Supporting Information

Title: Non-Polar Solvent a Key for Highly Regio-Selective SNAr Reaction in case of 2, 4-difluoronitrobenzene

Authors: Suresh Kumar Sythana, Surendra R. Naramreddy, Santosh Kavitake, Vinod Kumar CH.* and Pundlik R. Bhagat*

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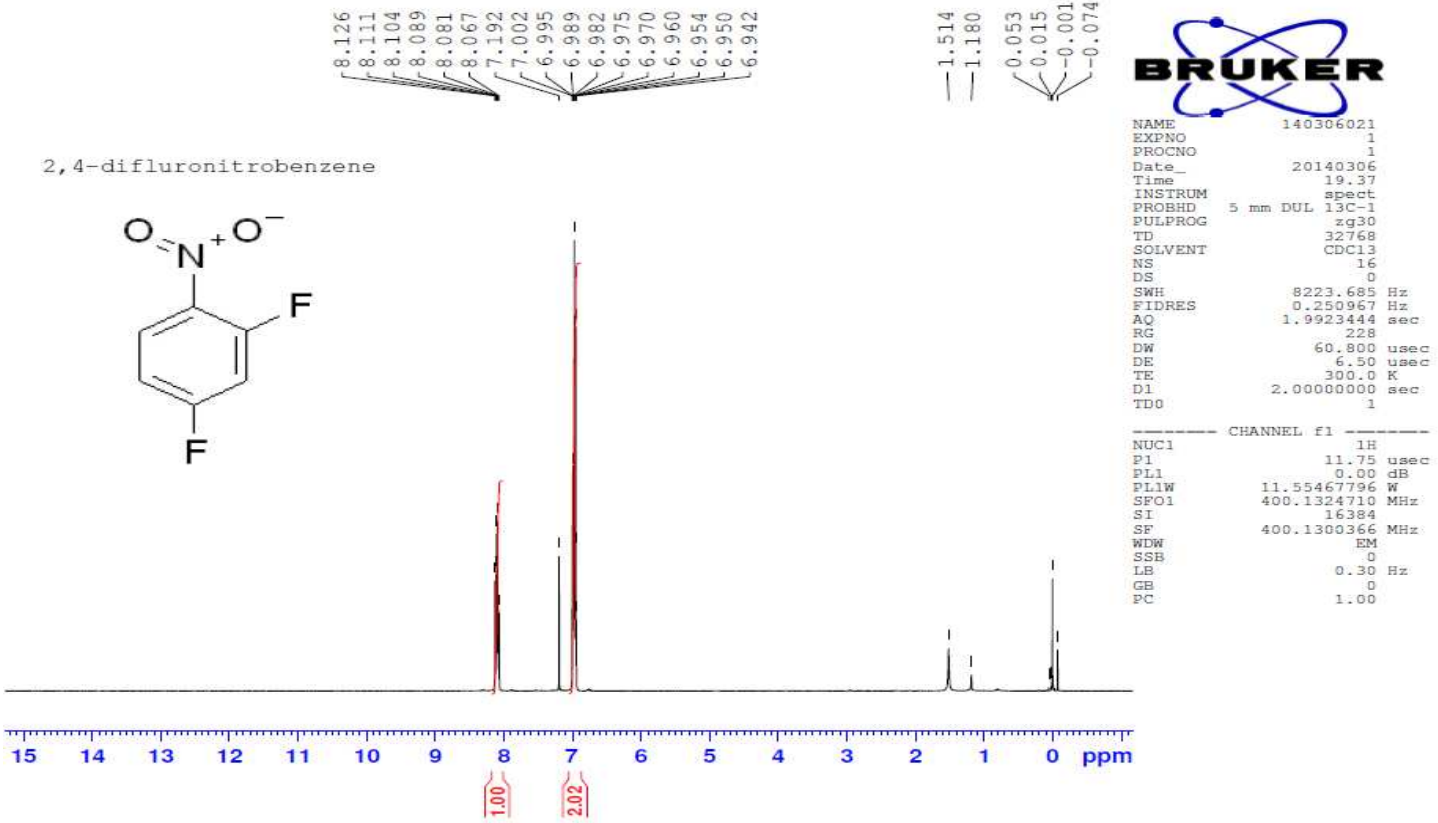
1. Spectral data ^{1}H NMR, ^{13} NMR, DEPT and HRMS

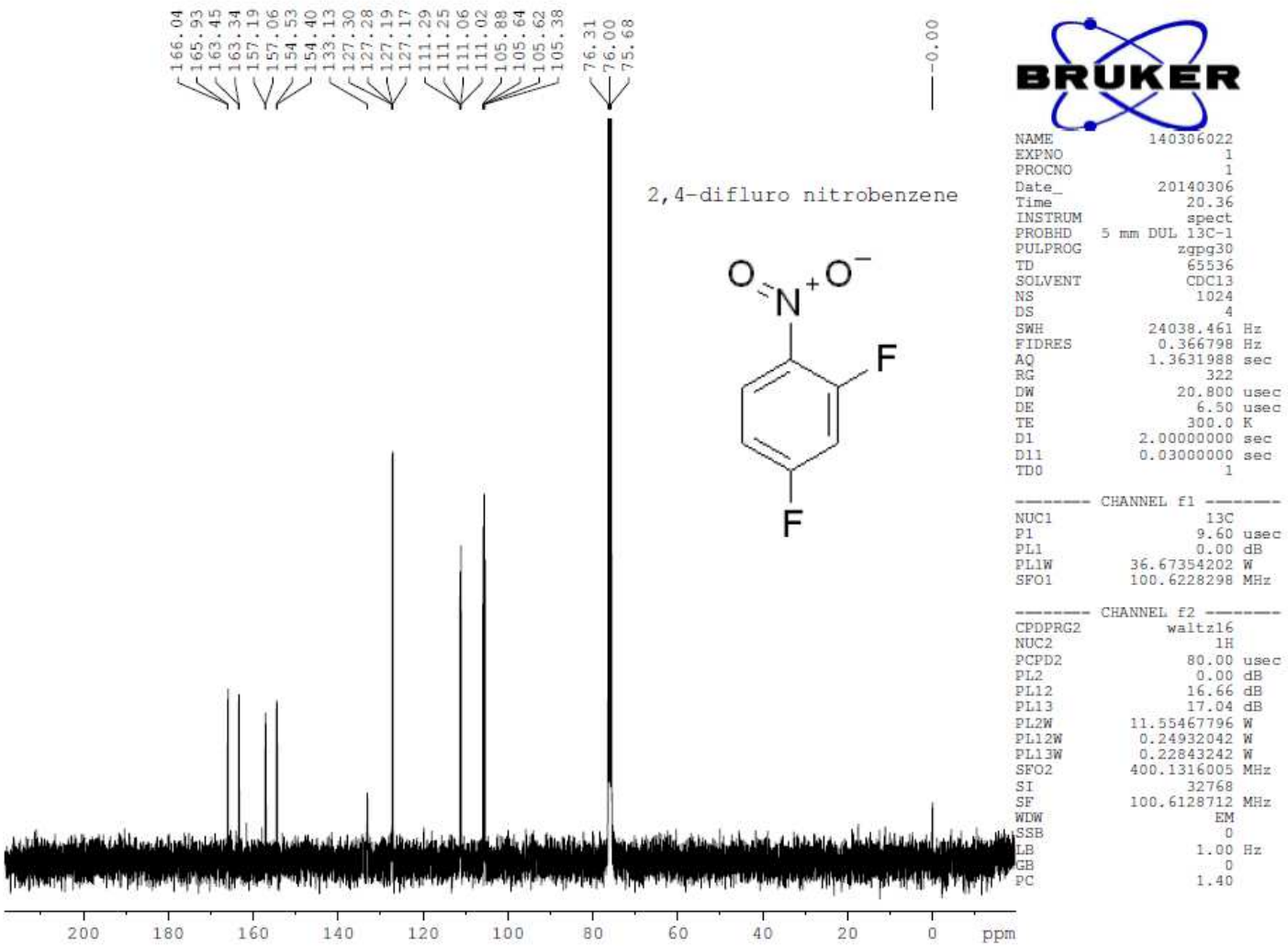
2, 4-difluoro-1-nitro-benzene, **1** (DFN Benzene) ^{1}H-NMR.



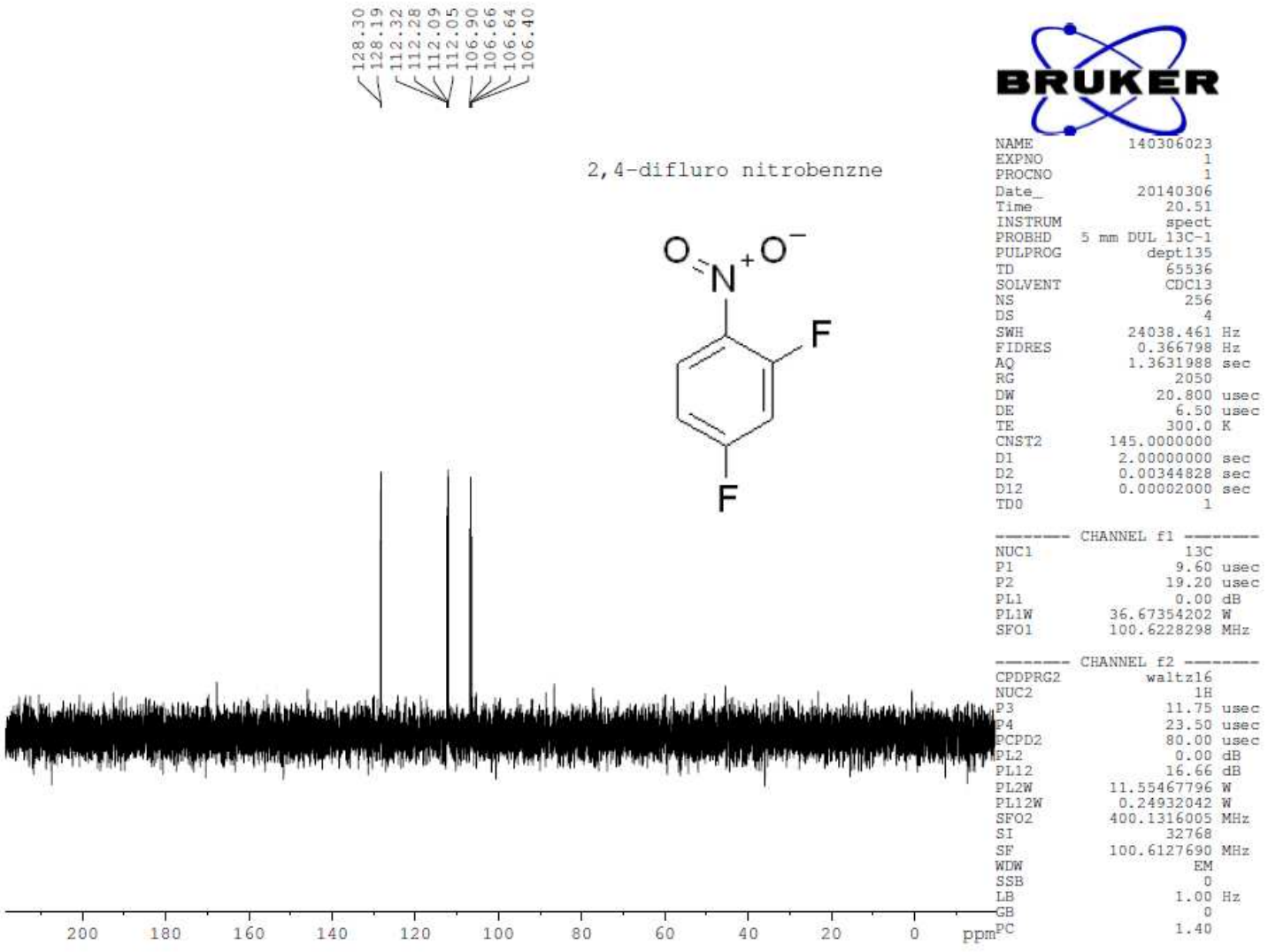
BRUKER

NAME	140306021
EXPNO	1
PROCNO	1
Date_	20140306
Time	19.37
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	32768
SOLVENT	CDC13
NS	16
DS	0
SWH	8223.685 Hz
FIDRES	0.250967 Hz
AQ	1.9923444 sec
RG	228
DW	60.800 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
-------- CHANNEL f1 --------	
NUC1	1H
P1	11.75 usec
PL1	0.00 dB
PL1W	11.55467796 W
SFO1	400.1324710 MHz
SI	16384
SF	400.1300366 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

2, 4-difluoro-1-nitro-benzene, **1** (DFN Benzene) ^{13}C-NMR.



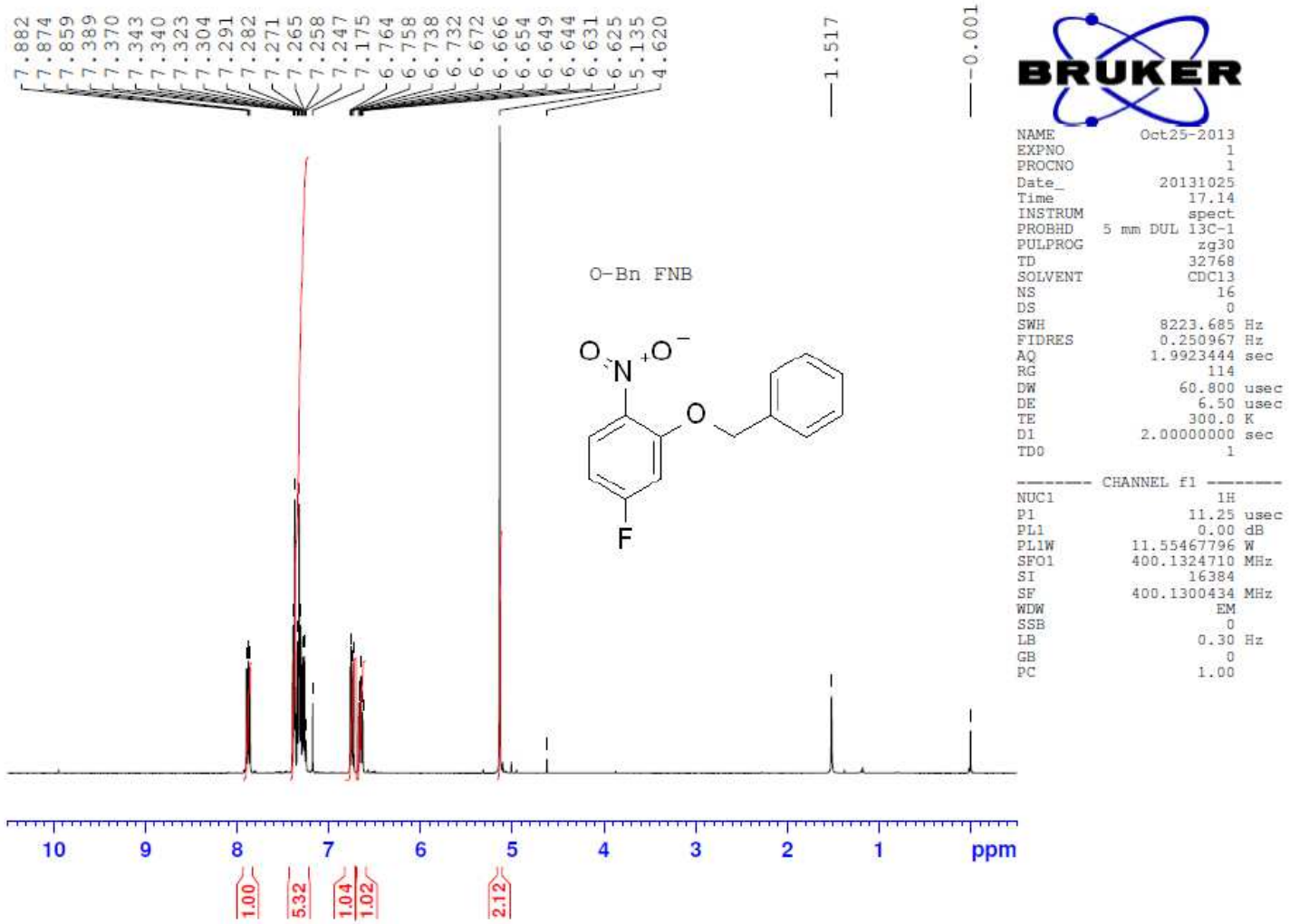
2,4-difluoro-1-nitro-benzene, **1** (DFN Benzene) DEPT-NMR.



BRUKER

NAME	140306023
EXPNO	1
PROCNO	1
Date_	20140306
Time	20.51
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	dept135
TD	65536
SOLVENT	CDC13
NS	256
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	300.0 K
CNST2	145.0000000
D1	2.00000000 sec
D2	0.00344828 sec
D12	0.00002000 sec
TD0	1
------- CHANNEL f1 -------	
NUC1	13C
P1	9.60 usec
P2	19.20 usec
PL1	0.00 dB
PL1W	36.67354202 W
SFO1	100.6228298 MHz
------- CHANNEL f2 -------	
CPDPRG2	waltz16
NUC2	1H
P3	11.75 usec
P4	23.50 usec
PCPD2	80.00 usec
PL2	0.00 dB
PL12	16.66 dB
PL2W	11.55467796 W
PL12W	0.24932042 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

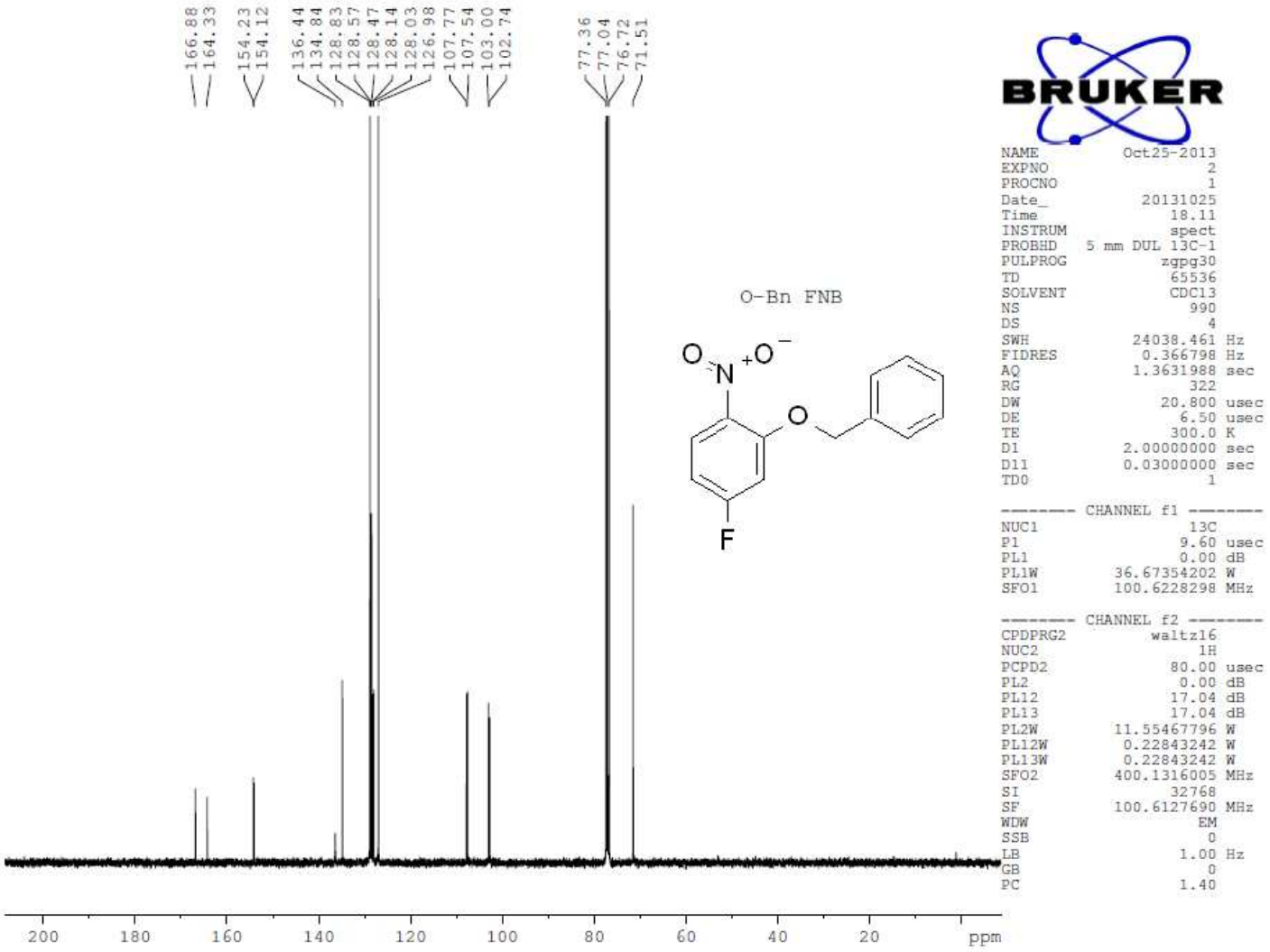
Product **3a** [(2-benzyloxy-4-fluoro-1-nitro-benzene) (O-Bn FNB)] ^{1}H-NMR



BRUKER

NAME	Oct25-2013
EXPNO	1
PROCNO	1
Date_	20131025
Time	17.14
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	0
SWH	8223.685 Hz
FIDRES	0.250967 Hz
AQ	1.9923444 sec
RG	114
DW	60.800 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
------- CHANNEL f1 -------	
NUC1	1H
P1	11.25 usec
PL1	0.00 dB
PL1W	11.55467796 W
SFO1	400.1324710 MHz
SI	16384
SF	400.1300434 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

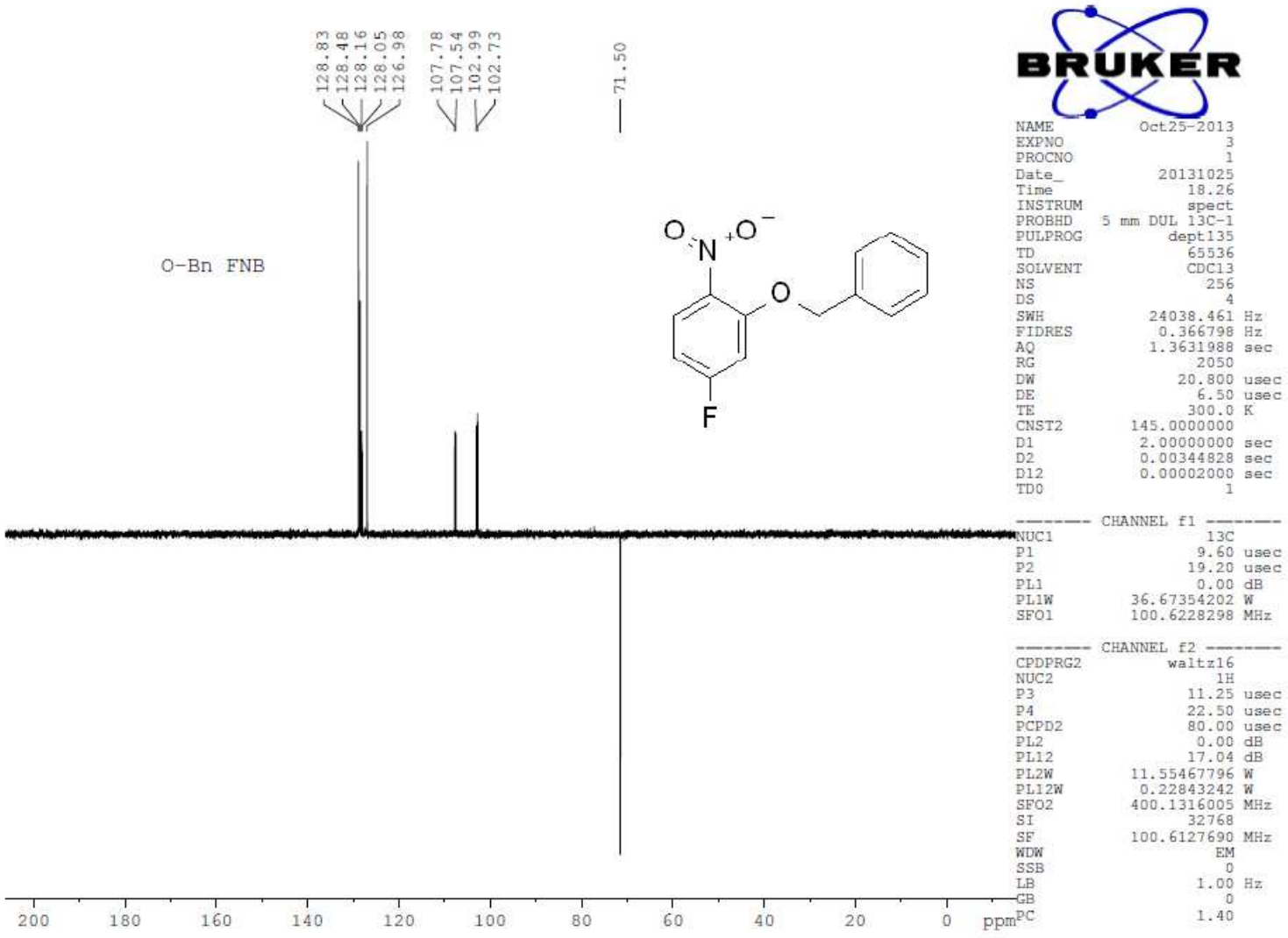
Product **3a** [(2-benzyloxy-4-fluoro-1-nitro-benzene) (O-Bn FNB)] ^{13}C-NMR



BRUKER

NAME	Oct25-2013
EXPNO	2
PROCNO	1
Date_	20131025
Time	18.11
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	990
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	322
DW	20.800 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
-------- CHANNEL f1 --------	
NUC1	13C
P1	9.60 usec
PL1	0.00 dB
PL1W	36.67354202 W
SFO1	100.6228298 MHz
-------- CHANNEL f2 --------	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	17.04 dB
PL13	17.04 dB
PL2W	11.55467796 W
PL12W	0.22843242 W
PL13W	0.22843242 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

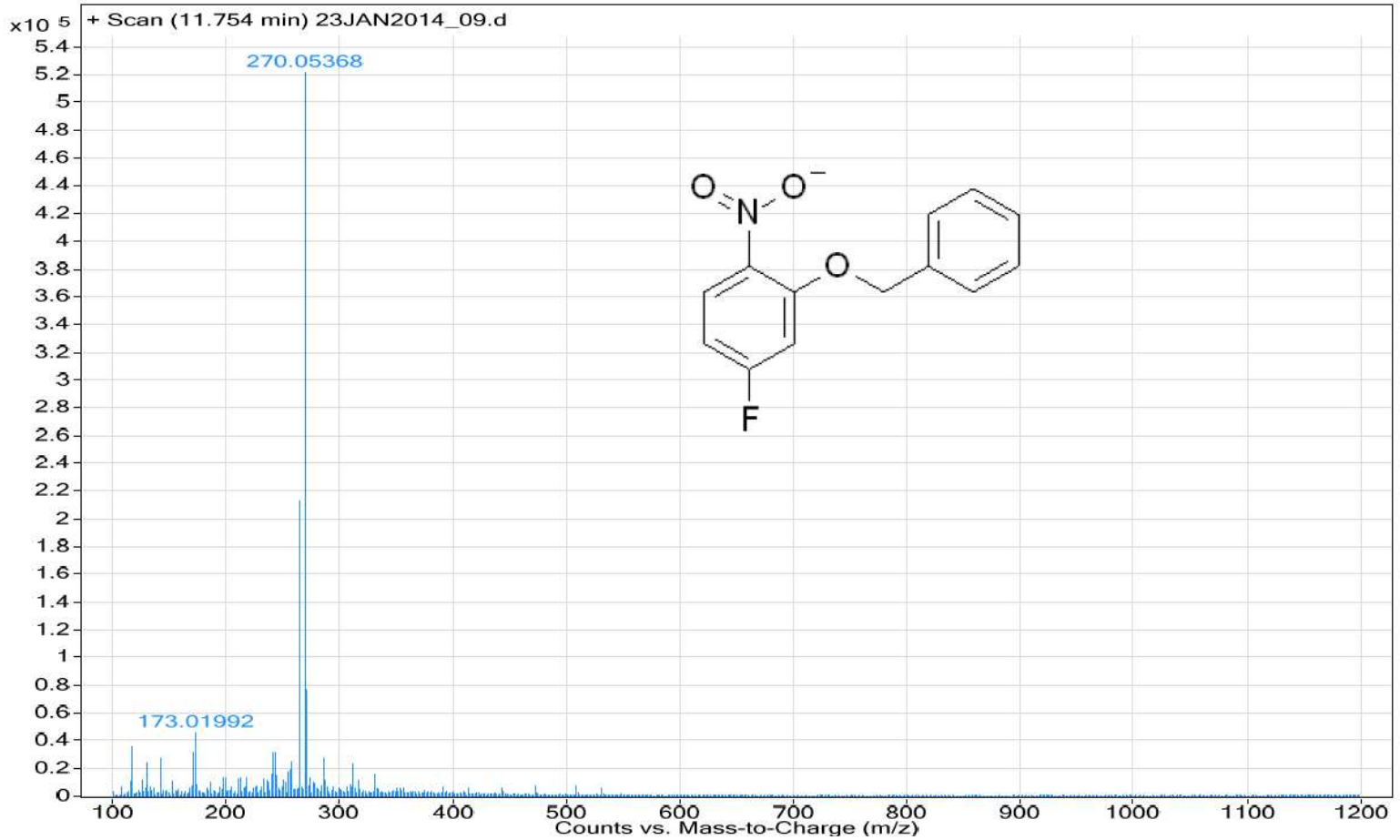
Product **3a** [(2-benzyloxy-4-fluoro-1-nitro-benzene) (O-Bn FNB)] DEPT-NMR



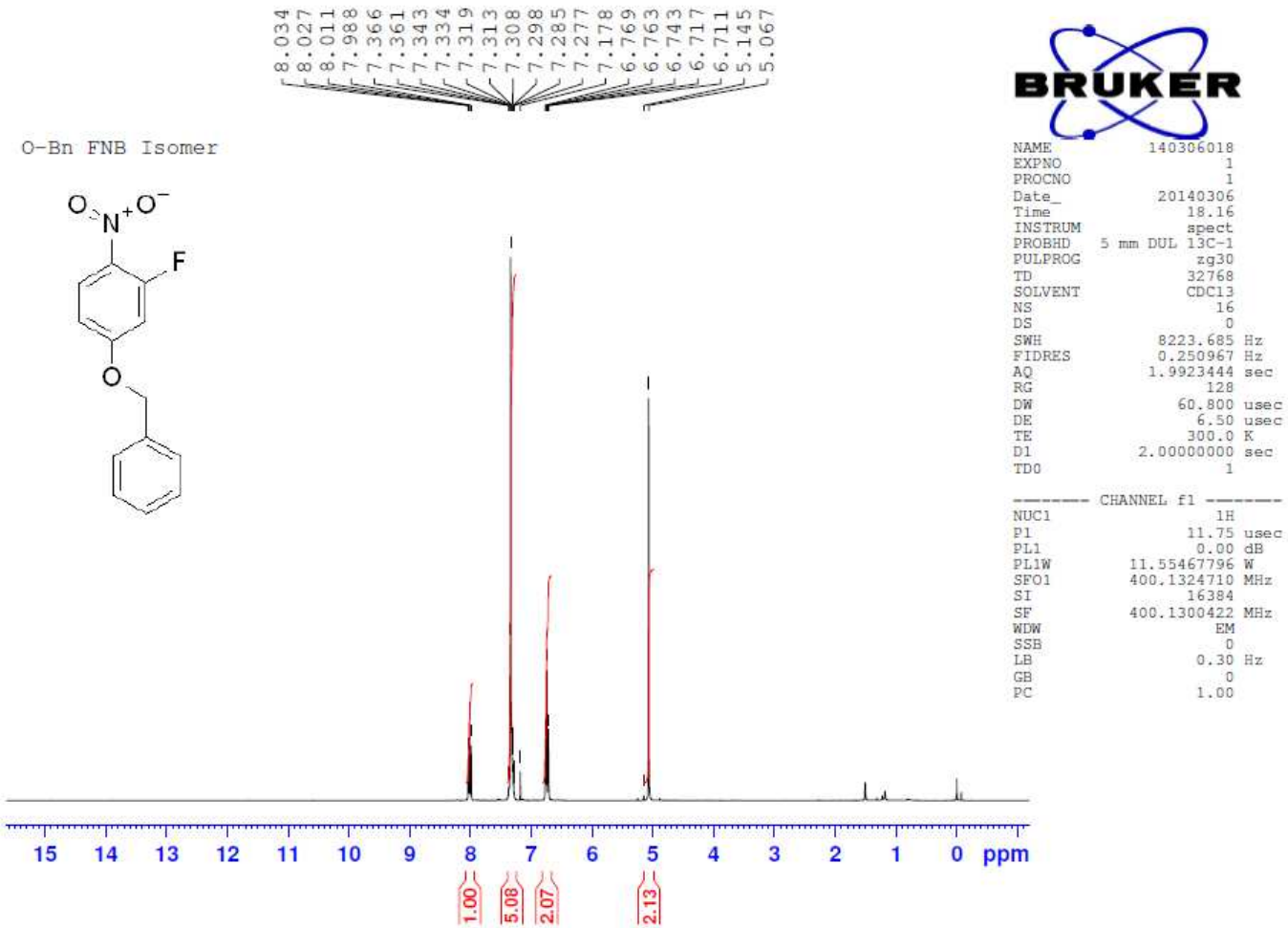
NAME	Oct25-2013
EXPNO	3
PROCNO	1
Date_	20131025
Time	18.26
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	dept135
TD	65536
SOLVENT	CDC13
NS	256
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	300.0 K
CNST2	145.0000000
D1	2.00000000 sec
D2	0.00344828 sec
D12	0.00002000 sec
TD0	1
------- CHANNEL f1 -------	
NUC1	13C
P1	9.60 usec
P2	19.20 usec
PL1	0.00 dB
PL1W	36.67354202 W
SFO1	100.6228298 MHz
------- CHANNEL f2 -------	
CPDPRG2	waltz16
NUC2	1H
P3	11.25 usec
P4	22.50 usec
PCPD2	80.00 usec
PL2	0.00 dB
PL12	17.04 dB
PL2W	11.55467796 W
PL12W	0.22843242 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Product **3a** [(2-benzyloxy-4-fluoro-1-nitro-benzene) (O-Bn FNB)] HRMS

Sample Name	O-Bn FBN	**Position**	P1-A9	**Instrument Name**	Q-TOF LCMS-01	**User Name**	Indira Jyothi
Inj Vol	1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	23JAN2014_09.d	**ACQ Method**	AZD1979_1.m	**Comment**		**Acquired Time**	1/23/2014 9:18:17 PM



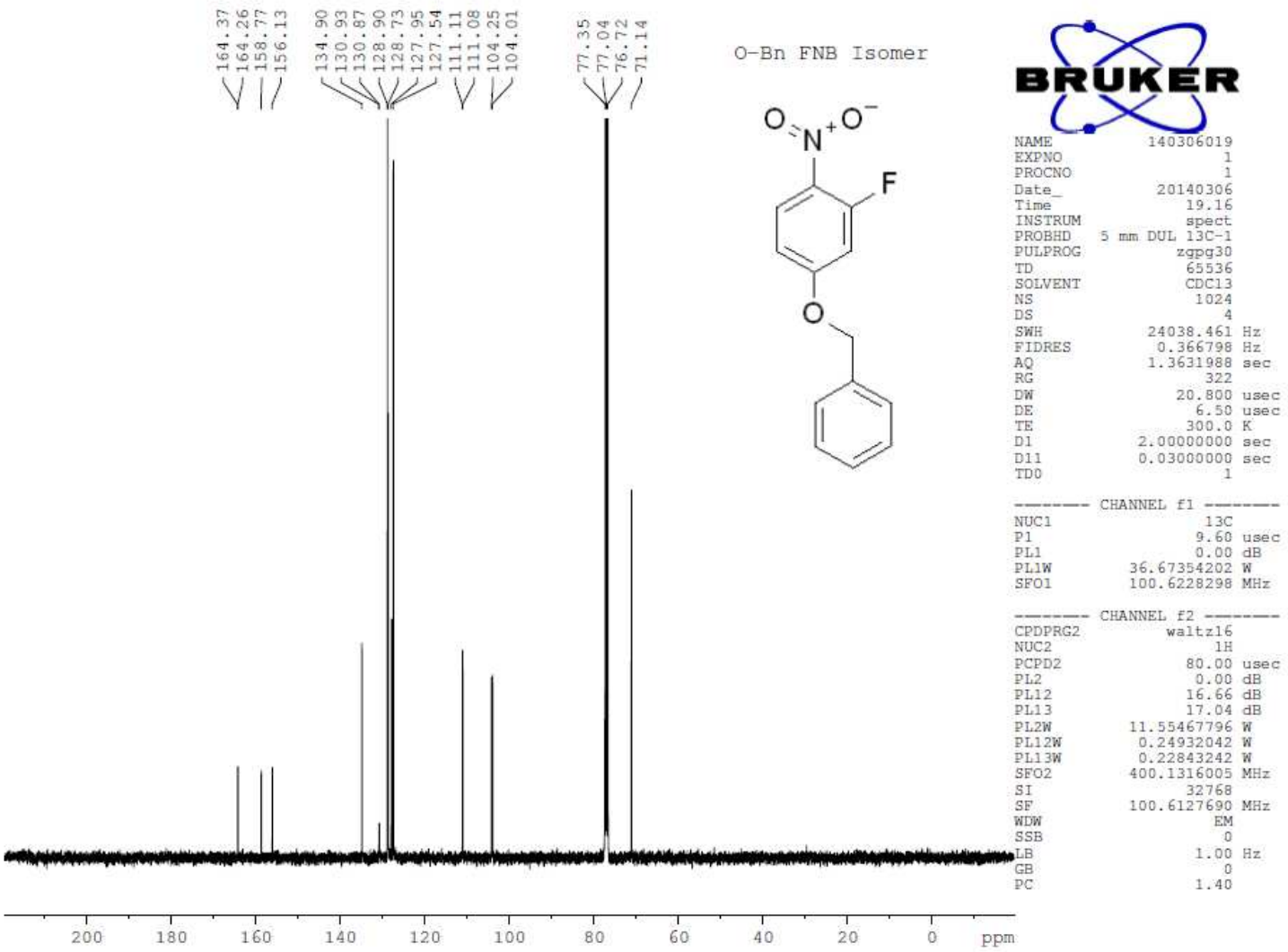
Product **3b** [(4-benzyloxy-2-fluoro-1-nitro-benzene) (O-Bn FNB Isomer)] ^{1}H-NMR



BRUKER

NAME	140306018
EXPNO	1
PROCNO	1
Date_	20140306
Time	18.16
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	32768
SOLVENT	CDC13
NS	16
DS	0
SWH	8223.685 Hz
FIDRES	0.250967 Hz
AQ	1.9923444 sec
RG	128
DW	60.800 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
------- CHANNEL f1 -------	
NUC1	1H
P1	11.75 usec
PL1	0.00 dB
PL1W	11.55467796 W
SFO1	400.1324710 MHz
SI	16384
SF	400.1300422 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

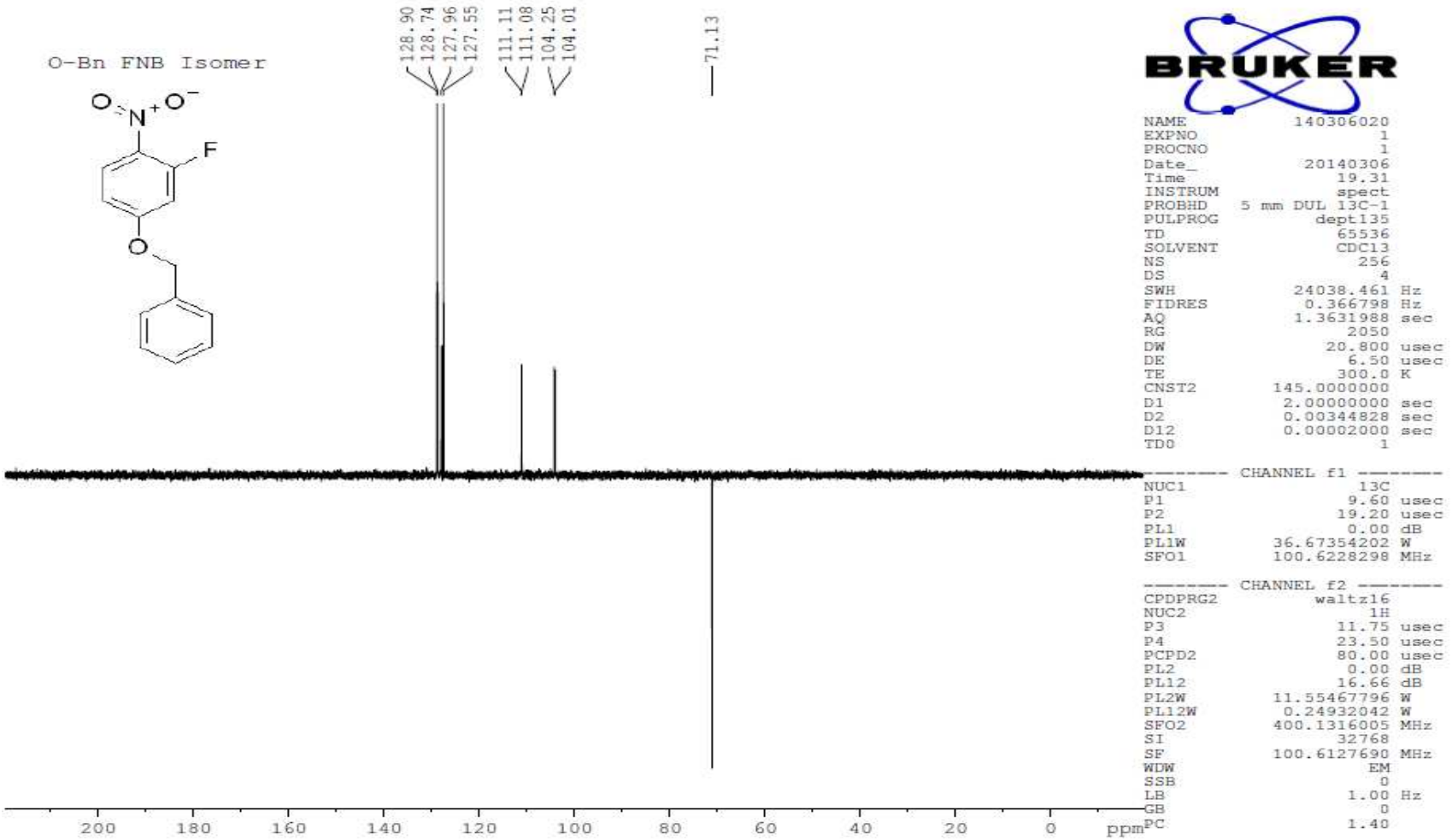
Product **3b** [(4-benzyloxy-2-fluoro-1-nitro-benzene) (O-Bn FNB Isomer)] ^{13}C-NMR



BRUKER

NAME	140306019
EXPNO	1
PROCNO	1
Date_	20140306
Time	19.16
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	322
DW	20.800 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
------- CHANNEL f1 -------	
NUC1	13C
P1	9.60 usec
PL1	0.00 dB
PL1W	36.67354202 W
SFO1	100.6228298 MHz
------- CHANNEL f2 -------	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	16.66 dB
PL13	17.04 dB
PL2W	11.55467796 W
PL12W	0.24932042 W
PL13W	0.22843242 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

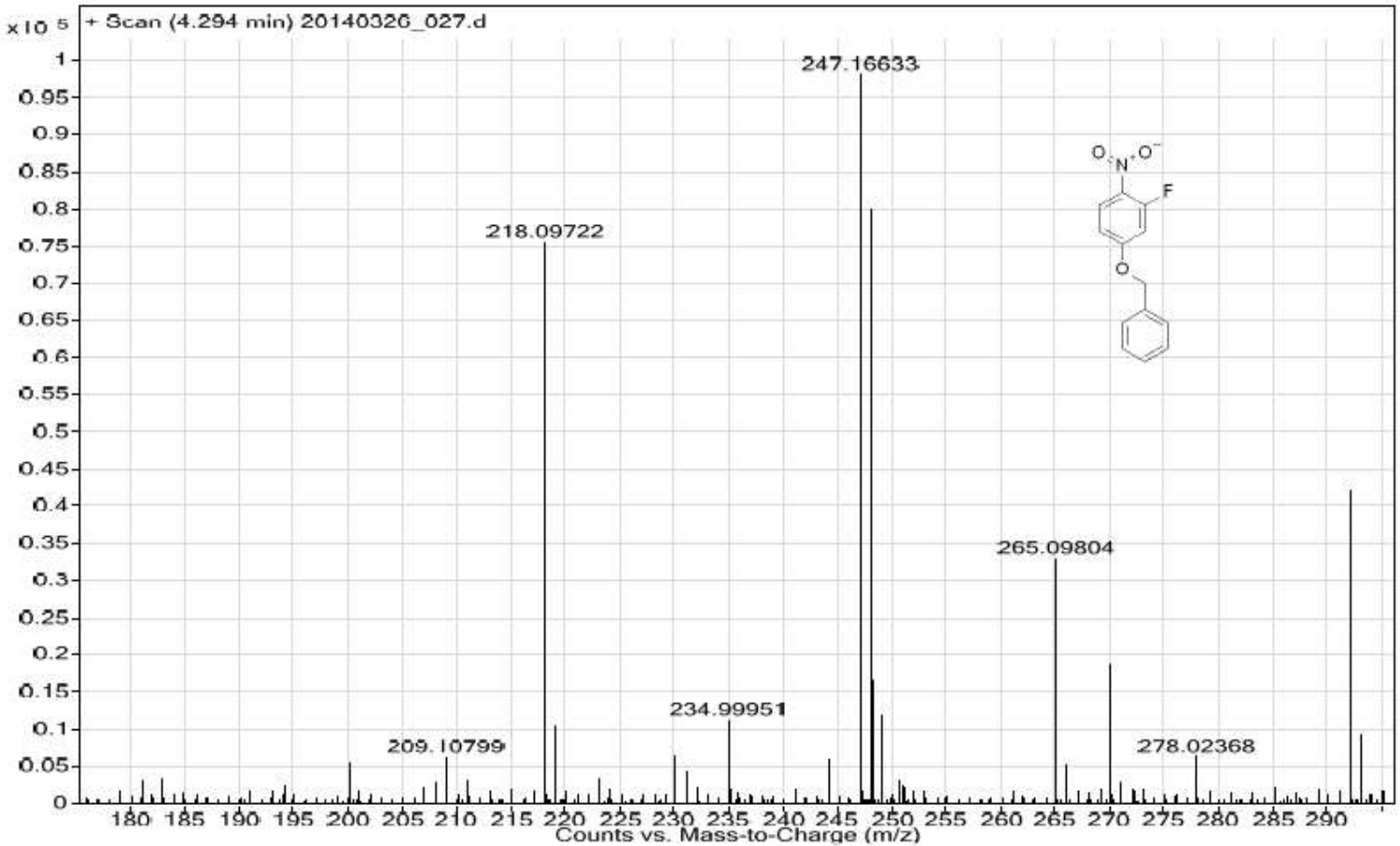
Product **3b** [(4-benzyloxy-2-fluoro-1-nitro-benzene) (O-Bn FNB Isomer)] DEPT-NMR



