Supporting Information

N,*N*-Diisopropyl-*N*-phosphonyl Imines Lead to Efficient Asymmetric Synthesis of Aziridine-2-Carboxylic Esters

Padmanabha V. Kattamuri,[a] Yiwen Xiong,[b] Yi Pan[*b] and Guigen Li[*a,c]

[a] *Department of Chemistry & Biochemistry, Texas Tech University,*

Lubbock, Texas 79409-1061, USA. E-mail: Guigen.Li@ttu.edu;

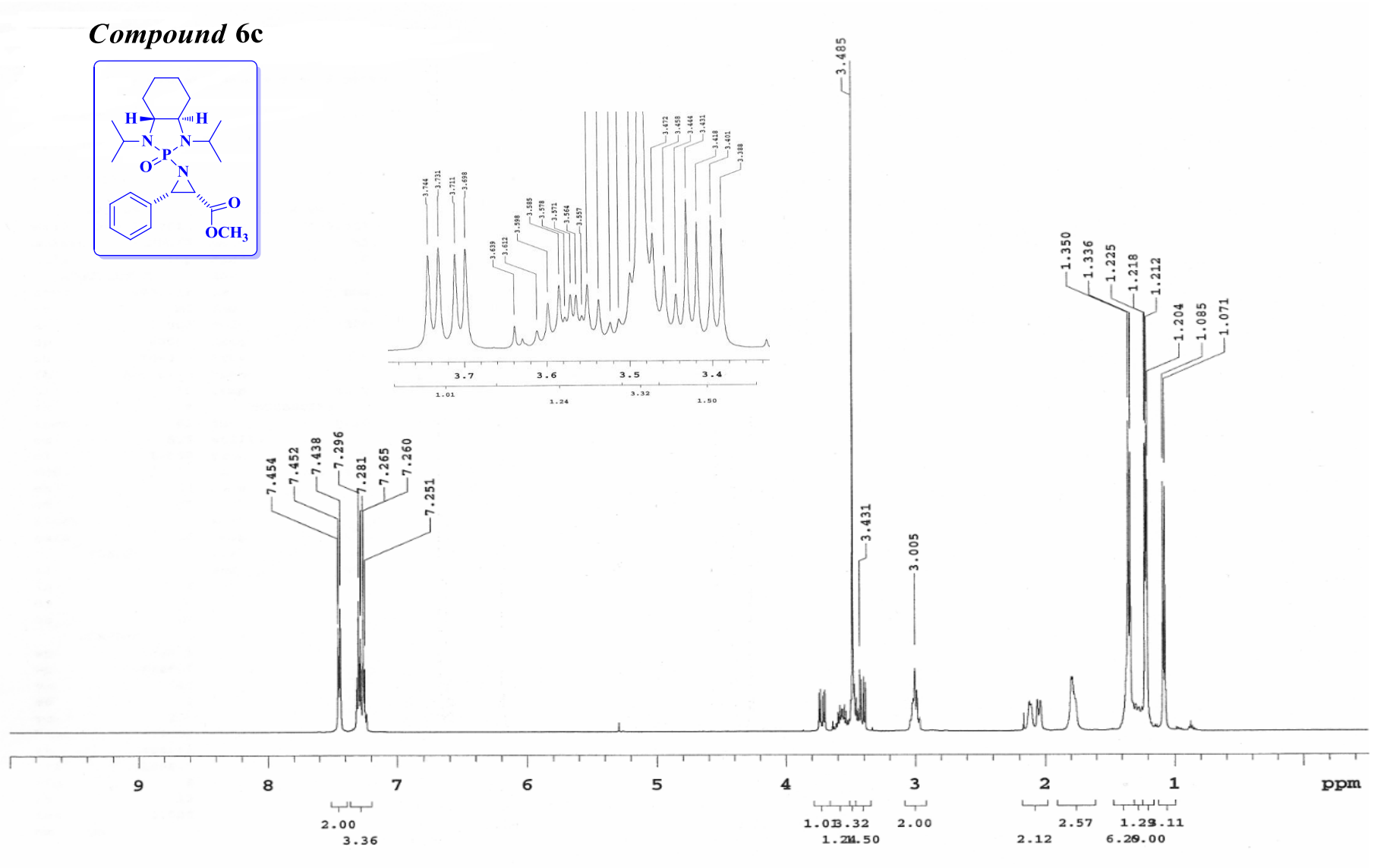
Fax: 001-806-742-1289; Tel: 001-806-742-3015

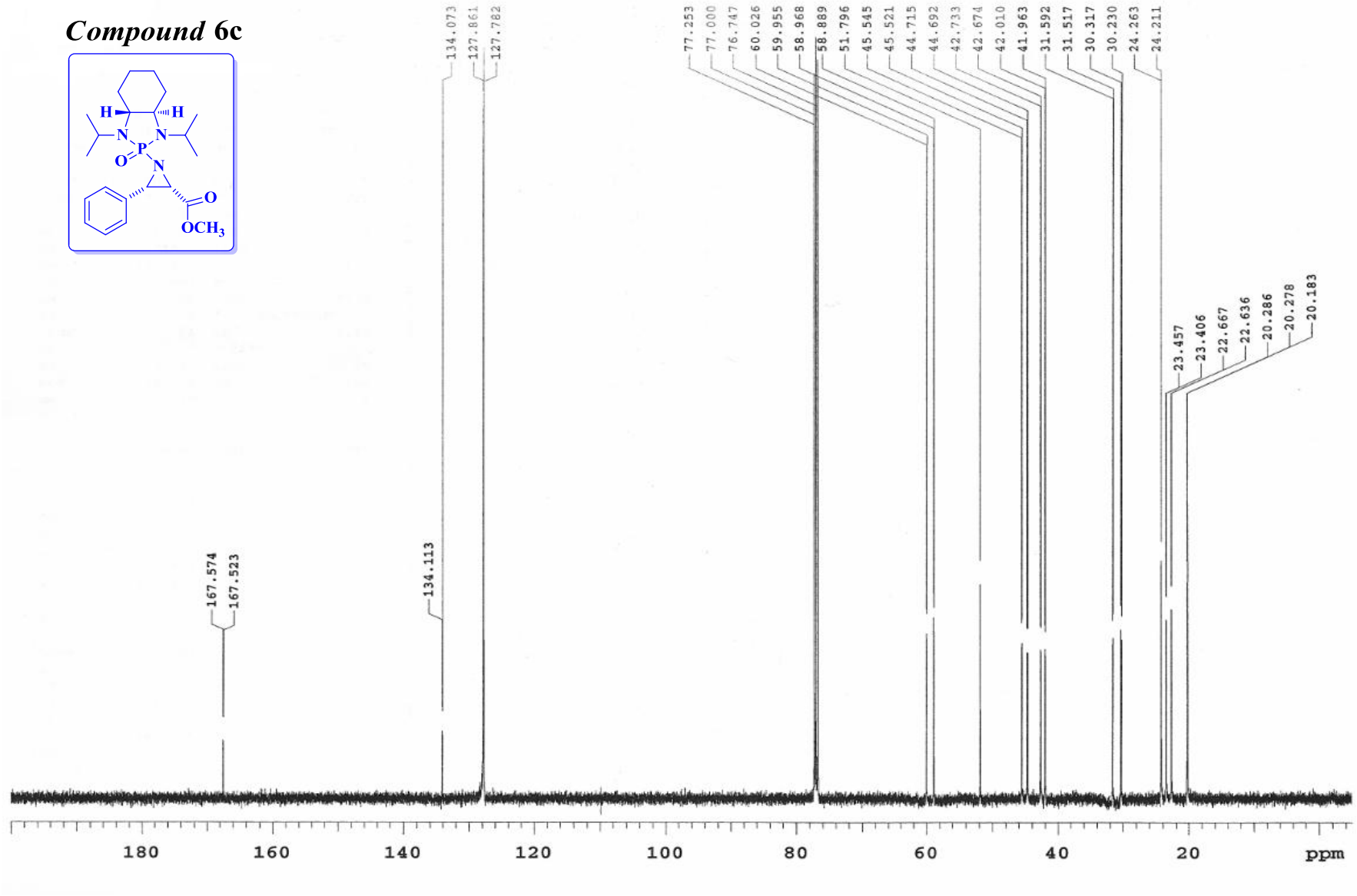
[b] *School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210093, P. R. China, E-mail: yipan@nju.edu.cn;*

[c] *Institute of Chemistry & BioMedical Sciences, Nanjing University, Nanjing 210093, P. R. China*

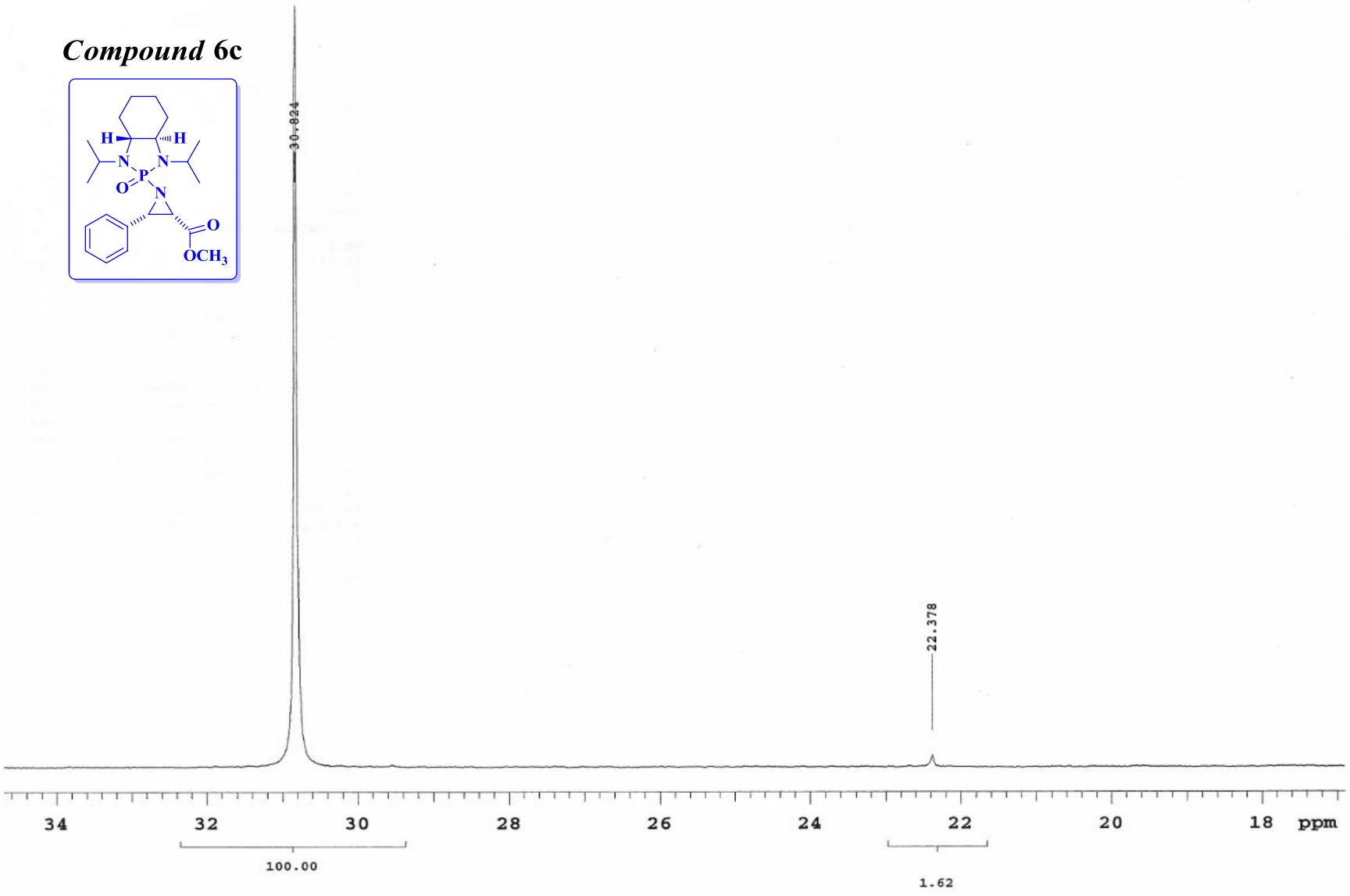
Table of Contents

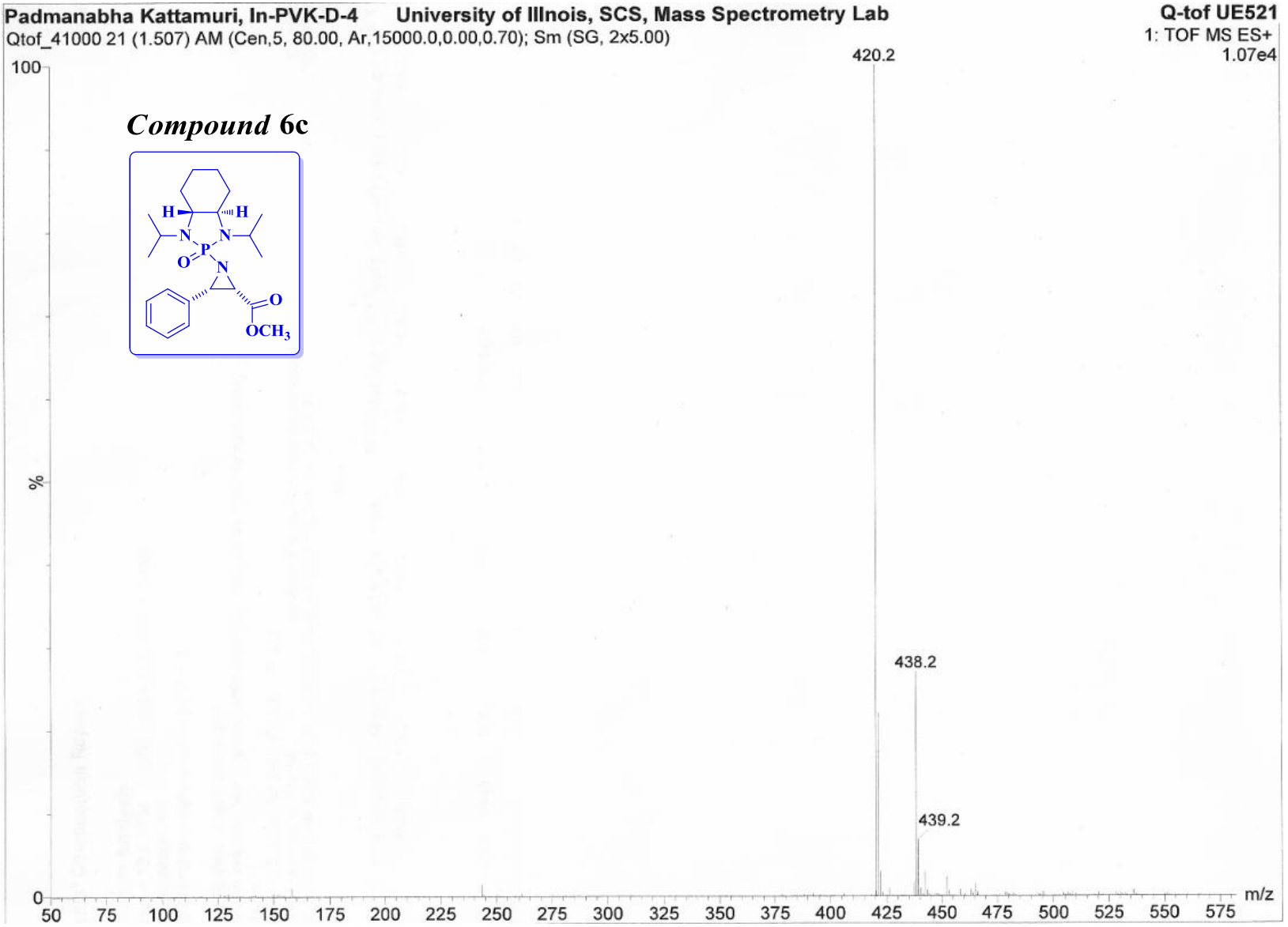
***Compound* 6c**





***Compound* 6c**



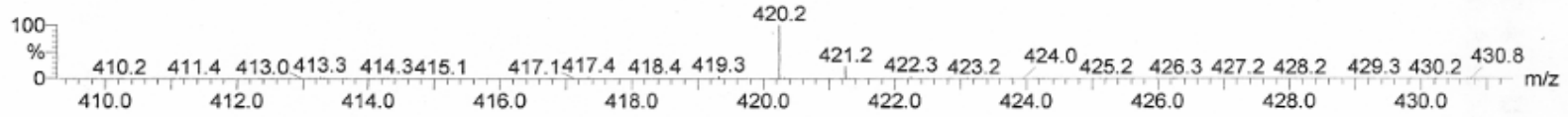


Elemental Composition Report **Page 1**

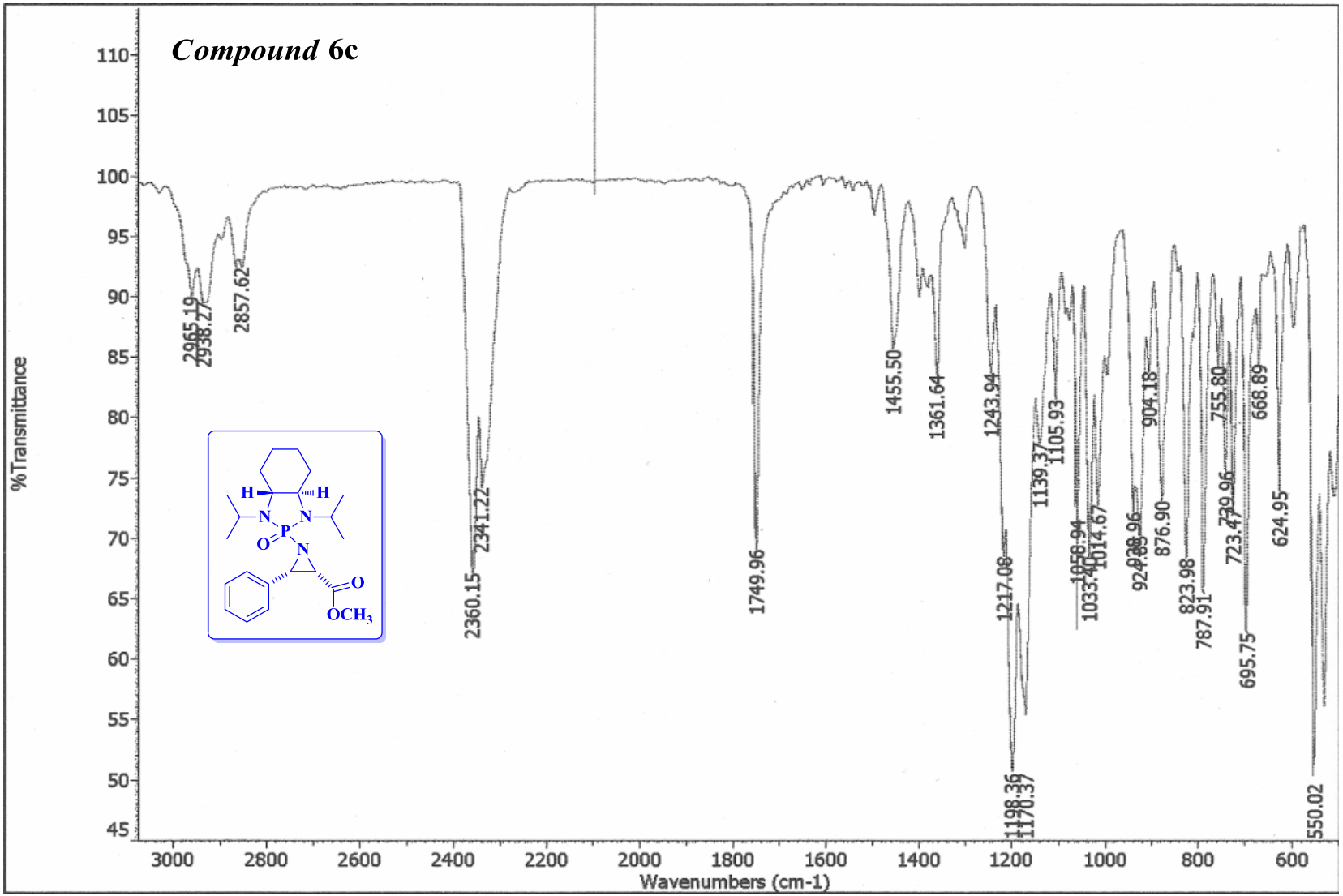
Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 600.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
88 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-250 N: 2-4 O: 2-4 P: 0-1

Padmanabha Kattamuri, In-PVK-D-4 University of Illnois, SCS, Mass Spectrometry Lab Q-tof UE521
Qtof_41000 29 (2.043) AM (Cen,3, 80.00, Ar,15000.0,716.46,0.70); Sm (SG, 2x5.00); Cm (28:30) 2: TOF MS ES+
1.27e+003



Minimum:				-1.5		
Maximum:		5.0	10.0	600.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
420.2425	420.2416	0.9	2.1	7.5	3.2	C22 H35 N3 O3 P



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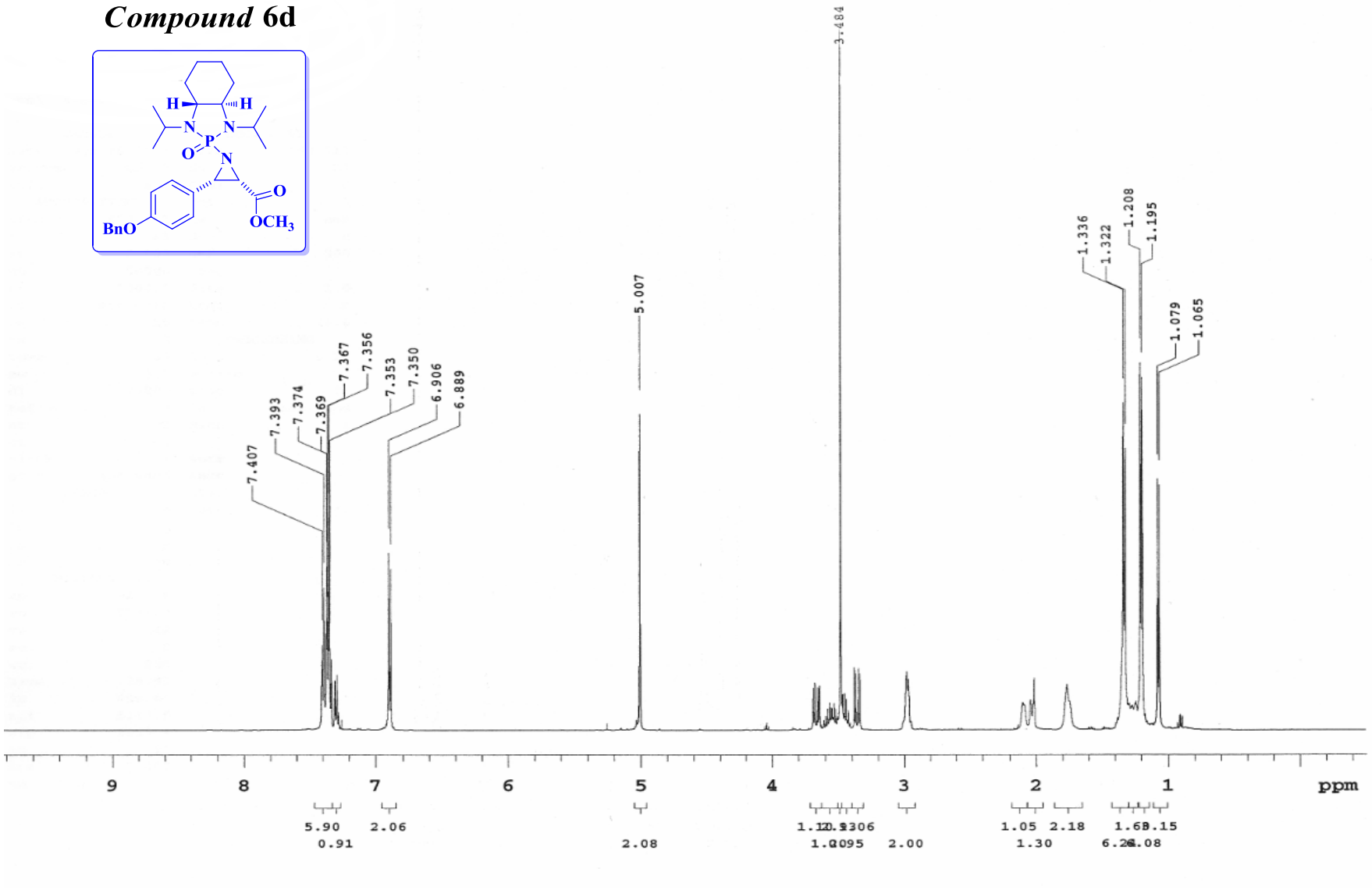
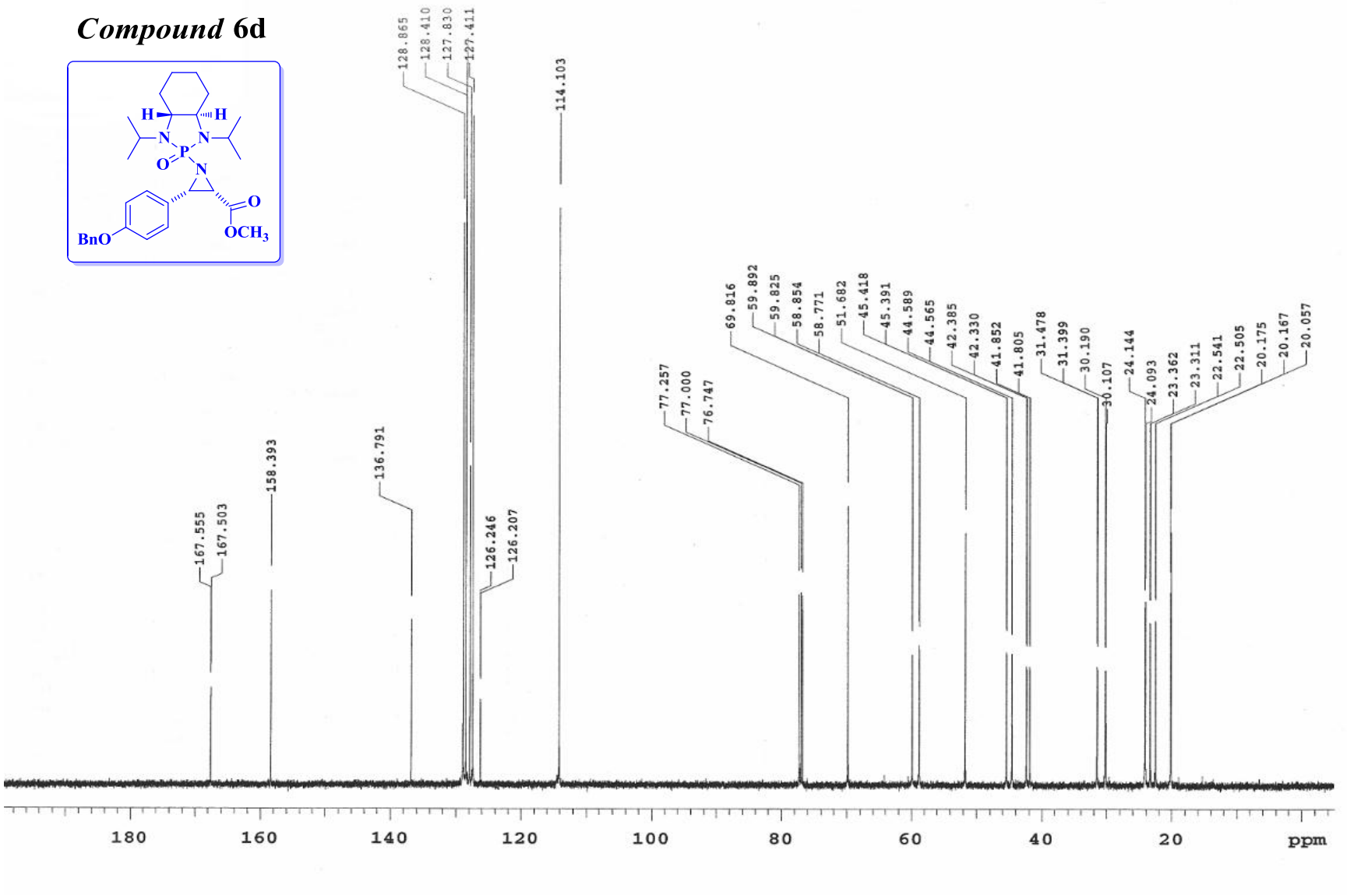
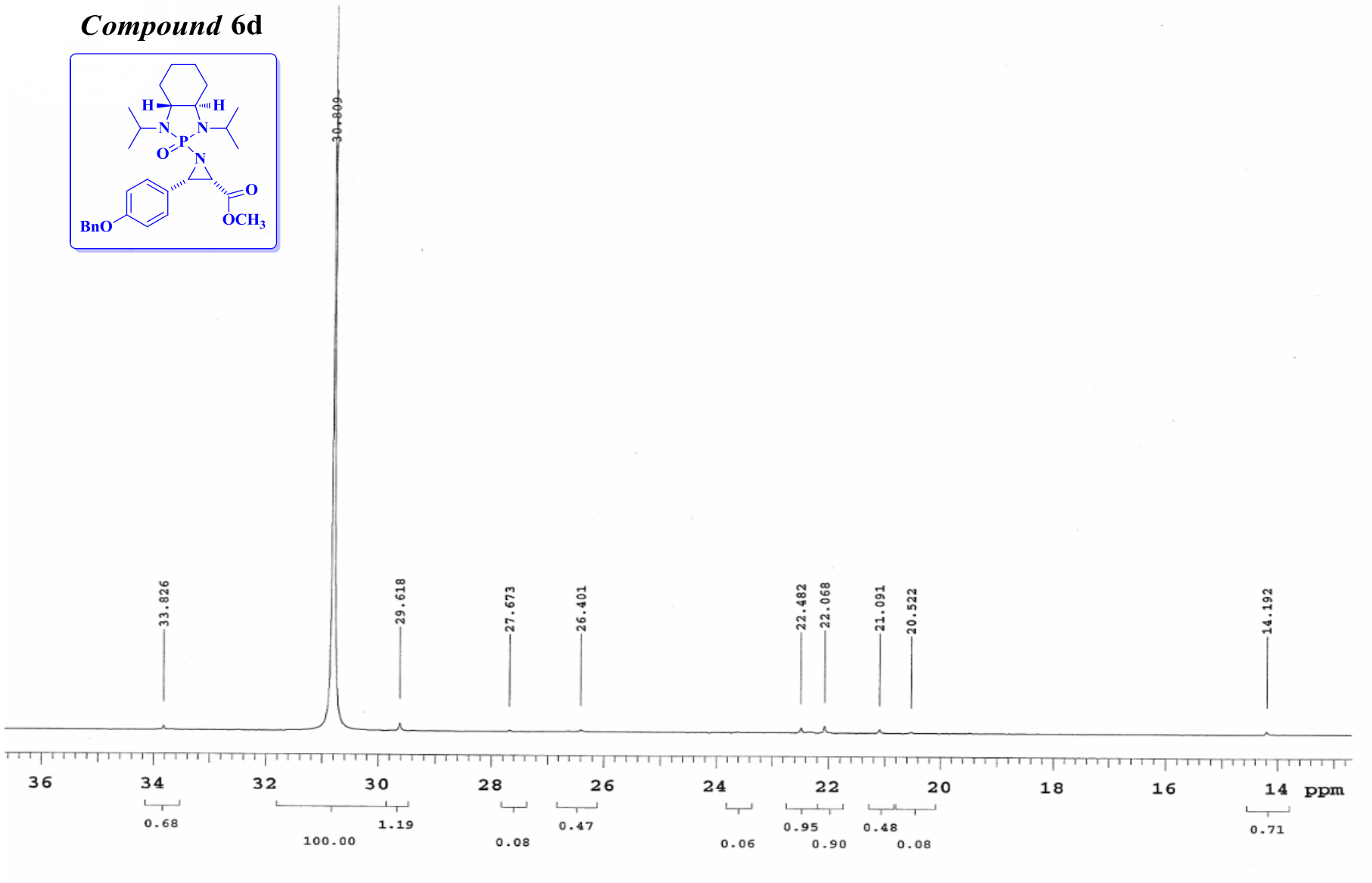
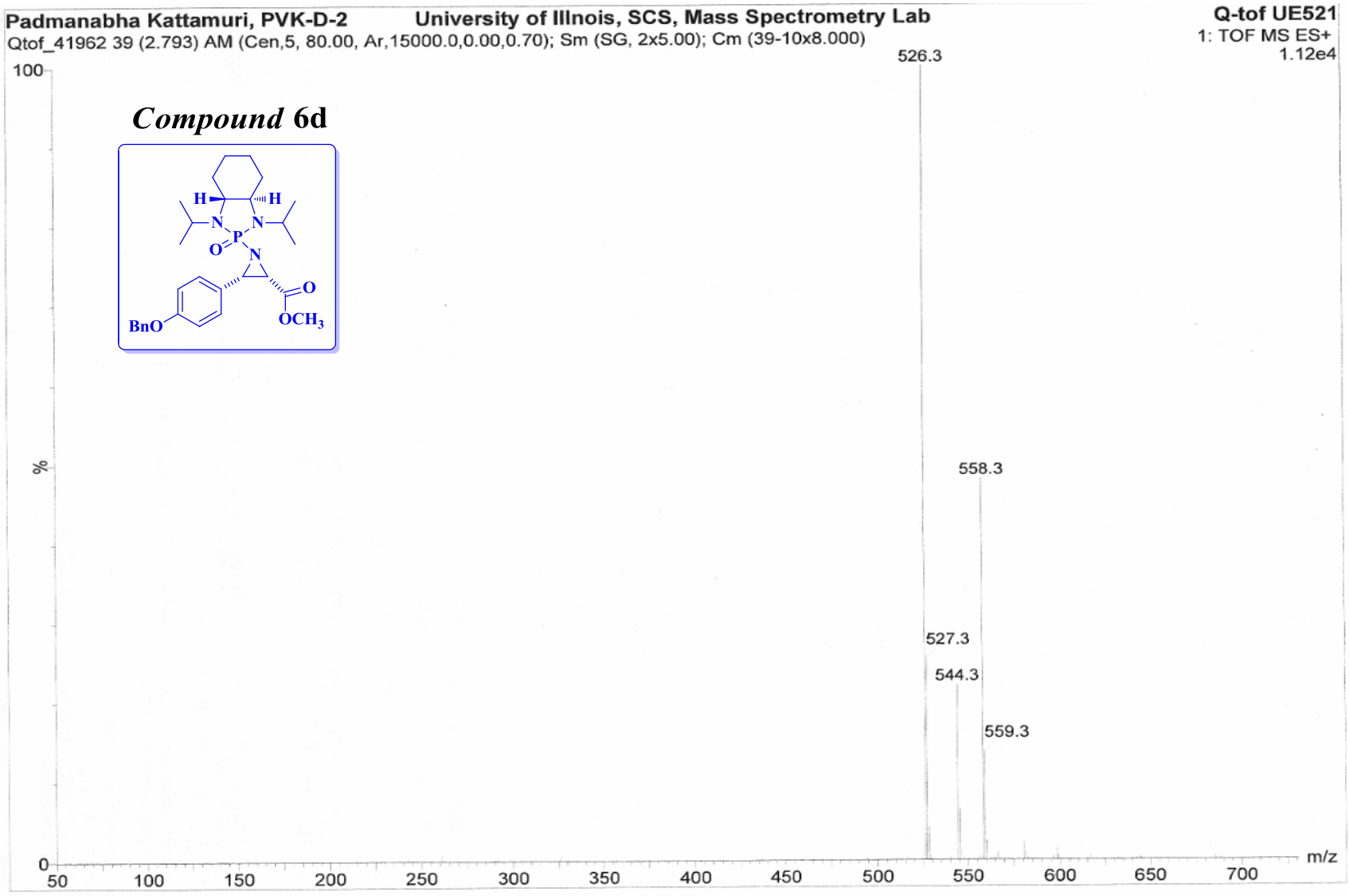








Elemental Composition Report

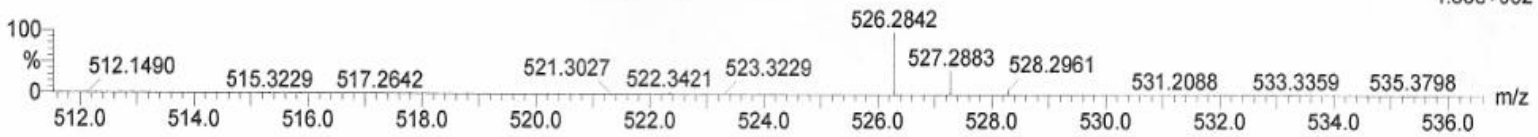
Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 600.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

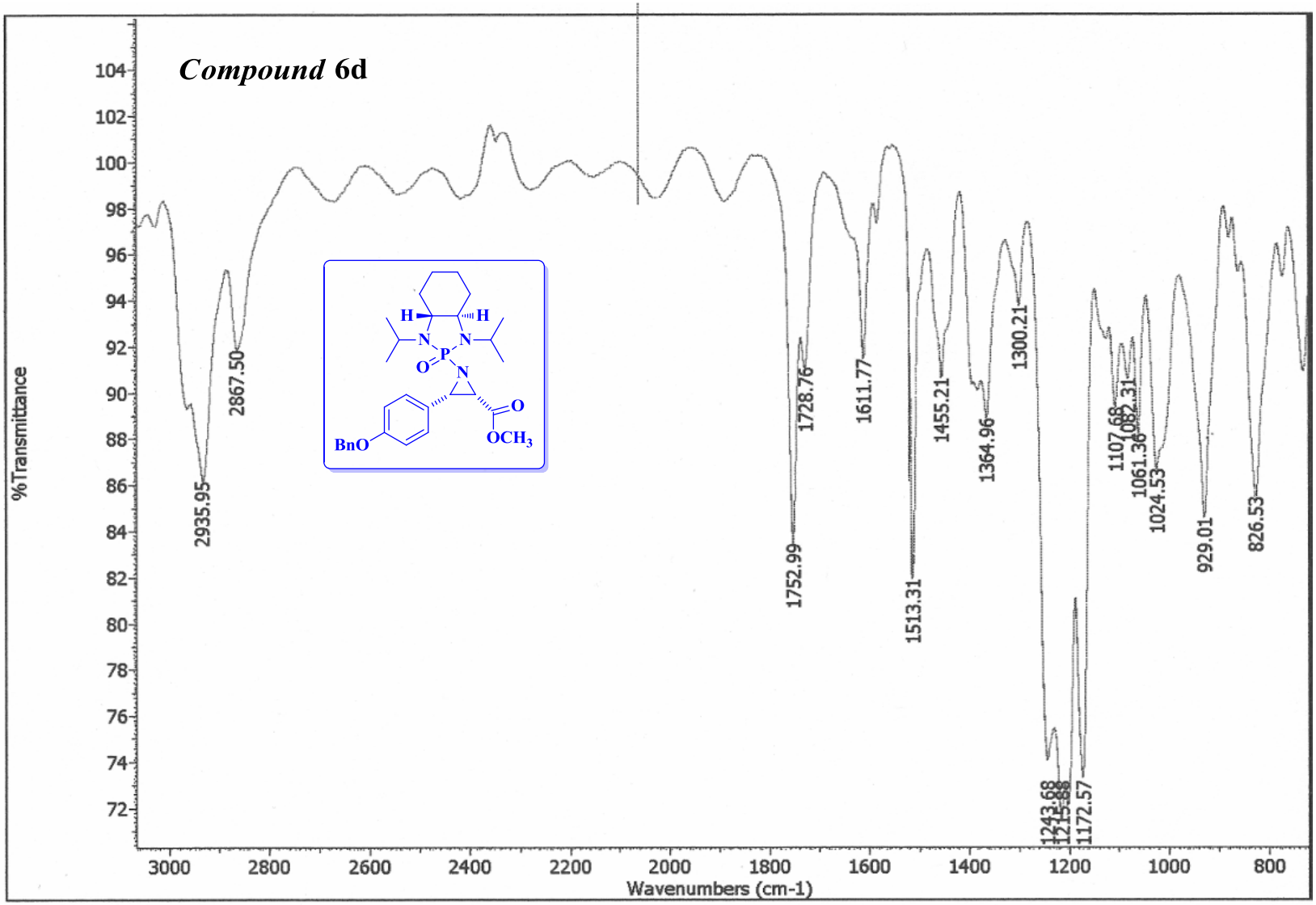
Monoisotopic Mass, Even Electron Ions
115 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-250 N: 2-4 O: 2-4 P: 0-1

Padmanabha Kattamuri, PVK-D-2 University of Illinois, SCS, Mass Spectrometry Lab
Qtof_41962 32 (2.257) AM (Cen,3, 80.00, Ar,15000.0,716.46,0.70); Sm (SG, 2x3.00); Cm (31:33)

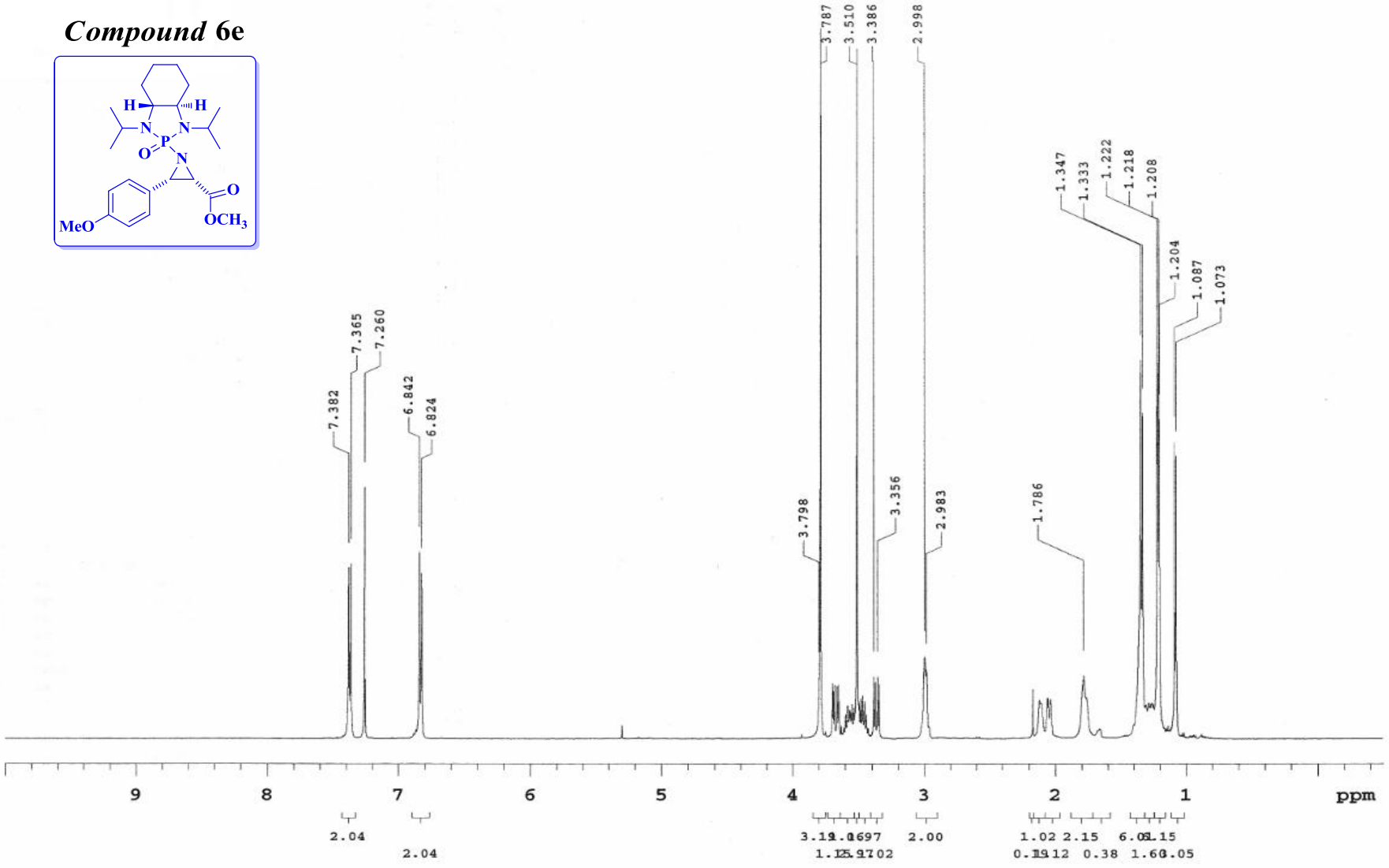
Q-tof UE521
2: TOF MS ES+
4.85e+002



	Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
Minimum:					-1.5		
Maximum:			5.0	10.0	600.0		
	526.2842	526.2835	0.7	1.3	11.5	1.2	C29 H41 N3 O4 P



***Compound* 6e**



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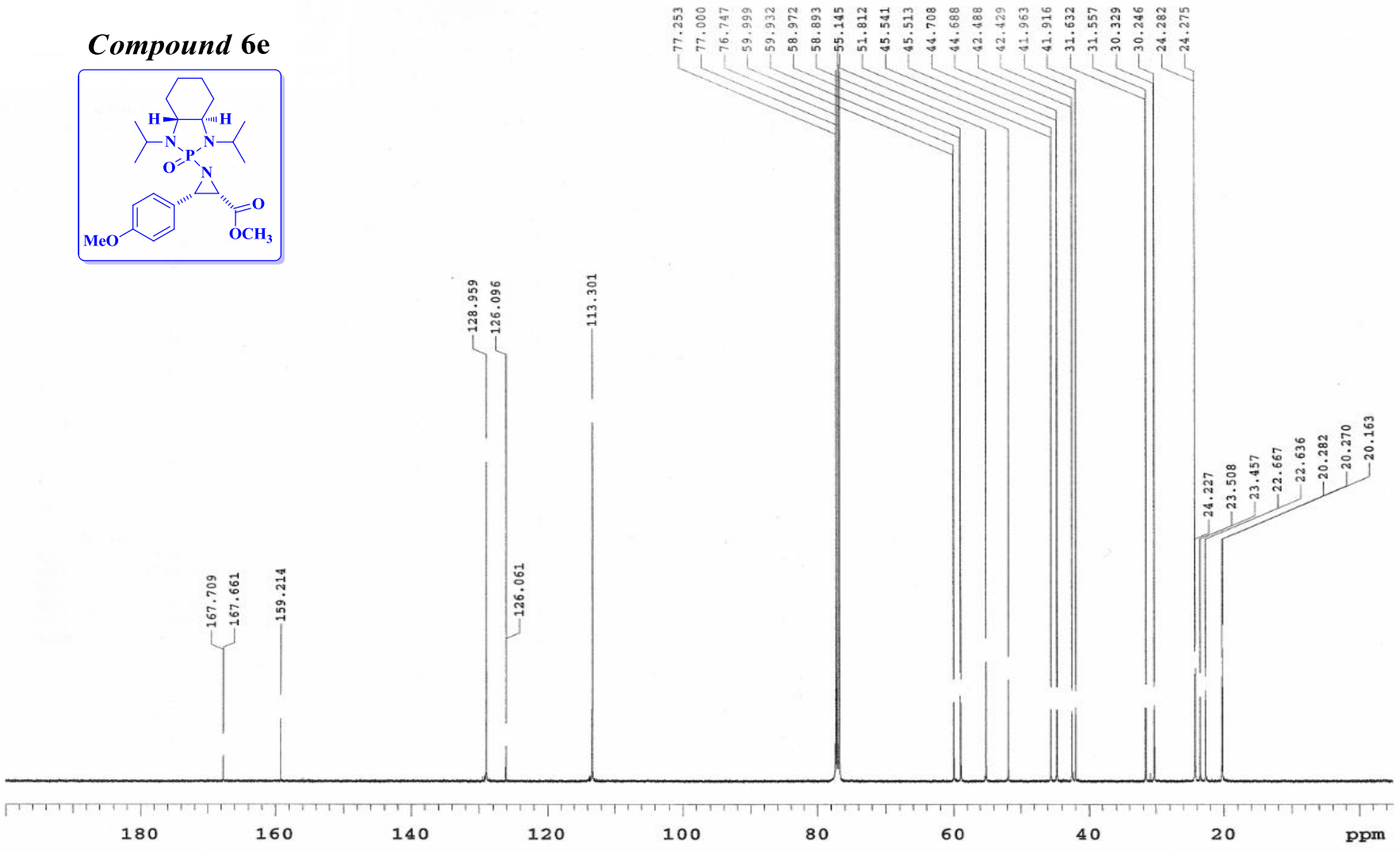
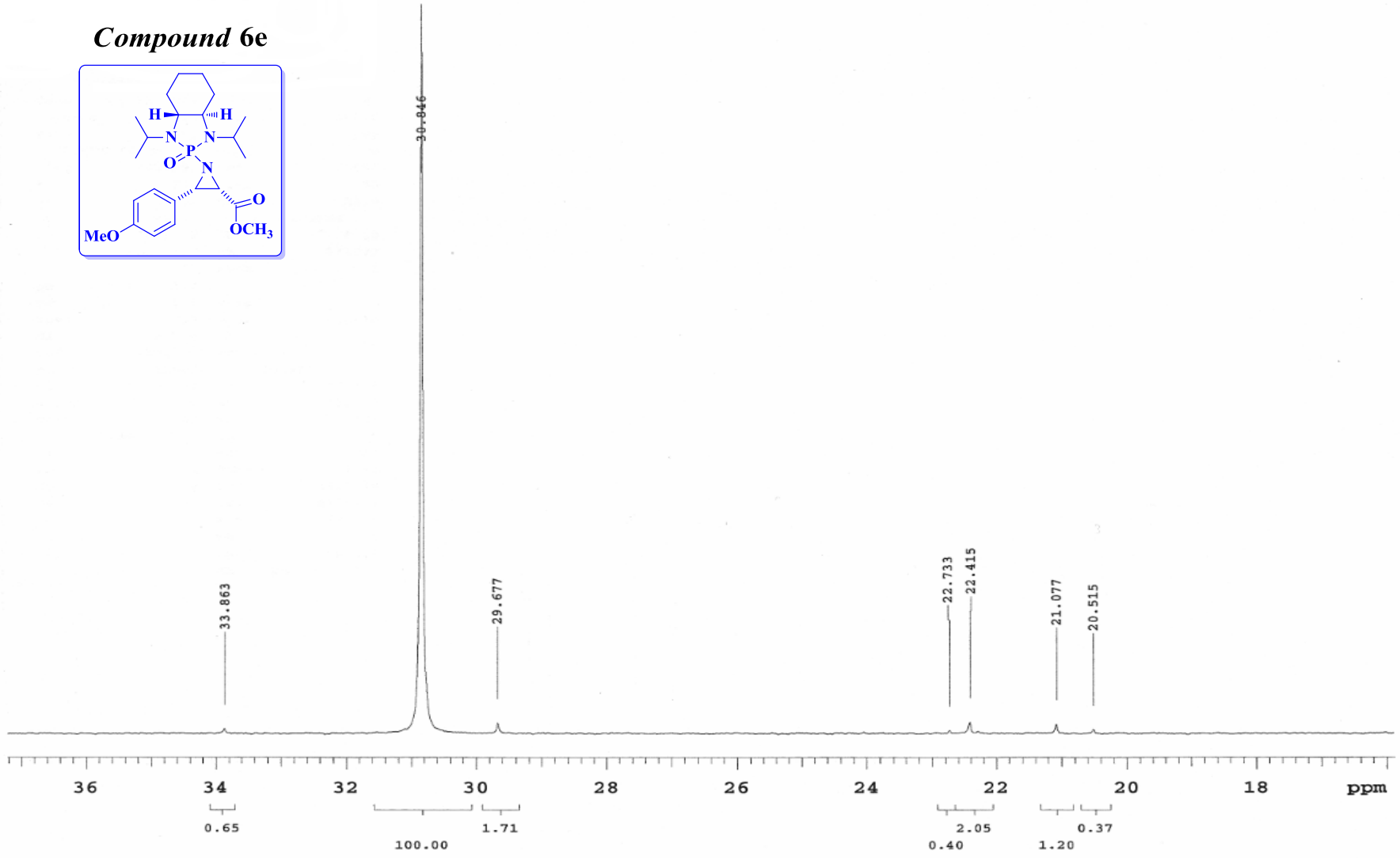
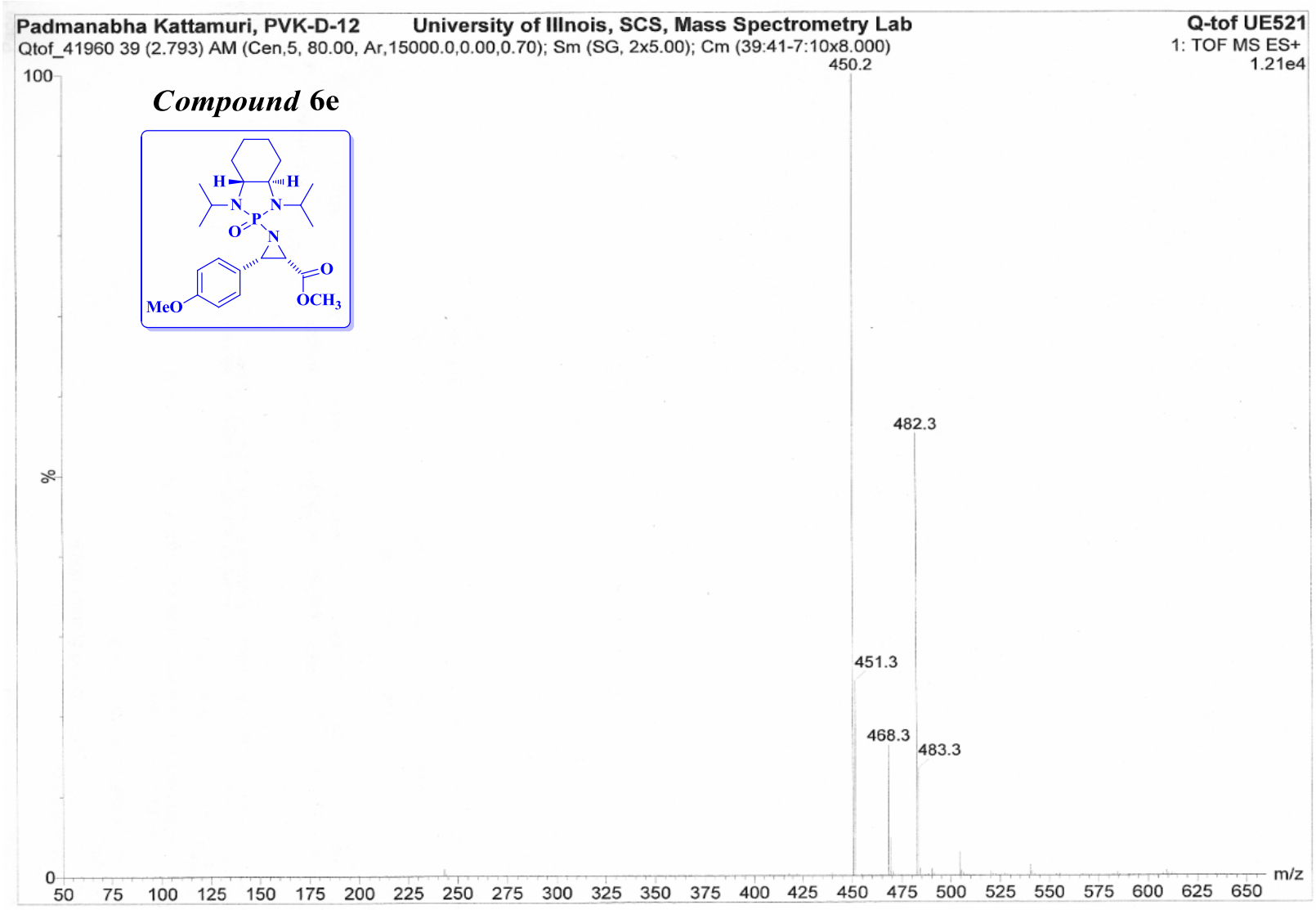





