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# Supporting Information

## Facile construction of novel heterocyclic compounds: Three-component, one-pot synthesis of 2-hydroxybenzoyl-1,2-dihydropyridine-3-carboxylates, ketones, pyridone-3-carboxylates, and benzopyrido-1,3-oxazole-4-carboxylates†

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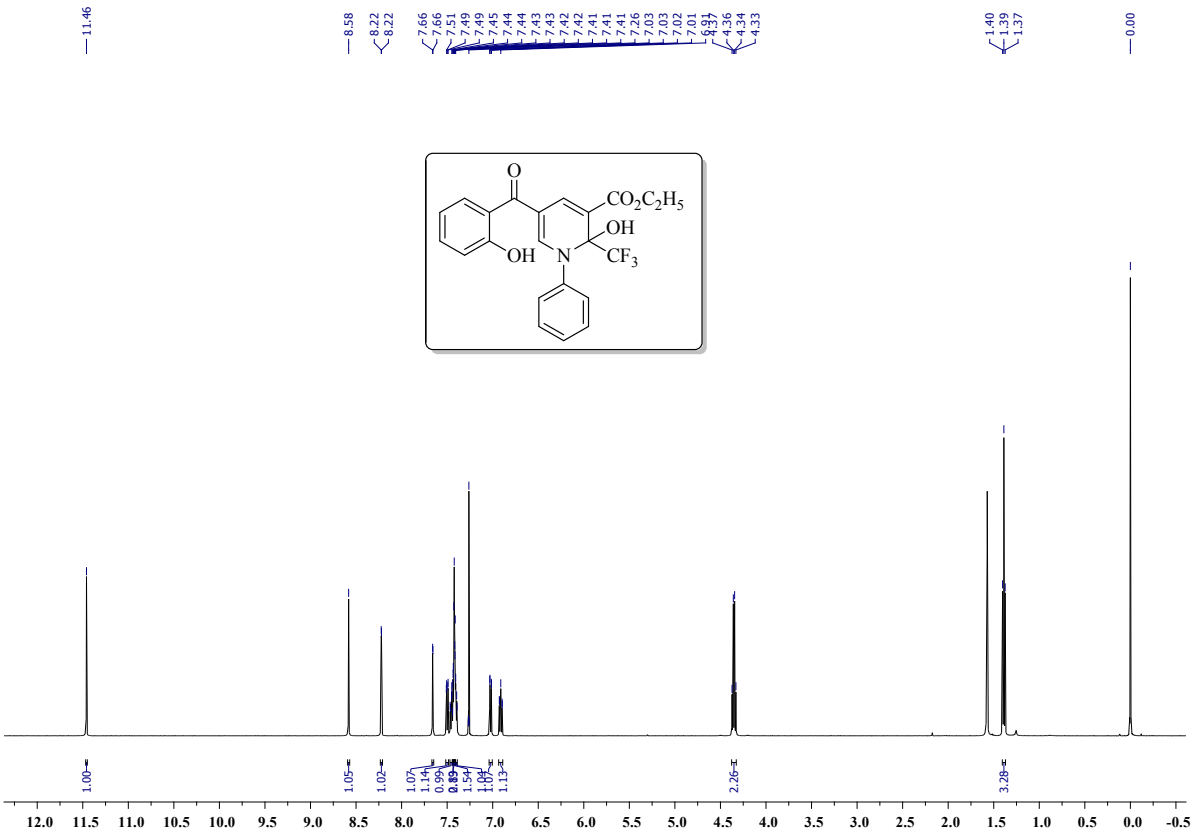
## Experimental section

### General

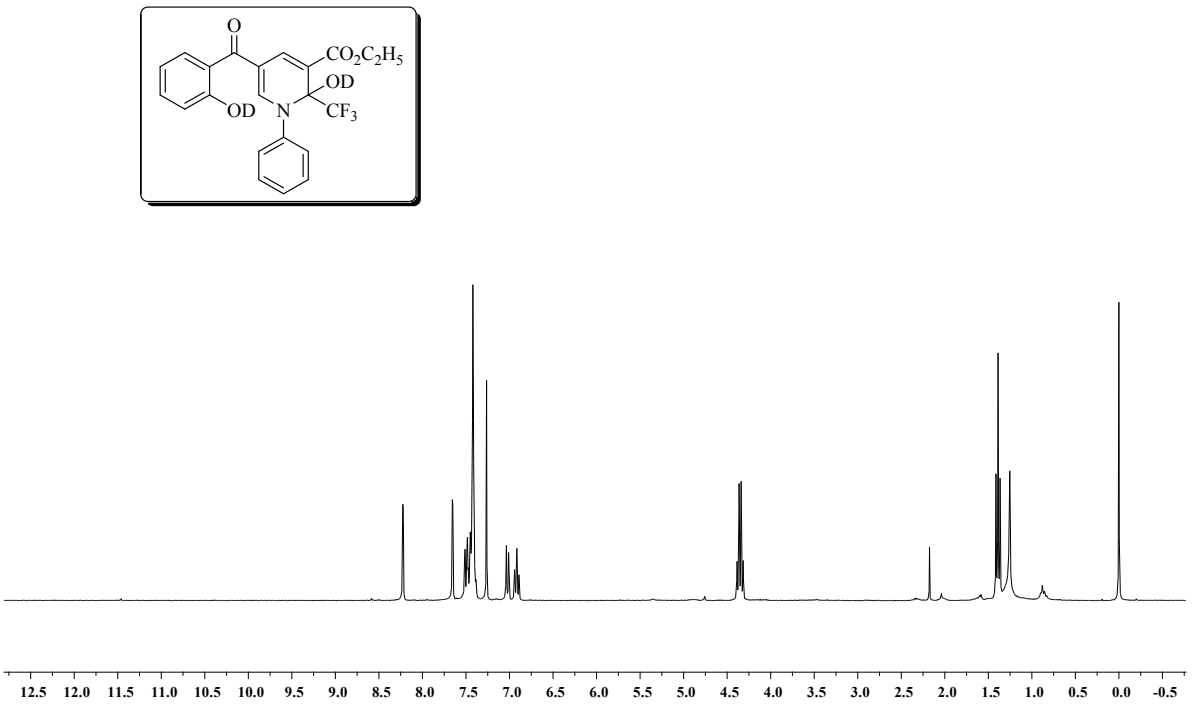
Ethyl 4,4,4-trifluoro-3-oxobutanoate, ethyl 4,4,4-trichloro-3-oxobutanoate, 1,1,1-trifluoropentane-2,4-dione, 4,4,4-trifluoro-1-phenylbutane-1,3-dione, 4,4,4-trifluoro-1-(furan-2-yl)butane-1,3-dione, and tryptamine were procured from Sigma-Aldrich. Benzylamine, aniline, 2-aminophenol, benzene-1,2-diamine, 2-aminobenzenethiol and solvents were obtained from local suppliers. 3-Formylchromenes were prepared as per the literature procedure. $^{1}H$ NMR and $^{13}C$ NMR spectra were recorded on a Varian Gemini 200 MHz and Avance 300 MHz spectrometer in $CDCl_3$ using TMS as internal standard. IR spectra were recorded on a Nicollet 740 FTIR spectrometer. Mass spectra were obtained on Agilent LCMS instrument. HRMS were measured on Agilent Technologies 6510, Q-TOFLC/MS ESI-Technique. Melting points were determined in open glass capillary tubes on a Metler FP 51 melting point apparatus and are uncorrected. All reactions were monitored by thin layer chromatography (TLC) on pre-coated silica gel 60 $F_{254}$ (mesh); spots were visualized under UV light. Merck silica gel (100-200 mesh) was used for chromatography.

### General procedure for the preparation of ethyl 2-hydroxy-5-(2-hydroxybenzoyl)-1-phenyl-2-(trifluoromethyl)-1,2-dihydropyridine-3-carboxylate (4a)

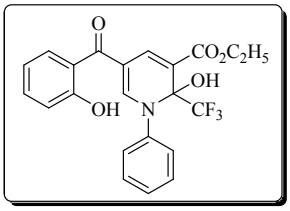
Ethyl 4,4,4-trifluoro-3-oxobutanoate (**3a**, 1.5 mmol) was added to a stirred solution of 4-oxo-4*H*-chromene-3-carbaldehyde (**1a**, 1 mmol) and aniline (**2a**, 1.2 mmol) in $CH_3CN$ (2 mL). The contents were stirred under reflux conditions for 2 h. After completion of the reaction (TLC), the residue was purified by column chromatography by using silica gel (100:200, ethyl acetate/hexane 2:98) afforded ethyl 2-hydroxy-5-(2-hydroxybenzoyl)-1-phenyl-2-(trifluoromethyl)-1,2-dihydropyridine-3-carboxylate **4a** as yellow solid.

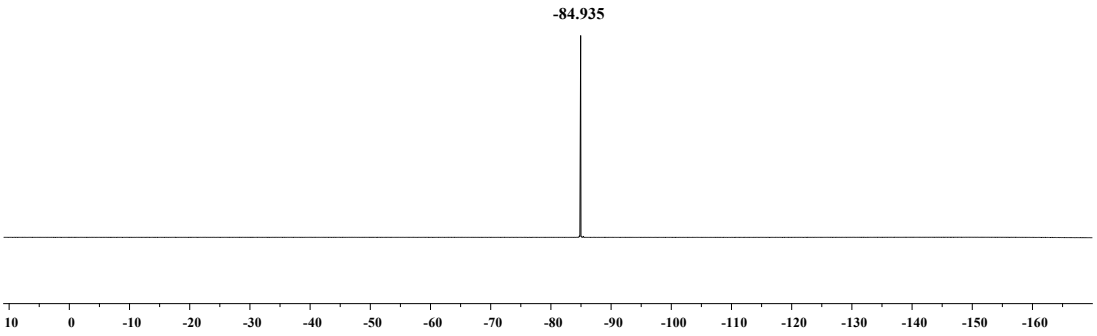



$^1$H NMR spectrum of compound **4a**

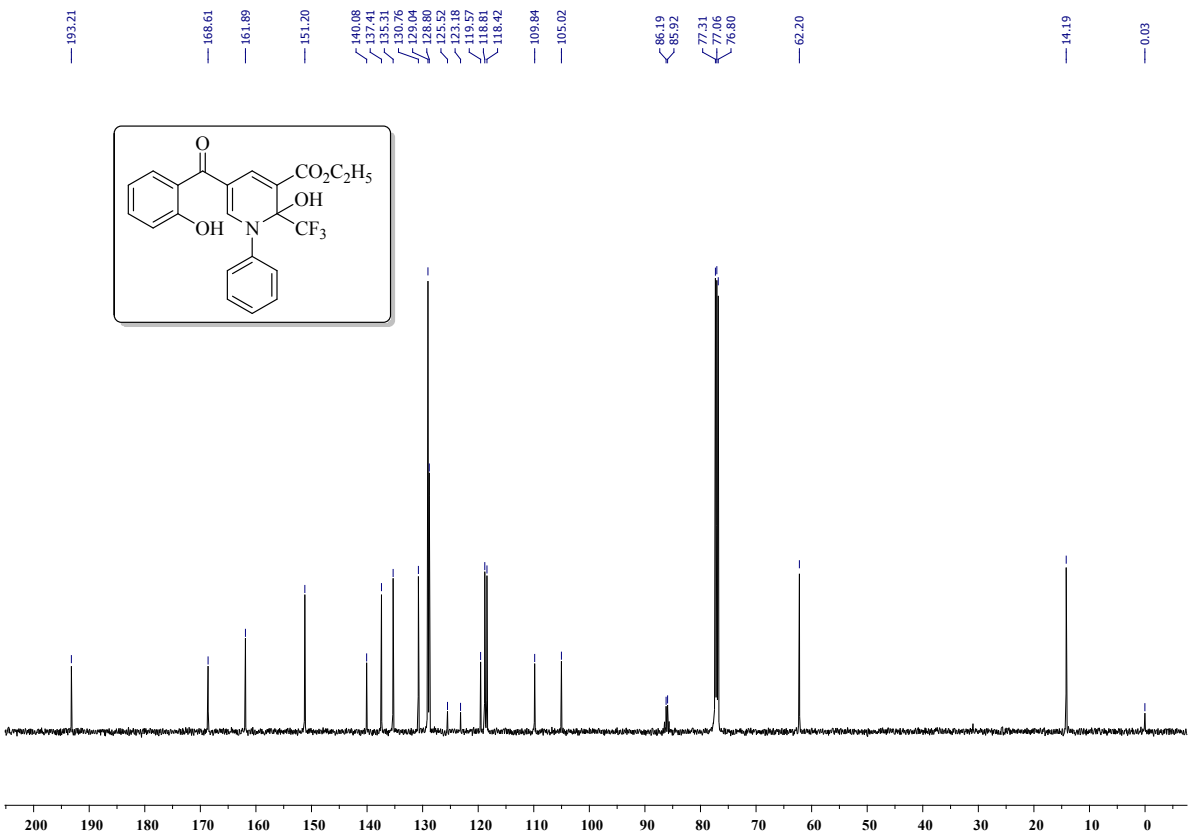



$^1$H NMR Spectrum of compound **4a** $D_2O$ exchange




$^{19}$F NMR Spectrum of compound **4a**




$^{13}$C NMR spectrum of compound **4a**

National Centre for Mass Spectrometry
CSIR-Indian Institute of Chemical Technology

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Sample Name K RAJ
Sample ID A:1
Date and Time 13-02-14 14:19:45

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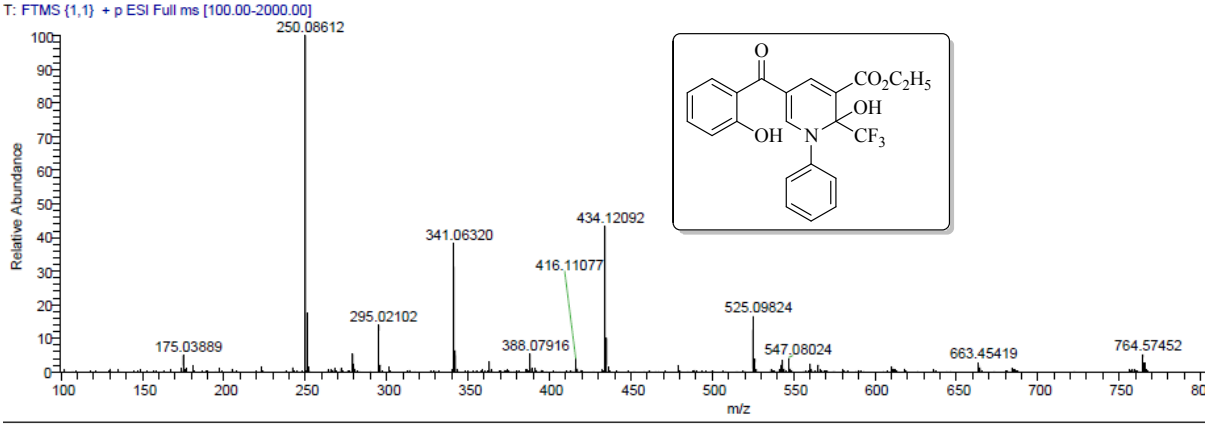


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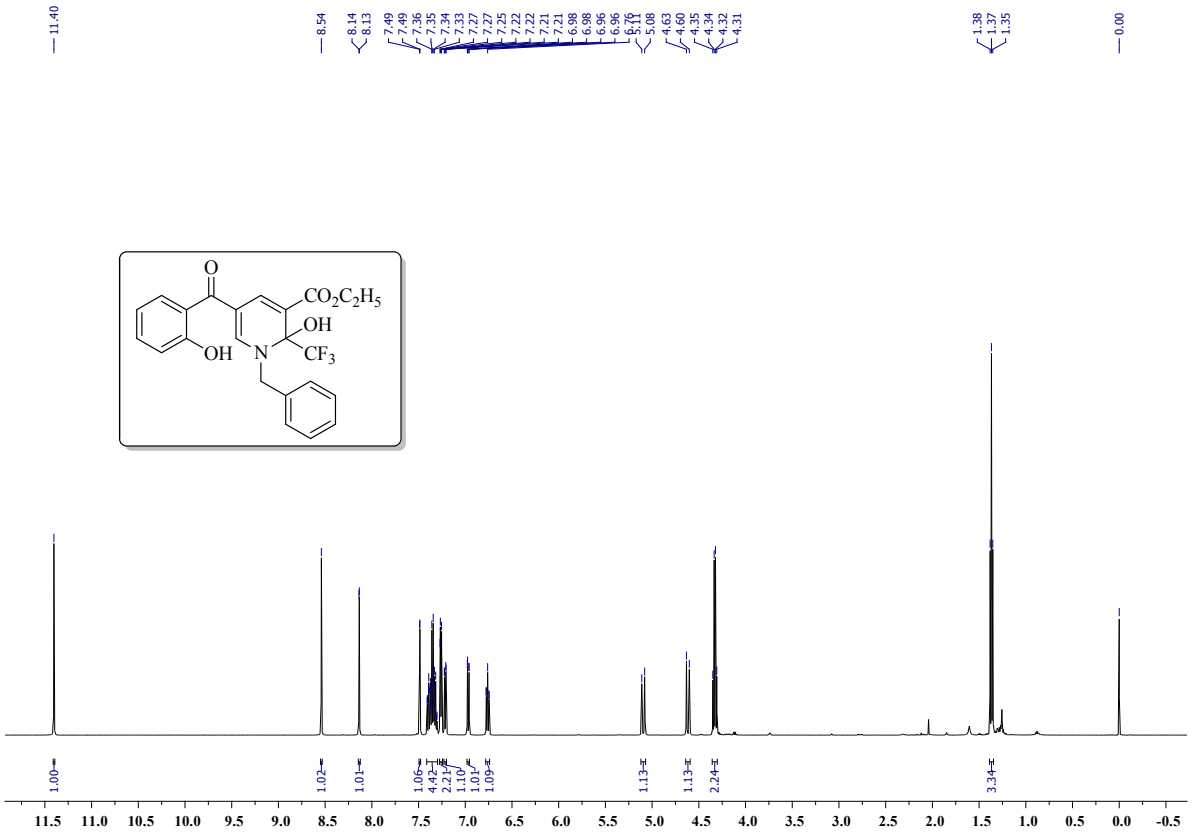
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]
m/z= 410.01-448.82

| m/z | Intensity | Relative | Theo. Mass | Delta (ppm) | RDB equiv. | Composition |
|---|---|---|---|---|---|---|
| 434.12098 | 15865634.0 | 100.00 | 434.12098 | -0.01 | 12.5 | $C_{22}H_{19}O_5NF_3$ |

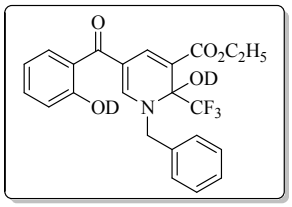
HRMS spectrum of compound **4a**

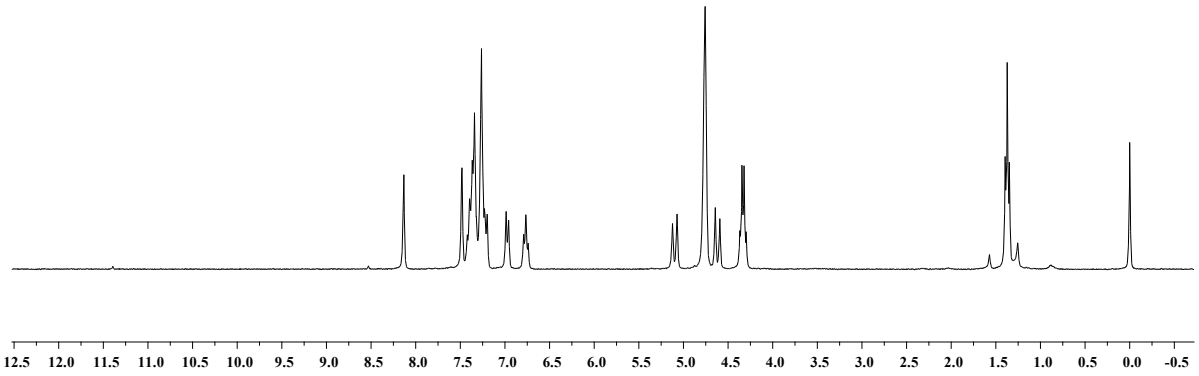
**General procedure for the preparation of 2-hydroxybenzoyl-2-(trifluoromethyl)-1,2-dihydropyridine-3-carboxylates 4b-k.**

Ethyl 4,4,4-trifluoro-3-oxobutanoate (**3a**, 1.5 mmol) was added to a stirred solution of 4-oxo-4*H*-chromene-3-carbaldehyde (**1a**, 1 mmol) and phenylmethanamine (**2b**, 1.2 mmol) in $CH_3CN$ (2 mL). The contents were stirred under reflux conditions for 2 h. After completion of the reaction (TLC), the residue was purified by column chromatography by using silica gel (100:200, ethyl acetate/hexane 2:98) afforded ethyl 1-benzyl-2-hydroxy-5-(2-hydroxybenzoyl)-2-(trifluoromethyl)-1,2-dihydropyridine-3-carboxylate **4b**. Similarly, compounds **4c-h** was prepared from corresponding 3-formylchromones **1a-c**, and benzylamines **2b-d**. However, compounds **4i-k** were prepared from corresponding 3-formylchromone **1a**, benzylamine **2b** and trifluoro containing 1,3-diketones such as 1,1,1-trifluoropentane-2,4-dione **3e**, 4,4,4-trifluoro-1-phenylbutane-1,3-dione **3f**, and 4,4,4-trifluoro-1-(furan-2-yl)butane-1,3-dione **3g**.

