

Preparation of a 12-membered Open-Cage Fullerendione through Silane/Borane Promoted Formation of Ketal Moieties and Oxidation of a Vicinal Fullerendiol

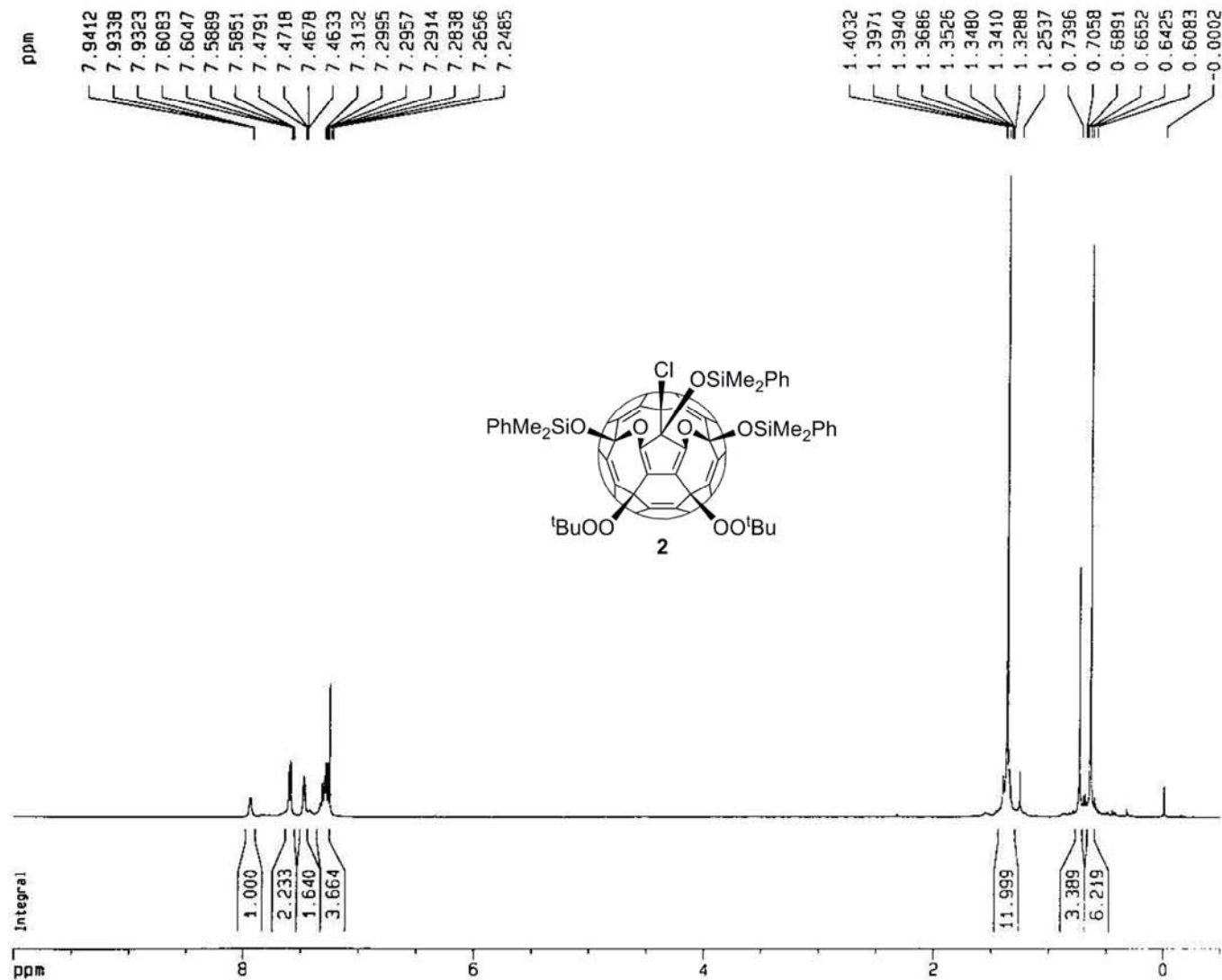
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 PROCNO 1

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F2 - Processing parameters
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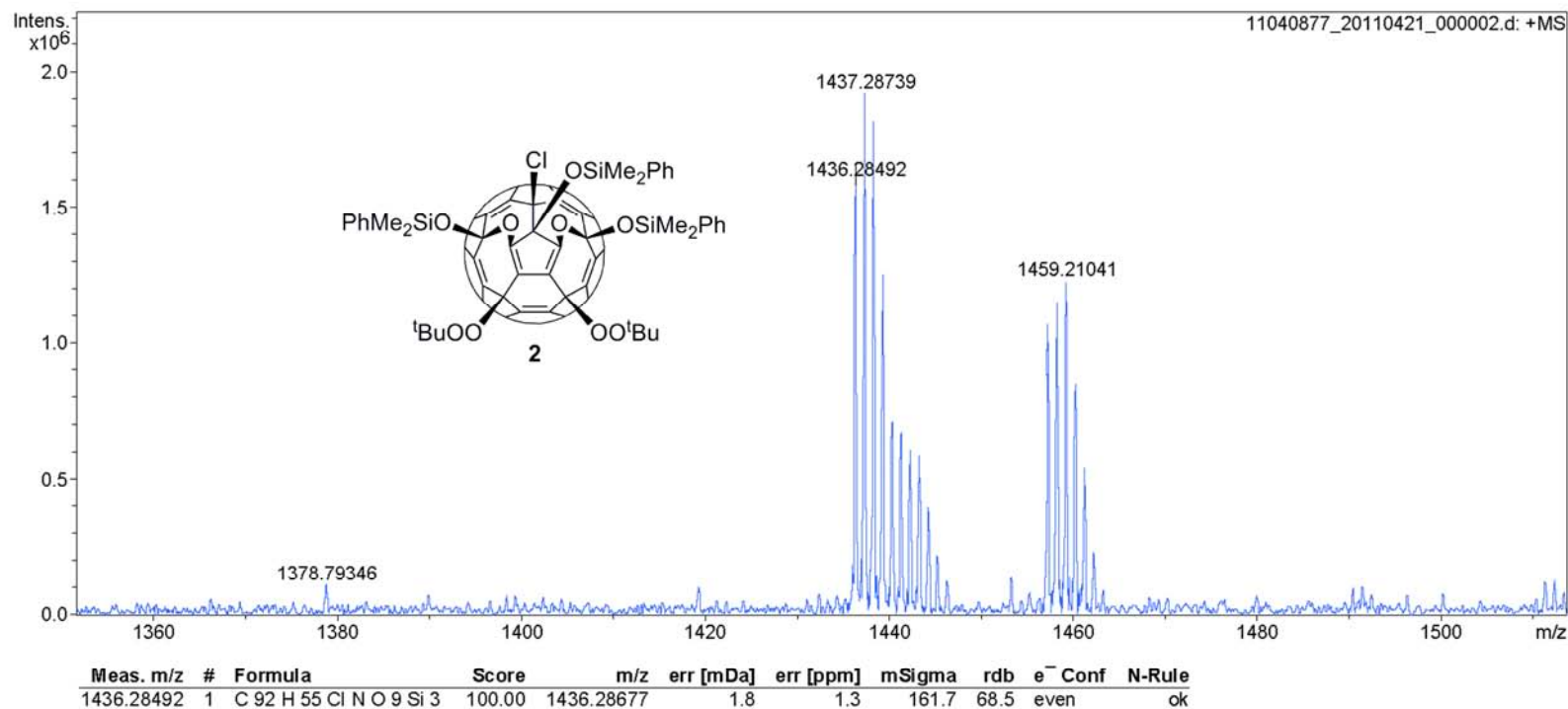
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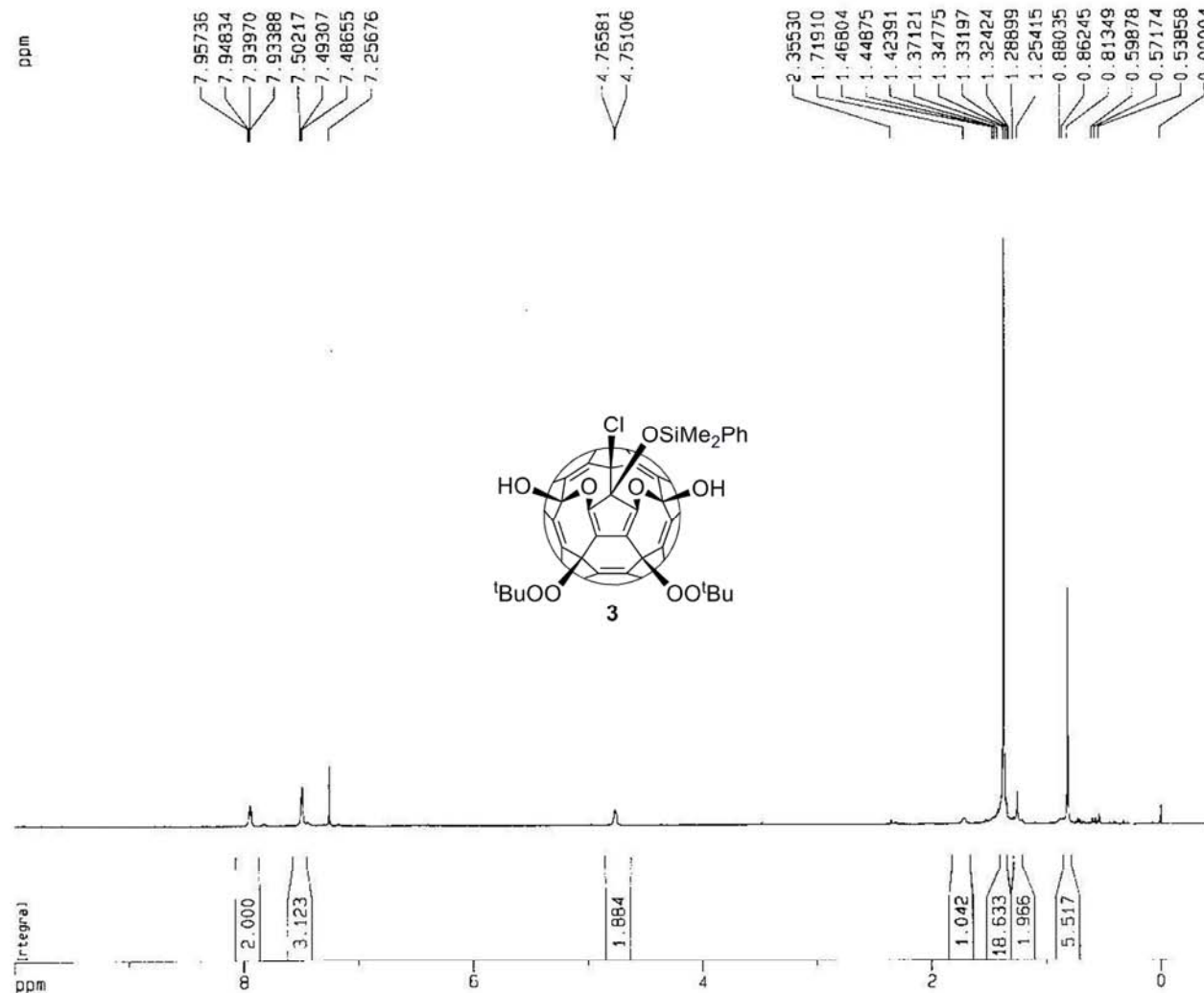
Peking University Mass Spectrometry Sample Analysis Report

Analysis Info

Analysis Name 11040877_20110421_000002.d
Sample 110417
Comment ESI Positive

Acquisition Date 4/21/2011 12:08:34 PM
Instrument Bruker Apex IV FTMS
Operator Peking University





Current Data Parameters
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EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

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PULPROG zg
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TE 300.0 K
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P1 3.00 usec
DE 98.57 usec
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F2 - Processing parameters

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1D NMR plot parameters

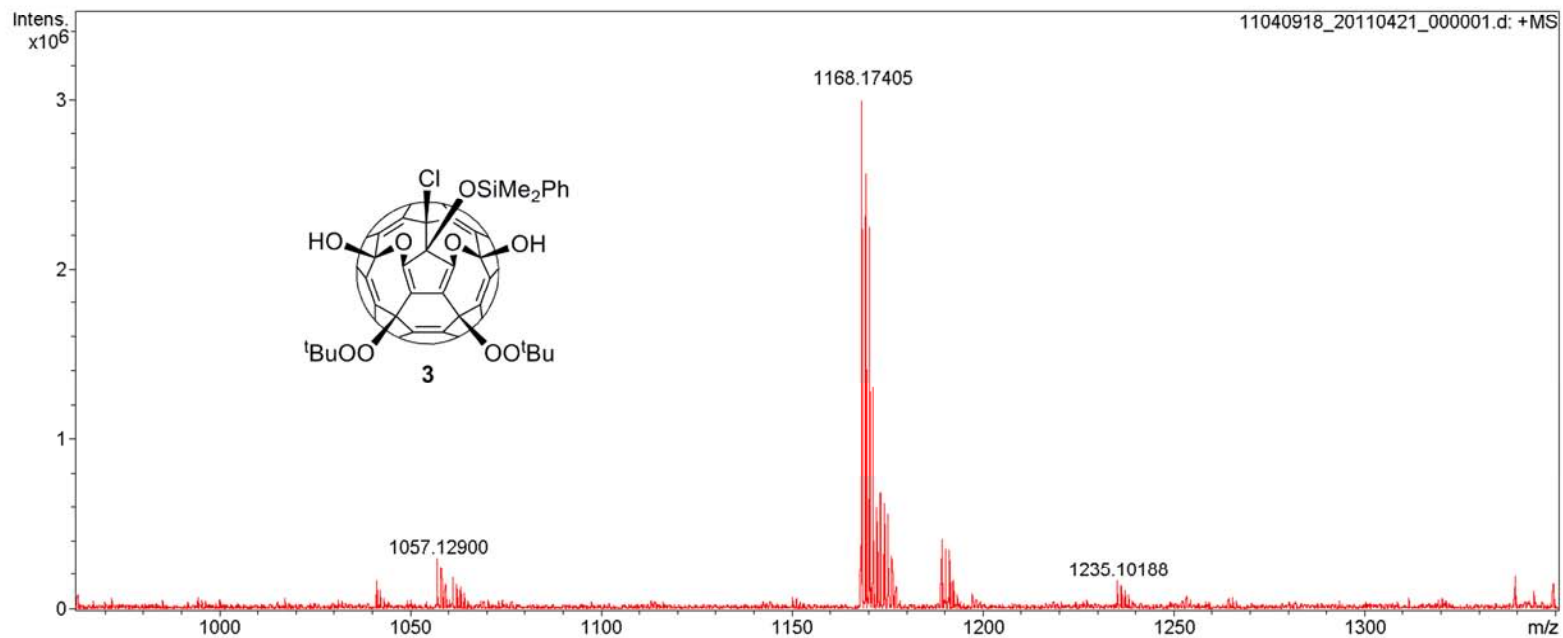
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Peking University Mass Spectrometry Sample Analysis Report

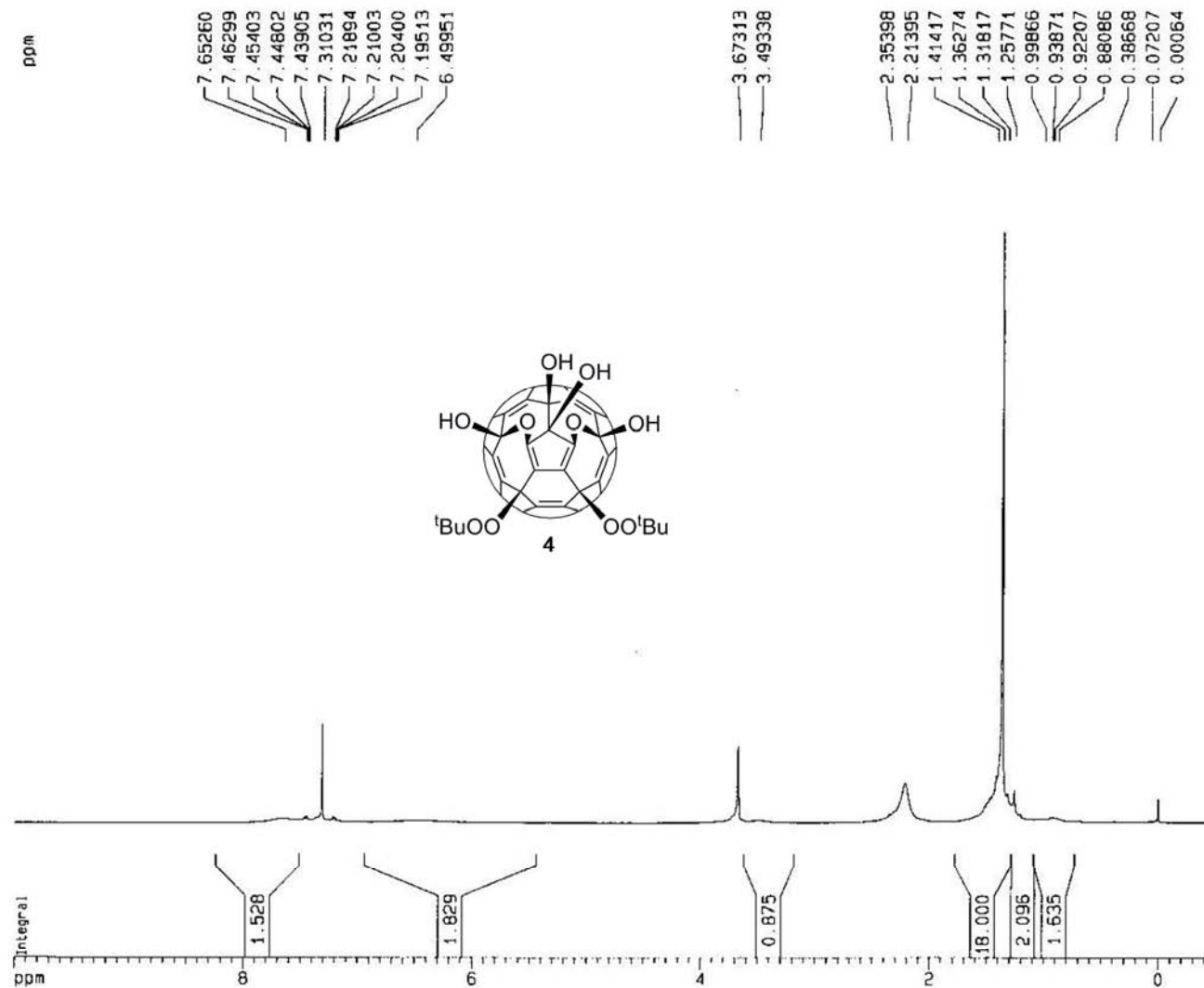
Analysis Info

Analysis Name 11040918_20110421_000001.d
Sample 110421
Comment ESI Positive

Acquisition Date 4/21/2011 5:08:13 PM
Instrument Bruker Apex IV FTMS
Operator Peking University



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
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Current Data Parameters
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EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

