Supporting Information

Design, synthesis and biological activity evaluation of regioisomeric spiro-(indoline-isoxazolidines) on the inhibition of TNF-alpha induced ICAM-1 expression on human endothelial cells.

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(S25-S68): **HPLC purity** information of novel final compounds **9a, 9c, 9h-9q, 9s, 7k, 7l** and selected known final compounds **10b, 10c, 10g, 10h, 8b, 8c, 8g, 8h, 8j**.

S25. HPLC purity data of novel final compounds **9a, 9c, 9h-9q, 9s, 7k, 7l** and selected known final compounds **10b, 10c, 10g, 10h, 8b, 8c, 8g, 8h, 8j** in tabular form.

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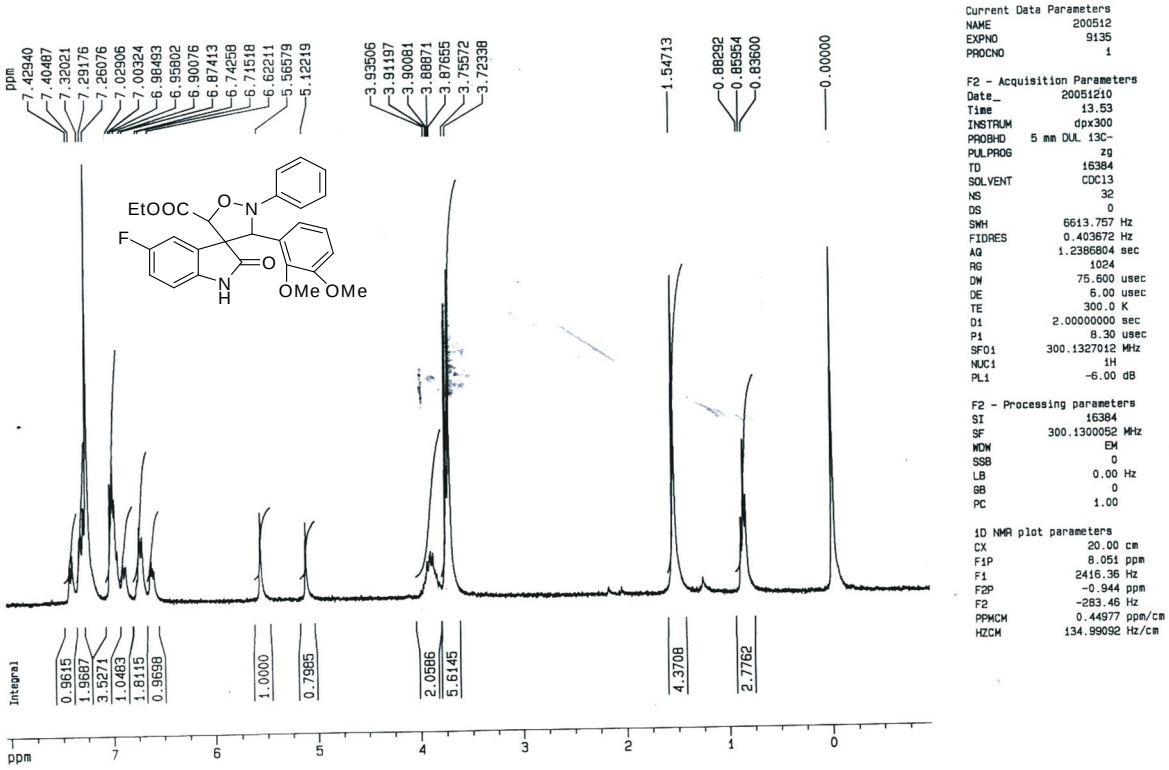
(S69-S84): **2D (cosy, hsqc, hmbc) and 1D (NOESY) NMR spectra** for compounds **10c, 8d, 9l and 7l**.

^{1}H NMR (Bruker AC-300 Avance, 300 MHz, $CDCl_3$) of compound 9k



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PULPROG	zg
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RG	1024
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D1	2.00000000 sec
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NUC1	1H
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F2 - Processing parameters

SI	16384
SF	300.1300052 MHz
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1D NMR plot parameters

CX	20.00 cm
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F1	2416.36 Hz
F2P	-0.944 ppm
F2	-283.46 Hz
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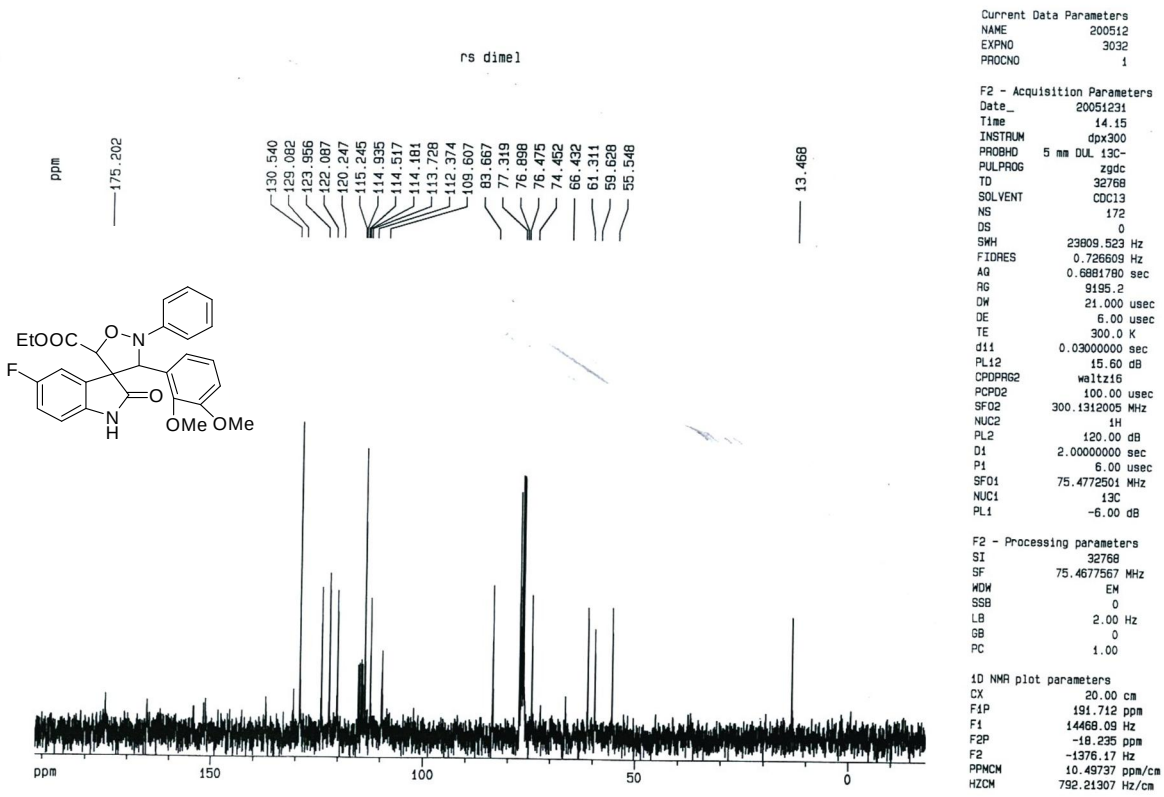
HZCM	134.99092 Hz/cm

^{13}C NMR (Bruker AC-300 Avance, 75.5 MHz, $CDCl_3$) of compound 9k



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TD 32768
SOLVENT CDCl3
NS 172
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SWH 23809.523 Hz
FIDRES 0.726609 Hz
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RG 9195.2
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DE 6.00 usec
TE 300.0 K
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PL12 15.60 dB
CPDPRG2 waltz16
PCPD2 100.00 usec
SFO2 300.1312005 MHz
NUC2 1H
PL2 120.00 dB
D1 2.00000000 sec
P1 6.00 usec
SFO1 75.4772501 MHz
NUC1 13C
PL1 -6.00 dB

F2 - Processing parameters
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WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 191.712 ppm
F1 14468.09 Hz
F2P -18.235 ppm
F2 -1376.17 Hz
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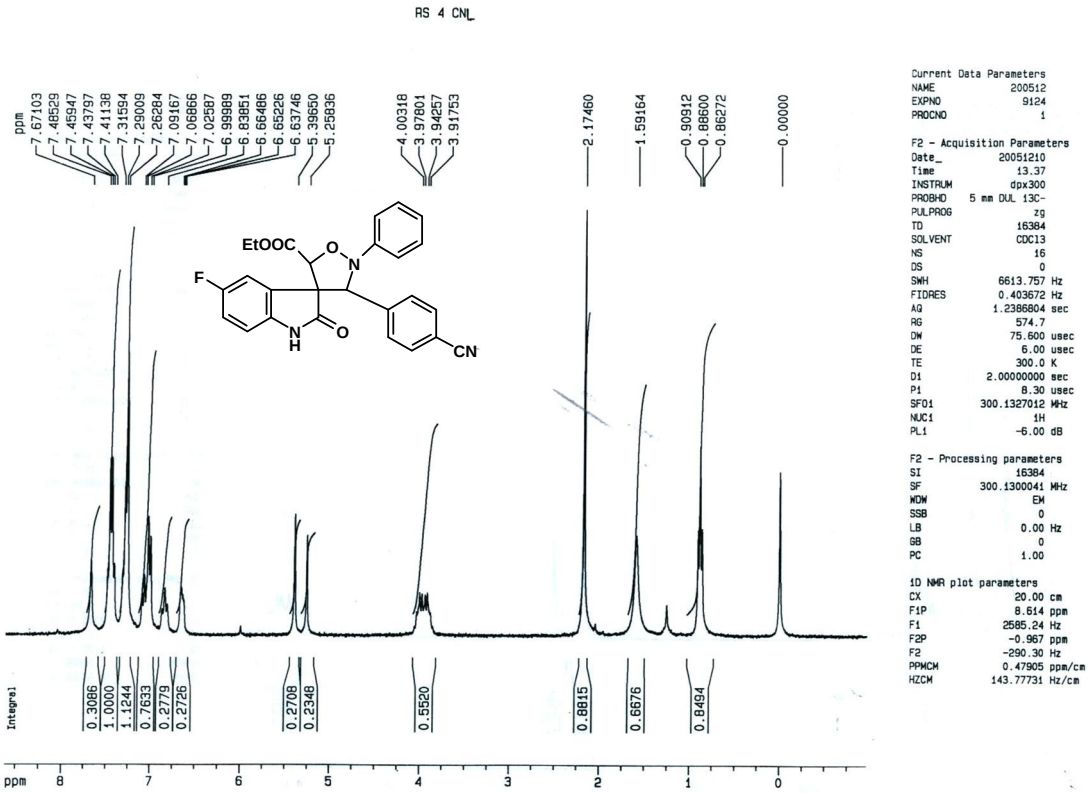
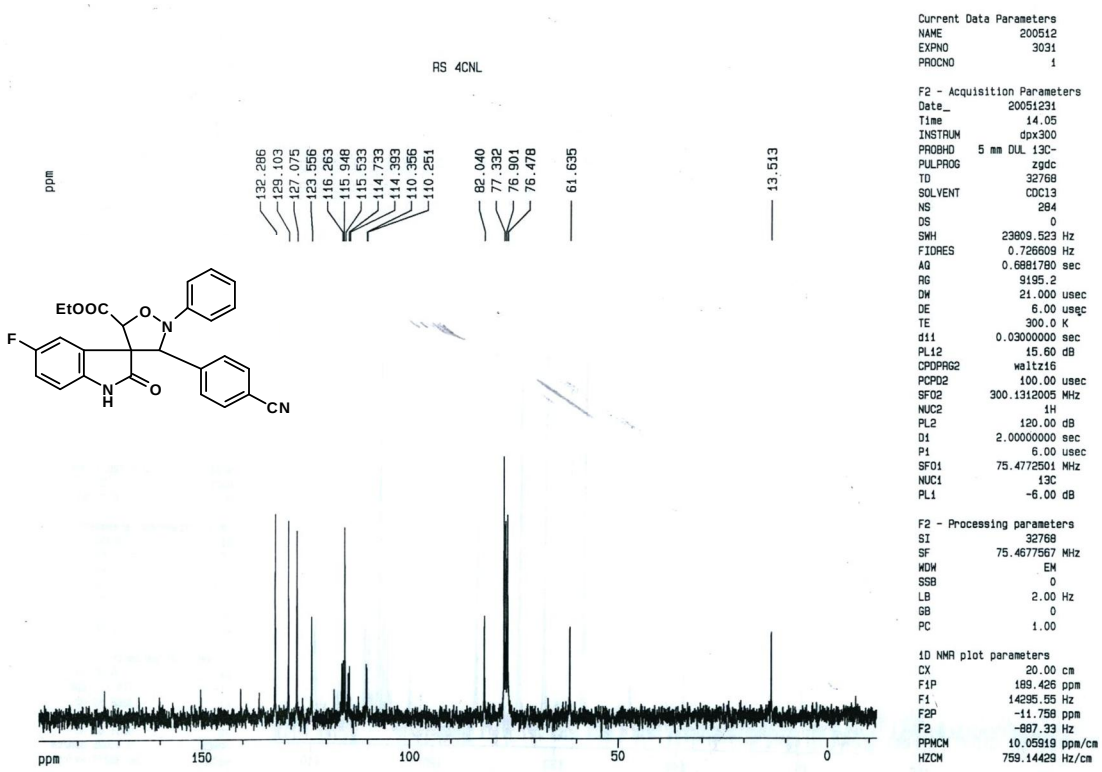
HZCM 792.21307 Hz/cm

^{1}H NMR (Bruker AC-300 Avance, 300 MHz, $CDCl_3$) of compound 9l



^{13}C NMR (Bruker AC-300 Avance, 75.5 MHz, $CDCl_3$) of compound 9l



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TD 32768
SOLVENT CDCl3
NS 284
DS 0
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 0.6881780 sec
RG 9195.2
DW 21.000 usec
DE 6.00 usec
TE 300.0 K
d11 0.03000000 sec
PL12 15.60 dB
CPDPRG2 waltz16
PCPD2 100.00 usec
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NUC2 1H
PL2 120.00 dB
D1 2.00000000 sec
P1 6.00 usec
SFO1 75.4772501 MHz
NUC1 13C
PL1 -6.00 dB

F2 - Processing parameters
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SF 75.4677567 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 189.426 ppm
F1 14295.55 Hz
F2P -11.758 ppm
F2 -887.33 Hz
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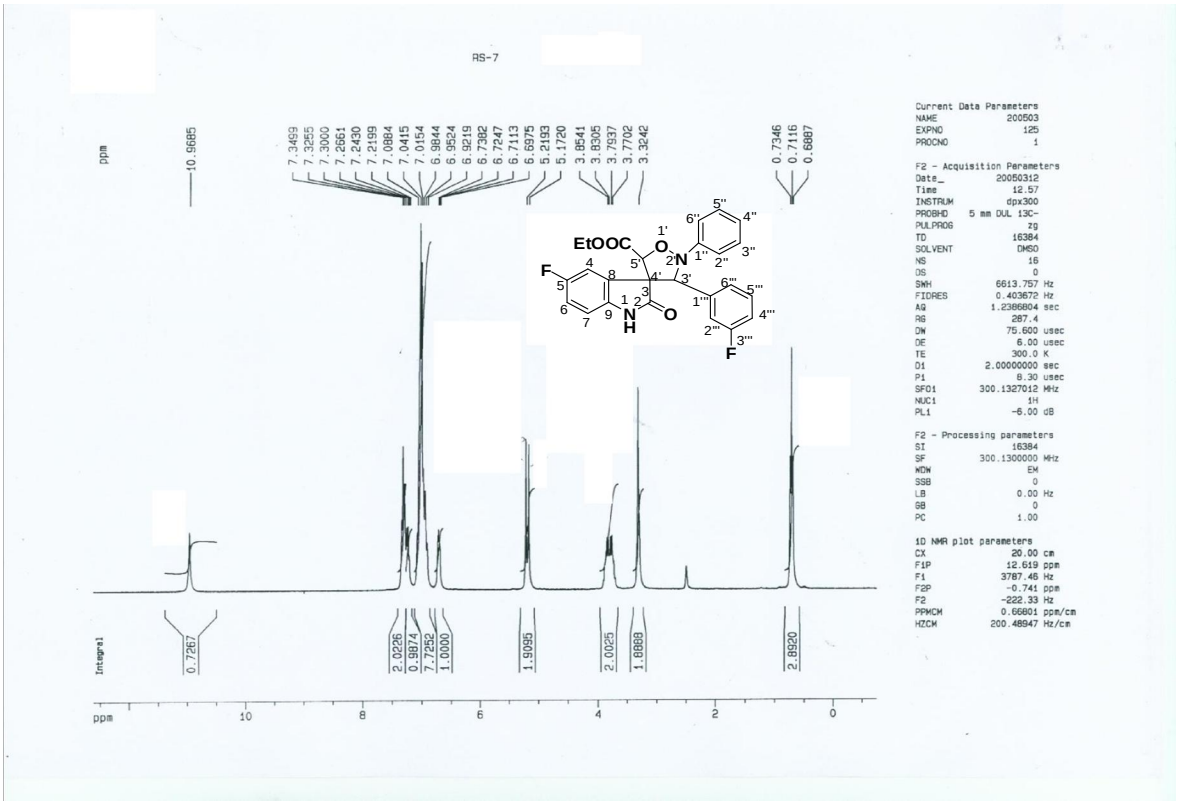
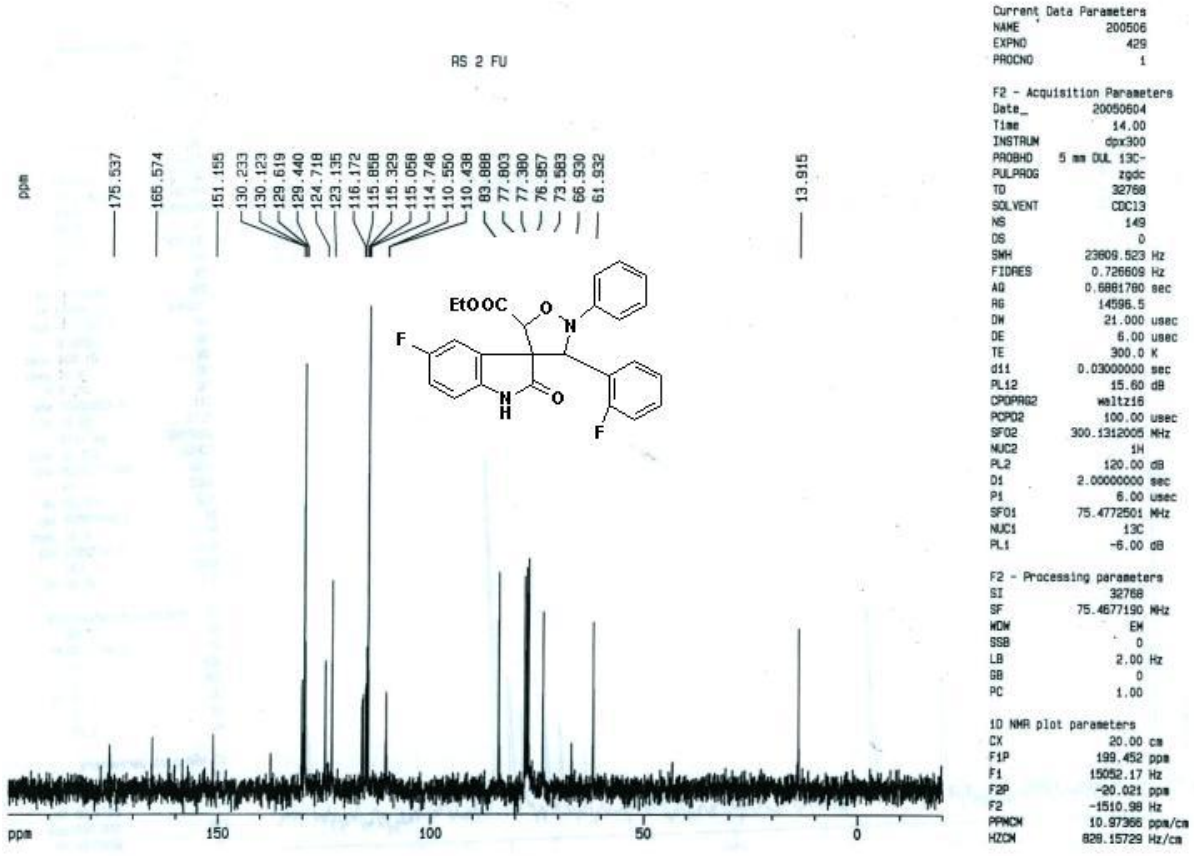
HZCM 759.14429 Hz/cm

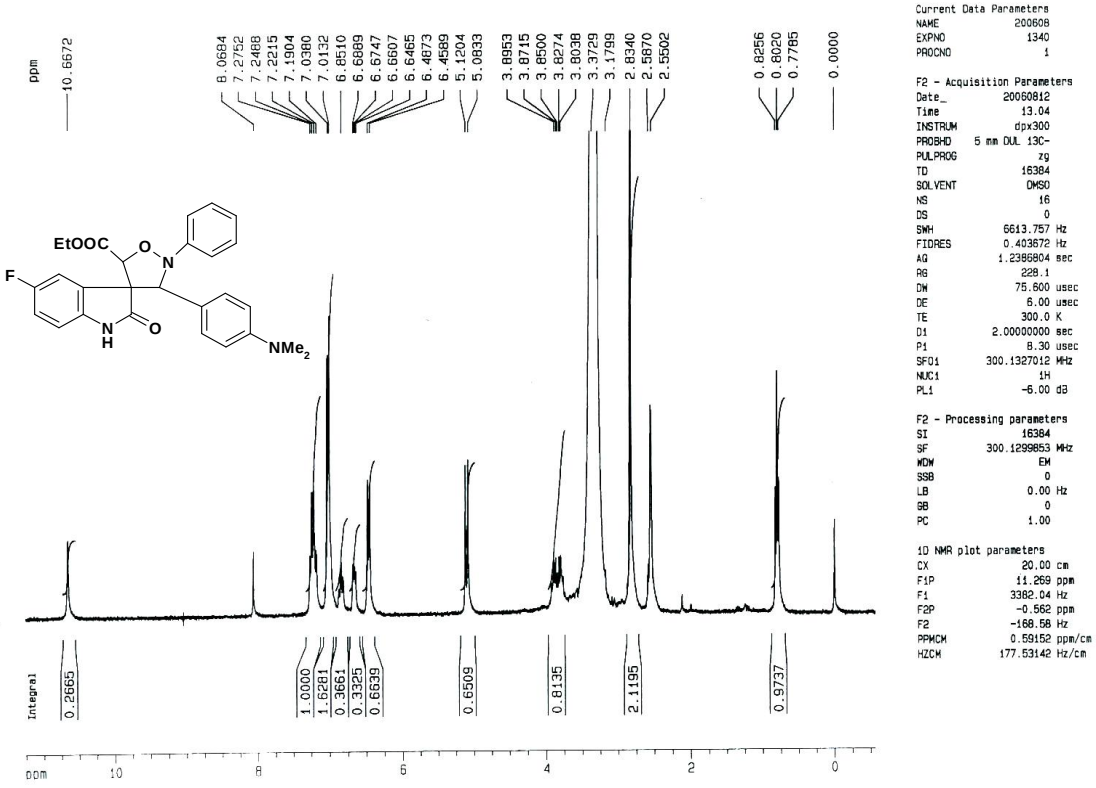
^{1}H NMR (Bruker AC-300 Avance, 300 MHz, $CDCl_3$) of compound 9n



^{13}C NMR (Bruker AC-300 Avance, 75.5 MHz, DMSO) of compound 9n



^{1}H NMR (Bruker AC-300 Avance, 300 MHz, DMSO) of compound 9o



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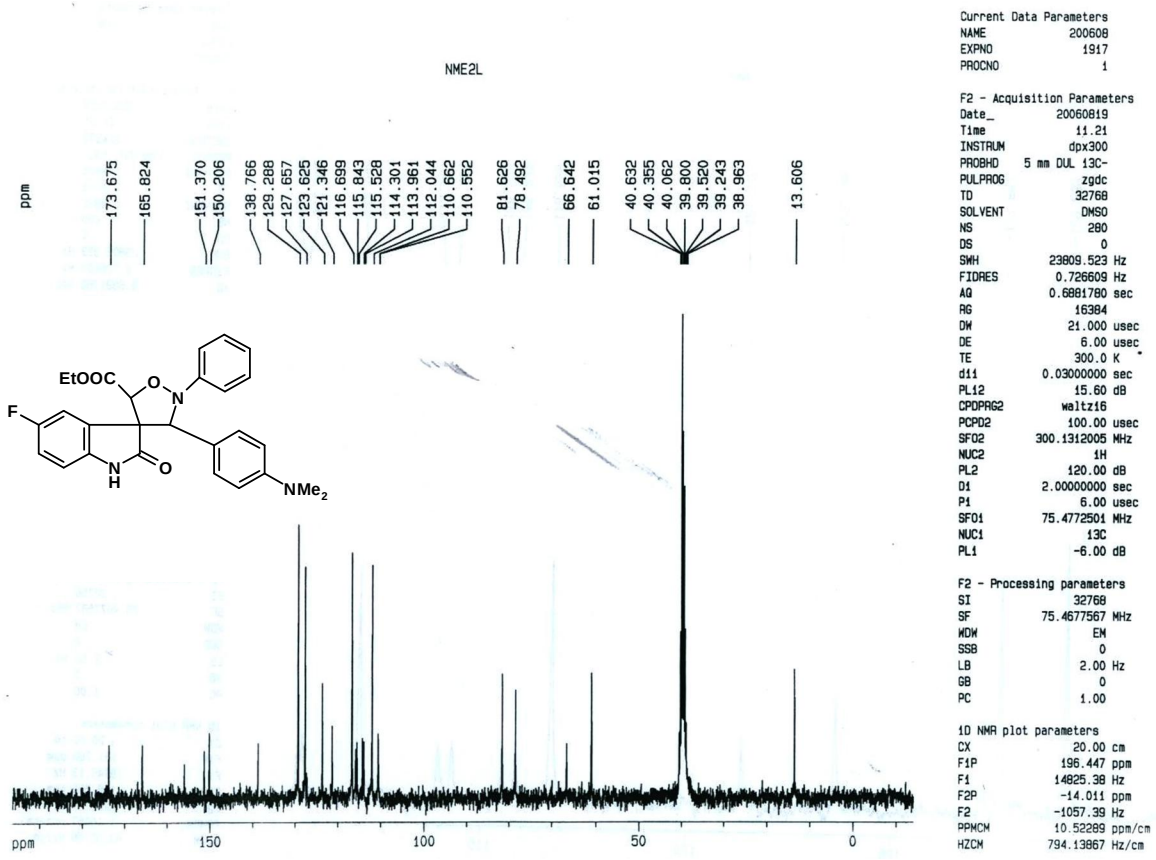
PULPROG zg
TD 16384
SOLVENT DMSO
NS 16
DS 0
SWH 6613.757 Hz
FIDRES 0.403672 Hz
AQ 1.2386804 sec
RG 228.1
DW 75.600 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
P1 8.30 usec
SFO1 300.1327012 MHz
NUC1 1H
PL1 -6.00 dB

F2 - Processing parameters
SI 16384
SF 300.1299853 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 11.269 ppm
F1 3382.04 Hz
F2P -0.562 ppm
F2 -168.58 Hz
PPMCM 0.59152 ppm/cm
HZCM 177.53142 Hz/cm

^{13}C NMR (Bruker AC-300 Avance, 75.5 MHz, DMSO) of compound 9o



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PROCNO 1

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Time 11.21
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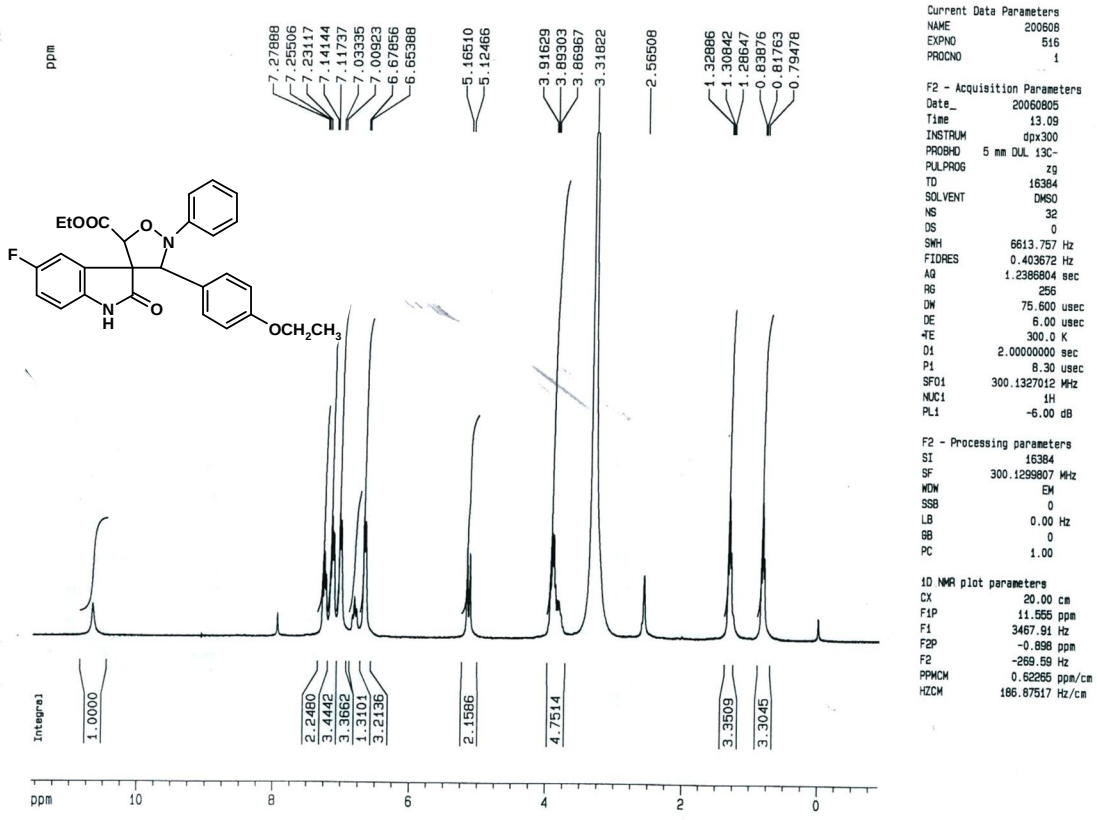
PULPROG zgdc
TD 32768
SOLVENT DMSO
NS 280
DS 0
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 0.6881780 sec
RG 16384
DW 21.000 usec
DE 6.00 usec
TE 300.0 K
d11 0.03000000 sec
PL12 15.60 dB
CPDPRG2 waltz16
PCPD2 100.00 usec
SFO2 300.1312005 MHz
NUC2 1H
PL2 120.00 dB
D1 2.00000000 sec
P1 6.00 usec
SFO1 75.4772501 MHz
NUC1 13C
PL1 -6.00 dB

F2 - Processing parameters
SI 32768
SF 75.4677567 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 196.447 ppm
F1 14825.38 Hz
F2P -14.011 ppm
F2 -1057.39 Hz
PPMCM 10.52289 ppm/cm
HZCM 794.13867 Hz/cm