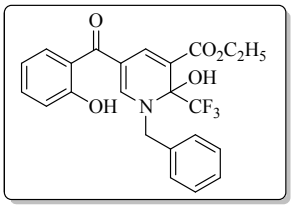


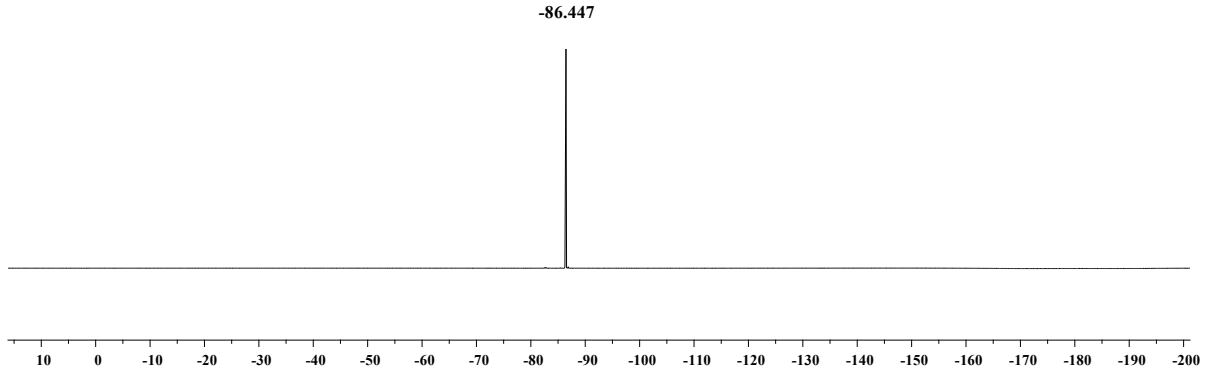

$^1$H NMR spectrum of compound **4b**



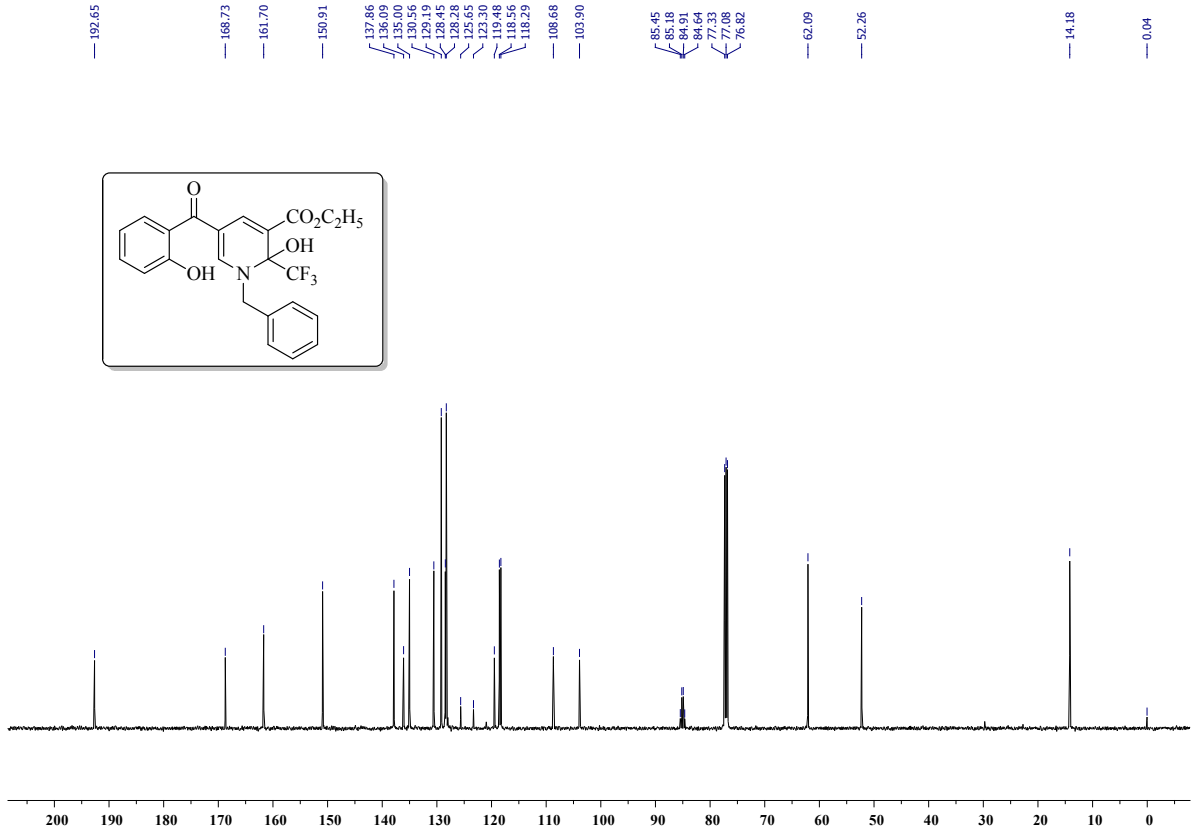




$^{1}$H NMR Spectrum of compound **4b** $D_2O$ exchange



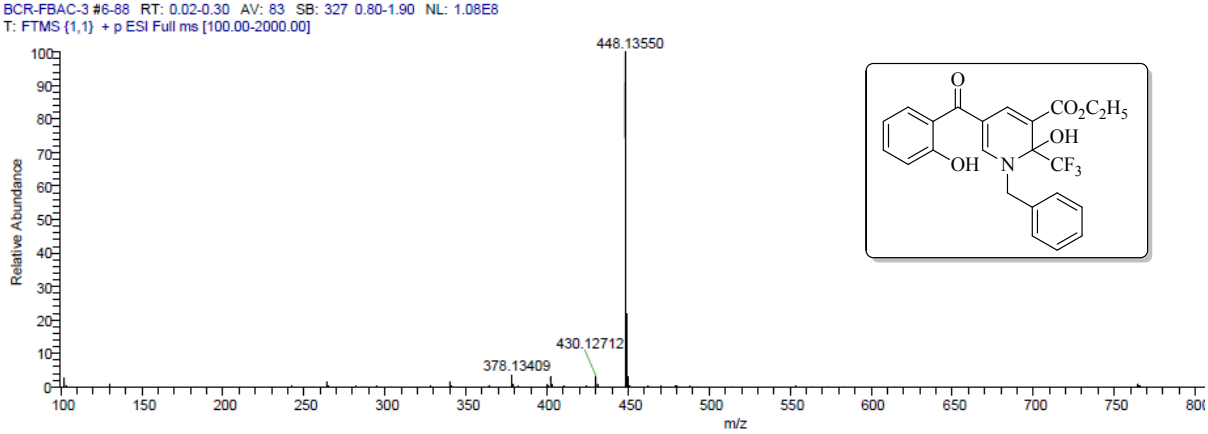




$^{19}$F NMR Spectrum of compound **4b**




$^{13}$C NMR spectrum of compound **4b**

National Centre for Mass Spectrometry

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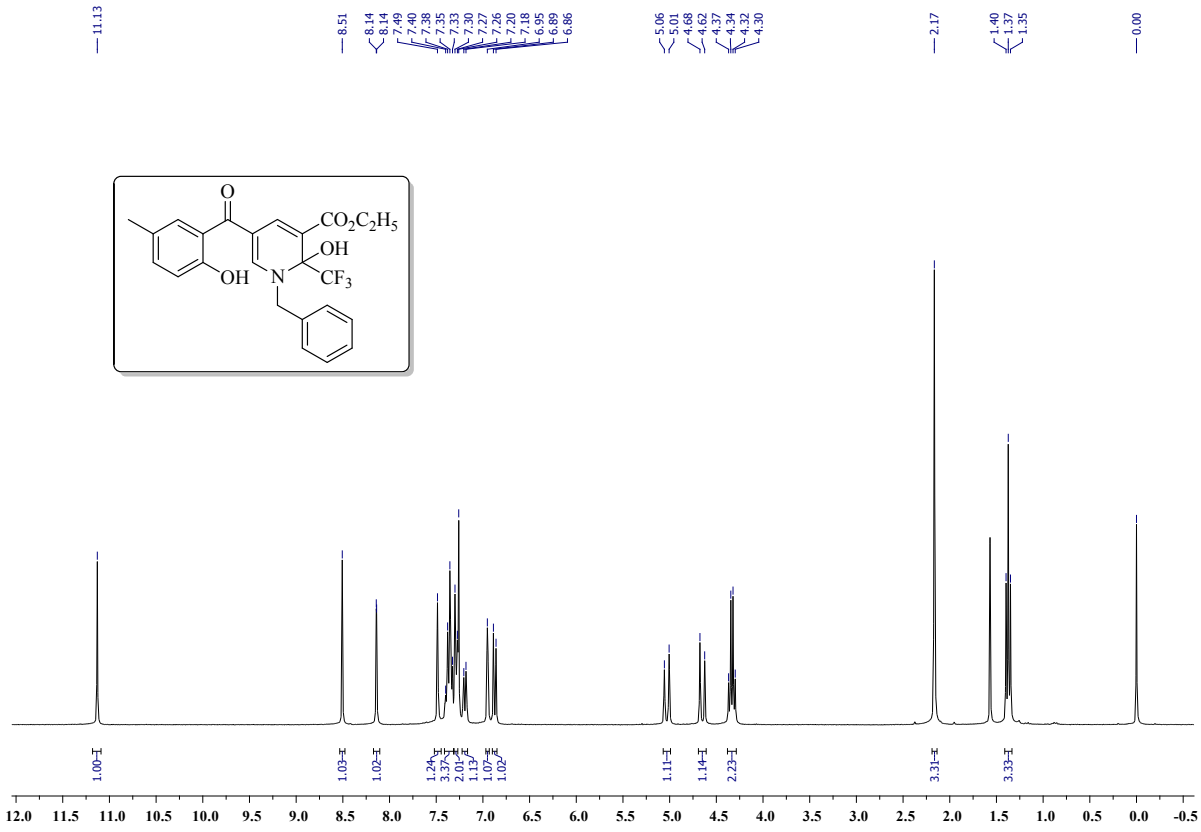
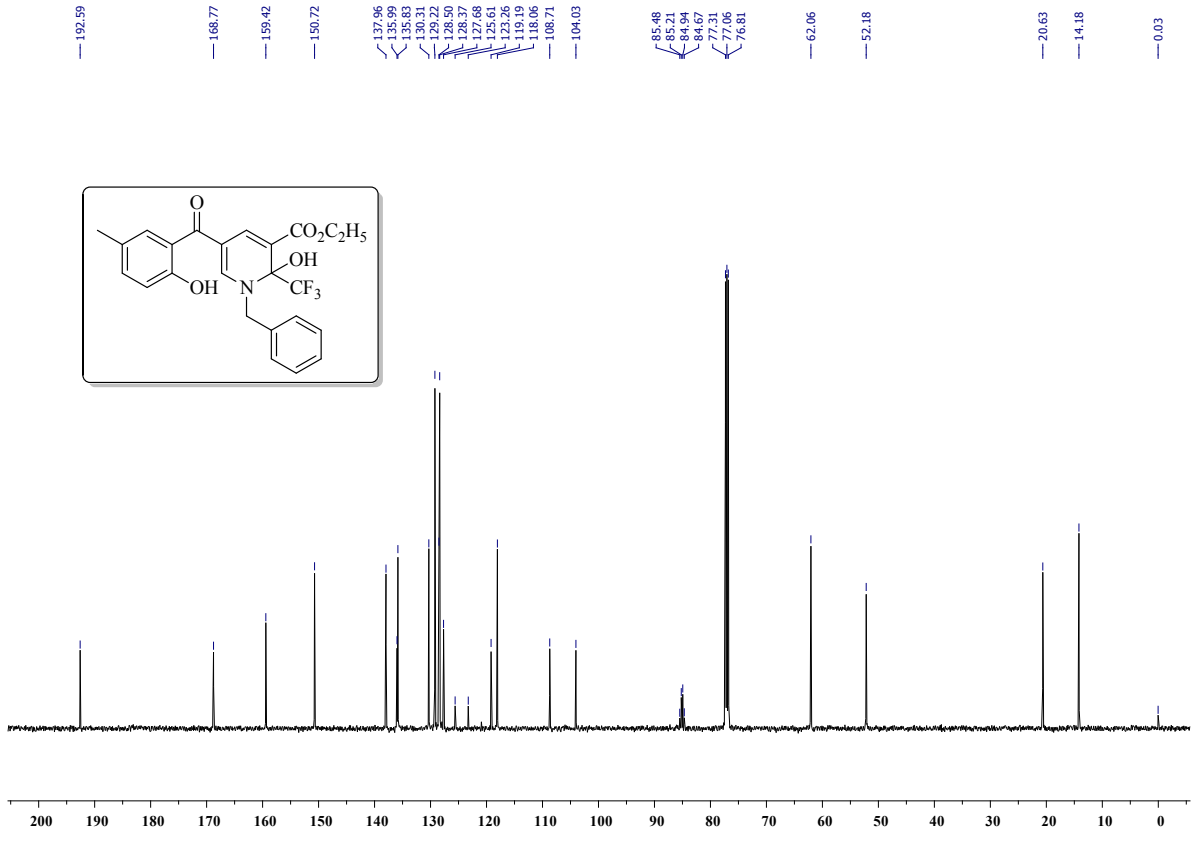
| m/z | Intensity | Relative | Theo. Mass | Delta (ppm) | RDB equiv. | Composition |
|---|---|---|---|---|---|---|
| 448.13554 | 93684040.0 | 100.00 | 448.13663 | -2.44 | 12.5 | $C_{23}H_{21}O_5NF_3$ |

HRMS spectrum of compound **4b**




$^{1}$H NMR spectrum of compound **4c**




$^{13}$C NMR spectrum of compound **4c**

National Centre for Mass Spectrometry
CSIR-Indian Institute of Chemical Technology

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Sample ID K-RAJKUMAR
Date and Time 30-09-14 16:25:42

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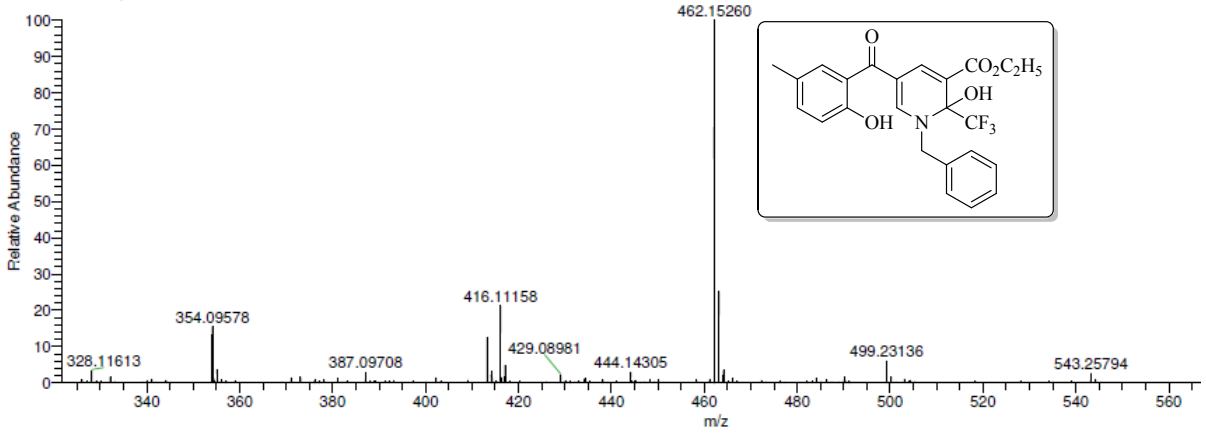


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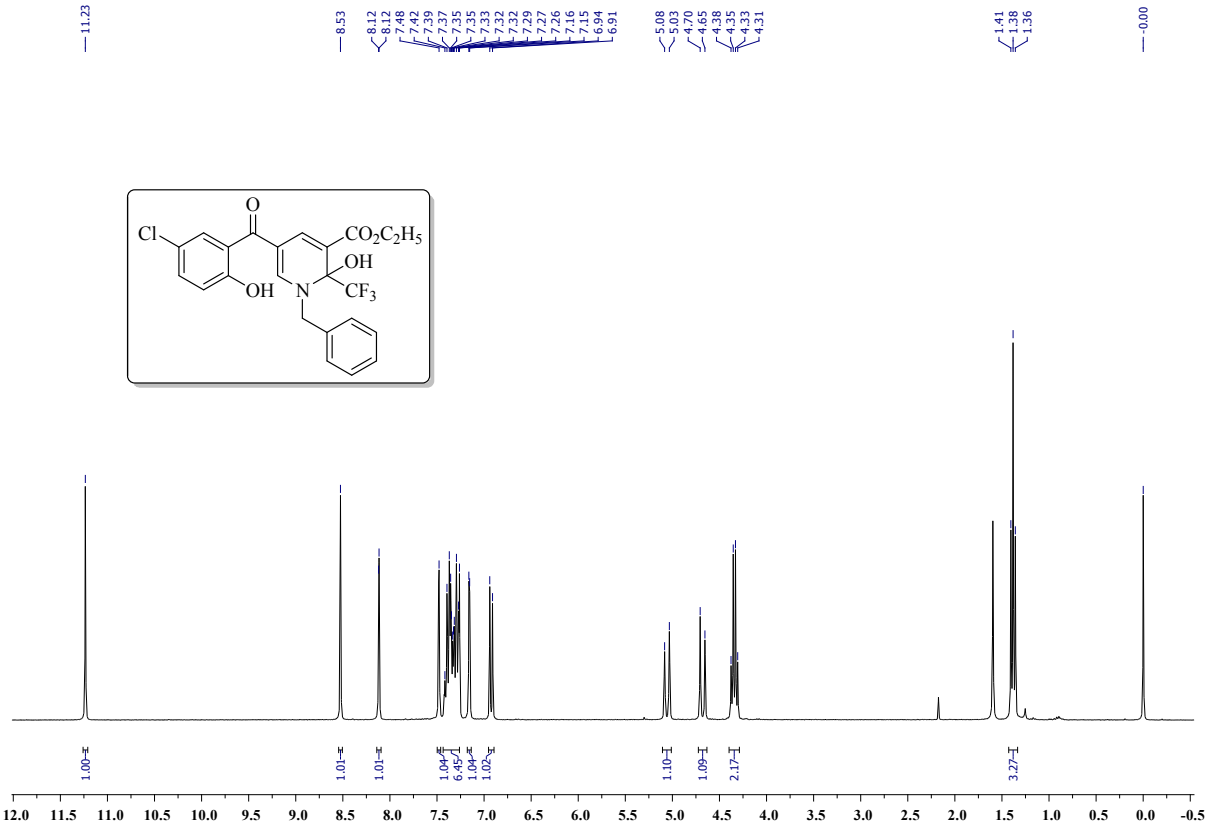
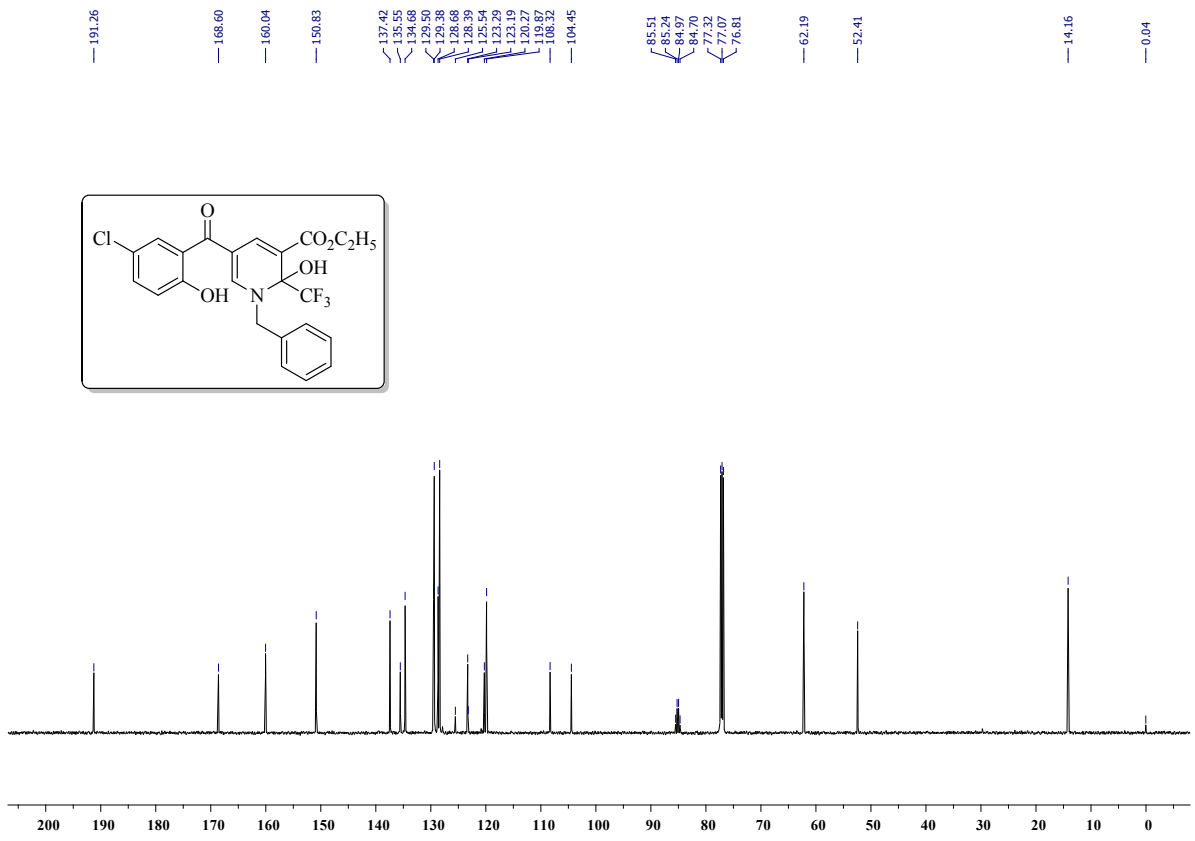
m/z= 456.45-470.92

| m/z | Intensity | Relative | Theo. Mass | Delta (ppm) | RDB equiv. | Composition |
|---|---|---|---|---|---|---|
| 462.15255 | 11256268.0 | 100.00 | 462.15228 | 0.27 | 12.5 | $C_{24}H_{23}O_5NF_3$ |

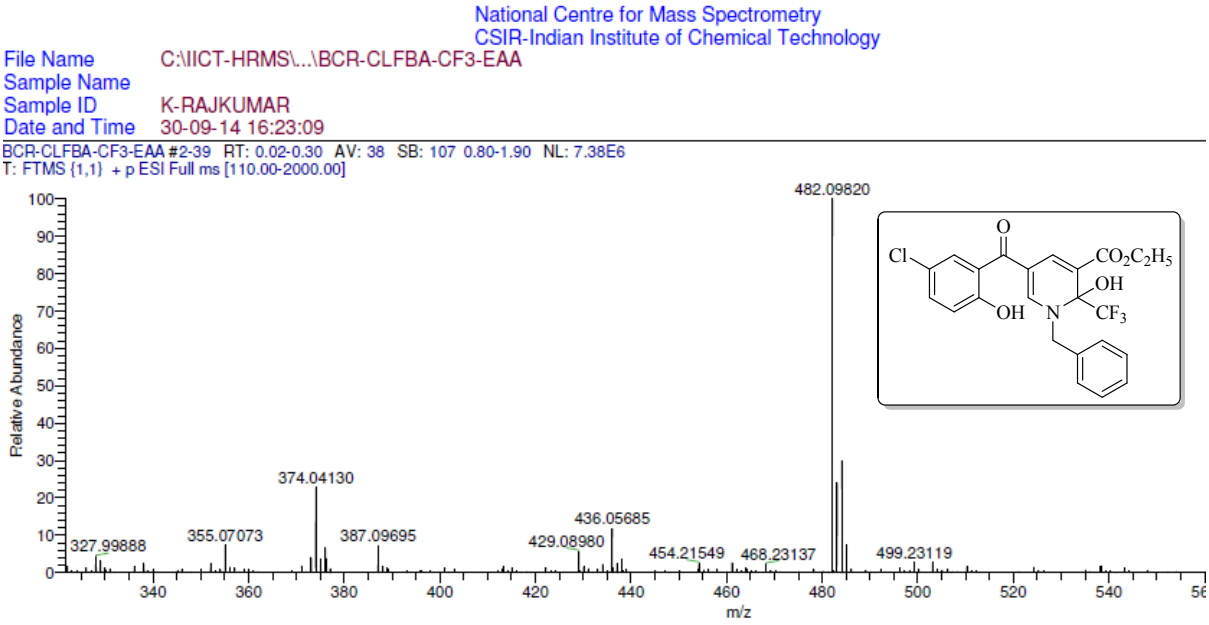
HRMS spectrum of compound **4c**




$^1$H NMR spectrum of compound **4d**




$^{13}$C NMR spectrum of compound **4d**

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m/z= 472.23-489.52

| m/z | Intensity | Relative | Theo. Mass | Delta (ppm) | RDB equiv. | Composition |
|---|---|---|---|---|---|---|
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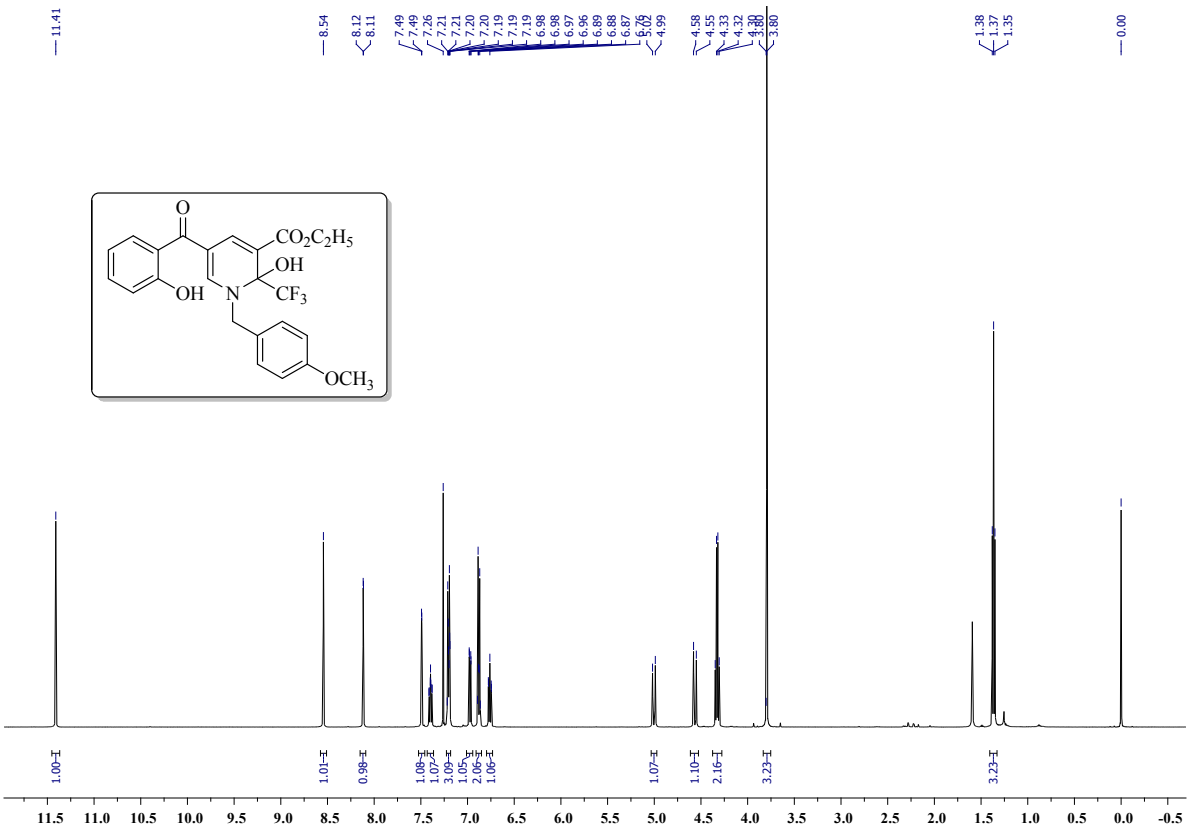
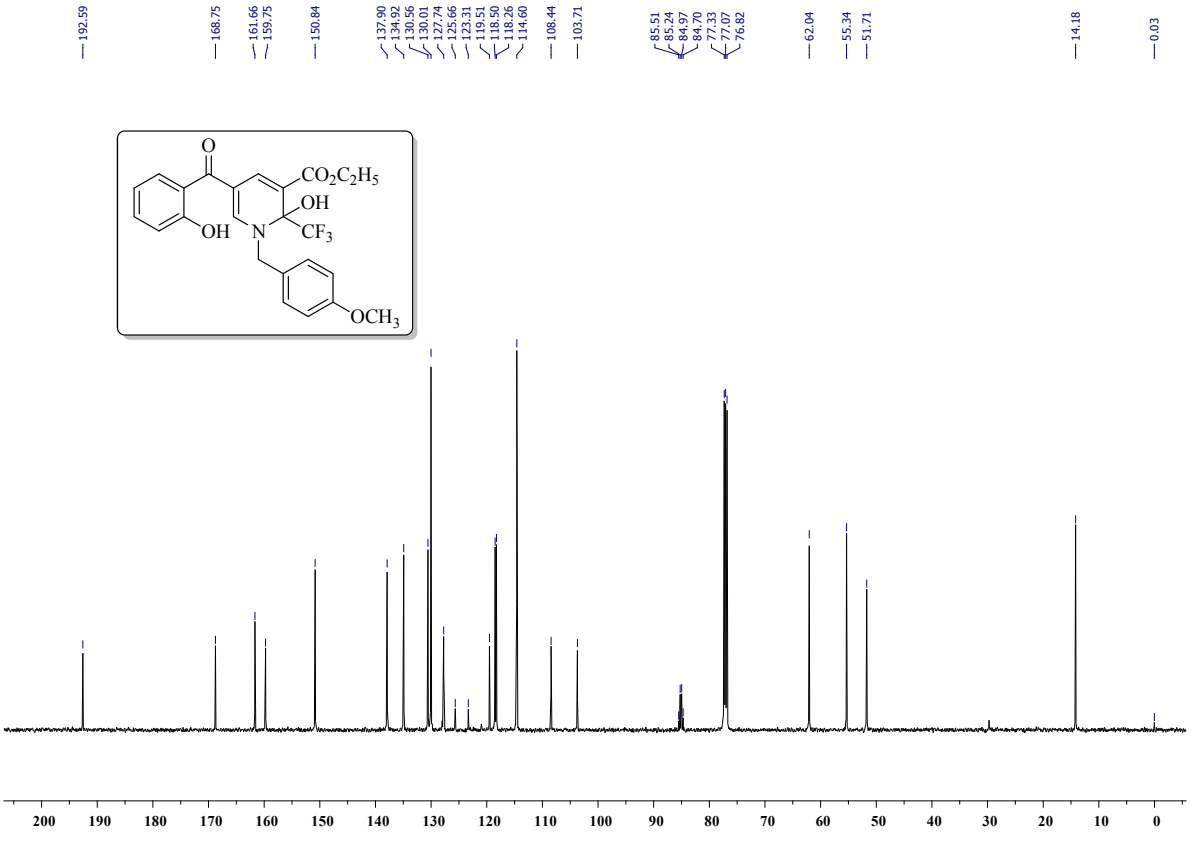
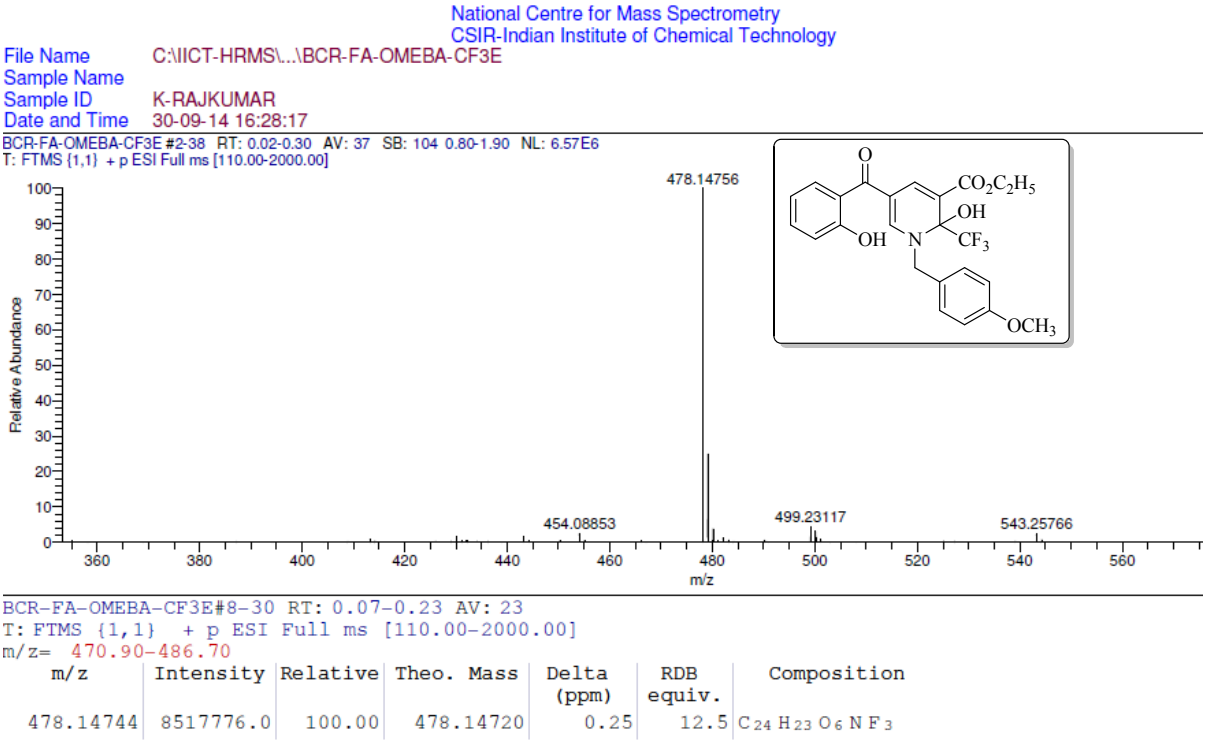
HRMS spectrum of compound **4d**