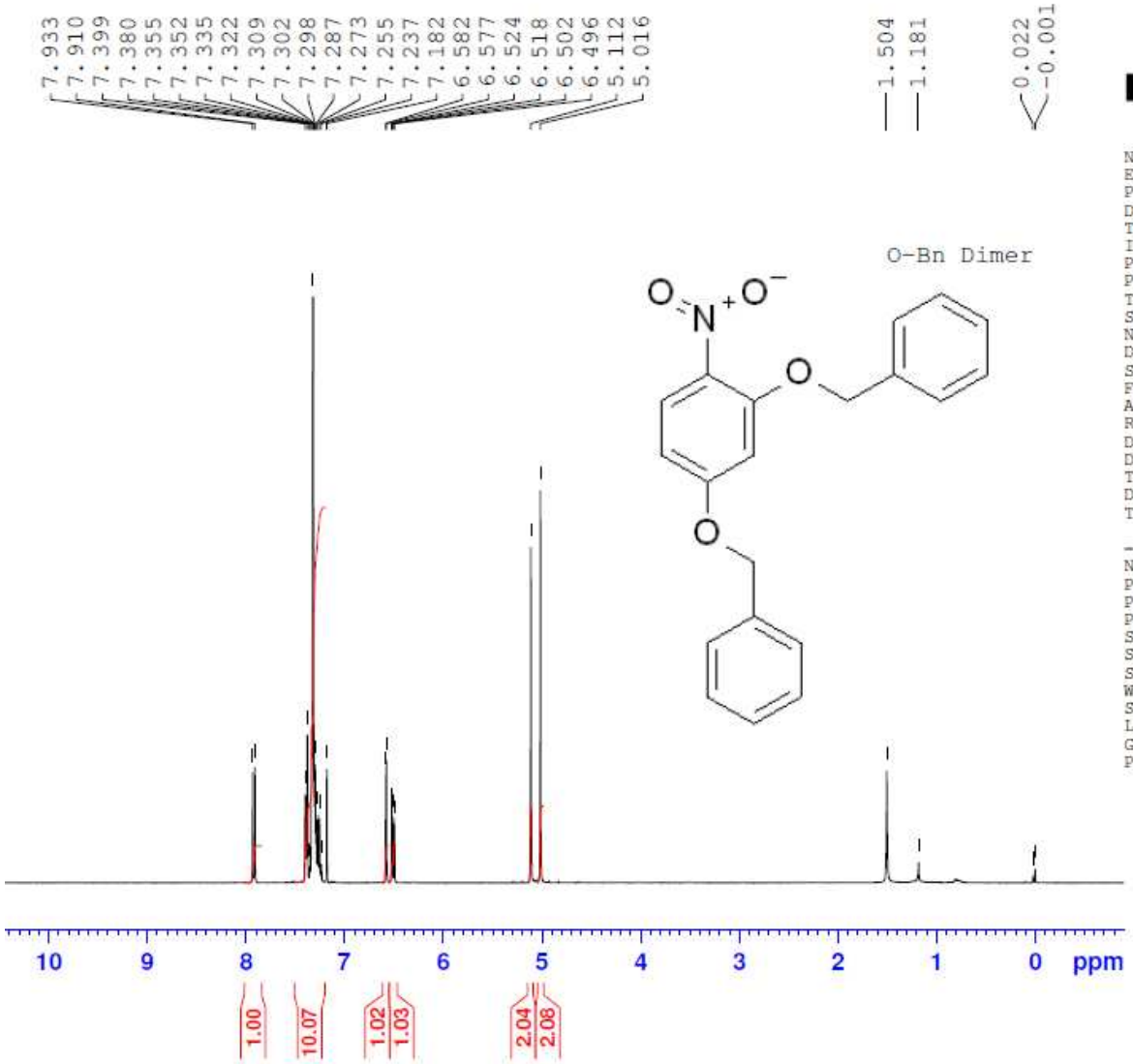
NAME	140306020
EXPNO	1
PROCNO	1
Date_	20140306
Time	19.31
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	dept135
TD	65536
SOLVENT	CDCl3
NS	256
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	300.0 K
CNST2	145.0000000
D1	2.00000000 sec
D2	0.00344828 sec
D12	0.00002000 sec
TD0	1
------- CHANNEL f1 -------	
NUC1	13C
P1	9.60 usec
P2	19.20 usec
PL1	0.00 dB
PL1W	36.67354202 W
SFO1	100.6228298 MHz
------- CHANNEL f2 -------	
CPDPRG2	waltz16
NUC2	1H
P3	11.75 usec
P4	23.50 usec
PCPD2	80.00 usec
PL2	0.00 dB
PL12	16.66 dB
PL2W	11.55467796 W
PL12W	0.24932042 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Product **3b** [(4-benzyloxy-2-fluoro-1-nitro-benzene) (O-Bn FNB Isomer)] HRMS

Sample Name	O-BN FNB ISOMER	**Position**	P1-C3	**Instrument Name**	Q-TOF LCMS-01	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	20140326_027.d	**ACQ Method**	BEH-C18_ACN_FA_C8_FA	**Comment**	O-BN FNB ISOMER	**Acquired Time**	3/26/2014 4:49:19 PM



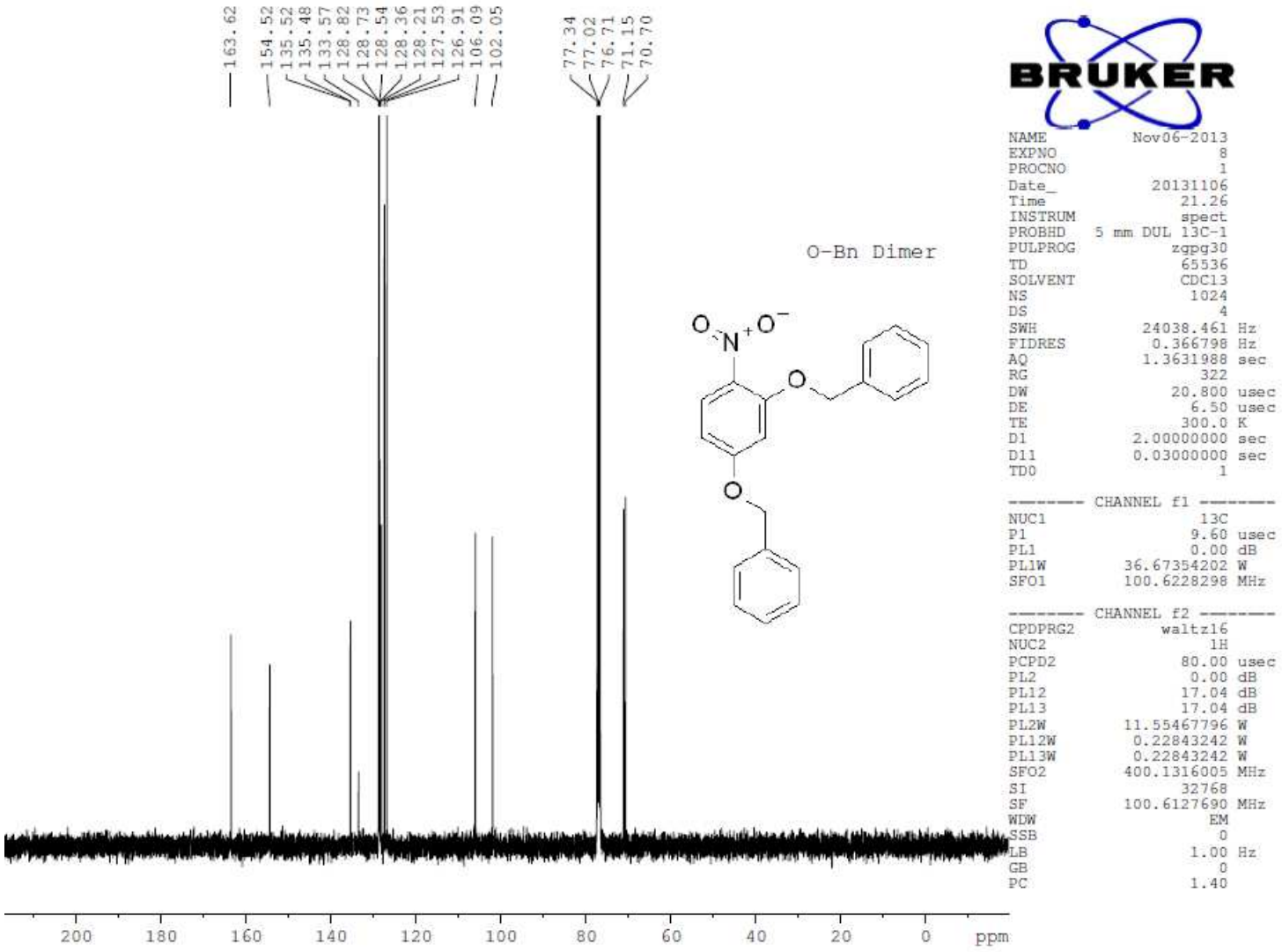
Product **3c** [(2,4-dibenzyloxy-1-nitro-benzene) (O-Bn Dimer)] ^{1}H-NMR



BRUKER

NAME	Nov06-2013
EXPNO	7
PROCNO	1
Date_	20131106
Time	20.26
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	0
SWH	8223.685 Hz
FIDRES	0.250967 Hz
AQ	1.9923444 sec
RG	144
DW	60.800 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
------- CHANNEL f1 -------	
NUC1	1H
P1	11.25 usec
PL1	0.00 dB
PL1W	11.55467796 W
SFO1	400.1324710 MHz
SI	16384
SF	400.1300407 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

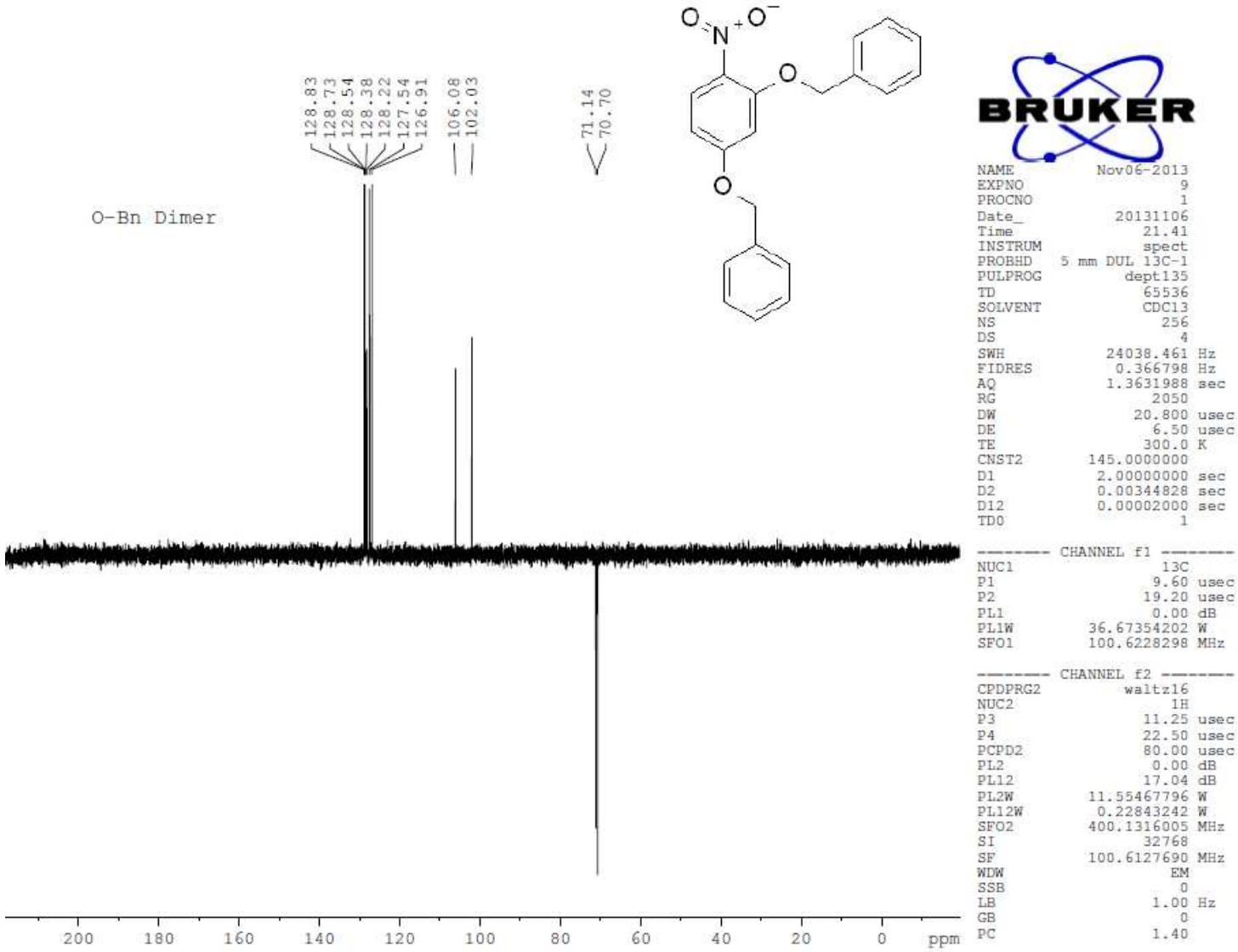
Product **3c** [(2,4-dibenzyloxy-1-nitro-benzene) (O-Bn Dimer)] ^{13}C-NMR



BRUKER

NAME	Nov06-2013
EXPNO	8
PROCNO	1
Date_	20131106
Time	21.26
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	322
DW	20.800 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
------- CHANNEL f1 -------	
NUC1	13C
P1	9.60 usec
PL1	0.00 dB
PL1W	36.67354202 W
SFO1	100.6228298 MHz
------- CHANNEL f2 -------	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	17.04 dB
PL13	17.04 dB
PL2W	11.55467796 W
PL12W	0.22843242 W
PL13W	0.22843242 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Product **3c** [(2,4-dibenzyloxy-1-nitro-benzene) (O-Bn Dimer)] DEPT-NMR

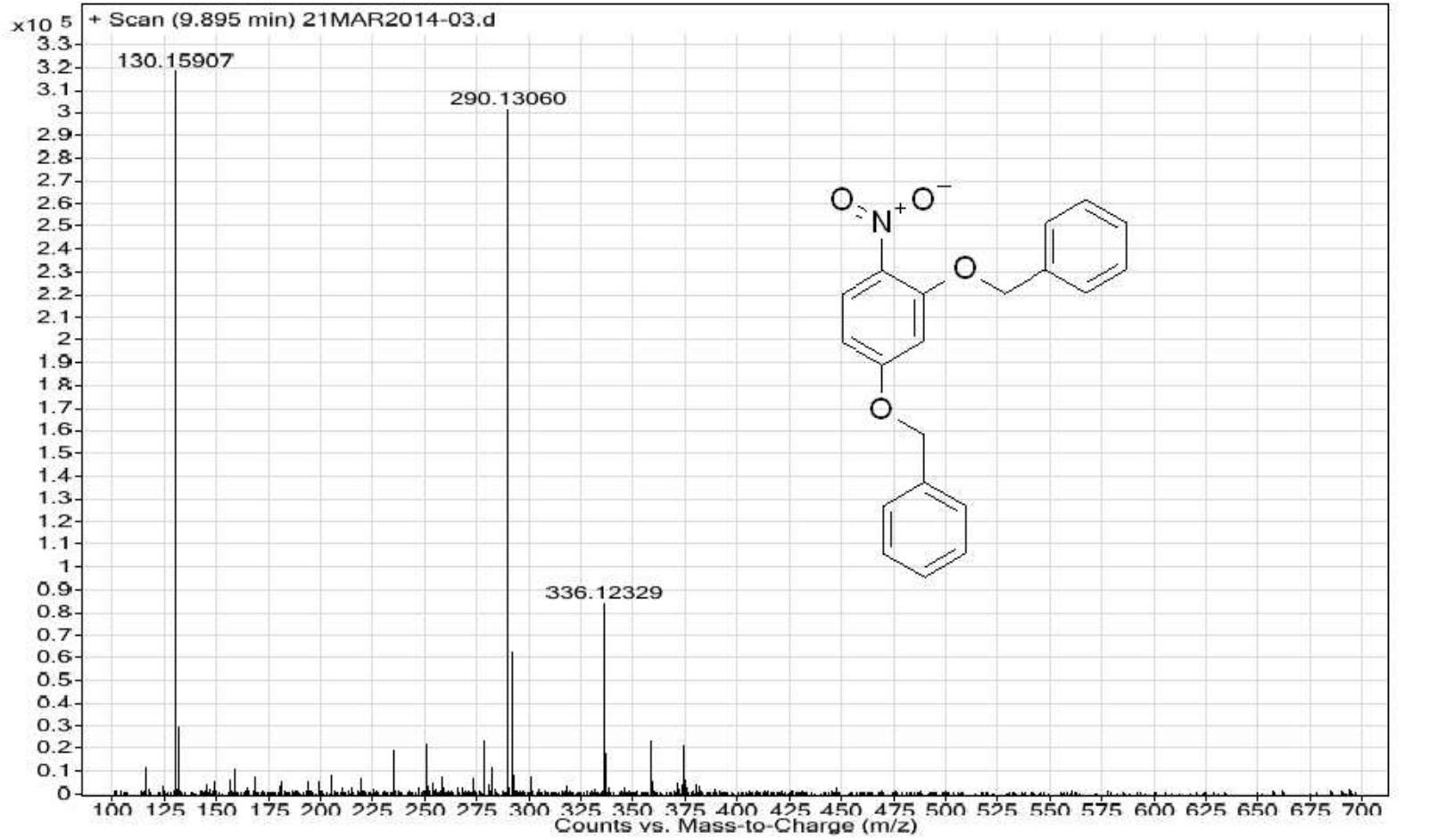


BRUKER

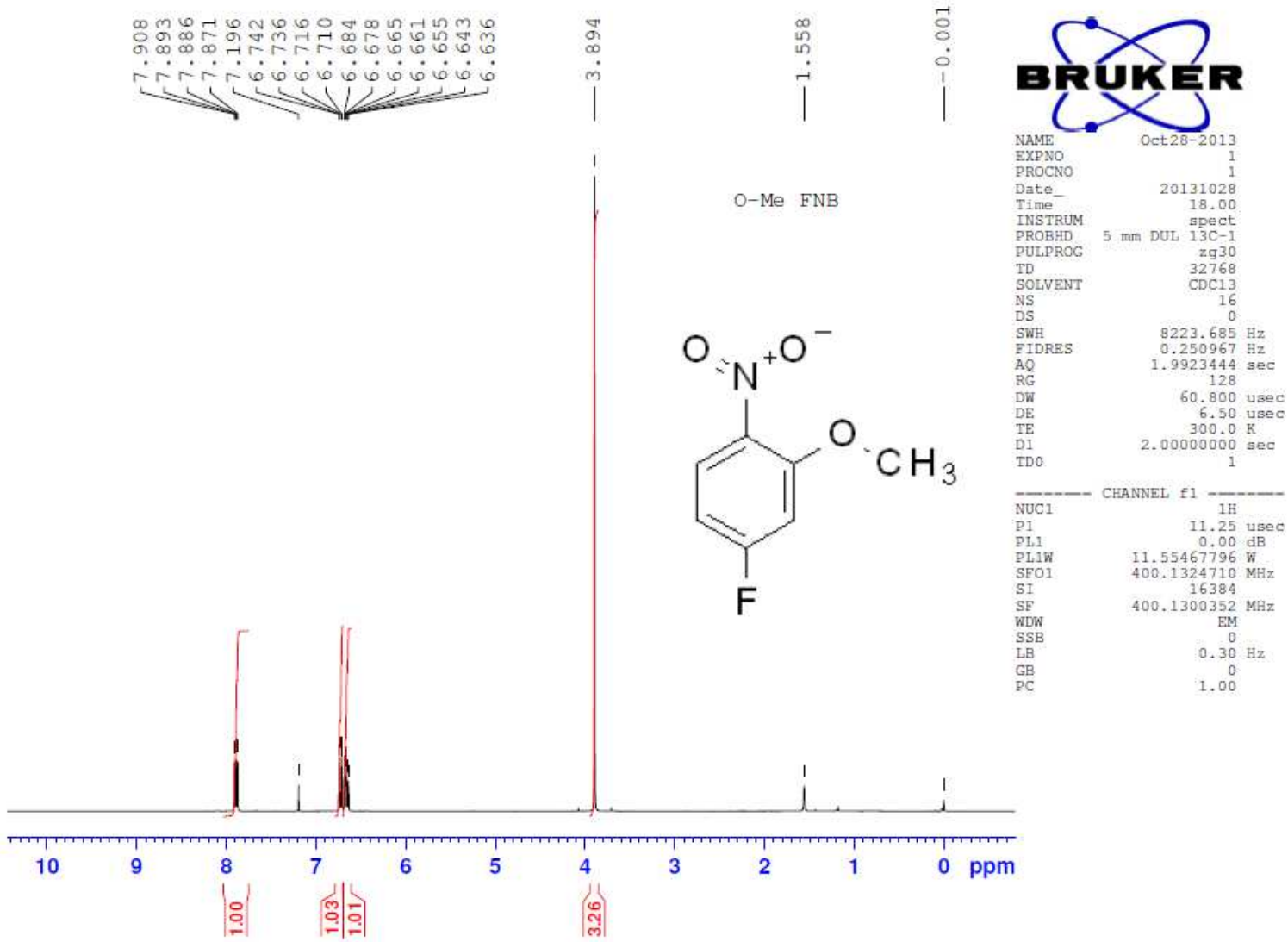
NAME	Nov06-2013	
EXPNO	9	
PROCNO	1	
Date_	20131106	
Time	21.41	
INSTRUM	spect	
PROBHD	5 mm DUL 13C-1	
PULPROG	dept135	
TD	65536	
SOLVENT	CDCl3	
NS	256	
DS	4	
SWH	24038.461	Hz
FIDRES	0.366798	Hz
AQ	1.3631988	sec
RG	2050	
DW	20.800	usec
DE	6.50	usec
TE	300.0	K
CNST2	145.0000000	
D1	2.00000000	sec
D2	0.00344828	sec
D12	0.00002000	sec
TD0	1	
------- CHANNEL f1 -------		
NUC1	13C	
P1	9.60	usec
P2	19.20	usec
PL1	0.00	dB
PL1W	36.67354202	W
SFO1	100.6228298	MHz
------- CHANNEL f2 -------		
CPDPRG2	waltz16	
NUC2	1H	
P3	11.25	usec
P4	22.50	usec
PCPD2	80.00	usec
PL2	0.00	dB
PL12	17.04	dB
PL2W	11.55467796	W
PL12W	0.22843242	W
SFO2	400.1316005	MHz
SI	32768	
SF	100.6127690	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

Product **3c** [(2,4-dibenzyloxy-1-nitro-benzene) (O-Bn Dimer)] HRMS

Sample Name	O-Bn dimer	**Position**	P1-A2	**Instrument Name**	Q-TOF LCMS-01	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	21MAR2014-03.d	**ACQ Method**	science1.m	**Comment**		**Acquired Time**	3/21/2014 2:55:48 PM



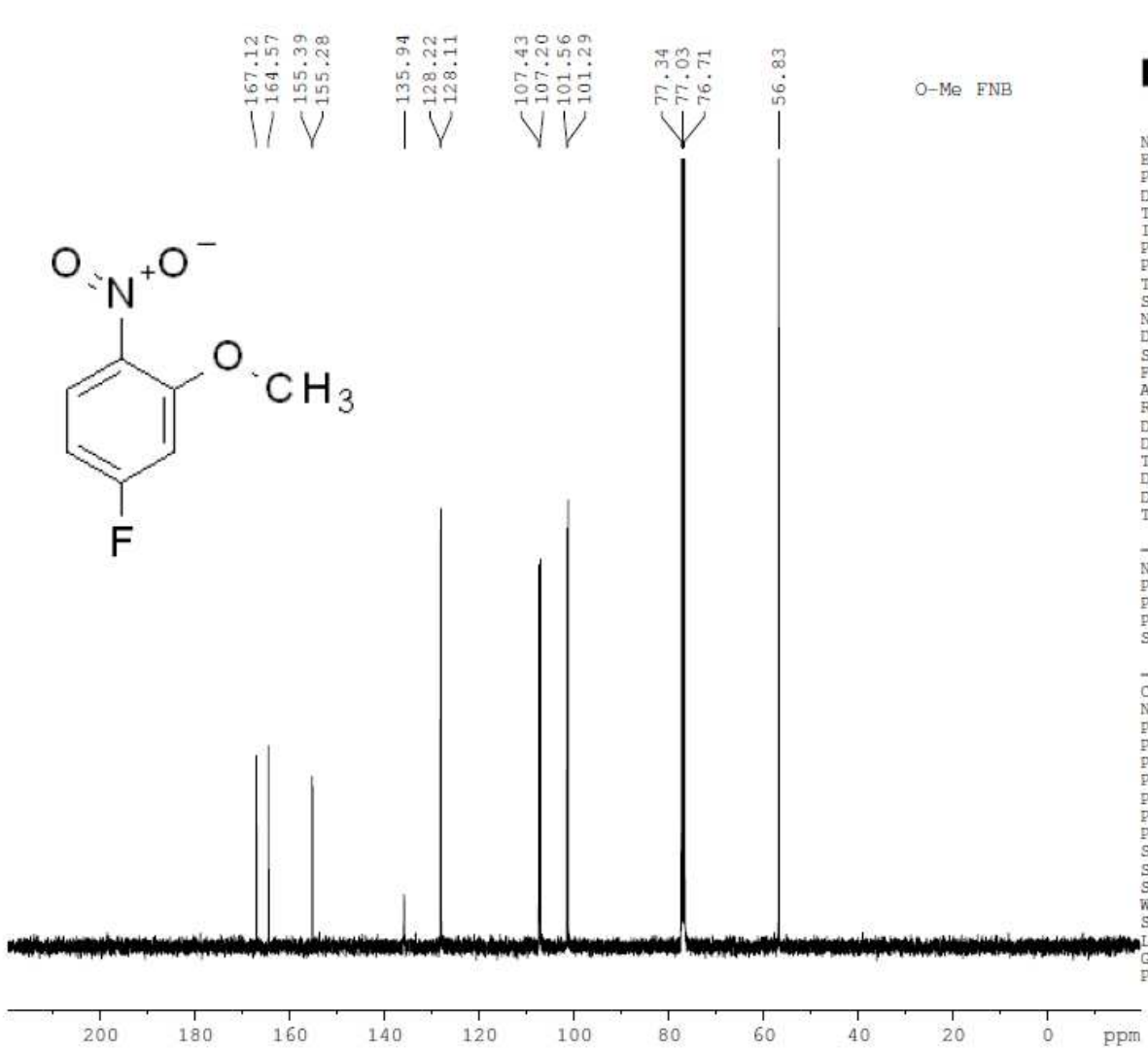
Product **4a** [(4-fluoro-2-methoxy-1-nitro-benzene) (O-Me FNB)] ^{1}H-NMR:



BRUKER

NAME	Oct28-2013
EXPNO	1
PROCNO	1
Date_	20131028
Time	18.00
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	32768
SOLVENT	CDC13
NS	16
DS	0
SWH	8223.685 Hz
FIDRES	0.250967 Hz
AQ	1.9923444 sec
RG	128
DW	60.800 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
------- CHANNEL f1 -------	
NUC1	1H
P1	11.25 usec
PL1	0.00 dB
PL1W	11.55467796 W
SFO1	400.1324710 MHz
SI	16384
SF	400.1300352 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

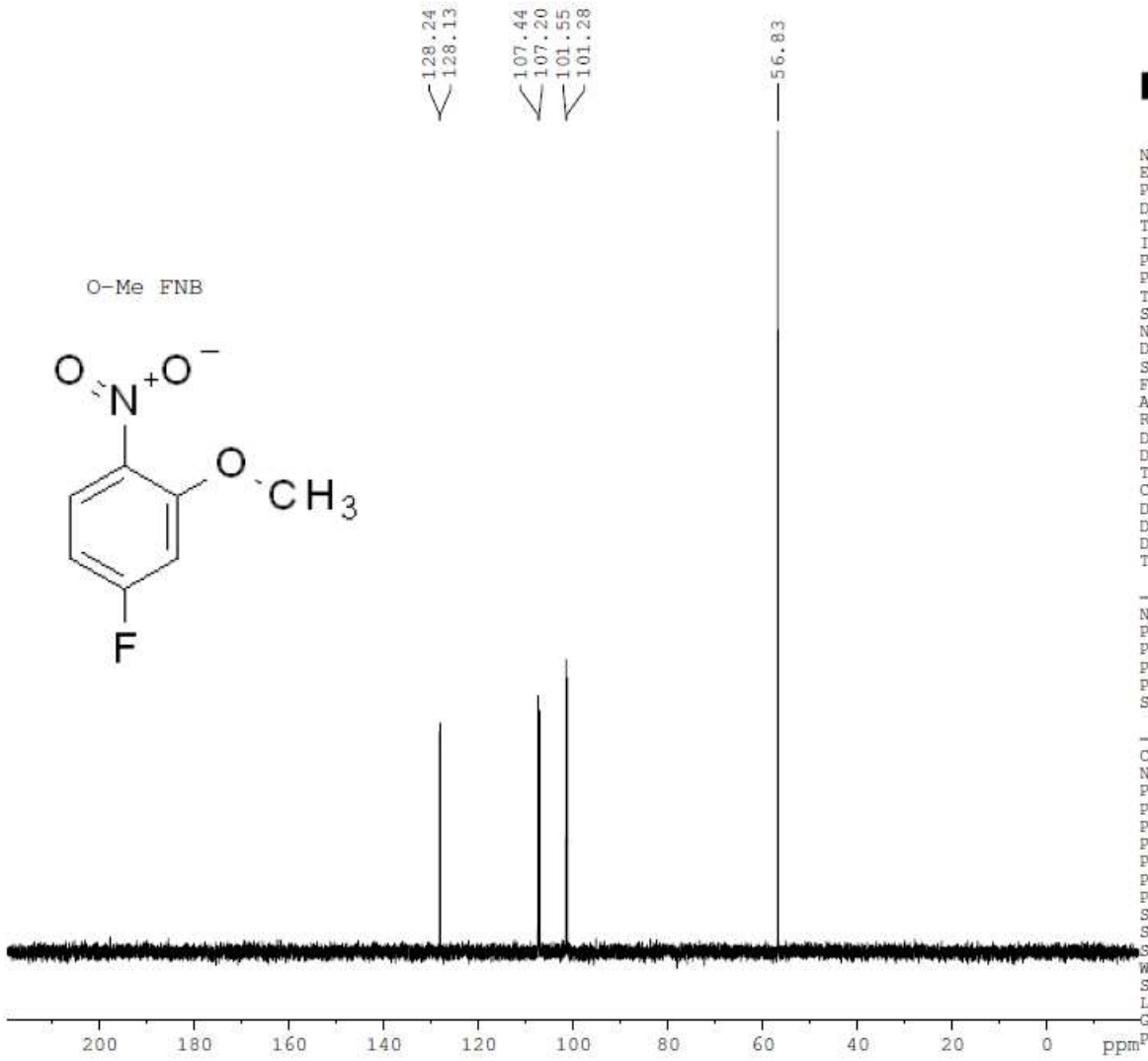
Product **4a** [(4-fluoro-2-methoxy-1-nitro-benzene) (O-Me FNB)] ^{13}C-NMR:



BRUKER

NAME	Oct28-2013
EXPNO	2
PROCNO	1
Date_	20131028
Time	18.59
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	322
DW	20.800 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
------- CHANNEL f1 -------	
NUC1	13C
P1	9.60 usec
PL1	0.00 dB
PL1W	36.67354202 W
SFO1	100.6228298 MHz
------- CHANNEL f2 -------	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	17.04 dB
PL13	17.04 dB
PL2W	11.55467796 W
PL12W	0.22843242 W
PL13W	0.22843242 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

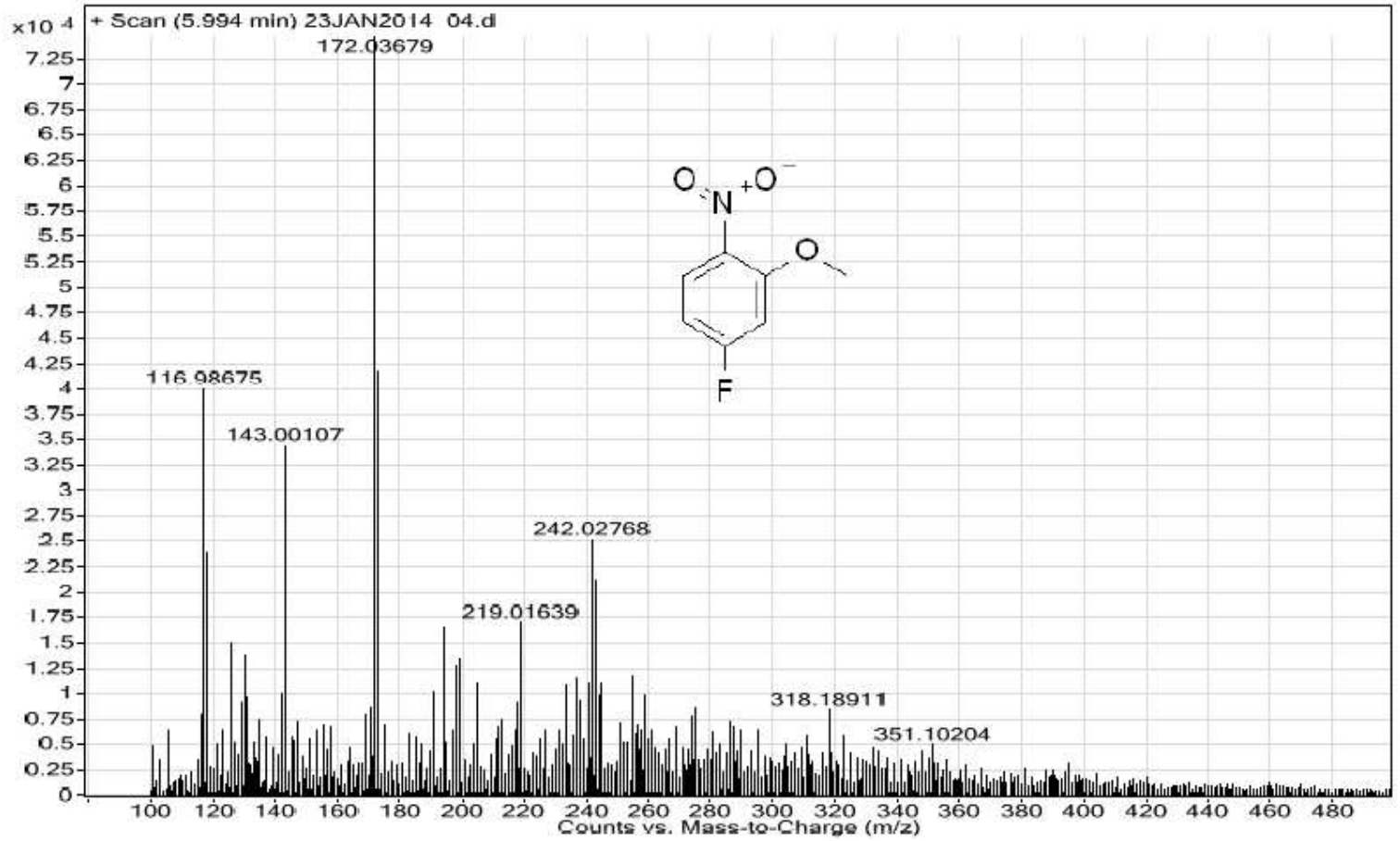
Product **4a** [(4-fluoro-2-methoxy-1-nitro-benzene) (O-Me FNB)] DEPT-NMR:



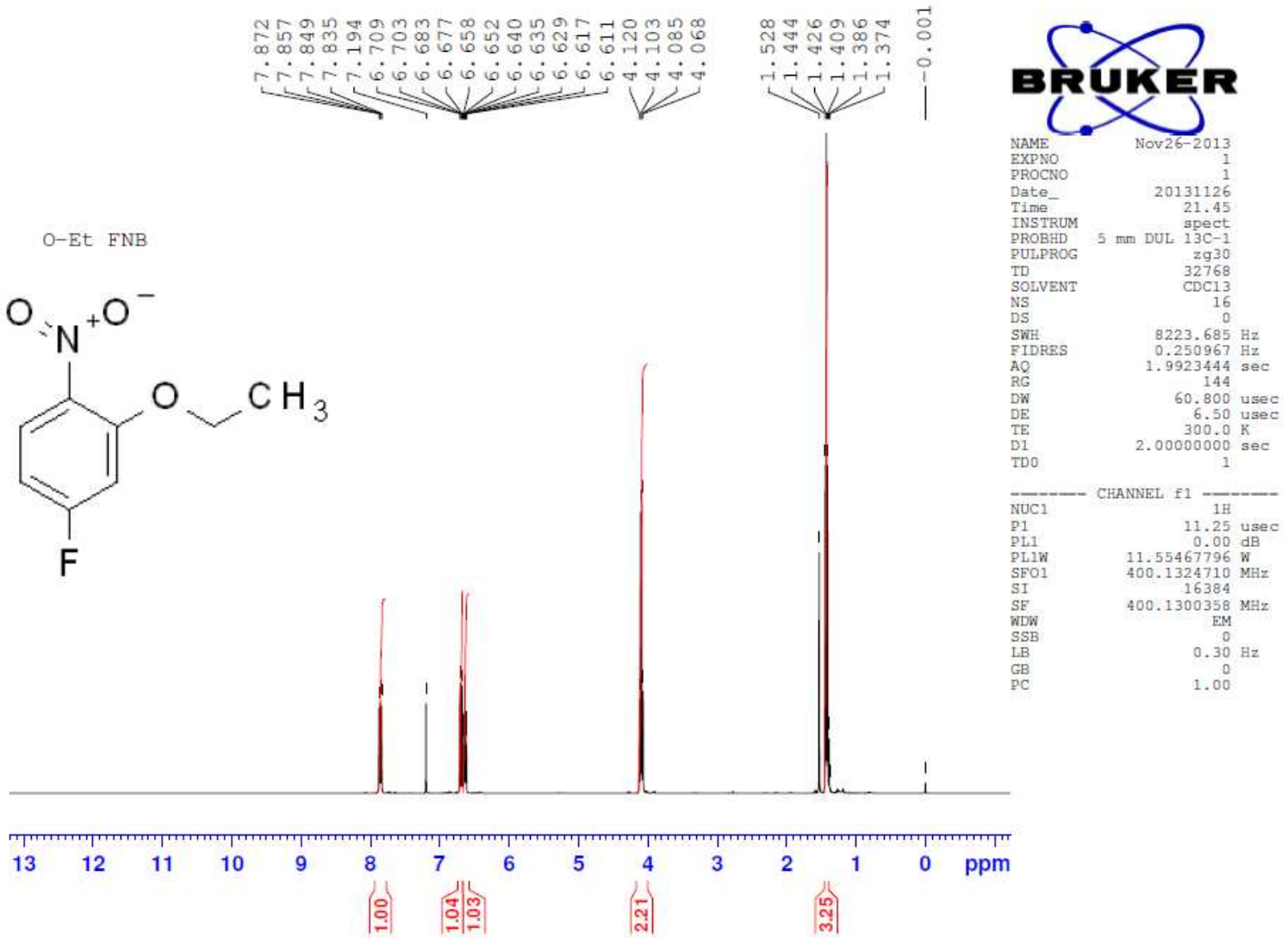
NAME	Oct28-2013
EXPNO	3
PROCNO	1
Date_	20131028
Time	19.14
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	dept135
TD	65536
SOLVENT	CDCl3
NS	256
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	300.0 K
CNST2	145.0000000
D1	2.00000000 sec
D2	0.00344828 sec
D12	0.00002000 sec
TD0	1
------- CHANNEL f1 -------	
NUC1	13C
P1	9.60 usec
P2	19.20 usec
PL1	0.00 dB
PL1W	36.67354202 W
SFO1	100.6228298 MHz
------- CHANNEL f2 -------	
CPDPRG2	waltz16
NUC2	1H
P3	11.25 usec
P4	22.50 usec
PCPD2	80.00 usec
PL2	0.00 dB
PL12	17.04 dB
PL2W	11.55467796 W
PL12W	0.22843242 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Product **4a** [(4-fluoro-2-methoxy-1-nitro-benzene) (O-Me FNB)] HRMS:

Sample Name	O-Me FBN	**Position**	P1-A4	**Instrument Name**	Q-TOF LCMS-01	**User Name**	Indira Jyothi
Inj Vol	1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	23JAN2014_04.d	**ACQ Method**	AZD1979_1.m	**Comment**		**Acquired Time**	1/23/2014 7:43:19 PM



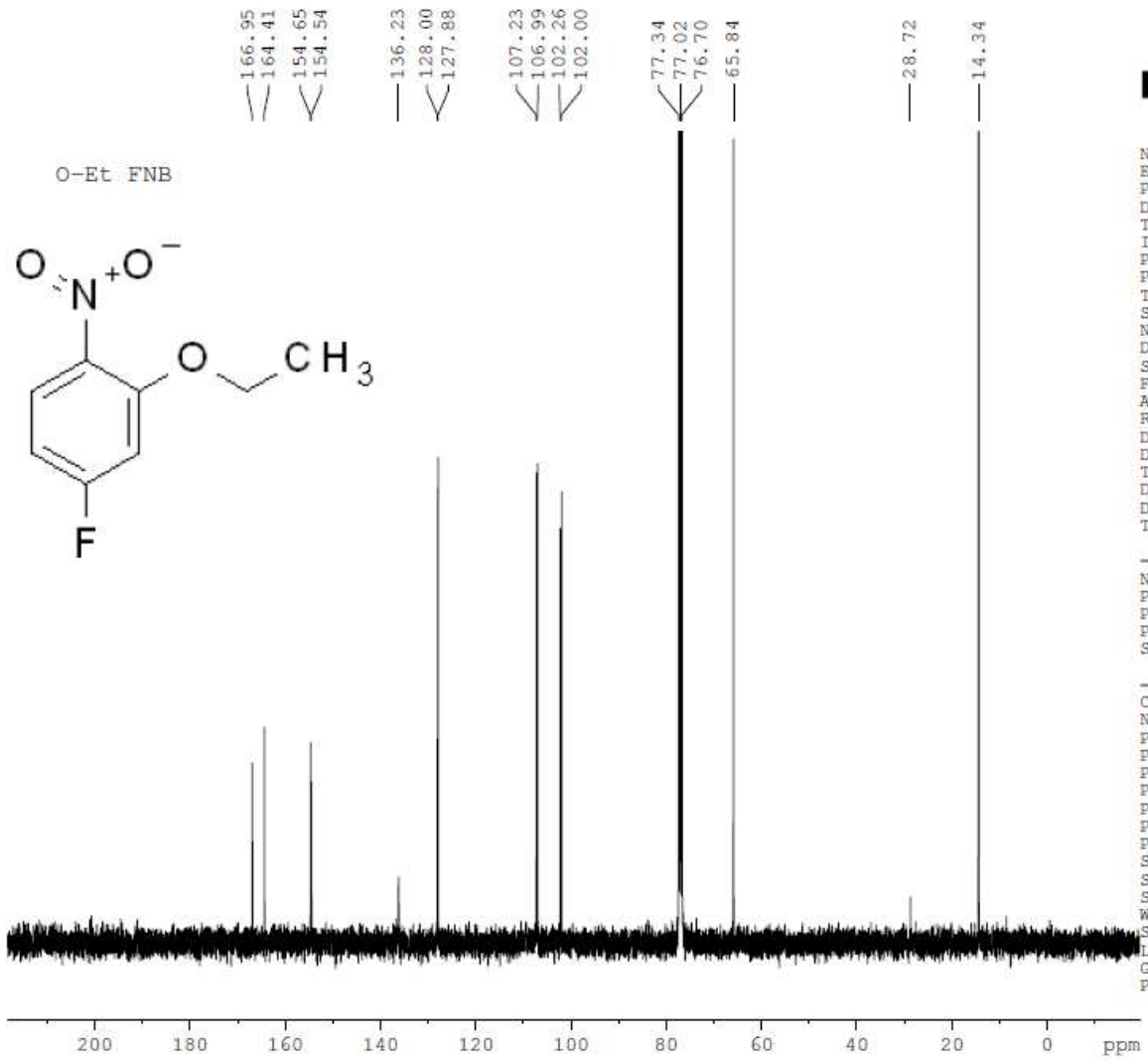
Product **5a** [(2-ethoxy-4-fluoro-1-nitro-benzene) (O-Et FNB)] ^{1}H-NMR



BRUKER

NAME	Nov26-2013
EXPNO	1
PROCNO	1
Date_	20131126
Time	21.45
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	32768
SOLVENT	CDC13
NS	16
DS	0
SWH	8223.685 Hz
FIDRES	0.250967 Hz
AQ	1.9923444 sec
RG	144
DW	60.800 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
------- CHANNEL f1 -------	
NUC1	1H
P1	11.25 usec
PL1	0.00 dB
PL1W	11.55467796 W
SFO1	400.1324710 MHz
SI	16384
SF	400.1300358 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