^{1}H NMR (Bruker AC-300 Avance, 300 MHz, DMSO) of compound 9p



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PROCNO 1

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PULPROG zg
TD 16384
SOLVENT DMSO
NS 32
DS 0
SWH 6613.757 Hz
FIDRES 0.403672 Hz
AQ 1.2386804 sec
RG 256
DW 75.600 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
P1 8.30 usec
SFO1 300.1327012 MHz
NUC1 1H
PL1 -6.00 dB

F2 - Processing parameters
SI 16384
SF 300.1299807 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 11.555 ppm
F1 3467.91 Hz
F2P -0.898 ppm
F2 -269.59 Hz
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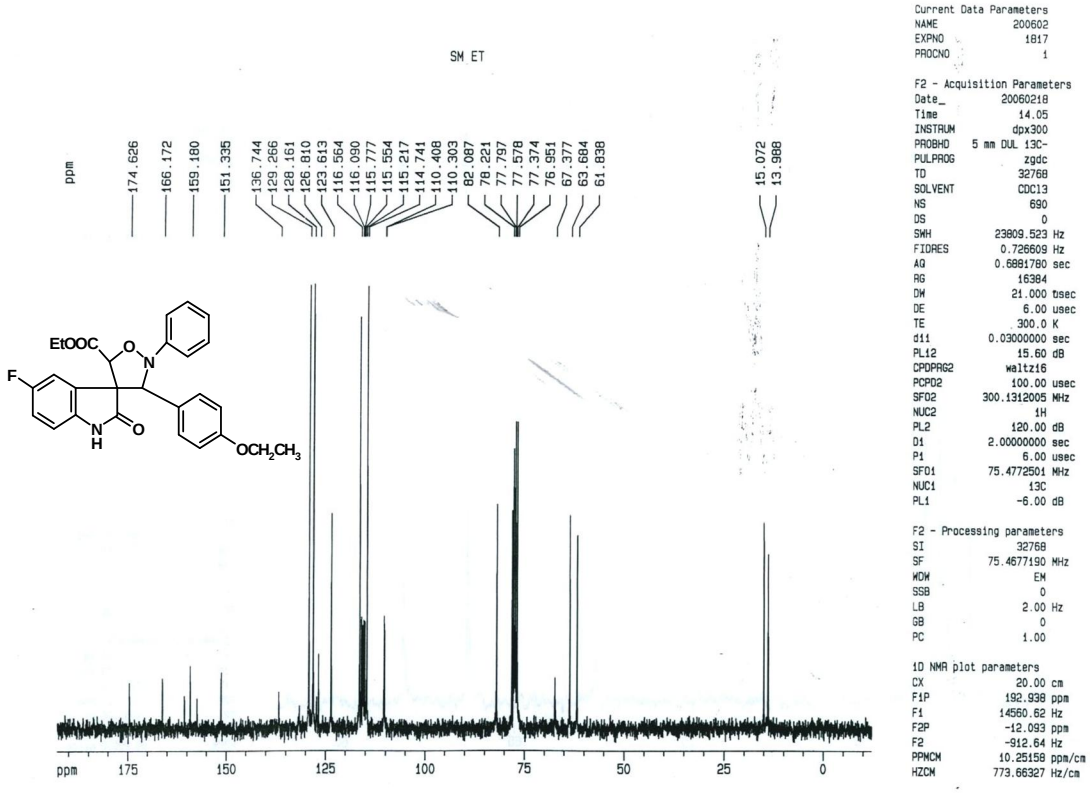
HZCM 186.87517 Hz/cm

^{13}C NMR (Bruker AC-300 Avance, 75.5 MHz, $CDCl_3$) of compound 9p



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EXPNO	1817
PROCNO	1

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PULPROG	zgdc
TD	32768
SOLVENT	CDCl3
NS	690
DS	0
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FIDRES	0.726609 Hz
AQ	0.6881780 sec
RG	16384
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DE	6.00 usec
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PL12	15.60 dB
CPDPRG2	waltz16
PCPD2	100.00 usec
SFO2	300.1312005 MHz
NUC2	1H
PL2	120.00 dB
D1	2.00000000 sec
P1	6.00 usec
SFO1	75.4772501 MHz
NUC1	13C
PL1	-6.00 dB

F2 - Processing parameters

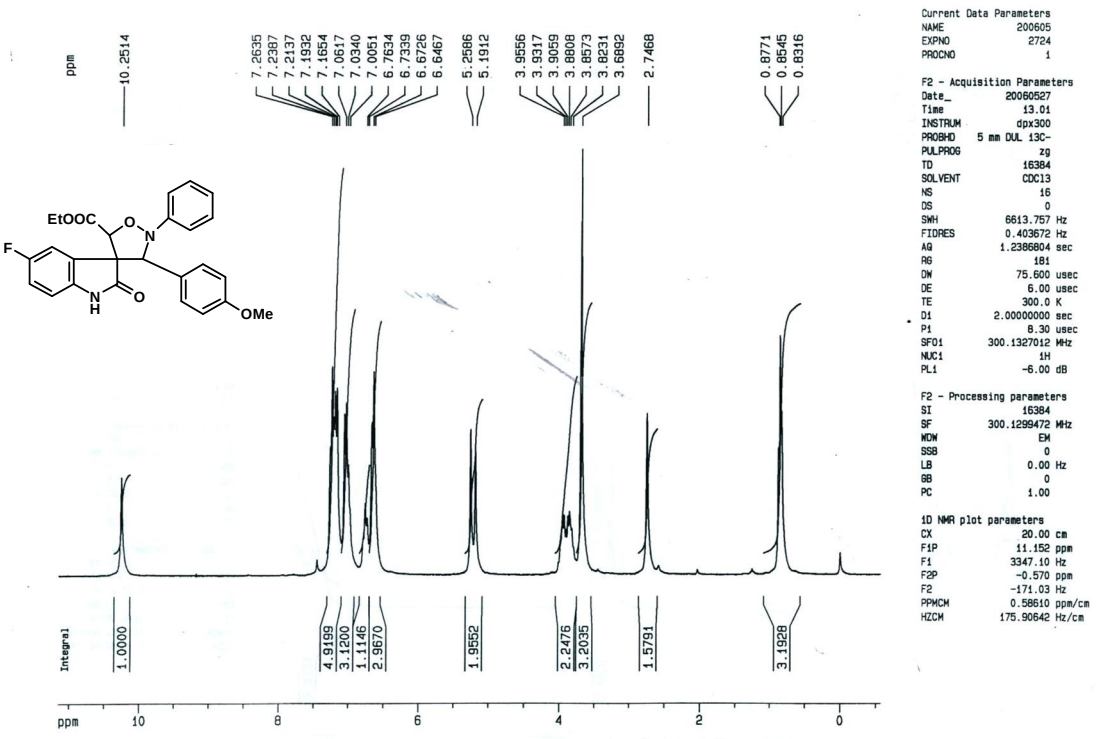
SI	32768
SF	75.4677190 MHz
WDW	EM
SSB	0
LB	2.00 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
F1P	192.938 ppm
F1	14560.62 Hz
F2P	-12.093 ppm
F2	-912.64 Hz
PPMCM	10.25158 ppm/cm
HZCM	773.66327 Hz/cm

Electronic Supplementary Material (ESI) for Medicinal Chemistry Communications

^{1}H NMR (Bruker AC-300 Avance, 300 MHz, mixture of $CDCl_3$ and DMSO) of compound 9q



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EXPNO	2724
PROCNO	1

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PULPROG	zg
TD	16384
SOLVENT	CDCl3
NS	16
DS	0
SWH	6613.757 Hz
FIDRES	0.403672 Hz
AQ	1.2386804 sec
RG	181
DW	75.600 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
P1	8.30 usec
SFO1	300.1327012 MHz
NUC1	1H
PL1	-6.00 dB

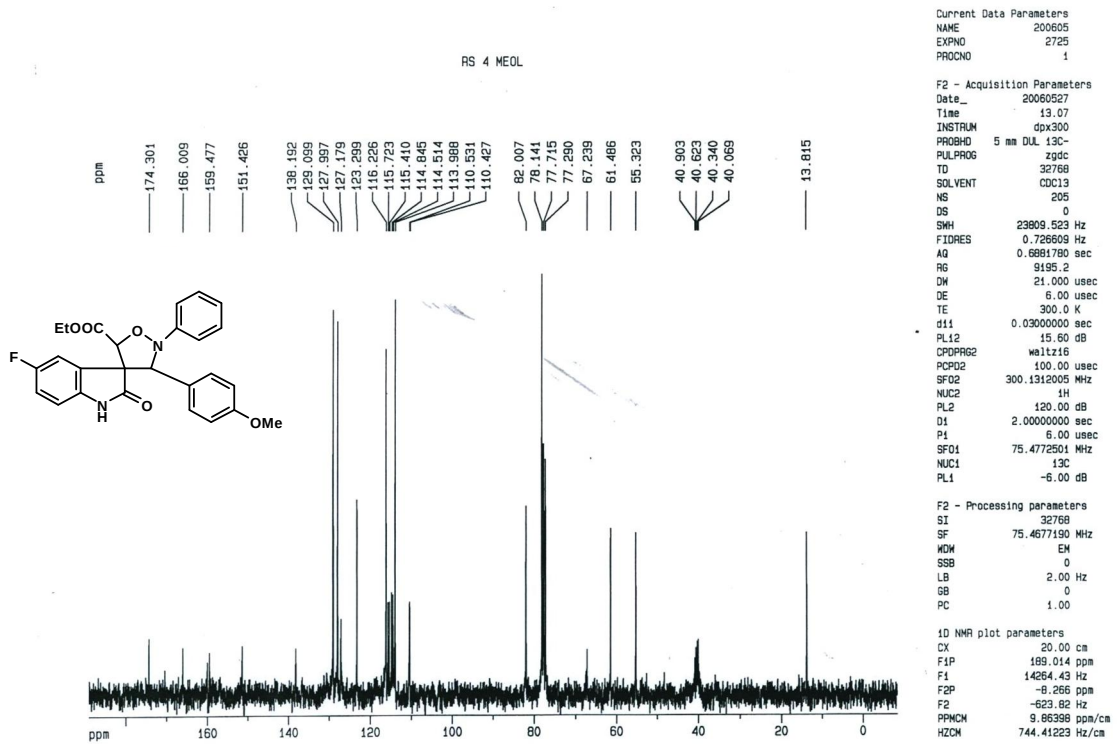
F2 - Processing parameters

SI	16384
SF	300.1299472 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

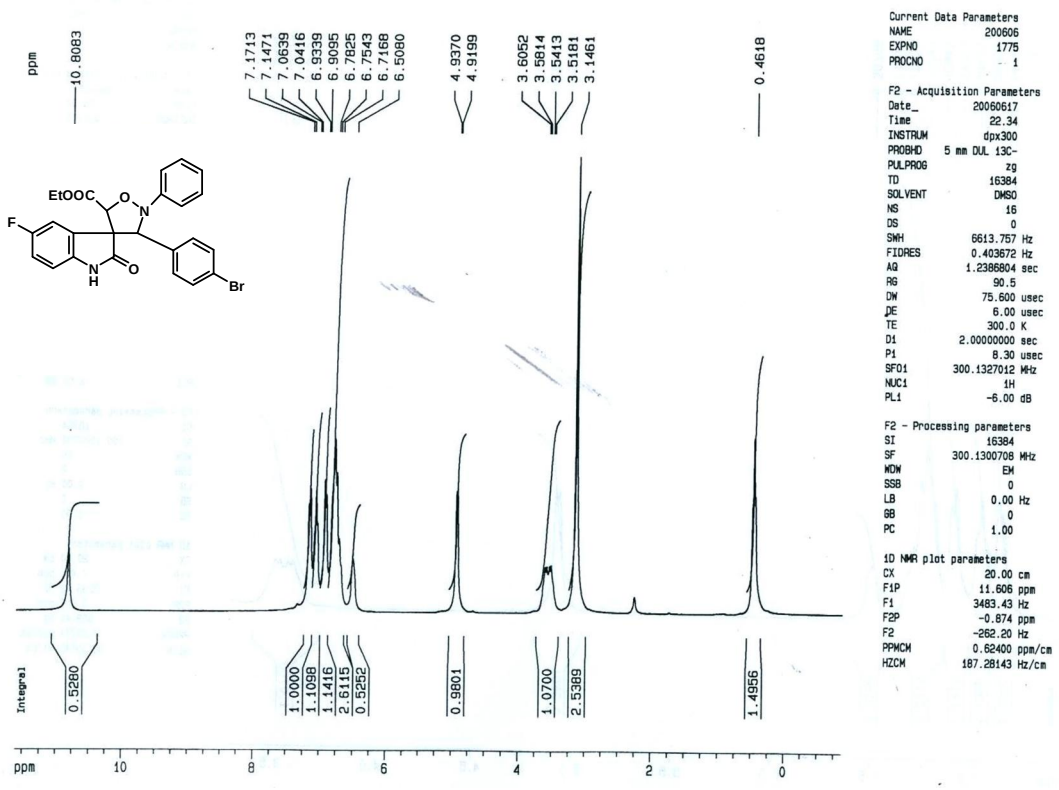
1D NMR plot parameters

CX	20.00 cm
F1P	11.152 ppm
F1	3347.10 Hz
F2P	-0.570 ppm
F2	-171.03 Hz
PPMCM	0.58610 ppm/cm
HZCM	175.90642 Hz/cm

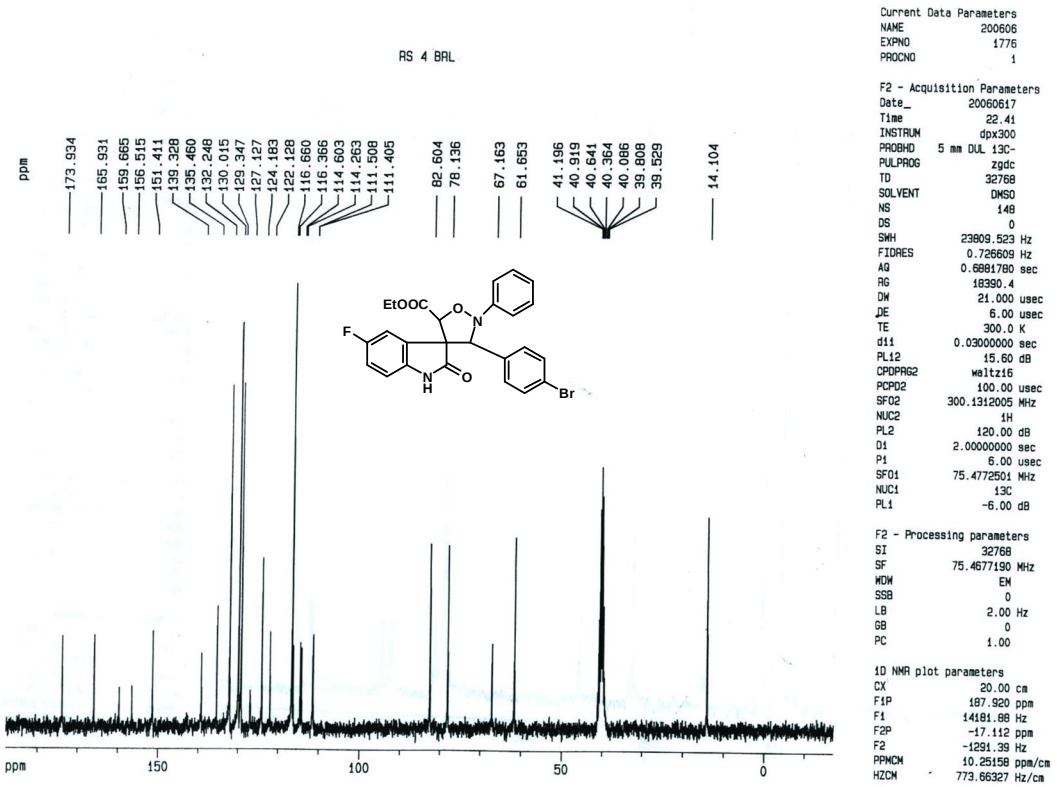
^{13}C NMR (Bruker AC-300 Avance, 75.5 MHz, mixture of $CDCl_3$ and DMSO) of compound 9q



^{1}H NMR (Bruker AC-300 Avance, 300 MHz, DMSO) of compound 9c



^{13}C NMR (Bruker AC-300 Avance, 75.5 MHz, DMSO) of compound 9c



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RG 18390.4
DW 21.000 usec
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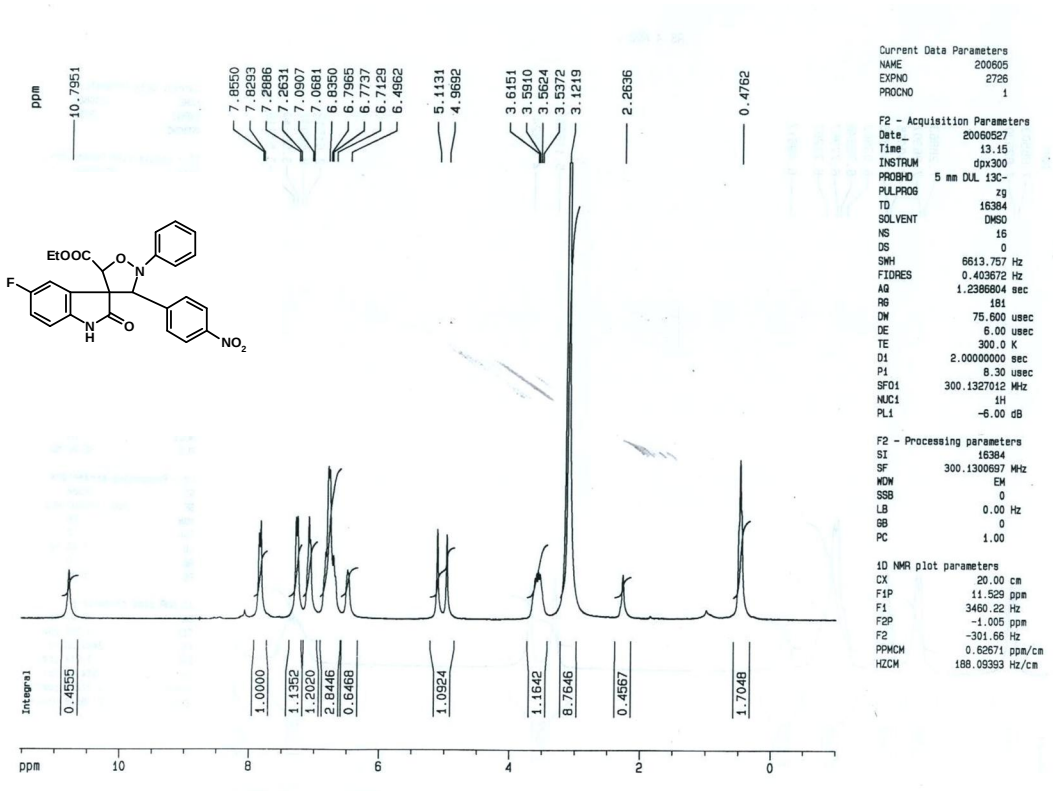
PL12 15.60 dB
CPDPRG2 waltz16
PCPD2 100.00 usec
SFO2 300.1312005 MHz
NUC2 1H
PL2 120.00 dB
D1 2.00000000 sec
P1 6.00 usec
SFO1 75.4772501 MHz
NUC1 13C
PL1 -6.00 dB

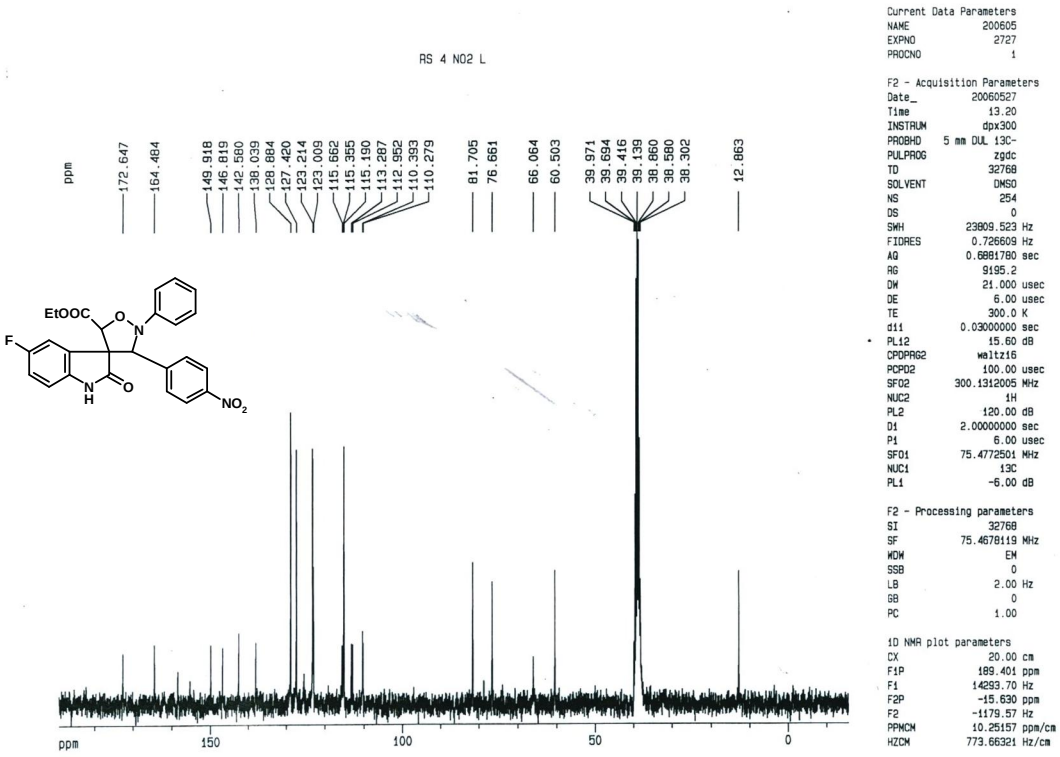
F2 - Processing parameters
SI 32768
SF 75.4677190 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 187.920 ppm
F1 14181.88 Hz
F2P -17.112 ppm
F2 -1291.39 Hz
PPMCM 10.25158 ppm/cm
HZCM 773.66327 Hz/cm

^{1}H NMR (Bruker AC-300 Avance, 300 MHz, DMSO) of compound 9e



^{13}C NMR (Bruker AC-300 Avance, 75.5 MHz, DMSO) of compound 9e

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PROCNO                     1

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PULPROG                zgdc
TD                     32768
SOLVENT                DMSO
NS                       254
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SWH                23809.523 Hz
FIDRES             0.726609 Hz
AQ                 0.6881780 sec
RG                    9195.2
DW                    21.000 usec
DE                     6.00 usec
TE                     300.0 K
d11                0.03000000 sec
PL12                   15.60 dB
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SFO2               300.1312005 MHz
NUC2                       1H
PL2                   120.00 dB
D1                 2.00000000 sec
P1                     6.00 usec
SFO1               75.4772501 MHz
NUC1                       13C
PL1                    -6.00 dB

F2 - Processing parameters
SI                     32768
SF                 75.4678119 MHz
WDW                       EM
SSB                        0
LB                      2.00 Hz
GB                         0
PC                      1.00

1D NMR plot parameters
CX                     20.00 cm
F1P                   189.401 ppm
F1                   14293.70 Hz
F2P                   -15.630 ppm
F2                   -1179.57 Hz
PPMCM                10.25157 ppm/cm
HZCM                 773.66321 Hz/cm
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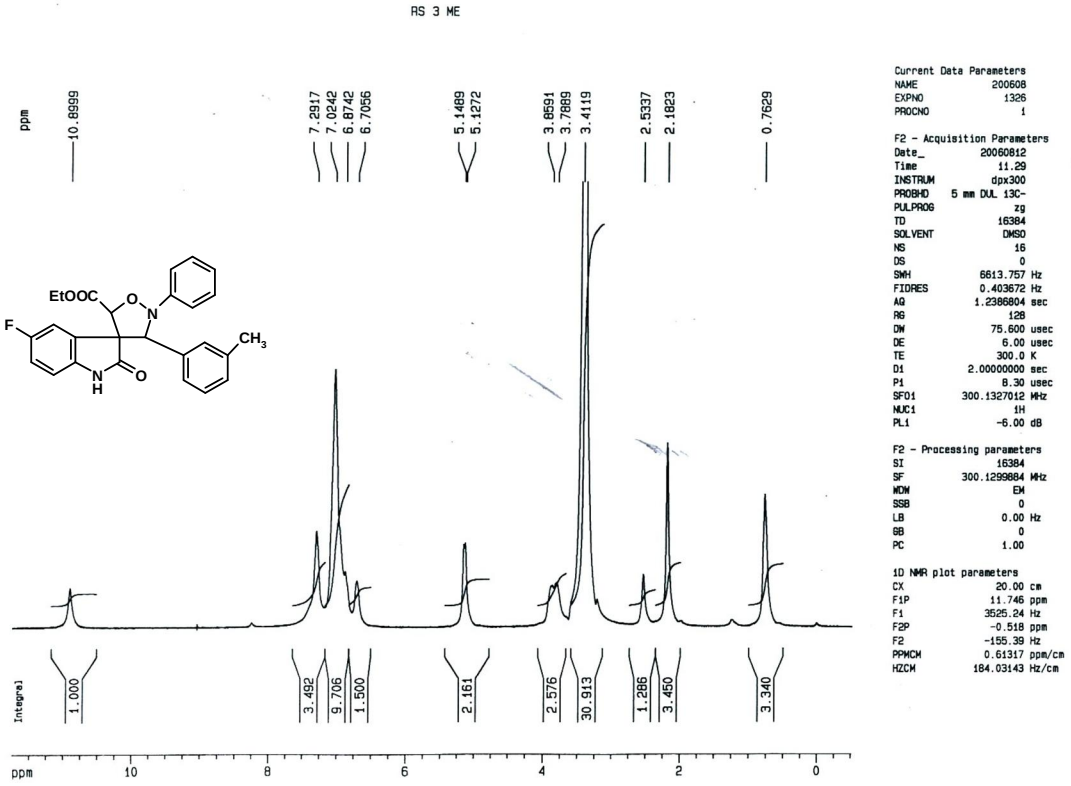
^{1}H NMR (Bruker AC-300 Avance, 300 MHz, DMSO) of compound 9h



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PROCNO 1

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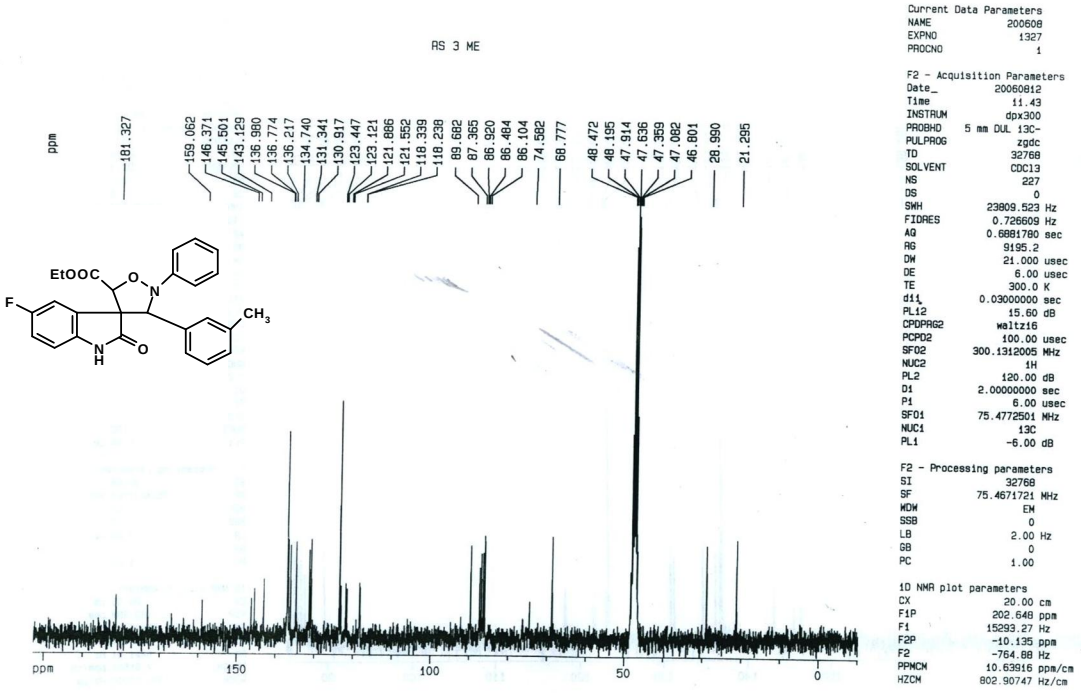
PULPROG zg
TD 16384
SOLVENT DMSO
NS 16
DS 0
SWH 6613.757 Hz
FIDRES 0.403672 Hz
AQ 1.2386804 sec
RG 128
DW 75.600 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
P1 8.30 usec
SFO1 300.1327012 MHz
NUC1 1H
PL1 -6.00 dB

F2 - Processing parameters
SI 16384
SF 300.1299884 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 11.746 ppm
F1 3525.24 Hz
F2P -0.518 ppm
F2 -155.39 Hz
PPMCM 0.61317 ppm/cm
HZCM 184.03143 Hz/cm

^{13}C NMR (Bruker AC-300 Avance, 75.5 MHz, $CDCl_3$) of compound 9h



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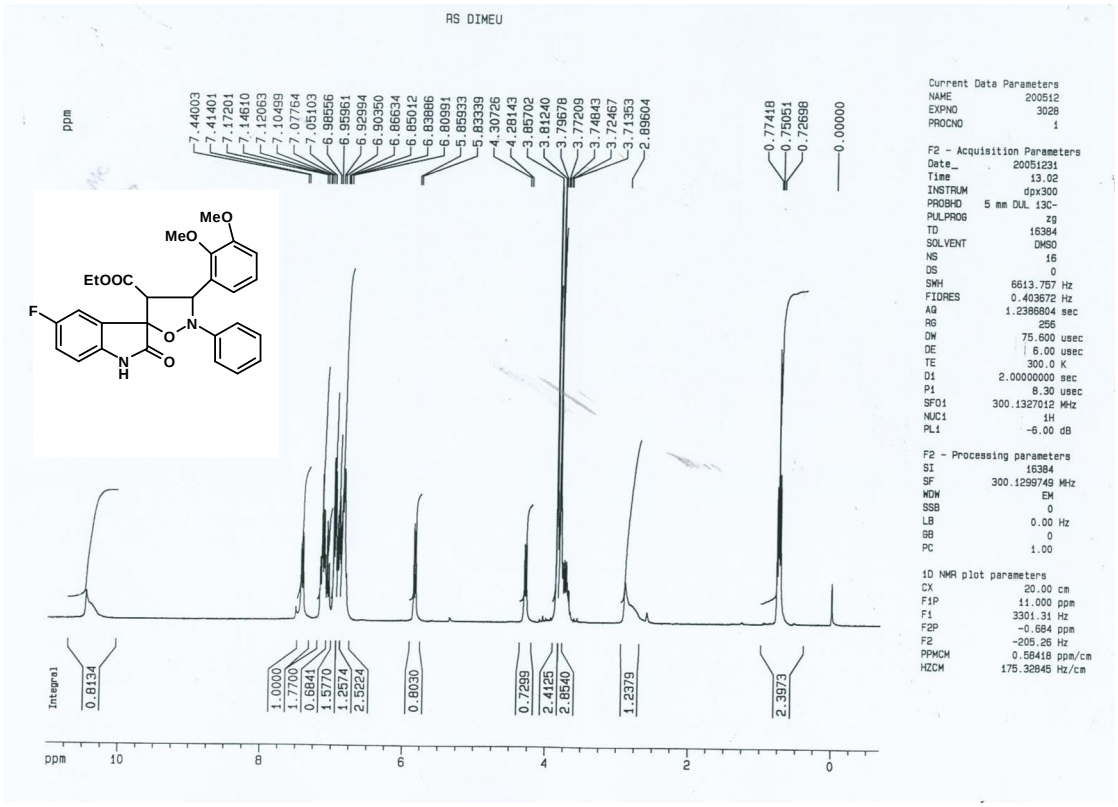
FIDRES 0.726609 Hz
AQ 0.6881780 sec
RG 9195.2
DW 21.000 usec
DE 6.00 usec
TE 300.0 K
d11 0.03000000 sec
PL12 15.60 dB
CPDPRG2 waltz16
PCPD2 100.00 usec
SF02 300.1312005 MHz
NUC2 1H
PL2 120.00 dB
D1 2.00000000 sec
P1 6.00 usec
SF01 75.4772501 MHz
NUC1 13C
PL1 -6.00 dB