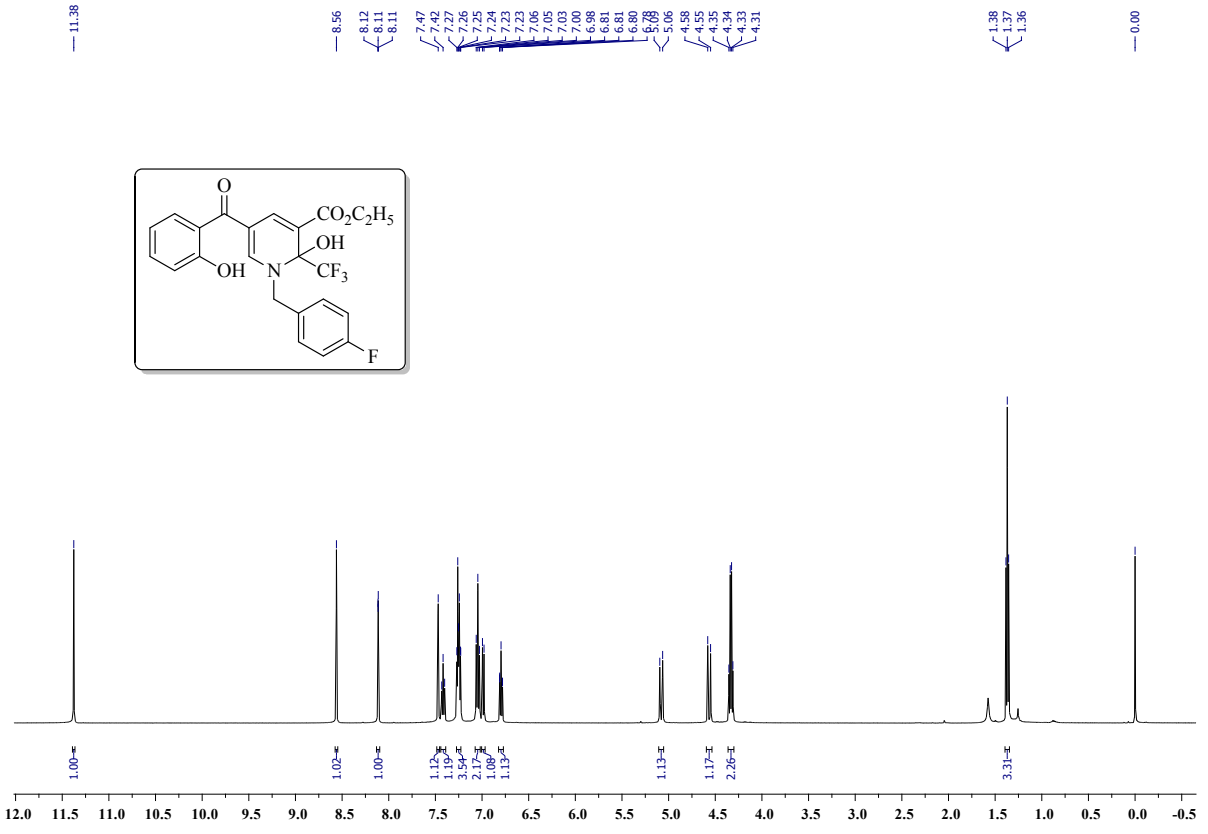

$^{1}$H NMR spectrum of compound **4e**



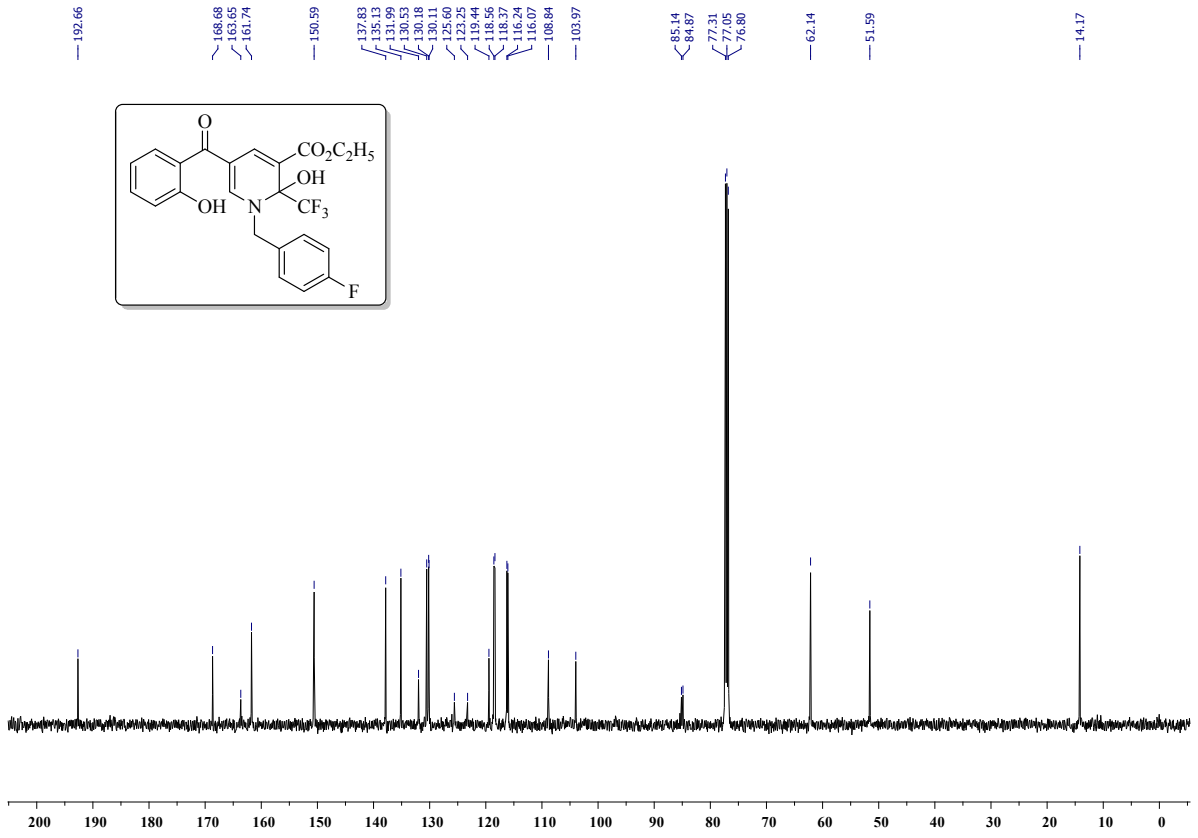

$^{13}$C NMR spectrum of compound **4e**



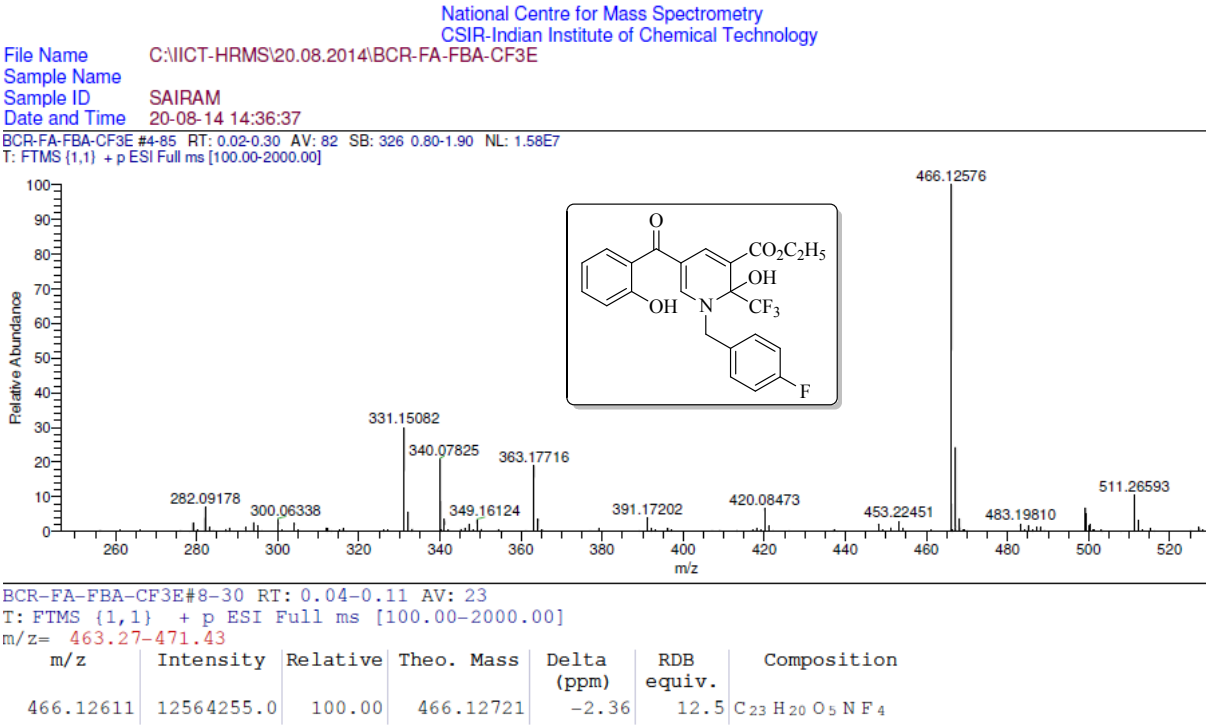

HRMS spectrum of compound **4e**



$^{1}$H NMR spectrum of compound **4f**




$^{13}$C NMR spectrum of compound **4f**

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|---|---|---|---|---|---|---|
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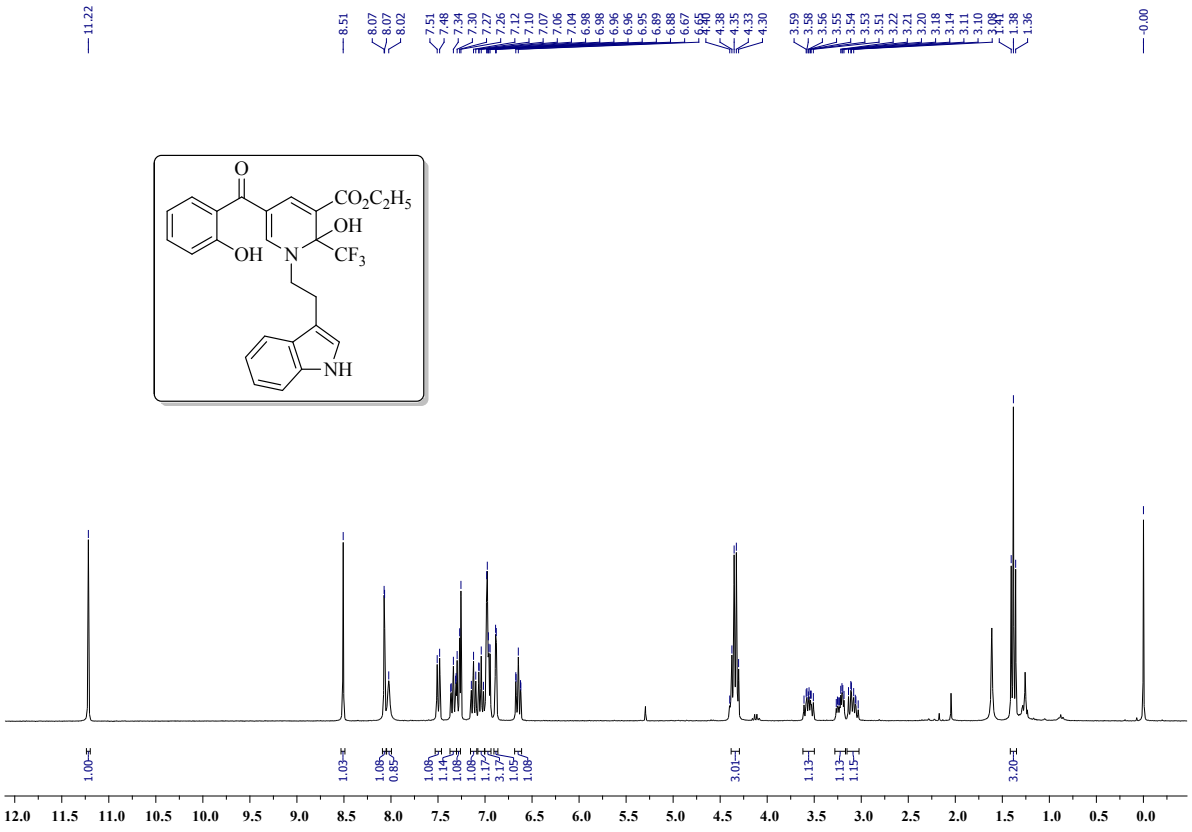
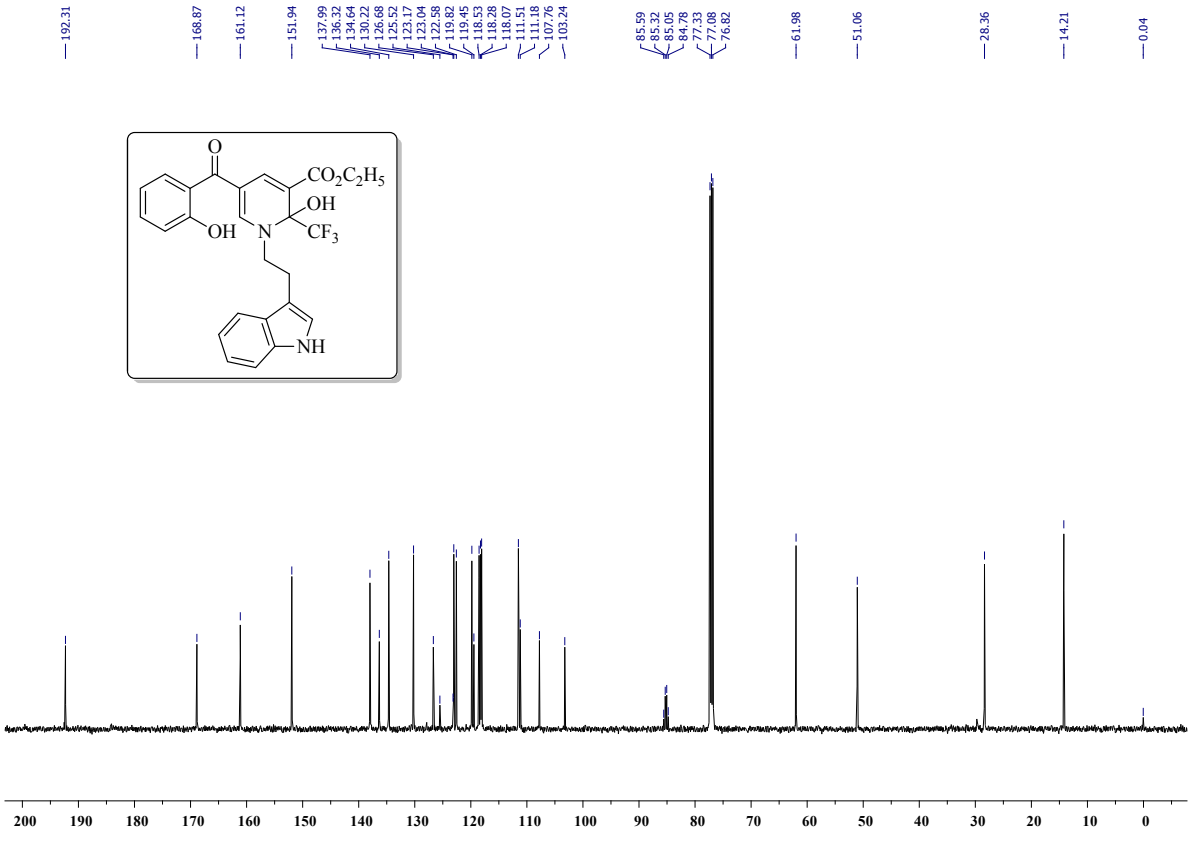
HRMS spectrum of compound **4f**




$^{1}$H NMR spectrum of compound **4g**




$^{13}$C NMR spectrum of compound **4g**

National Centre for Mass Spectrometry
CSIR-Indian Institute of Chemical Technology

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Date and Time 13-02-14 14:22:28

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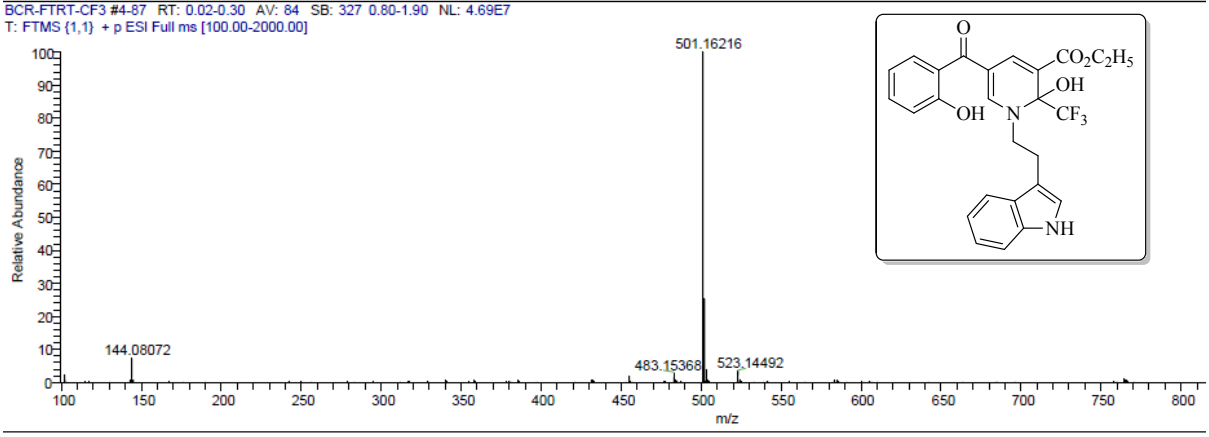


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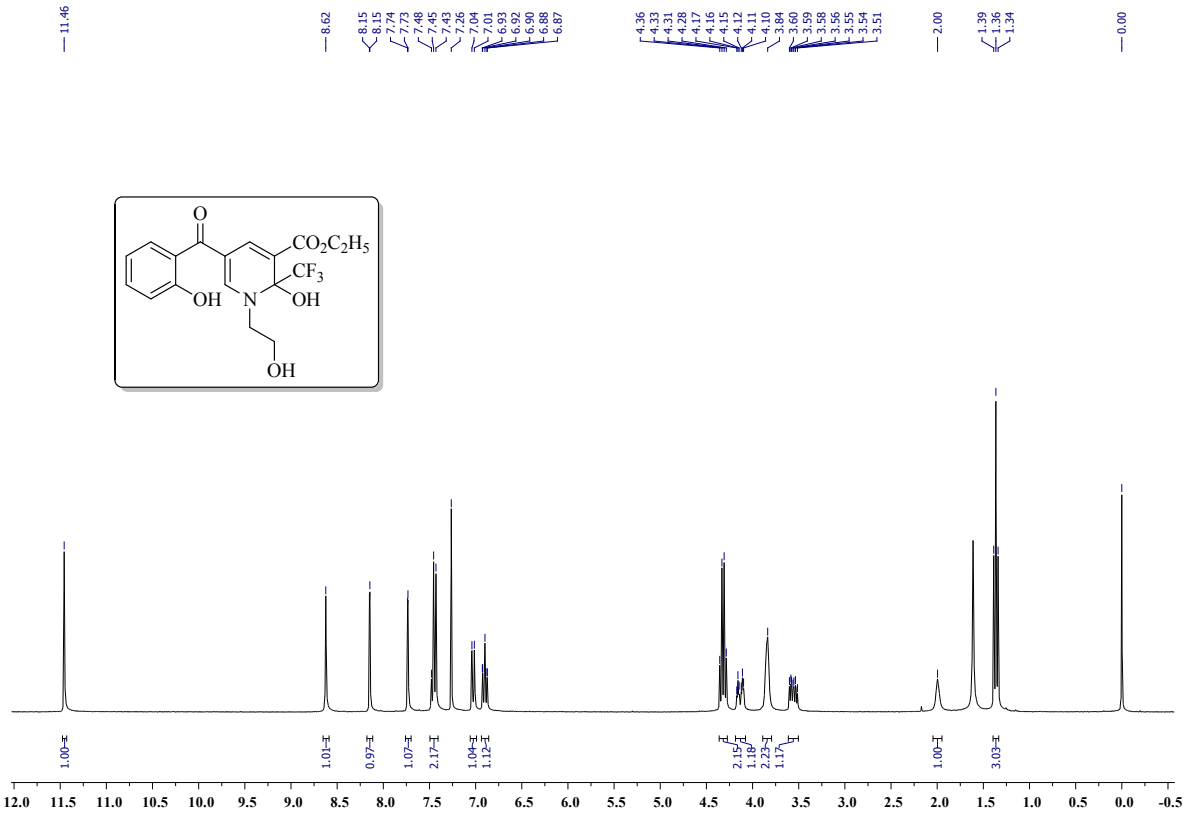
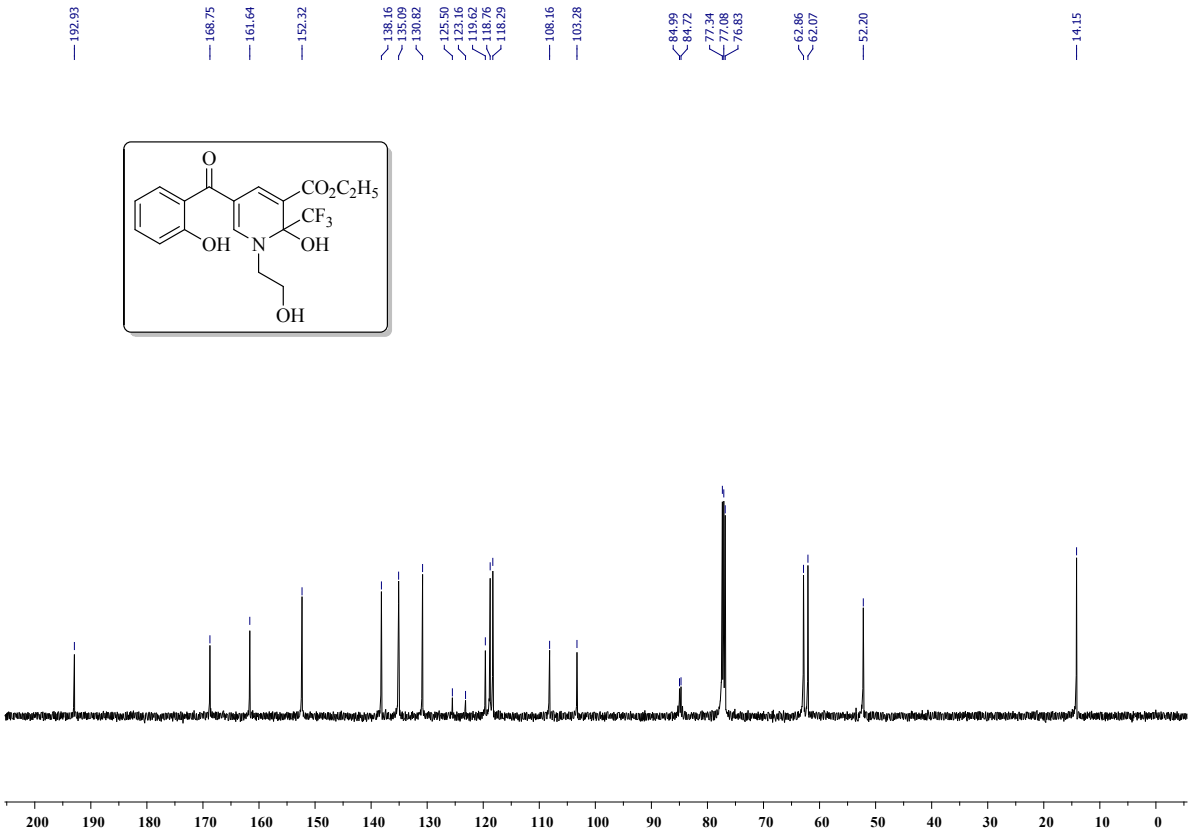
m/z= 460.30-535.18

| m/z | Intensity | Relative | Theo. Mass | Delta (ppm) | RDB equiv. | Composition |
|---|---|---|---|---|---|---|
| 501.16216 | 59884396.0 | 100.00 | 501.16318 | -2.04 | 14.5 | $C_{26}H_{24}O_5N_2F_3$ |

