Copies of spectra

Iodine catalyzed four-component reaction: A straightforward onepot synthesis of functionalized pyrroles under metal-free conditions

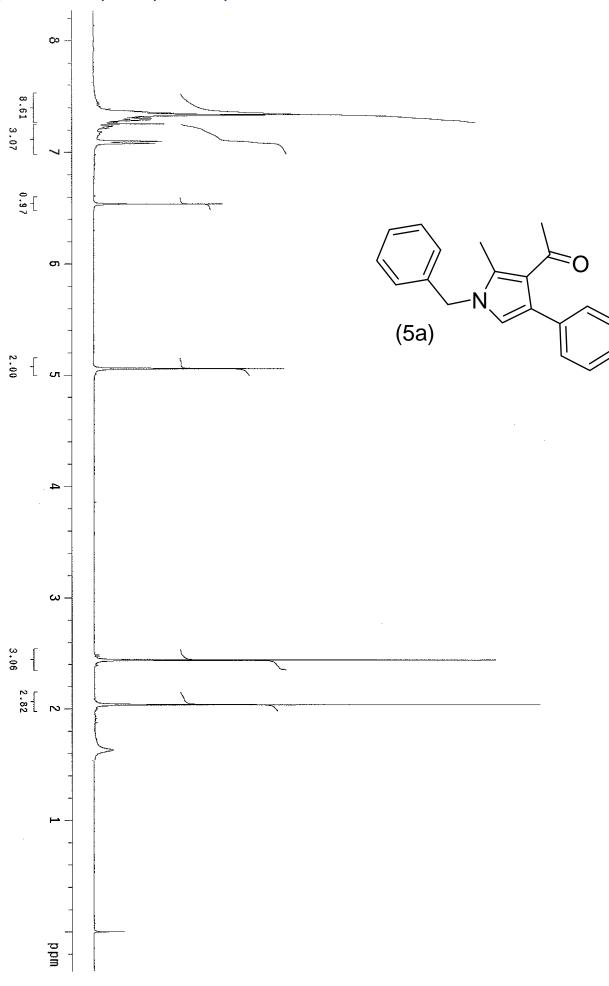
G. Rajeshwar Reddy, ^{a,b} T. Ram Reddy, ^a Suju C. Joseph, ^a K. Sateesh Reddy, ^a L. Srinivasula Reddy, ^a P. Mahesh Kumar, ^a and Manojit Pal^{c,*}

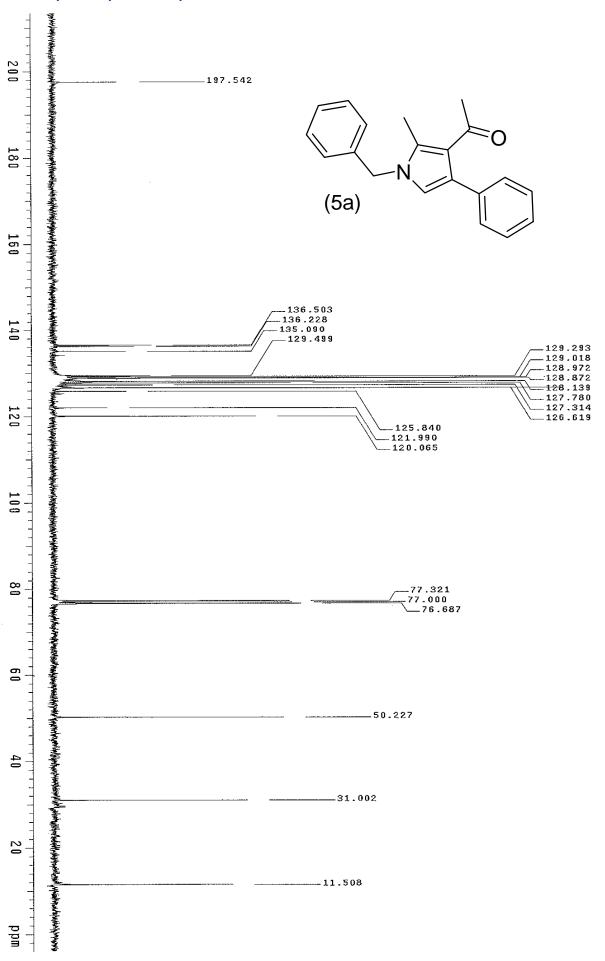
^aCustom Pharmaceutical Services, Dr. Reddy's Laboratories Limited, Bollaram Road Miyapur, Hyderabad 500 049, India

^bChemistry Division, Institute of Science and Technology, JNT University, Kukatpally, Hyderabad 500072, Andhra Pradesh, India

^cInstitute of Life Sciences, University of Hyderabad Campus, Gachibowli, Hyderabad 500 046, India.

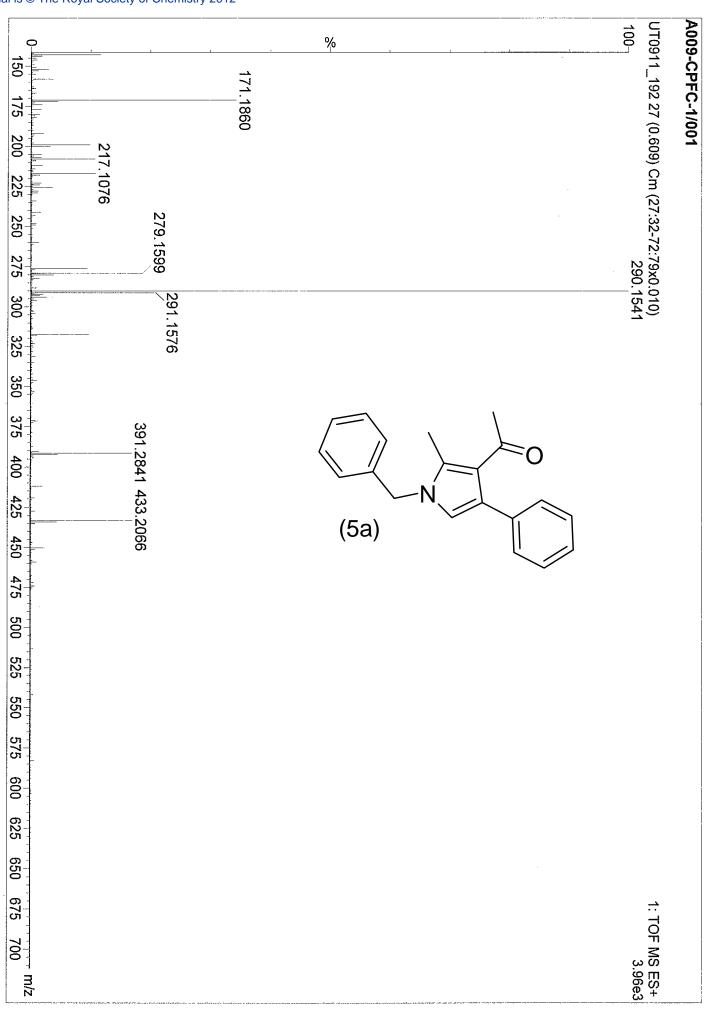
 $\hbox{E-mail: } \textit{manojitpal@rediffmail.com}$





NMR-400

A009-CPFC-1-001 in CDC13



Elemental Composition Report

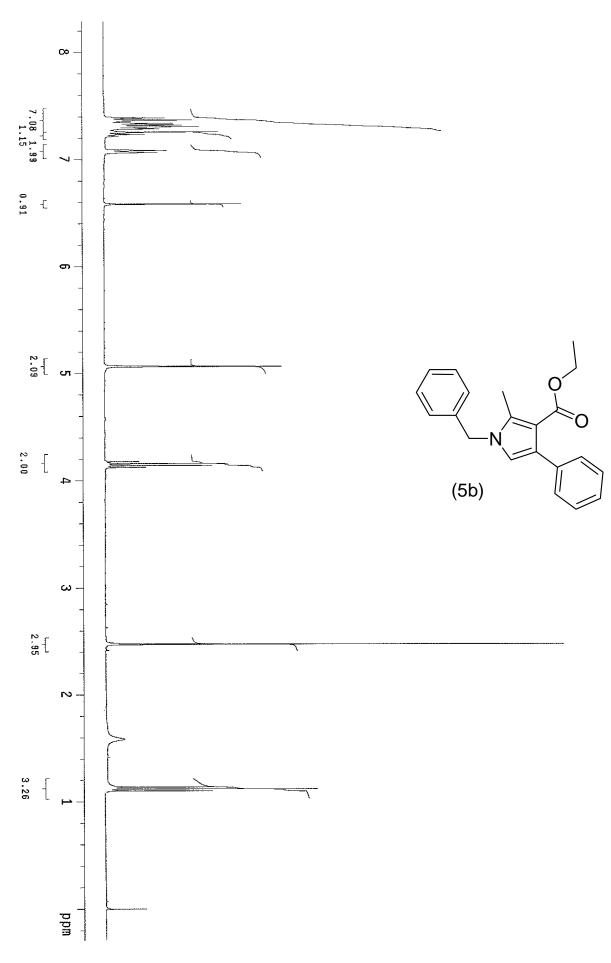
Single Mass Analysis Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0

Element prediction: Off Number of isotope peaks used for i-FIT = 4

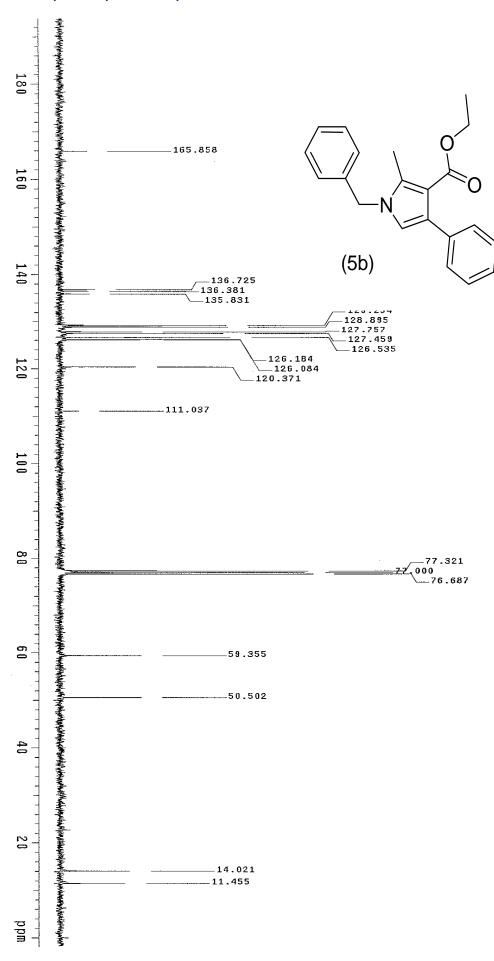
202 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass) Monoisotopic Mass, Even Electron lons

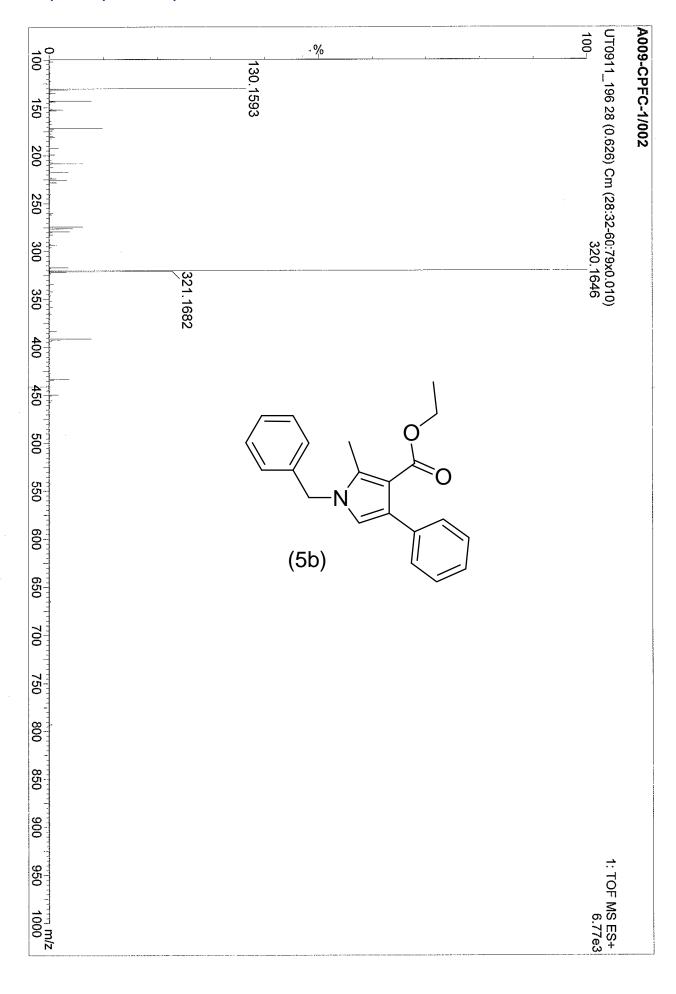
C: 0-70 H: 0-80 N: 0-5 O: 0-10 Elements Used:

290.1541	Mass	Minimum: Maximum:	0 160	%		100	UT0911_192;	A009-CPFC-1/001
290.1545	Calc. Mass		208.04002 180 200	_1.186			UT0911_192 27 (0.609) Cm (27:32-72:79x0.010)	001
~0.4	mDa	5.0	17.1076 226.0132 11.1.1.1.1.1.1.1.1.1.1.1.1.1.1.1.1.1.1				72:79x0.010)	
-1.4	Mdd	5.0	260	279.1599				
11.5	DBE	0.0 80.0	300	291.1576		290.1541		
28.2	i-FIT		320	o,				
C20 H20 N O	Formula		391.2841 433.2066 346.2772 390.1846 392.2895 434.2100 459.1676 512.9681 541.9564 582.9816 603.5248 346.2772 390.1846 392.2895 434.2100 459.1676 512.9681 541.9564 582.9816 603.5248 340 360 380 400 420 440 460 480 500 520 540 560 580 600 620		(5	āa)	>	\ -N
			582.9816 603.5248			3.80e+003	1: TOF MS ES+	









Calc. Mass

mDa

PPM

DBE

i-FIT

Formula

5. 0

5.0

80.0

320.1646

320.1651

-0.5

11.5

2.6

C21

H22

z 2 Maximum:

Elemental Composition Report

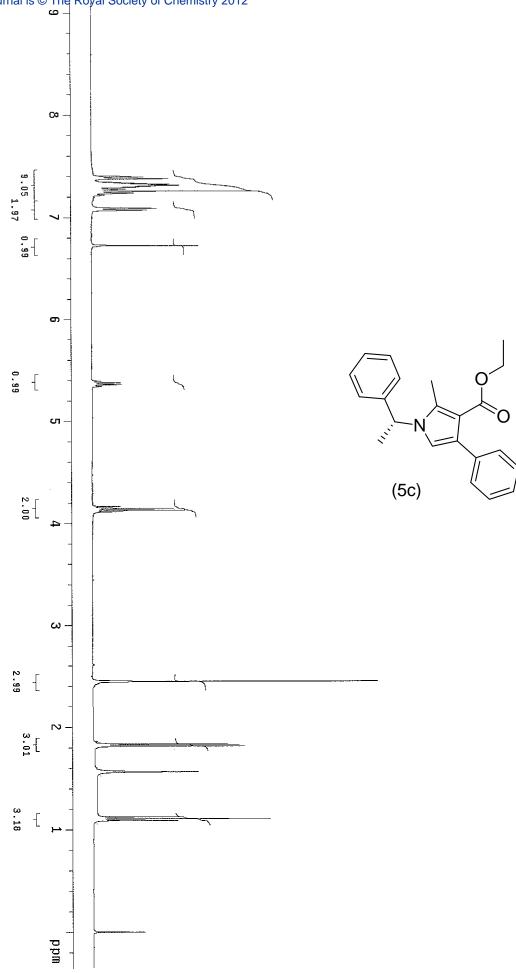
Single Mass Analysis Tolerance = 5.0 PPM /

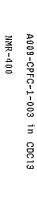
DBE: min = 0.0, max = 80.0

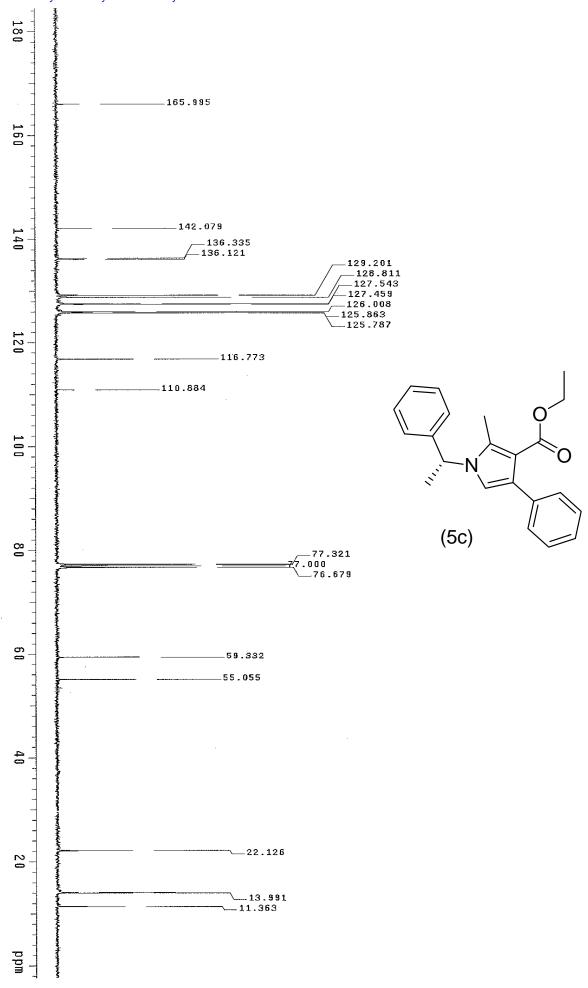
Element prediction: Off

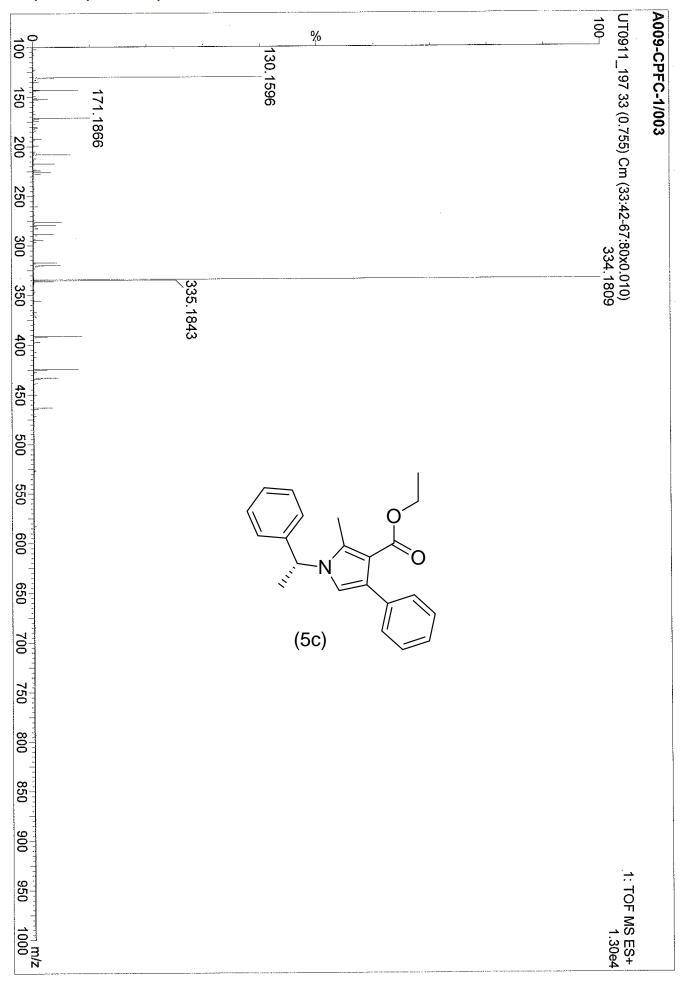
Monoisotopic Mass, Even Electron Ions
380 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used: Number of isotope peaks used for i-FIT = 4

Minimum:	100	5	%- 130.1593	1 .11	100-]	UT0911_196 28	C: 0-70 H: 0-80 N: 0-5 O: 0-10 Br: 0-1 A009-CPFC-1/002
	150 200	171.1866 208.0407 274.1237	w			UT0911_196 28 (0.626) Cm (28:32-60:79x0.010))-80 N: 0-5)2
	250	.0407 274.123				2-60:79x0.010)	O: 0-10 E
	300				320.1646	<u> </u>	3r. 0-1
0	350	22.1718 3	321.1682		46		
0.0	400	91.284743					
	450	3.2055449.					
	500	322.1718 391.2847433.2055449.3181 541.9619 582.9816					
	550	∕9 58:					
	600	2.9816					
	650	665.3156		/=	=\		O´
	700	36 7t			$\langle \rangle$).	
	750	8.3544				-N	
	908	792.6136			(5b)		Į.
	850	853.8426					
	900	902.7872					
	700 750 800 850 900 950 1000	982.48			Š	1: TOF MS ES+	
	1000	143 143				75e±003	









