Supporting Information

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

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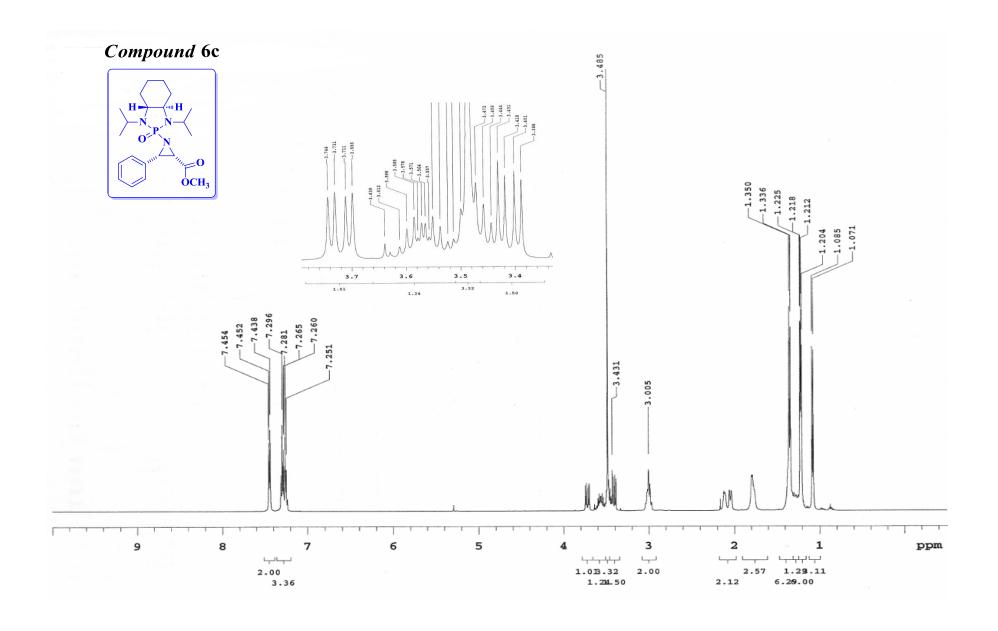
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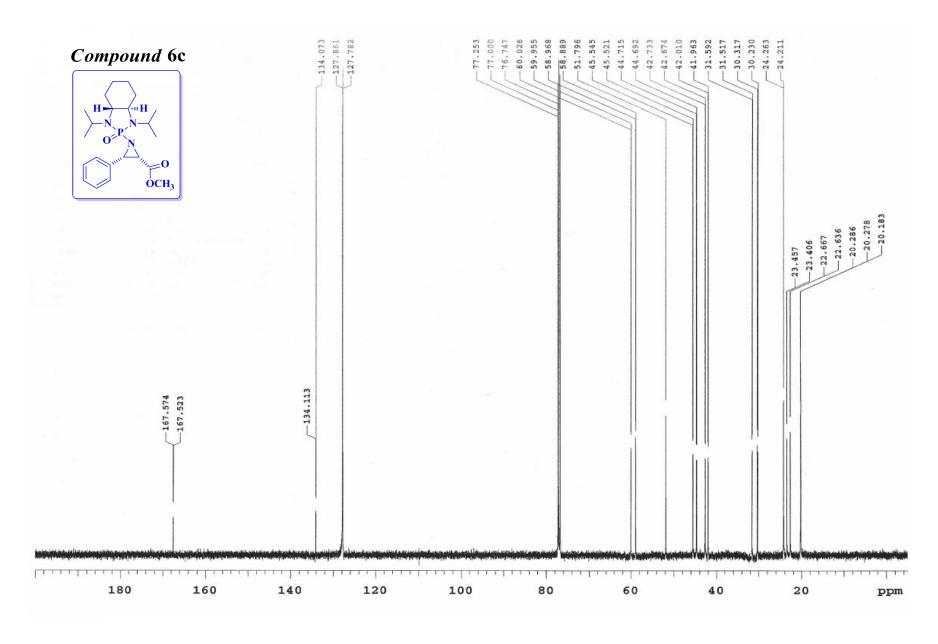
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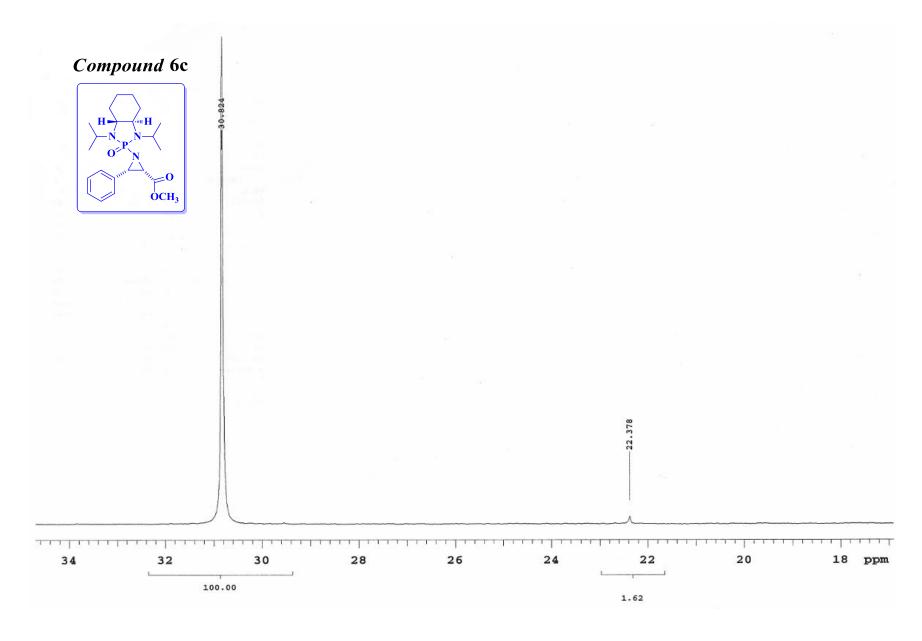
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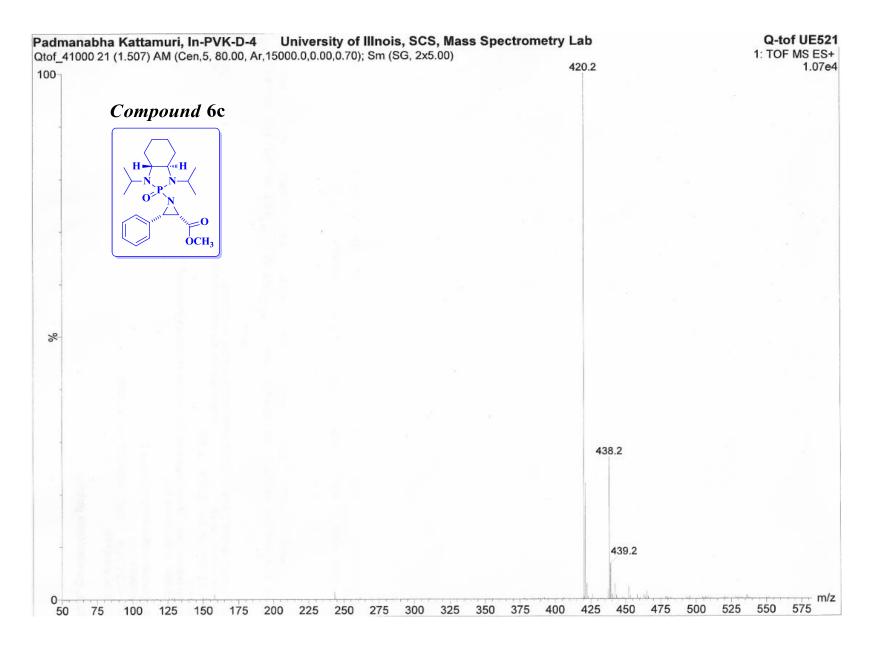
I. ¹H, ¹³C, ³¹P, HRMS and IR spectra of 6c to 6l S2-S62

II. ¹H, ¹³C, ³¹P, HRMS and IR spectra of 6m to 6v S63-S123

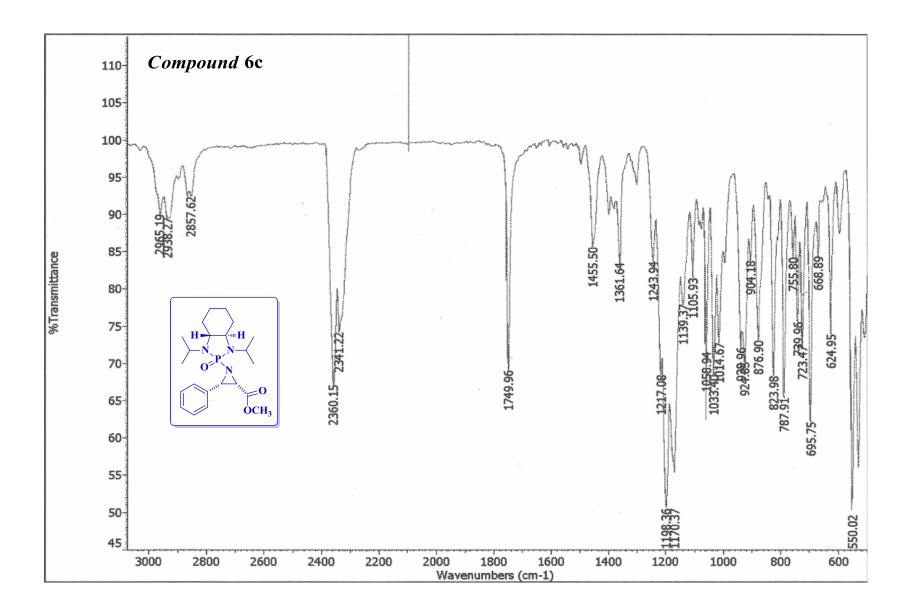


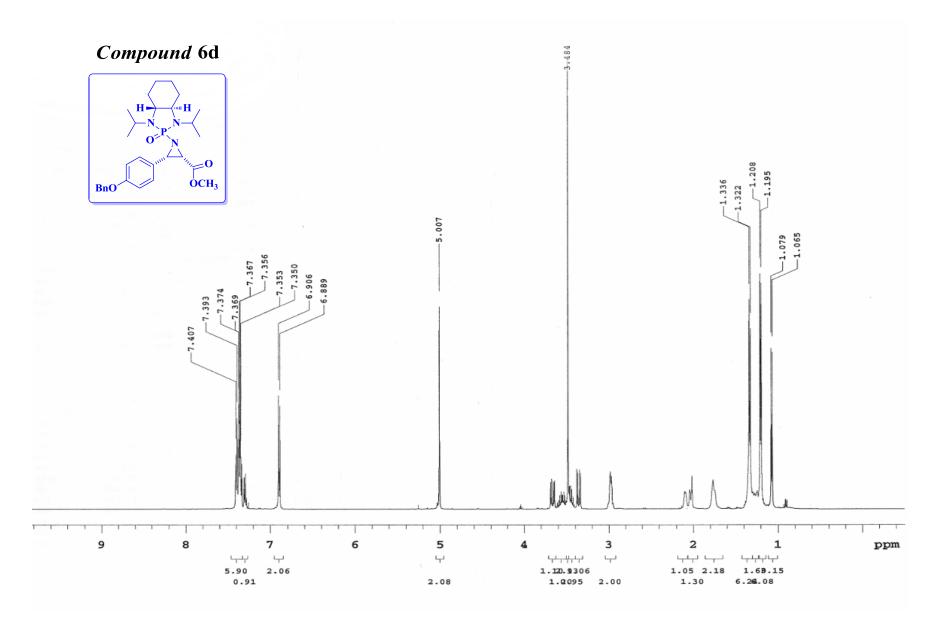


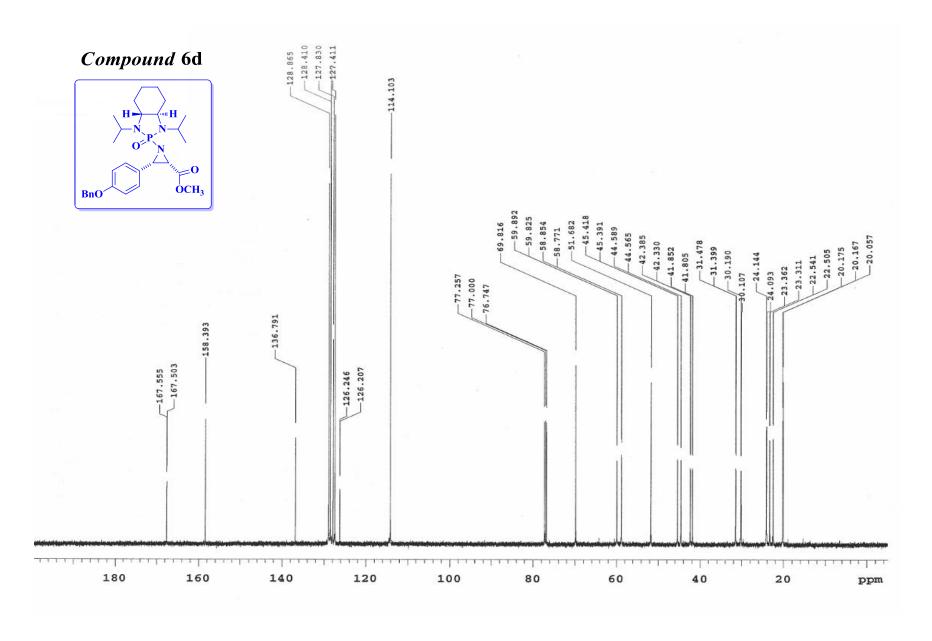


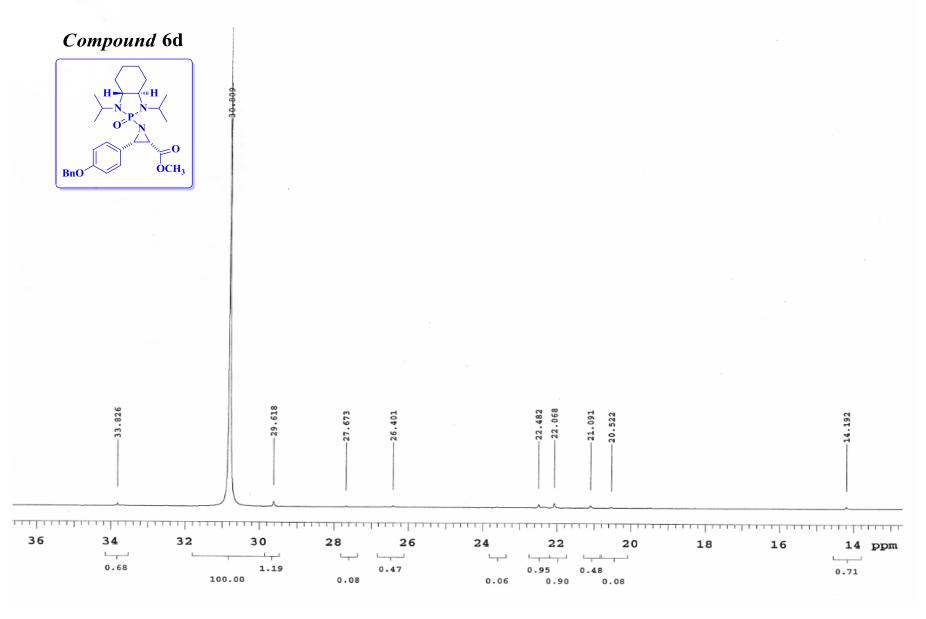


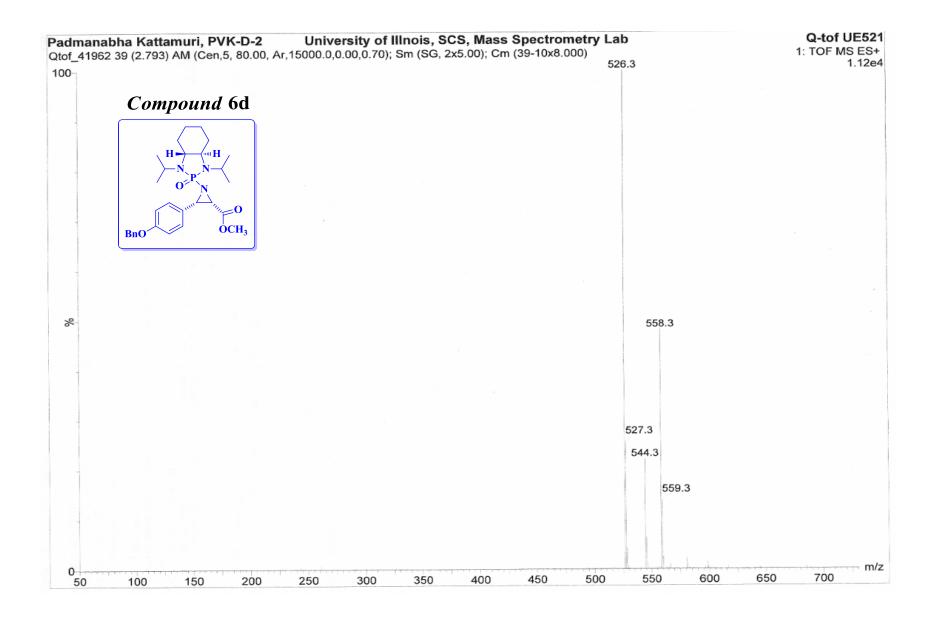
Page 1 **Elemental Composition Report** Single Mass Analysis Tolerance = 10.0 PPM / DBE: min = -1.5, max = 600.0 Element prediction: Off Number of isotope peaks used for i-FIT = 3 Monoisotopic Mass, Even Electron Ions 88 formula(e) evaluated with 1 results within limits (all results (up to 1000) for 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+003 420.2 100-% 421.2 422.3 423.2 424.0 425.2 426.3 427.2 428.2 429.3 430.2 430.8 410.2 411.4 413.0 413.3 414.3415.1 417.1417.4 418.4 419.3 0 412.0 418.0 410.0 414.0 416.0 420.0 422.0 424.0 426.0 428.0 430.0 -1.5 Minimum: 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