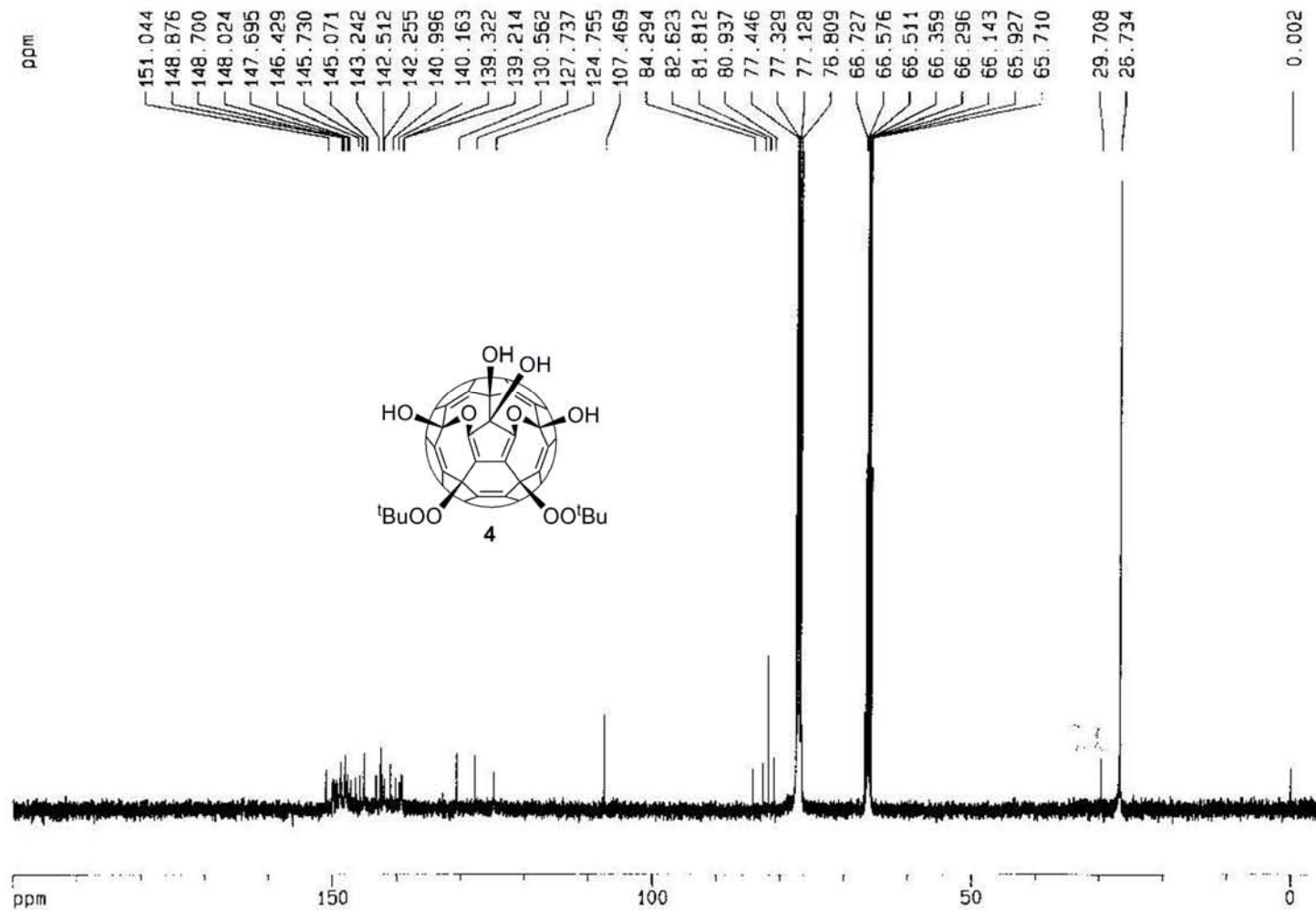
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AQ 2.5231860 sec
RG 1430
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DE 96.25 usec
TE 300.0 K
D1 2.00000000 sec
P1 3.00 usec
DE 96.25 usec
SF01 400.1319659 MHz
NUCLEUS 1H

F2 - Processing parameters

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SF 400.1299890 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00

1D NMR plot parameters

CX 20.00 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P -0.500 ppm
F2 -200.06 Hz
PPMCM 0.52500 ppm/cm
HZCM 210.06824 Hz/cm



Current Data Parameters
NAME c35898
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

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PULPROG zgdc
TD 32768
SOLVENT CDCl3
NS 16000
DS 2
SWH 25000.000 Hz
FIDRES 0.762939 Hz
AQ 0.6554100 sec
RG 8192
DW 20.000 usec
DE 25.00 usec
TE 300.0 K
D12 0.00002000 sec
DL5 22.20 dB
CPOPRG waltz16
P31 100.00 usec
D1 2.00000000 sec
P1 2.50 usec
DE 25.00 usec
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NUC1FUS 13C
D11 0.03000000 sec

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PC 1.00

1D NMR plot parameters

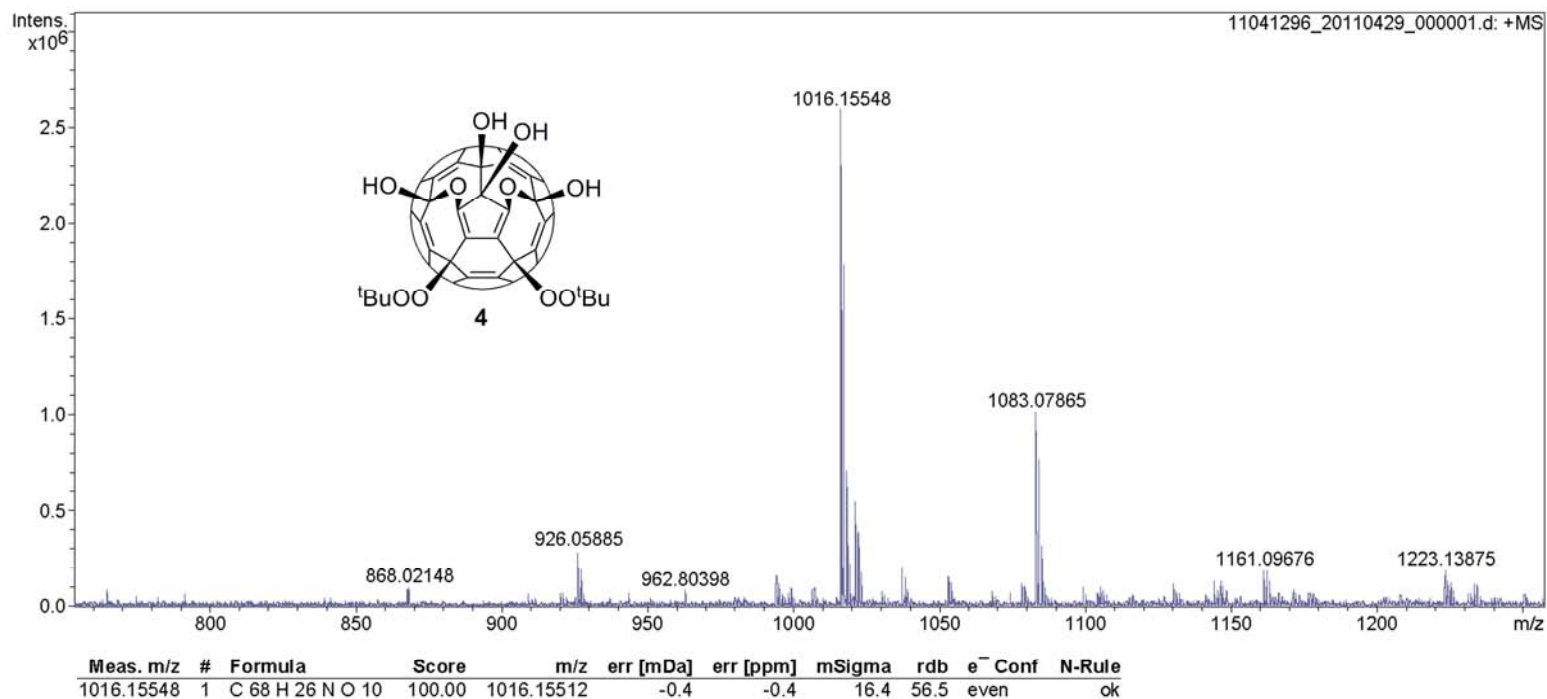
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F2P -5.000 ppm
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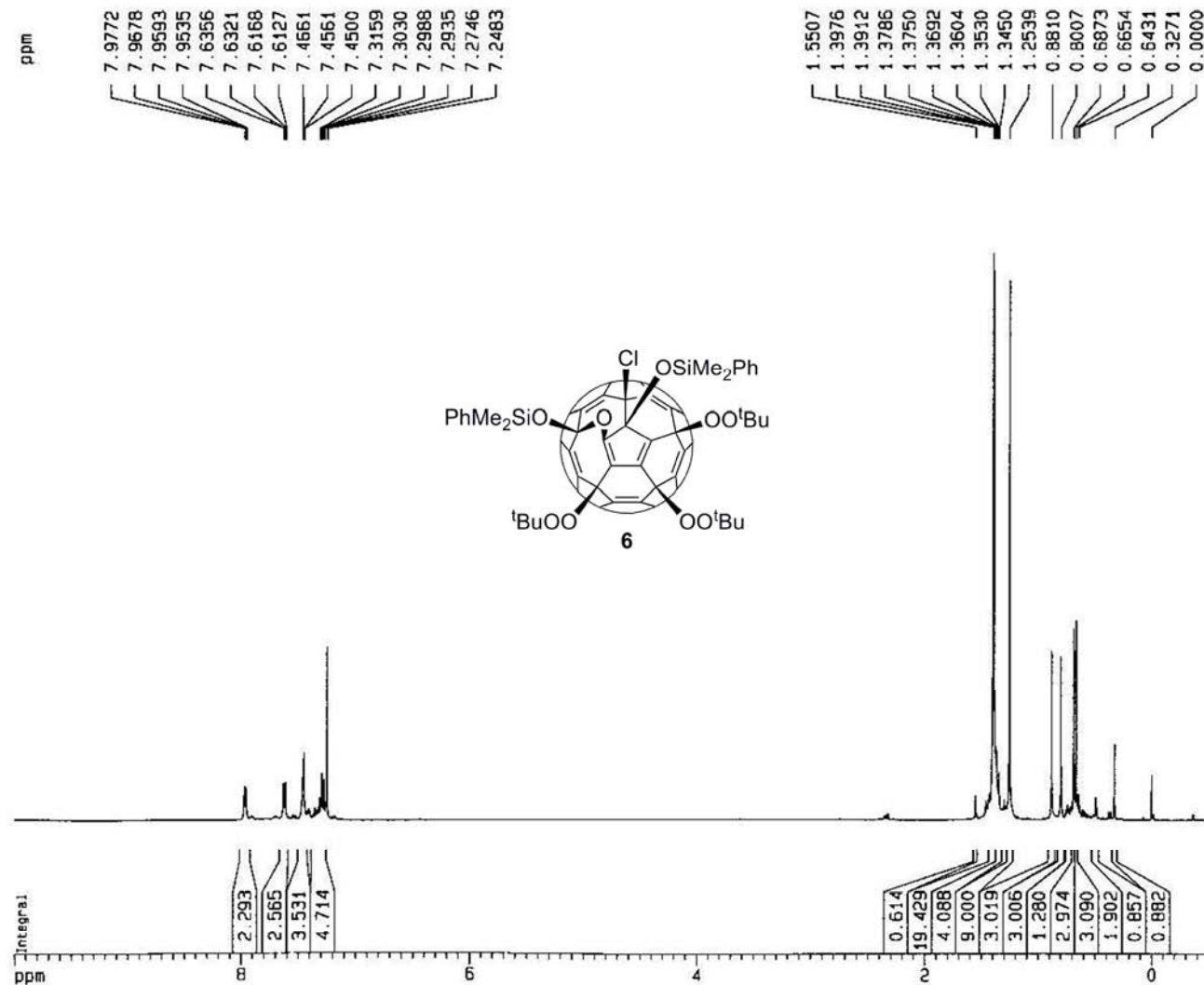
Peking University Mass Spectrometry Sample Analysis Report

Analysis Info

Analysis Name 11041296_20110429_000001.d
Sample 110429
Comment ESI Positive

Acquisition Date 4/29/2011 10:00:06 AM
Instrument Bruker Apex IV FTMS
Operator Peking University





Current Data Parameters

NAME h33141
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

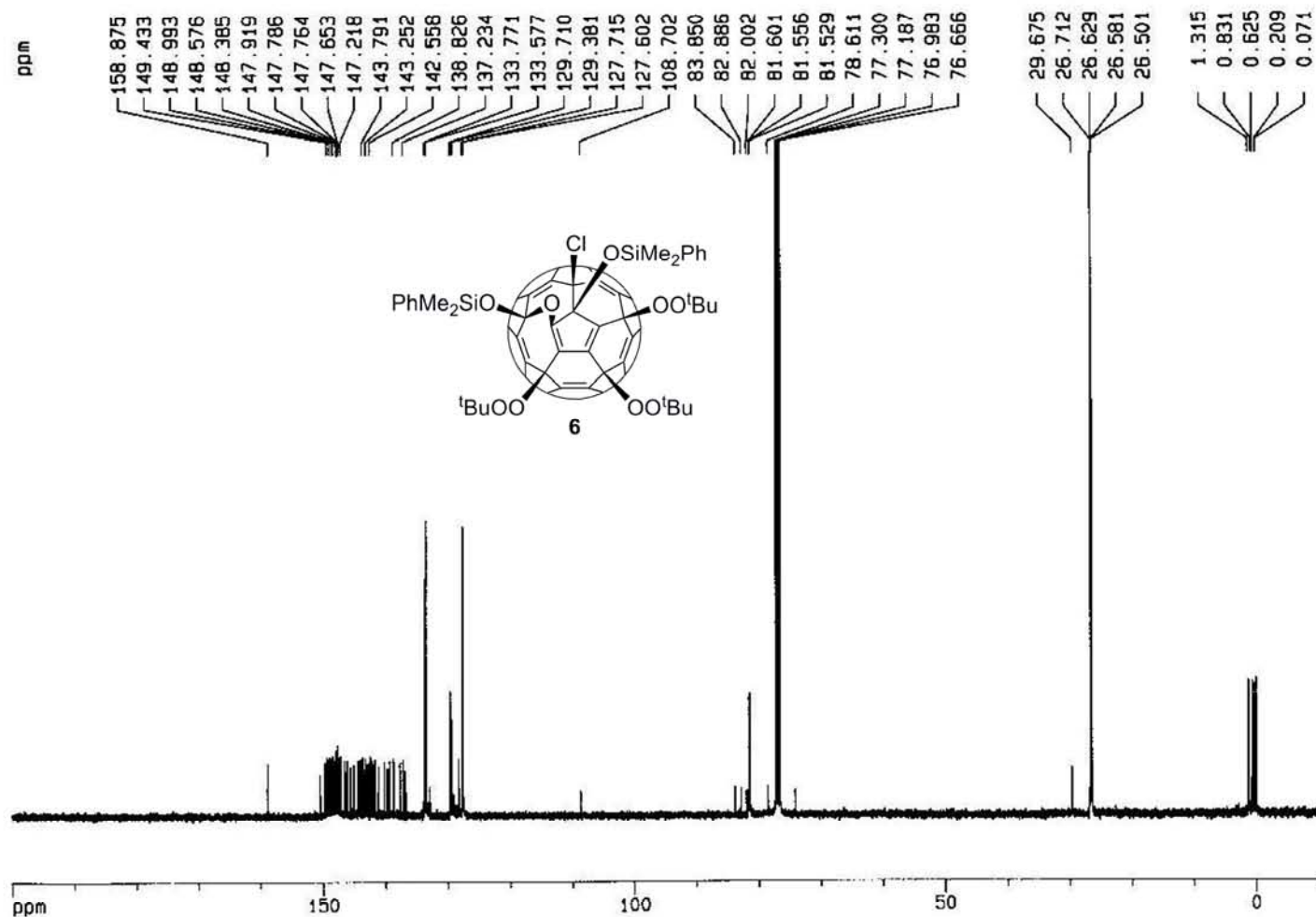
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PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2610421 sec
RG 512
DW 69.000 usec
DE 98.57 usec
TE 300.0 K
D1 2.00000000 sec
P1 3.00 usec
DE 98.57 usec
SF01 400.1319844 MHz
NUCLEUS 1H

F2 - Processing parameters

SI 16384
SF 400.1300149 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 4.00

1D NMR plot parameters

CX 20.00 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P -0.500 ppm
F2 -200.07 Hz
PPMCM 0.52500 ppm/cm
HZCM 210.06825 Hz/cm



Current Data Parameters
NAME c33141
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20061124
Time 11.14
INSTRUM ARX400
PROBHD 5 mm Multinu
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 3000
DS 2
SWH 25000.000 Hz
FIDRES 0.762939 Hz
AQ 0.6554100 sec
RG 8192
DM 20.000 usec
DE 25.00 usec
TE 300.0 K
D12 0.00002000 sec
DL5 22.20 dB
CPDPRG waltz16
P31 100.00 usec
D1 2.00000000 sec
P1 2.50 usec
DE 25.00 usec
SF01 100.6233680 MHz
NUCLEUS 13C
D11 0.03000000 sec

F2 - Processing parameters
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SSB 0
LB 0.50 Hz
GB 0
PC 1.00

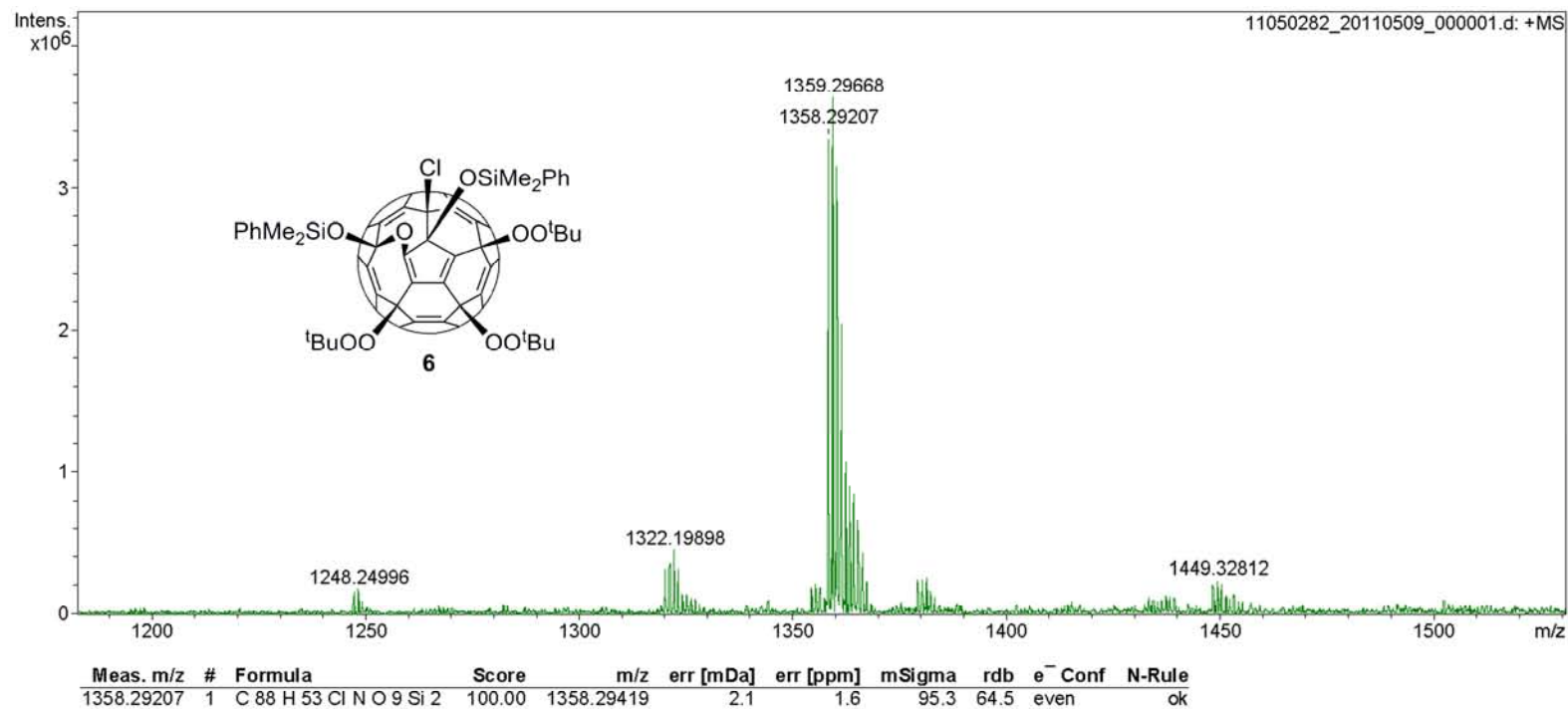
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F2 -1006.13 Hz
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HZCM 1056.43420 Hz/cm