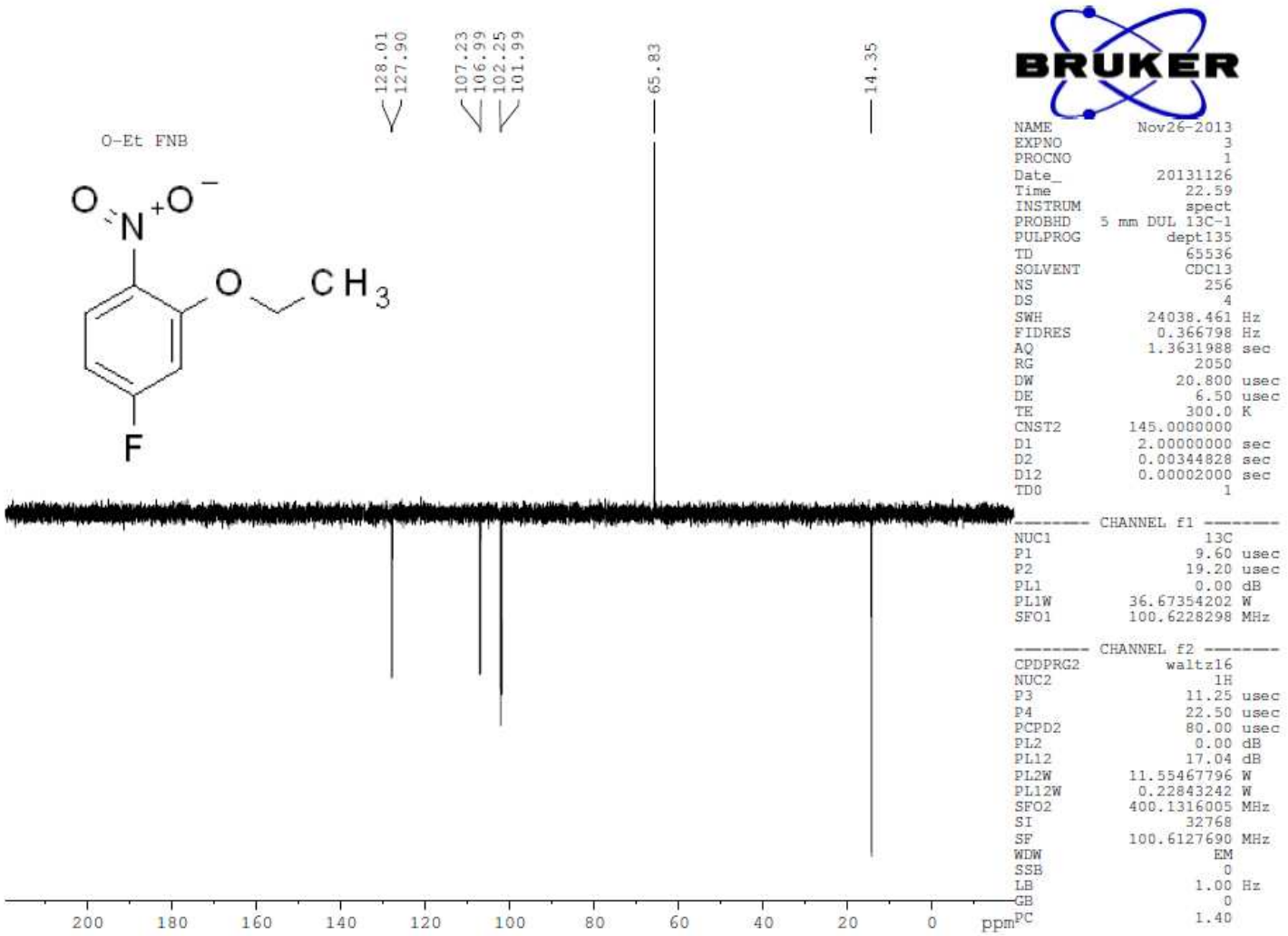
Product **5a** [(2-ethoxy-4-fluoro-1-nitro-benzene) (O-Et FNB)] ^{13}C–NMR



BRUKER

NAME	Nov26-2013
EXPNO	2
PROCNO	1
Date_	20131126
Time	22.44
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDC13
NS	1024
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	322
DW	20.800 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
------- CHANNEL f1 -------	
NUC1	13C
P1	9.60 usec
PL1	0.00 dB
PL1W	36.67354202 W
SFO1	100.6228298 MHz
------- CHANNEL f2 -------	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	17.04 dB
PL13	17.04 dB
PL2W	11.55467796 W
PL12W	0.22843242 W
PL13W	0.22843242 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Product **5a** [(2-ethoxy-4-fluoro-1-nitro-benzene) (O-Et FNB)] DEPT-NMR

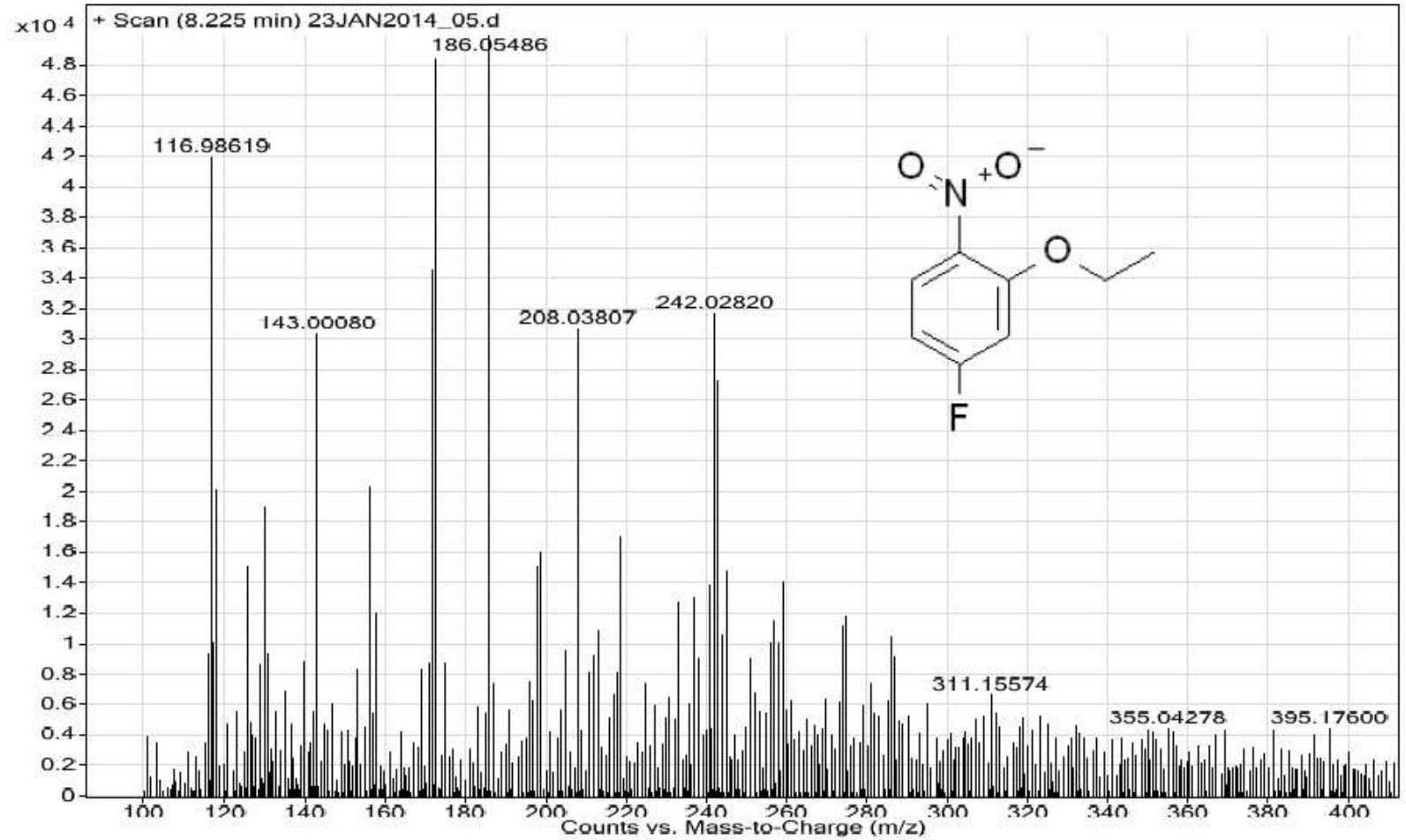


BRUKER

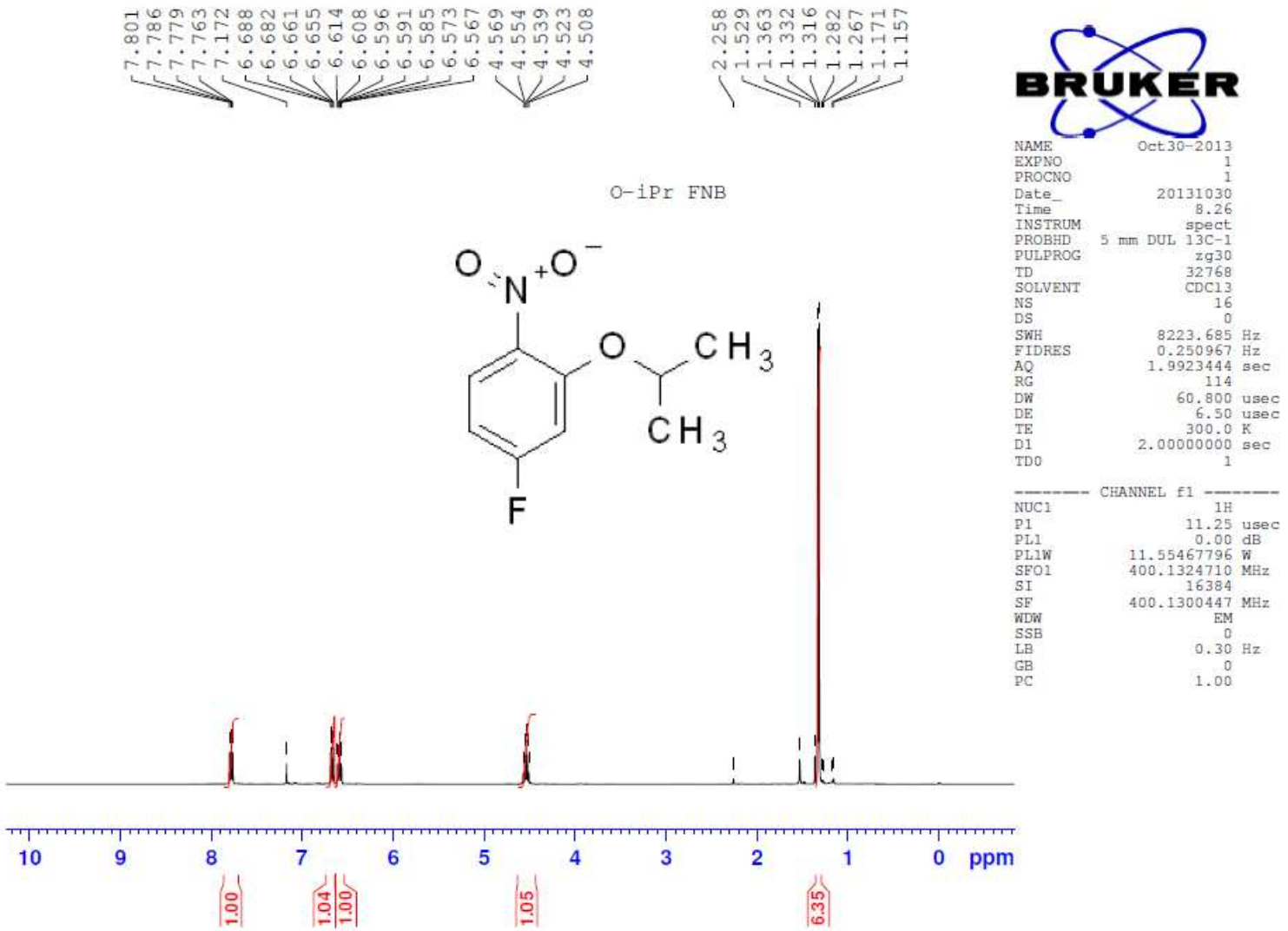
NAME	Nov26-2013
EXPNO	3
PROCNO	1
Date_	20131126
Time	22.59
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	dept135
TD	65536
SOLVENT	CDC13
NS	256
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	300.0 K
CNST2	145.0000000
D1	2.00000000 sec
D2	0.00344828 sec
D12	0.00002000 sec
TD0	1
------- CHANNEL f1 -------	
NUC1	13C
P1	9.60 usec
P2	19.20 usec
PL1	0.00 dB
PL1W	36.67354202 W
SFO1	100.6228298 MHz
------- CHANNEL f2 -------	
CPDPRG2	waltz16
NUC2	1H
P3	11.25 usec
P4	22.50 usec
PCPD2	80.00 usec
PL2	0.00 dB
PL12	17.04 dB
PL2W	11.55467796 W
PL12W	0.22843242 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Product **5a** [(2-ethoxy-4-fluoro-1-nitro-benzene) (O-Et FNB)] HRMS:

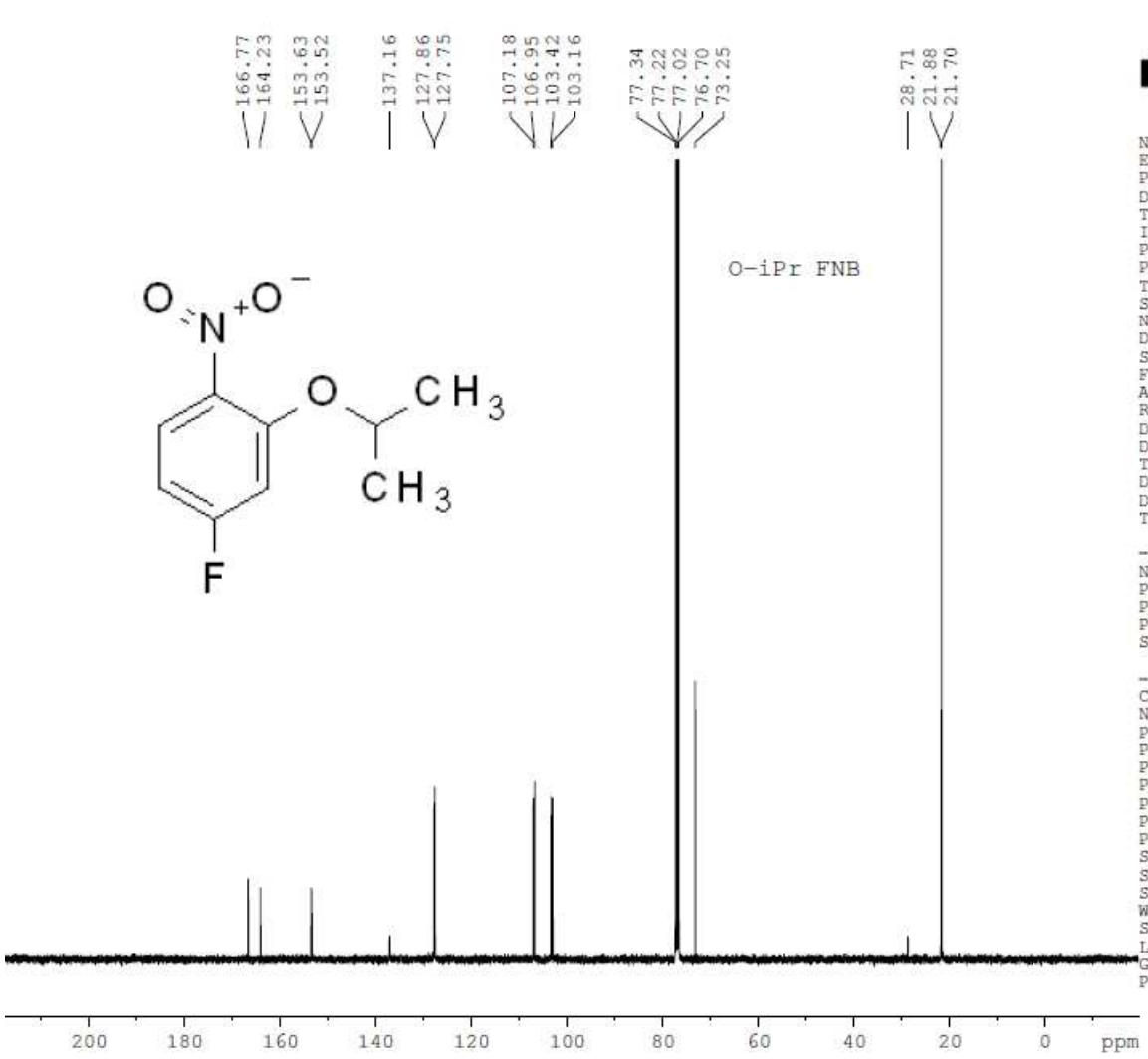
Sample Name	O-Et FBN	**Position**	P1-A5	**Instrument Name**	Q-TOF LCMS-01	**User Name**	Indira Jyothi
Inj Vol	1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	23JAN2014_05.d	**ACQ Method**	AZD1979_1.m	**Comment**		**Acquired Time**	1/23/2014 8:02:17 PM



Product **6a** [(4-fluoro-2-isopropoxy-1-nitro-benzene) (O-*i*Pr FNB)] ^{1}H-NMR



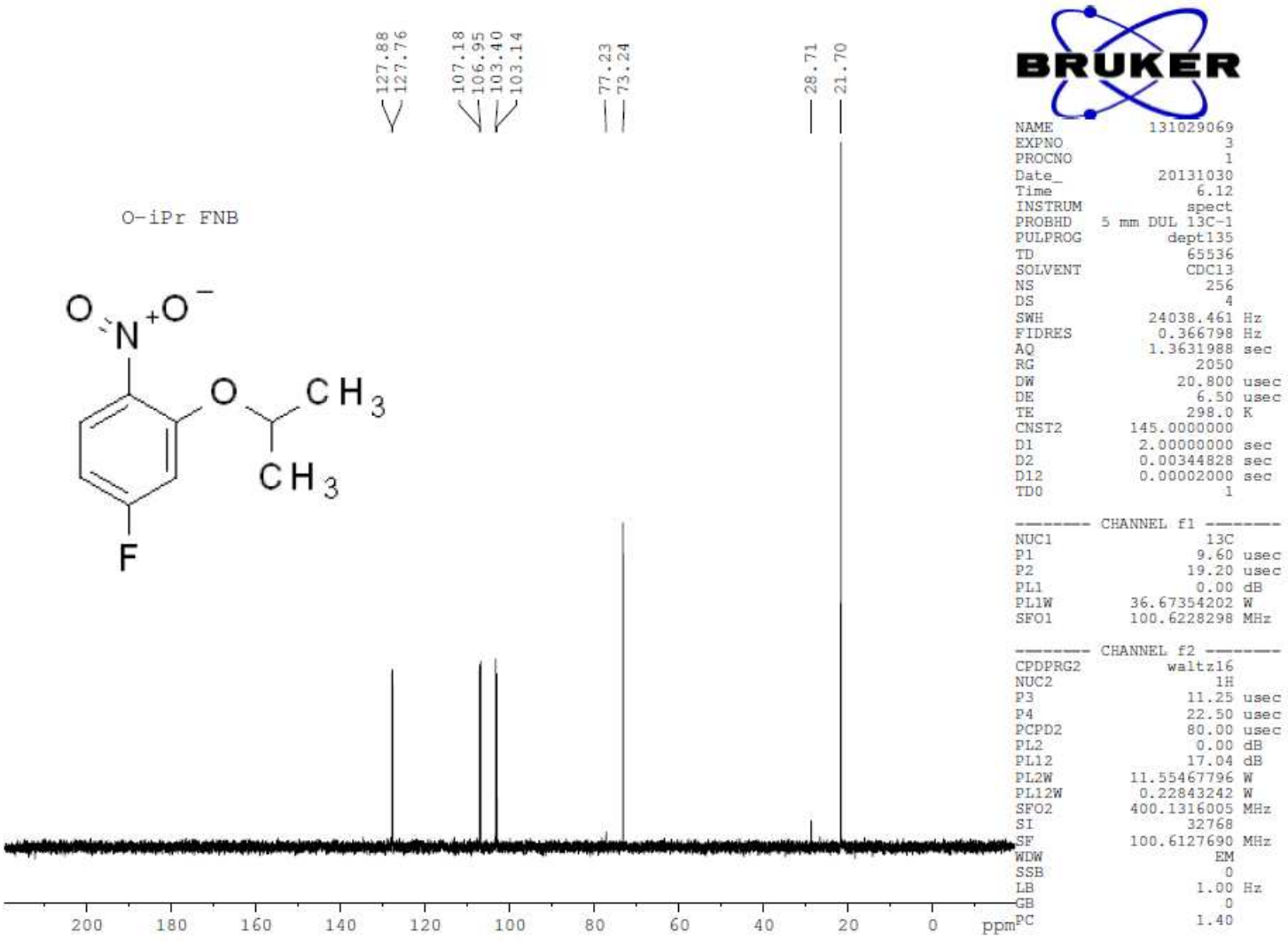
Product **6a** [(4-fluoro-2-isopropoxy-1-nitro-benzene) (O-*i*Pr FNB)] ^{13}C-NMR



BRUKER

NAME	131029069
EXPNO	2
PROCNO	1
Date_	20131030
Time	5.57
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	362
DW	20.800 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
------- CHANNEL f1 -------	
NUC1	13C
P1	9.60 usec
PL1	0.00 dB
PL1W	36.67354202 W
SFO1	100.6228298 MHz
------- CHANNEL f2 -------	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	17.04 dB
PL13	17.04 dB
PL2W	11.55467796 W
PL12W	0.22843242 W
PL13W	0.22843242 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Product **6a** [(4-fluoro-2-isopropoxy-1-nitro-benzene) (O-*i*Pr FNB)] DEPT-NMR

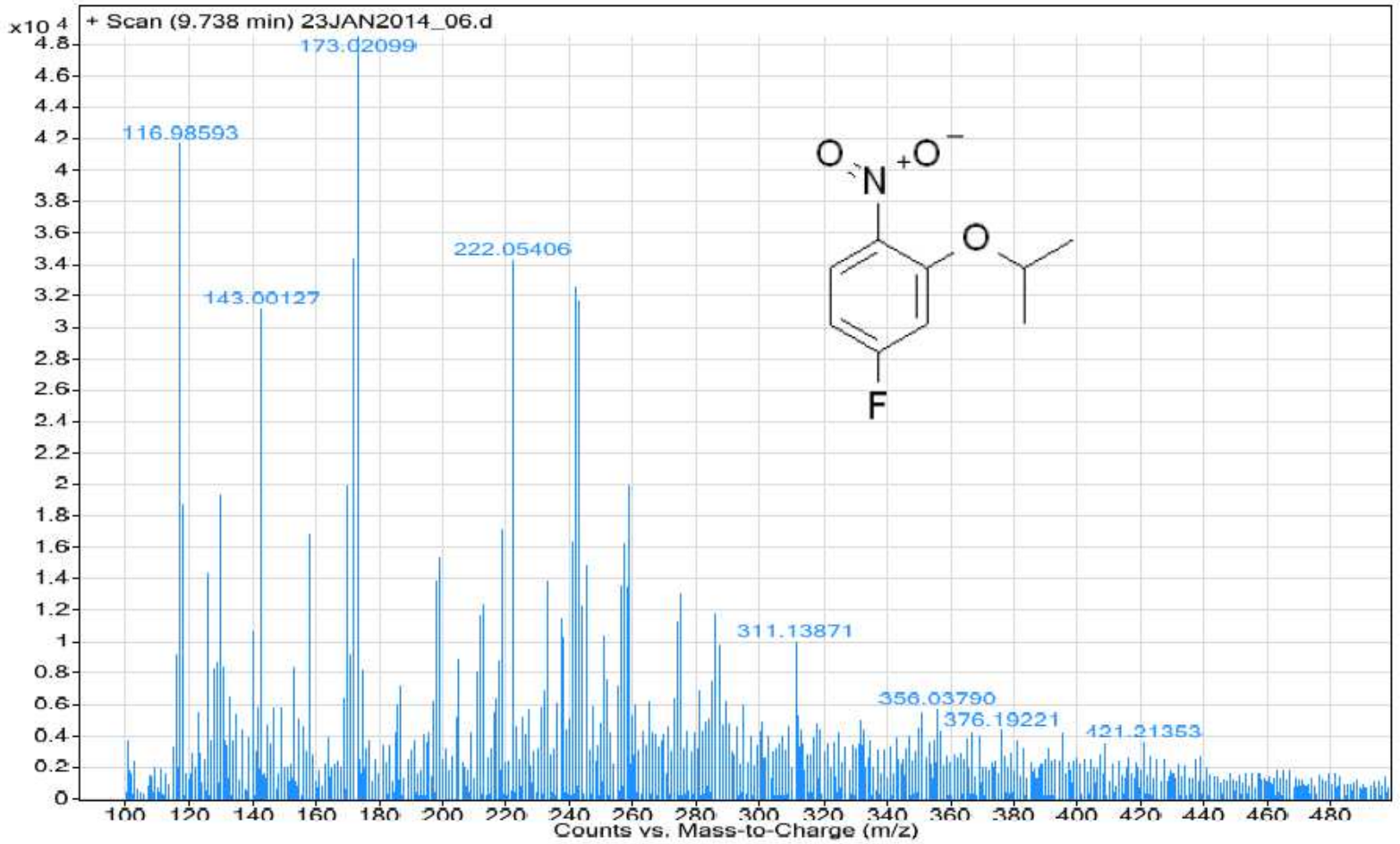


BRUKER

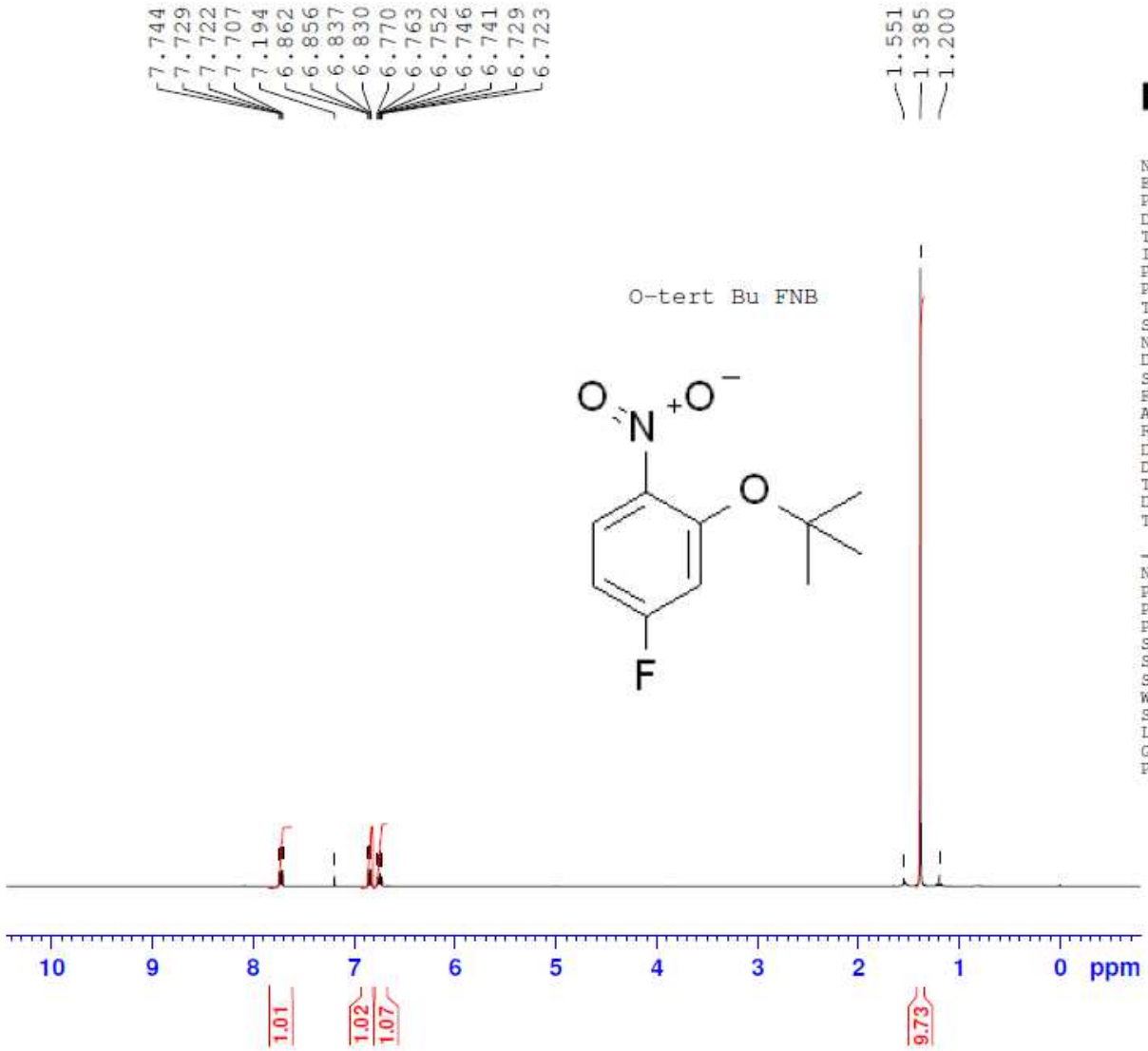
NAME	131029069
EXPNO	3
PROCNO	1
Date_	20131030
Time	6.12
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	dept135
TD	65536
SOLVENT	CDCl3
NS	256
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	298.0 K
CNST2	145.0000000
D1	2.00000000 sec
D2	0.00344828 sec
D12	0.00002000 sec
TD0	1
------- CHANNEL f1 -------	
NUC1	13C
P1	9.60 usec
P2	19.20 usec
PL1	0.00 dB
PL1W	36.67354202 W
SFO1	100.6228298 MHz
------- CHANNEL f2 -------	
CPDPRG2	waltz16
NUC2	1H
P3	11.25 usec
P4	22.50 usec
PCPD2	80.00 usec
PL2	0.00 dB
PL12	17.04 dB
PL2W	11.55467796 W
PL12W	0.22843242 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Product **6a** [(4-fluoro-2-isopropoxy-1-nitro-benzene) (O-*i*Pr FNB)] HRMS

Sample Name	O-ipr FBN	**Position**	P1-A6	**Instrument Name**	Q-TOF LCMS-01	**User Name**	Indira Jyothi
Inj Vol	1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	23JAN2014_06.d	**ACQ Method**	AZD1979_1.m	**Comment**		**Acquired Time**	1/23/2014 8:21:18 PM

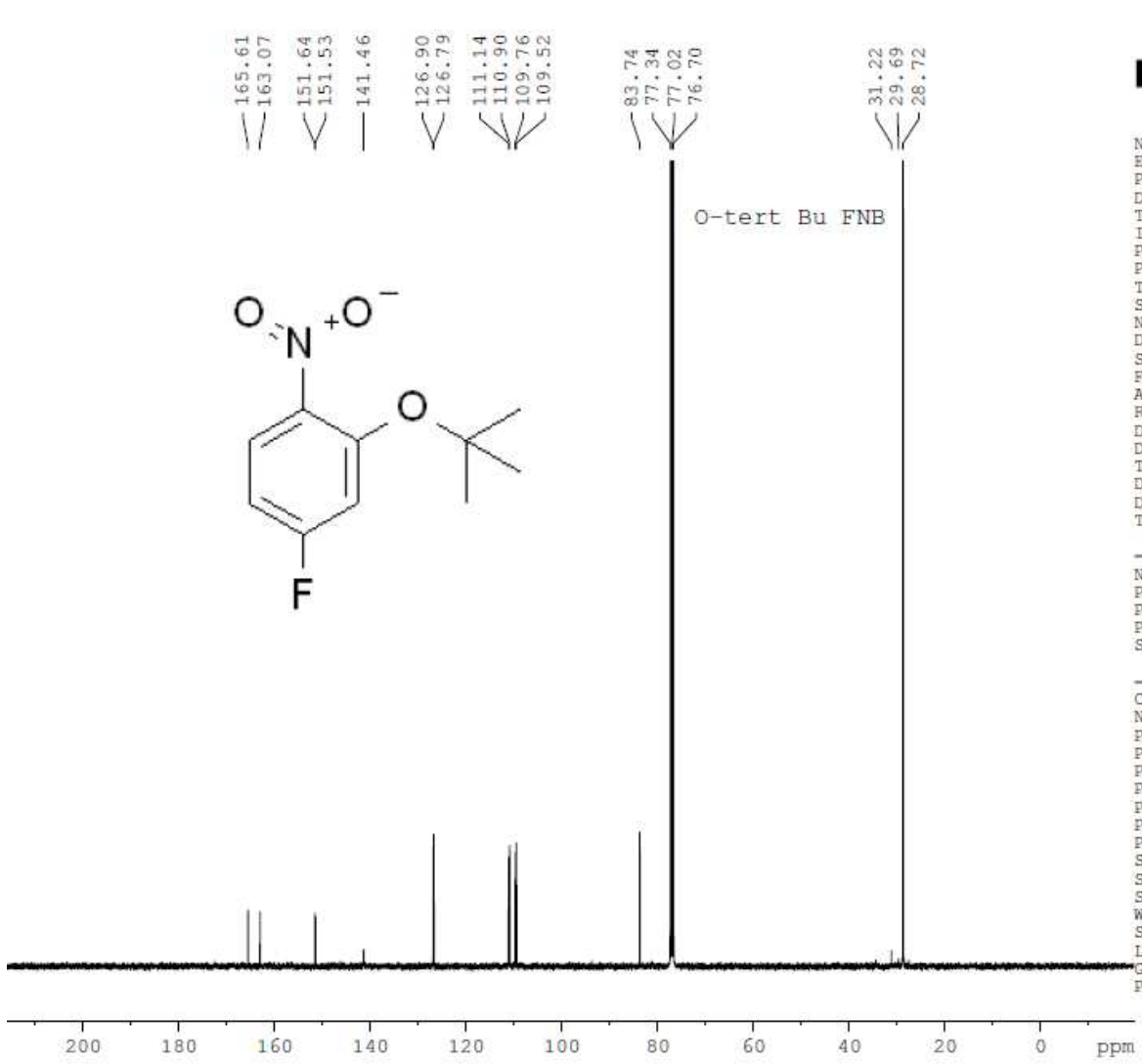


Product **7a** [(2-tert-butoxy-4-fluoro-1-nitro-benzene) (O-*tert.* Bu FNB)] ^{1}H-NMR:



NAME	Oct28-2013
EXPNO	4
PROCNO	1
Date_	20131028
Time	19.19
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	0
SWH	8223.685 Hz
FIDRES	0.250967 Hz
AQ	1.9923444 sec
RG	90.5
DW	60.800 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
-------- CHANNEL f1 --------	
NUC1	1H
P1	11.25 usec
PL1	0.00 dB
PL1W	11.55467796 W
SFO1	400.1324710 MHz
SI	16384
SF	400.1300357 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

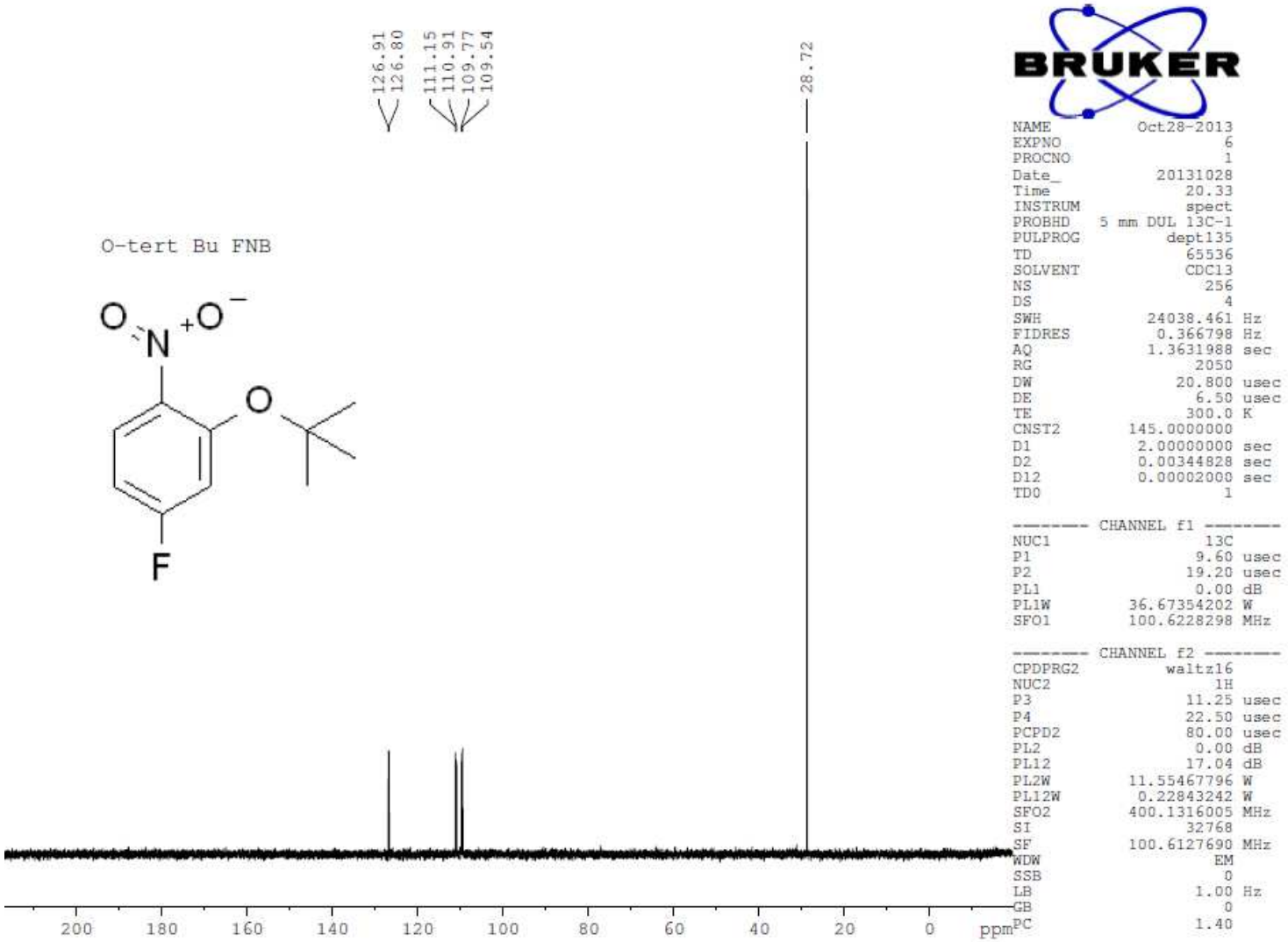
Product **7a** [(2-tert-butoxy-4-fluoro-1-nitro-benzene) (O-*tert.* Bu FNB)] ^{13}C-NMR:



BRUKER

NAME	Oct28-2013
EXPNO	5
PROCNO	1
Date_	20131028
Time	20.18
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	362
DW	20.800 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
------- CHANNEL f1 -------	
NUC1	13C
P1	9.60 usec
PL1	0.00 dB
PL1W	36.67354202 W
SFO1	100.6228298 MHz
------- CHANNEL f2 -------	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	17.04 dB
PL13	17.04 dB
PL2W	11.55467796 W
PL12W	0.22843242 W
PL13W	0.22843242 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Product **7a** [(2-tert-butoxy-4-fluoro-1-nitro-benzene) (O-*tert.* Bu FNB)] DEPT-NMR:

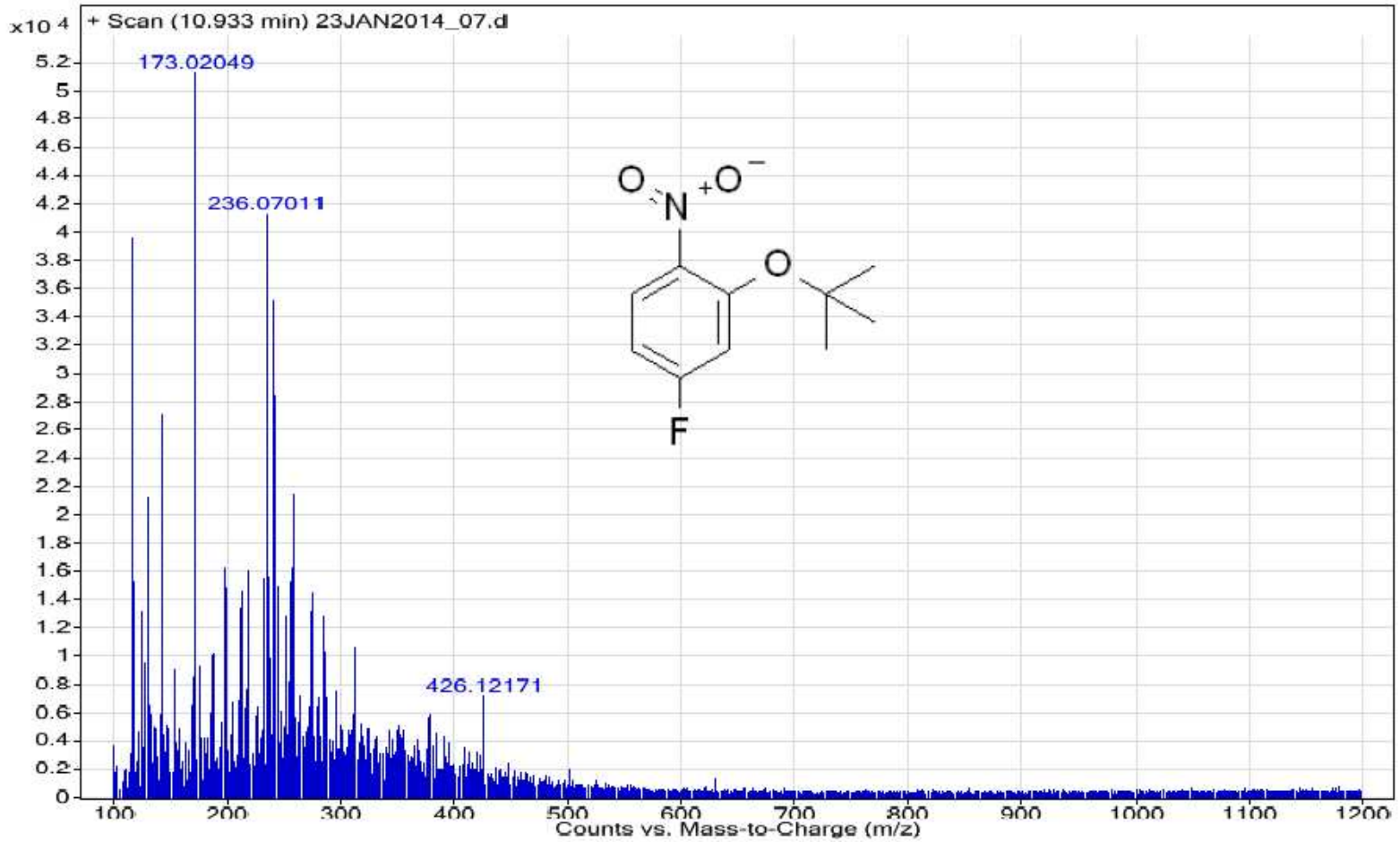


BRUKER

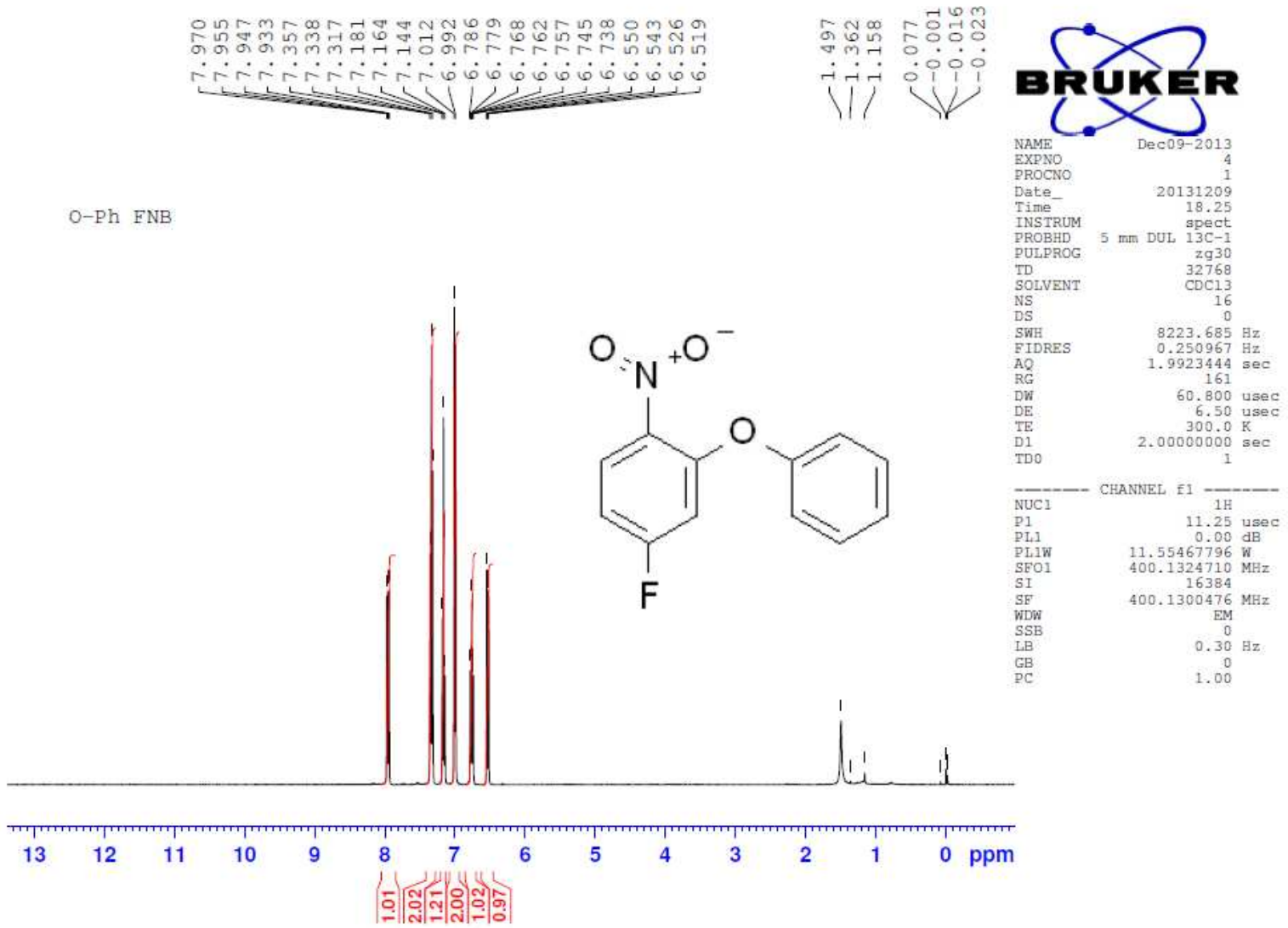
NAME	Oct28-2013
EXPNO	6
PROCNO	1
Date_	20131028
Time	20.33
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	dept135
TD	65536
SOLVENT	CDCl3
NS	256
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	300.0 K
CNST2	145.0000000
D1	2.00000000 sec
D2	0.00344828 sec
D12	0.00002000 sec
TD0	1
------- CHANNEL f1 -------	
NUC1	13C
P1	9.60 usec
P2	19.20 usec
PL1	0.00 dB
PL1W	36.67354202 W
SFO1	100.6228298 MHz
------- CHANNEL f2 -------	
CPDPRG2	waltz16
NUC2	1H
P3	11.25 usec
P4	22.50 usec
PCPD2	80.00 usec
PL2	0.00 dB
PL12	17.04 dB
PL2W	11.55467796 W
PL12W	0.22843242 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Product **7a** [(2-tert-butoxy-4-fluoro-1-nitro-benzene) (O-*tert.* Bu FNB)] HRMS:

