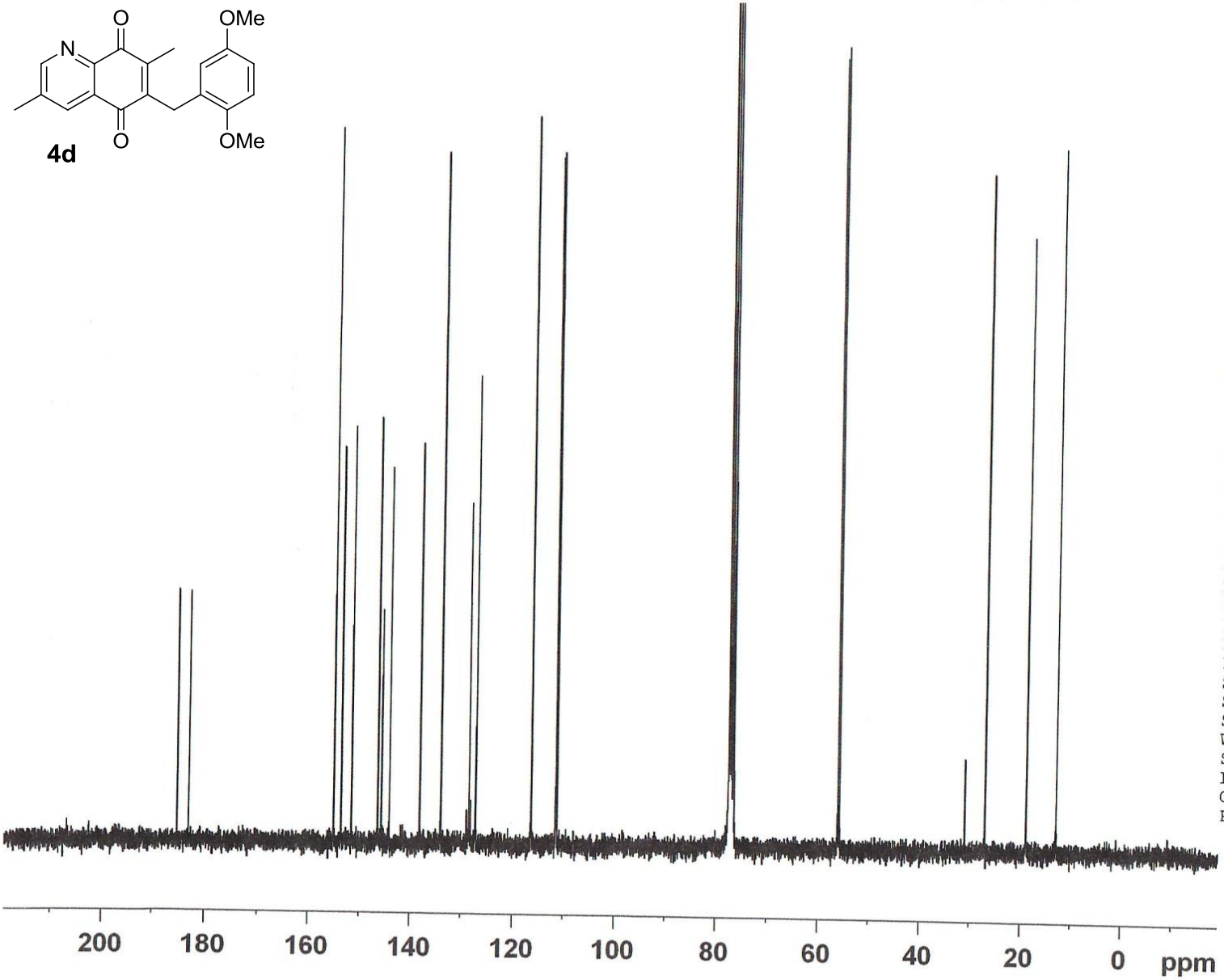
NAME	bb48.1038
EXPNO	10
PROCNO	1
Date_	20100920
Time	18.48
INSTRUM	spect
PROBHD	5 mm Dual 13C/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	1024
DW	27.800 usec
DE	6.50 usec
TE	298.3 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	5.50 usec
PL1	-6.00 dB
SFO1	75.4752953 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-3.00 dB
PL12	12.14 dB
PL13	20.50 dB
SFO2	300.1312005 MHz
SI	32768
SF	75.4677490 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



4d

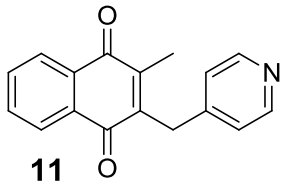
BRUKER

NAME	bb27.1023
EXPNO	12
PROCNO	1
Date_	20100612
Time	14.45
INSTRUM	spect
PROBHD	5 mm Dual 13C/
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	2
SWH	5411.255 Hz
FIDRES	0.165138 Hz
AQ	3.0278132 sec
RG	362
DW	92.400 usec
DE	6.50 usec
TE	298.5 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.00 usec
PL1	0.00 dB
SFO1	300.1314917 MHz
SI	16384
SF	300.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