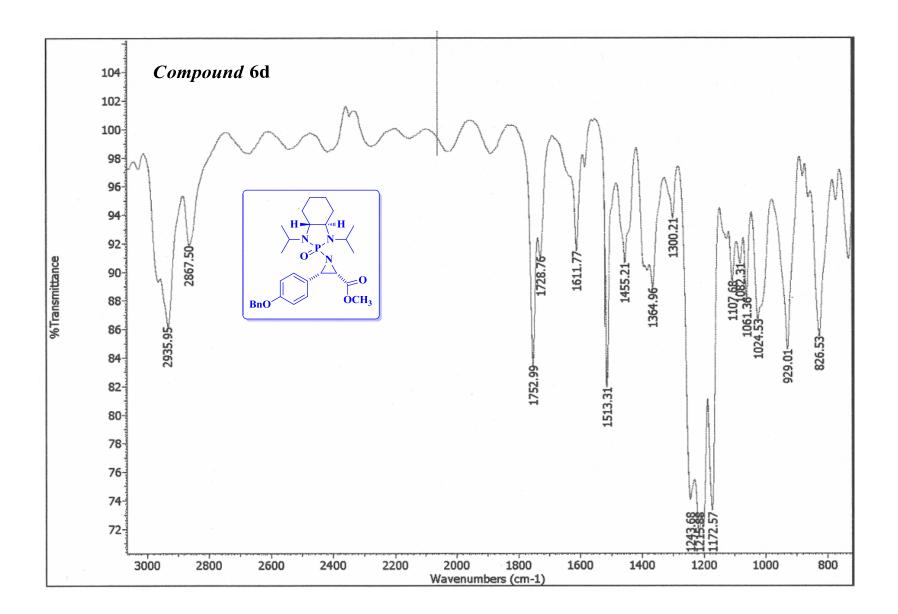


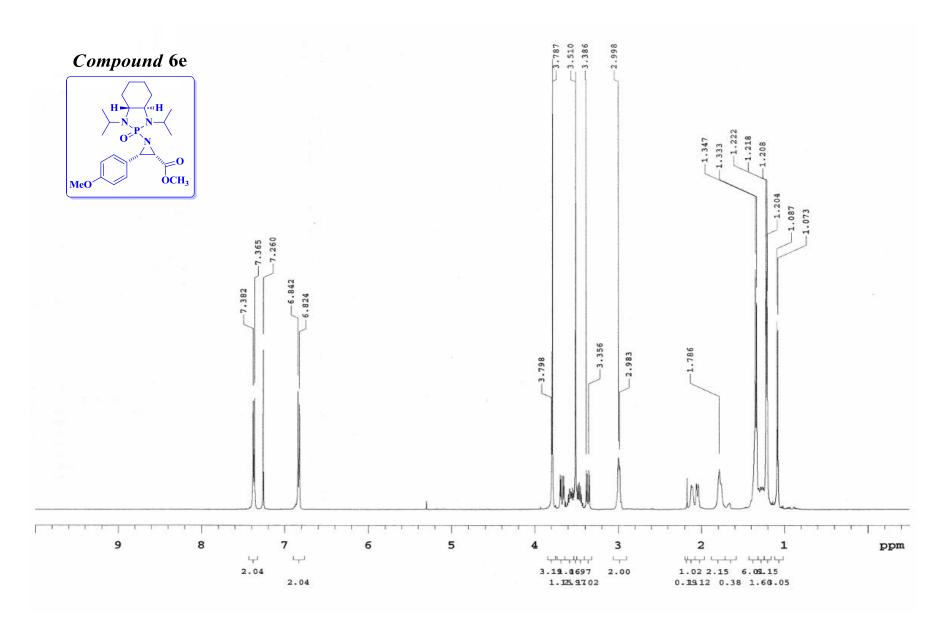


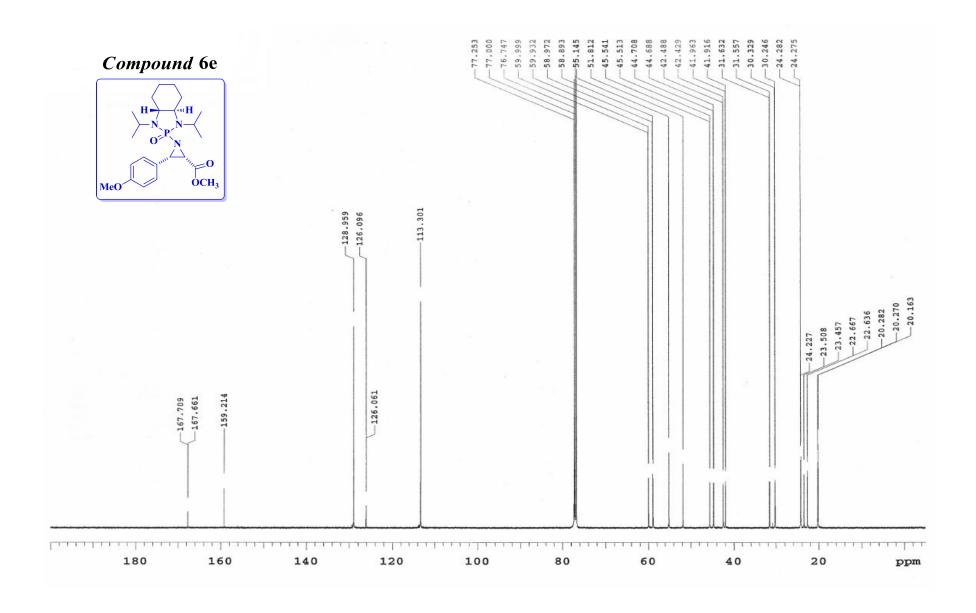


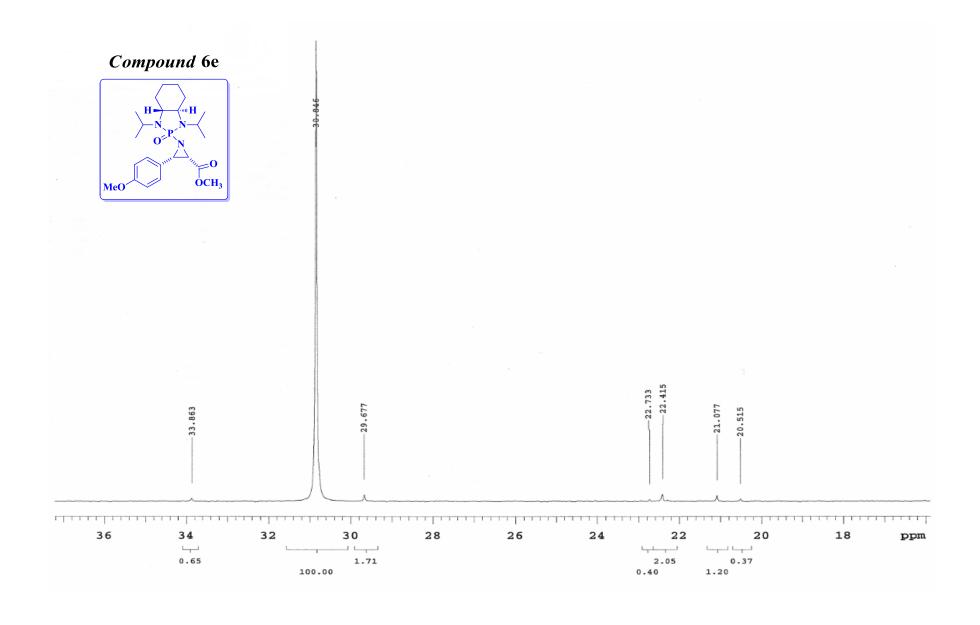


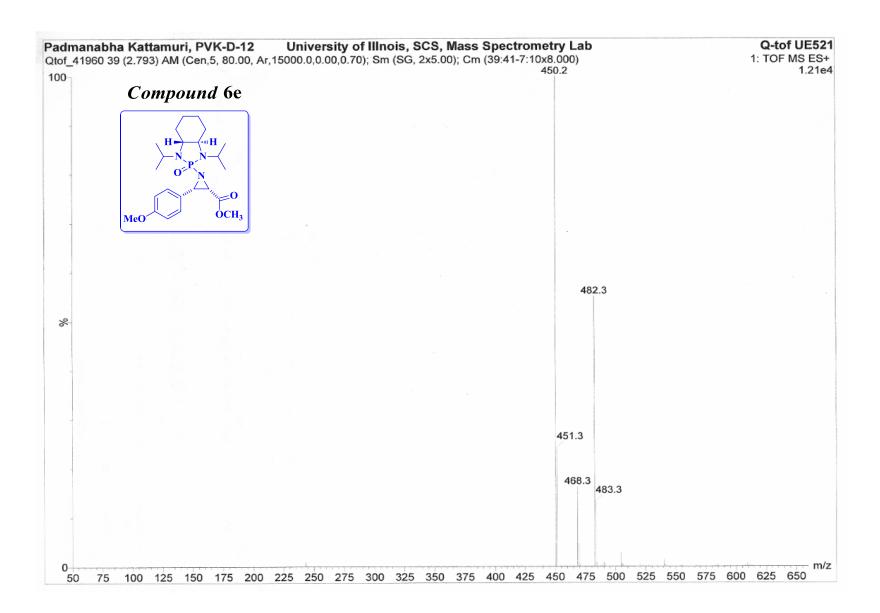
Elementa	al Composi	tion Re	eport										Page 1
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115 formula Elements Us C: 0-150	H: 0-250 N	with 1 re N: 2-4	sults within	P: 0-1			ach mass)	/ Lah					Q-tof UE521
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Qtof_41962 3	32 (2.257) AM (0	Cen,3, 80.		0.0,716.46,0.70); Sm (SG,	2x3.00); Cm	(31:33) 526.2842		528.296	1			2: TOF MS ES+ 4.85e+002
Qtof_41962 3	32 (2.257) AM (0	Cen,3, 80.	7.2642 518.0	521.3027 520.0); Sm (SG,	523.3229 524.0	(31:33) 526.2842		528.296	53	1.2088 532.0	533.3359	2: TOF MS ES+ 4.85e+002 535.3798 m/z
Qtof_41962 3	32 (2.257) AM (0	3229 51	7.2642	521.3027	522.3421	2x3.00); Cm 523.3229	(31:33) 526.2842 527.2	2883 5		53	111111		2: TOF MS ES+ 4.85e+002 535.3798 m/z
Qtof_41962 3 100 % 512.0 512.0 Minimum:	32 (2.257) AM (0	3229 51 516.0	7.2642 518.0	521.3027 520.0	522.3421 522.0 -1.5	2x3.00); Cm 523.3229	(31:33) 526.2842 527.2	2883 £		53	111111		2: TOF MS ES+ 4.85e+002 535.3798 m/z
Qtof_41962 3 100 % 512.0 512.0 Minimum: Maximum:	32 (2.257) AM (0 	3229 51 516.0	518.0 5.0	521.3027 520.0	522.3421 522.0 -1.5 600.0	523.3229 524.0	526.2842 527.2 526.0	2883 £		53	532.0		2: TOF MS ES+ 4.85e+002 535.3798 m/z



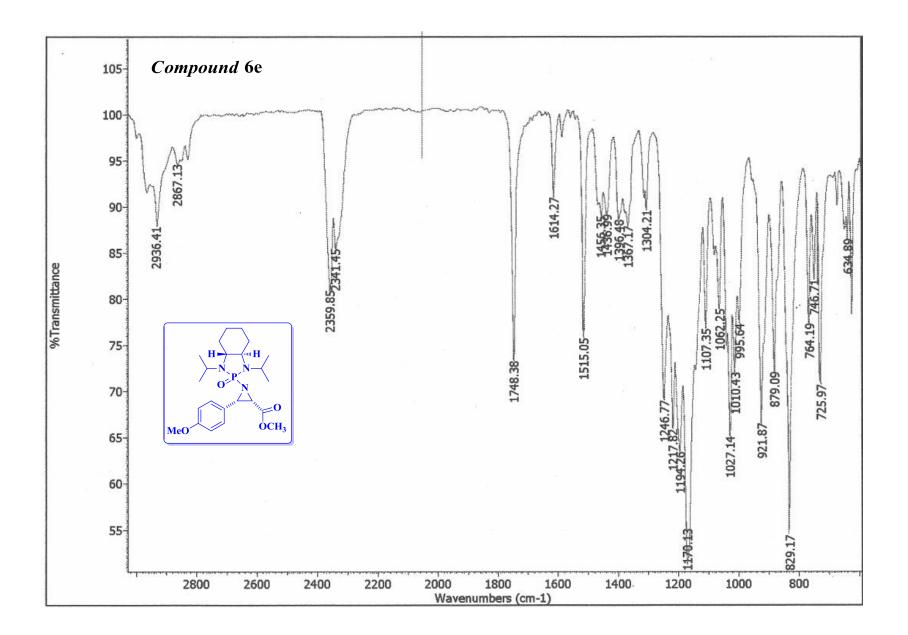


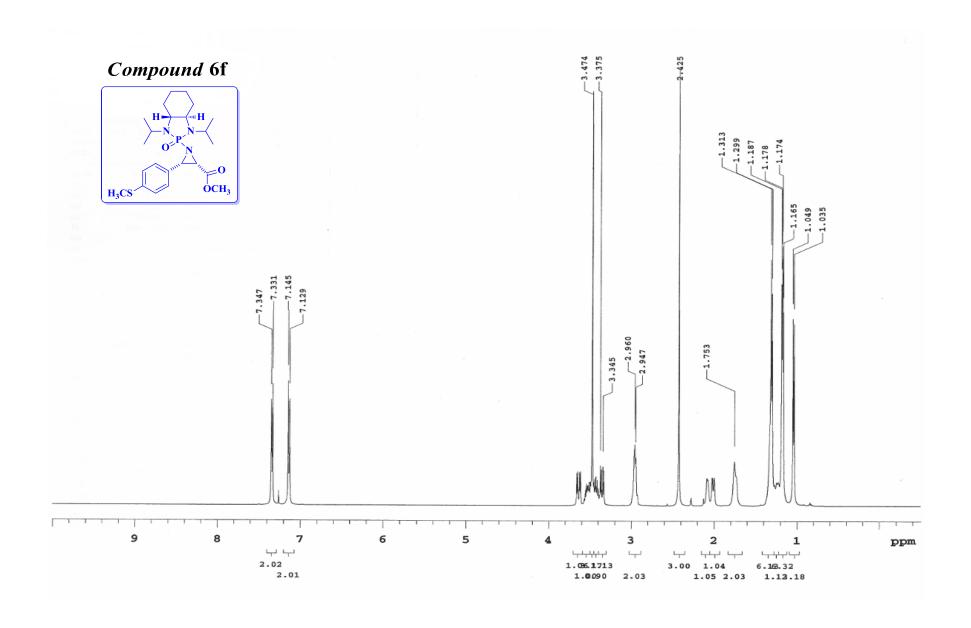


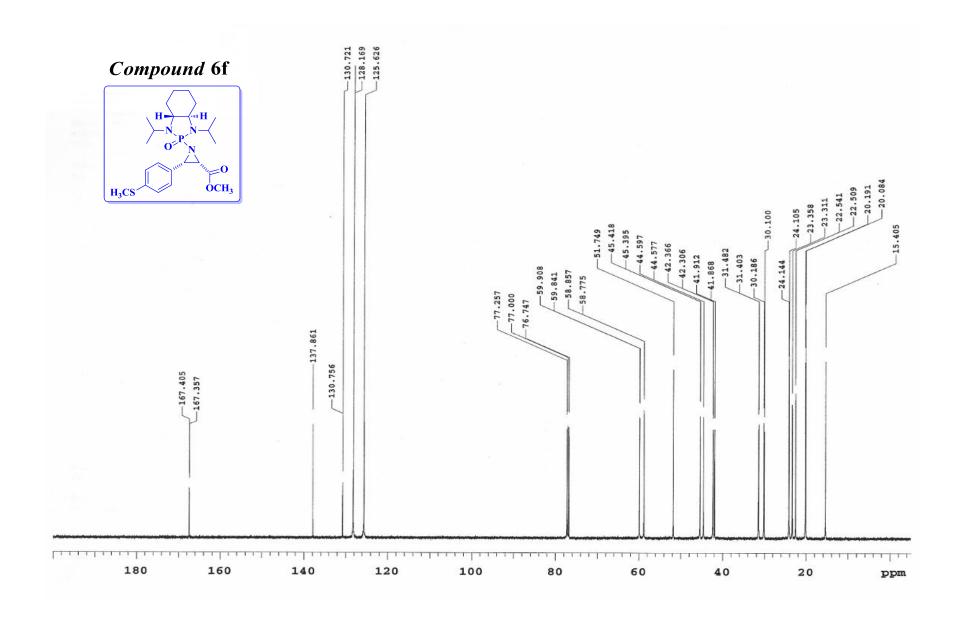


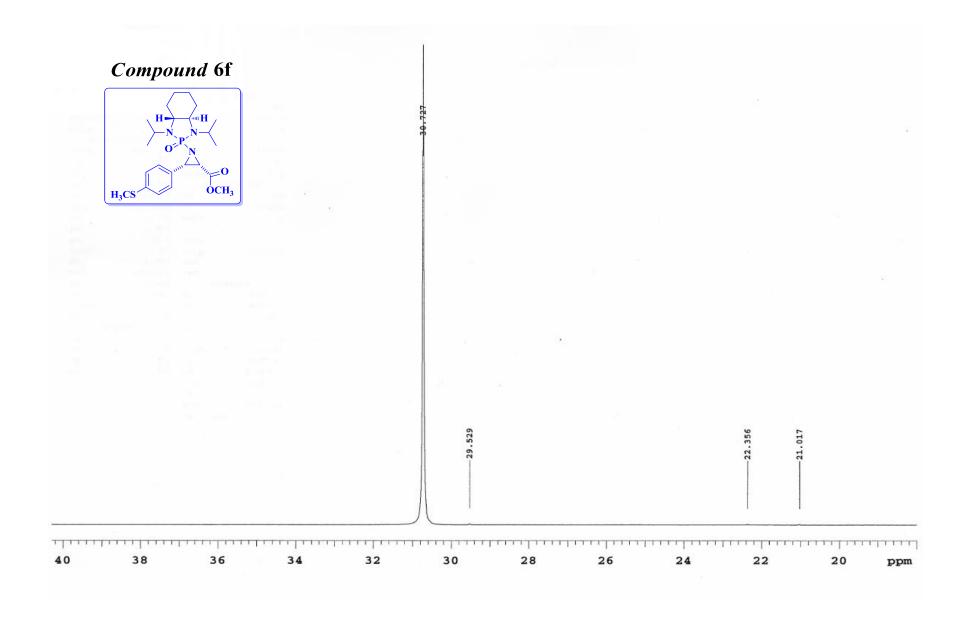


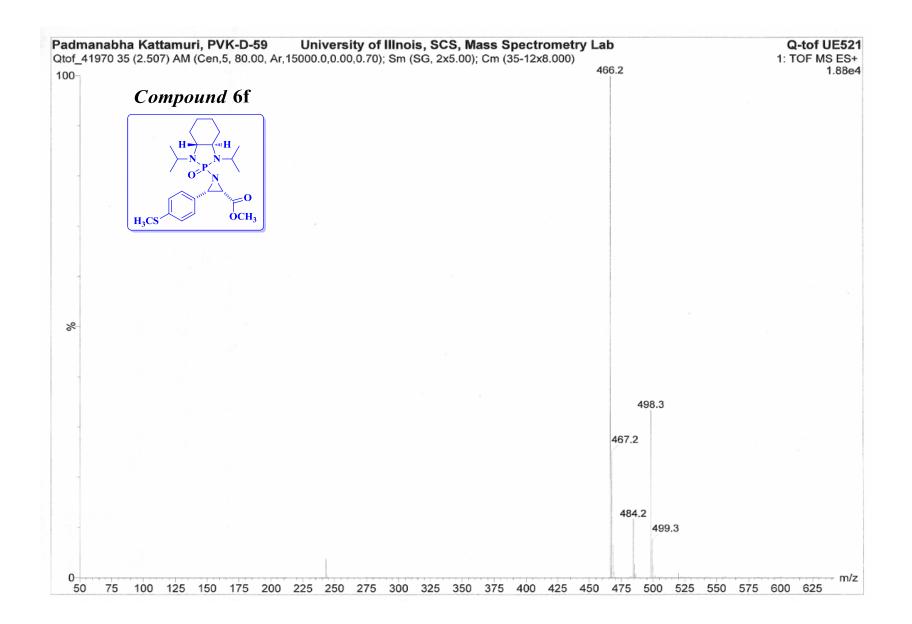
Page 1 **Elemental Composition Report** Single Mass Analysis Tolerance = 10.0 PPM / DBE: min = -1.5, max = 600.0 Element prediction: Off Number of isotope peaks used for i-FIT = 3 Monoisotopic Mass, Even Electron Ions 96 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass) Elements Used: C: 0-150 H: 0-250 N: 2-4 O: 2-4 P: 0-1 Q-tof UE521 University of Illnois, SCS, Mass Spectrometry Lab Padmanabha Kattamuri, PVK-D-12 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+003 450.2511 100 451.2556 440.2252.441.2330 444.2043 % 454.2676 457.2437 462.2901_{m/z} 434.2577.435.2588 448.2670 429.1815_430.3807 450.0 460.0 425.0 430.0 435.0 440.0 445.0 455.0 -1.5Minimum: 600.0 5.0 10.0 Maximum: Calc. Mass mDa. PPM DBE i-FIT Formula Mass 21.2 C23 H37 N3 O4 P 450.2511 450.2522 -1.1-2.47.5