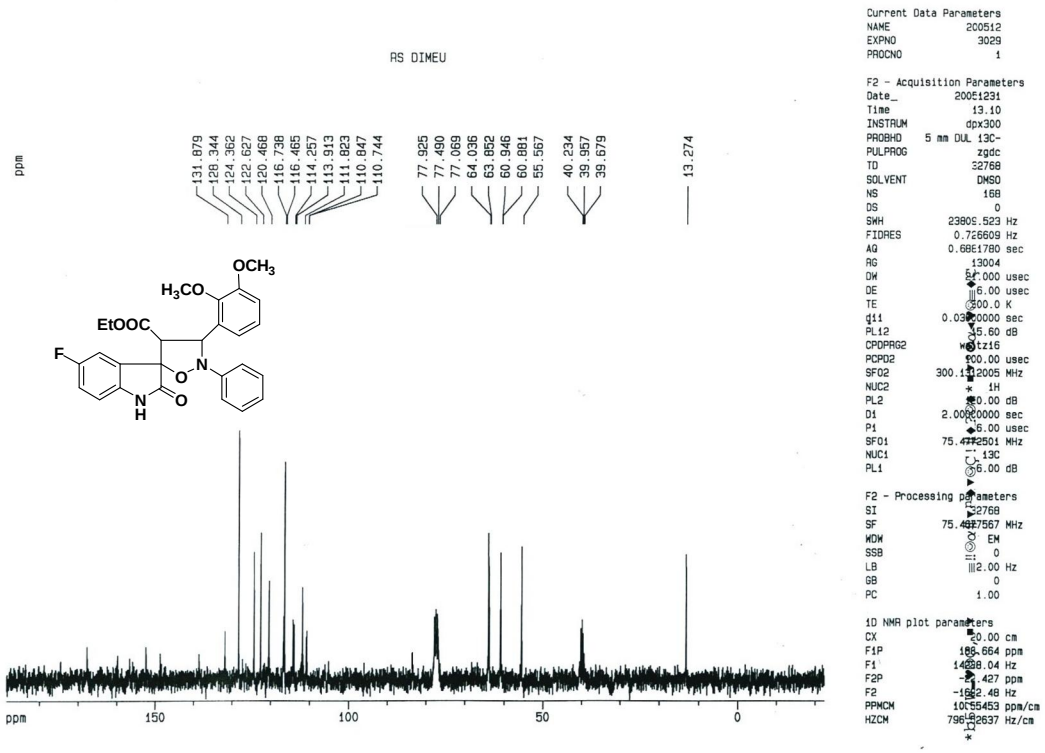
F2 - Processing parameters
SI 32768
SF 75.4671721 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 202.648 ppm
F1 15293.27 Hz
F2P -10.135 ppm
F2 -764.88 Hz
PPMCM 10.63916 ppm/cm
HZCM 802.90747 Hz/cm

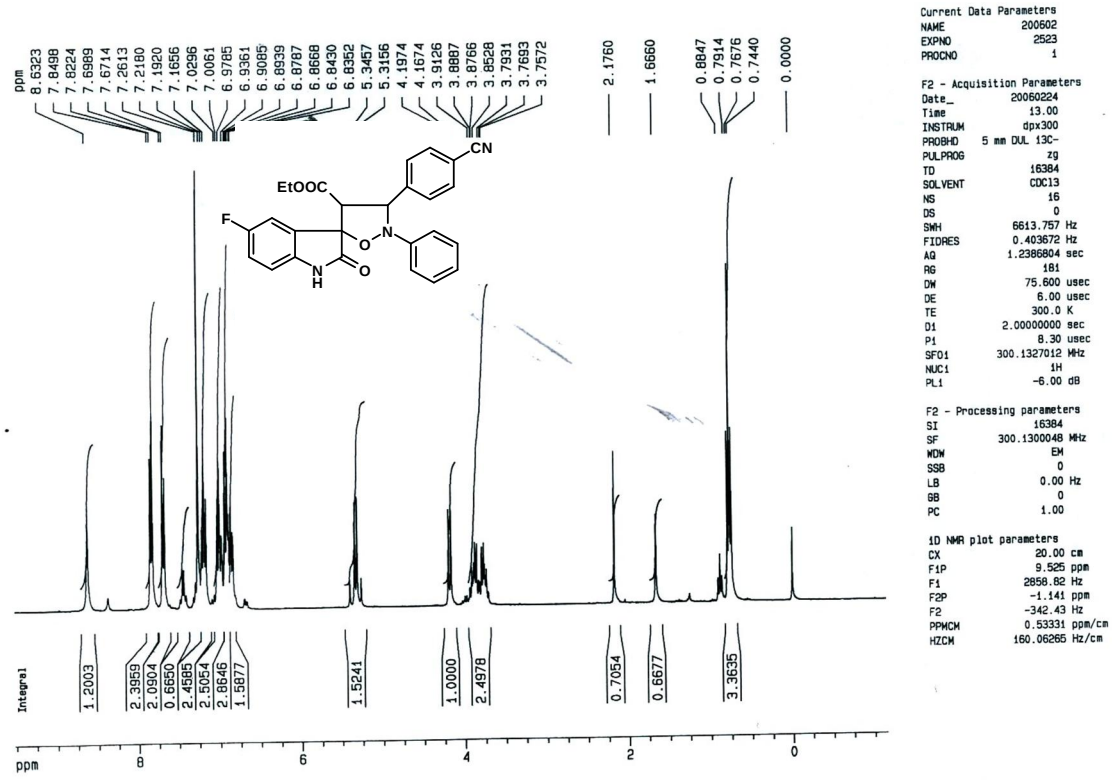
^{1}H NMR (Bruker AC-300 Avance, 300 MHz, DMSO) of compound 7k



^{13}C NMR (Bruker AC-300 Avance, 75.5 MHz, DMSO) of compound 7k



^{1}H NMR (Bruker AC-300 Avance, 300 MHz, $CDCl_3$) of compound 7l



Current Data Parameters

NAME	200602
EXPNO	2523
PROCNO	1

F2 - Acquisition Parameters

Date_	20060224
Time	13.00
INSTRUM	dpx300
PROBHD	5 mm DUL 13C-
PULPROG	zg
TD	16384
SOLVENT	CDCl3
NS	16
DS	0
SWH	6613.757 Hz
FIDRES	0.403672 Hz
AQ	1.2386804 sec
RG	181
DW	75.600 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
P1	8.30 usec
SFO1	300.1327012 MHz
NUC1	1H
PL1	-6.00 dB

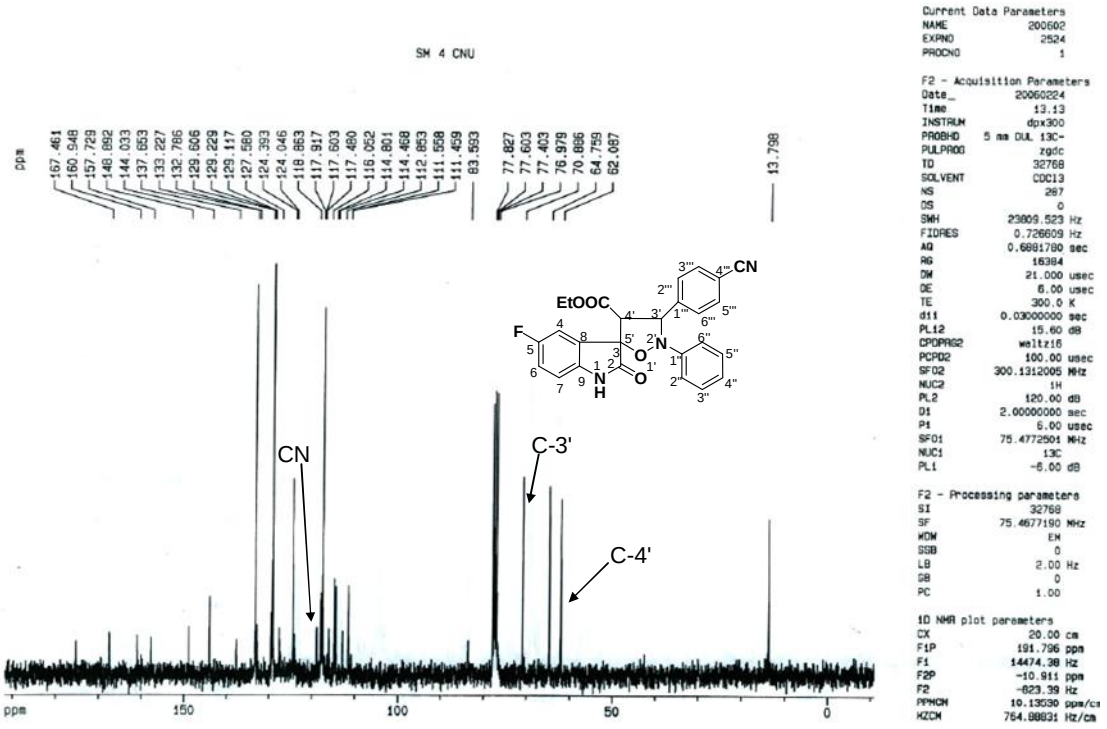
F2 - Processing parameters

SI	16384
SF	300.1300048 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
F1P	9.525 ppm
F1	2858.82 Hz
F2P	-1.141 ppm
F2	-342.43 Hz
PPMCM	0.53331 ppm/cm
HZCM	160.06265 Hz/cm

^{13}C NMR (Bruker AC-300 Avance, 75.5 MHz, $CDCl_3$) of compound 7l



Current Data Parameters
NAME 200602
EXPNO 2524
PROCNO 1

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Time 13.13
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PROBHD 5 mm DUL 13C-
PULPROG zgdc
TD 32768
SOLVENT CDCl3
NS 287
DS 0
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 0.6881790 sec
RG 16384
DW 21.000 usec
DE 6.00 usec
TE 300.0 K
d11 0.03000000 sec
PL12 15.60 dB
CPDPRG2 waltz16
PCPD2 100.00 usec
SFO2 300.1312005 MHz
NUC2 1H
PL2 120.00 dB
D1 2.00000000 sec
P1 6.00 usec
SFO1 75.4772501 MHz
NUC1 13C
PL1 -6.00 dB

F2 - Processing parameters
SI 32768
SF 75.4677190 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 191.796 ppm
F1 14474.38 Hz
F2P -10.911 ppm
F2 -823.39 Hz
PPMCM 10.13530 ppm/cm
HZCM 764.88831 Hz/cm

Part-B

HPLC purity information of novel final compounds

Compound	HPLC purity (20%Water / 80% Methanol)	HPLC purity (20%Water / 80% Acetonitrile)
9k	**100**	**99.3**
9l	**99.1**	**99.6**
9j	**100**	**99.4**
9m	**99.2**	**98.3**
9n	**99.4**	**98.2**
9i	**99.7**	**98.7**
9o	**97.5**	**98.2**
9p	**99.3**	**99.0**
9q	**99.3**	**100**
9c	**99.0**	**99.2**
9e	**98.5**	**99.3**
9r	**98.8**	**99.3**
9a	**99.0**	**98.7**
9h	**99.6**	**100**
9s	**99.1**	**99.6**
7k	**100**	**99.9**
7l	**98.1**	**100**

HPLC purity information of selected known final compounds

Compound	HPLC purity (20%Water / 80% Methanol)	HPLC purity (20%Water / 80% Acetonitrile)
10b	**99.4**	**100**
10c	**100**	**99.2**
10g	**100**	**99.2**
10h	**100**	**99.6**
8b	**100**	**98.2**
8c	**100**	**98.7**
8g	**100**	**99.6**
8h	**100**	**98.0**
8j	**100**	**99.6**

HPLC chromatograms of novel final compounds

Compound 9k: Solvent system: (20%water : 80%methanol)

Empower 2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	DiOMeL_20water_80methanol_2	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	20%water_80%Meth_1ml
Injection #:	1	Processing Method:	DiOMe_2
Injection Volume:	10.00 ul	Channel Name:	240.0nm
Run Time:	20.0 Minutes	Proc. Chnl. Descr.:	PDA 240.0 nm
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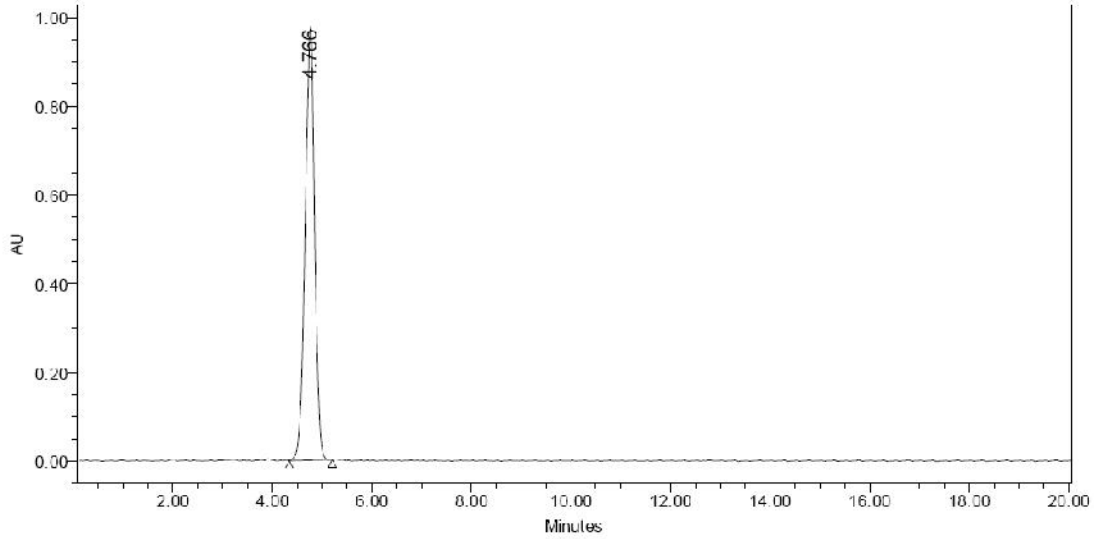
Date Processed:	5/3/2008 3:38:54 PM IST		



	RT	Area	% Area	Height
1	4.766	13034255	100.00	979794

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

Project Name: test_chemistry
Date Printed:
5/3/2008
3:39:27 PM Asia/Calcutta

Compound 9k:

Solvent system: (20%water : 80%Acetonitrile)

Empower 2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	DiOMeL_20water_80ACN_1	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	20_water_80_AcN_1ml
Injection #:	6	Processing Method:	DiOMeL_1
Injection Volume:	10.00 ul	Channel Name:	220.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	PDA 220.0 nm
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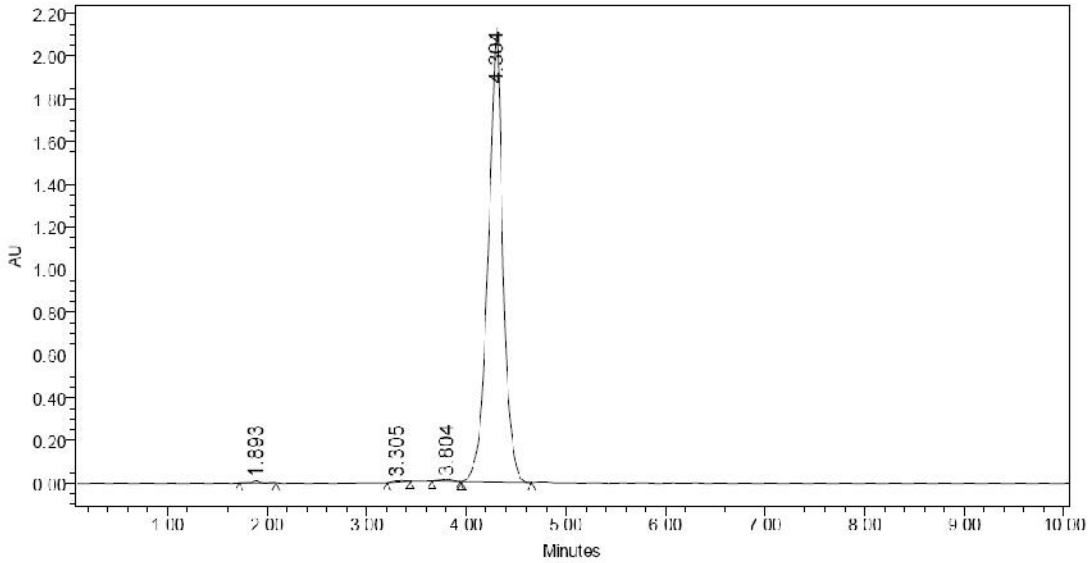

	RT	Area	% Area	Height
1	1.893	47634	0.21	8818
2	3.305	45465	0.20	5395
3	3.804	62430	0.28	6860
4	4.304	22028856	99.30	2118627

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

Project Name: test_chemistry
Date Printed: 5/8/2008
4:09:51 PM Asia/Calcutta

Compound 9l:
Solvent system: (20%water : 80%methanol)

Empower 2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	4CNL_20water_80methancl_1	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	20%water_80%Meth_1ml
Injection #:	3	Processing Method:	4CNL_1
Injection Volume:	10.00 ul	Channel Name:	235.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	PDA 235.0 nm
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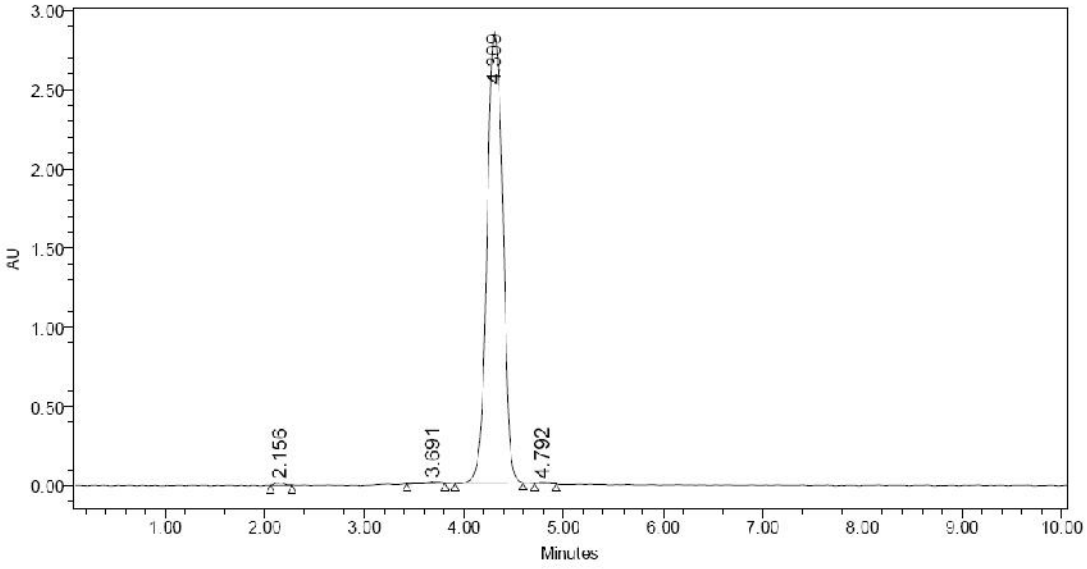

	RT	Area	% Area	Height
1	2.156	109801	0.35	16788
2	3.691	100748	0.32	10385
3	4.309	31401528	99.11	2853910
4	4.792	72579	0.23	7862

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

Project Name: test_chemistry
Date Printed:
5/6/2008
12:49:59 PM Asia/Calcutta

Compound 9l:

Solvent system: (20%water : 80%Acetonitrile)

Empower 2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	4CNL_20water_80ACN_2	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	20_water_80_AcN_1ml
Injection #:	2	Processing Method:	4CNL_2
Injection Volume:	10.00 ul	Channel Name:	240.0nm
Run Time:	20.0 Minutes	Proc. Chnl. Descr.:	PDA 240.0 nm
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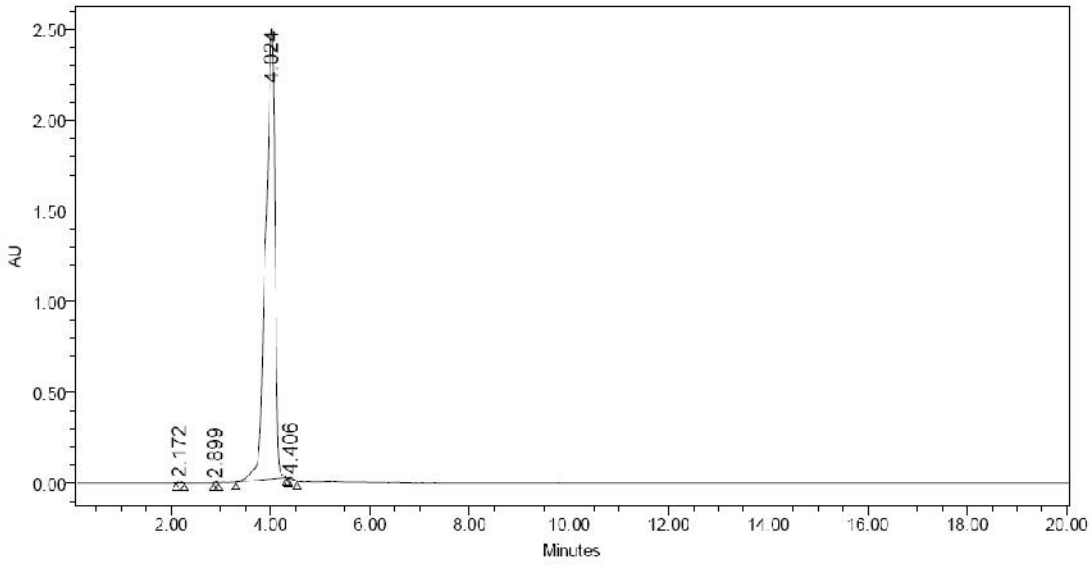
Date Processed:	5/7/2008 2:14:42 PM IST		



	RT	Area	% Area	Height
1	2.172	50940	0.16	13105
2	2.899	6748	0.02	1972
3	4.024	31742765	99.65	2485721
4	4.406	52616	0.17	9779

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

Project Name: test_chemistry
Date Printed:
5/7/2008
2:16:11 PM Asia/Calcutta

Compound 9j:
Solvent system: (20%water : 80%methanol)

Empower2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	3F-20water_80Methanol_1	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	20%water_80%Meth_1ml
Injection #:	1	Processing Method:	3F_1
Injection Volume:	10.00 ul	Channel Name:	220.0nm
Run Time:	30.0 Minutes	Proc. Chnl. Descr.:	PDA 220.0 nm
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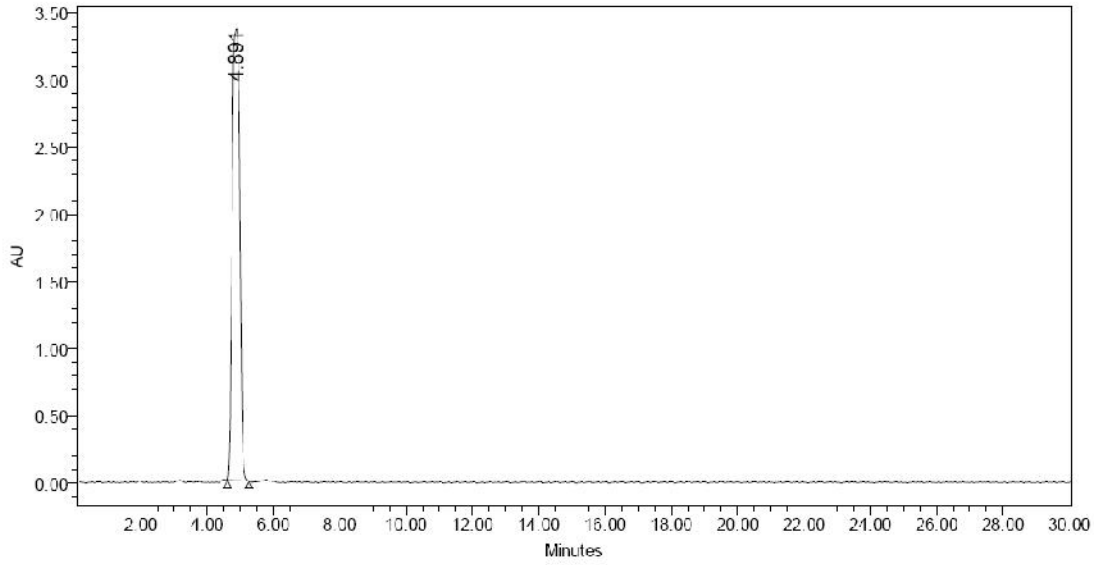
Date Processed:	5/2/2008 4:10:03 PM IST		



	RT	Area	% Area	Height
1	4.891	54562286	100.00	3370468

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

Project Name: test_chemistry
Date Printed:
5/2/2008
4:11:54 PM Asia/Calcutta

Compound 9j:

Solvent system: (20%water : 80%Acetonitrile)

Empower2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	3F_20water_80ACN_1	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	20_water_80_AcN_1ml
Injection #:	2	Processing Method:	3F_1_ACN
Injection Volume:	10.00 ul	Channel Name:	235.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	PDA 235.0 nm
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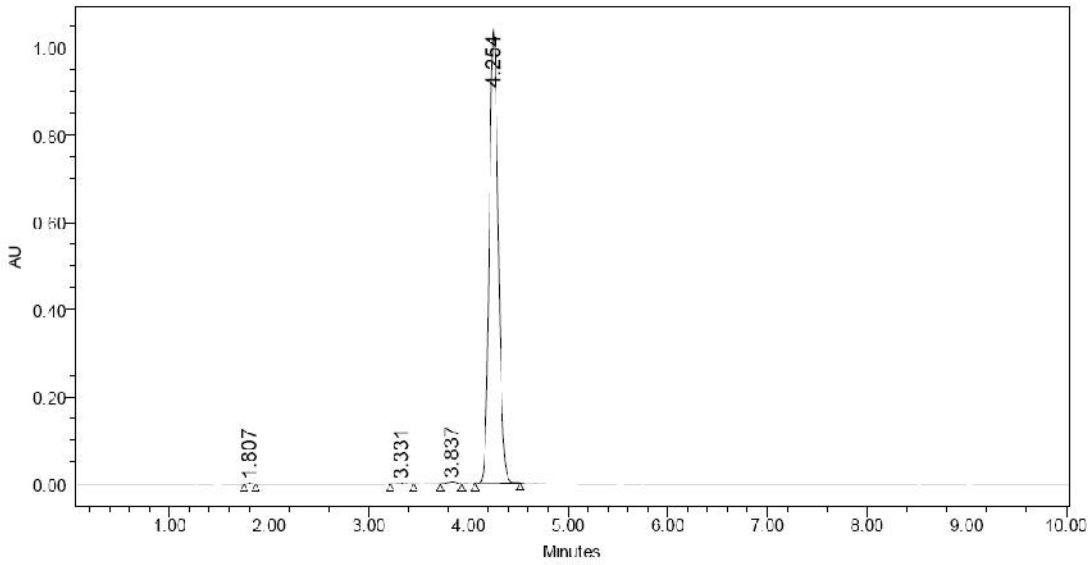

	RT	Area	% Area	Height
1	1.807	5833	0.09	1608
2	3.331	7231	0.11	896
3	3.837	23733	0.36	3950
4	4.254	6550451	99.44	1037974

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

Project Name: test_chemistry
Date Printed:
5/7/2008
3:36:59 PM Asia/Calcutta

Compound 9m:
Solvent system: (20%water : 80%methanol)

Empower 2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	DIF_20water_80methanol_f	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	20%water_80%Meth_1ml
Injection #:	2	Processing Method:	DIF_f
Injection Volume:	10.00 ul	Channel Name:	245.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	PDA 245.0 nm
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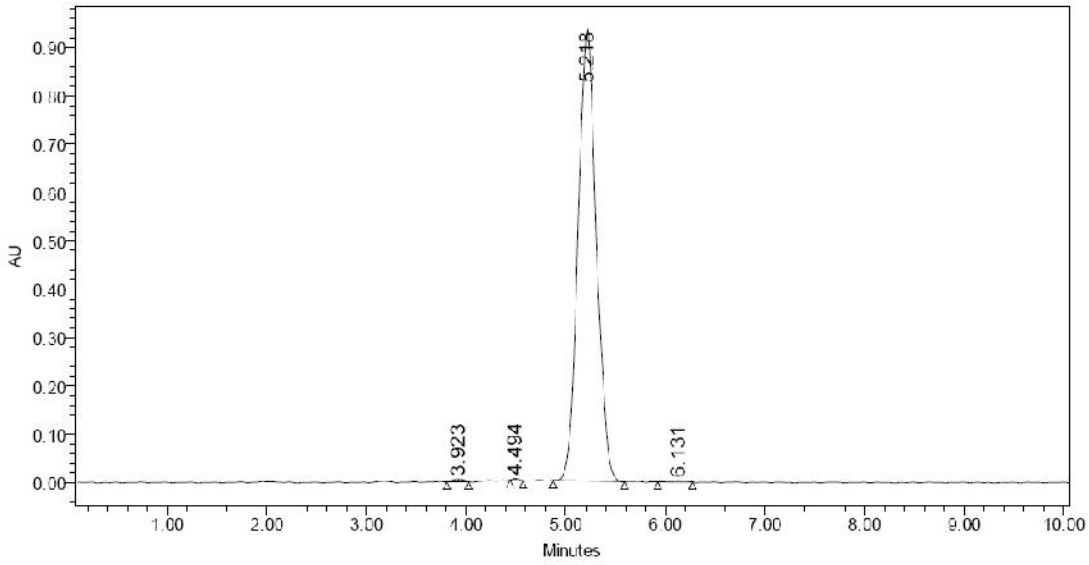
Date Processed:	5/6/2008 12:41:48 PM IST		



	RT	Area	% Area	Height
1	3.923	41842	0.35	5147
2	4.494	15357	0.13	3438
3	5.218	11955657	99.20	938043
4	6.131	38659	0.32	3236

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

Project Name: test_chemistry
Date Printed:
5/6/2008
12:42:31 PM Asia/Calcutta

Compound 9m:

Solvent system: (20%water : 80%Acetonitrile)