Padmanabha Kattamuri, PVK-D-12
University of Illnois, SCS, Mass Spectrometry Lab
Q-tof UE521
Qtof_41960 39 (2.793) AM (Cen,5, 80.00, Ar,15000.0,0.00,0.70); Sm (SG, 2x5.00); Cm (39:41-7:10x8.000)
1: TOF MS ES+
1.21e4
Compound 6e
MeO
OCH3
450.2
482.3
451.3
468.3
483.3
100
%
0
m/z
50 75 100 125 150 175 200 225 250 275 300 325 350 375 400 425 450 475 500 525 550 575 600 625 650

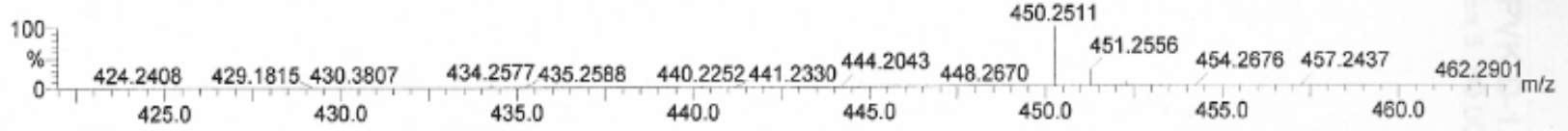
Elemental Composition Report

Single Mass Analysis

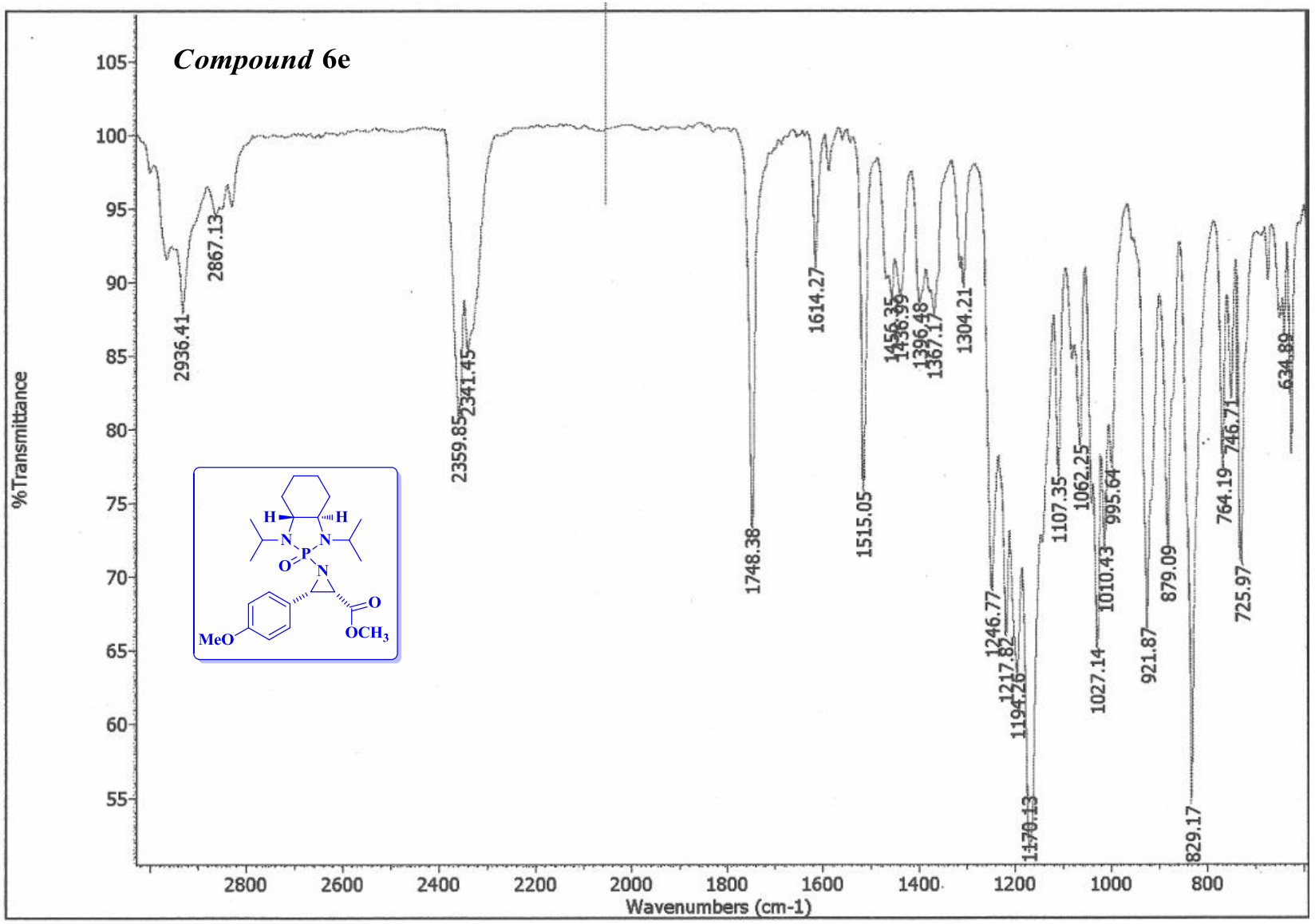
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 600.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
96 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-250 N: 2-4 O: 2-4 P: 0-1

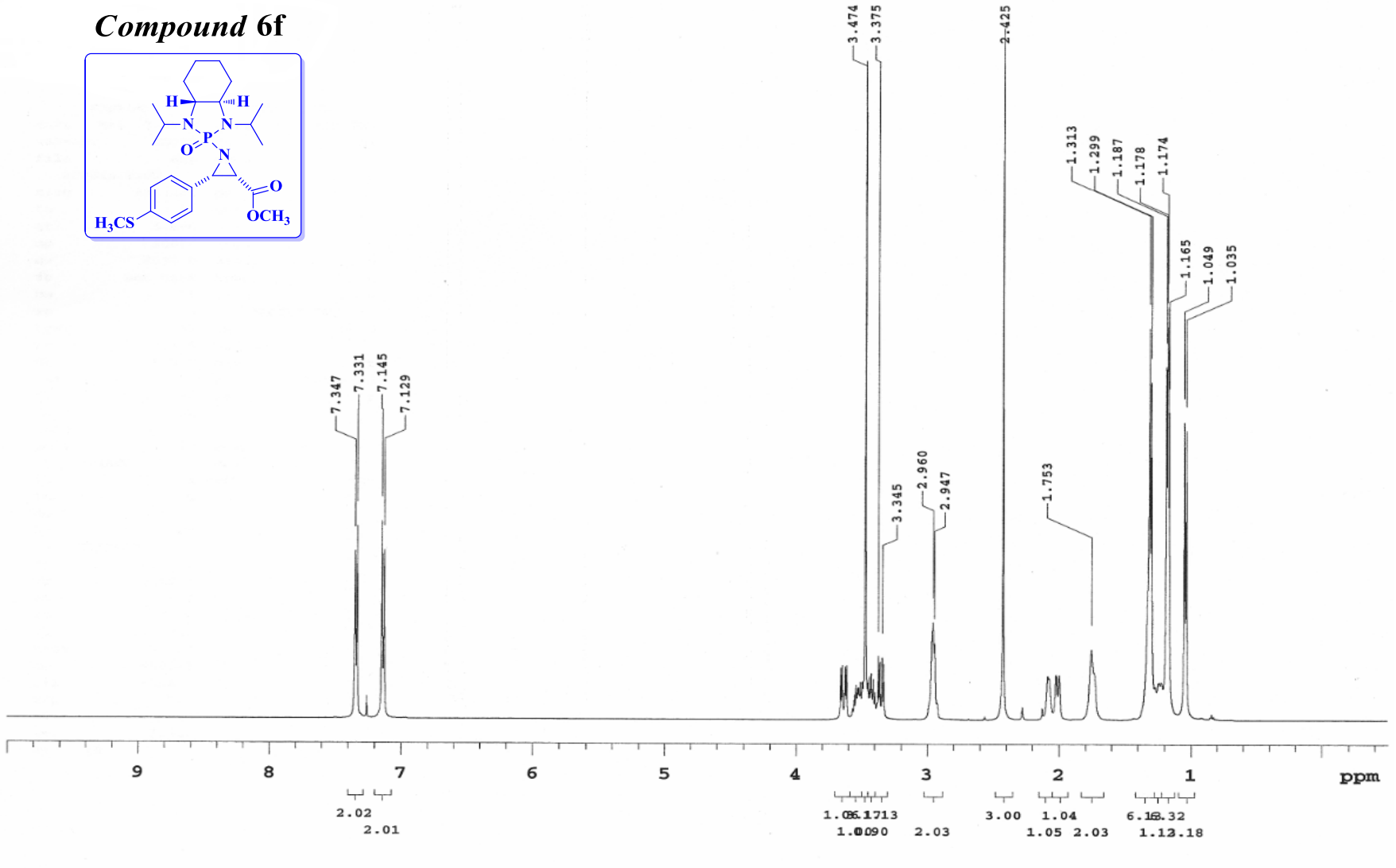
Padmanabha Kattamuri, PVK-D-12 University of Illinois, SCS, Mass Spectrometry Lab Q-tof UE521
Qtof_41960 52 (3.721) AM (Cen,3, 80.00, Ar,15000.0,716.46,0.70,LS 3); Sm (SG, 2x3.00); Cm (52:54) 1: TOF MS ES+
4.07e+003



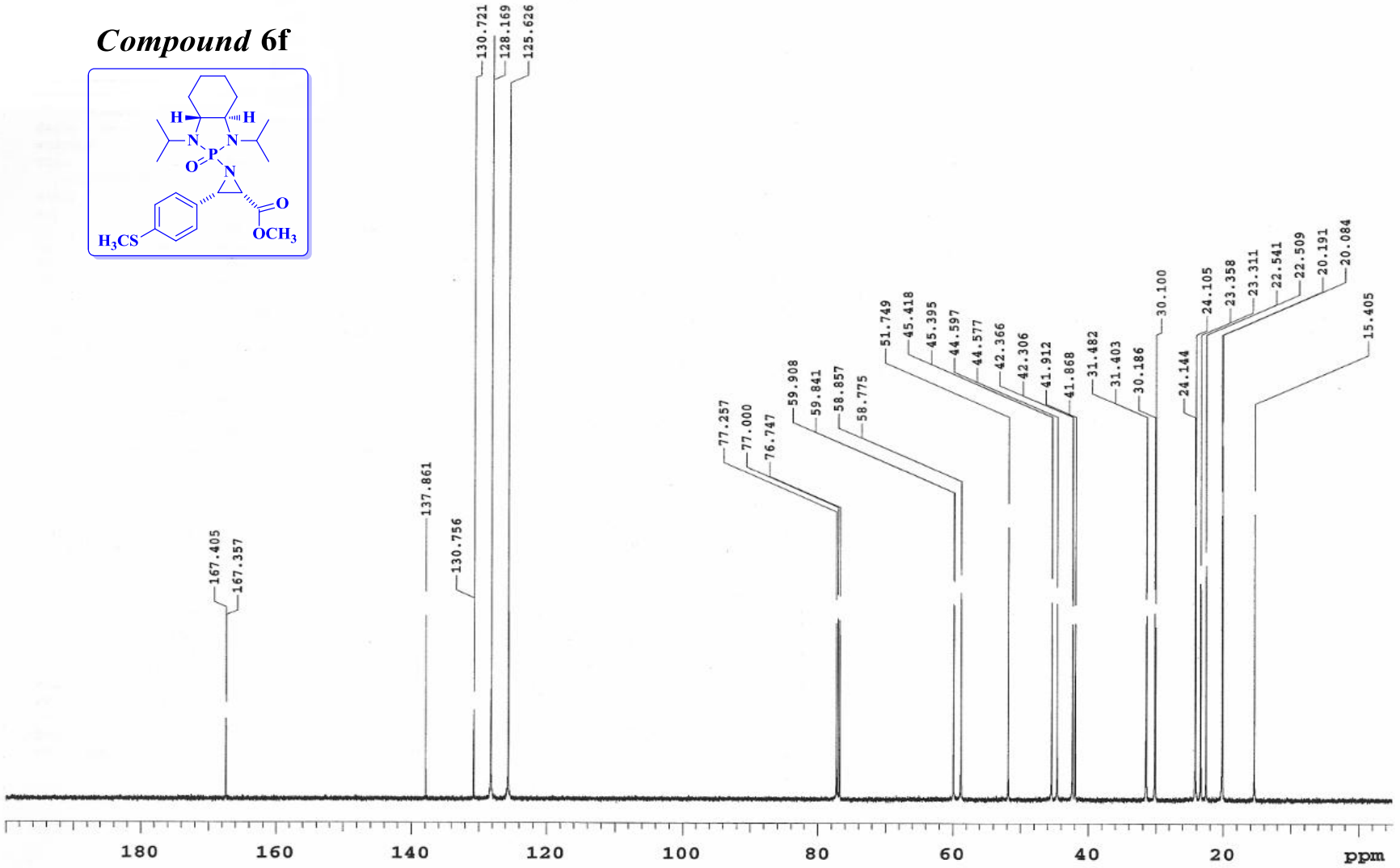
Minimum:				-1.5		
Maximum:		5.0	10.0	600.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
450.2511	450.2522	-1.1	-2.4	7.5	21.2	C23 H37 N3 O4 P



***Compound* 6f**



Compound 6f



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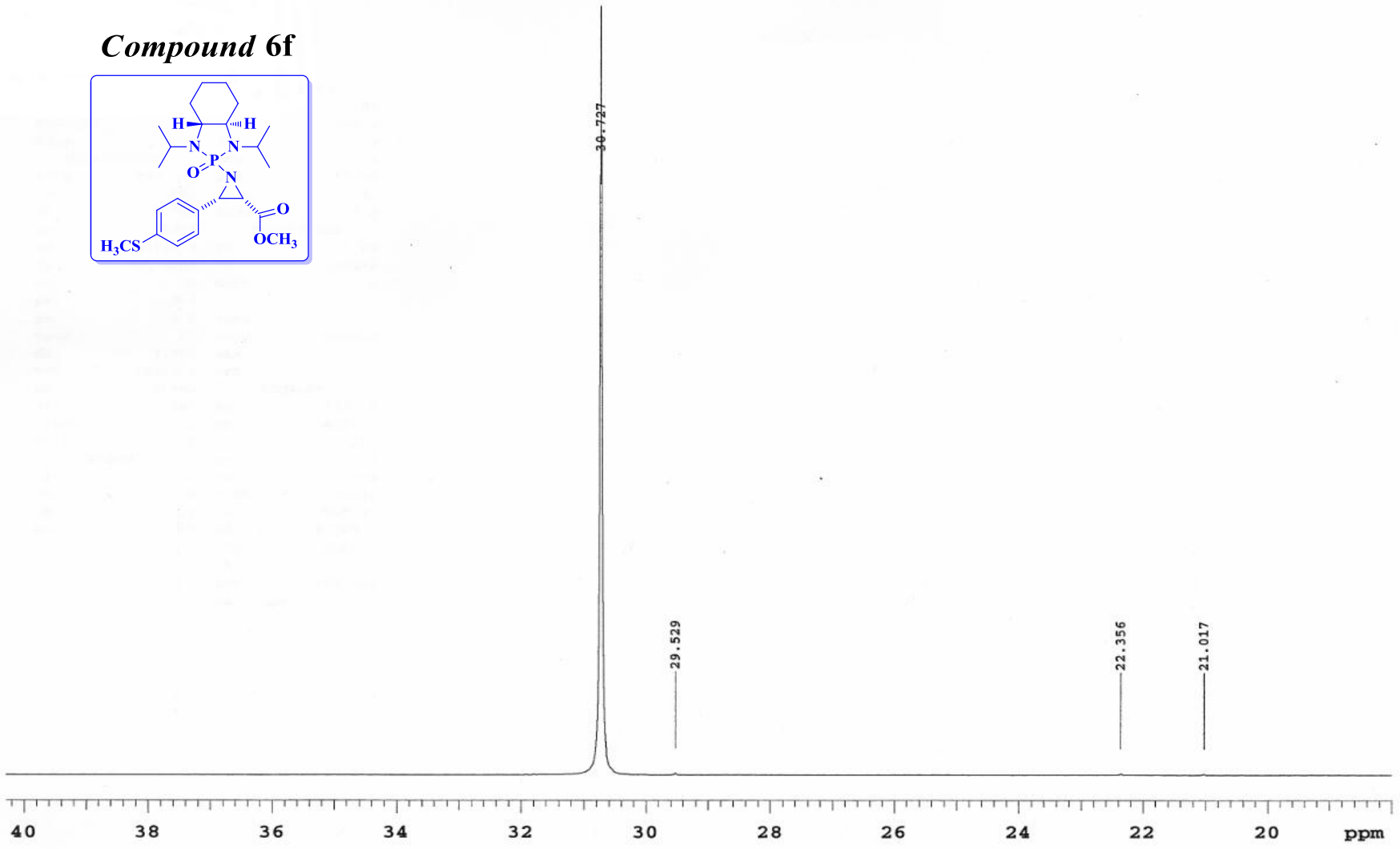
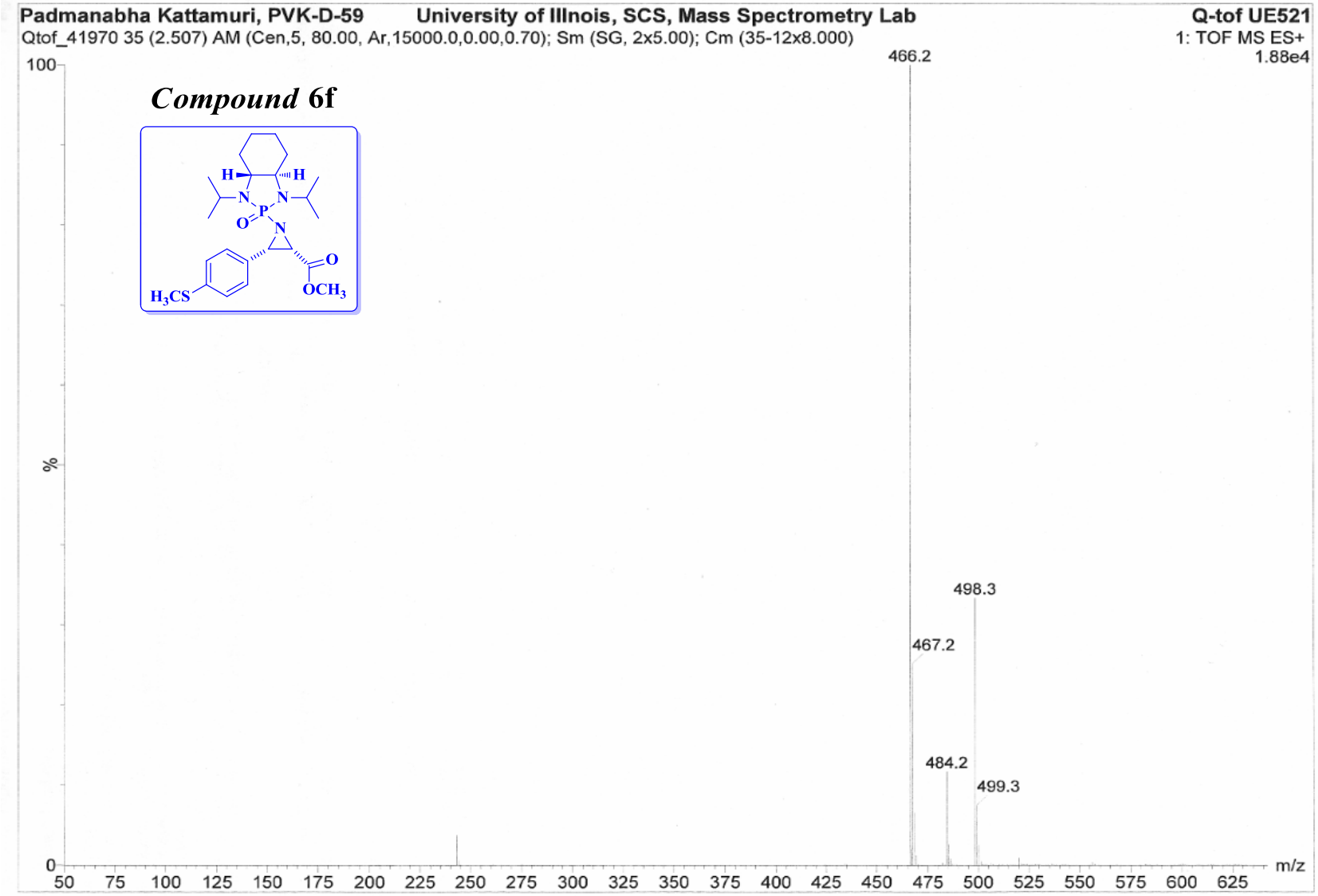




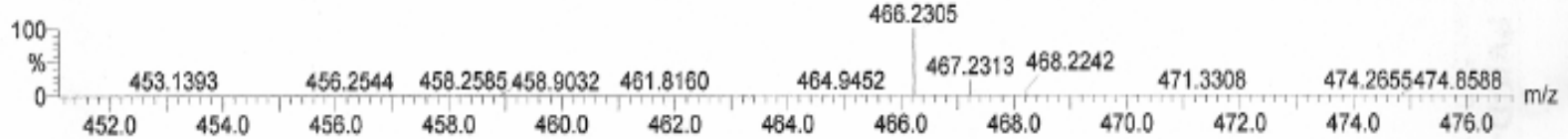
Elemental Composition Report

Single Mass Analysis

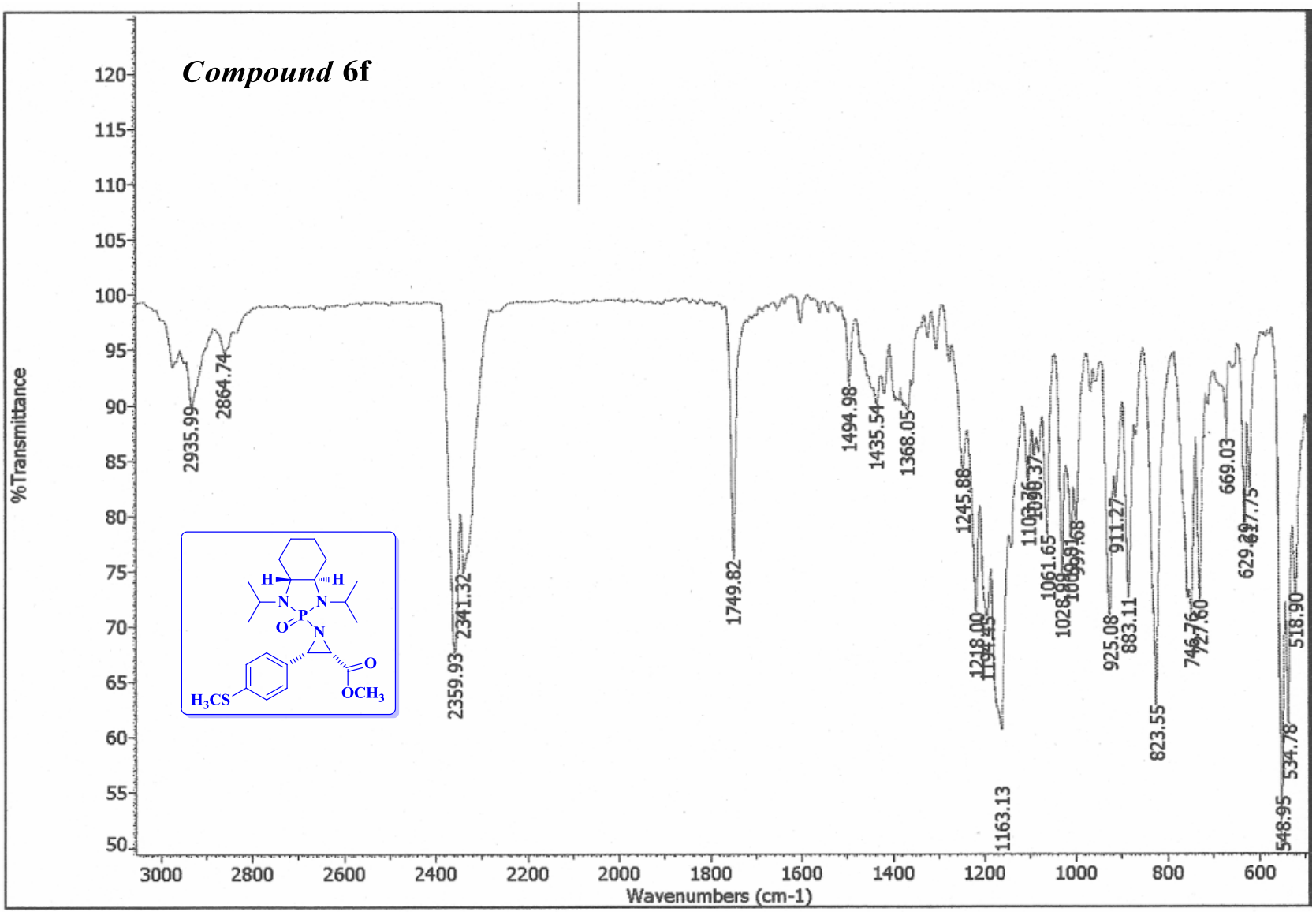
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 600.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
193 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-250 N: 2-4 O: 2-4 P: 0-1 S: 0-1

Padmanabha Kattamuri, PVK-D-59 University of Illinois, SCS, Mass Spectrometry Lab Q-tof UE521
Qtof_41970 29 (2.043) AM (Cen,3, 80.00, Ar,15000.0,716.46,0.70); Sm (SG, 2x3.00); Cm (28:29) 2: TOF MS ES+
3.20e+002

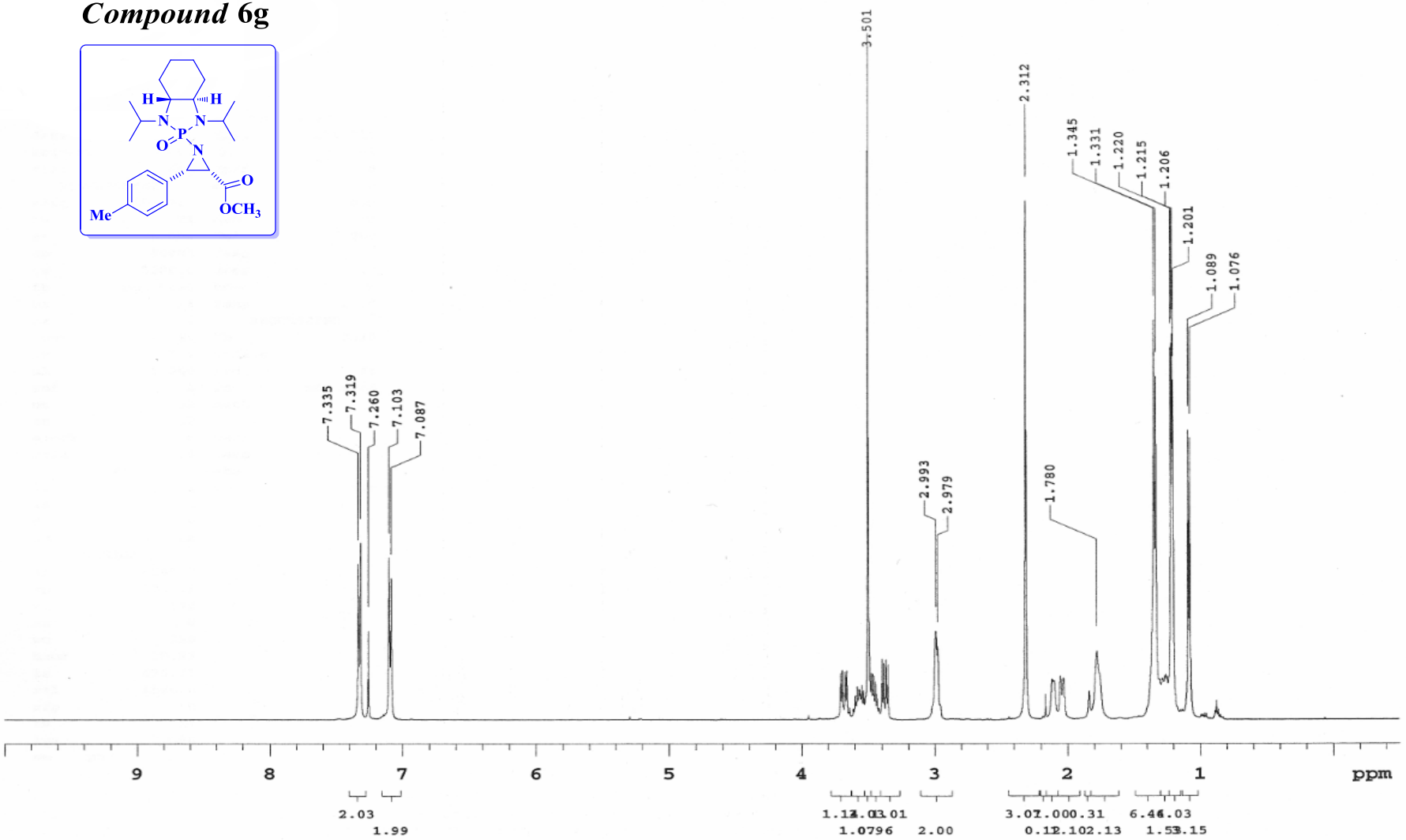


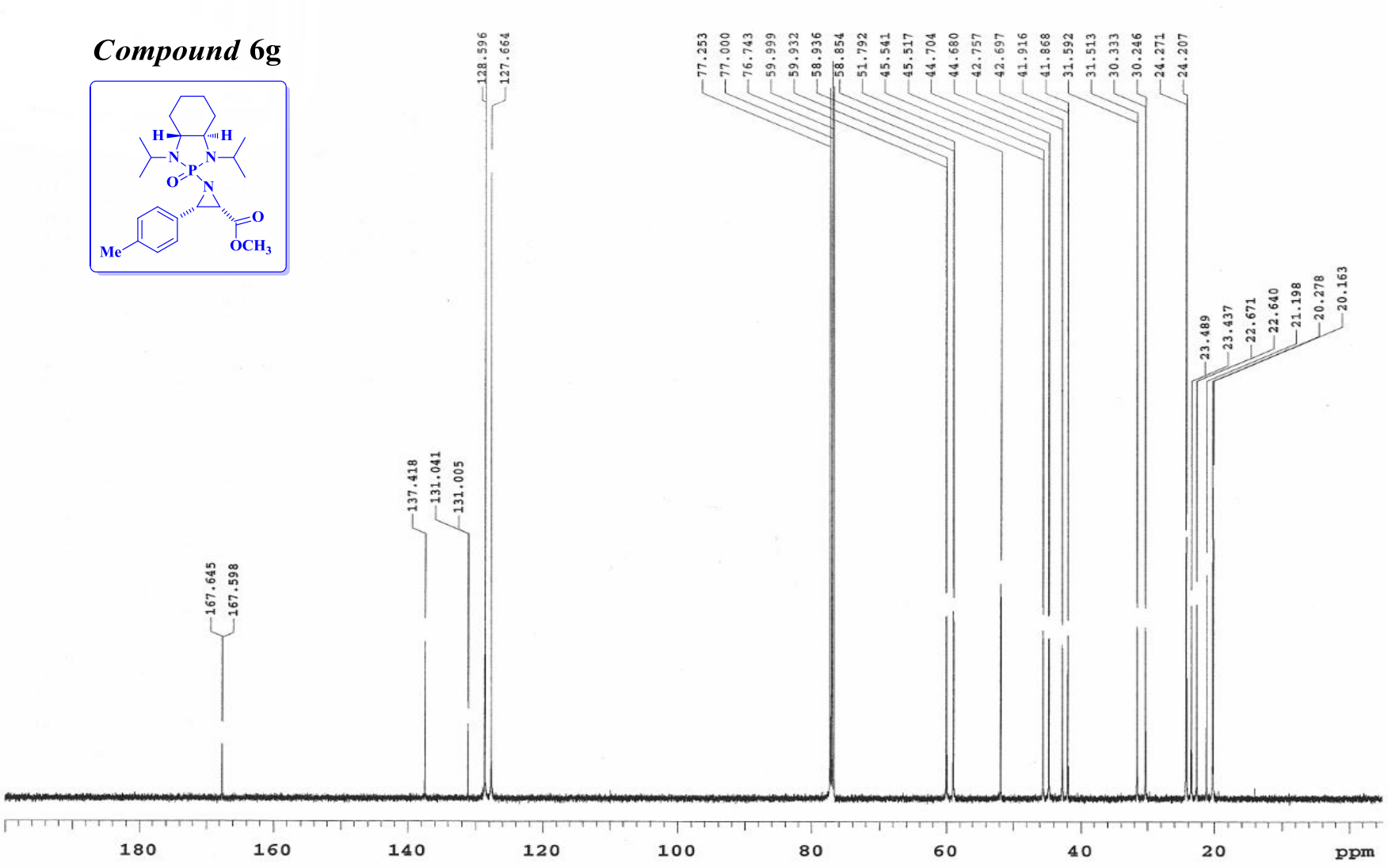
Minimum:				-1.5		
Maximum:		5.0	10.0	600.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
466.2305	466.2293	1.2	2.6	7.5	2.2	C23 H37 N3 O3 P S
	466.2260	4.5	9.7	12.5	5.7	C26 H33 N3 O3 P



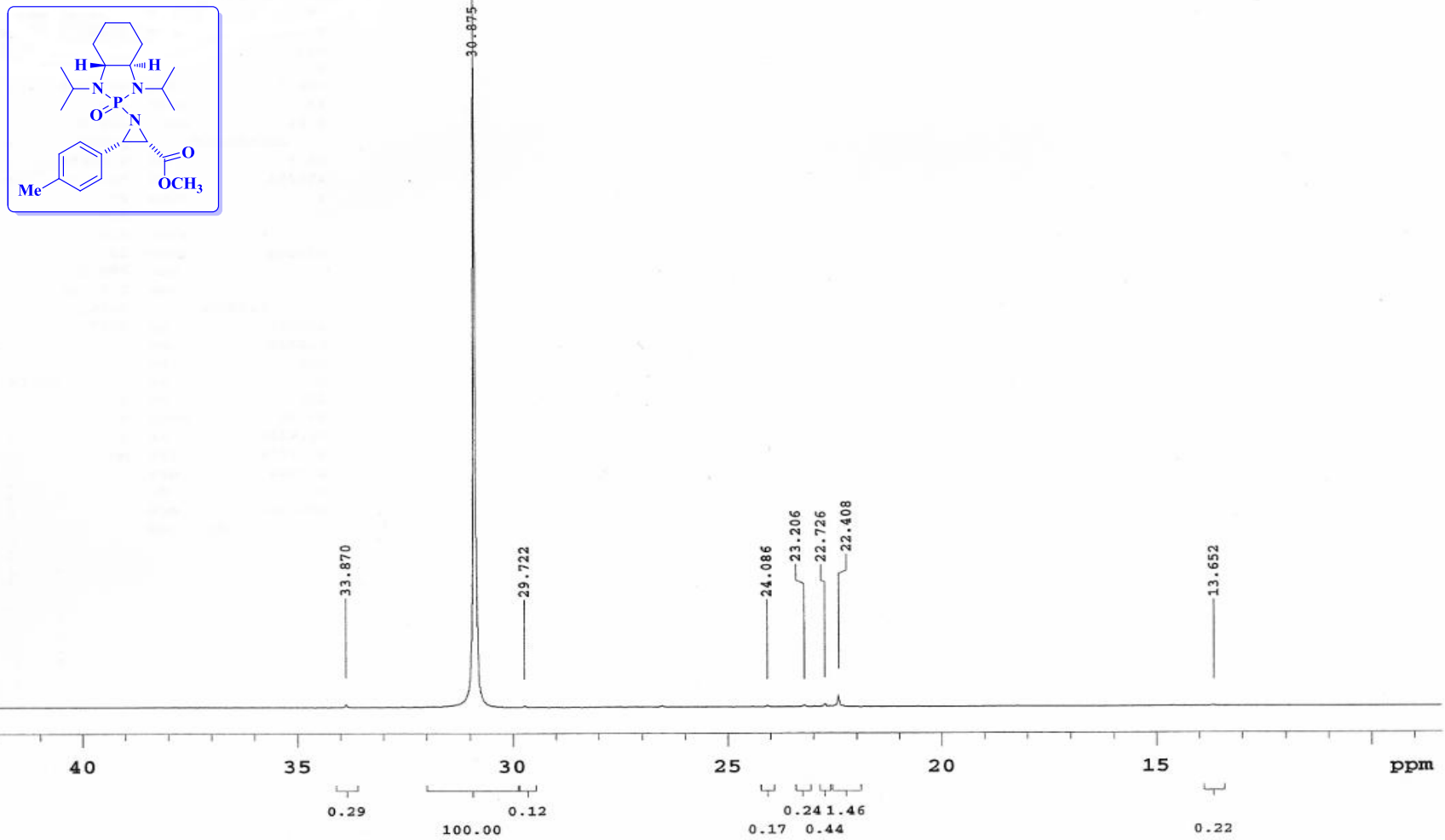
***Compound* 6g**

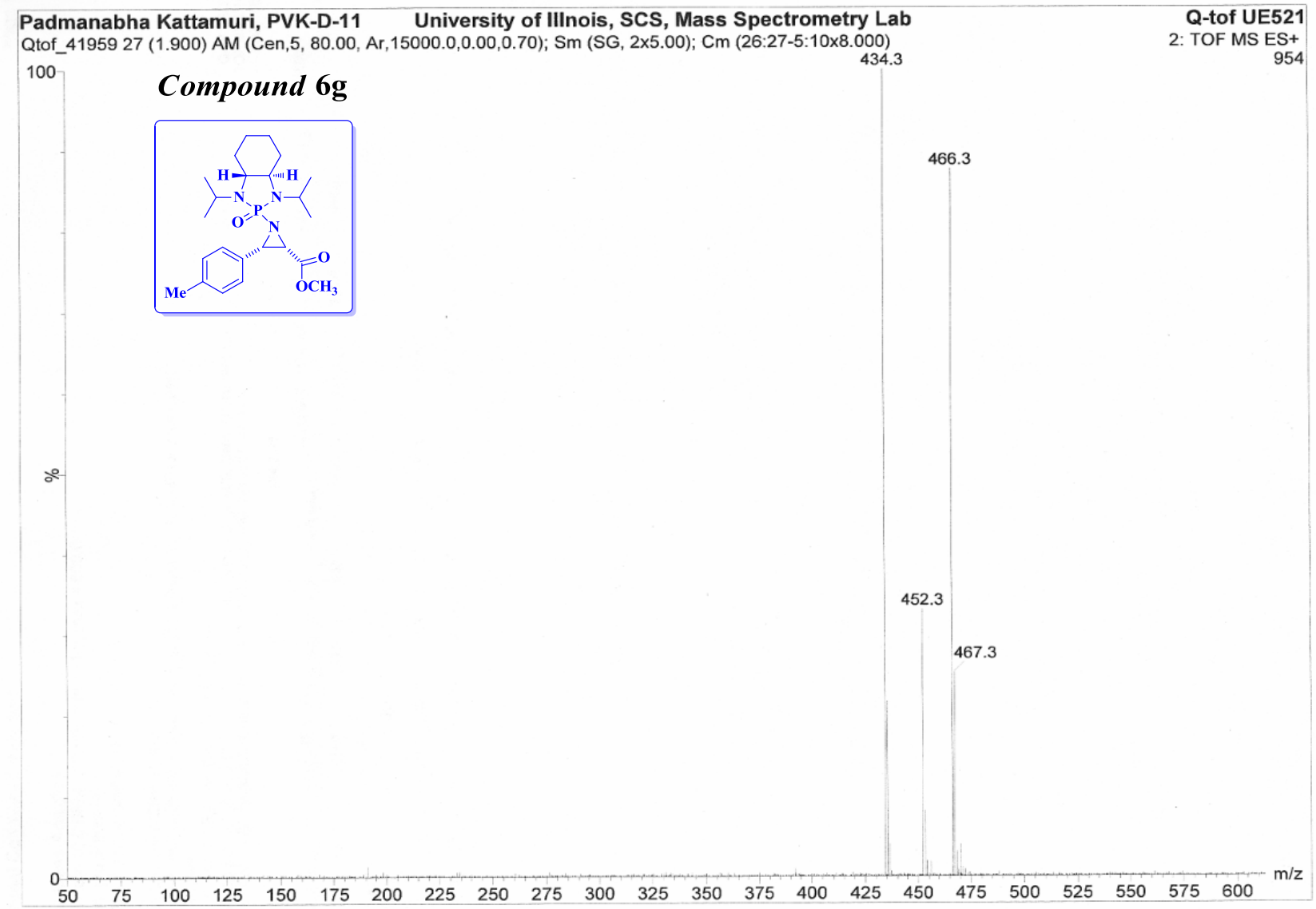
H
H
N
N
P
O
N
O
OCH3
Me


3.501
2.312
1.345
1.331
1.220
1.215
1.206
1.201
1.089
1.076
7.335
7.319
7.260
7.103
7.087
2.993
2.979
1.780
9
8
7
6
5
4
3
2
1
ppm
2.03
1.99
2.00
1.00
0.31
6.46
6.03
3.15



***Compound* 6g**


30.875
33.870
29.722
24.086
23.206
22.726
22.408
13.652
40
35
30
25
20
15
ppm
0.29
100.00
0.12
0.17
0.24
0.44
1.46
0.22



Elemental Composition Report

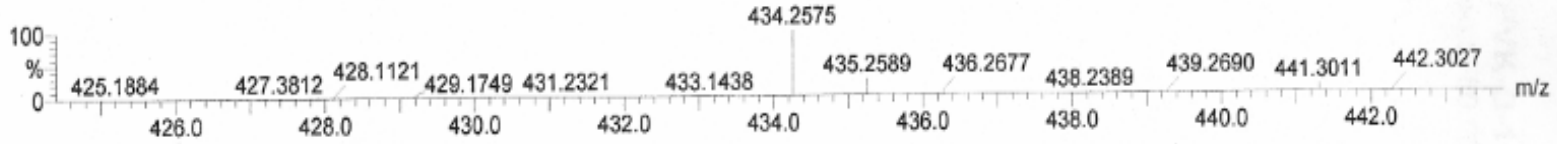
Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 600.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

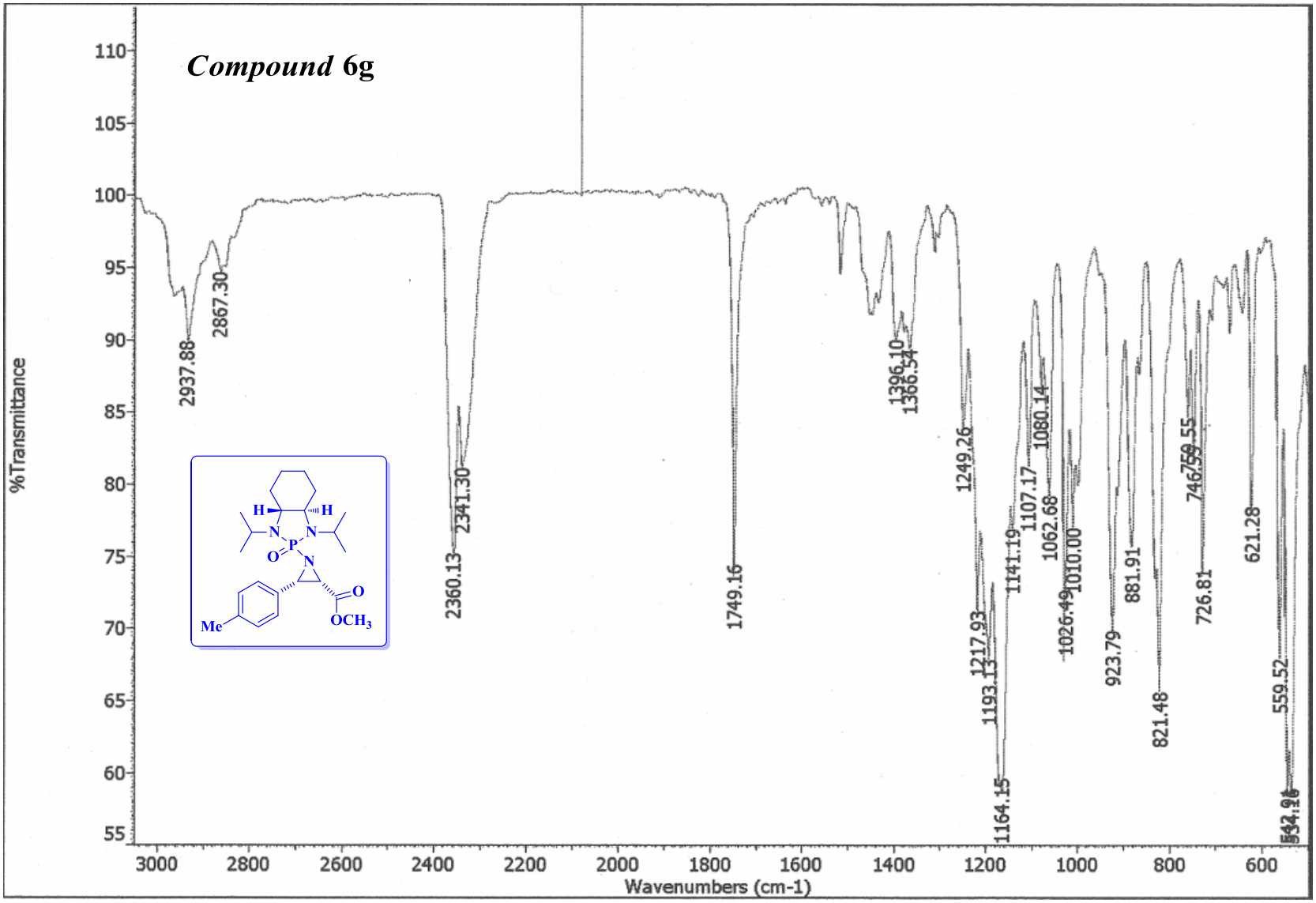
Monoisotopic Mass, Even Electron Ions
91 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-250 N: 2-4 O: 2-4 P: 0-1

Padmanabha Kattamuri, PVK-D-11 University of Illnois, SCS, Mass Spectrometry Lab
Qtof_41959 24 (1.686) AM (Cen,3, 80.00, Ar,15000.0,716.46,0.70); Sm (SG, 2x3.00); Cm (21:24)