Calc. Mass

mDa

ЬБМ

DBE

i-FIT

Formula

334.1809

334.1807

0.2

0.6

11.5

2.4

C22

H24

z

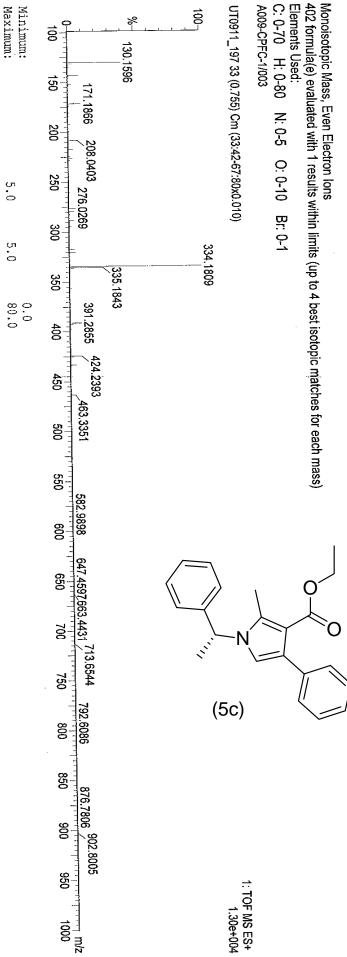
2

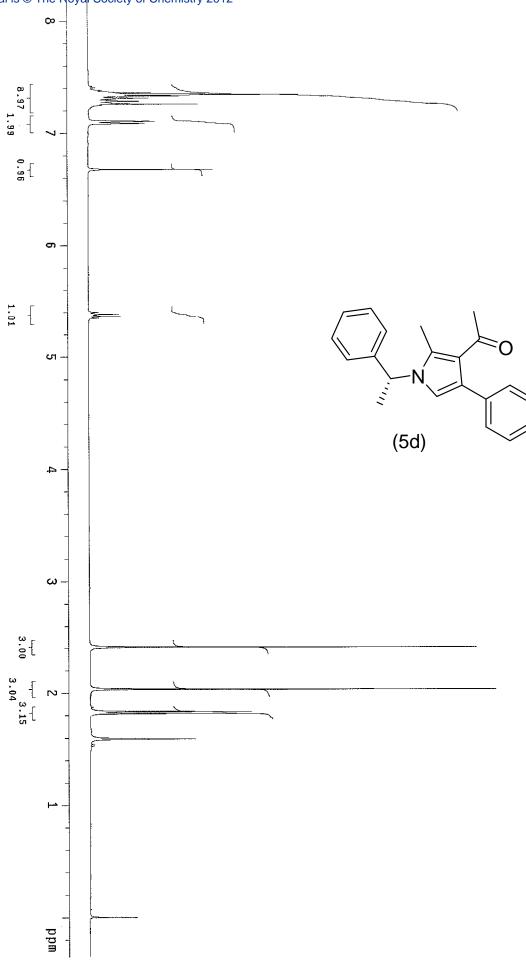
Elemental Composition Report

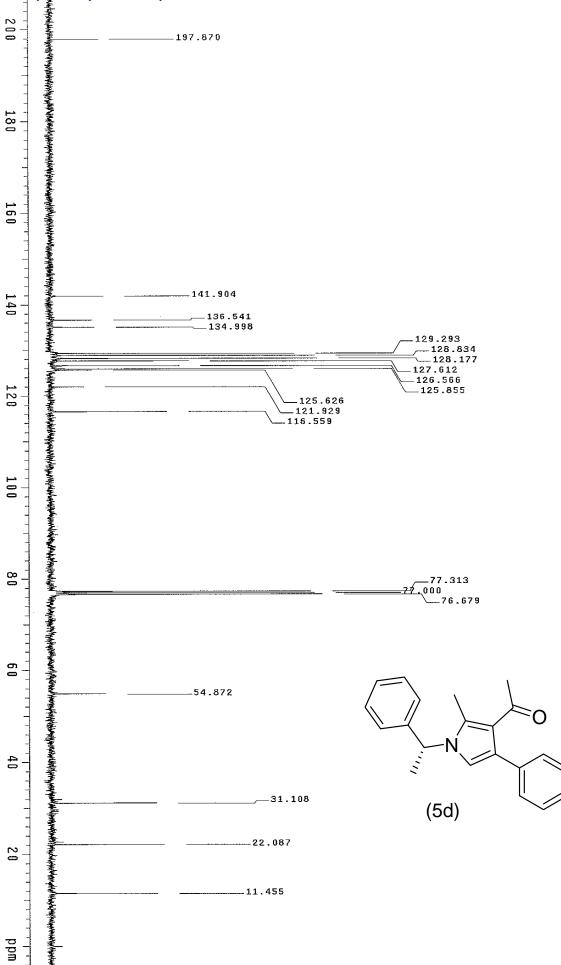
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4







Calc. Mass

mDa

PPM

JBE

304.1694

304.1701

-0.7

-2.3

11.5

ა 5

H22

z 0

Elemental Composition Report

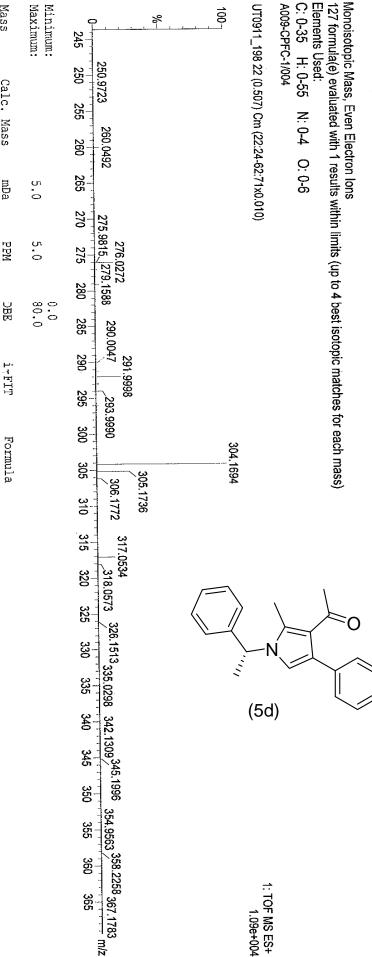
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0

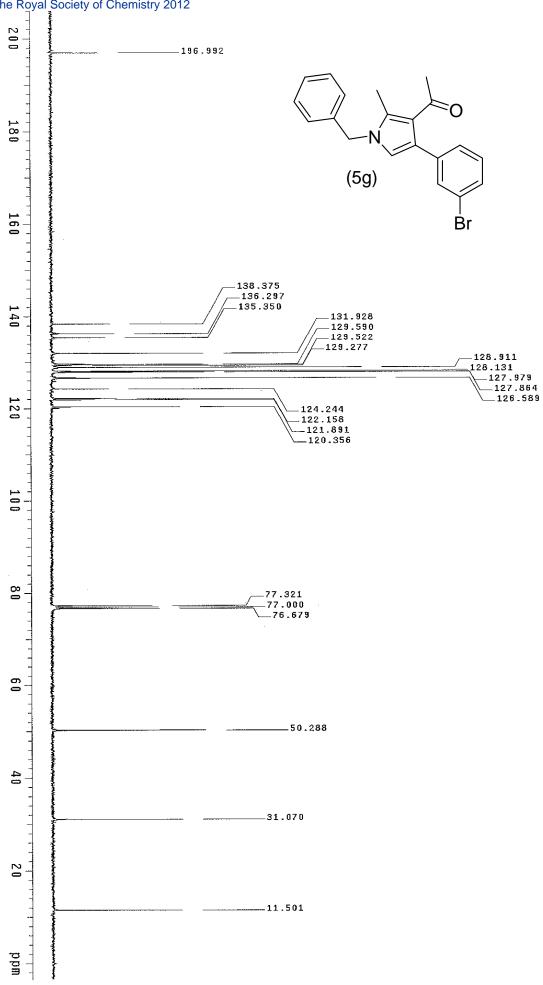
Element prediction: Off

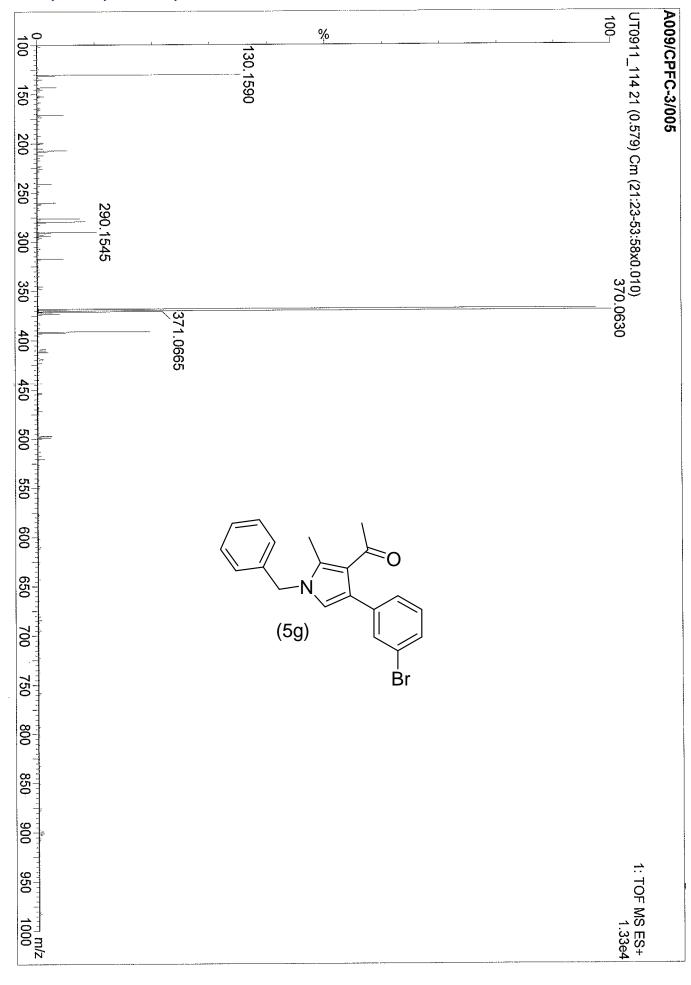
Number of isotope peaks used for i-FIT = 4

Elements Used: C: 0-35 H: 0-55 N: 0-4 O: 0-6









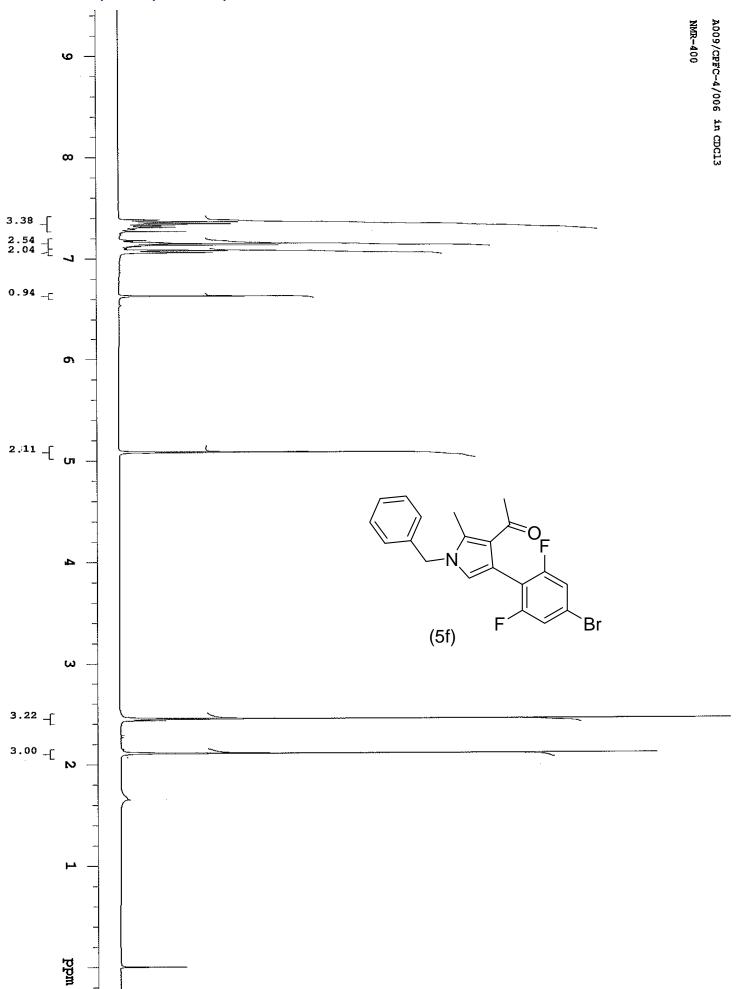
Elemental Composition Report

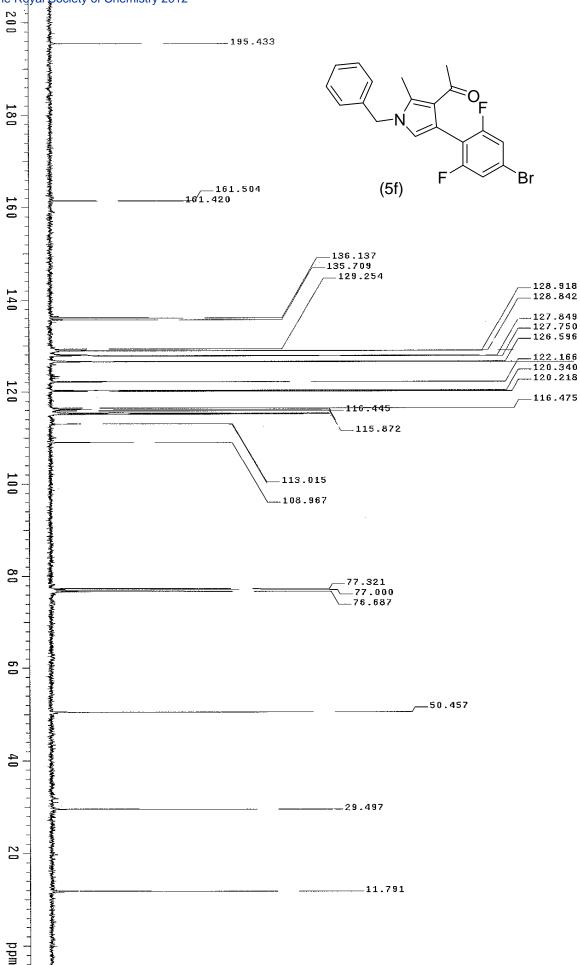
Single Mass Analysis

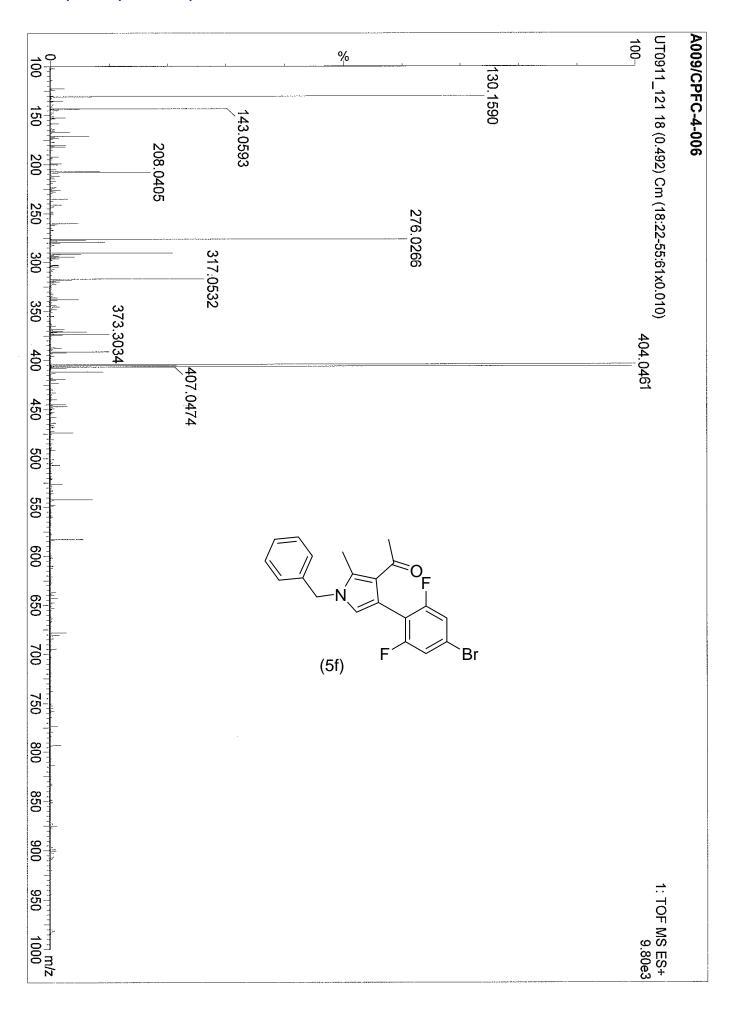
Element prediction: Off Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0

Number of isotope peaks used for i-FIT = 3.

Electronic Supplementary Material (ESI) for RSC Advances This journal is © The Royal Society of Chemistry 2012 Elements Used: 315 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass) Monoisotopic Mass, Even Electron lons UT0911_114 21 (0.579) Cm (21:23-53:58x0.010) ŝ C: 0-50 H: 0-65 A009/CPFC-3/005 331.2149 335.0 368,0650 Calc. Mass 335.1840 N: 0-5 O: 0-4 Br: 0-2 340.0 345.0 345.2707 mDa 5.0 -1.2 348,2715 350.0 5.0 -3.3 PPM 355.0 354.9543 80.0 0.0 11.5 BBE 360.0 367.2086 368.0638_370.0630 365.0 ω A i-FIT 370.0 371.0665 373,3047 8 Formula 375.0 H19 382.0793.384.0787 380.0 \mathbf{z} 0 385.0 路 390.0 391.2845 392,2869 (5g) 395.0 Br 400.0 398.9580 405.0 409.0920 412.0022 410.0 415.0 419.3098 420.0 1: TOF MS ES+ 1.33e+004 423,1993







404.0461

404.0462

-0.1

-0.2

11.5

ω.