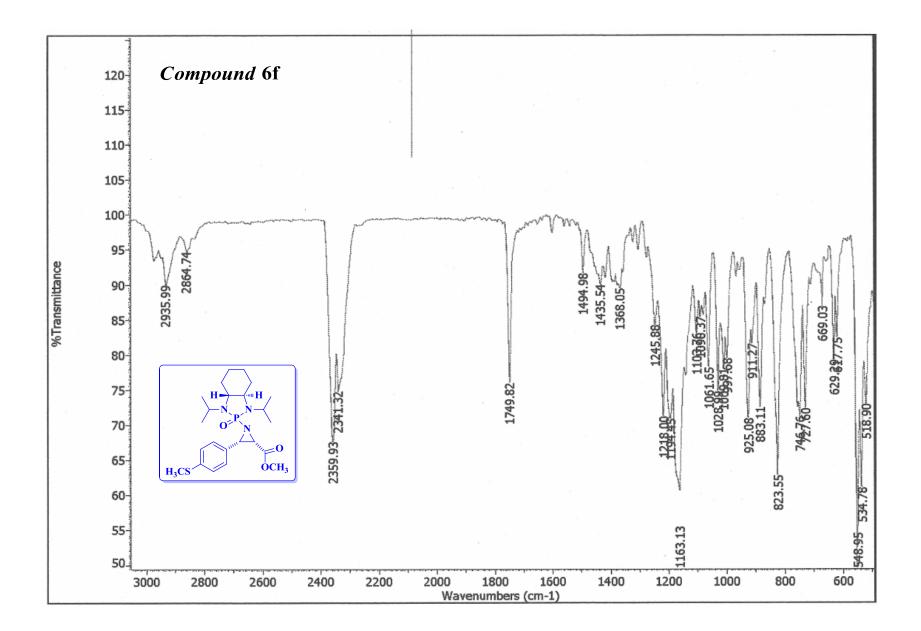


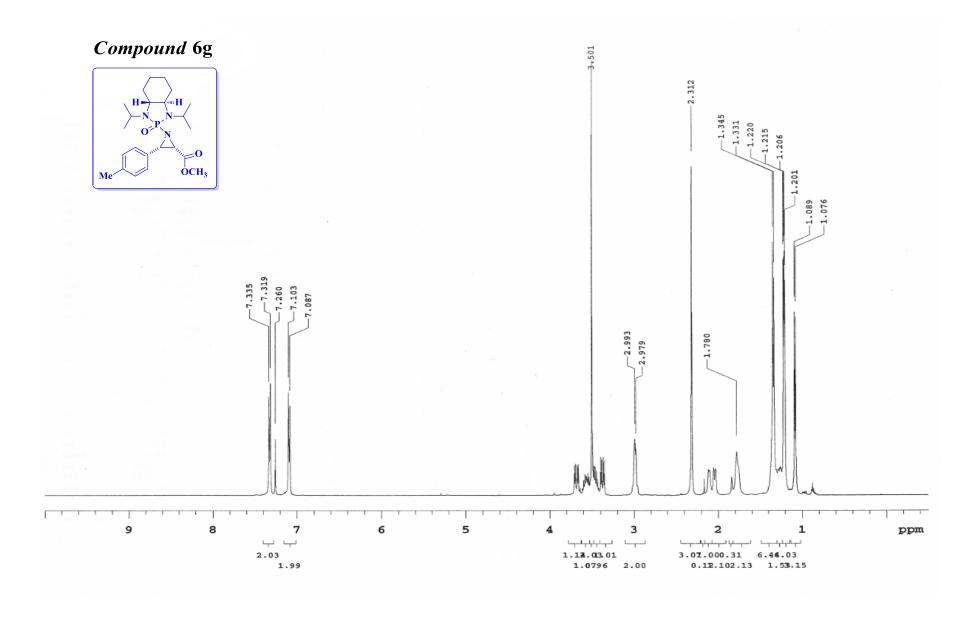


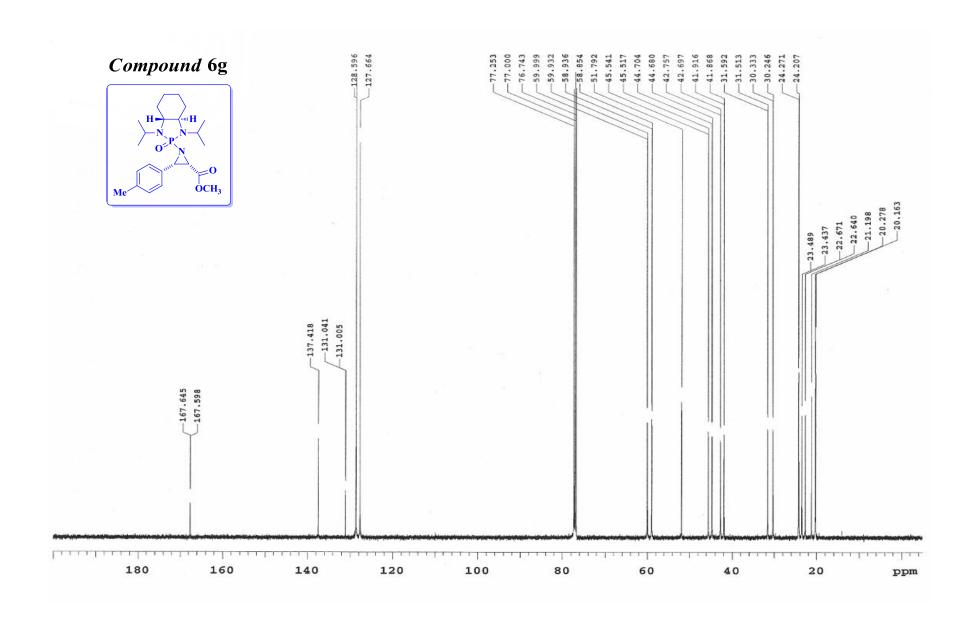


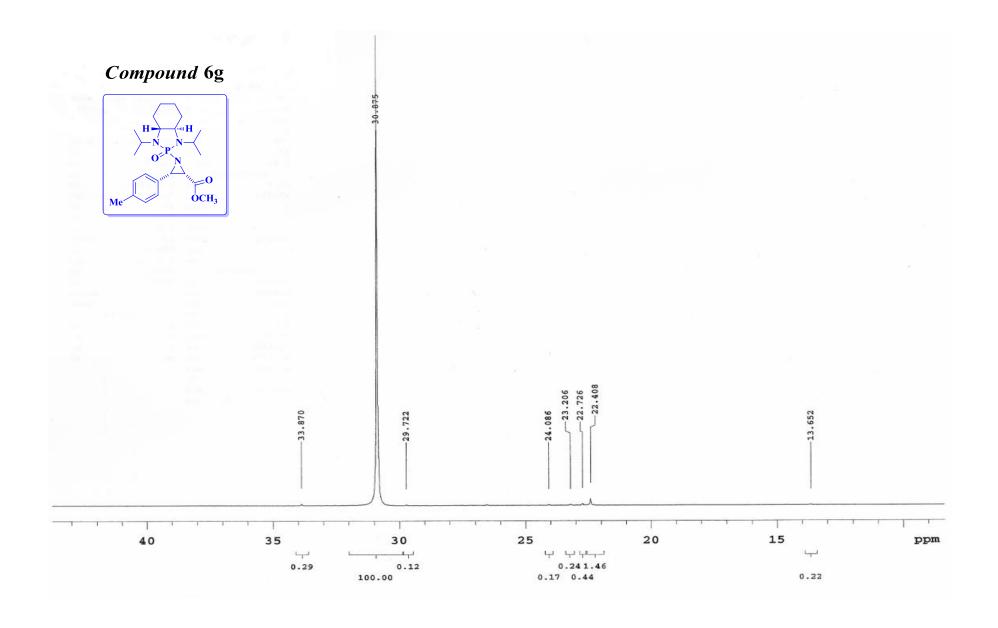


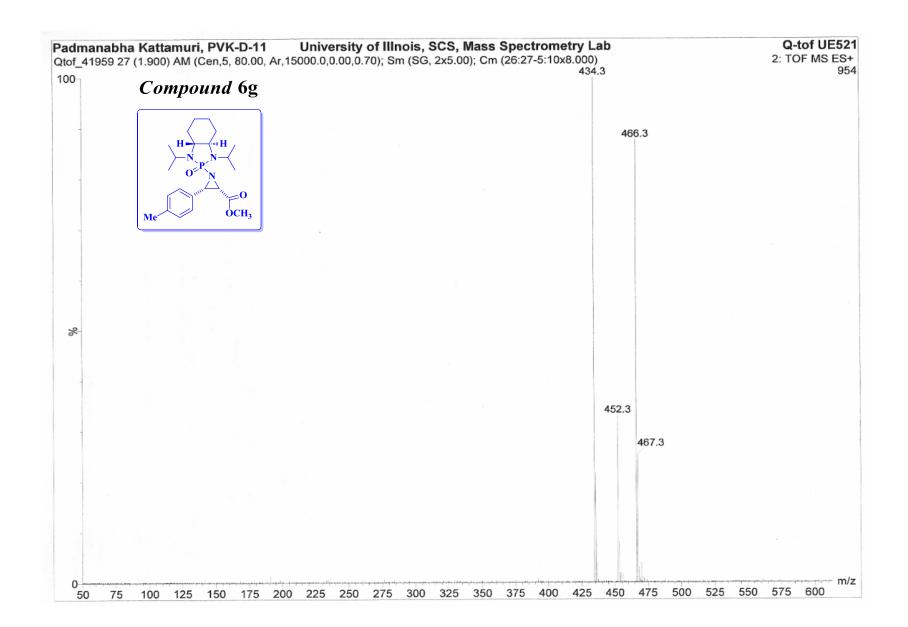
Page 1 Elemental Composition Report Single Mass Analysis Tolerance = 10.0 PPM / DBE: min = -1.5, max = 600.0 Element prediction: Off Number of isotope peaks used for i-FIT = 3 Monoisotopic Mass, Even Electron Ions 193 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass) Elements Used: C: 0-150 H: 0-250 N: 2-4 O: 2-4 P: 0-1 S: 0-1 University of Illnois, SCS, Mass Spectrometry Lab Padmanabha Kattamuri, PVK-D-59 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+002 466.2305 100-467.2313 468.2242 % 471.3308 474.2655474.8588 453.1393 456,2544 458,2585,458,9032 461,8160 464.9452 0-460.0 464.0 466.0 468.0 470.0 472.0 474.0 476.0 452.0 454.0 456.0 458.0 462.0 -1.5 Minimum: Maximum: 5.0 10.0 600.0 Calc. Mass PPM DBE i-FIT Formula Mass mDa 466.2305 466.2293 1.2 2.6 7.5 2.2 C23 H37 N3 03 5.7 C26 Н33 N3 03 466.2260 4.5 9.7 12.5