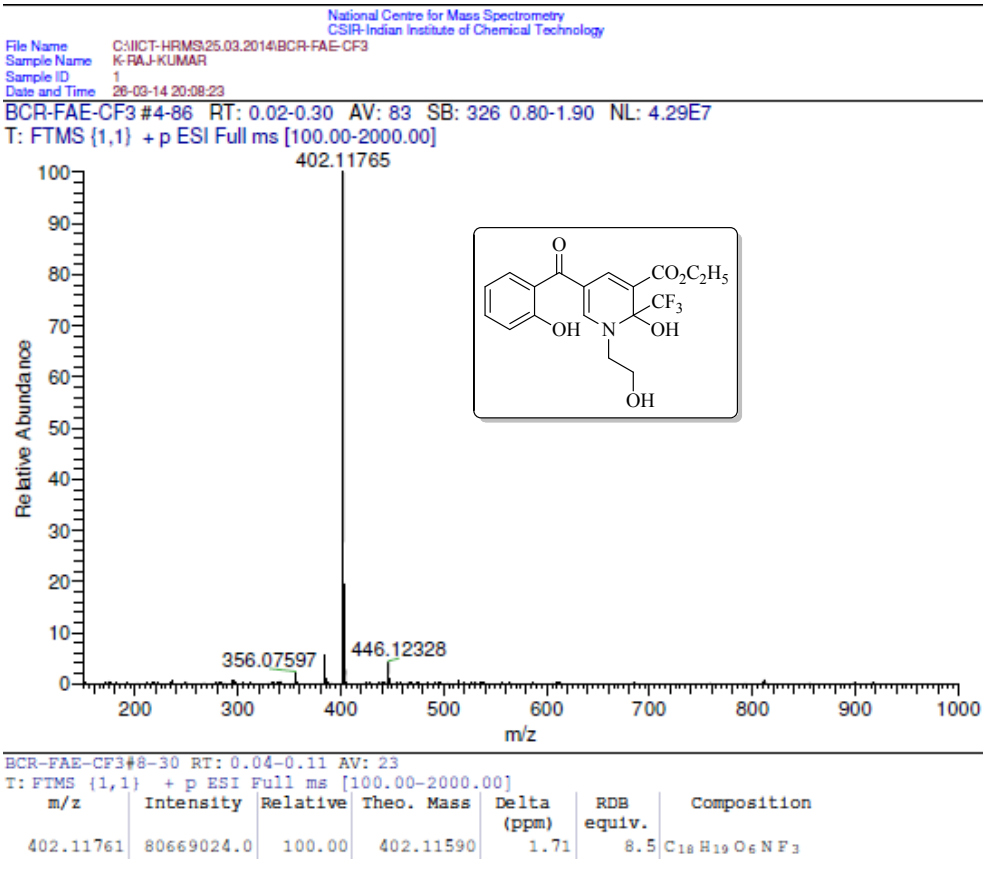
HRMS spectrum of compound **4g**



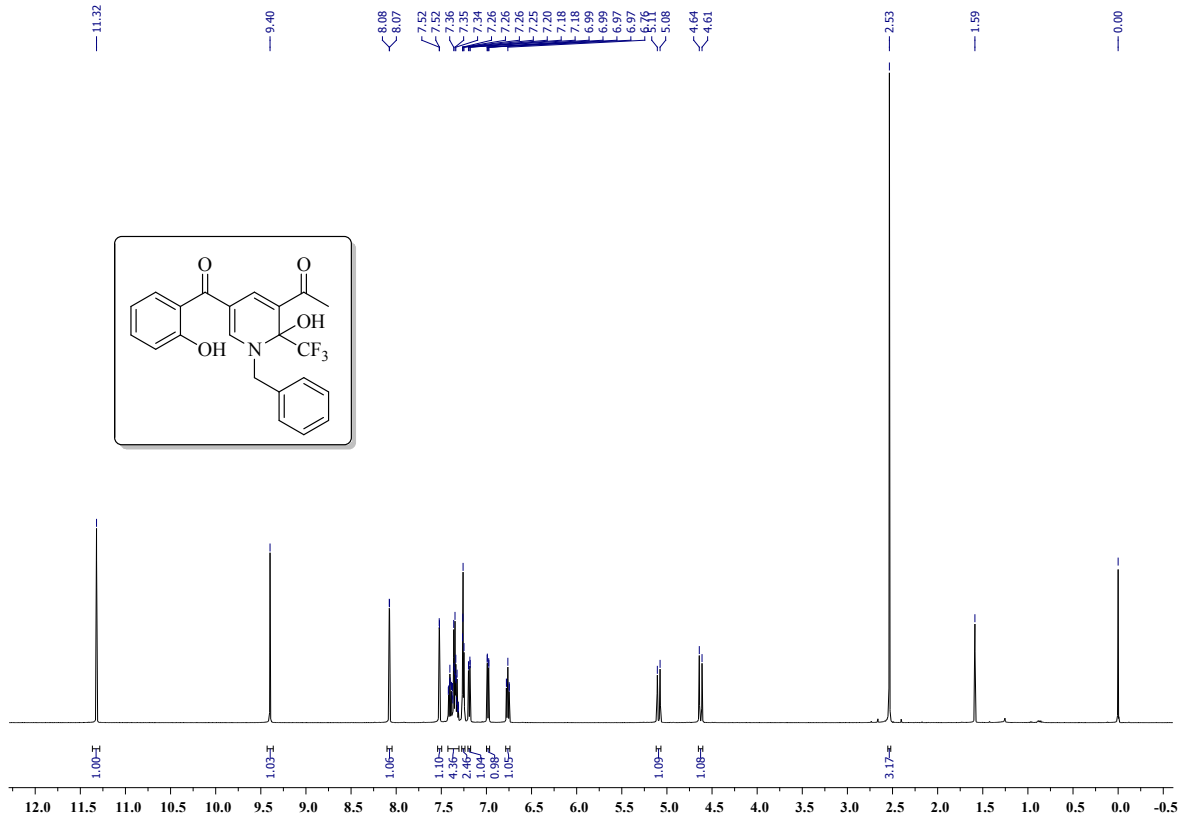

$^1$H NMR spectrum of compound **4h**



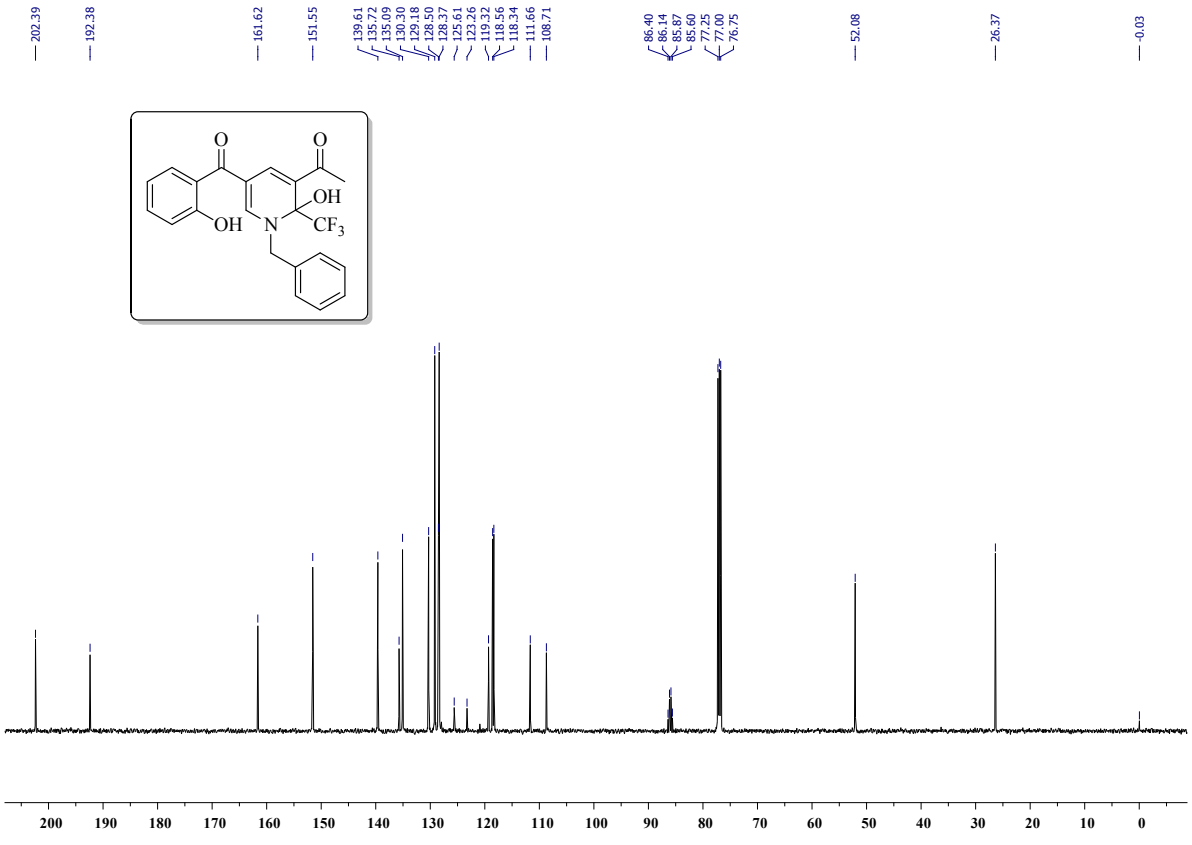

$^{13}$C NMR spectrum of compound **4h**



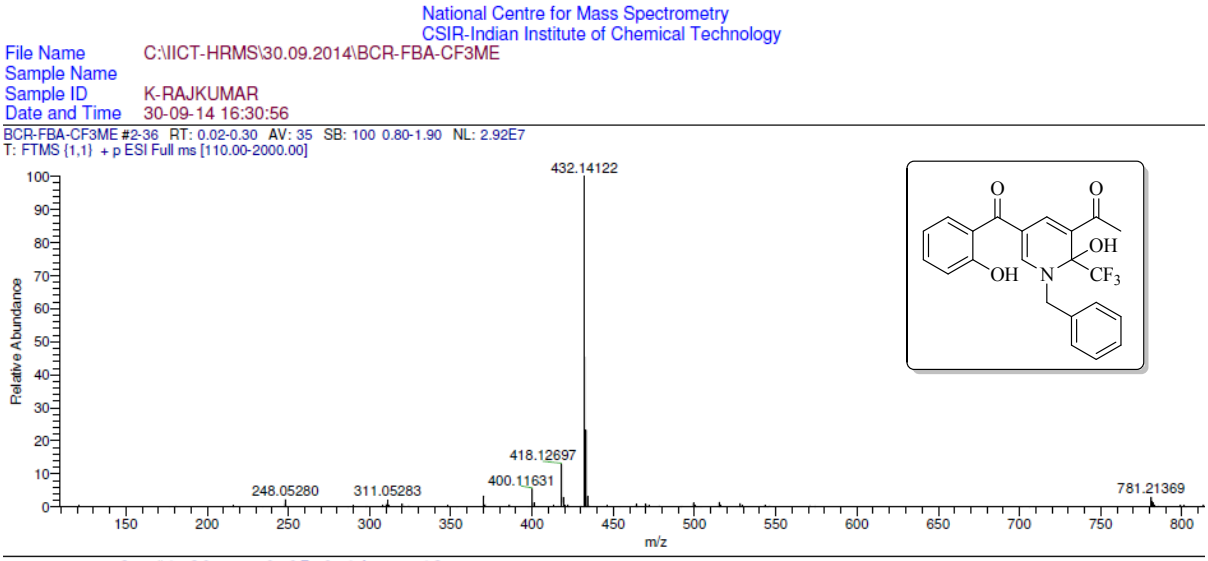

HRMS spectrum of compound **4h**



$^{1}$H NMR spectrum of compound **4i**



$^{13}$C NMR spectrum of compound **4i**

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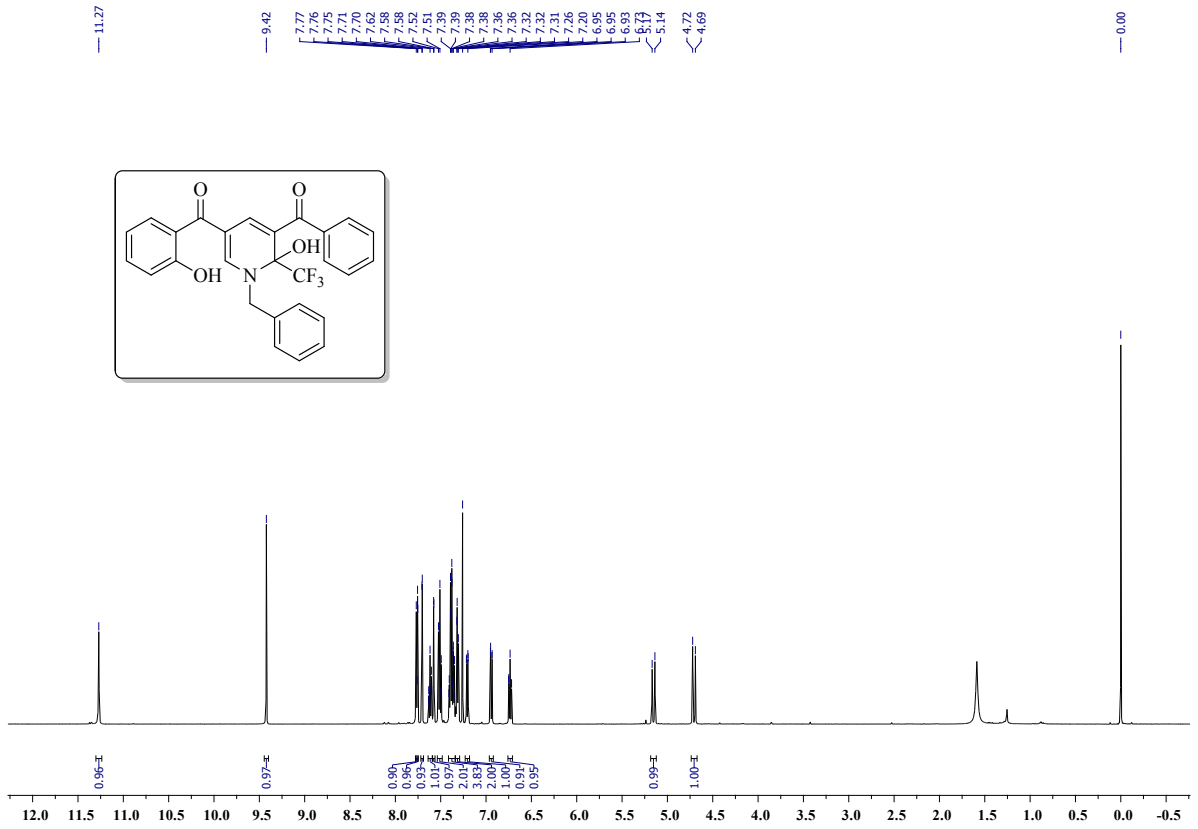
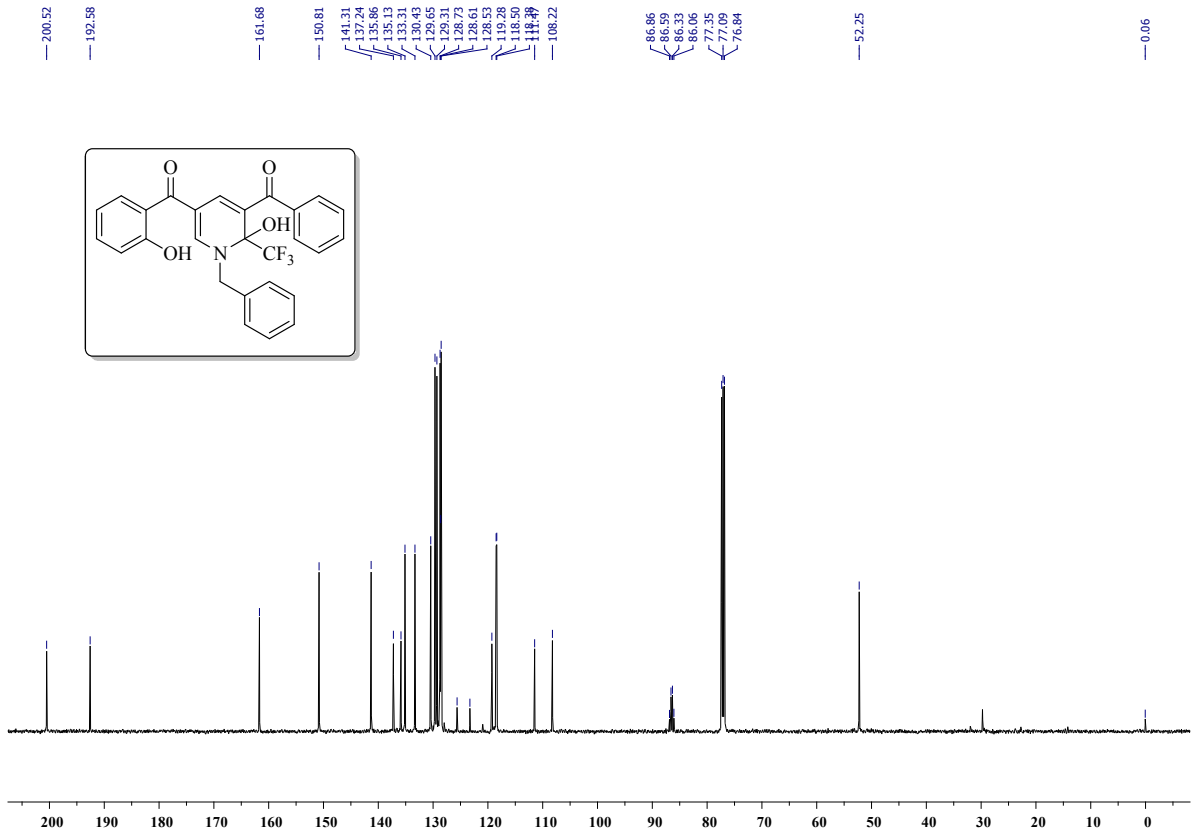
m/z= 410.92-445.68

| m/z | Intensity | Relative | Theo. Mass | Delta (ppm) | RDB equiv. | Composition |
|---|---|---|---|---|---|---|
| 432.14117 | 31840294.0 | 100.00 | 432.15189 | -10.72 | 9.0 | $C_{22}H_{24}O_4F_3Na$ |

HRMS spectrum of compound **4i**

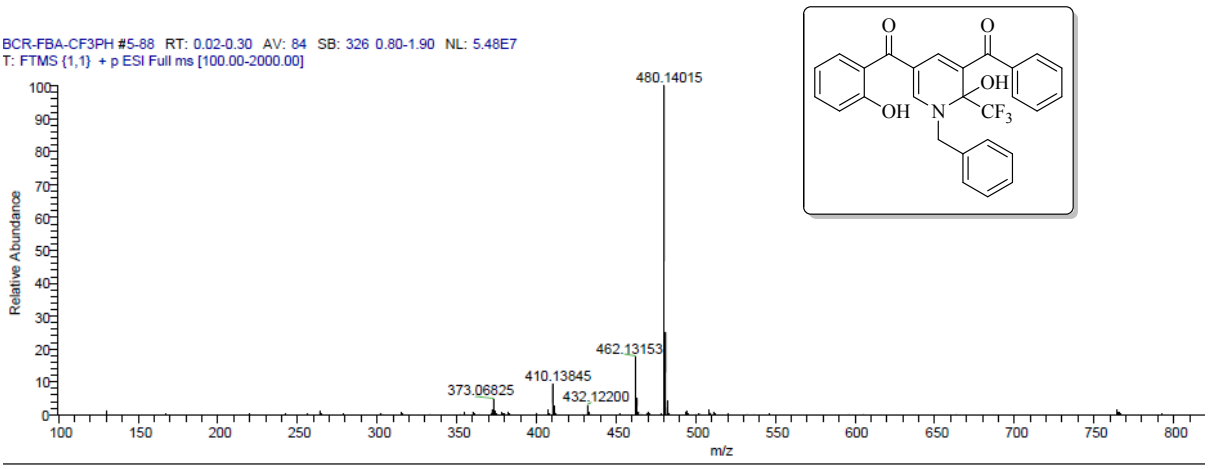



$^1$H NMR spectrum of compound **4j**




$^{13}$C NMR spectrum of compound **4j**

C:\IICT-HRMS\11.02.2014\BCR-FBA-CF3PH

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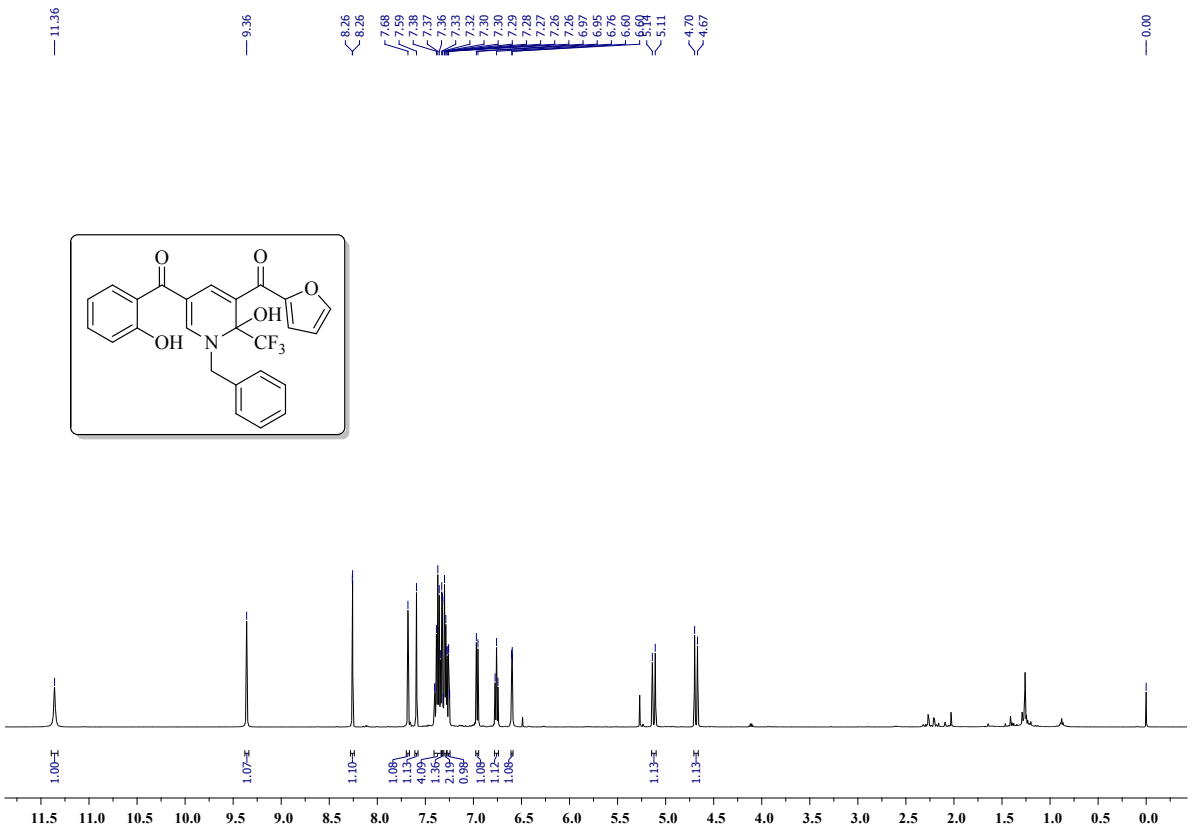
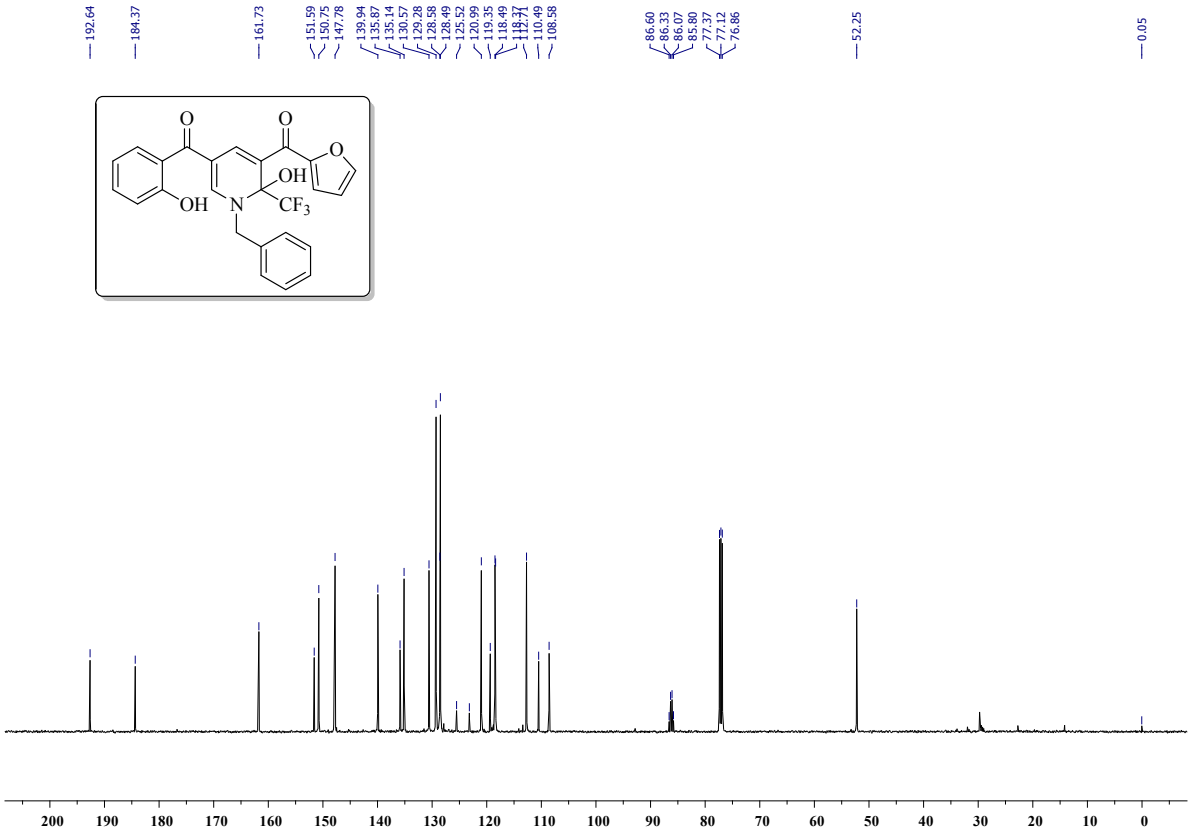
m/z= 474.51-483.80

| m/z | Intensity | Relative | Theo. Mass | Delta (ppm) | RDB equiv. | Composition |
|---|---|---|---|---|---|---|
| 480.14025 | 36078140.0 | 100.00 | 480.13931 | 1.95 | 13.5 | $C_{25}H_{22}O_4NF_3Na$ |

HRMS spectrum of compound 4**j**

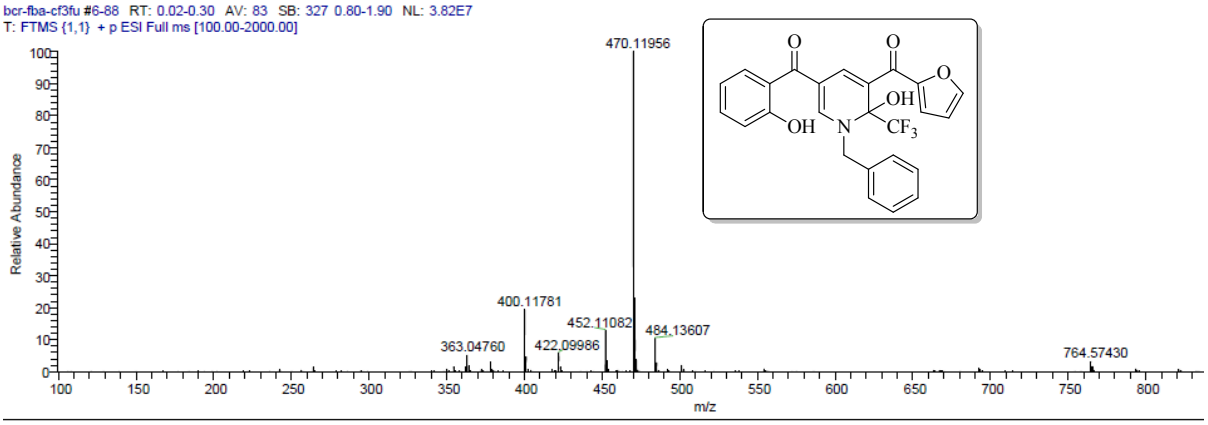


$^{1}$H NMR spectrum of compound **4k**



$^{13}$C NMR spectrum of compound **4k**

C:\IICT-HRMS\11.02.2014\bcr-fba-cf3fu



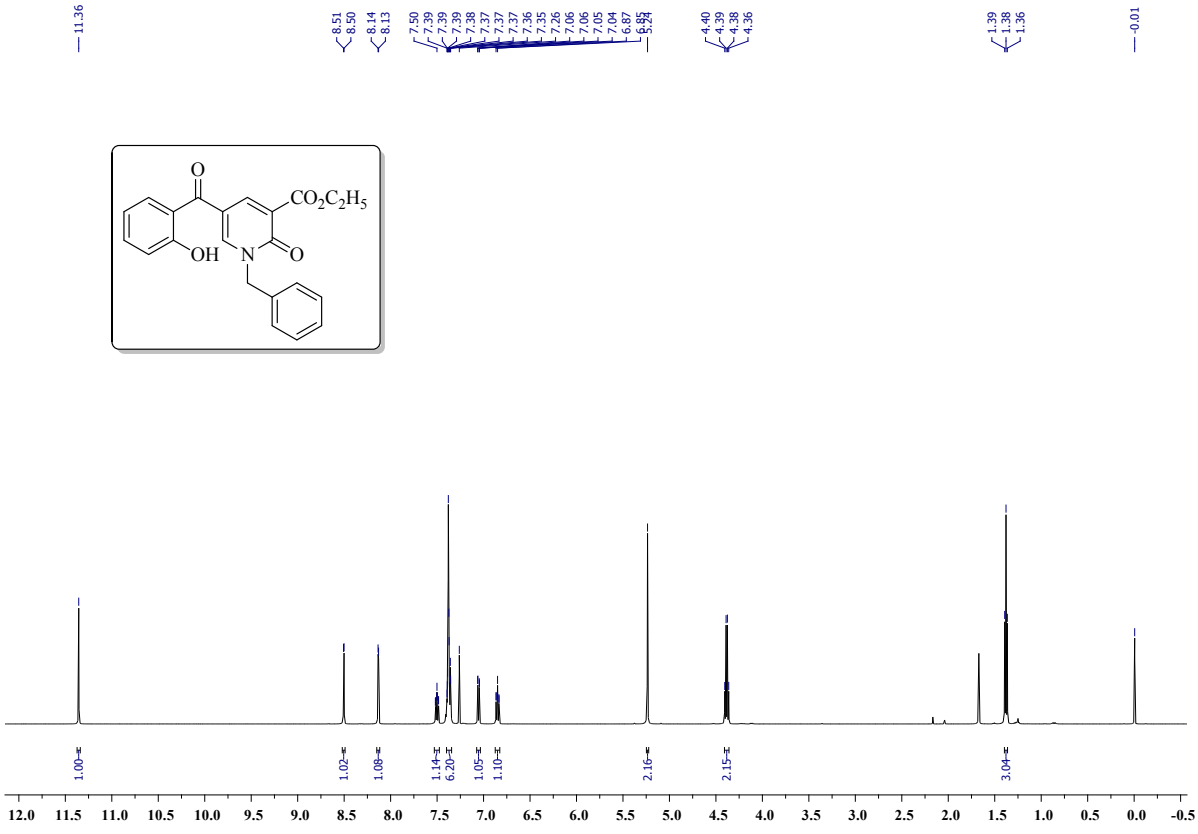

bcr-fba-cf3fu#8-30 RT: 0.03-0.10 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]

| m/z | Intensity | Relative | Theo. Mass | Delta (ppm) | RDB equiv. | Composition |
|---|---|---|---|---|---|---|
| 470.11978 | 32040270.0 | 100.00 | 470.12098 | -2.57 | 15.5 | $C_{25}H_{19}O_5NF_3$ |

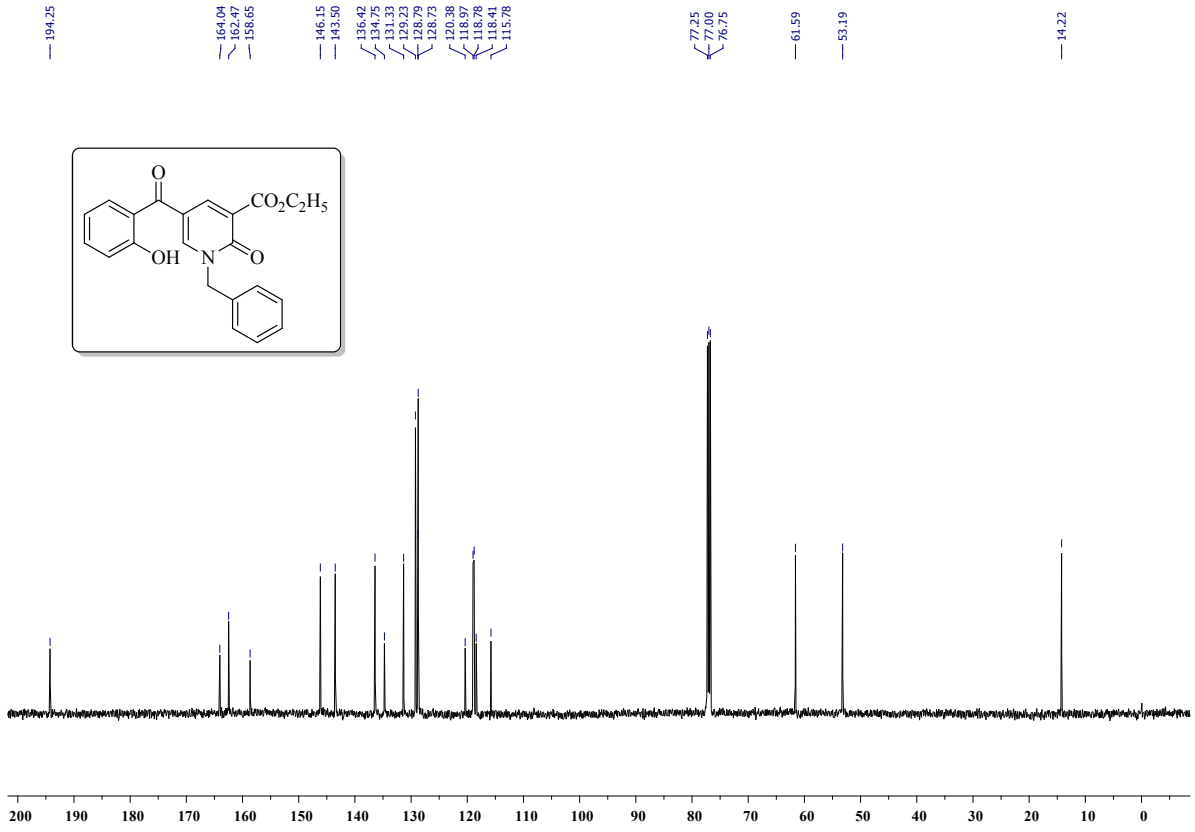
HRMS spectrum of compound **4k**

**General procedure for the preparation of 2-hydroxybenzoyl-1,2-dihydropyridone-3-carboxylates 5a-e**

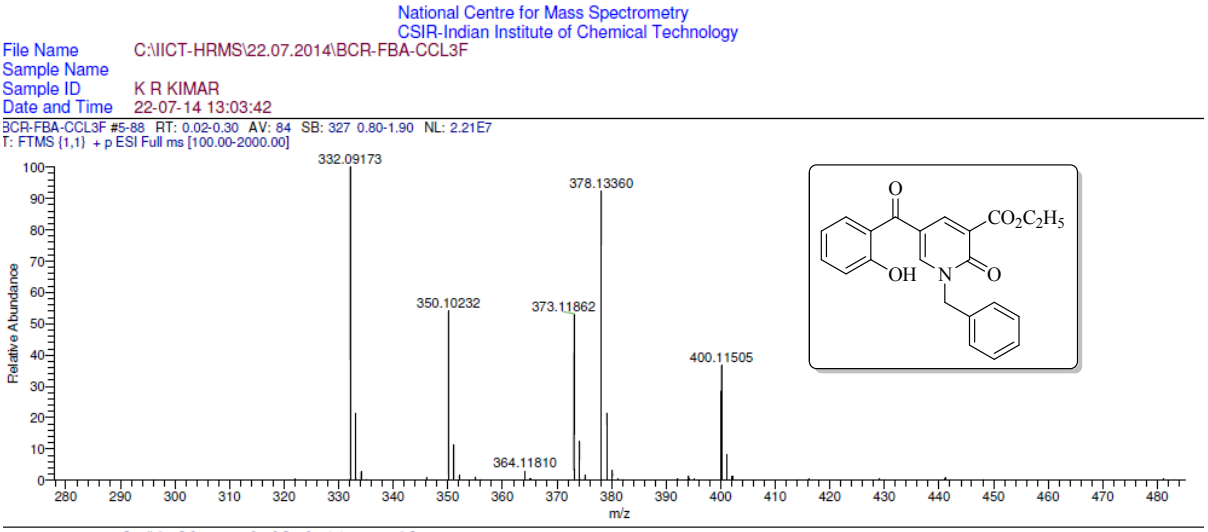
Ethyl 4,4,4-trichloro-3-oxobutanoate (**3h**, 1.5 mmol) was added to a stirred solution of 4-oxo-4*H*-chromene-3-carbaldehyde (**1a**, 1 mmol) and phenylmethanamine (**2b**, 1.2 mmol) in $CH_3CN$ (2 mL). The contents were stirred under reflux conditions for 6 h. After completion of the reaction (TLC), the residue was purified by column chromatography by using silica gel (100:200, ethyl acetate/hexane 24:76) afforded 2-hydroxybenzoyl-1,2-dihydropyridone-3-carboxylates **5a**. Similarly, compounds **5b-e** were prepared from corresponding 3-formylchromones **1a-c** and benzylamines **2b-d**.