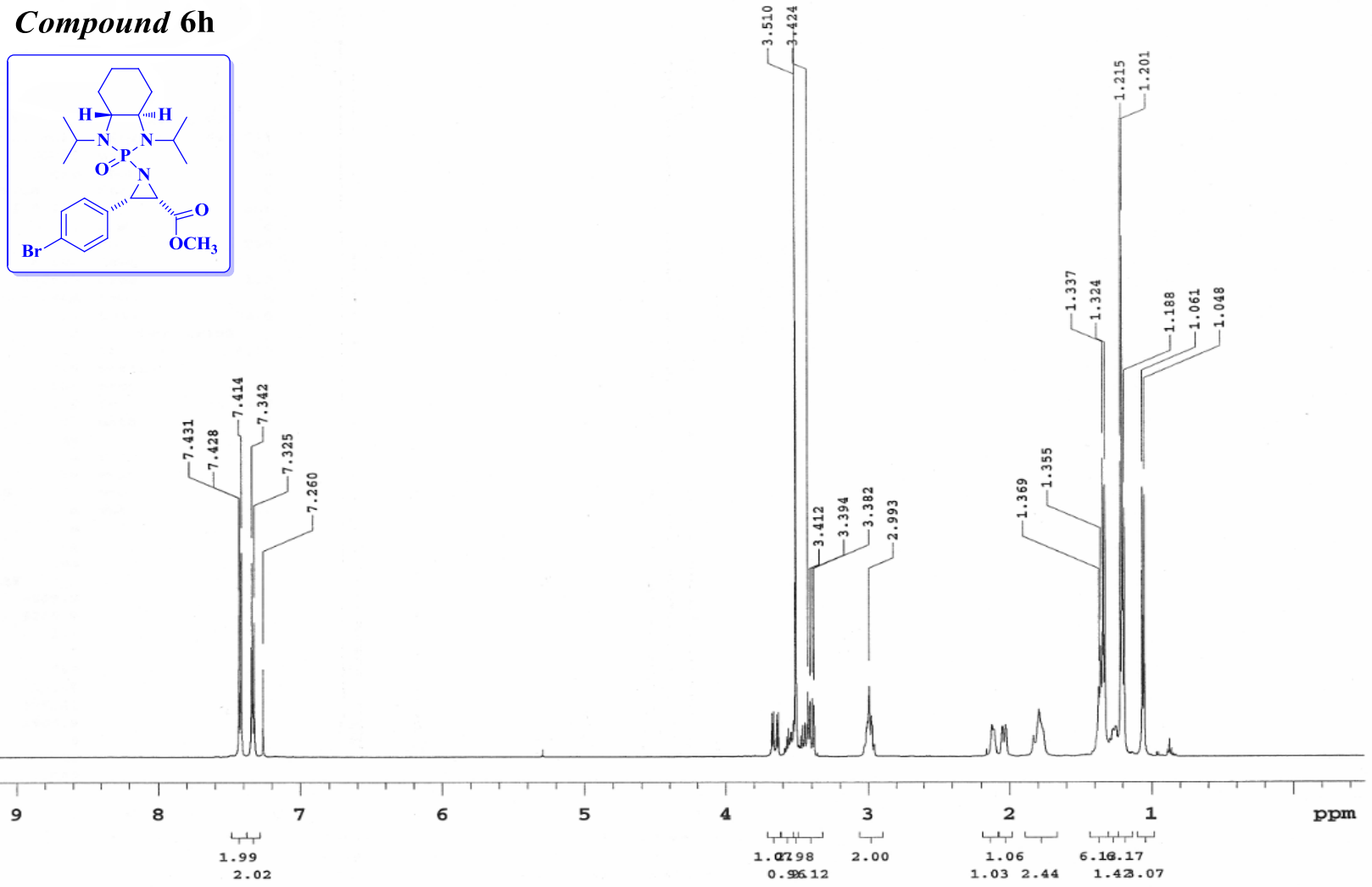
Q-tof UE521
2: TOF MS ES+
7.60e+002



Minimum:				-1.5		
Maximum:		5.0	10.0	600.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
434.2575	434.2573	0.2	0.5	7.5	0.5	C23 H37 N3 O3 P



***Compound* 6h**



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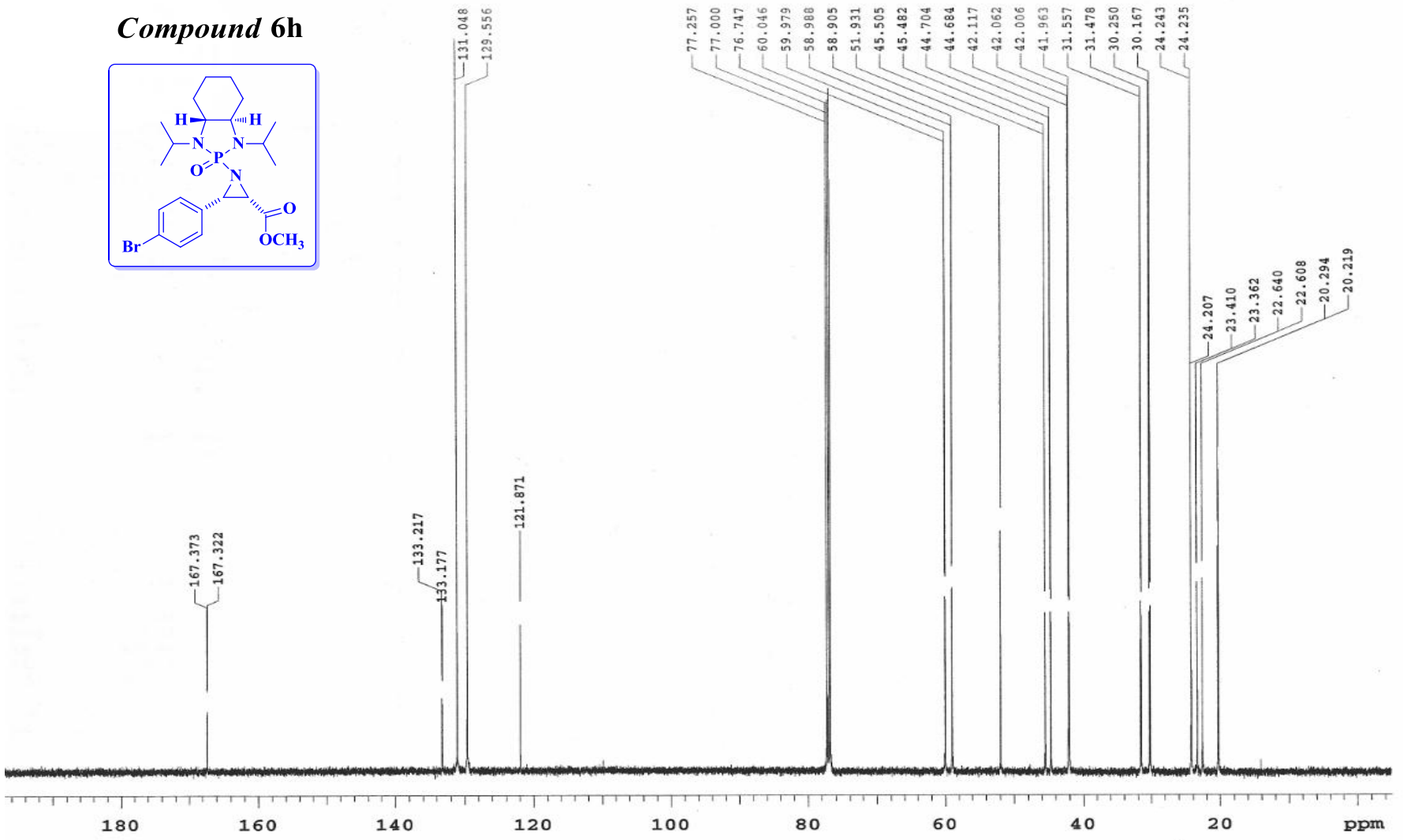

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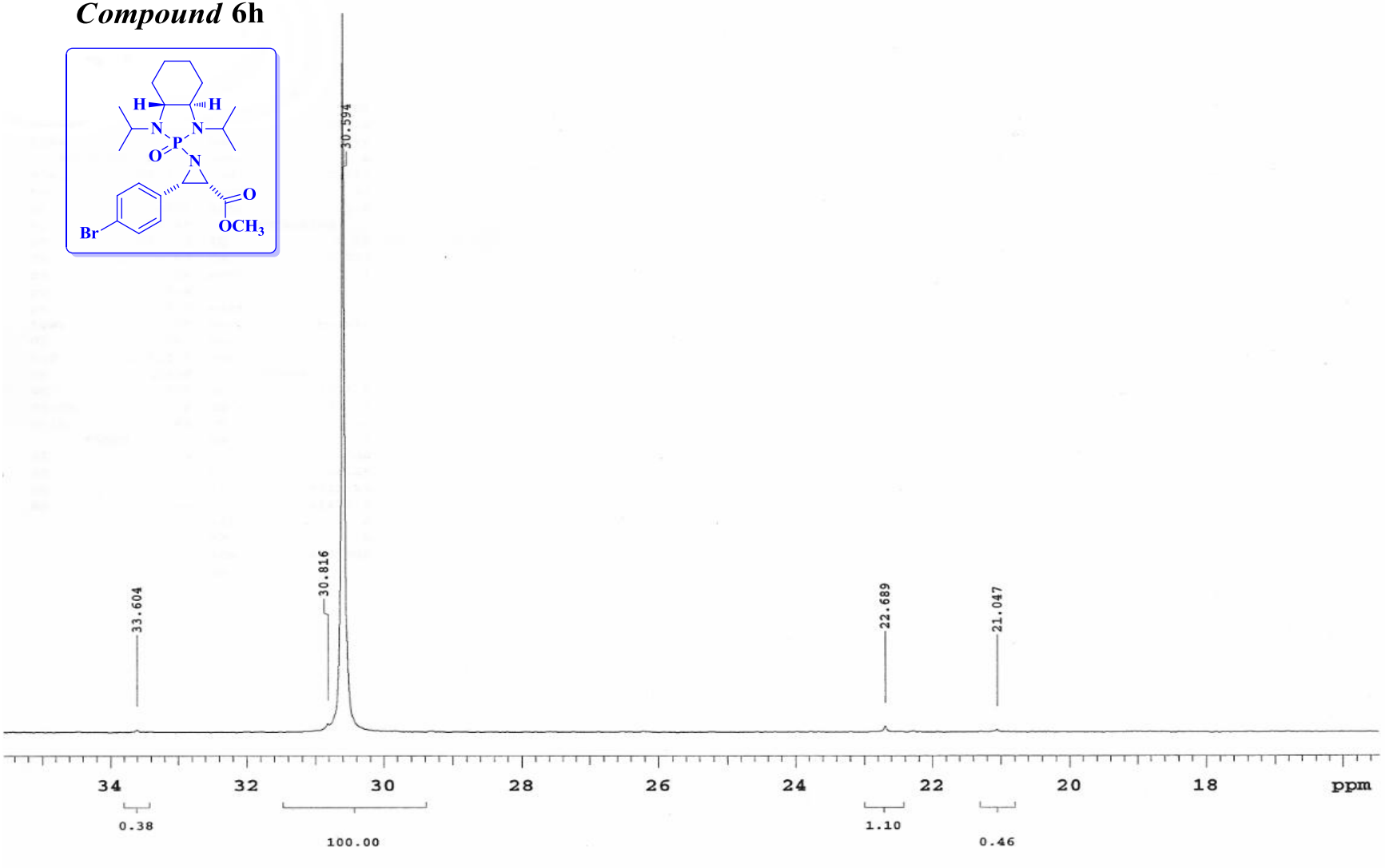
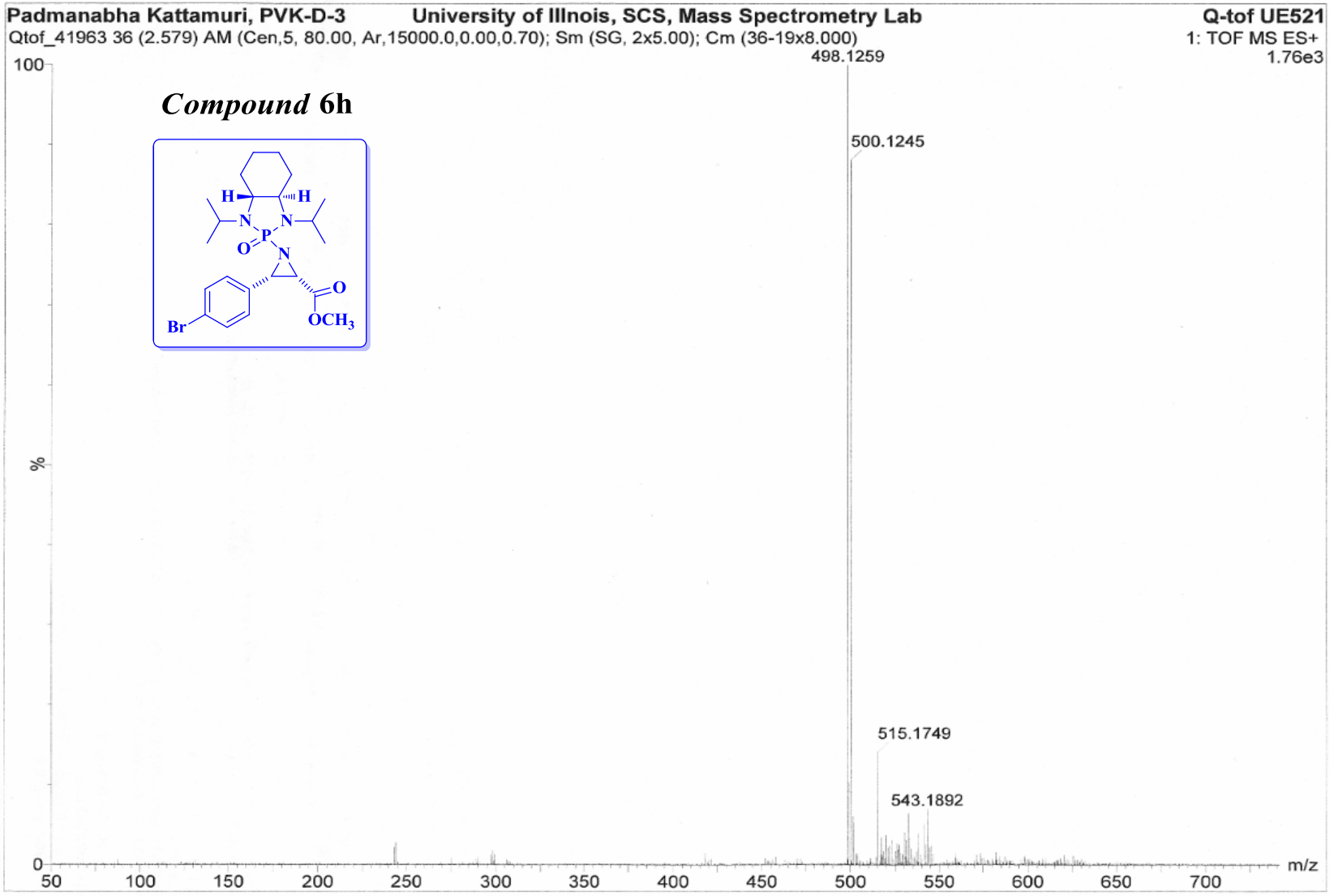




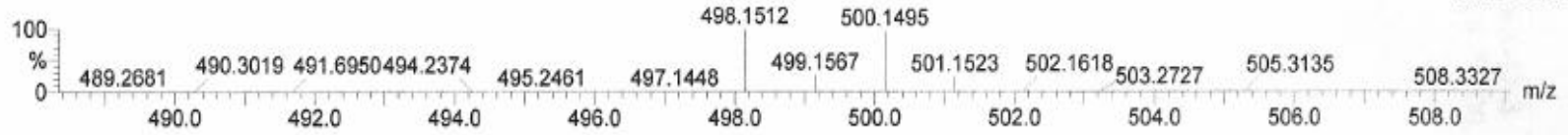
Elemental Composition Report

Single Mass Analysis

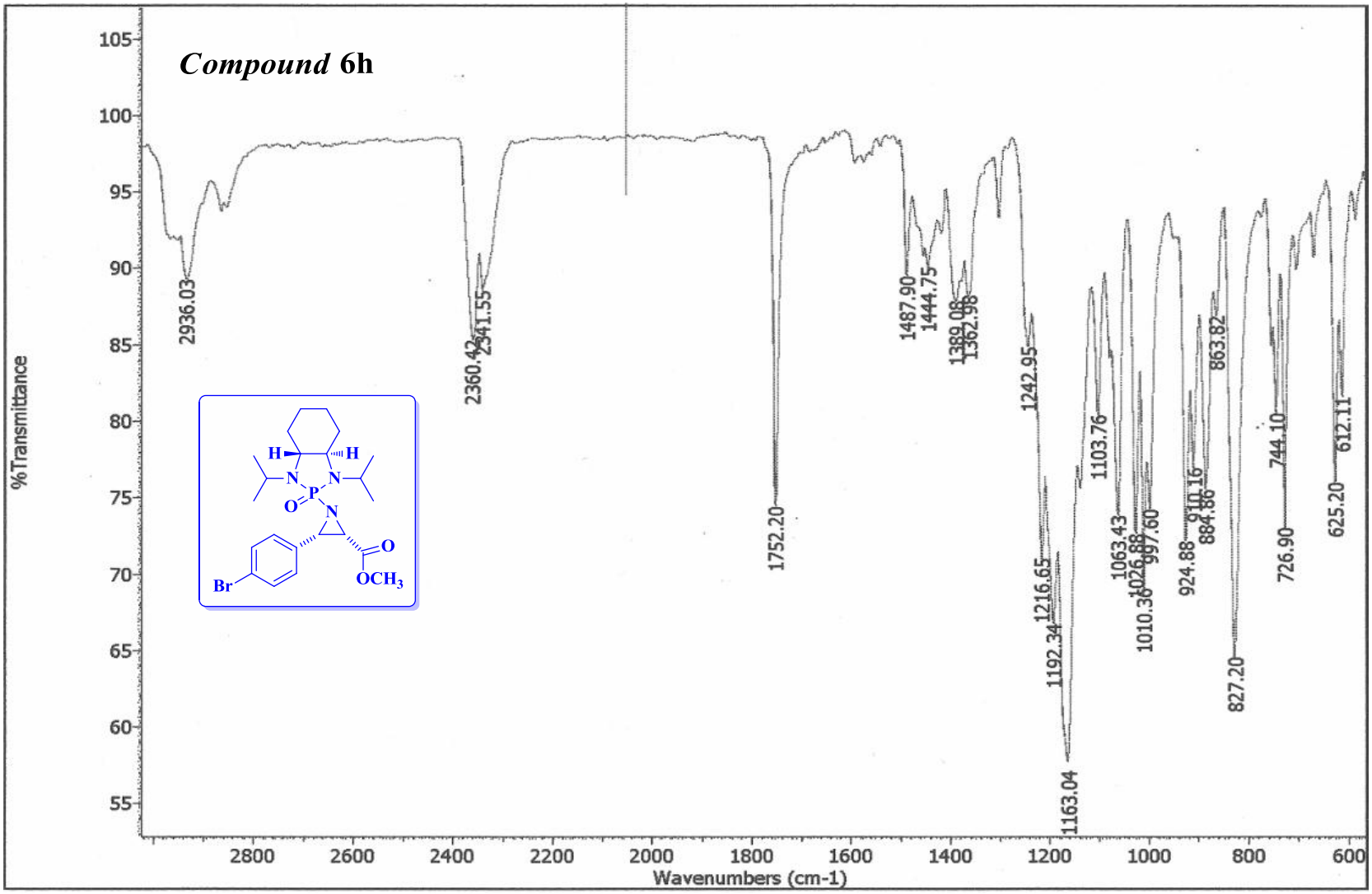
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 600.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

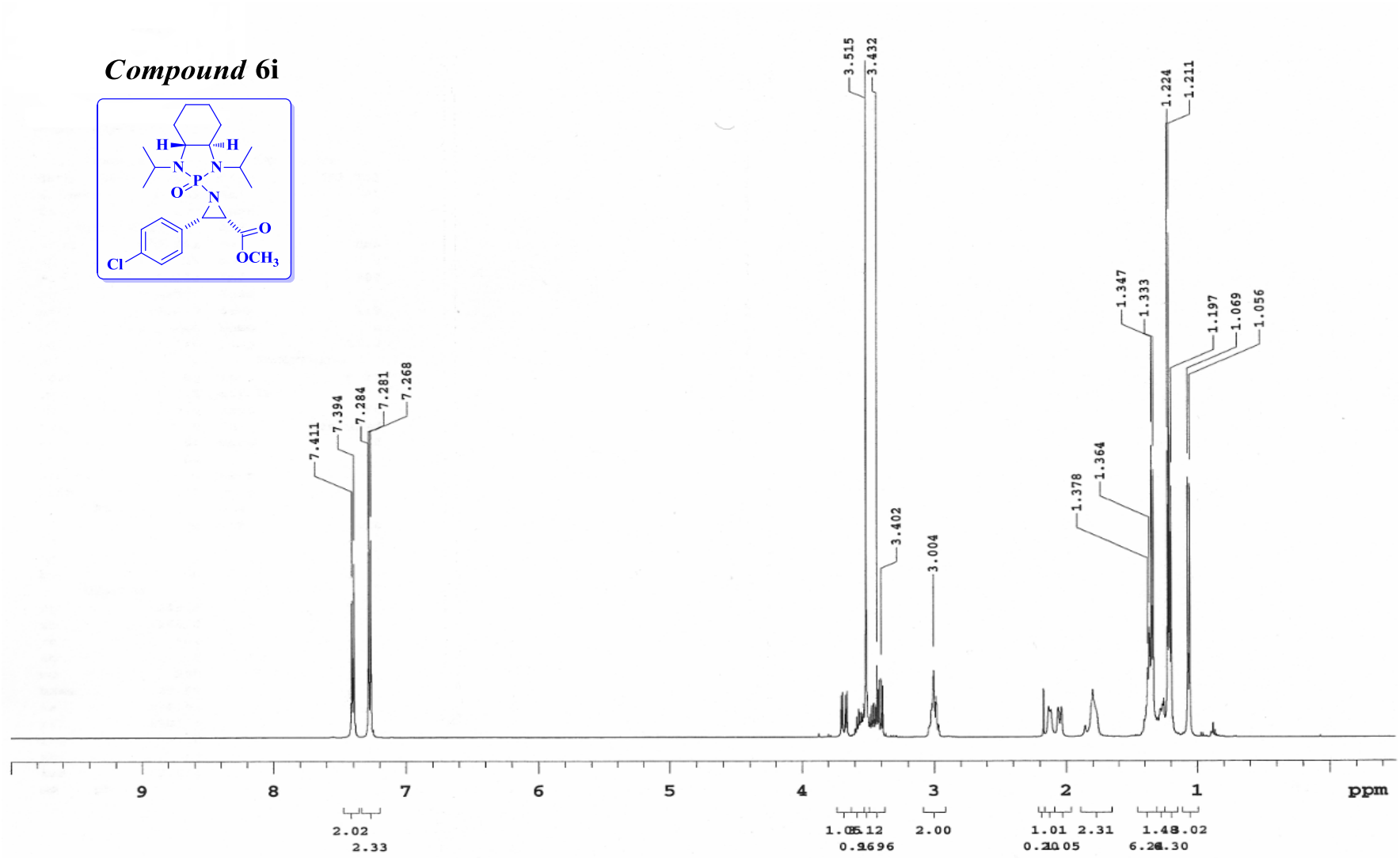
Monoisotopic Mass, Even Electron Ions
87 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-250 N: 2-4 O: 2-4 P: 0-1 Br: 1-1

Padmanabha Kattamuri, PVK-D-3 University of Illnois, SCS, Mass Spectrometry Lab Q-tof UE521
Qtof_41963 34 (2.400) AM (Cen,3, 80.00, Ar,15000.0,716.46,0.70); Sm (SG, 2x3.00); Cm (31:36) 2: TOF MS ES+
7.77e+002

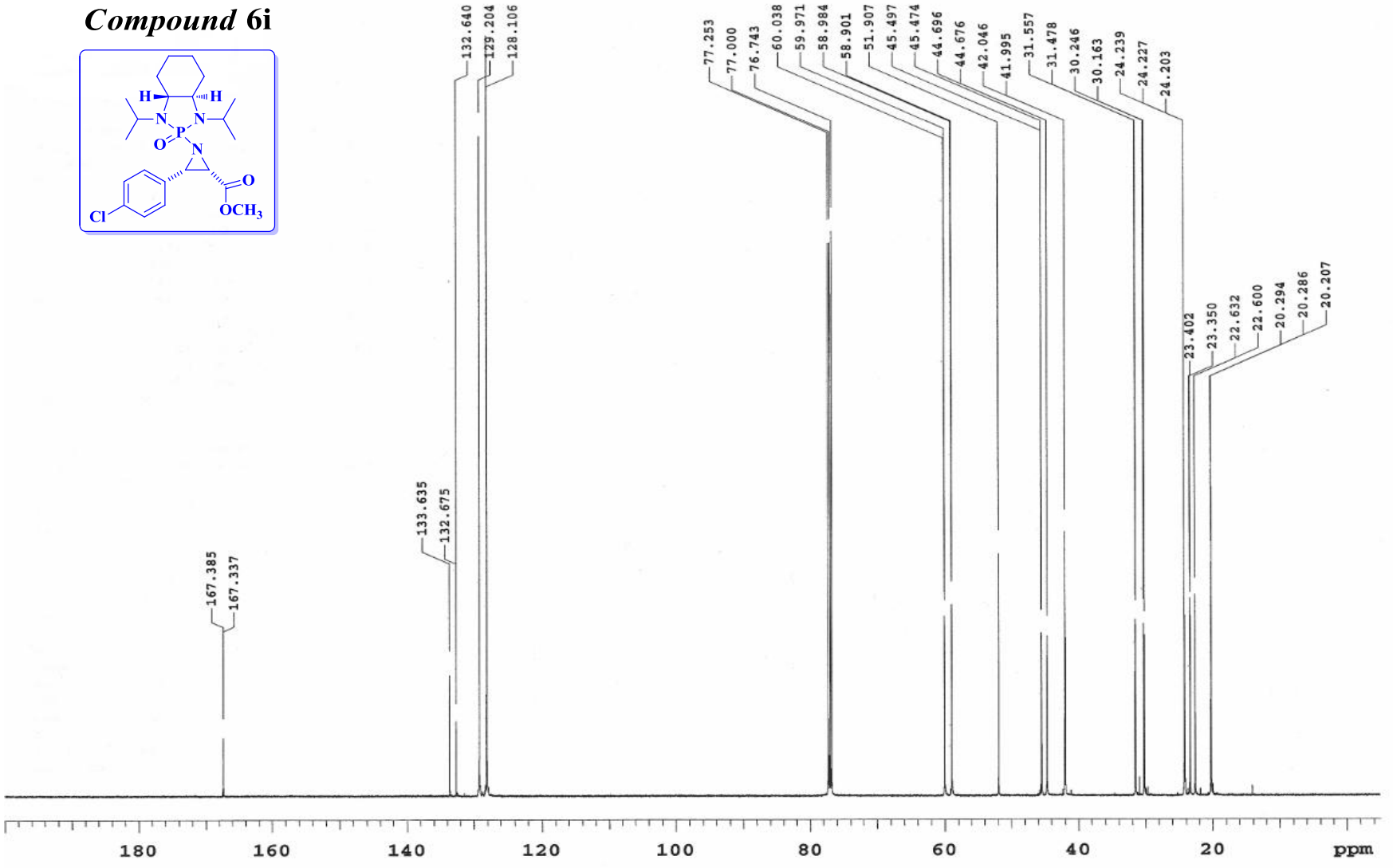


Minimum:				-1.5		
Maximum:		5.0	10.0	600.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
498.1512	498.1521	-0.9	-1.8	7.5	0.5	C22 H34 N3 O3 P Br

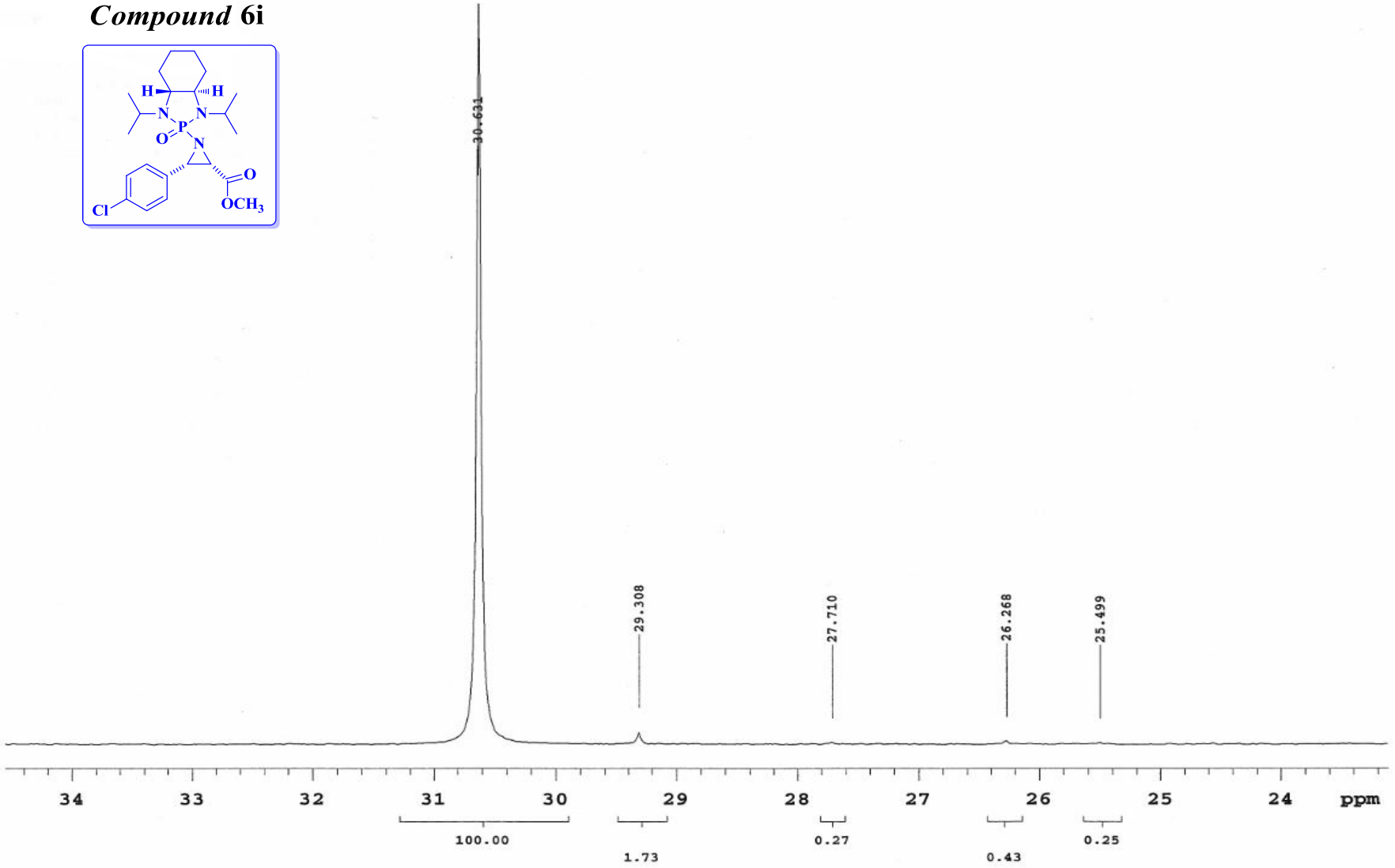


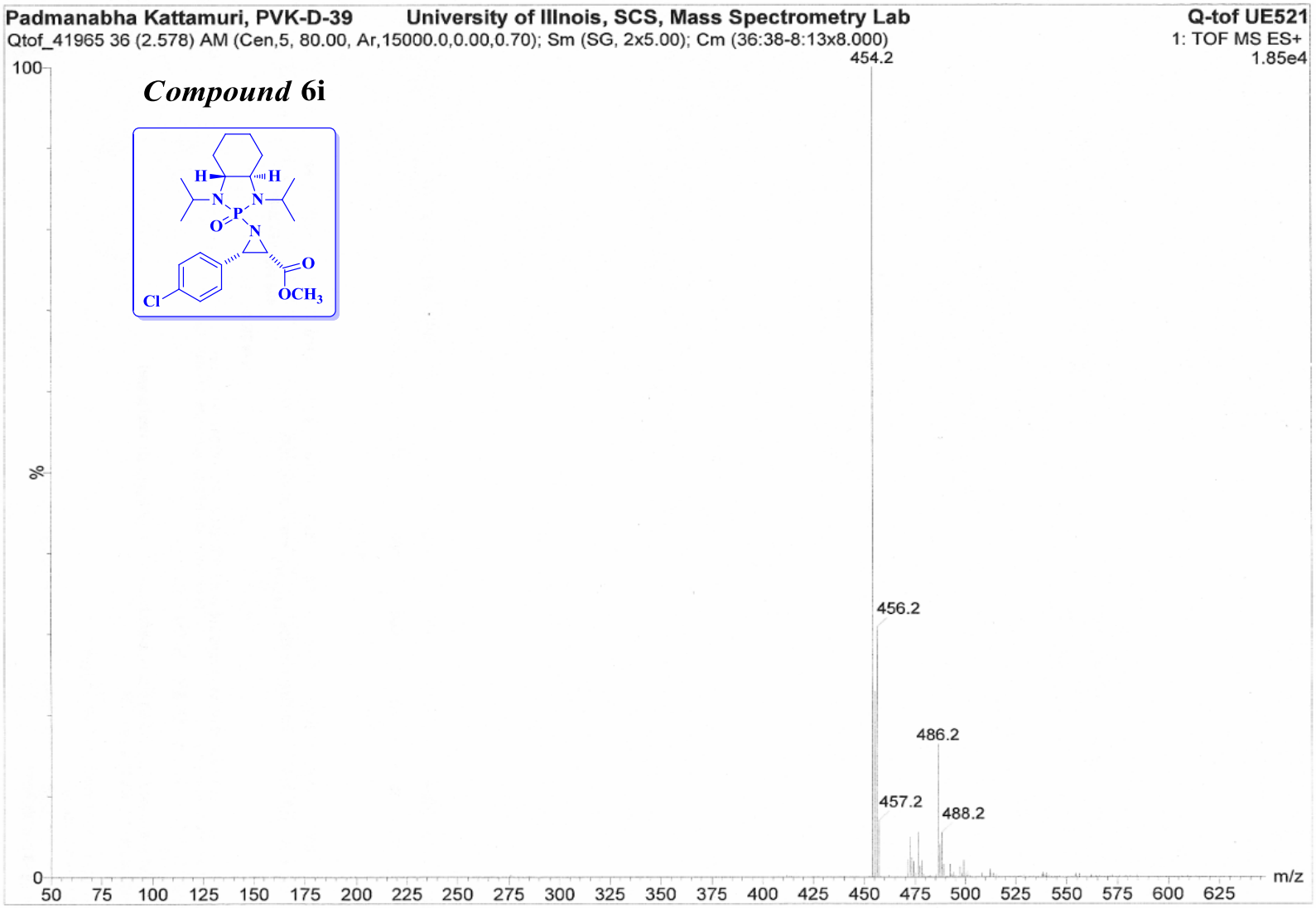


***Compound* 6i**



***Compound* 6i**




Padmanabha Kattamuri, PVK-D-39
University of Illnois, SCS, Mass Spectrometry Lab
Q-tof UE521
Qtof_41965 36 (2.578) AM (Cen,5, 80.00, Ar,15000.0,0.00,0.70); Sm (SG, 2x5.00); Cm (36:38-8:13x8.000)
1: TOF MS ES+
1.85e4
Compound 6i
454.2
456.2
486.2
457.2
488.2
100
%
0
m/z
50 75 100 125 150 175 200 225 250 275 300 325 350 375 400 425 450 475 500 525 550 575 600 625

Elemental Composition Report

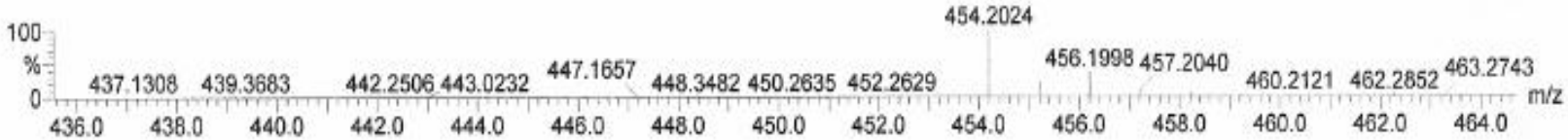
Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 600.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

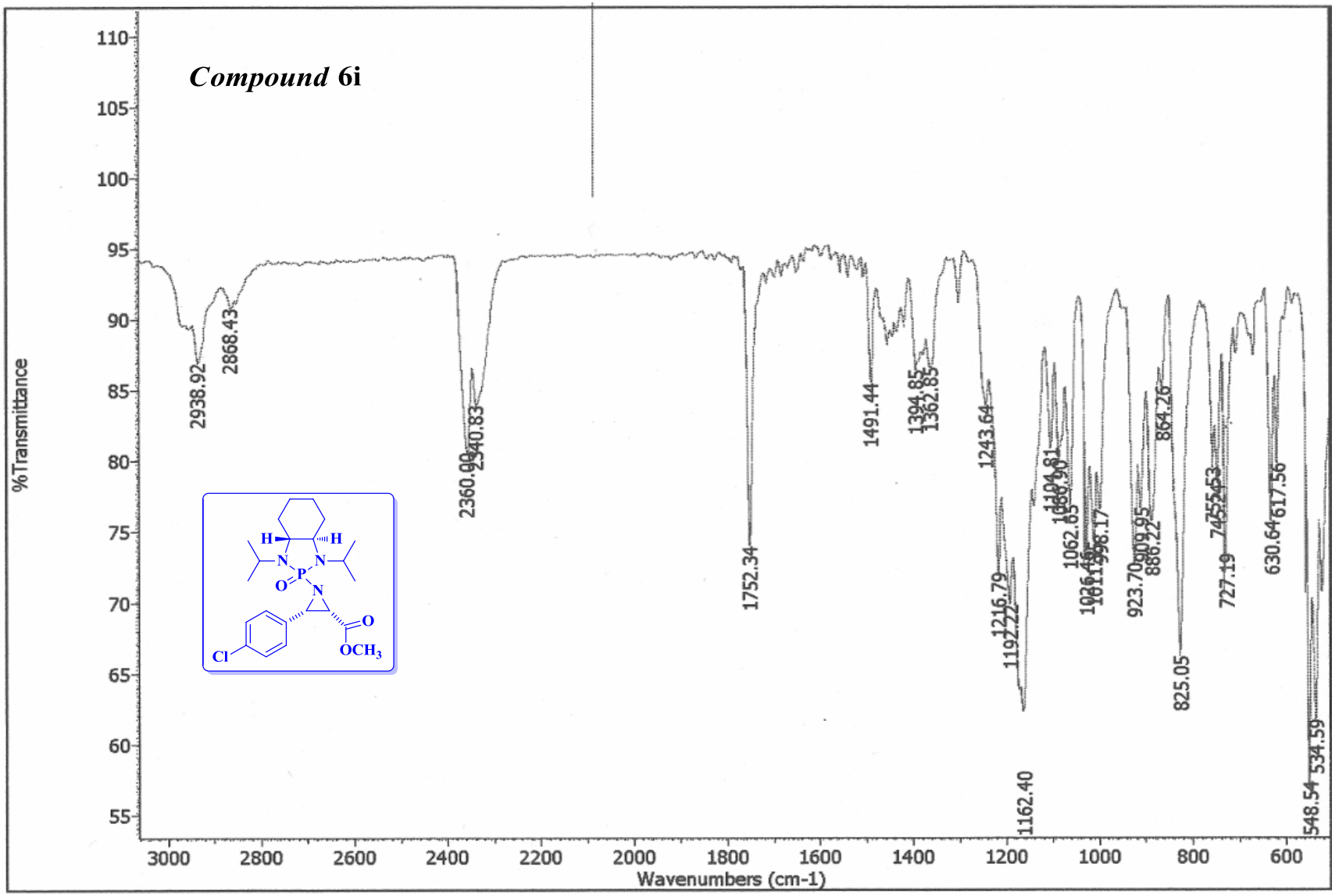
Monoisotopic Mass, Even Electron Ions
87 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-250 N: 2-4 O: 2-4 P: 0-1 Cl: 1-1

Padmanabha Kattamuri, PVK-D-39 University of Illinois, SCS, Mass Spectrometry Lab
Qtof_41965 51 (3.650) AM (Cen,3, 80.00, Ar,15000.0,716.46,0.70,LS 3); Sm (SG, 2x3.00); Cm (51:54)

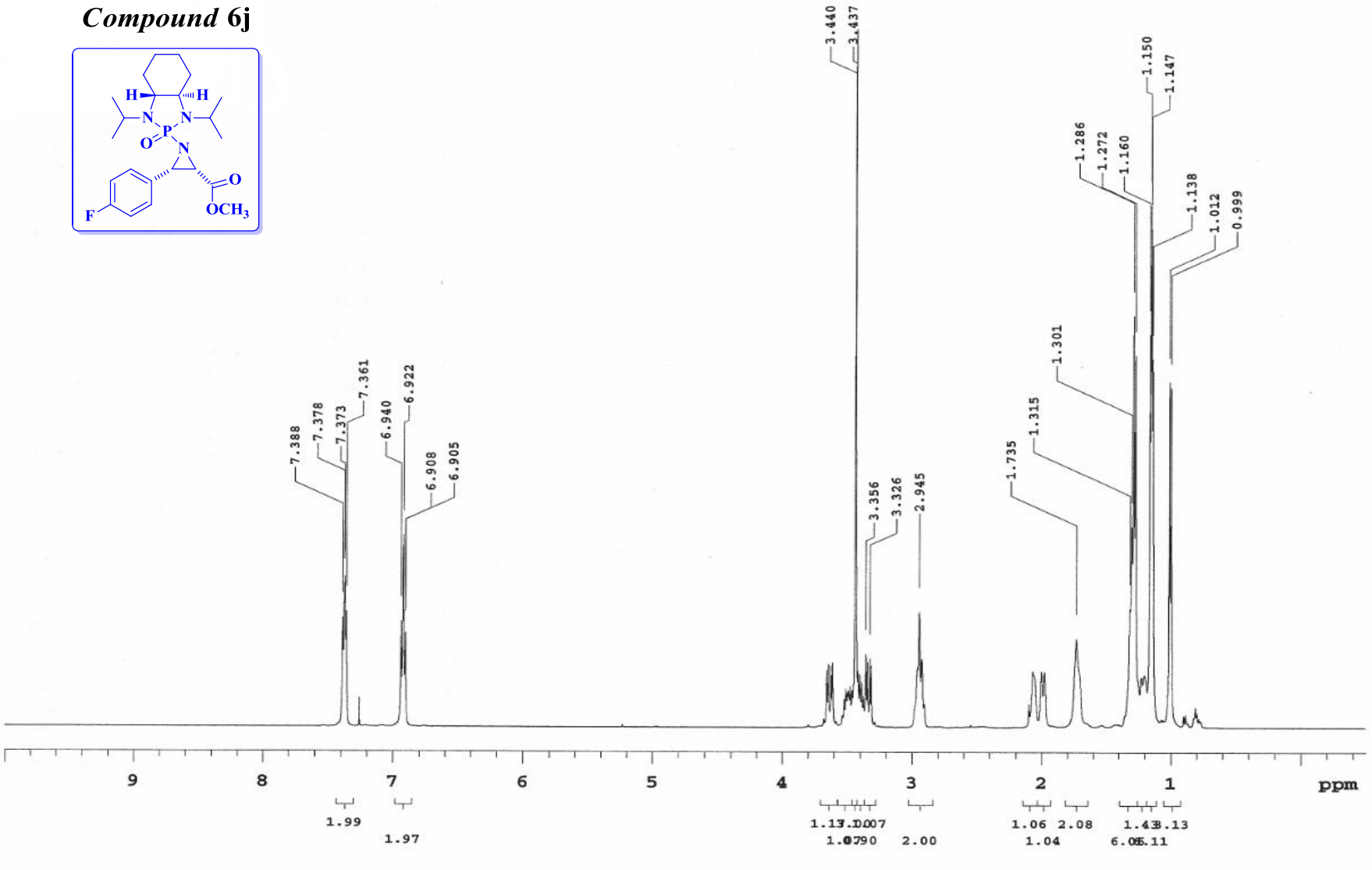
Q-tof UE521
1: TOF MS ES+
2.55e+003



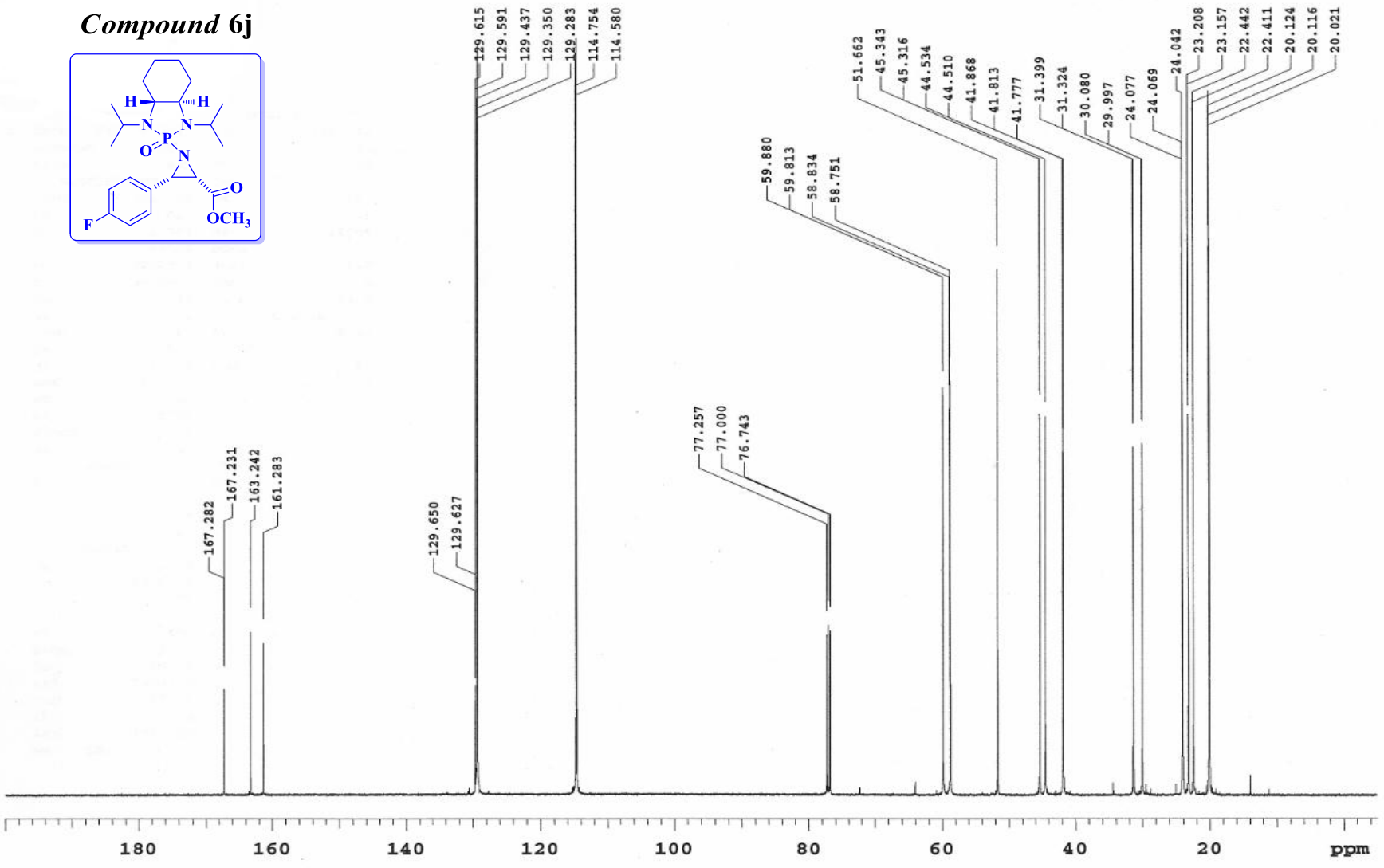
Minimum:				-1.5		
Maximum:		5.0	10.0	600.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
454.2024	454.2026	-0.2	-0.4	7.5	4.8	C22 H34 N3 O3 P Cl