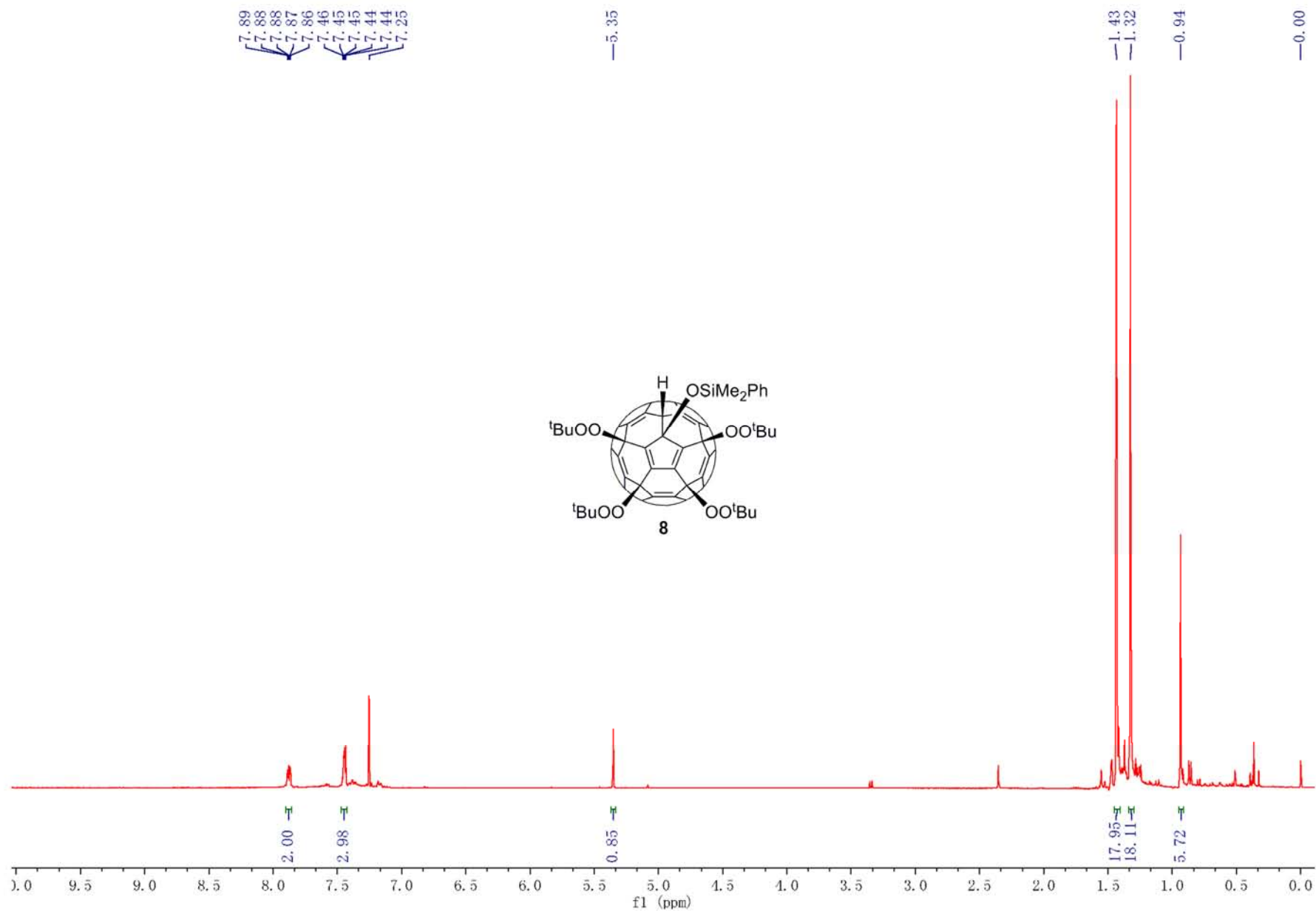
Peking University Mass Spectrometry Sample Analysis Report

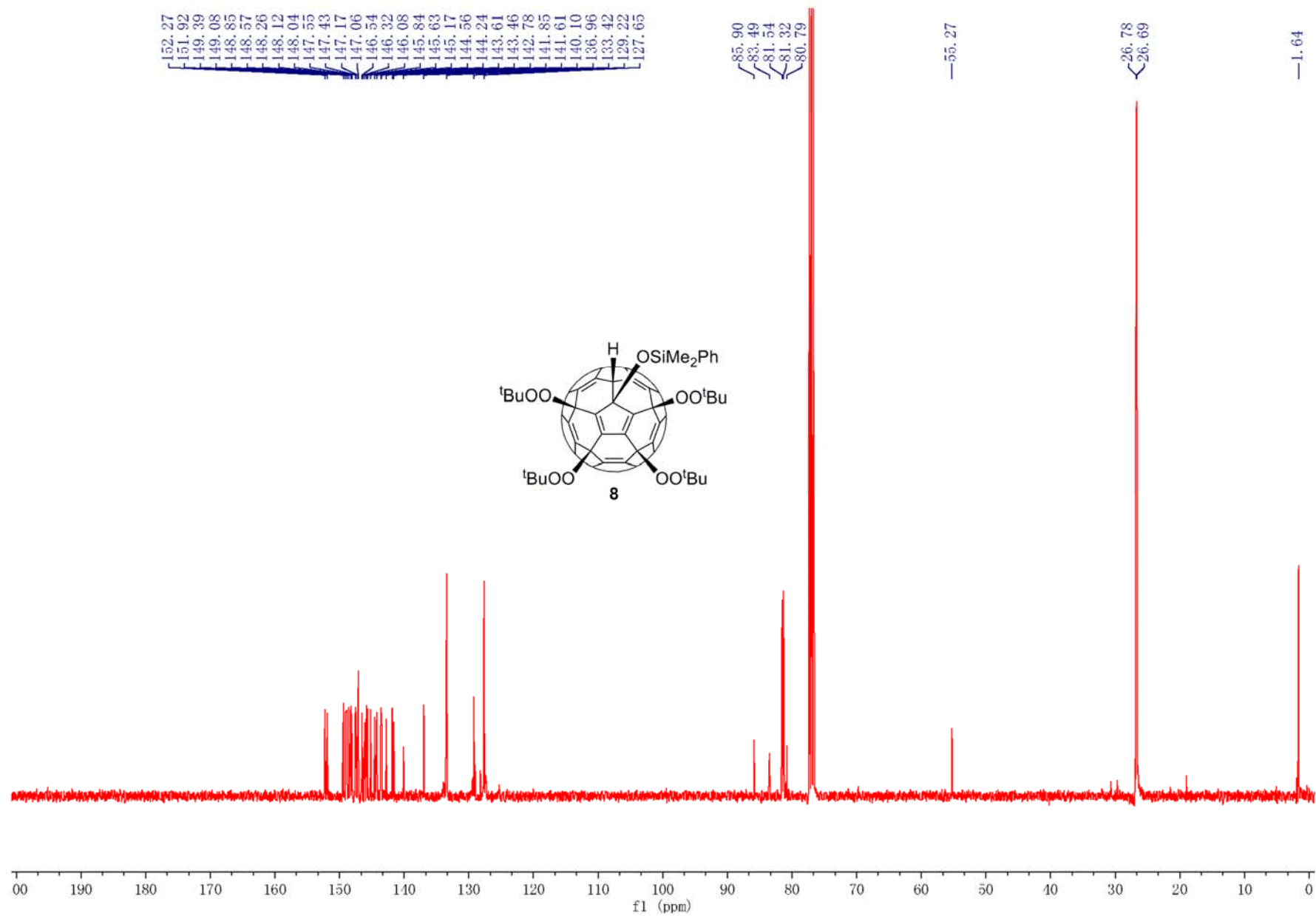
Analysis Info

Analysis Name 11050282_20110509_000001.d
 Sample 110507
 Comment ESI Positive

Acquisition Date 5/9/2011 9:33:48 AM
 Instrument Bruker Apex IV FTMS
 Operator Peking University





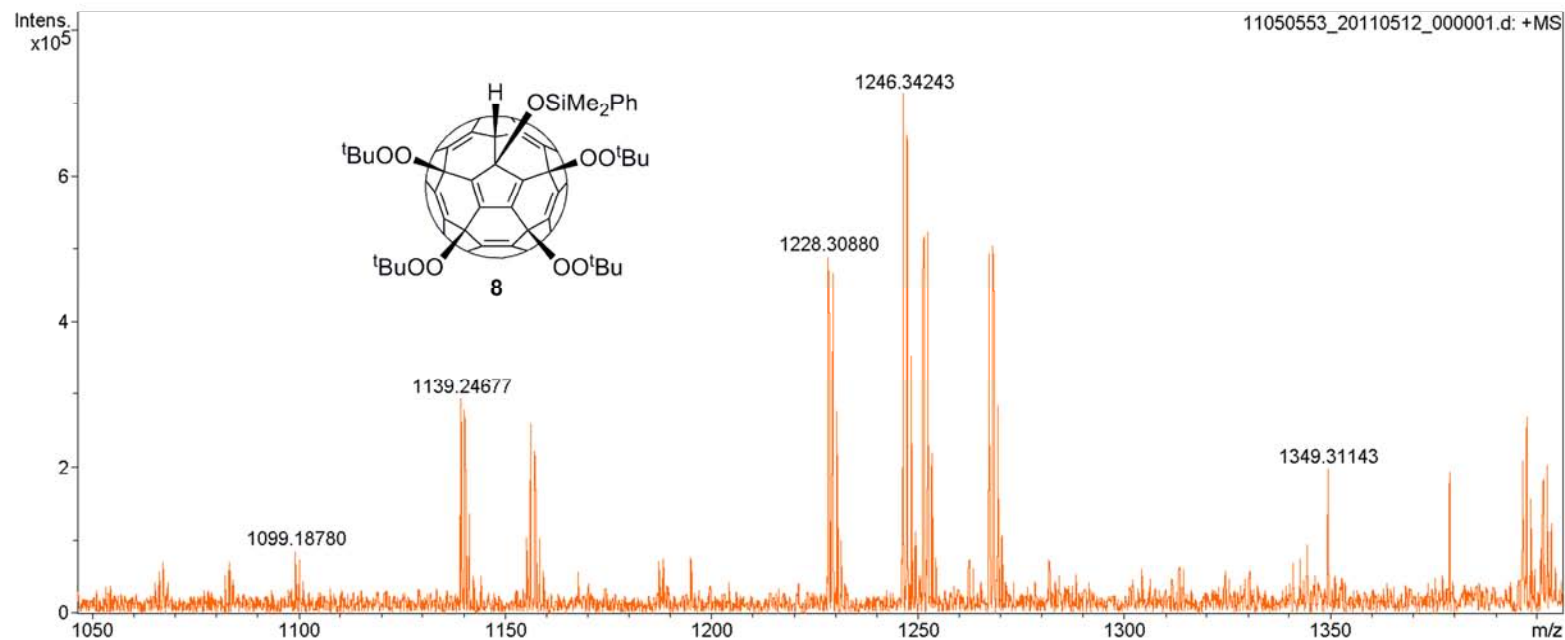


Peking University Mass Spectrometry Sample Analysis Report

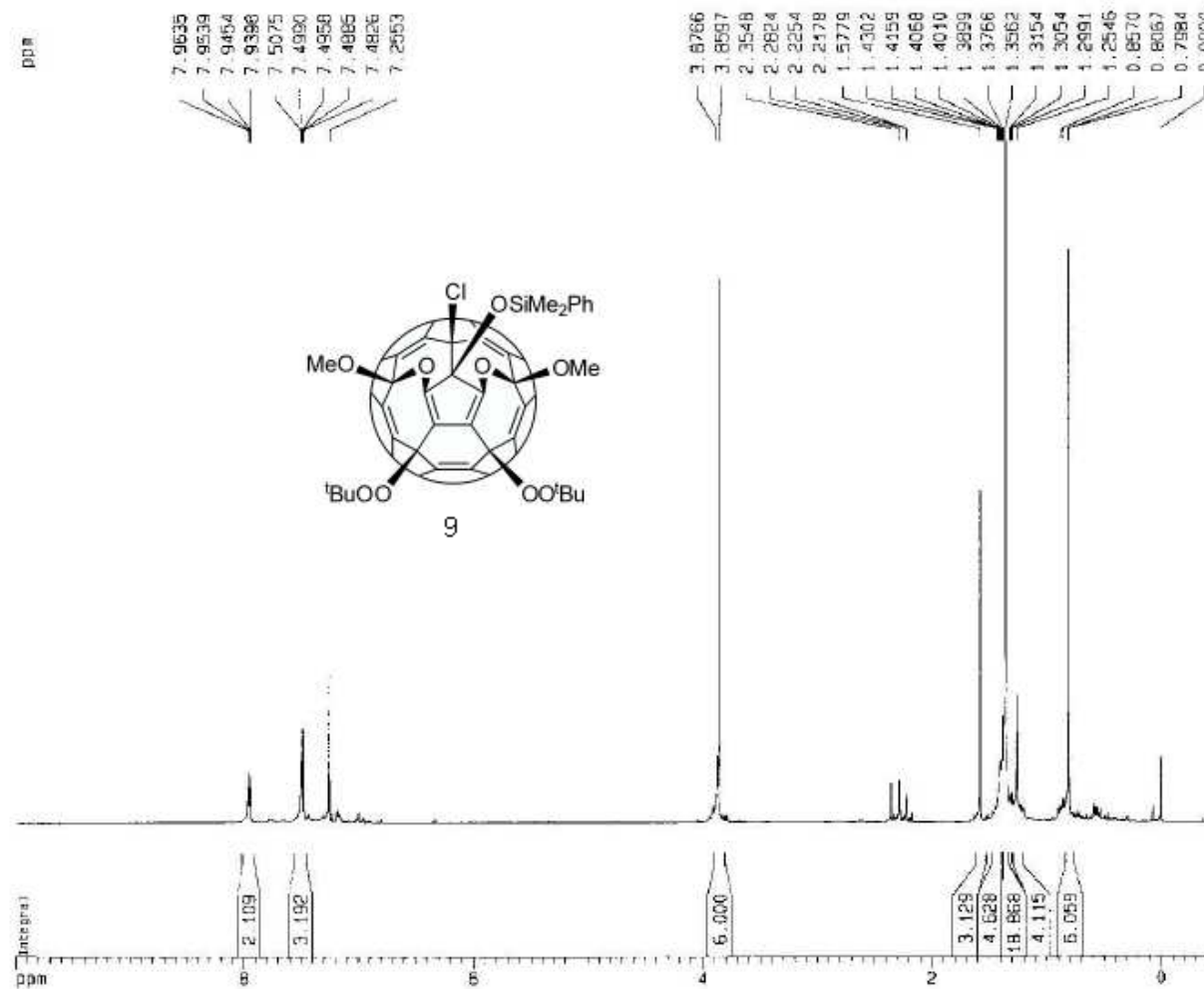
Analysis Info

Analysis Name 11050553_20110512_000001.d
Sample 110512
Comment ESI Positive

Acquisition Date 5/12/2011 11:24:52 AM
Instrument Bruker Apex IV FTMS
Operator Peking University



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
1228.30880	1	C 84 H 48 O 9 Si	100.00	1228.30621	-2.6	-2.1	34.2	62.0	odd	ok
1246.34243	1	C 84 H 52 N O 9 Si	100.00	1246.34059	-1.8	-1.5	296.1	60.5	even	ok



Current Data Parameters

NAME h36500
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

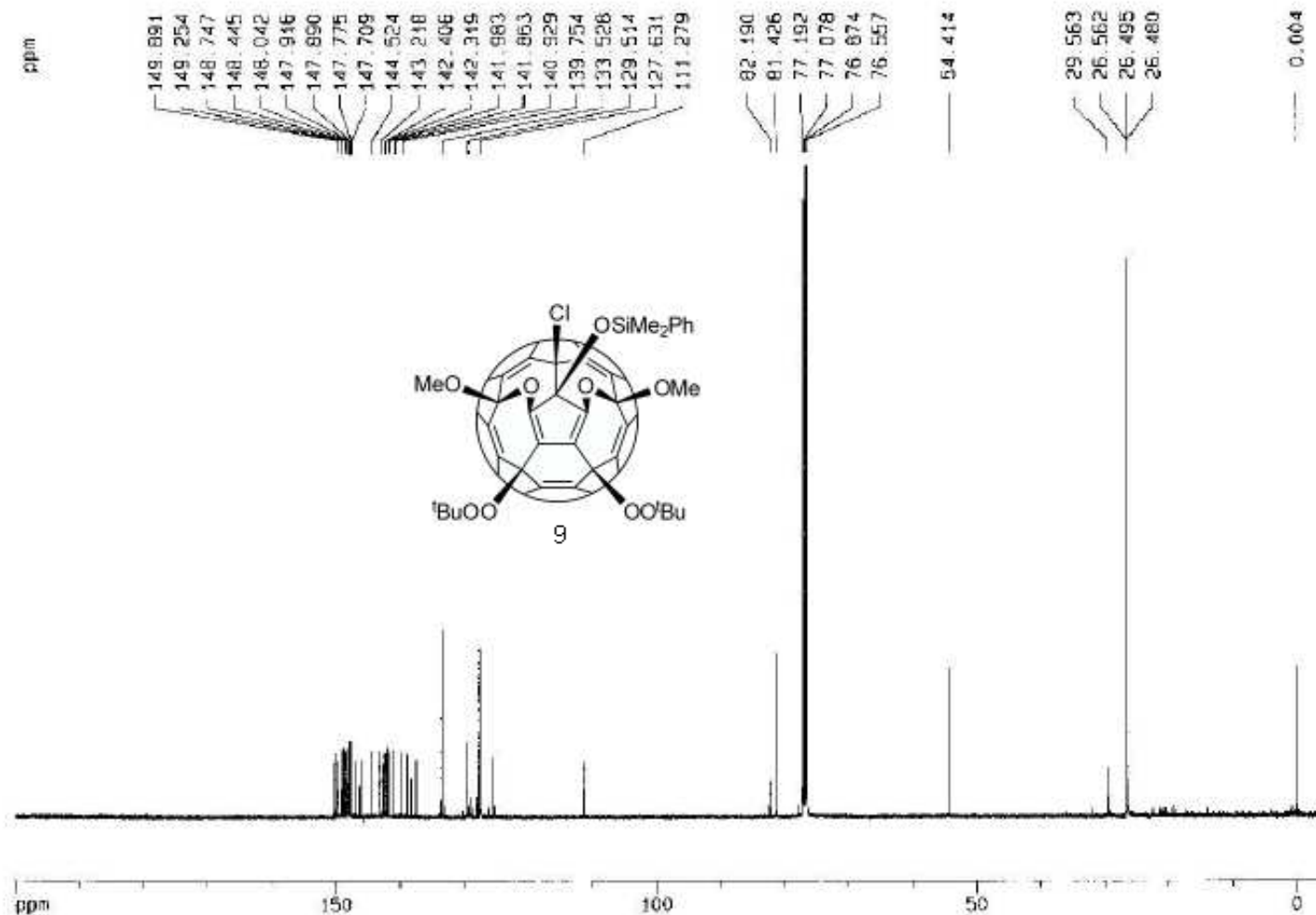
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Time 16.49
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PULPROG zg
TD 32768
SOLVENT CDCl₃
NS 32
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2610421 sec
RG 1024
DM 69.000 usec
DE 98.57 usec
TE 300.0 K
D1 2.00000000 sec
P1 3.00 usec
DE 98.57 usec
SFO1 400.1318844 MHz
NUCLEUS 1H

