Atom and Step Economic Multicomponent Synthesis of Highly Functionalized Novel N-alkyl Piperidines: Structural Elucidation through Spectral Studies and Single Crystallographic analysis

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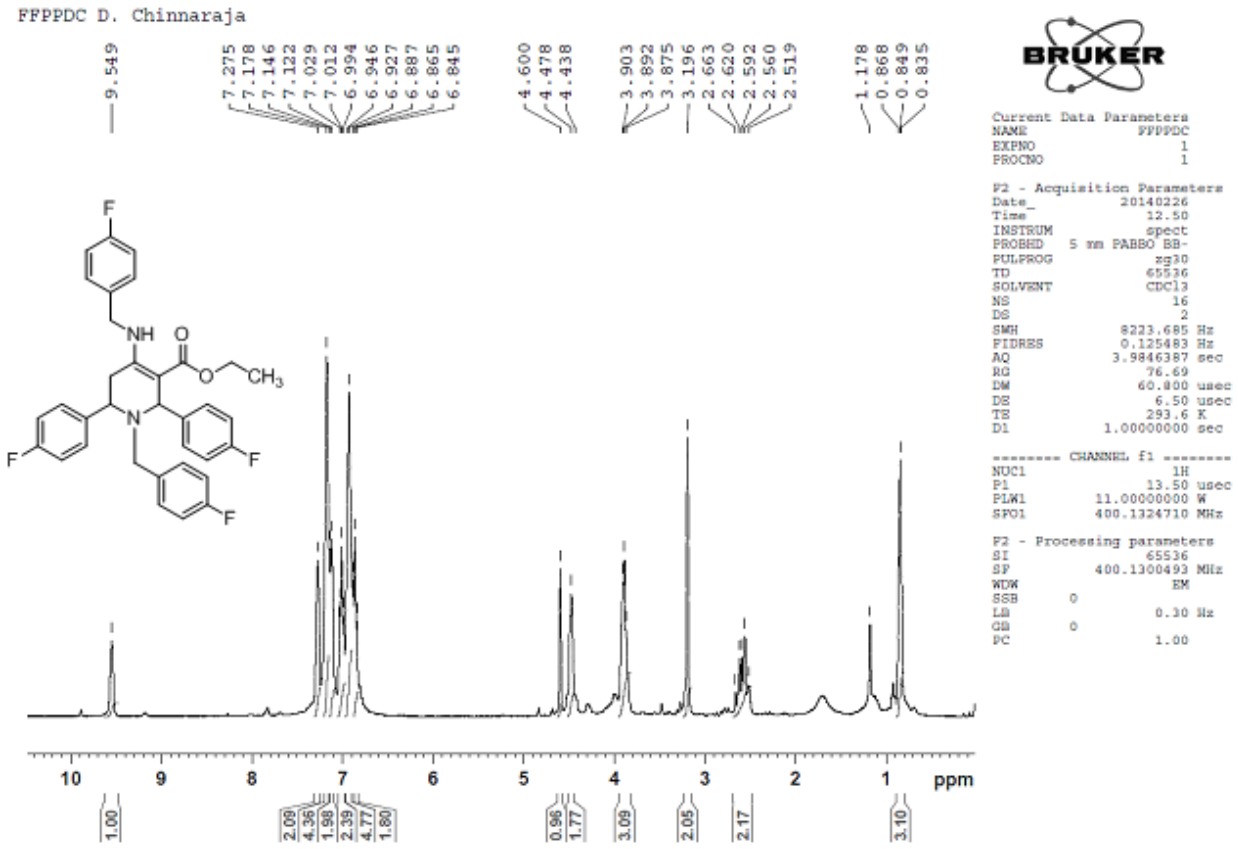
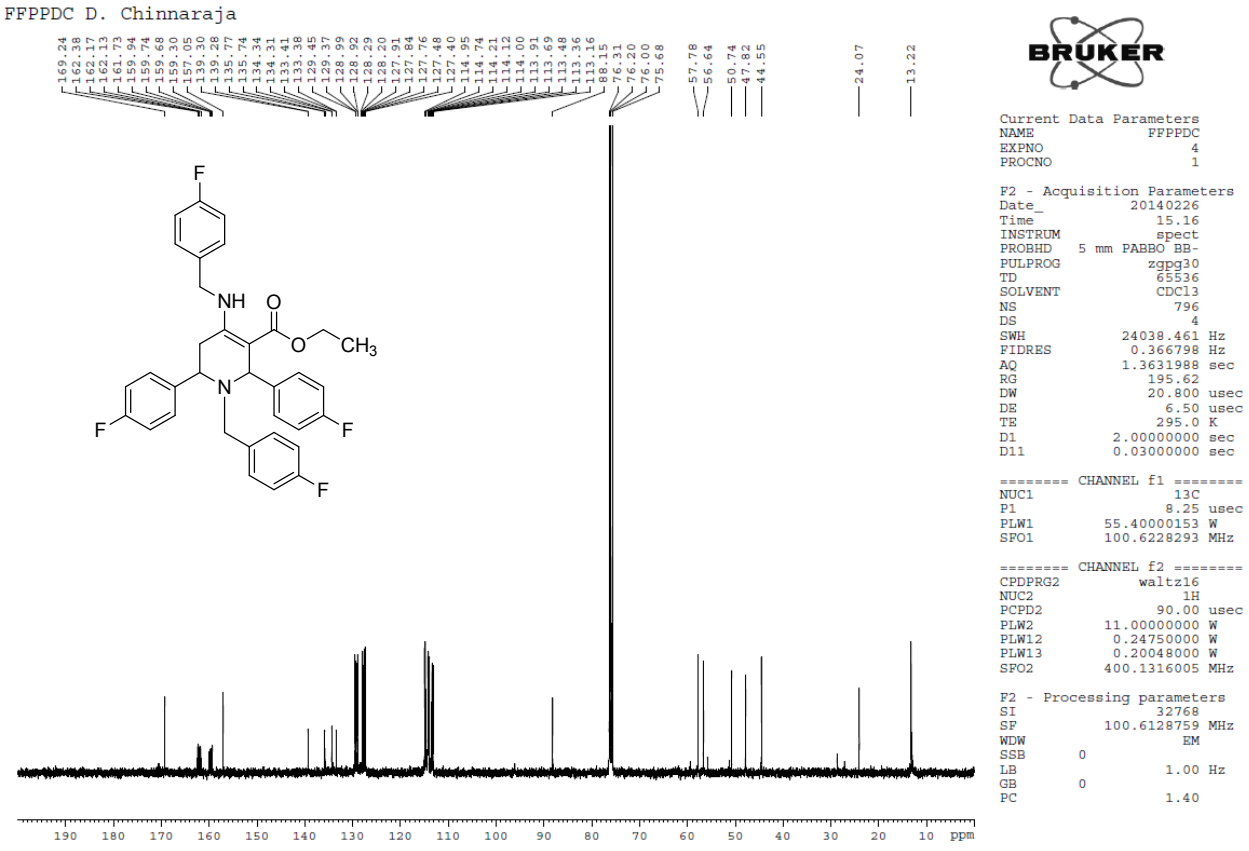
Supplementary data (^{1}H NMR, ^{13}C NMR, ^{1}H-^{1}H COSY, ^{1}H-^{13}C COSY, DEPT and HR-Mass spectra (**S1-S6)** the synthesized compound **7**