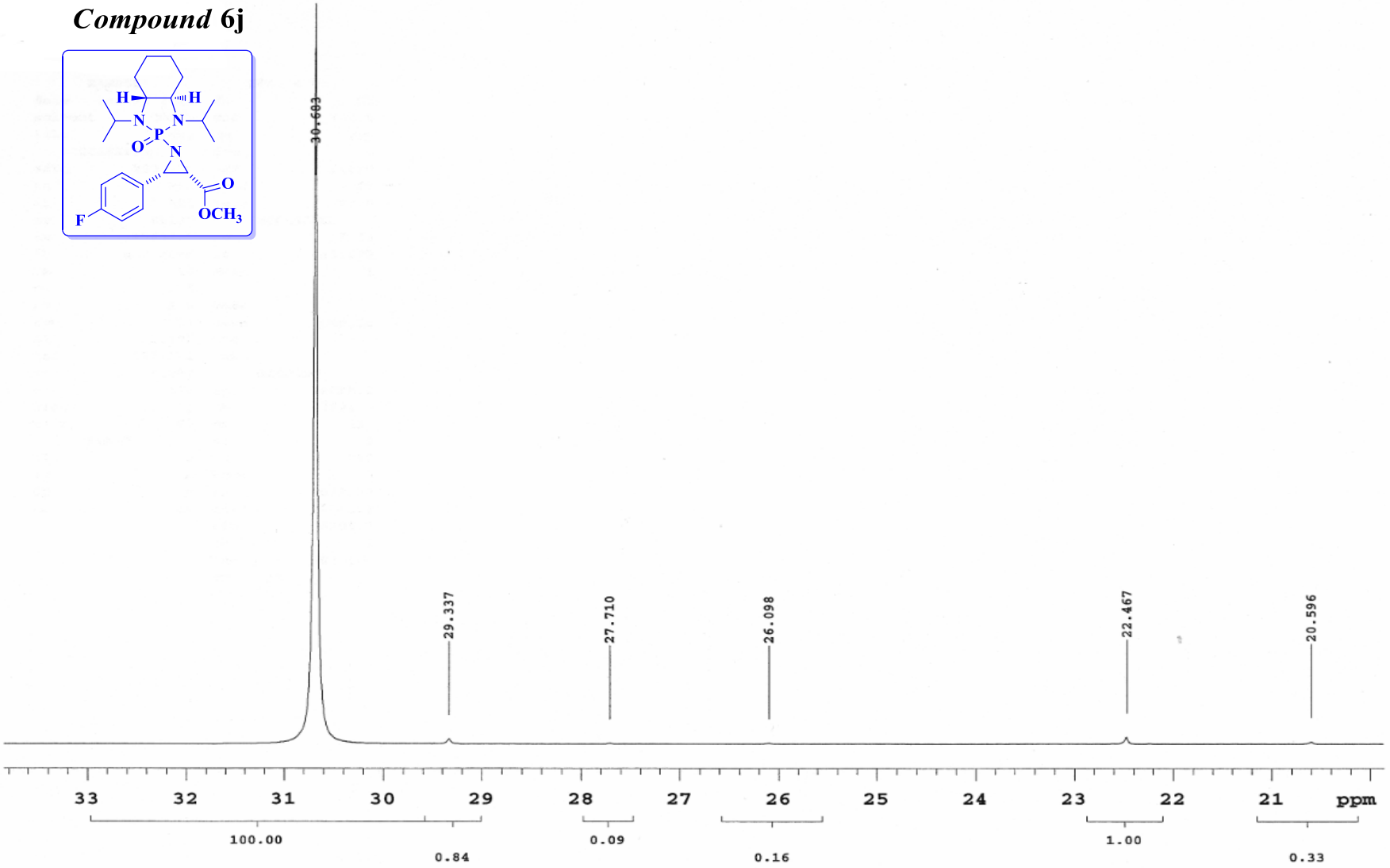
***Compound* 6j**



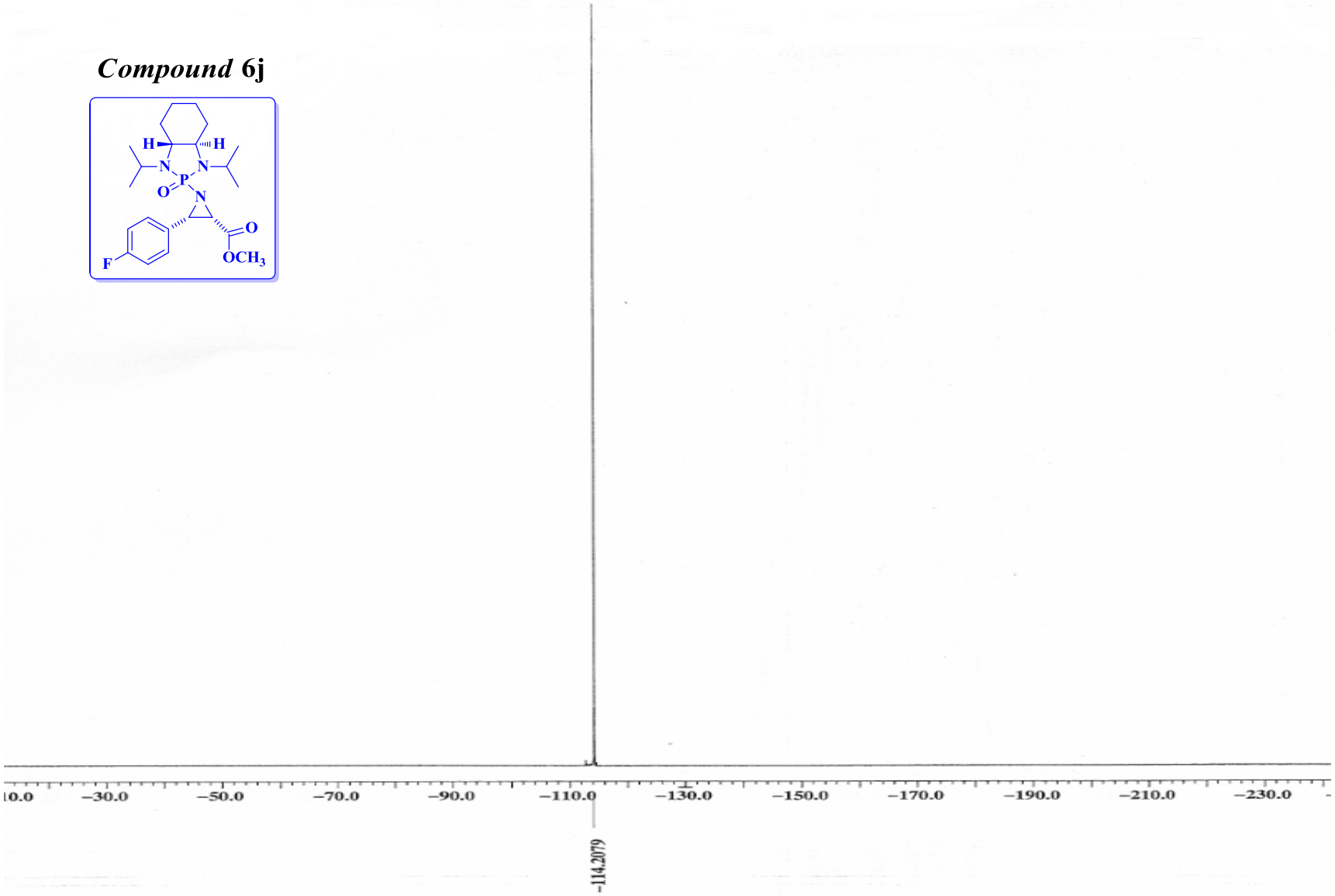
***Compound* 6j**

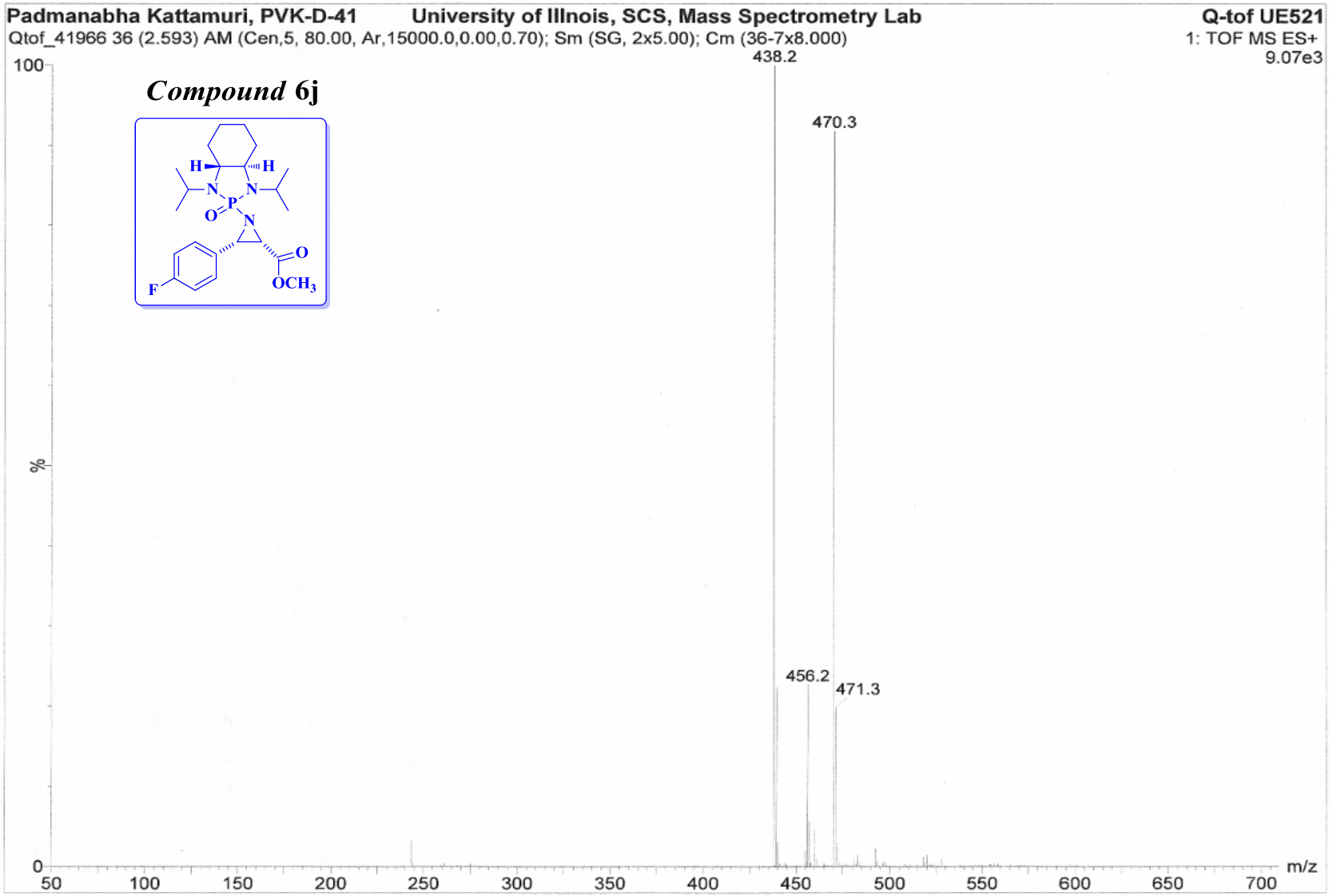


***Compound* 6j**



***Compound* 6j**





Elemental Composition Report

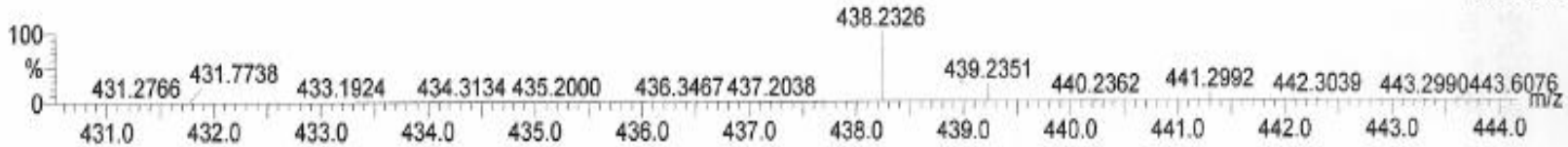
Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 600.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

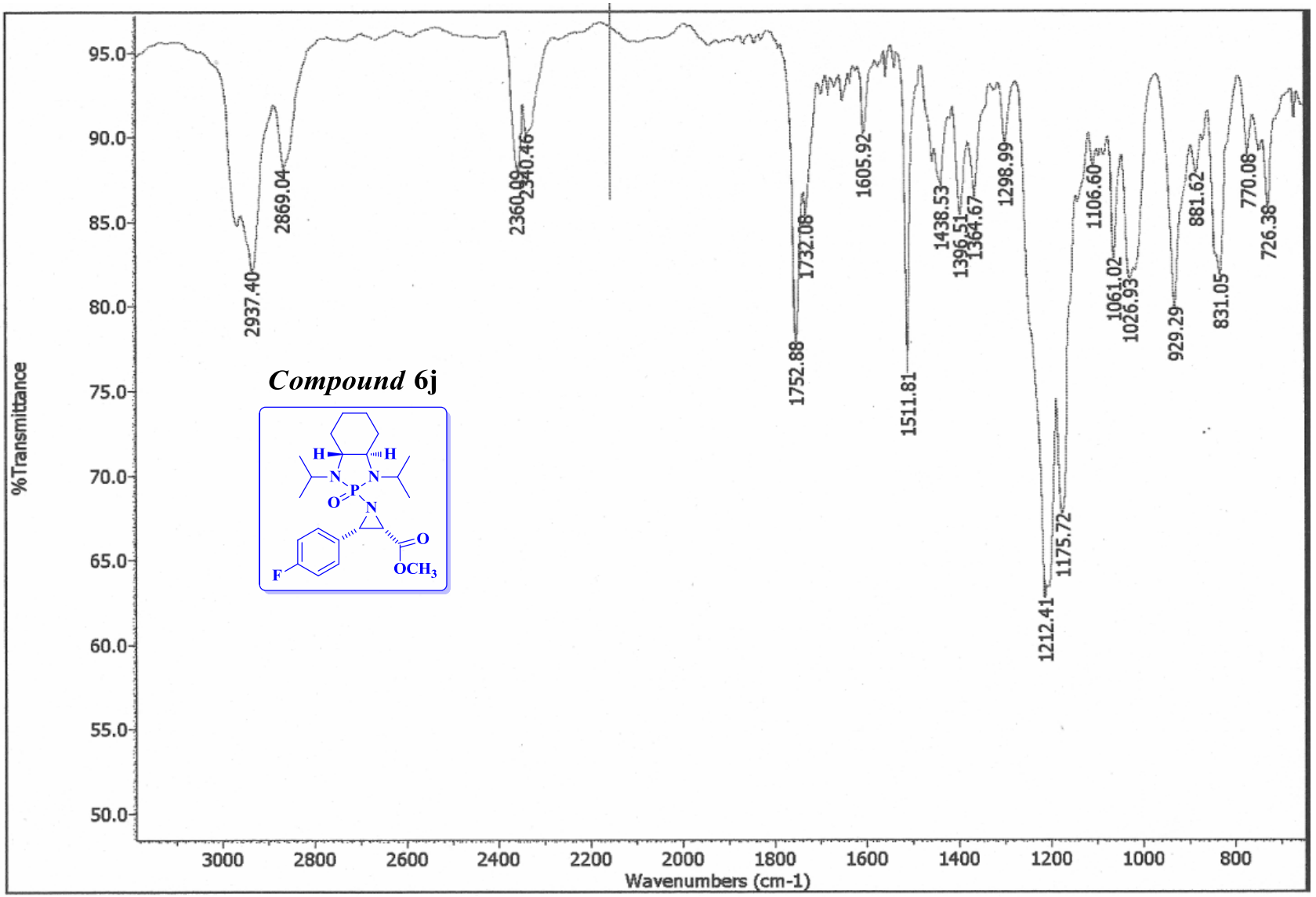
Monoisotopic Mass, Even Electron Ions
87 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-250 N: 2-4 O: 2-4 F: 1-1 P: 0-1

Padmanabha Kattamuri, PVK-D-41 University of Illnois, SCS, Mass Spectrometry Lab
Qtof_41966 32 (2.271) AM (Cen,3, 80.00, Ar,15000.0,716.46,0.70); Sm (SG, 2x3.00); Cm (30:33)

Q-tof UE521
2: TOF MS ES+
1.54e+003

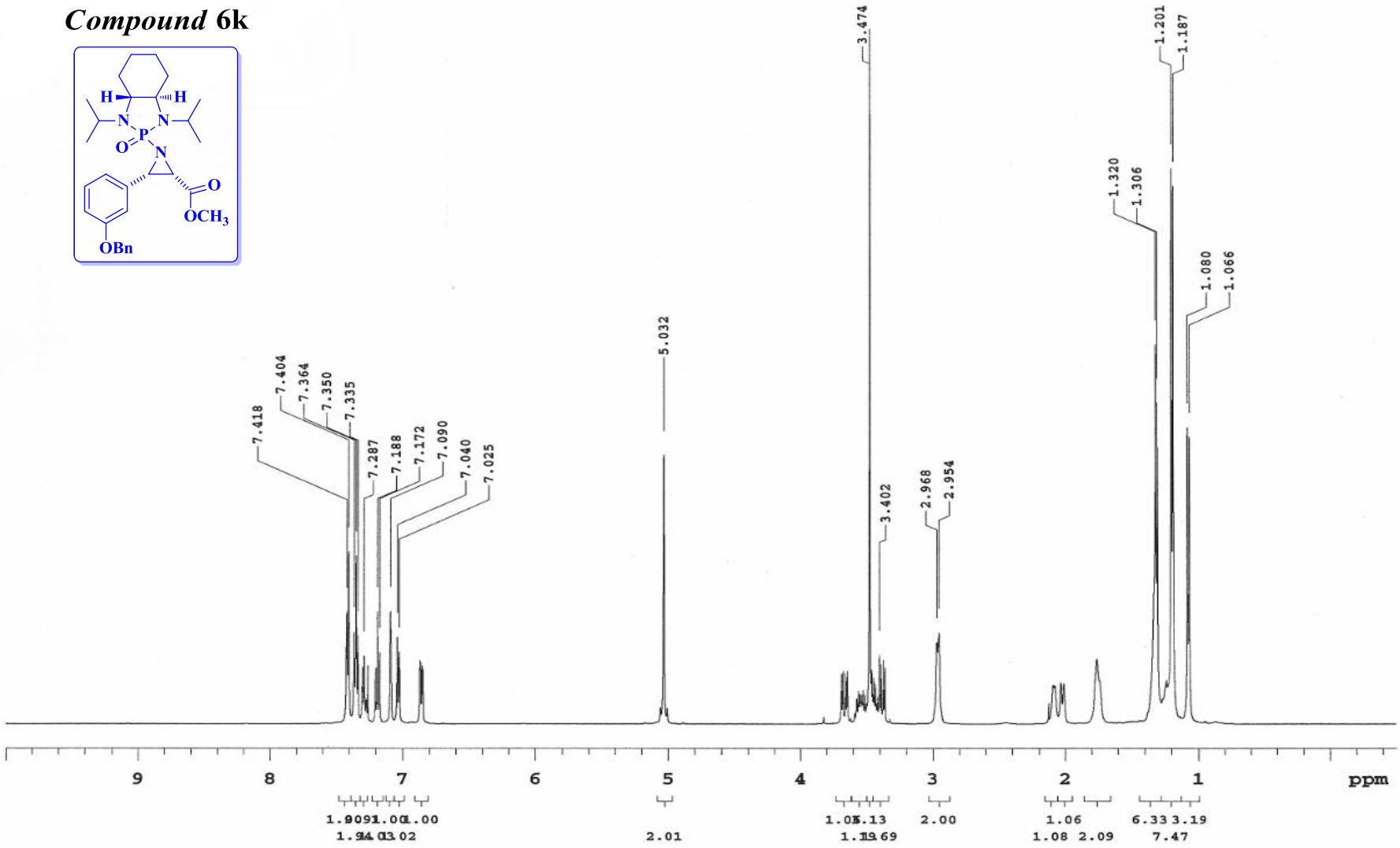


Minimum:				-1.5		
Maximum:		5.0	10.0	600.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
438.2326	438.2322	0.4	0.9	7.5	3.2	C22 H34 N3 O3 F P

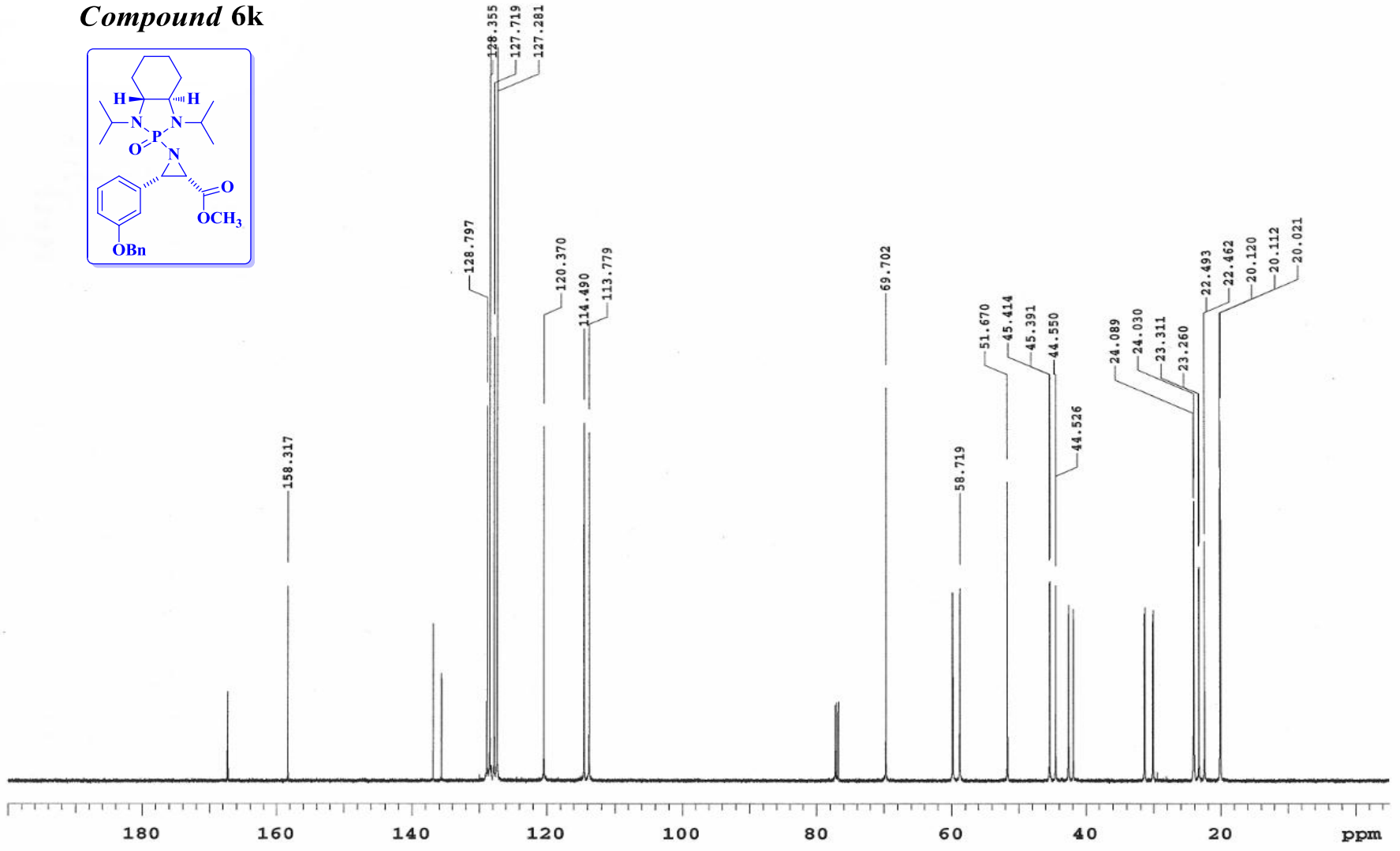


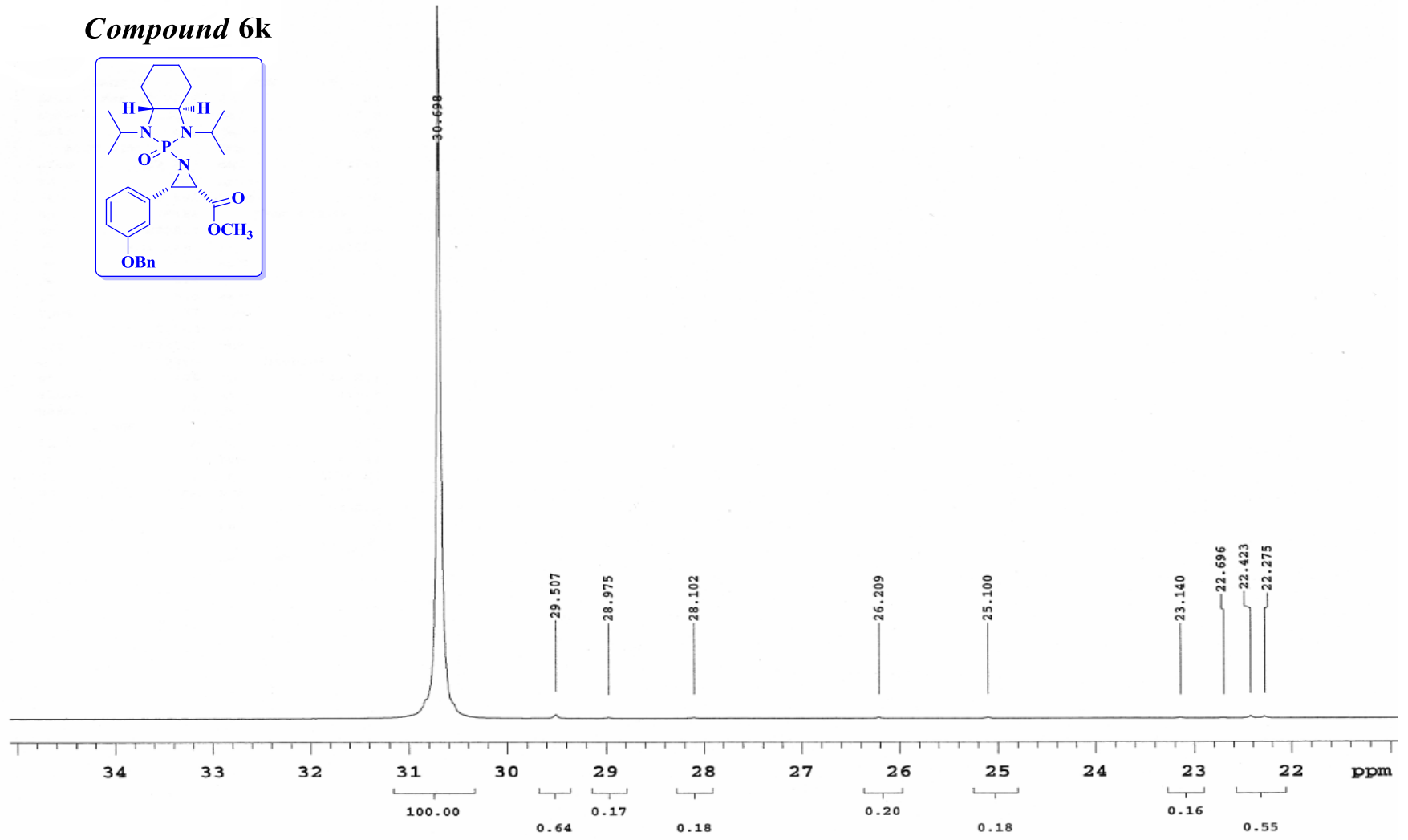
***Compound* 6k**

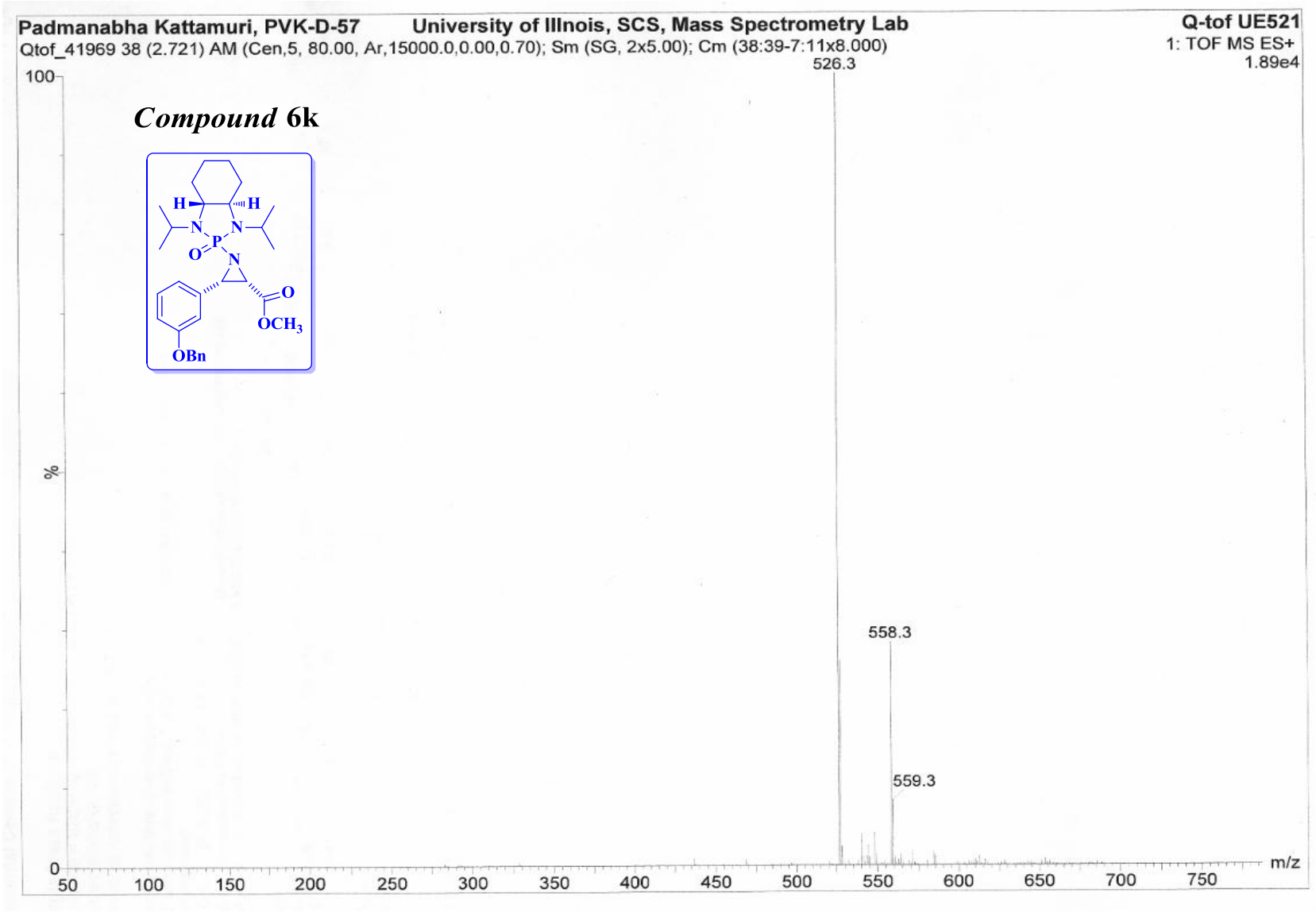
H
H
N
N
P
O
N
O
OCH3
OBn


7.418
7.404
7.364
7.350
7.335
7.287
7.188
7.172
7.090
7.040
7.025
5.032
3.474
3.402
2.968
2.954
1.320
1.306
1.201
1.187
1.080
1.066
9
8
7
6
5
4
3
2
1
ppm
1.90 1.00 1.00
1.94 1.03 1.02
2.01
1.05 5.13
1.13 3.69
2.00
1.06
1.08 2.09
6.33 3.19
7.47

***Compound* 6k**







Elemental Composition Report

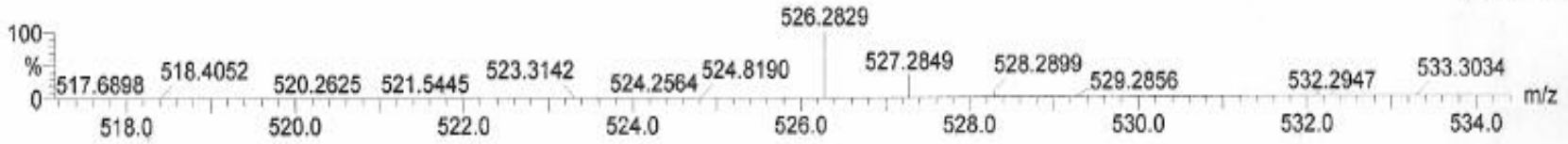
Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 600.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

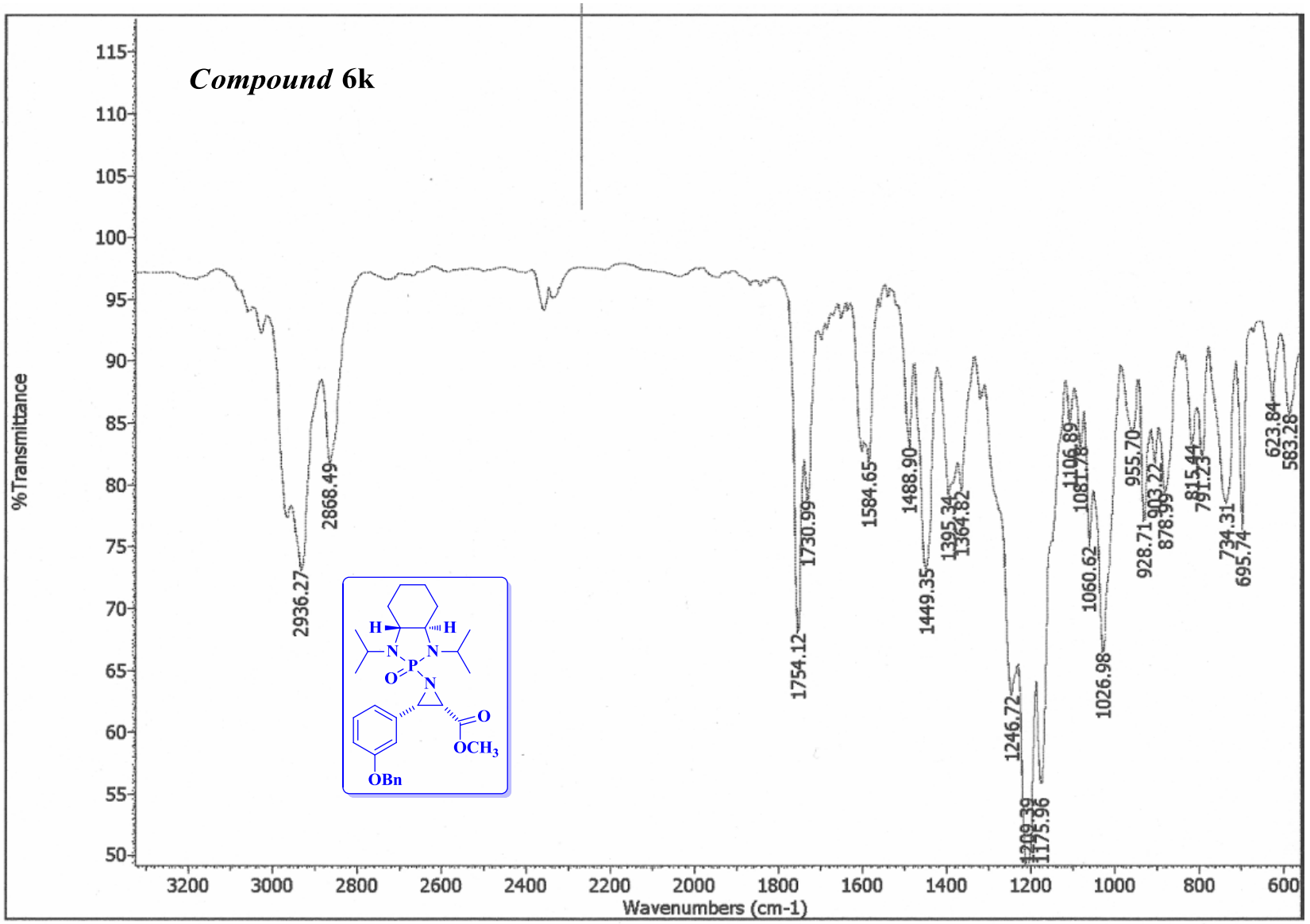
Monoisotopic Mass, Even Electron Ions
115 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-250 N: 2-4 O: 2-4 P: 0-1

Padmanabha Kattamuri, PVK-D-57 University of Illnois, SCS, Mass Spectrometry Lab
Qtof_41969 51 (3.650) AM (Cen,3, 80.00, Ar,15000.0,716.46,0.70,LS 3); Sm (SG, 2x3.00)

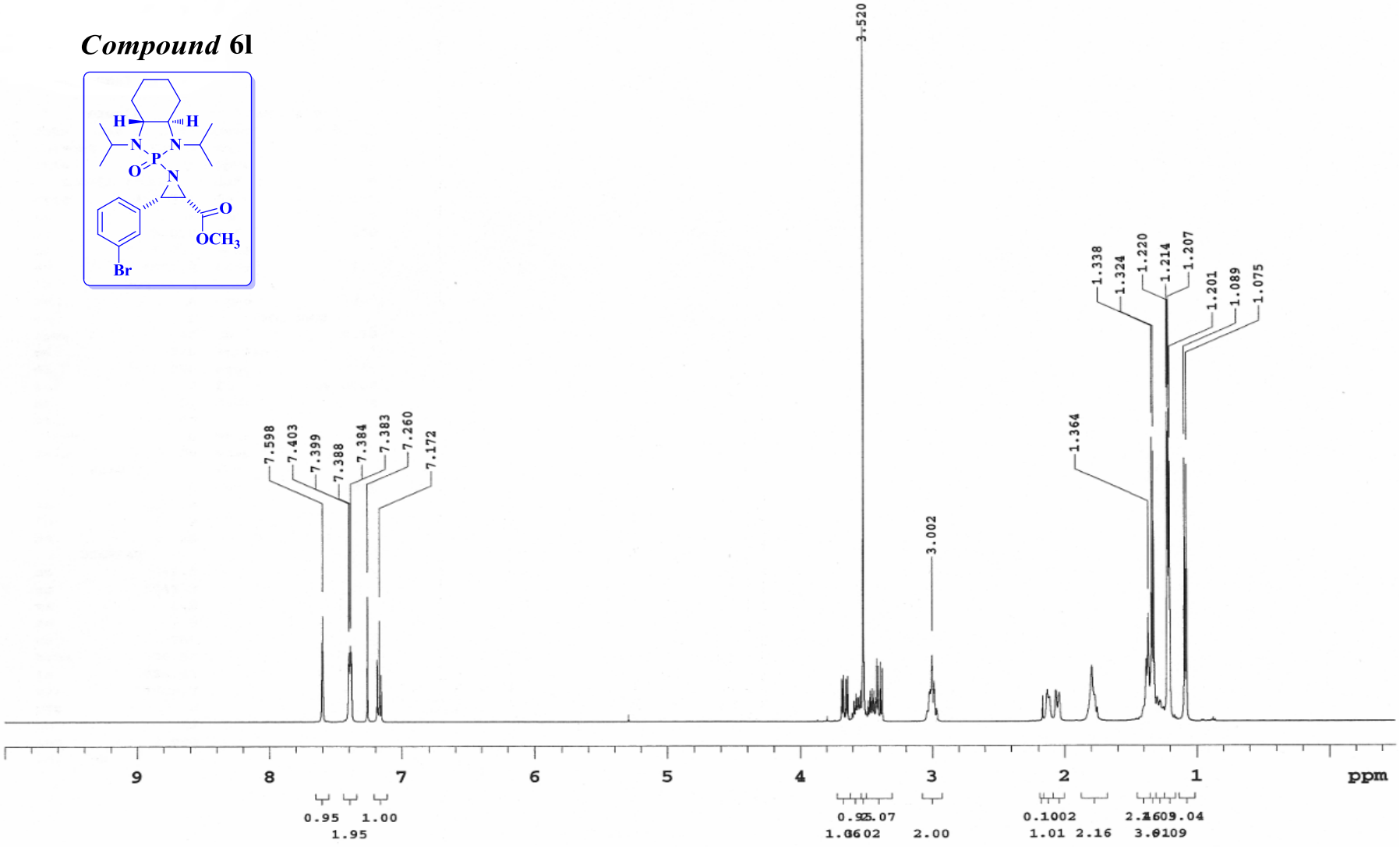
Q-tof UE521
1: TOF MS ES+
9.13e+002



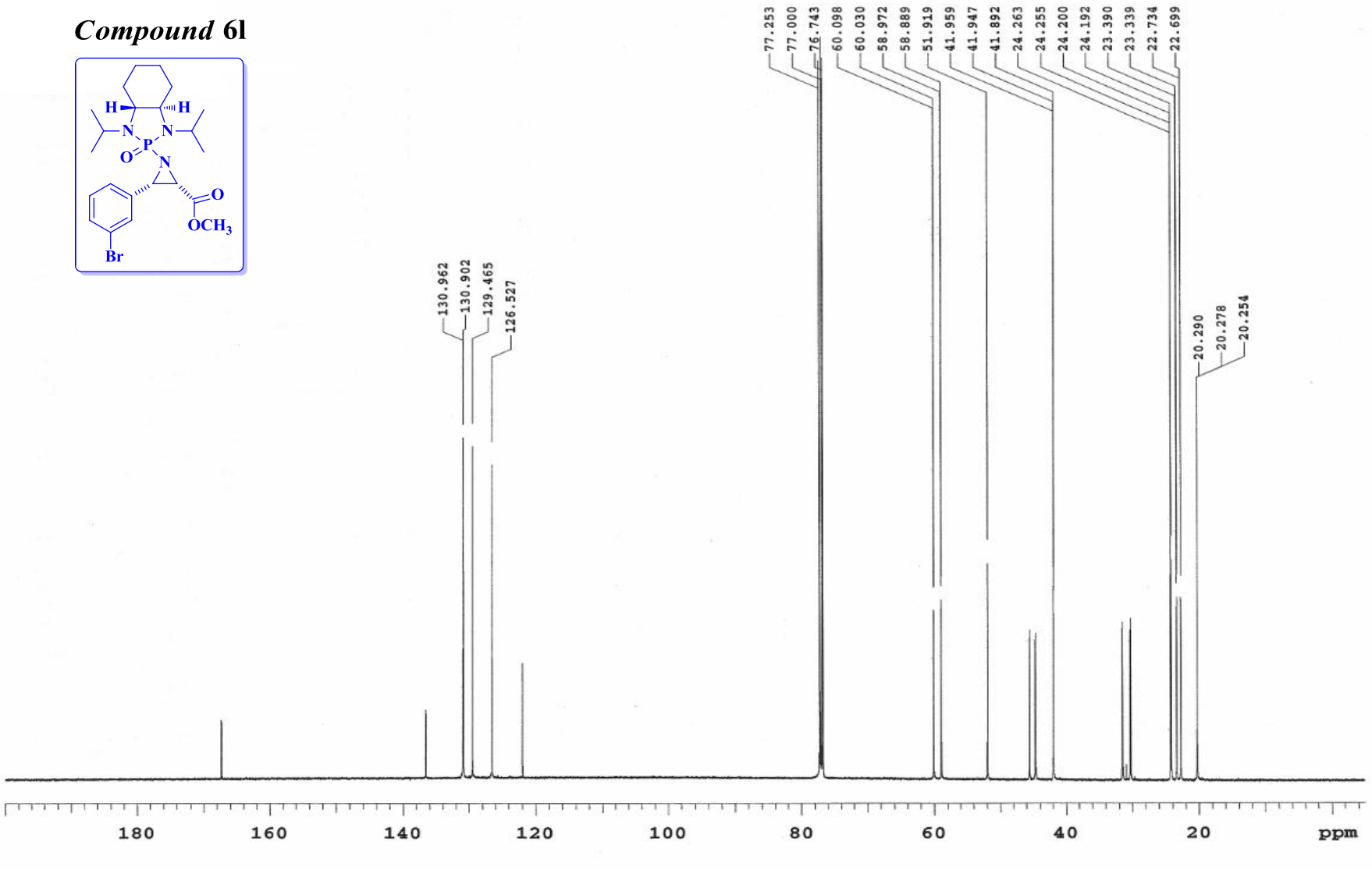
Minimum:				-1.5		
Maximum:		5.0	10.0	600.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
526.2829	526.2835	-0.6	-1.1	11.5	0.6	C29 H41 N3 O4 P



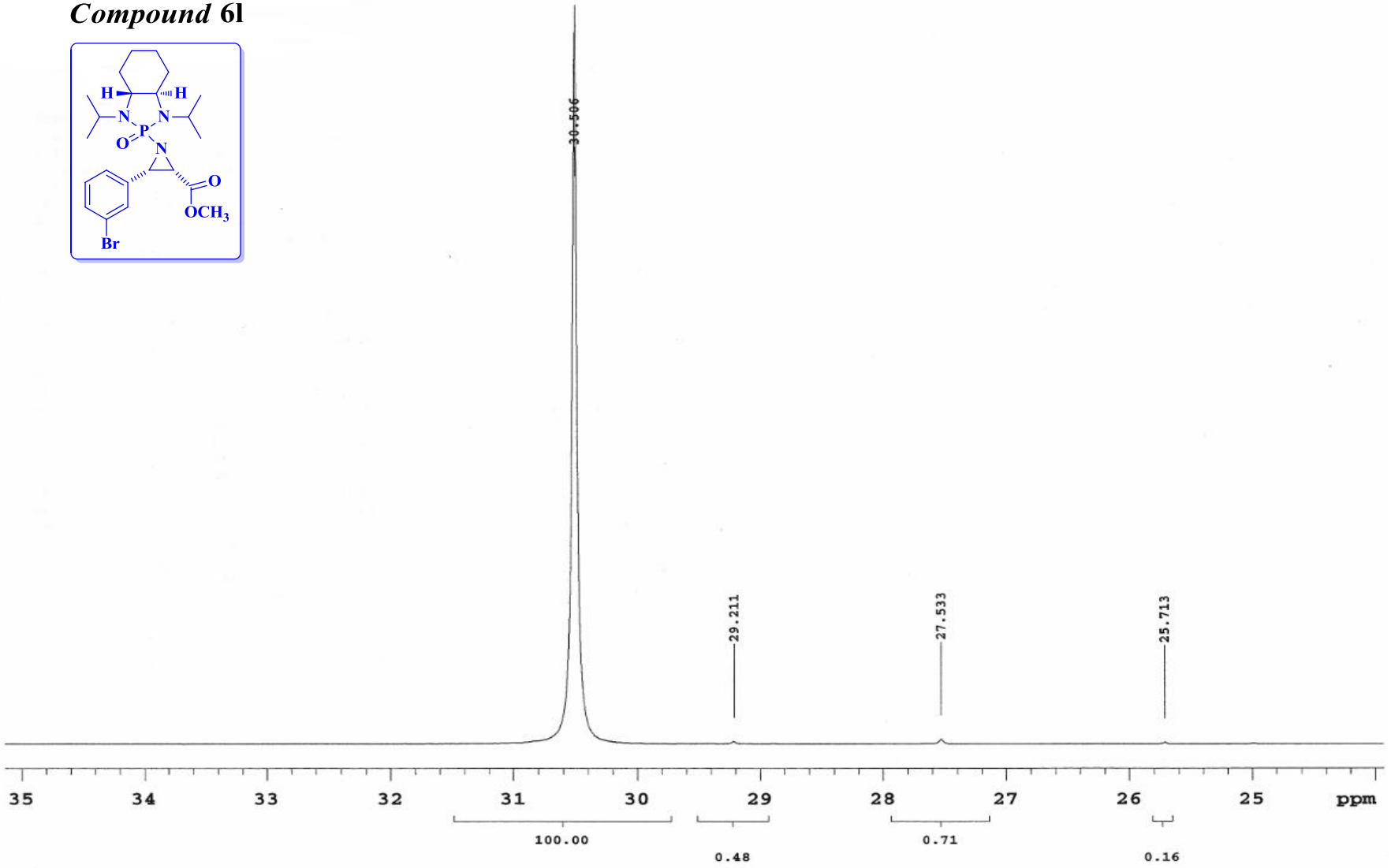
***Compound* 6l**

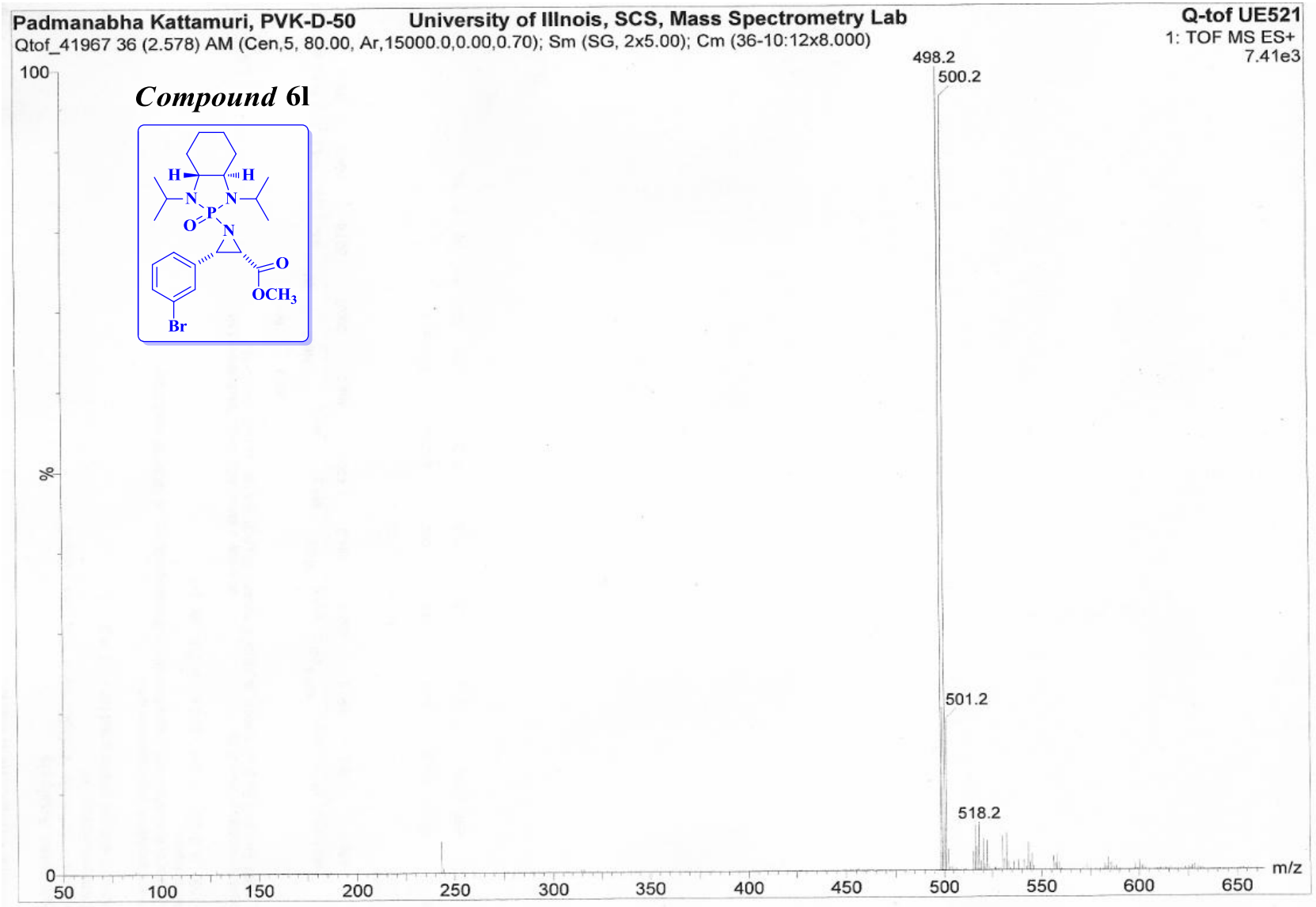


***Compound* 6l**



***Compound* 6l**




Padmanabha Kattamuri, PVK-D-50 University of Illnois, SCS, Mass Spectrometry Lab
Qtof_41967 36 (2.578) AM (Cen,5, 80.00, Ar,15000.0,0.00,0.70); Sm (SG, 2x5.00); Cm (36-10:12x8.000)
Q-tof UE521
1: TOF MS ES+
7.41e3
Compound 6l
498.2
500.2
501.2
518.2
100
%
0
50
100
150
200
250
300
350
400
450
500
550
600
650
m/z

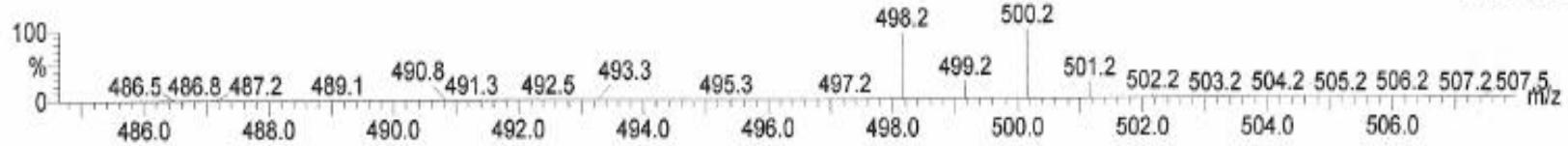
Elemental Composition Report

Single Mass Analysis

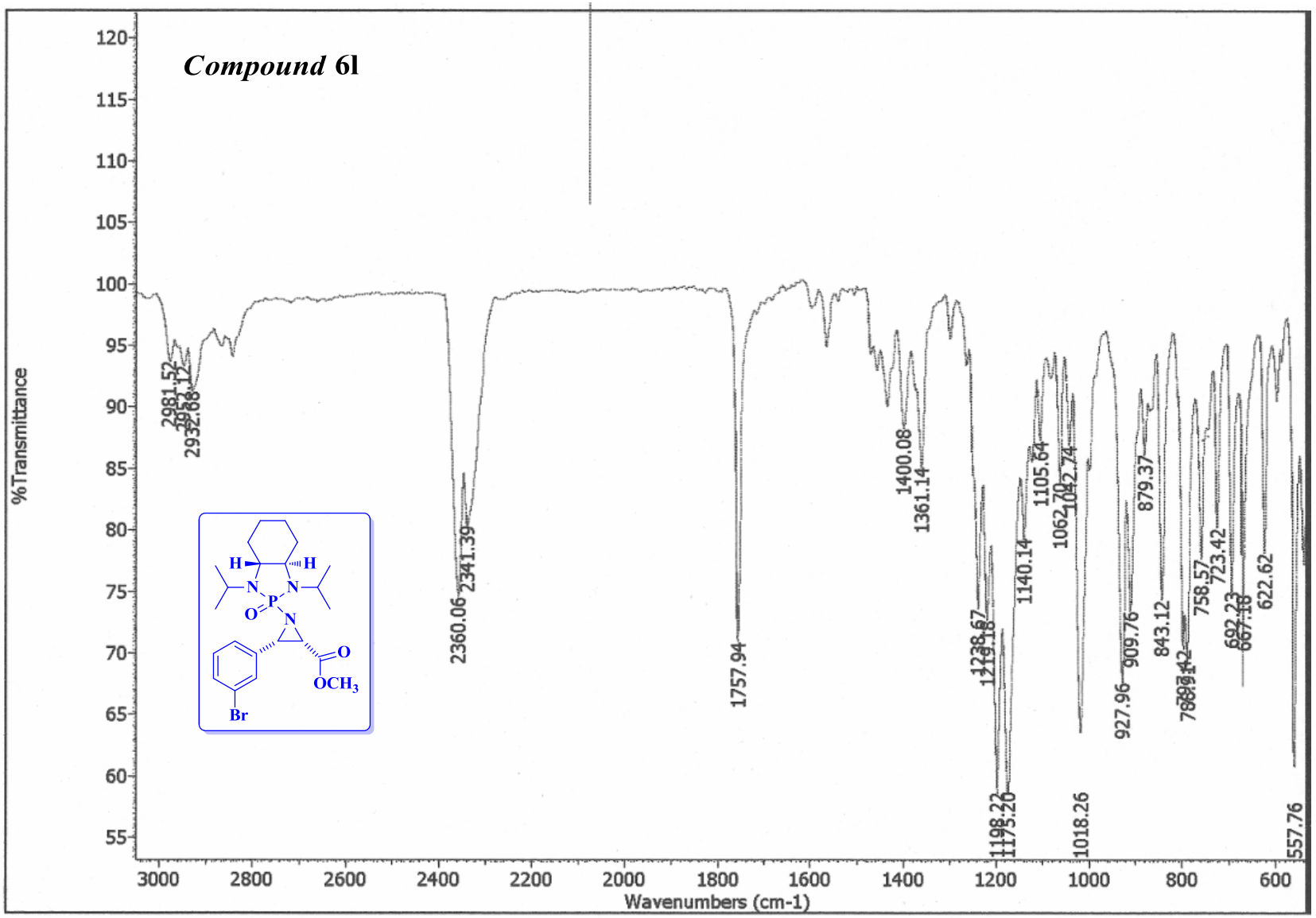
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 600.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
87 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-250 N: 2-4 O: 2-4 P: 0-1 Br: 1-1