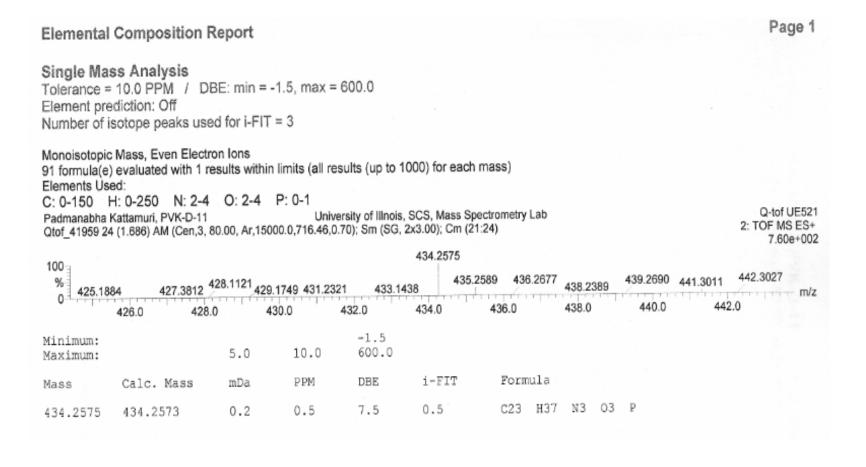


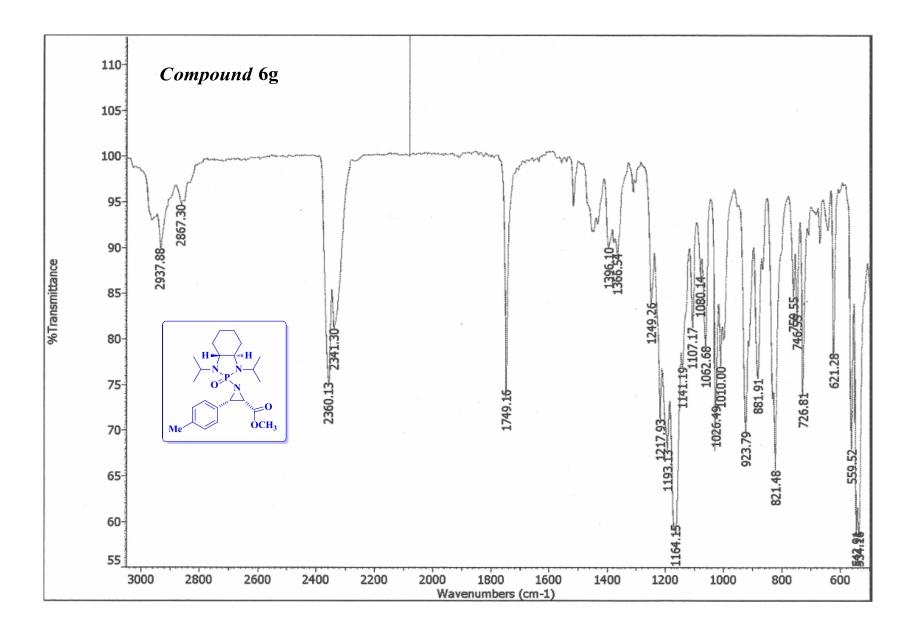


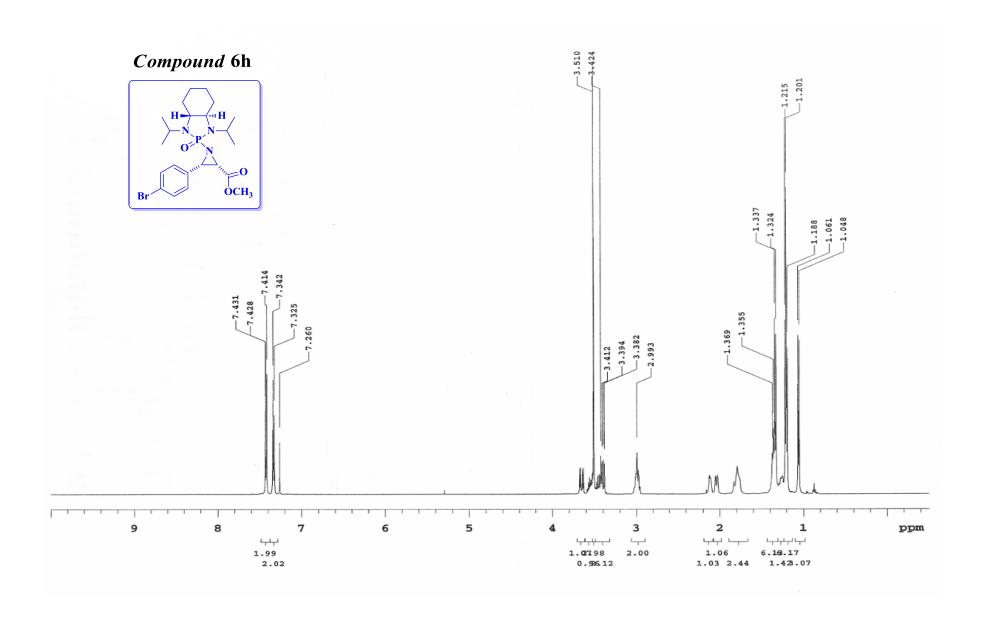


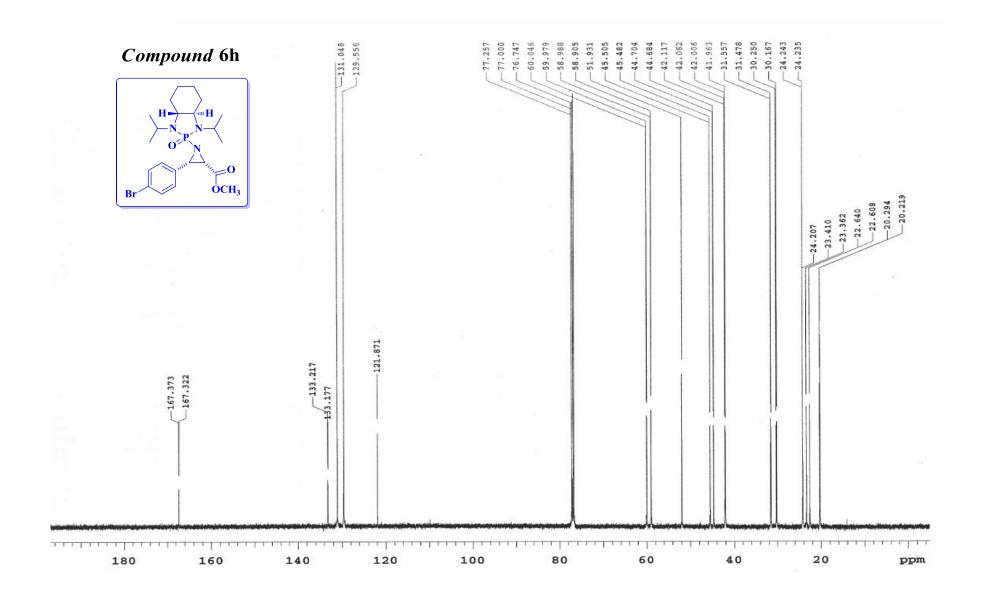


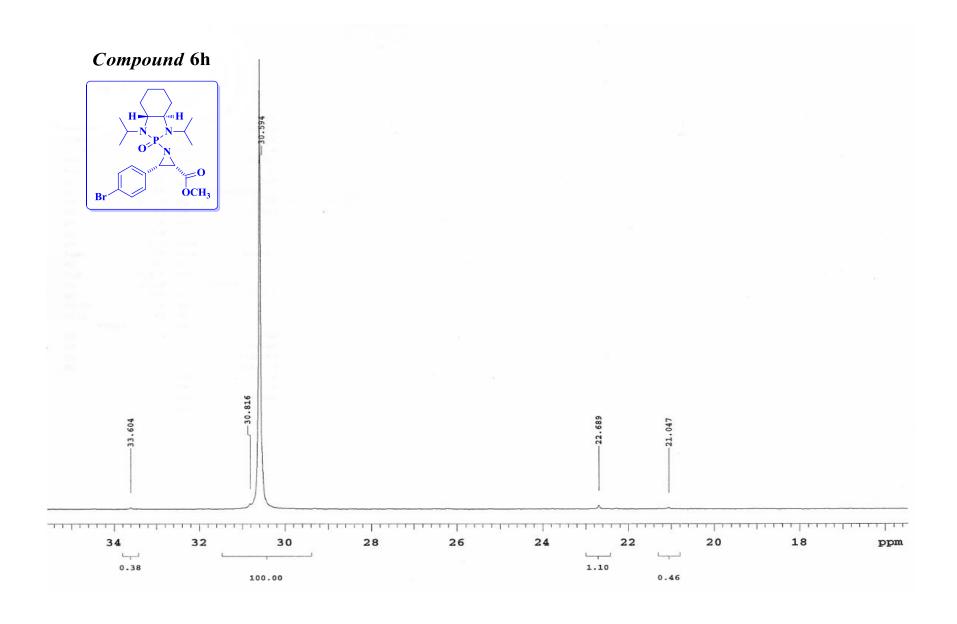


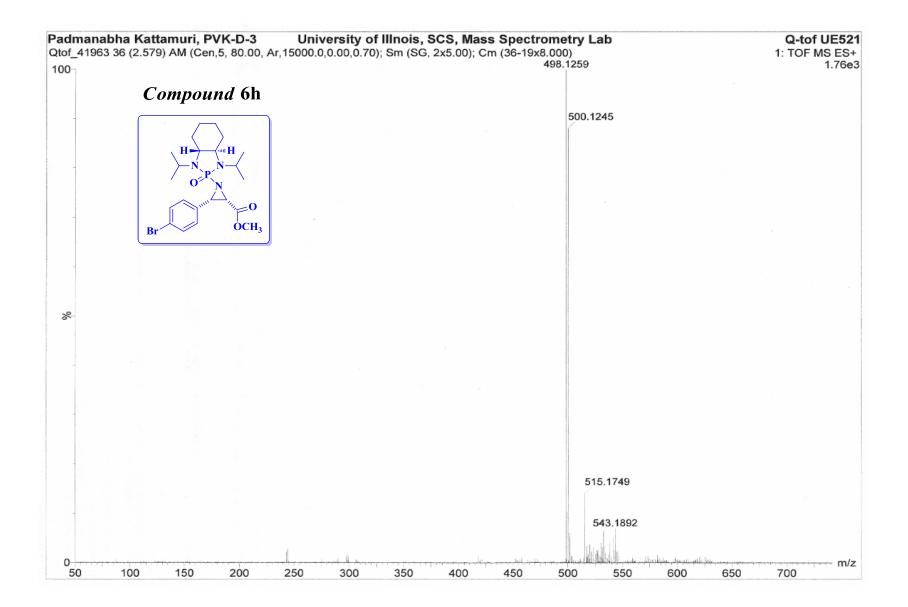


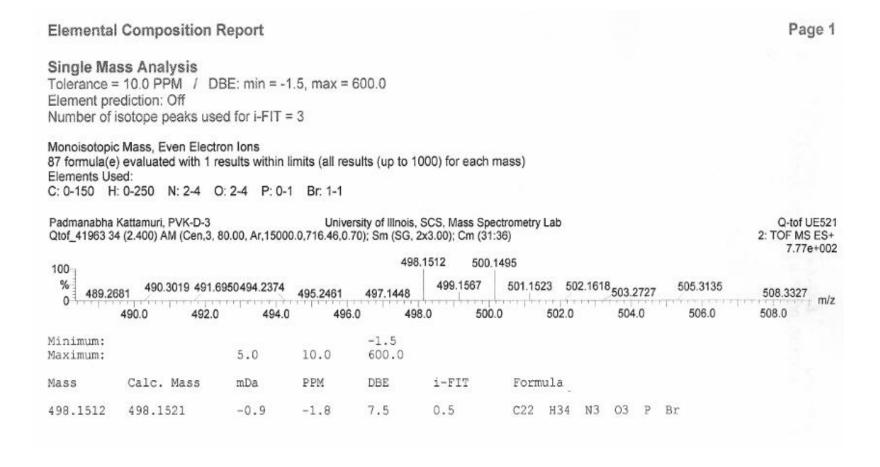


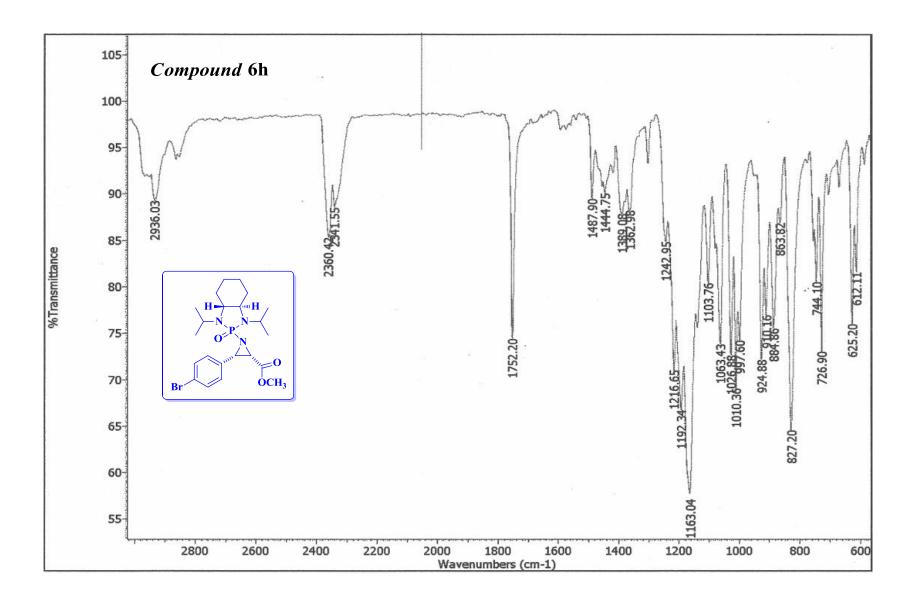


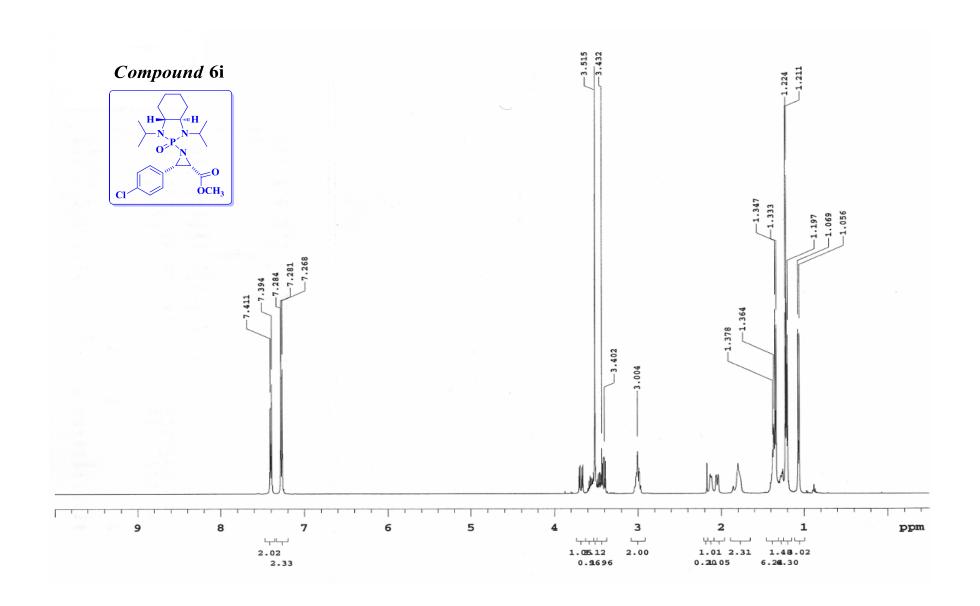


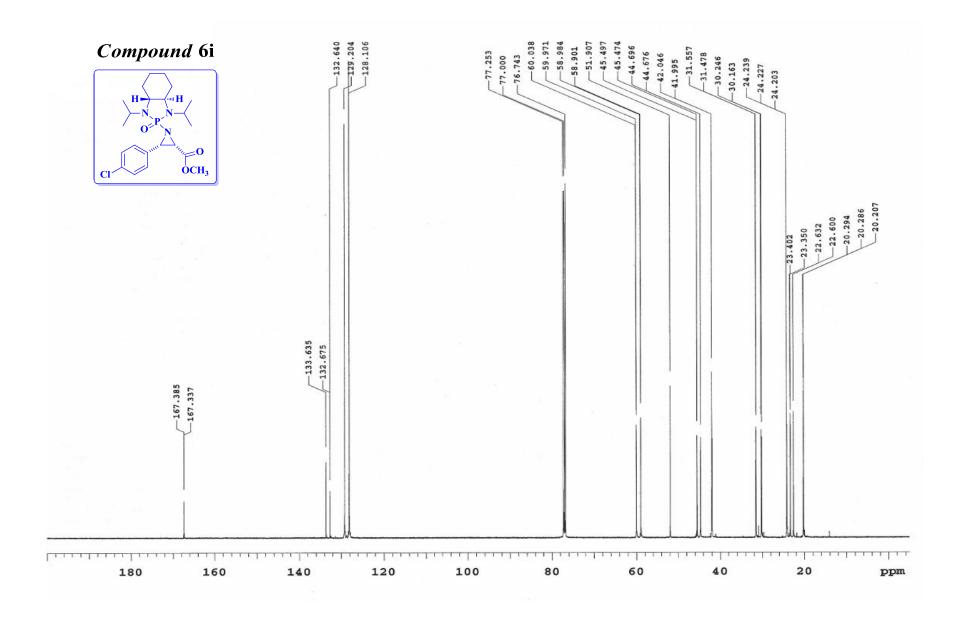


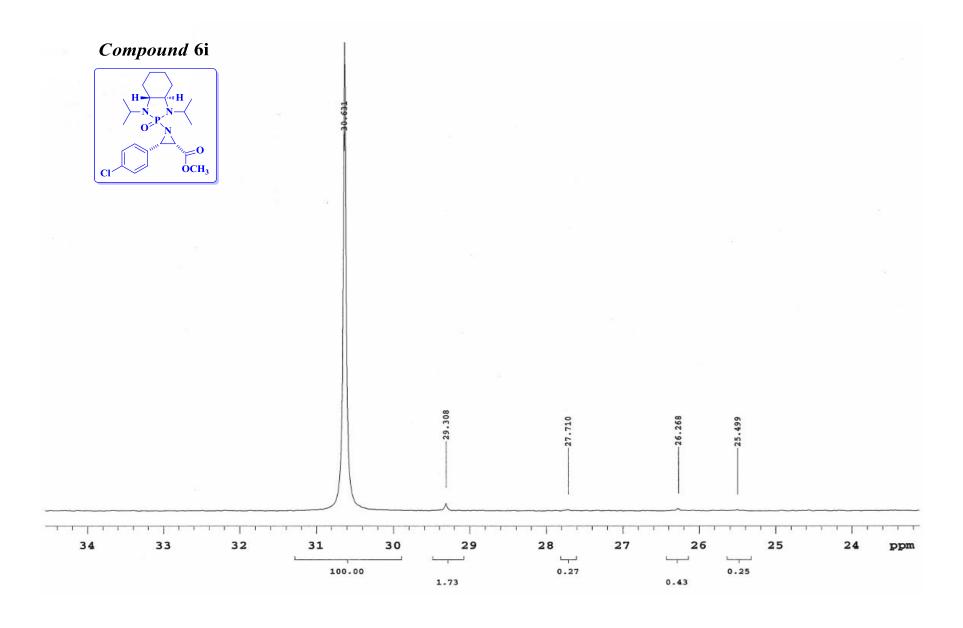


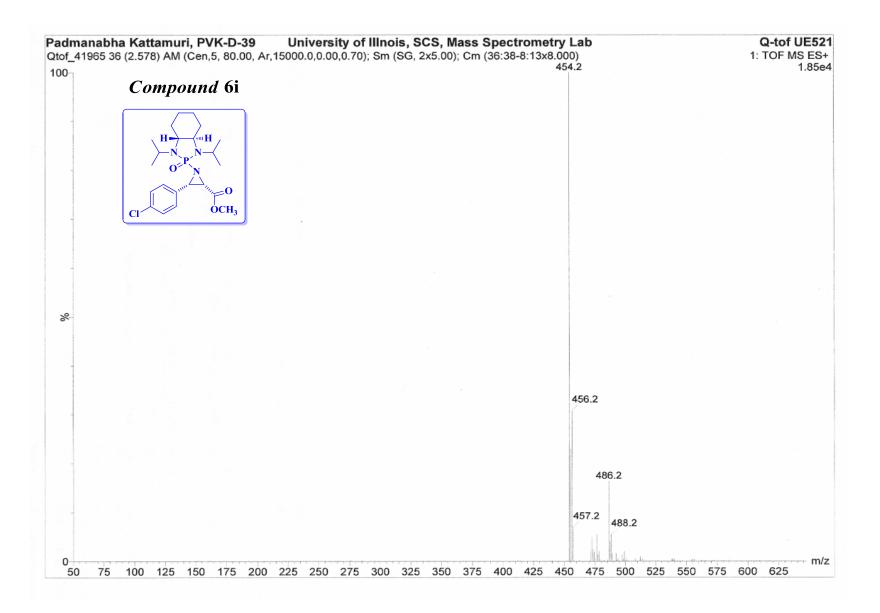




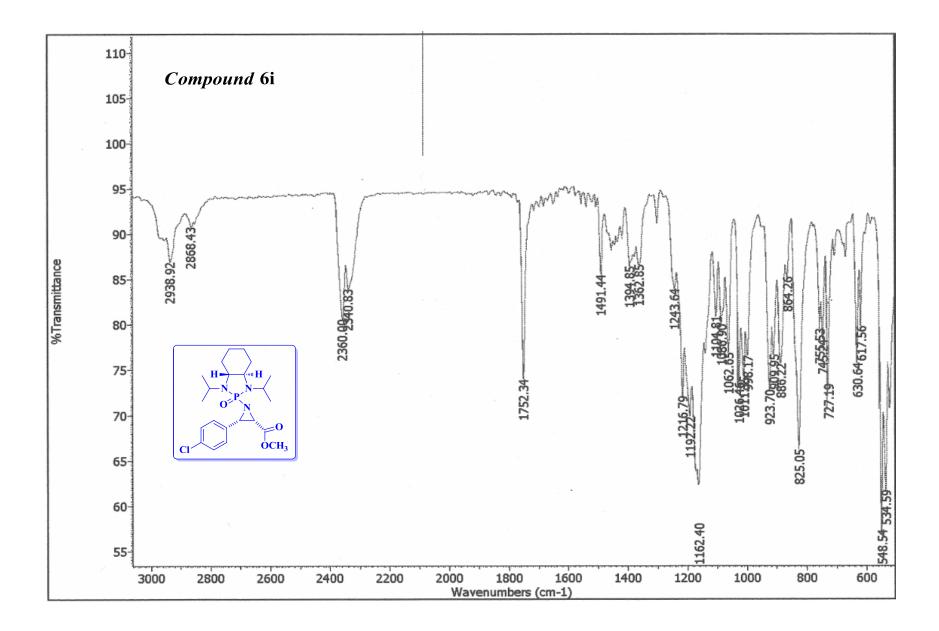


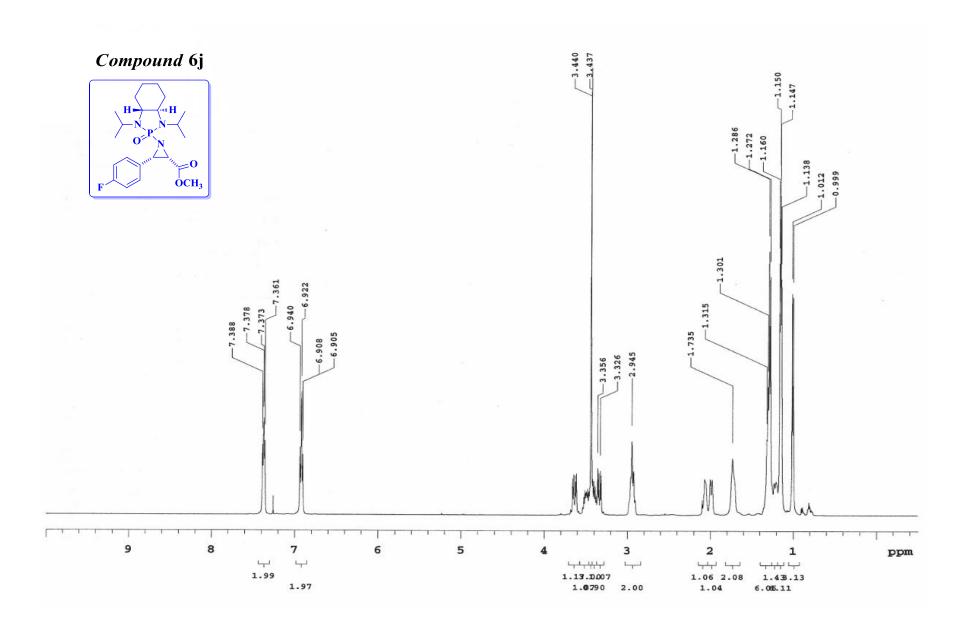


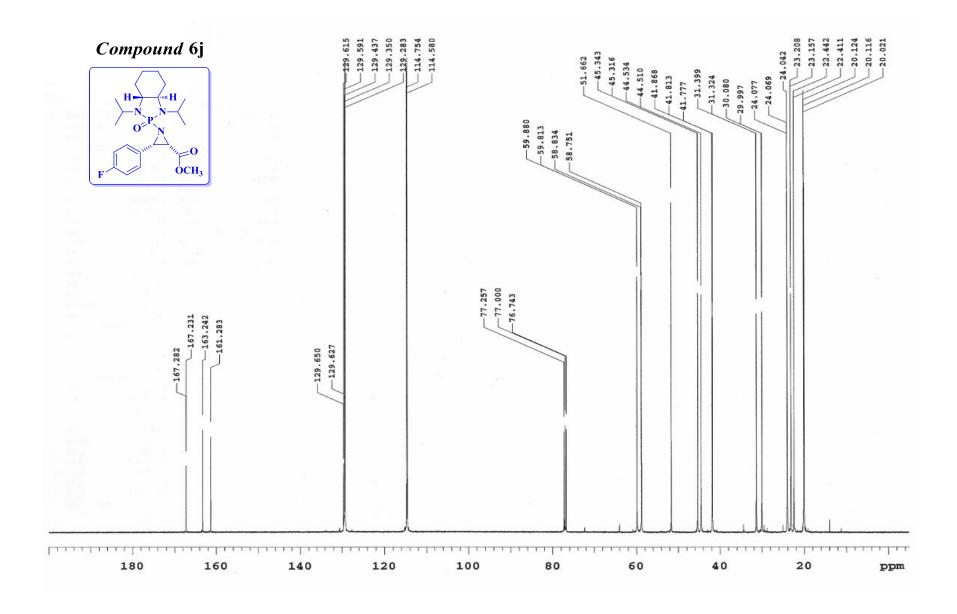


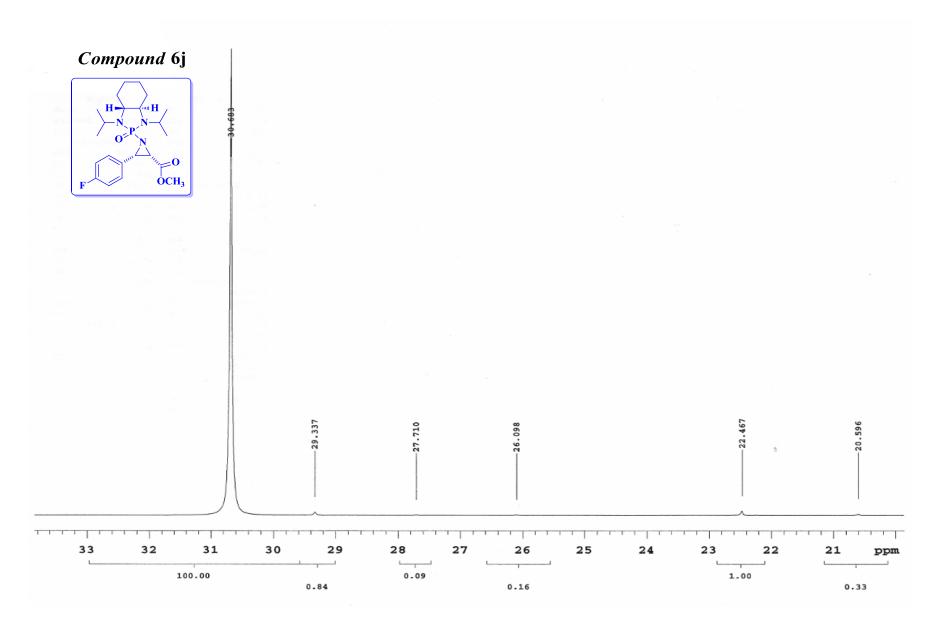


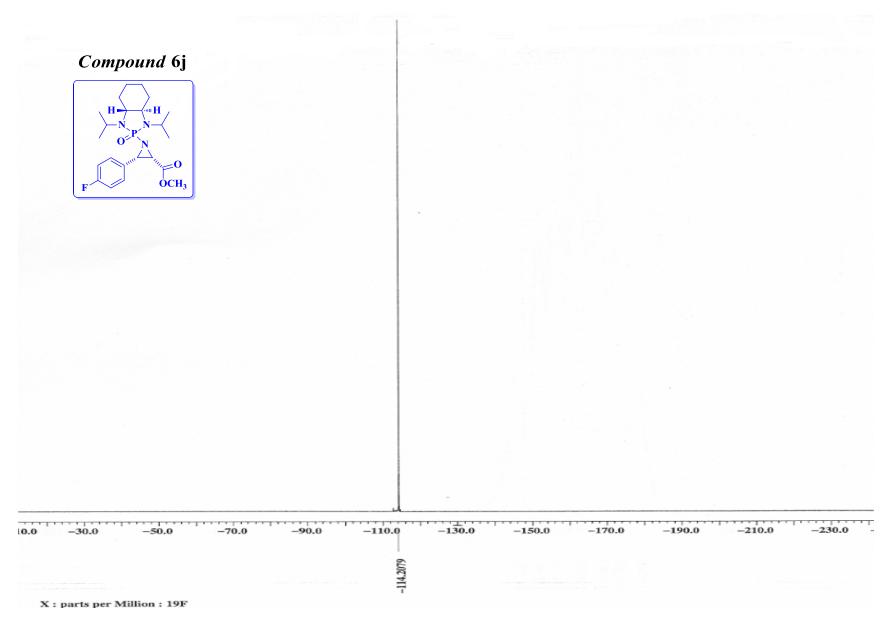
Elementa	l Comp	osition	Report											Page 1
Single Ma Tolerance Element pr Number of	= 10.0 P rediction:	PM / I	OBE: min		nax = 60	0.0								
Monoisotopi 87 formula(e Elements U C: 0-150 Padmanabha Qtof_41965 \$	e) evaluat sed: H: 0-250 Kattamuri	ed with 1 N: 2-4 , PVK-D-38	results wii 4 O: 2-4	4 P: 0-	Cl: 1	-1 ly of Illnois	s, SCS, Mass	Spectr	ometry Lab				1:	Q-tof UE521 TOF MS ES+ 2.55e+003
100 %- 437.1308 439.3683			442.2506.443.0232 447.165			7 448.3482 450.2635 452.26			456.1998 457,2040		460.2121	462.2852 463.2743		
436.0	438.0	440.0	442.0	444.0	446.0	448.0	450.0	452.0	454.0	456.0	458.0	460.0	462.0	464.0
Minimum: Maximum:			5.0	10	.0	-1.5 600.0								
Mass	Calc.	Mass	mDa	PP	М	DBE	i-FIT		Formula					
454.2024	454.2	026	-0.2	-0	. 4	7.5	4.8		C22 H3	N3	03 P (71		