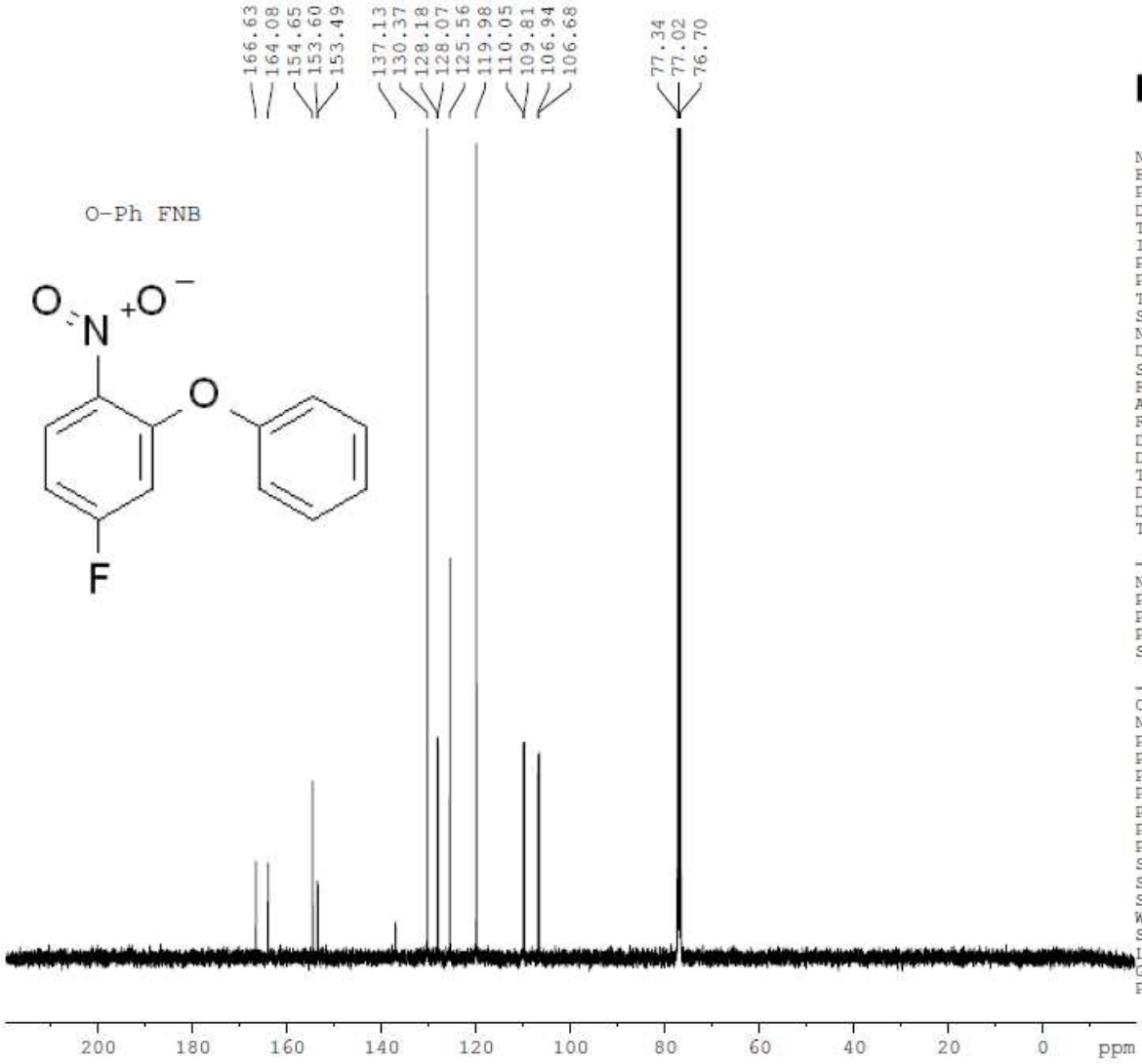
Sample Name	O-tert Bu FBN	**Position**	P1-A7	**Instrument Name**	Q-TOF LCMS-01	**User Name**	Indira Jyothi
Inj Vol	1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	23JAN2014_07.d	**ACQ Method**	AZD1979_1.m	**Comment**		**Acquired Time**	1/23/2014 8:40:18 PM



Product **8a** [(4-fluoro-1-nitro-2-phenoxy-benzene) (O-Ph FNB)] ^{1}H-NMR:



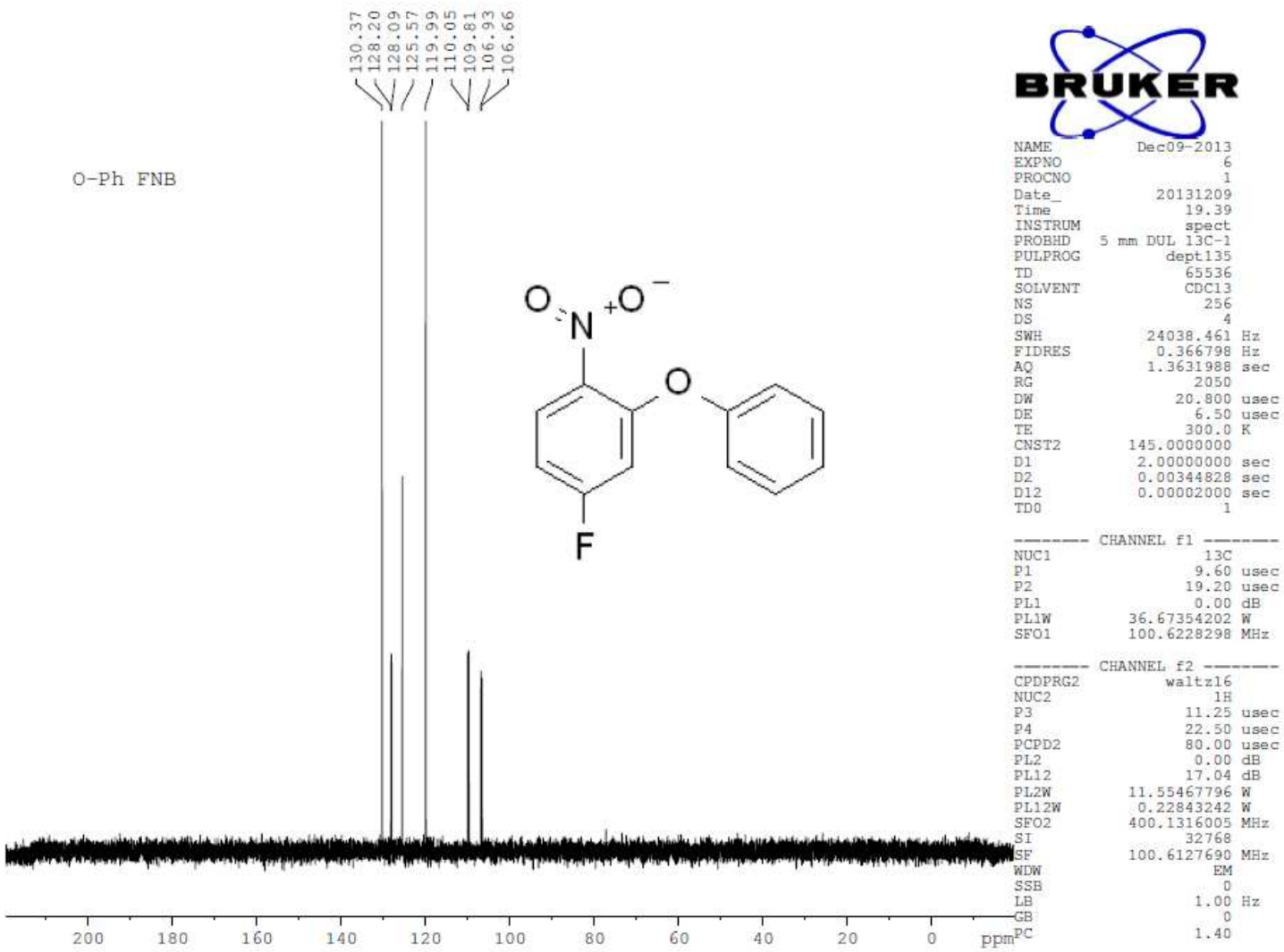
Product **8a** [(4-fluoro-1-nitro-2-phenoxy-benzene) (O-Ph FNB)] ^{13}C-NMR:



BRUKER

NAME	Dec09-2013
EXPNO	5
PROCNO	1
Date_	20131209
Time	19.24
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	406
DW	20.800 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
------- CHANNEL f1 -------	
NUC1	13C
P1	9.60 usec
PL1	0.00 dB
PL1W	36.67354202 W
SFO1	100.6228298 MHz
------- CHANNEL f2 -------	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	17.04 dB
PL13	17.04 dB
PL2W	11.55467796 W
PL12W	0.22843242 W
PL13W	0.22843242 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

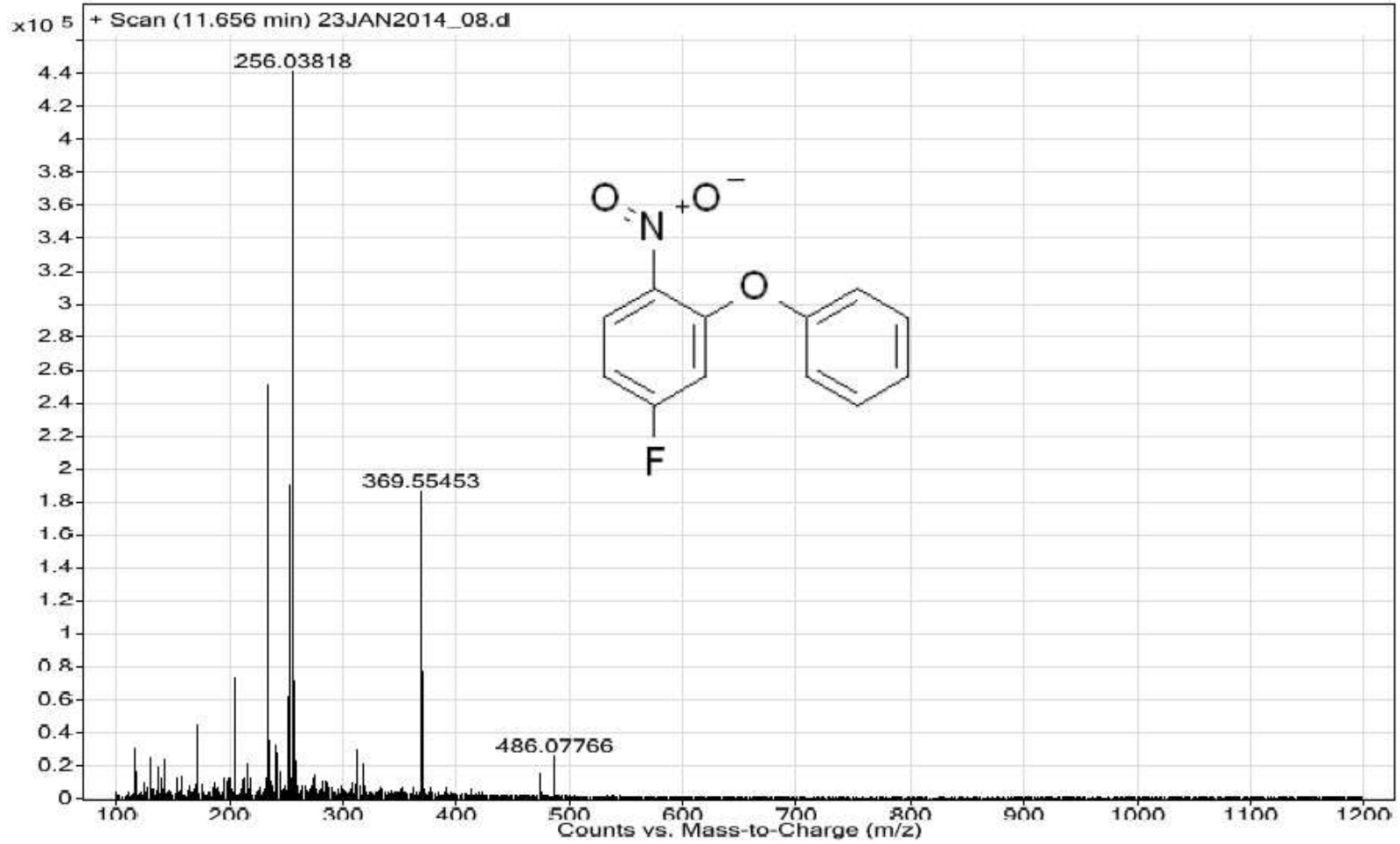
Product **8a** [(4-fluoro-1-nitro-2-phenoxy-benzene) (O-Ph FNB)] DEPT:



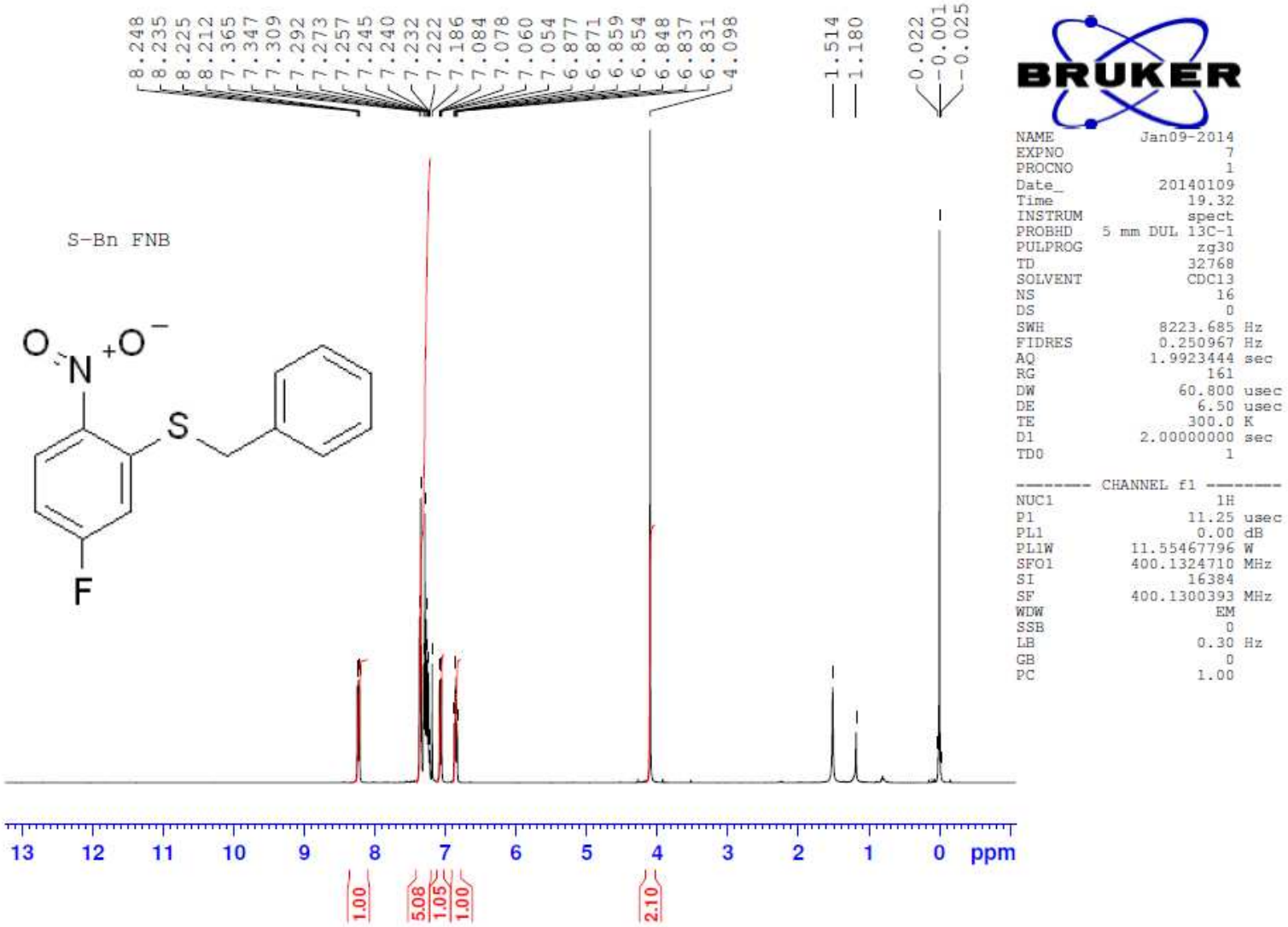
NAME	Dec09-2013
EXPNO	6
PROCNO	1
Date_	20131209
Time	19.39
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	dept135
TD	65536
SOLVENT	CDC13
NS	256
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	300.0 K
CNST2	145.0000000
D1	2.00000000 sec
D2	0.00344828 sec
D12	0.00002000 sec
TD0	1
-------- CHANNEL f1 --------	
NUC1	13C
P1	9.60 usec
P2	19.20 usec
PL1	0.00 dB
PL1W	36.67354202 W
SFO1	100.6228298 MHz
-------- CHANNEL f2 --------	
CPDPRG2	waltz16
NUC2	1H
P3	11.25 usec
P4	22.50 usec
PCPD2	80.00 usec
PL2	0.00 dB
PL12	17.04 dB
PL2W	11.55467796 W
PL12W	0.22843242 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Product **8a** [(4-fluoro-1-nitro-2-phenoxy-benzene) (O-Ph FNB)] HRMS:

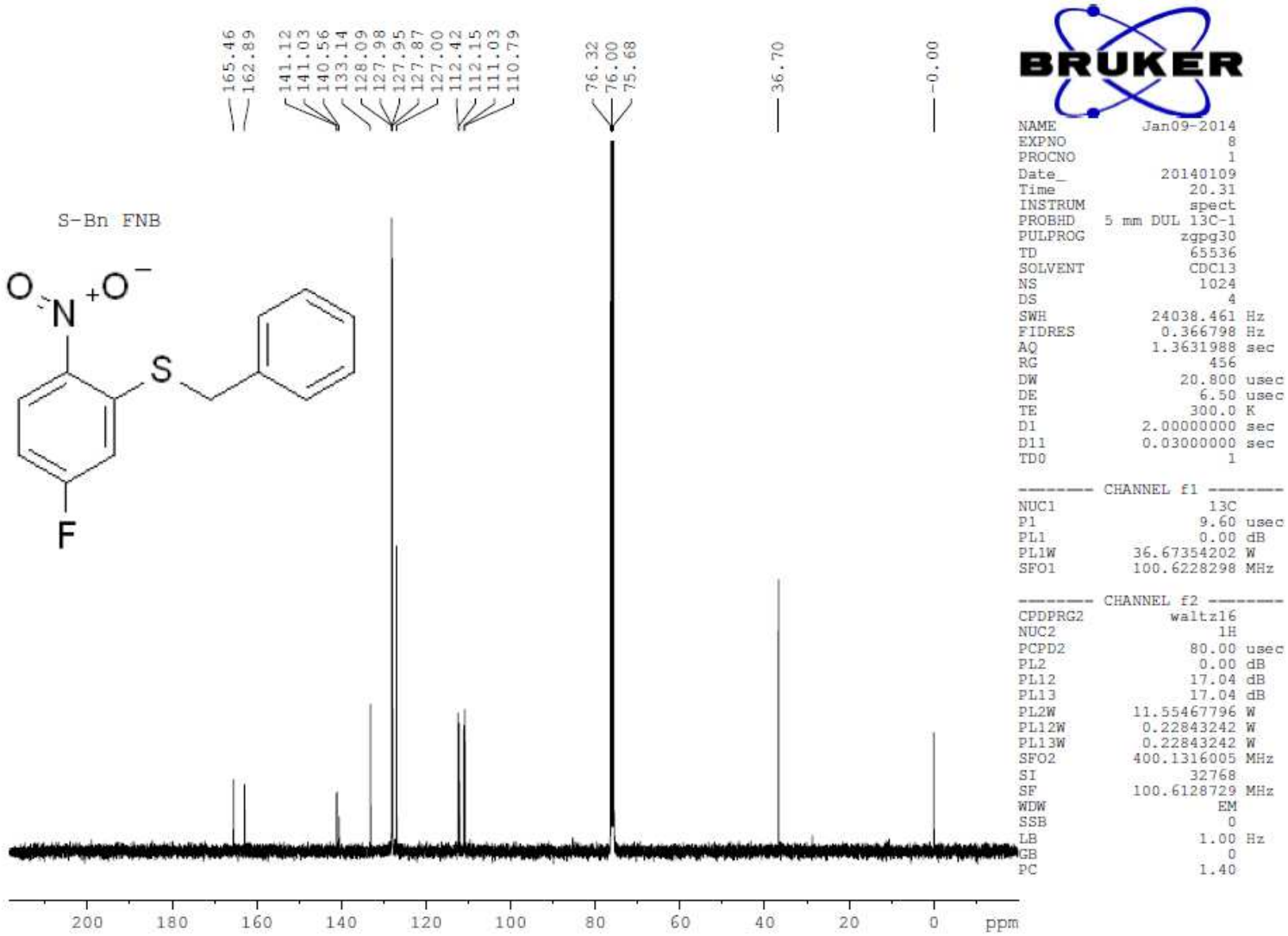
Sample Name	O-Ph FBN	**Position**	P1-A8	**Instrument Name**	Q-TOF LCMS-01	**User Name**	Indira Jyothi
Inj Vol	1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	23JAN2014_08.d	**ACQ Method**	AZD1979_1.m	**Comment**		**Acquired Time**	1/23/2014 8:59:16 PM



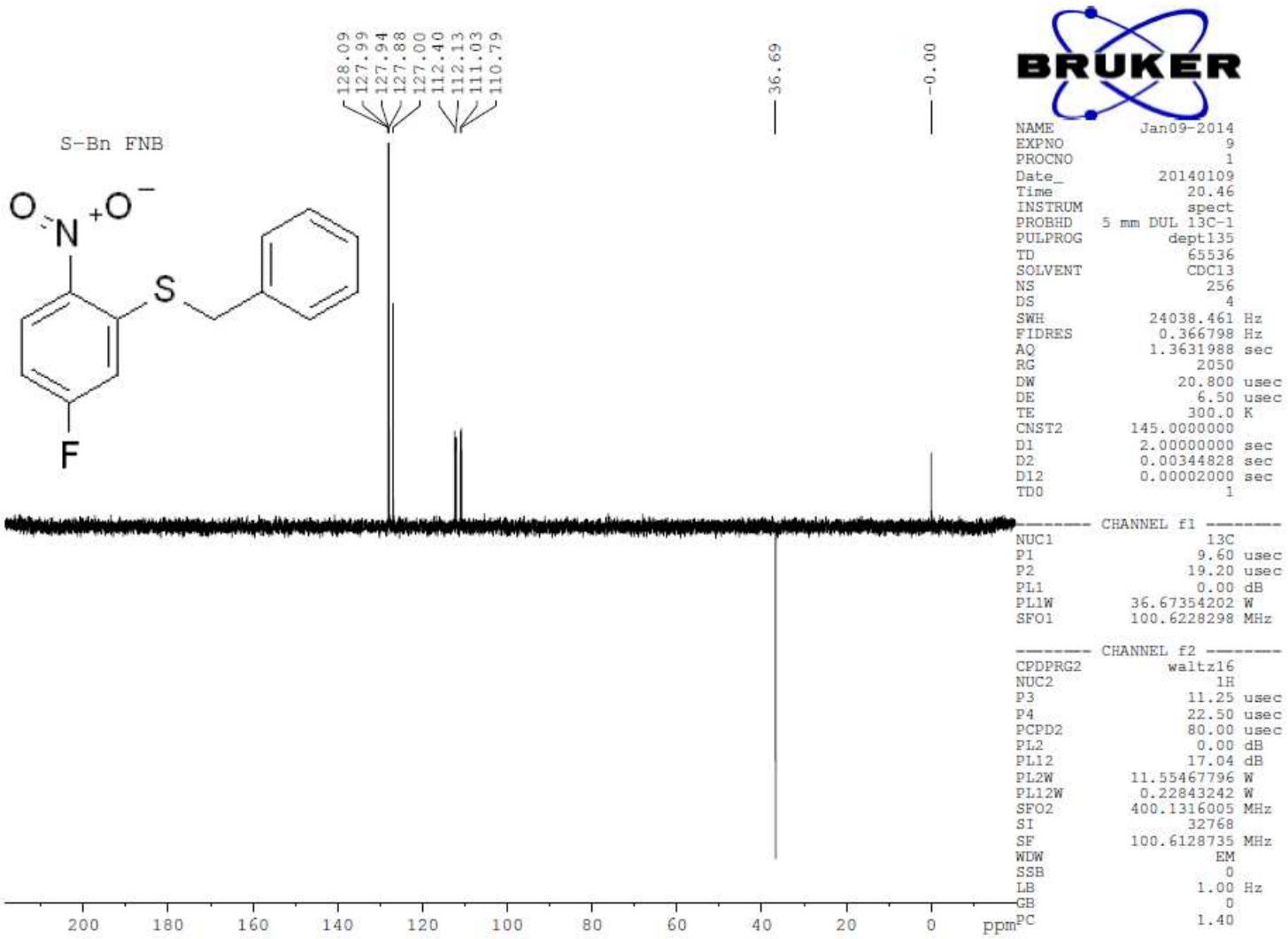
Product **9a** [(2-benzylsulfanyl-4-fluoro-1-nitro-benzene) (S-Bn FNB)] ^{1}H-NMR:



Product **9a** [(2-benzylsulfanyl-4-fluoro-1-nitro-benzene) (S-Bn FNB)] ^{13}C-NMR:

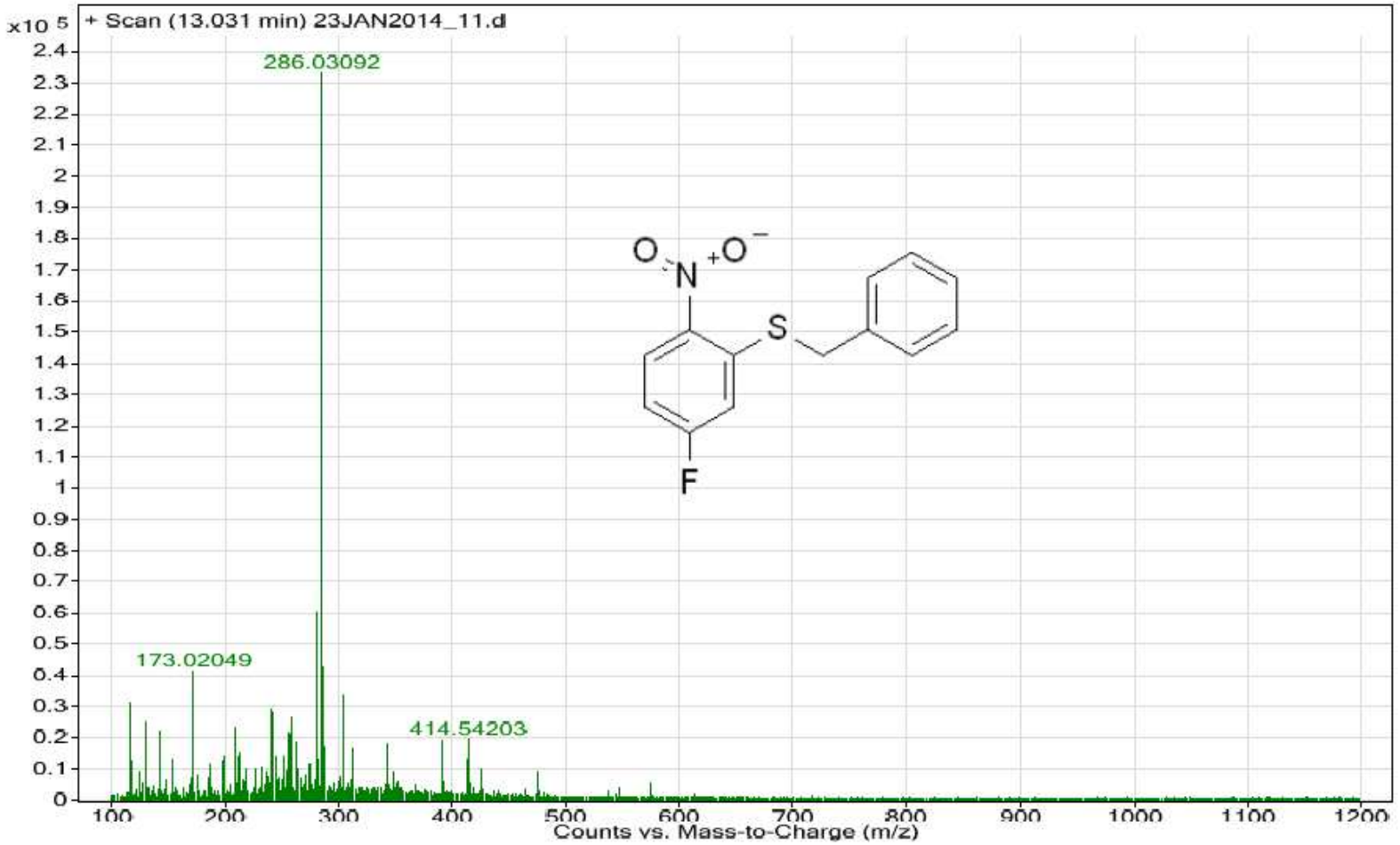


Product **9a** [(2-benzylsulfanyl-4-fluoro-1-nitro-benzene) (S-Bn FNB)] DEPT:

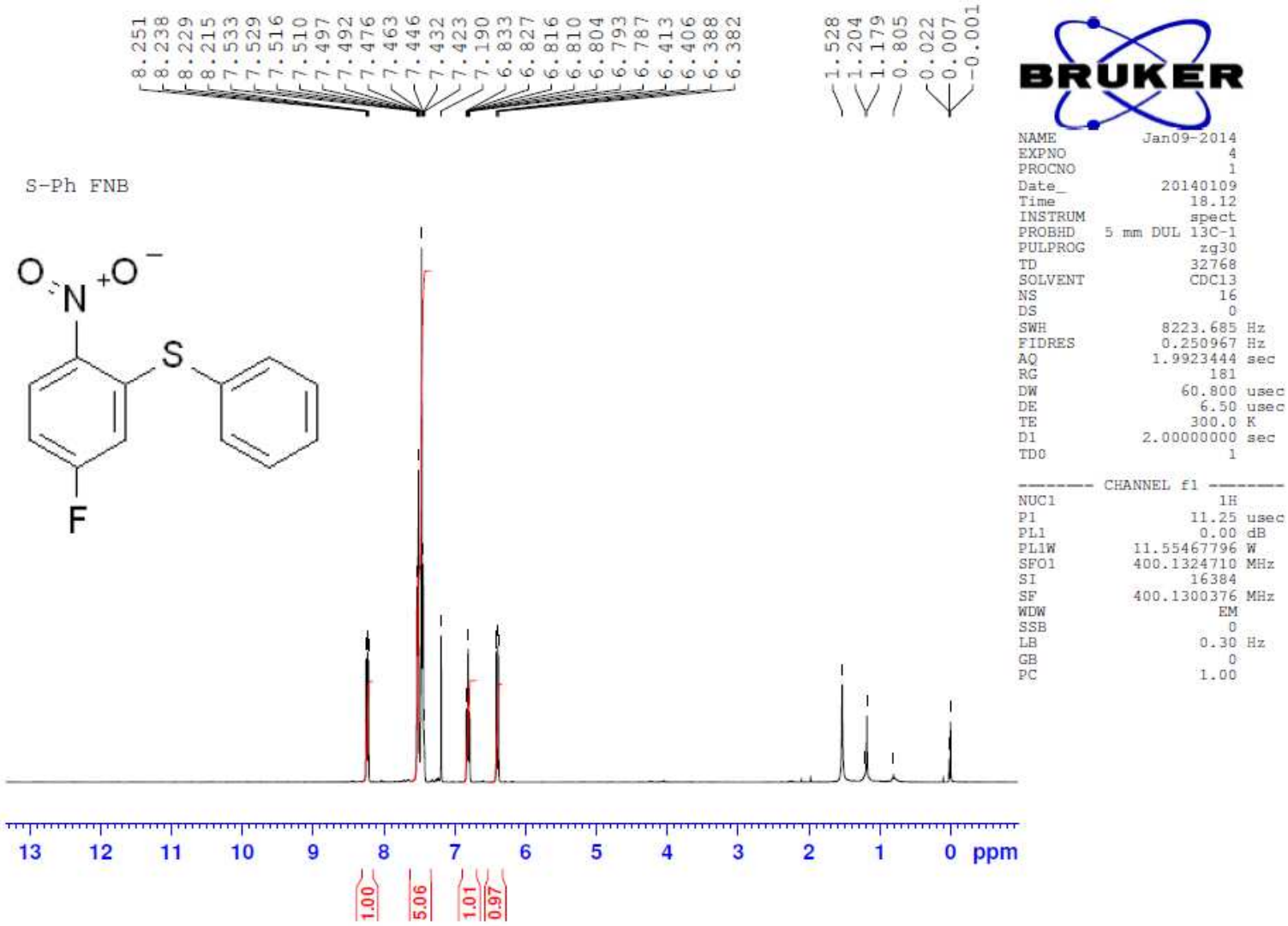


Product **9a** [(2-benzylsulfanyl-4-fluoro-1-nitro-benzene) (S-Bn FNB)] HRMS:

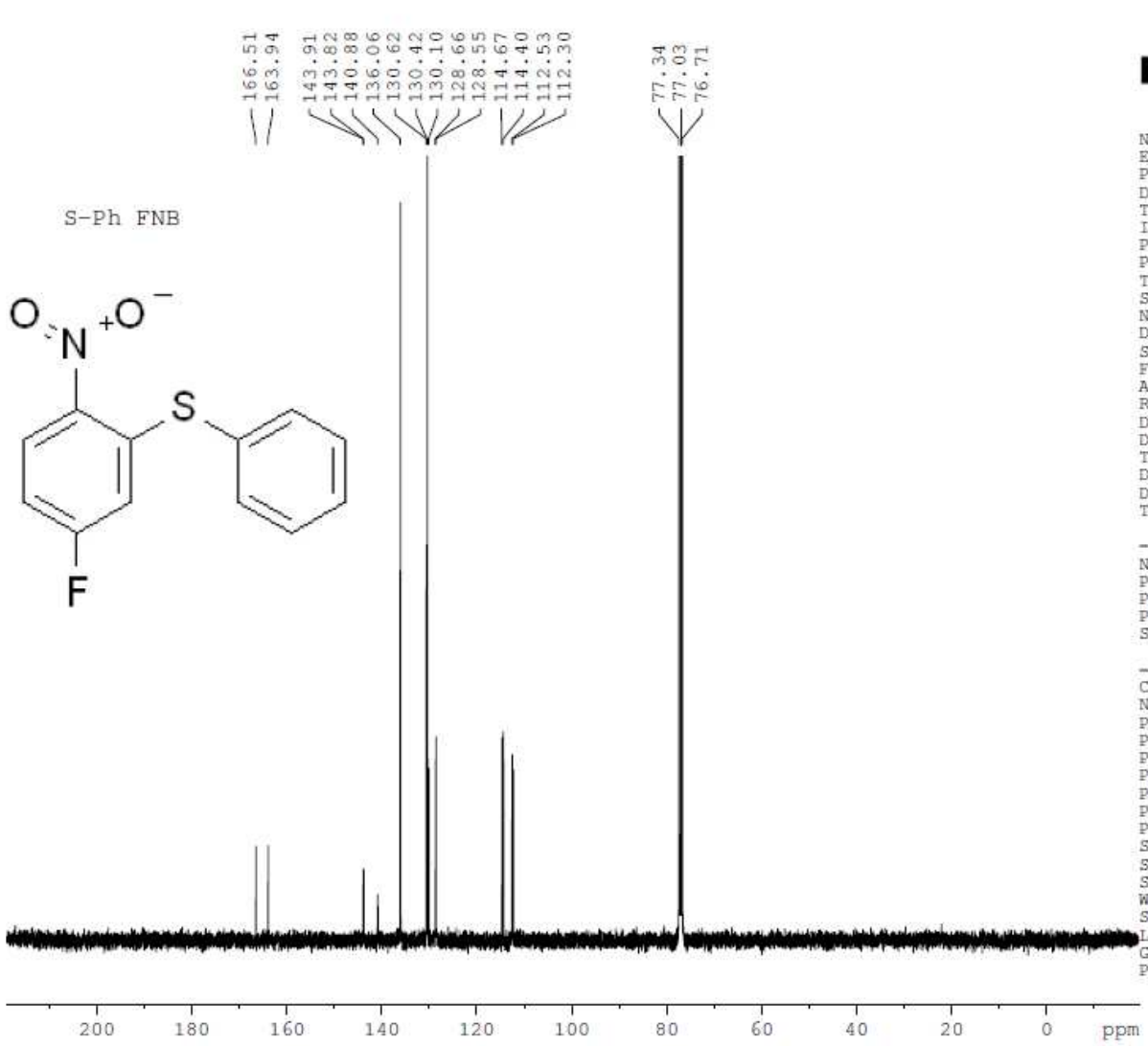
Sample Name	S-Bn FBN	**Position**	P1-B2	**Instrument Name**	Q-TOF LCMS-01	**User Name**	Indira Jyothi
Inj Vol	1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	23JAN2014_11.d	**ACQ Method**	AZD1979_1.m	**Comment**		**Acquired Time**	1/23/2014 9:56:13 PM



Product **10a** [(4-fluoro-1-nitro-2-phenylsulfanyl-benzene) (S-Ph FNB)] ^{1}H-NMR:



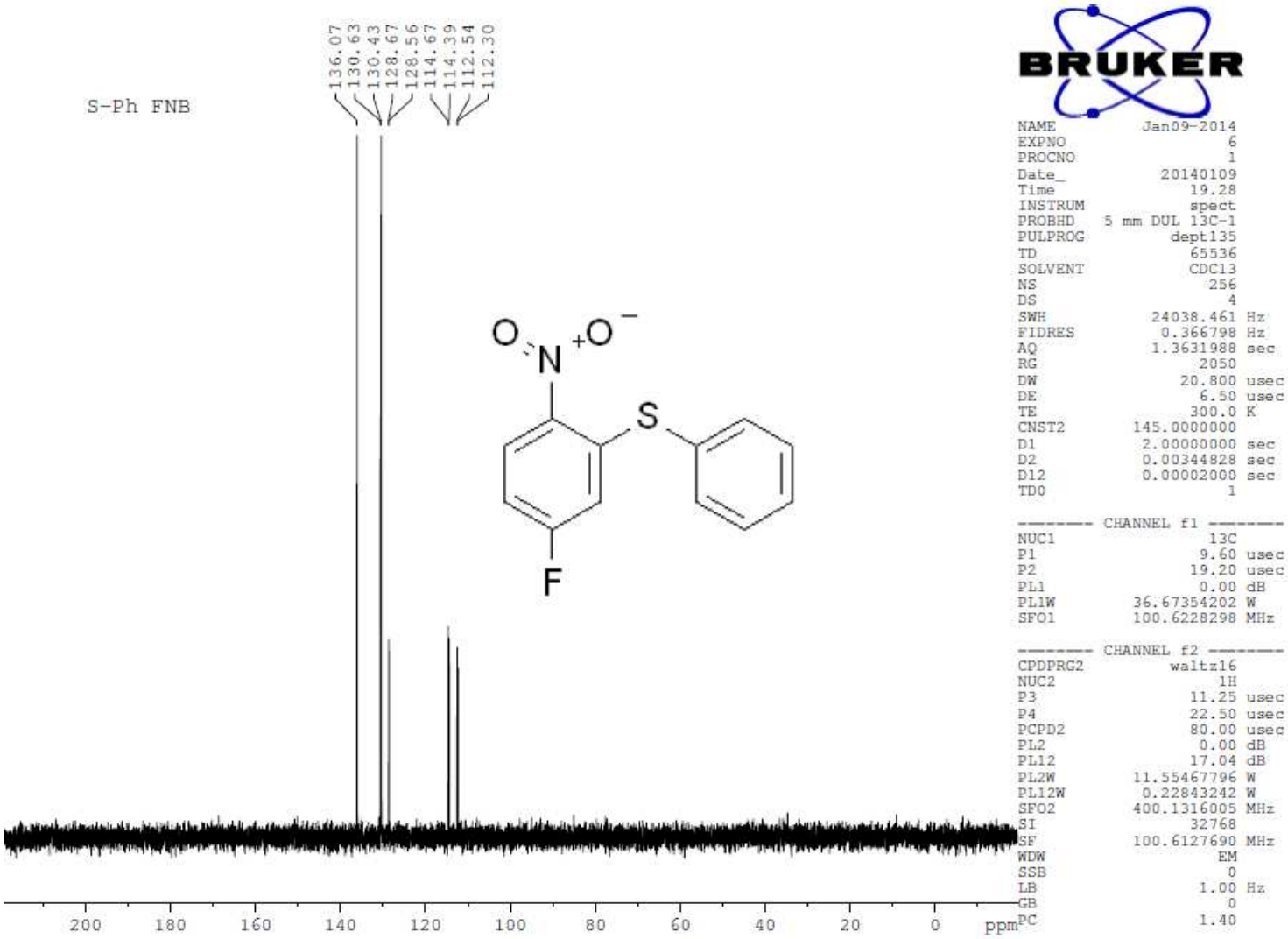
Product **10a** [(4-fluoro-1-nitro-2-phenylsulfanyl-benzene) (S-Ph FNB)] ^{13}C-NMR:



BRUKER

NAME	Jan09-2014
EXPNO	5
PROCNO	1
Date_	20140109
Time	19.13
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDC13
NS	1024
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	101
DW	20.800 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
------- CHANNEL f1 -------	
NUC1	13C
P1	9.60 usec
PL1	0.00 dB
PL1W	36.67354202 W
SFO1	100.6228298 MHz
------- CHANNEL f2 -------	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	17.04 dB
PL13	17.04 dB
PL2W	11.55467796 W
PL12W	0.22843242 W
PL13W	0.22843242 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Product **10a** [(4-fluoro-1-nitro-2-phenylsulfanyl-benzene) (S-Ph FNB)] DEPT-NMR:

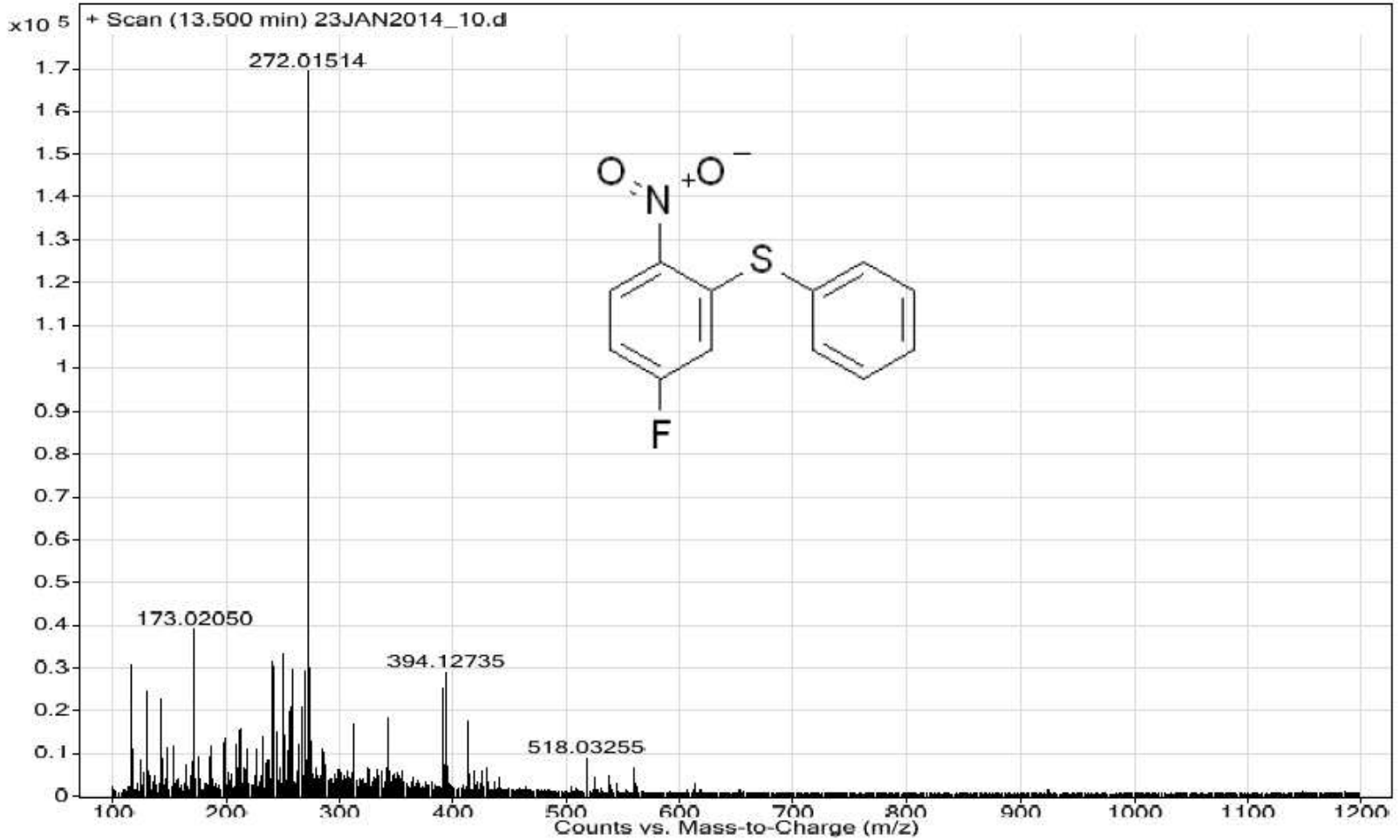


BRUKER

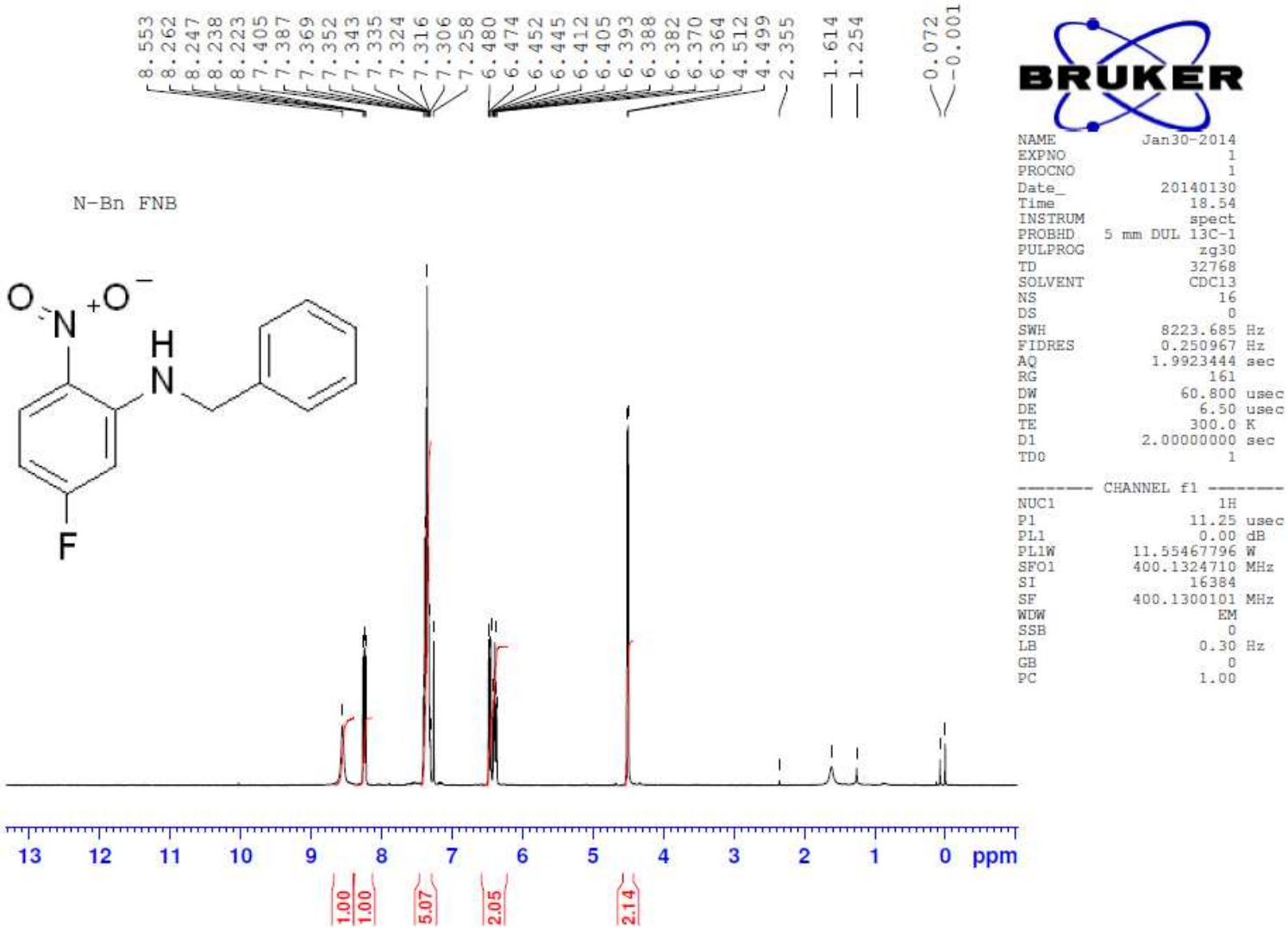
NAME	Jan09-2014
EXPNO	6
PROCNO	1
Date_	20140109
Time	19.28
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	dept135
TD	65536
SOLVENT	CDC13
NS	256
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	300.0 K
CNST2	145.0000000
D1	2.00000000 sec
D2	0.00344828 sec
D12	0.00002000 sec
TD0	1
------- CHANNEL f1 -------	
NUC1	13C
P1	9.60 usec
P2	19.20 usec
PL1	0.00 dB
PL1W	36.67354202 W
SFO1	100.6228298 MHz
------- CHANNEL f2 -------	
CPDPRG2	waltz16
NUC2	1H
P3	11.25 usec
P4	22.50 usec
PCPD2	80.00 usec
PL2	0.00 dB
PL12	17.04 dB
PL2W	11.55467796 W
PL12W	0.22843242 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Product **10a** [(4-fluoro-1-nitro-2-phenylsulfanyl-benzene) (S-Ph FNB)] HRMS:

Sample Name	S-Ph FBN	**Position**	P1-B1	**Instrument Name**	Q-TOF LCMS-01	**User Name**	Indira Jyothi
Inj Vol	1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	23JAN2014_10.d	**ACQ Method**	AZD1979_1.m	**Comment**		**Acquired Time**	1/23/2014 9:37:14 PM



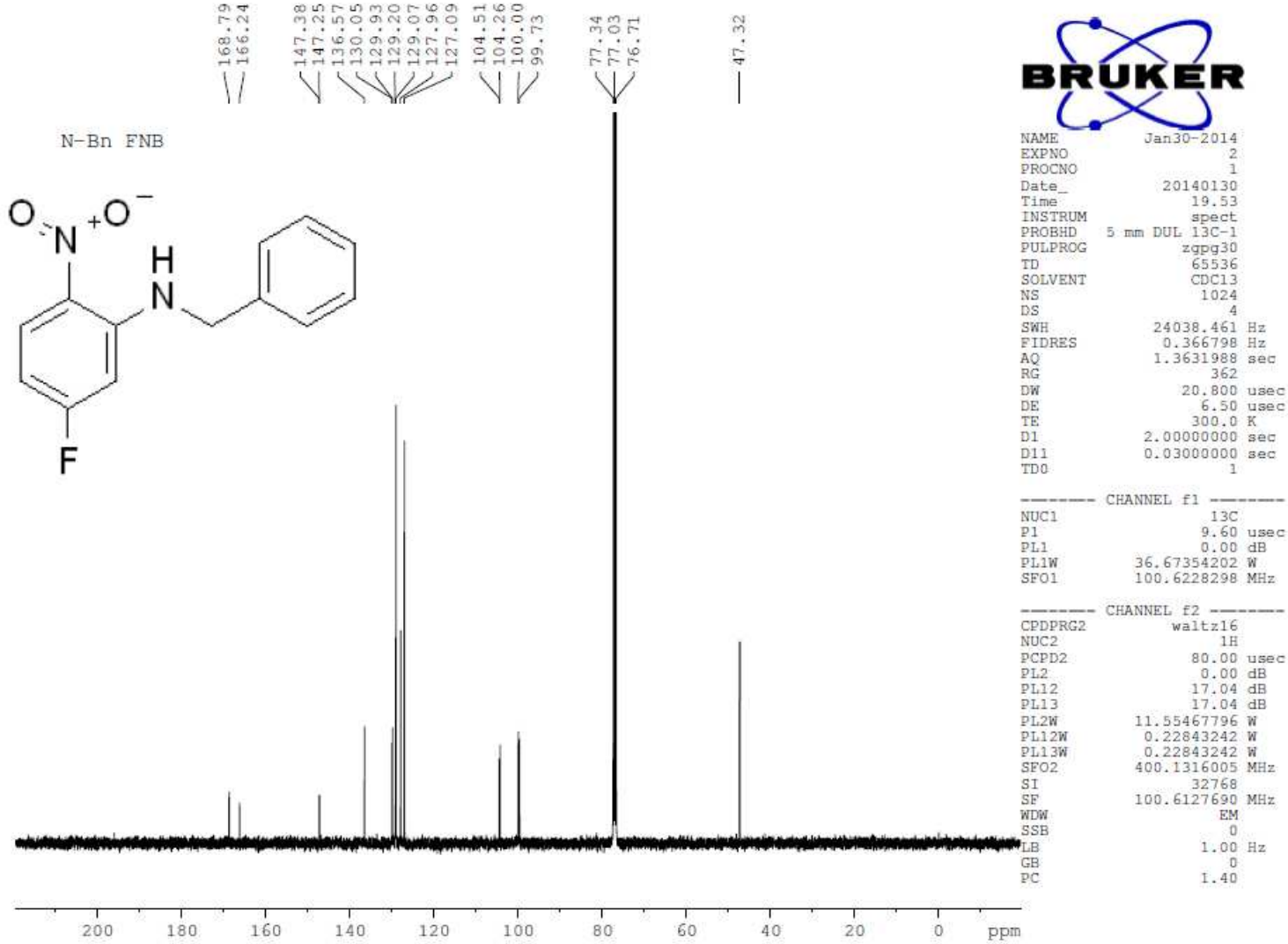
Product **11a** [(*N*-benzyl-5-fluoro-2-nitro-aniline) (*N*-Bn FNB)] ^{1}H-NMR:



BRUKER

NAME	Jan30-2014
EXPNO	1
PROCNO	1
Date_	20140130
Time	18.54
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	0
SWH	8223.685 Hz
FIDRES	0.250967 Hz
AQ	1.9923444 sec
RG	161
DW	60.800 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
------- CHANNEL f1 -------	
NUC1	1H
P1	11.25 usec
PL1	0.00 dB
PL1W	11.55467796 W
SFO1	400.1324710 MHz
SI	16384
SF	400.1300101 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

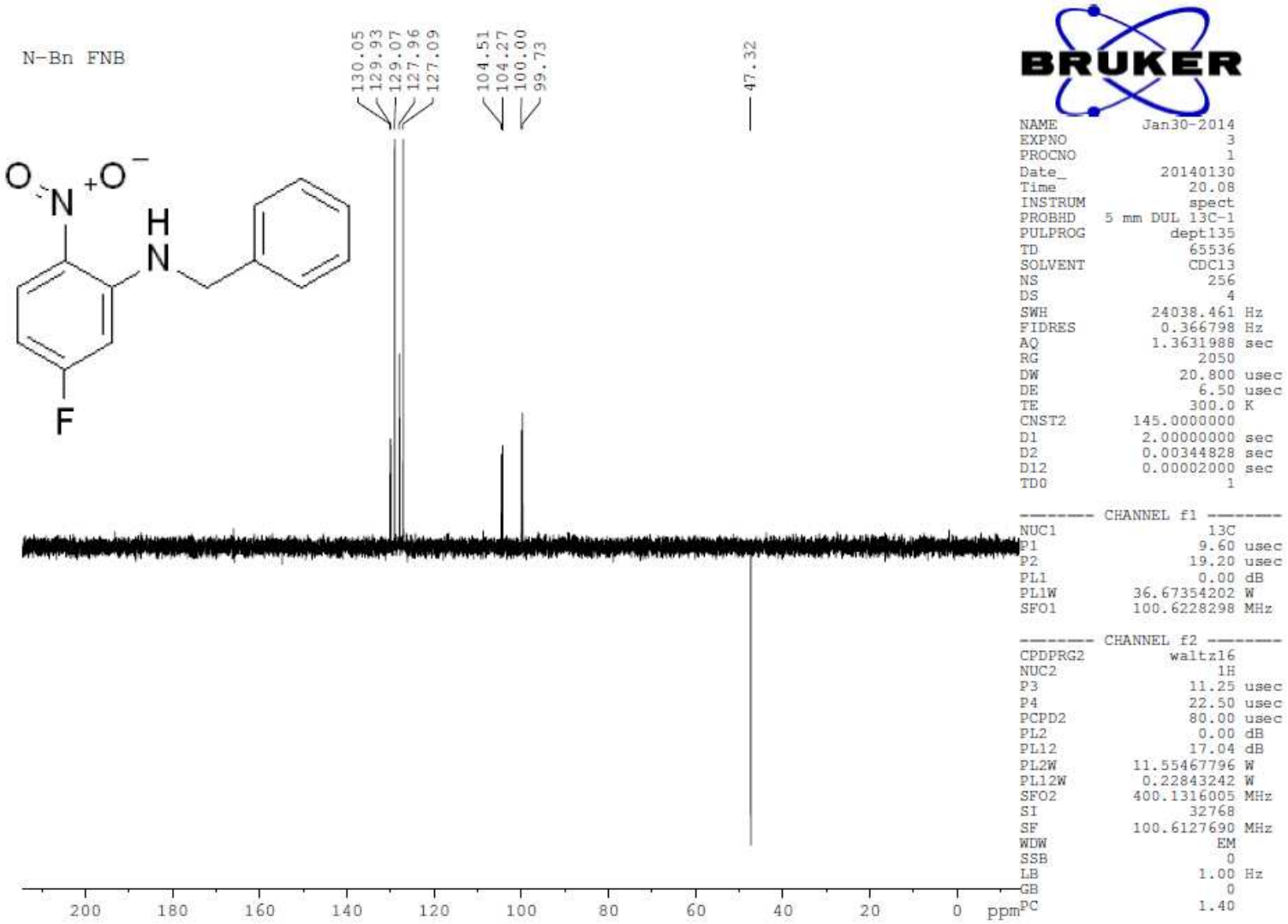
Product **11a** [(*N*-benzyl-5-fluoro-2-nitro-aniline) (*N*-Bn FNB)] ^{13}C-NMR:



BRUKER

NAME	Jan30-2014
EXPNO	2
PROCNO	1
Date_	20140130
Time	19.53
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	362
DW	20.800 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
------- CHANNEL f1 -------	
NUC1	13C
P1	9.60 usec
PL1	0.00 dB
PL1W	36.67354202 W
SFO1	100.6228298 MHz
------- CHANNEL f2 -------	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	17.04 dB
PL13	17.04 dB
PL2W	11.55467796 W
PL12W	0.22843242 W
PL13W	0.22843242 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Product **11a** [(*N*-benzyl-5-fluoro-2-nitro-aniline) (*N*-Bn FNB)] DEPT-NMR:

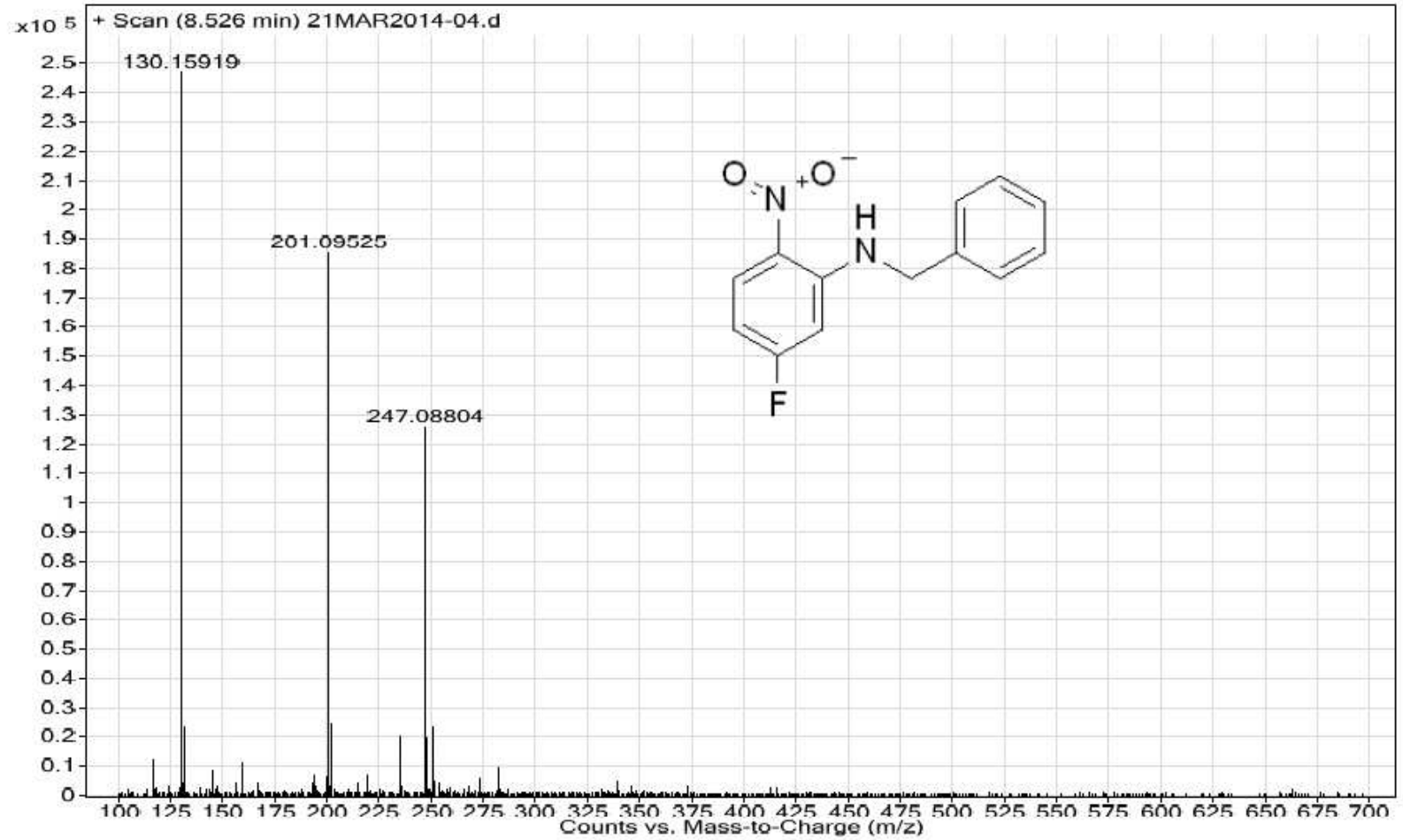


BRUKER

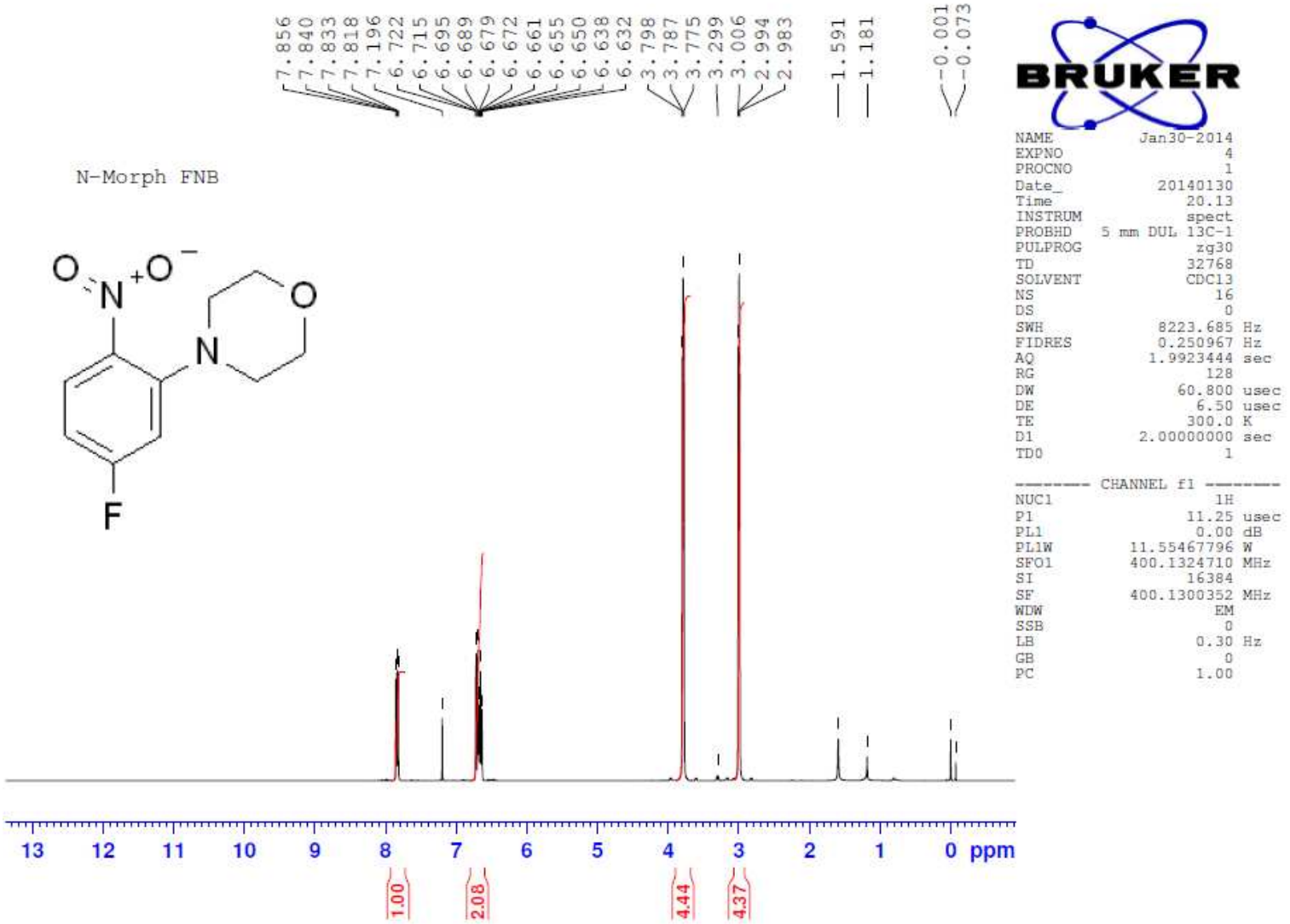
NAME	Jan30-2014
EXPNO	3
PROCNO	1
Date_	20140130
Time	20.08
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	dept135
TD	65536
SOLVENT	CDCl3
NS	256
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	300.0 K
CNST2	145.0000000
D1	2.00000000 sec
D2	0.00344828 sec
D12	0.00002000 sec
TD0	1
------- CHANNEL f1 -------	
NUC1	13C
P1	9.60 usec
P2	19.20 usec
PL1	0.00 dB
PL1W	36.67354202 W
SFO1	100.6228298 MHz
------- CHANNEL f2 -------	
CPDPRG2	waltz16
NUC2	1H
P3	11.25 usec
P4	22.50 usec
PCPD2	80.00 usec
PL2	0.00 dB
PL12	17.04 dB
PL2W	11.55467796 W
PL12W	0.22843242 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Product **11a** [(*N*-benzyl-5-fluoro-2-nitro-aniline) (*N*-Bn FNB)] HRMS:

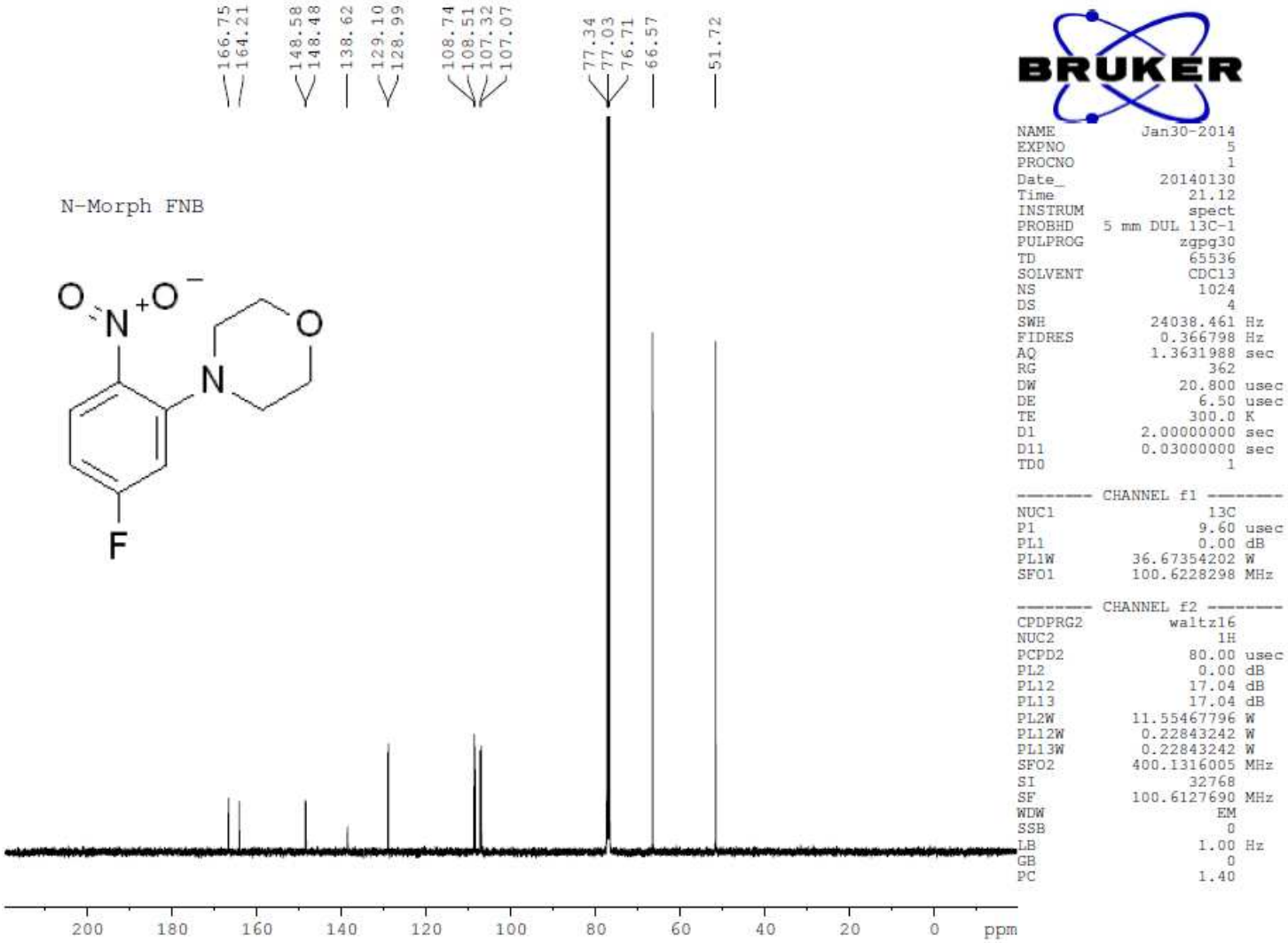
Sample Name	N-Bn FNB	**Position**	P1-A3	**Instrument Name**	Q-TOF LCMS-01	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	21MAR2014-04.d	**ACQ Method**	science1.m	**Comment**		**Acquired Time**	3/21/2014 3:14:39 PM



Product **12a** [(4-(5-fluoro-2-nitro-phenyl)morpholine) (*N*-Morph FNB)] ^{1}H-NMR:



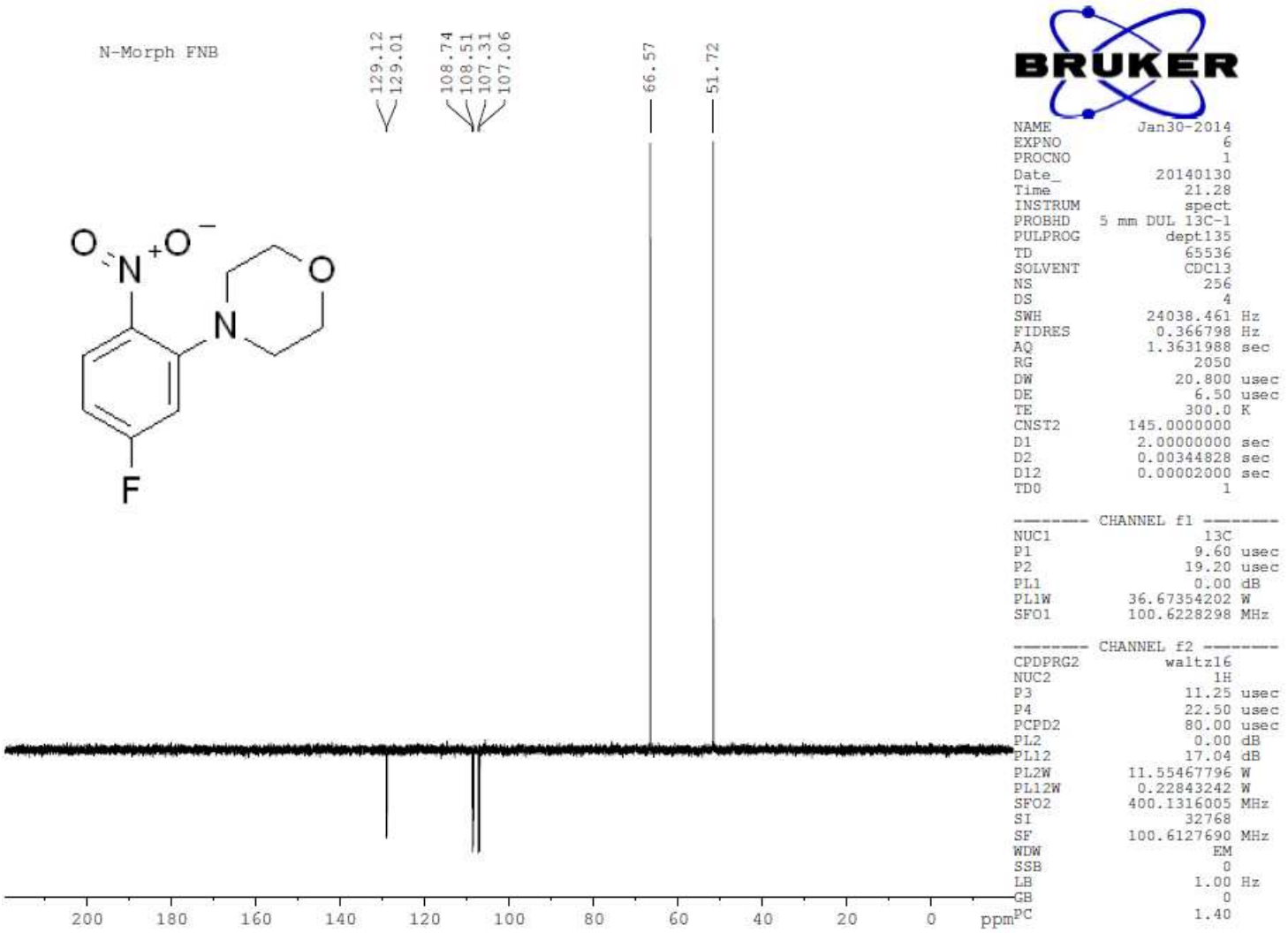
Product **12a** [(4-(5-fluoro-2-nitro-phenyl)morpholine) (*N*-Morph FNB)] ^{13}C-NMR:



BRUKER

NAME	Jan30-2014
EXPNO	5
PROCNO	1
Date_	20140130
Time	21.12
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	362
DW	20.800 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
------- CHANNEL f1 -------	
NUC1	13C
P1	9.60 usec
PL1	0.00 dB
PL1W	36.67354202 W
SFO1	100.6228298 MHz
------- CHANNEL f2 -------	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	17.04 dB
PL13	17.04 dB
PL2W	11.55467796 W
PL12W	0.22843242 W
PL13W	0.22843242 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Product **12a** [(4-(5-fluoro-2-nitro-phenyl)morpholine) (*N*-Morph FNB)] DEPT-NMR:

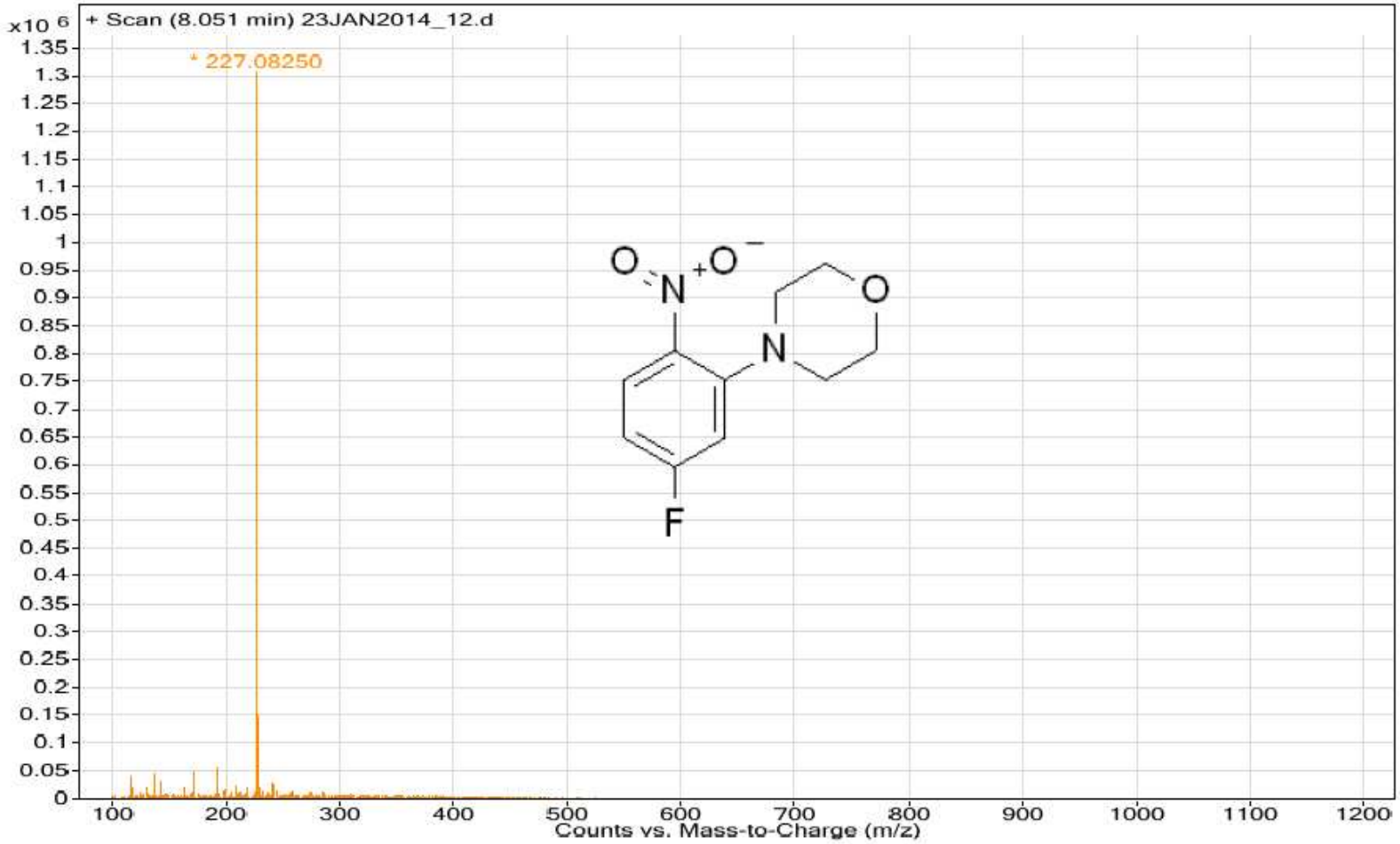


BRUKER

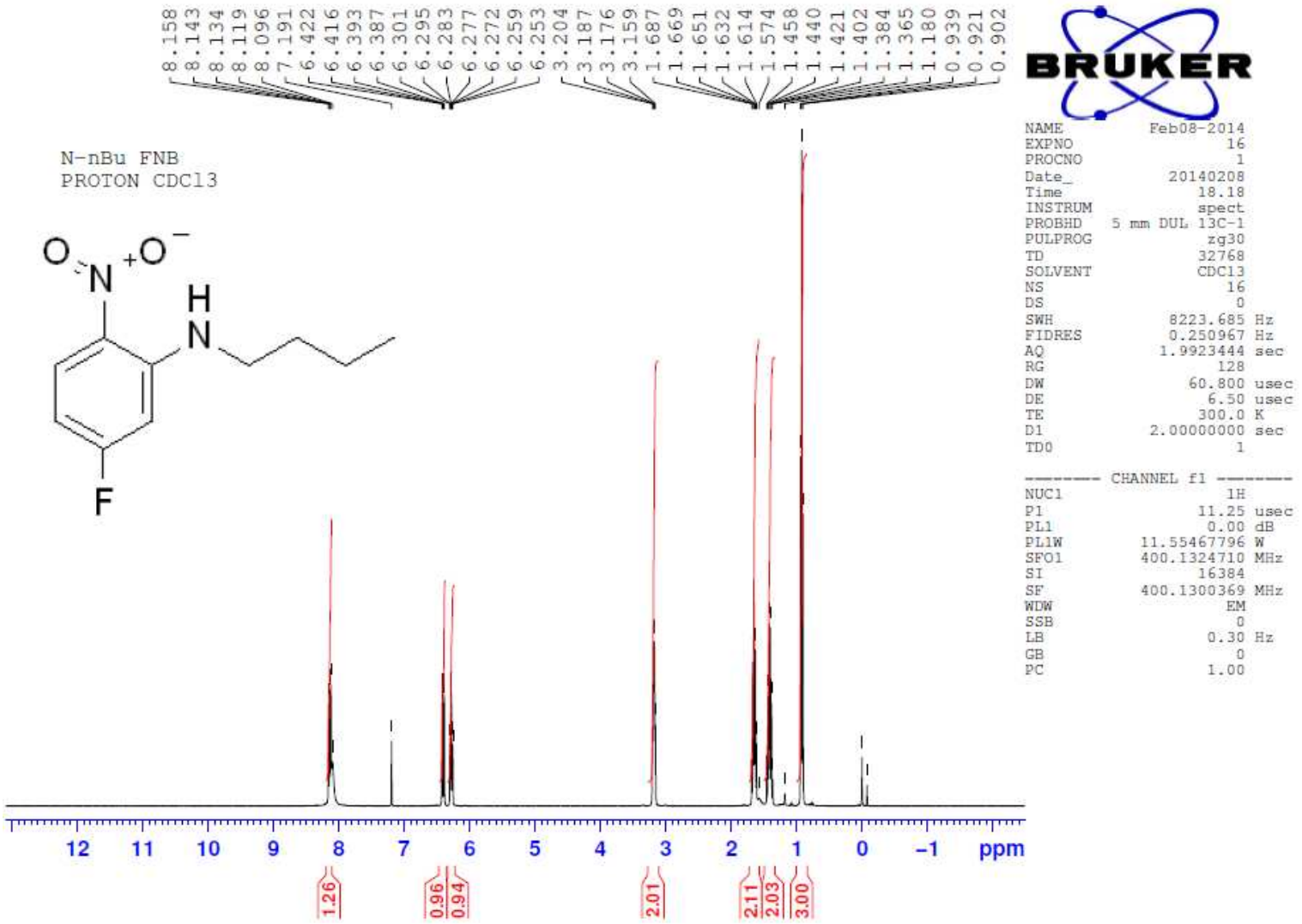
NAME	Jan30-2014
EXPNO	6
PROCNO	1
Date_	20140130
Time	21.28
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	dept135
TD	65536
SOLVENT	CDCl3
NS	256
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	300.0 K
CNST2	145.0000000
D1	2.00000000 sec
D2	0.00344828 sec
D12	0.00002000 sec
TD0	1
------- CHANNEL f1 -------	
NUC1	13C
P1	9.60 usec
P2	19.20 usec
PL1	0.00 dB
PL1W	36.67354202 W
SFO1	100.6228298 MHz
------- CHANNEL f2 -------	
CPDPRG2	waltz16
NUC2	1H
P3	11.25 usec
P4	22.50 usec
PCPD2	80.00 usec
PL2	0.00 dB
PL12	17.04 dB
PL2W	11.55467796 W
PL12W	0.22843242 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Product **12a** [(4-(5-fluoro-2-nitro-phenyl)morpholine) (*N*-Morph FNB)] HRMS:

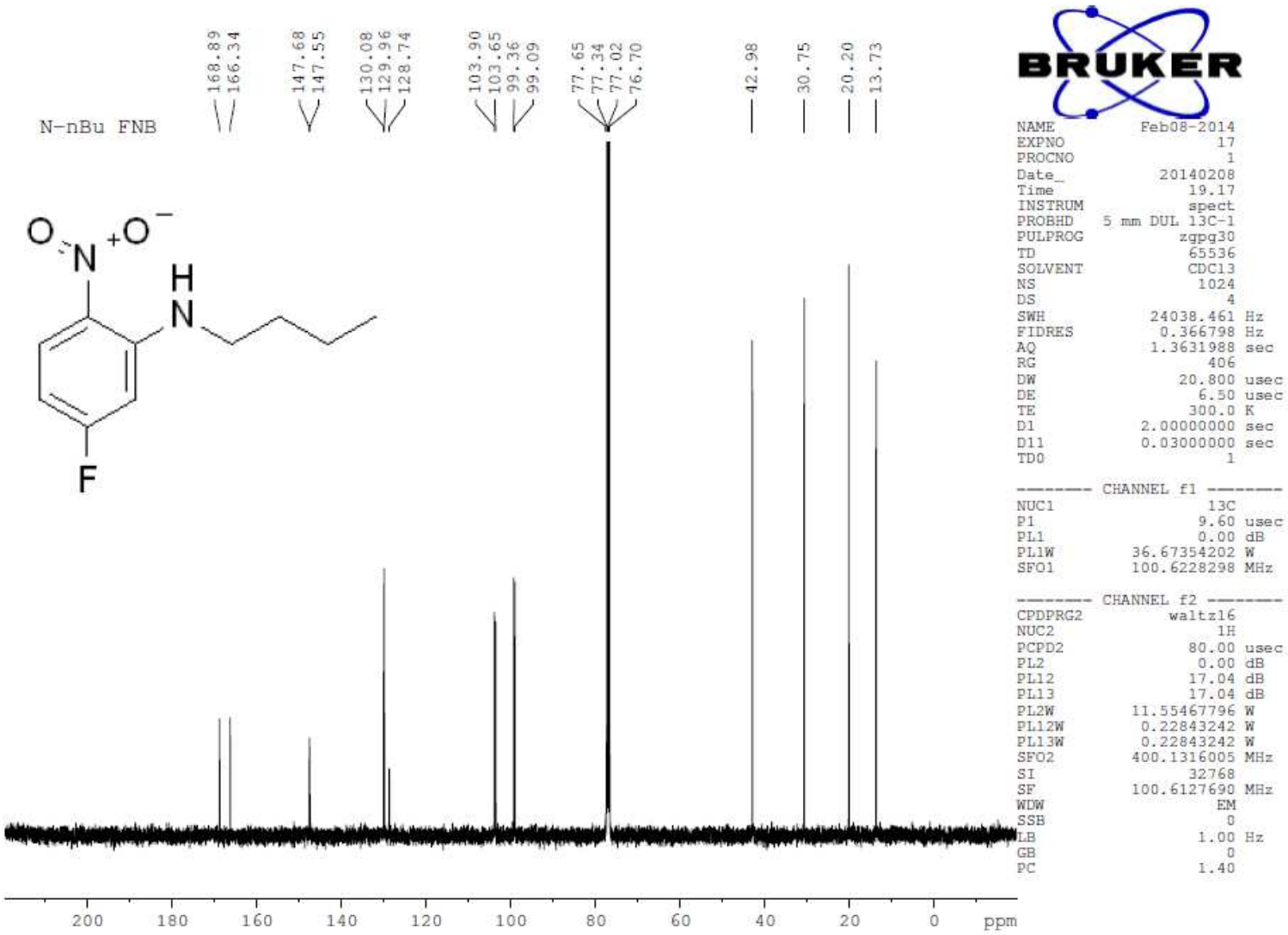
Sample Name	N-Morph FBN	**Position**	P1-B3	**Instrument Name**	Q-TOF LCMS-01	**User Name**	Indira Jyothi
Inj Vol	1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	23JAN2014_12.d	**ACQ Method**	AZD1979_1.m	**Comment**		**Acquired Time**	1/23/2014 10:15:15 PM



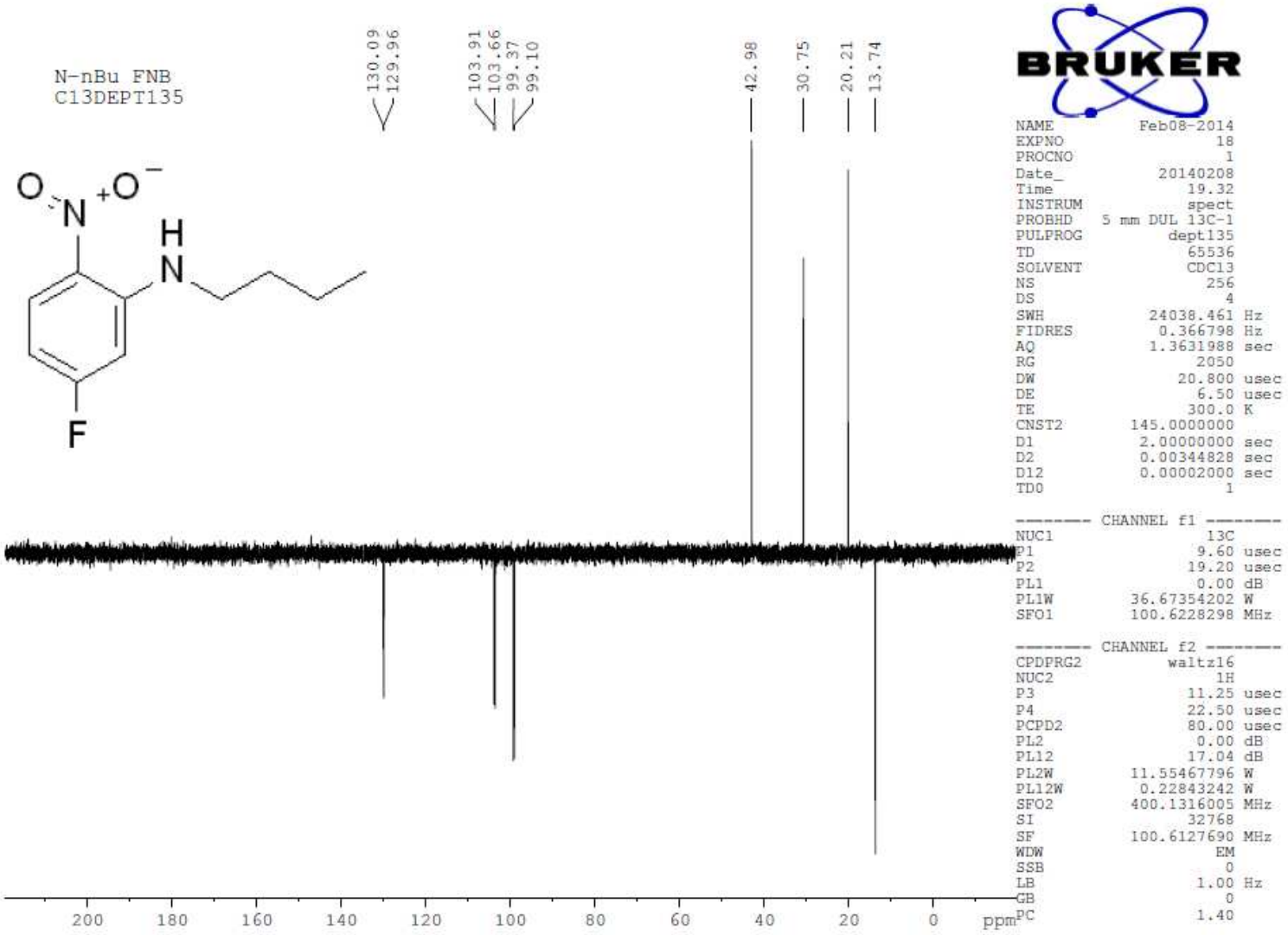
Product **13a** [(*N*-butyl-5-fluoro-2-nitro-aniline) (*N*-Bu FNB)] ^{1}H-NMR:



Product **13a** [(*N*-butyl-5-fluoro-2-nitro-aniline) (*N*-Bu FNB)] ^{13}C-NMR:



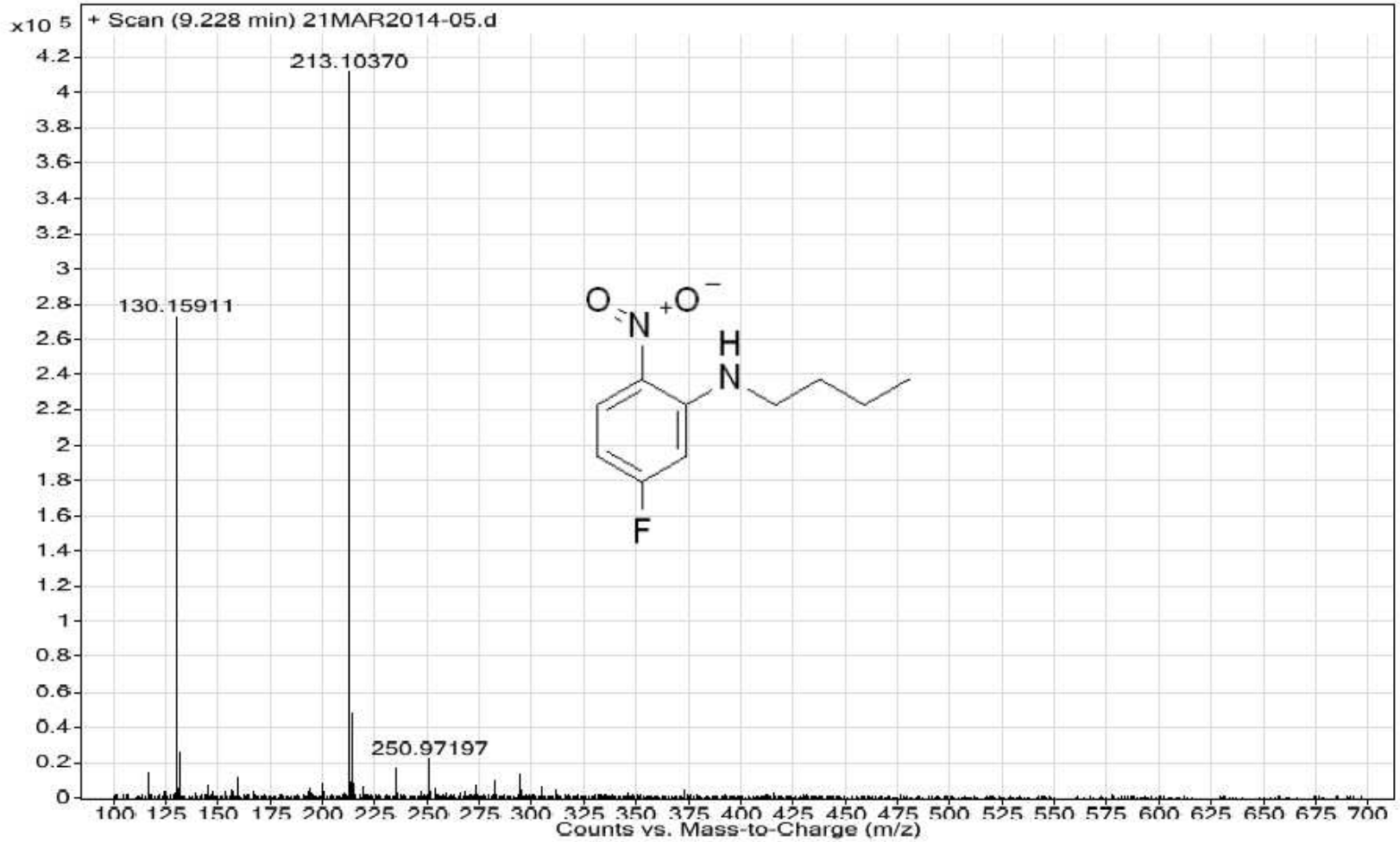
Product **13a** [(*N*-butyl-5-fluoro-2-nitro-aniline) (*N*-Bu FNB)] DEPT:



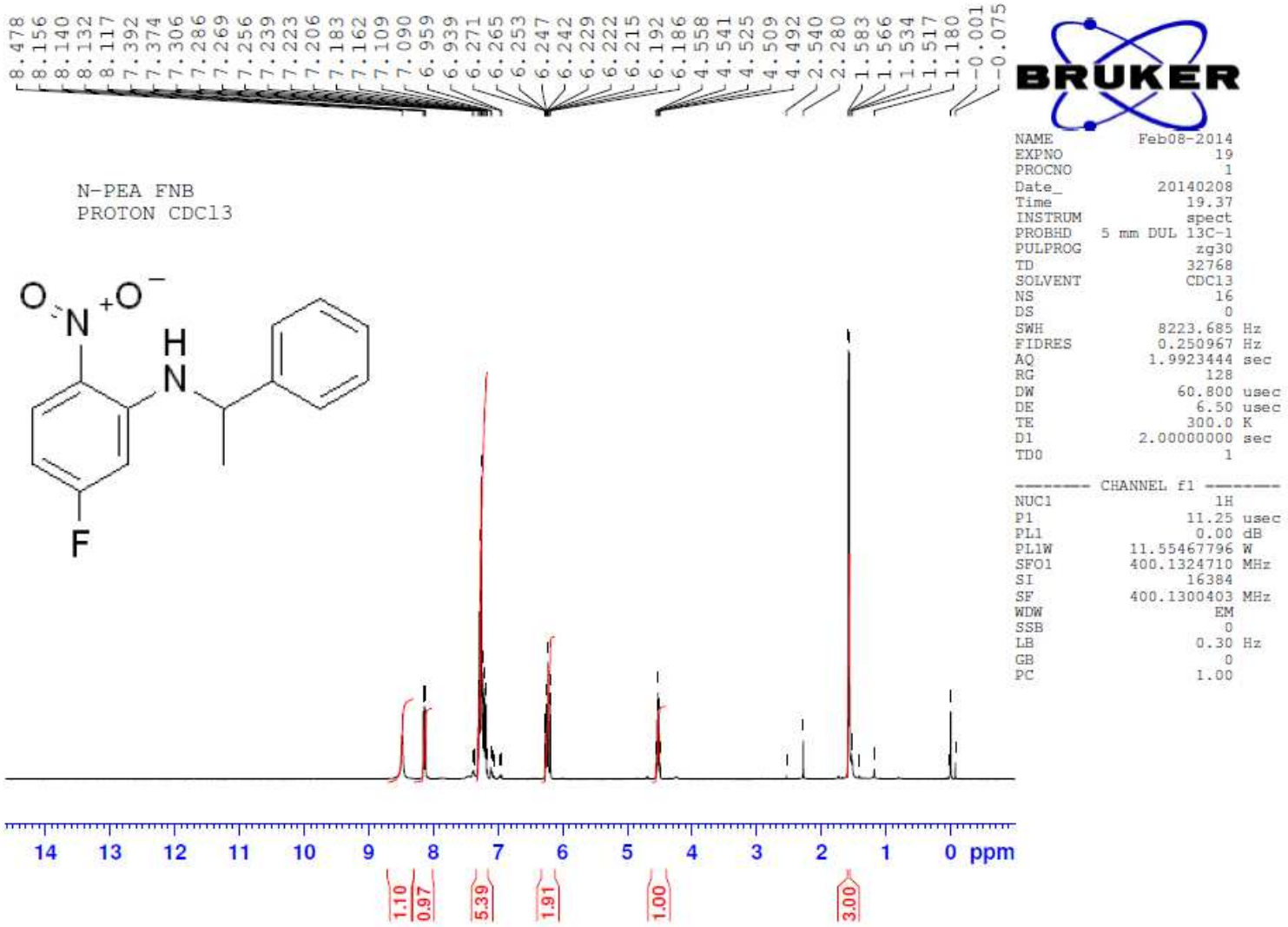
NAME	Feb08-2014
EXPNO	18
PROCNO	1
Date_	20140208
Time	19.32
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	dept135
TD	65536
SOLVENT	CDCl3
NS	256
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	300.0 K
CNST2	145.0000000
D1	2.00000000 sec
D2	0.00344828 sec
D12	0.00002000 sec
TD0	1
------- CHANNEL f1 -------	
NUC1	13C
P1	9.60 usec
P2	19.20 usec
PL1	0.00 dB
PL1W	36.67354202 W
SFO1	100.6228298 MHz
------- CHANNEL f2 -------	
CPDPRG2	waltz16
NUC2	1H
P3	11.25 usec
P4	22.50 usec
PCPD2	80.00 usec
PL2	0.00 dB
PL12	17.04 dB
PL2W	11.55467796 W
PL12W	0.22843242 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Product **13a** [(*N*-butyl-5-fluoro-2-nitro-aniline) (*N*-Bu FNB)] HRMS:

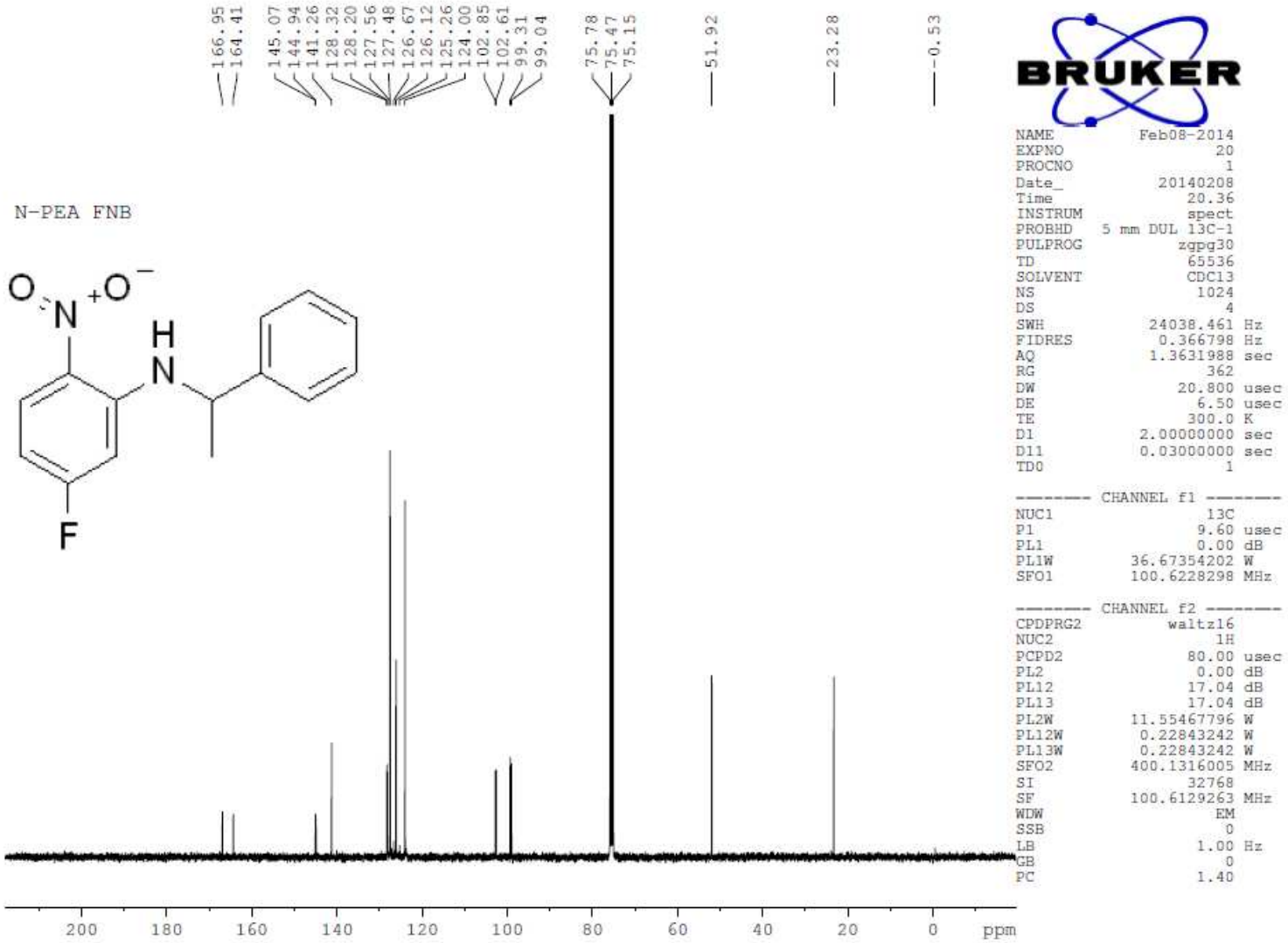
Sample Name	N-nBu FNB	**Position**	P1-A4	**Instrument Name**	Q-TOF LCMS-01	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	21MAR2014-05.d	**ACQ Method**	science1.m	**Comment**		**Acquired Time**	3/21/2014 3:33:33 PM



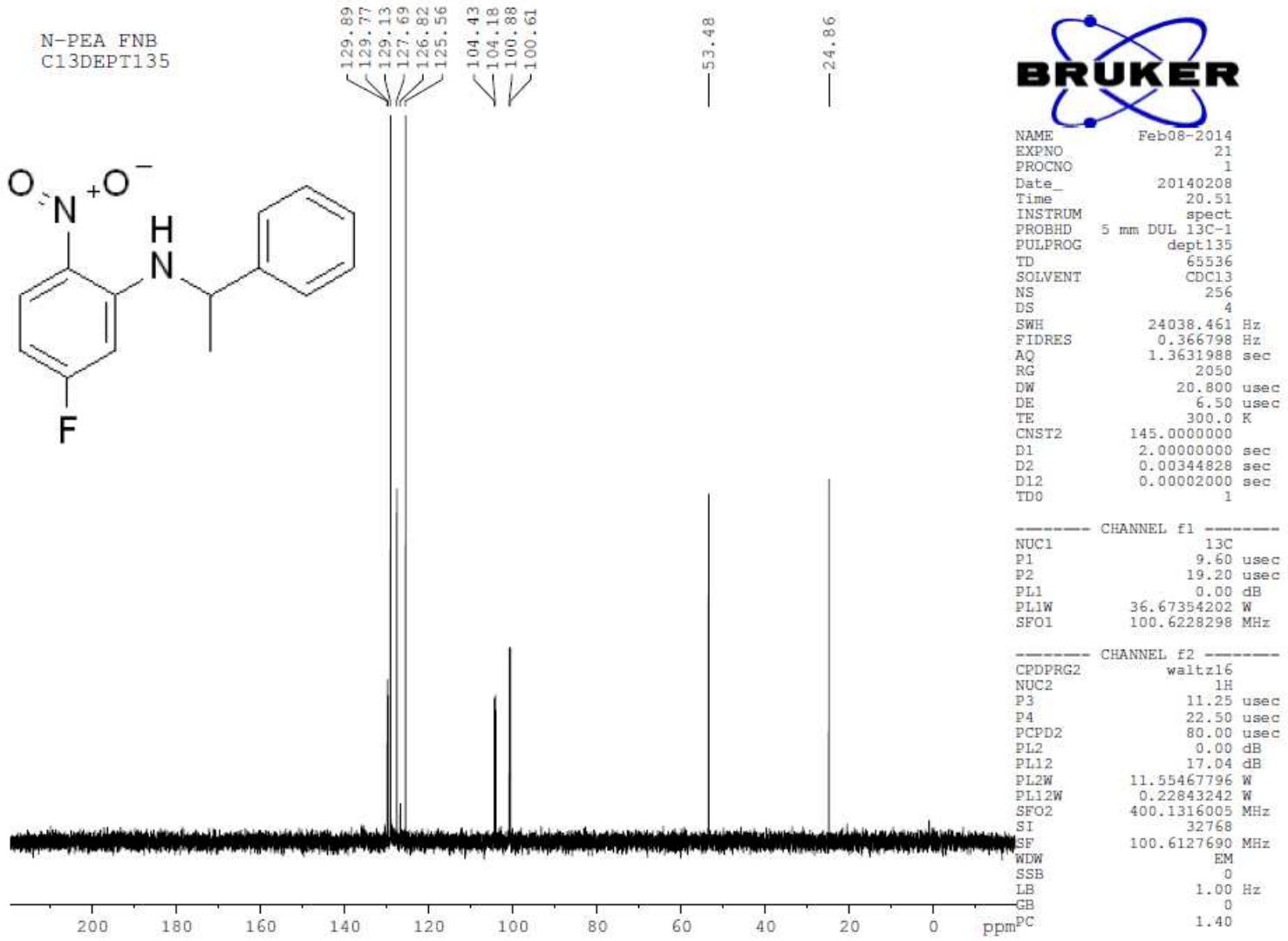
Product **14a** [(5-fluoro-2-nitro-*N*-(1-phenylethyl)amine) (*N*-PEA FNB)] ^{1}H-NMR:



Product **14a** [(5-fluoro-2-nitro-*N*-(1-phenylethyl)amine) (*N*-PEA FNB)] ^{13}C-NMR:

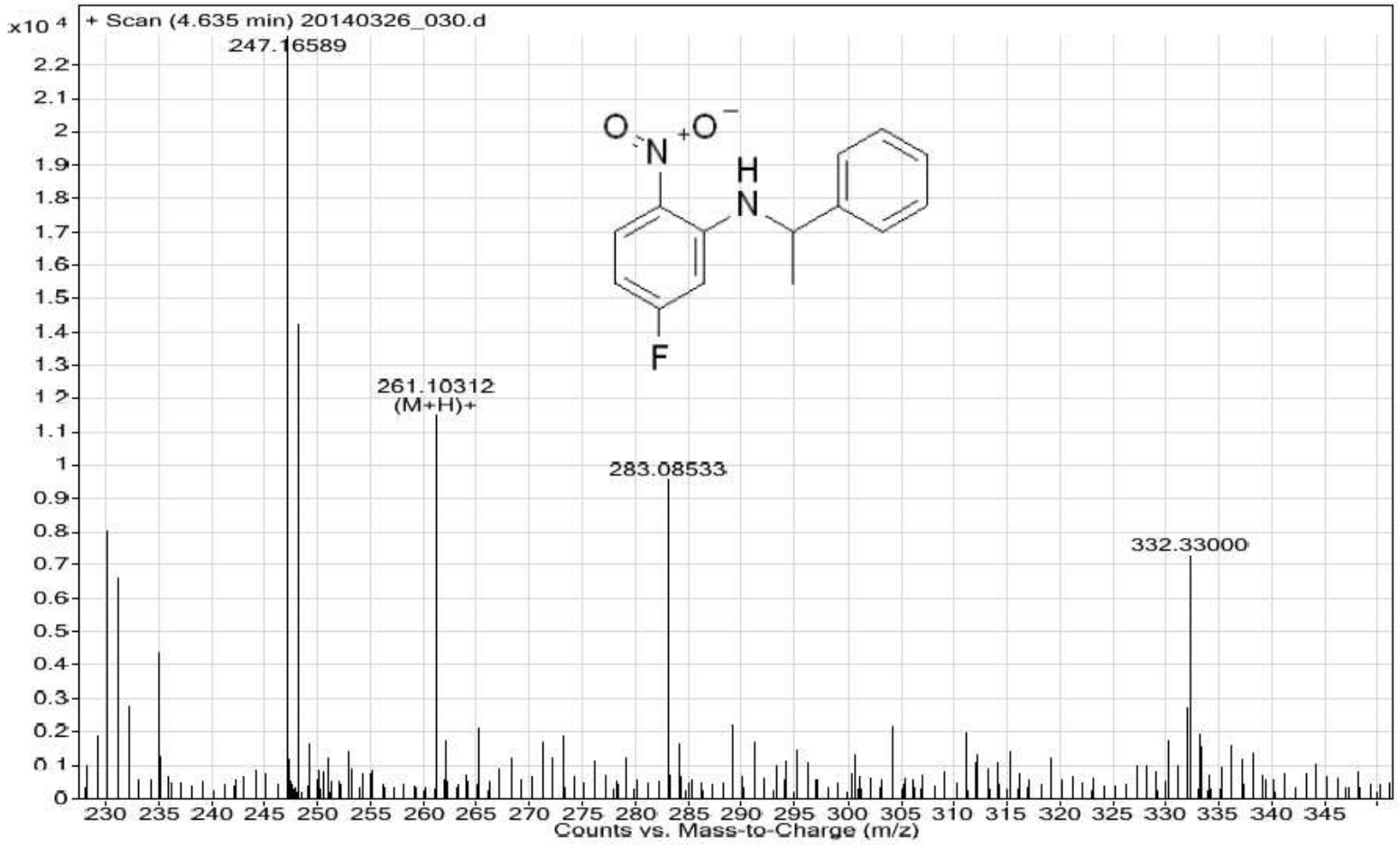


Product **14a** [(5-fluoro-2-nitro-*N*-(1-phenylethyl)amine) (*N*-PEA FNB)] DEPT-NMR:

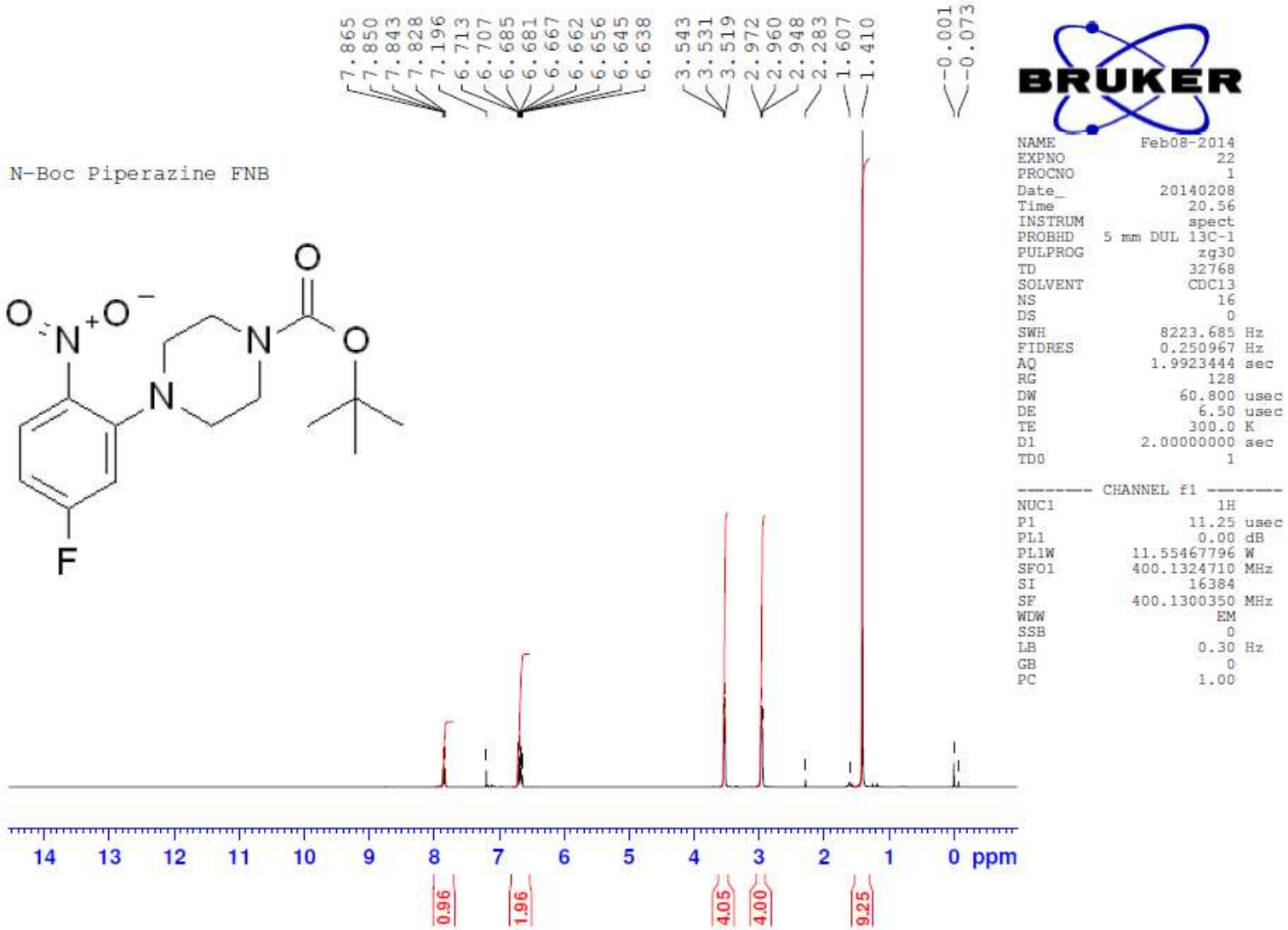


Product **14a** [(5-fluoro-2-nitro-*N*-(1-phenylethyl)amine) (*N*-PEA FNB)] HRMS:

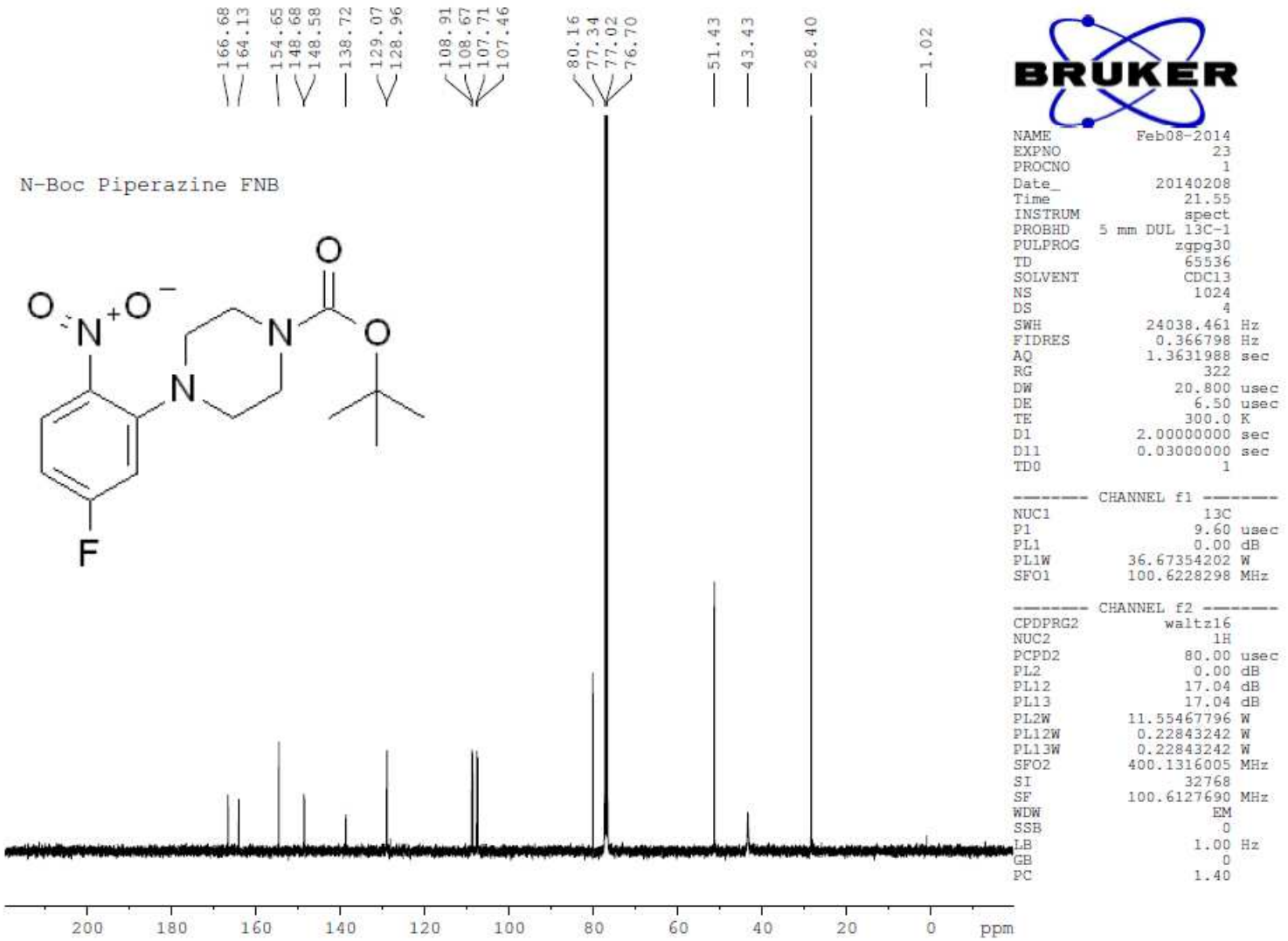
Sample Name	N-PEA FNB	**Position**	P1-C6	**Instrument Name**	Q-TOF LCMS-01	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	20140326_030.d	**ACQ Method**	BEH-C18_ACN_FA_C8_FA	**Comment**	N-PEA FNB	**Acquired Time**	3/26/2014 5:10:52 PM



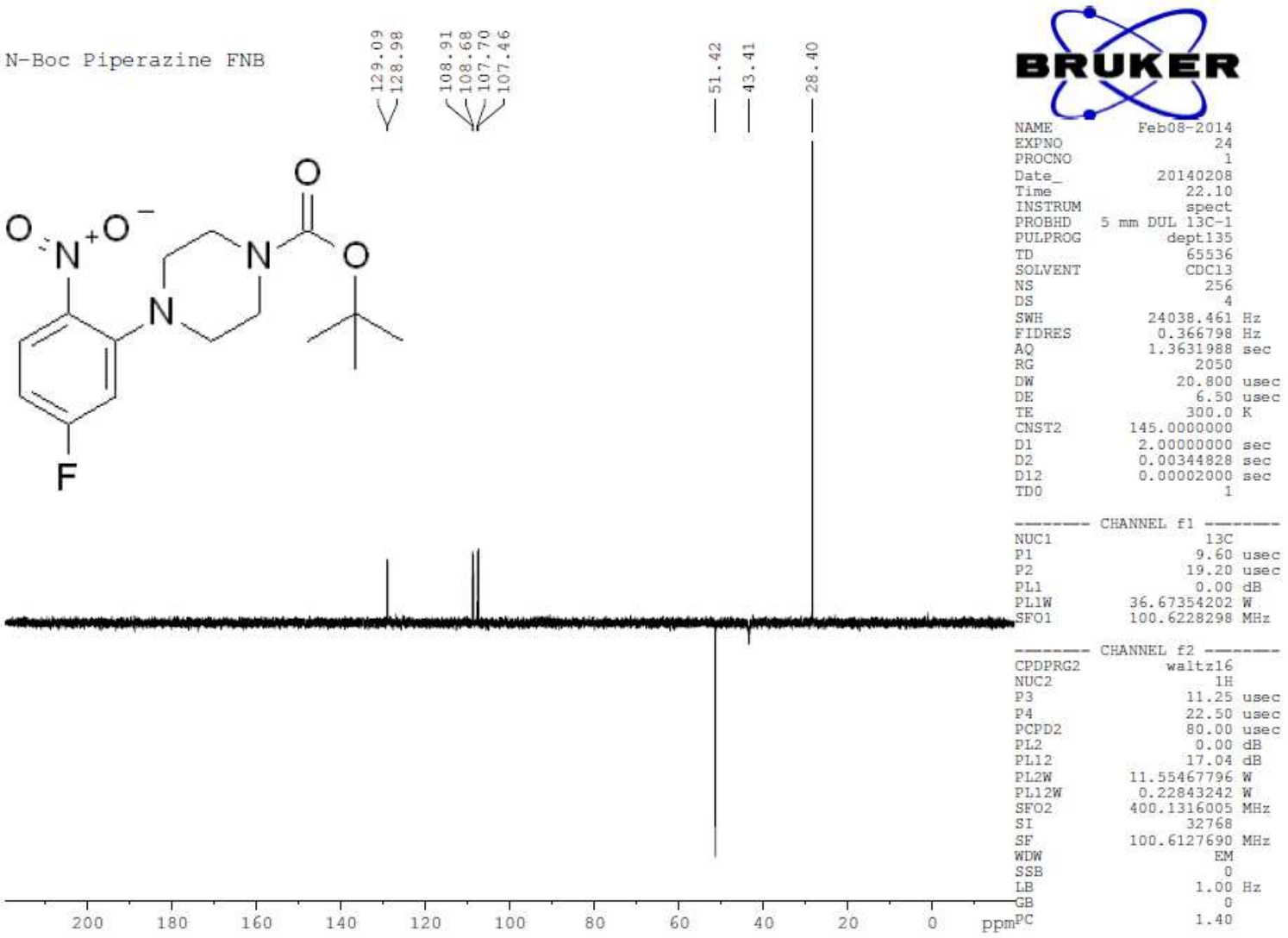
Product **15a** [(tert-butyl 4-(5-fluoro-2-nitro-phenyl)piperazine-1-carboxylate) (*N*-Boc Piperazine FNB)] ^{1}H-NMR:



Product **15a** [(tert-butyl 4-(5-fluoro-2-nitro-phenyl)piperazine-1-carboxylate) (*N*-Boc Piperazine FNB)] ^{13}C-NMR:

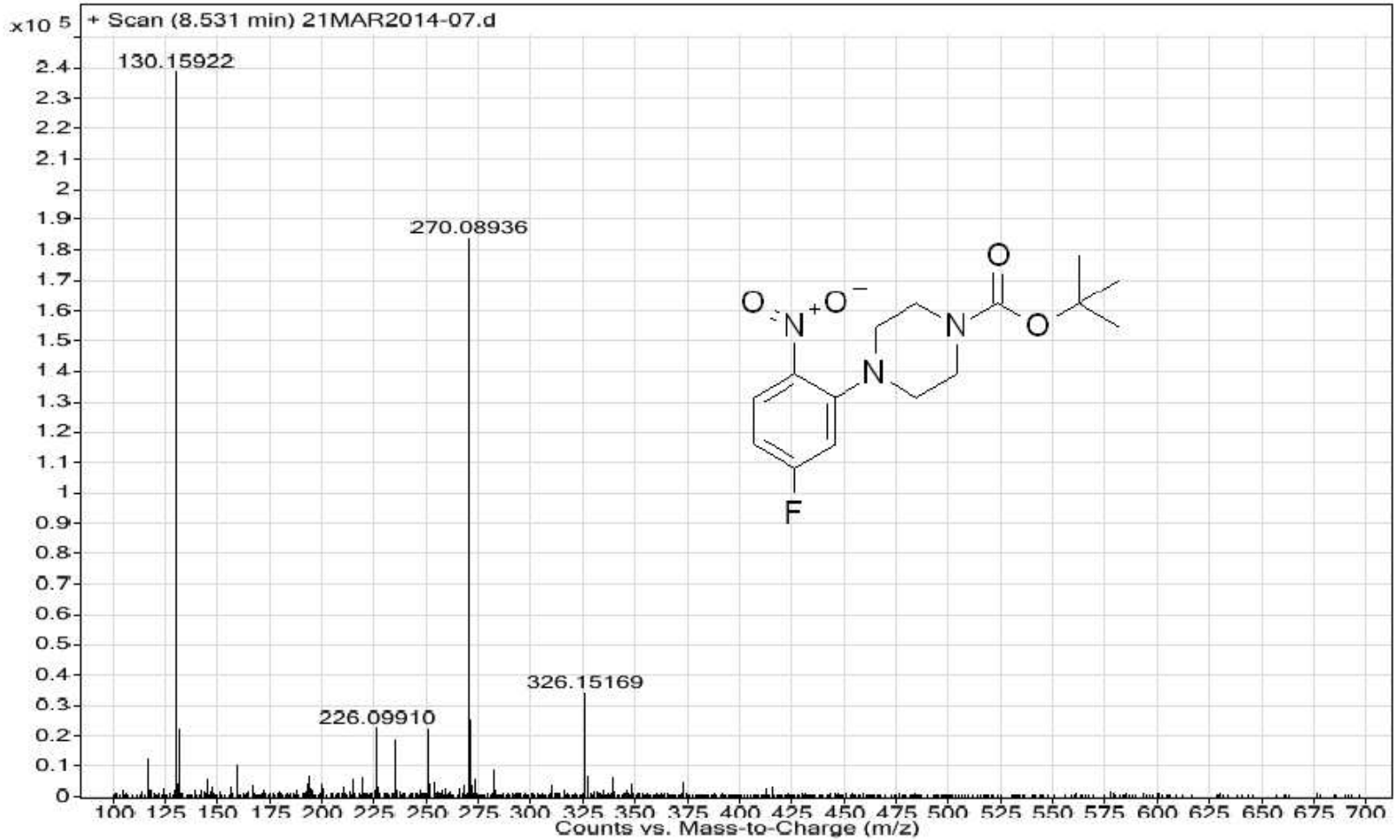


Product **15a** [(tert-butyl 4-(5-fluoro-2-nitro-phenyl)piperazine-1-carboxylate) (*N*-Boc Piperazine FNB)] DEPT-NMR:



Product **15a** [(tert-butyl 4-(5-fluoro-2-nitro-phenyl)piperazine-1-carboxylate) (*N*-Boc Piperazine FNB)] HRMS:

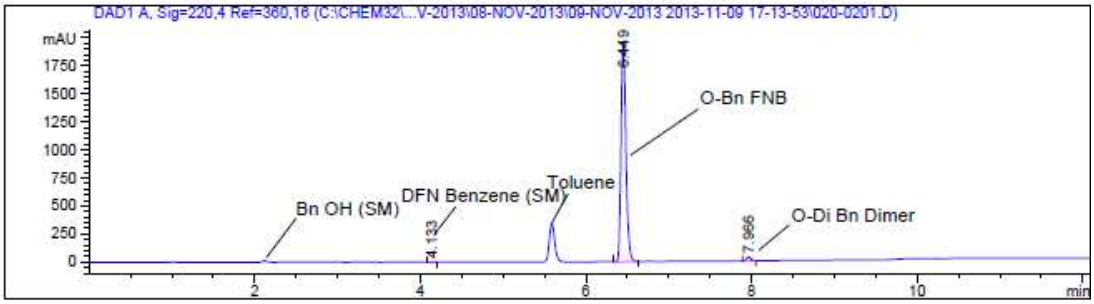
Sample Name	N-Boc pip FNB	**Position**	P1-A6	**Instrument Name**	Q-TOF LCMS-01	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	21MAR2014-07.d	**ACQ Method**	science1.m	**Comment**		**Acquired Time**	3/21/2014 4:11:22 PM



2. Solvent Screening in Method-A

Reaction profile in Toluene (Method-A)

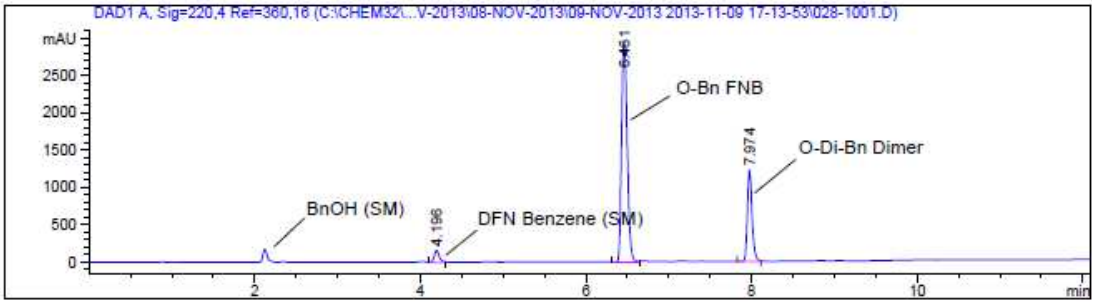
```
Data File C:\CHEM32\...CD2\NOV-2013\08-NOV-2013\09-NOV-2013 2013-11-09 17-13-53\020-0201.D
Sample Name: Toluene-O-Bn FNB

    ======================================================================
    Acq. Operator   : Sagar                          Seq. Line :   2
    Acq. Instrument : PRDB-LC-22                      Location : Vial 20
    Injection Date  : 09/11/2013 05:39:12 PM             Inj :   1
                                                    Inj Volume : 4 µl
    Acq. Method     : C:\Chem32\PRDB-LC-22\Data\2013-BCL2 CD2\Nov-2013\08-NOV-2013\09-NOV-2013
                      2013-11-09 17-13-53\ATLANTIST3_BCL-2_CD2_1.M
    Last changed    : 24/10/2013 02:27:28 PM by Sagar
    Analysis Method : C:\CHEM32\PRDB-LC-22\DATA\2013-BCL2 CD2\NOV-2013\08-NOV-2013\08-NOV-2013
                      2013-11-08 13-53-49\03-KPWL 686-084 RS 3.D\DA.M (ATLANTIST3_BCL-2_CD2_1.M)
    Last changed    : 24/10/2013 02:27:28 PM by Sagar
    Sample Info     : Toluene-O-Bn FNB
```




```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=220,4 Ref=360,16

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   4.133 MM R  0.0673    6.87718    1.70186   0.0840
       2   6.449 MM R  0.0625 8040.75586 1965.88416  98.2355
       3   7.966 MM R  0.0638  137.55057   35.96042   1.6805

    Totals :                  8185.18361 2003.53644

    ======================================================================
                            *** End of Report ***
```

Reaction profile in Tetrahydrofuran (Method-A):

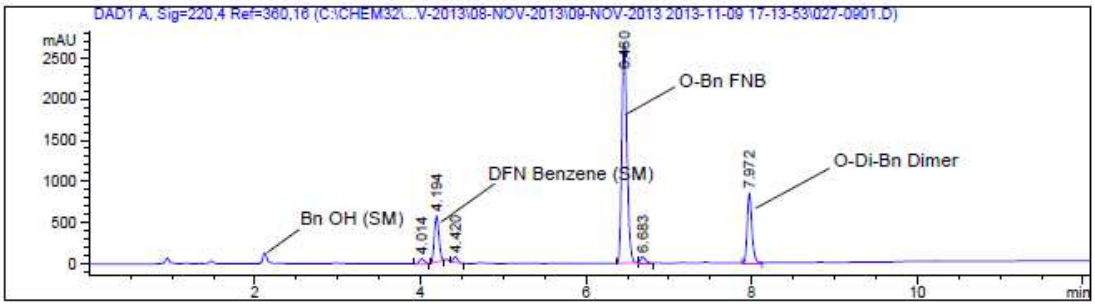
```
Data File C:\CHEM32\...CD2\NOV-2013\08-NOV-2013\09-NOV-2013 2013-11-09 17-13-53\028-1001.D
Sample Name: THF-O-Bn FNB

    ======================================================================
    Acq. Operator   : Sagar                          Seq. Line :  10
    Acq. Instrument : PRDB-LC-22                     Location : Vial 28
    Injection Date  : 09/11/2013 07:48:23 PM            Inj :   1
                                                    Inj Volume : 4 µl
    Acq. Method     : C:\Chem32\PRDB-LC-22\Data\2013-BCL2 CD2\Nov-2013\08-NOV-2013\09-NOV-2013
                      2013-11-09 17-13-53\ATLANTIST3_BCL-2_CD2_1.M
    Last changed    : 24/10/2013 02:27:28 PM by Sagar
    Analysis Method : C:\CHEM32\PRDB-LC-22\DATA\2013-BCL2 CD2\NOV-2013\08-NOV-2013\08-NOV-2013
                      2013-11-08 13-53-49\03-KPWL 686-084 RS 3.D\DA.M (ATLANTIST3_BCL-2_CD2_1.M)
    Last changed    : 24/10/2013 02:27:28 PM by Sagar
    Sample Info     : THF-O-Bn FNB
```




```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=220,4 Ref=360,16

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   4.196 MM R  0.0725  705.73828  162.22139   3.6201
       2   6.461 MM R  0.0789 1.39793e4  2952.57593  71.7071
       3   7.974 MM R  0.0656 4809.95508 1221.98132  24.6728

    Totals :                  1.94950e4  4336.77864


    ======================================================================
                            *** End of Report ***
```

Reaction profile in Acetonitrile (Method-A):

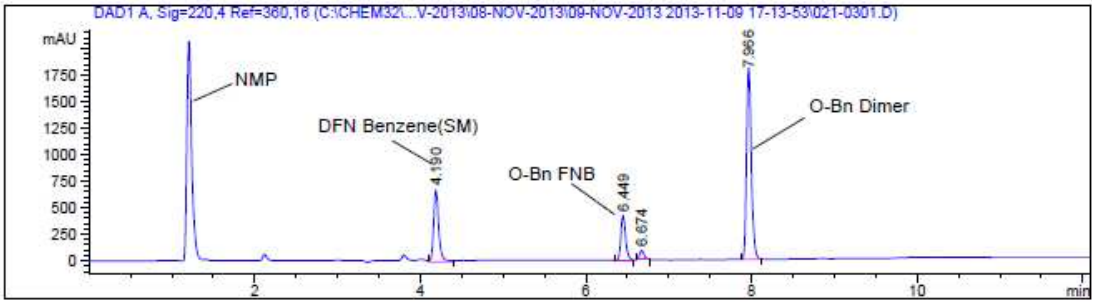
```
Data File C:\CHEM32\...CD2\NOV-2013\08-NOV-2013\09-NOV-2013 2013-11-09 17-13-53\027-0901.D
Sample Name: ACN-O-Bn FNB

    ======================================================================
    Acq. Operator   : Sagar                          Seq. Line :   9
    Acq. Instrument : PRDB-LC-22                     Location : Vial 27
    Injection Date  : 09/11/2013 07:32:13 PM            Inj :   1
                                                    Inj Volume : 4 µl
    Acq. Method     : C:\Chem32\PRDB-LC-22\Data\2013-BCL2 CD2\Nov-2013\08-NOV-2013\09-NOV-2013
                      2013-11-09 17-13-53\ATLANTIST3_BCL-2_CD2_1.M
    Last changed    : 24/10/2013 02:27:28 PM by Sagar
    Analysis Method : C:\CHEM32\PRDB-LC-22\DATA\2013-BCL2 CD2\NOV-2013\08-NOV-2013\08-NOV-2013
                      2013-11-08 13-53-49\03-KPWL 686-084 RS 3.D\DA.M (ATLANTIST3_BCL-2_CD2_1.M)
    Last changed    : 24/10/2013 02:27:28 PM by Sagar
    Sample Info     : ACN-O-Bn FNB
```




```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=220,4 Ref=360,16

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   4.014 MM R  0.0853  303.96866   67.92220   1.6847
       2   4.194 MM R  0.0632 2140.68433  564.59363  11.8642
       3   4.420 MM R  0.0577  241.56987   69.83508   1.3388
       4   6.460 MM R  0.0690 1.16515e4  2686.89062  64.5757
       5   6.683 MM R  0.0695  316.97665   76.02736   1.7568
       6   7.972 MM R  0.0660 3388.46362  855.09491  18.7798

    Totals :                  1.80432e4  4320.36379

    ======================================================================
                              *** End of Report ***
```