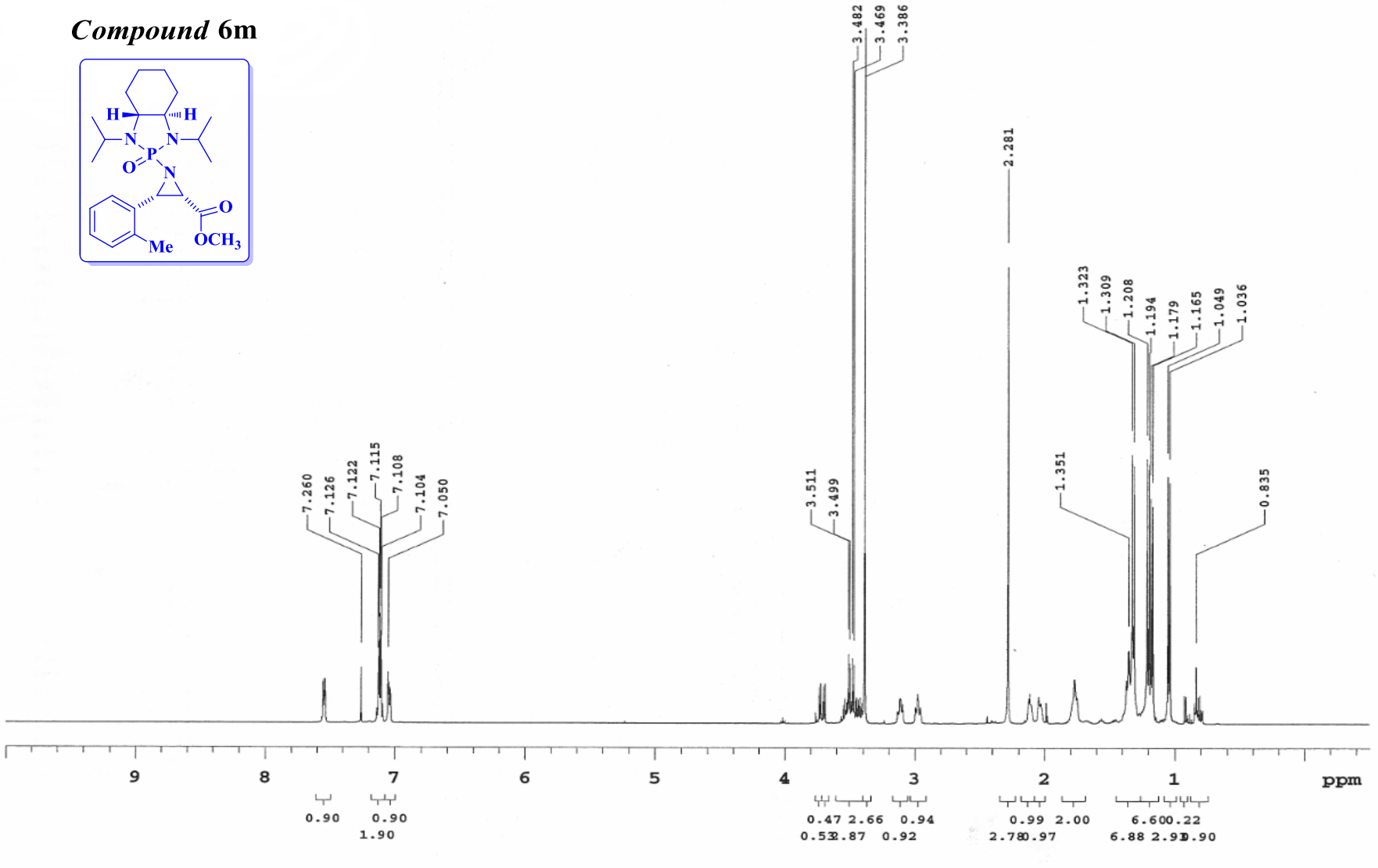
Padmanabha Kattamuri, PVK-D-50 University of Illinois, SCS, Mass Spectrometry Lab Q-tof UE521
Qtof_41967 50 (3.579) AM (Cen,3, 80.00, Ar,15000.0,716.46,0.70,LS 3); Sm (SG, 2x3.00); Cm (50:52) 1: TOF MS ES+
2.13e+003

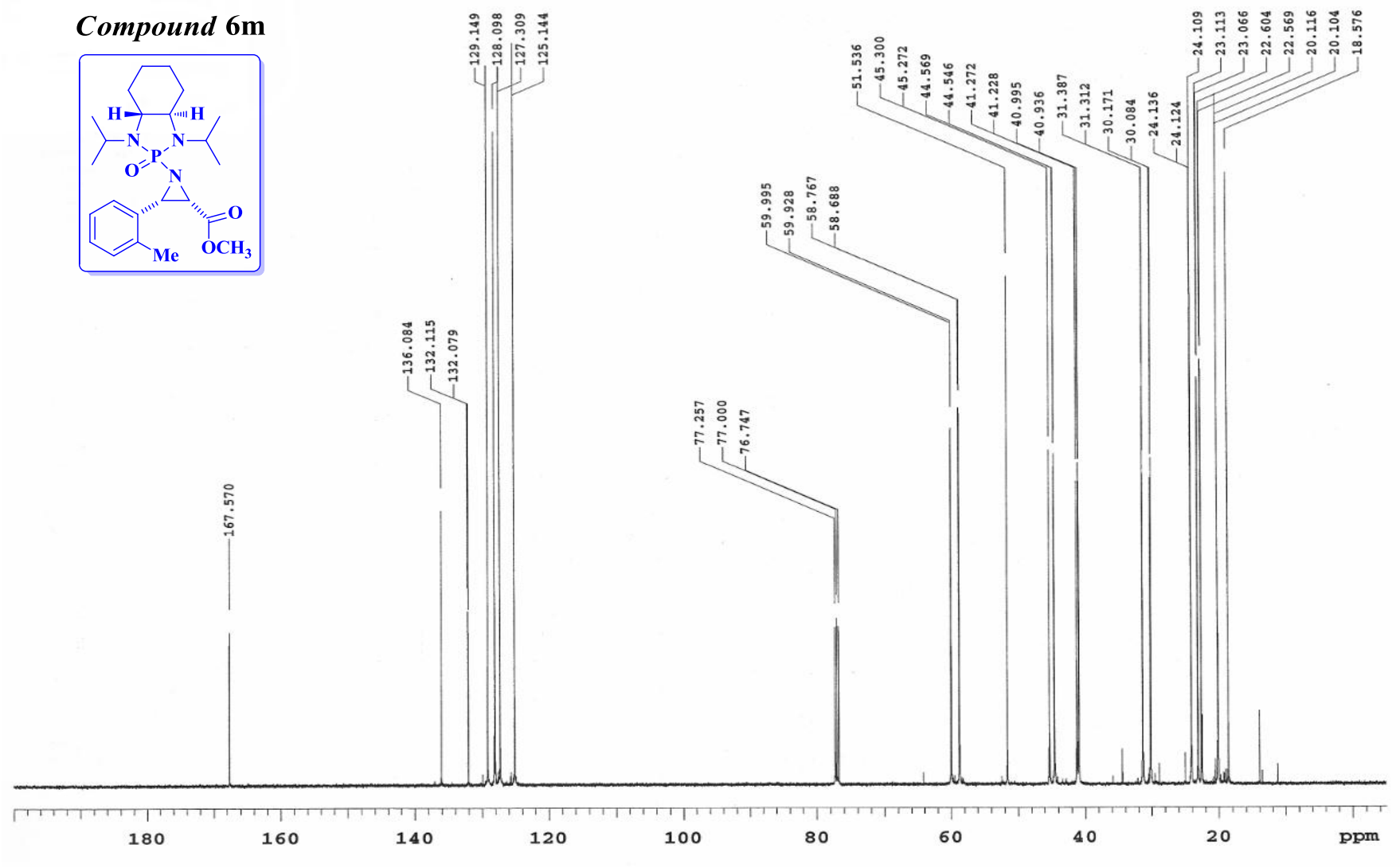


Minimum:				-1.5		
Maximum:		5.0	10.0	600.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
498.1522	498.1521	0.1	0.2	7.5	0.7	C22 H34 N3 O3 P Br

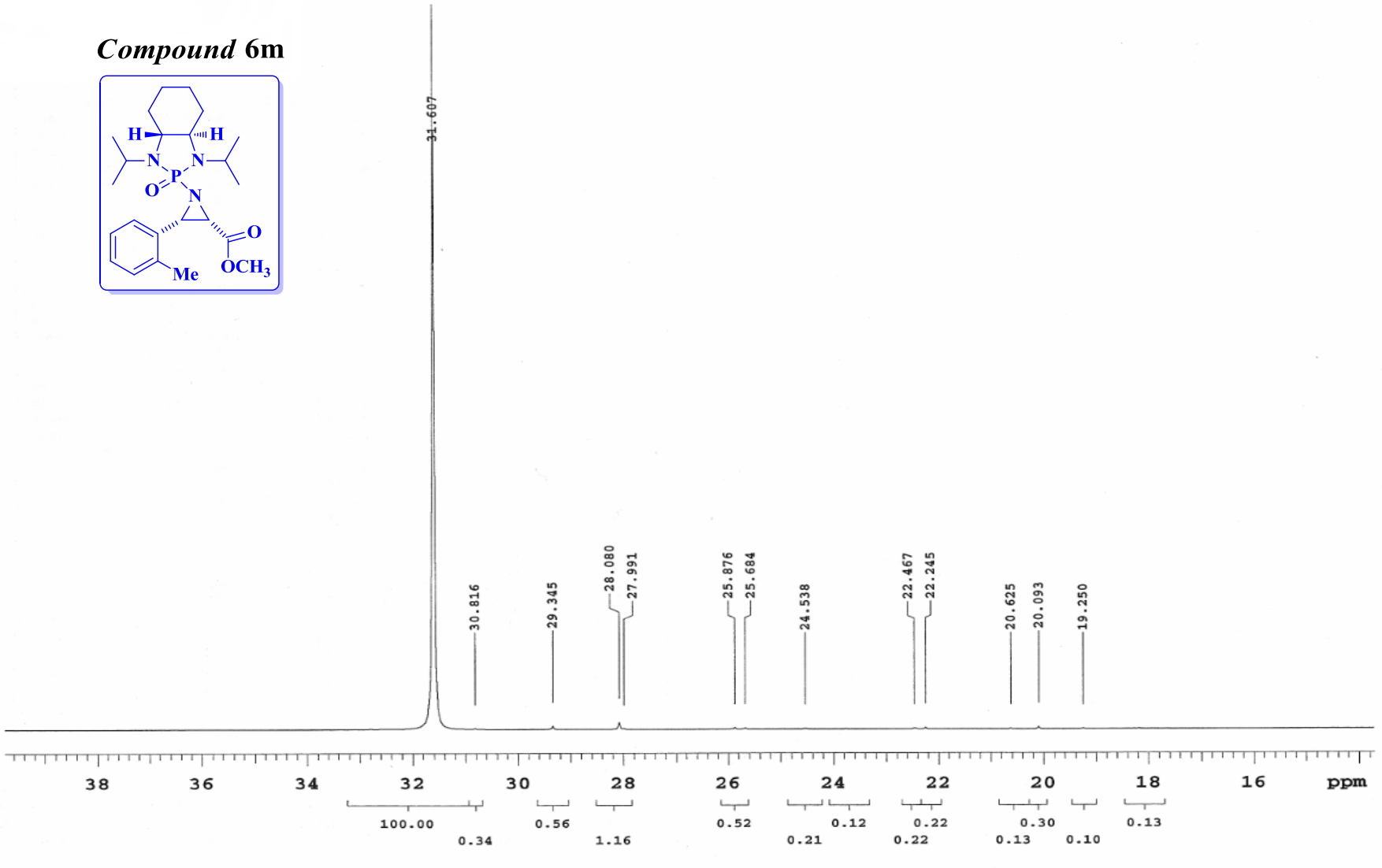


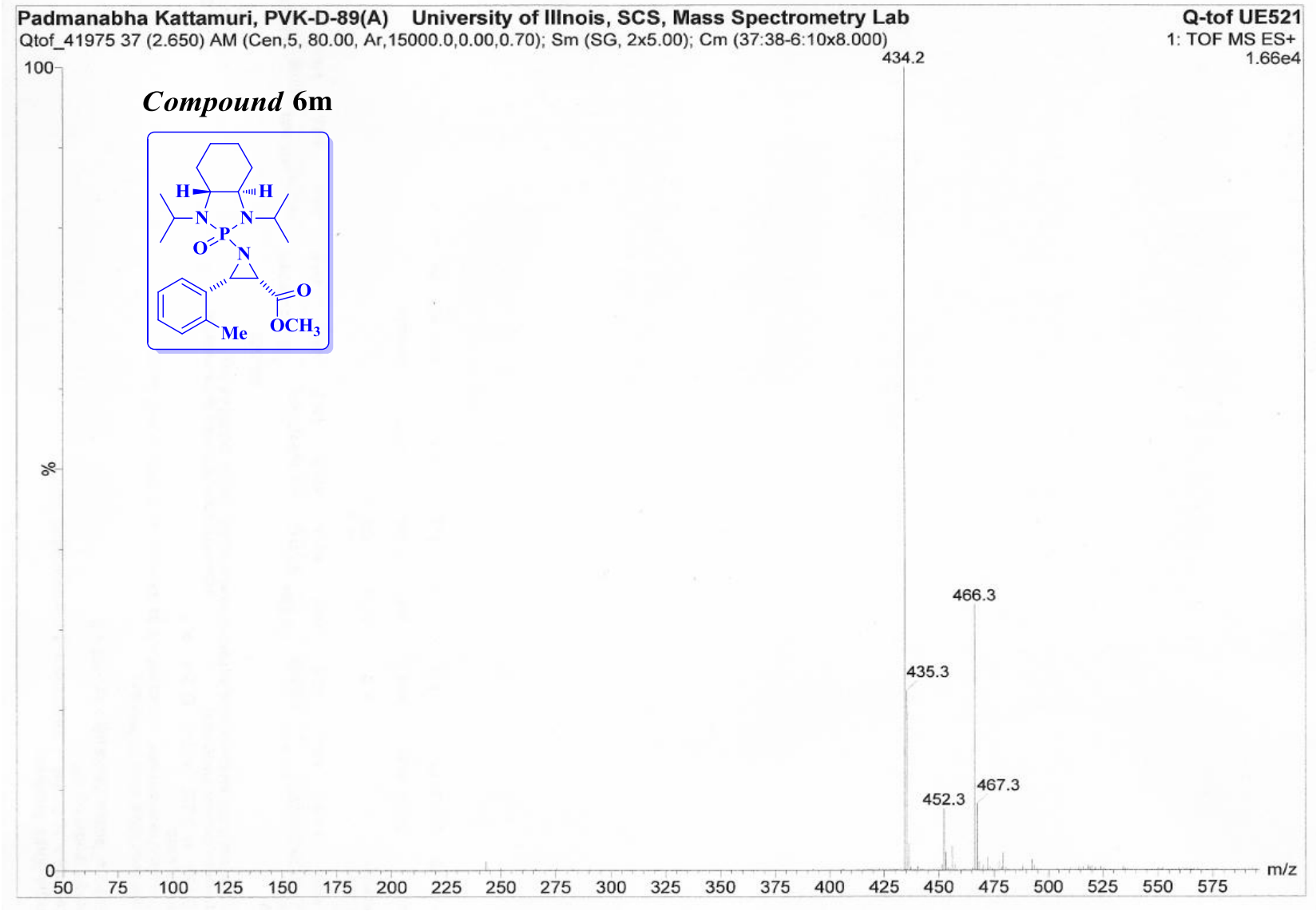
***Compound* 6m**





***Compound* 6m**





Elemental Composition Report

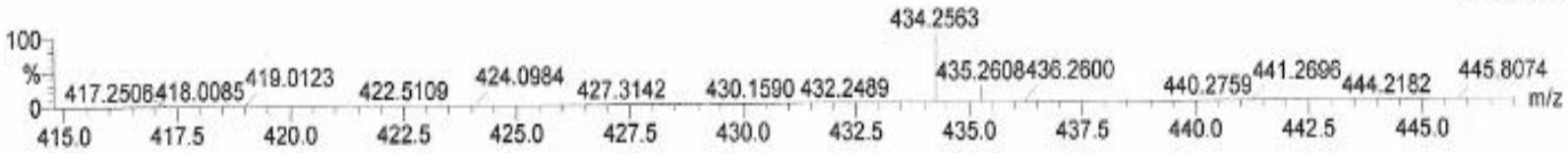
Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 600.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

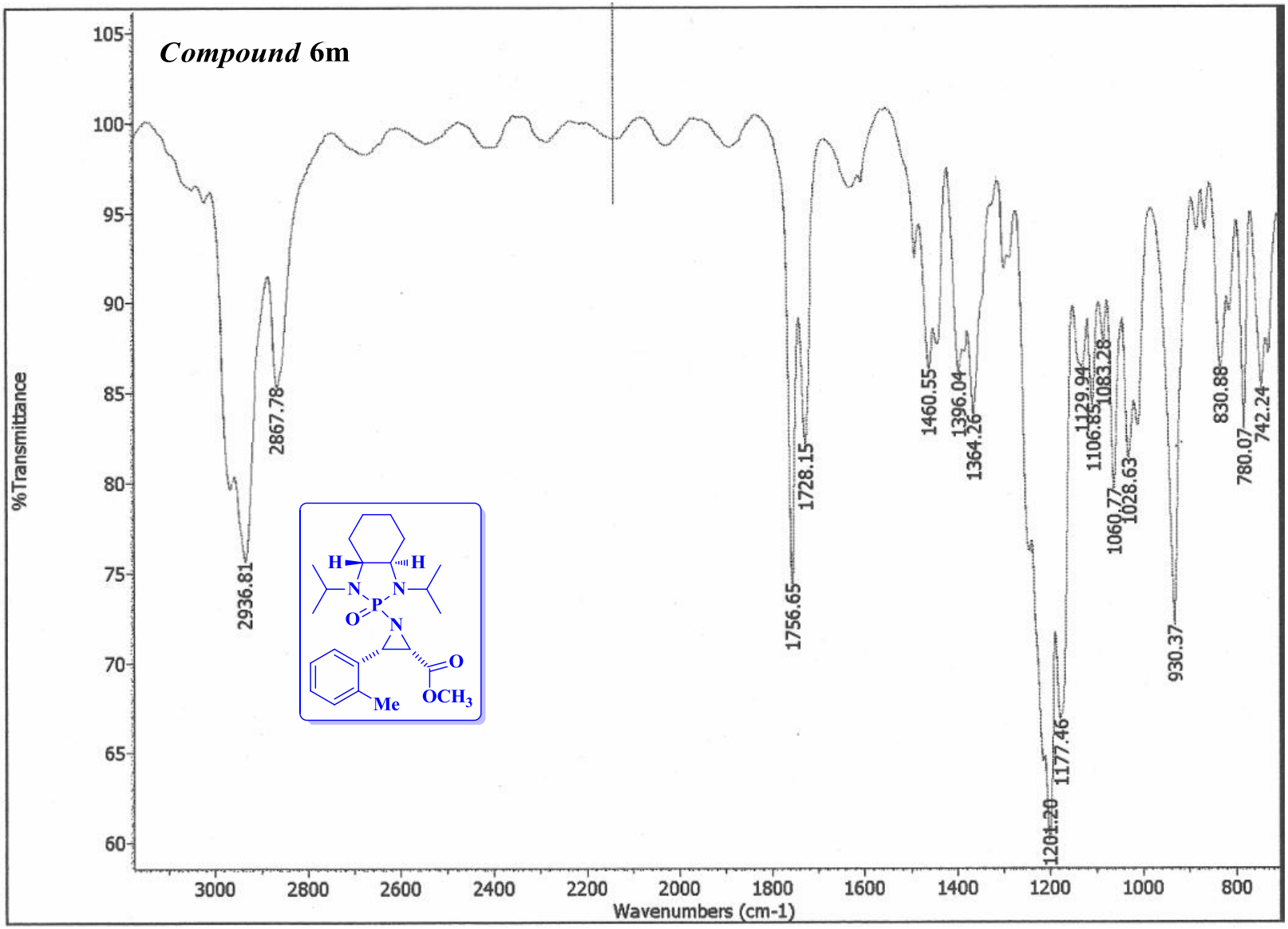
Monoisotopic Mass, Even Electron Ions
91 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-250 N: 2-4 O: 2-4 P: 0-1

Padmanabha Kattamuri, PVK-D-89(A) University of Illinois, SCS, Mass Spectrometry Lab
Qtof_41975 52 (3.722) AM (Cen,3, 80.00, Ar,15000.0,716.46,0.70,LS 3); Sm (SG, 2x3.00); Cm (52)

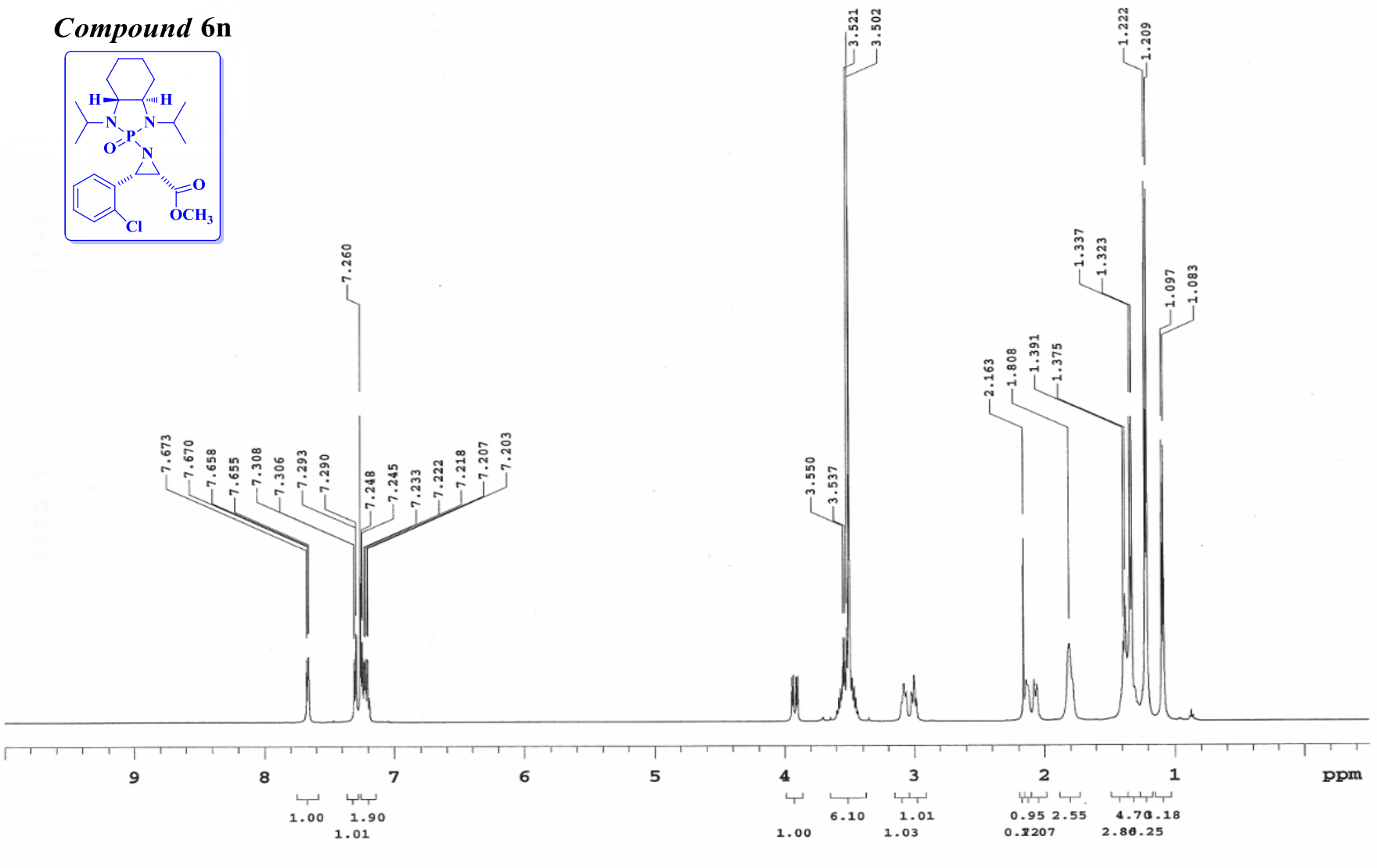
Q-tof UE521
1: TOF MS ES+
1.40e+003



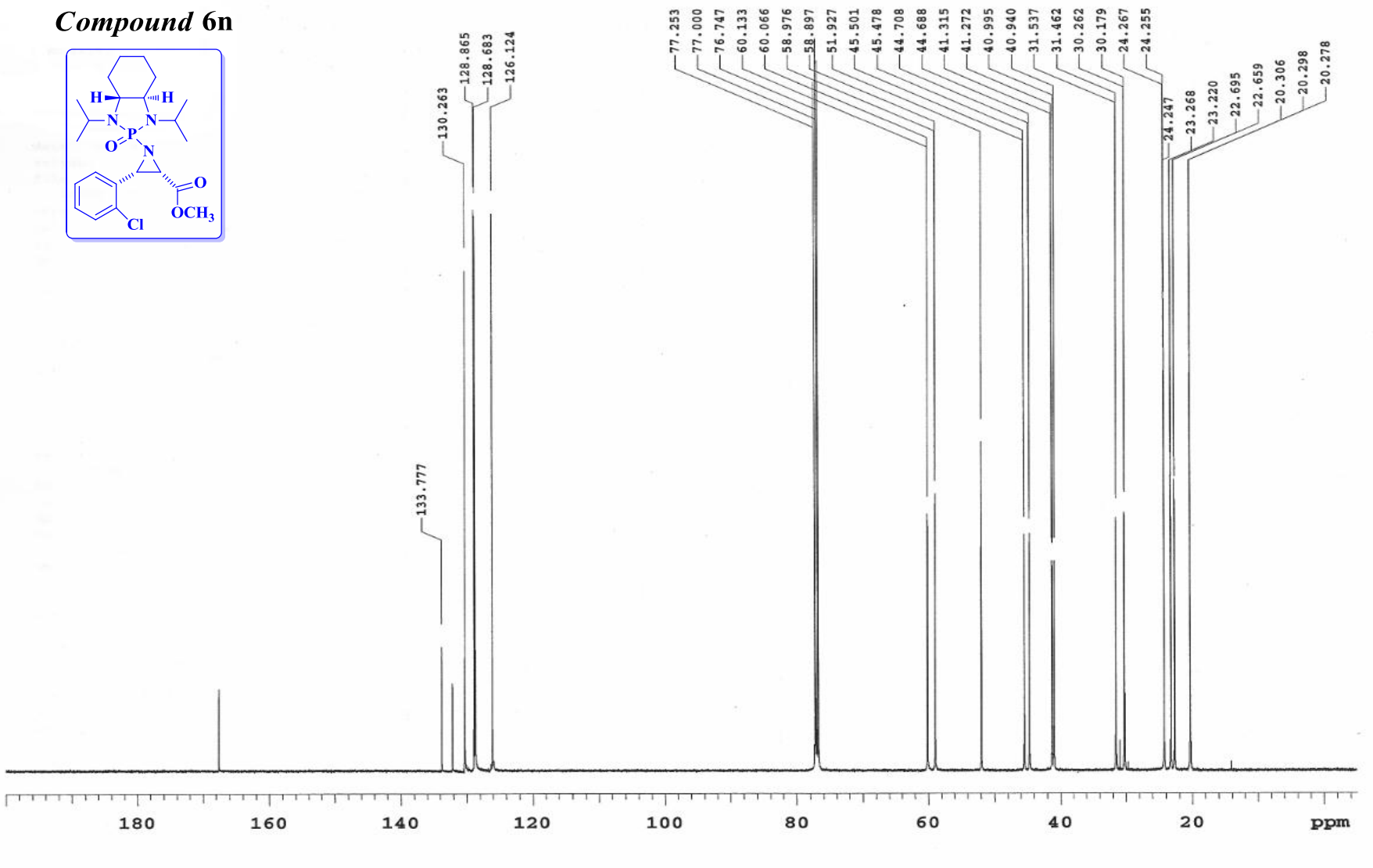
Minimum:				-1.5		
Maximum:		5.0	10.0	600.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
434.2563	434.2573	-1.0	-2.3	7.5	3.5	C23 H37 N3 O3 P



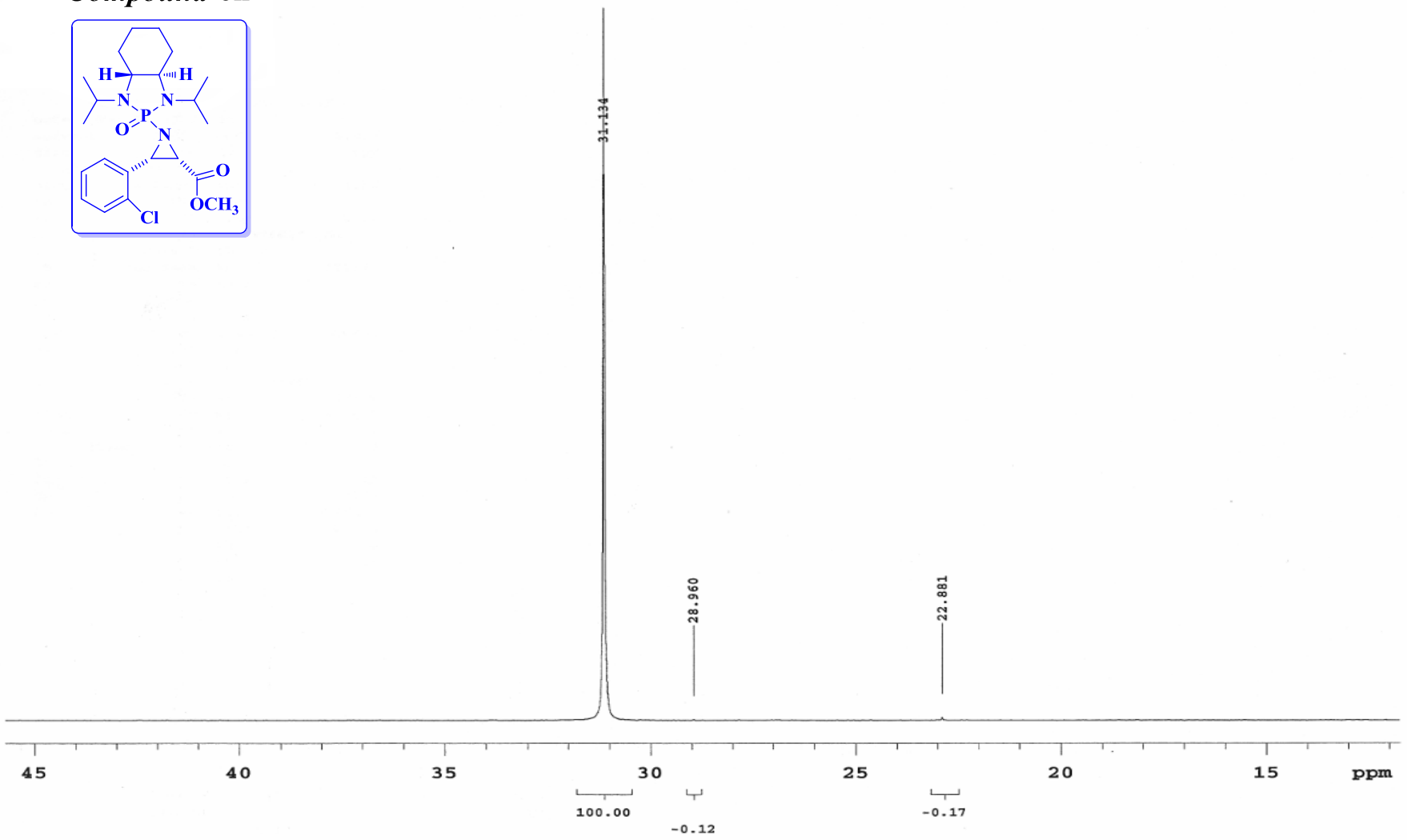
***Compound* 6n**

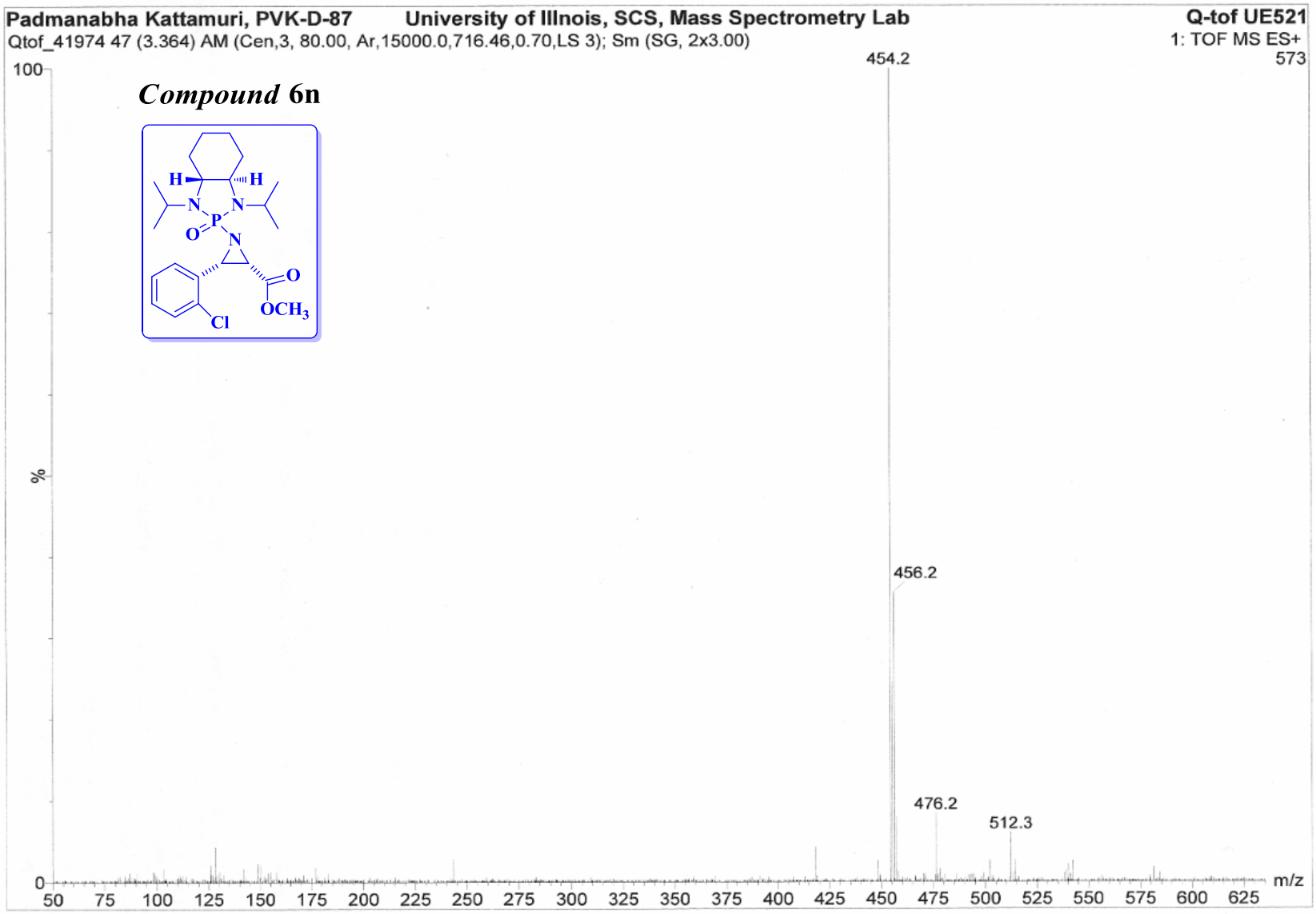


***Compound* 6n**



***Compound* 6n**





Elemental Composition Report

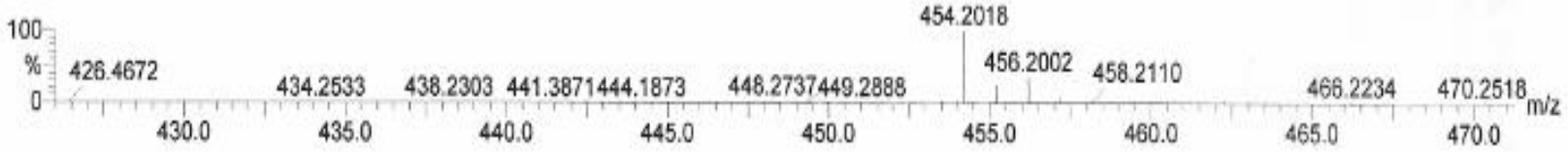
Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 600.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

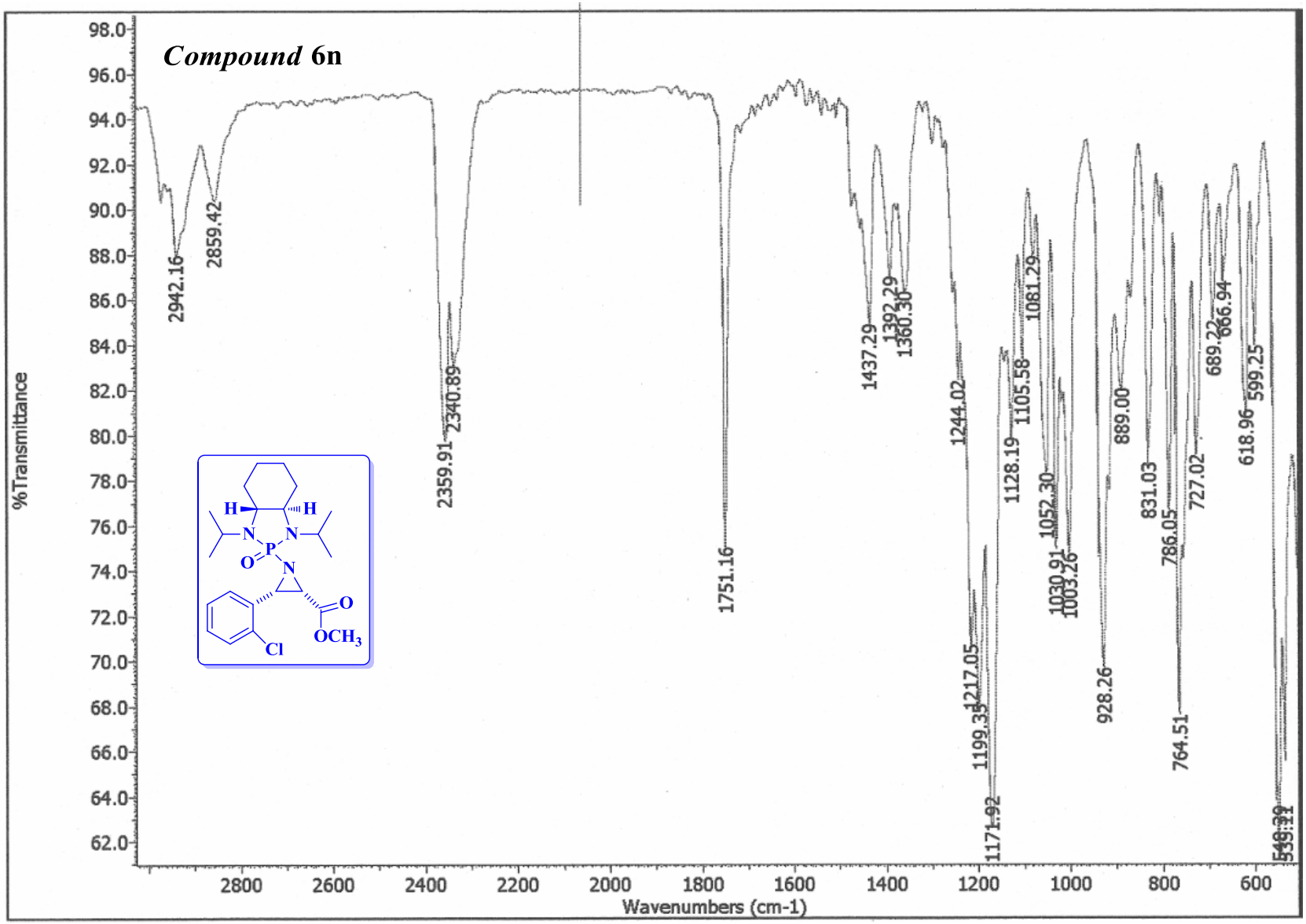
Monoisotopic Mass, Even Electron Ions
87 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-250 N: 2-4 O: 2-4 P: 0-1 Cl: 1-1

Padmanabha Kattamuri, PVK-D-87 University of Illinois, SCS, Mass Spectrometry Lab
Qtof_41974 47 (3.364) AM (Cen,3, 80.00, Ar,15000.0,716.46,0.70,LS 3); Sm (SG, 2x3.00)

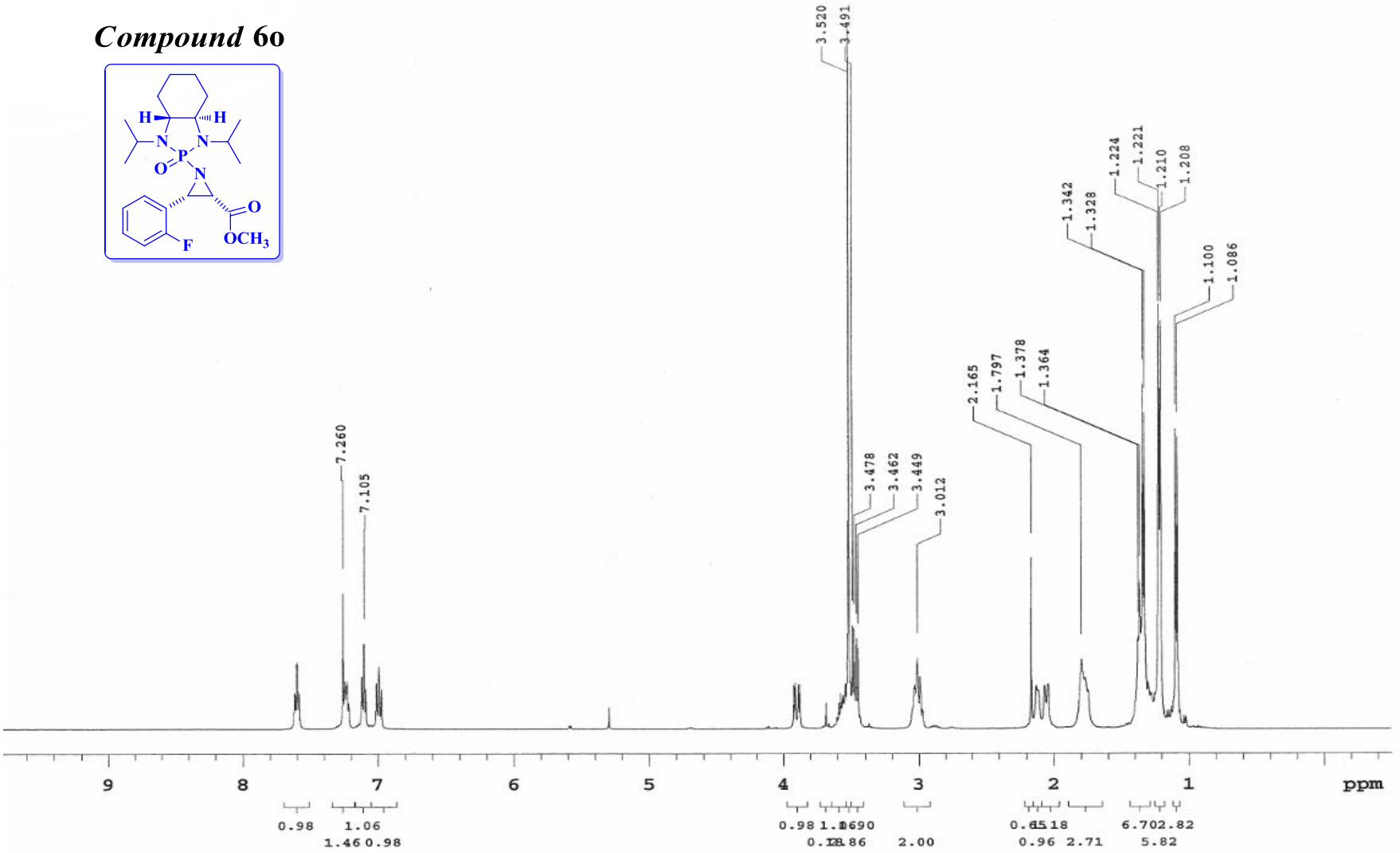
Q-tof UE521
1: TOF MS ES+
5.73e+002



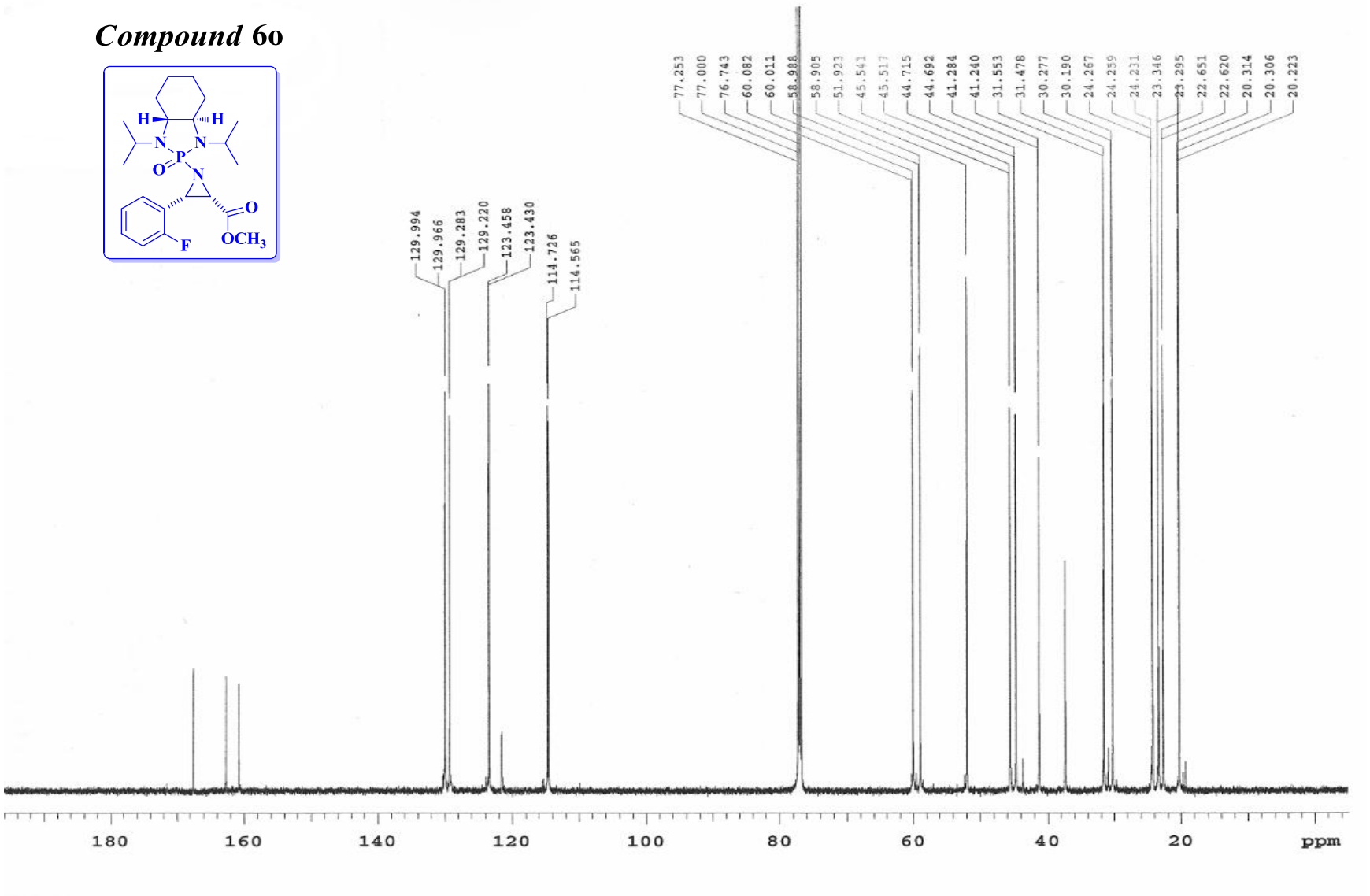
Minimum:				-1.5		
Maximum:		5.0	10.0	600.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
454.2018	454.2026	-0.8	-1.8	7.5	0.2	C22 H34 N3 O3 P Cl