Empower2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	DiF_20water_80ACN_1	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	20_water_80_AcN_1ml
Injection #:	7	Processing Method:	DiF_1
Injection Volume:	10.00 ul	Channel Name:	227.0nm@1
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	PDA 227.0 nm
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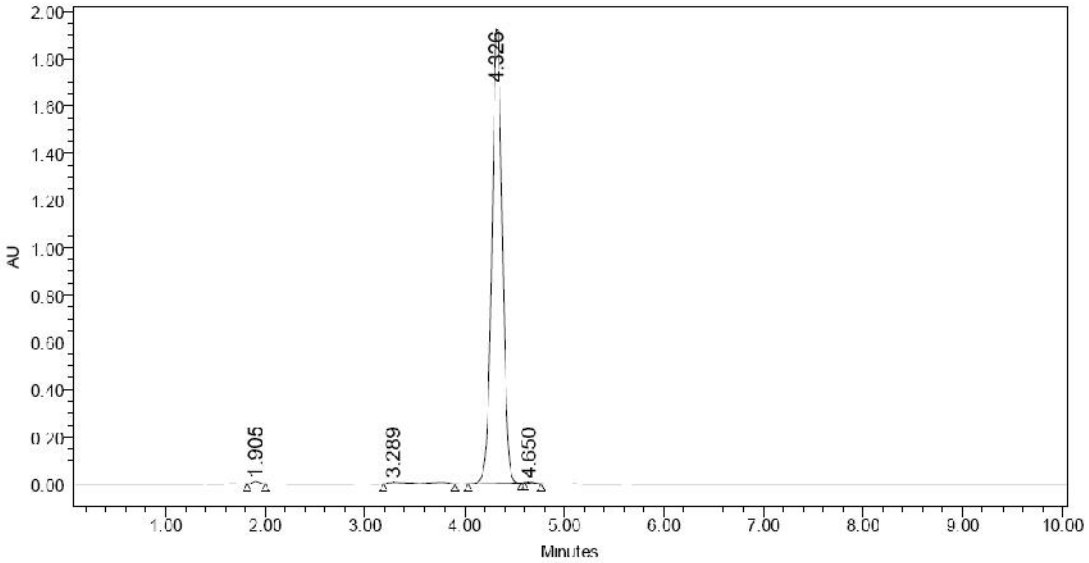
Date Processed:	5/7/2008 5:25:59 PM IST		



	RT	Area	% Area	Height
1	1.905	45960	0.32	10352
2	3.289	166681	1.18	6304
3	4.326	14111566	98.35	1938895
4	4.650	21465	0.15	3838

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

Project Name: test_chemistry
Date Printed: 5/7/2008
5:26:40 PM Asia/Calcutta

Compound 9n:

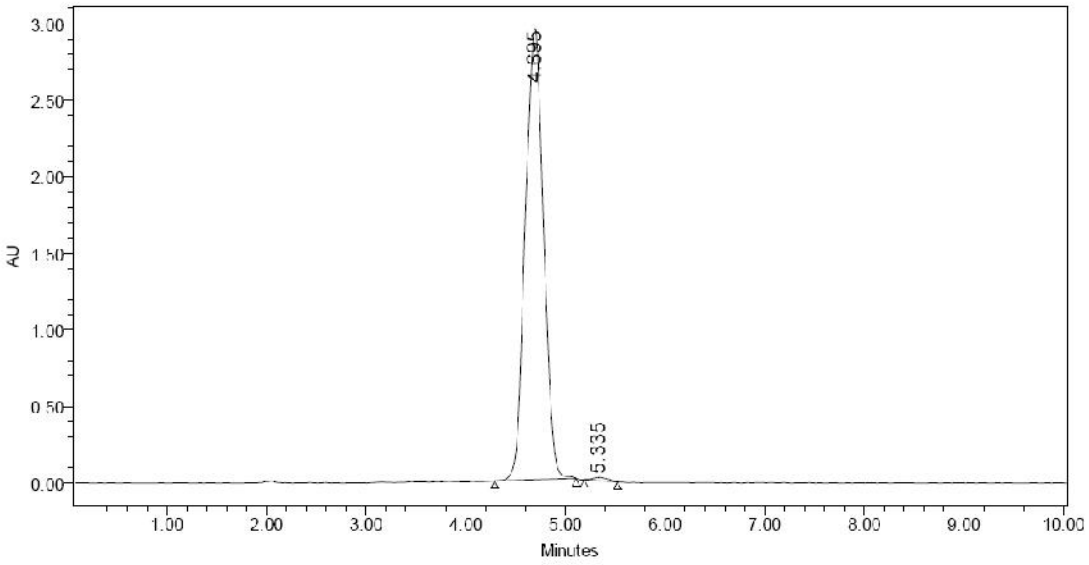
Solvent system: (20%water : 80%methanol)

Empower 2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	2F_20water_80methanol_2	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	20%water_80%Meth_1ml
Injection #:	2	Processing Method:	2F_2
Injection Volume:	10.00 ul	Channel Name:	240.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	PDA 240.0 nm
Date Acquired:	5/6/2008 3:26:51 PM IST		
Date Processed:	5/6/2008 3:50:52 PM IST		



	RT	Area	% Area	Height
1	4.695	37571391	99.41	2952545
2	5.335	224007	0.59	21552

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

Project Name: test_chemistry
Date Printed:
5/6/2008
3:51:21 PM Asia/Calcutta

Compound 9n:

Solvent system: (20%water : 80%Acetonitrile)

Empower2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	2F_20water_80ACN_1	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	20_water_80_AcN_1ml
Injection #:	8	Processing Method:	2F_1
Injection Volume:	10.00 ul	Channel Name:	210.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	PDA 210.0 nm
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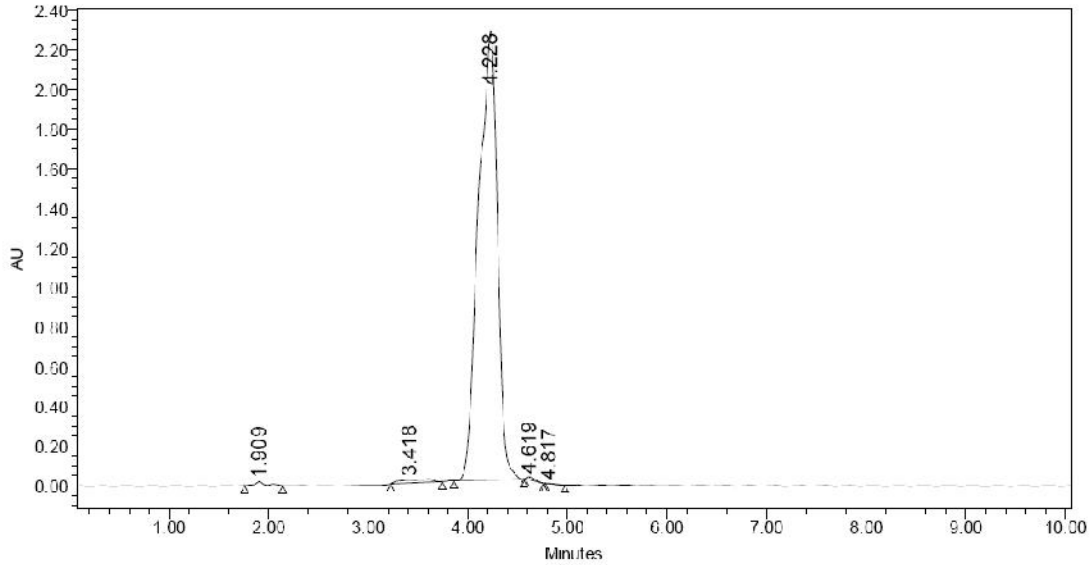
Date Processed:	5/8/2008 4:22:01 PM IST		



	RT	Area	% Area	Height
1	1.909	121253	0.40	18153
2	3.418	325595	1.07	14741
3	4.228	29947122	98.27	2261158
4	4.619	69026	0.23	13474
5	4.817	10993	0.04	1085

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

Project Name: test_chemistry
Date Printed:
5/8/2008
4:22:32 PM Asia/Calcutta

Compound 9i:
Solvent system: (20%water : 80%methanol)

Empower 2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	4F_20water_80methanol_1	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	20%water_80%Meth_1ml
Injection #:	2	Processing Method:	4F_1
Injection Volume:	10.00 ul	Channel Name:	250.0nm
Run Time:	15.0 Minutes	Proc. Chnl. Descr.:	PDA 250.0 nm
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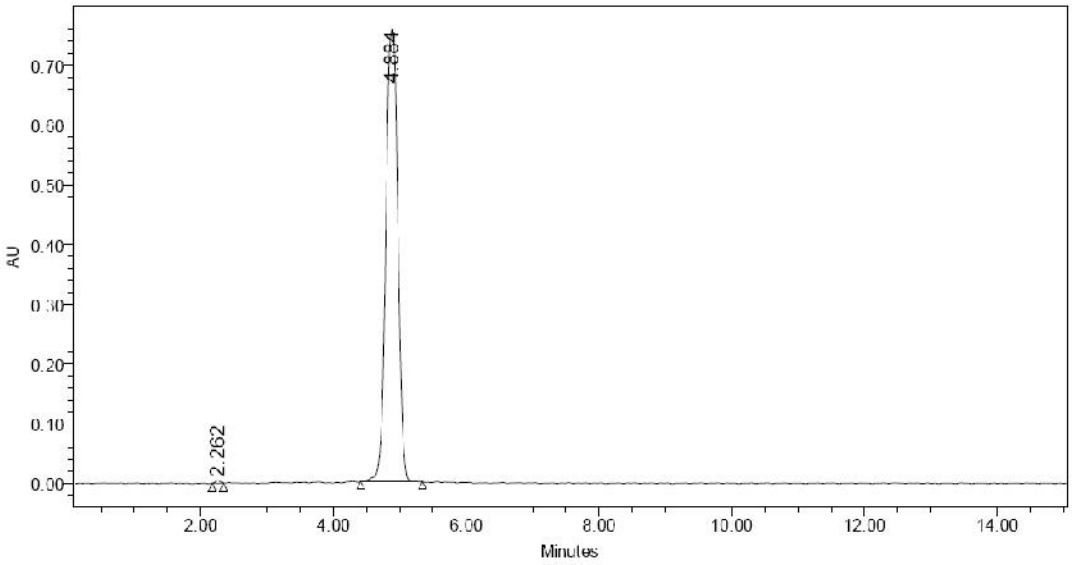

	RT	Area	% Area	Height
1	2.262	23194	0.24	4877
2	4.884	9620647	99.76	760653

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

Project Name: test_chemistry
Date Printed:
5/5/2008
3:09:58 PM Asia/Calcutta

Compound 9i:
Solvent system: (20%water : 80%Acetonitrile)

Empower 2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	4F_20water_80ACN_2	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	20_water_80_AcN_1ml
Injection #:	2	Processing Method:	4F_2
Injection Volume:	10.00 ul	Channel Name:	254.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	PDA 254.0 nm
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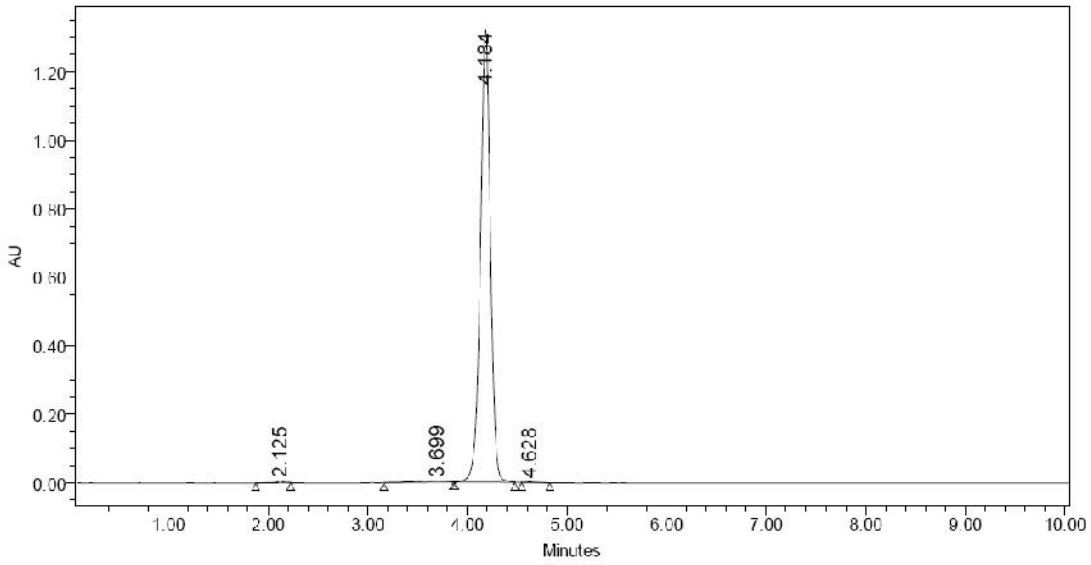


	RT	Area	% Area	Height
1	2.125	23709	0.25	4587
2	3.699	82561	0.88	3934
3	4.184	9308759	98.74	1325722
4	4.628	12098	0.13	1639

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

Project Name: test_chemistry
Date Printed:
5/8/2008
3:59:22 PM Asia/Calcutta

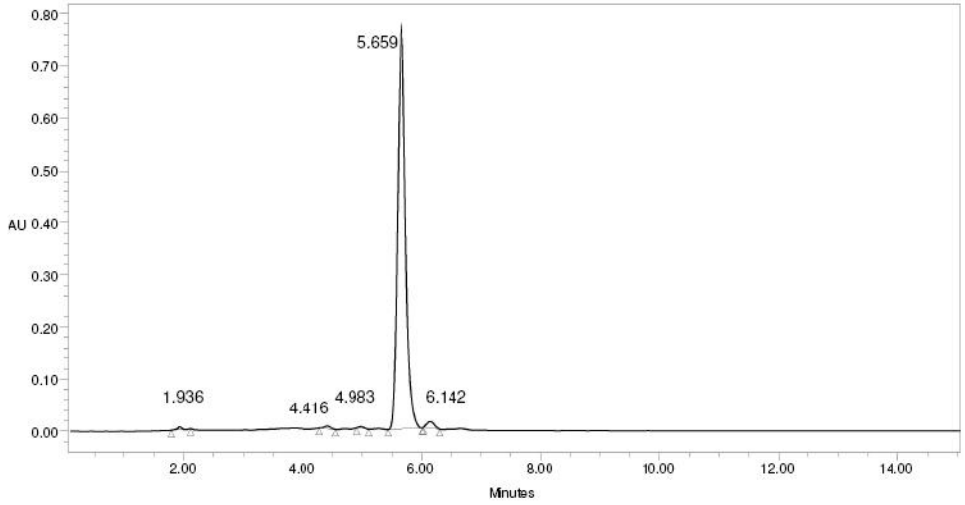
Compound 9o:
Solvent system: (20%water : 80%methanol)

Empower 2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	NMe2_20w ater_80MeOH_1	Acquired By:	System
Sample Type:	Unknow n	Sample Set Name:	
Vial:	1	Acq. Method Set:	20_w ater_80_AcN_1ml
Injection #:	11	Processing Method:	NMe2_1
Injection Volume:	10.00 ul	Channel Name:	257.8nm
Run Time:	15.0 Minutes	Proc. Chnl. Descr.:	PDA 257.8 nm
Date Acquired:	5/8/2008 3:44:30 PM IST		
Date Processed:	5/8/2008 4:41:03 PM IST		



	RT	Area	% Area	Height
1	1.936	27982	0.36	5136
2	4.416	37569	0.48	5032
3	4.983	21075	0.27	3300
4	5.659	7603933	97.56	776220
5	6.142	103164	1.32	11912

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 10021002
Page: 1 of 1

Project Name: test_chemistry
Date Printed: 5/8/2008
4:42:07 PM Asia/Calcutta

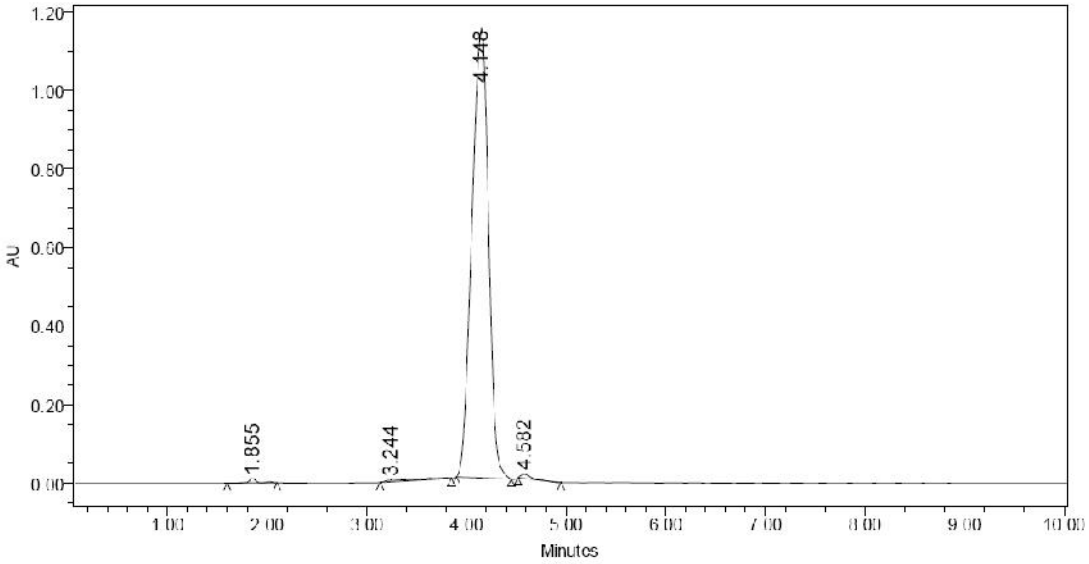
Compound 9o:
Solvent system: (20%water : 80%Acetonitrile)

Empower2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	NMe2_20water_80ACN_1	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	20_water_80_AcN_1ml
Injection #:	10	Processing Method:	NMe2_1
Injection Volume:	10.00 ul	Channel Name:	230.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	PDA 230.0 nm
Date Acquired:	5/8/2008 3:32:50 PM IST		
Date Processed:	5/8/2008 4:28:11 PM IST		



	RT	Area	% Area	Height
1	1.855	58234	0.43	11117
2	3.244	102567	0.76	3657
3	4.148	13287843	98.27	1145289
4	4.582	72557	0.54	10781

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

Project Name: test_chemistry
Date Printed:
5/8/2008
4:28:54 PM Asia/Calcutta

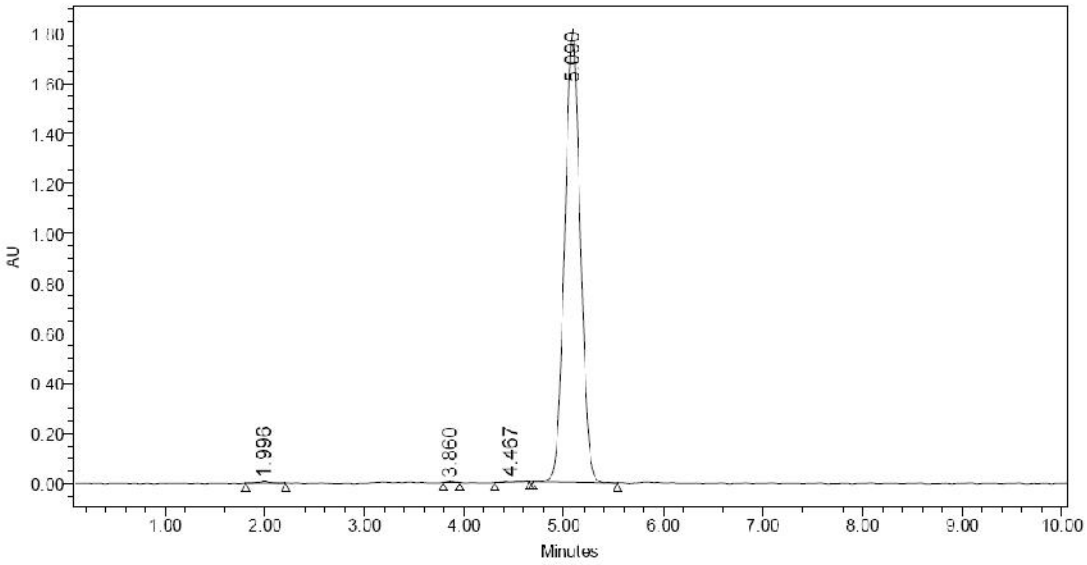
Compound 9p:
Solvent system: (20%water : 80%methanol)

Empower 2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	4OEt-20water_80Methanol_1	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	20%water_80%Meth_1ml
Injection #:	1	Processing Method:	4OEt_1
Injection Volume:	10.00 ul	Channel Name:	238.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	PDA 238.0 nm
Date Acquired:	5/2/2008 12:08:31 PM IST		
Date Processed:	5/2/2008 12:25:42 PM IST		



	RT	Area	% Area	Height
1	1.996	43519	0.22	6363
2	3.860	18297	0.09	3085
3	4.467	66808	0.34	7071
4	5.090	19810893	99.35	1812011

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

Project Name: test_chemistry
Date Printed:
5/2/2008
12:26:34 PM Asia/Calcutta

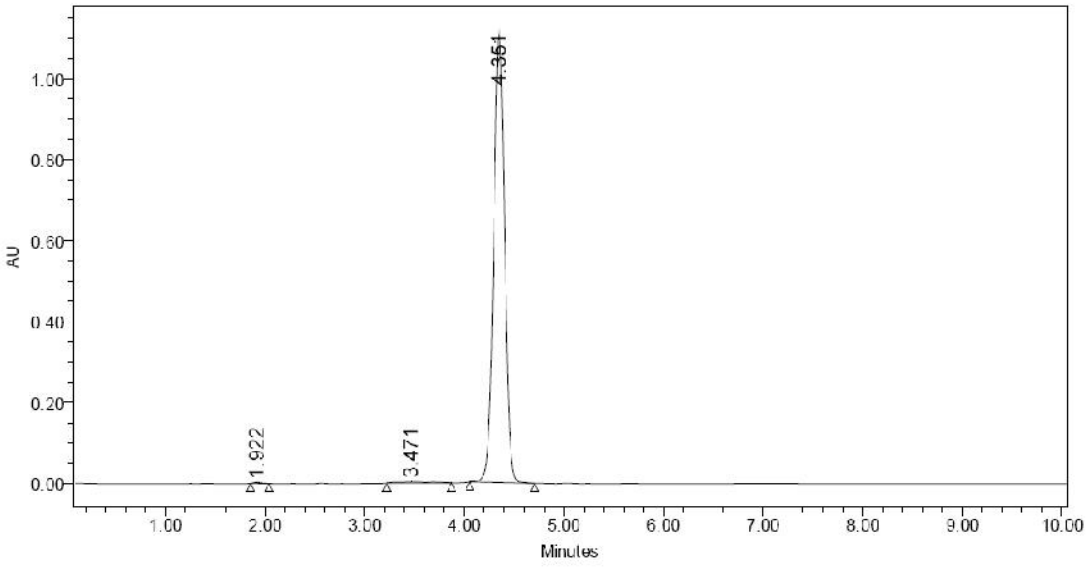
Compound 9p:
Solvent system: (20%water : 80%Acetonitrile)

Empower 2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	4OEt_20water_80ACN_1	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	20_water_80_AcN_1ml
Injection #:	3	Processing Method:	4OEt_1_ACn
Injection Volume:	10.00 ul	Channel Name:	240.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	PDA 240.0 nm
Date Acquired:	5/7/2008 3:27:23 PM IST		
Date Processed:	5/7/2008 5:02:11 PM IST		



	RT	Area	% Area	Height
1	1.922	14293	0.17	2947
2	3.471	69106	0.80	2574
3	4.351	8504537	99.03	1120326

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

Project Name: test_chemistry
Date Printed:
5/7/2008
5:02:54 PM Asia/Calcutta

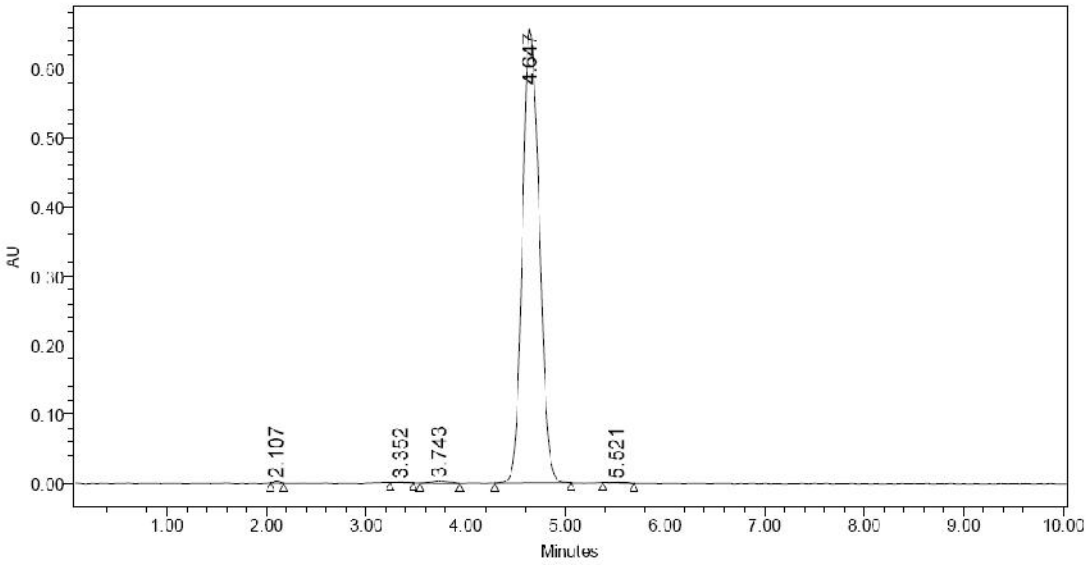
Compound 9q:
Solvent system: (20%water : 80%methanol)

Empower 2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	4-OMe_20water_80methanol_1	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	20%water_80%Meth_1ml
Injection #:	1	Processing Method:	4OMe_f
Injection Volume:	10.00 ul	Channel Name:	254.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	PDA 254.0 nm
Date Acquired:	5/1/2008 3:35:49 PM IST		
Date Processed:	5/1/2008 4:44:32 PM IST		



	RT	Area	% Area	Height
1	2.107	10799	0.14	2610
2	3.352	2984	0.04	413
3	3.743	33671	0.43	2999
4	4.647	7767013	99.31	657923
5	5.521	6826	0.09	684

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

Project Name: test_chemistry
Date Printed:
5/1/2008
4:46:09 PM Asia/Calcutta

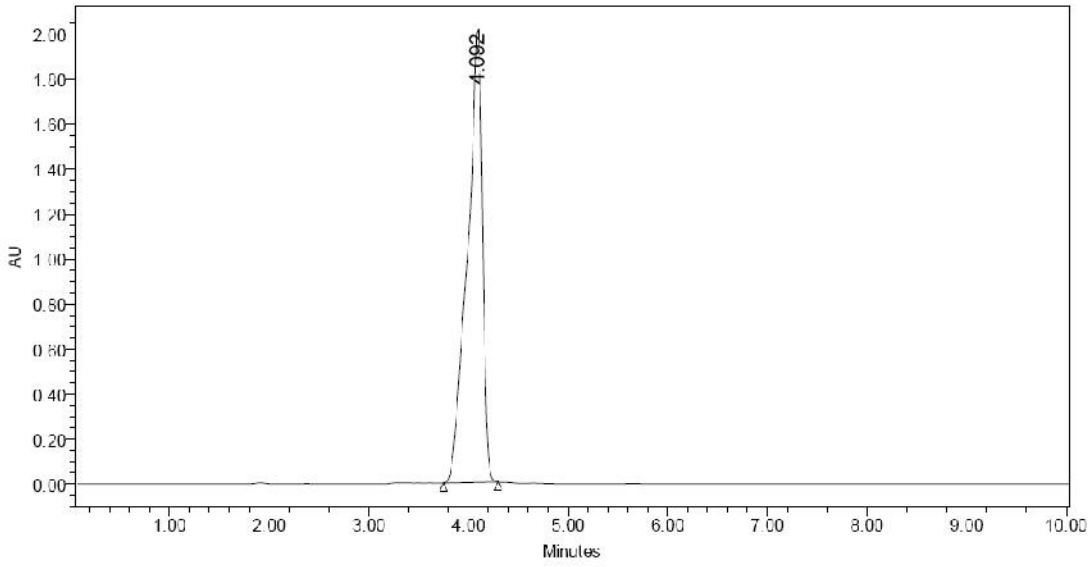
Compound 9q:
Solvent system: (20%water : 80%Acetonitrile)

Empower 2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	4OMe_20water_80ACN_1	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	20_water_80_AcN_1ml
Injection #:	5	Processing Method:	4OMe_1
Injection Volume:	10.00 ul	Channel Name:	232.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	PDA 232.0 nm
Date Acquired:	5/7/2008 4:32:32 PM IST		
Date Processed:	5/7/2008 5:18:53 PM IST		



	RT	Area	% Area	Height
1	4.092	21113857	100.00	2031703

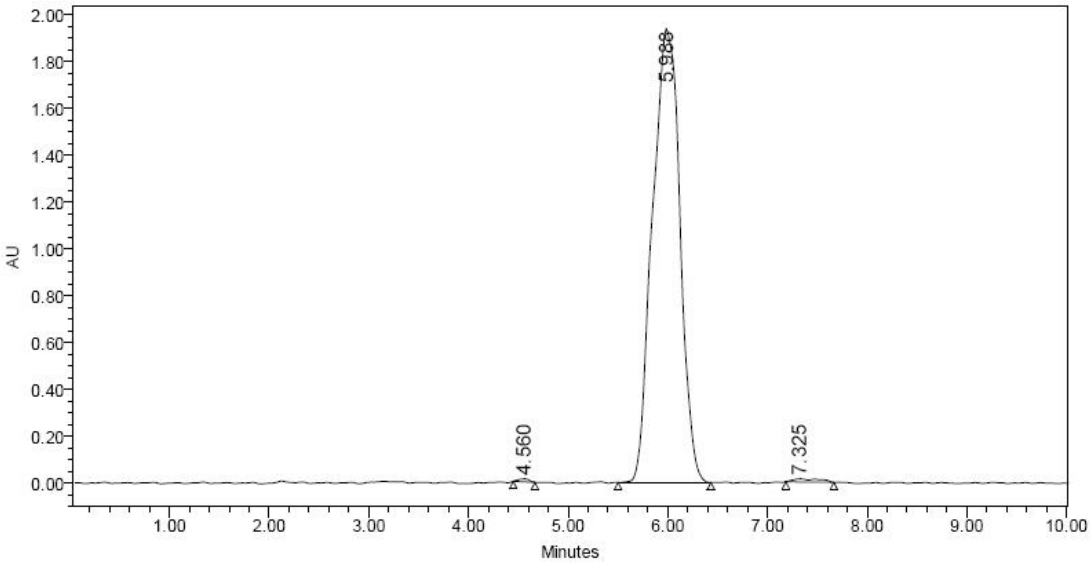
Compound 9c:
Solvent system: (20%water : 80%methanol)