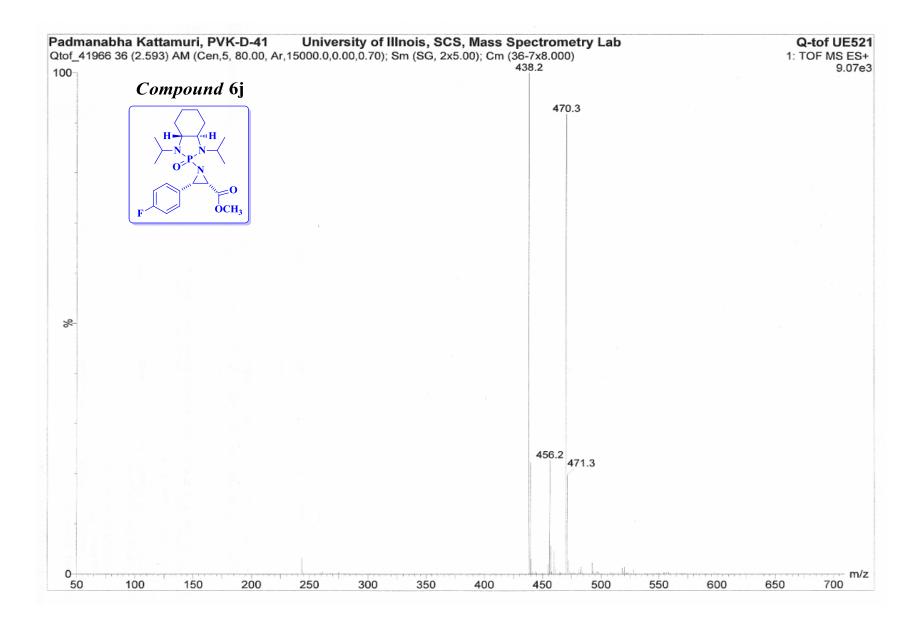


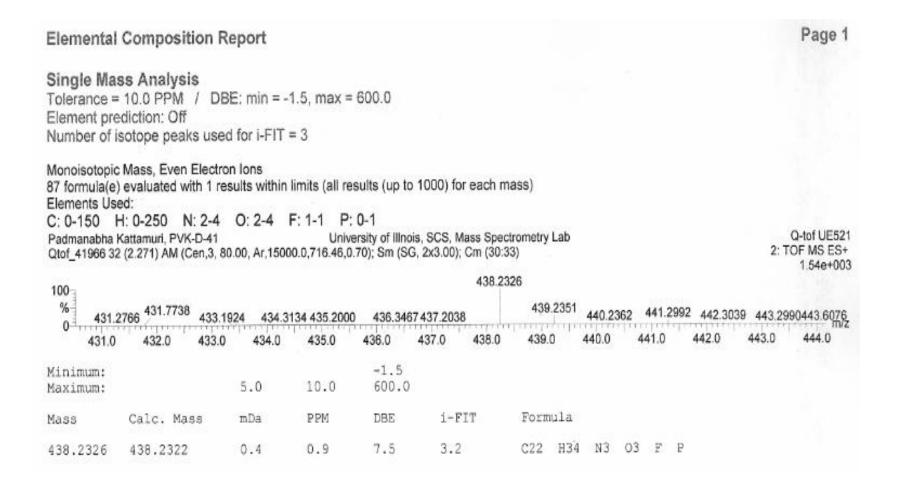


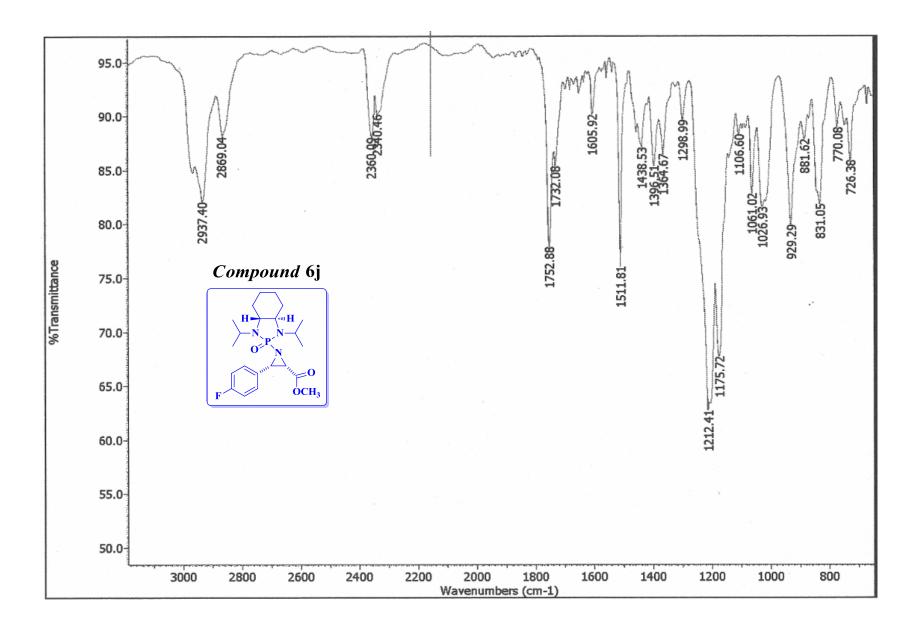


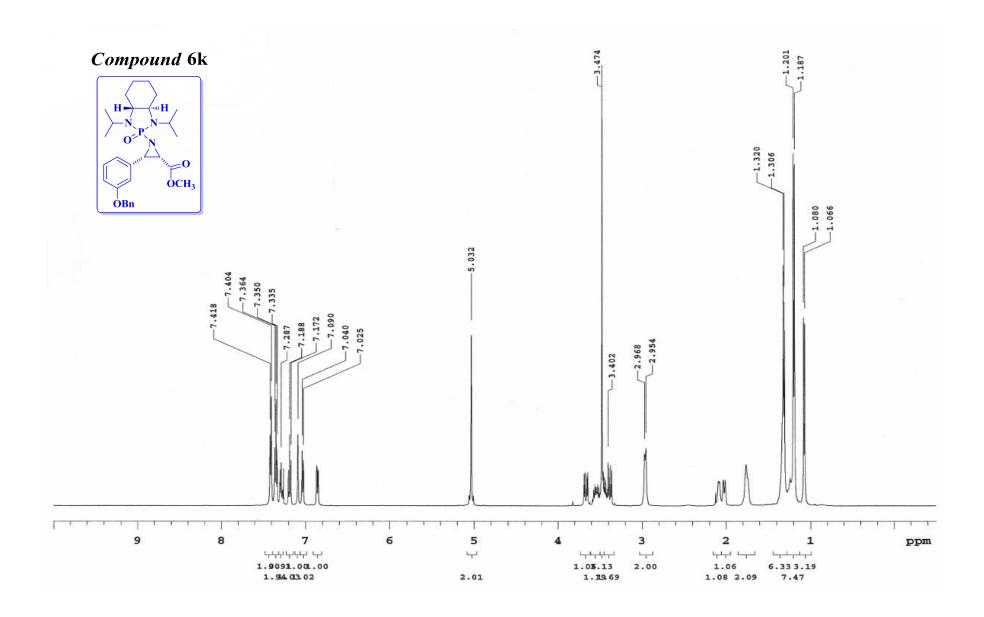


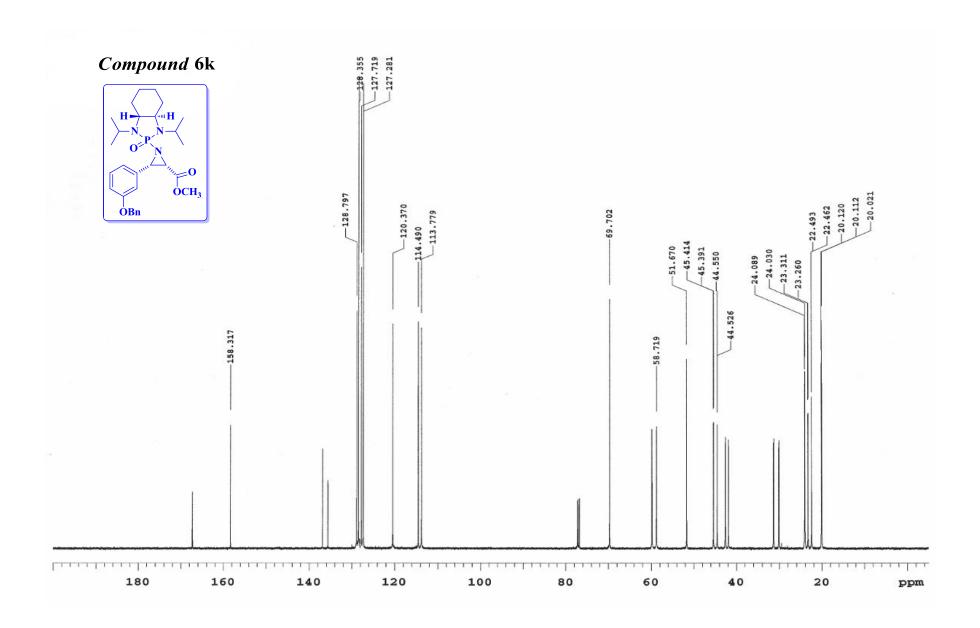


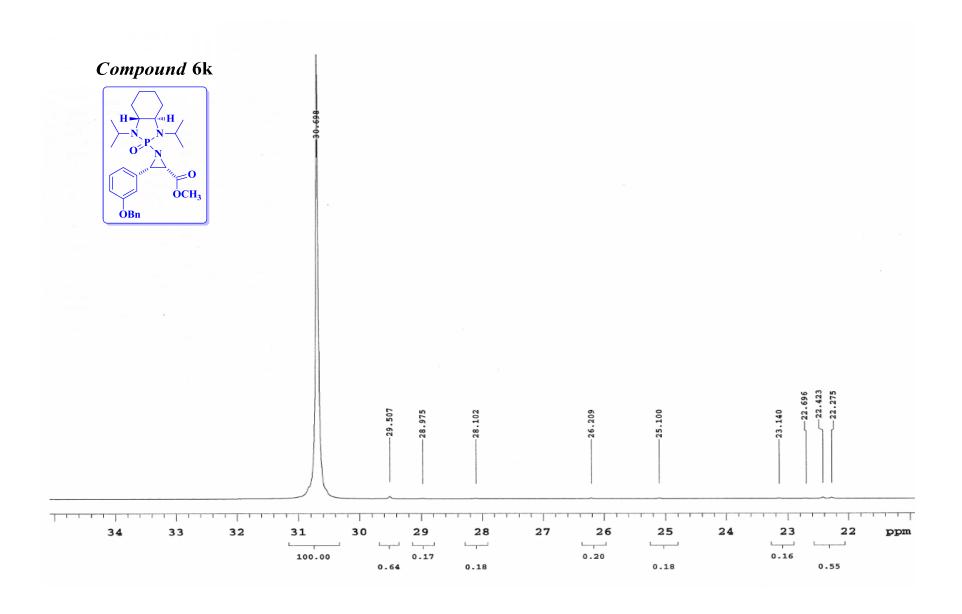


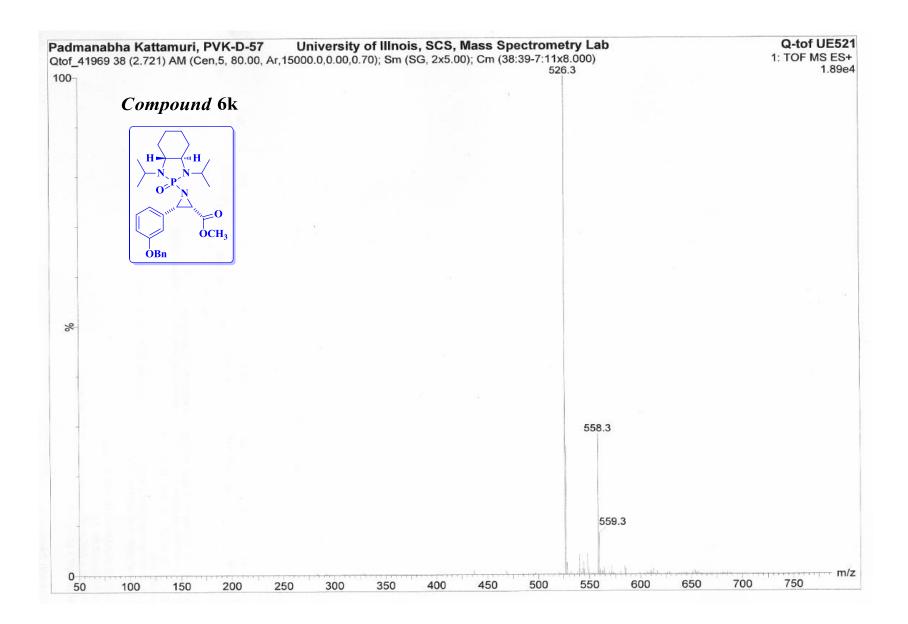




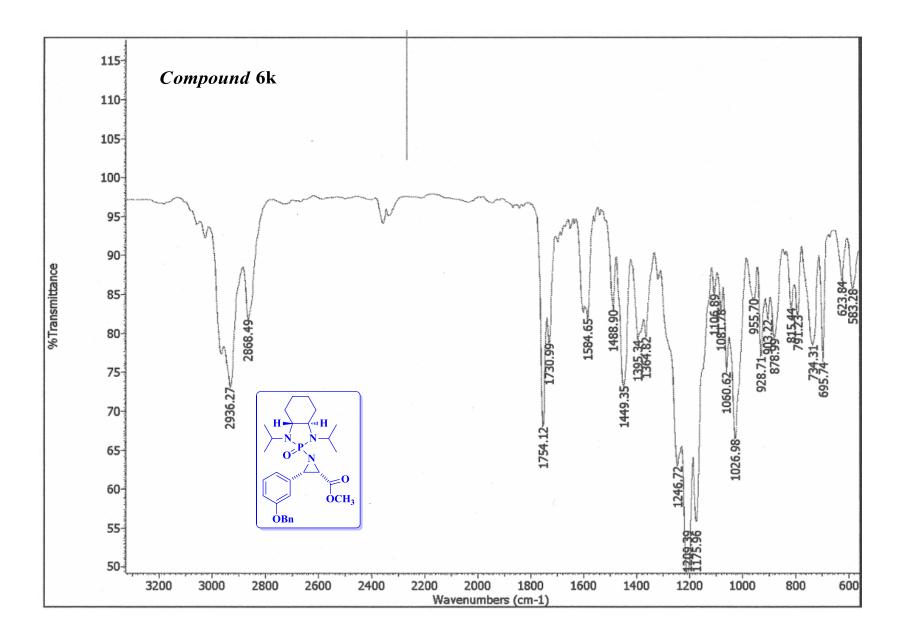


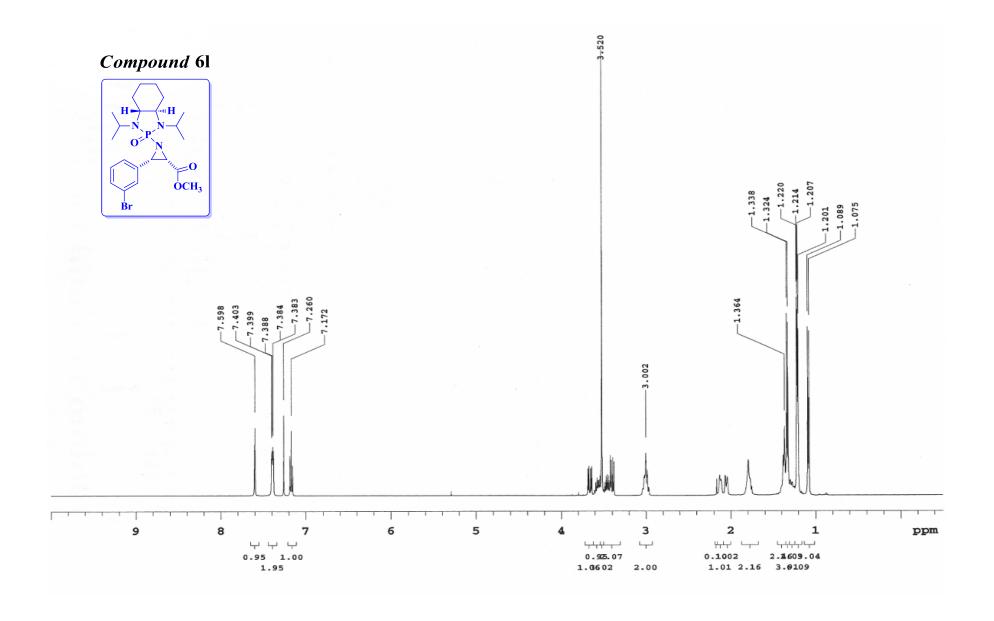


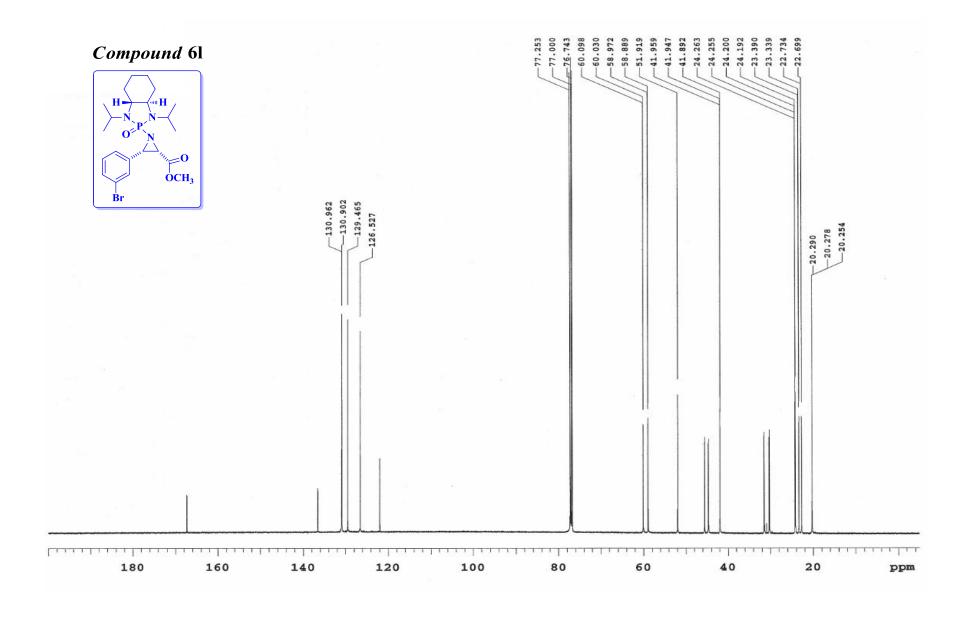