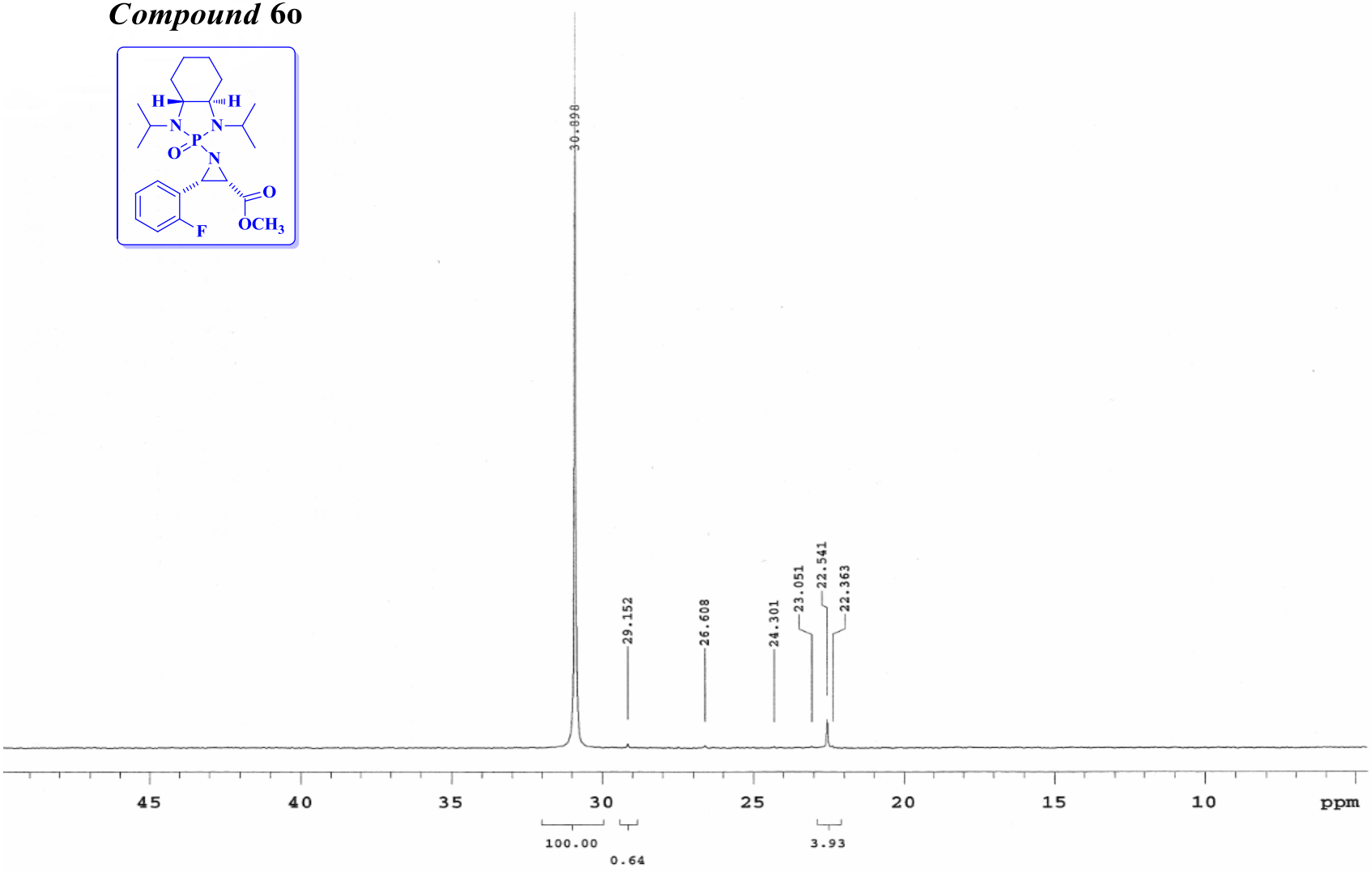
***Compound* 6o**



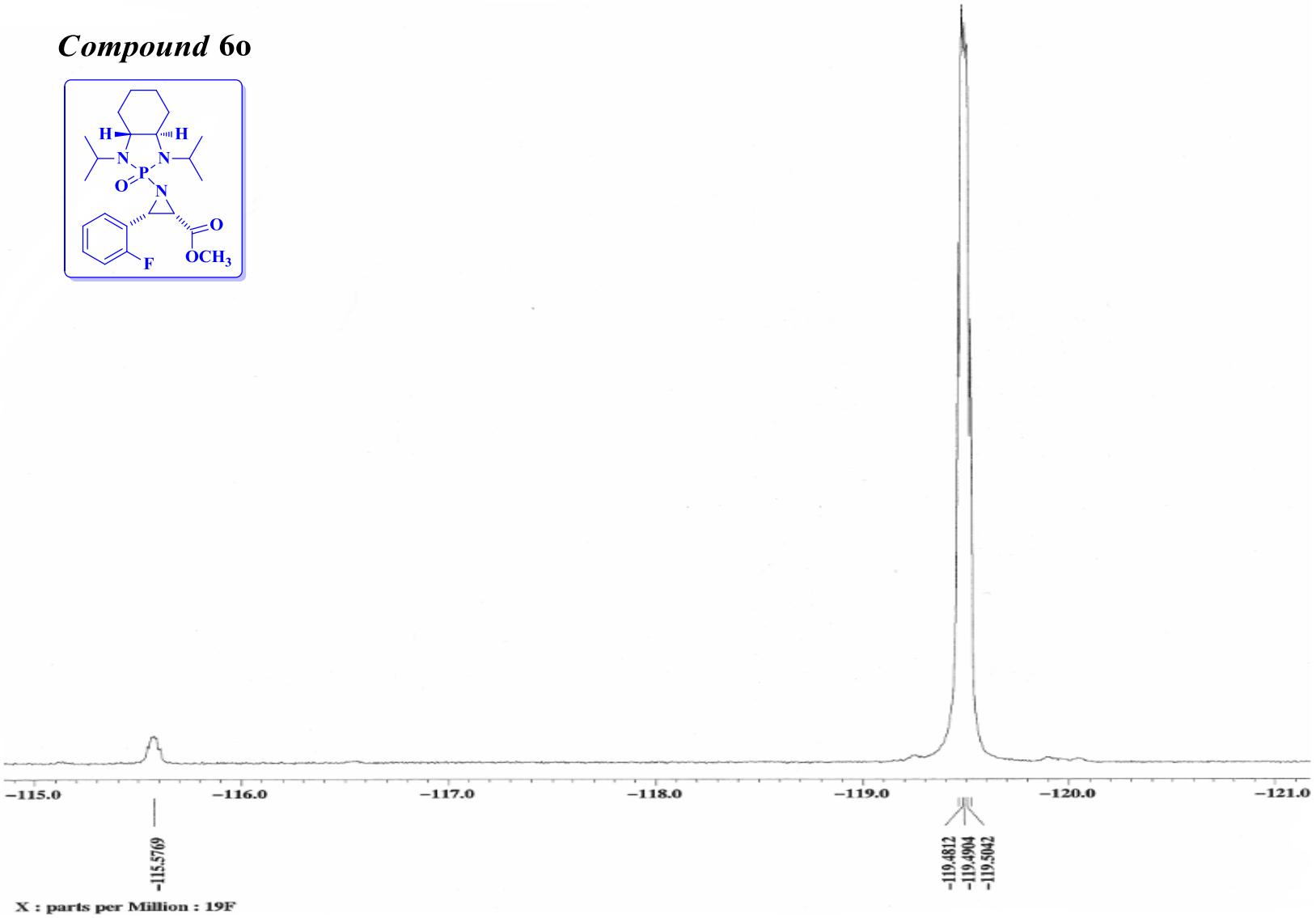
***Compound* 6o**

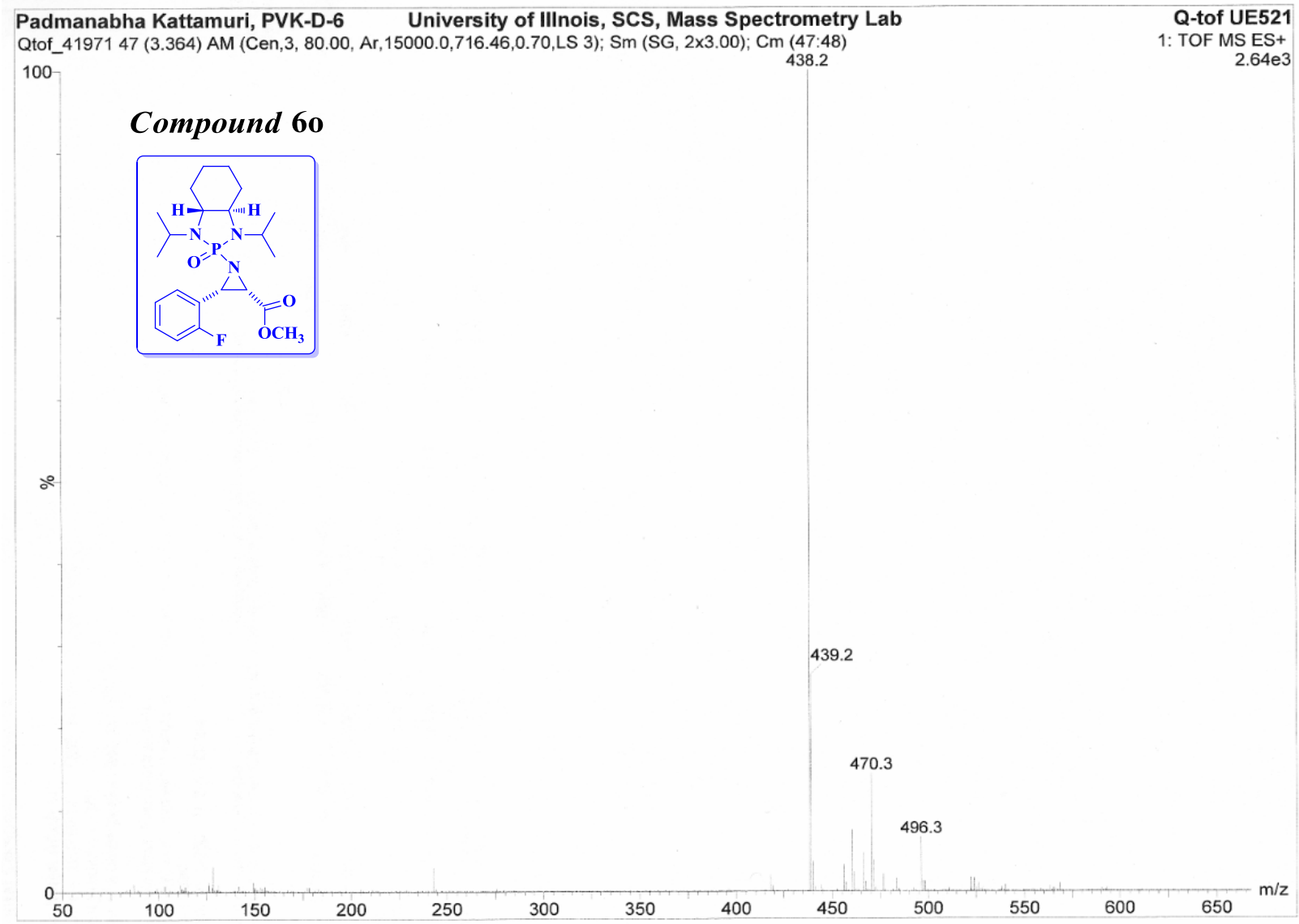


***Compound* 6o**



***Compound* 6o**





Elemental Composition Report

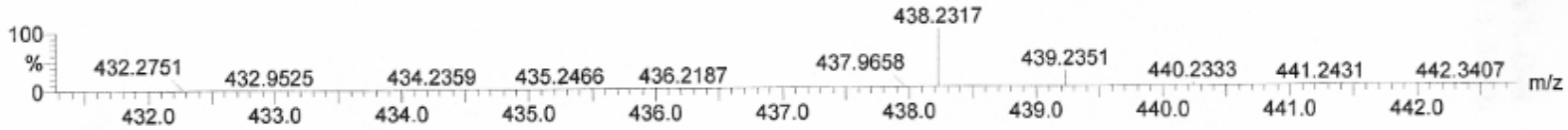
Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 600.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

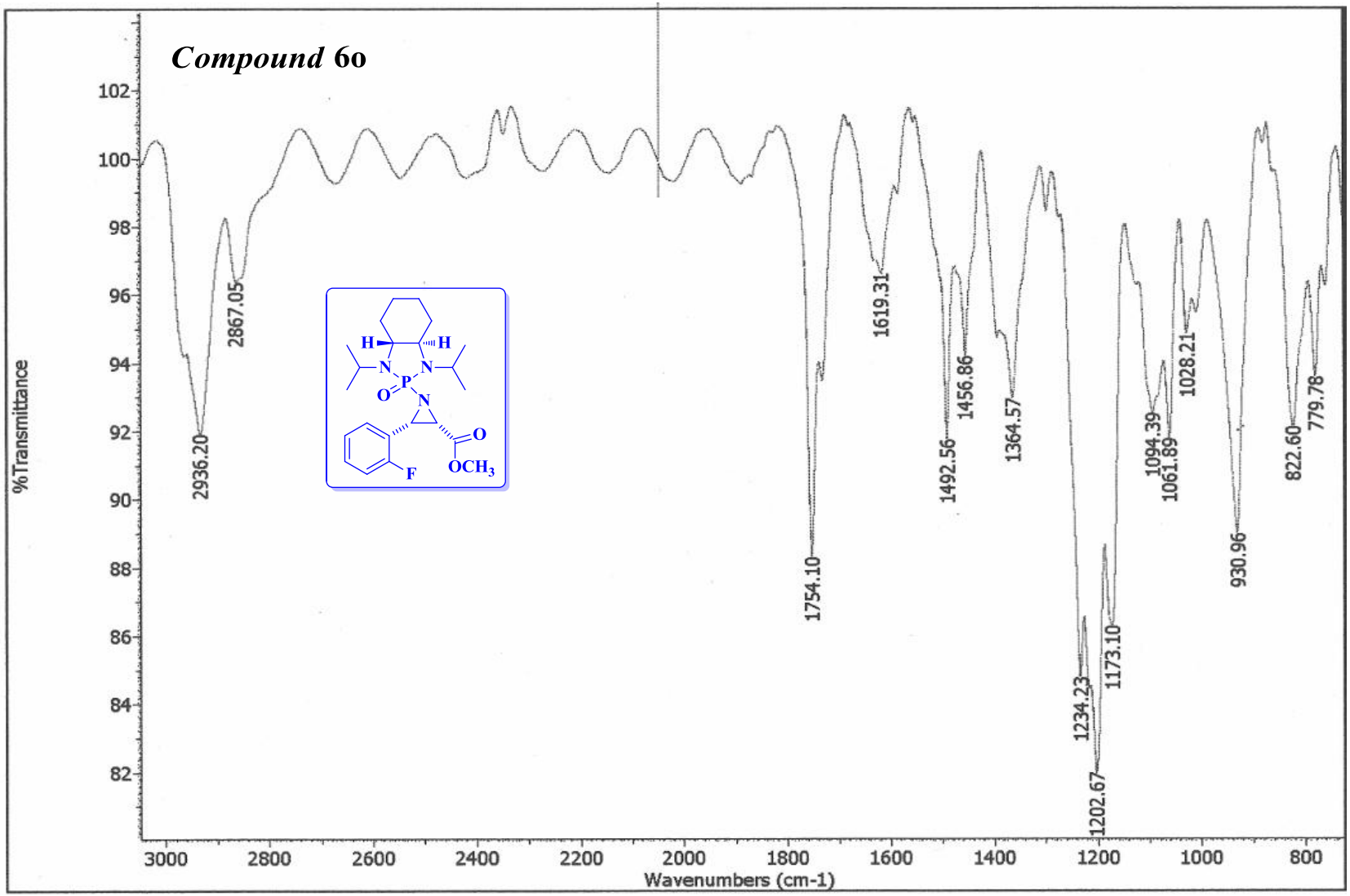
Monoisotopic Mass, Even Electron Ions
169 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-250 N: 2-4 O: 2-4 P: 0-1 S: 0-1 F: 1-1

Padmanabha Kattamuri, PVK-D-6 University of Illnois, SCS, Mass Spectrometry Lab
Qtof_41971 47 (3.364) AM (Cen,3, 80.00, Ar,15000.0,716.46,0.70,LS 3); Sm (SG, 2x3.00); Cm (47:48)

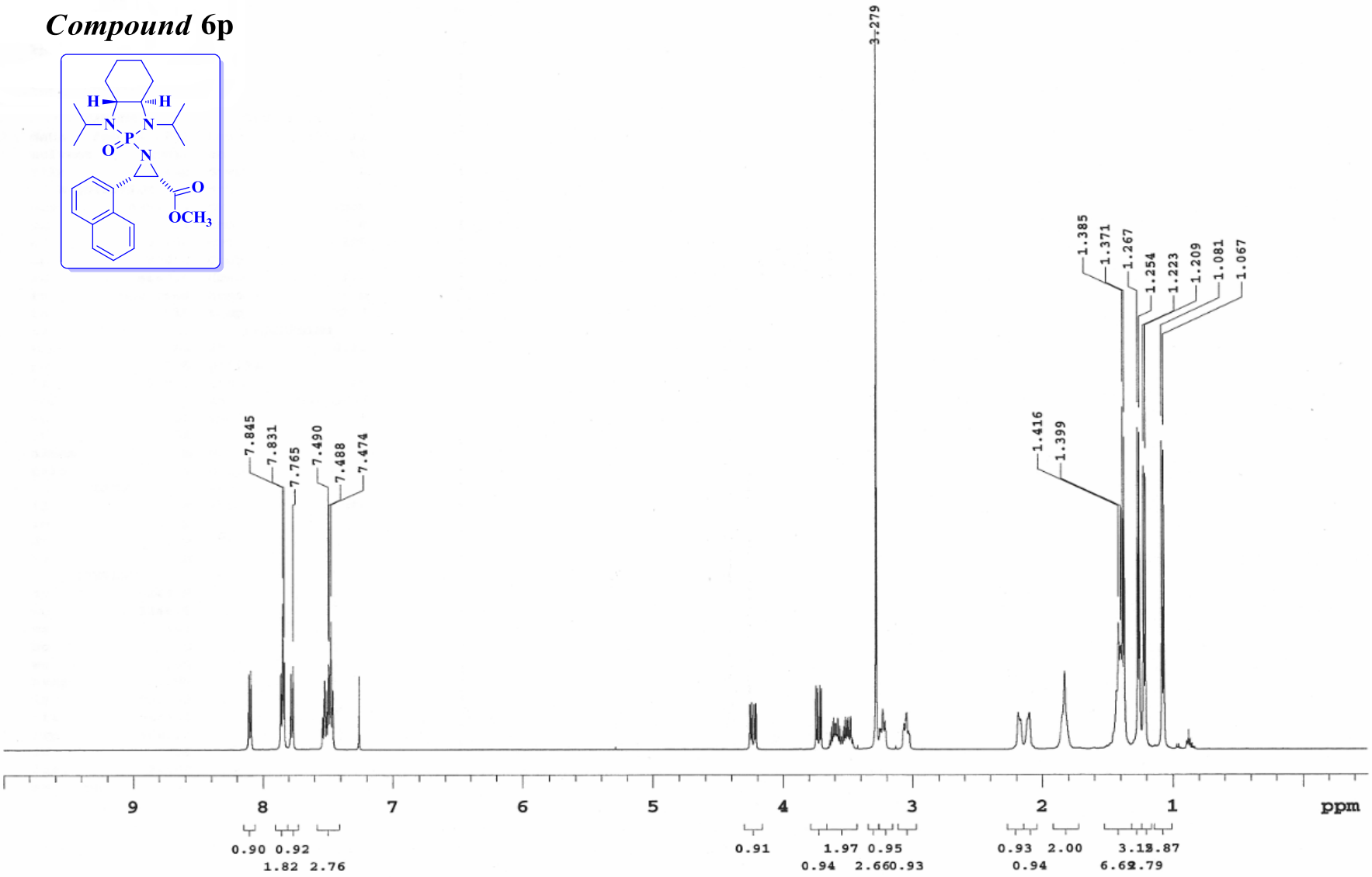
Q-tof UE521
1: TOF MS ES+
2.64e+003



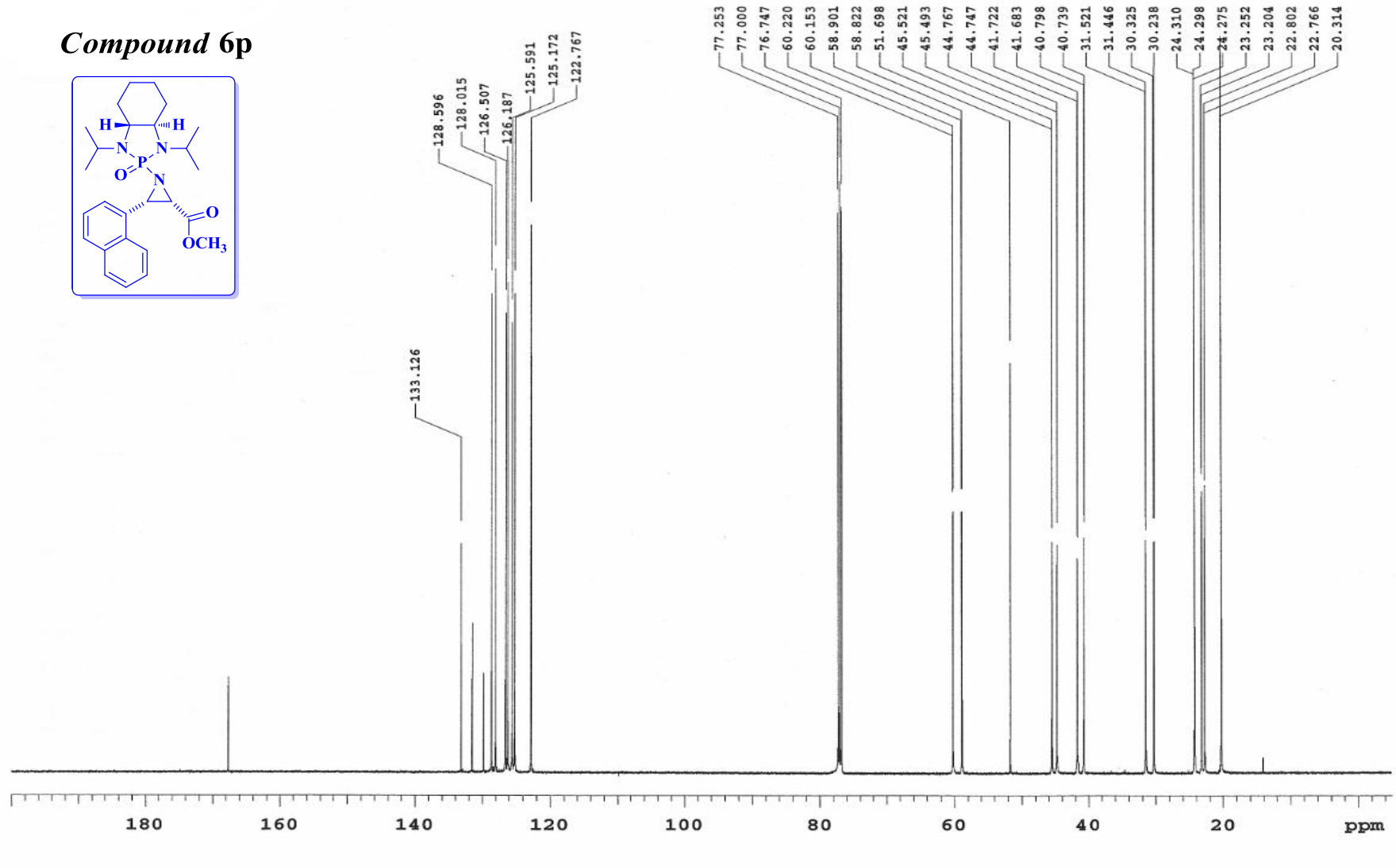
Minimum:				-1.5		
Maximum:		5.0	10.0	600.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
438.2317	438.2322	-0.5	-1.1	7.5	0.3	C22 H34 N3 O3 P F
	438.2356	-3.9	-8.9	2.5	61.5	C19 H38 N3 O3 P S F



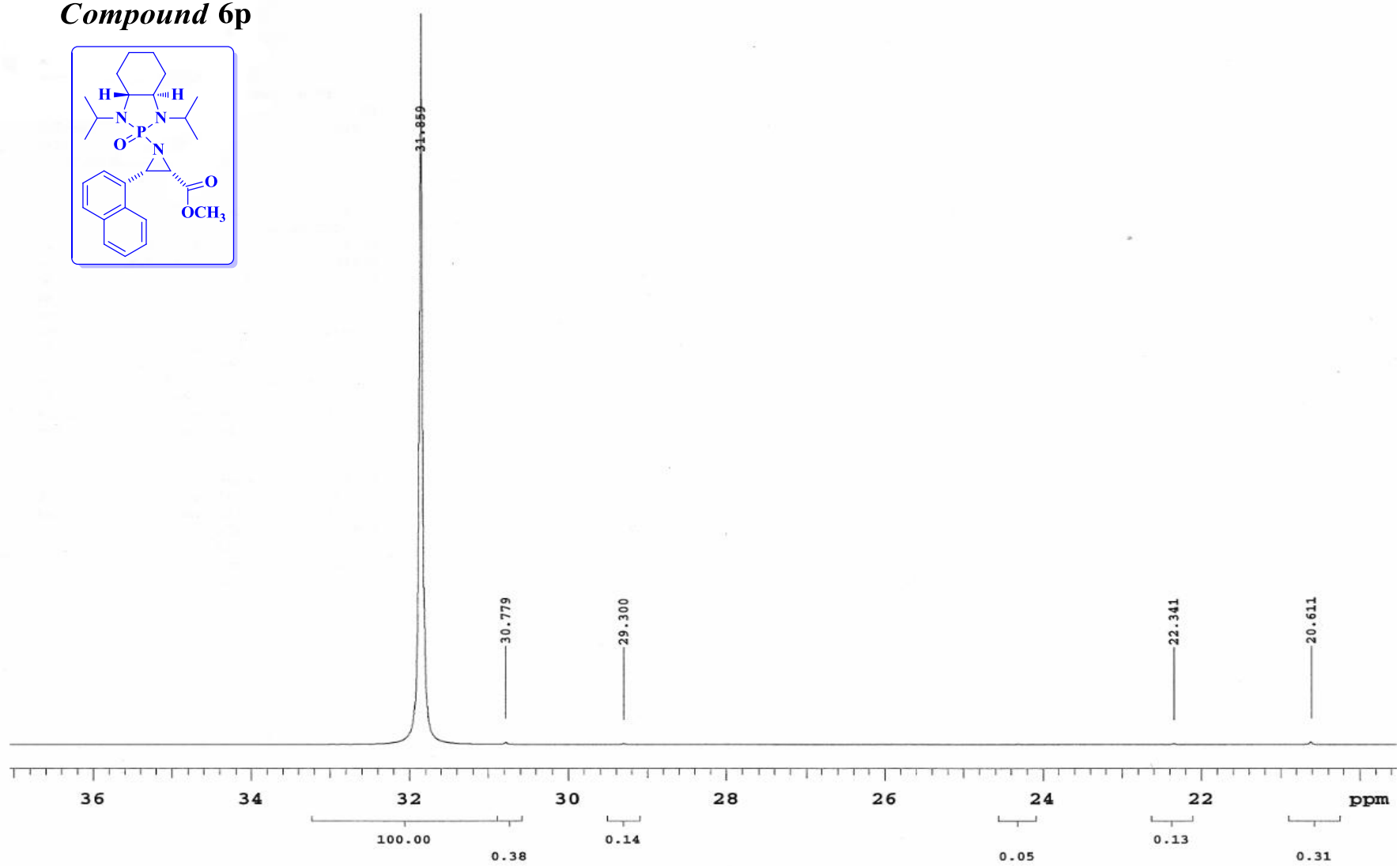
***Compound* 6p**

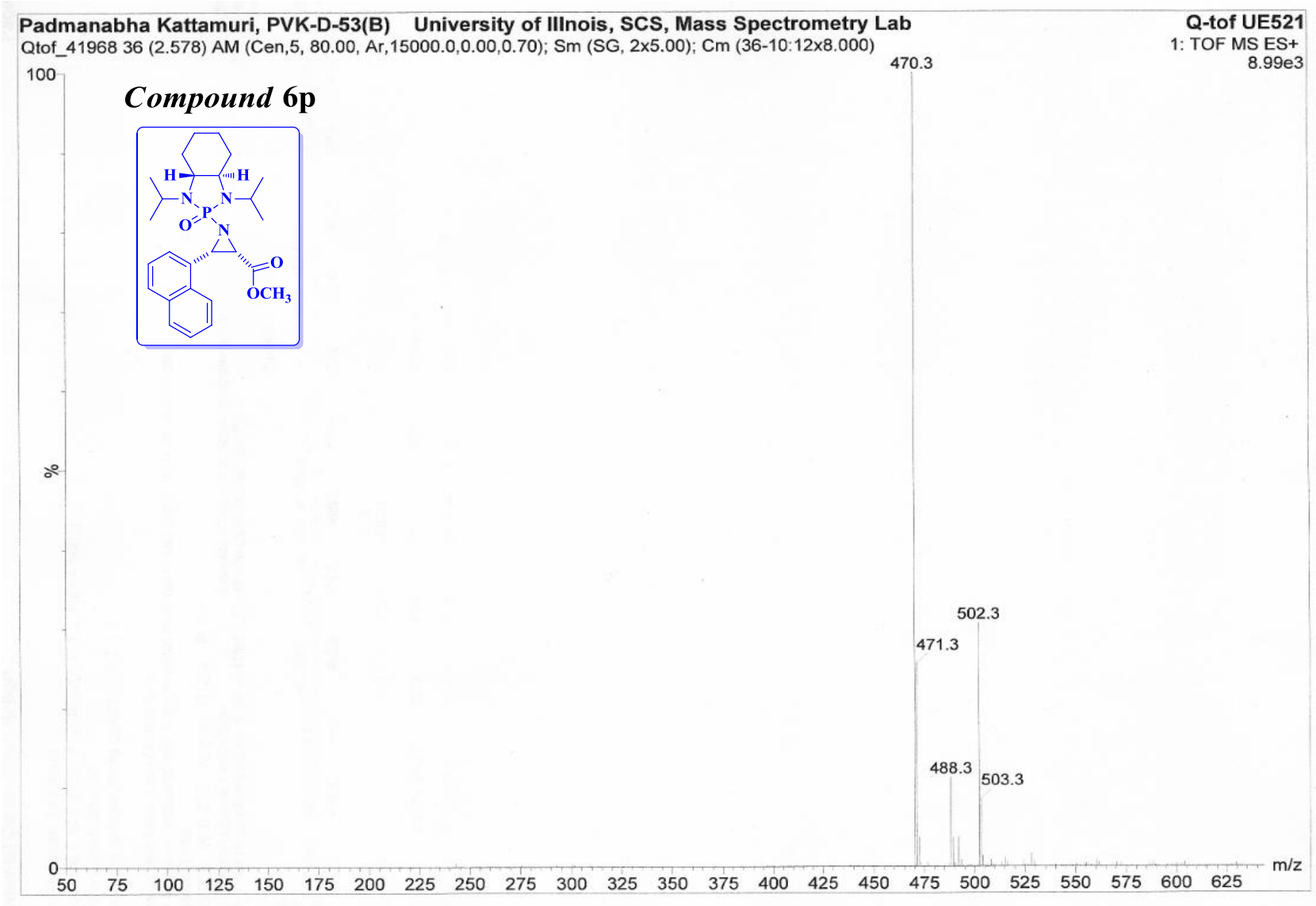


***Compound* 6p**



***Compound* 6p**





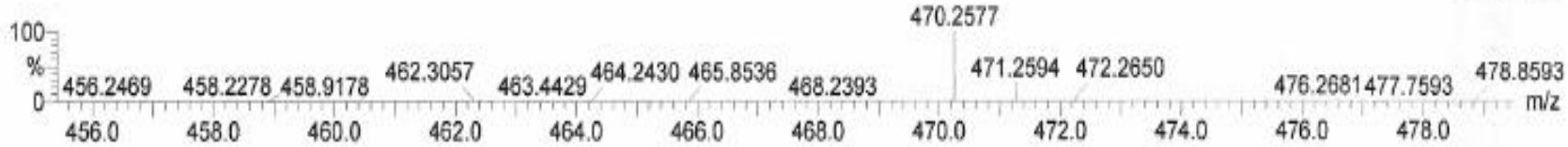
Elemental Composition Report

Single Mass Analysis

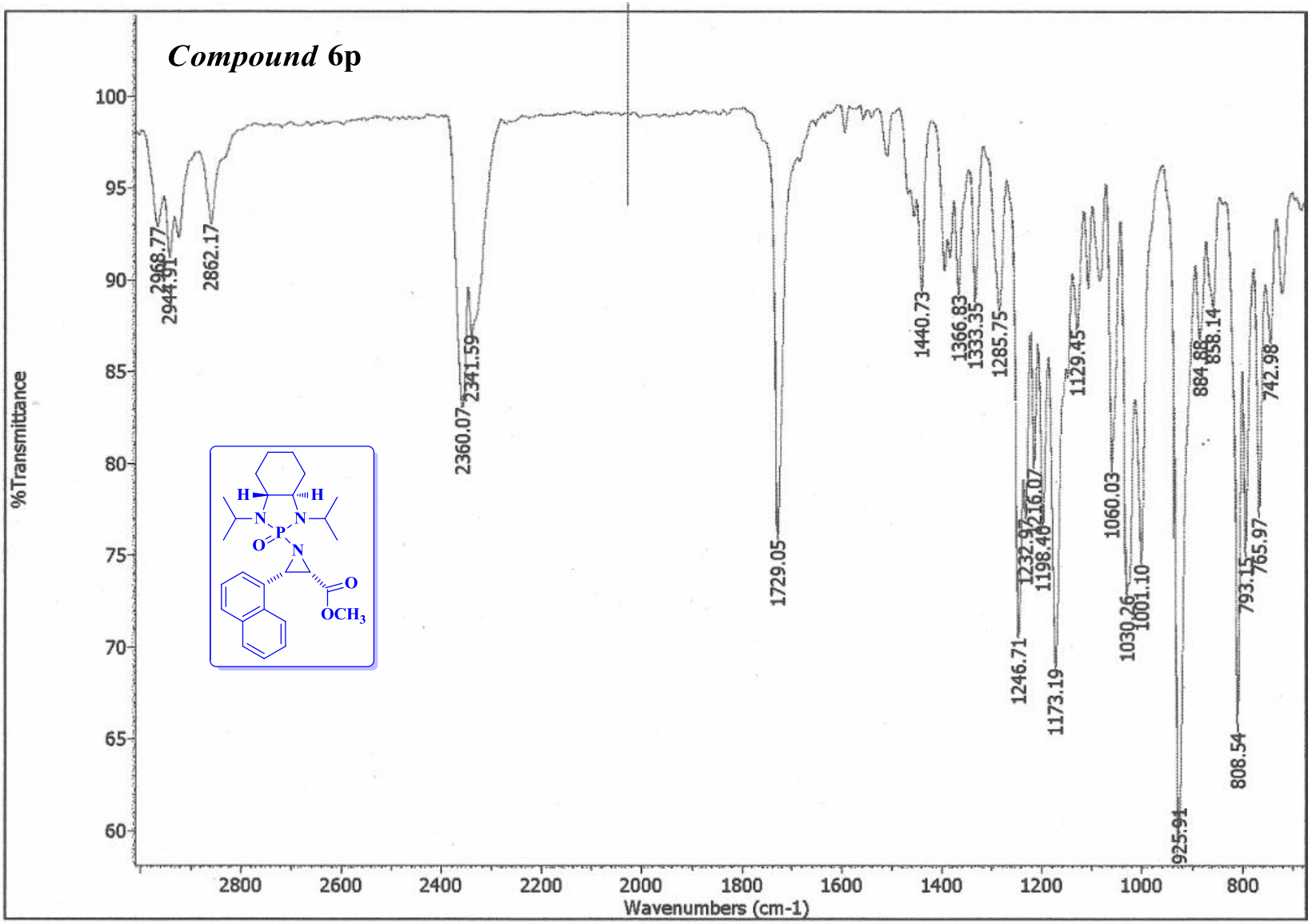
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 600.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
103 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-250 N: 2-4 O: 2-4 P: 0-1

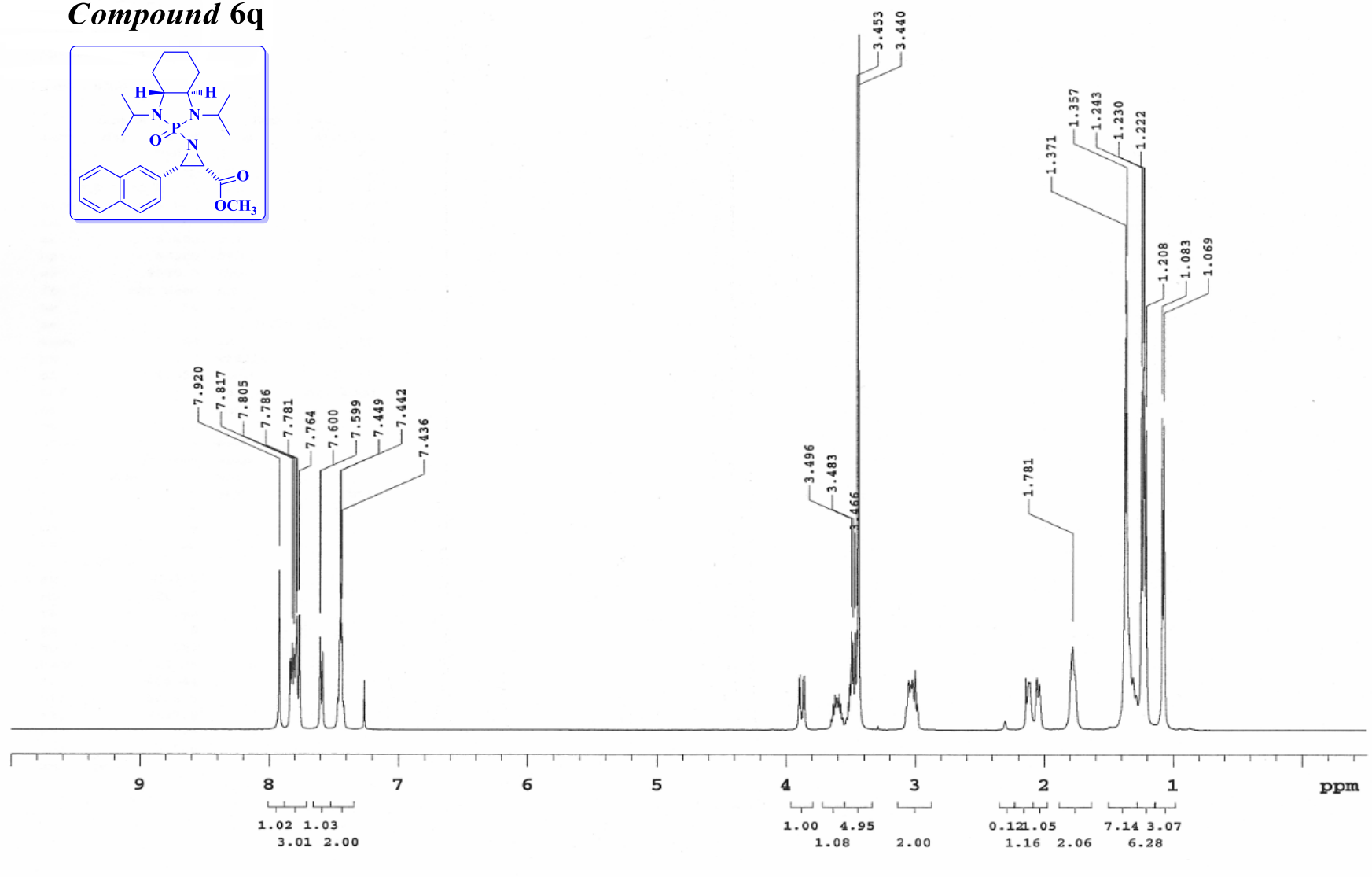
Padmanabha Kattamuri, PVK-D-53(B) University of Illnois, SCS, Mass Spectrometry Lab Q-tof UE521
Qtof_41968 54 (3.864) AM (Cen,3, 80.00, Ar,15000.0,716.46,0.70,LS 3); Sm (SG, 2x3.00) 1: TOF MS ES+
4.97e+002



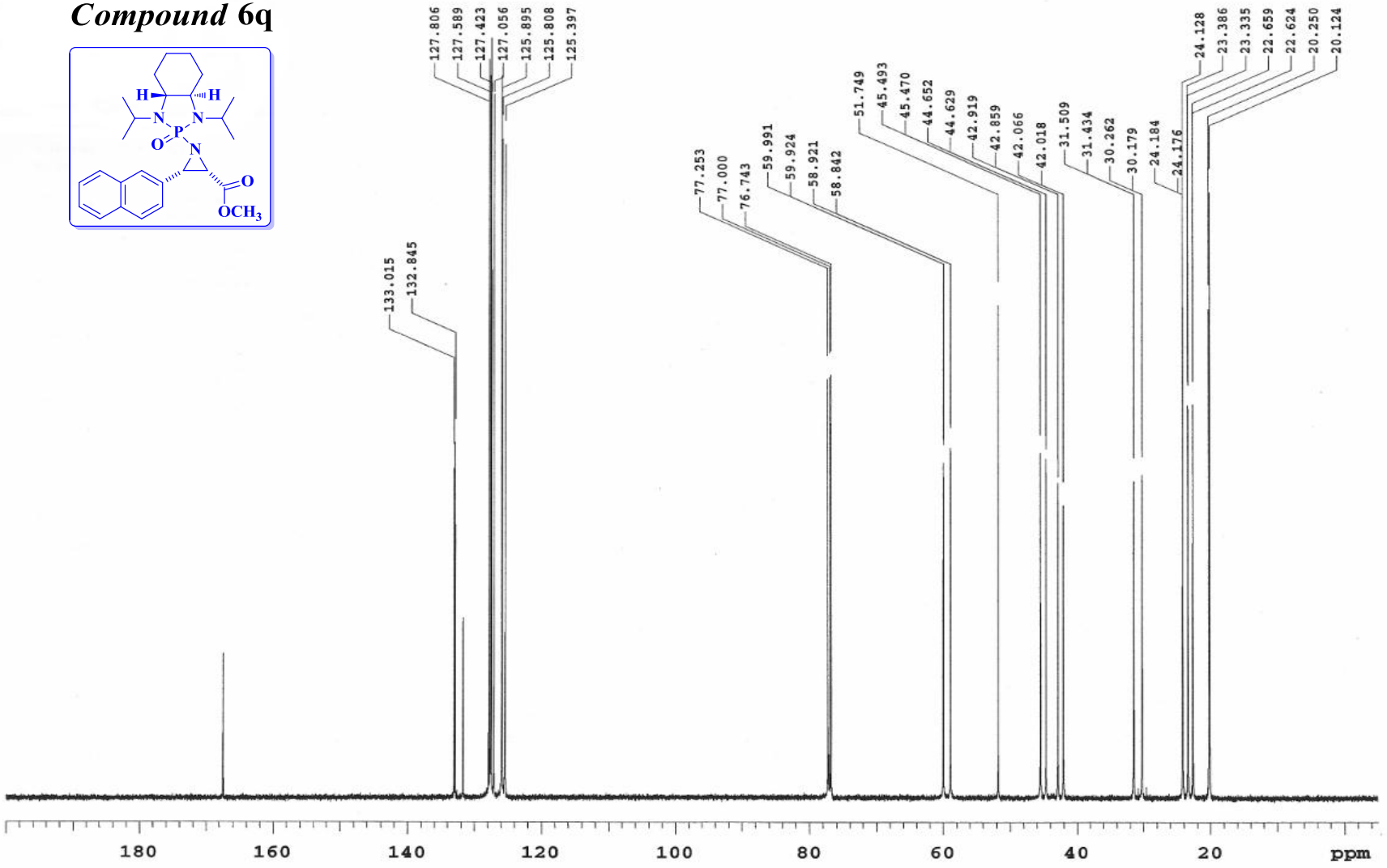
Minimum:				-1.5		
Maximum:		5.0	10.0	600.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
470.2577	470.2573	0.4	0.9	10.5	0.9	C26 H37 N3 O3 P



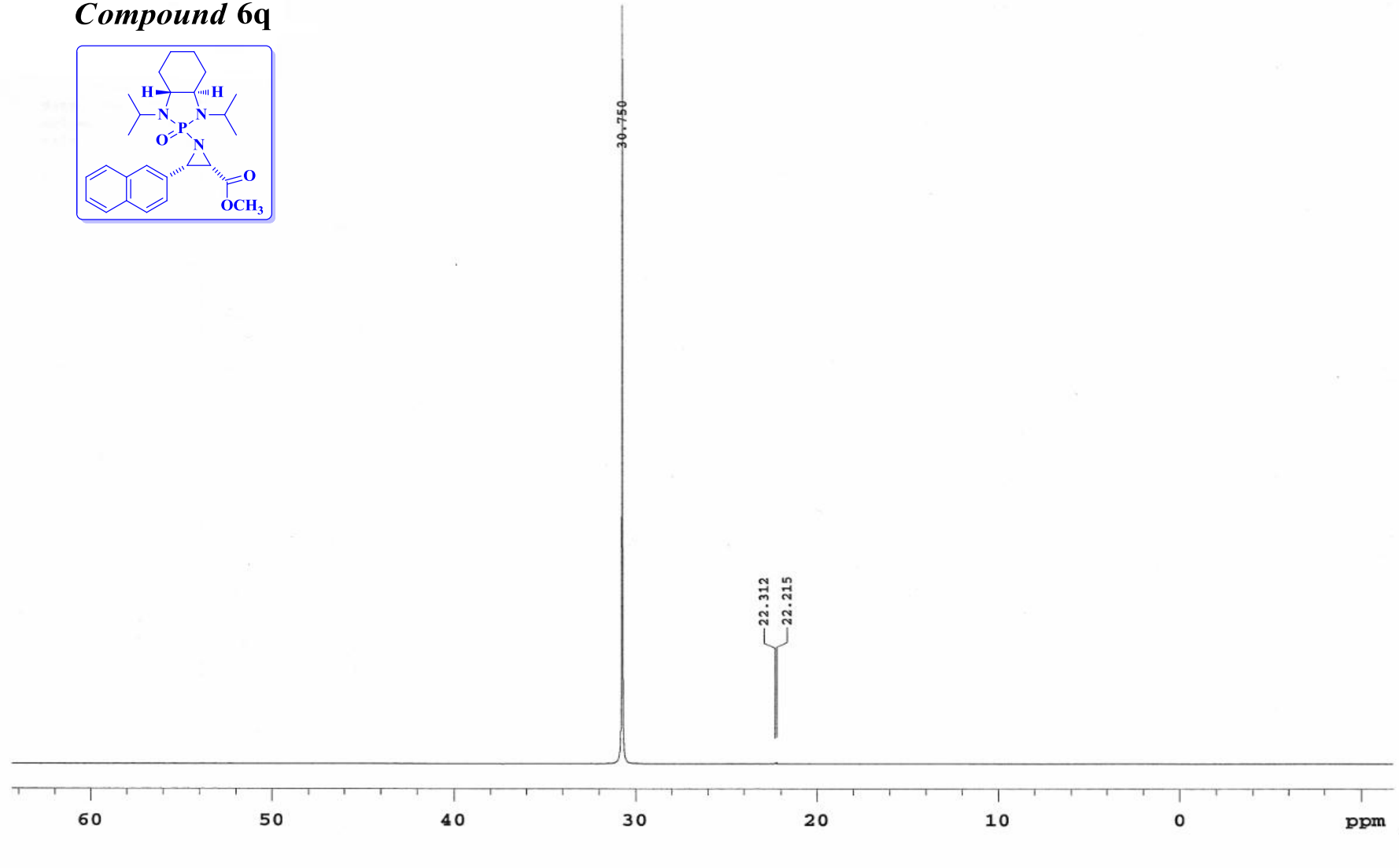
***Compound* 6q**

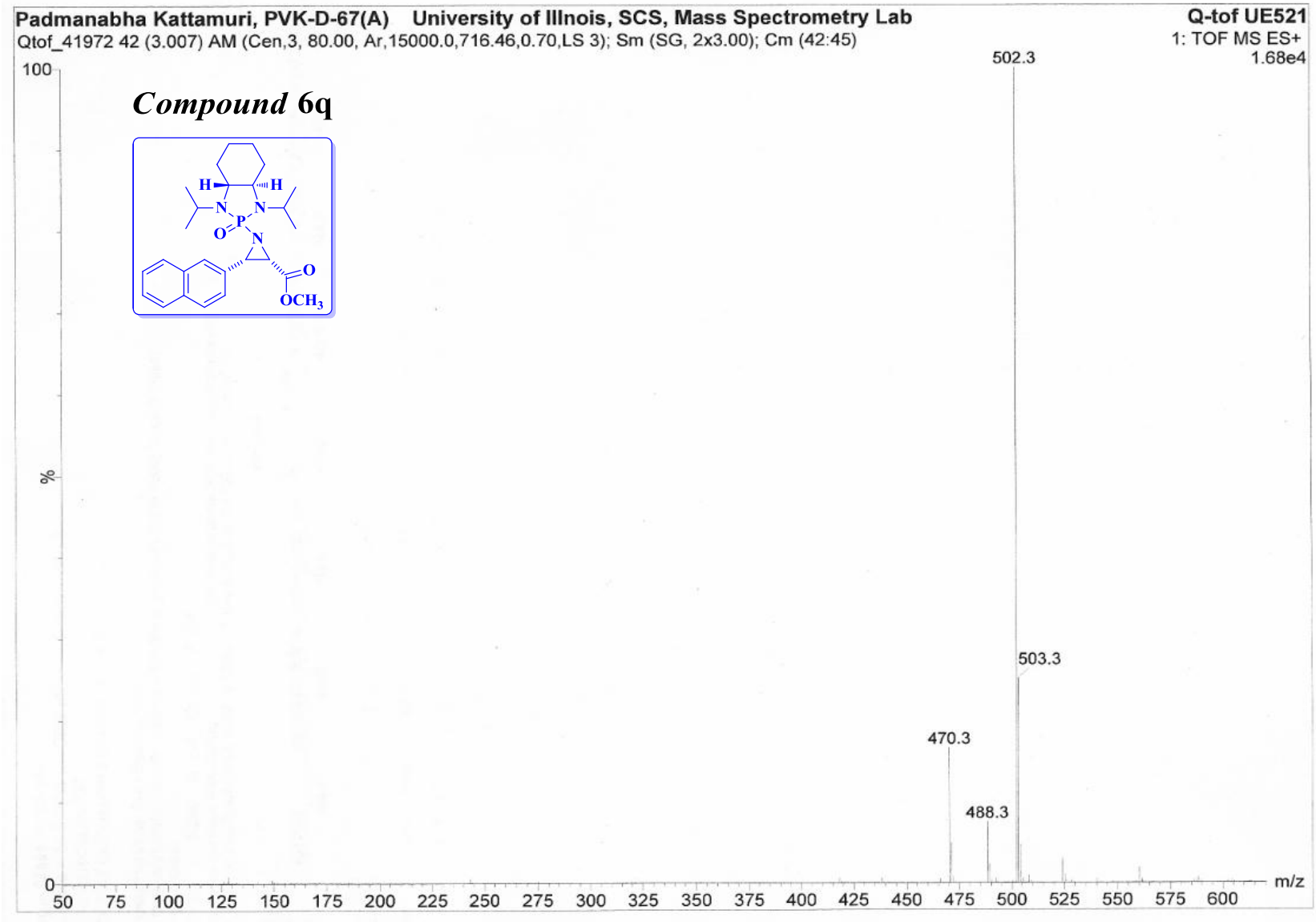


***Compound* 6q**



***Compound* 6q**





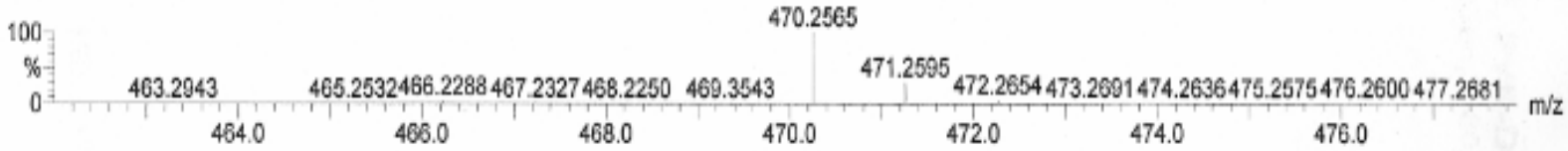
Elemental Composition Report

Single Mass Analysis

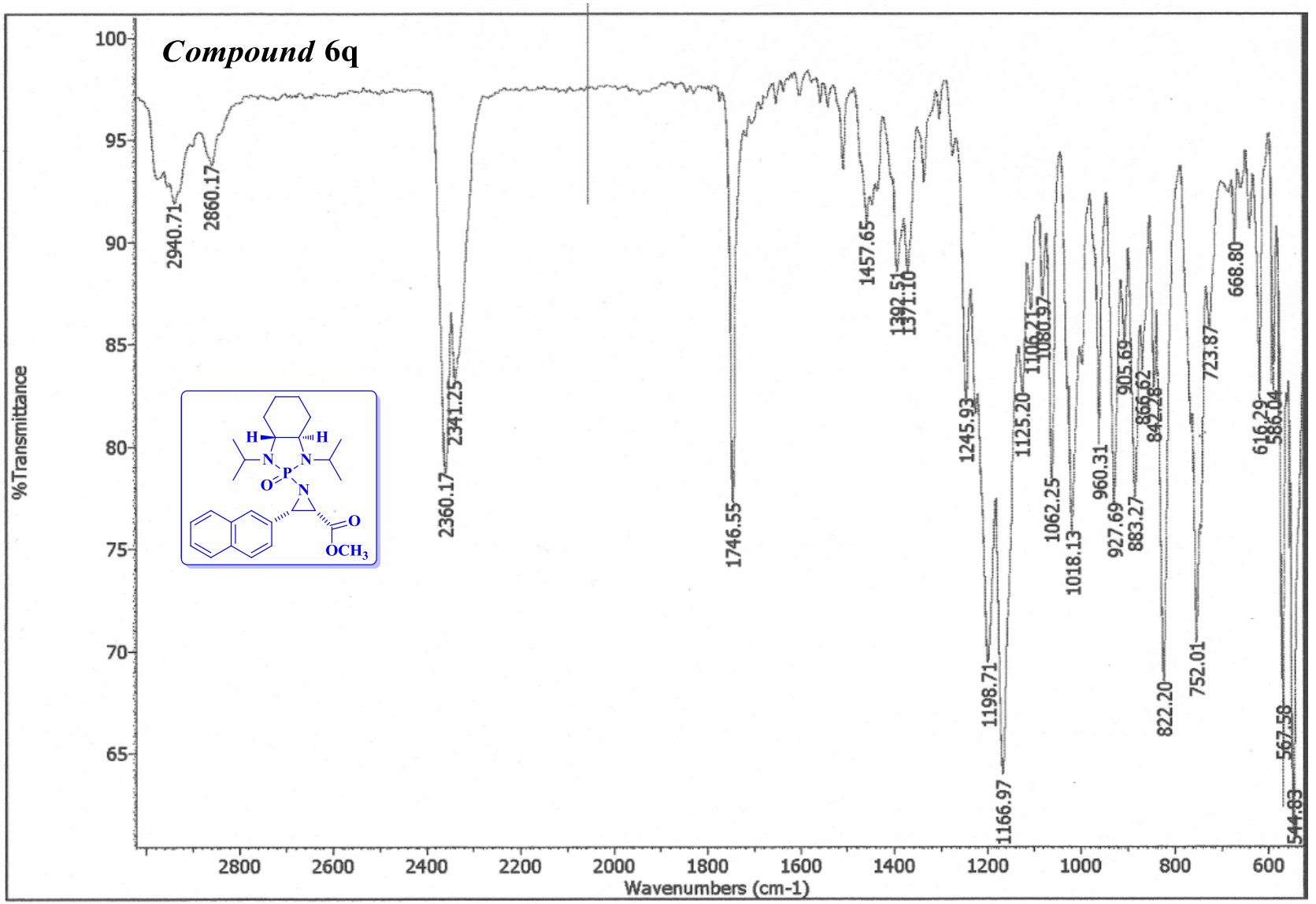
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 600.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
103 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-250 N: 2-4 O: 2-4 P: 0-1