Reaction profile in *N*-Methyl Pyrrolidone (Method-A):

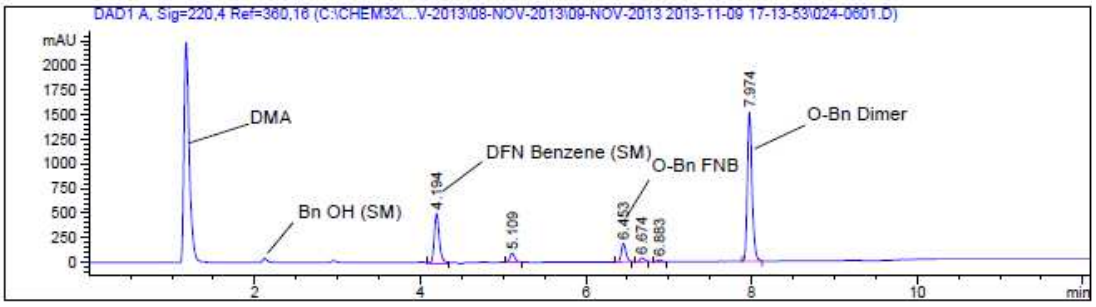
```
Data File C:\CHEM32\...CD2\NOV-2013\08-NOV-2013\09-NOV-2013 2013-11-09 17-13-53\021-0301.D
Sample Name: NMP-O-Bn FNB

    ======================================================================
    Acq. Operator   : Sagar                          Seq. Line :   3
    Acq. Instrument : PRDB-LC-22                      Location : Vial 21
    Injection Date  : 09/11/2013 05:55:23 PM             Inj :   1
                                                    Inj Volume : 4 µl
    Acq. Method     : C:\Chem32\PRDB-LC-22\Data\2013-BCL2 CD2\Nov-2013\08-NOV-2013\09-NOV-2013
                      2013-11-09 17-13-53\ATLANTIST3_BCL-2_CD2_1.M
    Last changed    : 24/10/2013 02:27:28 PM by Sagar
    Analysis Method : C:\CHEM32\PRDB-LC-22\DATA\2013-BCL2 CD2\NOV-2013\08-NOV-2013\08-NOV-2013
                      2013-11-08 13-53-49\03-KPWL 686-084 RS 3.D\DA.M (ATLANTIST3_BCL-2_CD2_1.M)
    Last changed    : 24/10/2013 02:27:28 PM by Sagar
    Sample Info     : NMP-O-Bn FNB
```




```
    ======================================================================
                               Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=220,4 Ref=360,16

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   4.190 VB    0.0645 2941.90527  679.59021  24.0067
       2   6.449 MM R  0.0674 1731.89343  428.30161  14.1327
       3   6.674 MM R  0.0647  340.59973   87.67644   2.7794
       4   7.966 MM R  0.0661 7240.13770 1825.56921  59.0813

    Totals :                  1.22545e4  3021.13747


    ======================================================================
                               *** End of Report ***
```

Reaction profile in Dimethyl acetamide (Method-A):

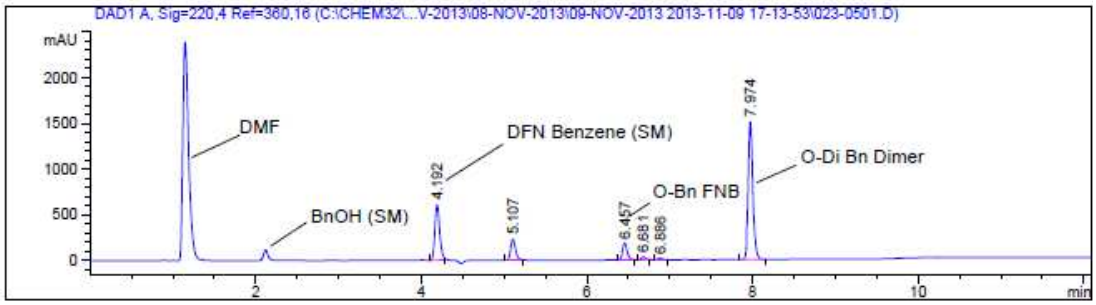
```
Data File C:\CHEM32\...CD2\NOV-2013\08-NOV-2013\09-NOV-2013 2013-11-09 17-13-53\024-0601.D
Sample Name: DMA-O-Bn FNB

    ======================================================================
    Acq. Operator   : Sagar                          Seq. Line :   6
    Acq. Instrument : PRDB-LC-22                     Location : Vial 24
    Injection Date  : 09/11/2013 06:43:46 PM              Inj :   1
                                                   Inj Volume : 4 µl
    Acq. Method     : C:\Chem32\PRDB-LC-22\Data\2013-BCL2 CD2\Nov-2013\08-NOV-2013\09-NOV-2013
                      2013-11-09 17-13-53\ATLANTIST3_BCL-2_CD2_1.M
    Last changed    : 24/10/2013 02:27:28 PM by Sagar
    Analysis Method : C:\CHEM32\PRDB-LC-22\DATA\2013-BCL2 CD2\NOV-2013\08-NOV-2013\08-NOV-2013
                      2013-11-08 13-53-49\03-KPWL 686-084 RS 3.D\DA.M (ATLANTIST3_BCL-2_CD2_1.M)
    Last changed    : 24/10/2013 02:27:28 PM by Sagar
    Sample Info     : DMA-O-Bn FNB
```




```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=220,4 Ref=360,16

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   4.194 MM R  0.0875 2118.56152  504.10254  22.4753
       2   5.109 MM R  0.0682  375.45181   91.77794   3.9831
       3   6.453 MM R  0.0641  716.72705  186.39850   7.6036
       4   6.674 MM R  0.0822  171.11533   40.04478   1.8153
       5   6.883 MM R  0.0707   88.92309   20.95343   0.9434
       6   7.974 MM R  0.0654 5955.41650 1517.01563  63.1794

    Totals :                  9426.19530 2360.29281

    ======================================================================
                              *** End of Report ***
```

Reaction profile in Dimethyl formamide (Method-A):

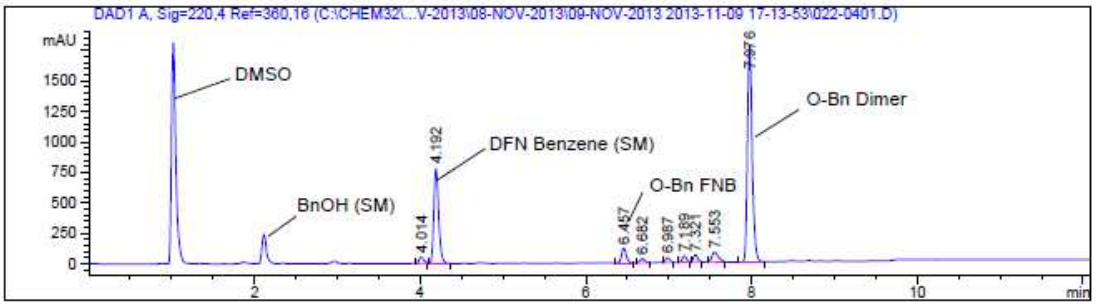
```
Data File C:\CHEM32\...CD2\NOV-2013\08-NOV-2013\09-NOV-2013 2013-11-09 17-13-53\023-0501.D
Sample Name: DMF-O-Bn FNB

    ======================================================================
    Acq. Operator   : Sagar                          Seq. Line :   5
    Acq. Instrument : PRDB-LC-22                     Location : Vial 23
    Injection Date  : 09/11/2013 06:27:38 PM            Inj :   1
                                                    Inj Volume : 4 µl
    Acq. Method     : C:\Chem32\PRDB-LC-22\Data\2013-BCL2 CD2\Nov-2013\08-NOV-2013\09-NOV-2013
                      2013-11-09 17-13-53\ATLANTIST3_BCL-2_CD2_1.M
    Last changed    : 24/10/2013 02:27:28 PM by Sagar
    Analysis Method : C:\CHEM32\PRDB-LC-22\DATA\2013-BCL2 CD2\NOV-2013\08-NOV-2013\08-NOV-2013
                      2013-11-08 13-53-49\03-KPWL 686-084 RS 3.D\DA.M (ATLANTIST3_BCL-2_CD2_1.M)
    Last changed    : 24/10/2013 02:27:28 PM by Sagar
    Sample Info     : DMF-O-Bn FNB
```




```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=220,4 Ref=360,16

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   4.192 MM R  0.0665 2437.58643  610.71094  23.7956
       2   5.107 MM R  0.0681  945.60681  231.28413   9.2309
       3   6.457 MM R  0.0654  734.38184  187.07715   7.1690
       4   6.681 MM R  0.0595  104.16990   29.17670   1.0169
       5   6.886 MM R  0.0642   71.40524   18.53735   0.6971
       6   7.974 MM R  0.0654 5950.72412 1517.27893  58.0906

    Totals :                  1.02439e4  2594.06520

    ======================================================================
                              *** End of Report ***
```

Reaction profile in Dimethyl sulfoxide (Method-A):

```
Data File C:\CHEM32\...CD2\NOV-2013\08-NOV-2013\09-NOV-2013 2013-11-09 17-13-53\022-0401.D
Sample Name: DMSO-O-Bn FNB

    ======================================================================
    Acq. Operator   : Sagar                          Seq. Line :   4
    Acq. Instrument : PRDB-LC-22                     Location : Vial 22
    Injection Date  : 09/11/2013 06:11:29 PM              Inj :   1
                                                   Inj Volume : 4 µl
    Acq. Method     : C:\Chem32\PRDB-LC-22\Data\2013-BCL2 CD2\Nov-2013\08-NOV-2013\09-NOV-2013
                      2013-11-09 17-13-53\ATLANTIST3_BCL-2_CD2_1.M
    Last changed    : 24/10/2013 02:27:28 PM by Sagar
    Analysis Method : C:\CHEM32\PRDB-LC-22\DATA\2013-BCL2 CD2\NOV-2013\08-NOV-2013\08-NOV-2013
                      2013-11-08 13-53-49\03-KPWL 686-084 RS 3.D\DA.M (ATLANTIST3_BCL-2_CD2_1.M)
    Last changed    : 24/10/2013 02:27:28 PM by Sagar
    Sample Info     : DMSO-O-Bn FNB
```

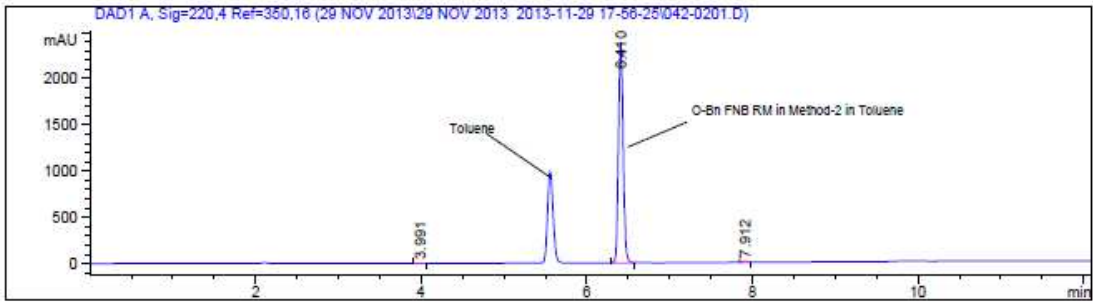



```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=220,4 Ref=360,16

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   4.014 MM R  0.0619  207.81573   55.95644   1.7161
       2   4.192 MM R  0.0677 3183.22070  783.87292  26.2857
       3   6.457 MM R  0.0669  497.26263  123.84898   4.1062
       4   6.682 MM R  0.0672  134.27525   33.32367   1.1088
       5   6.987 MM R  0.0600  139.71515   38.83951   1.1537
       6   7.189 MM R  0.0568  172.15765   50.49361   1.4216
       7   7.321 MM R  0.0571  193.32916   56.43207   1.5964
       8   7.553 MM R  0.0901  429.51593   79.47179   3.5468
       9   7.976 MM R  0.0663 7152.79395 1798.88318  59.0648

    Totals :                  1.21101e4  3021.12217
```

3. Solvent Screening in Method-B

Reaction profile in Toluene at 0 °C(Method-B):

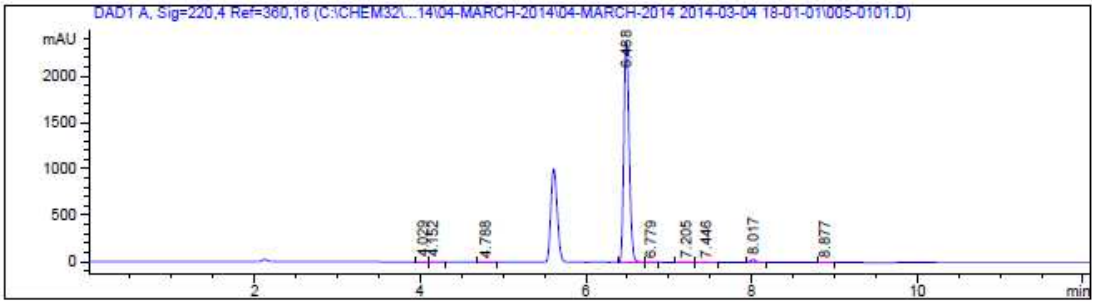
```
Data File C:\CHEM32\2\DATA\29 NOV 2013\29 NOV 2013  2013-11-29 17-56-25\042-0201.D
Sample Name: M2-Toluene-O-Bn FNB

    ======================================================================
    Acq. Operator   : Sagar                          Seq. Line :   2
    Acq. Instrument : PRDB-LC-23                      Location : Vial 42
    Injection Date  : 29/11/2013 06:31:15 PM             Inj :   1
                                                    Inj Volume : 4 µl
    Acq. Method     : C:\Chem32\2\DATA\29 NOV 2013\29 NOV 2013  2013-11-29 17-56-25\SURESH_
                      SCIENCE_METHOD.M
    Last changed    : 29/11/2013 05:56:19 PM by Sagar
    Analysis Method : C:\CHEM32\2\METHODS\SCIENCE.M
    Last changed    : 30/11/2013 01:34:36 PM by Sagar
                      (modified after loading)
    Sample Info     : M2-Toluene-O-Bn FNB
```




```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=220,4 Ref=350,16

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   3.991 MM R  0.0657   11.67699    2.96273   0.1229
       2   6.410 MM R  0.0657 9442.83887 2394.63525  99.3823
       3   7.912 MM R  0.0608   47.01827   12.89701   0.4948

    Totals :                  9501.53413 2410.49500

    ======================================================================
                              *** End of Report ***
```

Reaction profile in Toluene at 22 °C(Method-B):

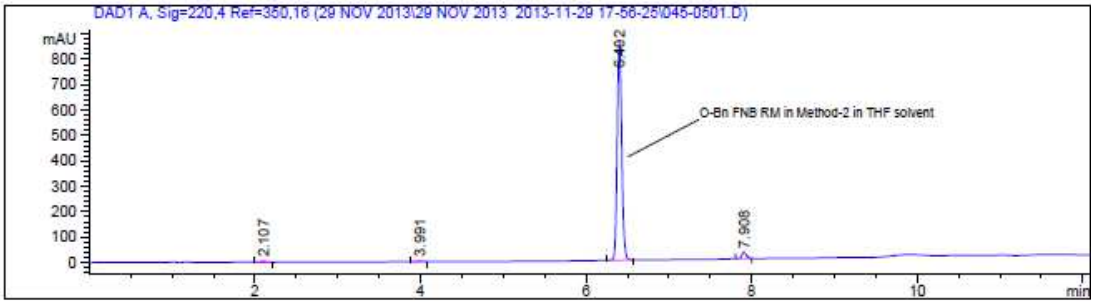
```
Data File C:\CHEM32\...RCH-2014\04-MARCH-2014\04-MARCH-2014 2014-03-04 18-01-01\005-0101.D
Sample Name: O-Bn FNB RM-Method-2

    ======================================================================
    Acq. Operator   : Purushottam                    Seq. Line :   1
    Acq. Instrument : PRDB-LC-22                     Location : Vial 5
    Injection Date  : 04/03/2014 06:04:18 PM            Inj :   1
                                                   Inj Volume : 4 µl
    Acq. Method     : C:\Chem32\PRDB-LC-22\Data\2014-BCL2BU\March-2014\04-MARCH-2014\04-MARCH-
                      2014 2014-03-04 18-01-01\ATLANTIST3_BCL-2_CD2_BINARY.M
    Last changed    : 20/01/2014 03:19:21 PM by Suresh
    Analysis Method : C:\CHEM32\1\METHODS\ATLANTIST3_BCL-2_CD2_BINARY.M
    Last changed    : 20/01/2014 03:19:21 PM by Suresh
    Sample Info     : O-Bn FNB RM
                      Method-2 at 22 deg C
```




```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=220,4 Ref=360,16

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   4.029 BV    0.0663   14.40367    3.34203   0.1330
       2   4.152 VB    0.0698   11.42721    2.38980   0.1055
       3   4.788 BB    0.0702    9.44655    2.03309   0.0872
       4   6.488 VV    0.0698 1.05818e4  2384.91821  97.7056
       5   6.779 VV    0.0706   14.12796    2.91072   0.1304
       6   7.205 BV    0.0899   32.58521    5.14250   0.3009
       7   7.446 VB    0.0869   14.49213    2.38320   0.1338
       8   8.017 BB    0.0644  136.49785   32.89495   1.2603
       9   8.877 BB    0.0636   15.50638    3.80455   0.1432

    Totals :                  1.08303e4  2439.81904
```

Reaction profile in Tetrahydrofuran at 0 °C (Method-B):

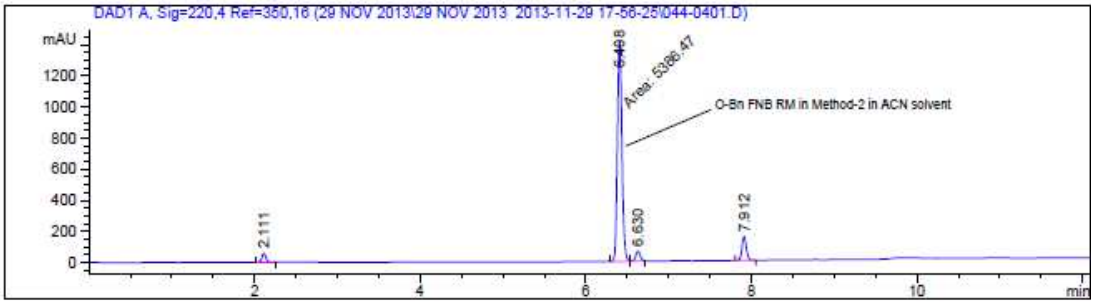
```
Data File C:\CHEM32\2\DATA\29 NOV 2013\29 NOV 2013  2013-11-29 17-56-25\045-0501.D
Sample Name: M-2-THF-O-Bn FNB

    ======================================================================
    Acq. Operator   : Sagar                          Seq. Line :   5
    Acq. Instrument : PRDB-LC-23                     Location : Vial 45
    Injection Date  : 29/11/2013 07:19:57 PM            Inj :   1
                                                    Inj Volume : 4 µl
    Acq. Method     : C:\Chem32\2\DATA\29 NOV 2013\29 NOV 2013  2013-11-29 17-56-25\SURESH_
                      SCIENCE_METHOD.M
    Last changed    : 29/11/2013 05:56:19 PM by Sagar
    Analysis Method : C:\CHEM32\2\METHODS\SCIENCE.M
    Last changed    : 30/11/2013 01:34:36 PM by Sagar
                      (modified after loading)
    Sample Info     : M-2-THF-O-Bn FNB
```




```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=220,4 Ref=350,16

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   2.107 MM R  0.0842   19.26171    3.81164   0.5652
       2   3.991 MM R  0.0735   14.99372    3.40122   0.4400
       3   6.402 MM R  0.0629 3277.57739  868.05334  96.1810
       4   7.908 MM R  0.0610   95.88615   26.20187   2.8138

    Totals :                  3407.71898  901.46807


    ======================================================================
                            *** End of Report ***
```

Reaction profile in Acetonitrile at 0 °C (Method-B):

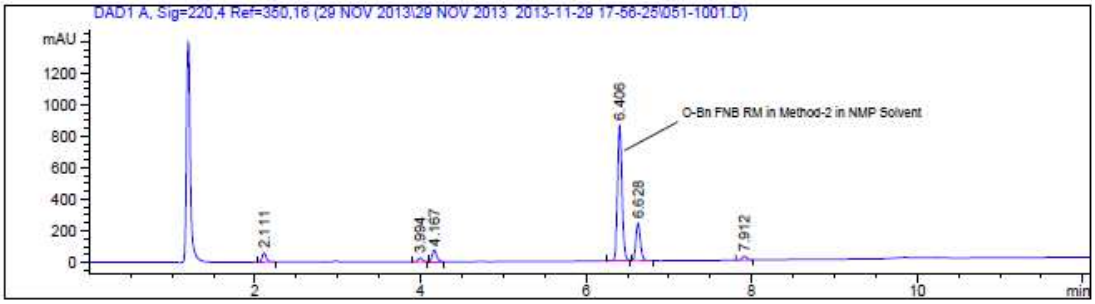
```
Data File C:\CHEM32\2\DATA\29 NOV 2013\29 NOV 2013  2013-11-29 17-56-25\044-0401.D
Sample Name: M-2-ACN-O-Bn FNB

    ======================================================================
    Acq. Operator   : Sagar                          Seq. Line :   4
    Acq. Instrument : PRDB-LC-23                     Location : Vial 44
    Injection Date  : 29/11/2013 07:03:43 PM            Inj :   1
                                                    Inj Volume : 4 µl
    Acq. Method     : C:\Chem32\2\DATA\29 NOV 2013\29 NOV 2013  2013-11-29 17-56-25\SURESH_
                      SCIENCE_METHOD.M
    Last changed    : 29/11/2013 05:56:19 PM by Sagar
    Analysis Method : C:\CHEM32\2\METHODS\SCIENCE.M
    Last changed    : 30/11/2013 01:34:36 PM by Sagar
                      (modified after loading)
    Sample Info     : M-2-ACN-O-Bn FNB
```




```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=220,4 Ref=350,16

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   2.111 MM R  0.0598  210.78899   58.72299   3.2889
       2   6.408 MF    0.0630 5386.46826 1425.44666  84.0451
       3   6.630 FM R  0.0625  243.11568   64.87424   3.7933
       4   7.912 MM R  0.0613  568.65143  154.64748   8.8727

    Totals :                  6409.02435 1703.69137


    ======================================================================
                              *** End of Report ***
```

Reaction profile in *N*-Methyl pyrrolidone at 0 °C (Method-B):

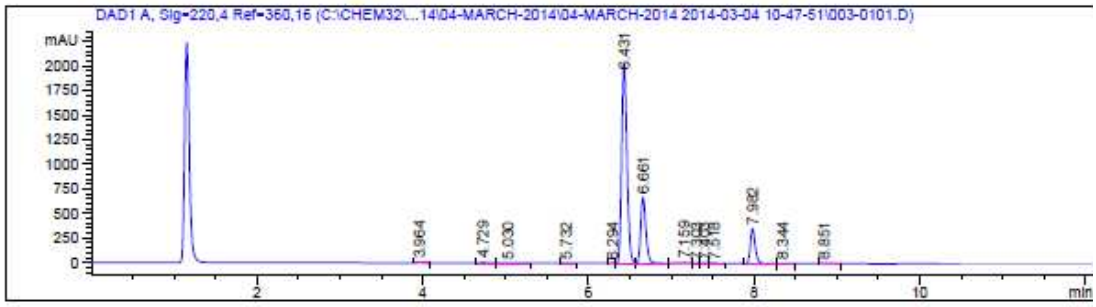
```
Data File C:\CHEM32\2\DATA\29 NOV 2013\29 NOV 2013  2013-11-29 17-56-25\051-1001.D
Sample Name: M-2-NMP-O-Bn FNB

    ======================================================================
    Acq. Operator   : Sagar                          Seq. Line :  10
    Acq. Instrument : PRDB-LC-23                      Location : Vial 51
    Injection Date  : 29/11/2013 08:41:05 PM             Inj :   1
                                                     Inj Volume : 4 µl
    Acq. Method     : C:\Chem32\2\DATA\29 NOV 2013\29 NOV 2013  2013-11-29 17-56-25\SURESH_
                      SCIENCE_METHOD.M
    Last changed    : 29/11/2013 05:56:19 PM by Sagar
    Analysis Method : C:\CHEM32\2\METHODS\SCIENCE.M
    Last changed    : 30/11/2013 01:34:36 PM by Sagar
                      (modified after loading)
    Sample Info     : M-2-NMP-O-Bn FNB
```




```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=220,4 Ref=350,16

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   2.111 MM R  0.0574  203.87834   59.23055   4.2272
       2   3.994 MM R  0.0793   95.29228   24.52273   1.9758
       3   4.167 MM R  0.0630  280.31244   74.16983   5.8120
       4   6.406 MM R  0.0629 3262.67529  864.74438  67.6485
       5   6.628 MM R  0.0618  884.71045  238.42064  18.3436
       6   7.912 MM R  0.0657   96.11639   24.36506   1.9929

    Totals :                  4822.98520 1285.45320

    ======================================================================
                              *** End of Report ***
```

Reaction profile in Dimethyl acetamide at 0 °C (Method-B):

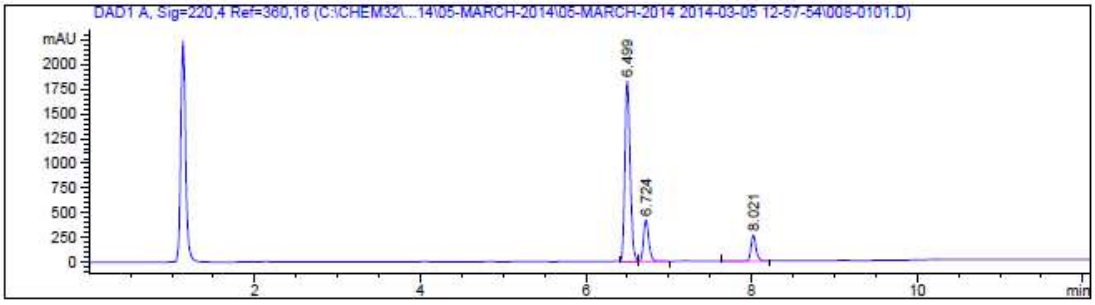
```
Data File C:\CHEM32\...RCH-2014\04-MARCH-2014\04-MARCH-2014 2014-03-04 10-47-51\003-0101.D
Sample Name: O-Bn FNB Isomer

======================================================================
Acq. Operator    : Purushottam                    Seq. Line :   1
Acq. Instrument  : PRDB-LC-22                      Location : Vial 3
Injection Date   : 04/03/2014 10:51:11 AM             Inj :   1
                                                  Inj Volume : 4 µl
Acq. Method      : C:\Chem32\PRDB-LC-22\Data\2014-BCL2BU\March-2014\04-MARCH-2014\04-MARCH-
                   2014 2014-03-04 10-47-51\ATLANTIST3_BCL-2_CD2_BINARY.M
Last changed     : 20/01/2014 03:19:21 PM by Suresh
Analysis Method  : C:\CHEM32\1\METHODS\ATLANTIST3_BCL-2_CD2_BINARY.M
Last changed     : 20/01/2014 03:19:21 PM by Suresh
Sample Info      : O-Bn FNB Isomer
                   DMA solvent-Method-2
```




```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=220,4 Ref=360,16

Peak RetTime Type  Width     Area      Height     Area
  #   [min]      [min]    [mAU*s]     [mAU]        %
----|-------|----|-------|----------|----------|--------|
   1   3.964 BB    0.0661   11.71194    2.72997   0.0872
   2   4.729 BB    0.0755   24.97823    5.07076   0.1859
   3   5.030 BB    0.1256   10.69203    1.18086   0.0796
   4   5.732 BB    0.0671    5.16181    1.17906   0.0384
   5   6.294 BV    0.0592    5.79711    1.56653   0.0432
   6   6.431 VV    0.0672 8908.22070 2031.69983  66.3096
   7   6.661 VB    0.0663 2897.64844  671.86694  21.5690
   8   7.159 BV    0.0967   51.41387    7.25398   0.3827
   9   7.303 VV    0.0641    9.58623    2.23368   0.0714
  10   7.403 VV    0.0680   16.14429    3.62358   0.1202
  11   7.518 VV    0.0663   18.22129    4.22370   0.1356
  12   7.982 VB    0.0616 1443.82117  354.03098  10.7473
  13   8.344 BV    0.0759    7.73105    1.50693   0.0575
  14   8.851 VB    0.0640   23.16448    5.63211   0.1724

Totals :                  1.34343e4  3093.79891
```

Reaction profile in Dimethyl acetamide at 22 °C (Method-B):

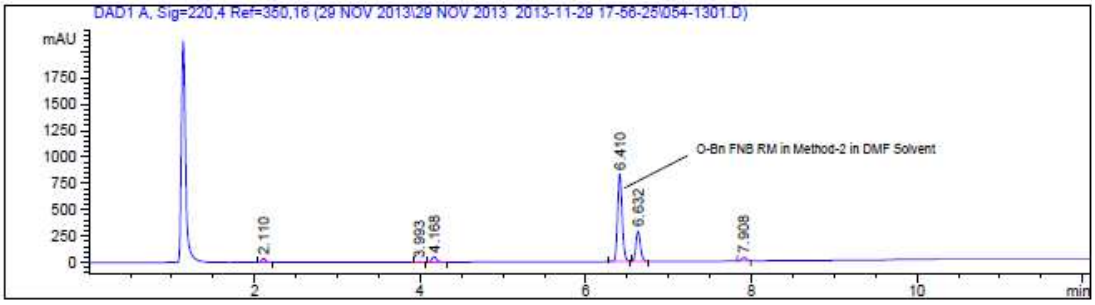
```
Data File C:\CHEM32\...RCH-2014\05-MARCH-2014\05-MARCH-2014 2014-03-05 12-57-54\008-0101.D
Sample Name: O-Bn FNB RM-Method-2

    ======================================================================
    Acq. Operator   : Suresh                          Seq. Line :   1
    Acq. Instrument : PRDB-LC-22                       Location : Vial 8
    Injection Date  : 05/03/2014 01:01:13 PM              Inj :   1
                                                     Inj Volume : 4 µl
    Acq. Method     : C:\Chem32\PRDB-LC-22\Data\2014-BCL2BU\March-2014\05-MARCH-2014\05-MARCH-
                      2014 2014-03-05 12-57-54\ATLANTIST3_BCL-2_CD2_BINARY.M
    Last changed    : 20/01/2014 03:19:21 PM by Suresh
    Analysis Method : C:\CHEM32\1\METHODS\ATLANTIST3_BCL-2_CD2_BINARY.M
    Last changed    : 20/01/2014 03:19:21 PM by Suresh
    Sample Info     : O-Bn FNB RM in DMA
                      Method-2 at 22 deg C
```




```
    ======================================================================
                               Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=220,4 Ref=360,16

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   6.499 VV    0.0676 8062.13721 1822.74524  73.2276
       2   6.724 VV    0.0675 1849.35266  419.25974  16.7975
       3   8.021 VB    0.0648 1098.21265  262.48175   9.9750

    Totals :                  1.10097e4  2504.48672

    ======================================================================
                               *** End of Report ***
```

Reaction profile in Dimethyl formamide at 0 °C (Method-B):

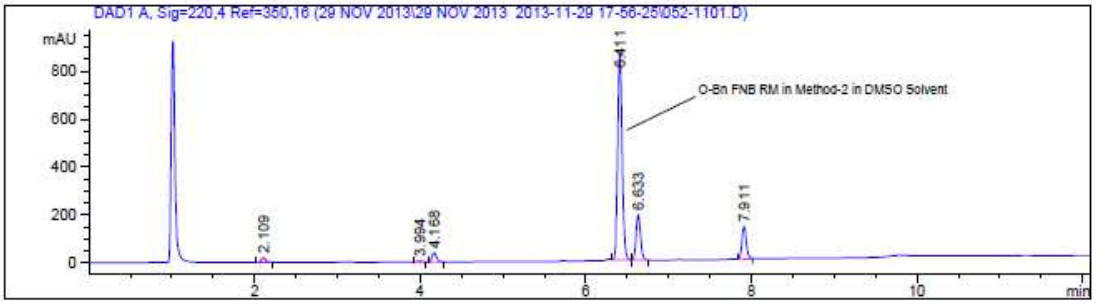
```
Data File C:\CHEM32\2\DATA\29 NOV 2013\29 NOV 2013  2013-11-29 17-56-25\054-1301.D
Sample Name: M-2-DMF-O-Bn FNB

    ======================================================================
    Acq. Operator   : Sagar                          Seq. Line :  13
    Acq. Instrument : PRDB-LC-23                     Location : Vial 54
    Injection Date  : 29/11/2013 09:29:34 PM              Inj :  1
                                                    Inj Volume : 4 µl
    Acq. Method     : C:\Chem32\2\DATA\29 NOV 2013\29 NOV 2013  2013-11-29 17-56-25\SURESH_
                      SCIENCE_METHOD.M
    Last changed    : 29/11/2013 05:56:19 PM by Sagar
    Analysis Method : C:\CHEM32\2\METHODS\SCIENCE.M
    Last changed    : 30/11/2013 01:34:36 PM by Sagar
                      (modified after loading)
    Sample Info     : M-2-DMF-O-Bn FNB
```




```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=220,4 Ref=350,16

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   2.110 MM R  0.0564  120.79497   35.67378   2.5600
       2   3.993 MM R  0.0746    8.98819    2.00817   0.1905
       3   4.168 MM R  0.0650  205.95616   52.77039   4.3648
       4   6.410 MM R  0.0633 3154.95947  831.34491  66.8627
       5   6.632 MM R  0.0631 1097.12854  289.66092  23.2513
       6   7.908 MM R  0.0634  130.73755   34.39297   2.7707

    Totals :                  4718.56488 1245.85114

    ======================================================================
                              *** End of Report ***
```

Reaction profile in Dimethyl sulfoxide at 22 °C (Method-B):

```
Data File C:\CHEM32\2\DATA\29 NOV 2013\29 NOV 2013  2013-11-29 17-56-25\052-1101.D
Sample Name: M-2-DMSO-O-Bn FNB

    ======================================================================
    Acq. Operator   : Sagar                          Seq. Line :  11
    Acq. Instrument : PRDB-LC-23                      Location : Vial 52
    Injection Date  : 29/11/2013 08:57:14 PM             Inj :  1
                                                     Inj Volume : 4 µl
    Acq. Method     : C:\Chem32\2\DATA\29 NOV 2013\29 NOV 2013  2013-11-29 17-56-25\SURESH_
                      SCIENCE_METHOD.M
    Last changed    : 29/11/2013 05:56:19 PM by Sagar
    Analysis Method : C:\CHEM32\2\METHODS\SCIENCE.M
    Last changed    : 30/11/2013 01:34:36 PM by Sagar
                      (modified after loading)
    Sample Info     : M-2-DMSO-O-Bn FNB
```

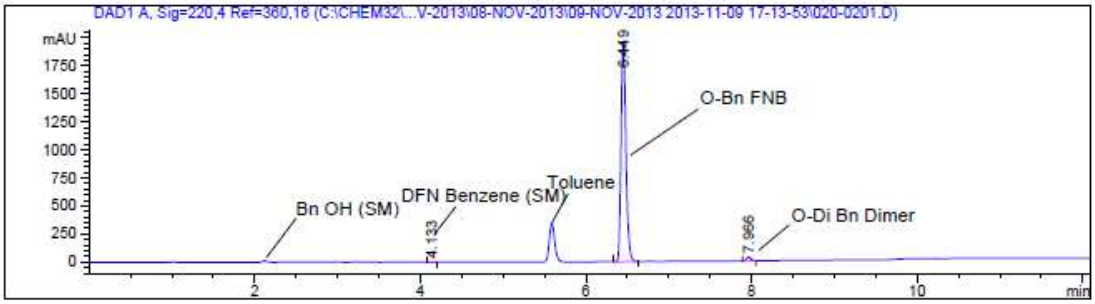



```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=220,4 Ref=350,16

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]    [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   2.109 MM R  0.0618   76.99293   20.77941   1.6358
       2   3.994 MM R  0.0653   18.22349    4.65188   0.3872
       3   4.168 MM R  0.0643  147.30528   38.18768   3.1296
       4   6.411 MM R  0.0548 3249.83203  869.54395  69.0449
       5   6.633 MM R  0.0618  711.13989  191.80905  15.1087
       6   7.911 MM R  0.0608  503.84494  137.95410  10.6939

    Totals :                  4706.83857 1262.92607


    ======================================================================
                              *** End of Report ***
```

4. Role of potassium ion (HPLC Chromatograms)

Reaction profile KO*t*Bu without 18-crown-6 (Method-A)

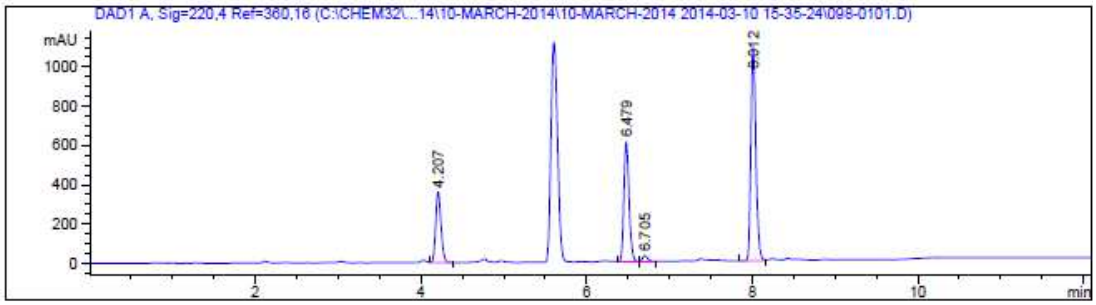
```
Data File C:\CHEM32\...CD2\NOV-2013\08-NOV-2013\09-NOV-2013 2013-11-09 17-13-53\020-0201.D
Sample Name: Toluene-O-Bn FNB

    ======================================================================
    Acq. Operator   : Sagar                          Seq. Line :   2
    Acq. Instrument : PRDB-LC-22                     Location : Vial 20
    Injection Date  : 09/11/2013 05:39:12 PM            Inj :   1
                                                    Inj Volume : 4 µl
    Acq. Method     : C:\Chem32\PRDB-LC-22\Data\2013-BCL2 CD2\Nov-2013\08-NOV-2013\09-NOV-2013
                      2013-11-09 17-13-53\ATLANTIST3_BCL-2_CD2_1.M
    Last changed    : 24/10/2013 02:27:28 PM by Sagar
    Analysis Method : C:\CHEM32\PRDB-LC-22\DATA\2013-BCL2 CD2\NOV-2013\08-NOV-2013\08-NOV-2013
                      2013-11-08 13-53-49\03-KPWL 686-084 RS 3.D\DA.M (ATLANTIST3_BCL-2_CD2_1.M)
    Last changed    : 24/10/2013 02:27:28 PM by Sagar
    Sample Info     : Toluene-O-Bn FNB
```




```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=220,4 Ref=360,16

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   4.133 MM R  0.0673    6.87718    1.70186   0.0840
       2   6.449 MM R  0.0625 8040.75586 1965.88416  98.2355
       3   7.966 MM R  0.0638  137.55057   35.96042   1.6805

    Totals :                  8185.18361 2003.53644

    ======================================================================
                              *** End of Report ***
```

Reaction profile KO*t*Bu with 18-crown-6 (Method-A)

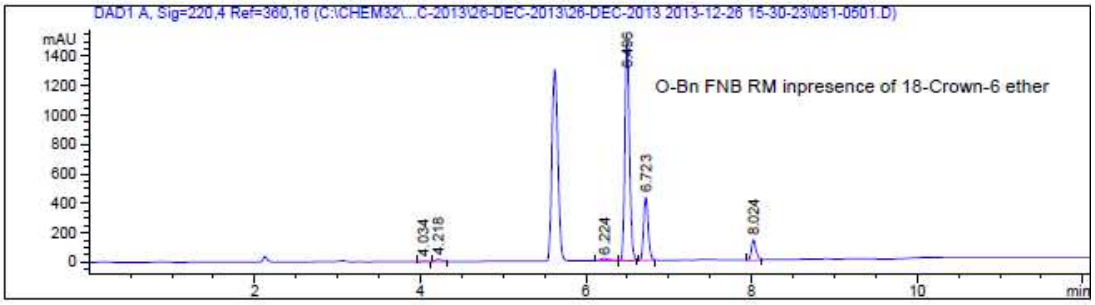
```
Data File C:\CHEM32\...RCH-2014\10-MARCH-2014\10-MARCH-2014 2014-03-10 15-35-24\098-0101.D
Sample Name: O-Bn FNB (18-Crown-6)

    ======================================================================
    Acq. Operator   : Suresh                          Seq. Line :   1
    Acq. Instrument : PRDB-LC-22                        Location : Vial 98
    Injection Date  : 10/03/2014 03:38:42 PM              Inj :   1
                                                      Inj Volume : 4 µl
    Acq. Method     : C:\Chem32\PRDB-LC-22\Data\2014-BCL2BU\March-2014\10-MARCH-2014\10-MARCH-
                      2014 2014-03-10 15-35-24\ATLANTIST3_BCL-2_CD2_BINARY.M
    Last changed    : 20/01/2014 03:19:21 PM by Suresh
    Analysis Method : C:\CHEM32\1\METHODS\ATLANTIST3_BCL-2_CD2_BINARY.M
    Last changed    : 20/01/2014 03:19:21 PM by Suresh
    Sample Info     : O-Bn FNB (18-Crown-6) KOtBu
                      Method-1, Toluene
```




```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=220,4 Ref=360,16

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   4.207 VV    0.0700 1608.14917  360.59845  17.9090
       2   6.479 VV    0.0665 2654.32446  612.60583  29.5597
       3   6.705 VV    0.0696  146.89816   31.99645   1.6359
       4   8.012 BV    0.0648 4570.16211 1092.51453  50.8953

    Totals :                   8979.53391 2097.71526


    ======================================================================
                              *** End of Report ***
```

Reaction profile KO*t*Bu with 18-crown-6 (Method-B)

```
Data File C:\CHEM32\...CD2\DEC-2013\26-DEC-2013\26-DEC-2013 2013-12-26 15-30-23\081-0501.D
Sample Name: O-Bn FNB + 18-Crown-6

    ======================================================================
    Acq. Operator    : Suresh                          Seq. Line :   5
    Acq. Instrument  : PRDB-LC-22                       Location : Vial 81
    Injection Date   : 26/12/2013 04:37:54 PM             Inj :   1
                                                      Inj Volume : 4 µl
    Acq. Method      : C:\Chem32\PRDB-LC-22\Data\2013-BCL2 CD2\Dec-2013\26-DEC-2013\26-DEC-2013
                       2013-12-26 15-30-23\ATLANTIST3_BCL-2_CD2_BINARY.M
    Last changed     : 17/12/2013 02:17:22 PM by Suresh
    Analysis Method  : C:\CHEM32\1\METHODS\ATLANTIST3_BCL-2_CD2_1.M
    Last changed     : 27/12/2013 02:36:00 PM by Suresh
                       (modified after loading)
    Sample Info      : O-Bn FNB + 18-Crown-6
                       Method-2
```

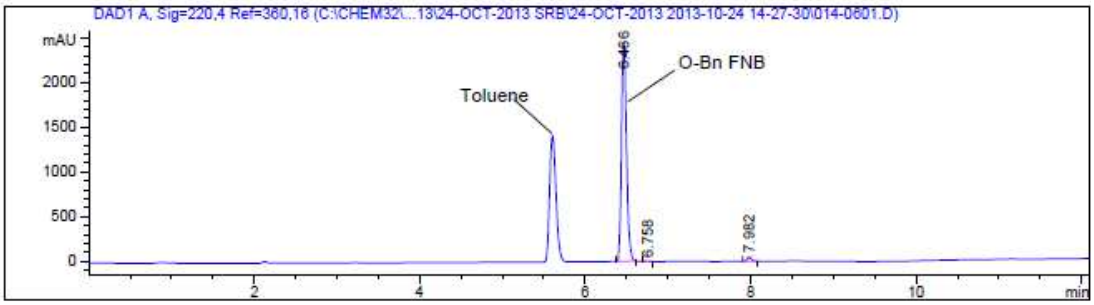



```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=220,4 Ref=360,16

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   4.034 MM R  0.0802   25.49193    5.30070   0.3139
       2   4.218 MM R  0.0679   63.87980   15.67214   0.7867
       3   6.224 MM R  0.1144  108.60382   15.81946   1.3375
       4   6.496 MM R  0.0641 5742.53711 1493.81177  70.7209
       5   6.723 MM R  0.0634 1642.51746  431.95059  20.2281
       6   8.024 MM R  0.0646  536.96643  138.58374   6.6129

    Totals :                  8119.99655 2101.13840

    ======================================================================
```

5. Reaction profile for O, S, *N* -nucelophiles (HPLC Chromatograms)

3a-Reaction profile (Method-A)