F2 - Processing parameters

SF 16384
SF 400.1300113 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 4.00

1D NMR plot parameters

CX 20.00 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P -0.500 ppm
F2 -200.07 Hz
PPMCM 0.52500 ppm/cm
HZCM 210.06825 Hz/cm



Current Data Parameters
NAME c30500
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070917
Time 17.01
INSTRUM AFX400
PROBHD 5 mm Multinu
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 8000
DS 2
SWH 25000.000 Hz
FIDRES 0.762939 Hz
AQ 0.6554100 sec
RG 8192
DM 20.000 usec
DE 25.00 usec
TE 300.0 K
D12 0.00002000 sec
DL5 22.20 dB
COPRPG waltz16
P31 100.00 usec
D1 2.00000000 sec
P1 2.50 usec
DE 25.00 usec
SFO1 100.623080 MHz
NUCLEUS 13C
D11 0.03000000 sec

F2 - Processing parameters
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SSB 0
LB 0.50 Hz
GB 0
PC 1.00

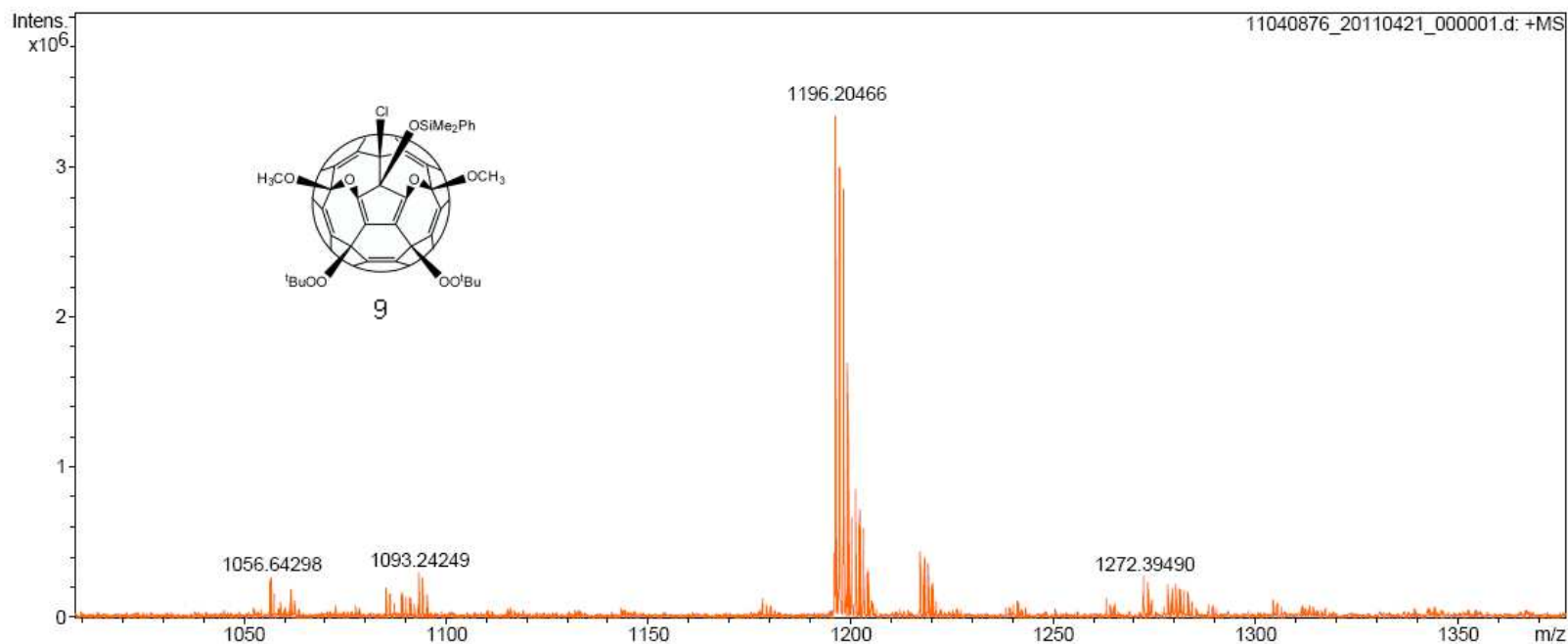
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F1 20122.56 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PRGCM 10.25000 ppm/cm
HZCM 1035.28113 Hz/cm

Peking University Mass Spectrometry Sample Analysis Report

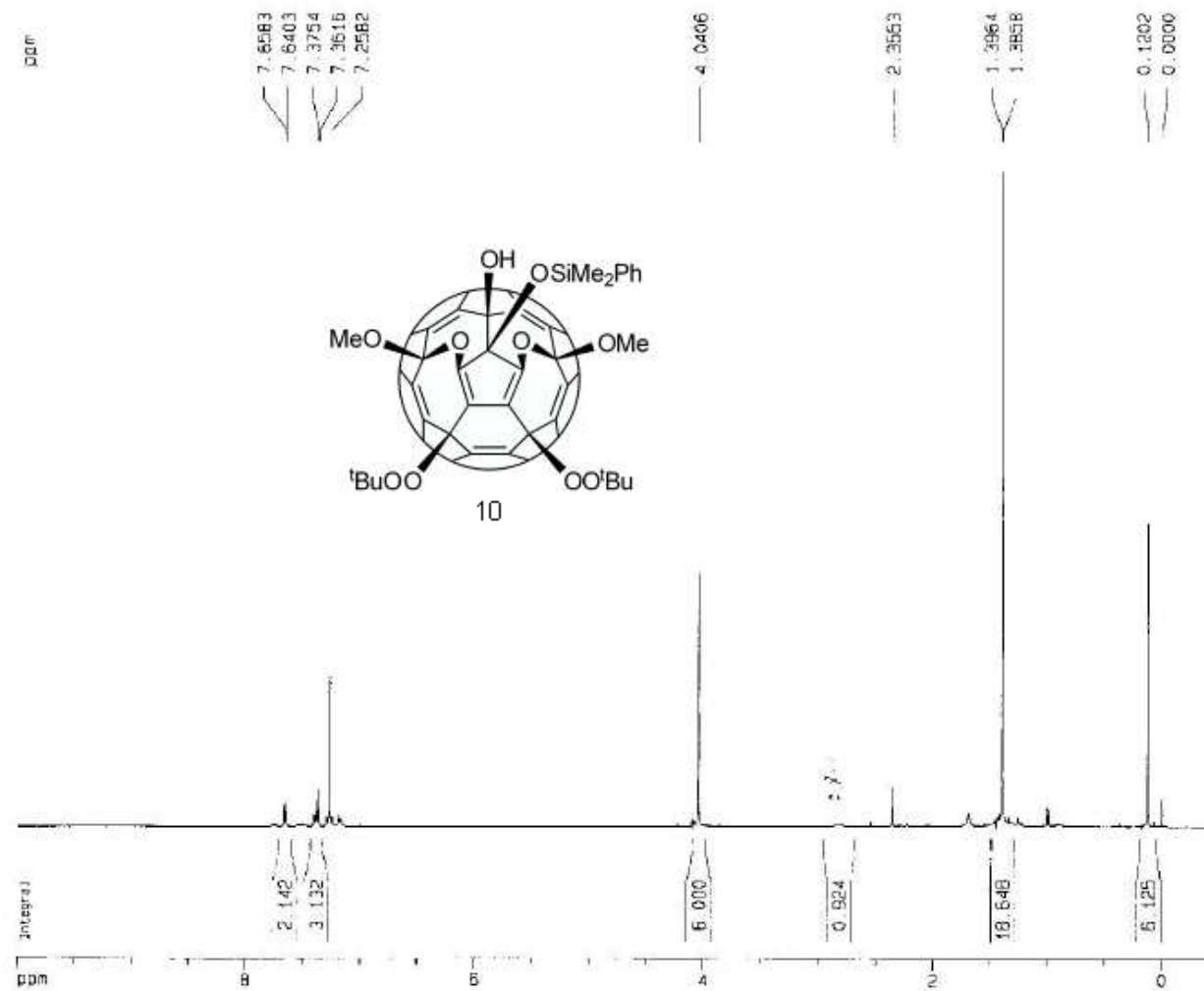
Analysis Info

Analysis Name 11040876_20110421_000001.d
Sample 110416
Comment ESI Positive

Acquisition Date 4/21/2011 11:55:53 AM
Instrument Bruker Apex IV FTMS
Operator Peking University



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule
1196.20466	1	C ₇₈ H ₃₉ ClN ₉ Si ₉	100.00	1196.20771	3.1	2.6	109.3	60.5	even		ok



Current Data Parameters
NAME H36602
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

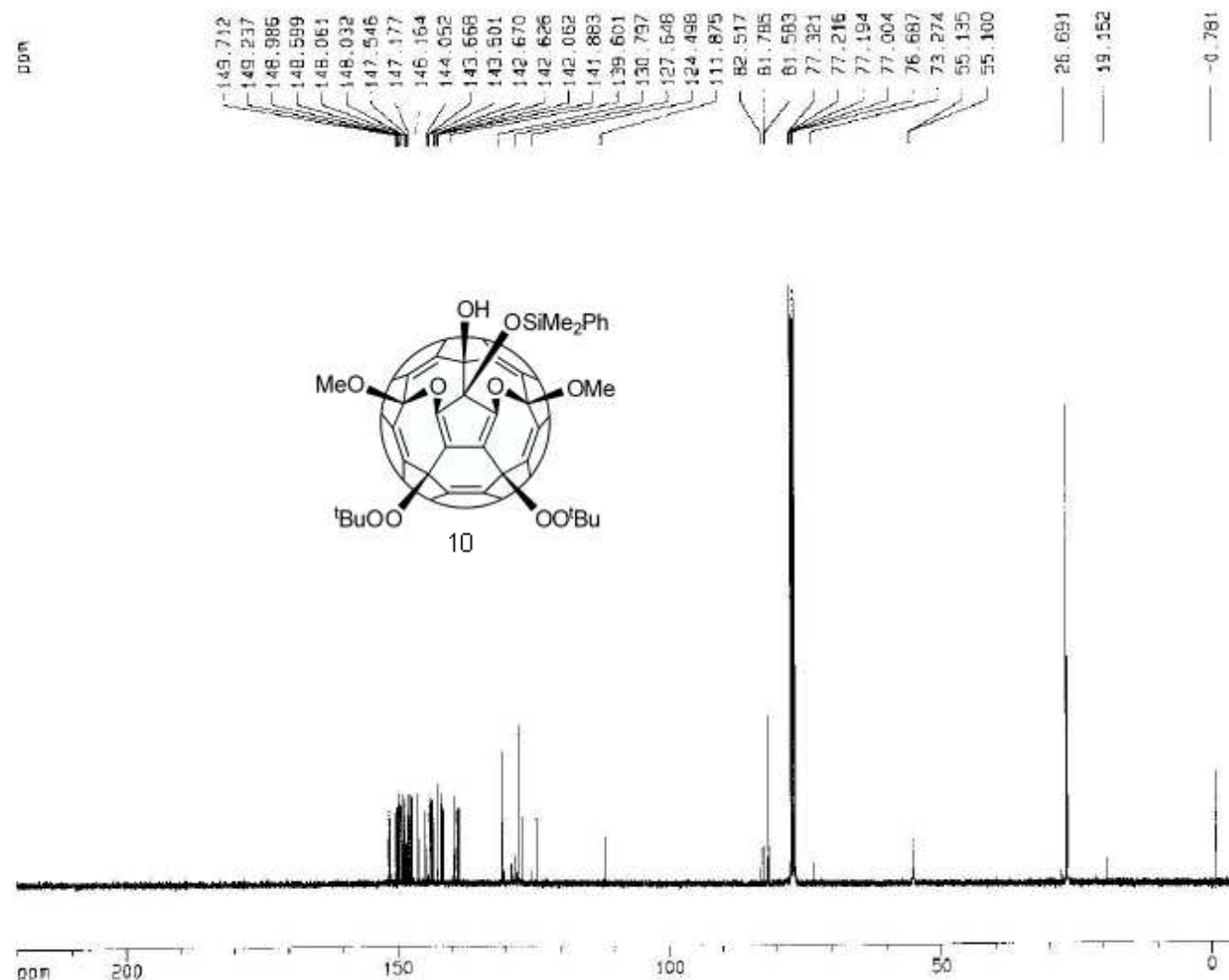
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PULPROG zg
TD 32768
SOLVENT CDCl₃
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SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 715
DW 78.000 usec
DE 97.50 usec
TE 300.0 K
D1 2.00000000 sec
P1 3.00 usec
DE 97.50 usec
SFO1 400.1324000 MHz
NUCLEUS 1H

F2 - Processing parameters

SI 16384
SF 400.1300102 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 0.50

1D NMR plot parameters

CX 20.00 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P -0.500 ppm
F2 -200.07 Hz
PPMCM 0.52500 ppm/cm
HZCM 210.06825 Hz/cm



Current Data Parameters
NAME C36602
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

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Time 11.24
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PULPROG zgpg
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SOLVENT CDCl3
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SMH 27777.777 Hz
FIDRES 0.847710 Hz
AQ 0.5898740 sec
RG 8192
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DE 25.71 usec
TE 300.0 K
D12 0.00002000 sec
OL5 24.00 dB
CPDPRG waltz16
P31 100.00 usec
B1 2.00000000 sec
P1 4.00 usec
DE 25.71 usec
SF01 100.6240000 MHz
NUCLEUS 13C
D11 0.03000000 sec

F2 - Processing parameters

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PC 0.30

1D NMR plot parameters

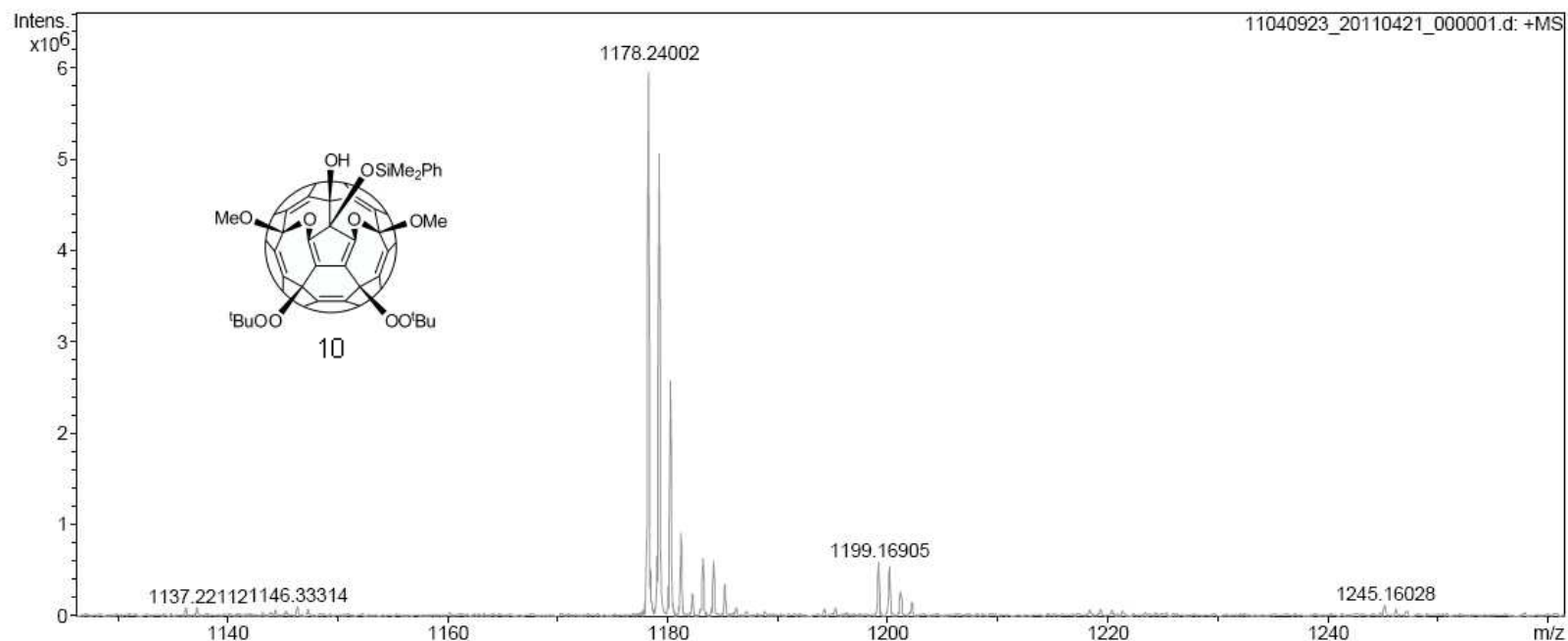
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F2 -503.07 Hz
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Peking University Mass Spectrometry Sample Analysis Report