$^1$H NMR spectrum of compound **5a**



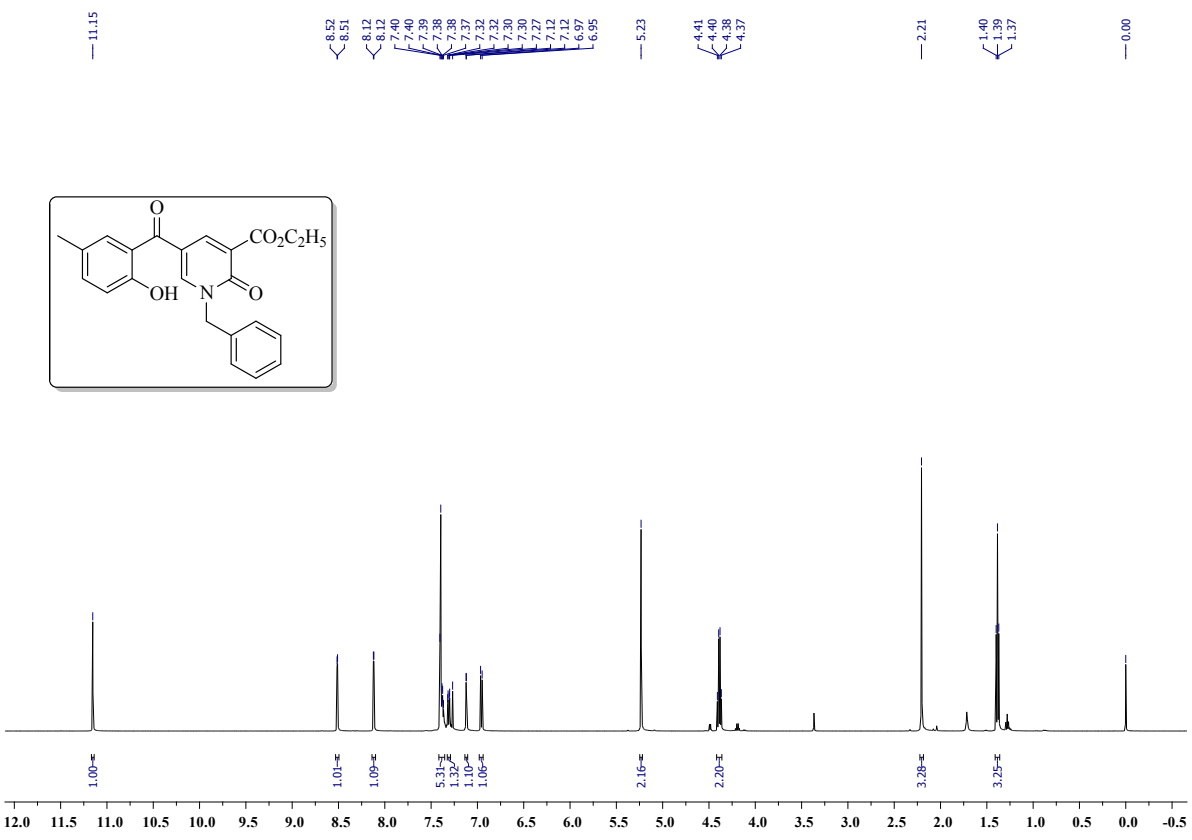

$^{13}$C NMR spectrum of compound **5a**



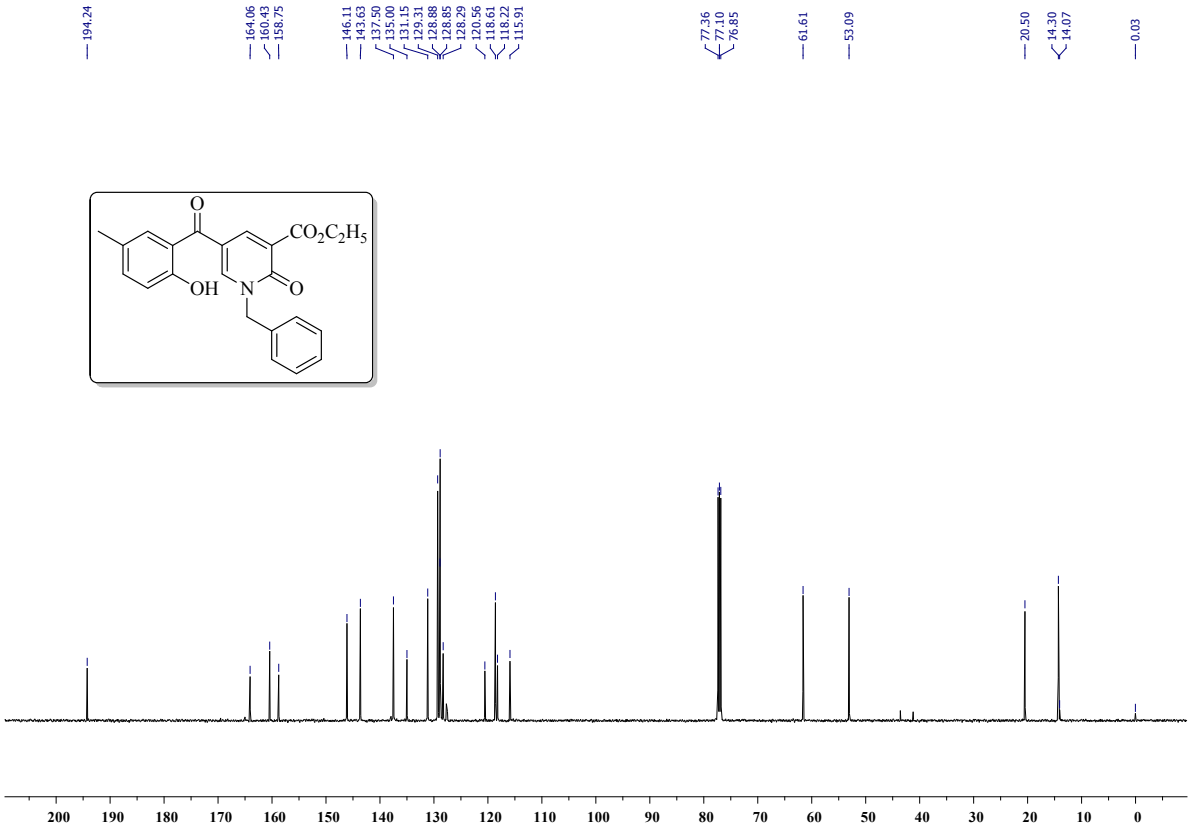

BCR-FBA-CCL3F#8-30 RT: 0.03-0.11 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]
m/z= 393.68-406.57

| m/z | Intensity | Relative | Theo. Mass | Delta (ppm) | RDB equiv. | Composition |
|---|---|---|---|---|---|---|
| 400.11483 | 324511.3 | 100.00 | 400.11554 | -1.79 | 13.5 | $C_{22}H_{19}O_5NNa$ |

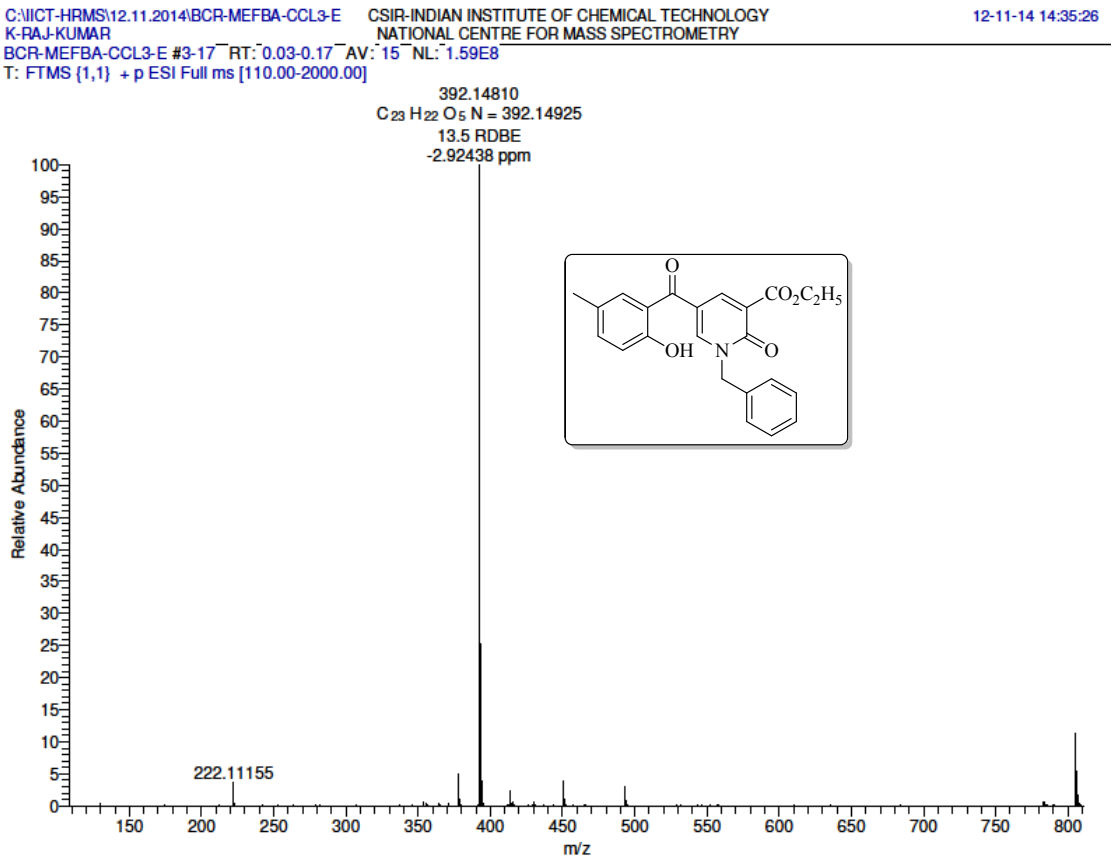
HRMS spectrum of compound **5a**



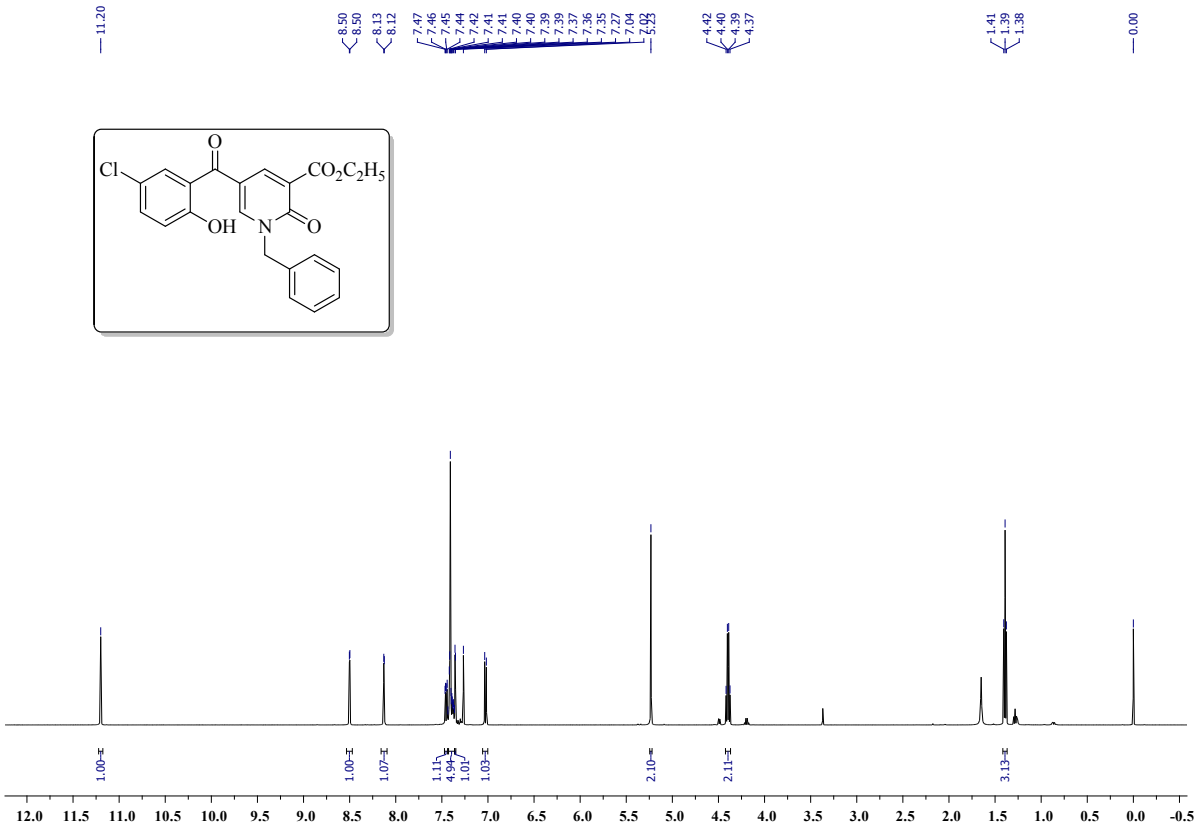

$^{1}$H NMR spectrum of compound **5b**



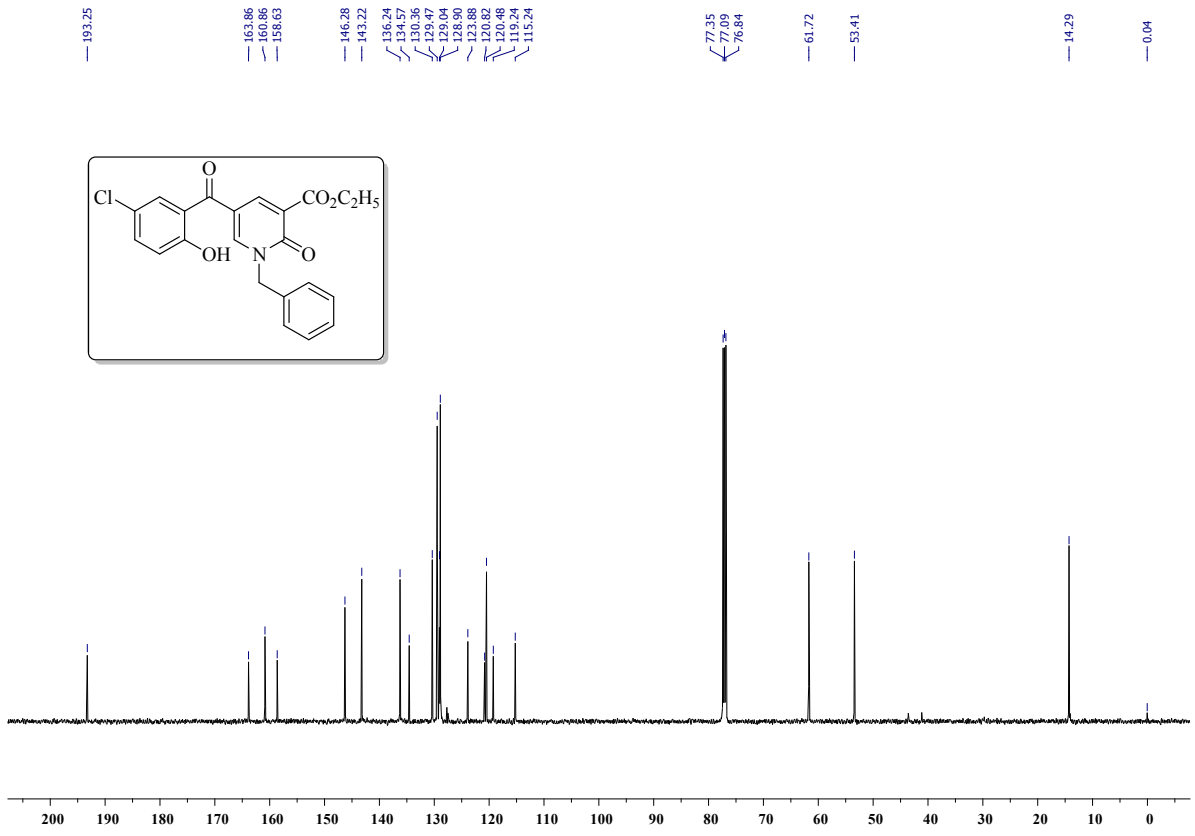

$^{13}$C NMR spectrum of compound **5b**



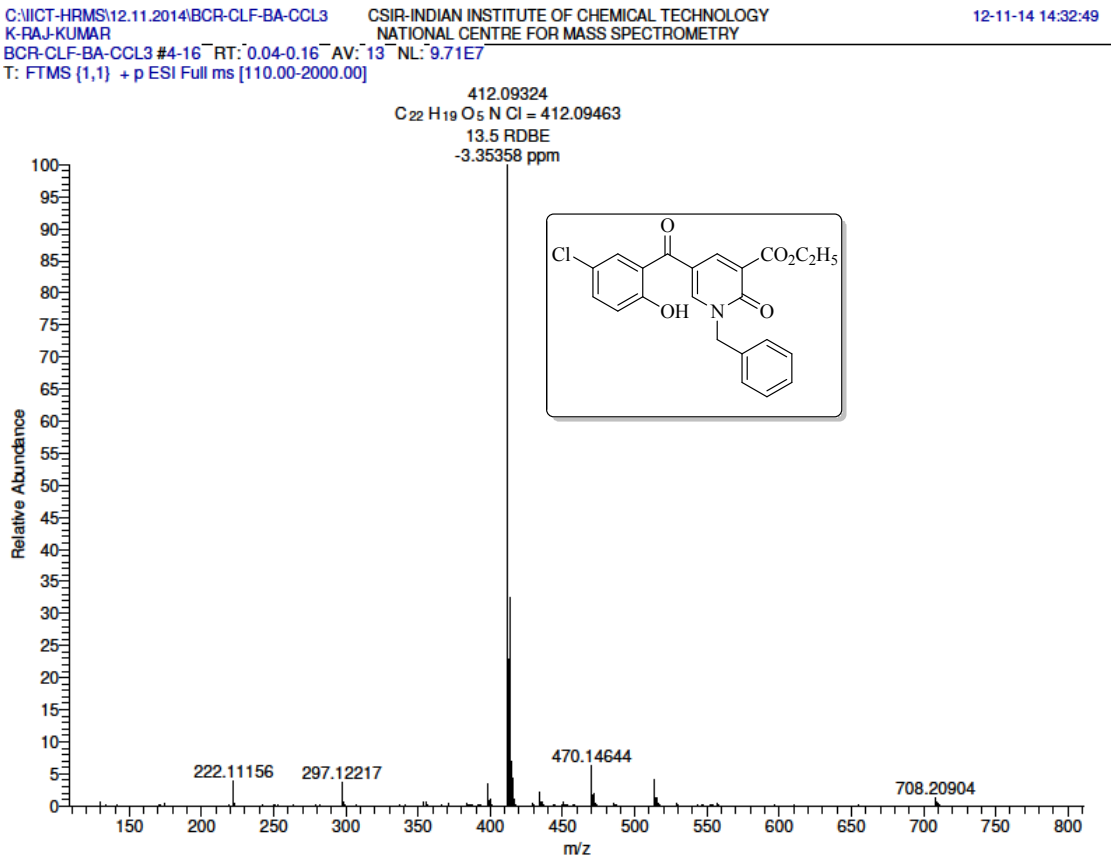

HRMS spectrum of compound **5b**



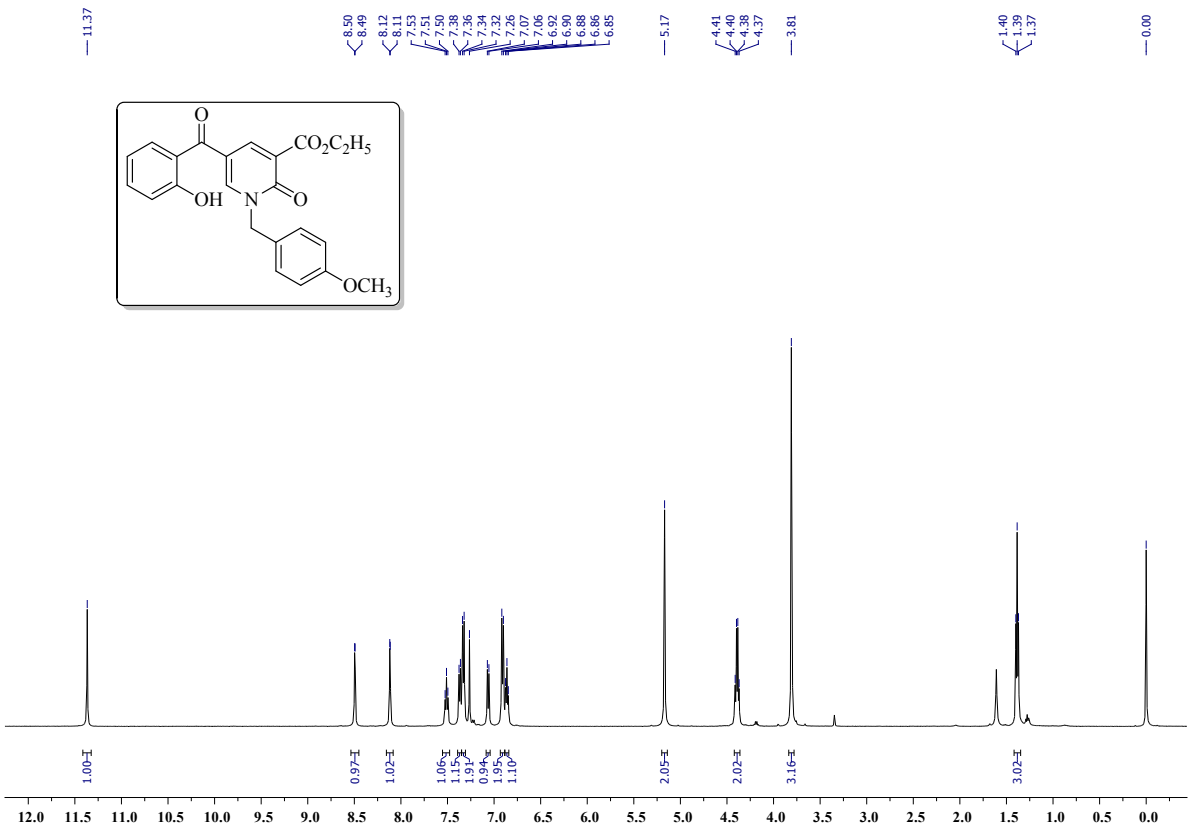

$^{1}$H NMR spectrum of compound **5c**



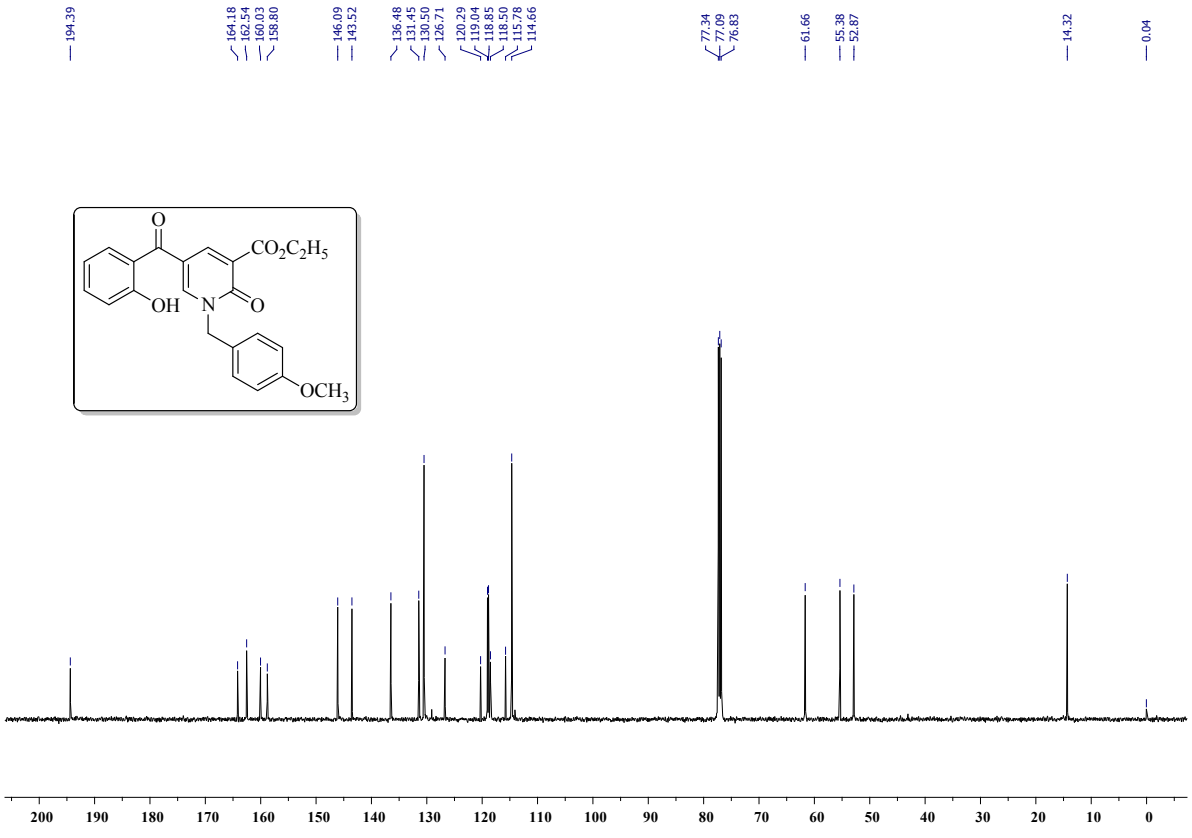

$^{13}$C NMR spectrum of compound **5c**




HRMS spectrum of compound **5c**




$^{1}$H NMR spectrum of compound **5d**

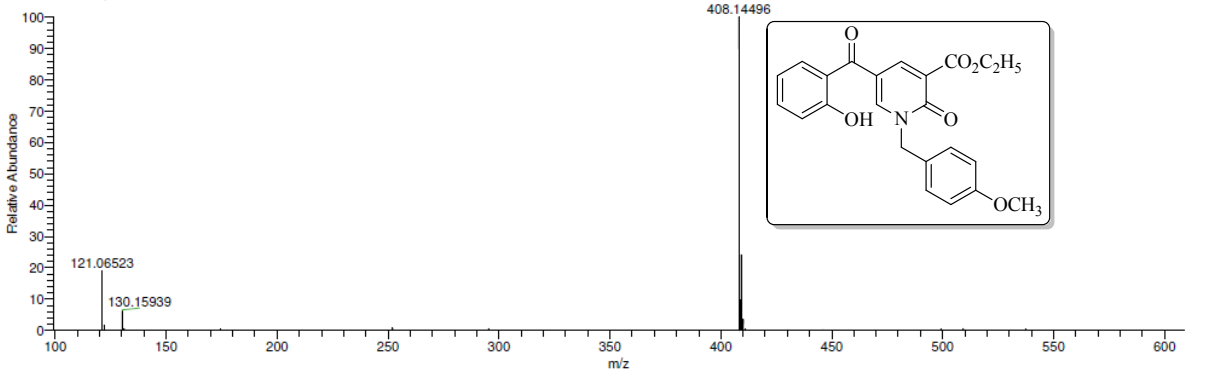



$^{13}$C NMR spectrum of compound **5d**

National Centre for Mass Spectrometry
CSIR-Indian Institute of Chemical Technology