Empower2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	4Br_20water_80methanol_2	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	20%water_80%Meth_1ml
Injection #:	2	Processing Method:	4Br_2
Injection Volume:	10.00 ul	Channel Name:	228.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	PDA 228.0 nm
Date Acquired:	5/1/2008 6:01:22 PM IST		
Date Processed:	5/1/2008 7:41:21 PM IST		



	RT	Area	% Area	Height
1	4.560	94843	0.25	12612
2	5.988	37107059	99.06	1940395
3	7.325	256079	0.68	13101

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

Project Name: test_chemistry
Date Printed: 5/1/2008
7:42:08 PM Asia/Calcutta

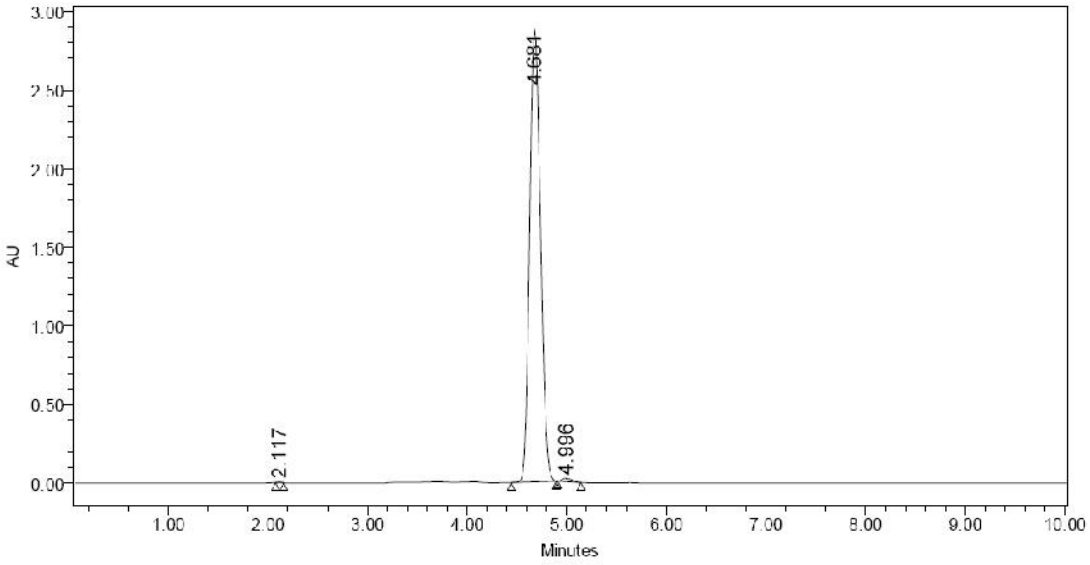
Compound 9c:
Solvent system: (20%water : 80%Acetonitrile)

Empower 2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	4Br_20water_80ACN_1	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	20_water_80_AcN_1ml
Injection #:	6	Processing Method:	4Br_1
Injection Volume:	10.00 ul	Channel Name:	235.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	PDA 235.0 nm
Date Acquired:	5/7/2008 4:44:31 PM IST		
Date Processed:	5/7/2008 5:23:22 PM IST		



	RT	Area	% Area	Height
1	2.117	11225	0.05	3657
2	4.681	21853348	99.28	2887672
3	4.996	147390	0.67	21891

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

Project Name: test_chemistry
Date Printed:
5/7/2008
5:23:57 PM Asia/Calcutta

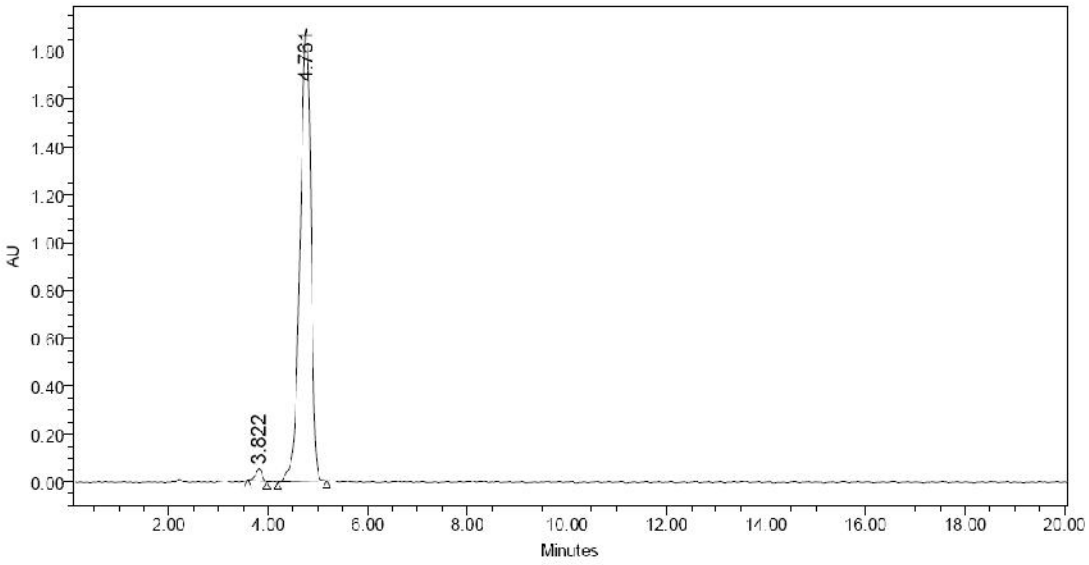
Compound 9e:
Solvent system: (20%water : 80%methanol)

Empower 2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	4NO2_20water_80methanol_1	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	20%water_80%Meth_1ml
Injection #:	2	Processing Method:	4NO2_1
Injection Volume:	10.00 ul	Channel Name:	230.0nm
Run Time:	20.0 Minutes	Proc. Chnl. Descr.:	PDA 230.0 nm
Date Acquired:	5/2/2008 7:04:20 PM IST		
Date Processed:	5/2/2008 7:43:05 PM IST		



	RT	Area	% Area	Height
1	3.822	443604	1.50	52427
2	4.761	29181366	98.50	1893972

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

Project Name: test_chemistry
Date Printed:
5/2/2008
7:43:54 PM Asia/Calcutta

Compound 9e:

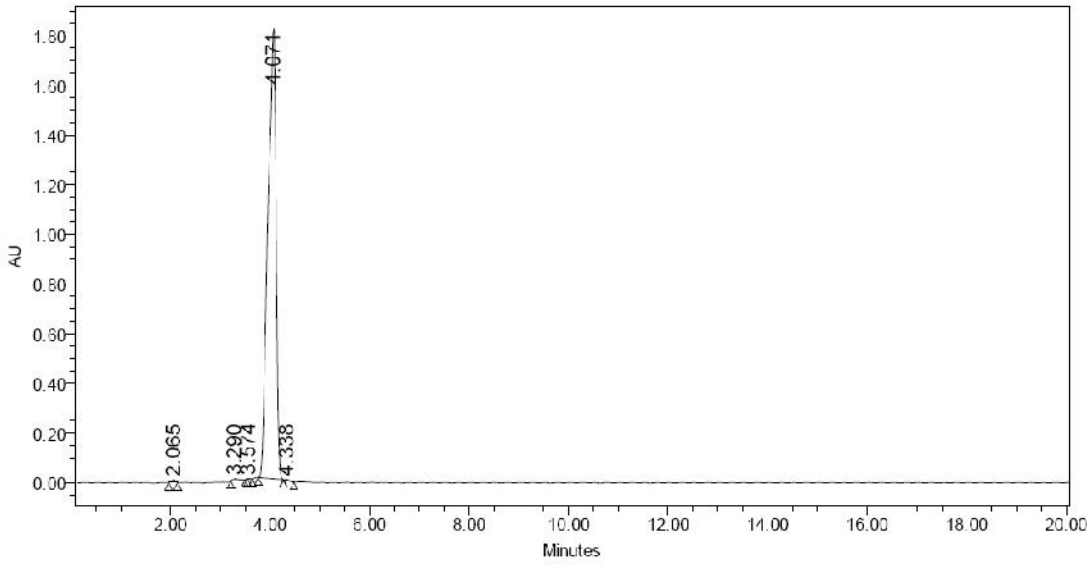
Solvent system: (20%water : 80%Acetonitrile)

Empower 2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	4NO2_20water_80ACN_1	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	20_water_80_AcN_1ml
Injection #:	4	Processing Method:	4NO2_1
Injection Volume:	10.00 ul	Channel Name:	215.0nm
Run Time:	20.0 Minutes	Proc. Chnl. Descr.:	PDA 215.0 nm
Date Acquired:	5/8/2008 1:04:19 PM IST		
Date Processed:	5/8/2008 4:06:28 PM IST		



	RT	Area	% Area	Height
1	2.065	43735	0.21	11071
2	3.290	58837	0.29	6979
3	3.574	2383	0.01	723
4	4.071	20246426	99.36	1829056
5	4.338	24544	0.12	3996

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

Project Name: test_chemistry
Date Printed:
5/8/2008
4:07:02 PM Asia/Calcutta

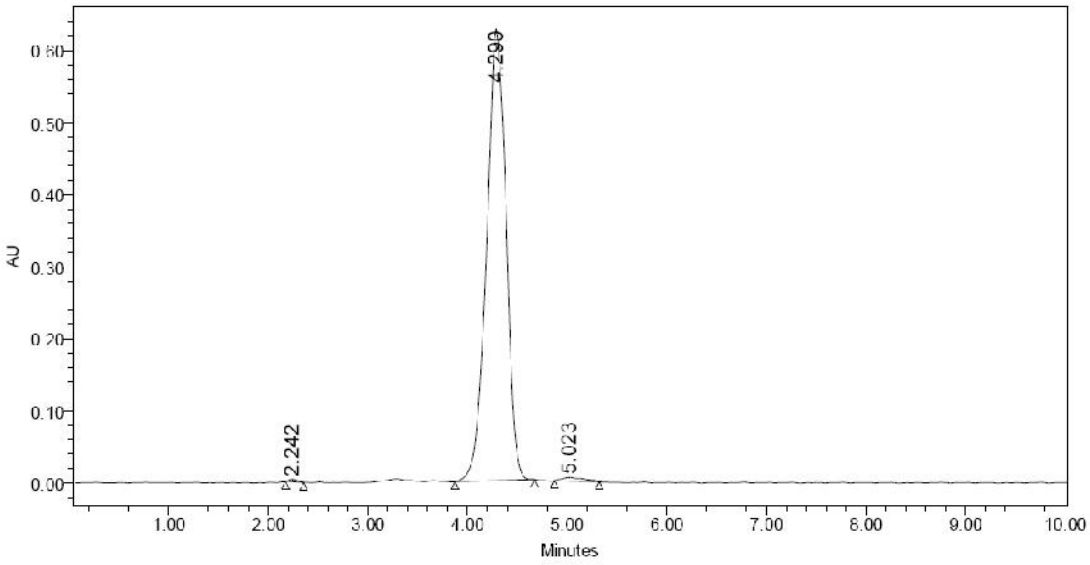
Compound 9r:
Solvent system: (20%water : 80%methanol)

Empower 2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	TriOMe_20water_80methanol_2	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	20%water_80%Meth_1ml
Injection #:	2	Processing Method:	TriOme4
Injection Volume:	10.00 ul	Channel Name:	250.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	PDA 250.0 nm
Date Acquired:	5/1/2008 12:53:31 PM IST		
Date Processed:	5/1/2008 1:14:50 PM IST		



	RT	Area	% Area	Height
1	2.242	20610	0.24	3450
2	4.290	8511300	98.87	626794
3	5.023	78728	0.89	5039

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

Project Name: test_chemistry
Date Printed:
5/1/2008
1:20:47 PM Asia/Calcutta

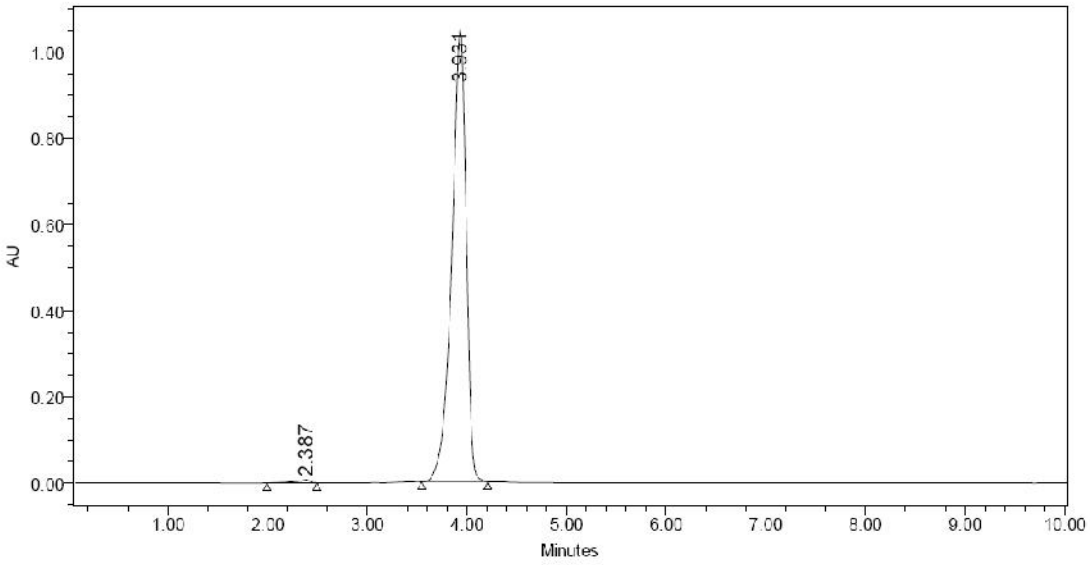
Compound 9r:
Solvent system: (20%water : 80%Acetonitrile)

Empower 2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	TriOMe_20water_80ACN_1	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	20_water_80_AcN_1ml
Injection #:	3	Processing Method:	TriOMe_1
Injection Volume:	10.00 ul	Channel Name:	265.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	PDA 265.0 nm
Date Acquired:	5/7/2008 4:09:40 PM IST		
Date Processed:	5/7/2008 5:12:33 PM IST		



	RT	Area	% Area	Height
1	2.387	69068	0.65	7248
2	3.931	10537917	99.35	1051752

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

Project Name: test_chemistry
Date Printed:
5/7/2008
5:13:14 PM Asia/Calcutta

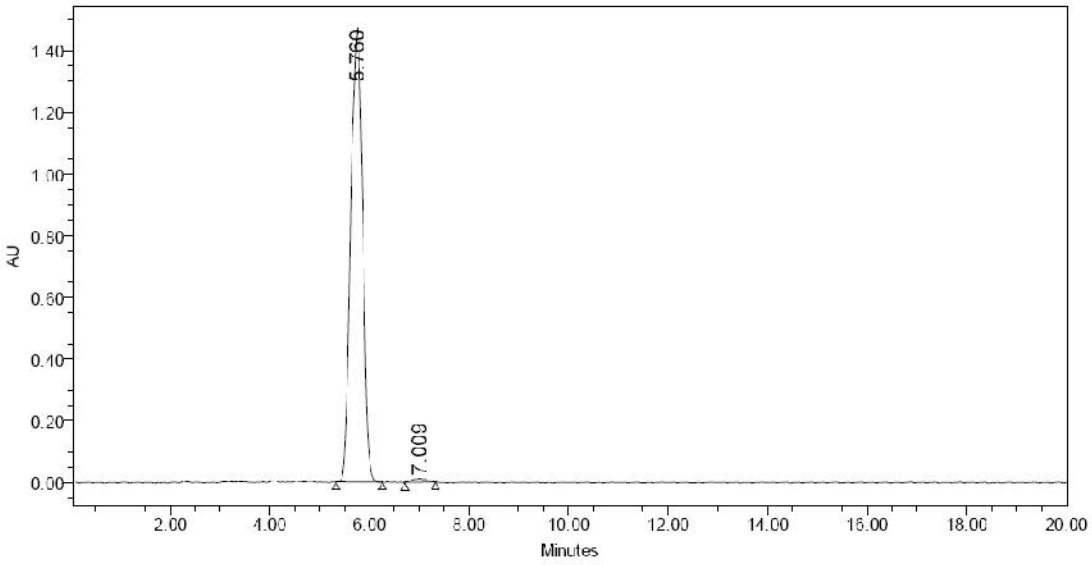
Compound 9a:
Solvent system: (20%water : 80%methanol)

Empower 2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	4Cl_20water_80methanol_1	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	20%water_80%Meth_1ml
Injection #:	2	Processing Method:	4Cl_1
Injection Volume:	10.00 ul	Channel Name:	240.0nm
Run Time:	20.0 Minutes	Proc. Chnl. Descr.:	PDA 240.0 nm
Date Acquired:	5/3/2008 3:36:16 PM IST		
Date Processed:	5/3/2008 4:02:38 PM IST		



	RT	Area	% Area	Height
1	5.760	24389264	99.02	1469362
2	7.009	242335	0.98	12306

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

Project Name: test_chemistry
Date Printed:
5/3/2008
4:03:19 PM Asia/Calcutta

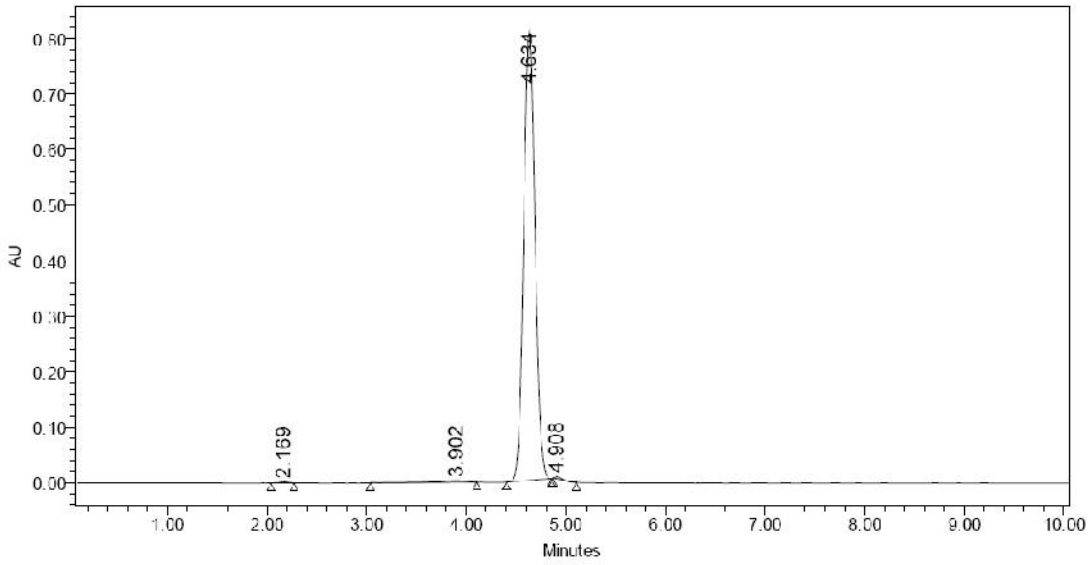
Compound 9a:
Solvent system: (20%water : 80%Acetonitrile)

Empower 2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	4Cl_20water_80ACN_1	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	20_water_80_AcN_1ml
Injection #:	7	Processing Method:	4Cl_1
Injection Volume:	10.00 ul	Channel Name:	270.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	PDA 270.0 nm
Date Acquired:	5/8/2008 2:36:30 PM IST		
Date Processed:	5/8/2008 4:15:56 PM IST		



	RT	Area	% Area	Height
1	2.169	12750	0.20	2341
2	3.902	53011	0.82	3314
3	4.634	6408207	98.71	814740
4	4.908	17768	0.27	2969

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

Project Name: test_chemistry
Date Printed:
5/8/2008
4:16:34 PM Asia/Calcutta

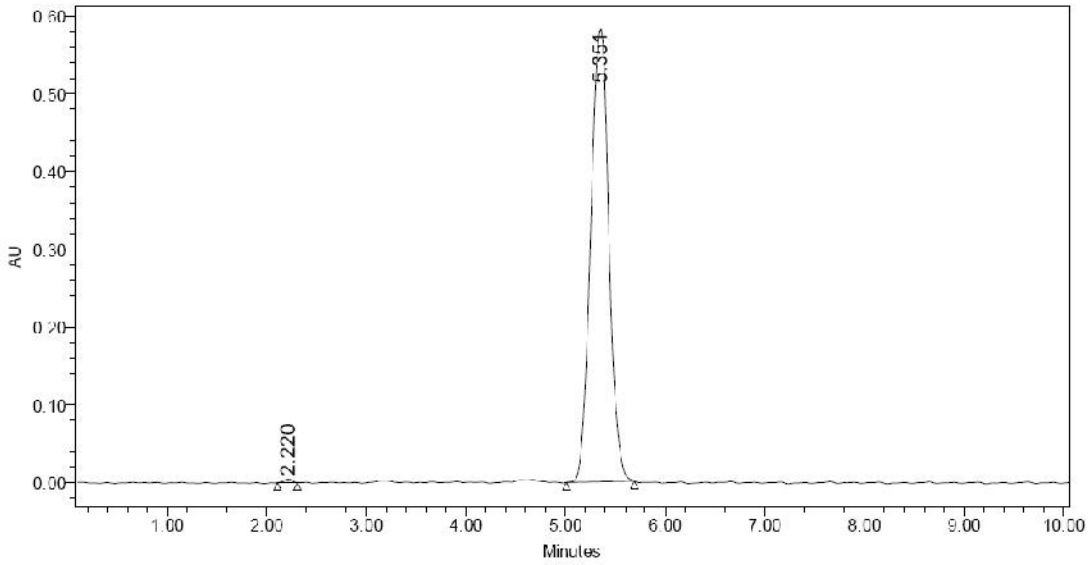
Compound 9h:
Solvent system: (20%water : 80%methanol)

Empower 2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	3Me_20water_80methanol_2	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	20%water_80%Meth_1ml
Injection #:	2	Processing Method:	3Me_4
Injection Volume:	10.00 ul	Channel Name:	240.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	PDA 240.0 nm
Date Acquired:	5/1/2008 5:12:35 PM IST		
Date Processed:	5/1/2008 5:30:39 PM IST		



	RT	Area	% Area	Height
1	2.220	25855	0.35	4500
2	5.351	7412608	99.65	583990

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

Project Name: test_chemistry
Date Printed:
5/1/2008
5:31:41 PM Asia/Calcutta

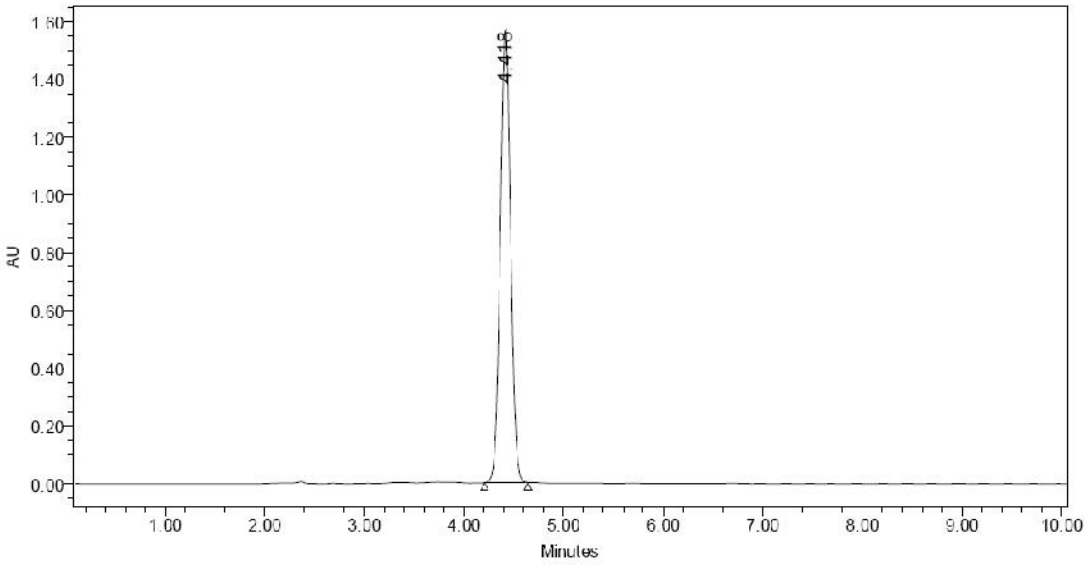
Compound 9h:
Solvent system: (20%water : 80%Acetonitrile)

Empower 2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	3Me_20water_80ACN_1	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	20_water_80_AcN_1ml
Injection #:	4	Processing Method:	3Me_1
Injection Volume:	10.00 ul	Channel Name:	240.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	PDA 240.0 nm
Date Acquired:	5/7/2008 4:21:14 PM IST		
Date Processed:	5/7/2008 5:15:32 PM IST		



	RT	Area	% Area	Height
1	4.418	11327805	100.00	1580045

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

Project Name: test_chemistry
Date Printed:
5/7/2008
5:16:12 PM Asia/Calcutta

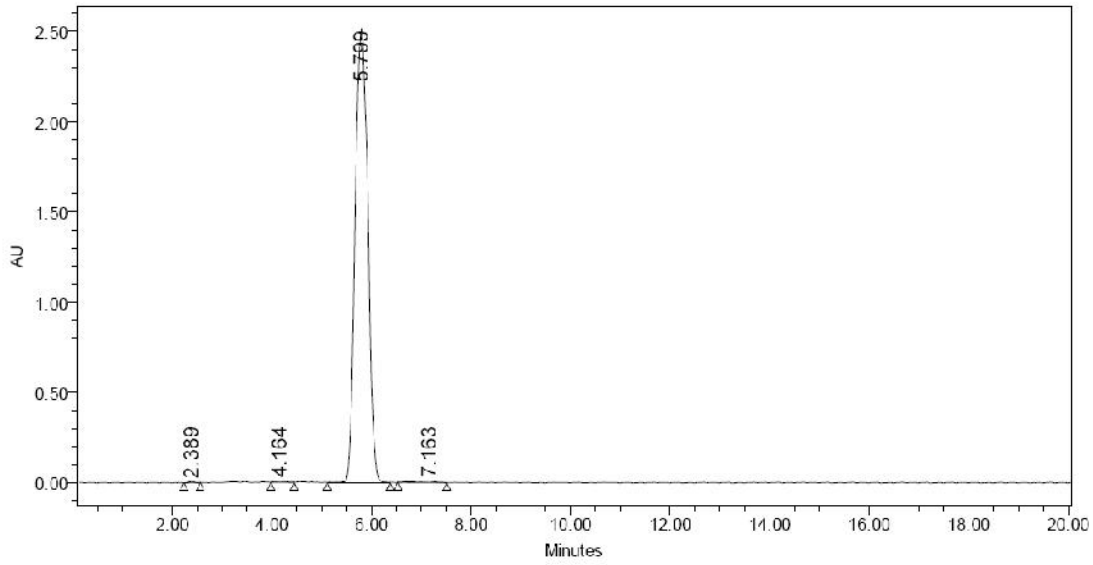
Compound 9s:
Solvent system: (20%water : 80%methanol)

Empower 2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	4CF3_20water_80methanol_1	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	20%water_80%Meth_1ml
Injection #:	3	Processing Method:	4CF3_1
Injection Volume:	10.00 ul	Channel Name:	235.0nm
Run Time:	20.0 Minutes	Proc. Chnl. Descr.:	PDA 235.0 nm
Date Acquired:	5/3/2008 3:59:16 PM IST		
Date Processed:	5/3/2008 5:00:30 PM IST		



	RT	Area	% Area	Height
1	2.389	52777	0.12	6695
2	4.164	83655	0.19	5991
3	5.799	44804327	99.14	2514598
4	7.163	252652	0.56	9006

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

Project Name: test_chemistry
Date Printed:
5/3/2008
5:01:14 PM Asia/Calcutta

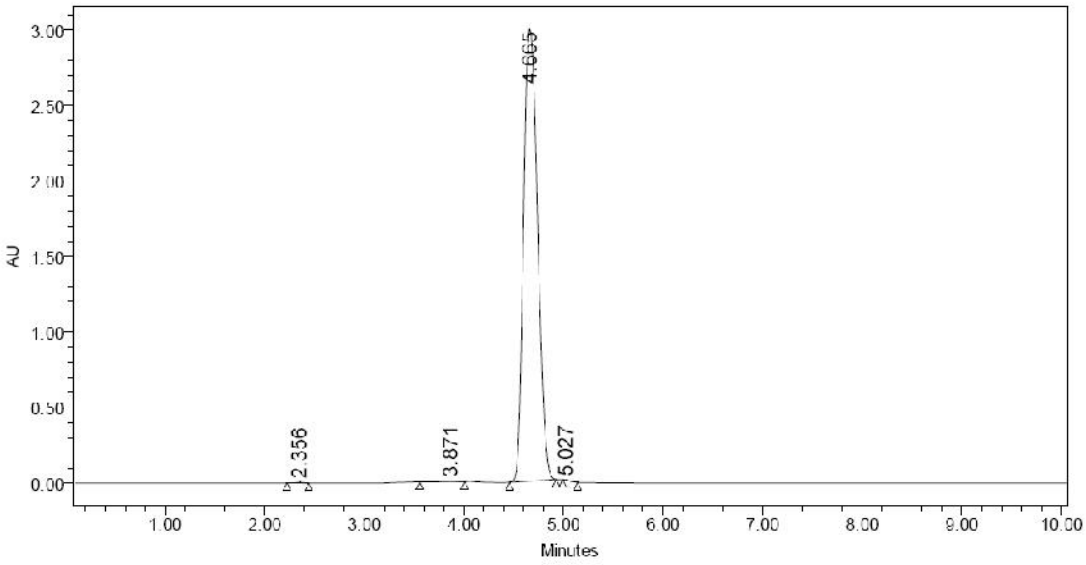
Compound 9s:
Solvent system: (20%water : 80%Acetonitrile)

Empower2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	4CF3_20water_80ACN_1	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	20_water_80_AcN_1ml
Injection #:	9	Processing Method:	4CF3_1
Injection Volume:	10.00 ul	Channel Name:	252.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	PDA 252.0 nm
Date Acquired:	5/8/2008 3:21:17 PM IST		
Date Processed:	5/8/2008 4:25:45 PM IST		



	RT	Area	% Area	Height
1	2.356	21884	0.07	4374
2	3.871	76042	0.26	5452
3	4.665	29437042	99.65	3008367
4	5.027	6169	0.02	1315

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

Project Name: test_chemistry
Date Printed:
5/8/2008
4:26:17 PM Asia/Calcutta

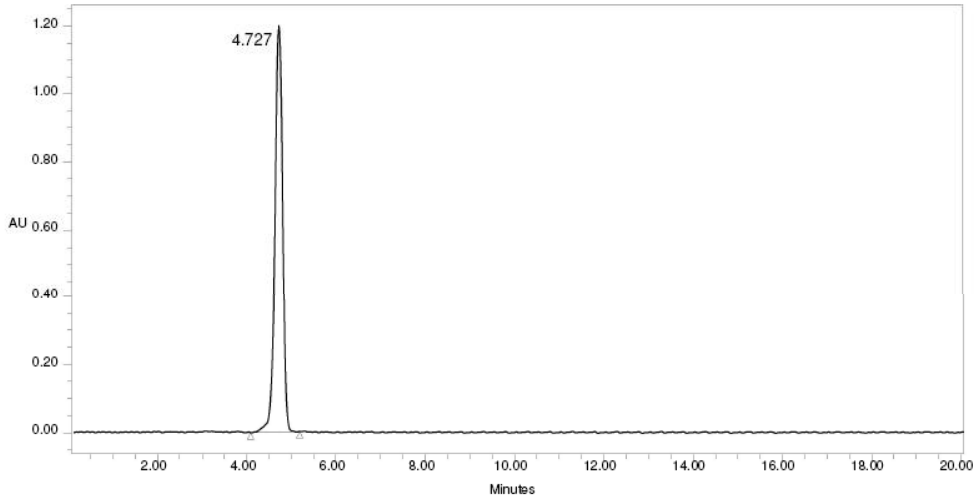
Compound 7k:
Solvent system: (20%water : 80%methanol)