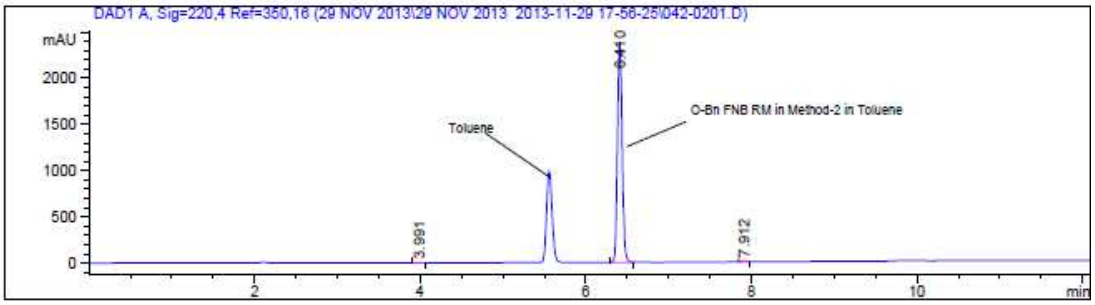
```
Data File C:\CHEM32\...OCT-2013\24-OCT-2013 SRB\24-OCT-2013 2013-10-24 14-27-30\014-0601.D
Sample Name: O-Bn FNB RM

=====================================================================
Acq. Operator   : Sagar                          Seq. Line :   6
Acq. Instrument : PRDB-LC-22                     Location : Vial 14
Injection Date  : 24/10/2013 03:58:13 PM             Inj :   1
                                                 Inj Volume : 4 µl
Acq. Method     : C:\Chem32\PRDB-LC-22\Data\2013-BCL2 CD2\Oct-2013\24-OCT-2013 SRB\24-OCT-
                  2013 2013-10-24 14-27-30\ATLANTIST3_BCL-2_CD2_1.M
Last changed    : 24/10/2013 02:27:28 PM by Sagar
Analysis Method : C:\CHEM32\1\METHODS\BCL-2 WASH.M
Last changed    : 25/10/2013 01:35:10 PM by Sagar
                  (modified after loading)
Sample Info     : O-Bn FNB RM
```




```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=220,4 Ref=360,16

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.466 MM R  0.0696 1.02821e4  2463.32935  98.0933
   2   6.758 MM R  0.0693   10.73059    2.58043   0.1024
   3   7.982 MM R  0.0641  189.12881   49.15940   1.8043

Totals :                  1.04820e4  2515.06918

=====================================================================
                        *** End of Report ***
```

3a-Reaction profile (Method-B)

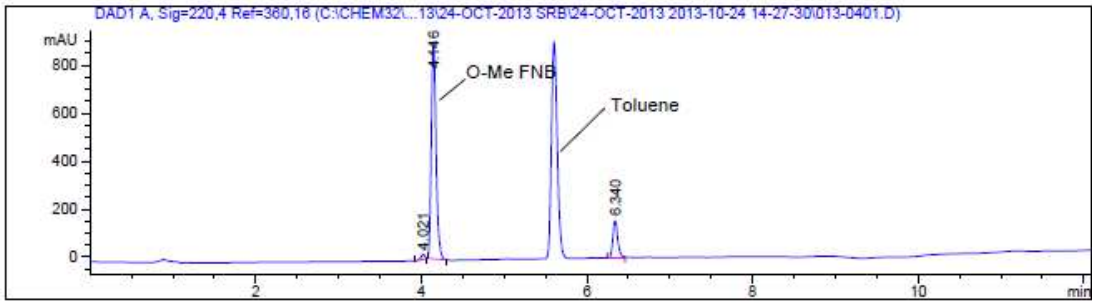
```
Data File C:\CHEM32\2\DATA\29 NOV 2013\29 NOV 2013  2013-11-29 17-56-25\042-0201.D
Sample Name: M2-Toluene-O-Bn FNB

    ======================================================================
    Acq. Operator   : Sagar                          Seq. Line :   2
    Acq. Instrument : PRDB-LC-23                      Location : Vial 42
    Injection Date  : 29/11/2013 06:31:16 PM             Inj :   1
                                                    Inj Volume : 4 µl
    Acq. Method     : C:\Chem32\2\DATA\29 NOV 2013\29 NOV 2013  2013-11-29 17-56-25\SURESH_
                      SCIENCE_METHOD.M
    Last changed    : 29/11/2013 05:56:19 PM by Sagar
    Analysis Method : C:\CHEM32\2\METHODS\SCIENCE.M
    Last changed    : 30/11/2013 01:34:36 PM by Sagar
                      (modified after loading)
    Sample Info     : M2-Toluene-O-Bn FNB
```




```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=220,4 Ref=350,16

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   3.991 MM R  0.0657   11.67699    2.96273   0.1229
       2   6.410 MM R  0.0657 9442.83887 2394.63525  99.3823
       3   7.912 MM R  0.0608   47.01827   12.89701   0.4948

    Totals :                  9501.53413 2410.49500

    ======================================================================
                              *** End of Report ***
```

4a-Reaction profile (Method-A)

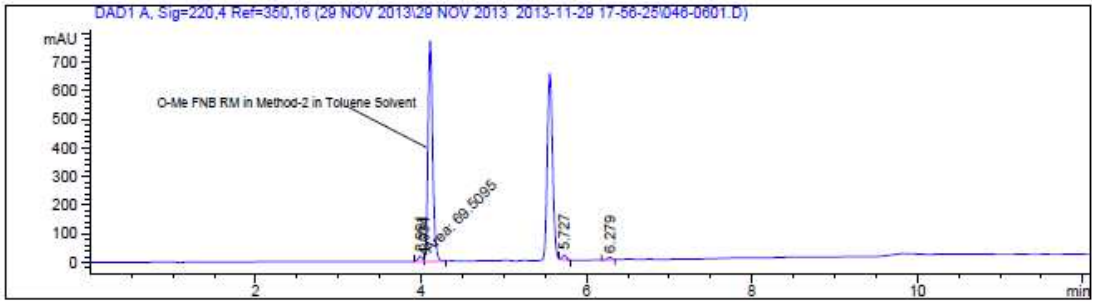
```
Data File C:\CHEM32\...OCT-2013\24-OCT-2013 SRB\24-OCT-2013 2013-10-24 14-27-30\013-0401.D
Sample Name: O-Me FNB RM

    ======================================================================
    Acq. Operator   : Sagar                          Seq. Line :   4
    Acq. Instrument : PRDB-LC-22                     Location : Vial 13
    Injection Date  : 24/10/2013 03:26:02 PM            Inj :   1
                                                    Inj Volume : 4 µl
    Acq. Method     : C:\Chem32\PRDB-LC-22\Data\2013-BCL2 CD2\Oct-2013\24-OCT-2013 SRB\24-OCT-
                      2013 2013-10-24 14-27-30\ATLANTIST3_BCL-2_CD2_1.M
    Last changed    : 24/10/2013 02:27:28 PM by Sagar
    Analysis Method : C:\CHEM32\1\METHODS\BCL-2 WASH.M
    Last changed    : 25/10/2013 01:35:10 PM by Sagar
                      (modified after loading)
    Sample Info     : O-Me FNB RM
```




```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=220,4 Ref=360,16

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   4.021 MM R  0.0761   69.34348   20.18332   1.6122
       2   4.146 MM R  0.0484 3578.04321  909.26440  83.1877
       3   6.340 MM R  0.0695  653.78113  156.85577  15.2001

    Totals :                  4301.16782 1086.30350


    ======================================================================
                              *** End of Report ***
```

4a-Reaction profile (Method-B)

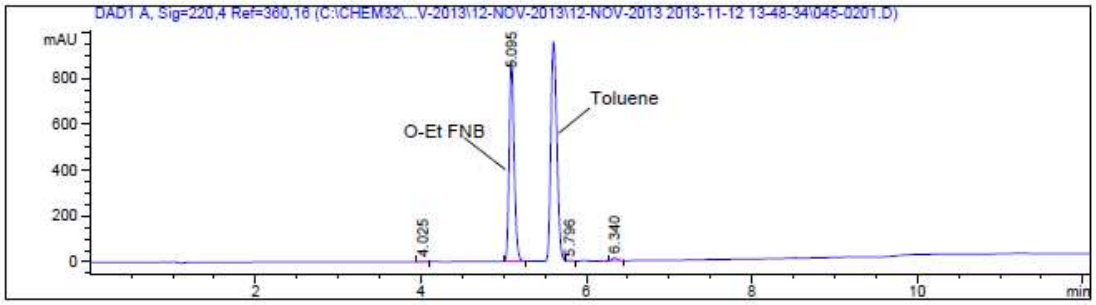
```
Data File C:\CHEM32\2\DATA\29 NOV 2013\29 NOV 2013  2013-11-29 17-56-25\046-0601.D
Sample Name: M-2-Toluene-O-Me FNB

    ========================================================================
    Acq. Operator    : Sagar                          Seq. Line :   6
    Acq. Instrument  : PRDB-LC-23                      Location : Vial 46
    Injection Date   : 29/11/2013 07:36:13 PM             Inj :   1
                                                     Inj Volume : 4 µl
    Acq. Method      : C:\Chem32\2\DATA\29 NOV 2013\29 NOV 2013  2013-11-29 17-56-25\SURESH_
                       SCIENCE_METHOD.M
    Last changed     : 29/11/2013 05:56:19 PM by Sagar
    Analysis Method  : C:\CHEM32\2\METHODS\SCIENCE.M
    Last changed     : 30/11/2013 01:34:36 PM by Sagar
                       (modified after loading)
    Sample Info      : M-2-Toluene-O-Me FNB
```




```
    ========================================================================
                              Area Percent Report
    ========================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=220,4 Ref=350,16

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   3.991 MF T  0.0637   69.50954   18.18840   2.1830
       2   4.034 FM R 3.61e-3 3022.34277    9.03829  94.9200
       3   5.727 MM R  0.0582   58.97605   16.89148   1.8522
       4   6.279 MM R  0.0646   33.26682    8.58670   1.0448

    Totals :                  3184.09518   52.70487


    ========================================================================
                              *** End of Report ***
```

5a-Reaction profile (Method-A)

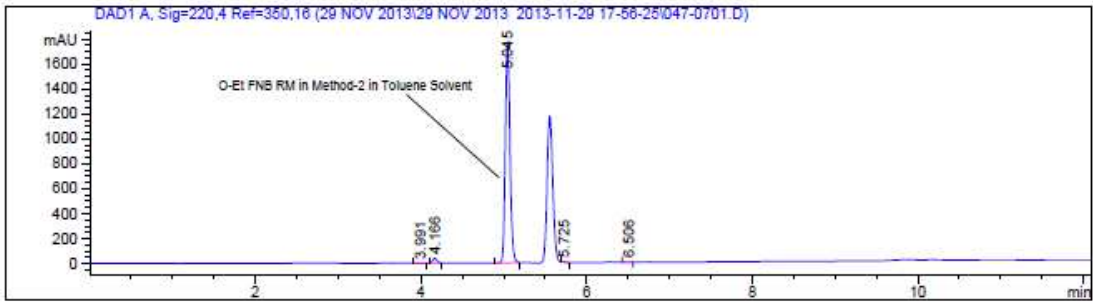
```
Data File C:\CHEM32\...CD2\NOV-2013\12-NOV-2013\12-NOV-2013 2013-11-12 13-48-34\045-0201.D
Sample Name: O-Et FNB RM

    ========================================================================
    Acq. Operator   : Suresh                          Seq. Line :   2
    Acq. Instrument : PRDB-LC-22                       Location : Vial 45
    Injection Date  : 12/11/2013 02:14:02 PM              Inj :   1
                                                     Inj Volume : 4 µl
    Acq. Method     : C:\Chem32\PRDB-LC-22\Data\2013-BCL2 CD2\Nov-2013\12-NOV-2013\12-NOV-2013
                      2013-11-12 13-48-34\ATLANTIST3_BCL-2_CD2_1.M
    Last changed    : 12/11/2013 11:40:18 AM by Suresh
    Analysis Method : C:\CHEM32\PRDB-LC-22\DATA\2013-BCL2 CD2\NOV-2013\14-NOV-2013\14-NOV-2013
                      2013-11-15 19-01-21\034-0601.D\DA.M (ATLANTIST3_BCL-2_CD2_1.M)
    Last changed    : 12/11/2013 11:40:18 AM by Suresh
    Sample Info     : O-Et FNB RM
                      After 2 hrs
```




```
    ========================================================================
                              Area Percent Report
    ========================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=220,4 Ref=360,16

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   4.025 MM R  0.0699    6.62577    1.58073   0.1791
       2   5.095 MM R  0.0621 3640.00635  875.16632  98.3752
       3   5.796 MM R  0.0479    2.94597    1.02478   0.0796
       4   6.340 MM R  0.0680   50.54704   12.38812   1.3661

    Totals :                  3700.12513  890.15996

    ========================================================================
                              *** End of Report ***
```

5a-Reaction profile (Method-B)

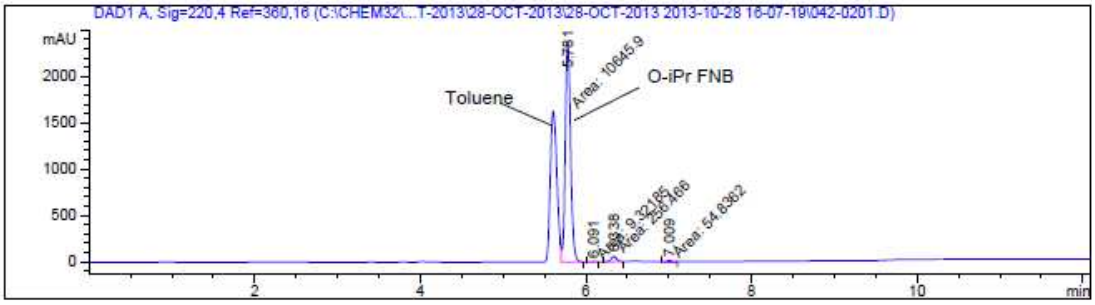
```
Data File C:\CHEM32\2\DATA\29 NOV 2013\29 NOV 2013  2013-11-29 17-56-25\047-0701.D
Sample Name: M-2-Toluene-O-Et FNB

    ======================================================================
    Acq. Operator   : Sagar                          Seq. Line :   7
    Acq. Instrument : PRDB-LC-23                     Location : Vial 47
    Injection Date  : 29/11/2013 07:52:23 PM            Inj :   1
                                                    Inj Volume : 4 µl
    Acq. Method     : C:\Chem32\2\DATA\29 NOV 2013\29 NOV 2013  2013-11-29 17-56-25\SURESH_
                      SCIENCE_METHOD.M
    Last changed    : 29/11/2013 05:56:19 PM by Sagar
    Analysis Method : C:\CHEM32\2\METHODS\SCIENCE.M
    Last changed    : 30/11/2013 01:34:36 PM by Sagar
                      (modified after loading)
    Sample Info     : M-2-Toluene-O-Et FNB
```




```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=220,4 Ref=350,16

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   3.991 MM R  0.0639    9.29233    2.42352   0.1311
       2   4.166 MM R  0.0614  132.94873   36.08504   1.8758
       3   5.045 MM R  0.0650 6922.42871 1774.83813  97.6697
       4   5.725 MM R  0.0499   14.59854    4.87806   0.2060
       5   6.506 MM R  0.0736    8.32561    1.88657   0.1175

    Totals :                  7087.59392 1820.11132


    ======================================================================
                              *** End of Report ***
```

6a-Reaction profile (Method-A)

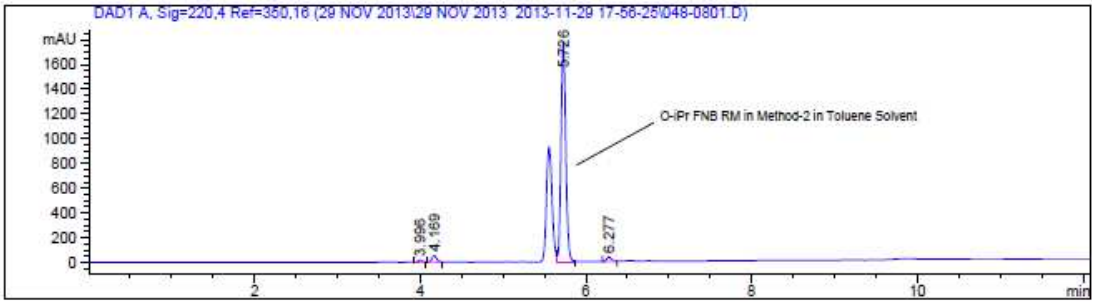
```
Data File C:\CHEM32\...CD2\OCT-2013\28-OCT-2013\28-OCT-2013 2013-10-28 16-07-19\042-0201.D
Sample Name: O-iPr FBN RM

    ======================================================================
    Acq. Operator   : Sagar                          Seq. Line :   2
    Acq. Instrument : PRDB-LC-22                     Location : Vial 42
    Injection Date  : 28/10/2013 04:27:56 PM            Inj :   1
                                                    Inj Volume : 4 µl
    Acq. Method     : C:\Chem32\PRDB-LC-22\Data\2013-BCL2 CD2\Oct-2013\28-OCT-2013\28-OCT-2013
                      2013-10-28 16-07-19\ATLANTIST3_BCL-2_CD2_1.M
    Last changed    : 24/10/2013 02:27:28 PM by Sagar
    Analysis Method : C:\CHEM32\1\METHODS\BCL-2 WASH.M
    Last changed    : 28/10/2013 02:09:32 PM by Sagar
                      (modified after loading)
    Sample Info     : O-iPr FBN RM
```




```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=220,4 Ref=360,16

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   5.781 FM    0.0741 1.06459e4  2395.10718  97.0763
       2   6.091 MM    0.0788    9.32185    1.97047   0.0850
       3   6.338 MM    0.0700  256.46622   61.07615   2.3386
       4   7.009 MM    0.0696   54.83624   13.13385   0.5000

    Totals :                  1.09665e4  2471.28766


    ======================================================================
                            *** End of Report ***
```

6a-Reaction profile (Method-B)

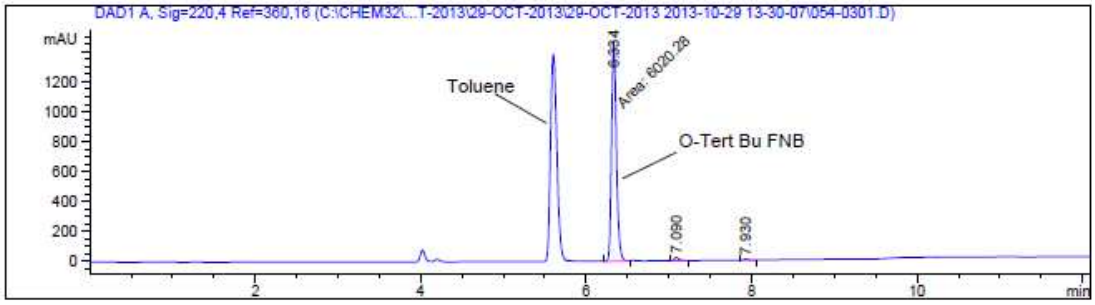
```
Data File C:\CHEM32\2\DATA\29 NOV 2013\29 NOV 2013  2013-11-29 17-56-25\048-0801.D
Sample Name: M-2-Toluene-O-iPr FNB

    ======================================================================
    Acq. Operator   : Sagar                          Seq. Line :   8
    Acq. Instrument : PRDB-LC-23                      Location : Vial 48
    Injection Date  : 29/11/2013 08:08:37 PM             Inj :   1
                                                     Inj Volume : 4 µl
    Acq. Method     : C:\Chem32\2\DATA\29 NOV 2013\29 NOV 2013  2013-11-29 17-56-25\SURESH_
                      SCIENCE_METHOD.M
    Last changed    : 29/11/2013 05:56:19 PM by Sagar
    Analysis Method : C:\CHEM32\2\METHODS\SCIENCE.M
    Last changed    : 30/11/2013 01:34:36 PM by Sagar
                      (modified after loading)
    Sample Info     : M-2-Toluene-O-iPr FNB
```




```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=220,4 Ref=350,16

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   3.996 MM R  0.0633   61.10439   16.09744   0.8121
       2   4.169 MM R  0.0636  200.49081   52.50299   2.6645
       3   5.726 FM R  0.0661 7095.99561 1788.98486  94.3042
       4   6.277 MM R  0.0726  166.98772   38.31123   2.2192

    Totals :                  7524.57853 1895.89652

    ======================================================================
                              *** End of Report ***
```

7a-Reaction profile (Method-A)

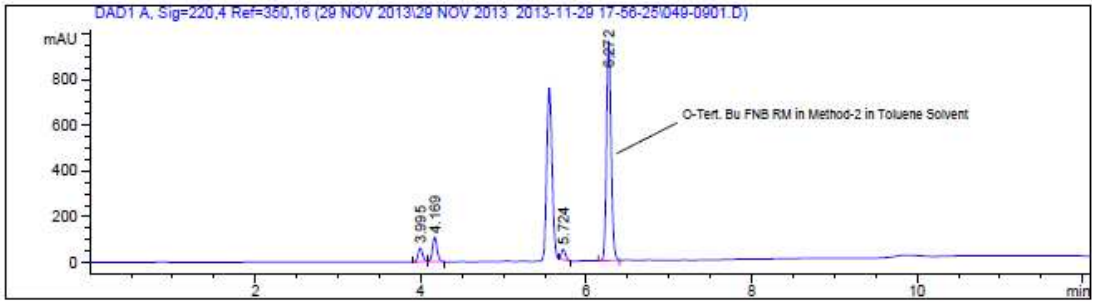
```
Data File C:\CHEM32\...CD2\OCT-2013\29-OCT-2013\29-OCT-2013 2013-10-29 13-30-07\054-0301.D
Sample Name: O-Tert Bu FNB RM

======================================================================
Acq. Operator   : Sagar                        Seq. Line :   3
Acq. Instrument : PRDB-LC-22                    Location : Vial 54
Injection Date  : 29/10/2013 02:05:41 PM           Inj :   1
                                               Inj Volume : 4 µl
Acq. Method     : C:\Chem32\PRDB-LC-22\Data\2013-BCL2 CD2\Oct-2013\29-OCT-2013\29-OCT-2013
                  2013-10-29 13-30-07\ATLANTIST3_BCL-2_CD2_1.M
Last changed    : 24/10/2013 02:27:28 PM by Sagar
Analysis Method : C:\CHEM32\1\METHODS\BCL-2 WASH.M
Last changed    : 05/11/2013 01:43:42 PM by Sagar
                  (modified after loading)
Sample Info     : O-Tert Bu FNB RM
```




```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=220,4 Ref=360,16

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.334 MM    0.0678 6020.28027 1480.92847  97.5723
   2   7.090 MM R  0.0745  104.31441   23.32751   1.6907
   3   7.930 MM R  0.0828   45.47598    9.15381   0.7370

Totals :                  6170.07066 1513.40979

======================================================================
                        *** End of Report ***
```

7a-Reaction profile (Method-B)

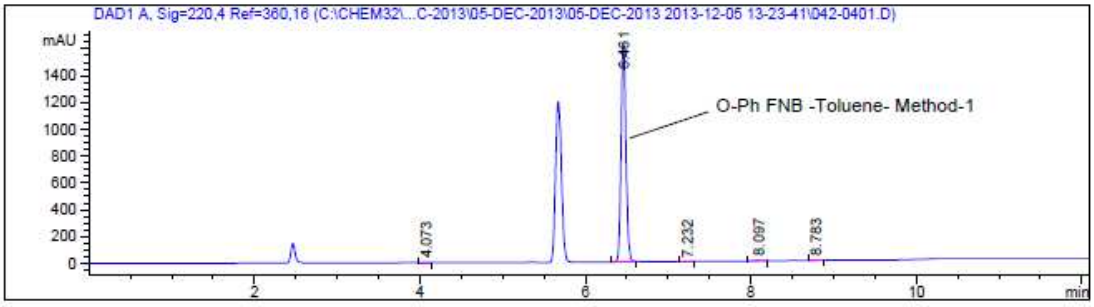
```
Data File C:\CHEM32\2\DATA\29 NOV 2013\29 NOV 2013  2013-11-29 17-56-25\049-0901.D
Sample Name: M-2-Toluene-O-Tert Bu FNB

    ======================================================================
    Acq. Operator   : Sagar                          Seq. Line :   9
    Acq. Instrument : PRDB-LC-23                      Location : Vial 49
    Injection Date  : 29/11/2013 08:24:51 PM             Inj :   1
                                                    Inj Volume : 4 µl
    Acq. Method     : C:\Chem32\2\DATA\29 NOV 2013\29 NOV 2013  2013-11-29 17-56-25\SURESH_
                      SCIENCE_METHOD.M
    Last changed    : 29/11/2013 05:56:19 PM by Sagar
    Analysis Method : C:\CHEM32\2\METHODS\SCIENCE.M
    Last changed    : 30/11/2013 01:34:36 PM by Sagar
                      (modified after loading)
    Sample Info     : M-2-Toluene-O-Tert Bu FNB
```




```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=220,4 Ref=350,16

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   3.995 MM R  0.0625  226.86348   60.47741   5.0186
       2   4.169 MM R  0.0640  413.49066  107.69834   9.1471
       3   5.724 MM R  0.0580  160.49353   46.09598   3.5504
       4   6.272 MM R  0.0644 3719.60278  962.36243  82.2839

    Totals :                  4520.45045 1176.63415


    ======================================================================
                            *** End of Report ***
```

8a-Reaction profile (Method-A)

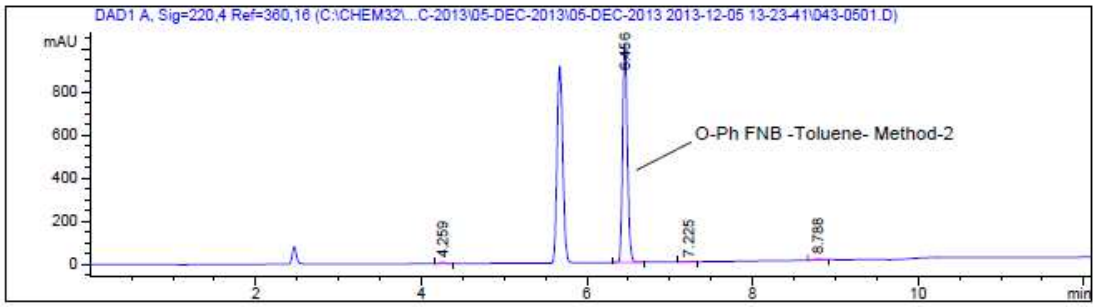
```
Data File C:\CHEM32\...CD2\DEC-2013\05-DEC-2013\05-DEC-2013 2013-12-05 13-23-41\042-0401.D
Sample Name: O-Ph FNB-Toluene-Method-1

    ======================================================================
    Acq. Operator   :                                Seq. Line :   4
    Acq. Instrument : PRDB-LC-22                      Location : Vial 42
    Injection Date  : 05/12/2013 02:15:30 PM             Inj :   1
                                                    Inj Volume : 4 µl
    Acq. Method     : C:\Chem32\PRDB-LC-22\Data\2013-BCL2 CD2\Dec-2013\05-DEC-2013\05-DEC-2013
                      2013-12-05 13-23-41\ATLANTIST3_BCL-2_CD2_BINARY.M
    Last changed    : 05/12/2013 01:12:48 PM by Sagar
    Analysis Method : C:\CHEM32\1\METHODS\ATLANTIST3_BCL-2_CD2_1.M
    Last changed    : 29/11/2013 10:41:26 AM by Suresh
    Sample Info     : O-Ph FNB-Toluene-Method-1
```




```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=220,4 Ref=360,16

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]       [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   4.073 MM R  0.0768   10.85634    2.35455   0.1614
       2   6.461 MM R  0.0963 6628.63330 1637.96716  98.5431
       3   7.232 MM R  0.0906   16.61663    3.05509   0.2470
       4   8.097 MM R  0.1116   48.46064    7.23995   0.7204
       5   8.783 MM R  0.1030   22.06980    3.57133   0.3281

    Totals :                  6726.63671 1654.18808

    ======================================================================
                              *** End of Report ***
```

8a-Reaction profile (Method-B)

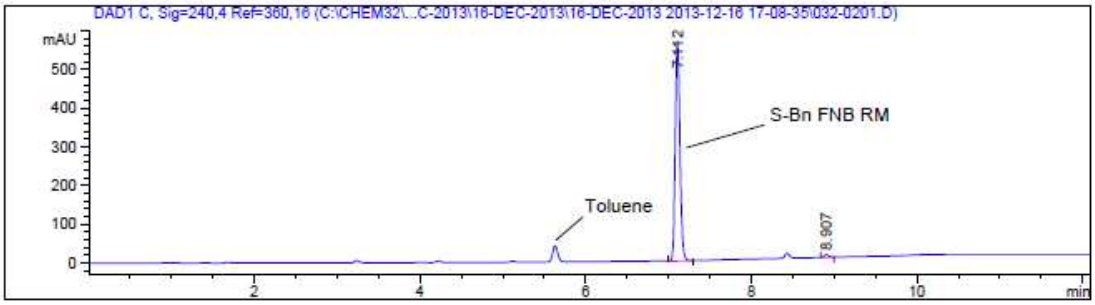
```
Data File C:\CHEM32\...CD2\DEC-2013\05-DEC-2013\05-DEC-2013 2013-12-05 13-23-41\043-0501.D
Sample Name: O-Ph FNB-Toluene-Method-2

    ======================================================================
    Acq. Operator   :                              Seq. Line :   5
    Acq. Instrument : PRDB-LC-22                    Location : Vial 43
    Injection Date  : 05/12/2013 02:31:39 PM           Inj :   1
                                                   Inj Volume : 4 µl
    Acq. Method     : C:\Chem32\PRDB-LC-22\Data\2013-BCL2 CD2\Dec-2013\05-DEC-2013\05-DEC-2013
                      2013-12-05 13-23-41\ATLANTIST3_BCL-2_CD2_BINARY.M
    Last changed    : 05/12/2013 01:12:48 PM by Sagar
    Analysis Method : C:\CHEM32\1\METHODS\ATLANTIST3_BCL-2_CD2_1.M
    Last changed    : 29/11/2013 10:41:26 AM by Suresh
    Sample Info     : O-Ph FNB-Toluene-Method-2
```




```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=220,4 Ref=360,16

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   4.259 MM R  0.0698   29.73720    7.10383   0.7202
       2   6.456 MM R  0.0667 4058.90210 1013.54749  98.3058
       3   7.225 MM R  0.1119   12.13470    1.80786   0.2939
       4   8.788 MM R  0.1153   28.07806    4.05722   0.6800

    Totals :                  4128.85206 1026.51639


    ======================================================================
                              *** End of Report ***
```

9a-Reaction profile (Method-B)

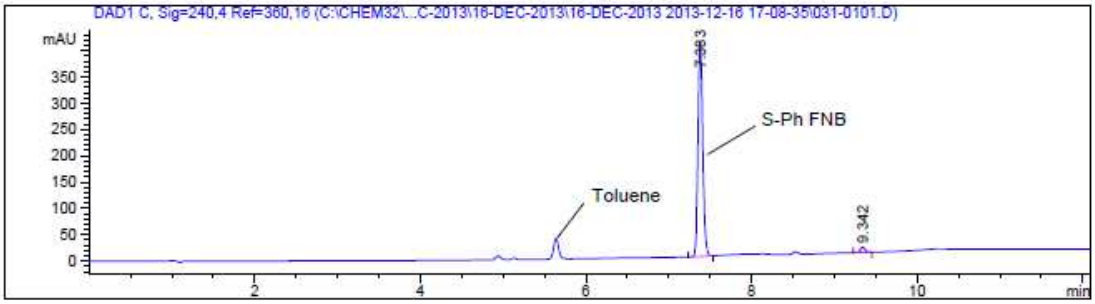
```
Data File C:\CHEM32\...CD2\DEC-2013\16-DEC-2013\16-DEC-2013 2013-12-16 17-08-35\032-0201.D
Sample Name: S-Bn FNB RM

    ======================================================================
    Acq. Operator   : Suresh                          Seq. Line :   2
    Acq. Instrument : PRDB-LC-22                       Location : Vial 32
    Injection Date  : 16/12/2013 05:34:02 PM              Inj :   1
                                                      Inj Volume : 4 µl
    Acq. Method     : C:\Chem32\PRDB-LC-22\Data\2013-BCL2 CD2\Dec-2013\16-DEC-2013\16-DEC-2013
                      2013-12-16 17-08-35\ATLANTIST3_BCL-2_CD2_BINARY.M
    Last changed    : 10/12/2013 08:03:23 AM by Suresh
    Analysis Method : C:\CHEM32\1\METHODS\ATLANTIST3_BCL-2_CD2_1.M
    Last changed    : 29/11/2013 10:41:26 AM by Suresh
    Sample Info     : S-Bn FNB RM-Toluene
                      Method-2
```




```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 C, Sig=240,4 Ref=360,16

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   7.112 MM R  0.0868 2233.78076  566.65515  98.7462
       2   8.907 MM R  0.0663   28.36357    7.13100   1.2538

    Totals :                  2262.14434  573.78615

    ======================================================================
                            *** End of Report ***
```

10a-Reaction profile (Method-B)

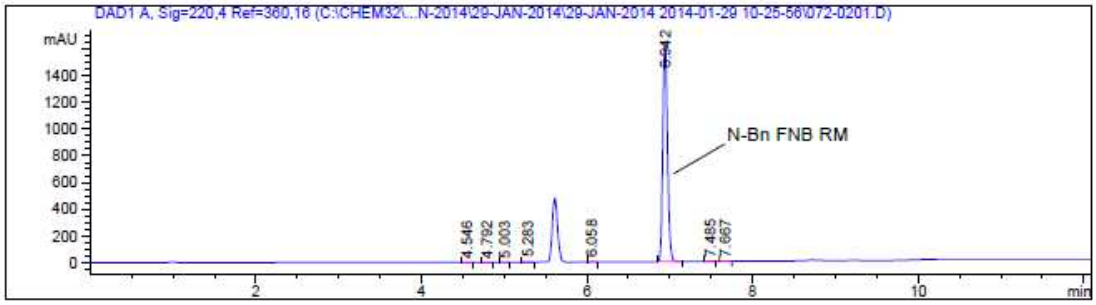
```
Data File C:\CHEM32\...CD2\DEC-2013\16-DEC-2013\16-DEC-2013 2013-12-16 17-08-35\031-0101.D
Sample Name: S-Ph FNB RM

    ======================================================================
    Acq. Operator   : Suresh                          Seq. Line :   1
    Acq. Instrument : PRDB-LC-22                       Location : Vial 31
    Injection Date  : 16/12/2013 05:17:52 PM             Inj :   1
                                                     Inj Volume : 4 µl
    Acq. Method     : C:\Chem32\PRDB-LC-22\Data\2013-BCL2 CD2\Dec-2013\16-DEC-2013\16-DEC-2013
                      2013-12-16 17-08-35\ATLANTIST3_BCL-2_CD2_BINARY.M
    Last changed    : 10/12/2013 08:03:23 AM by Suresh
    Analysis Method : C:\CHEM32\1\METHODS\ATLANTIST3_BCL-2_CD2_1.M
    Last changed    : 29/11/2013 10:41:26 AM by Suresh
    Sample Info     : S-Ph FNB RM-Toluene
                      Method-2
```




```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 C, Sig=240,4 Ref=360,16

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   7.383 MM R  0.0956 1627.50757  409.08466  97.6940
       2   9.342 MM R  0.0631   38.41548   10.14124   2.3060

    Totals :                  1665.92305  419.22590


    ======================================================================
                              *** End of Report ***
```

11a-Reaction profile (Method-B)

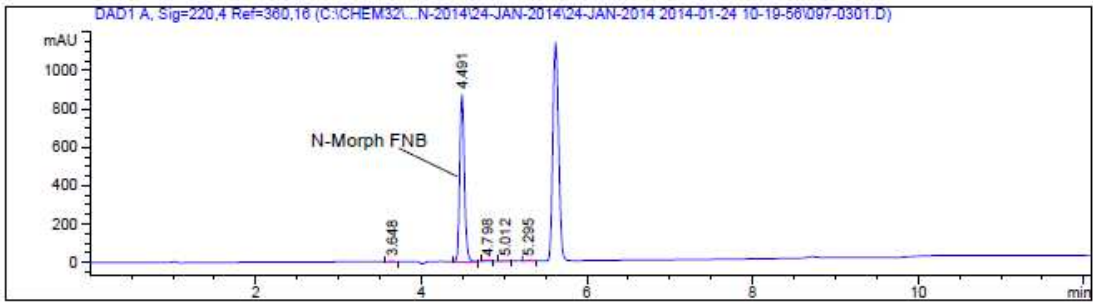
```
Data File C:\CHEM32\...2BU\JAN-2014\29-JAN-2014\29-JAN-2014 2014-01-29 10-25-56\072-0201.D
Sample Name: N-Bn FNB RM

    ======================================================================
    Acq. Operator   : Suresh                          Seq. Line :   2
    Acq. Instrument : PRDB-LC-22                       Location : Vial 72
    Injection Date  : 29/01/2014 10:45:21 AM              Inj :   1
                                                      Inj Volume : 4 µl
    Acq. Method     : C:\Chem32\PRDB-LC-22\Data\2014-BCL2BU\JAN-2014\29-JAN-2014\29-JAN-2014
                      2014-01-29 10-25-56\ATLANTIST3_BCL-2_CD2_BINARY.M
    Last changed    : 20/01/2014 03:19:21 PM by Suresh
    Analysis Method : C:\CHEM32\1\METHODS\ATLANTIST3_BCL-2_CD2_1.M
    Last changed    : 29/01/2014 05:05:15 PM by Suresh
                      (modified after loading)
    Sample Info     : N-Bn FNB RM
```




```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=220,4 Ref=360,16

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   4.546 MM R  0.0640    5.07555    1.32165   0.0787
       2   4.792 MM R  0.0603    5.65409    1.56324   0.0877
       3   5.003 MM R  0.0610    3.34008 9.12461e-1   0.0518
       4   5.283 MM R  0.0738    8.35852    1.88730   0.1296
       5   6.058 MM R  0.0626   10.49271    2.79492   0.1627
       6   6.942 MM R  0.0646 6401.19727 1652.58569  99.2320
       7   7.485 MM R  0.0594    7.23704    2.02942   0.1122
       8   7.667 FM R  0.0928    9.38102    1.68479   0.1454

    Totals :                  6450.73628 1664.77948
```

12a-Reaction profile (Method-B)

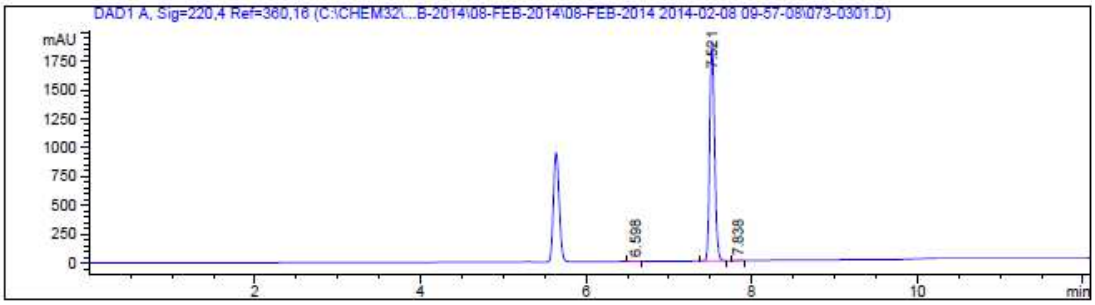
```
Data File C:\CHEM32\...2BU\JAN-2014\24-JAN-2014\24-JAN-2014 2014-01-24 10-19-56\097-0301.D
Sample Name: N-Morph FNB RM

    ======================================================================
    Acq. Operator    : Suresh                          Seq. Line :   3
    Acq. Instrument : PRDB-LC-22                        Location : Vial 97
    Injection Date  : 24/01/2014 10:55:39 AM              Inj :   1
                                                      Inj Volume : 4 µl
    Acq. Method     : C:\Chem32\PRDB-LC-22\Data\2014-BCL2BU\JAN-2014\24-JAN-2014\24-JAN-2014
                      2014-01-24 10-19-56\ATLANTIST3_BCL-2_CD2_BINARY.M
    Last changed    : 20/01/2014 03:19:21 PM by Suresh
    Analysis Method : C:\CHEM32\1\METHODS\ATLANTIST3_BCL-2_CD2_1.M
    Last changed    : 29/01/2014 05:05:15 PM by Suresh
                      (modified after loading)
    Sample Info     : N-Morph FNB RM
```




```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=220,4 Ref=360,16

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   3.648 MM R  0.0644    8.48174    2.19623   0.2489
       2   4.491 MM R  0.0644 3374.02319  872.77716  99.0294
       3   4.798 MM R  0.0637    8.24687    2.15717   0.2421
       4   5.012 MM R  0.0707    4.91451    1.15801   0.1442
       5   5.295 MM R  0.0825   11.42455    2.30889   0.3353

    Totals :                  3407.09086  880.59746

    ======================================================================
                              *** End of Report ***
```

13a-Reaction profile (Method-B)

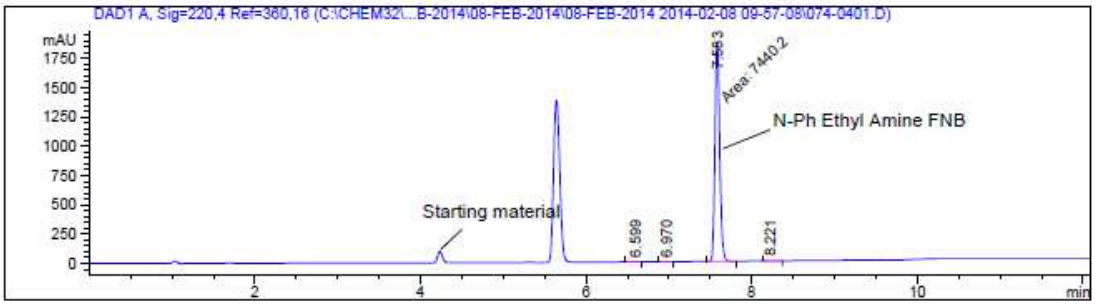
```
Data File C:\CHEM32\...2BU\FEB-2014\08-FEB-2014\08-FEB-2014 2014-02-08 09-57-08\073-0301.D
Sample Name: N-nBu FNB RM

    ======================================================================
    Acq. Operator   : Suresh                        Seq. Line :   3
    Acq. Instrument : PRDB-LC-22                     Location : Vial 73
    Injection Date  : 08/02/2014 10:32:39 AM              Inj :   1
                                                   Inj Volume : 4 µl
    Acq. Method     : C:\Chem32\PRDB-LC-22\Data\2014-BCL2BU\FEB-2014\08-FEB-2014\08-FEB-2014
                      2014-02-08 09-57-08\ATLANTIST3_BCL-2_CD2_BINARY.M
    Last changed    : 20/01/2014 03:19:21 PM by Suresh
    Analysis Method : C:\CHEM32\1\METHODS\ATLANTIST3_BCL-2_CD2_1.M
    Last changed    : 06/02/2014 10:37:49 AM by Suresh
                      (modified after loading)
    Sample Info     : N-nBu FNB RM
```




```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=220,4 Ref=360,16

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   6.598 MM R  0.0918   10.02706    1.81994   0.1286
       2   7.521 MM R  0.0681 7777.87988 1904.91626  99.7715
       3   7.838 MM R  0.0636    7.78480    2.04047   0.0999

    Totals :                  7795.69174 1908.77667


    ======================================================================
                              *** End of Report ***
```

14a-Reaction profile (Method-B)

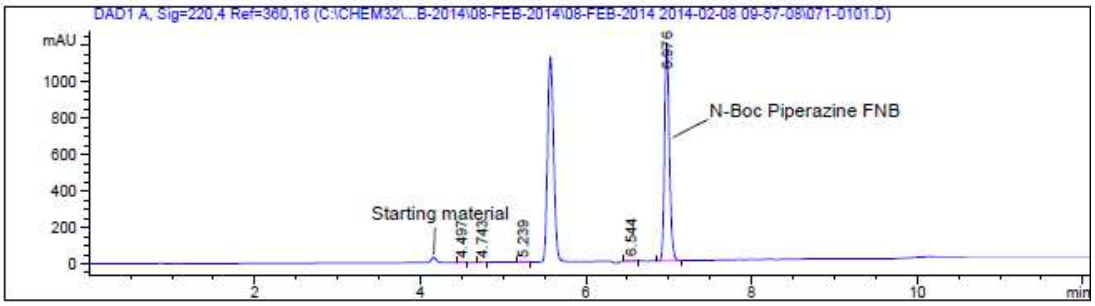
```
Data File C:\CHEM32\...2BU\FEB-2014\08-FEB-2014\08-FEB-2014 2014-02-08 09-57-08\074-0401.D
Sample Name: N-PEA FNB RM

    ======================================================================
    Acq. Operator   : Suresh                          Seq. Line :   4
    Acq. Instrument : PRDB-LC-22                       Location : Vial 74
    Injection Date  : 08/02/2014 10:48:42 AM              Inj :   1
                                                      Inj Volume : 4 µl
    Acq. Method     : C:\Chem32\PRDB-LC-22\Data\2014-BCL2BU\FEB-2014\08-FEB-2014
                      2014-02-08 09-57-08\ATLANTIST3_BCL-2_CD2_BINARY.M
    Last changed    : 20/01/2014 03:19:21 PM by Suresh
    Analysis Method : C:\CHEM32\1\METHODS\ATLANTIST3_BCL-2_CD2_1.M
    Last changed    : 06/02/2014 10:37:49 AM by Suresh
                      (modified after loading)
    Sample Info     : N-PEA FNB RM
```




```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=220,4 Ref=360,16

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   6.599 MM R  0.0852   16.05501    3.13955   0.2147
       2   6.970 MM R  0.0770    8.62692    1.86640   0.1154
       3   7.583 MM T  0.0656 7440.19580 1889.82202  99.5095
       4   8.221 MM R  0.1171   11.99358    1.70680   0.1604

    Totals :                  7476.87131 1896.53476

    ======================================================================
                              *** End of Report ***
```

15a-Reaction profile (Method-B)

```
Data File C:\CHEM32\...2BU\FEB-2014\08-FEB-2014\08-FEB-2014 2014-02-08 09-57-08\071-0101.D
Sample Name: N-Boc Piperazine FNB RM

    ======================================================================
    Acq. Operator   : Suresh                          Seq. Line :   1
    Acq. Instrument : PRDB-LC-22                       Location : Vial 71
    Injection Date  : 08/02/2014 10:00:29 AM             Inj :   1
                                                     Inj Volume : 4 µl
    Acq. Method     : C:\Chem32\PRDB-LC-22\Data\2014-BCL2BU\FEB-2014\08-FEB-2014\08-FEB-2014
                      2014-02-08 09-57-08\ATLANTIST3_BCL-2_CD2_BINARY.M
    Last changed    : 20/01/2014 03:19:21 PM by Suresh
    Analysis Method : C:\CHEM32\1\METHODS\ATLANTIST3_BCL-2_CD2_1.M
    Last changed    : 06/02/2014 10:37:49 AM by Suresh
                      (modified after loading)
    Sample Info     : N-Boc Piperazine FNB RM
```




```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=220,4 Ref=360,16

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   4.497 MM R  0.0645    8.28076    2.13923   0.1688
       2   4.743 MM R  0.0650   10.03082    2.57027   0.2044
       3   5.239 MM R  0.0753   14.13667    3.13079   0.2881
       4   6.544 MM R  0.0908   13.47295    2.47230   0.2746
       5   6.976 MM R  0.0671 4860.49219 1206.89221  99.0641

    Totals :                  4906.41339 1217.20480


    ======================================================================
                              *** End of Report ***
```