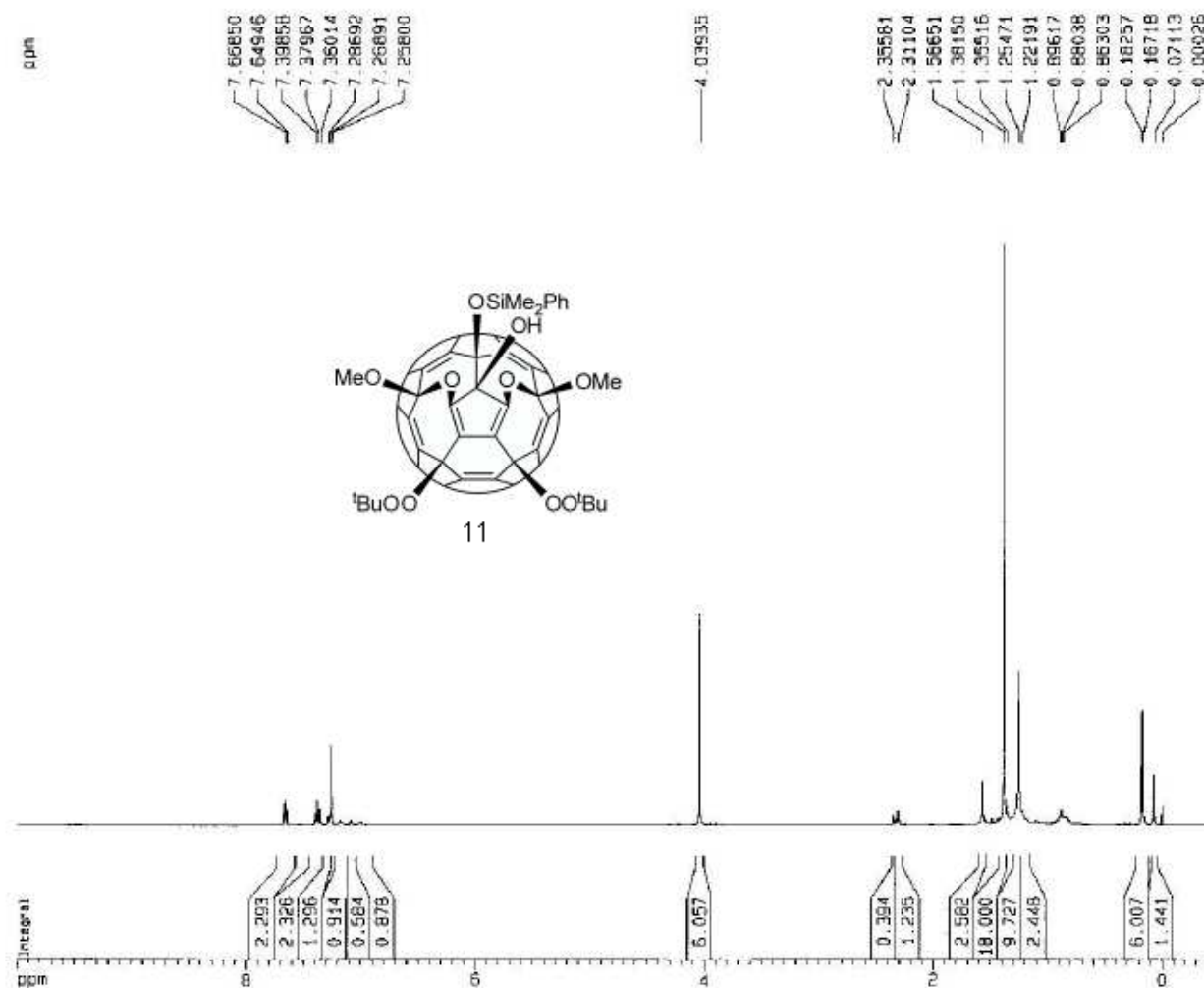
Analysis Info

Analysis Name 11040923_20110421_000001.d
 Sample 110419
 Comment ESI Positive

Acquisition Date 4/21/2011 4:41:45 PM
 Instrument Bruker Apex IV FTMS
 Operator Peking University



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
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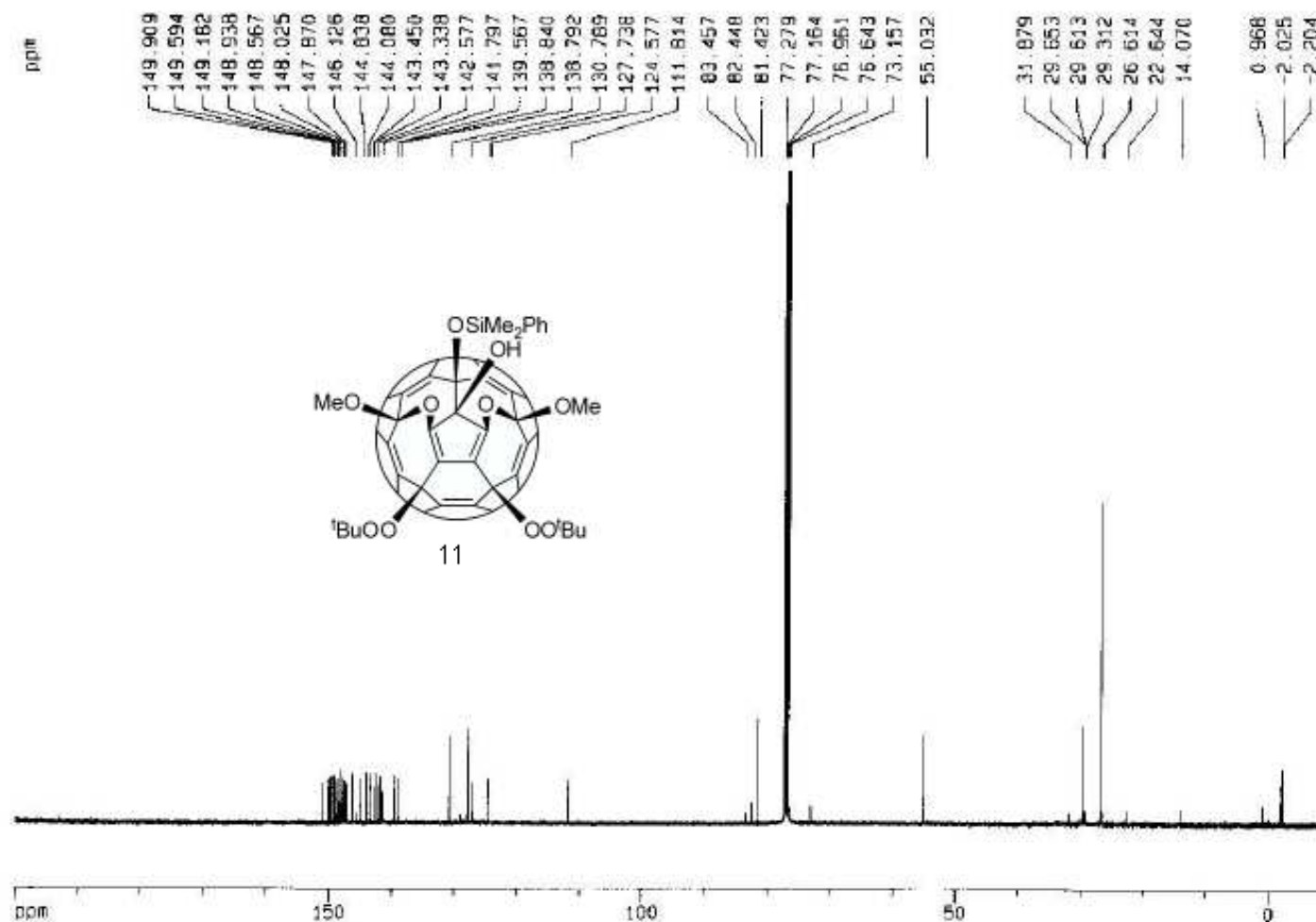


Current Data Parameters
NAME h36885
EXPNO 1
PROCNO 1

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PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2610421 sec
RG 1024
DW 69.000 usec
DE 98.57 usec
TE 300.0 K
D1 2.0000000 sec
P1 3.00 usec
DE 98.57 usec
SFO1 400.1318844 MHz
NUCLEUS 1H

F2 - Processing parameters
SI 16384
SF 400.1300100 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 4.00

1D NMR plot parameters
CX 20.00 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P -0.500 ppm
F2 -200.07 Hz
PPMCM 0.52500 ppm/cm
HZCM 210.06825 Hz/cm



Current Data Parameters
NAME c36885
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20071023
Time 15.50
INSTRUM ARX400
PROBHD 5 mm Multinu
PULPROG zgpg
TD 32768
SOLVENT CDCl₃
NS 5000
DS 2
SWH 25000.000 Hz
FIDRES 0.762939 Hz
AQ 0.5954100 sec
RG 8192
DM 20.000 usec
DE 20.00 usec
TE 300.0 K
D12 0.0002000 sec
BLS 22.20 dB
CPDPRG waltz16
P31 100.00 usec
Q1 2.00000000 sec
P1 2.50 usec
DE 25.00 usec
SFO1 100.6233680 MHz
NUCLEUS 13C
Q11 0.03600000 sec

F2 - Processing parameters

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SSB 0
LB 0.50 Hz
GB 0
PC 1.00

1D NMR plot parameters

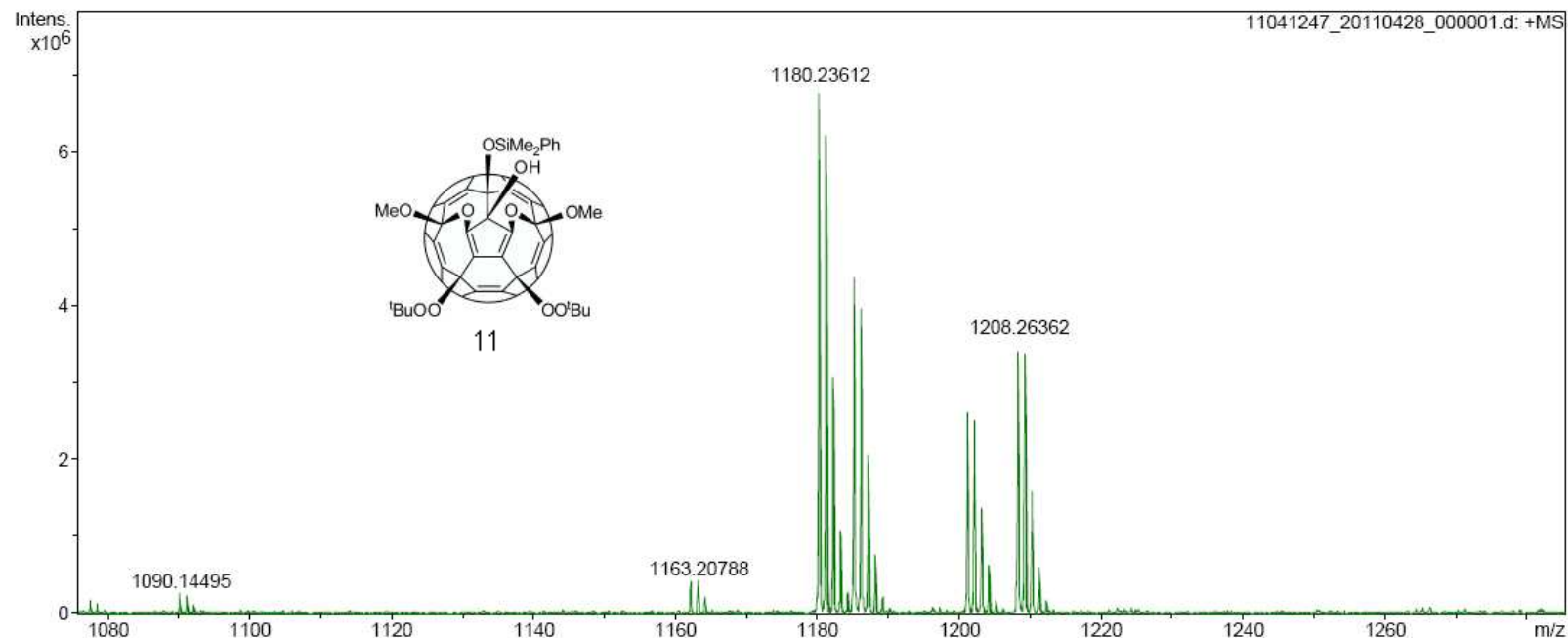
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F1P 200.000 ppm
F1 20122.55 Hz
F2P -10.000 ppm
F2 -1006.13 Hz
PPMCM 10.50000 ppm/cm
HZCM 1056.43420 Hz/cm

Peking University Mass Spectrometry Sample Analysis Report

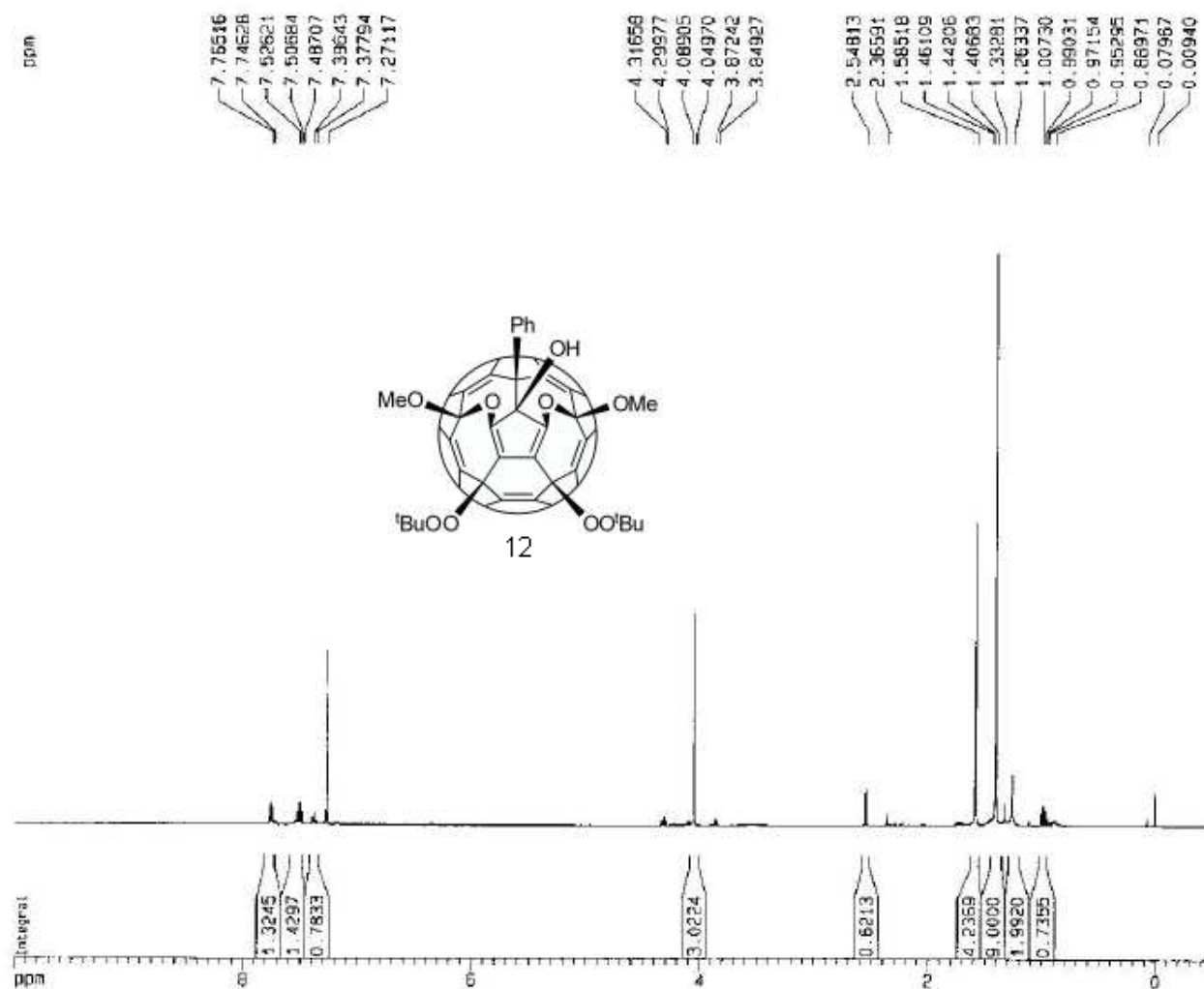
Analysis Info

Analysis Name 11041247_20110428_000001.d
 Sample 110427
 Comment ESI Positive

Acquisition Date 4/28/2011 5:59:43 PM
 Instrument Bruker Apex IV FTMS
 Operator Peking University



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule
1180.23612	1	C 76 H 39 N Na O 12	100.00	1180.23645	0.3	0.3	53.8	57.5	even		ok
	2	C 79 H 39 N Na O 8 Si	83.86	1180.23371	-2.4	-2.0	6.2	61.5	even		ok
	3	C 78 H 38 N O 12	28.93	1180.23885	2.7	2.3	41.0	60.5	even		ok
	4	C 72 H 43 N Na O 13 Si	16.44	1180.23959	3.5	2.9	34.9	52.5	even		ok
	5	C 74 H 42 N O 13 Si	0.90	1180.24199	5.9	5.0	22.0	55.5	even		ok



Current Data Parameters
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EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

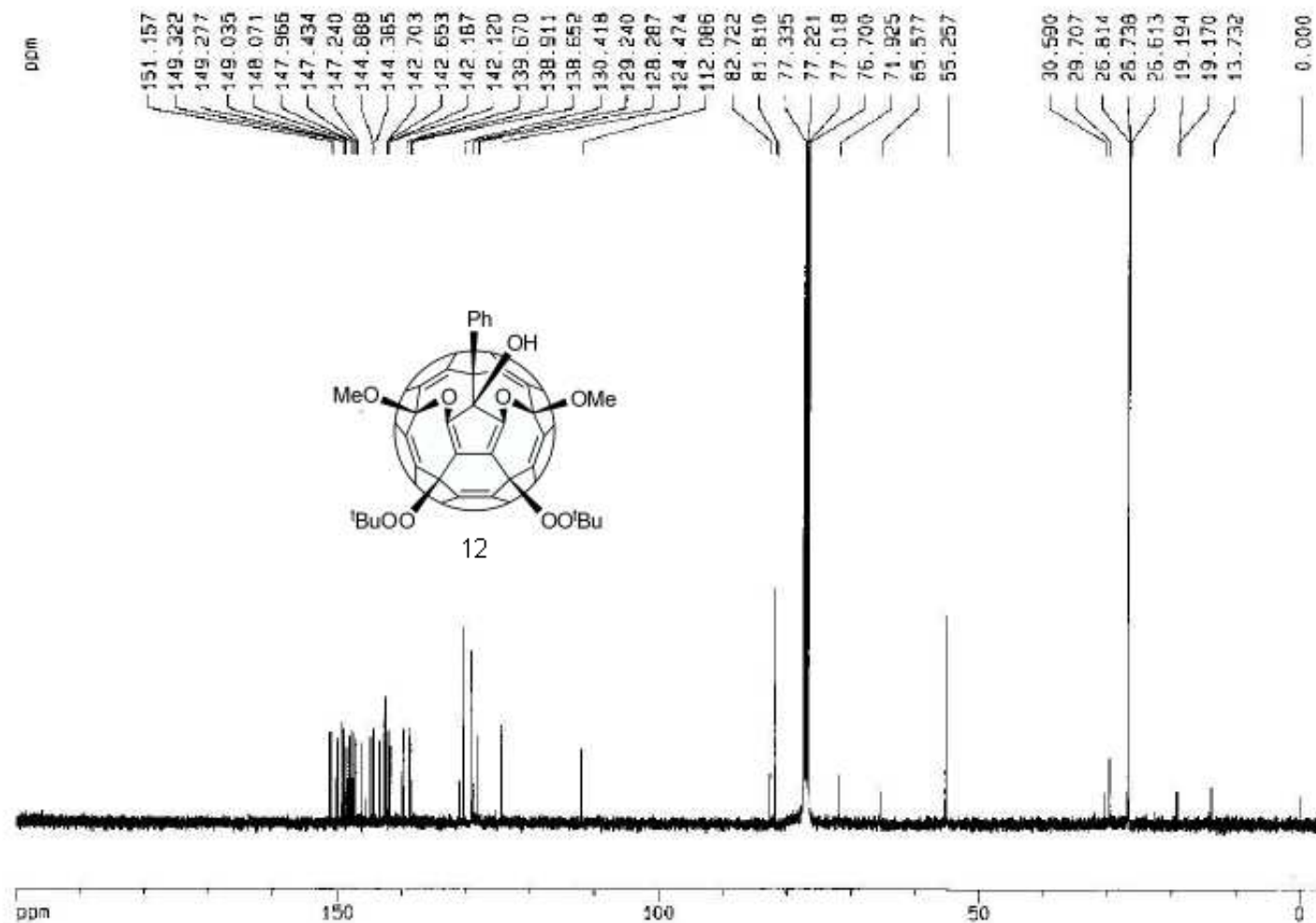
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Time 17.15
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PROBHD 5 mm Multinu
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2610421 sec
RG 2860
DW 69.000 usec
DE 98.57 usec
TE 300.0 K
D1 2.00000000 sec
P1 3.00 usec
DE 98.57 usec
SFO1 400.1318844 MHz
NUCLEUS 1H