Empower 2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	DiOMeU_20w ater_80methanol_1	Acquired By:	System
Sample Type:	Unknow n	Sample Set Name:	
Vial:	1	Acq. Method Set:	20%w ater_80%Meth_1ml
Injection #:	2	Processing Method:	2,3DiOMeU_1
Injection Volume:	10.00 ul	Channel Name:	235.0nm
Run Time:	20.0 Minutes	Proc. Chnl. Descr.:	PDA 235.0 nm
Date Acquired:	5/3/2008 12:49:50 PM IST		
Date Processed:	5/3/2008 3:18:15 PM IST		



	RT	Area	% Area	Height
1	4.727	14400640	100.00	1200797

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 10021002
Page: 1 of 1

Project Name: test_chemistry
Date Printed: 5/3/2008
3:19:50 PM Asia/Calcutta

Compound 7k:
Solvent system: (20%water : 80%Acetonitrile)

Empower 2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	DiOMeU_20water_80ACN_1	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	20_water_80_AcN_1ml
Injection #:	3	Processing Method:	DiOMe_1
Injection Volume:	10.00 ul	Channel Name:	240.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	PDA 240.0 nm
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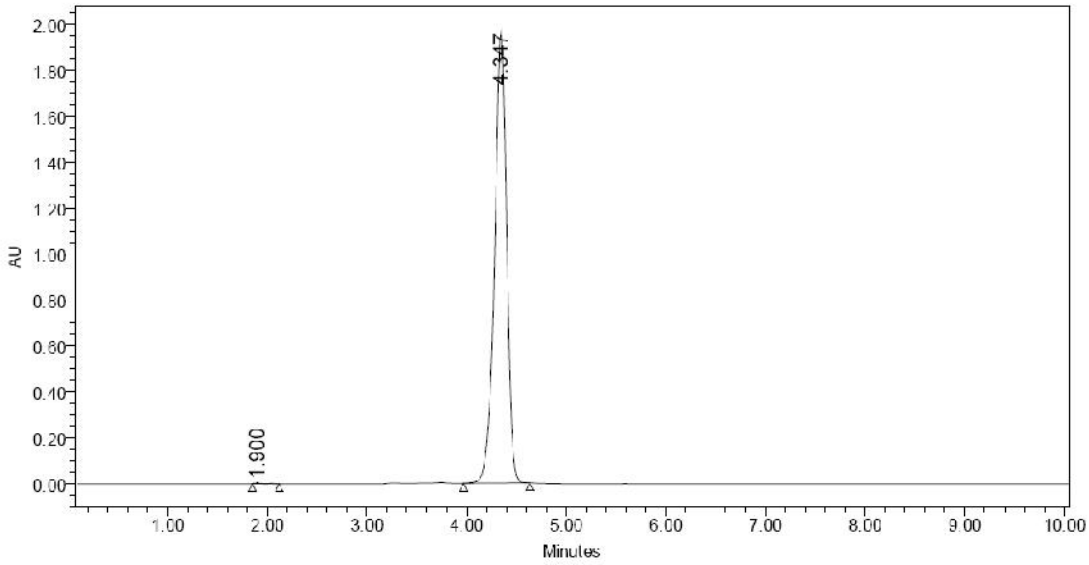


	RT	Area	% Area	Height
1	1.900	13968	0.08	2655
2	4.347	16613455	99.92	1979937

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

Project Name: test_chemistry
Date Printed:
5/8/2008
4:03:01 PM Asia/Calcutta

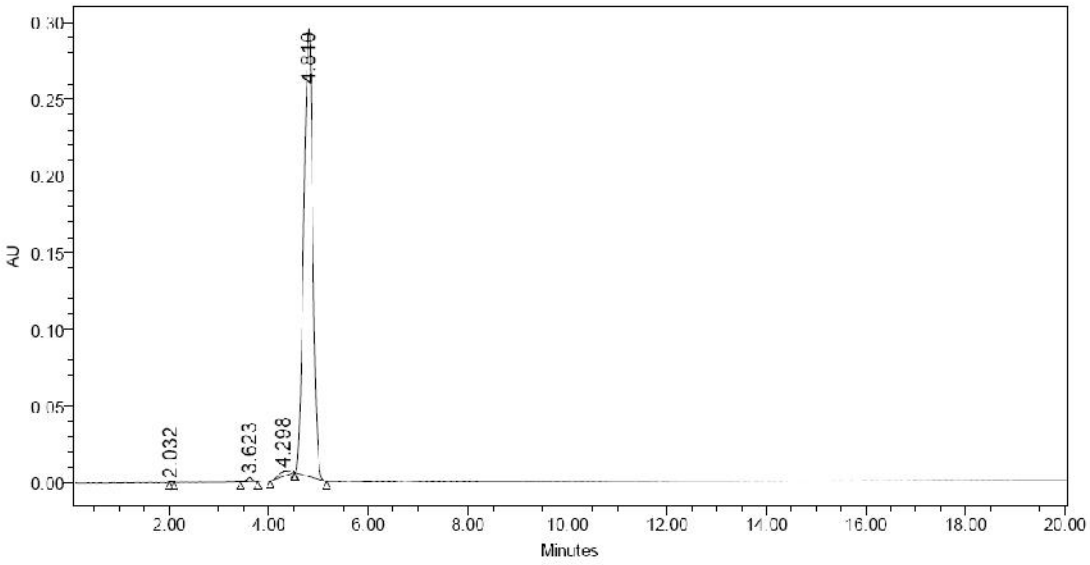
Compound 7l:
Solvent system: (20%water : 80%methanol)

Empower2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	4CNU-20water_80Methanol_1	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	20%water_80%Meth_1ml
Injection #:	1	Processing Method:	4CNU3
Injection Volume:	10.00 ul	Channel Name:	332.0nm
Run Time:	20.0 Minutes	Proc. Chnl. Descr.:	PDA 332.0 nm
Date Acquired:	5/2/2008 4:27:34 PM IST		
Date Processed:	5/2/2008 4:54:29 PM IST		



	RT	Area	% Area	Height
1	2.032	588	0.02	159
2	3.623	22832	0.60	2928
3	4.298	47372	1.25	2820
4	4.810	3715082	98.13	292349

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

Project Name: test_chemistry
Date Printed:
5/2/2008
4:55:46 PM Asia/Calcutta

Compound 7l:

Solvent system: (20%water : 80%Acetonitrile)

Empower 2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	4CNU_20water_80ACN_2	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	20_water_80_AcN_1ml
Injection #:	2	Processing Method:	4CNU_2
Injection Volume:	10.00 ul	Channel Name:	260.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	PDA 260.0 nm
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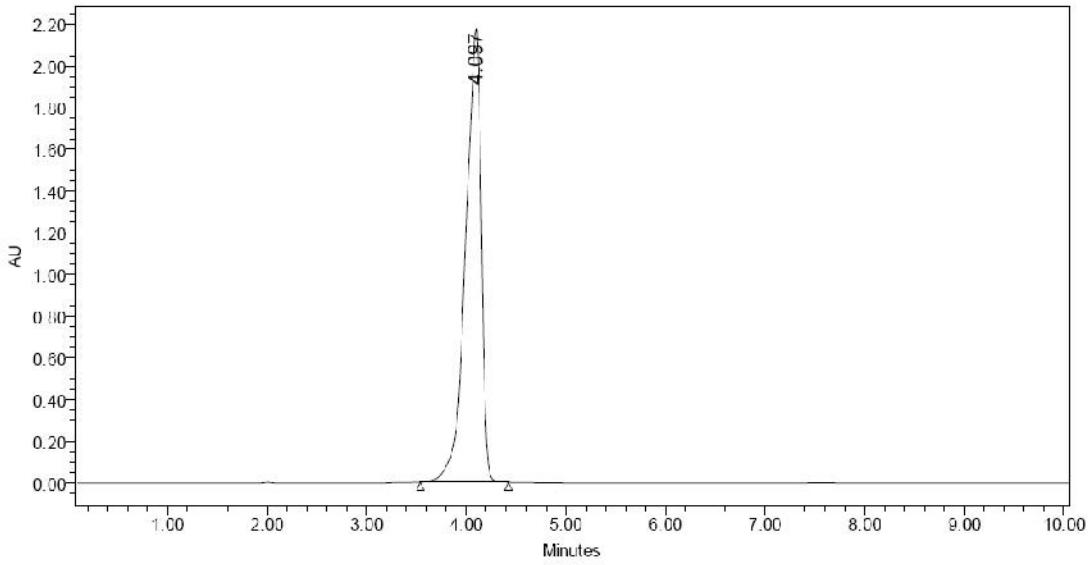


	RT	Area	% Area	Height
1	4.097	23775220	100.00	2193275

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

Project Name: test_chemistry
Date Printed:
5/7/2008
5:10:20 PM Asia/Calcutta

HPLC chromatograms of selected known final compounds

Compound 10b:

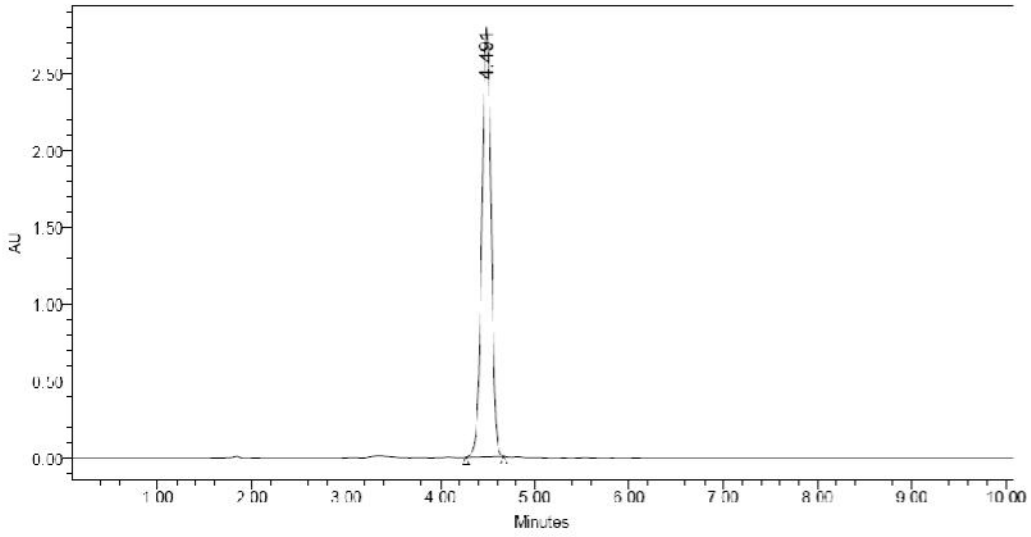
Solvent system: (20%water : 80%Acetonitrile)

Empower 2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	7b_20water_80AcN_1	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	02_Water_80AcN_1ml
Injection #:	2	Processing Method:	7b_20water_80AcN
Injection Volume:	10.00 ul	Channel Name:	220.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	PDA 220.0 nm
Date Acquired:	6/5/2008 3:32:28 PM IST		
Date Processed:	6/5/2008 4:26:35 PM IST		



	RT	Area	% Area	Height
1	4.491	19275306	100.00	2787201

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

Project Name: test_chemistry
Date Printed:
6/5/2008
4:27:19 PM Asia/Calcutta

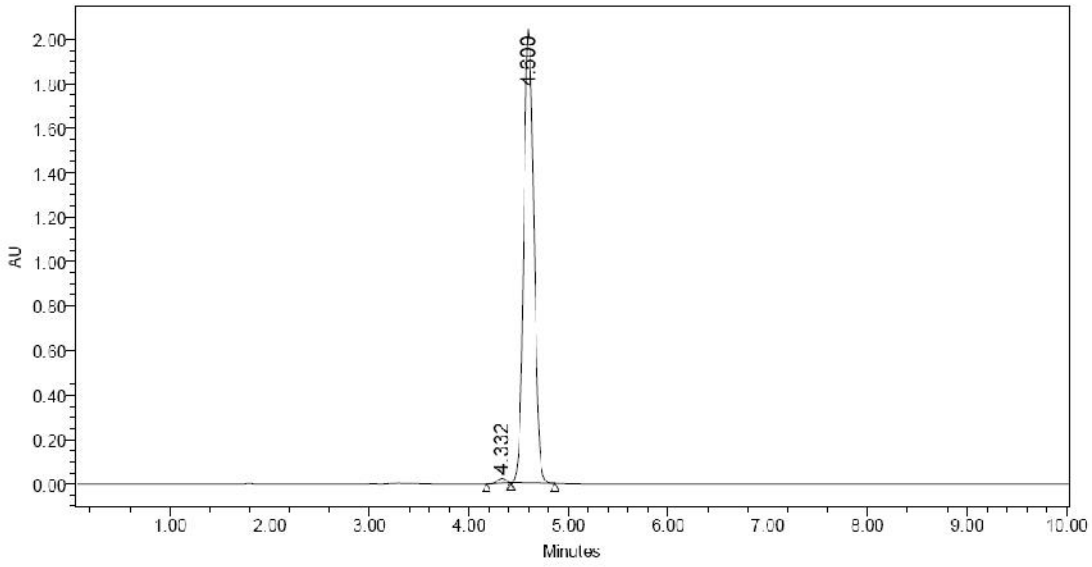
Compound 10c:
Solvent system: (20%water : 80%Acetonitrile)

Empower 2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	7c_20water_80AcN_1	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	02_Water_80AcN_1ml
Injection #:	4	Processing Method:	7c_20water_80AcN
Injection Volume:	10.00 ul	Channel Name:	240.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	PDA 240.0 nm
Date Acquired:	6/5/2008 4:13:42 PM IST		
Date Processed:	6/5/2008 4:36:36 PM IST		



	RT	Area	% Area	Height
1	4.332	114601	0.78	20982
2	4.600	14563614	99.22	2042523

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

Project Name: test_chemistry
Date Printed:
6/5/2008
4:37:43 PM Asia/Calcutta

Compound 10g:
Solvent system: (20%water : 80%Acetonitrile)

Empower 2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	7g_20water_80AcN_1	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	02_Water_80AcN_1ml
Injection #:	5	Processing Method:	7g_20water_80AcN
Injection Volume:	10.00 ul	Channel Name:	270.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	PDA 270.0 nm
Date Acquired:	6/5/2008 5:47:40 PM IST		
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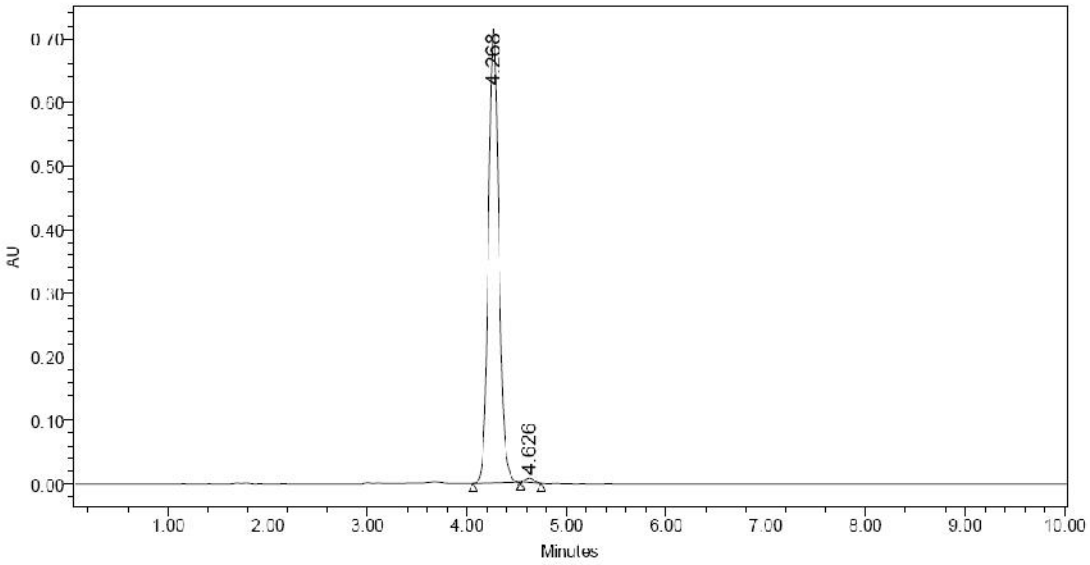

	RT	Area	% Area	Height
1	4.268	5227950	99.21	717131
2	4.626	41870	0.79	7087

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

Project Name: test_chemistry
Date Printed:
6/5/2008
5:58:58 PM Asia/Calcutta

Compound 10h:
Solvent system: (20%water : 80%Acetonitrile)

Empower 2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	7h_20water_80AcN_1	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	02_Water_80AcN_1ml
Injection #:	3	Processing Method:	7h_20water_80AcN
Injection Volume:	10.00 ul	Channel Name:	254.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	PDA 254.0 nm
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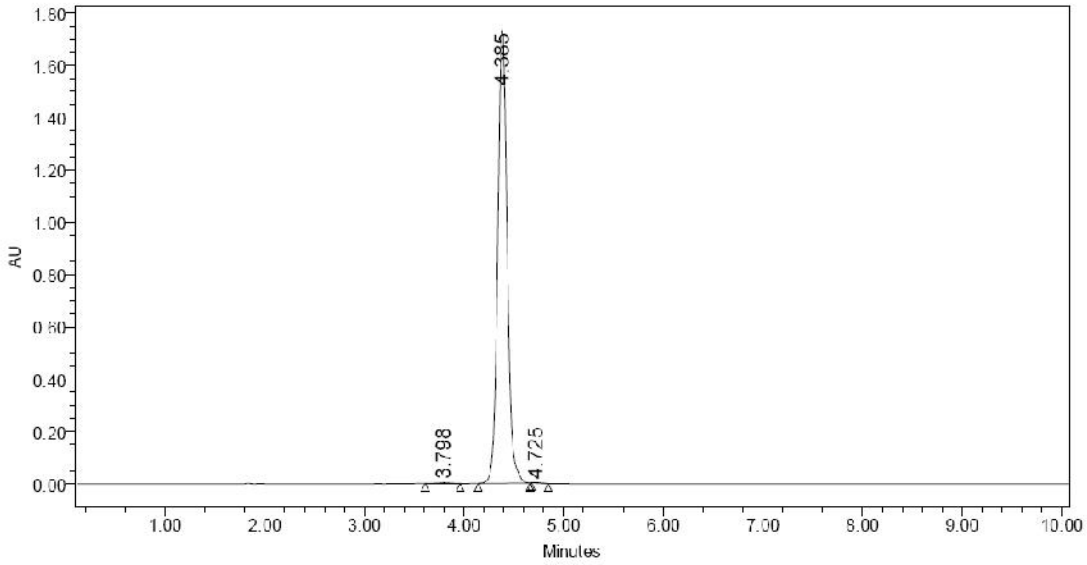
Date Processed:	6/5/2008 4:32:42 PM IST		



	RT	Area	% Area	Height
1	3.798	28527	0.25	2613
2	4.385	11426521	99.67	1745140
3	4.725	9012	0.08	1797

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

Project Name: test_chemistry
Date Printed: 6/5/2008
4:33:23 PM Asia/Calcutta

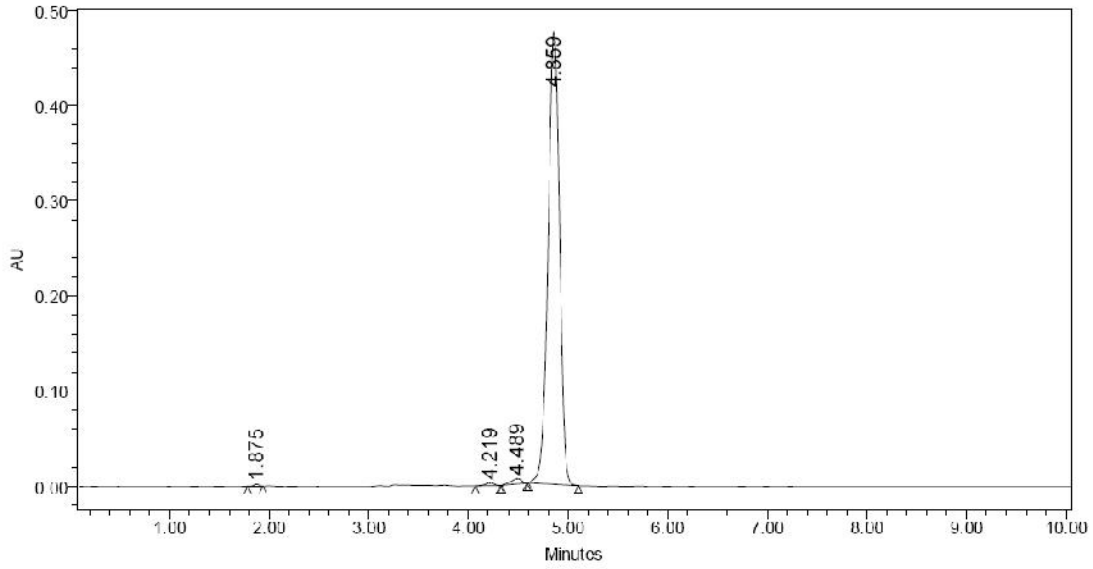
Compound 8b:
Solvent system: (20%water : 80%Acetonitrile)

Empower 2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	8b_20water_80AcN_1	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	02_Water_80AcN_1ml
Injection #:	1	Processing Method:	8b_20water_80AcN
Injection Volume:	10.00 ul	Channel Name:	250.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	PDA 250.0 nm
Date Acquired:	6/5/2008 4:52:37 PM IST		
Date Processed:	6/5/2008 5:18:52 PM IST		



	RT	Area	% Area	Height
1	1.875	8350	0.22	2106
2	4.219	18148	0.47	2989
3	4.489	40197	1.05	5549
4	4.859	3764071	98.26	476488

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

Project Name: test_chemistry
Date Printed:
6/5/2008
5:20:03 PM Asia/Calcutta

Compound 8c:
Solvent system: (20%water : 80%Acetonitrile)

Empower 2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	8c_20water_80AcN_1	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	02_Water_80AcN_1ml
Injection #:	1	Processing Method:	8c_20water_80AcN_1
Injection Volume:	10.00 ul	Channel Name:	220.0nm
Run Time:	20.0 Minutes	Proc. Chnl. Descr.:	PDA 220.0 nm
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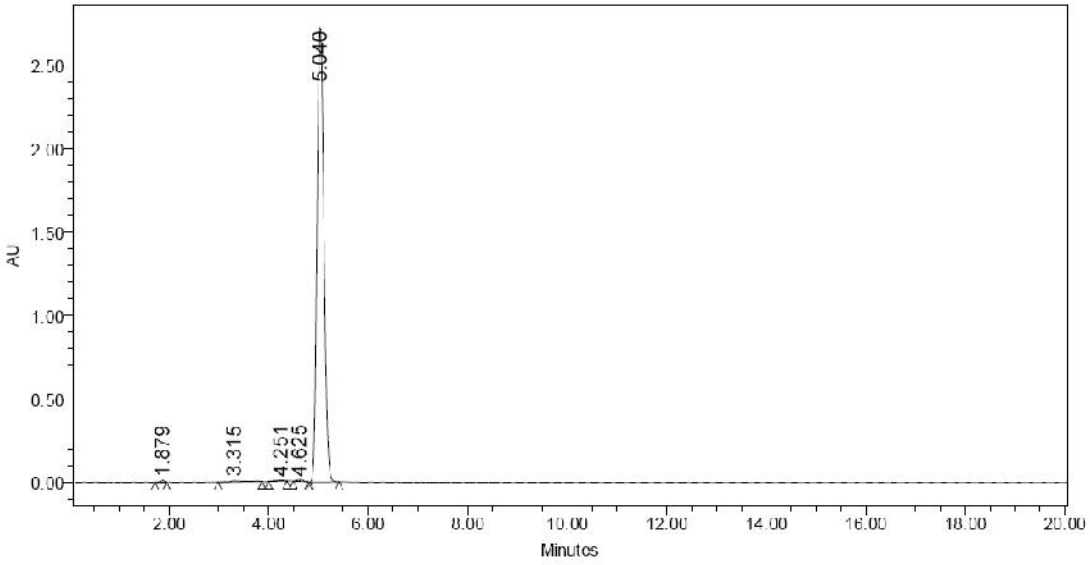
Date Processed:	6/5/2008 2:29:28 PM IST		



	RT	Area	% Area	Height
1	1.879	46446	0.17	9976
2	3.315	120767	0.45	7232
3	4.251	73646	0.28	5205
4	4.625	97688	0.37	10044
5	5.040	26303040	98.73	2730969

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

Project Name: test_chemistry
Date Printed:
6/5/2008
2:30:52 PM Asia/Calcutta

Compound 8g:
Solvent system: (20%water : 80%Acetonitrile)

Empower 2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	8g_20water_80AcN_1	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	02_Water_80AcN_1ml
Injection #:	2	Processing Method:	8g_20water_80AcN
Injection Volume:	10.00 ul	Channel Name:	290.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	PDA 290.0 nm
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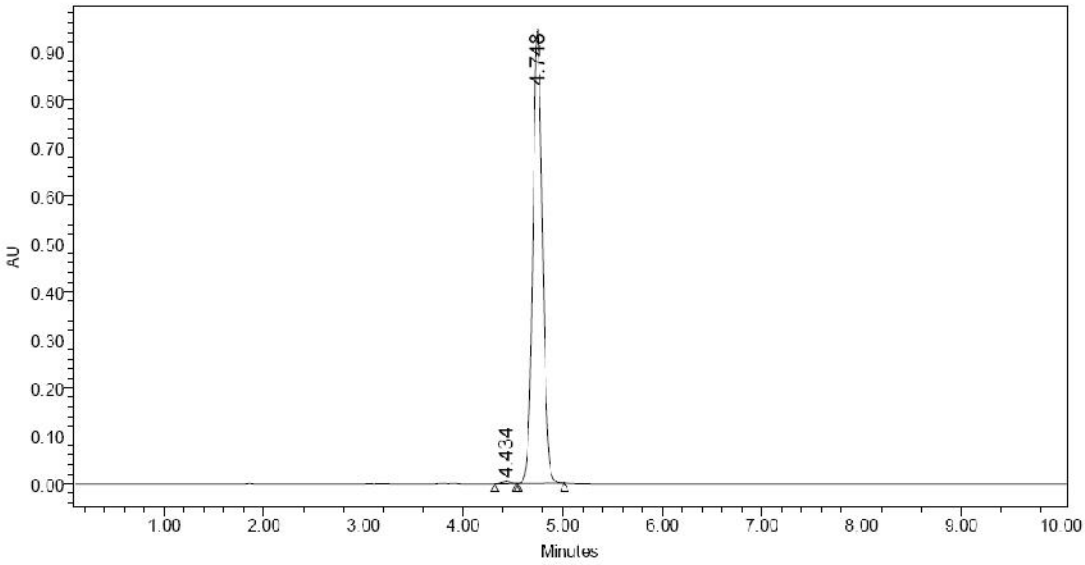
Date Processed:	6/5/2008 5:25:30 PM IST		



	RT	Area	% Area	Height
1	4.434	22443	0.35	3646
2	4.748	6396268	99.65	942269

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

Project Name: test_chemistry
Date Printed:
6/5/2008
5:26:10 PM Asia/Calcutta

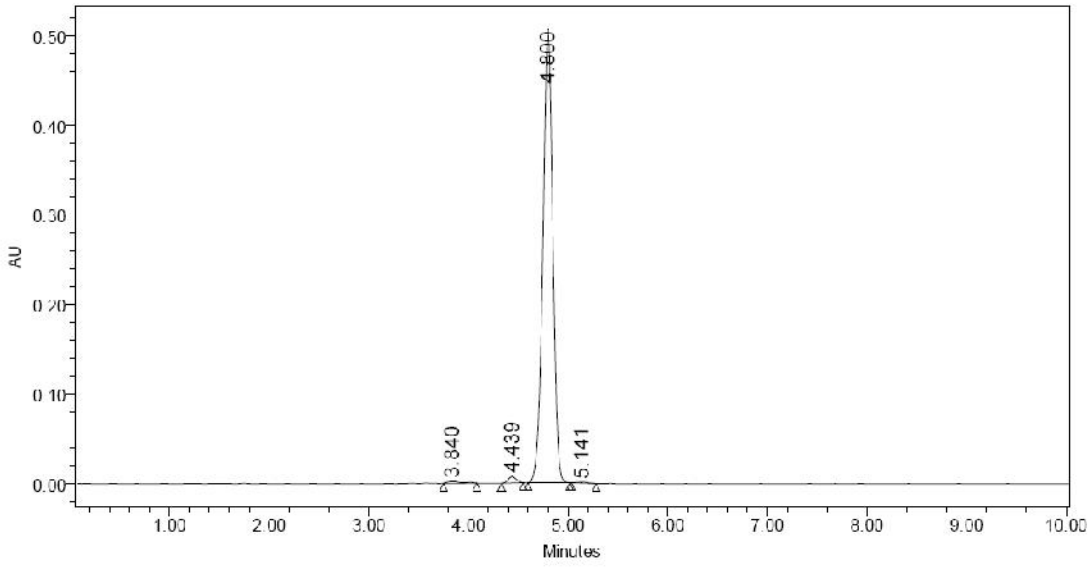
Compound 8h:
Solvent system: (20%water : 80%Acetonitrile)

Empower 2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	8h_20water_80AcN_1	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	02_Water_80AcN_1ml
Injection #:	3	Processing Method:	8h_20water_80AcN
Injection Volume:	10.00 ul	Channel Name:	254.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	PDA 254.0 nm
Date Acquired:	6/5/2008 5:16:10 PM IST		
Date Processed:	6/5/2008 5:29:08 PM IST		



	RT	Area	% Area	Height
1	3.840	21005	0.59	2119
2	4.439	41262	1.17	7247
3	4.800	3470142	98.03	504206
4	5.141	7479	0.21	1080