C20

H17

z

0

Ŧ2 ᄧ

425.0

430.0

435.0

440.0

445.0

450.0

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0

Element prediction: Off

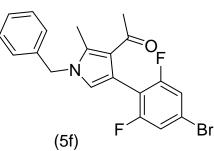
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron lons 390 formula(e) evaluated with 2 results within limits (up to 4 best isotopic matches for each mass)

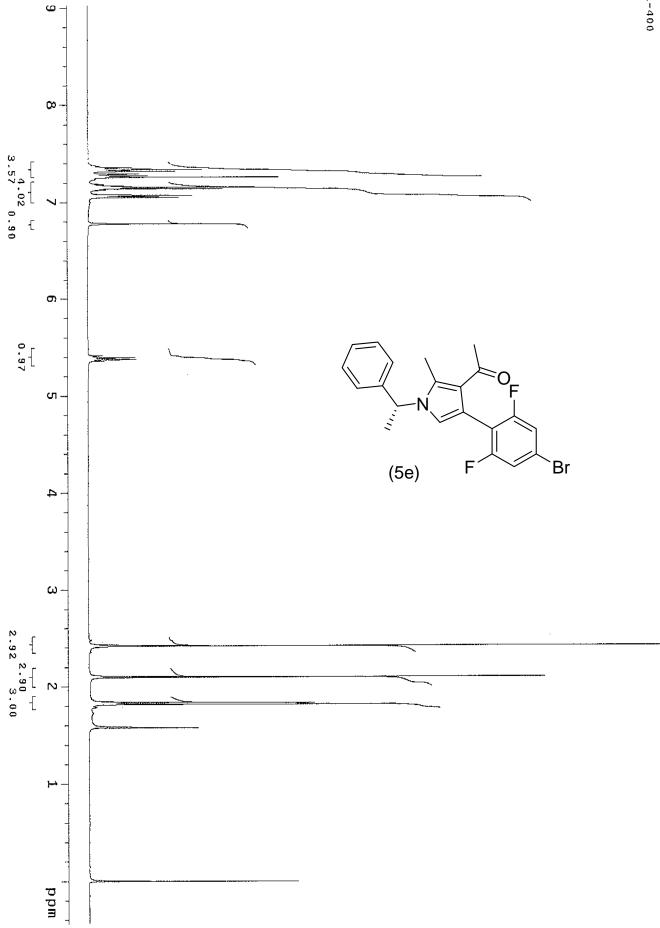
Elements Used:

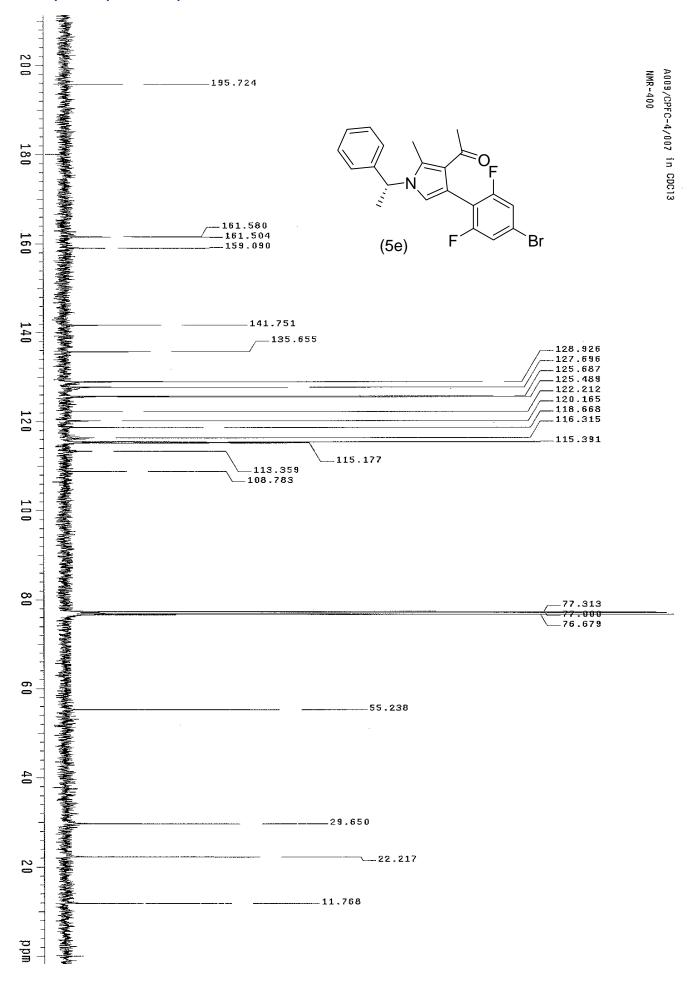
C: 0-50 H: 0-65 N: 0-2 O: 0-4 F: 0-2 Br: 0-1

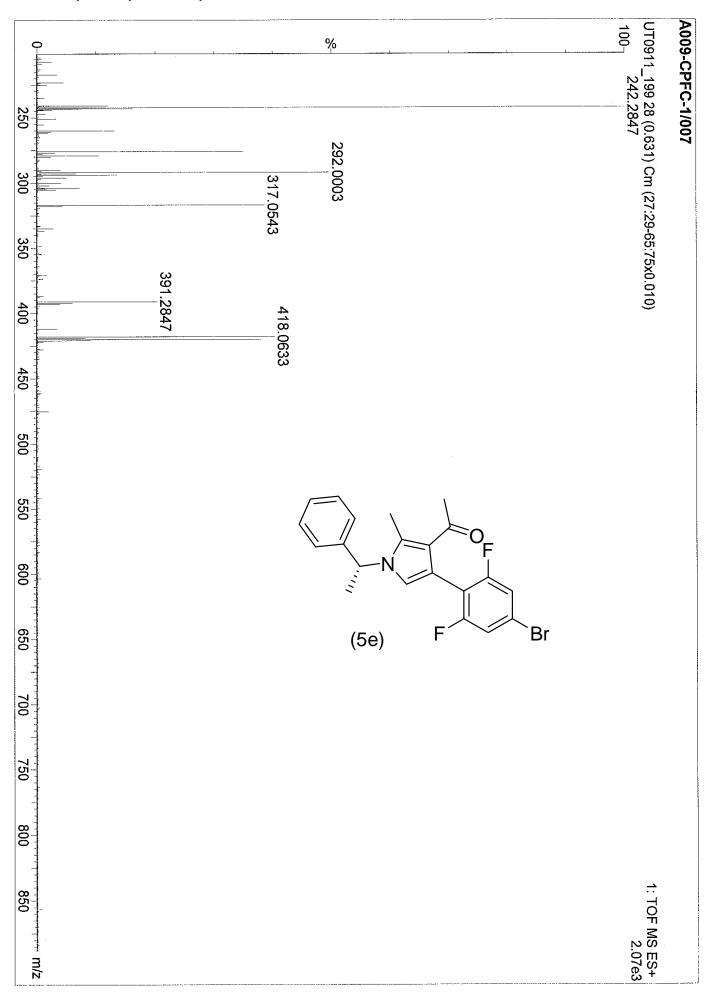
Mass Maximum: Minimum: UT0911_121 18 (0.492) Cm (18:22-55:61x0.010) 8 A009/CPFC-4-006 % 373.3034 375.0 Calc. 377.9114 380.0 Mass 385.0 387.9431 mDa 5.0 390.0 391.2838 PPM 5.0 395.0 396.0274 0.0 DBE 400.0 403.2896 404.0461,406.0443 i-FIT 405.0 407.0474 410.0 412.0002 Formula 415.0 419.3091 420.0



423.2032 432,9466 439.8624 445.0721447.0717 452.9034454.3470_{m/z} 1: TOF MS ES+ 9.80e+003







Calc. Mass

mDa

PPM

DBE

i-FIT

Formula

418.0633

418.0618

1.5

ა. 6

2 3

C21

H19

z 0

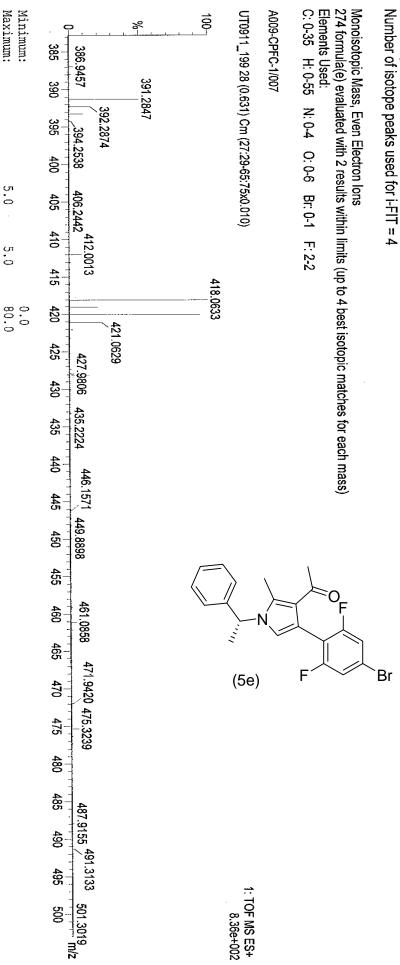
Вг

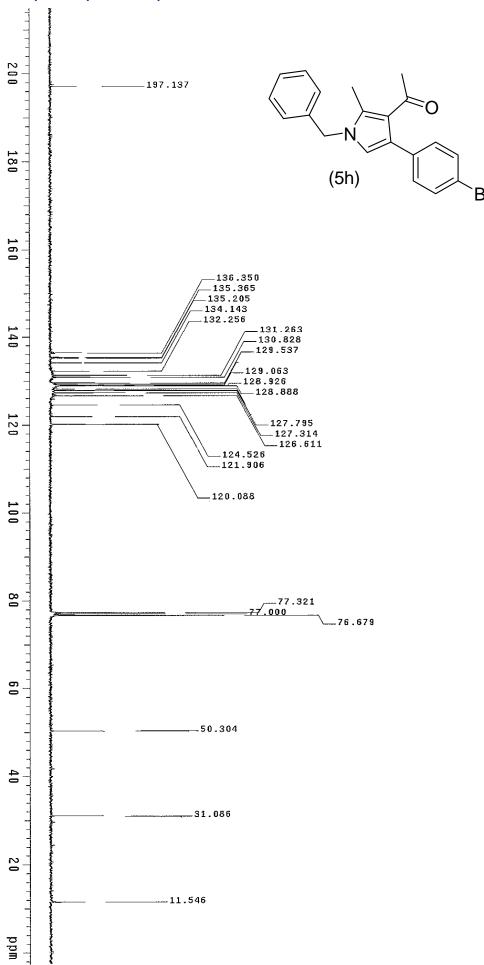
F2

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0

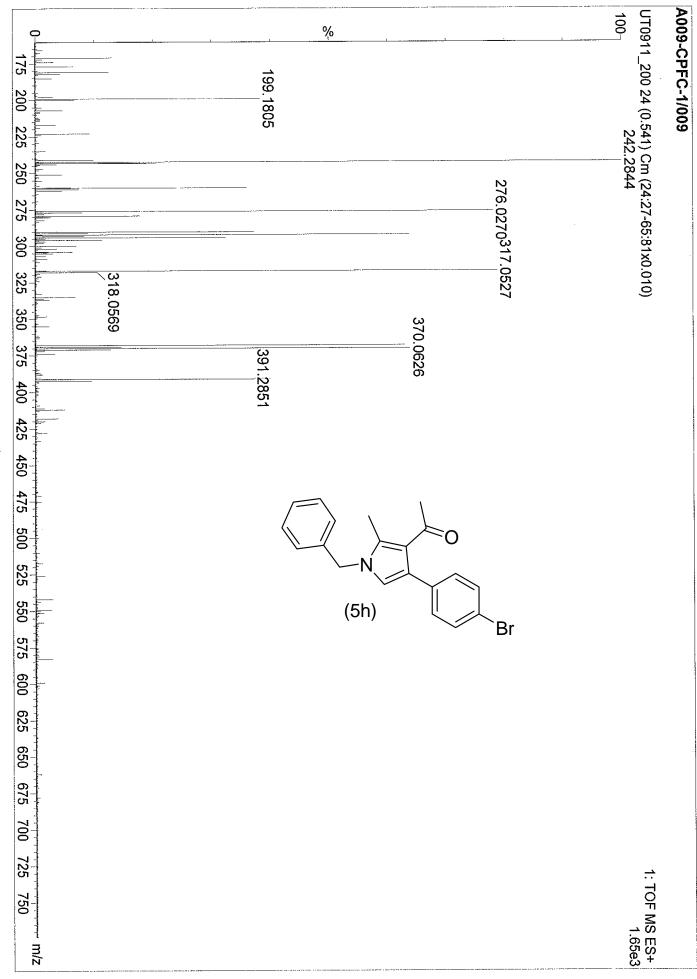
Element prediction: Off





NMR-400

A009-CPFC-4-009 in CDC13



Calc. Mass

mDa

PPM

DBE

i-FIT

Formula

Maximum:

370.0626

370.0650

-0.3

-0.8

11.5

1.4

C20

H19

z 0

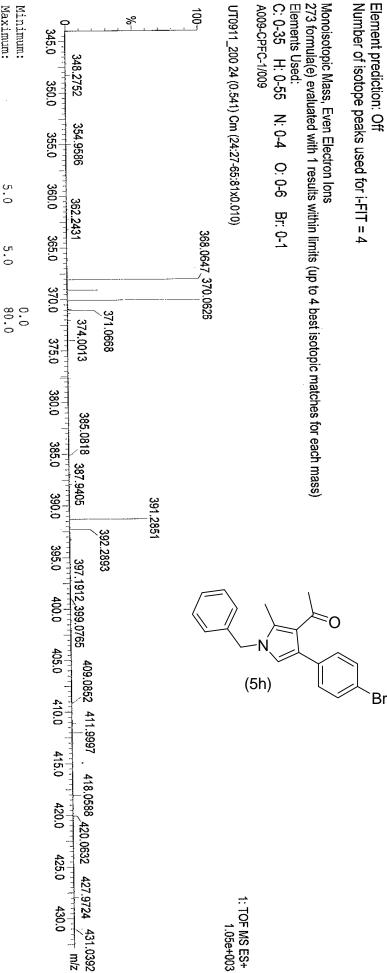
8

Elemental Composition Report

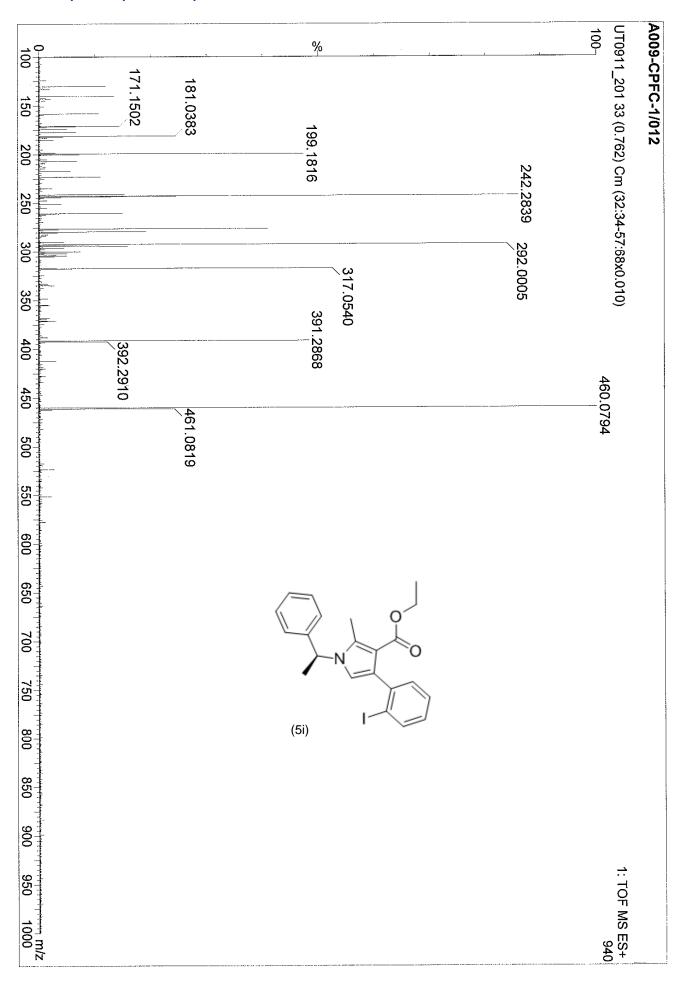
Single Mass Analysis
Tolerance = 5.0 PPM /

Element prediction: Off DBE: min = 0.0, max = 80.0

C: 0-35 H: 0-55 UT0911_200 24 (0.541) Cm (24:27-65:81x0.010) A009-CPFC-1/009 N: 0-4 O: 0-6 Br: 0-1



A009-CPFC-2-012 in CDC13 NMR-400



Н

650

8

750

800

90

950

734.4391

763.5085

835,7822 883,7720 850

969.6360

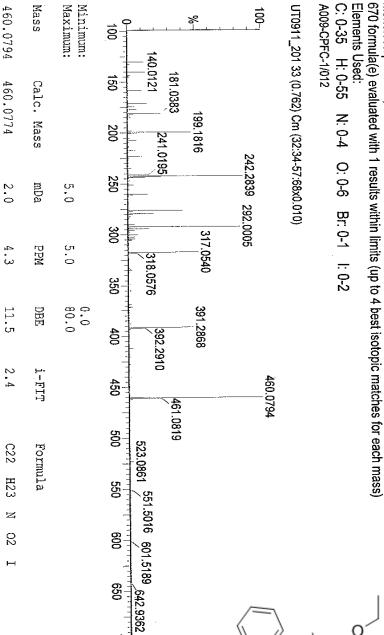
(5i)

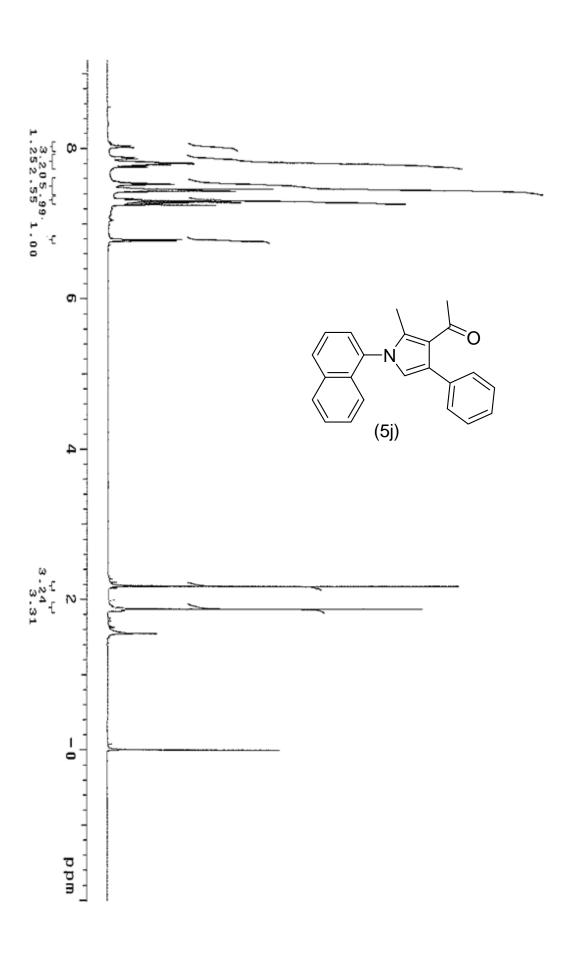
1: TOF MS ES+ 9.40e+002

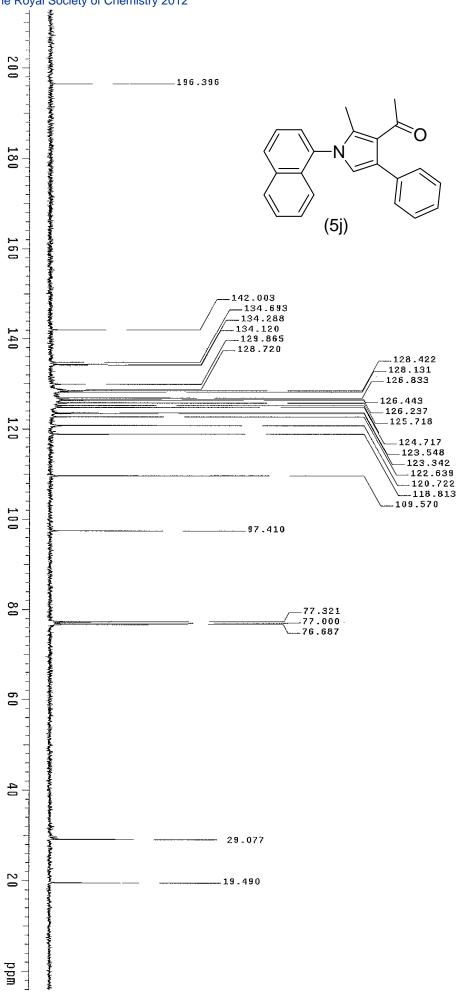
Elemental Composition Report

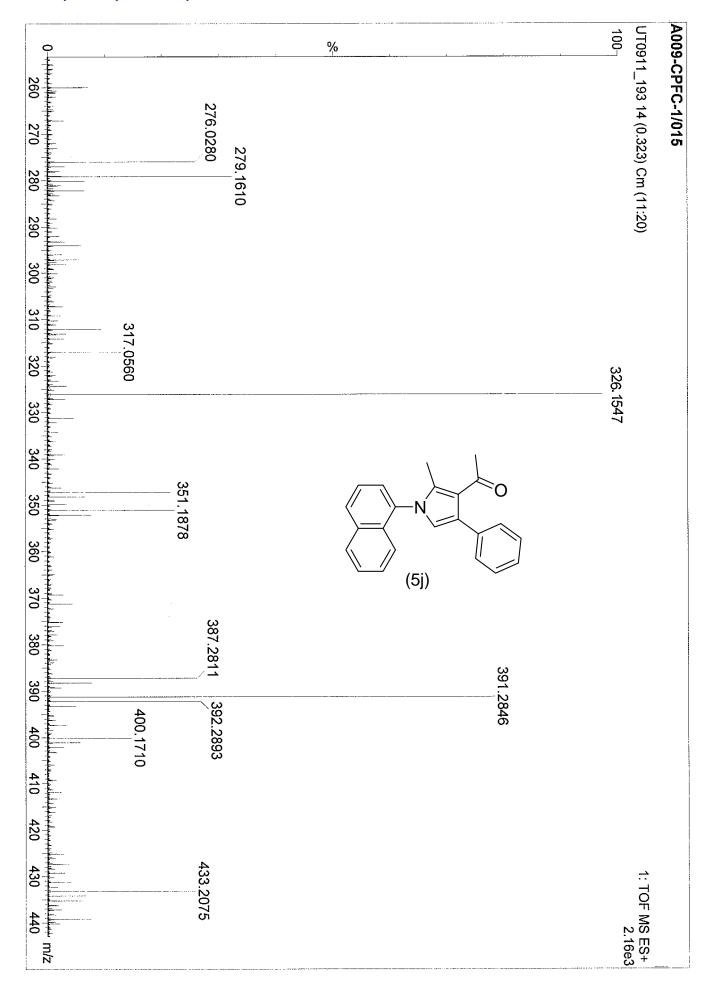
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0

Elements Used: Monoisotopic Mass, Even Electron Ions Number of isotope peaks used for i-FIT = 4 Element prediction: Off









Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron lons 223 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Mass Minimum: Elements Used: Maximum: UT0911_193 14 (0.323) Cm (11:20) C: 0-70 H: 0-80 326.1547 9 A009-CPFC-1/015 * 300.0 300.1126 326.1545 Calc. Mass 305.0 N: 0-5 O: 0-10 307.2213 310.0 0.2 mDa 5.0 312,1399 313.1442 315.0 0.6 5.0 PPM317.0560 318.0544 14.5 0.0 BE 320.0 324,2910 9.1 i-FIT 325.0 326,1547 327.2184 C23 Formula 330.0 331.2156 H20 334,2519 z 335.0 0 339,0980 340.0 (5j)

346.2823

352.2674

352.1921

347.2497

351.1878

1: TOF MS ES+ 4.83e+002

345.0

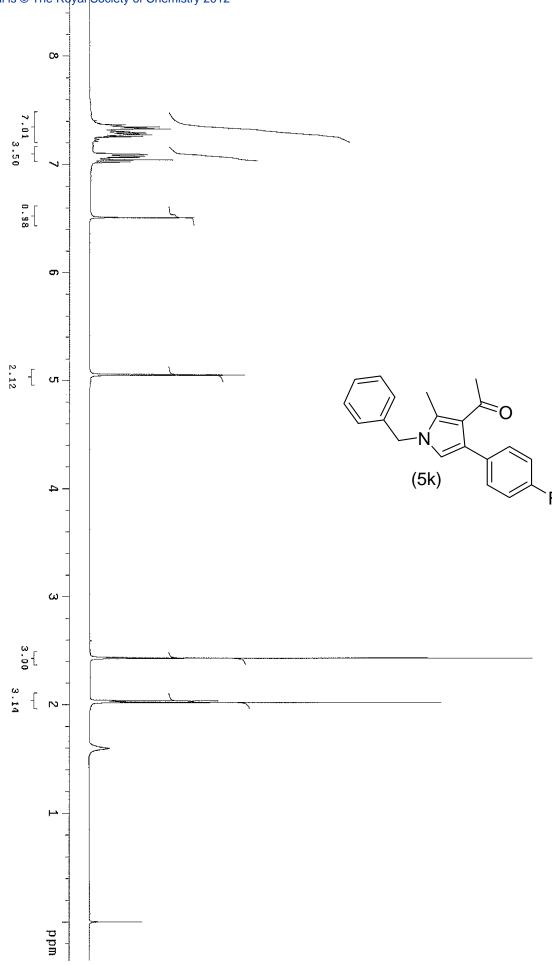
350.0

355.0

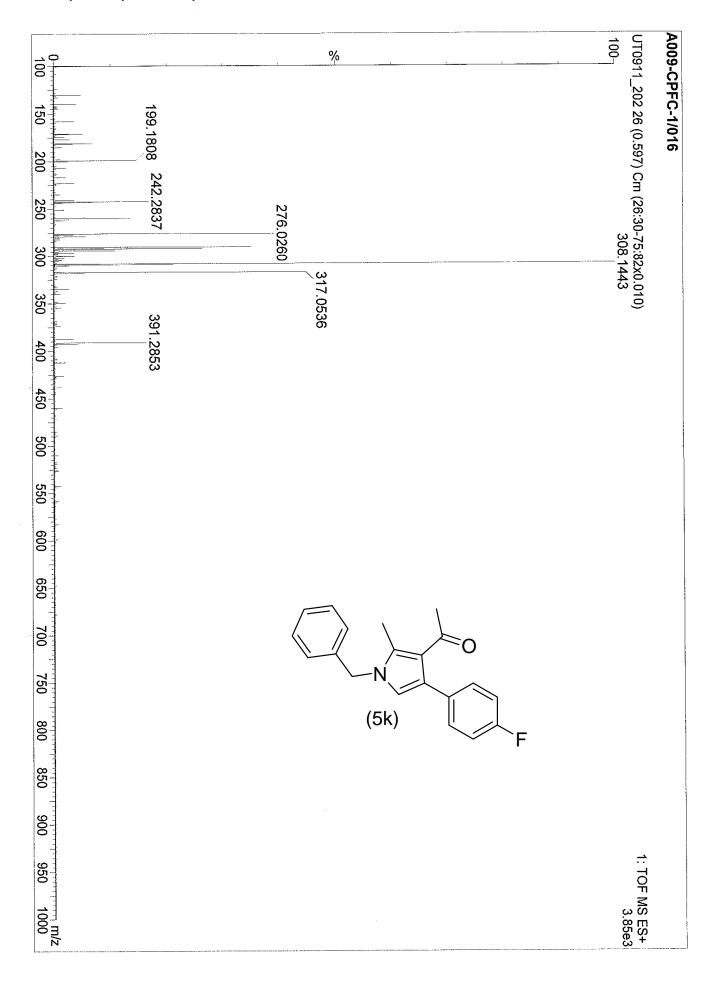
360.0

361.1698

m/z



A009-CPFC-1-016 in CDC13



Elemental Composition Report

Single Mass Analysis

Element prediction: Off Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0

Number of isotope peaks used for i-FIT = 4

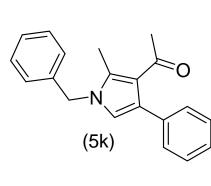
Monoisotopic Mass, Even Electron lons

Elements Used: 249 formula(e) evaluated with 2 results within limits (up to 4 best isotopic matches for each mass)

C: 0-35 H: 0-55 N: 0-4 O: 0-6 F: 0-1

UT0911_202 26 (0.597) Cm (26:30-75:82x0.010) A009-CPFC-1/016

100			308.1443		
<u> </u>		276.0260	317.0536		
> ·	199,1808 242,2837	42.2837	318.0556	391.2853 _392.2849	2849 4
100	150 200	250	300 350	400	450
Minimum: Maximum:		5.0	5.0	0.0	
Mass	Calc. Mass	mDa	Mdd	DBE	i-FIT
308.1443	308.1451	-0.8	-2.6	11.5	ა დ



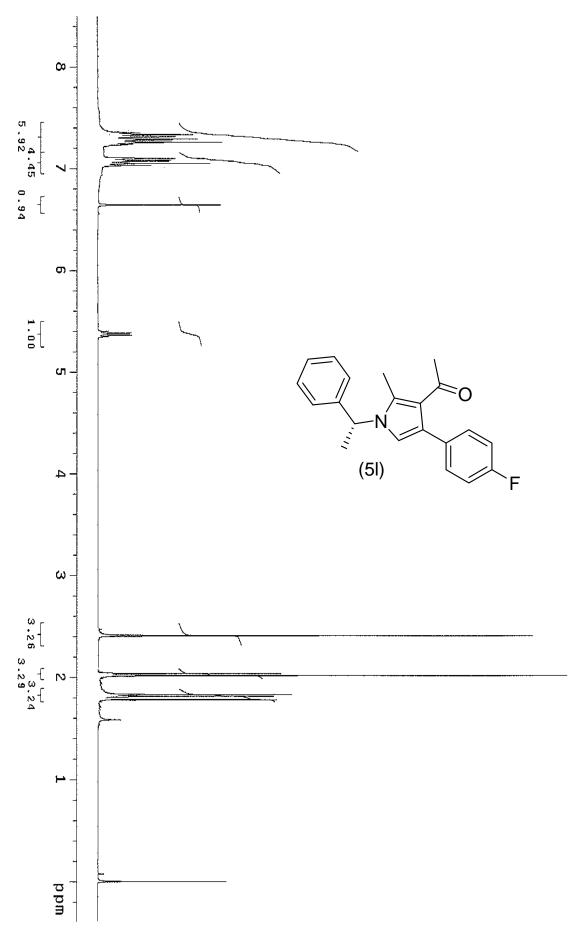
C20

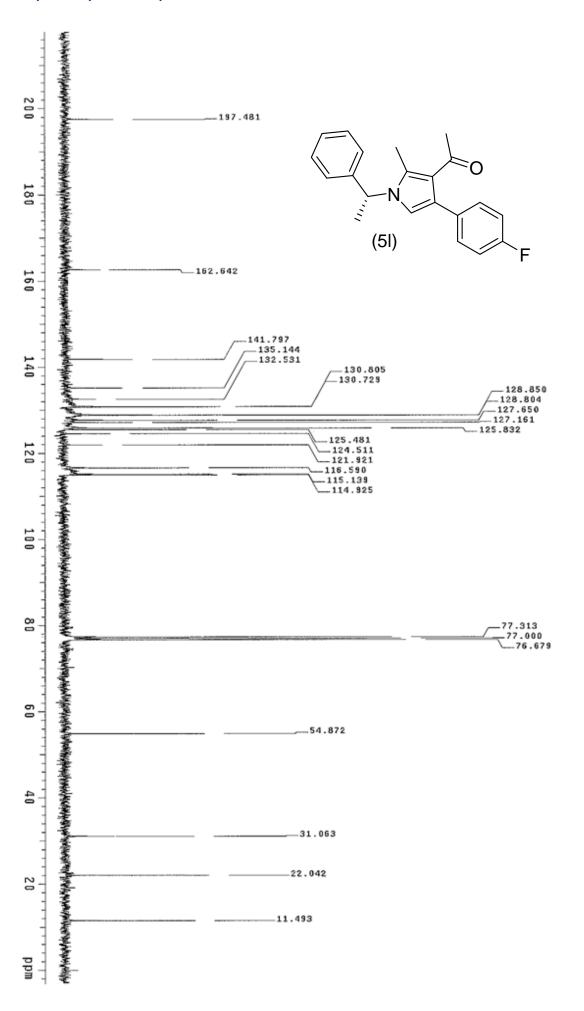
H19

z 0

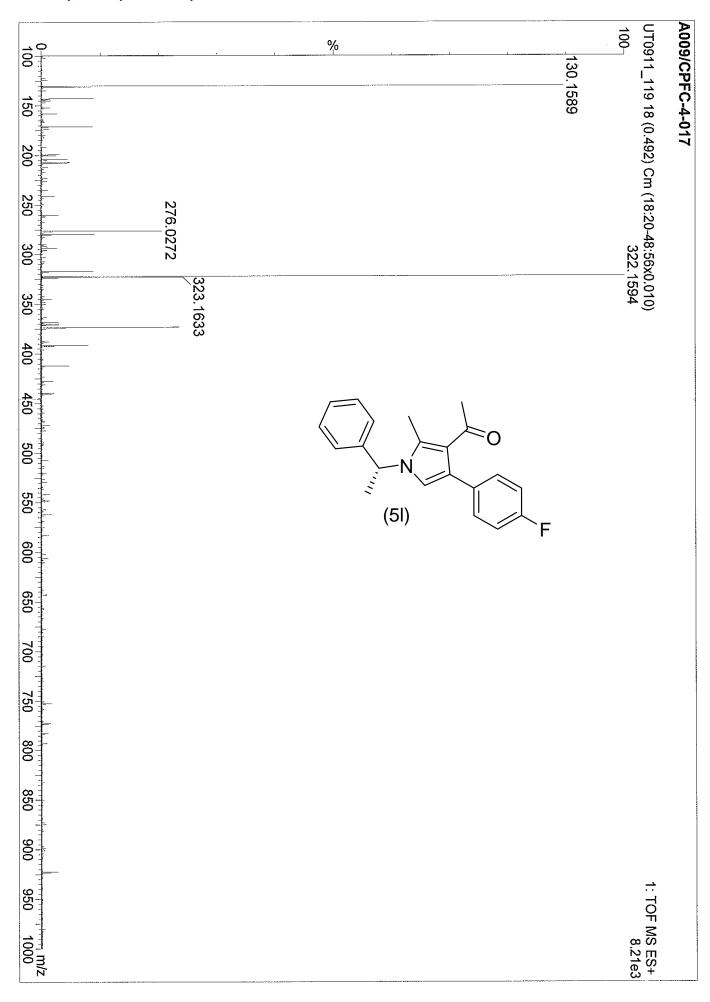
щ

1: TOF MS ES+ 3.85e+003





A009-CPFC-1-017 in CDC13



Mass

Calc. Mass

mDa

PPM

DBE

i-EIT

Formula

322,1594

322.1607

-1.3

-4.0

11.5

0. ნ

C21

H21

и 0

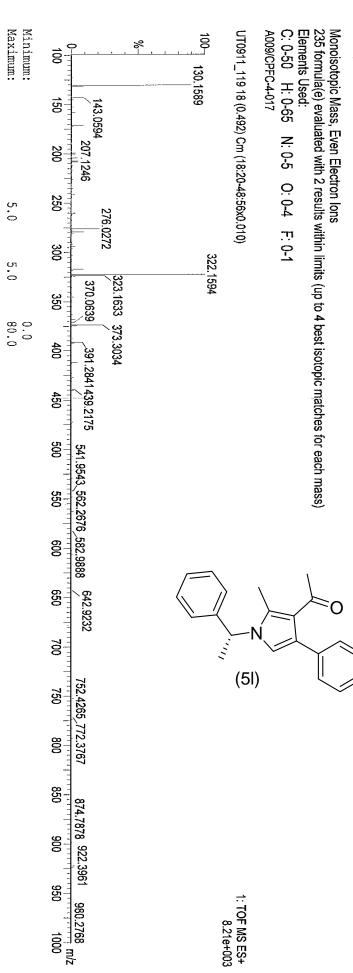
퍼

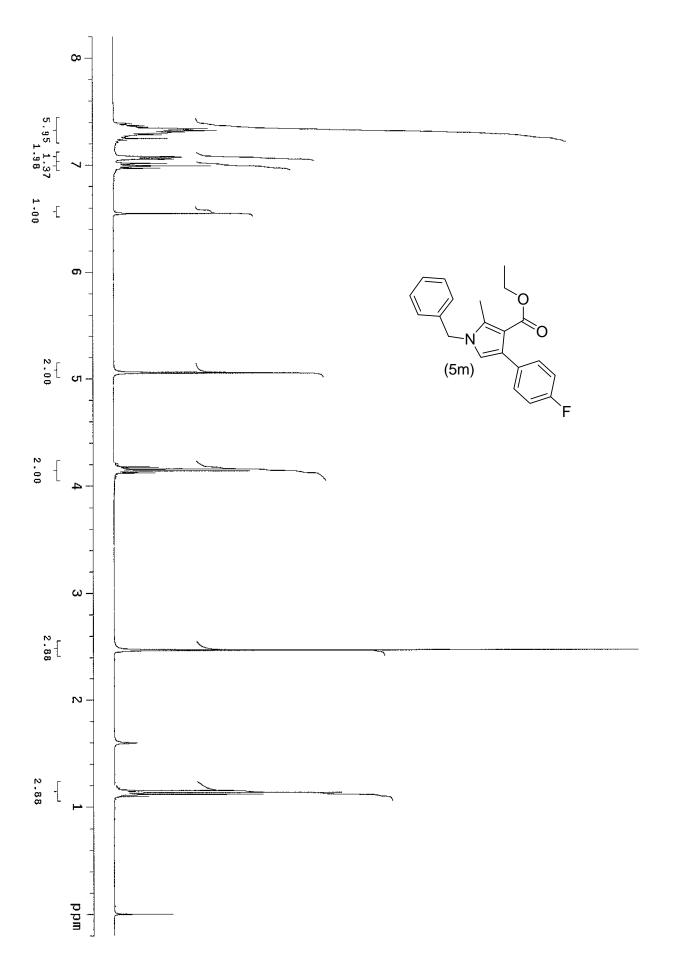
Elemental Composition Report

Single Mass Analysis

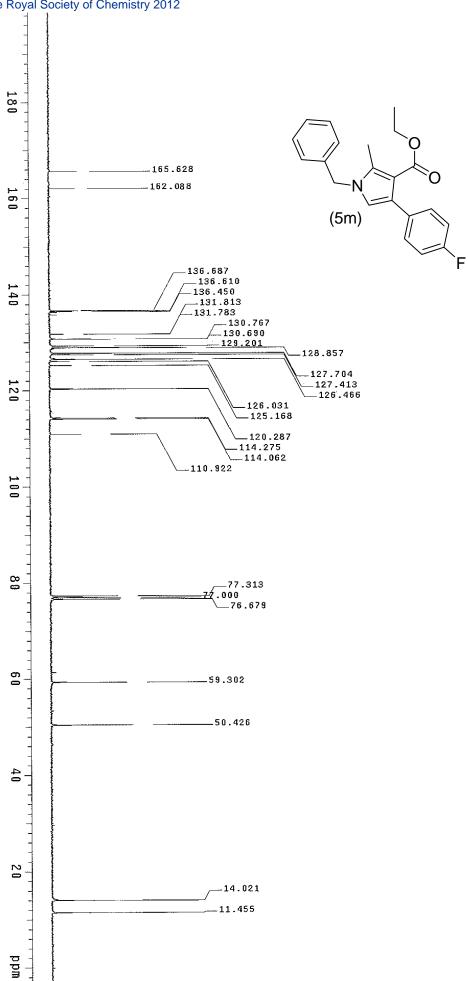
Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0 Element prediction: Off

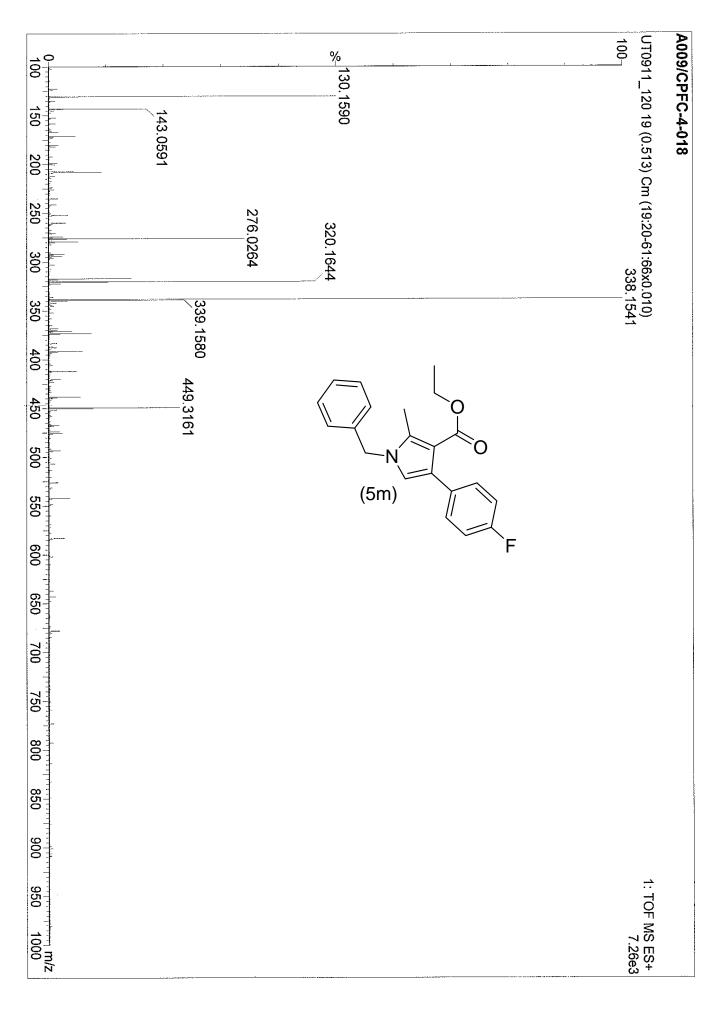
Number of isotope peaks used for i-FIT = 3











Mass

Calc.