F2 - Processing parameters

SI 15384
SF 400.1300051 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 4.00

1D NMR plot parameters

CX 20.00 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P -0.500 ppm
F2 -200.07 Hz
PPMCM 0.52500 ppm/cm
HZCM 210.06825 Hz/cm



Current Data Parameters
NAME c38936
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20071026
Time 17.17
INSTRUM ARX400
PROBHD 5 mm Multinu
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 15000
DS 2
SWH 25000.000 MHz
FIDRES 0.762939 MHz
AQ 0.6004100 sec
RG 8192
DN 20.000 usec
DE 25.00 usec
TE 300.0 K
D12 0.00002000 sec
OL5 22.20 dB
COPROG waltz16
R31 100.00 usec
D1 2.00000000 sec
P1 2.50 usec
DE 25.00 usec
SFO1 100.6233680 MHz
NUCLEUS 13C
D11 0.03000000 sec

F2 - Processing parameters

SI 32768
SF 100.6127665 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.00

1D NMR plot parameters

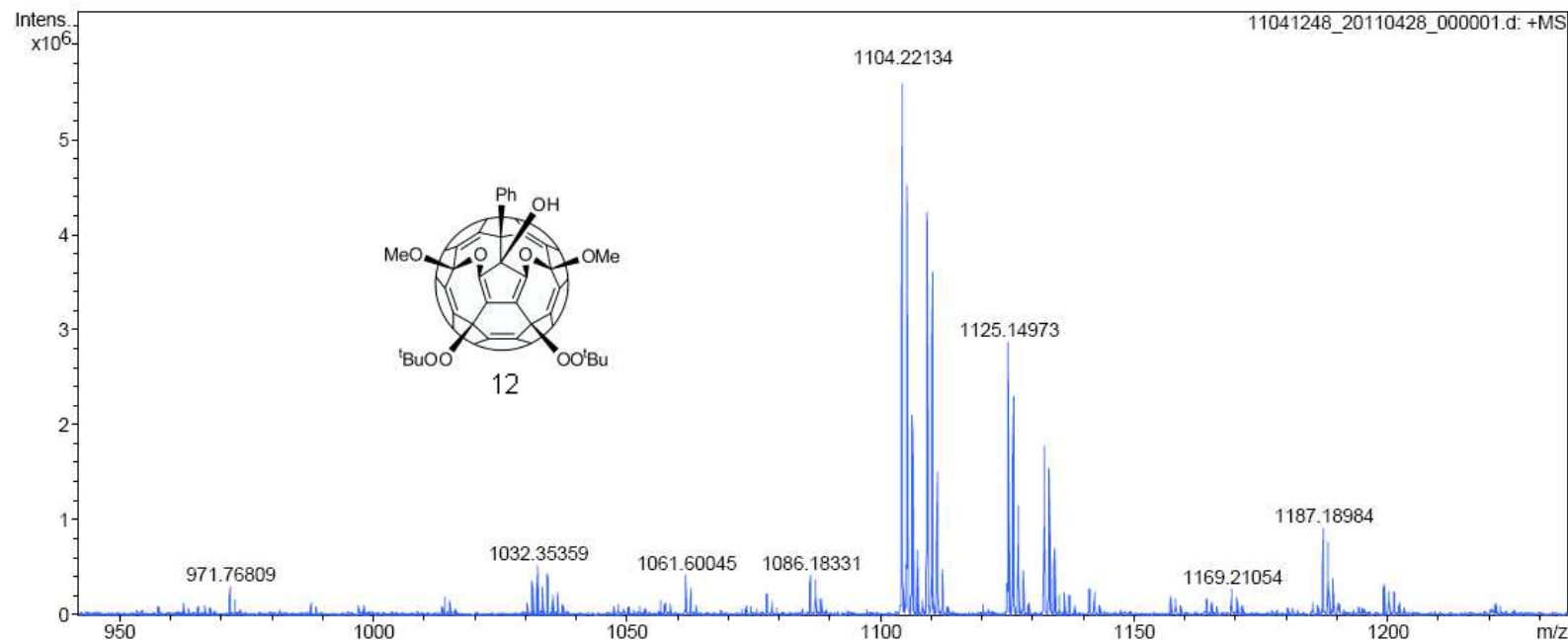
CX 20.00 cm
F1P 200.000 ppm
F1 20122.55 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCK 10.25000 ppm/cm
HZCM 1031.28101 Hz/cm

Peking University Mass Spectrometry Sample Analysis Report

Analysis Info

Analysis Name 11041248_20110428_000001.d
Sample 110428
Comment ESI Positive

Acquisition Date 4/28/2011 6:08:33 PM
Instrument Bruker Apex IV FTMS
Operator Peking University



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule
1104.22134	1	C ₇₆ H ₃₄ N ₄ O ₉	100.00	1104.22281	1.5	1.3	9.2	60.5	even		ok

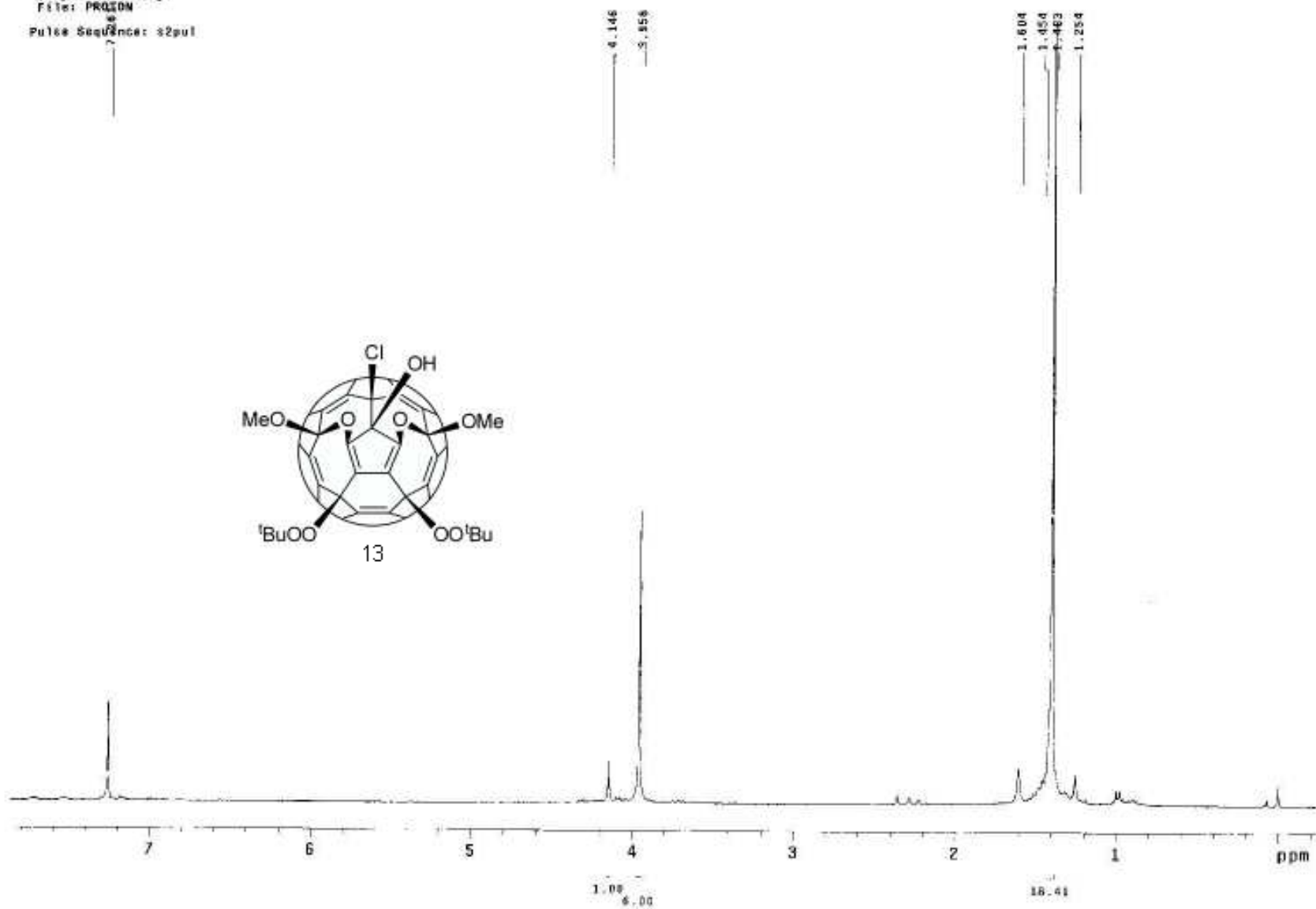
gy-970828-1

Archive directory: /export/home/vnmr1/vnmr6ys/data

Sample directory:

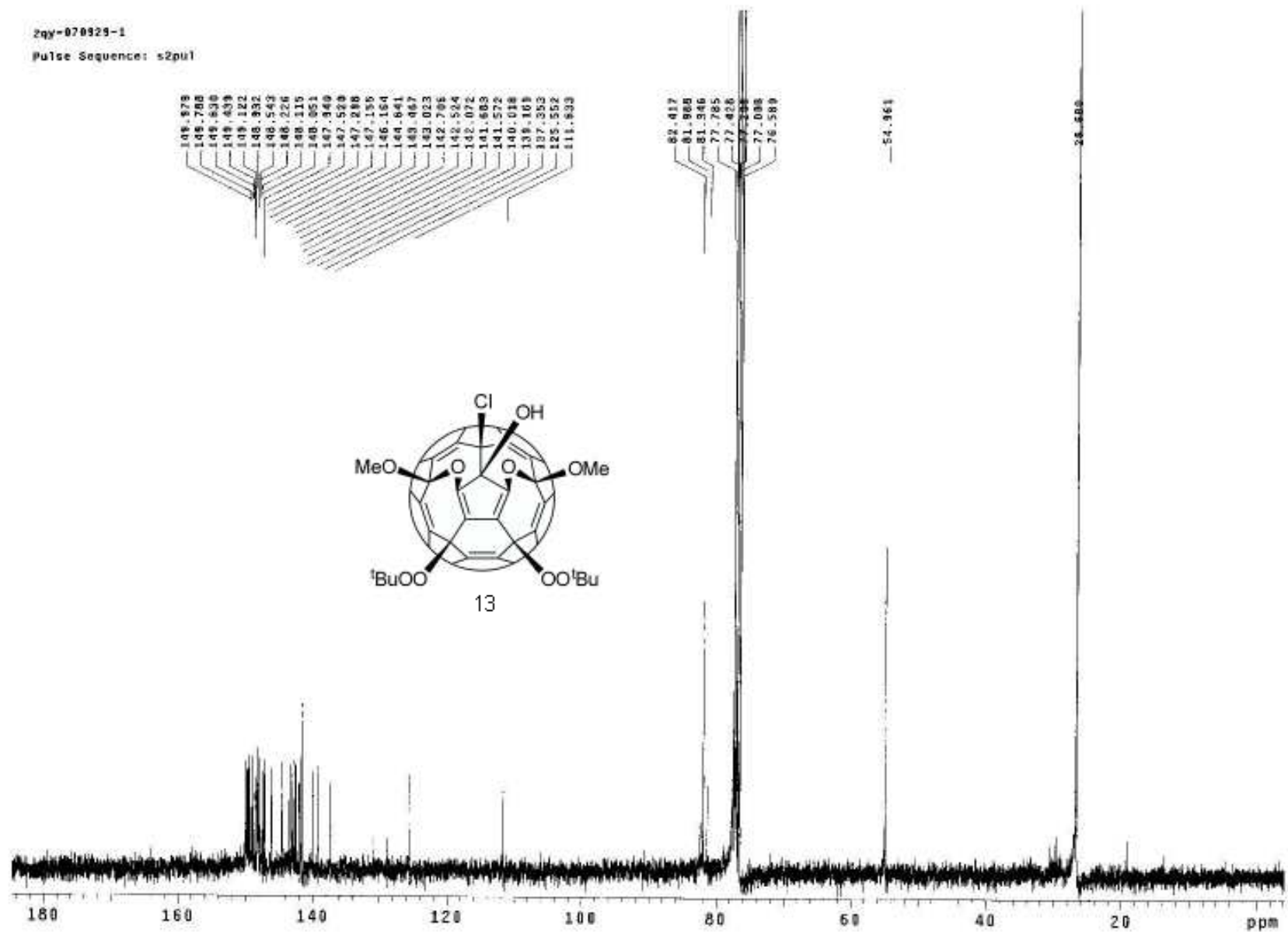
File: PRQSDM

Pulse Sequence: zgpg30



2qy-070929-1

Pulse Sequence: s2pul

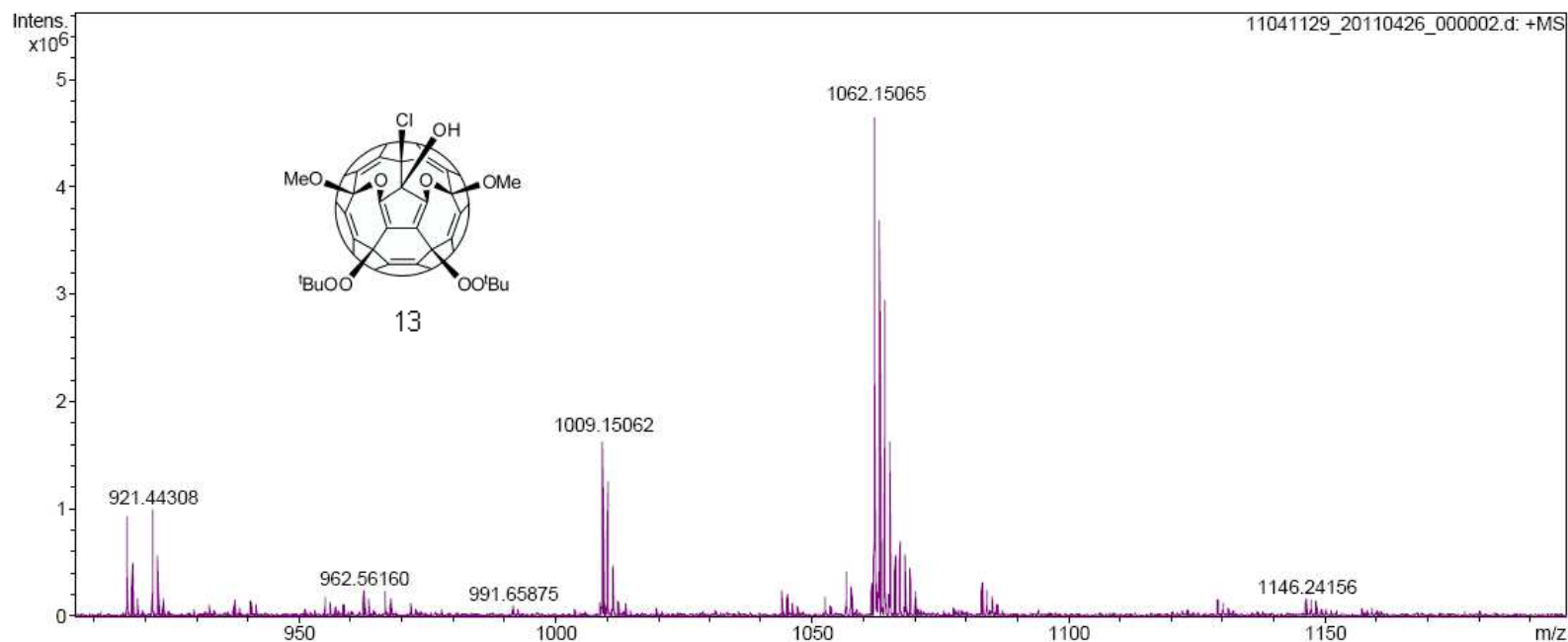


Peking University Mass Spectrometry Sample Analysis Report

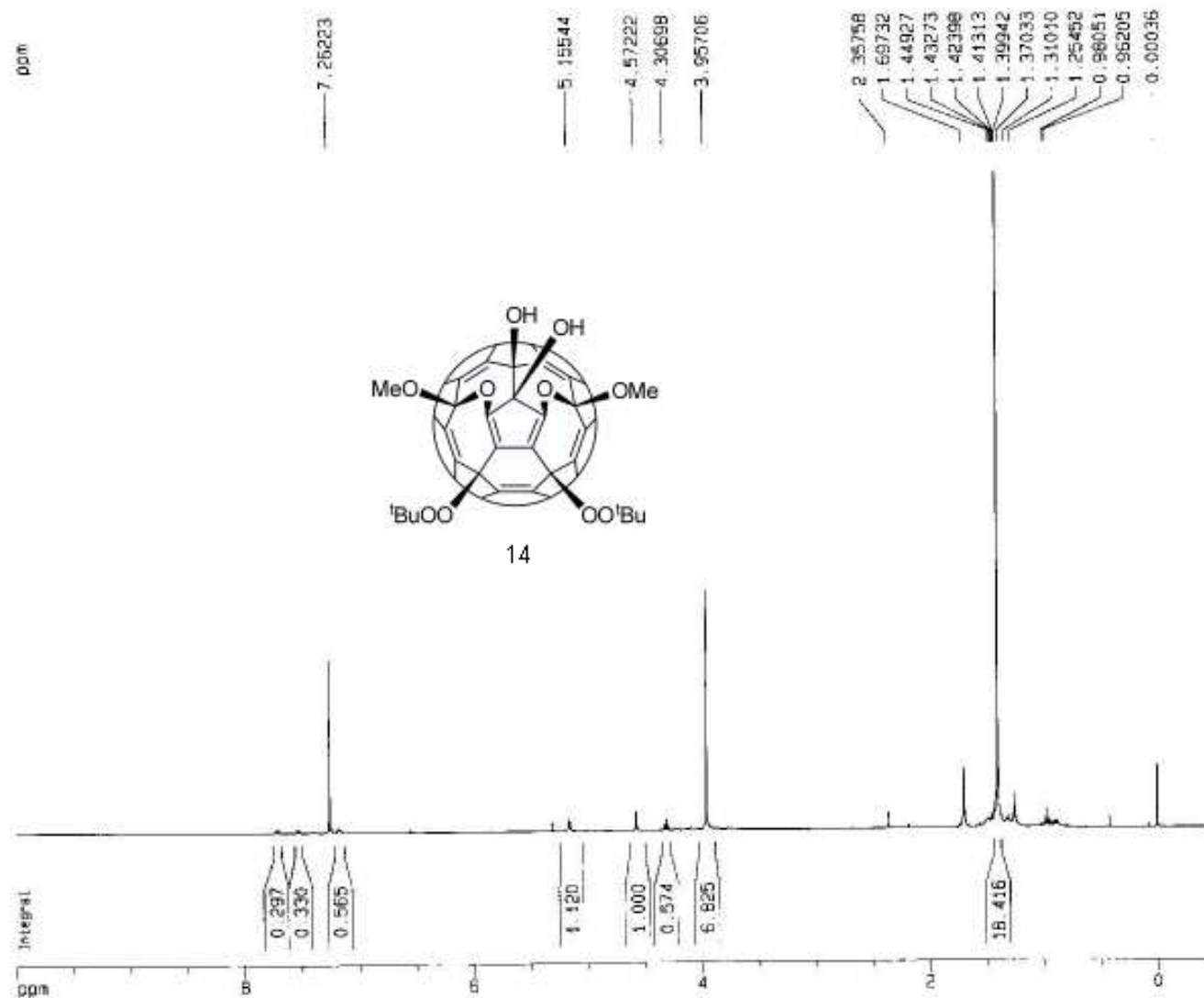
Analysis Info

Analysis Name 11041129_20110426_000002.d
 Sample 110406
 Comment ESI Positive

Acquisition Date 4/26/2011 4:06:47 PM
 Instrument Bruker Apex IV FTMS
 Operator Peking University