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

Project Name: test_chemistry
Date Printed:
6/5/2008
5:29:54 PM Asia/Calcutta

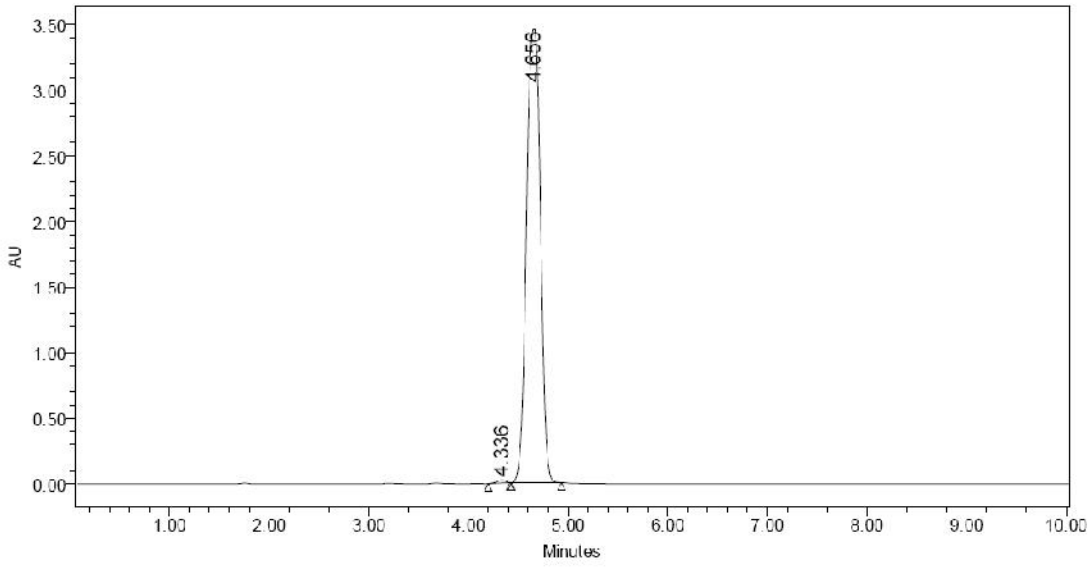
Compound 8j:
Solvent system: (20%water : 80%Acetonitrile)

Empower 2 software

Default Individual Report

SAMPLE INFORMATION

Sample Name:	8j_20water_80AcN_1	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	02_Water_80AcN_1ml
Injection #:	4	Processing Method:	8j_20water_80AcN
Injection Volume:	10.00 ul	Channel Name:	230.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	PDA 230.0 nm
Date Acquired:	6/5/2008 5:35:14 PM IST		
Date Processed:	6/5/2008 5:49:20 PM IST		

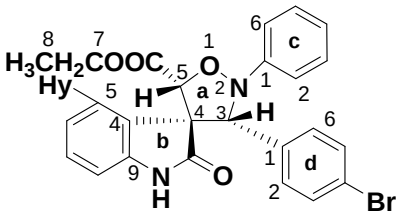


	RT	Area	% Area	Height
1	4.336	133162	0.39	22387
2	4.656	33622196	99.61	3479083

Reported by User: System
Report Method: Default Individual Report
Report Method ID: 1002
Page: 1 of 1

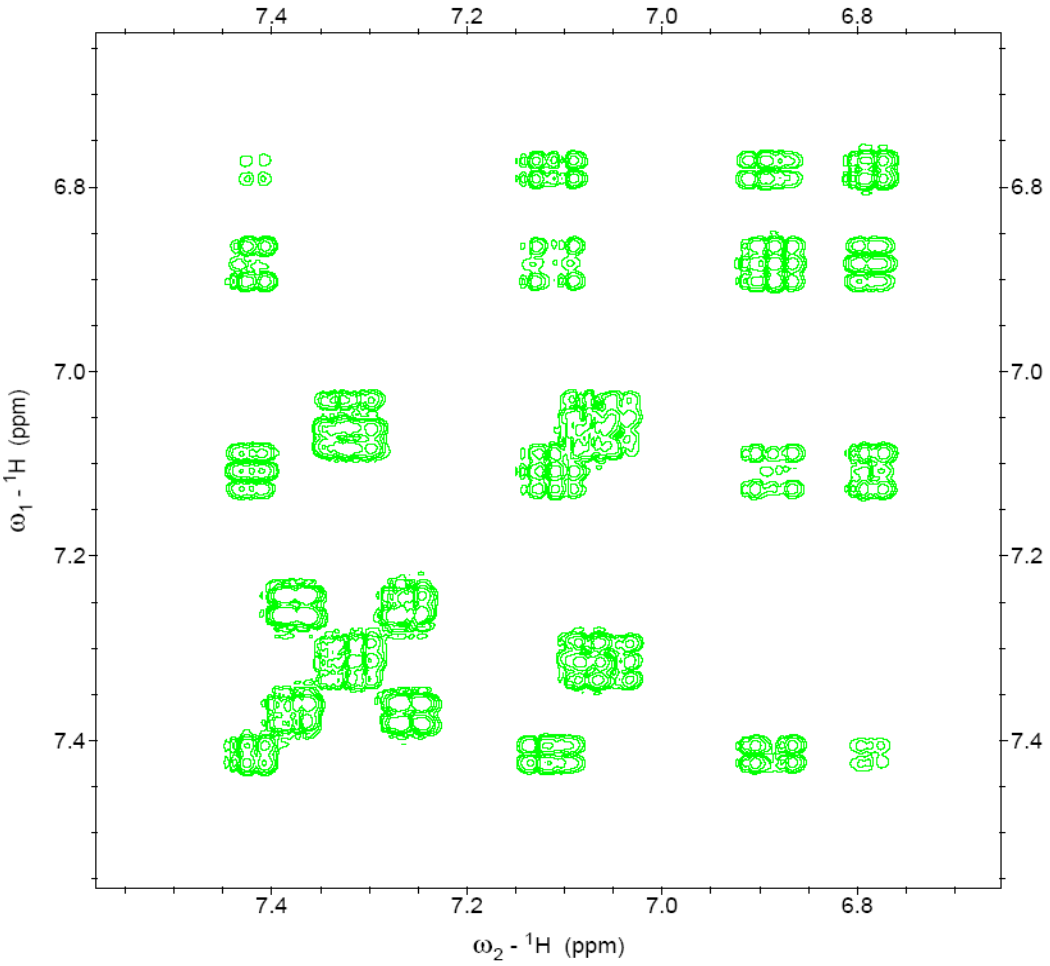
Project Name: test_chemistry
Date Printed:
6/5/2008
5:50:12 PM Asia/Calcutta

2D (cosy, hsqc, hmbc) and 1D (NOESY) NMR spectra for compounds 10c, 8d, 9l and 7l

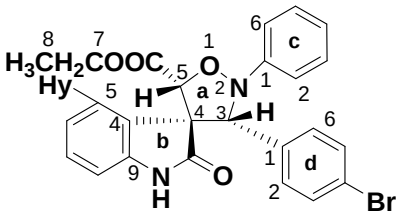


10c

Spectrum: cosy
User: CEO Date: Tue May 17 08:46:09 2011
Positive contours: low 7.00e+006 levels 5 factor 2.00
Negative contours: low -1.00e+007 levels 1 factor 1.40

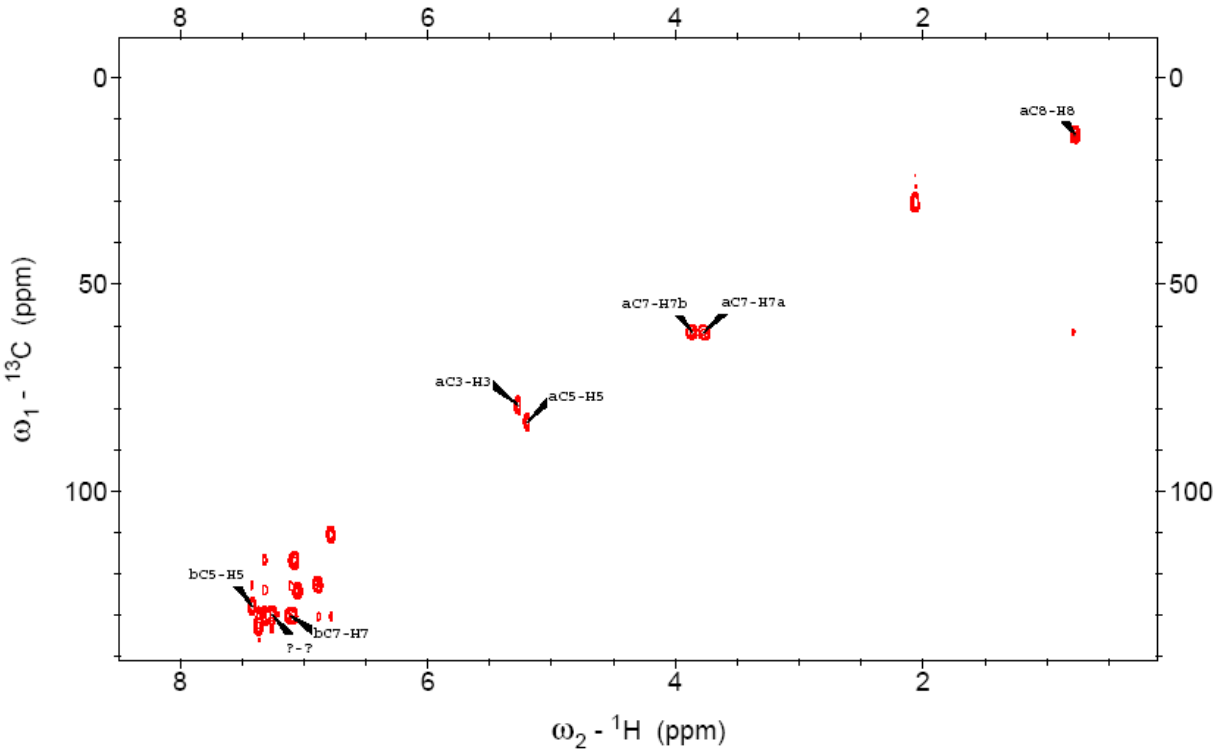


* The numbering of carbon atoms and the ring numbers shown here are limited to the assignment of spectra here only. It should not be confused with the assignment in experimental part.

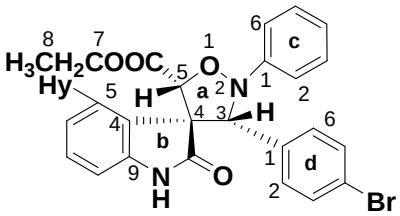


10c

Spectrum: hsqc
User: CEO Date: Tue May 17 08:45:45 2011
Positive contours: low 3.00e+006 levels 5 factor 2.00
Negative contours: low -1.00e+007 levels 1 factor 1.40

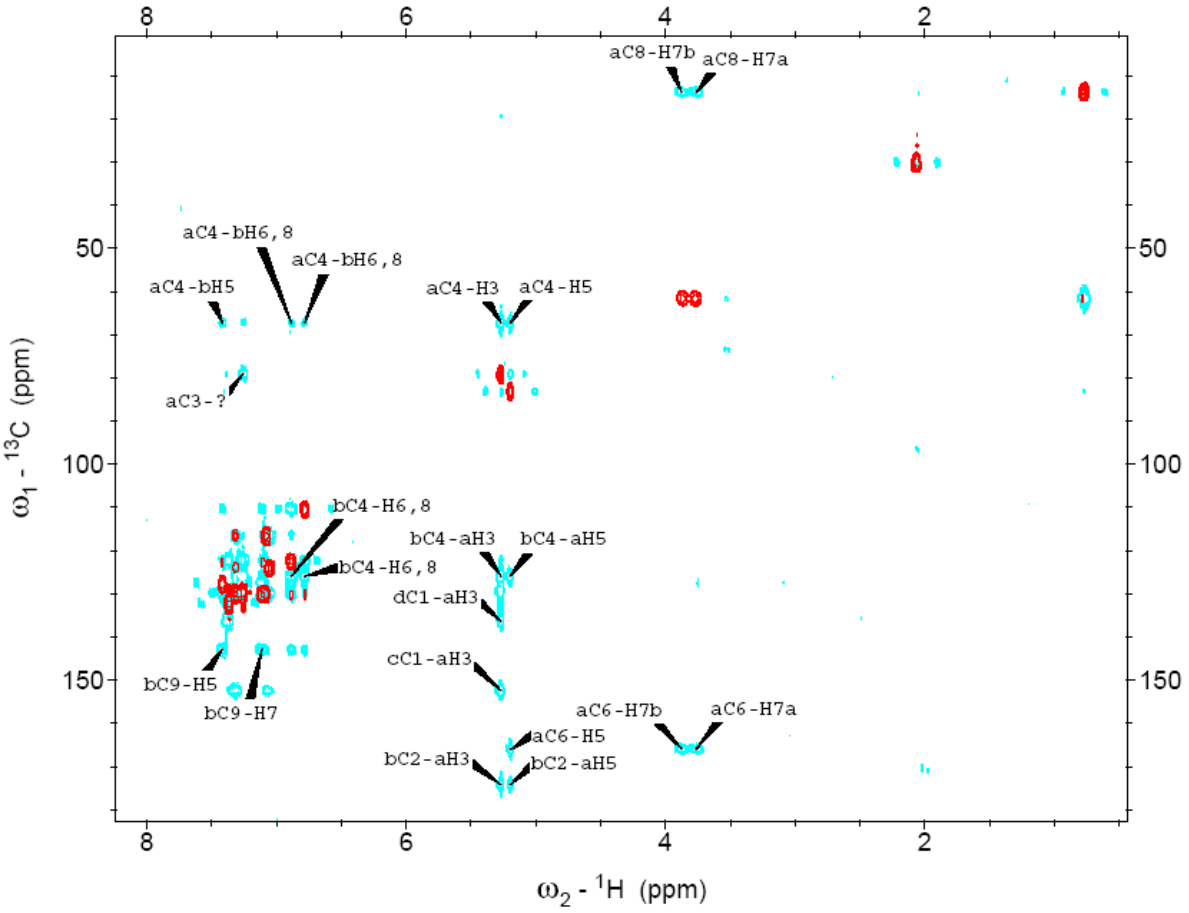


* The numbering of carbon atoms and the ring numbers shown here are limited to the assignment of spectra here only. It should not be confused with the assignment in experimental part.

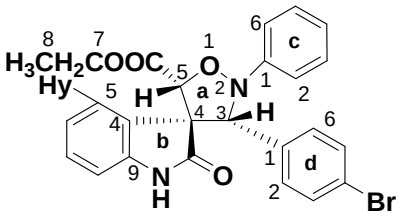


10c

Spectrum: hmbc
User: CEO Date: Tue May 17 08:44:32 2011
Positive contours: low 7.00e+005 levels 6 factor 1.40
Negative contours: low -1.00e+007 levels 1 factor 1.40

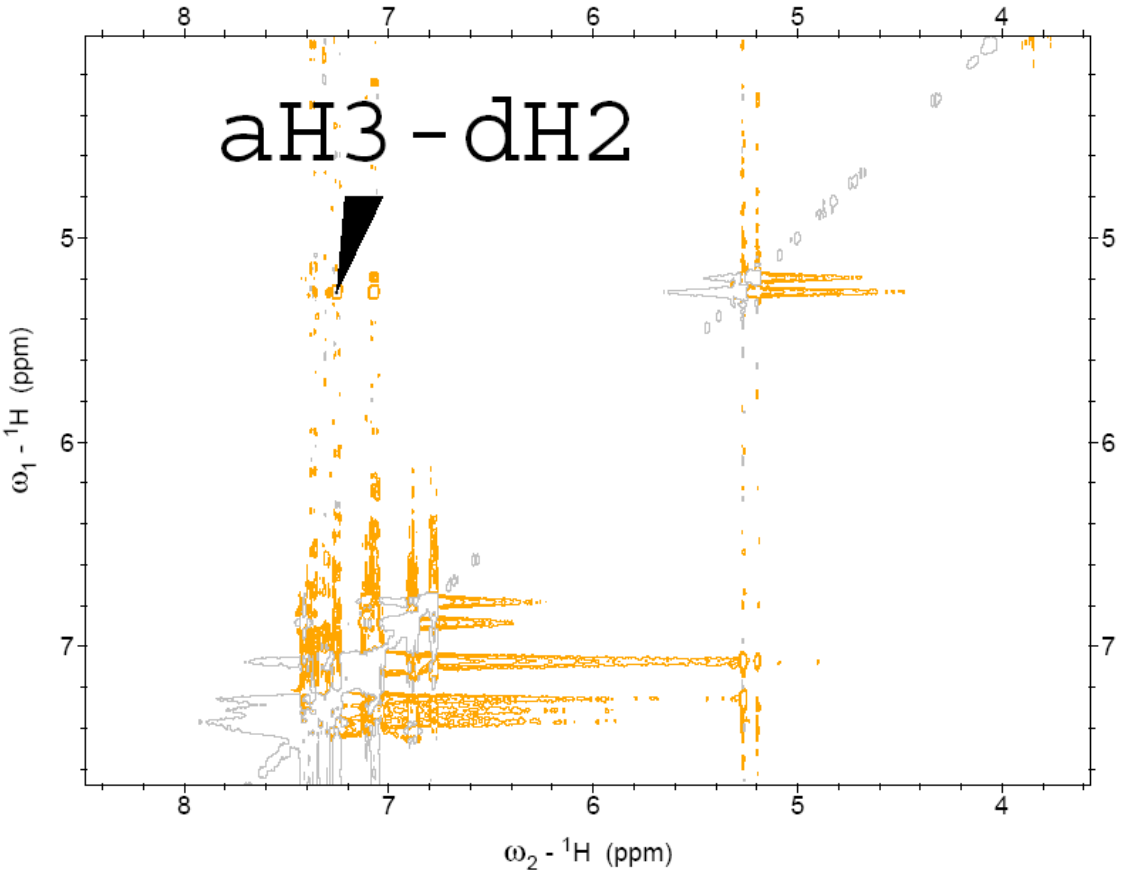


* The numbering of carbon atoms and the ring numbers shown here are limited to the assignment of spectra here only. It should not be confused with the assignment in experimental part.

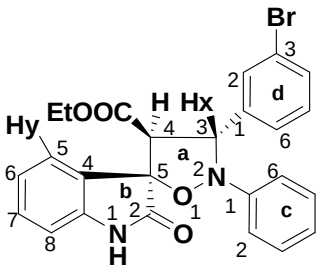


10c

Spectrum: noesy800
User: CEO Date: Tue May 17 08:52:45 2011
Positive contours: low 7.00e+004 levels 5 factor 1.40
Negative contours: low -1.00e+005 levels 1 factor 1.40

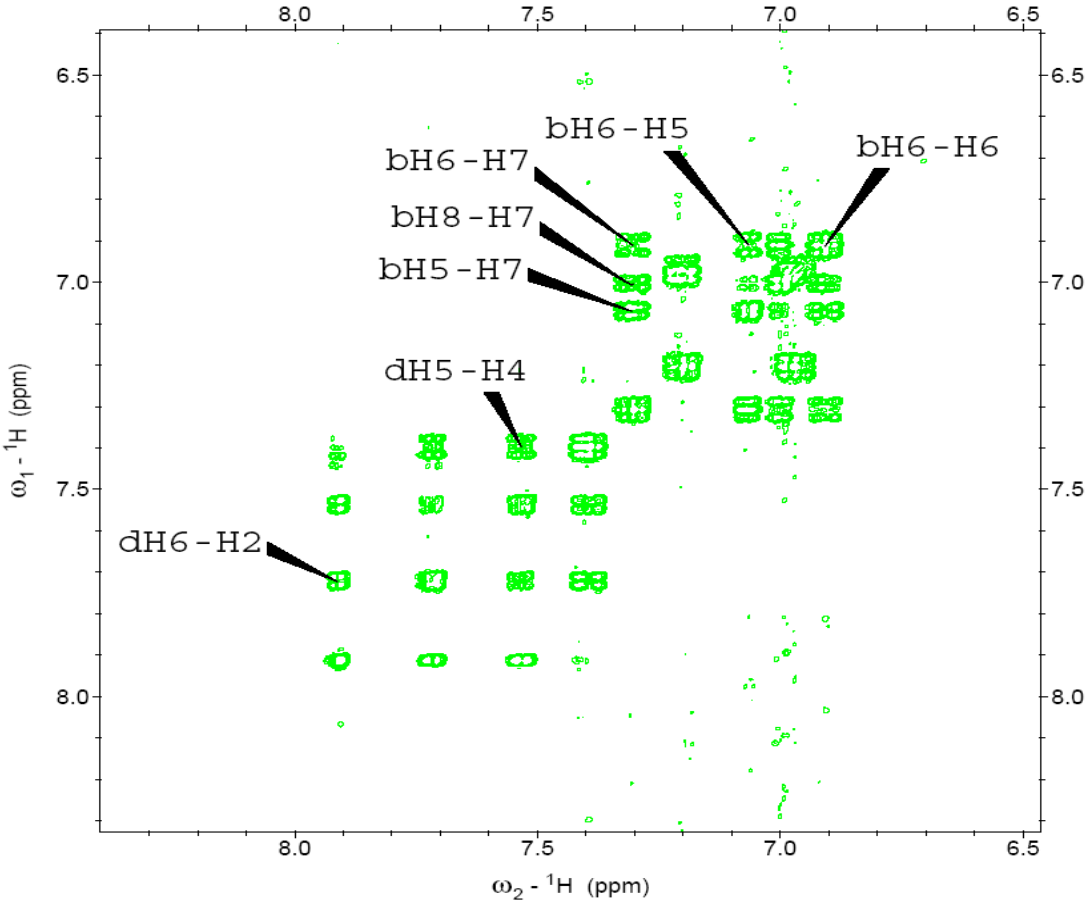


* The numbering of carbon atoms and the ring numbers shown here are limited to the assignment of spectra here only. It should not be confused with the assignment in experimental part.

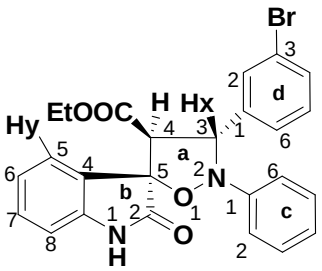


8d

Spectrum: cosy
User: CEO Date: Tue May 17 09:00:05 2011
Positive contours: low 3.00e+006 levels 5 factor 1.80
Negative contours: low -1.00e+007 levels 1 factor 1.40

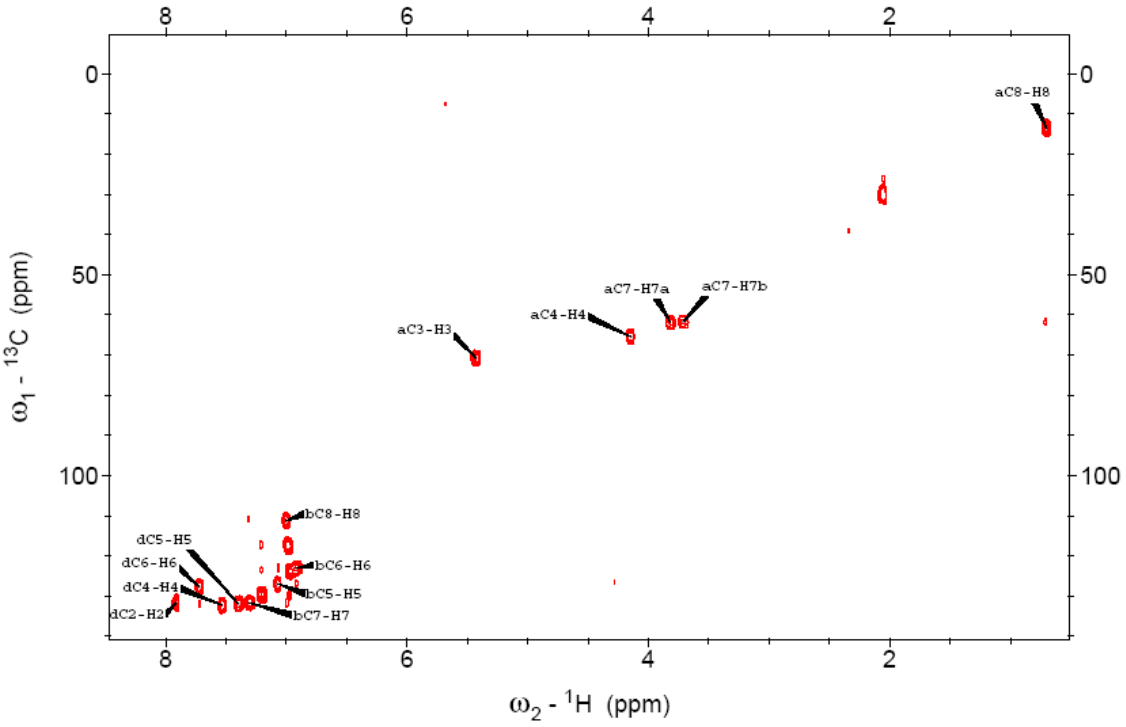


* The numbering of carbon atoms and the ring numbers shown here are limited to the assignment of spectra here only. It should not be confused with the assignment in experimental part.

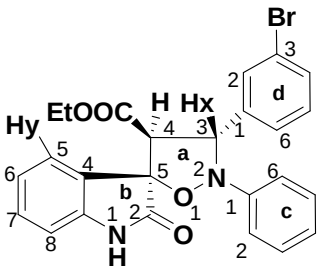


8d

Spectrum: hsqc
User: CEO Date: Tue May 17 08:59:37 2011
Positive contours: low 3.00e+006 levels 5 factor 1.80
Negative contours: low -1.00e+007 levels 1 factor 1.40

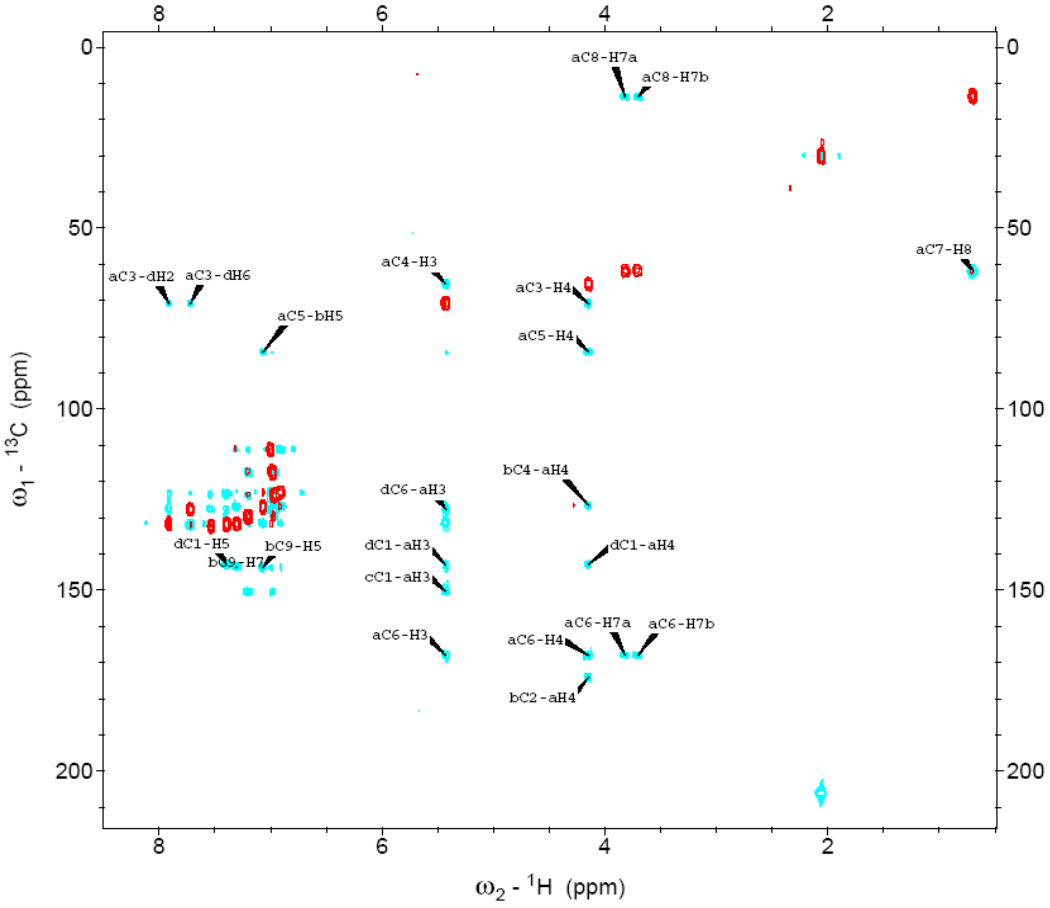


* The numbering of carbon atoms and the ring numbers shown here are limited to the assignment of spectra here only. It should not be confused with the assignment in experimental part.

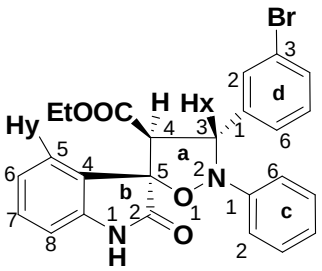


8d

Spectrum: hmbc
User: CEO Date: Tue May 17 08:59:06 2011
Positive contours: low 3.00e+006 levels 5 factor 2.00
Negative contours: low -1.00e+007 levels 1 factor 1.40

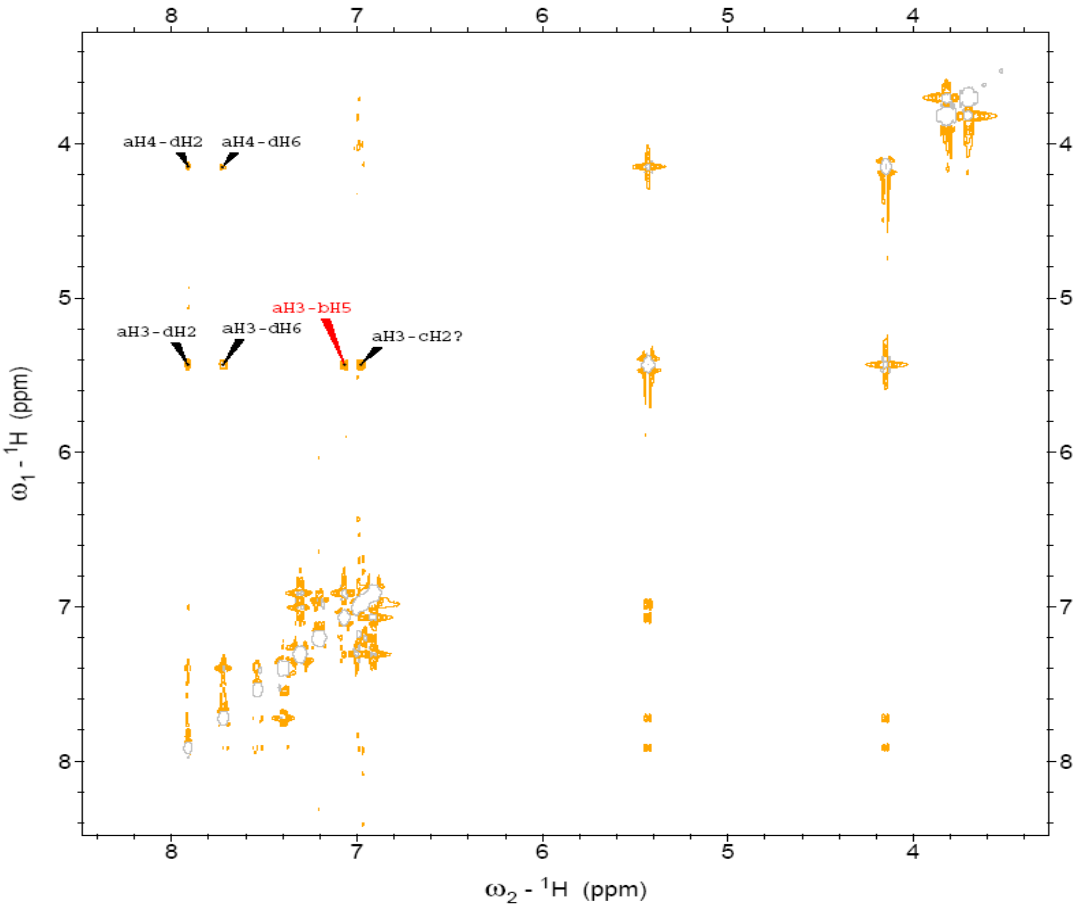


* The numbering of carbon atoms and the ring numbers shown here are limited to the assignment of spectra here only. It should not be confused with the assignment in experimental part.