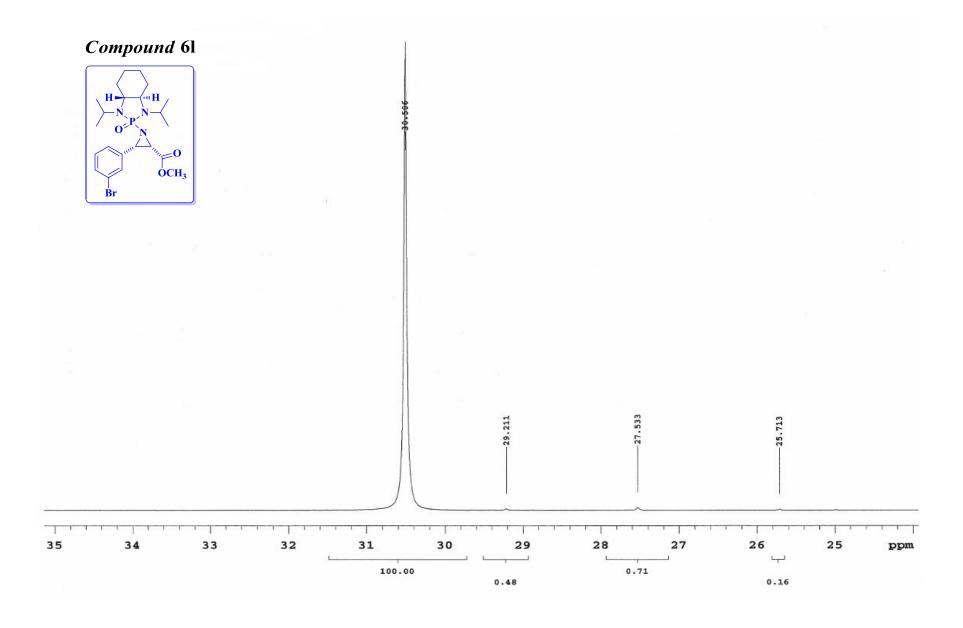


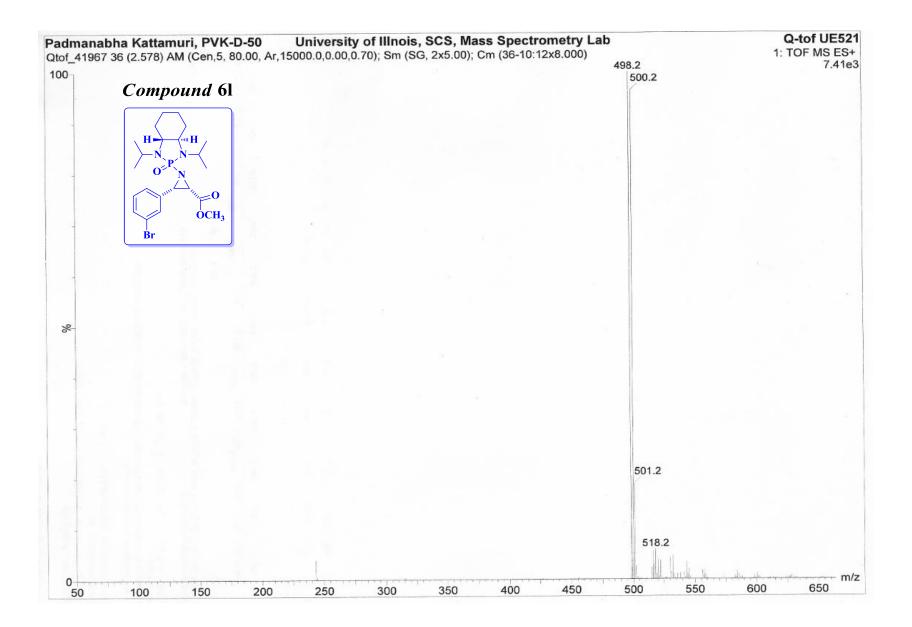
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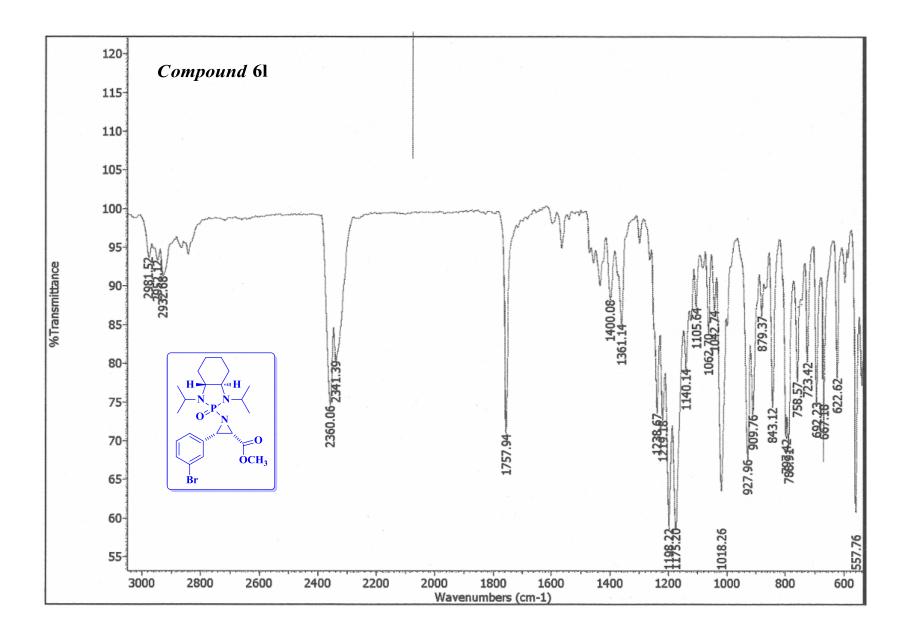


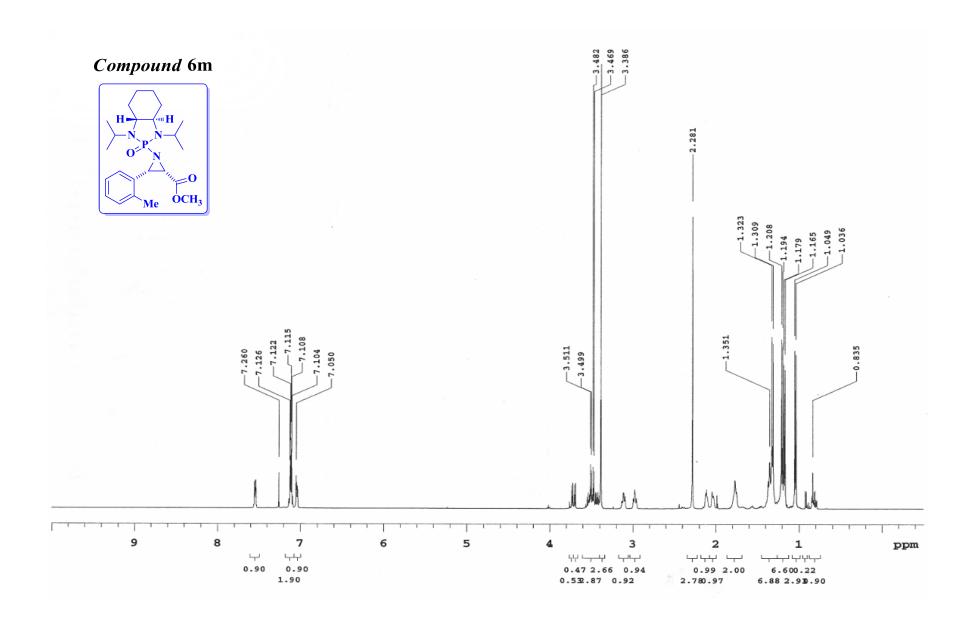


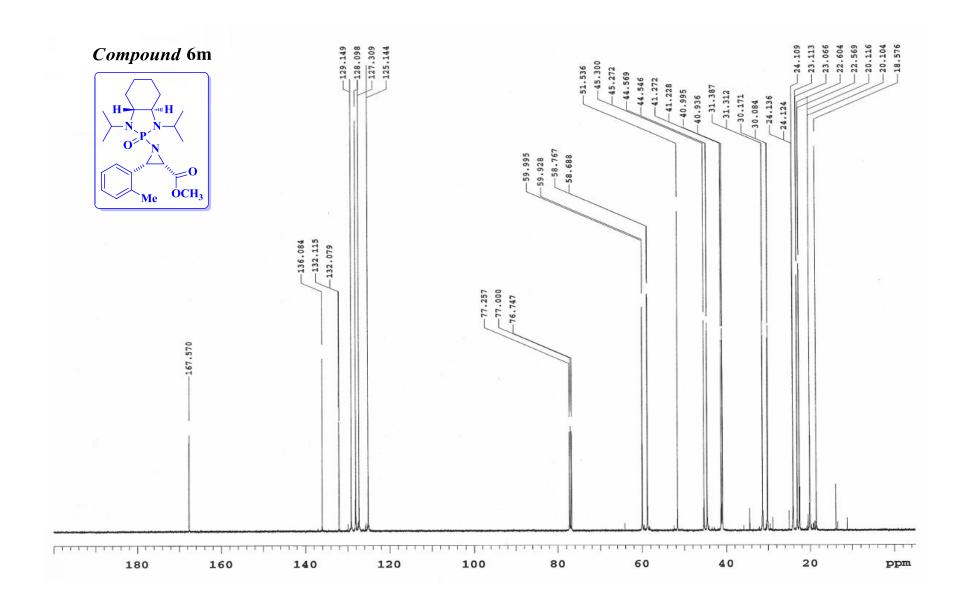


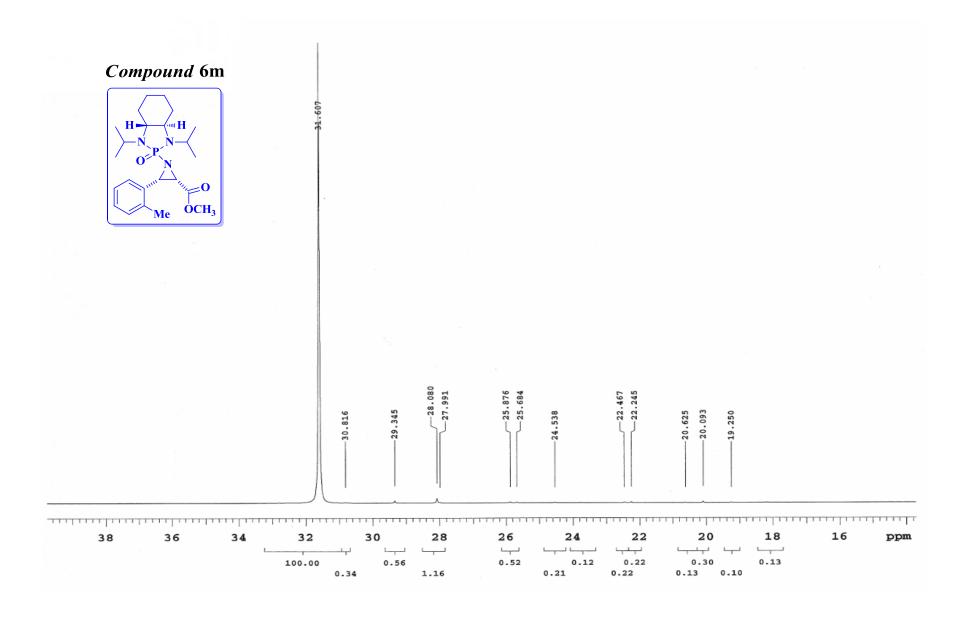


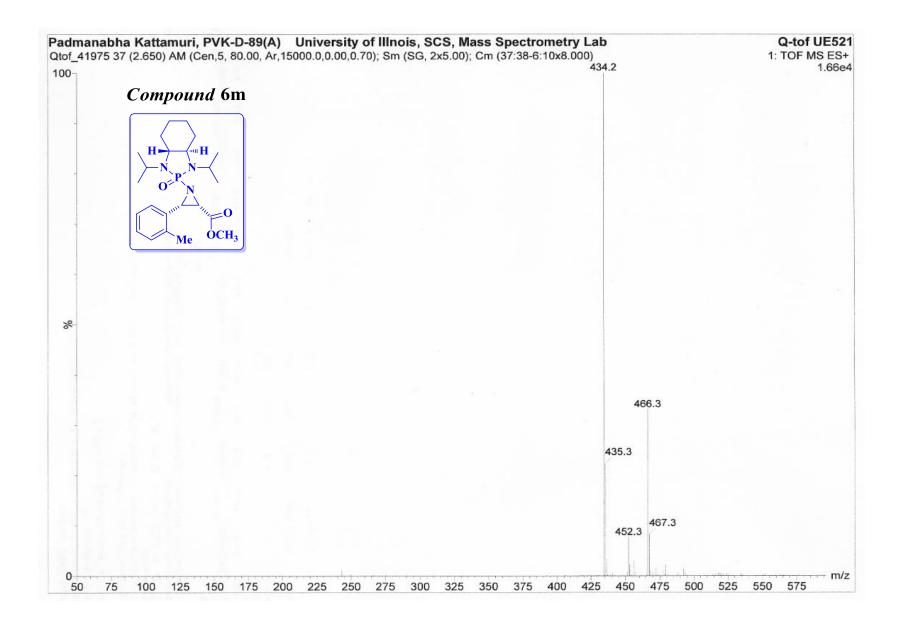
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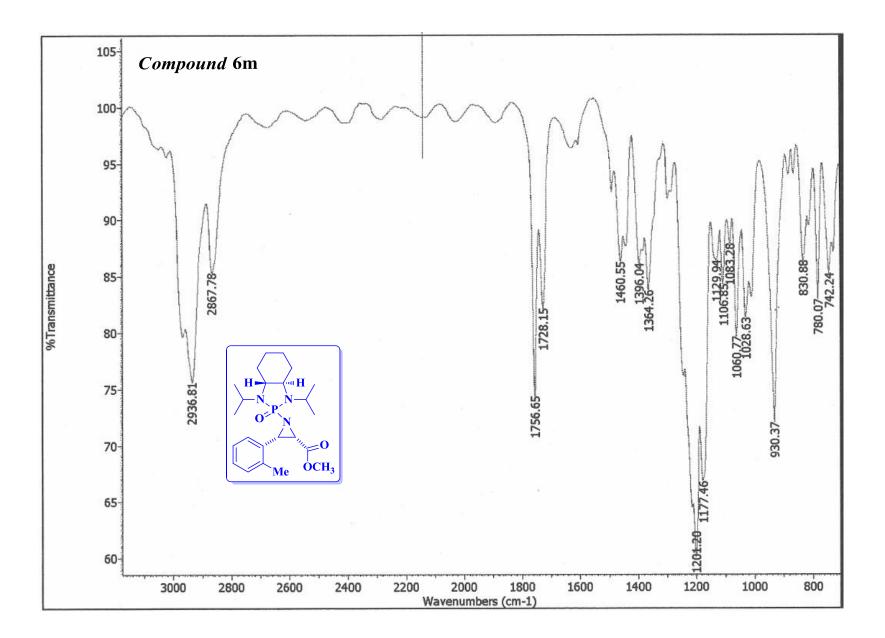