Mass

mDa

PPM

i-FIT

Formula

5.0

5.0

338.1541

338.1556

-1.5

-4.4

11.5

0.9

C21

H21

z

2

ᅿ

Minimum:

8

Maximum:

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0 Element prediction: Off

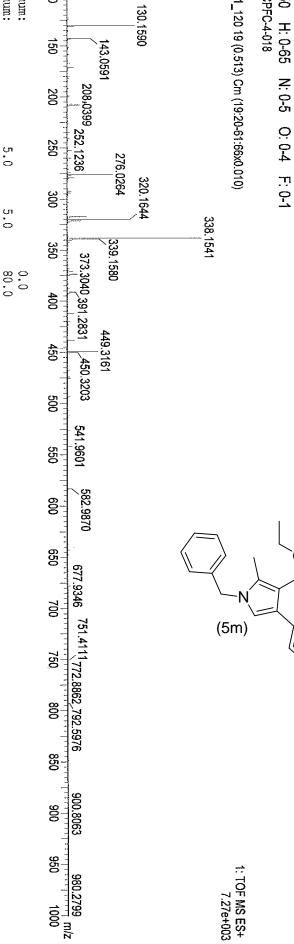
Monoisotopic Mass, Even Electron Ions Number of isotope peaks used for i-FIT = 3

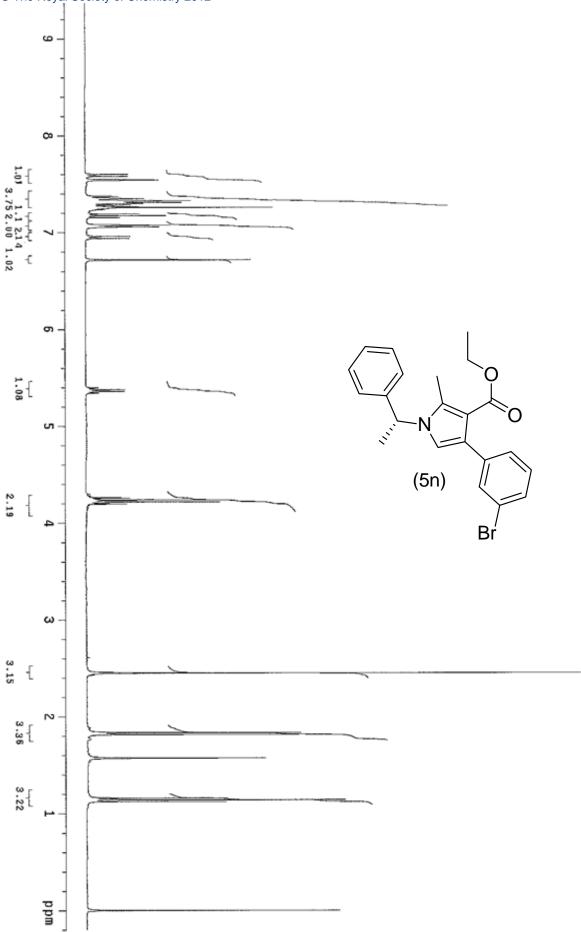
Elements Used: 246 formula(e) evaluated with 2 results within limits (up to 4 best isotopic matches for each mass)

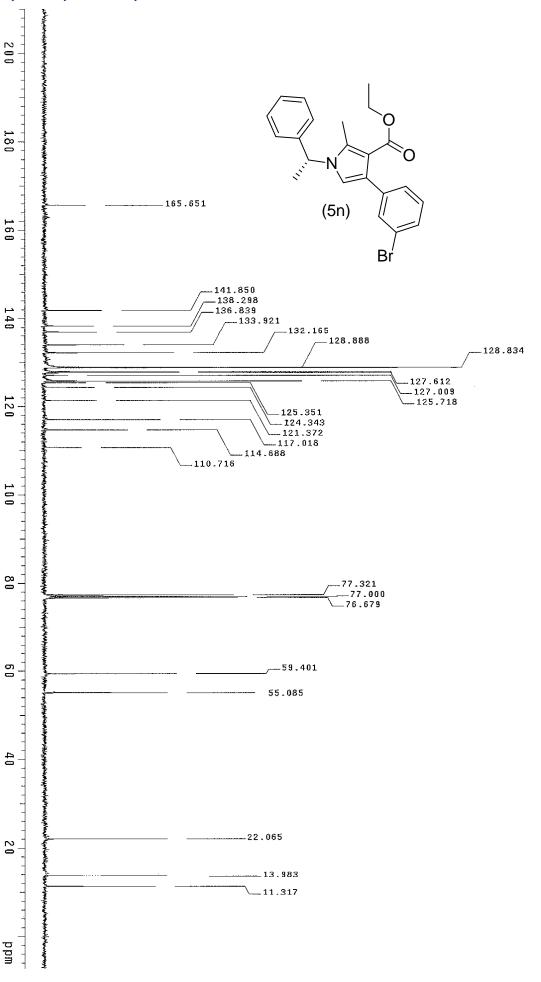
A009/CPFC-4-018 C: 0-50 H: 0-65 UT0911_120 19 (0.513) Cm (19:20-61:66x0.010)

8

*

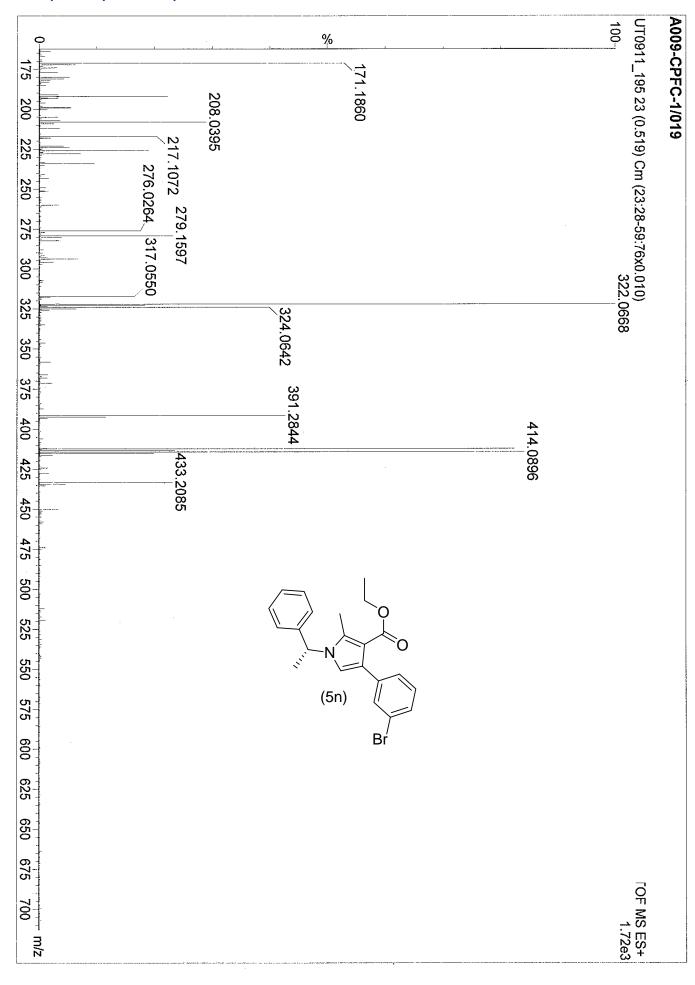






A009/CPFC-3/019 in CDC13

NMR-400



8

540

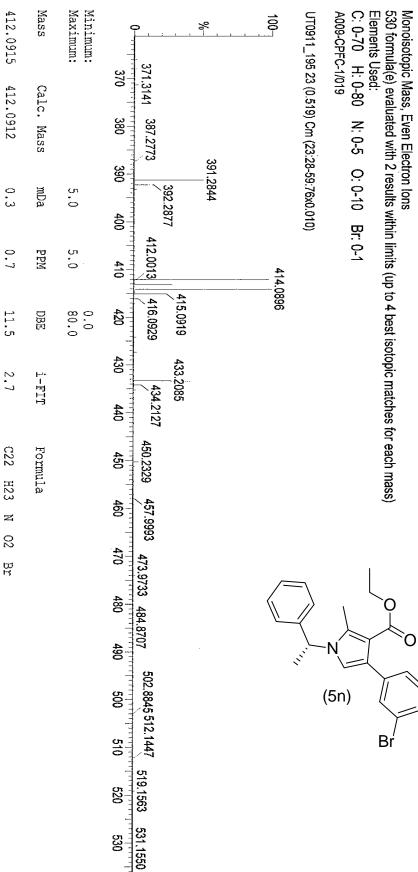
Elemental Composition Report

Single Mass Analysis

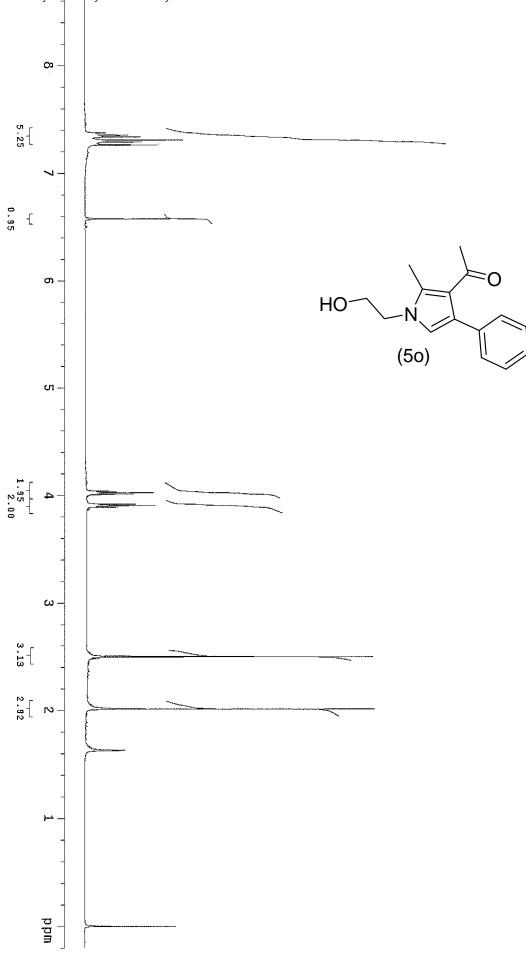
Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0

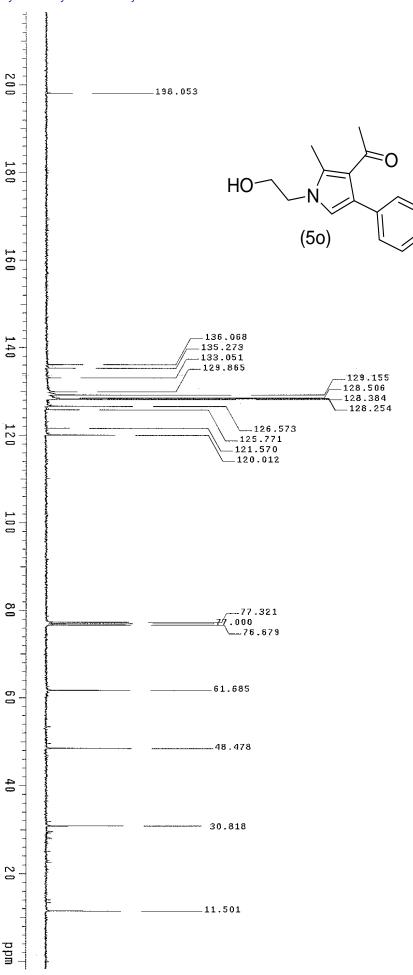
Element prediction: Off

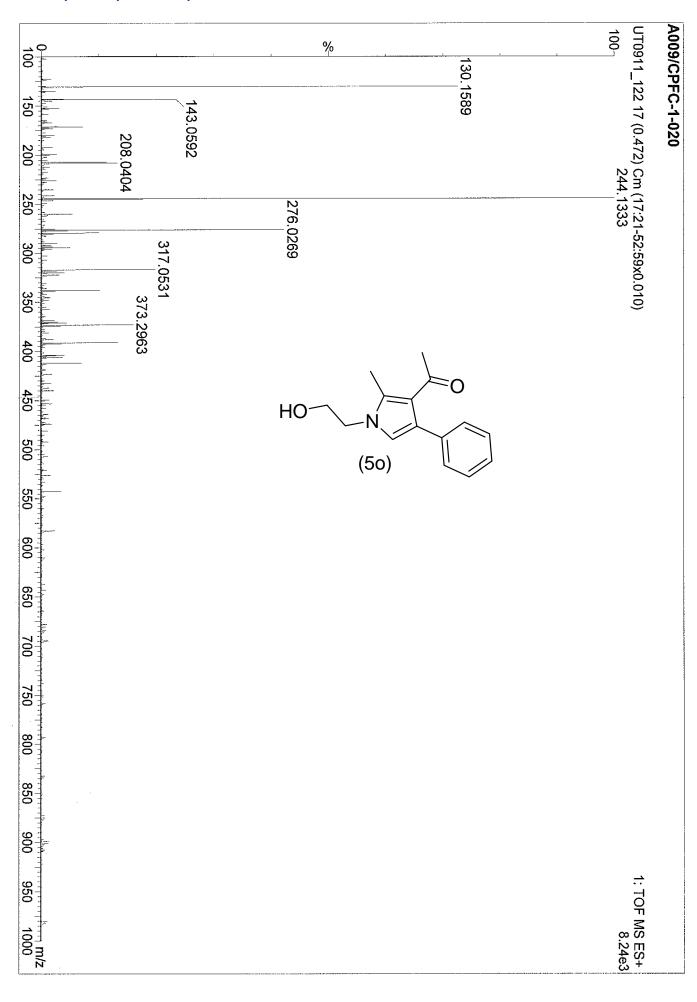
Number of isotope peaks used for i-FIT = 4



1: TOF MS ES+ 1.45e+003







Elemental Composition Report

Single Mass Analysis

Element prediction: Off Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0

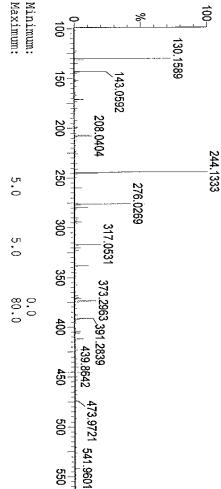
Number of isotope peaks used for i-FIT = 3

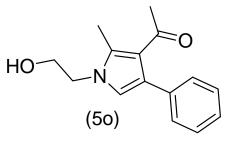
213 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass) Monoisotopic Mass, Even Electron lons

C: 0-50 H: 0-65 N: 0-2 O: 0-4 F: 0-2 Br: 0-1 Elements Used:

A009/CPFC-1-020

UT0911_122 17 (0.472) Cm (17:21-52:59x0.010)





1: TOF MS ES+ 8.24e+003

244.1338 Calc. Mass mDa -0.5 -2.0PPM 7.5 踞 i-FIT C15Formula H18 z 8

500

55

60

650

70

750

8

850

900

950

980.2875

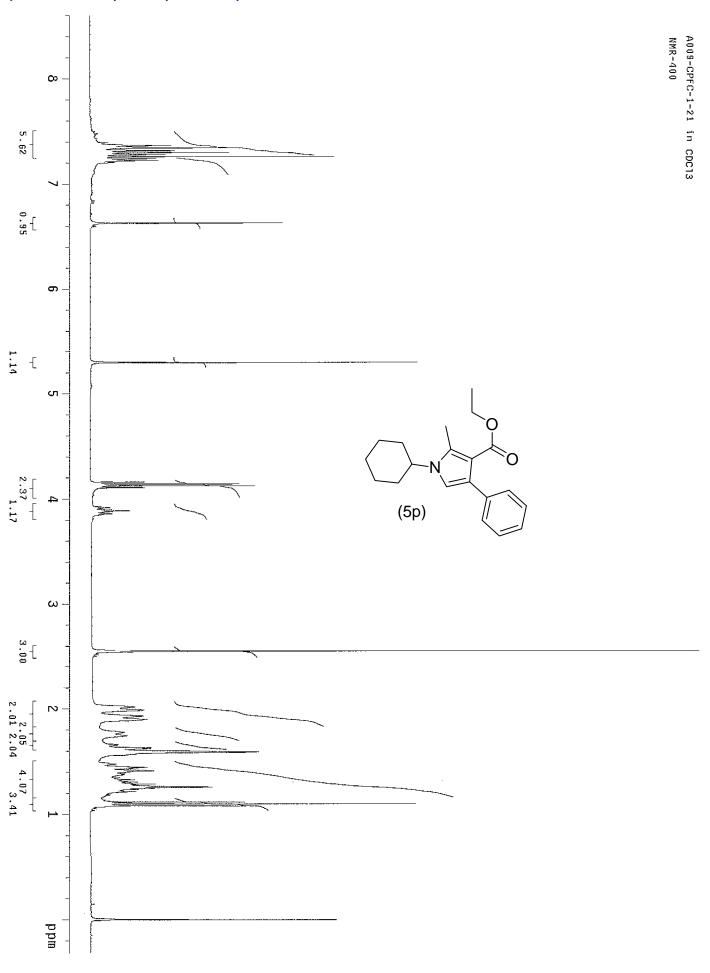
582.9906

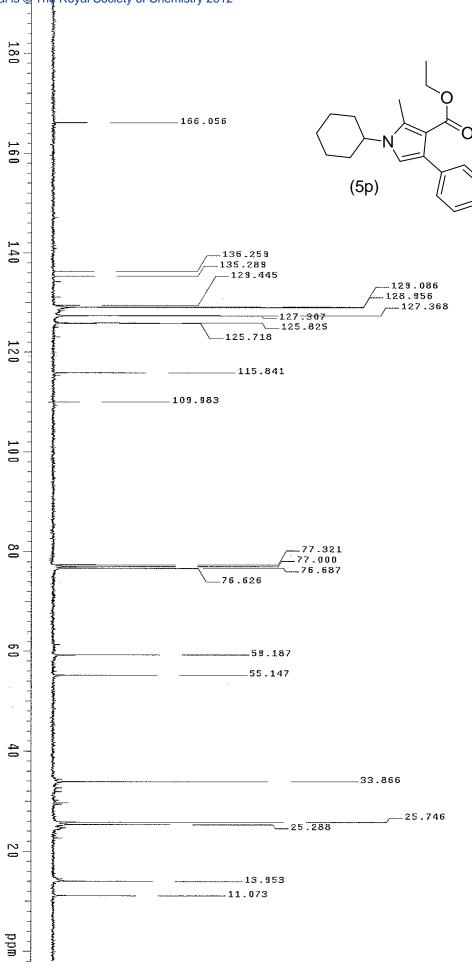
677.9393694.6121758.2247

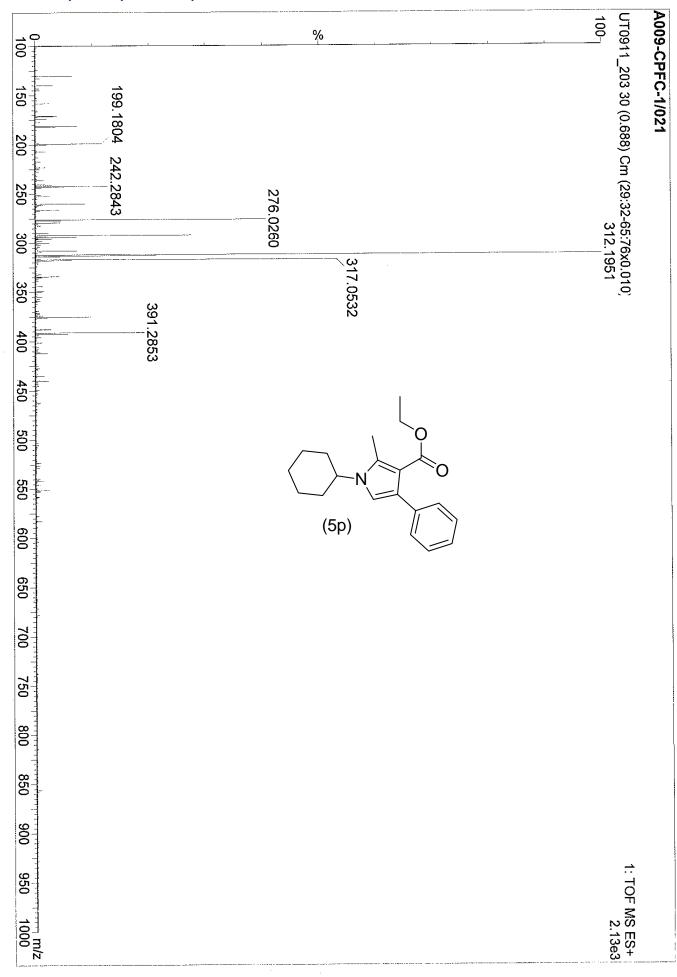
874.7864 898.7846

Mass

244.1333







Mass

Calc. Mass

mDa

PPM

DBE

i-FIT

Formula

5.0

5·0

Maximum:

312,1951

312.1964

-4.2

œ 5

C20

H26

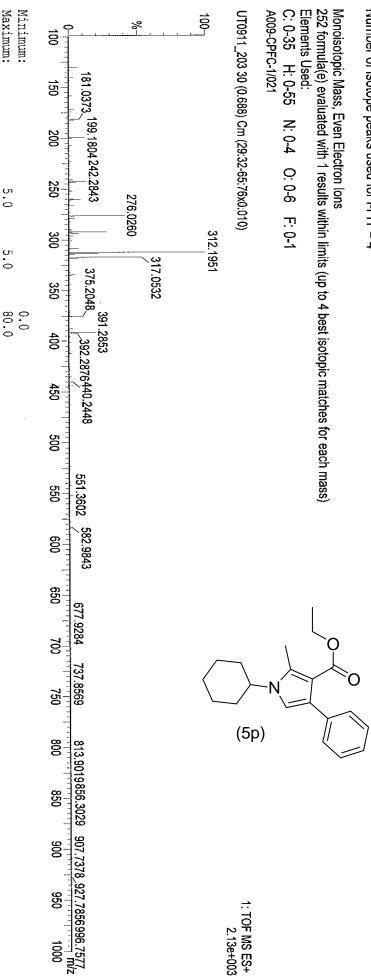
z 2

Elemental Composition Report

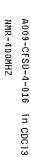
Single Mass Analysis

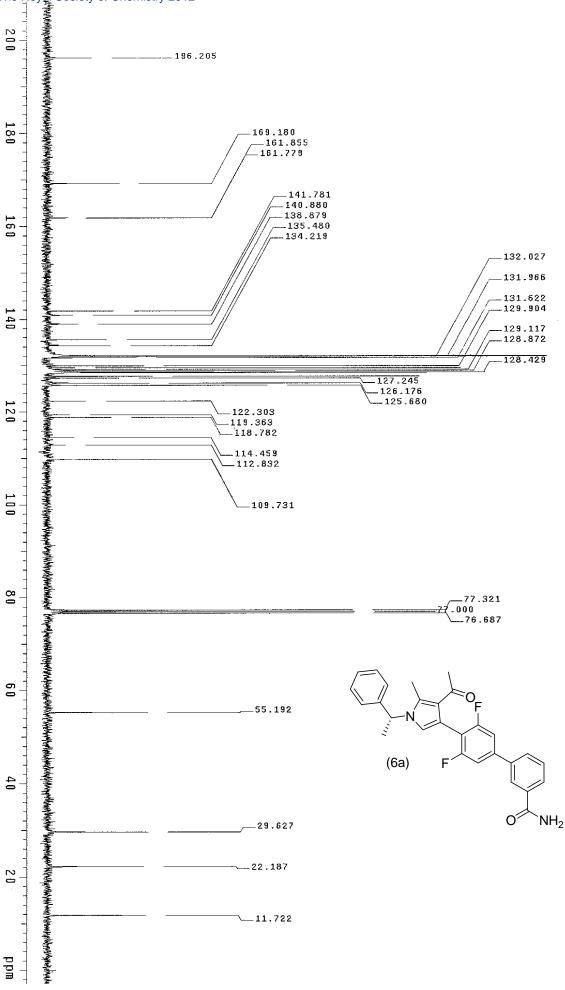
Element prediction: Off Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0