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule
1062.15065	1	C 70 H 29 Cl N O 9	100.00	1062.15254	1.9	1.8	65.3	56.5	even		ok

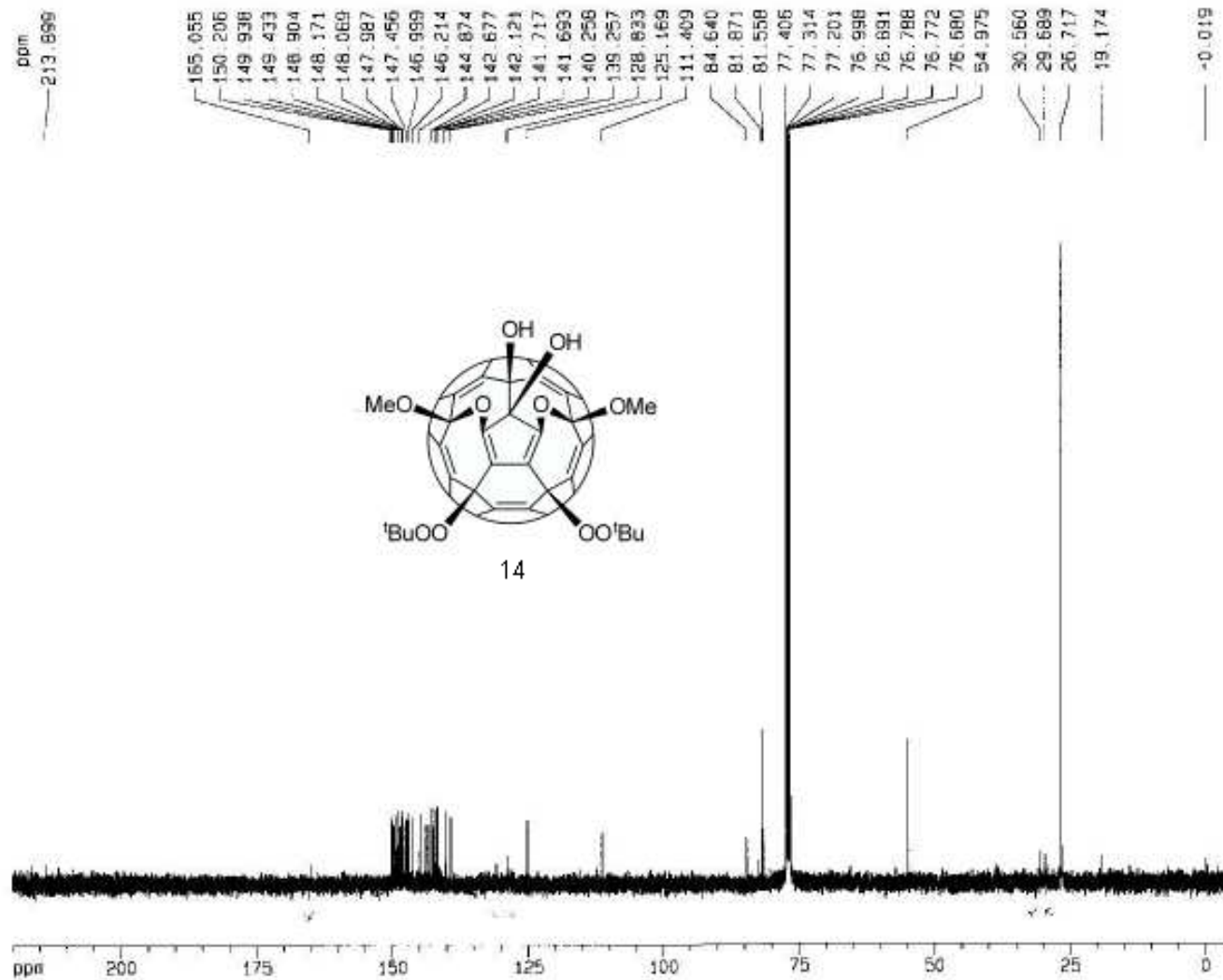


Current Data Parameters
 NAME H37567
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20071217
 Time 11.32
 INSTRUM ARX400
 PROBHD 5 mm Multinu
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 30
 DS 0
 SWH 6410.256 Hz
 FIDRES 0.195625 Hz
 AQ 2.5559540 sec
 RG 2860
 CW 78.000 usec
 DE 97.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 P1 3.00 usec
 DE 97.50 usec
 SFO1 400.1324000 MHz
 NUCLEUS 1H

F2 - Processing parameters
 SI 16384
 SF 400.1300095 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 0.50

1D NMR plot parameters
 CX 20.00 cm
 F1P 10.000 ppm
 F1 4001.30 Hz
 F2P -0.500 ppm
 F2 -200.07 Hz
 PPMCM 0.52500 ppm/cm
 HZCM 210.06825 Hz/cm



Current Data Parameters
NAME C37567
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20071217
Time 11.46
INSTRUM ARX400
PROBHD 5 mm Multinu
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 3051
DS 0
SMH 27777.777 Hz
FIDRES 0.847710 Hz
AQ 0.5898740 sec
RG 8192
DM 18.000 usec
DE 25.71 usec
TE 300.0 K
D12 0.00002000 sec
DL5 22.20 dB
CPDPRG waltz16
P31 100.00 usec
D1 2.00000000 sec
P1 3.00 usec
DE 25.71 usec
SF01 100.6240000 MHz
NUCLEUS 13C
D11 0.03000000 sec

F2 - Processing parameters

SI 32768
SF 100.6127713 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 0.30

1D NMR plot parameters

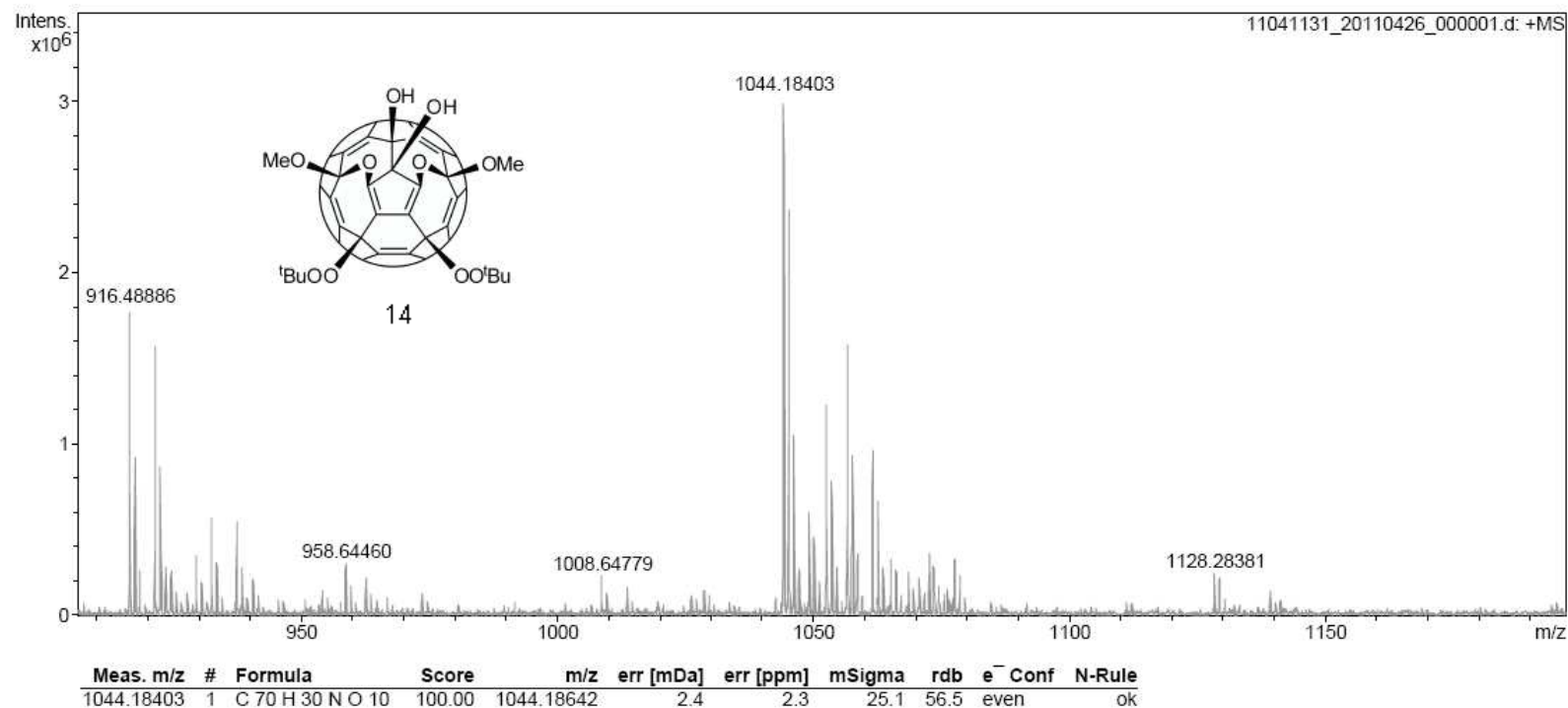
CX 20.00 cm
F1P 220.000 ppm
F1 22134.81 Hz
F2P -5.000 ppm
F2 -503.07 Hz
PPMCM 11.25000 ppm/cm
HZCM 1131.89368 Hz/cm

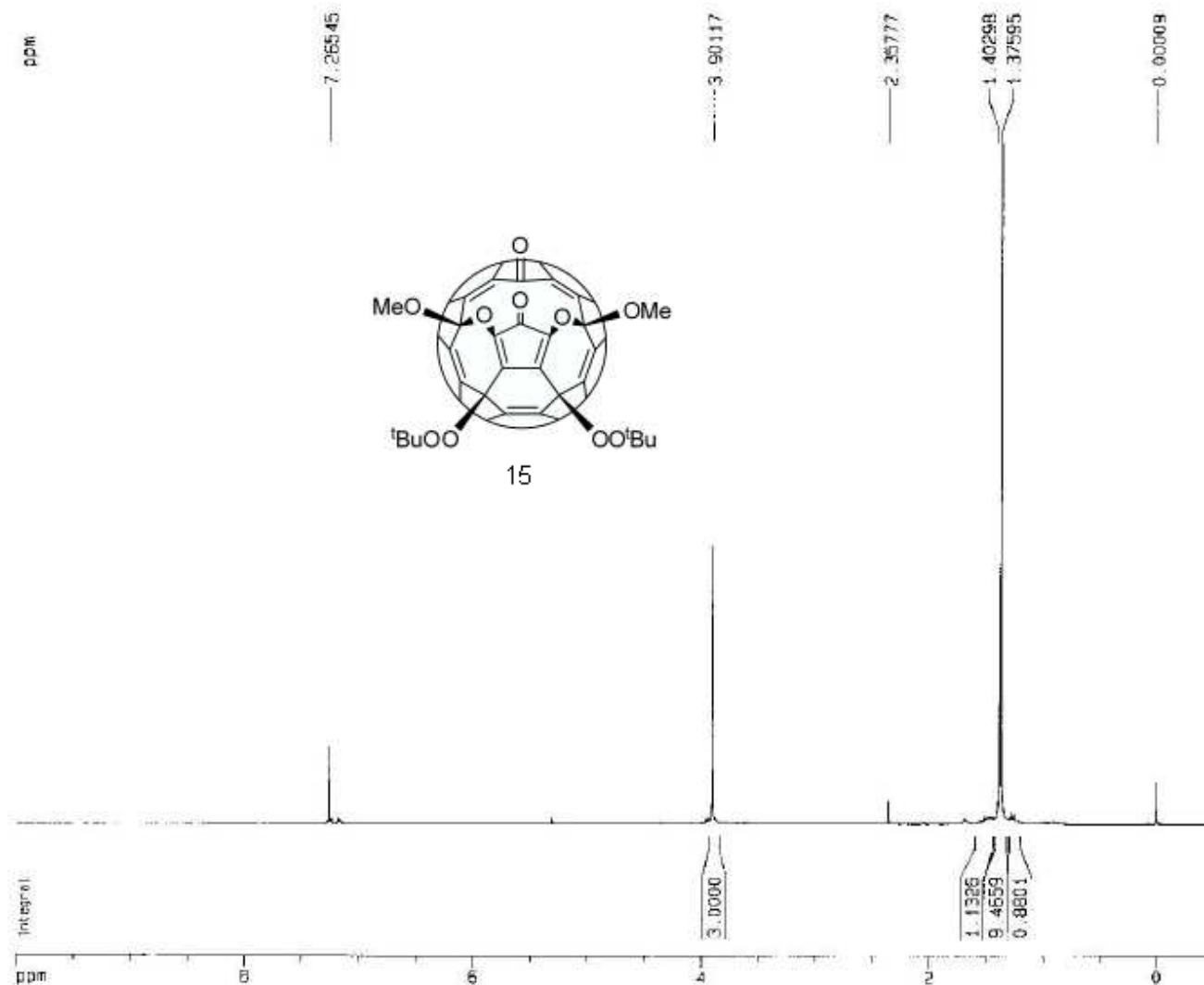
Peking University Mass Spectrometry Sample Analysis Report

Analysis Info

Analysis Name 11041131_20110426_000001.d
Sample 110426
Comment ESI Positive

Acquisition Date 4/26/2011 4:08:21 PM
Instrument Bruker Apex IV FTMS
Operator Peking University



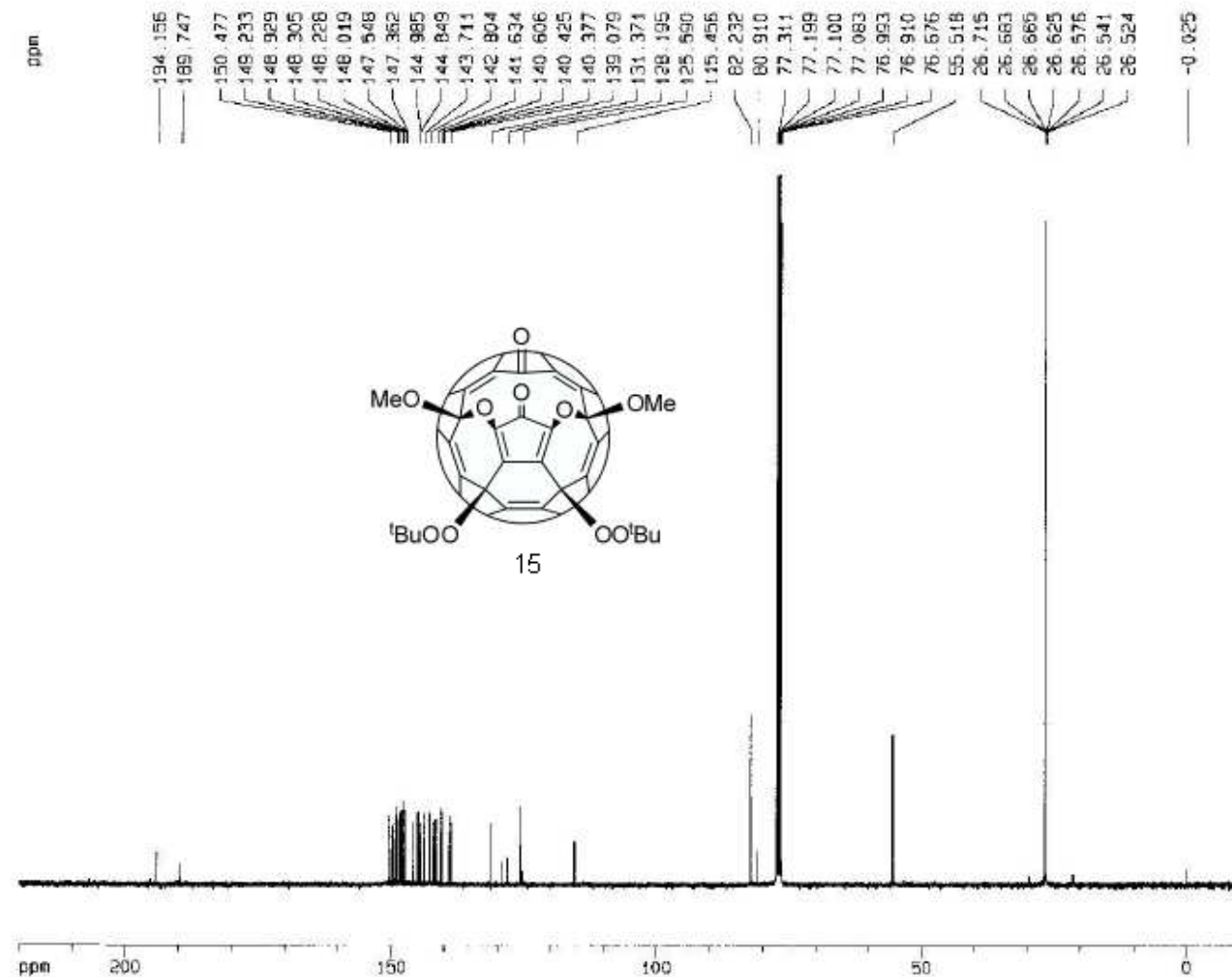


Current Data Parameters
 NAME H38071
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080123
 Time 11.28
 INSTRUM ARX400
 PROBHD 5 mm Multinu
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 64
 DS 0
 SWH 6410.256 Hz
 FIDRES 0.195625 Hz
 AQ 2.5559540 sec
 RG 1024
 DM 78.000 usec
 DE 97.50 usec
 TE 300.0 K
 D1 2.0000000 sec
 P1 3.00 usec
 DE 97.50 usec
 SF01 400.1324000 MHz
 NUCLEUS 1H

F2 - Processing parameters
 SI 32768
 SF 400.1300083 MHz
 WDM no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 0.50

1D NMR plot parameters
 CX 20.00 cm
 F1P 10.000 ppm
 F1 4001.30 Hz
 F2P -0.500 ppm
 F2 -200.07 Hz
 PPMCM 0.52500 ppm/cm
 HZCM 210.06625 Hz/cm



Current Data Parameters
NAME C38971
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