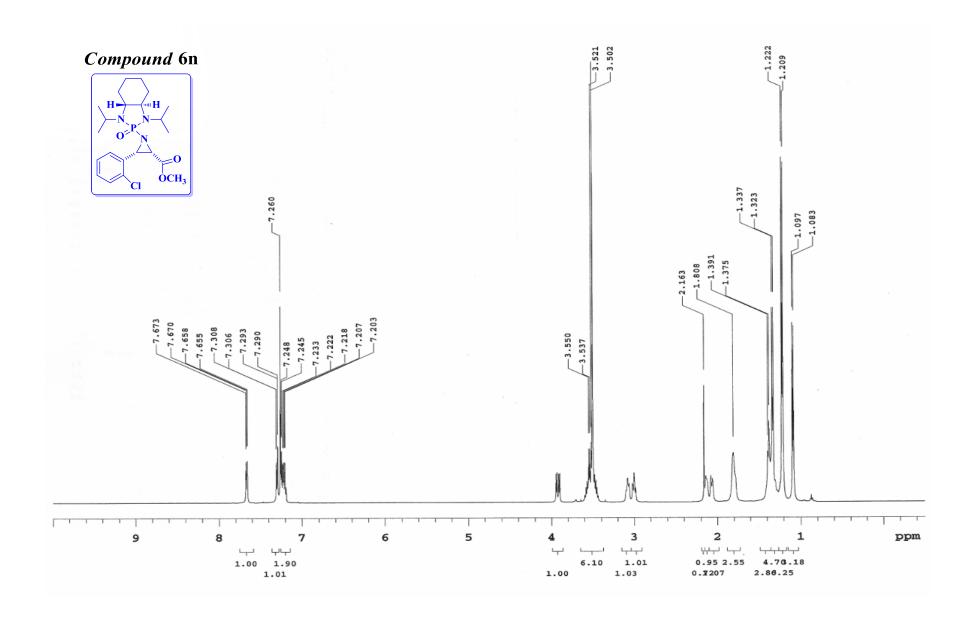


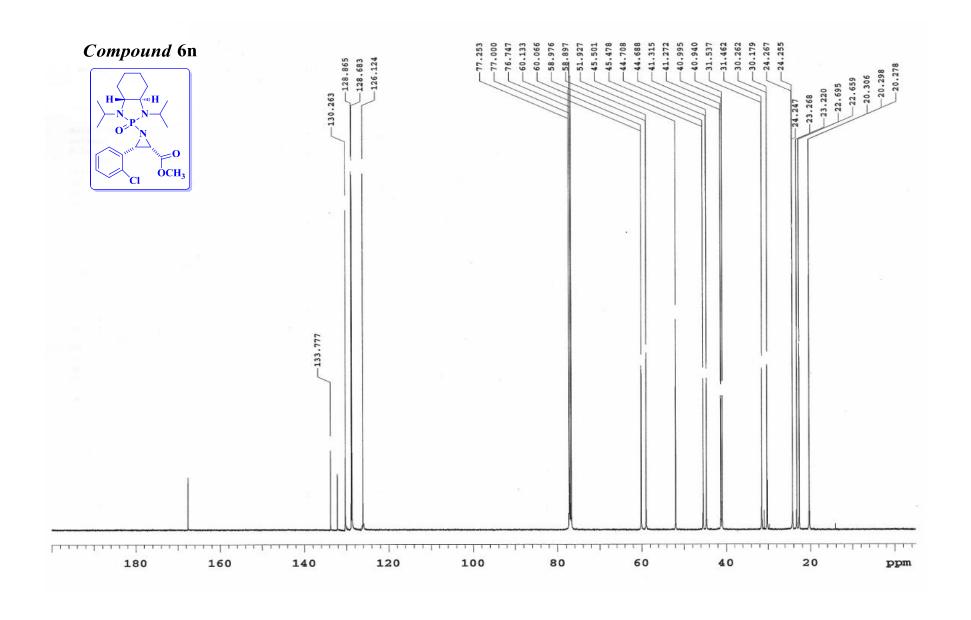


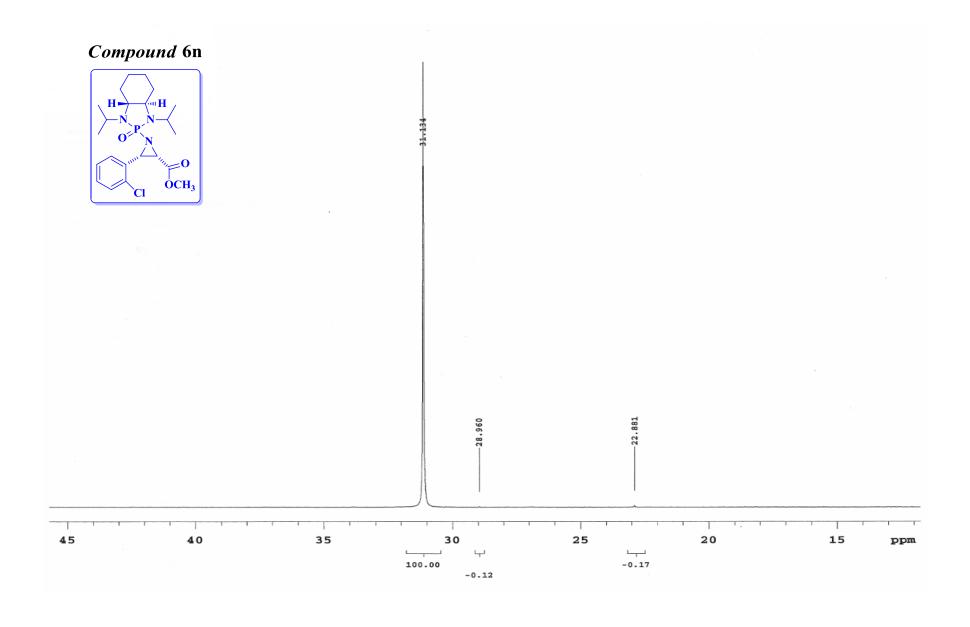


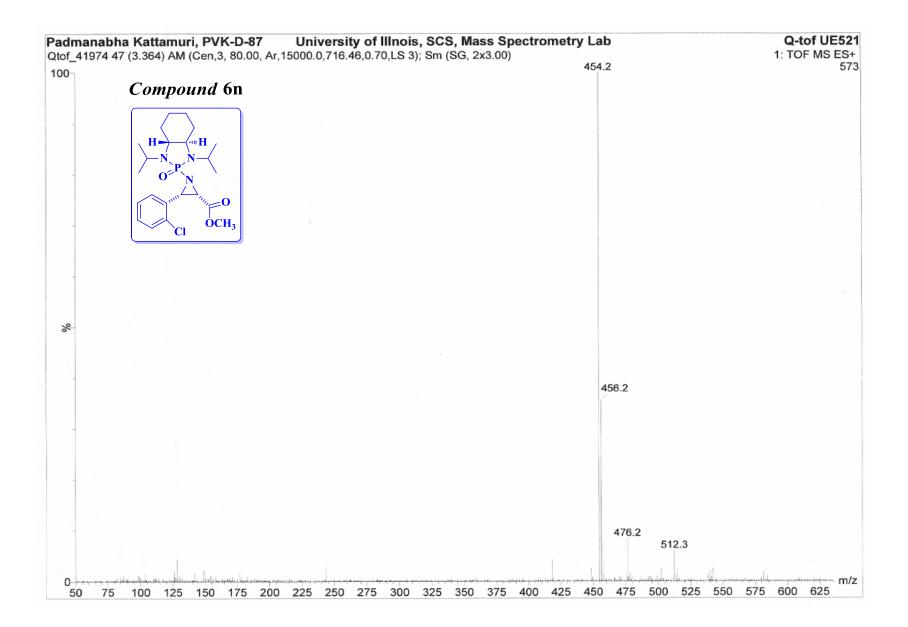
Page 1 Elemental Composition Report Single Mass Analysis Tolerance = 10.0 PPM / DBE: min = -1.5, max = 600.0 Element prediction: Off Number of isotope peaks used for i-FIT = 3 Monoisotopic Mass, Even Electron Ions 91 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass) Elements Used: C: 0-150 H: 0-250 N: 2-4 O: 2-4 P: 0-1 Q-tof UE521 University of Illnois, SCS, Mass Spectrometry Lab Padmanabha Kattamuri, PVK-D-89(A) 1: TOF MS ES+ 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) 1.40e+003 434.2563 100 440.2759 441.2696 444.2182 435.2608436.2600 445.8074 417.2506418.0085 419.0123 427.3142 430.1590 432.2489 422.5109 m/z 0 427.5 430.0 432.5 437.5 440.0 442.5 445.0 422.5 425.0 435.0 417.5 420.0 415.0 -1.5 Minimum: 600.0 5.0 10.0 Maximum: i-FIT Formula PPM DBE Calc. Mass mDa Mass -1.0-2.3 7.5 3.5 C23 H37 N3 O3 P 434.2573 434.2563



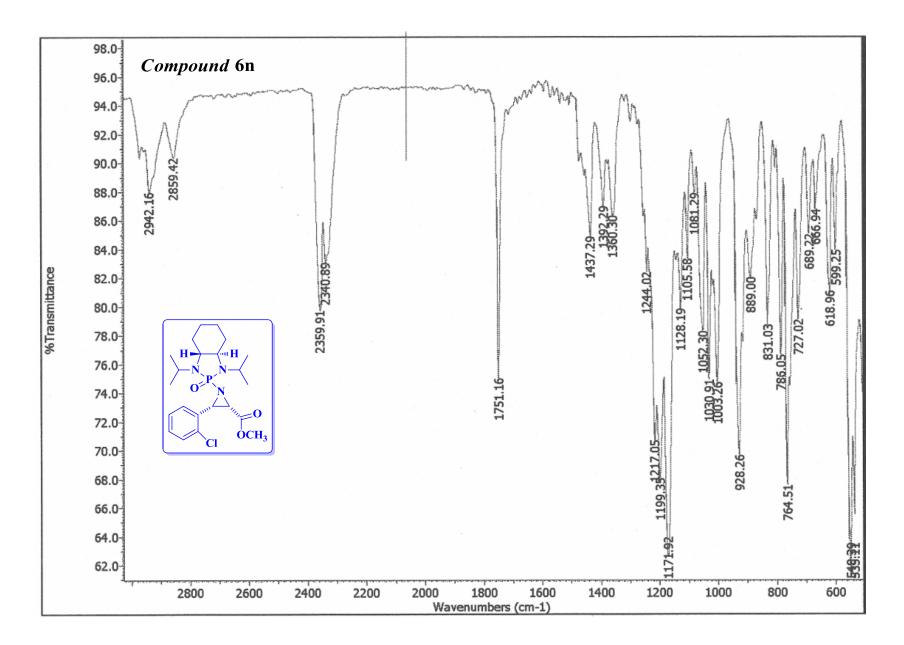


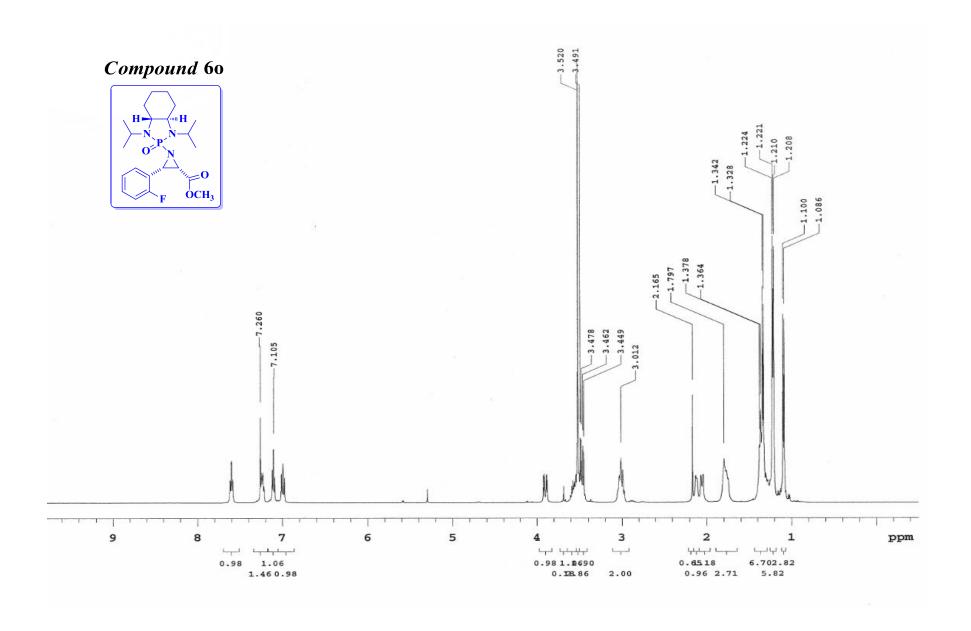


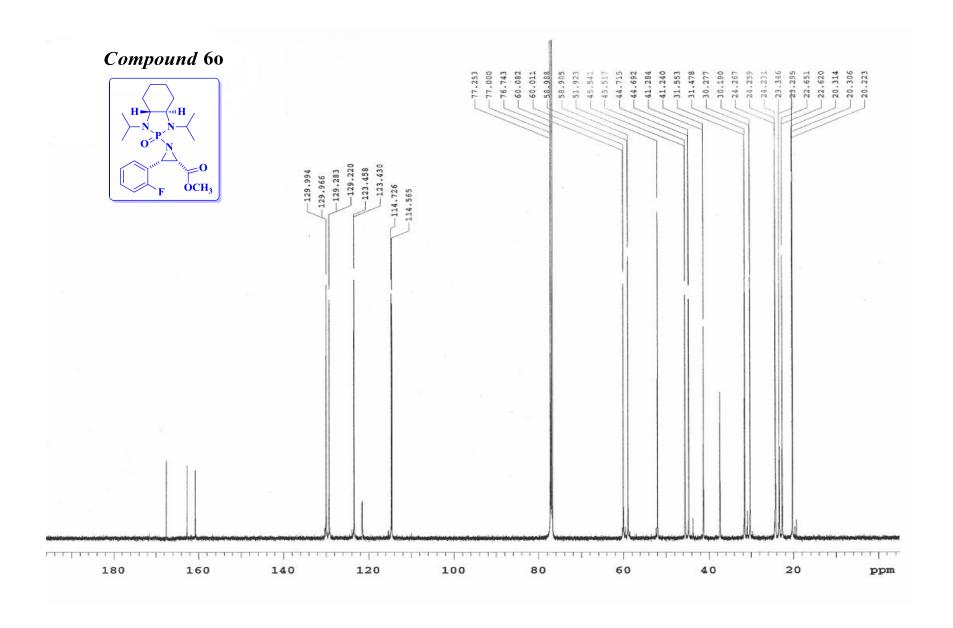


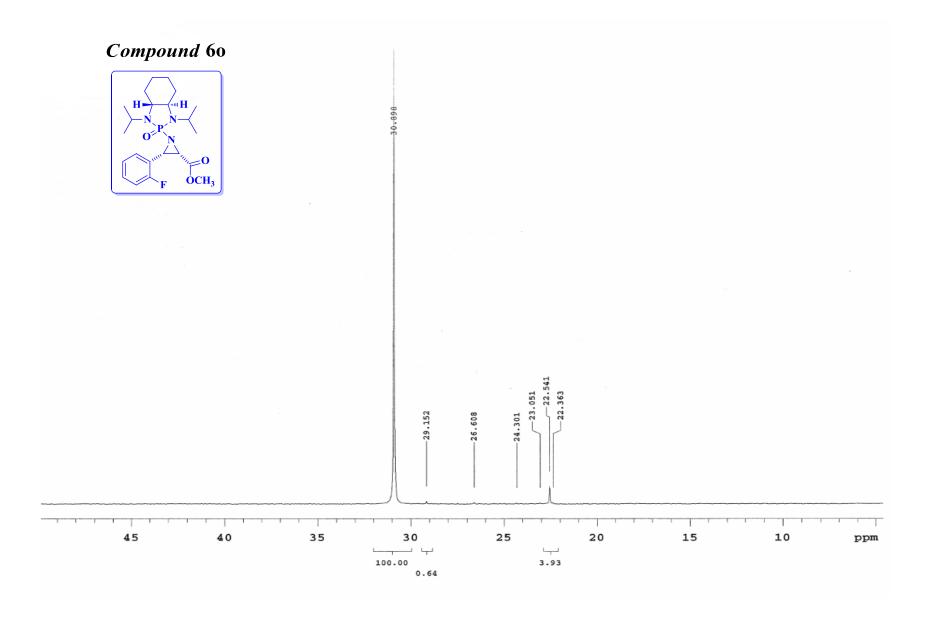


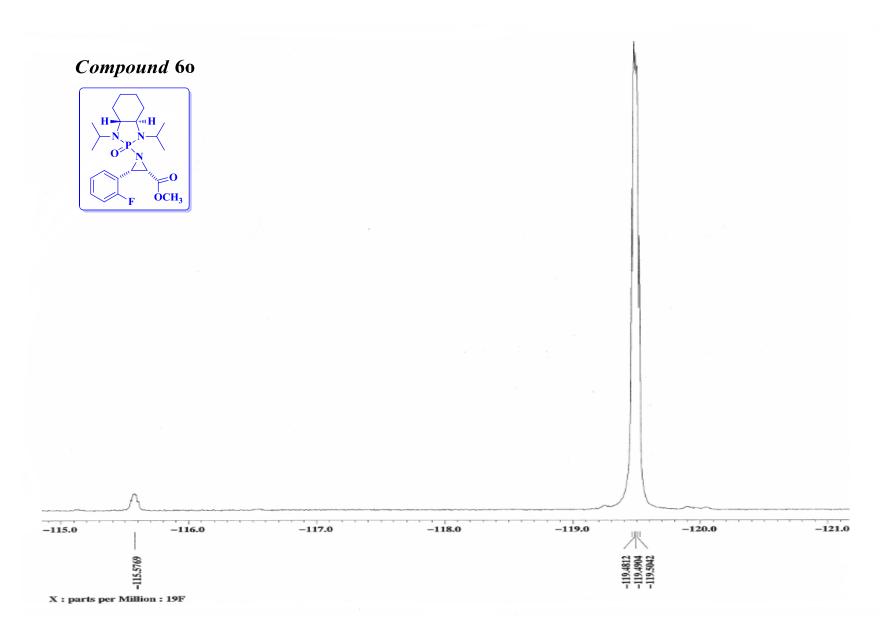
Elemental Composition Report Page 1 Single Mass Analysis Tolerance = 10.0 PPM / DBE: min = -1.5, max = 600.0 Element prediction: Off Number of isotope peaks used for i-FIT = 3 Monoisotopic Mass, Even Electron Ions 87 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass) Elements Used: C: 0-150 H: 0-250 N: 2-4 O: 2-4 P: 0-1 Cl: 1-1 University of Illnois, SCS, Mass Spectrometry Lab Padmanabha Kattamuri, PVK-D-87 Q-tof UE521 Qtof_41974 47 (3.364) AM (Cen.3, 80.00, Ar,15000.0,716.46,0.70,LS 3); Sm (SG, 2x3.00) 1: TOF MS ES+ 5.73e+002 454.2018 100 456.2002 % 426.4672 458,2110 0 434.2533 448.2737449.2888 438.2303 441.3871444.1873 470.2518_{m/z} 466.2234 435.0 440.0 430.0 445.0 450.0 455.0 460.0 465.0 470.0 Minimum: -1.5 5.0 Maximum: 10.0 600.0 Calc. Mass PPM 1-FIT Mass mDa DBE Formula 454.2018 454.2026 -0.8 -1.8 7.5 0.2 H34 N3 O3 P C1 C22