File Name C:\IICT-HRMS\...\BCR-FA-OMEBA-CL3E
Sample Name
Sample ID K-RAJKUMAR
Date and Time 08-09-14 22:07:18

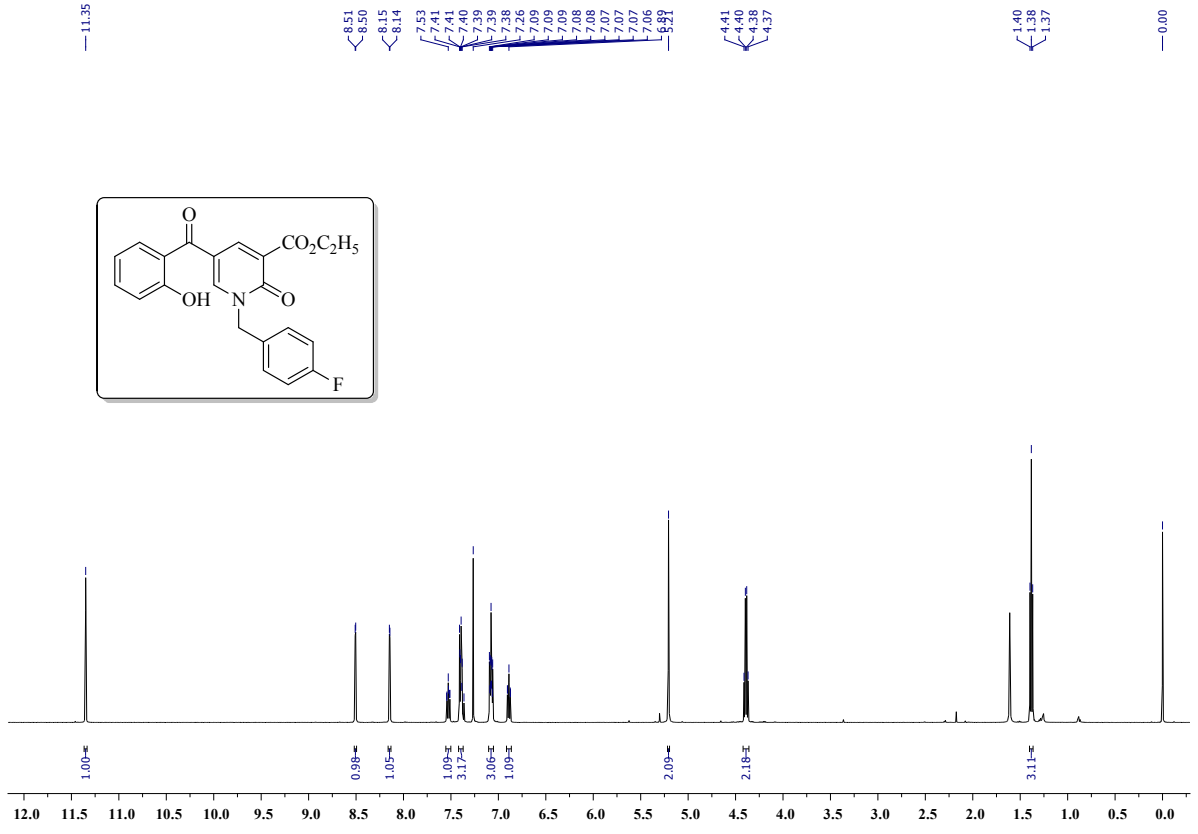
BCR-FA-OMEBA-CL3E #6-89 RT: 0.02-0.30 AV: 84 SB: 326 0.80-1.90 NL: 1.23E8
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]



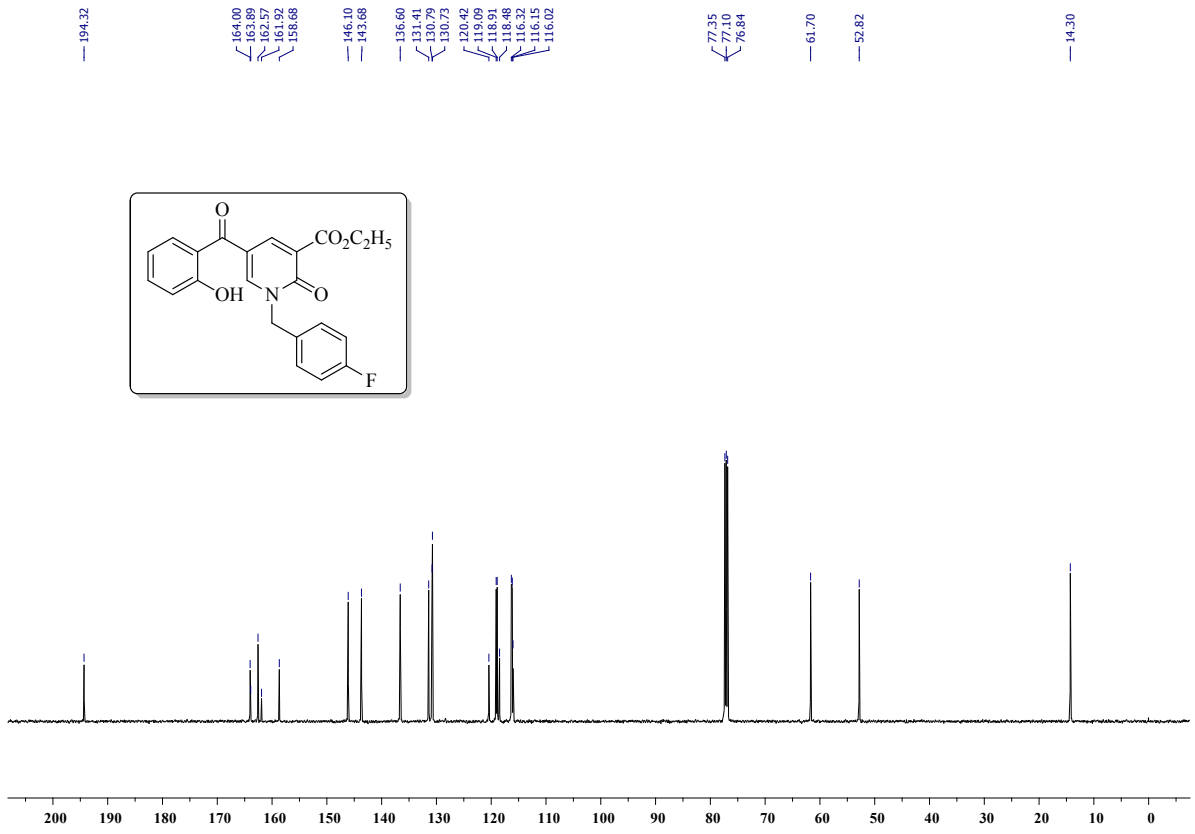

BCR-FA-OMEBA-CL3E#8-30 RT: 0.03-0.10 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]
m/z= 376.88-451.13

| m/z | Intensity | Relative | Theo. Mass | Delta (ppm) | RDB equiv. | Composition |
|---|---|---|---|---|---|---|
| 408.14495 | 102210776.0 | 100.00 | 408.14416 | 1.91 | 13.5 | $C_{23}H_{22}O_6N$ |

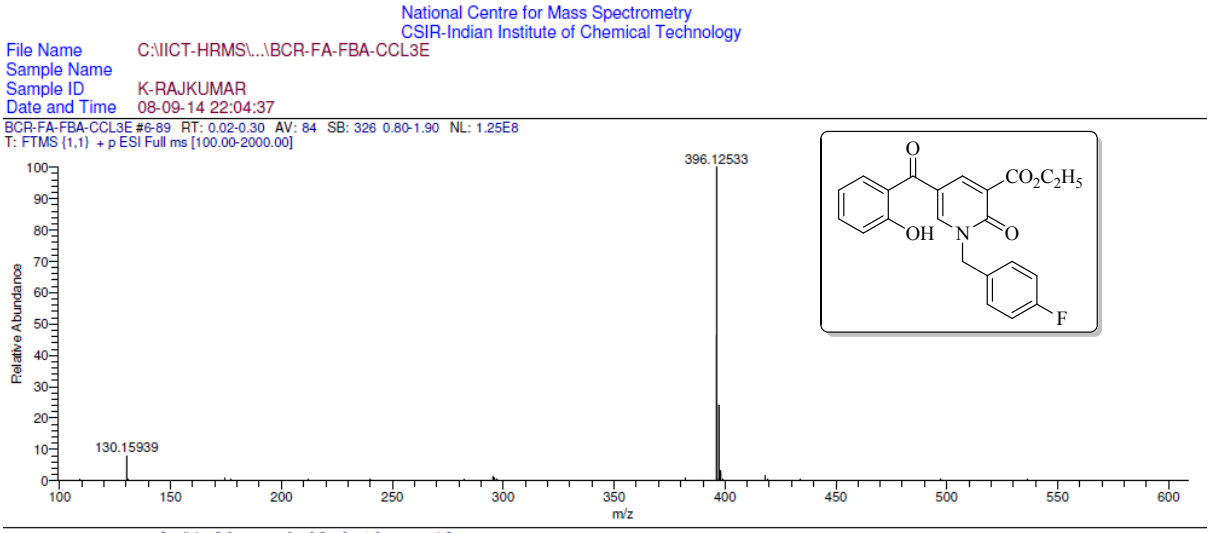
HRMS spectrum of compound **5d**




$^1$H NMR spectrum of compound **5e**




$^{13}$C NMR spectrum of compound **5e**

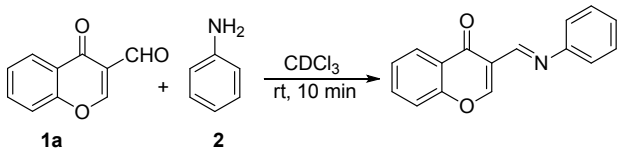



BCR-FA-FBA-CCL3E#8-30 RT: 0.03-0.10 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]
m/z= 372.59-420.44

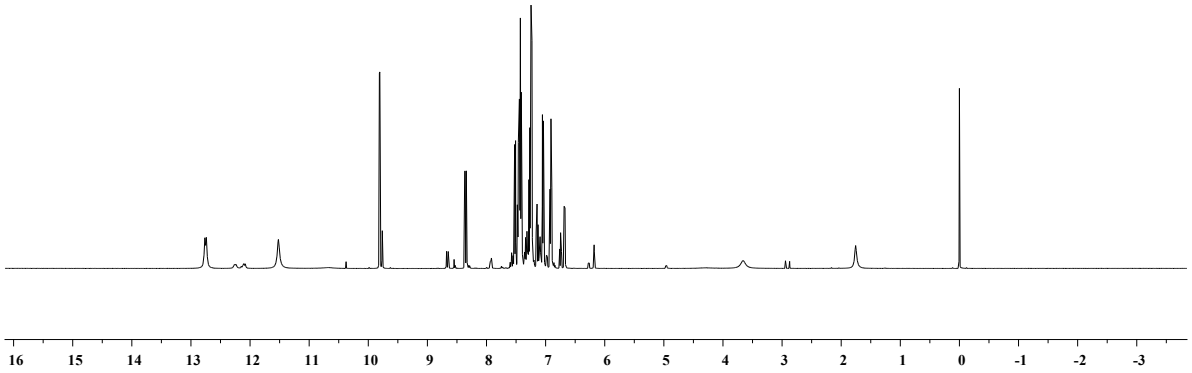
| m/z | Intensity | Relative | Theo. Mass | Delta (ppm) | RDB equiv. | Composition |
|---|---|---|---|---|---|---|
| 396.12530 | 114008704.0 | 100.00 | 396.12418 | 2.84 | 13.5 | $C_{22}H_{19}O_5NF$ |

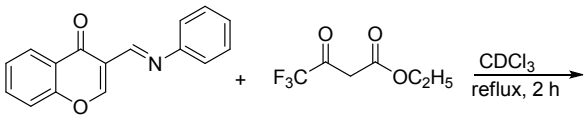
HRMS spectrum of compound **5e**

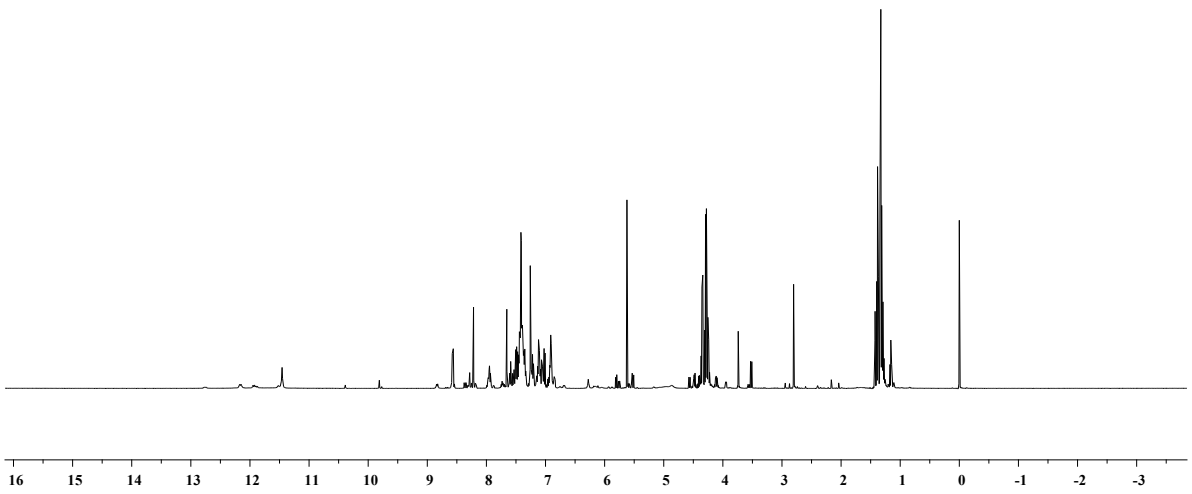
**$^1$H NMR-Monitoring Reactions between 3-formylchromone, aniline/benzylamine and 4,4,4-trifluoro-3-oxobutanoate.**

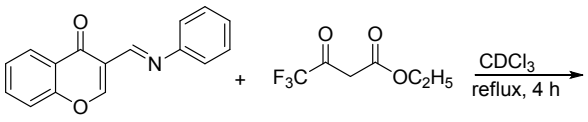


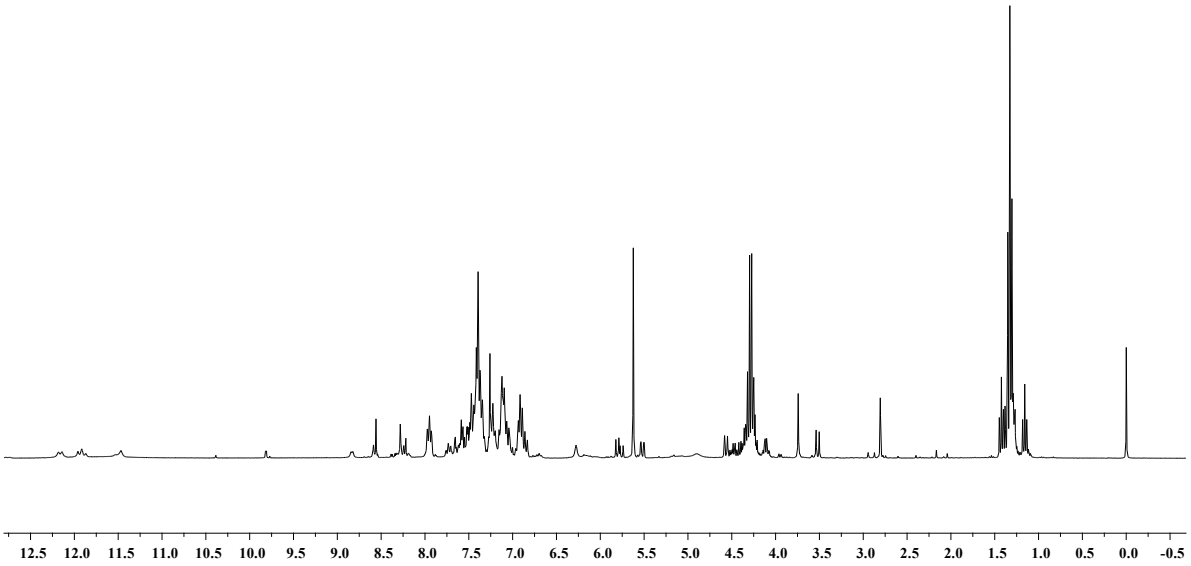

**1a** **2**

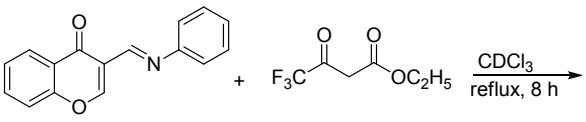


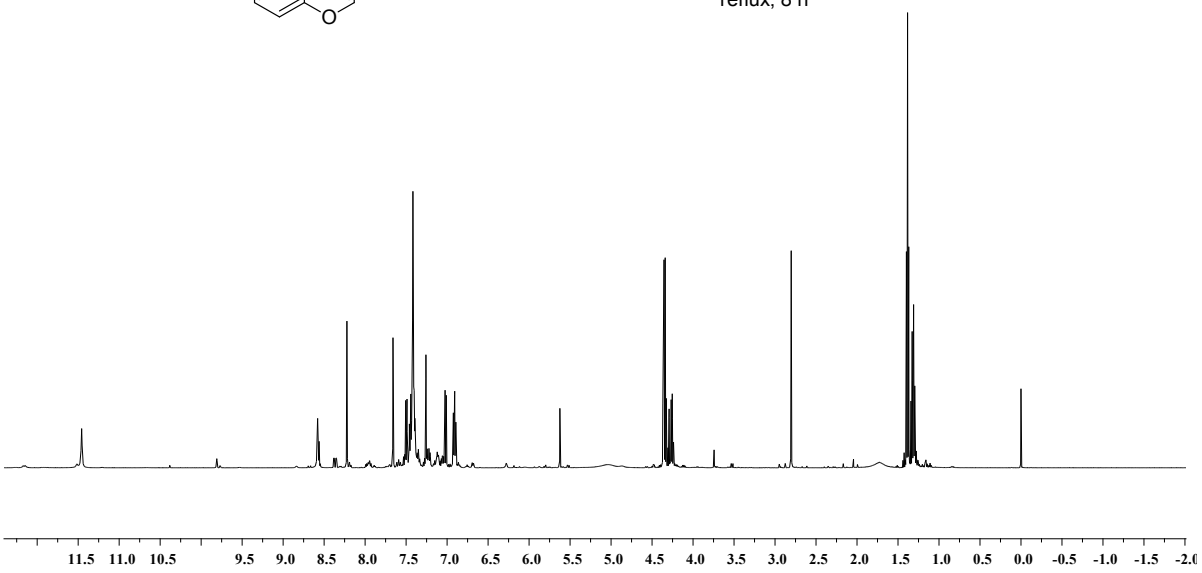



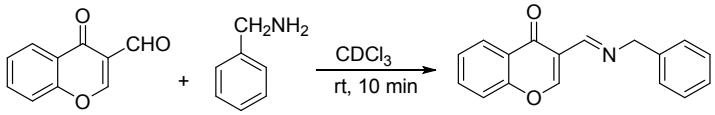



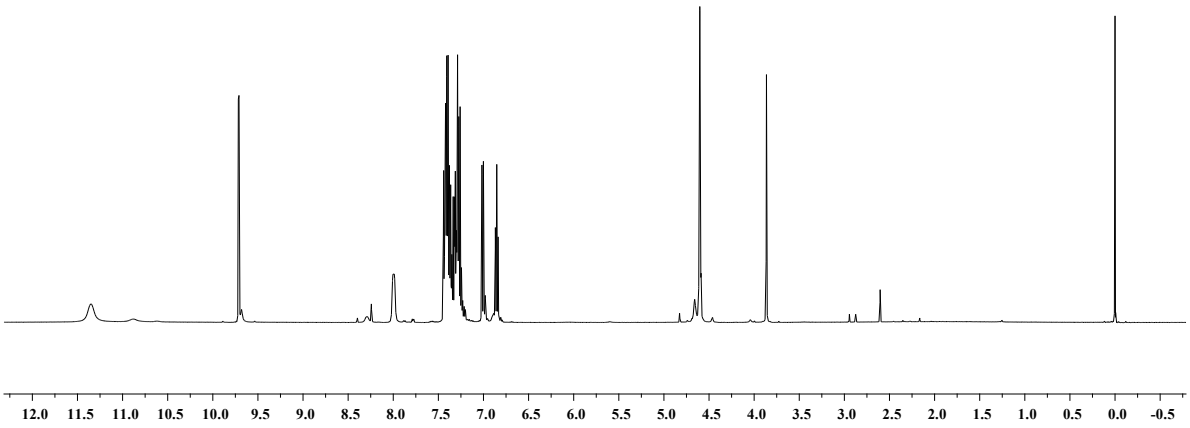

O
N
O
+
F3C
O
O
OC2H5
CDCl3
reflux, 4 h

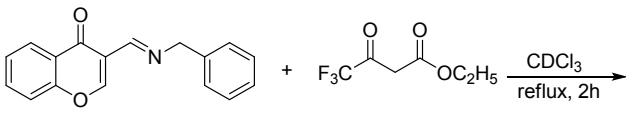

12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

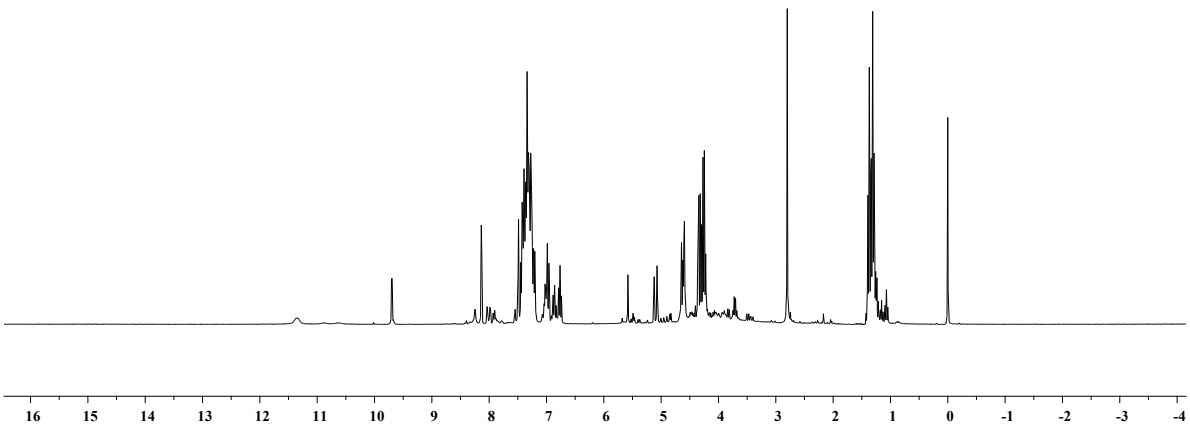

O
N
O
+
F3C
O
O
OC2H5
CDCl3
reflux, 8 h

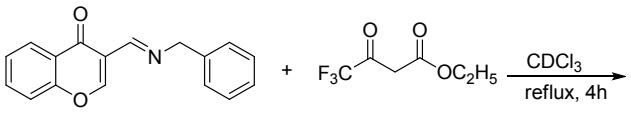

11.5 11.0 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5

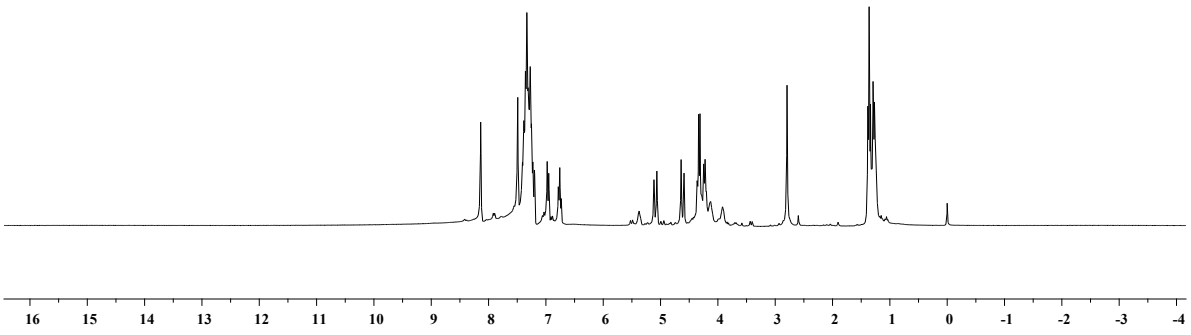

O
CHO
O
1a
+
CH2NH2
2a
CDCl3
rt, 10 min
O
N
O

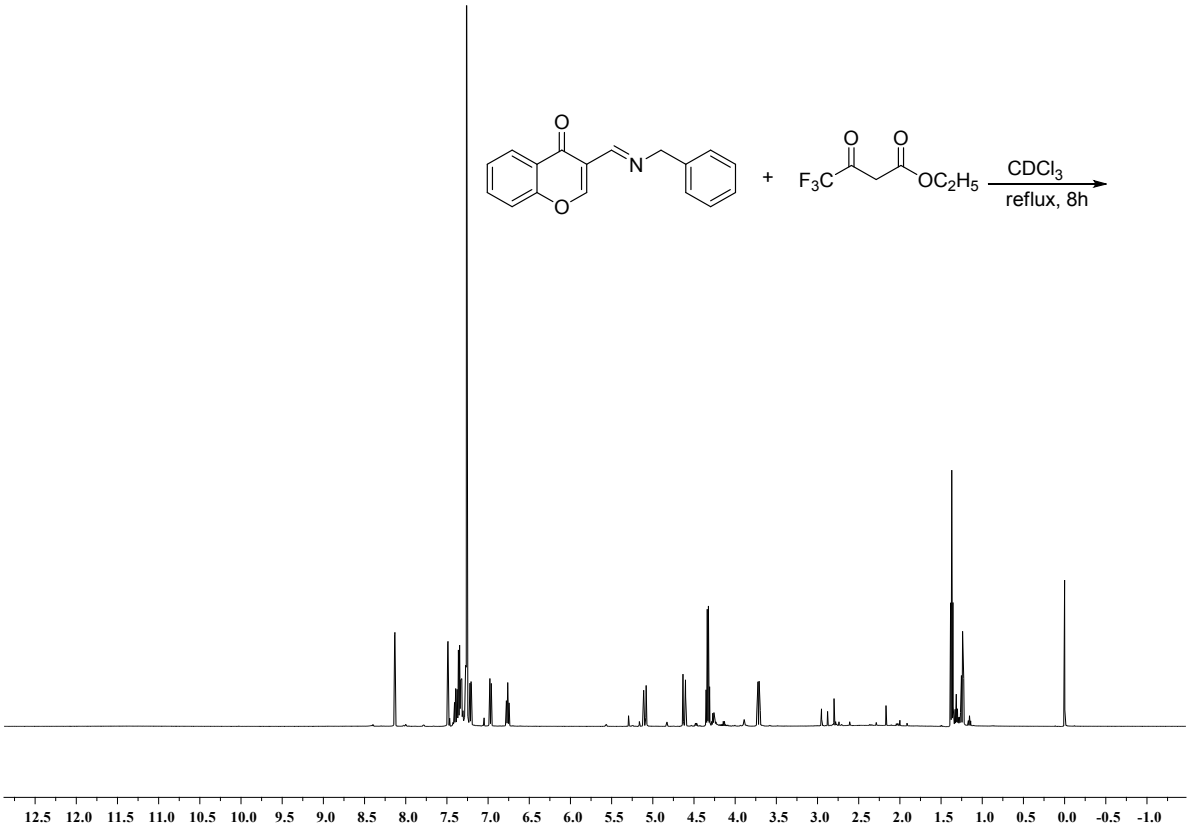

12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5


O
N
O
+
O
O
F3C
OC2H5
CDCl3
reflux, 2h


16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4

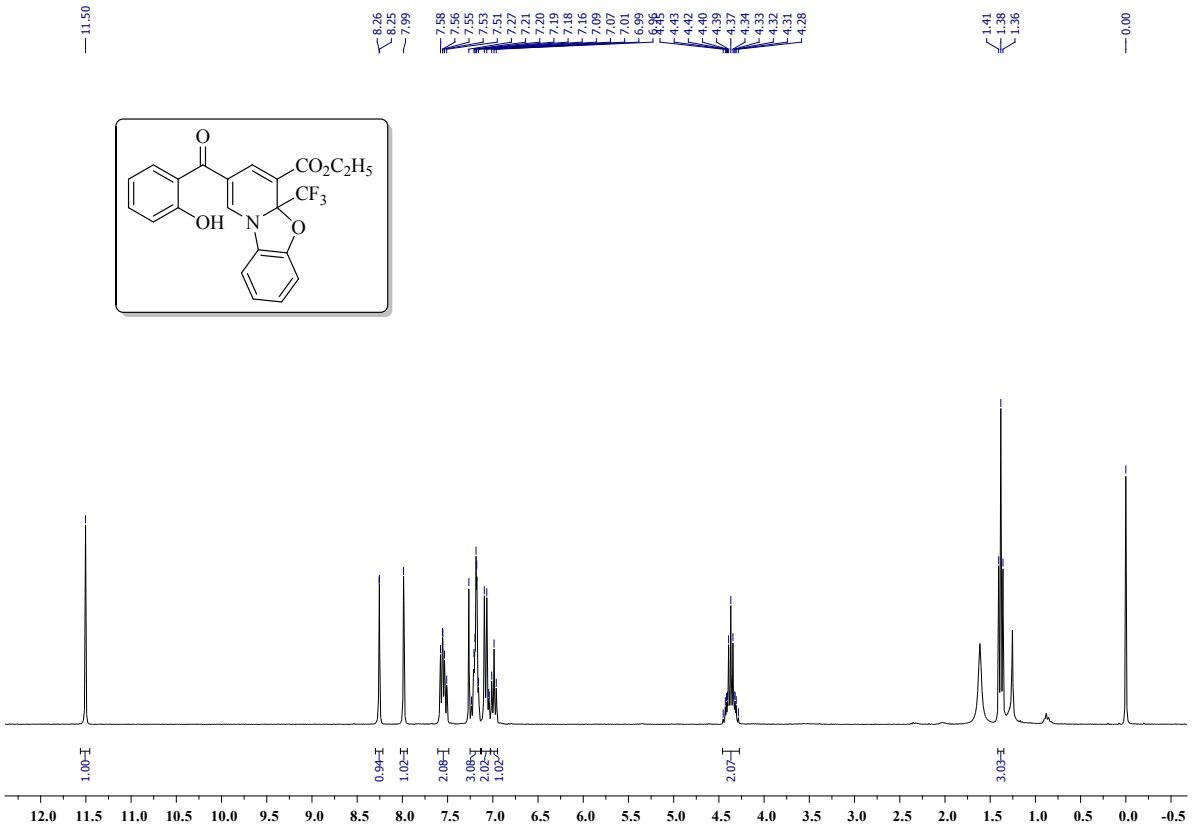

O
N
O
+
F3C
O
O
OC2H5
CDCl3
reflux, 4h


16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4

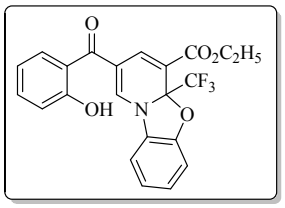

O
N
O
+
F3C
O
O
OC2H5
CDCl3
reflux, 8h
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0