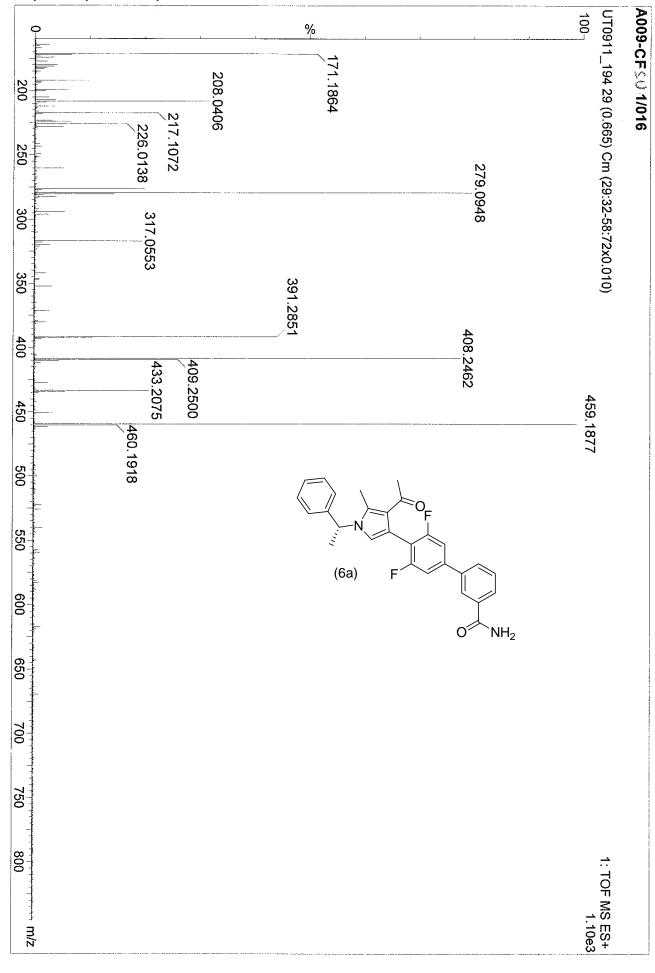
Number of isotope peaks used for i-FIT = 4



udd







459.1884

-0.7

-1.5

16.5

1.8

C28

H25

N2

02

E2

Calc.

Mass

mDa

PPM

DBE

i-FIT

Formula

5. O

5.0

80.0 0.0

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

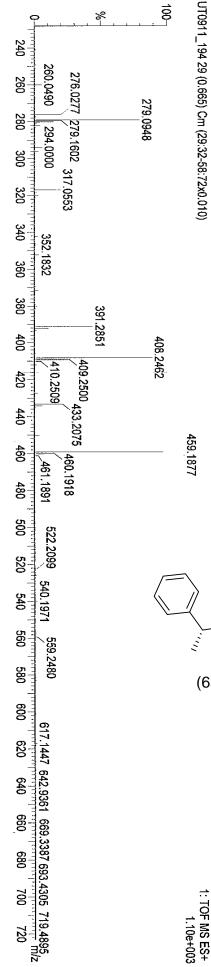
Monoisotopic Mass, Even Electron Ions

296 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

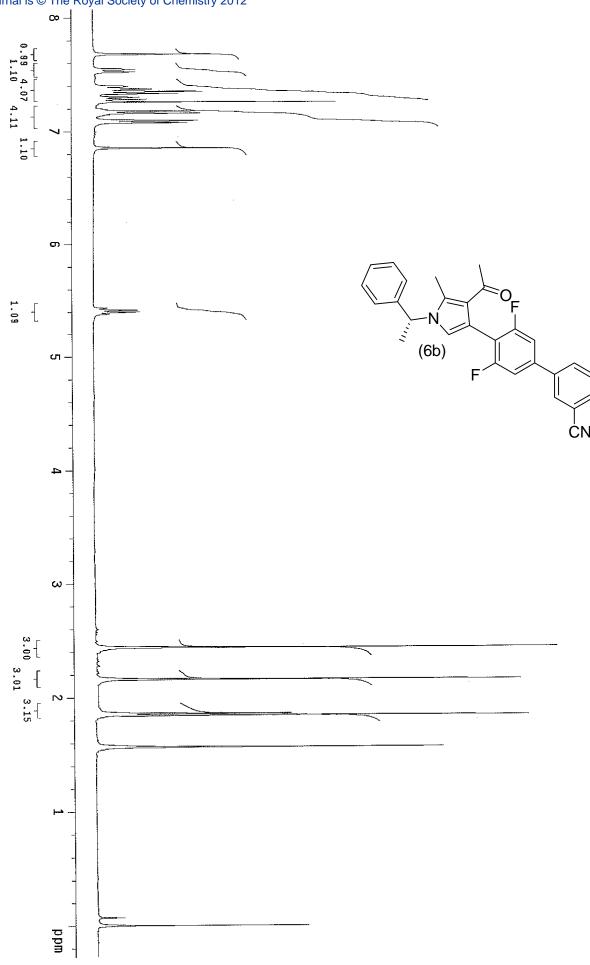
Elements Used: C: 0-70 H: 0-80 N: 0-5 O: 0-10 F: 2-2

A009-CFSu-1/016

UT0911_194 29 (0.665) Cm (29:32-58:72x0.010)

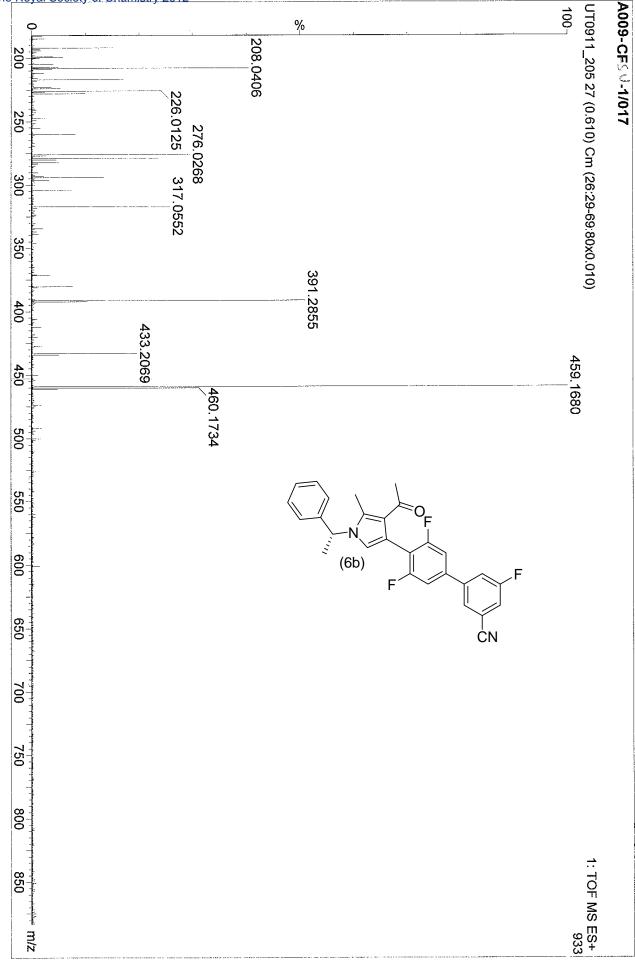


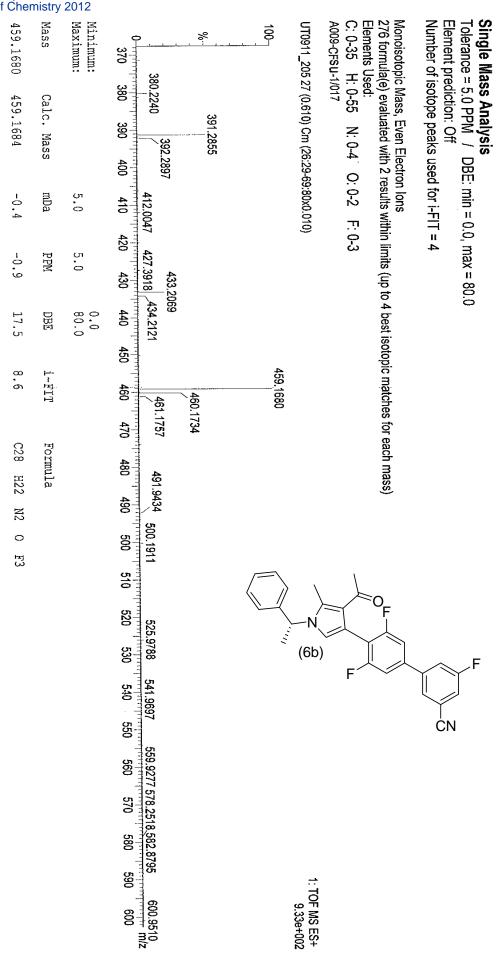


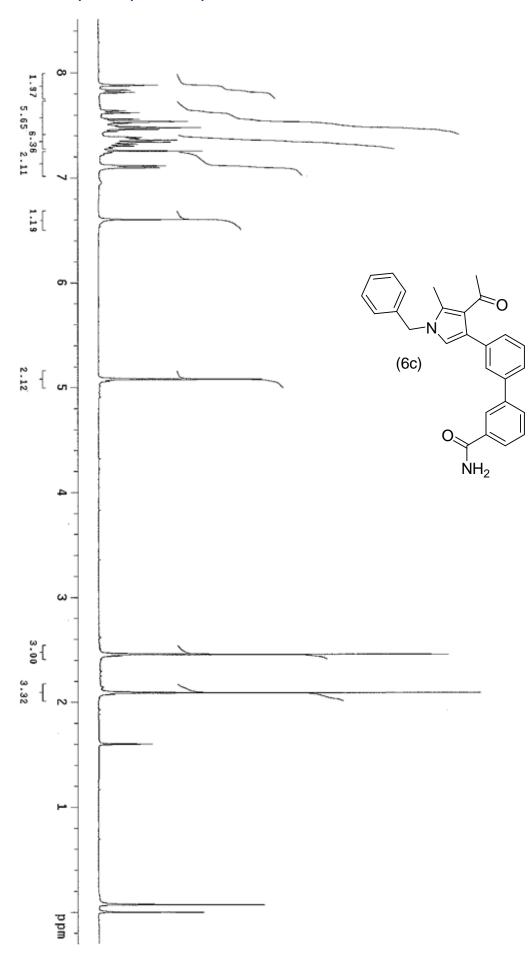


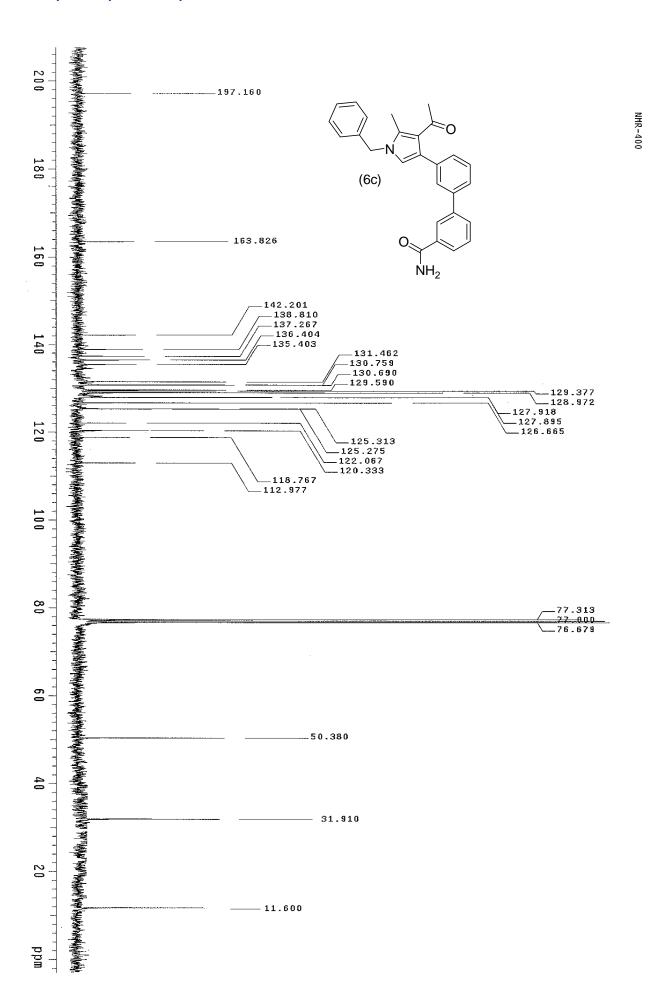
A009-CFSU-3-017 in CDC13

NMR-400

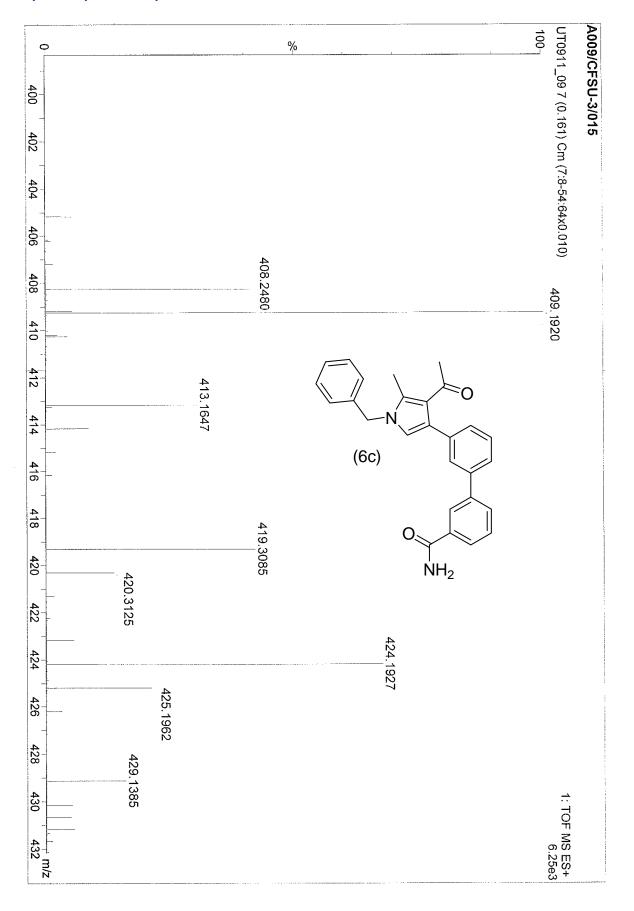








A009-CFSU-3-015 in CDC13



Single Mass Analysis

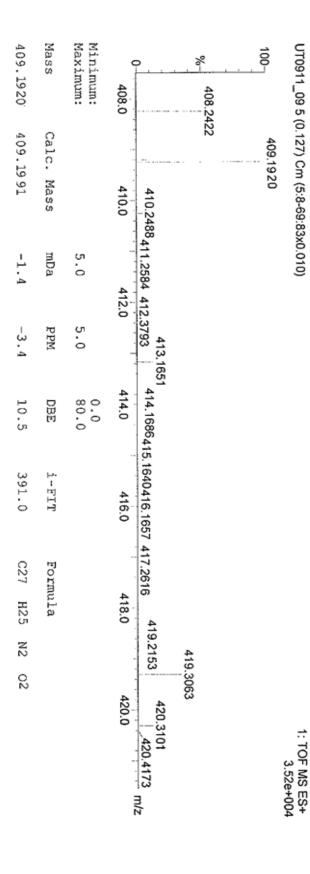
Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0

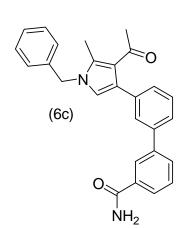
Element prediction: Off

Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron lons 120 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

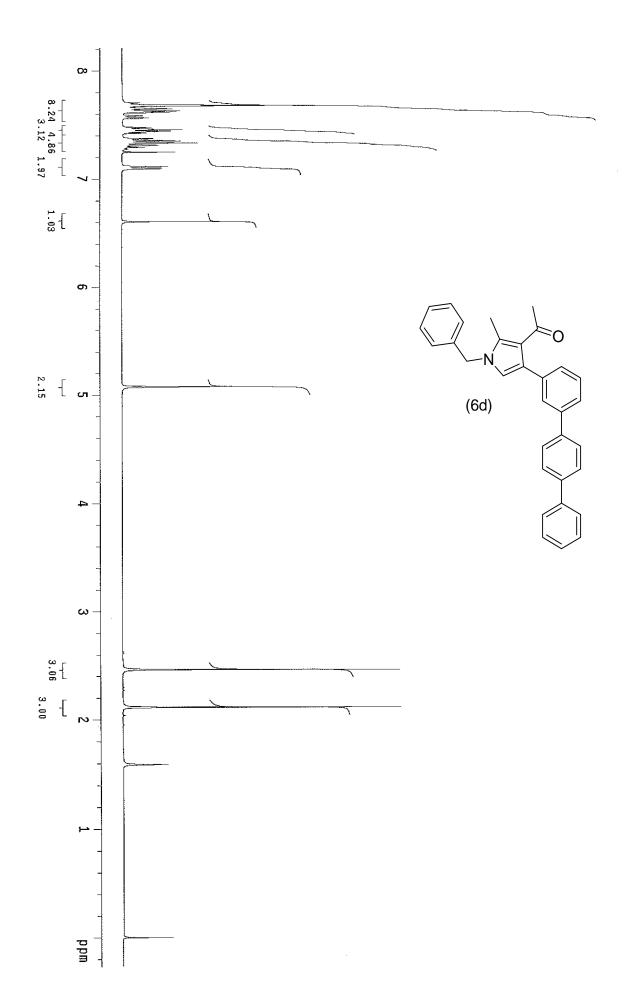
Elements Used: C: 0-35 H: 0-A009/CFSU-3/015 H: 0-45 N: 0-4 O: 0-5

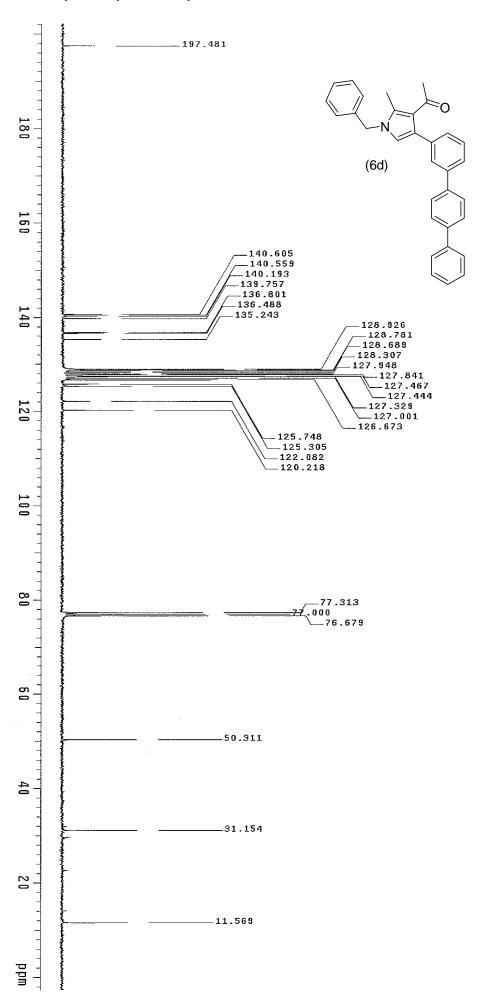


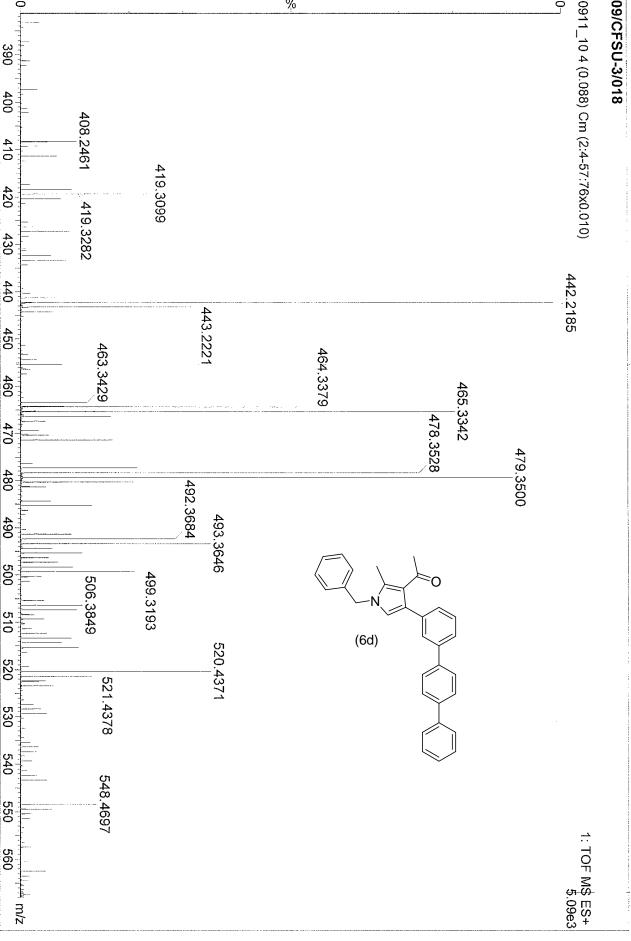




NMR-400







Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = 0.0, max = 80.0 Element prediction: Off