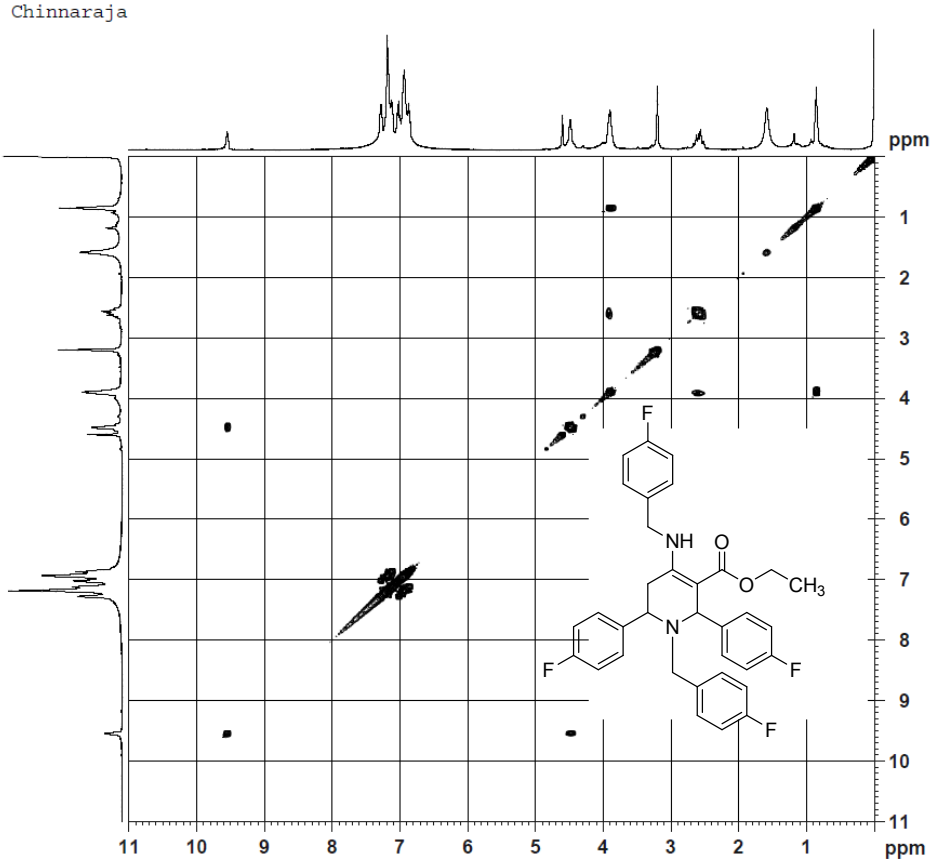


^{1}H NMR spectrum of compound-**7**



^{13}C NMR spectrum of compound-**7**

FAFBA D. Chinnaraja



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PROCNO                    1

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TD                     2048
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DS                        8
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RG                    61.57
DW                  109.000 usec
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TE                   294.0 K
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D11               0.03000000 sec
D12               0.00002000 sec
D13               0.00000400 sec
D16               0.00020000 sec
IN0               0.00021800 sec

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P1                     13.50 usec
P17                  2500.00 usec
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SPO1           400.1319057 MHz

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GPZ1                10.00 %
P16                 1000.00 usec

F1 - Acquisition parameters
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FIDRES           35.837154 Hz
SW                  11.464 ppm
FnMODE                   QF

F2 - Processing parameters
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SF             400.1300437 MHz
WDW                   QSINE
SSB          0
LB           0 Hz
GB           0
PC                      1.40