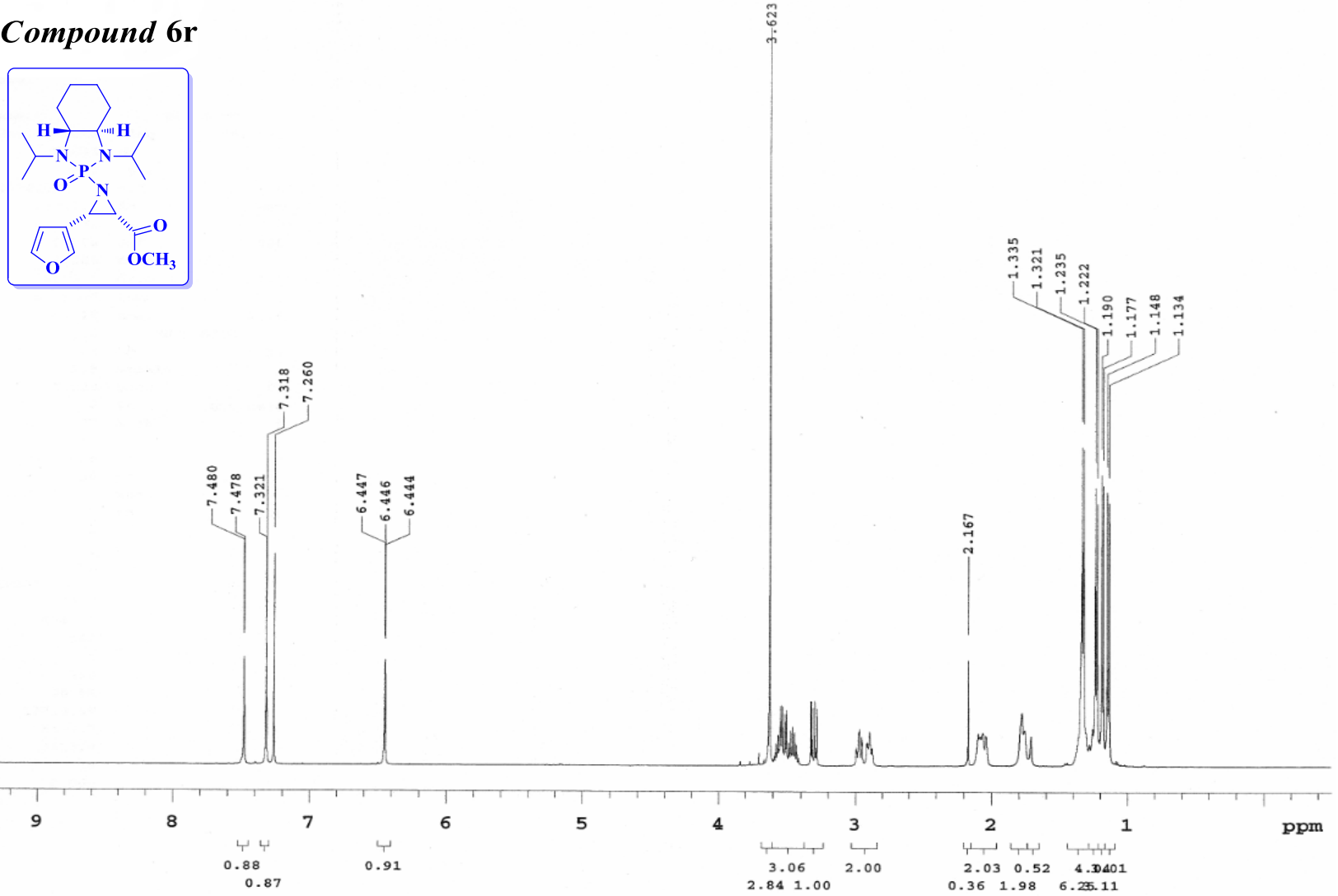
Padmanabha Kattamuri, PVK-D-67(A) University of Illinois, SCS, Mass Spectrometry Lab Q-tof UE521
Qtof_41972 42 (3.007) AM (Cen,3, 80.00, Ar,15000.0,716.46,0.70,LS 3); Sm (SG, 2x3.00); Cm (42:45) 1: TOF MS ES+
2.78e+003



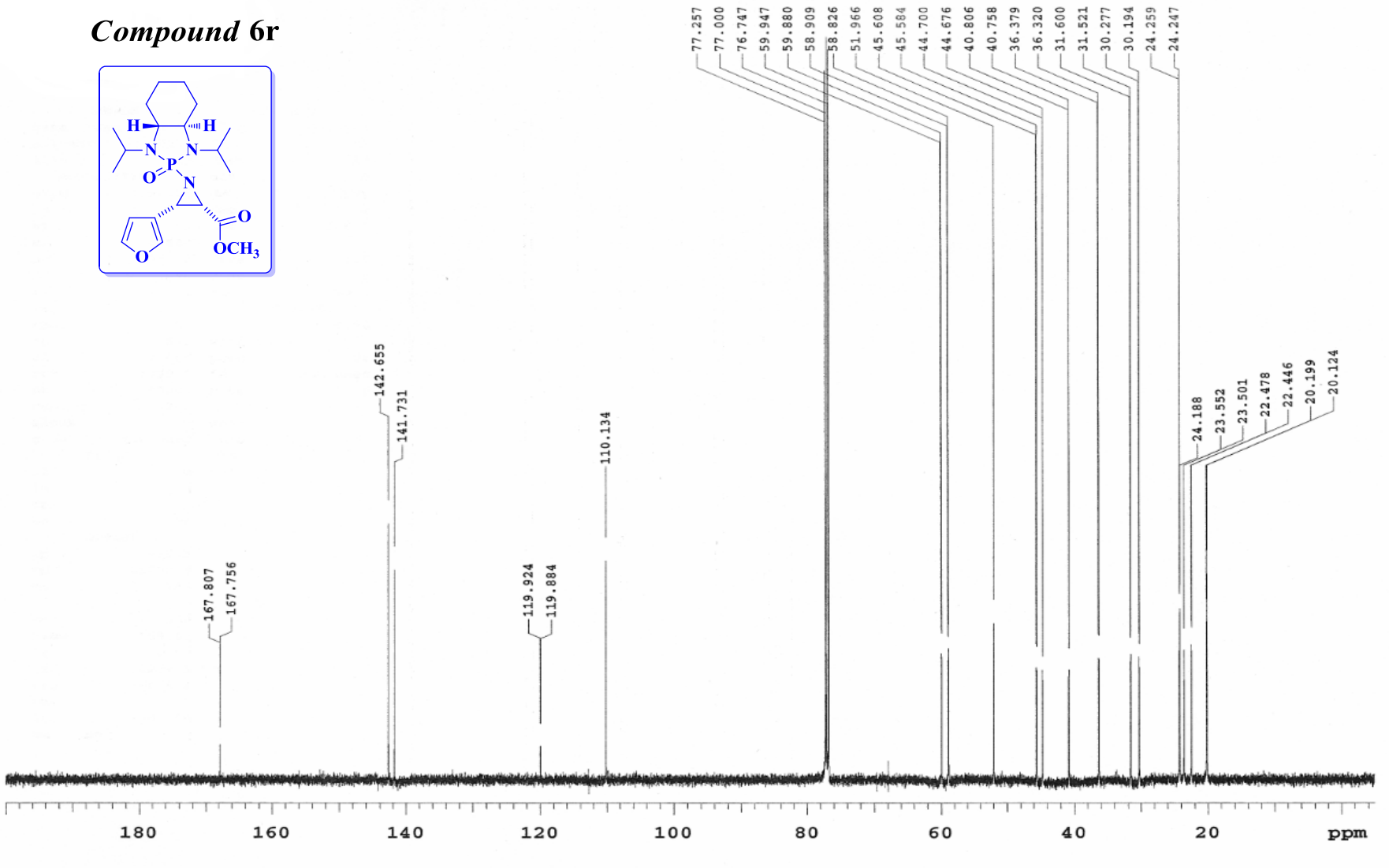
Minimum:				-1.5		
Maximum:		5.0	10.0	600.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
470.2565	470.2573	-0.8	-1.7	10.5	1.1	C26 H37 N3 O3 P



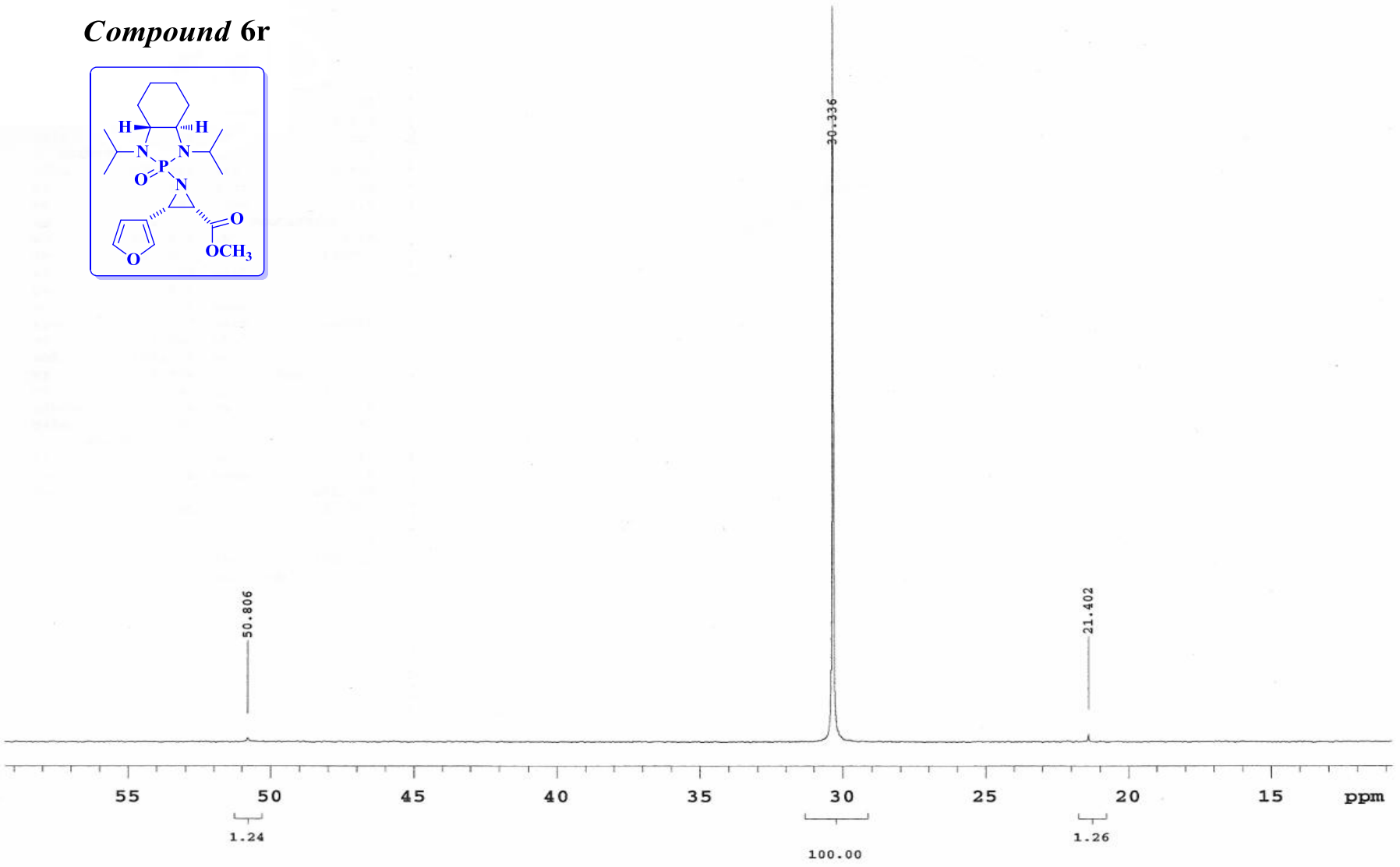
***Compound* 6r**

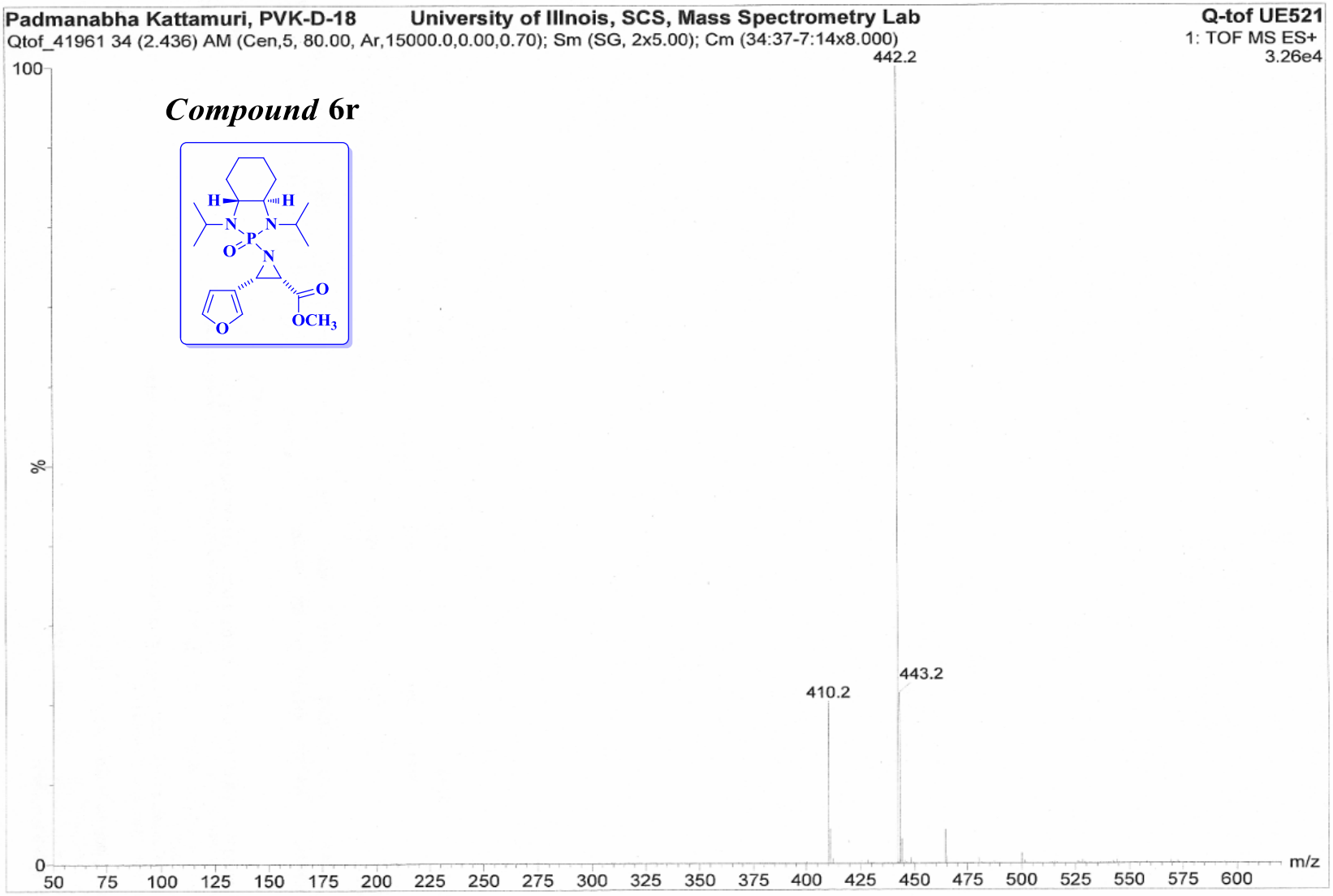


***Compound* 6r**



***Compound* 6r**




Padmanabha Kattamuri, PVK-D-18
University of Illnois, SCS, Mass Spectrometry Lab
Q-tof UE521
Qtof_41961 34 (2.436) AM (Cen,5, 80.00, Ar,15000.0,0.00,0.70); Sm (SG, 2x5.00); Cm (34:37-7:14x8.000)
1: TOF MS ES+
3.26e4
Compound 6r
442.2
443.2
410.2
100
%
0
m/z
50 75 100 125 150 175 200 225 250 275 300 325 350 375 400 425 450 475 500 525 550 575 600

Elemental Composition Report

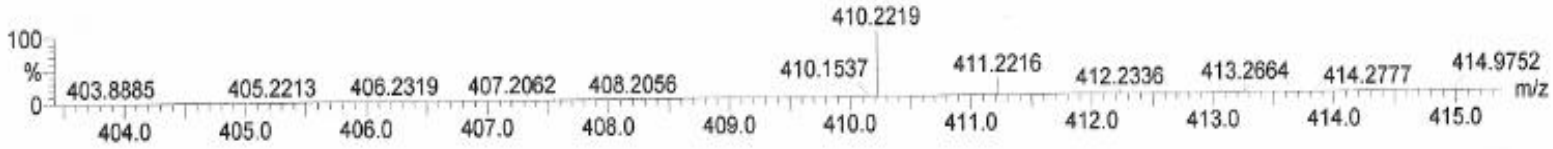
Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 600.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

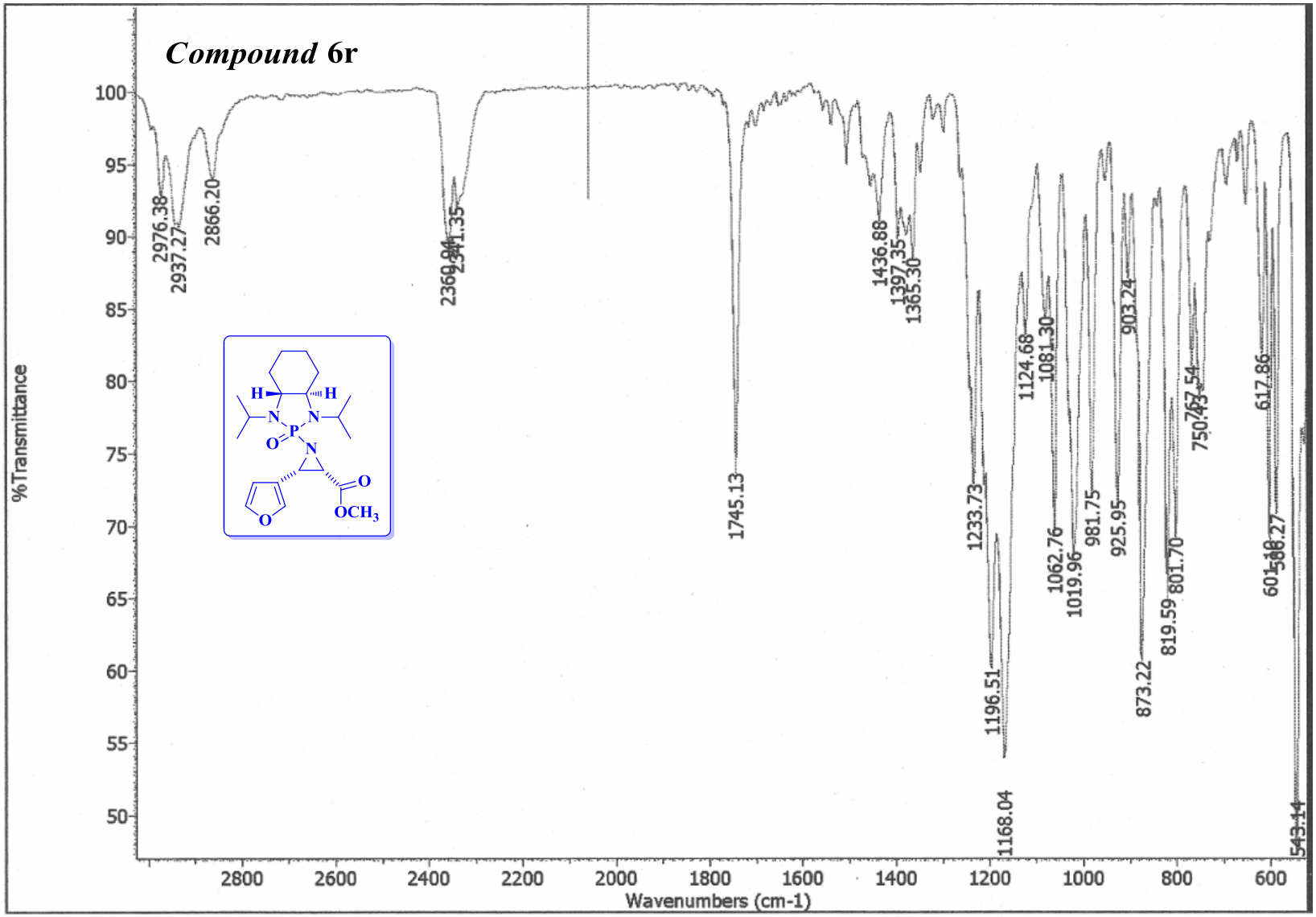
Monoisotopic Mass, Even Electron Ions
90 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-250 N: 2-4 O: 2-4 P: 0-1

Padmanabha Kattamuri, PVK-D-18 University of Illinois, SCS, Mass Spectrometry Lab
Qtof_41961 29 (2.043) AM (Cen,3, 80.00, Ar,15000.0,716.46,0.70); Sm (SG, 2x3.00); Cm (27:30)

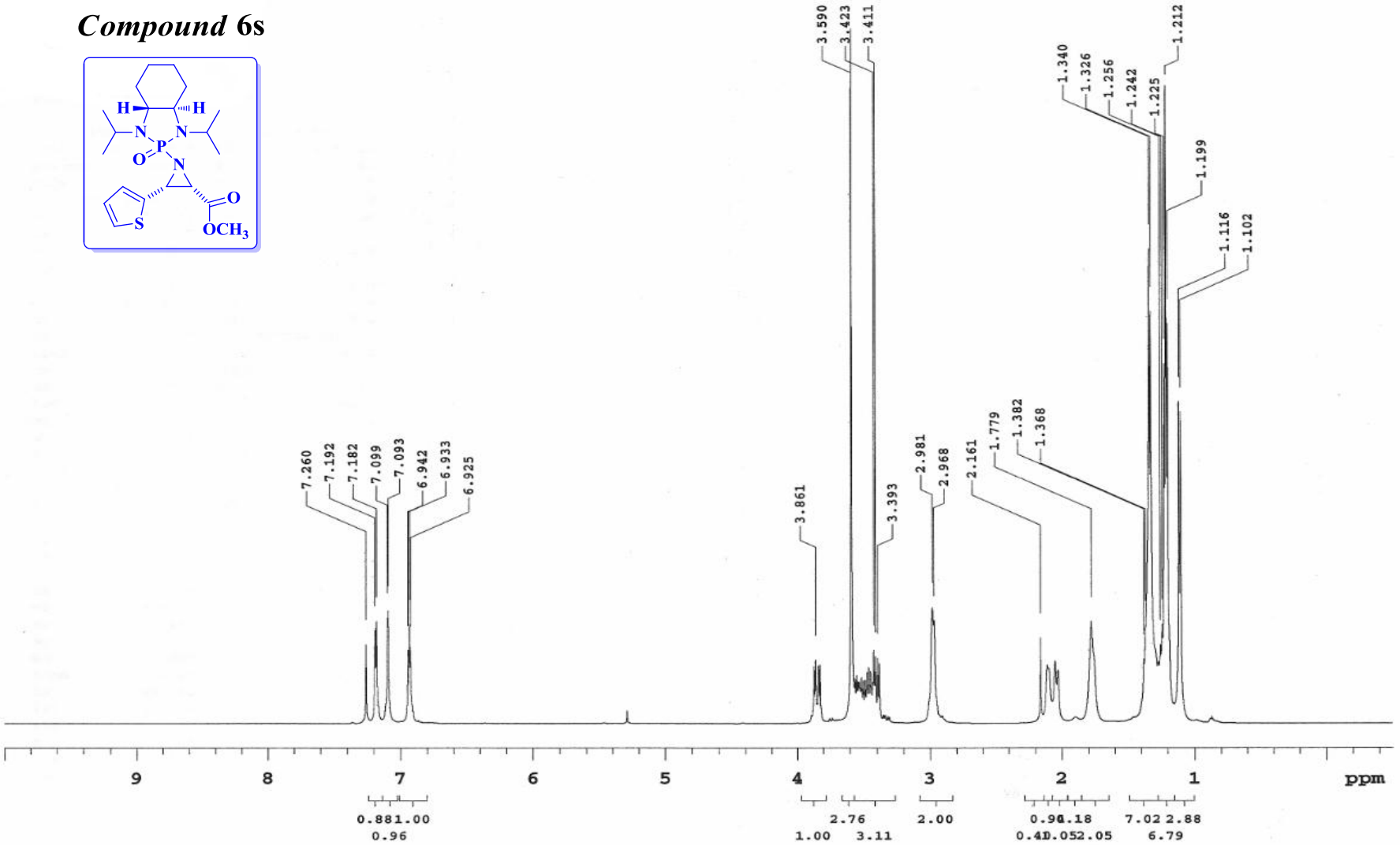
Q-tof UE521
2: TOF MS ES+
4.96e+002



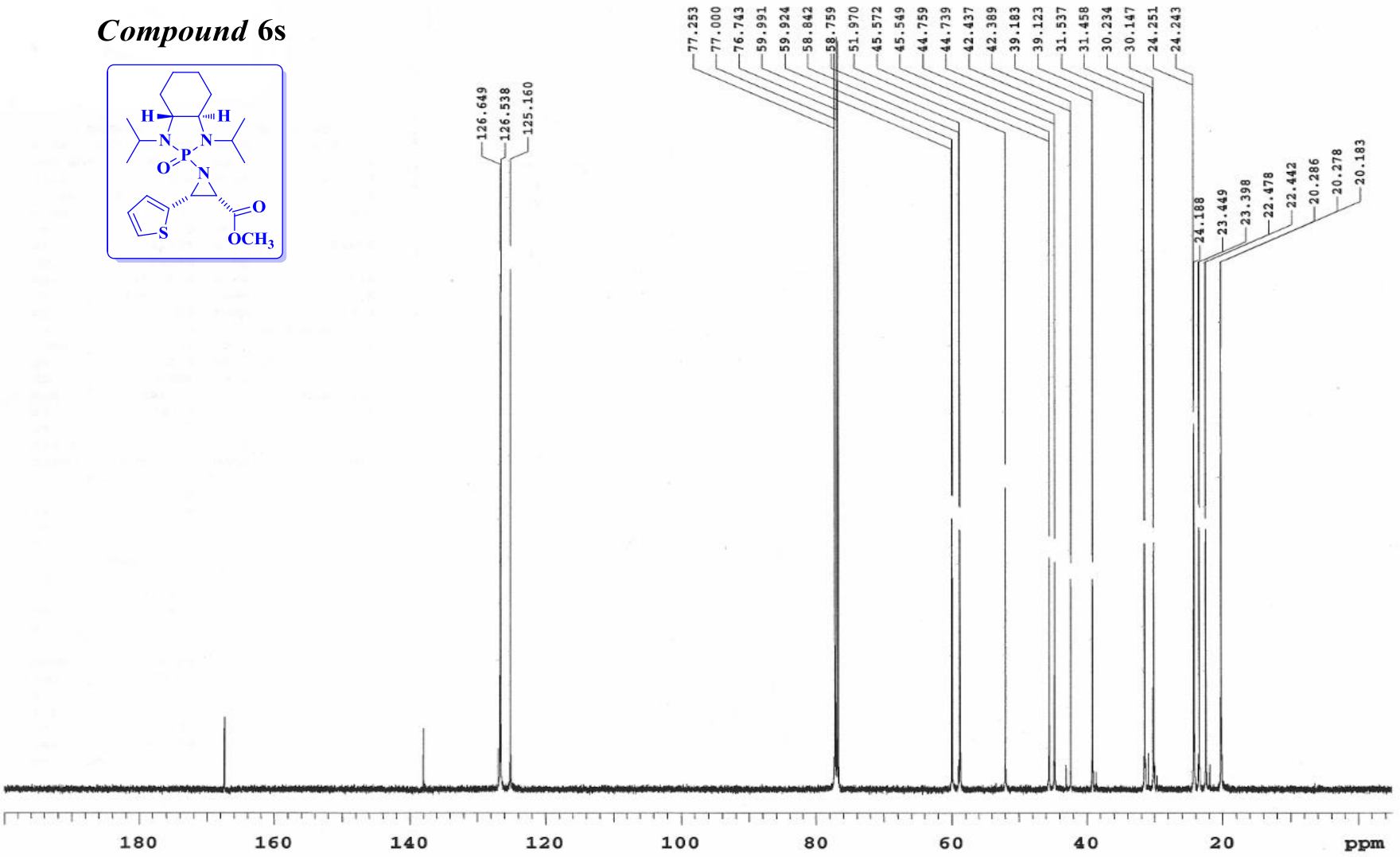
Minimum:				-1.5		
Maximum:		5.0	10.0	600.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
410.2219	410.2209	1.0	2.4	6.5	0.7	C20 H33 N3 O4 P



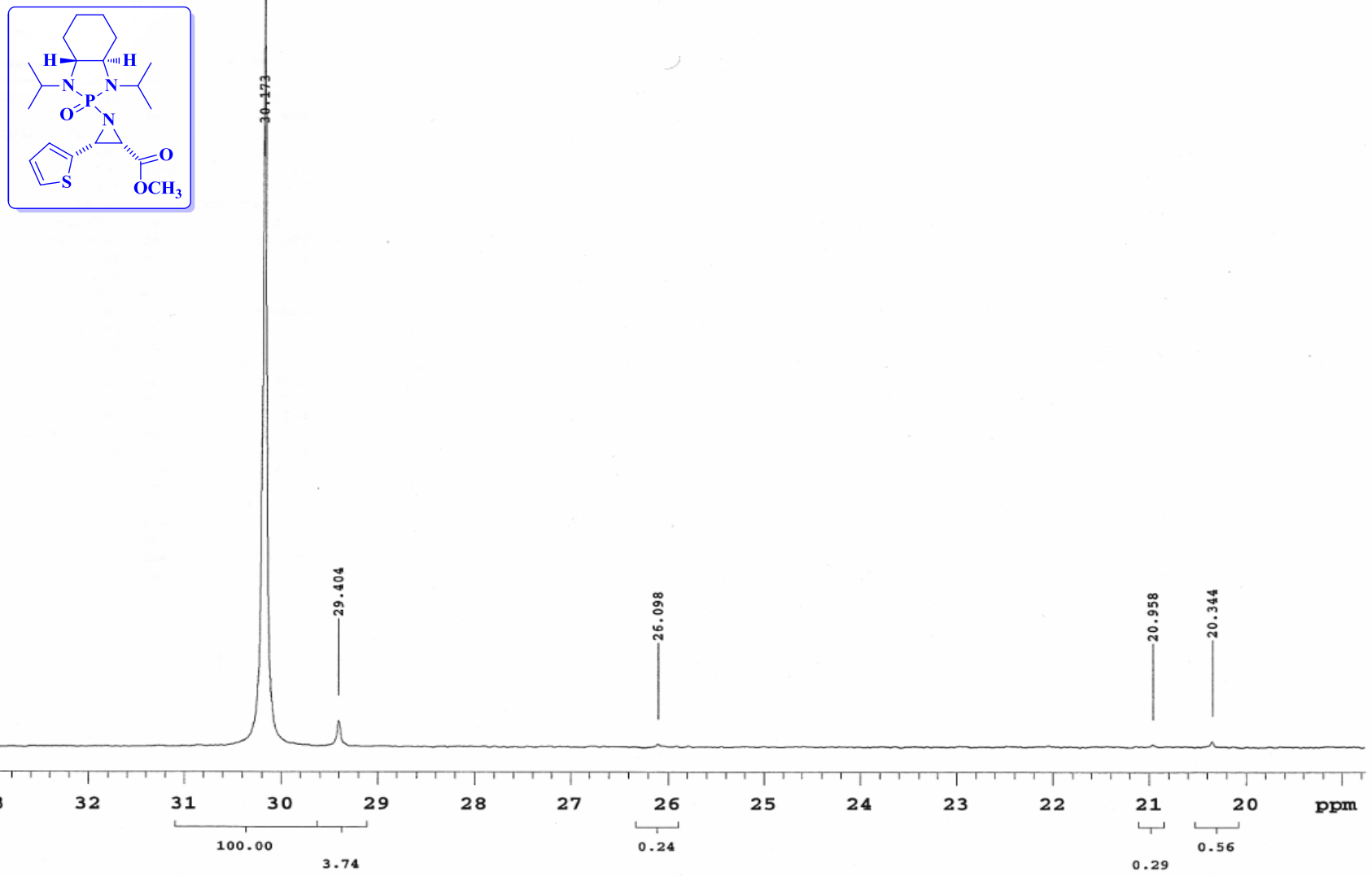
***Compound* 6s**

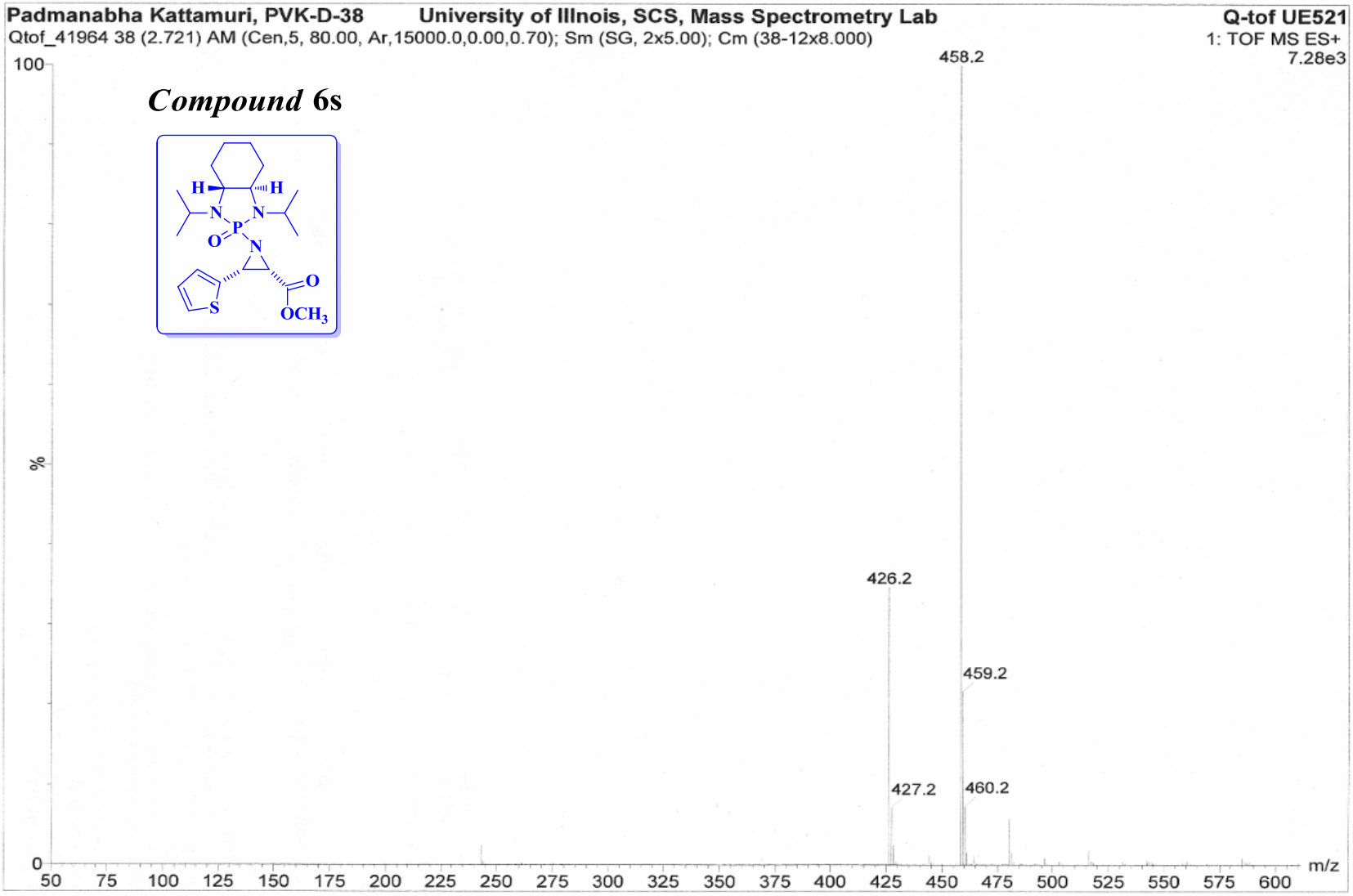


***Compound* 6s**



***Compound* 6s**





Elemental Composition Report

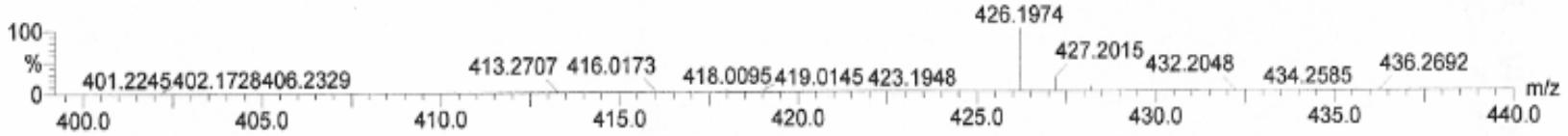
Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 600.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

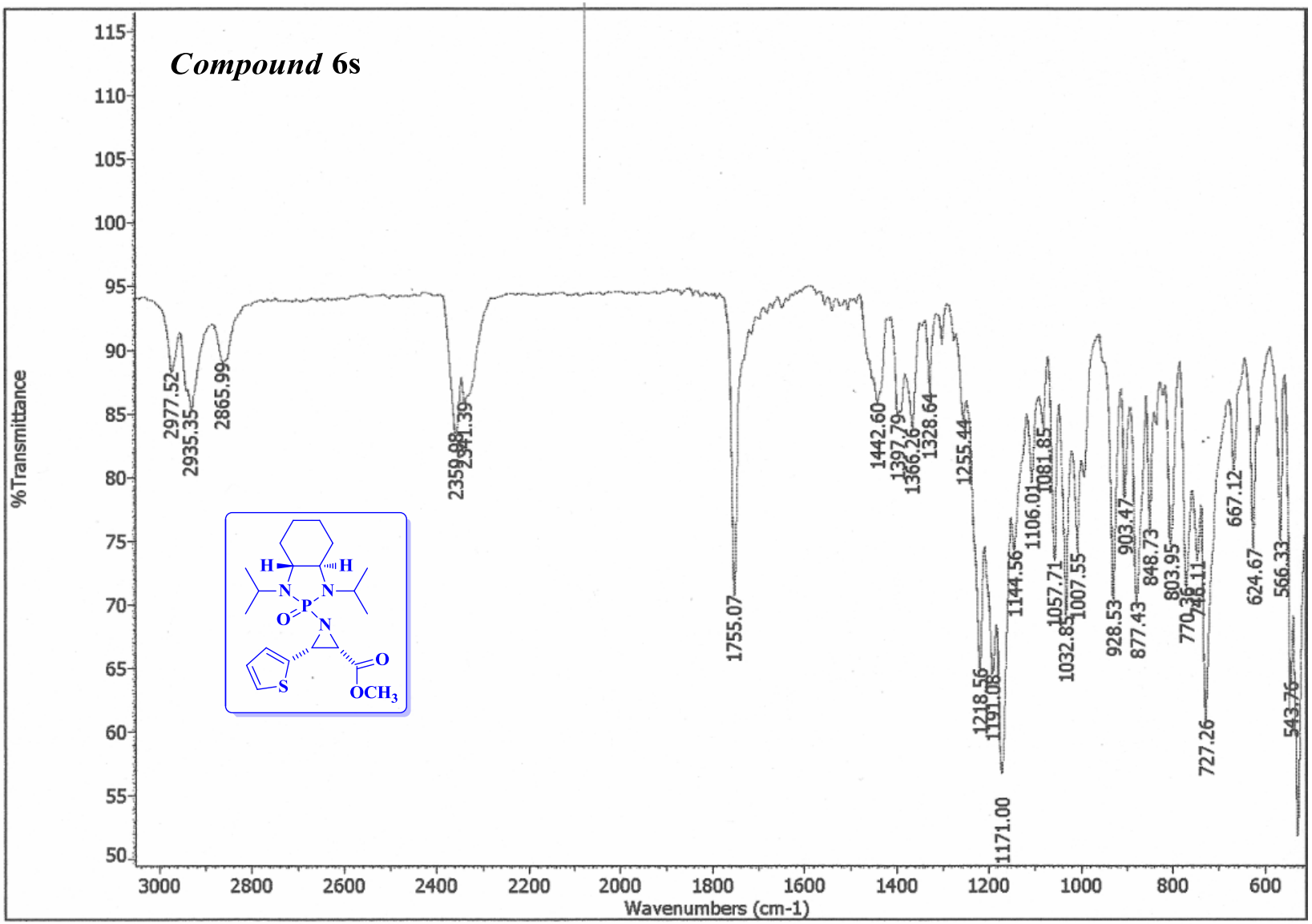
Monoisotopic Mass, Even Electron Ions
178 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-250 N: 2-4 O: 2-4 P: 0-1 S: 0-1

Padmanabha Kattamuri, PVK-D-38 University of Illnois, SCS, Mass Spectrometry Lab
Qtof_41964 47 (3.364) AM (Cen,3, 80.00, Ar,15000.0,716.46,0.70,LS 3); Sm (SG, 2x3.00); Cm (47:49)

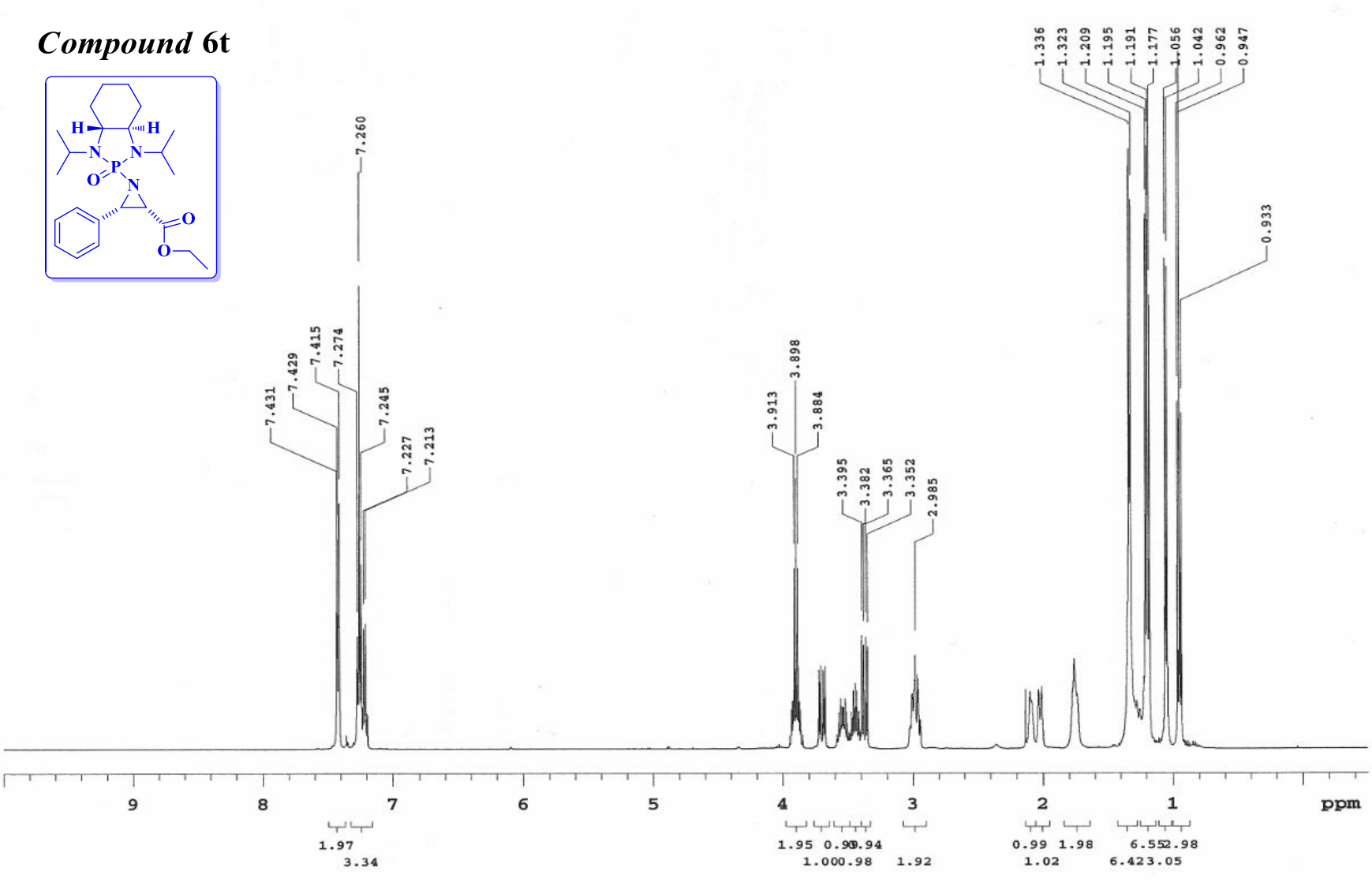
Q-tof UE521
1: TOF MS ES+
2.45e+003



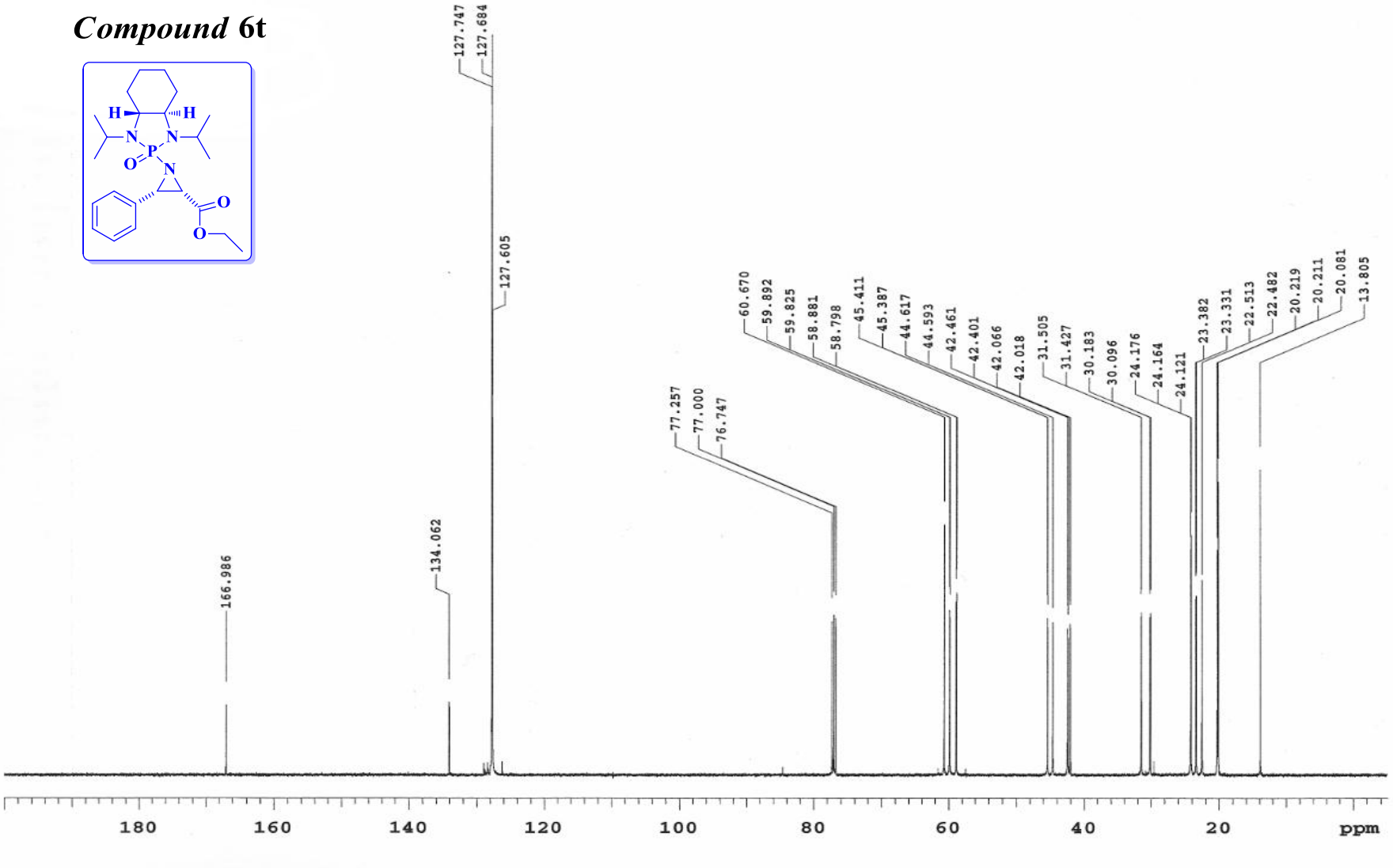
Minimum:				-1.5		
Maximum:		5.0	10.0	600.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
426.1974	426.1980	-0.6	-1.4	6.5	6.2	C20 H33 N3 O3 P S
	426.1947	2.7	6.3	11.5	26.8	C23 H29 N3 O3 P