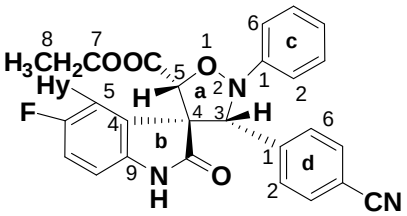


8d

Spectrum: noesy300
User: CEO Date: Tue May 17 09:00:50 2011
Positive contours: low 1.00e+005 levels 5 factor 1.80
Negative contours: low -1.00e+006 levels 1 factor 1.40

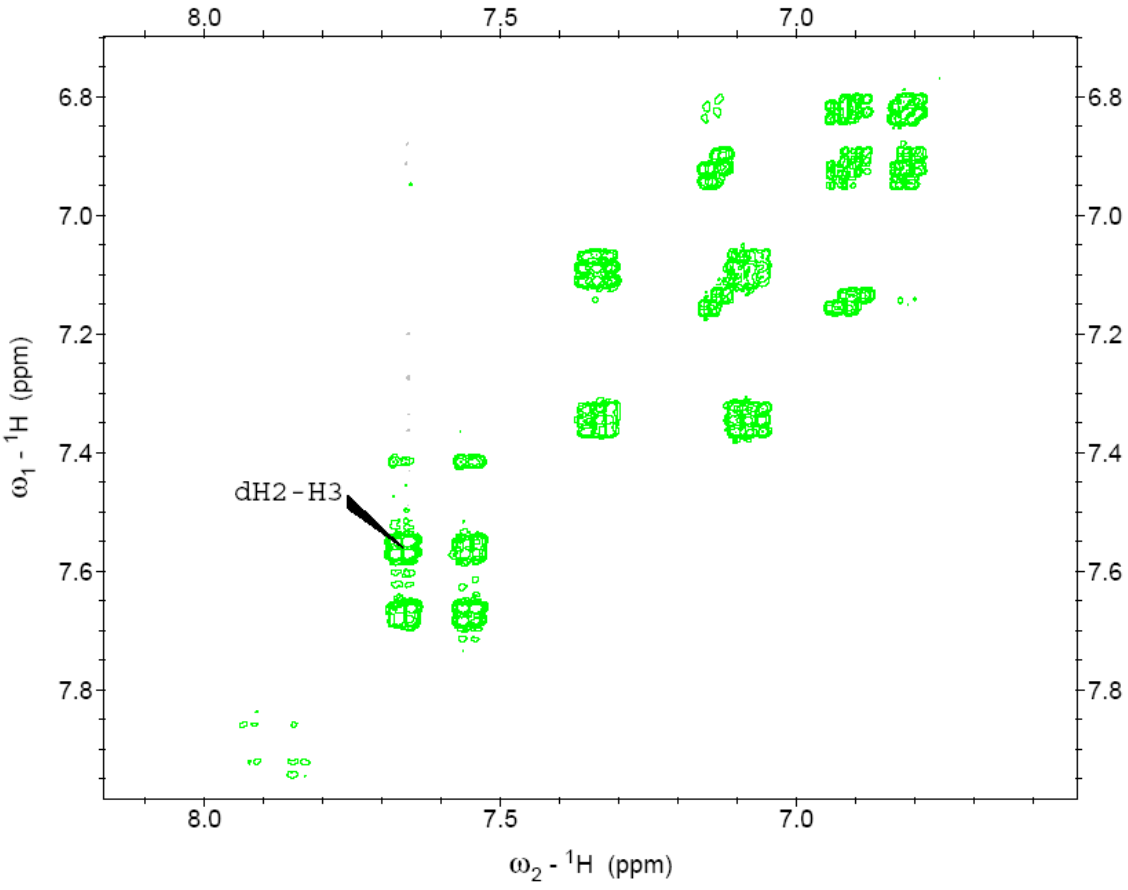


* The numbering of carbon atoms and the ring numbers shown here are limited to the assignment of spectra here only. It should not be confused with the assignment in experimental part.

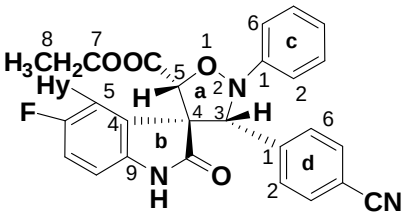


9l

Spectrum: cosy
User: CEO Date: Tue May 17 09:08:01 2011
Positive contours: low 5.00e+006 levels 5 factor 2.00
Negative contours: low -3.00e+006 levels 1 factor 2.00

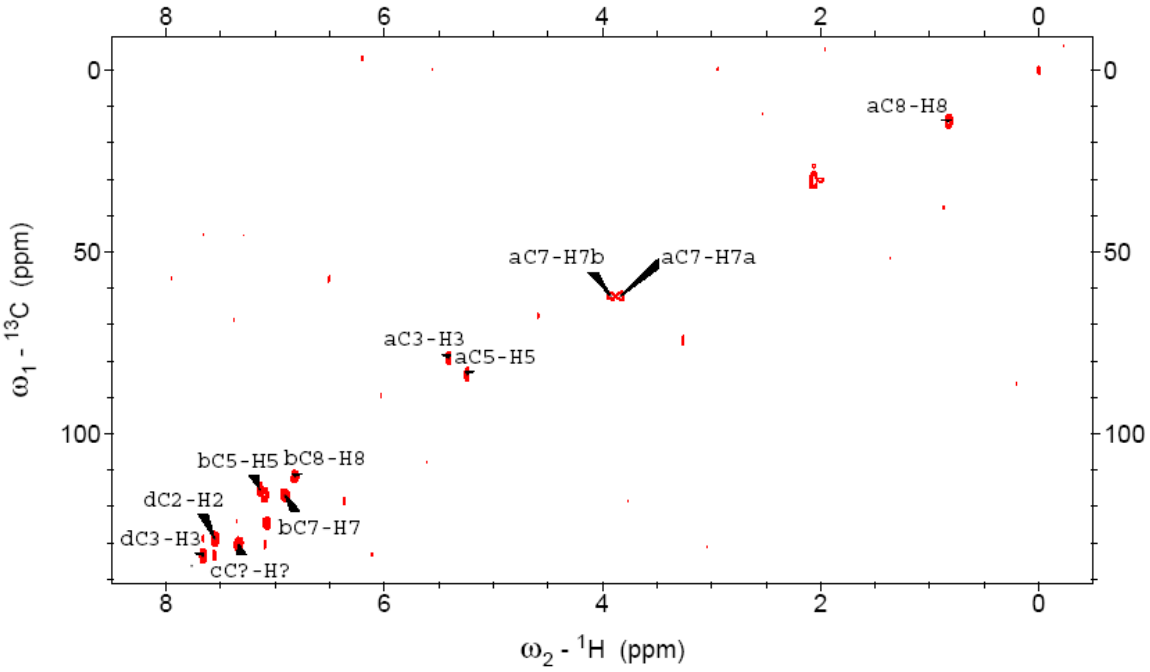


* The numbering of carbon atoms and the ring numbers shown here are limited to the assignment of spectra here only. It should not be confused with the assignment in experimental part.

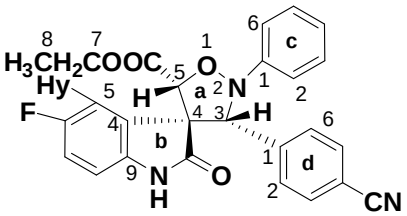


9l

Spectrum: hsqc
User: CEO Date: Tue May 17 09:07:37 2011
Positive contours: low 2.70e+006 levels 8 factor 1.50
Negative contours: low -5.00e+006 levels 1 factor 1.40

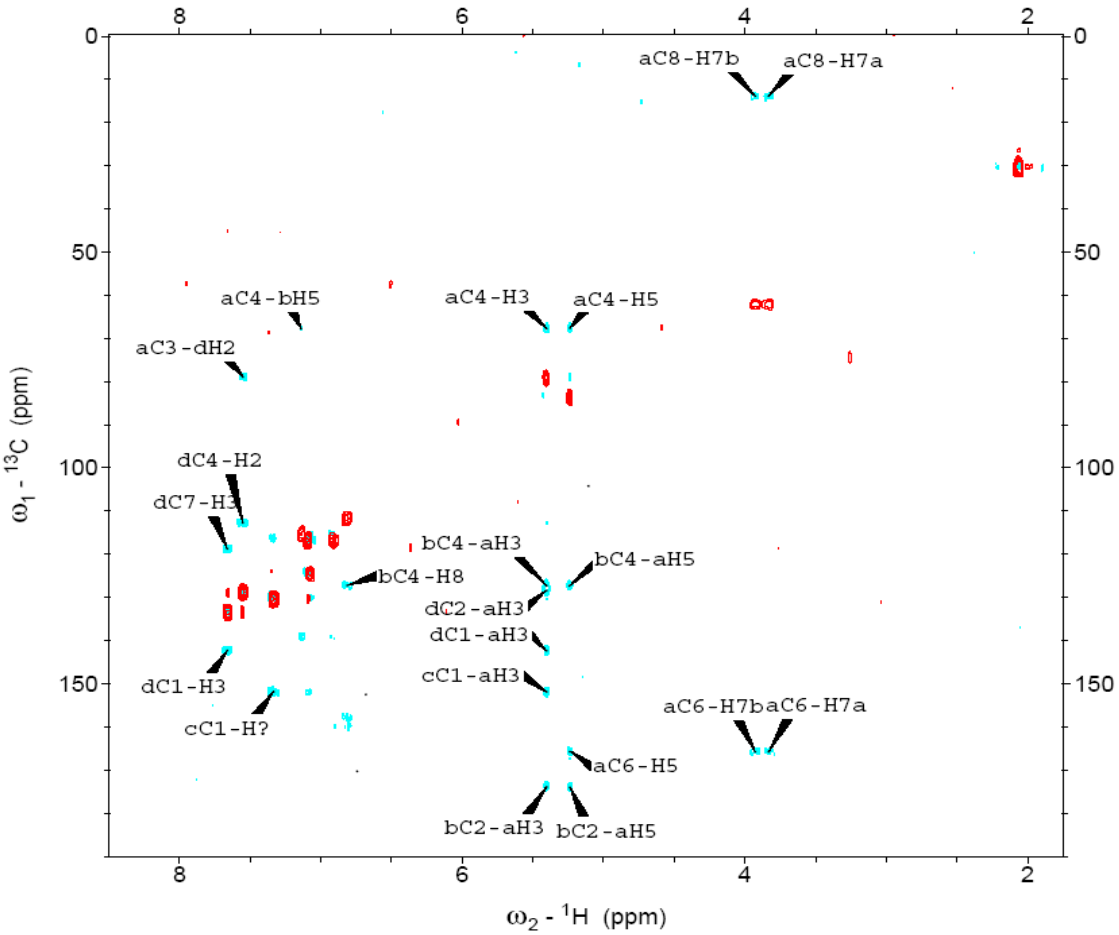


* The numbering of carbon atoms and the ring numbers shown here are limited to the assignment of spectra here only. It should not be confused with the assignment in experimental part.

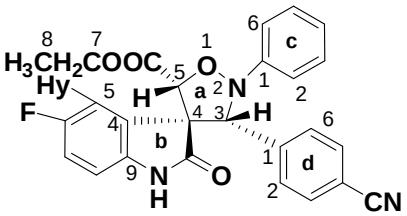


9l

Spectrum: hmbc
User: CEO Date: Tue May 17 09:06:23 2011
Positive contours: low 3.00e+006 levels 5 factor 1.70
Negative contours: low -5.00e+006 levels 1 factor 1.40

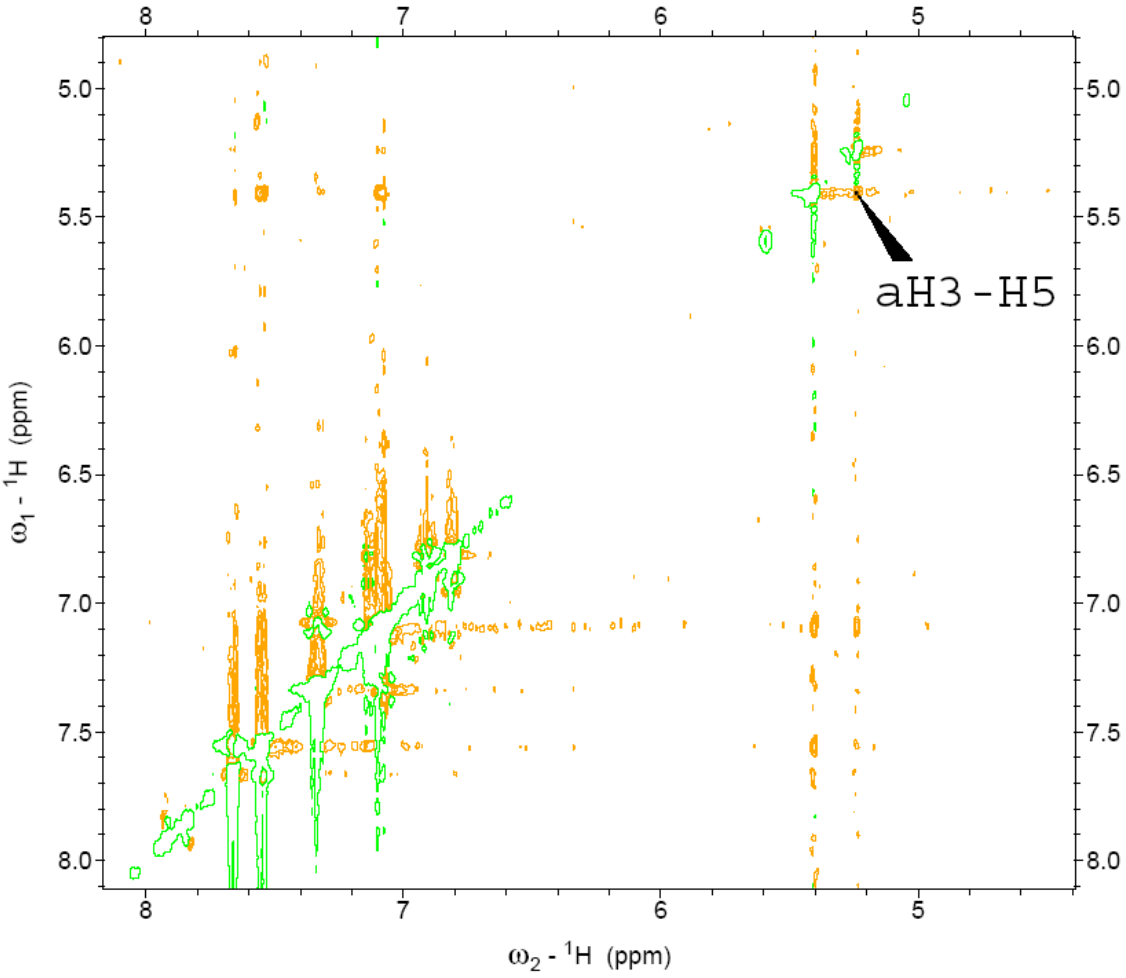


* The numbering of carbon atoms and the ring numbers shown here are limited to the assignment of spectra here only. It should not be confused with the assignment in experimental part.



9l

Spectrum: noesy300
User: CEO Date: Tue May 17 09:11:08 2011
Positive contours: low 3.00e+004 levels 5 factor 1.80
Negative contours: low -5.00e+004 levels 1 factor 1.40



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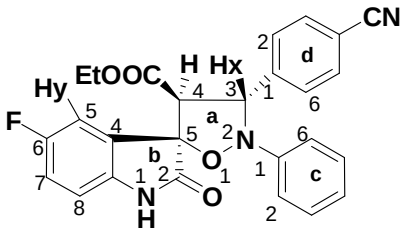
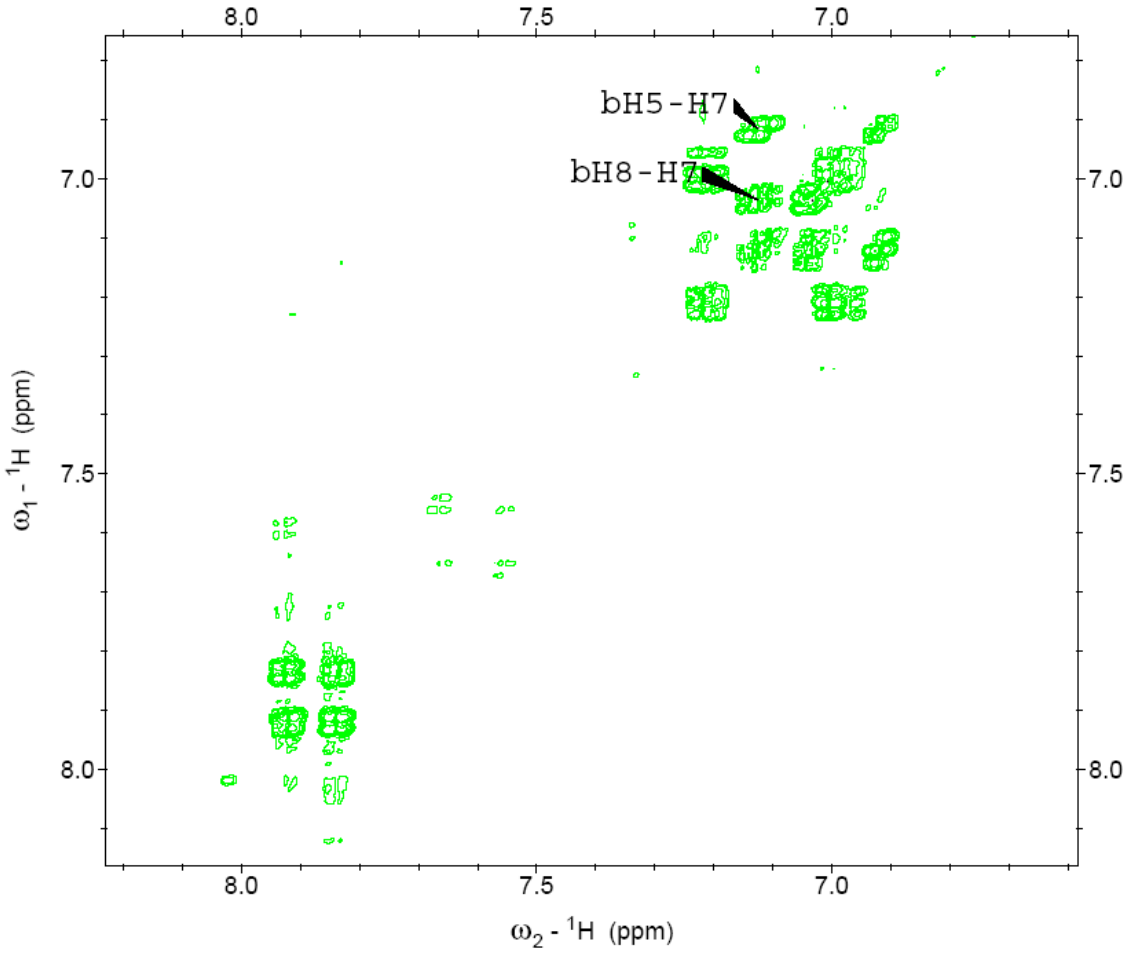
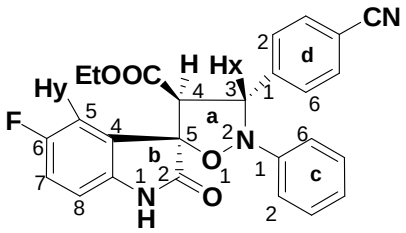


7l

Spectrum: cosy
User: CEO Date: Tue May 17 09:15:46 2011
Positive contours: low 7.00e+006 levels 5 factor 2.00
Negative contours: low -4.46e+008 levels 1 factor 1.40

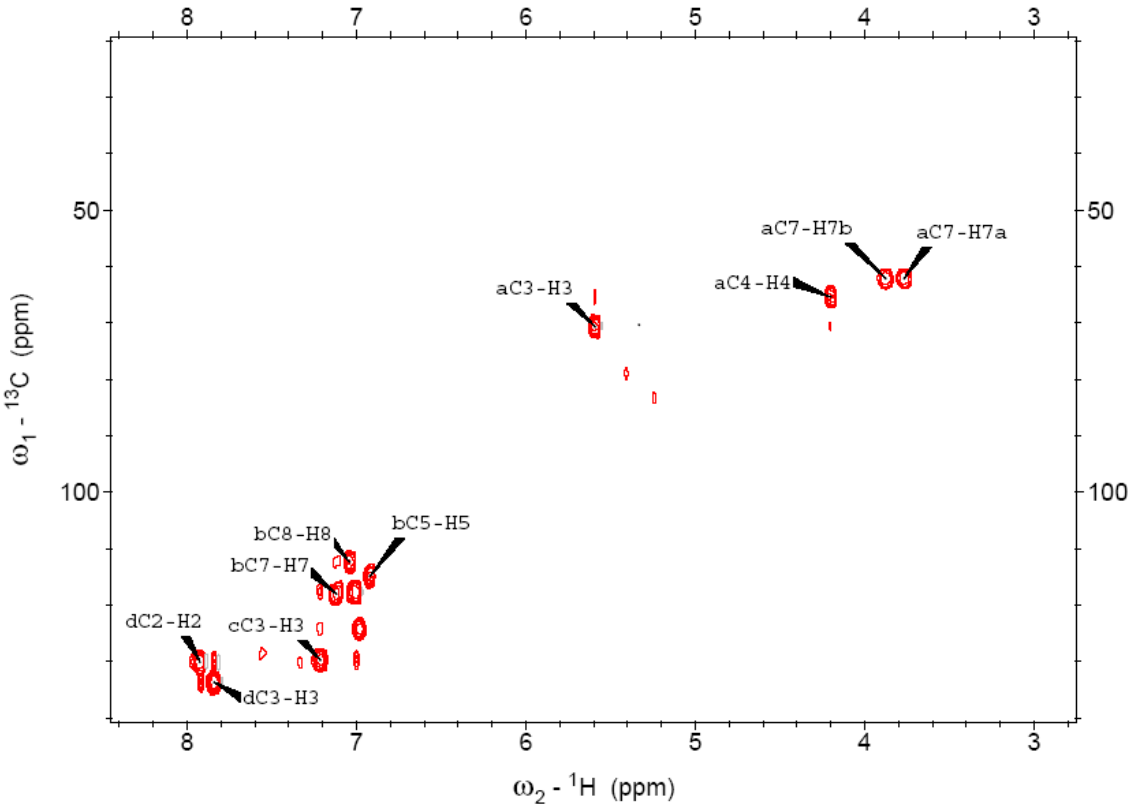


* The numbering of carbon atoms and the ring numbers shown here are limited to the assignment of spectra here only. It should not be confused with the assignment in experimental part.

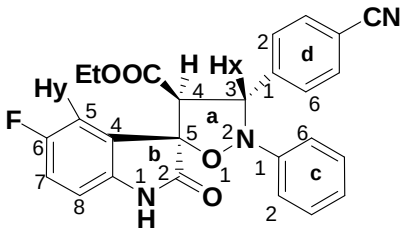


7l

Spectrum: hsqc
User: CEO Date: Tue May 17 09:15:20 2011
Positive contours: low 4.00e+006 levels 5 factor 1.80
Negative contours: low -6.00e+006 levels 1 factor 1.40

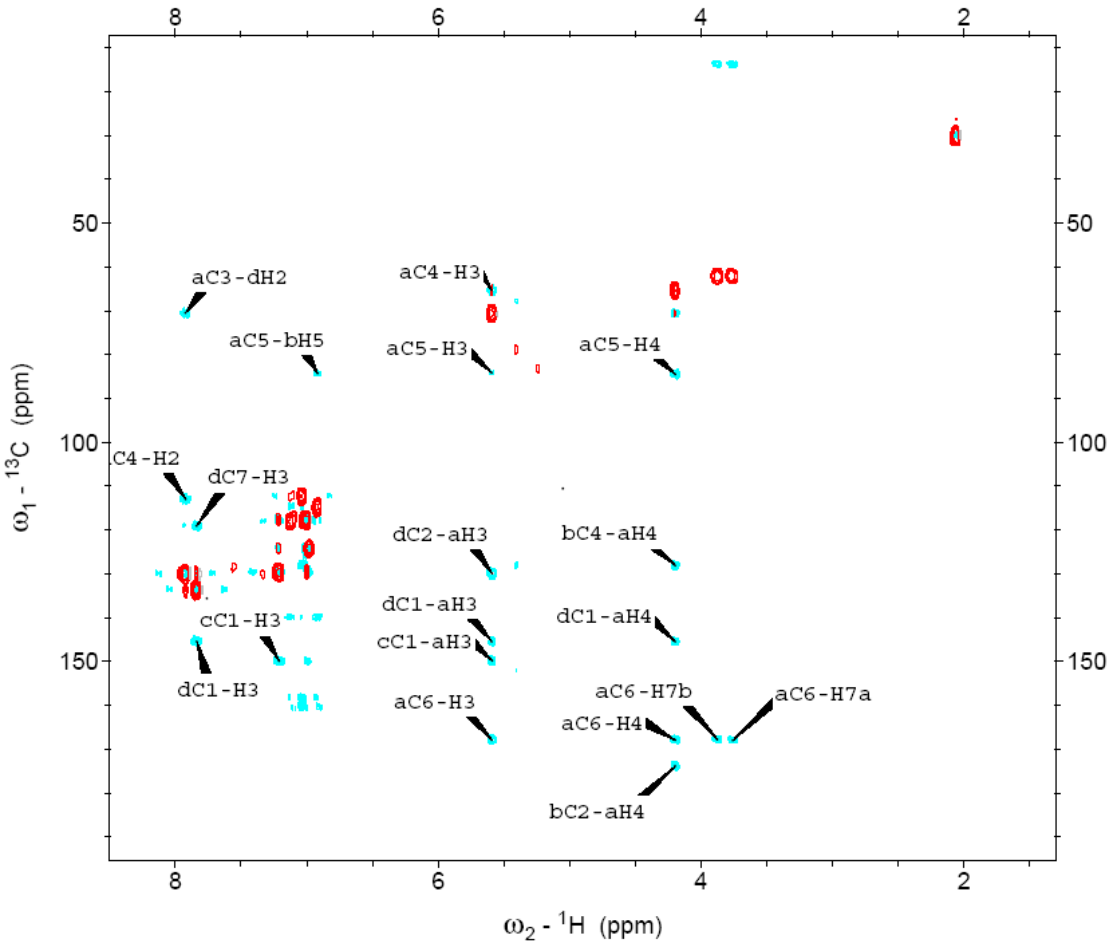


* The numbering of carbon atoms and the ring numbers shown here are limited to the assignment of spectra here only. It should not be confused with the assignment in experimental part.

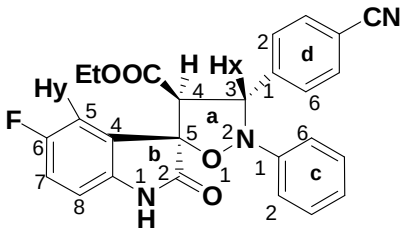


7l

Spectrum: hmbc
User: CEO Date: Tue May 17 09:14:51 2011
Positive contours: low 4.00e+006 levels 5 factor 1.80
Negative contours: low -1.00e+007 levels 1 factor 1.40

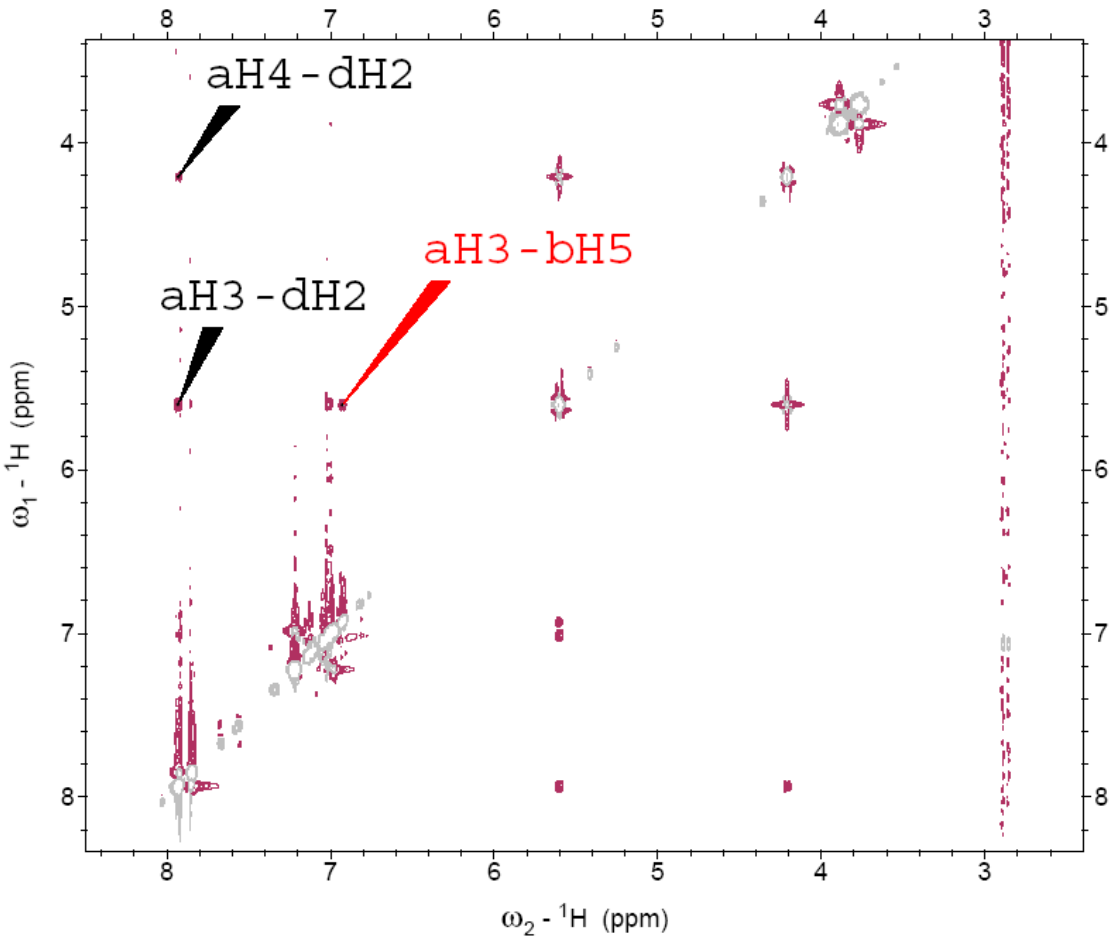


* The numbering of carbon atoms and the ring numbers shown here are limited to the assignment of spectra here only. It should not be confused with the assignment in experimental part.



7l

Spectrum: noesy300
User: CEO Date: Tue May 17 09:16:21 2011
Positive contours: low 2.00e+005 levels 5 factor 1.60
Negative contours: low -1.00e+006 levels 5 factor 1.40



* The numbering of carbon atoms and the ring numbers shown here are limited to the assignment of spectra here only. It should not be confused with the assignment in experimental part.