F1 - Processing parameters
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MC2                     QF
SF             400.1300437 MHz
WDW           States-TPPI
SSB          0
LB           0 Hz
GB           0
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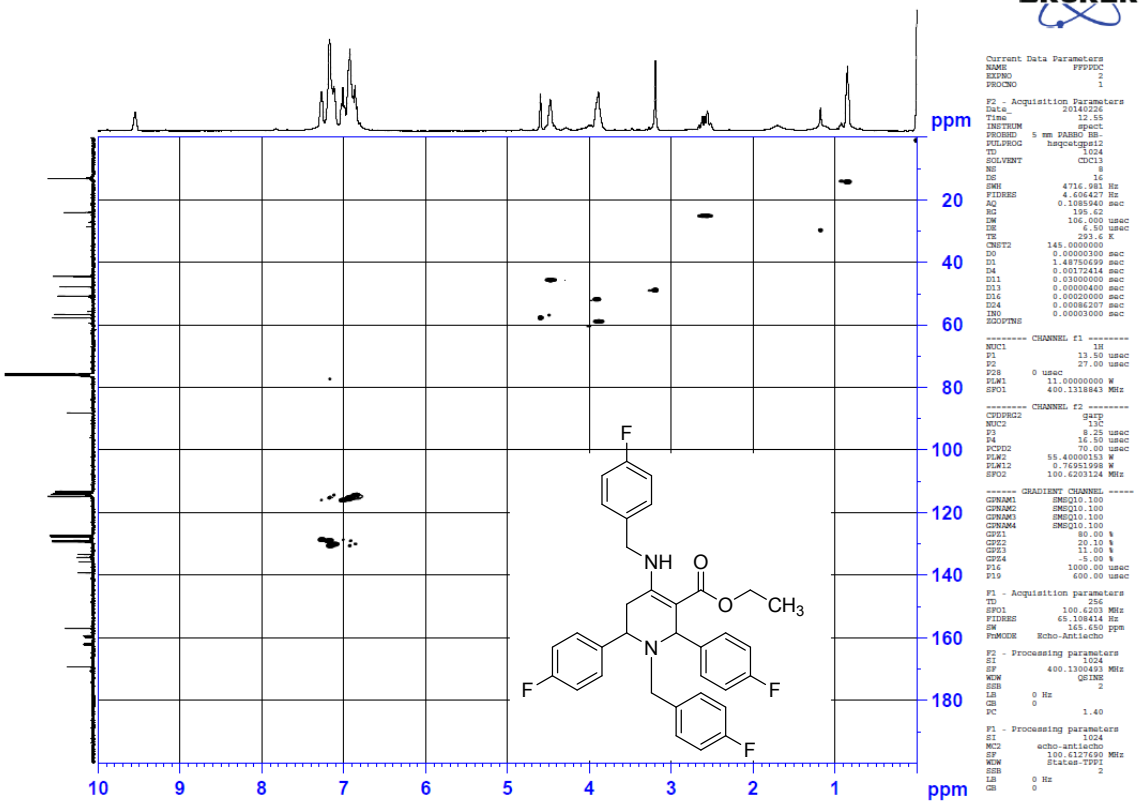
^{1}H-^{1}H COSY spectrum of compound-7

FFPPDC D. Chinnaraja



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PROCNO 1

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TD 1024
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NS 8
DS 16
SWH 4716.981 Hz
FIDRES 4.606427 Hz
AQ 0.1085940 sec
RG 195.62
DW 106.000 usec
DE 6.50 usec
TE 293.6 K
CNST2 145.0000000
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D1 1.48750699 sec
D4 0.00172414 sec
D11 0.03000000 sec
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EGOPTNS

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P2 27.00 usec
P28 0 usec
PLW1 11.00000000 W
SFO1 400.1318843 MHz

-------- CHANNEL f2 --------
CPDPRG2 garp
NUC2 13C
P3 8.25 usec
P4 16.50 usec
PCPD2 70.00 usec
PLW2 55.40000153 W
PLW12 0.76951998 W
SFO2 100.6203124 MHz

------ GRADIENT CHANNEL -----
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GPNAM2 SMSQ10.100
GPNAM3 SMSQ10.100
GPNAM4 SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
GPZ3 11.00 %
GPZ4 -5.00 %
P16 1000.00 usec
P19 600.00 usec