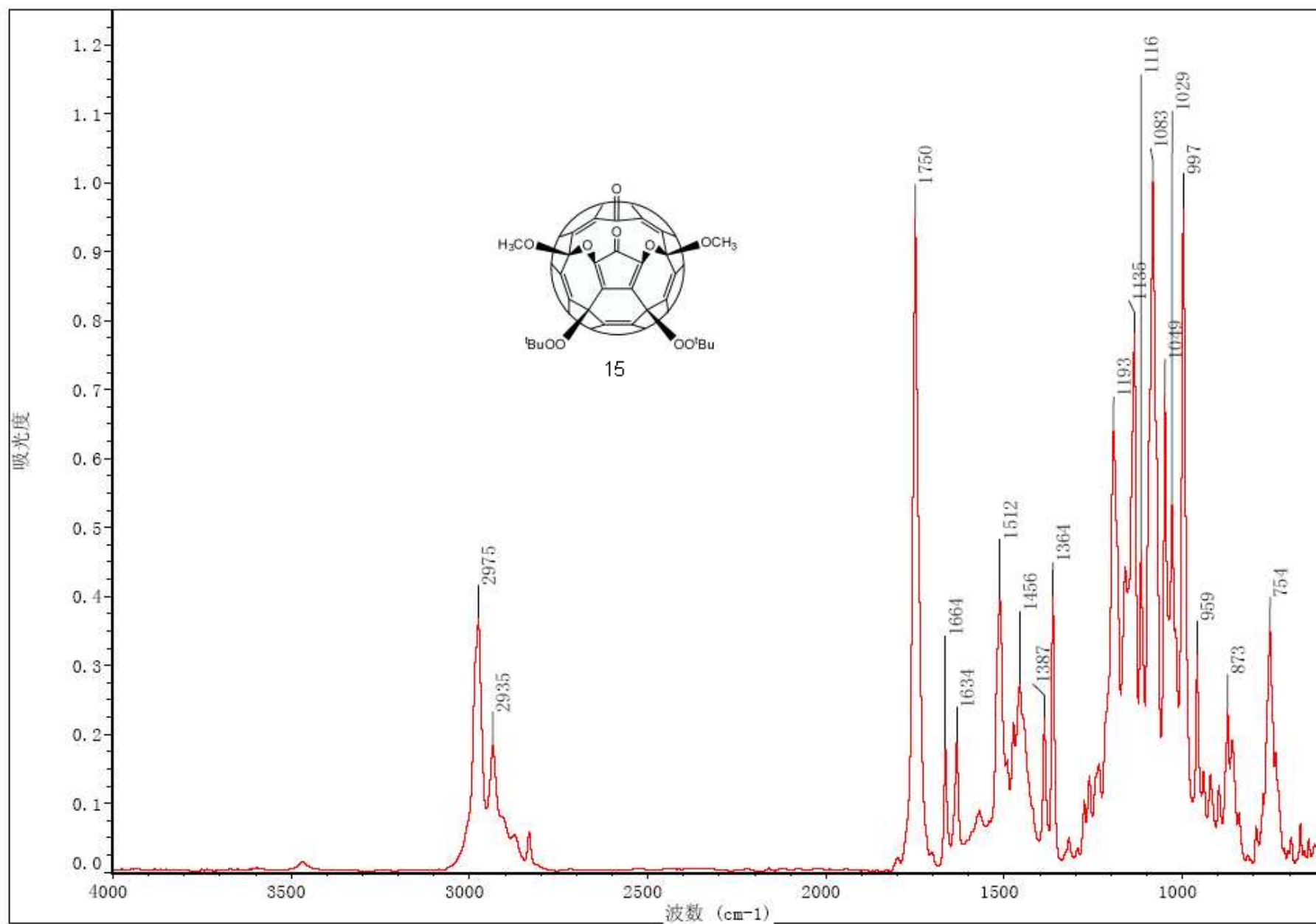
Date_ 20080123
Time 11:31
INSTRUM ARX400
PROBHD 5 mm Multinu
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 4373
DS 0
SWH 27777.777 Hz
FIDRES 0.847710 Hz
AQ 0.5888740 sec
RG 4096
DM 18.000 usec
DE 25.71 usec
TE 300.0 K
D12 0.00002000 sec
CL5 22.20 dB
CPDPRG waltz16
P31 100.00 usec
D1 2.00000000 sec
P1 3.00 usec
DE 25.71 usec
SF01 100.6240000 MHz
NUCLEUS 13C
D11 0.03000000 sec

F2 - Processing parameters

SI 32768
SF 100.6127738 MHz
WDW EN
SSB 0
LB 0.50 Hz
GB 0
PC 0.30

1D NMR plot parameters

CX 20.00 cm
F1P 220.000 ppm
F1 22134.81 Hz
F2P -10.000 ppm
F2 -1006.13 Hz
PPMCM 11.50000 ppm/cm
HZCM 1157.04587 Hz/cm

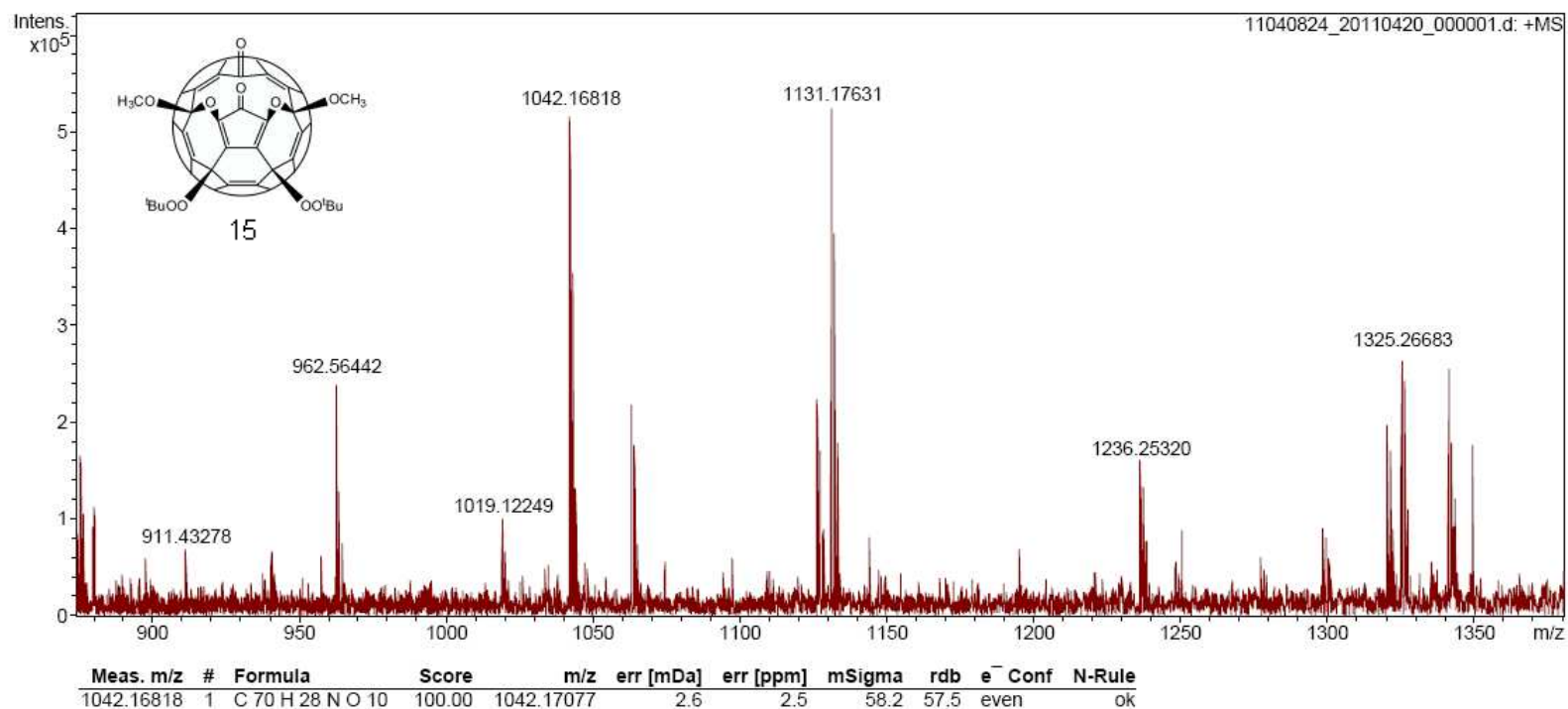


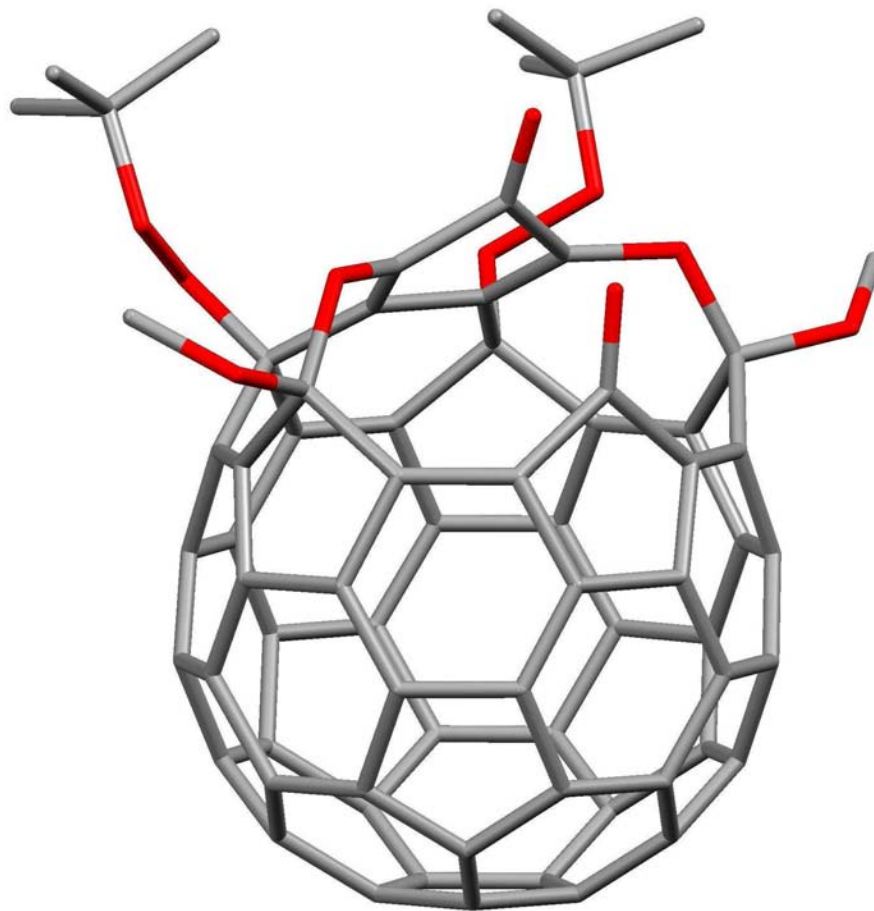
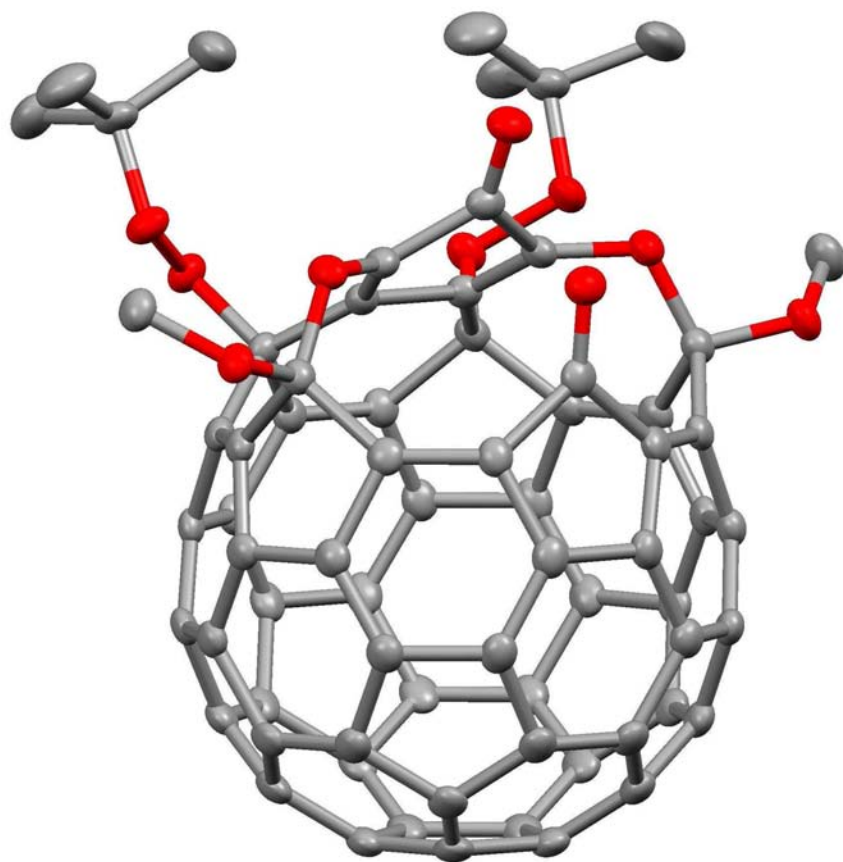
Peking University Mass Spectrometry Sample Analysis Report

Analysis Info

Analysis Name 11040824_20110420_000001.d
Sample 110418
Comment ESI Positive

Acquisition Date 4/20/2011 11:57:23 AM
Instrument Bruker Apex IV FTMS
Operator Peking University





Single-crystal X ray structure of 15. Ellipsoids (left) were drawn at the 50% level; for clarity hydrogen atoms were not shown. Color key:
gray, carbon; red, oxygen.

24y-080124-triOMe-300m

Archive directory: /export/home/vnmr1/vnmr/sys/data
Sample directory:
File: PROTON

Pulse Sequence: s2pu1

7.274

4.077

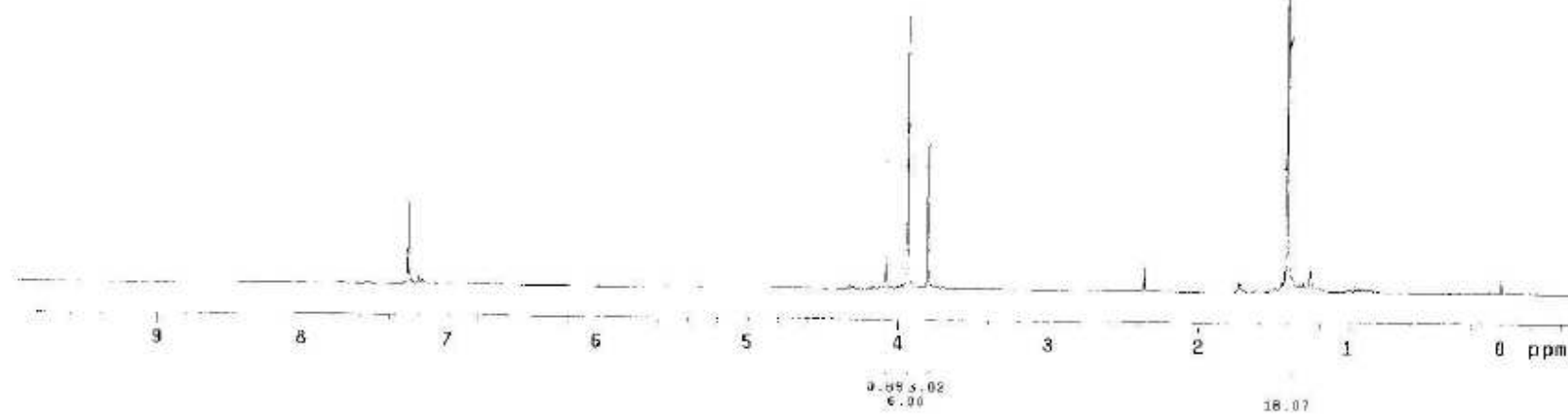
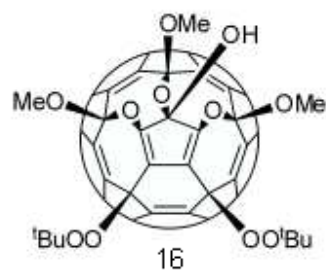
3.937

3.802

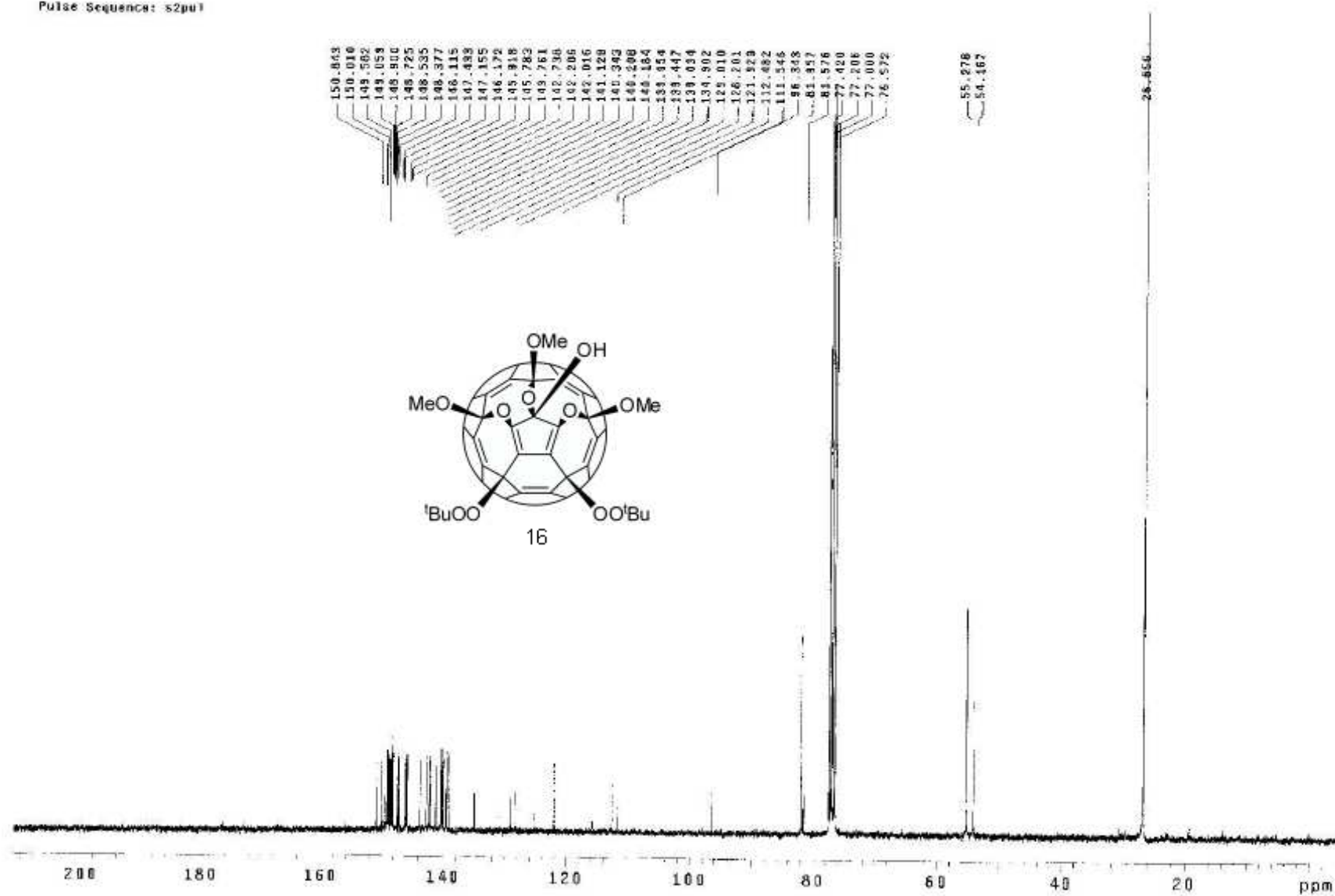
2.362

1.411

1.255



zcy-080124-triOMe-n
Pulse Sequence: s2pul



Peking University Mass Spectrometry Sample Analysis Report

Analysis Info

Analysis Name 11041020_20110425_000001.d
Sample 110423
Comment ESI Positive

Acquisition Date 4/25/2011 5:15:17 PM
Instrument Bruker Apex IV FTMS
Operator Peking University