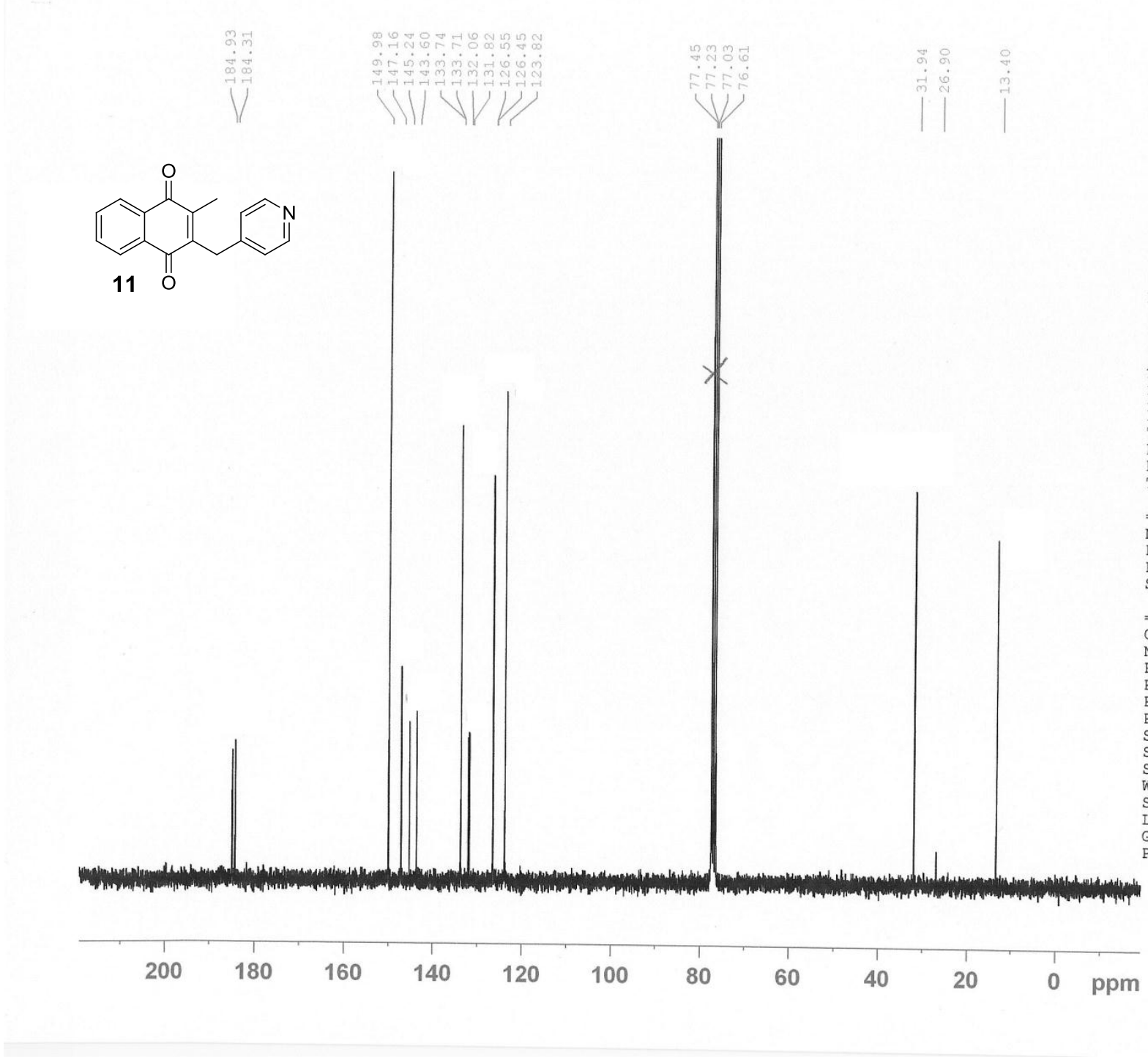
BRUKER

NAME	bb27.1023
EXPNO	10
PROCNO	1
Date_	20100612
Time	13.51
INSTRUM	spect
PROBHD	5 mm Dual 13C/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	4096
DS	4
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	5792.6
DW	27.800 usec
DE	6.50 usec
TE	298.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	5.50 usec
PL1	-6.00 dB
SFO1	75.4752953 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	15.78 dB
PL13	20.50 dB
SFO2	300.1312005 MHz
SI	32768
SF	75.4677490 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



11

NAME	LJ186K.1017
EXPNO	22
PROCNO	1
Date_	20100430
Time	2.34
INSTRUM	spect
PROBHD	5 mm Dual 13C/
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	2
SWH	5411.255 Hz
FIDRES	0.165138 Hz
AQ	3.0278132 sec
RG	362
DW	92.400 usec
DE	6.50 usec
TE	297.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.00 usec
PL1	0.00 dB
SFO1	300.1314917 MHz
SI	16384
SF	300.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



BRUKER

NAME	LJ186K.1017
EXPNO	20
PROCNO	1
Date_	20100430
Time	2.15
INSTRUM	spect
PROBHD	5 mm Dual 13C/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	800
DS	4
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	2580.3
DW	27.800 usec
DE	6.50 usec
TE	297.5 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	5.50 usec
PL1	-6.00 dB
SFO1	75.4752953 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	15.78 dB
PL13	20.50 dB
SFO2	300.1312005 MHz
SI	32768
SF	75.4677490 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40