F1 - Acquisition parameters
TD 256
SFO1 100.6203 MHz
FIDRES 65.108414 Hz
SW 165.650 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 400.1300493 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
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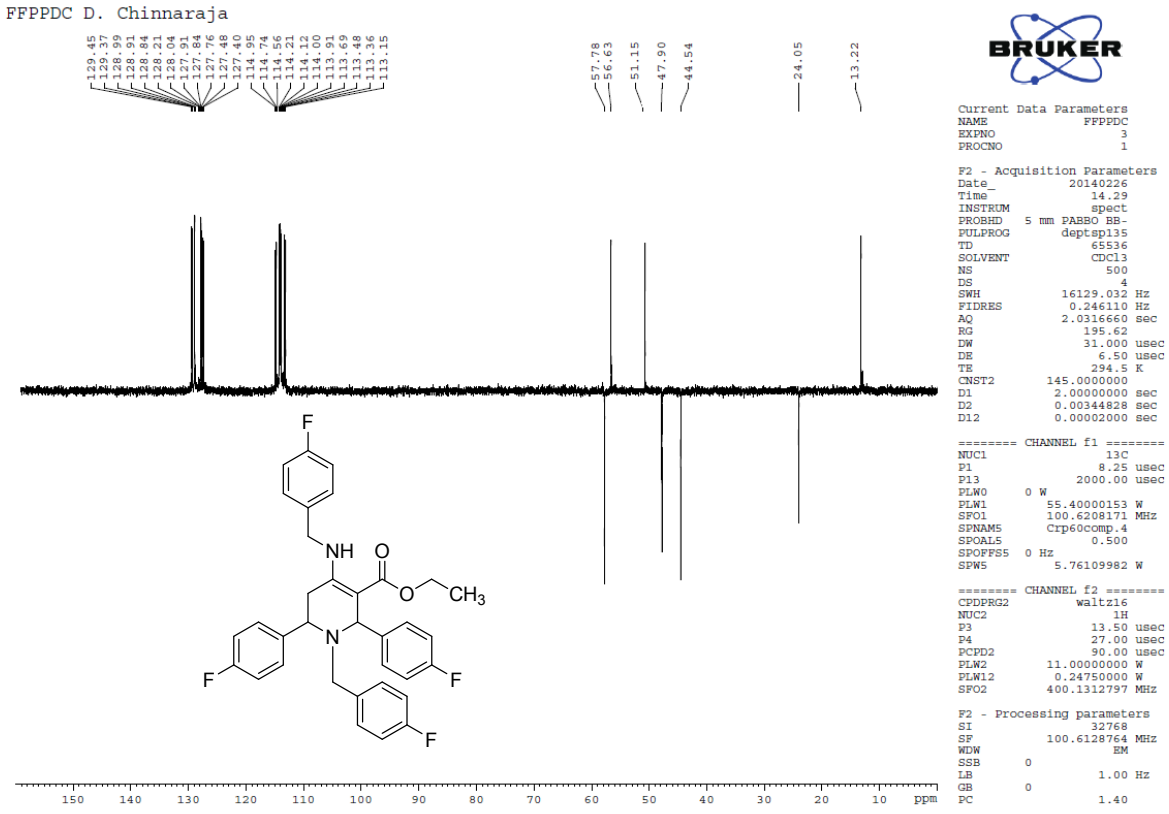
MC2 echo-antiecho
SF 100.6127690 MHz
WDW States-TPPI
SSB 2
LB 0 Hz
GB 0

^{1}H-^{13}C COSY spectrum of compound-7



DEPT spectrum compound-7

BRUKER MAXIS HRMS REPORT

School of Chemistry
University of Hyderabad

Analysis Info

Analysis Name	D:\Data\2013\Dr.NAGARAJAN\DEC\TFACLF-R.d	Acquisition Date	12/19/2013 12:00:25 PM
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Sample Name	TFACLF-CHCL3-ACN	Instrument	maXis 10138
Comment			