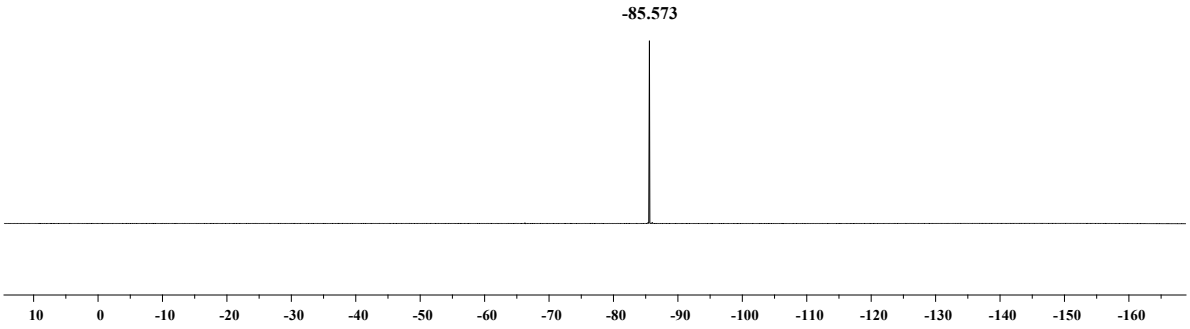
**General procedure for the preparation of 2-hydroxy-benzoyl-trifluoromethyl-benzopyrido-1,3-oxazole-4-carboxylates 7a-f.**

Ethyl 4,4,4-trifluoro-3-oxobutanoate (**3a**, 1.5 mmol) was added to a stirred solution of 4-oxo-4*H*-chromene-3-carbaldehyde (**1a**, 1 mmol) and 2-aminophenol (**6a**, 1.2 mmol) in $CH_3CN$ (2 mL). The contents were stirred under reflux conditions for 4 h. After completion of the reaction (TLC), the residue was purified by column chromatography by using silica gel (100:200, ethyl acetate/hexane 8:92) afforded 2-hydroxybenzoyl-trifluoromethyl-benzopyrido-1,3-oxazole-4-carboxylate **7a**. Similarly, compounds **7b-f** were prepared from corresponding 3-formylchromones **1a-c** and 2-aminophenols **6a-c**.

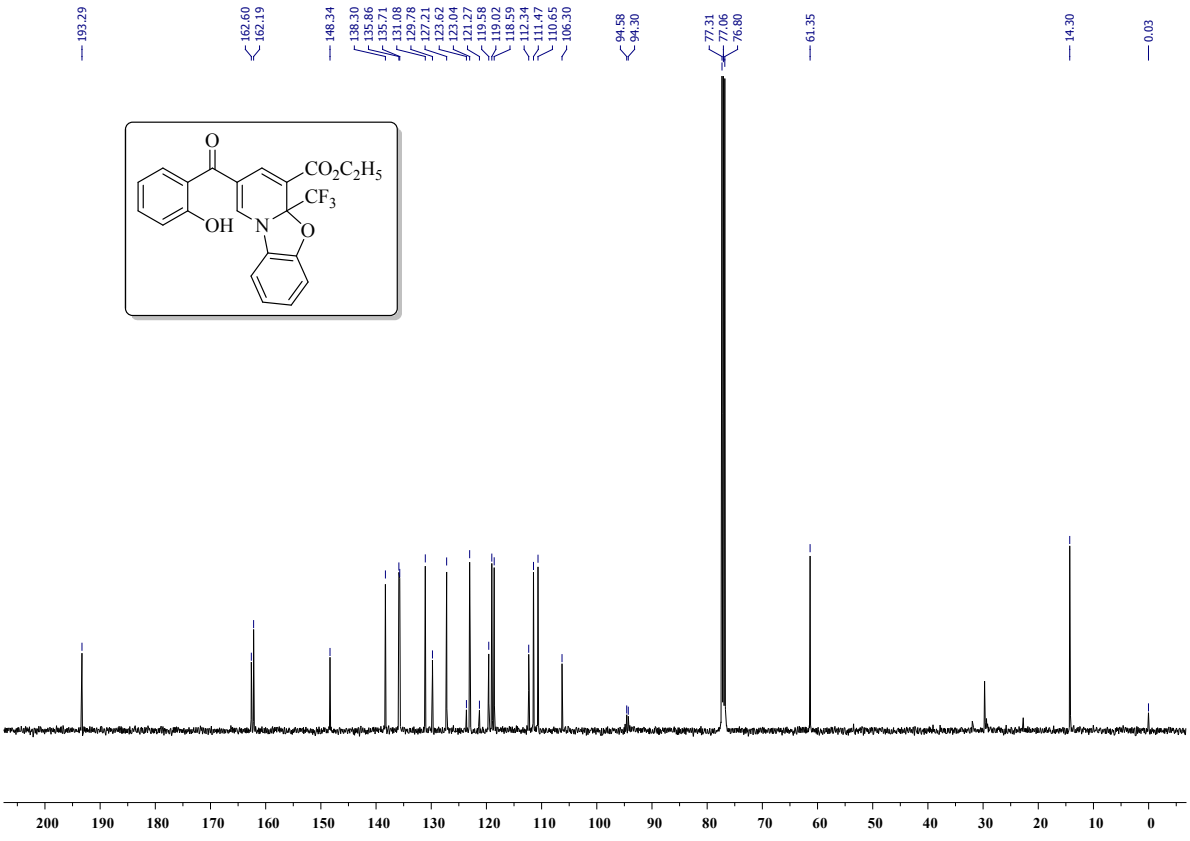



$^1$H NMR spectrum of compound **7a**




$^{19}$F NMR spectrum of compound **7a**

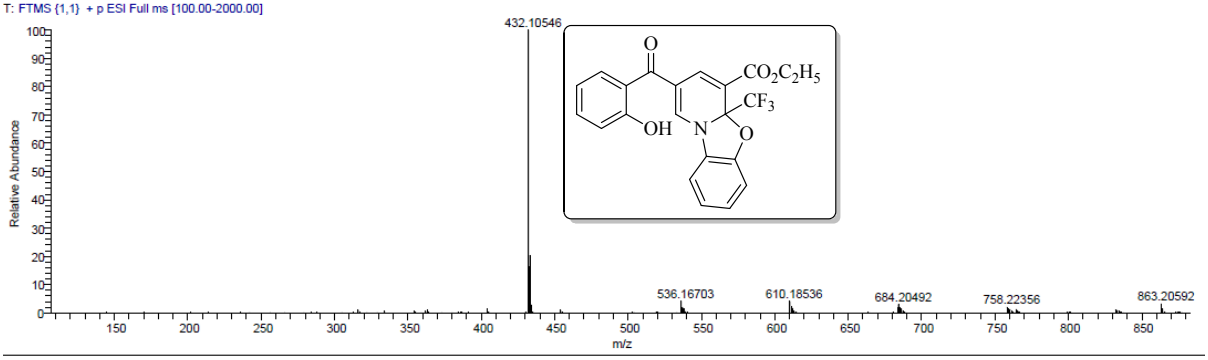



$^{13}$C NMR spectrum of compound **7a**

National Centre for Mass Spectrometry
CSIR-Indian Institute of Chemical Technology

File Name C:\IICT-HRMS\05.02.2014\BCR-FAP-CF3
Sample Name CH-DYAKAR
Sample ID 1
Date and Time 05-02-14 19:27:06

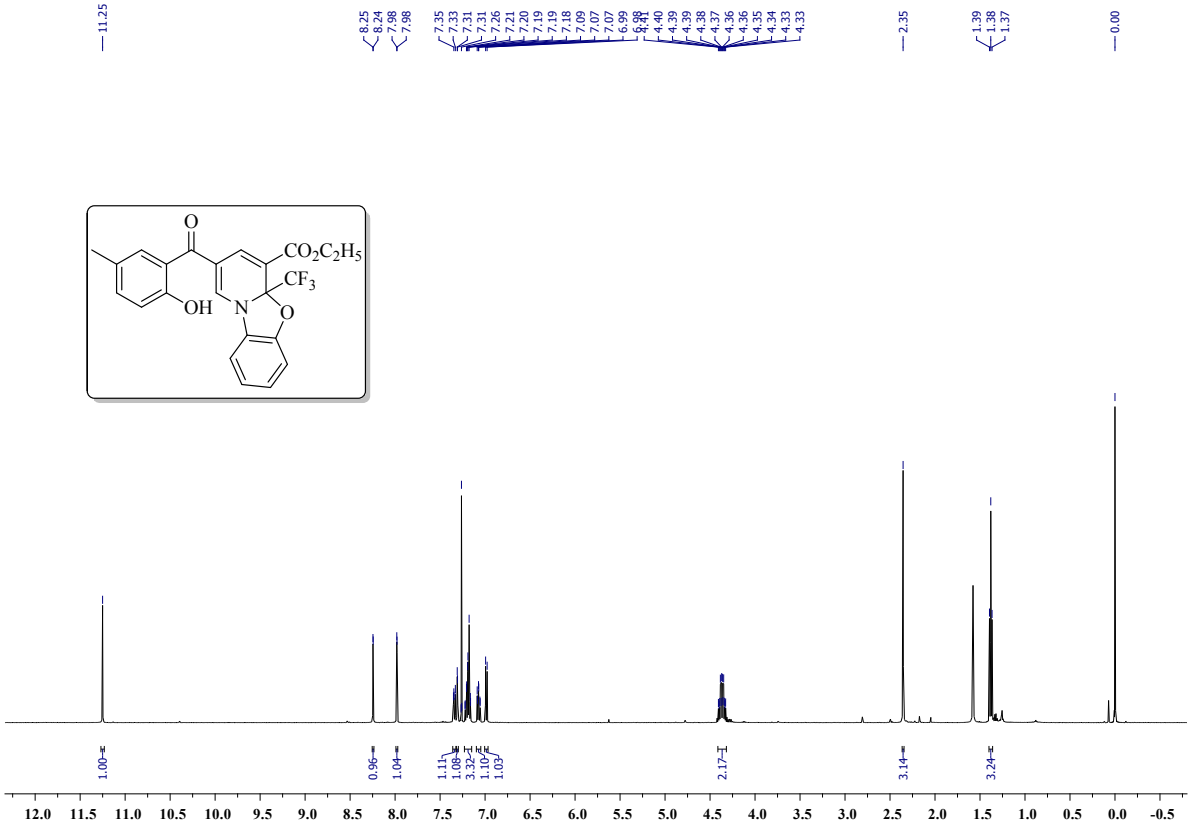
BCR-FAP-CF3 #4-62 RT: 0.02-0.21 AV: 59 SB: 420 0.57-1.99 NL: 2.45E7
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]



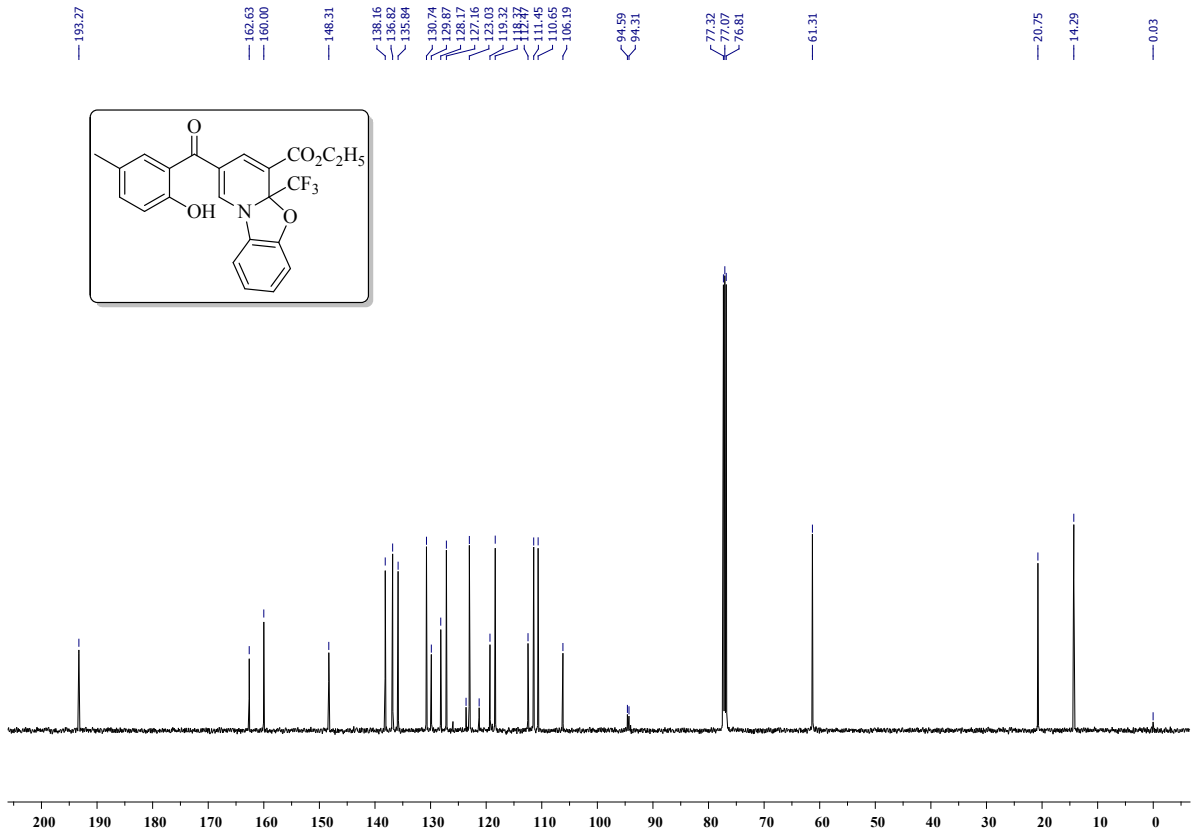

BCR-FAP-CF3#8-30 RT: 0.03-0.10 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]
m/z= 407.53-451.40

| m/z | Intensity | Relative | Theo. Mass | Delta (ppm) | RDB equiv. | Composition |
|---|---|---|---|---|---|---|
| 432.10529 | 34783576.0 | 100.00 | 432.10533 | -0.10 | 13.5 | $C_{22}H_{17}O_5NF_3$ |
| 433.10965 | 6887484.5 | 19.80 | | | | |

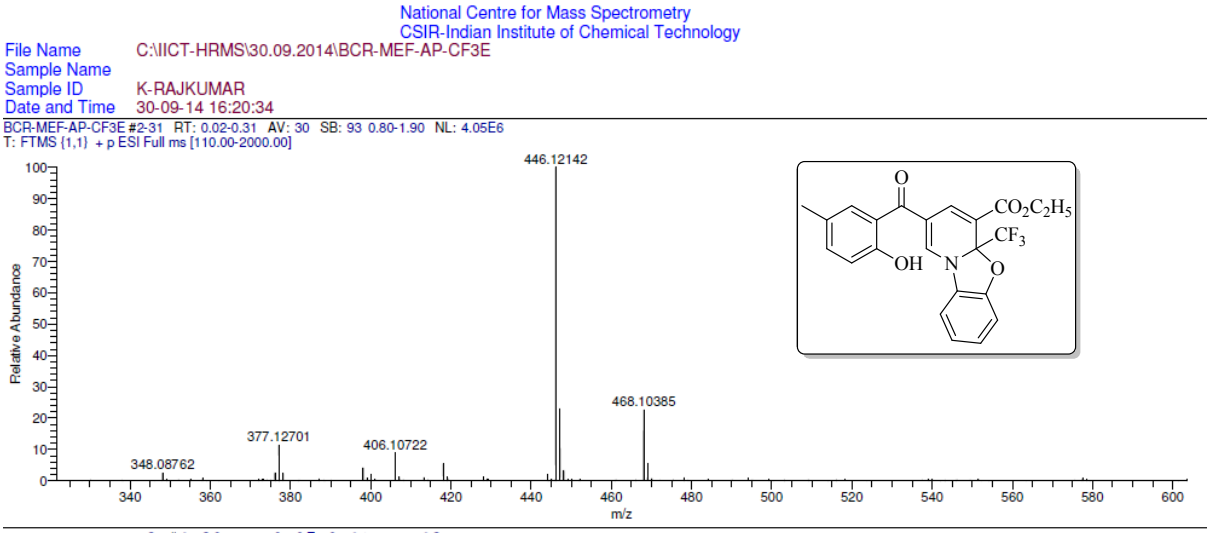
HRMS spectrum of compound **7a**




$^1$H NMR spectrum of compound 7**b**



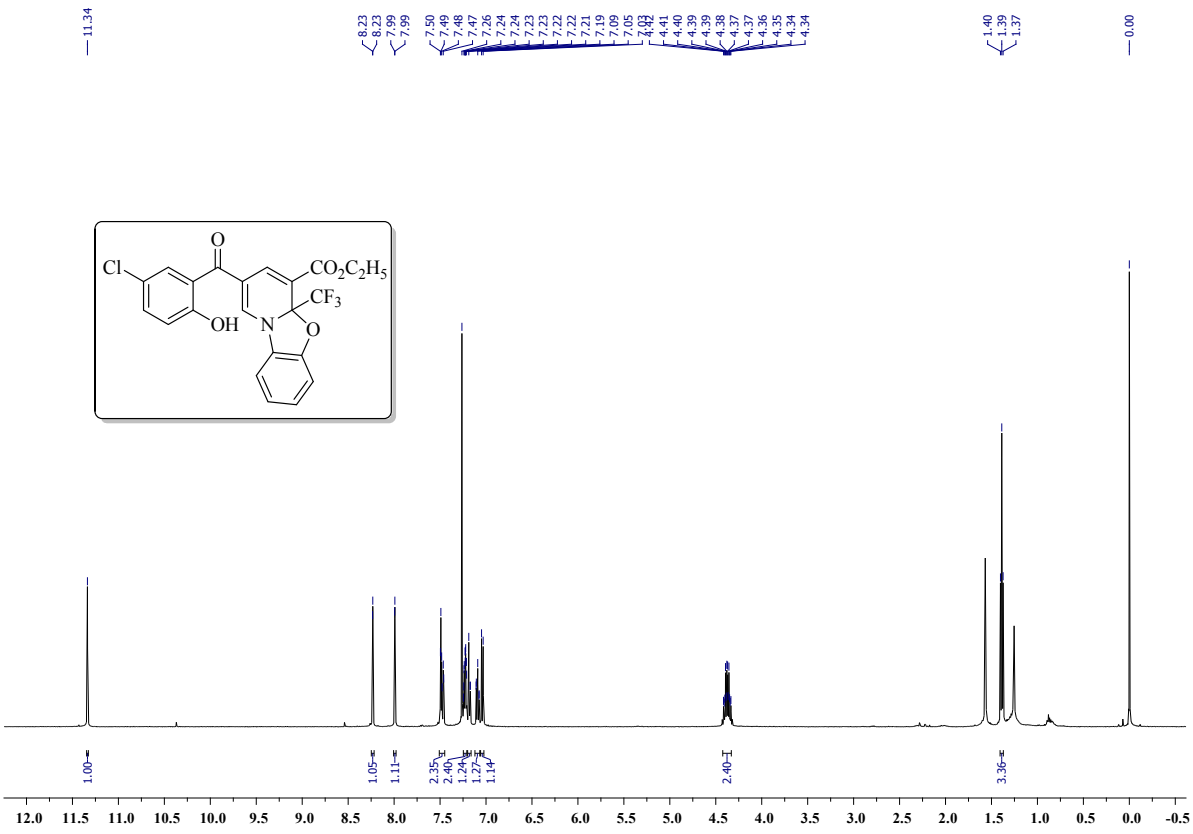

$^{13}$C NMR spectrum of compound 7**b**



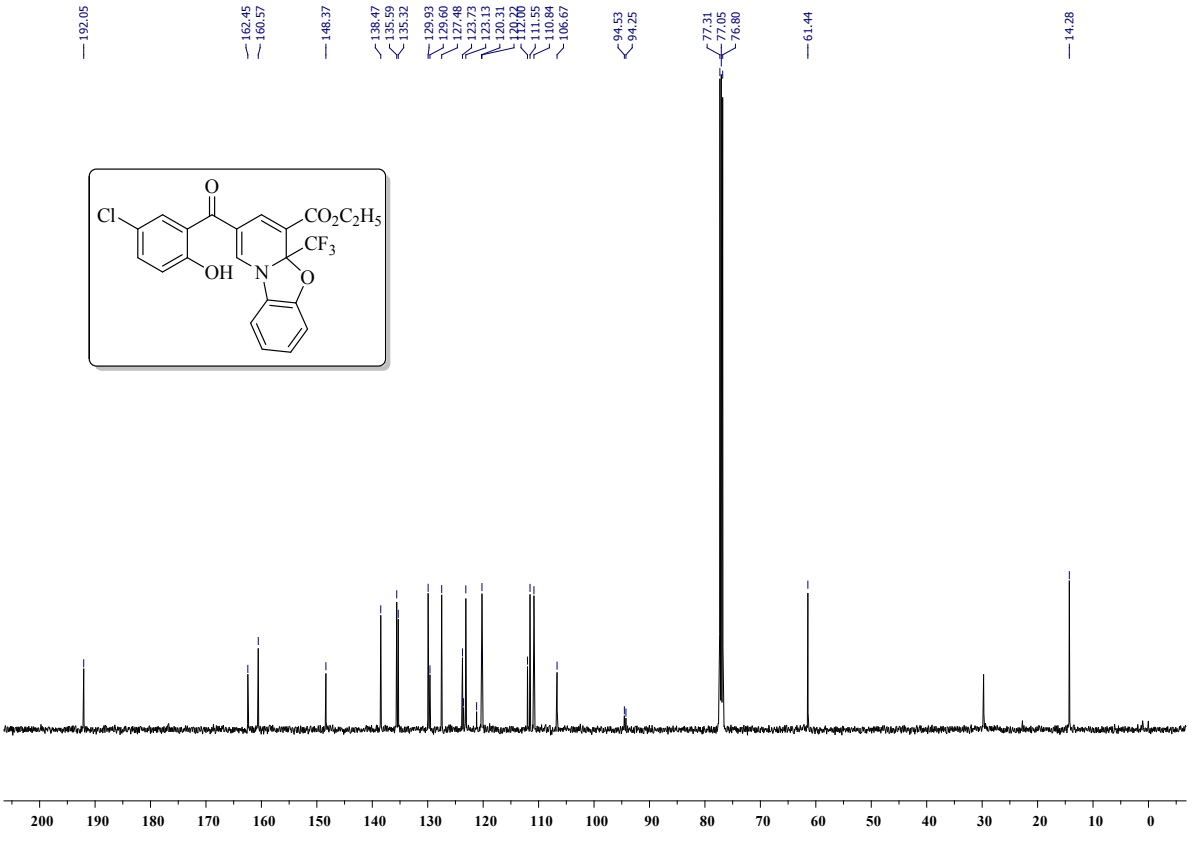

BCR-MEF-AP-CF3E#8-30 RT: 0.07-0.29 AV: 23
T: FTMS {1,1} + p ESI Full ms [110.00-2000.00]
m/z= 439.17-452.13

| m/z | Intensity | Relative | Theo. Mass | Delta (ppm) | RDB equiv. | Composition |
|---|---|---|---|---|---|---|
| 446.12146 | 3677234.8 | 100.00 | 446.12098 | 0.48 | 13.5 | $C_{23}H_{19}O_5NF_3$ |