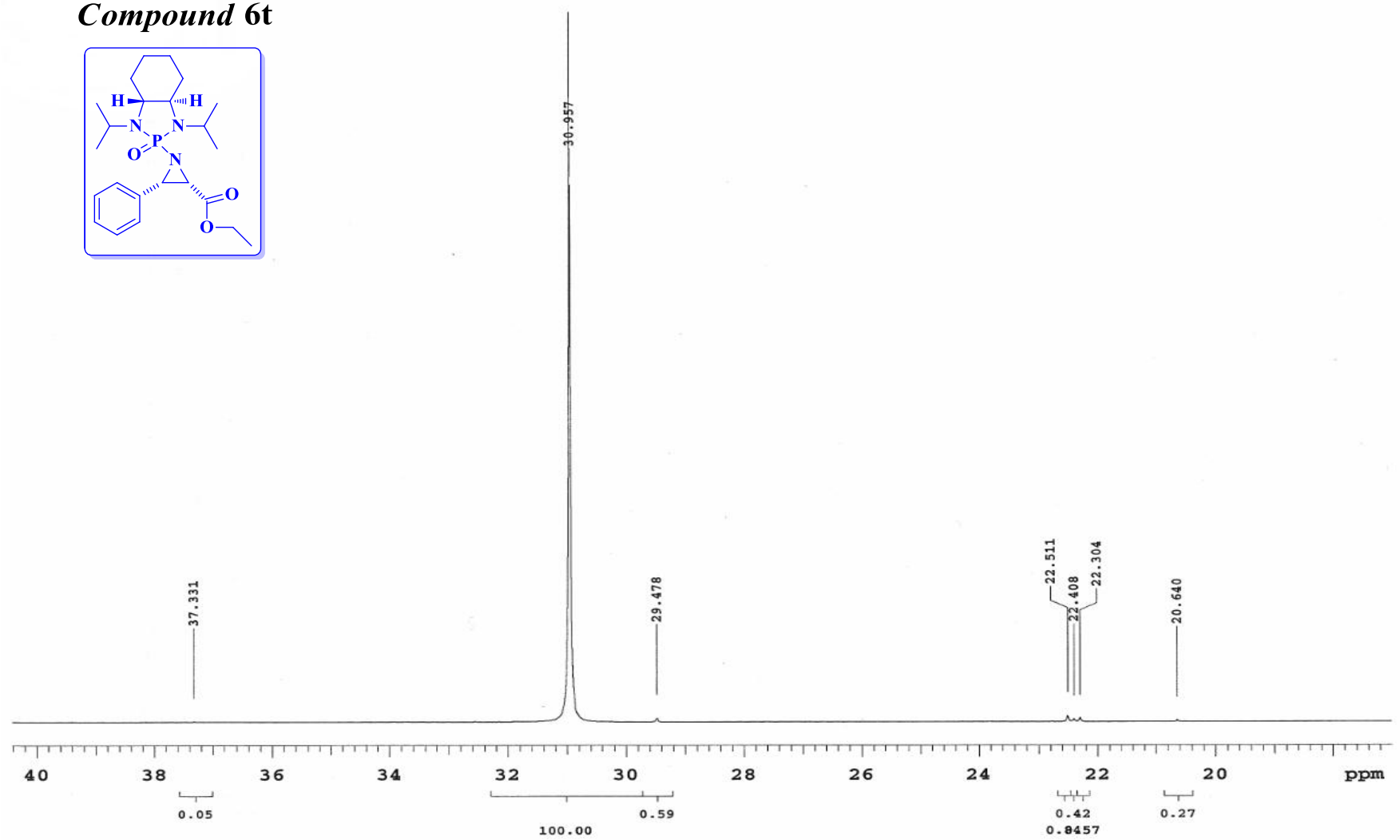
***Compound* 6t**

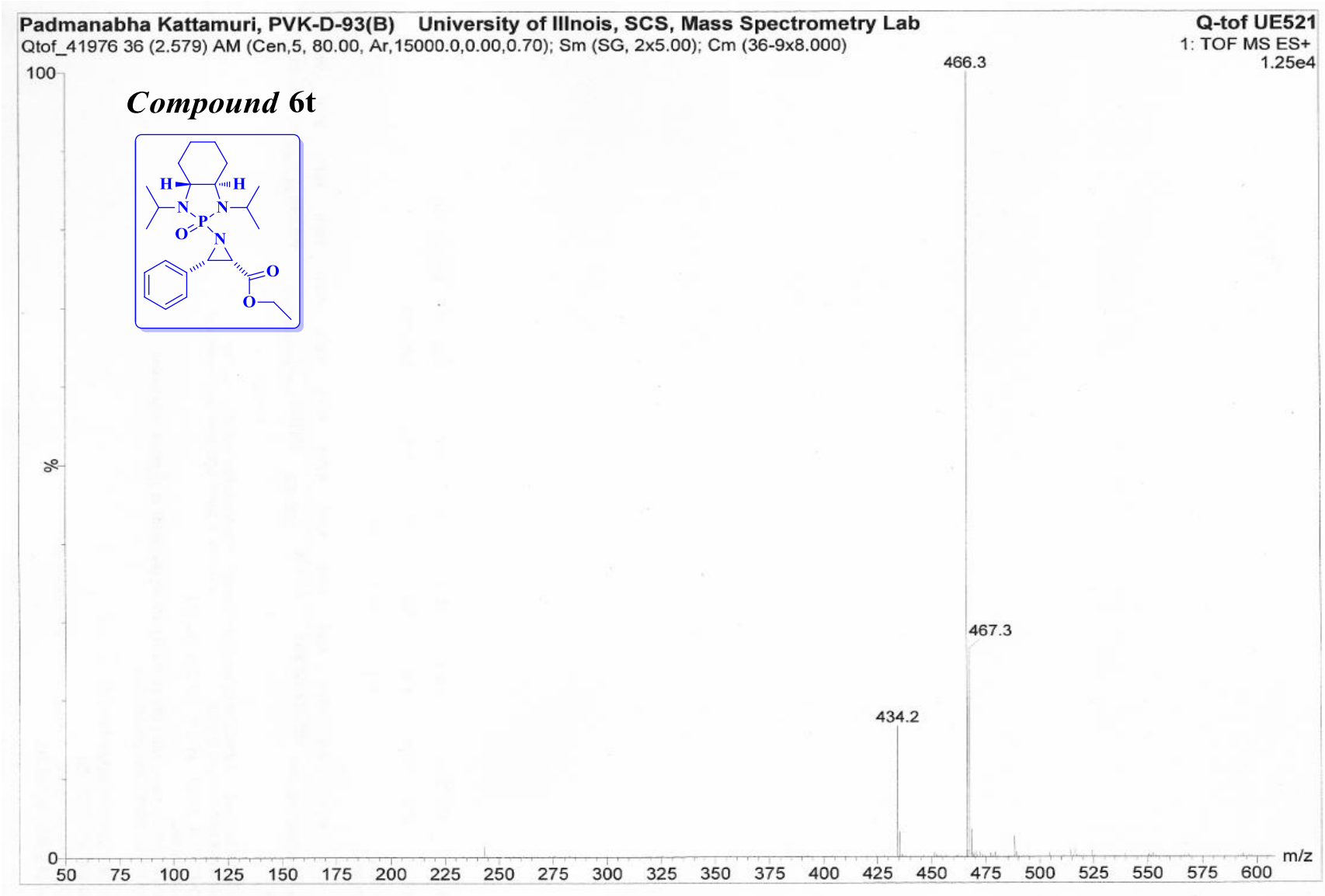


***Compound* 6t**



***Compound* 6t**





Elemental Composition Report

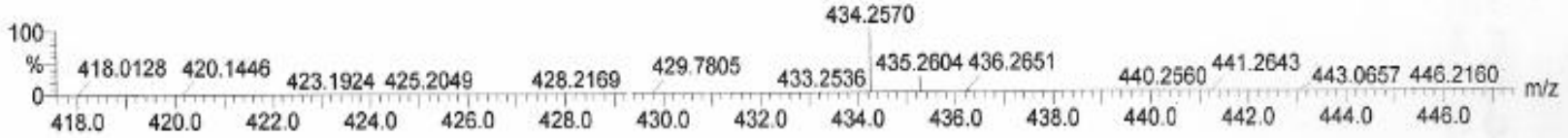
Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 600.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

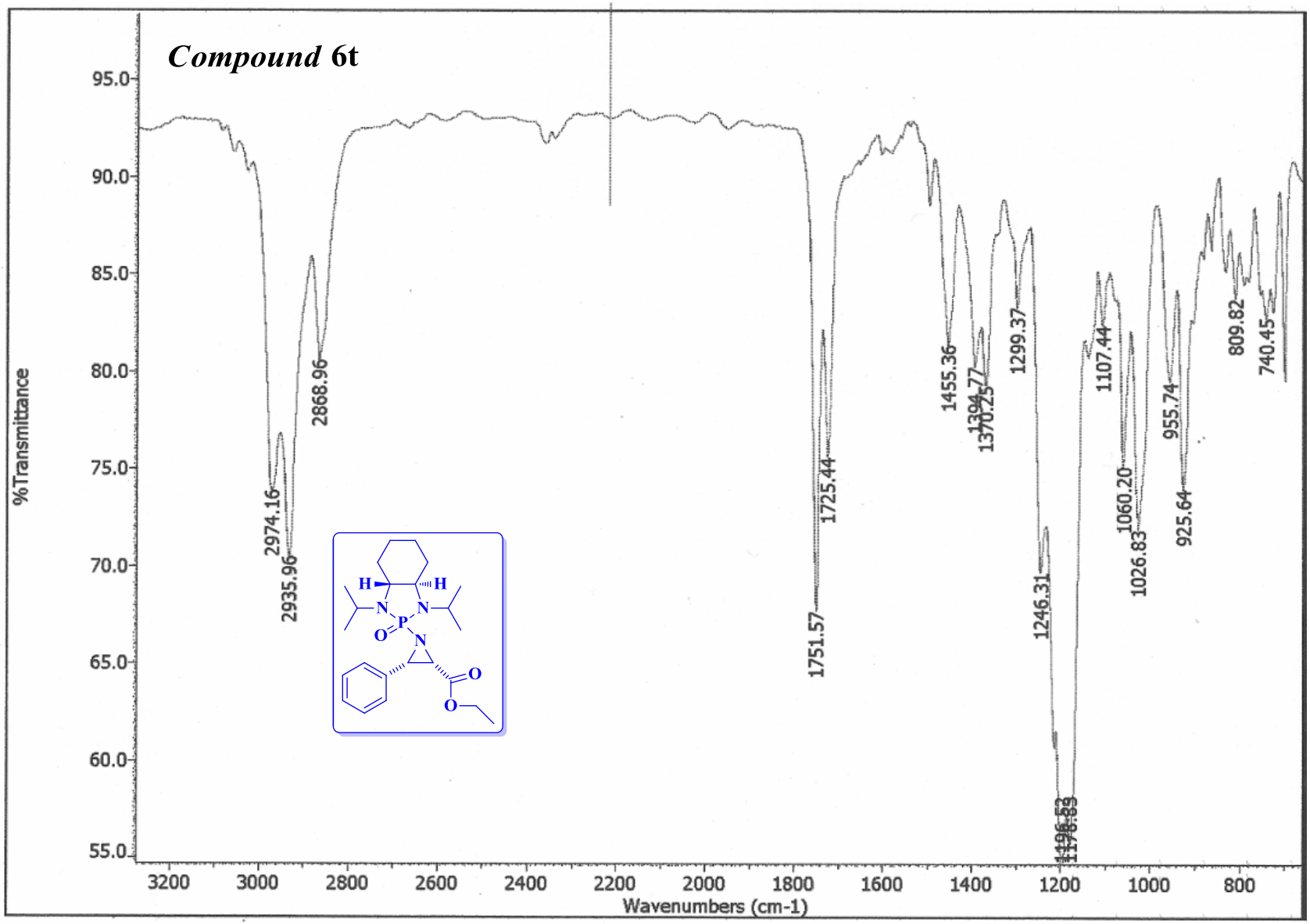
Monoisotopic Mass, Even Electron Ions
91 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-250 N: 2-4 O: 2-4 P: 0-1

Padmanabha Kattamuri, PVK-D-93(B) University of Illinois, SCS, Mass Spectrometry Lab
Qtof_41976 51 (3.650) AM (Cen,3, 80.00, Ar,15000.0,716.46,0.70,LS 3); Sm (SG, 2x3.00); Cm (51:52)

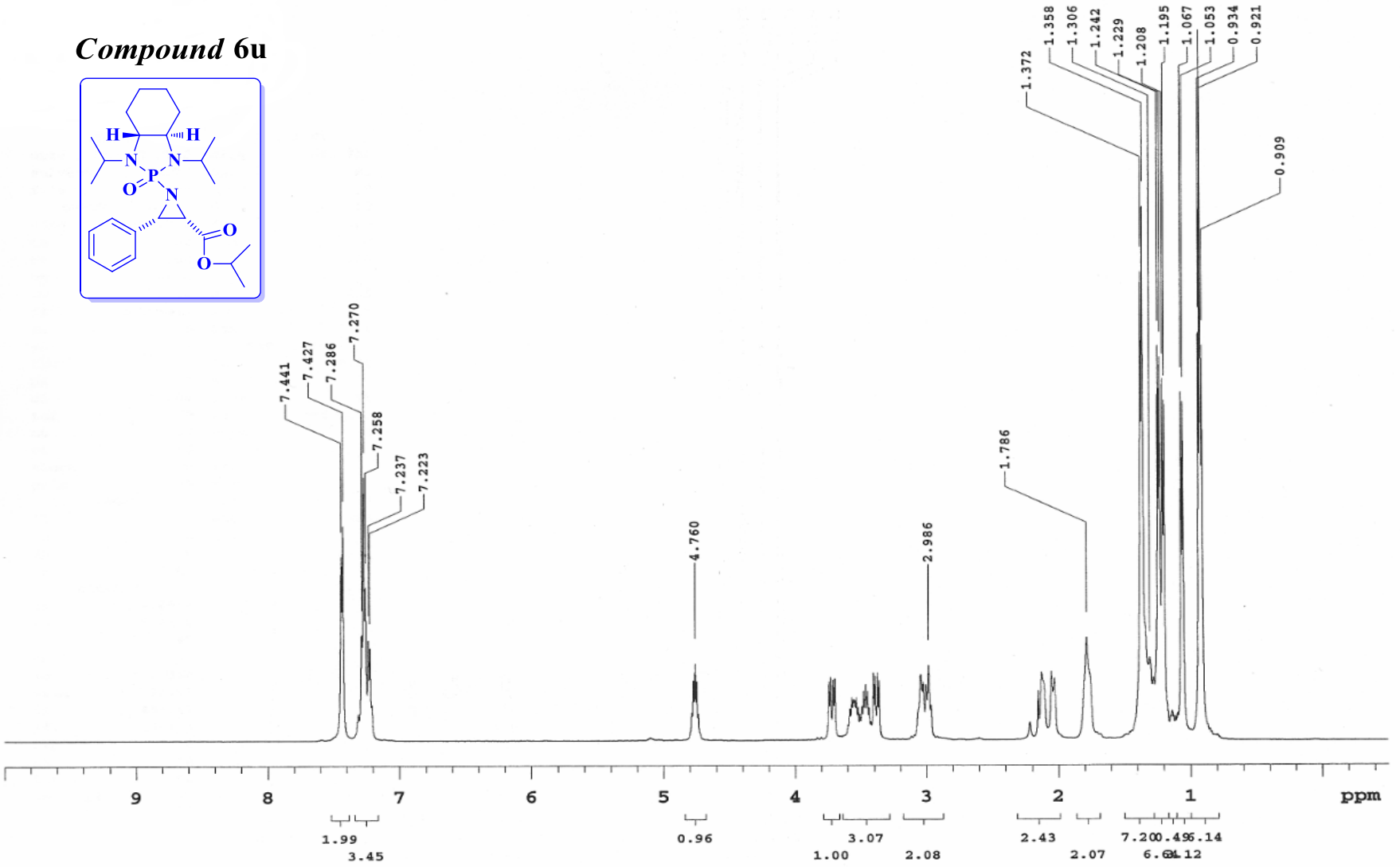
Q-tof UE521
1: TOF MS ES+
1.89e+003



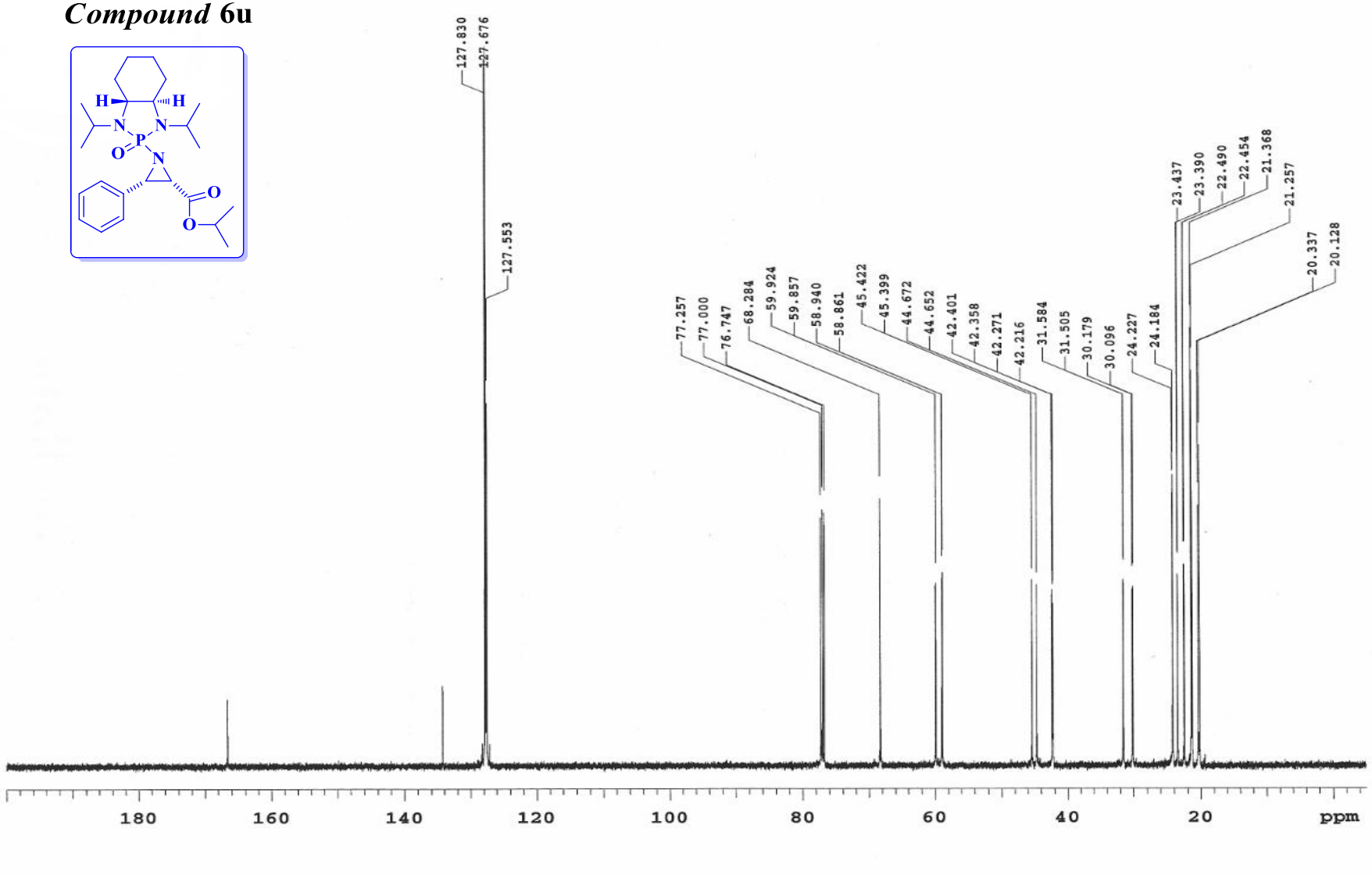
Minimum:				-1.5		
Maximum:		5.0	10.0	600.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
434.2570	434.2573	-0.3	-0.7	7.5	3.5	C23 H37 N3 O3 P



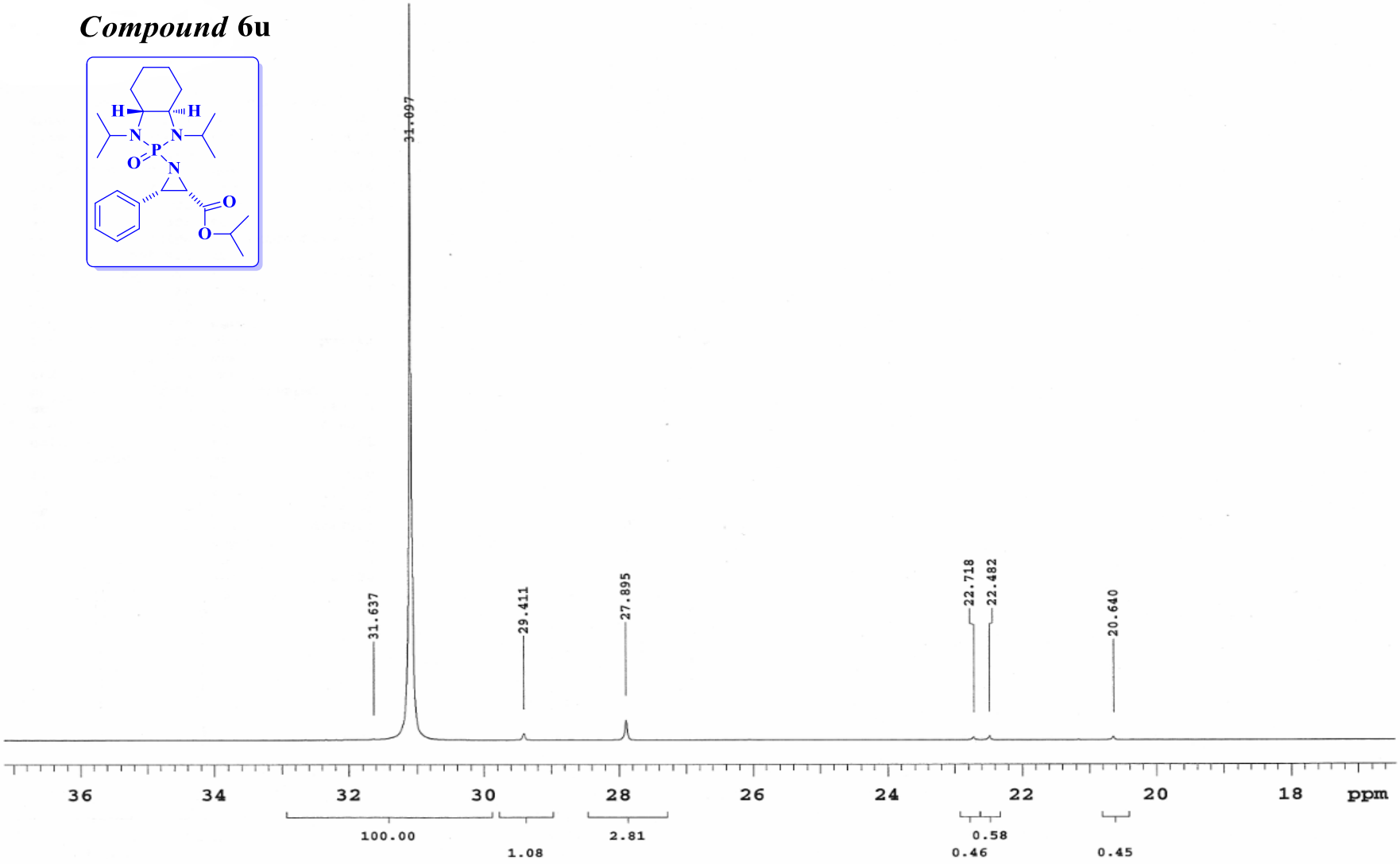
***Compound* 6u**

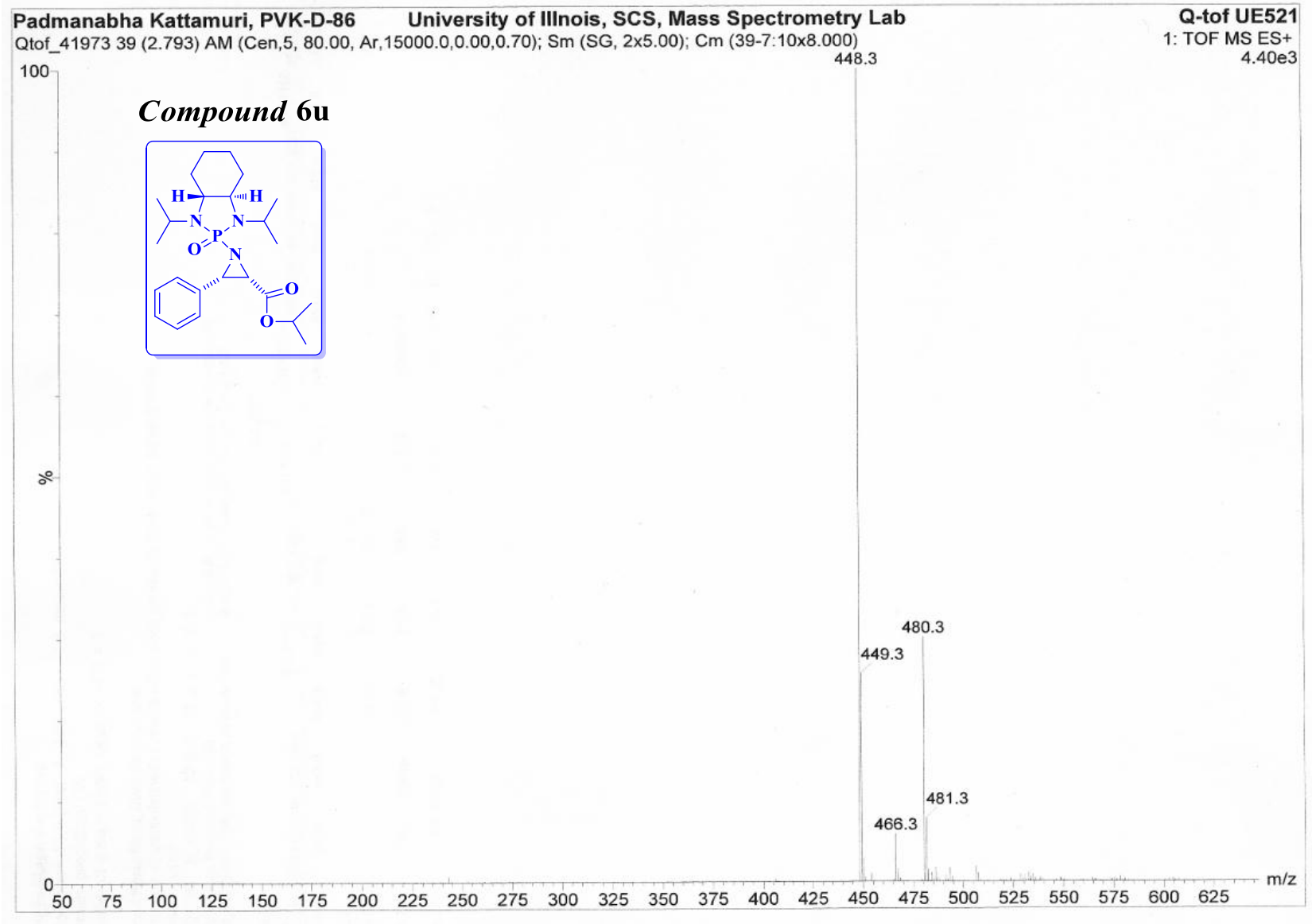


***Compound* 6u**


127.830
127.676
127.553
77.257
77.000
76.747
68.284
59.924
59.857
58.940
58.861
45.422
45.399
44.672
44.652
42.401
42.358
42.271
42.216
31.584
31.505
30.179
30.096
24.227
24.184
23.437
23.390
22.490
22.454
21.368
21.257
20.337
20.128
180
160
140
120
100
80
60
40
20
ppm

***Compound* 6u**





Elemental Composition Report

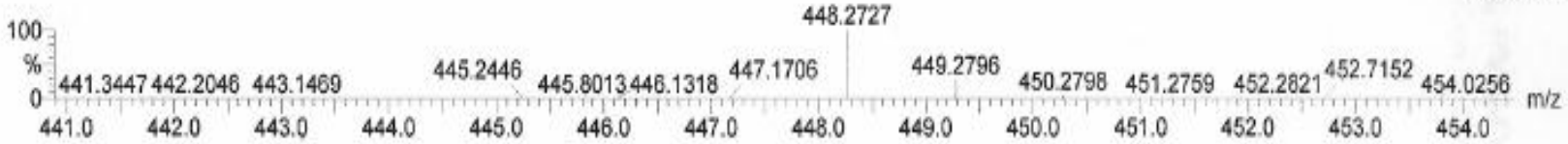
Page 1

Single Mass Analysis

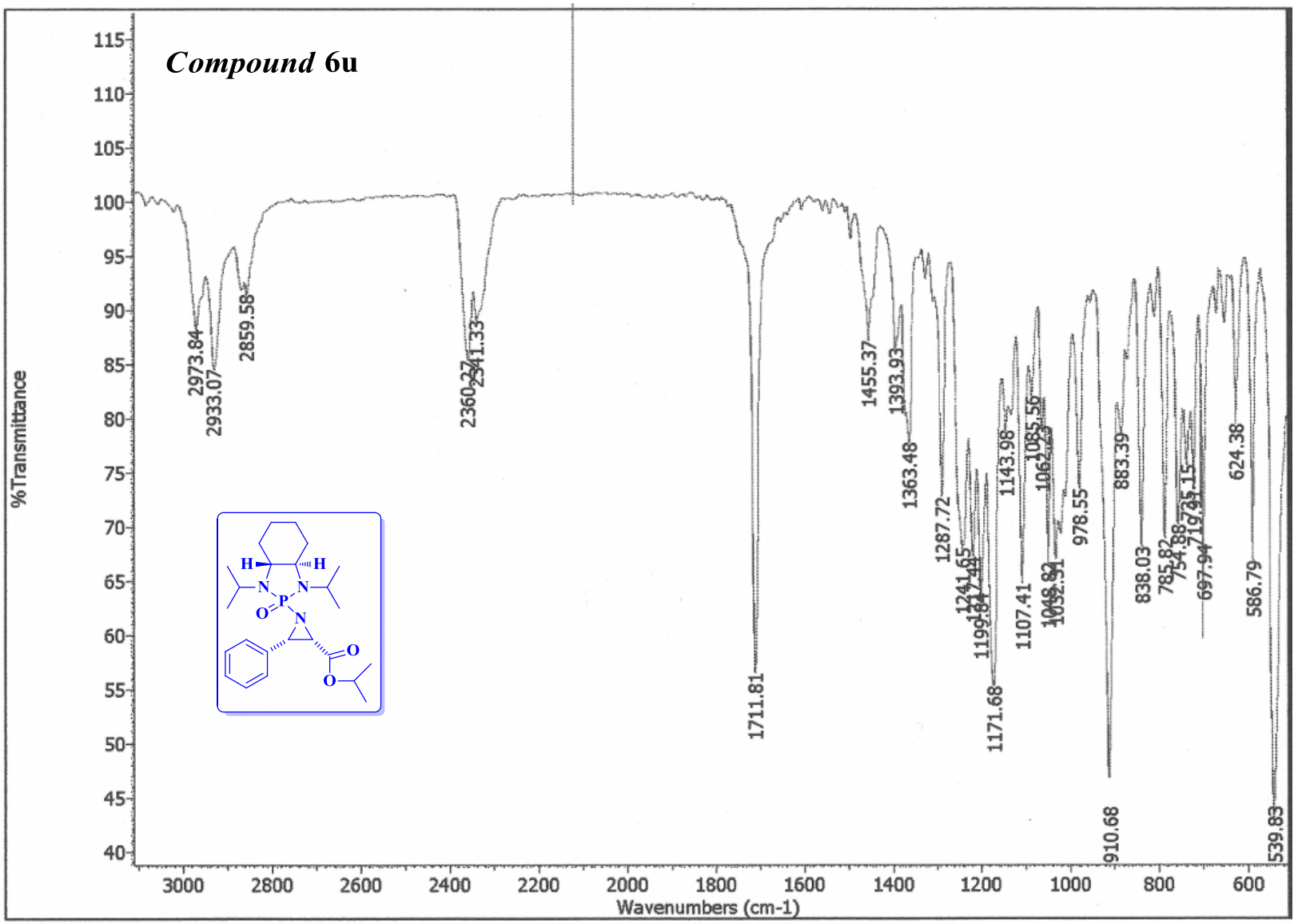
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 600.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
94 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-250 N: 2-4 O: 2-4 P: 0-1

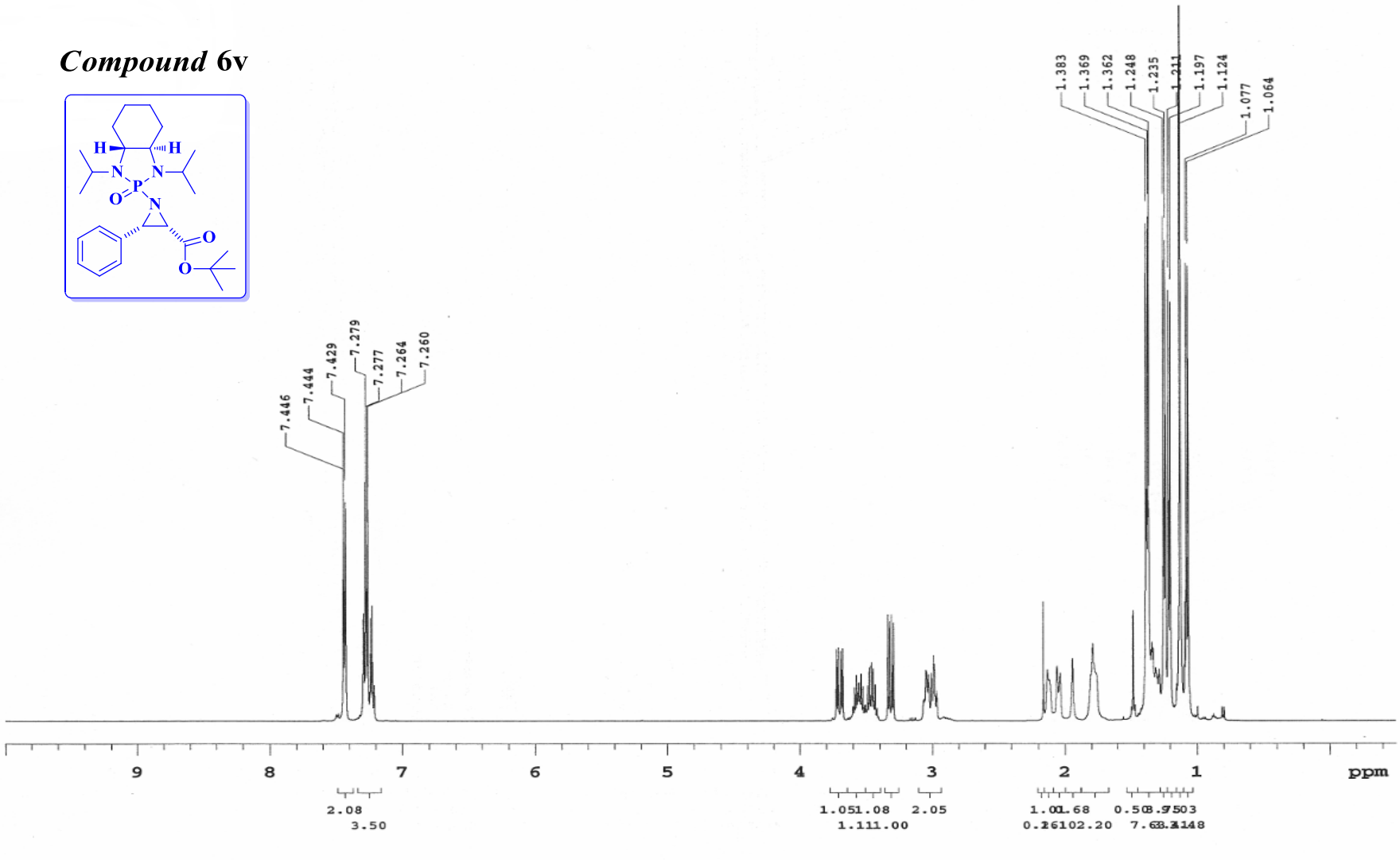
Padmanabha Kattamuri, PVK-D-86 University of Illnois, SCS, Mass Spectrometry Lab Q-tof UE521
Qtof_41973 51 (3.650) AM (Cen,3, 80.00, Ar,15000.0,716.46,0.70,LS 3); Sm (SG, 2x3.00); Cm (51:52) 1: TOF MS ES+
1.49e+003

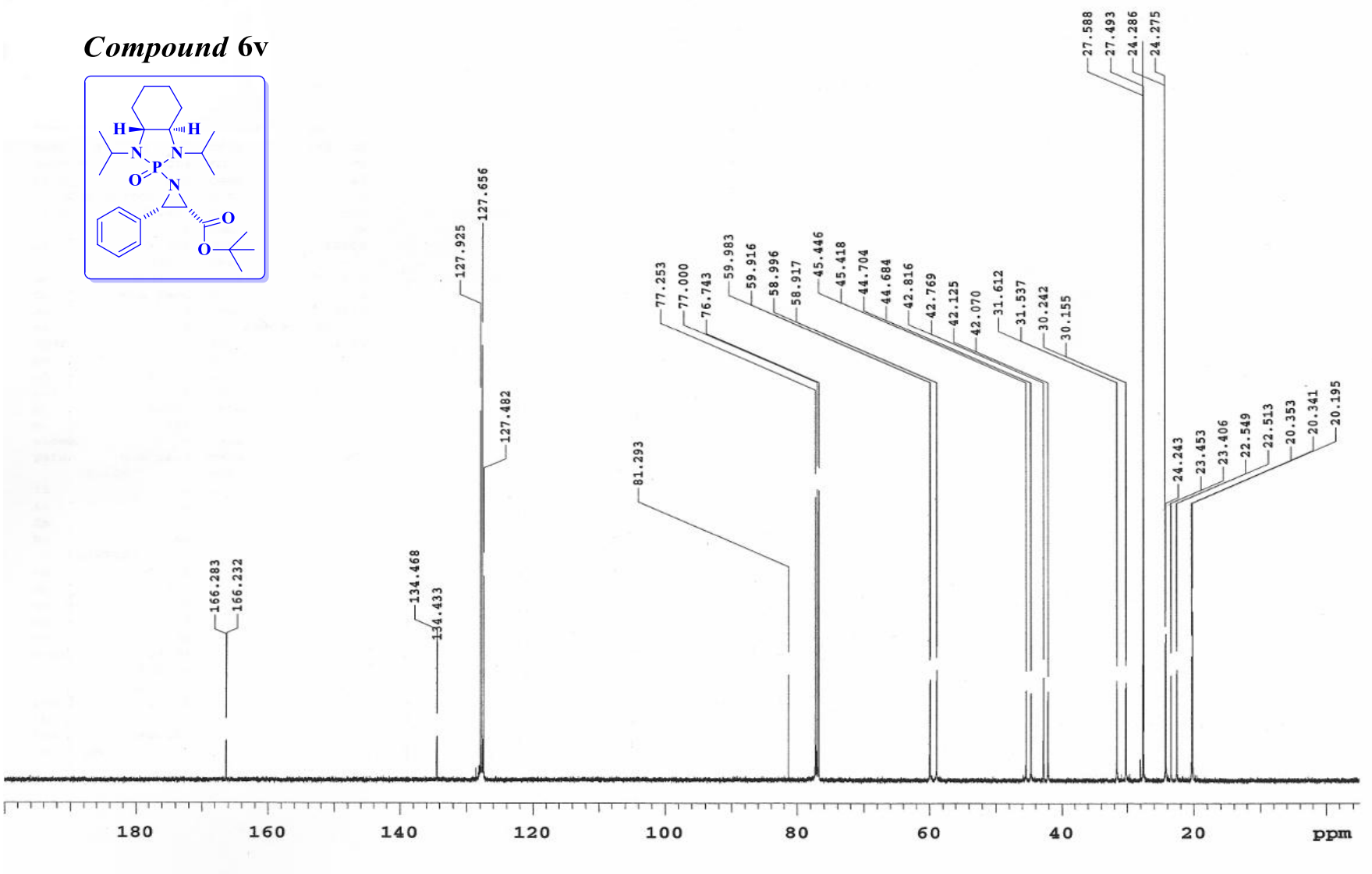


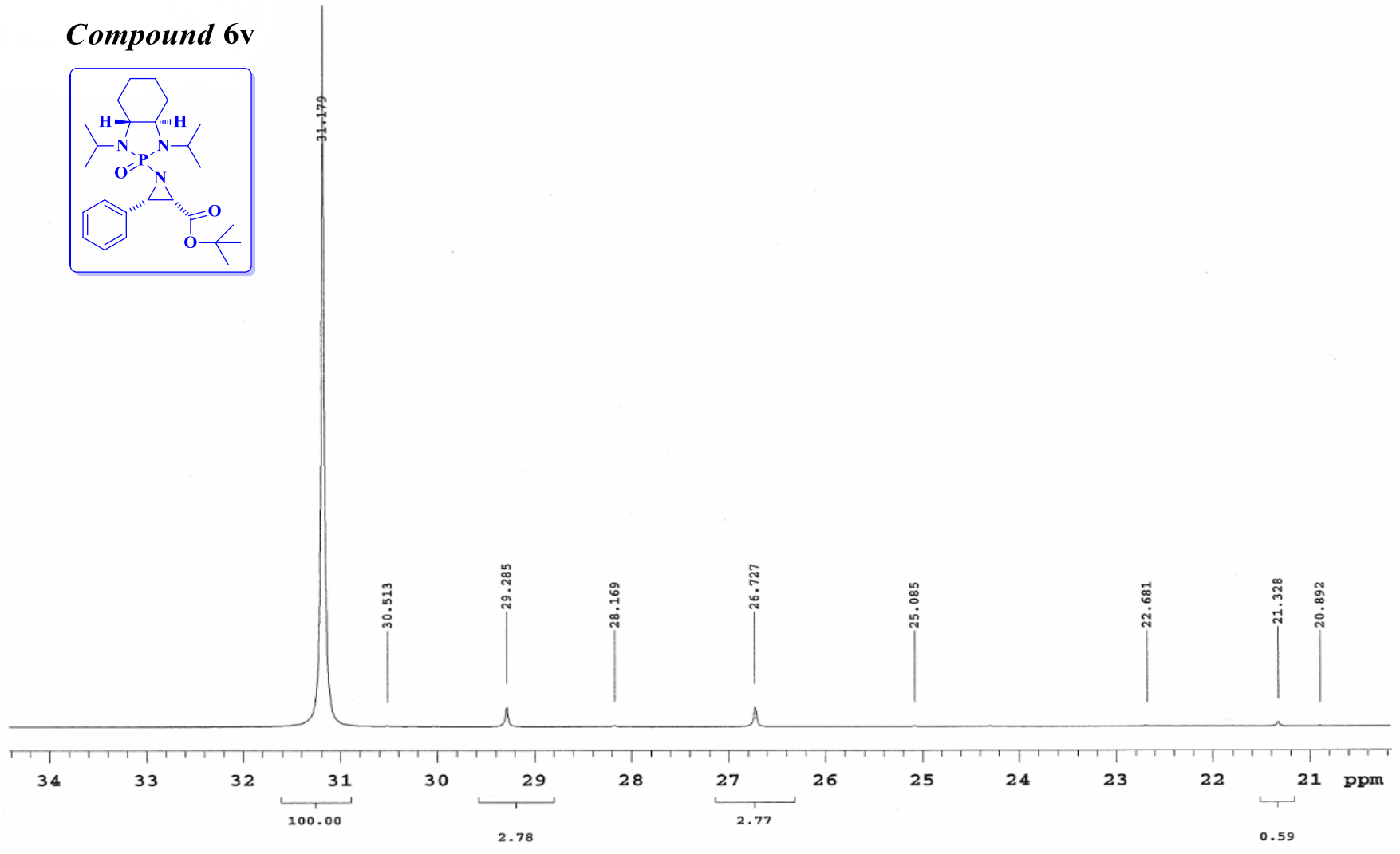
Minimum:				-1.5		
Maximum:		5.0	10.0	600.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
448.2727	448.2729	-0.2	-0.4	7.5	2.2	C24 H39 N3 O3 P

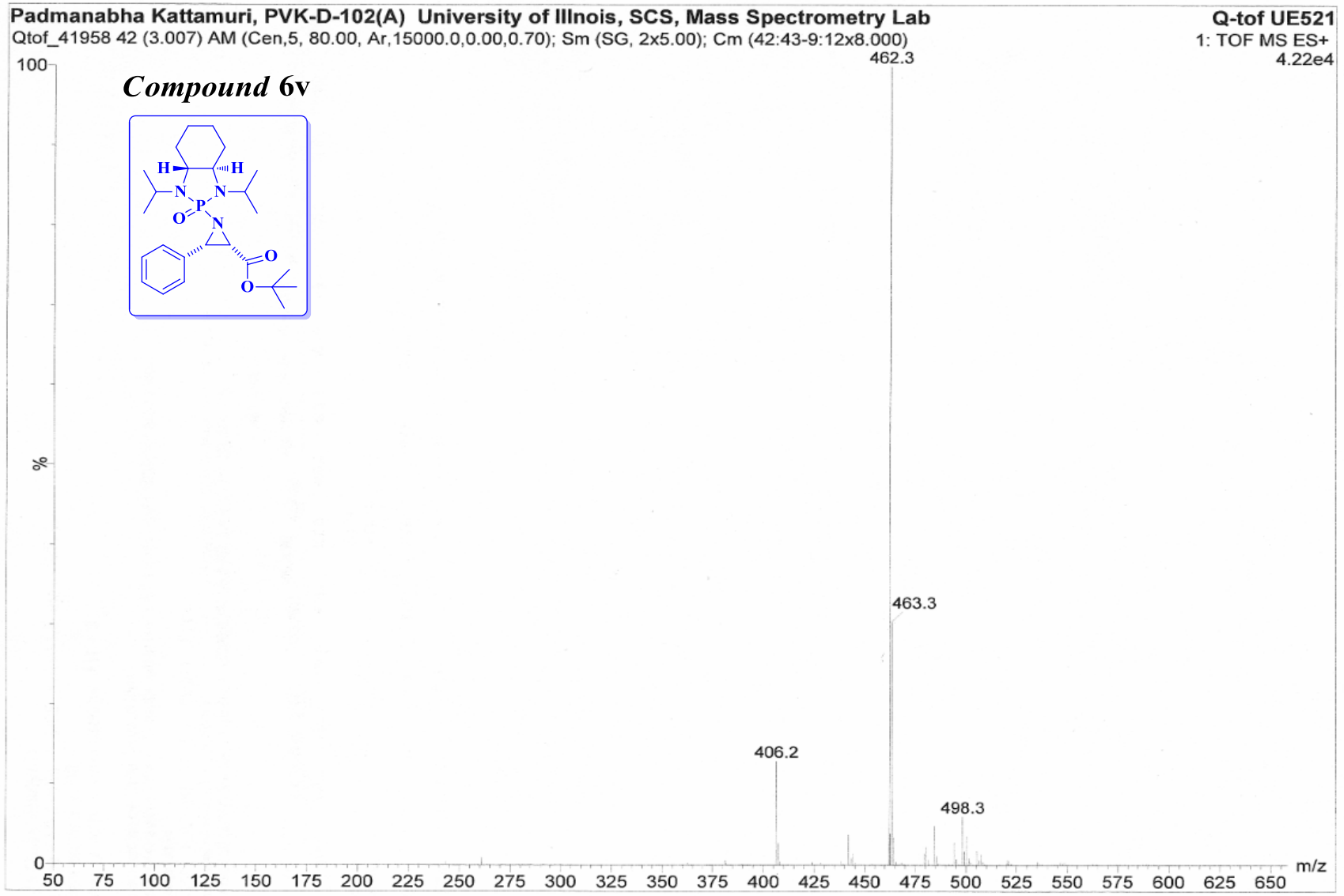


***Compound* 6v**









Elemental Composition Report

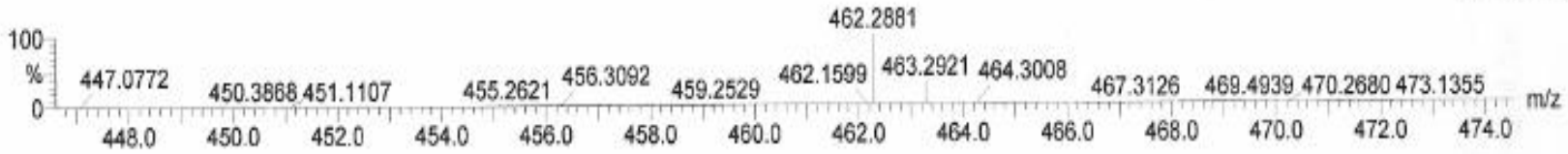
Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 600.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
97 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-250 N: 2-4 O: 2-4 P: 0-1

Padmanabha Kattamuri, PVK-D-102(A) University of Illnois, SCS, Mass Spectrometry Lab
Qtof_41958 39 (2.757) AM (Cen,3, 80.00, Ar,15000.0,716.46,0.70); Sm (SG, 2x3.00); Cm (39)

Q-tof UE521
2: TOF MS ES+
4.93e+002



Minimum:				-1.5		
Maximum:		5.0	10.0	600.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
462.2881	462.2886	-0.5	-1.1	7.5	0.5	C25 H41 N3 O3 P