Acquisition Parameter

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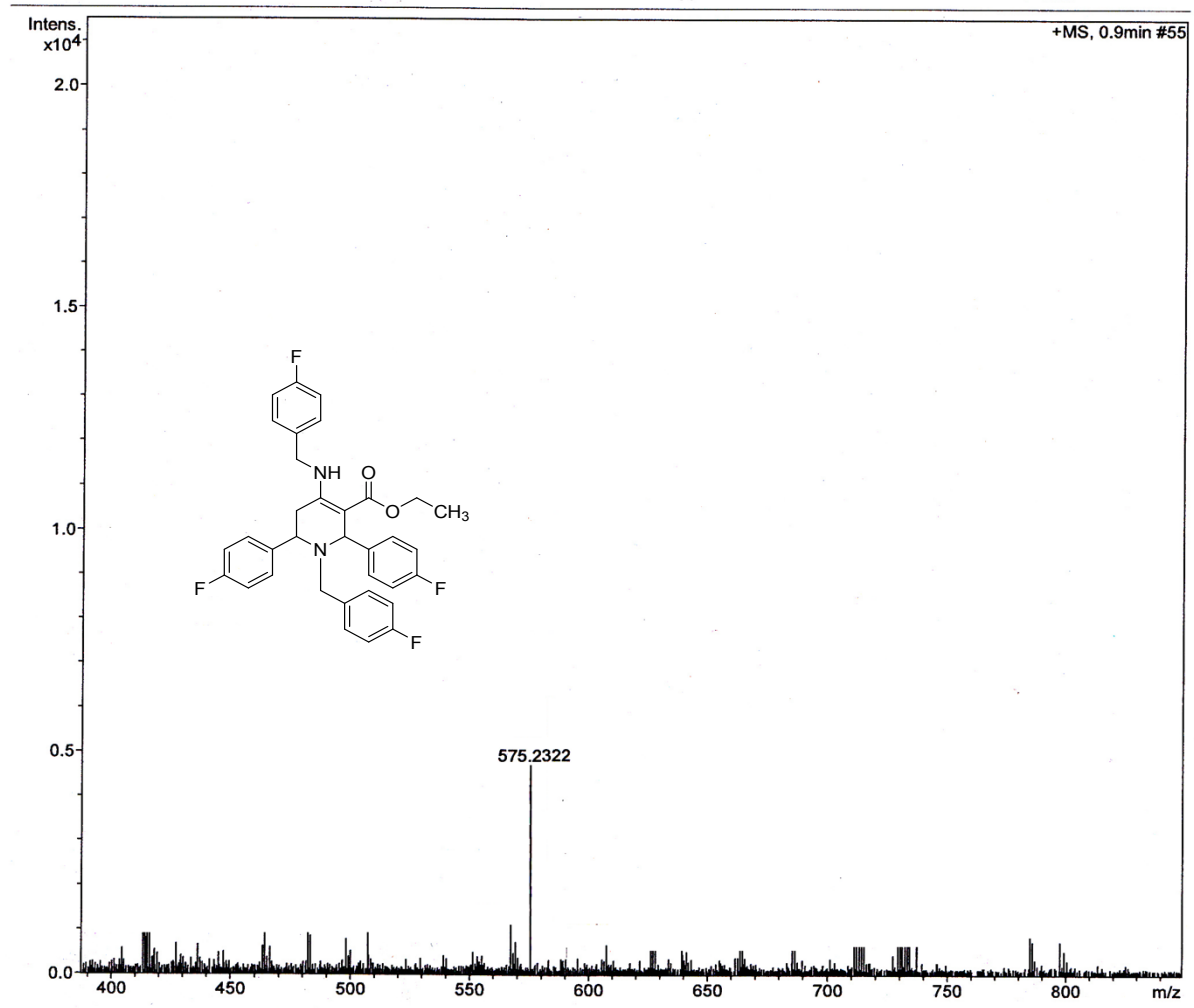
Scan End	2580 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



Bruker Compass DataAnalysis 4.0 printed: 12/19/2013 12:02:54 PM Page 1 of 1

HR-Mass spectrum of compound-7