Number of isotope peaks used for i-FIT = 4

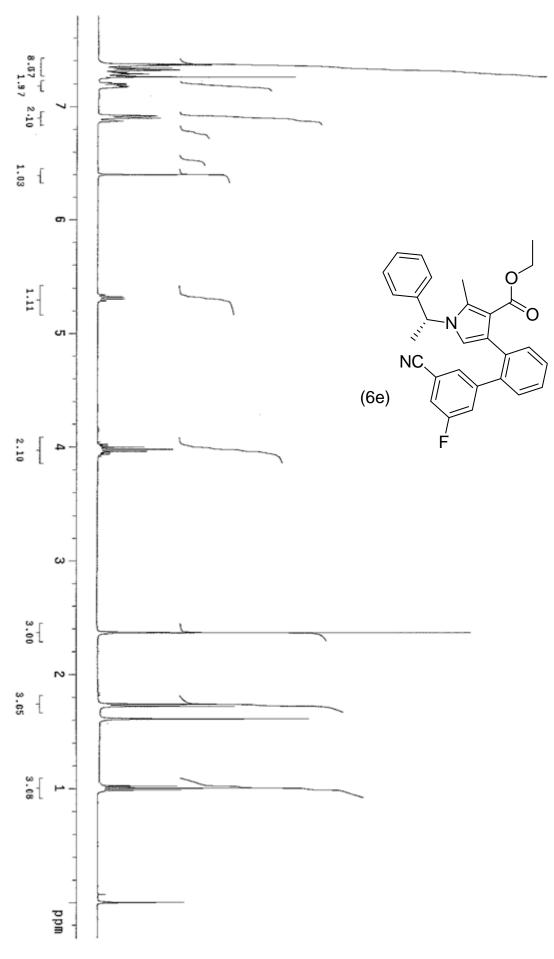
Monoisotopic Mass, Even Electron Ions

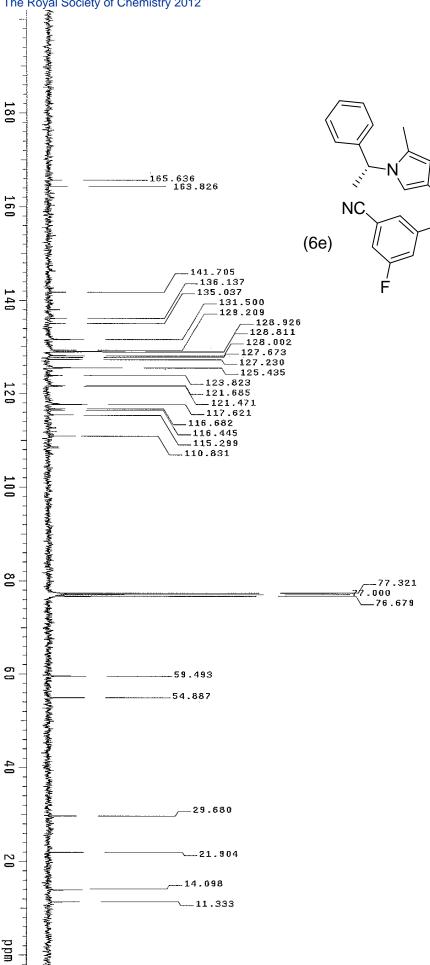
91 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass) Elements Used:

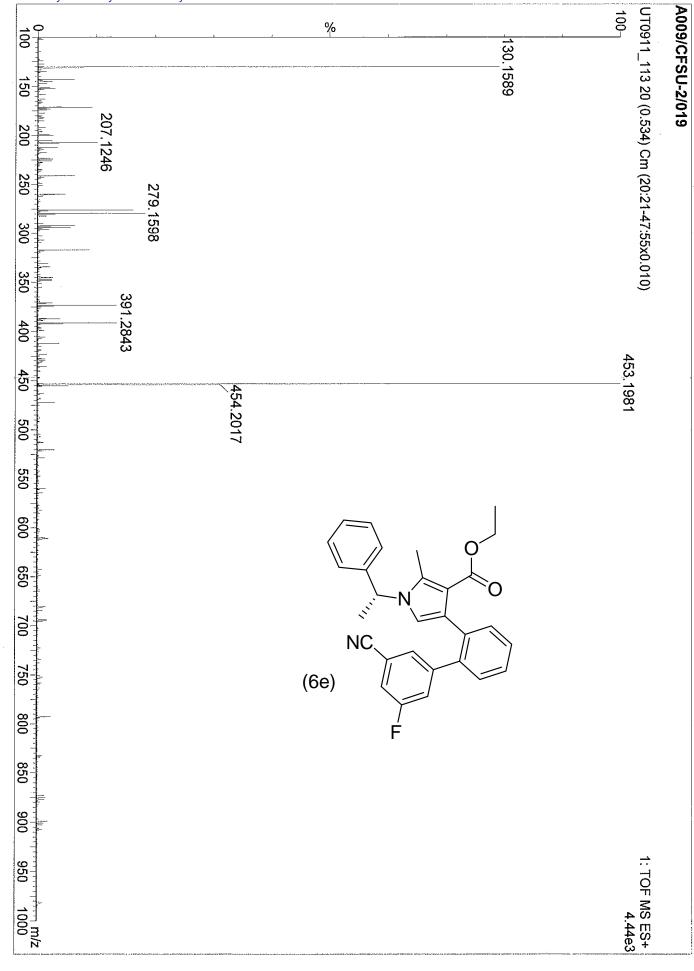
(6d)

C: 0-35 H: 0-45 N: 0-3 O: 0-5
A009/CFSU-3/018









453,1978

0.3

0.7

17.5

ယ ယ

C29

H26

Ν2

2 щ Calc. Mass

mDa

PPM

DBE

i-FIT

Formula

5.0

5.0

0.0

Elemental Composition Report

Single Mass Analysis

Element prediction: Off Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron lons 322 formula(e) evaluated with 2 results within limits (up to 4 best isotopic matches for each mass)

A009/CFSU-2/019 Elements Used: C: 0-50 H: 0-65 UT0911_113 20 (0.534) Cm (20:21-47:55x0.010) N: 0-5 O: 0-4 F: 0-1

8

130,1589

8

용

200

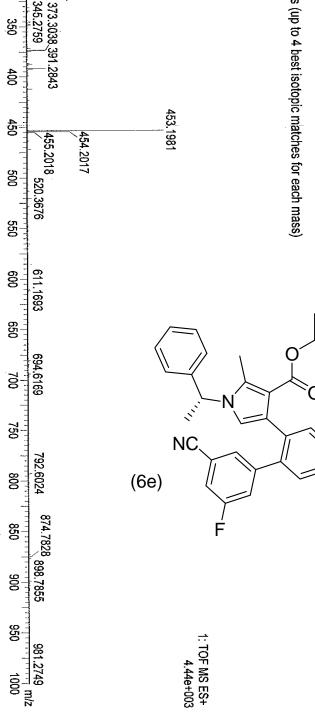
250

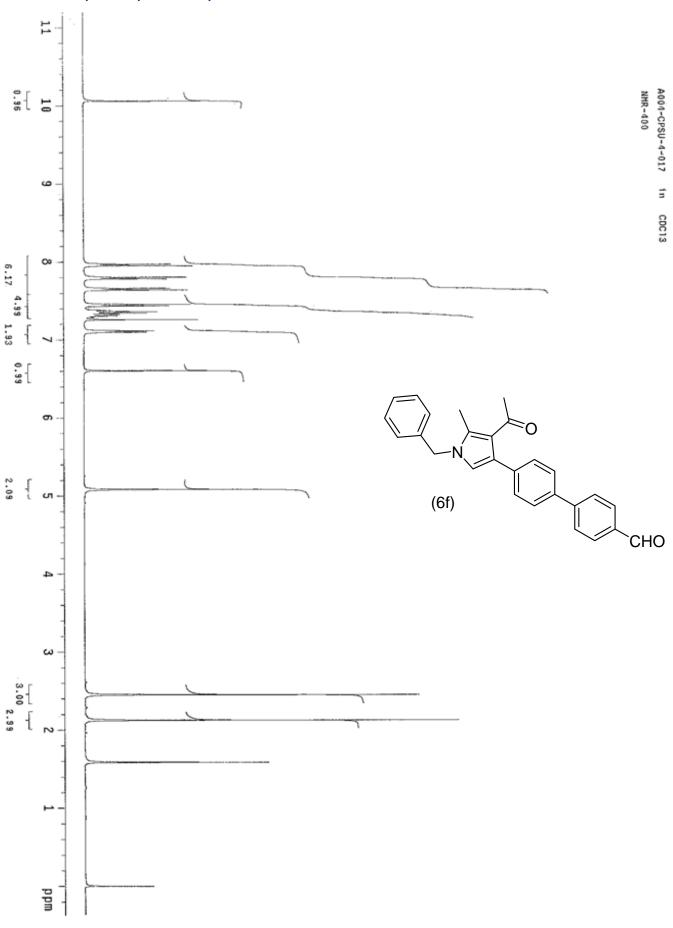
300

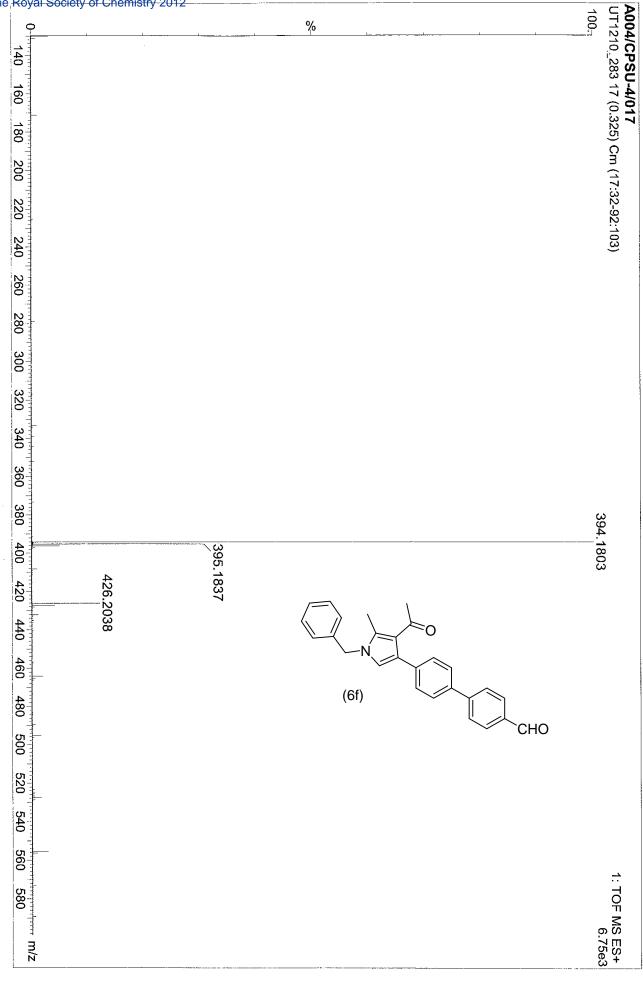
350

207,1246

279.1598







394.1807

-0.4

-1.0

16.5 DBE

0.1

C27

H24

z

02

Calc.

Mass

mDa

PPM

i-FIT

Formula

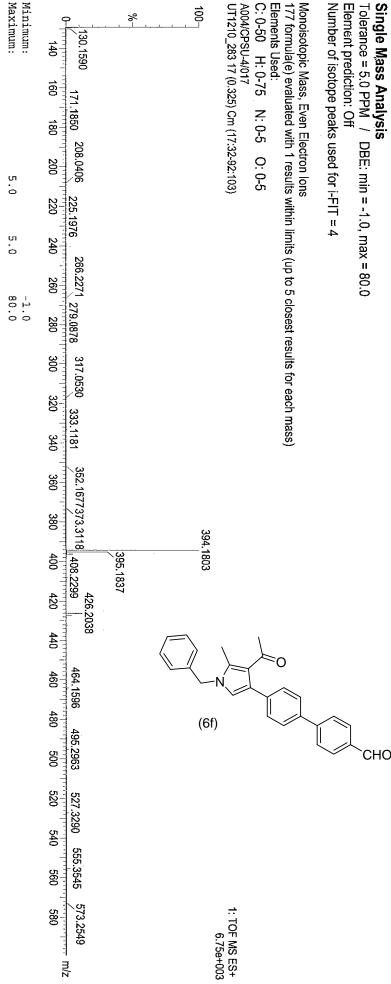
Elemental Composition Report

Element prediction: Off Single Mass Analysis

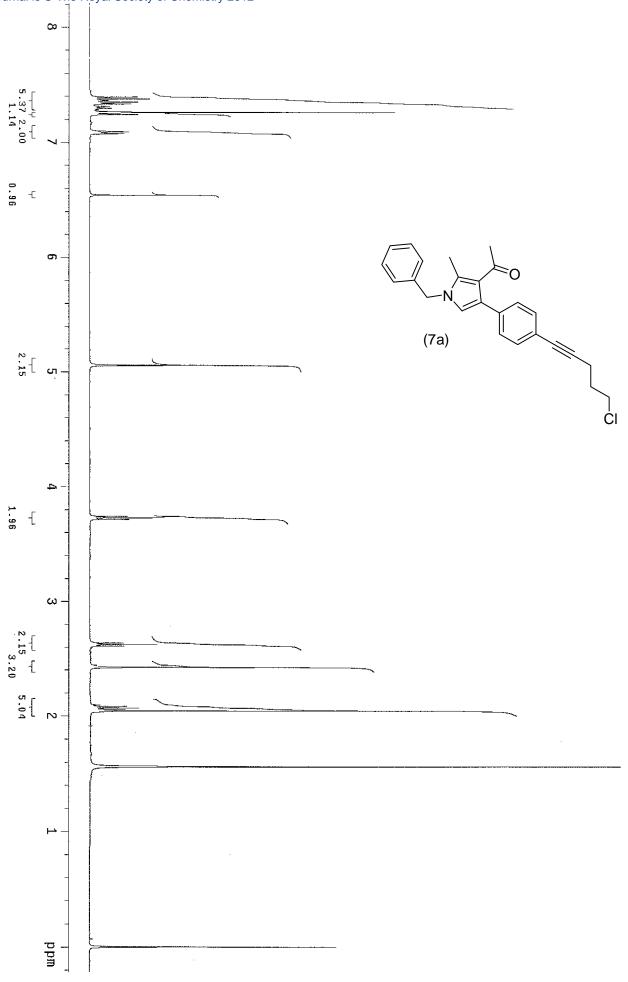
Number of isotope peaks used for i-FIT = 4 Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0

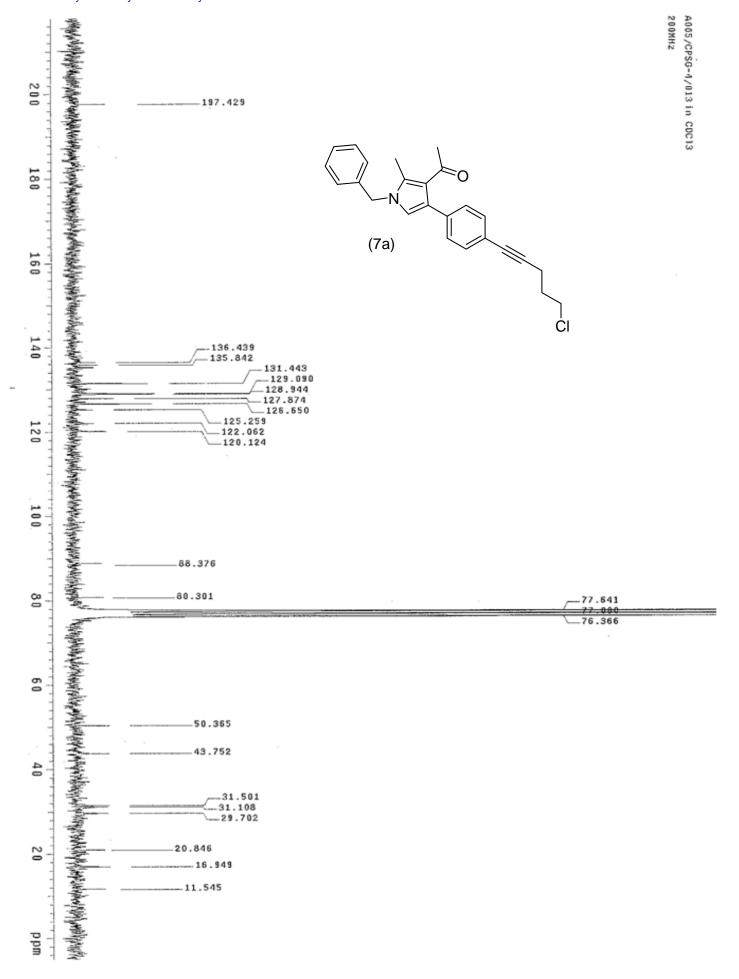
Elements Used: C: 0-50 H: 0-75 A004/CPSU-4/017 N: 0-5 O: 0-5

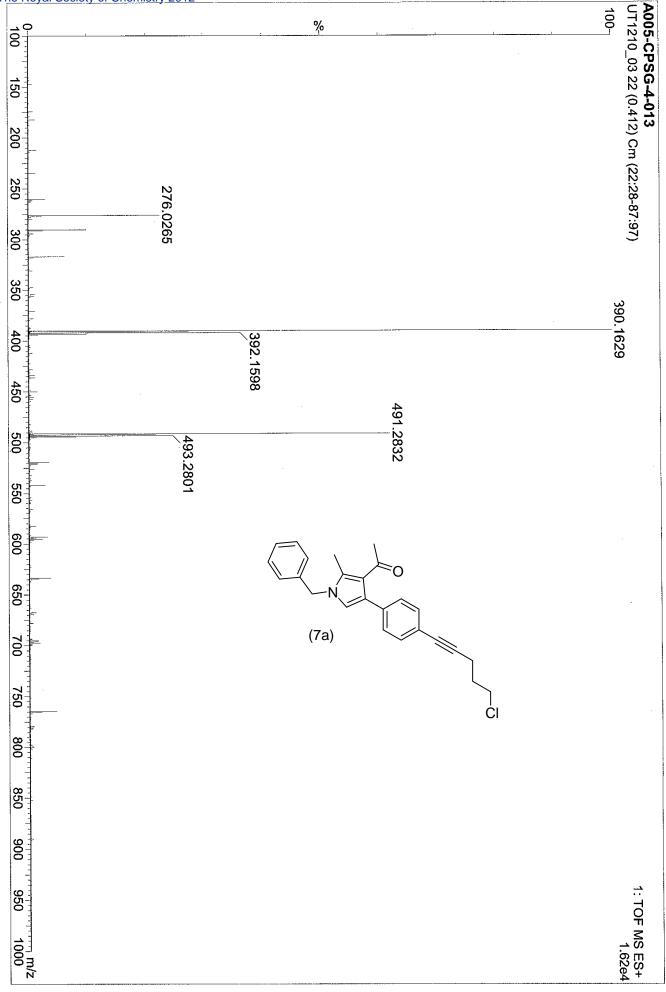
UT1210_283 17 (0.325) Cm (17:32-92:103)