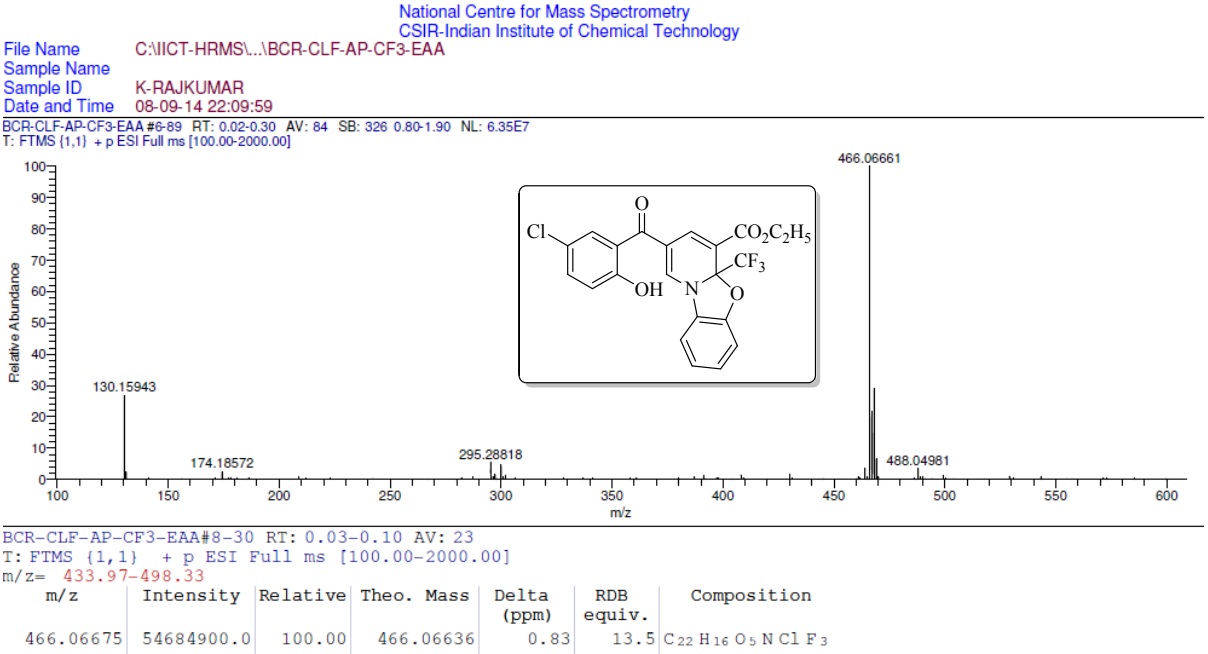
HRMS spectrum of compound 7**b**




$^{1}$H NMR spectrum of compound **7c**



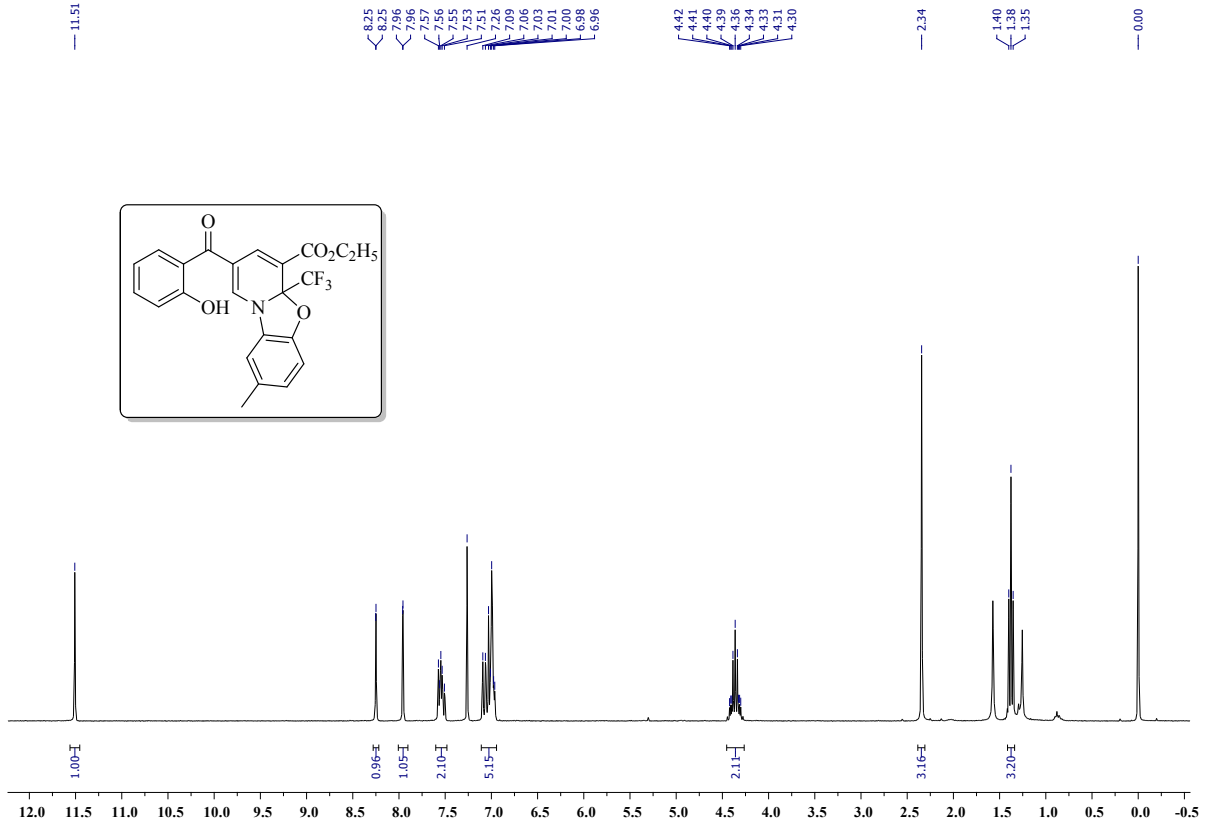

$^{13}$C NMR spectrum of compound 7**c**



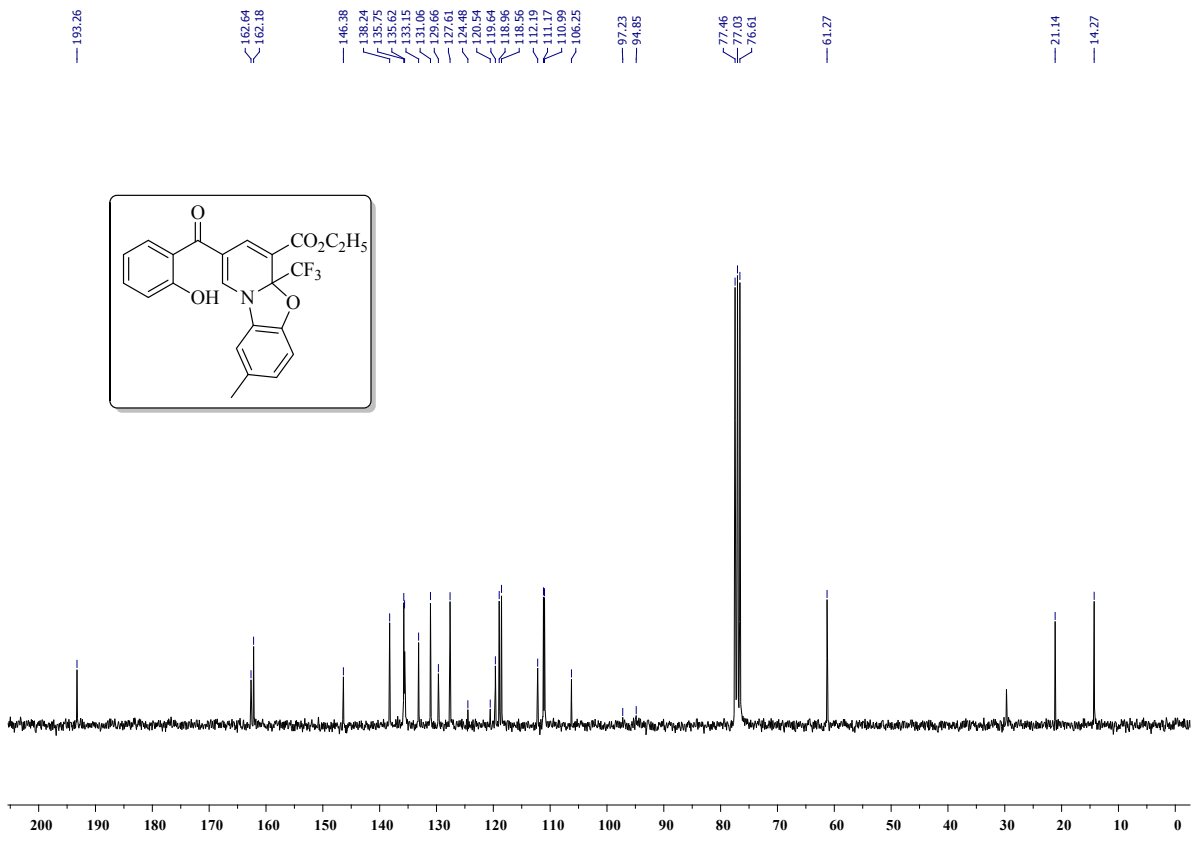

BCR-CLF-AP-CF3-EAA#8-30 RT: 0.03-0.10 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]
m/z= 433.97-498.33

| m/z | Intensity | Relative | Theo. Mass | Delta (ppm) | RDB equiv. | Composition |
|---|---|---|---|---|---|---|
| 466.06675 | 54684900.0 | 100.00 | 466.06636 | 0.83 | 13.5 | $C_{22}H_{16}O_5NClF_3$ |

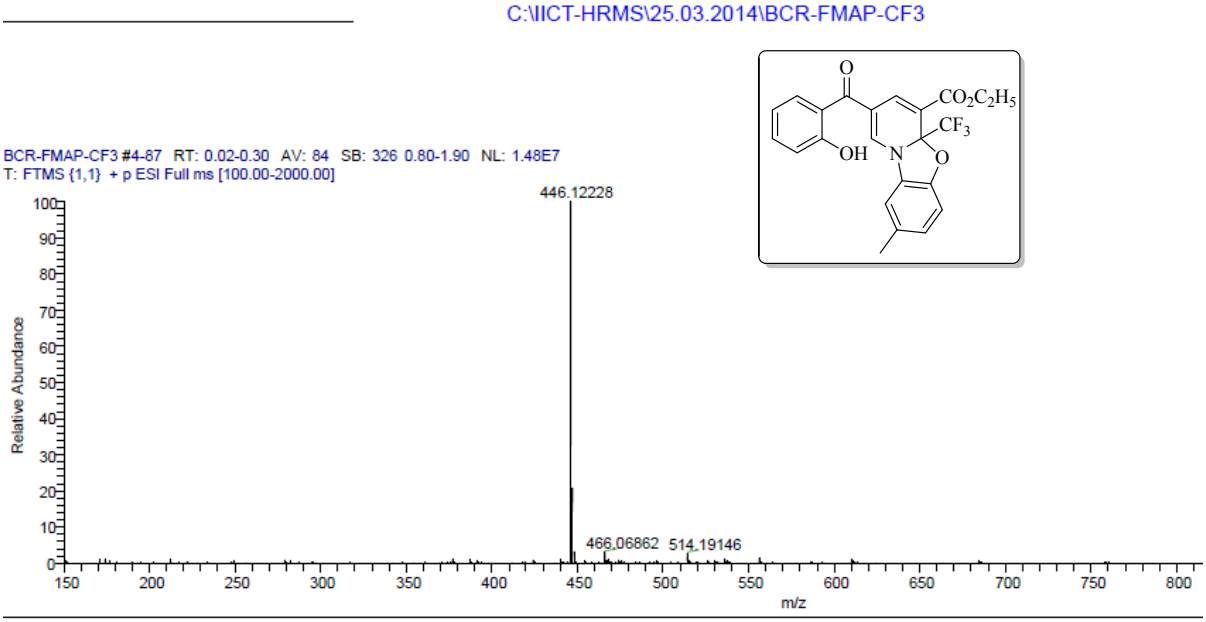
HRMS spectrum of compound 7**c**




$^{1}$H NMR spectrum of compound 7**d**



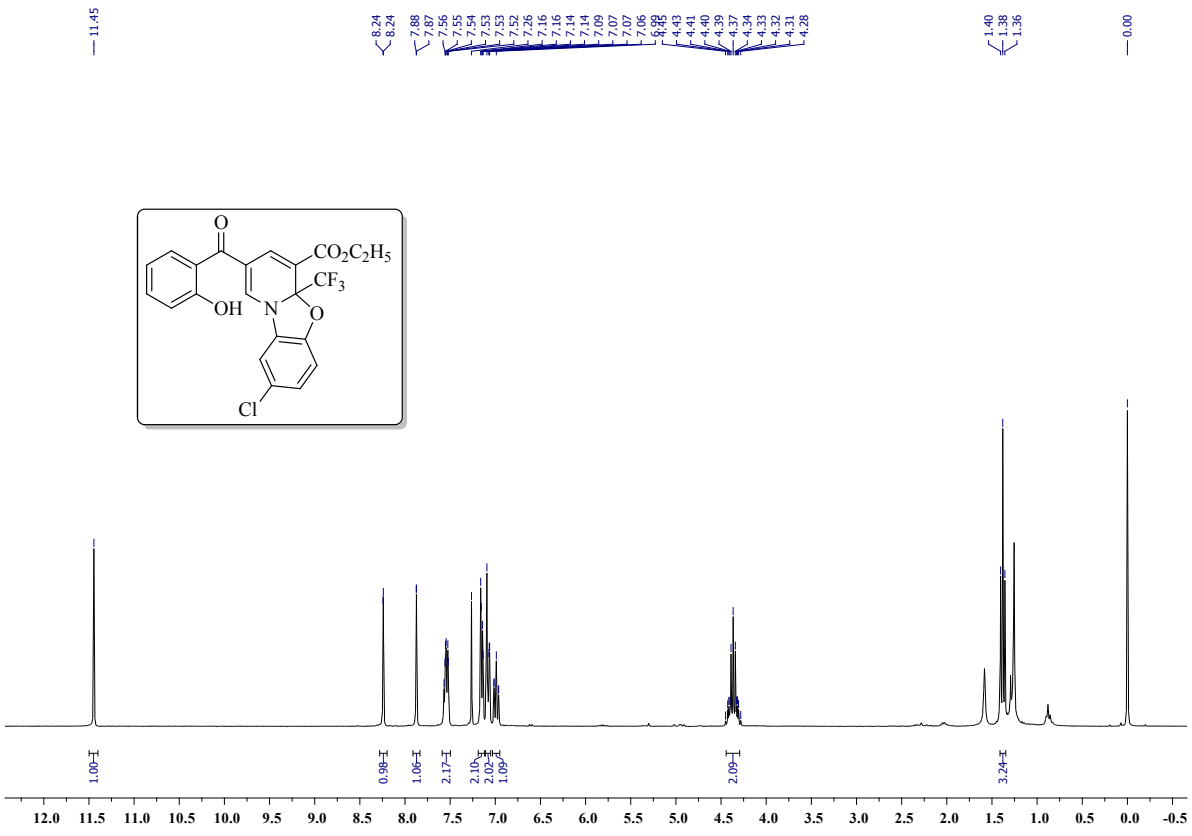

$^{13}$C NMR spectrum of compound 7**d**



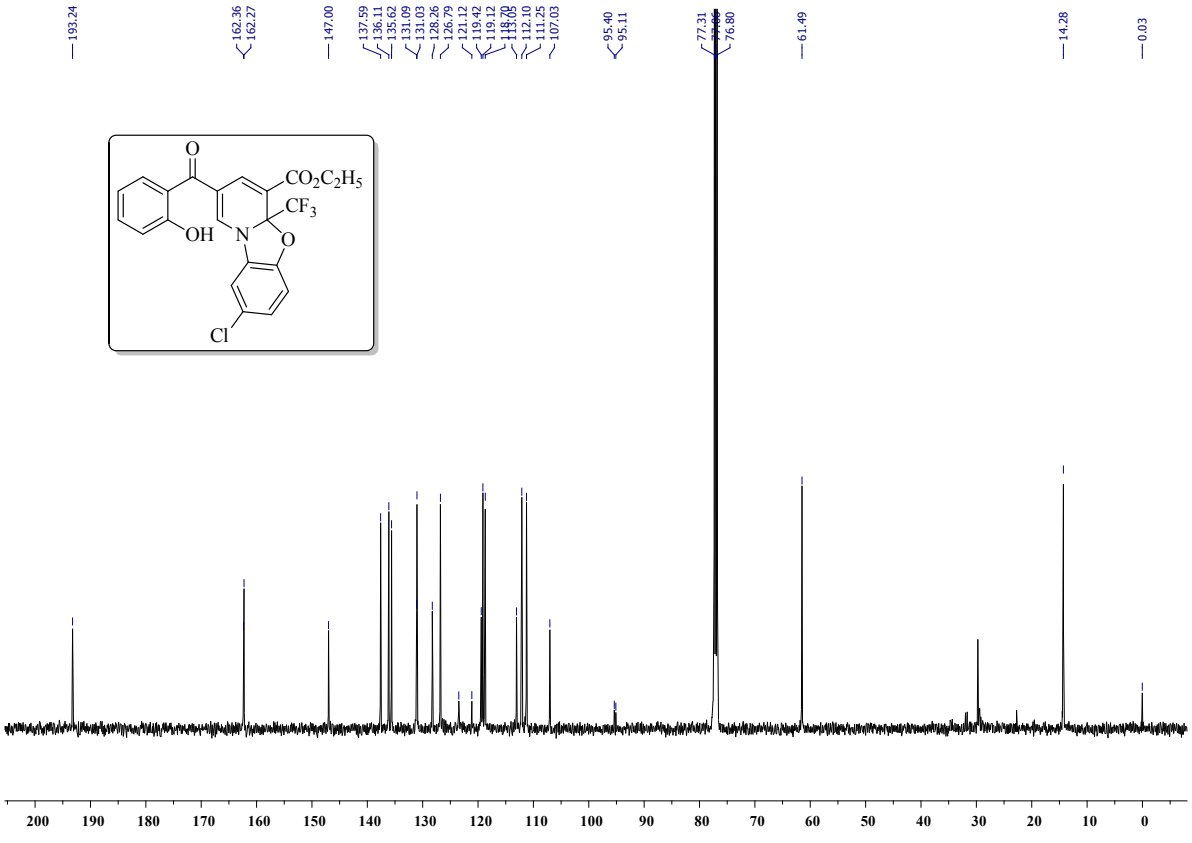

BCR-FMAP-CF3#8-30 RT: 0.03-0.11 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]

| m/z | Intensity | Relative | Theo. Mass | Delta (ppm) | RDB equiv. | Composition |
|---|---|---|---|---|---|---|
| 446.12232 | 44656400.0 | 100.00 | 446.12098 | 3.01 | 13.5 | $C_{23}H_{19}O_5NF_3$ |

HRMS spectrum of compound 7**d**



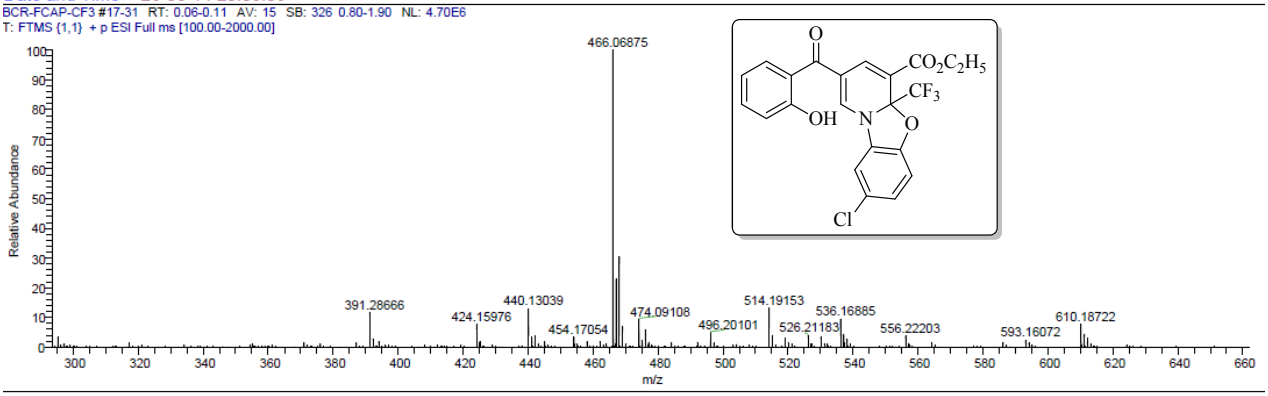

$^{1}$H NMR spectrum of compound 7**e**




$^{13}$C NMR spectrum of compound 7**e**

National Centre for Mass Spectrometry
CSIR-Indian Institute of Chemical Technology

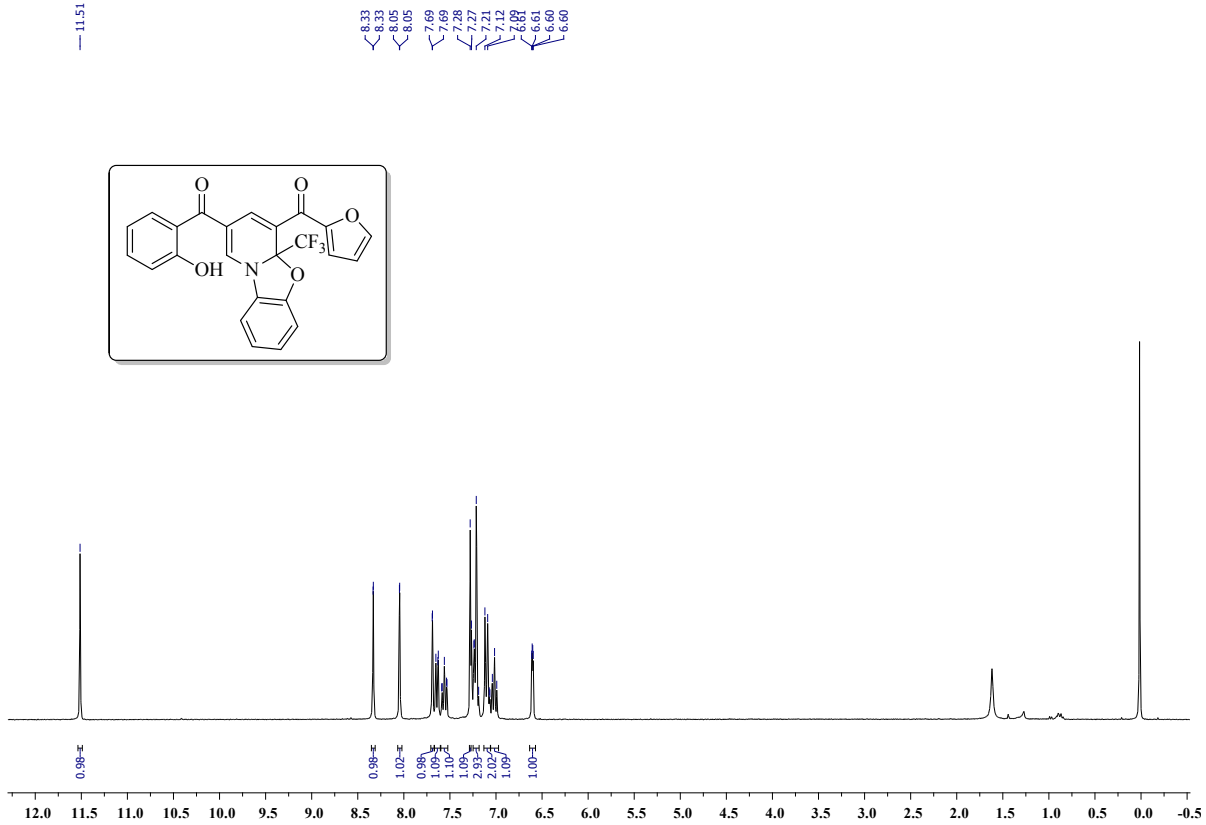
File Name C:\IICT-HRMS\25.03.2014\BCR-FCAP-CF3
Sample Name K-RAJ-KUMAR
Sample ID 1
Date and Time 26-03-14 20:03:09



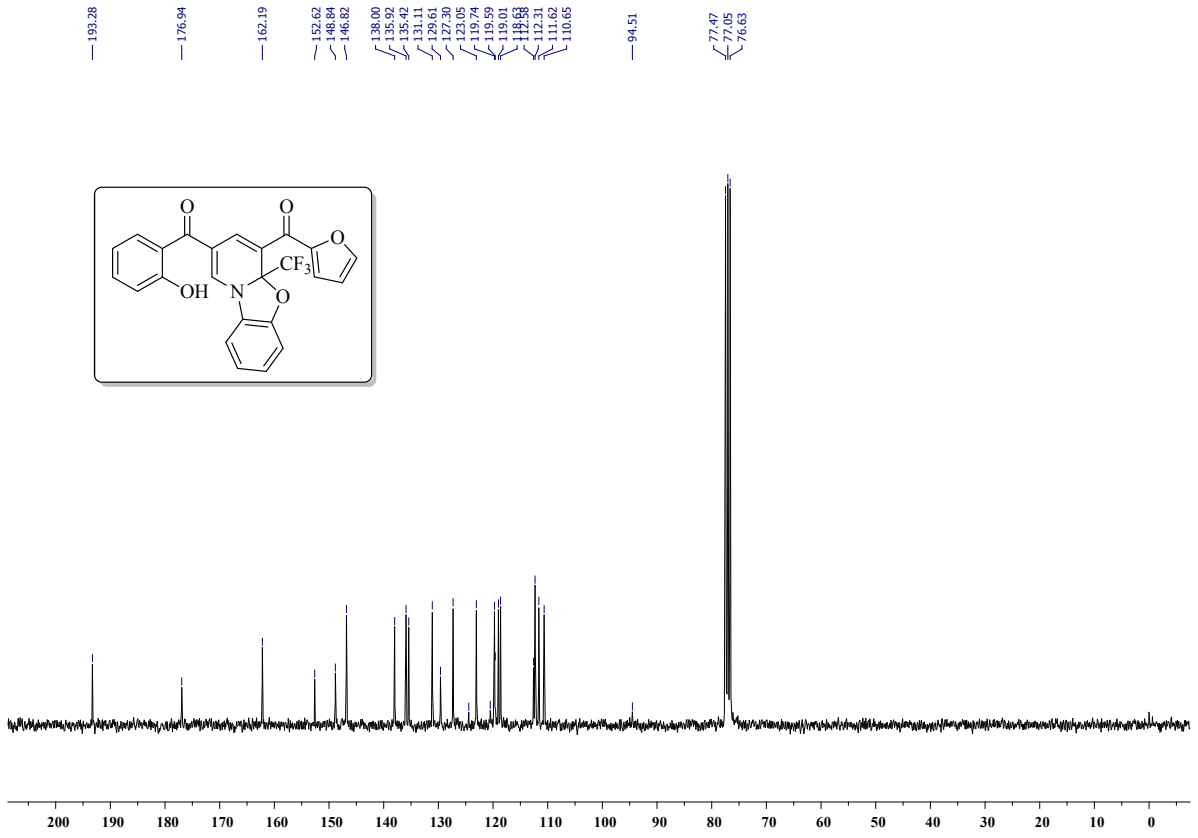

BCR-FCAP-CF3#8-30 RT: 0.03-0.11 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]
m/z= 463.67-470.70

| m/z | Intensity | Relative | Theo. Mass | Delta (ppm) | RDB equiv. | Composition |
|---|---|---|---|---|---|---|
| 466.06885 | 3698194.3 | 100.00 | 466.06636 | 5.34 | 13.5 | $C_{22}H_{16}O_5NClF_3$ |

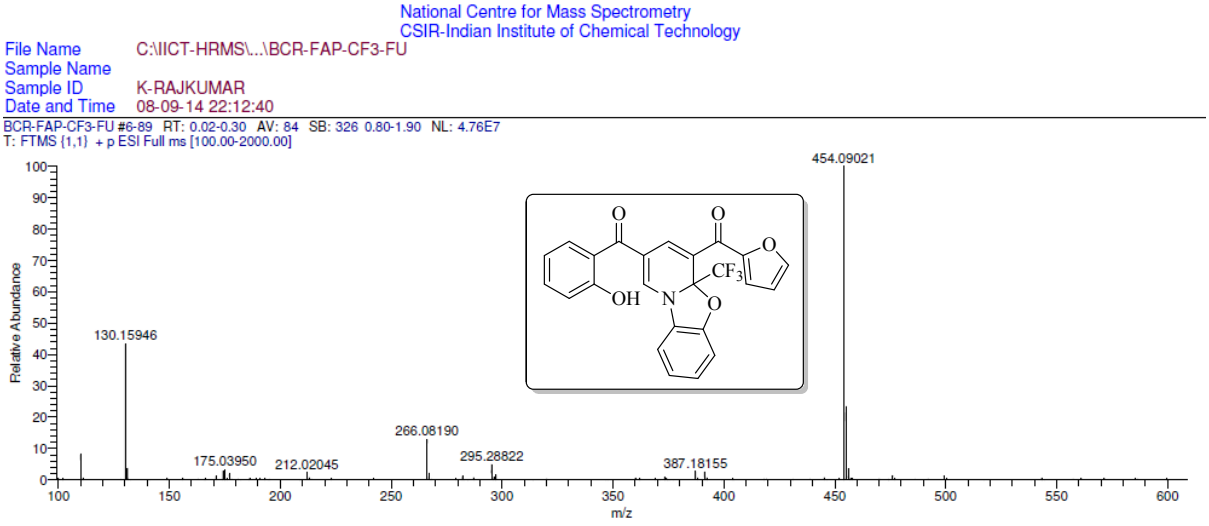
HRMS spectrum of compound 7**e**




$^1$H NMR spectrum of compound 7**f**




$^{13}$C NMR spectrum of compound 7**f**




BCR-FAP-CF3-FU#8-30 RT: 0.03-0.10 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]
m/z= 438.26-472.58

| m/z | Intensity | Relative | Theo. Mass | Delta (ppm) | RDB equiv. | Composition |
|---|---|---|---|---|---|---|
| 454.09022 | 45002360.0 | 100.00 | 454.08968 | 1.18 | 16.5 | $C_{24}H_{15}O_5NF_3$ |

HRMS spectrum of compound 7**f**