Mass

Calc. Mass

mDa

PPM

DBE

i-FIT

Formula

ហ 0

5.0

390.1629

390.1625

0.4

1.0

13.5

ა 4

C25

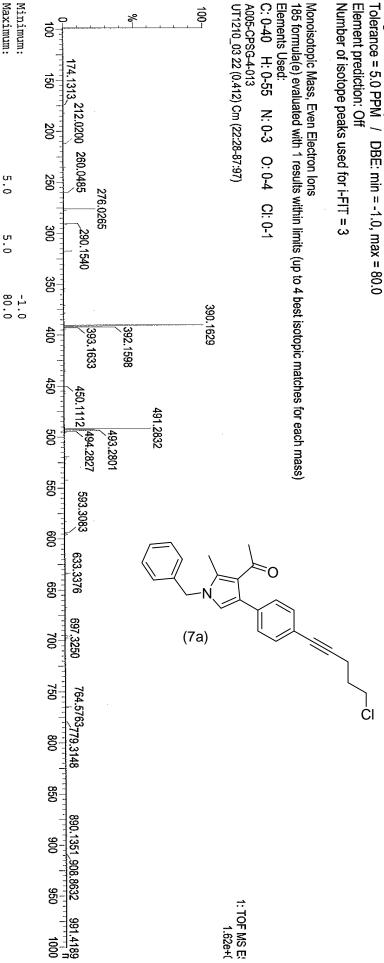
H25

z

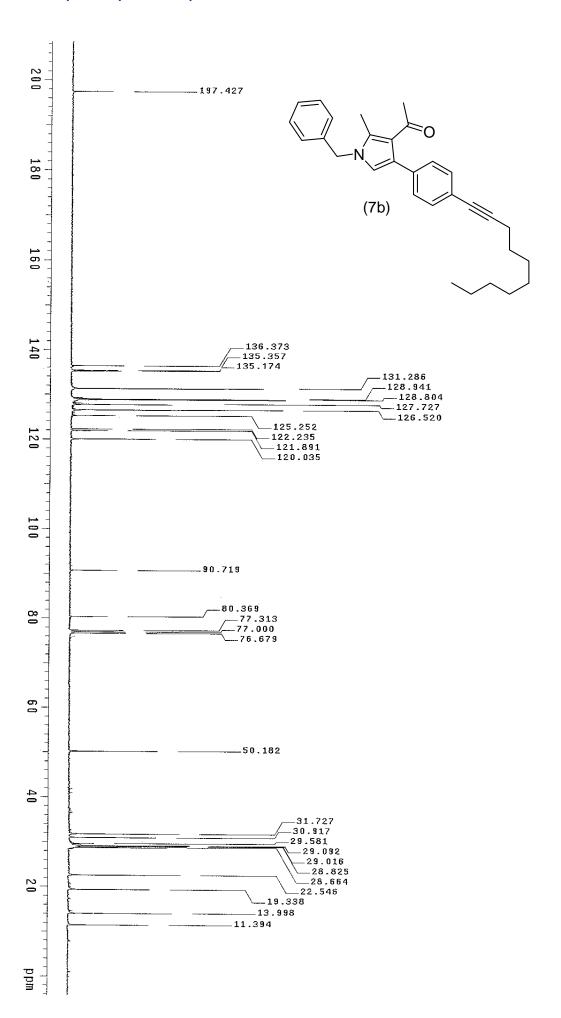
0 Ω Maximum:

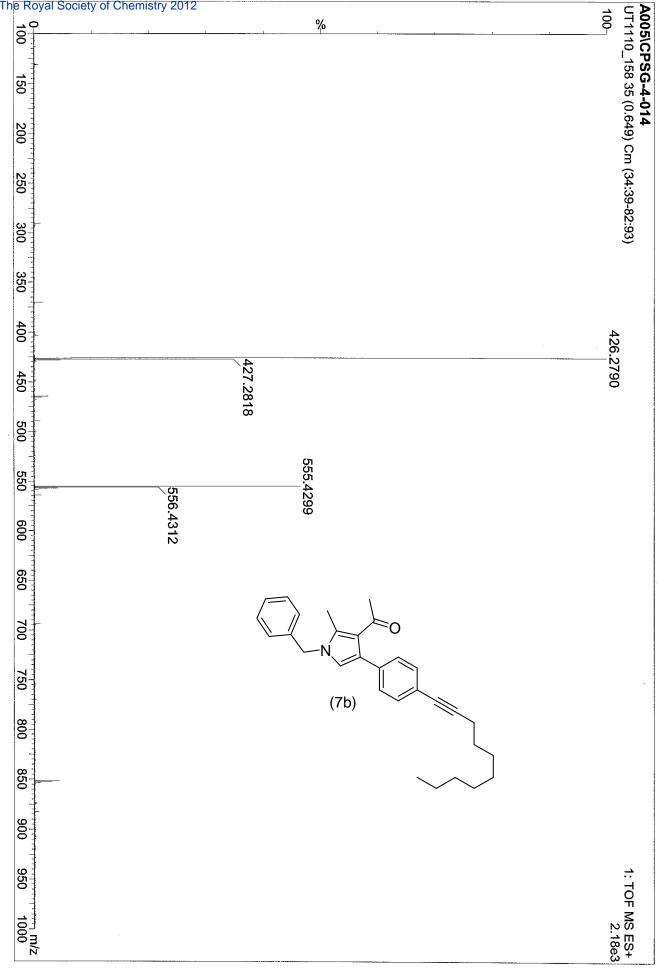
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM /



NMR-400





426.2797

-0.7

13.5

0.1

C30

H36

z

0

Calc. Mass

mDa

PPM

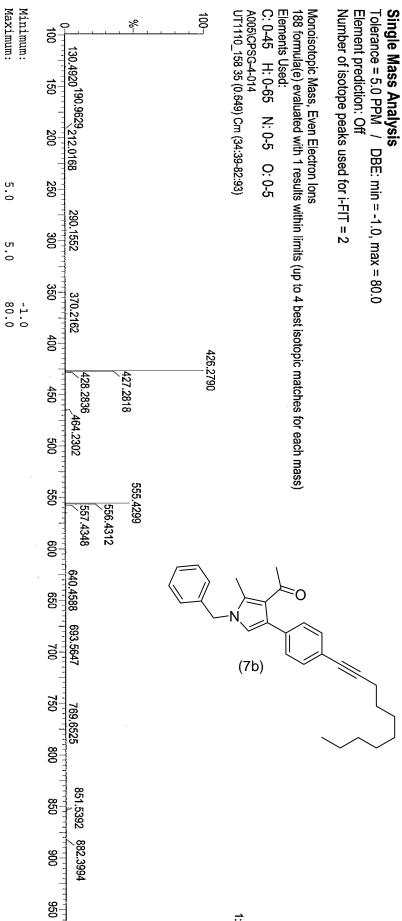
BEG

i-FIT

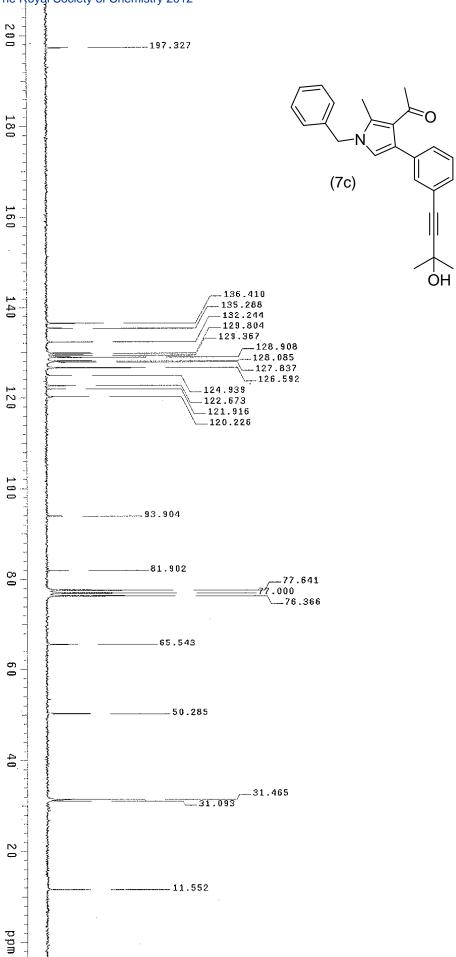
Formula

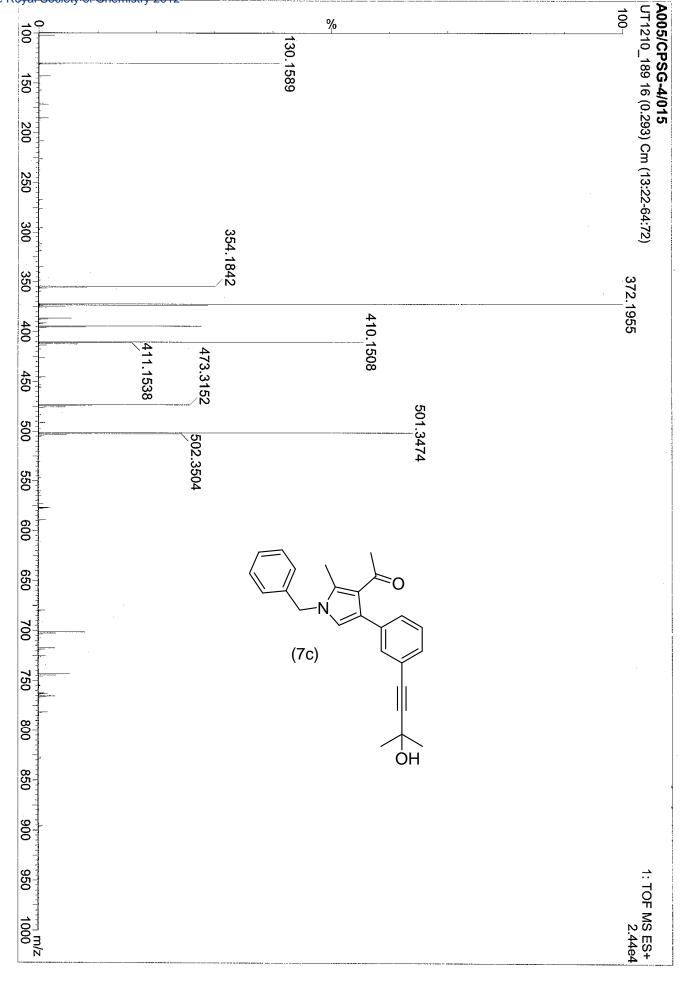
Elemental Composition Report

Monoisotopic Mass, Even Electron lons



1: TOF MS ES+ 2.18e+003





Single Mass Analysis

Element prediction: Off Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0

Number of isotope peaks used for i-FIT = 3

A005/CPSG-4/015 UT1210_189 16 (0.293) Cm (13:22-64:72) C: 0-35 H: 0-60 Elements Used: N: 0-4 O: 0-4

9

%

130,1589

8

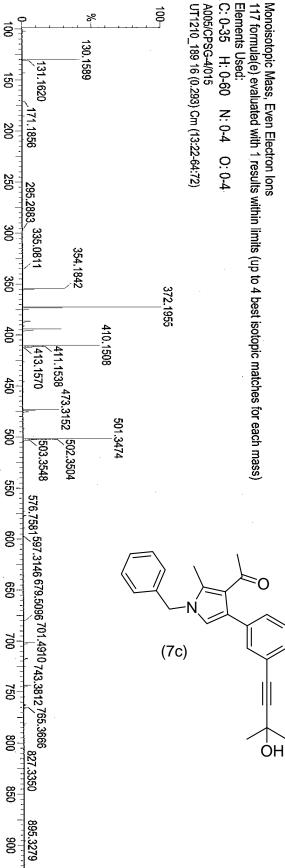
엸

250

950

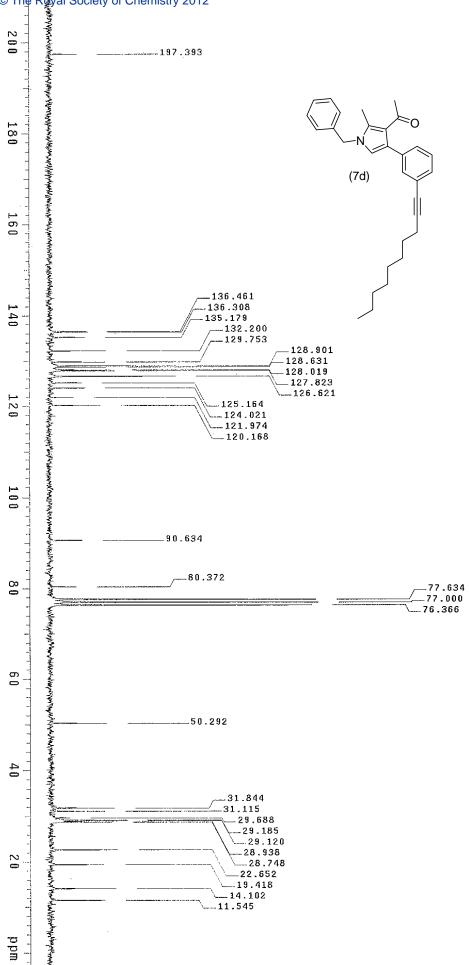
131.1620

171.1856 200



1: TOF MS ES+ 2.44e+004

Minimum: Maximum: Mass 372.1955 372.1964 Calc. Mass -0.9 mDa 5.0 -2.4 PPM 5.0 -1.0 80.0 13.5 DBE 2.2 i-FIT C25 Formula H26 z 2



Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -1.0, max = 80.0

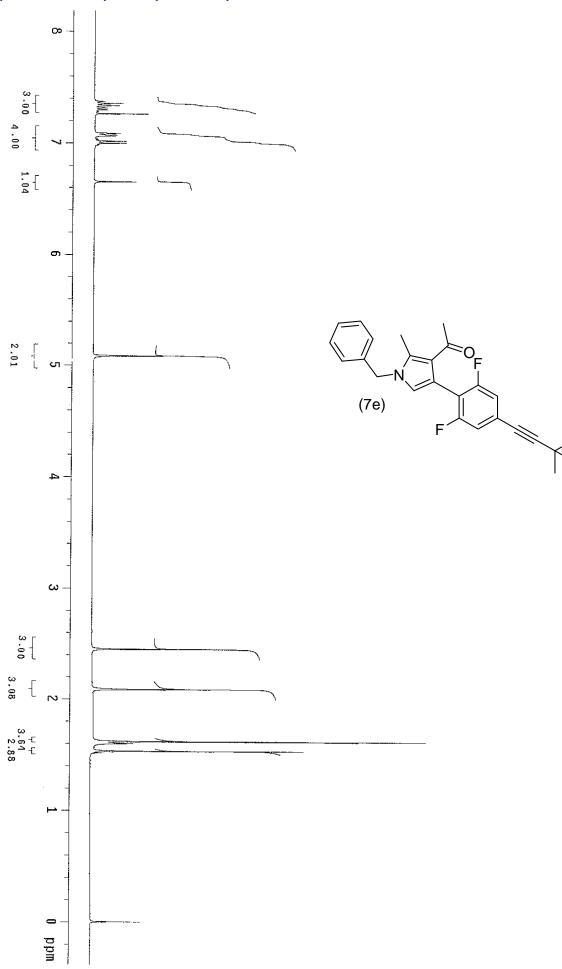
Element prediction: Off

Number of isotope peaks used for i-FIT = 3

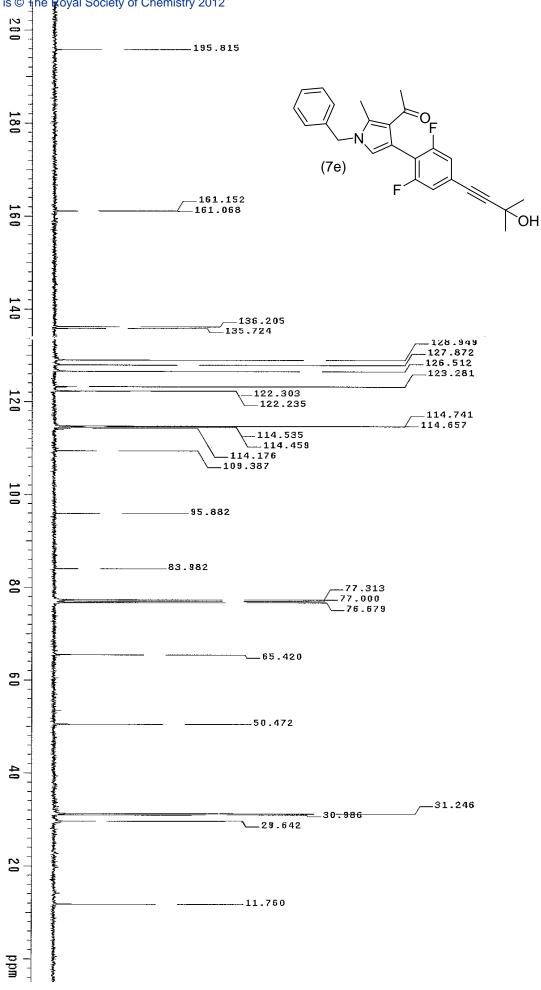
Monoisotopic Mass, Even Electron lons 94 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

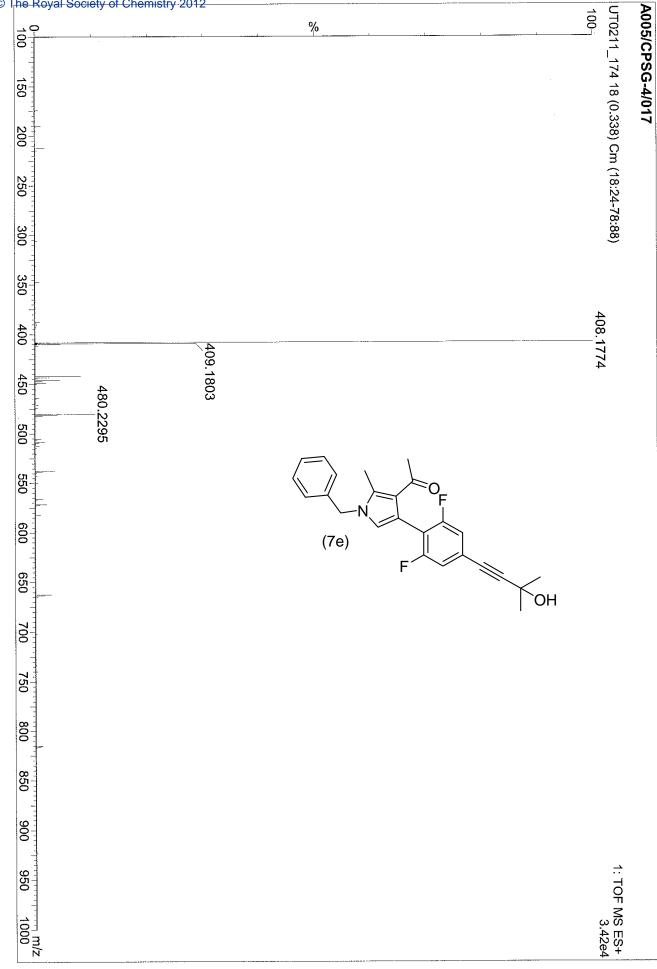
Minimum: Maximum: Elements Used: C: 0-40 H: 0-55 UT1210_05 30 (0.560) Cm (28:34-89:101) 9 A005-CPSG-3-016 8 166.0648 182.0405 150 426.2797 Calc. Mass N: 0-3 O: 0-4 200 260.0481 5.0 ১ ০ mDa 250 276.0268 317.0531358.1809 300 PPM 4.7 10.0 350 DBE -1.0 80.0 13.5 400 426.2817 2.4 i-FIT 427.2847 428.2873 450 499.3676 C30Formula 500 527.4008 H36 528.4042 550 z 0 582.9823 60 636.8941 719.1482 764.5704 650 700 (7d) 750 798.2875 88 851.5541 874.5609 850 900 950 957.8420 1: TOF MS ES+ 2.00e+004 985,1068 m/z

OH



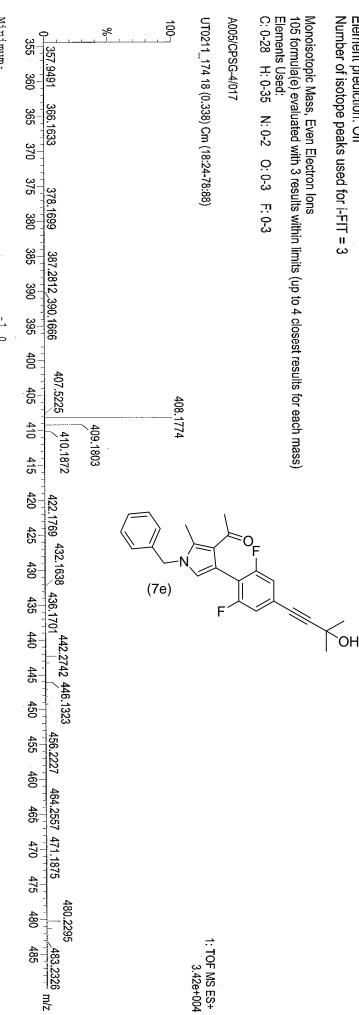






Single Mass Analysis

Element prediction: Off Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0



	U 12	
408.1774	Mass	Minimum: Maximum:
408.1775	Calc. Mass	
-0.1	mDa	5.0
-0.2	PPM	5.0
13.5	DBE	*1.0 80.0
1.6	i-FIT	

C25

H24

z

2

F2

Formula

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