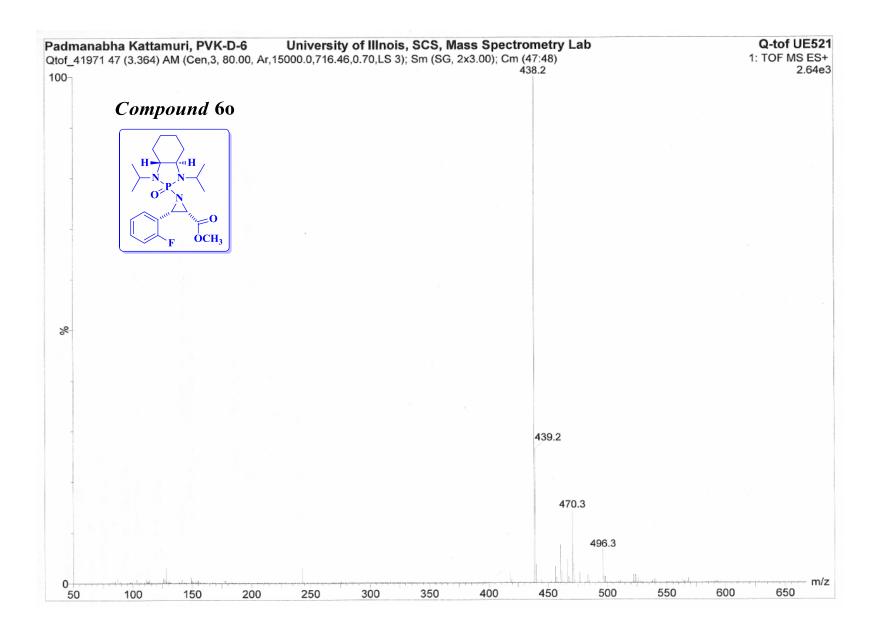




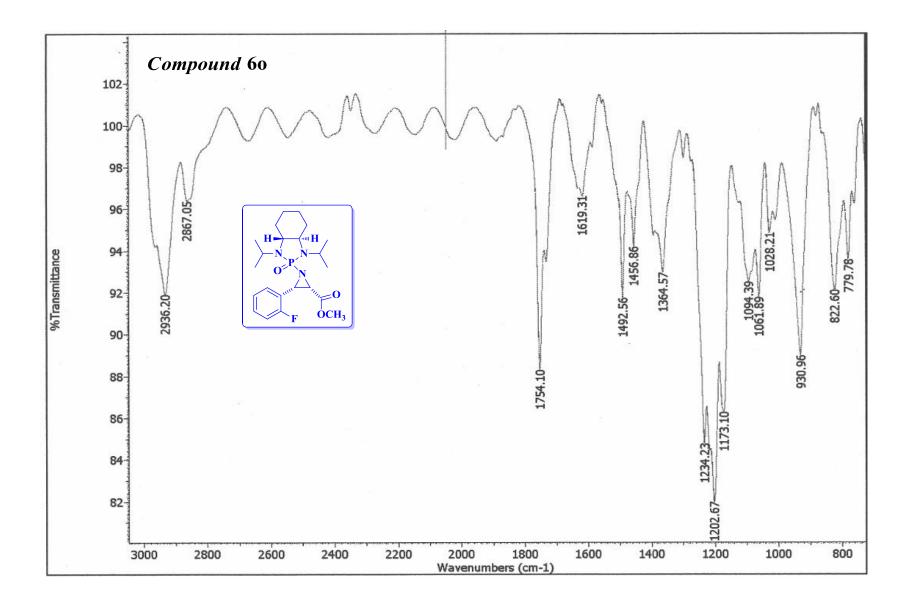


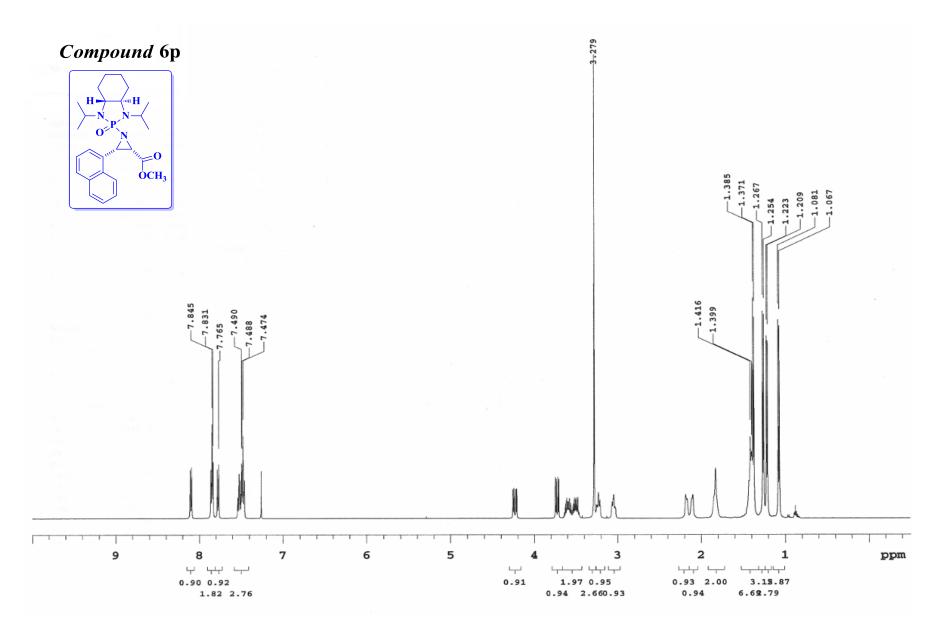


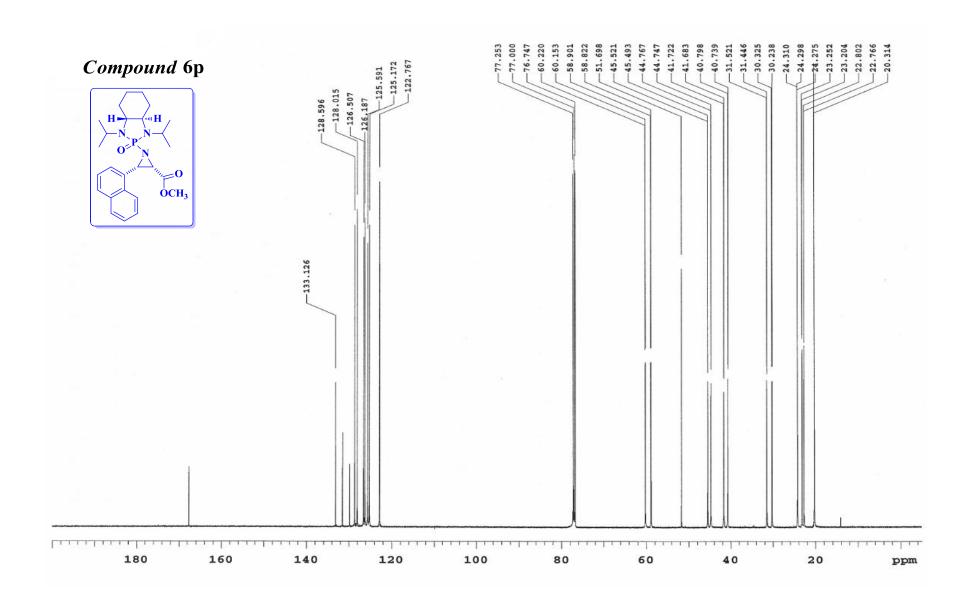


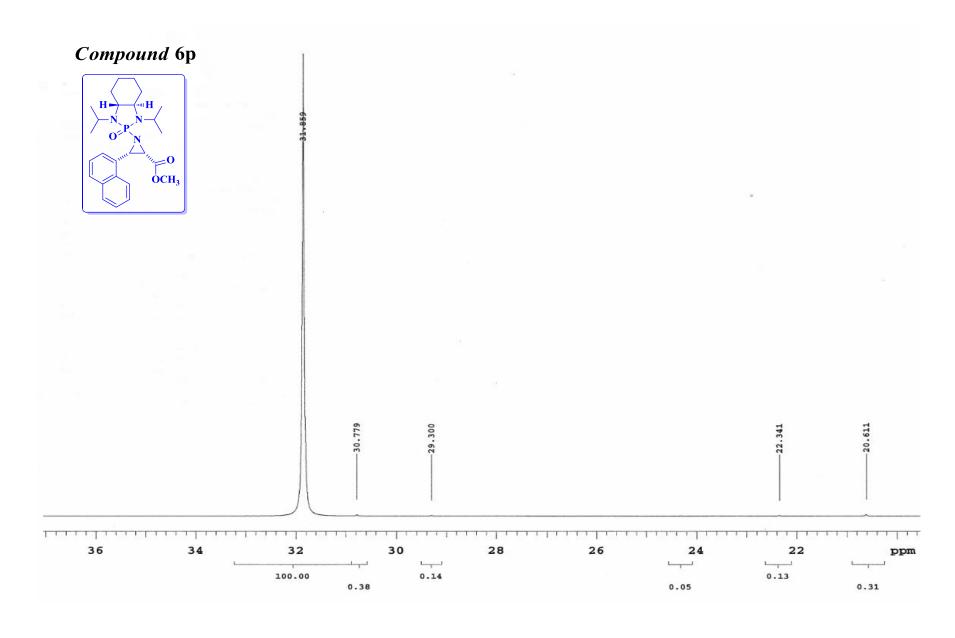


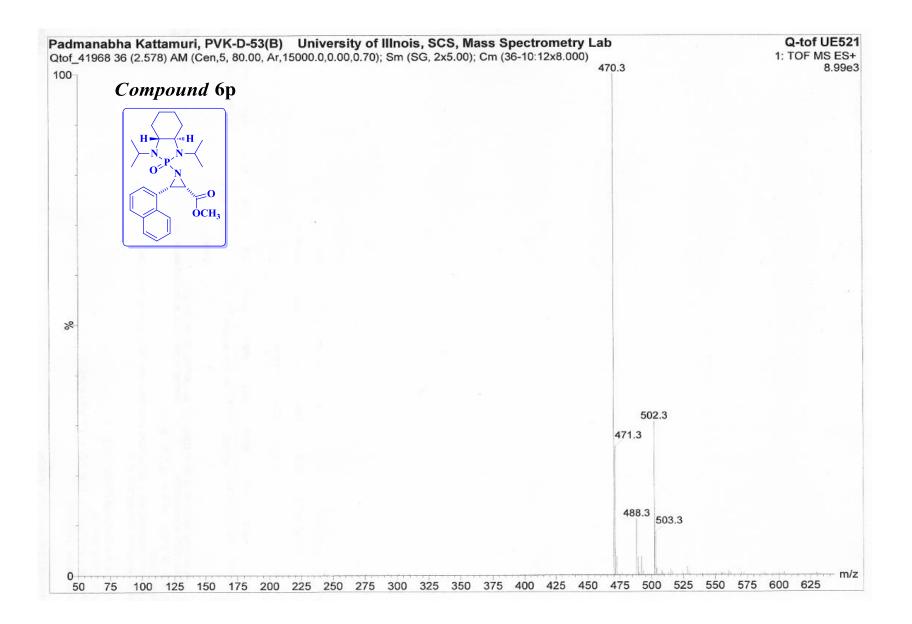
Elemental	Composition R	eport									Pag	ge 1
Tolerance = Element pre	ss Analysis = 10.0 PPM / DE ediction: Off isotope peaks use	BE: min = -1.		00.0								
169 formula(Elements Us	c Mass, Even Electro (e) evaluated with 2 r sed: I: 0-250 N: 2-4 O	esults within I			1000) for ea	nch mass)						
Padmanabha Qtof_41971 4	Kattamuri, PVK-D-6 7 (3.364) AM (Cen,3, 8	0.00, Ar,15000.	Univers 0,716.46,0.7	sity of Illnois, on (3), Sm (3)	SCS, Mass 5 SG, 2x3.00);	Spectrometry Cm (47:48)	y Lab				Q-tof L 1: TOF MS	
100						438.231	7				2.040	5.000
	.2751 432.9525	434.2359	435.2466	436.2187		9658	439.2	4	40.2333	441.2431	442.3407	m/z
	32.0 433.0	434.0	435.0	436.0	437.0	438.0	439.0		0.0	441.0	442.0	
Minimum: Maximum:		5.0	10.0	-1.5 600.0								
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	For	mula					
438.2317	438.2322 438.2356	-0.5 -3.9	-1.1 -8.9	7.5 2.5	0.3 61.5	C22 C19		13 03 13 03	P F P S	F		



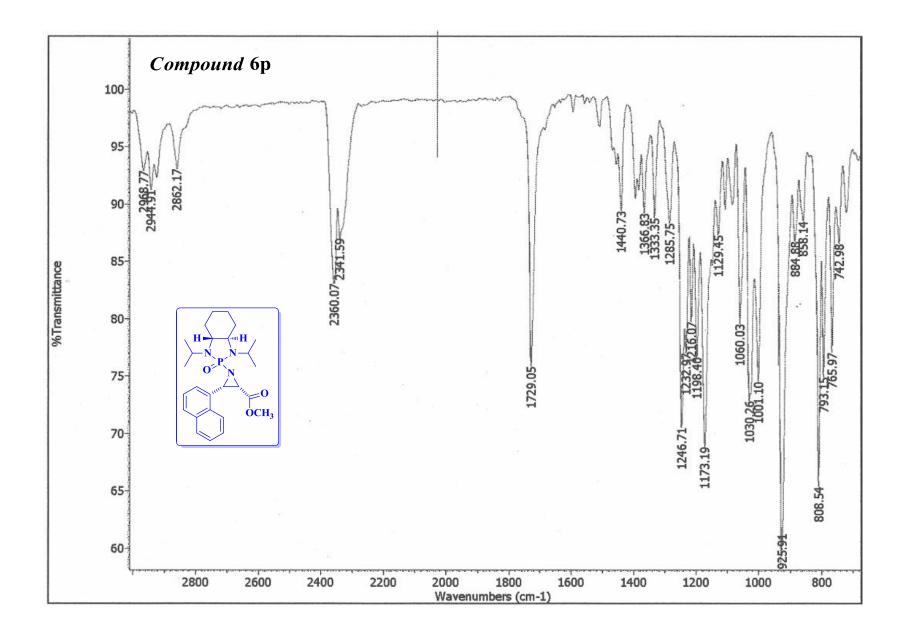


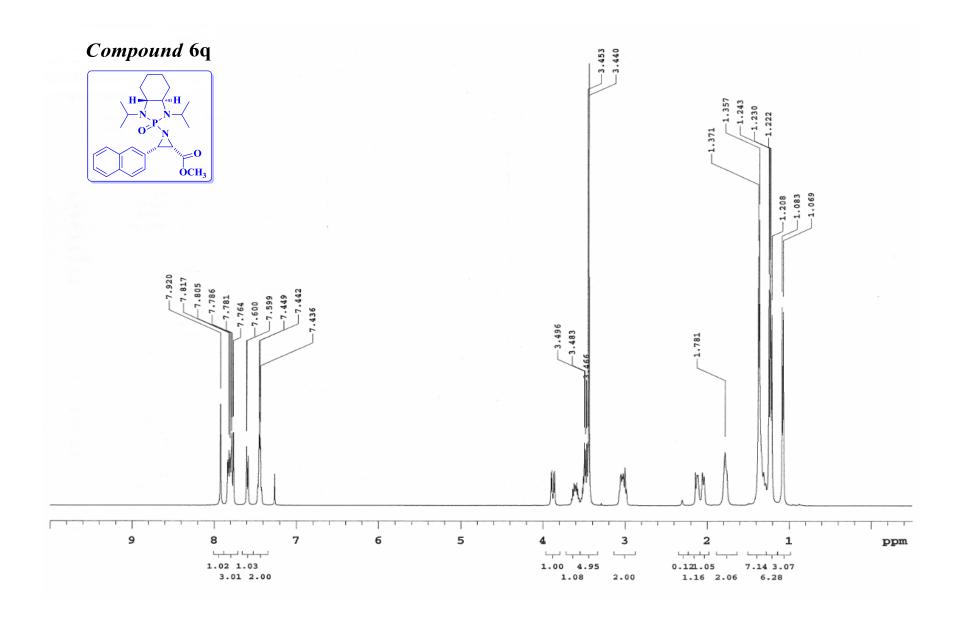


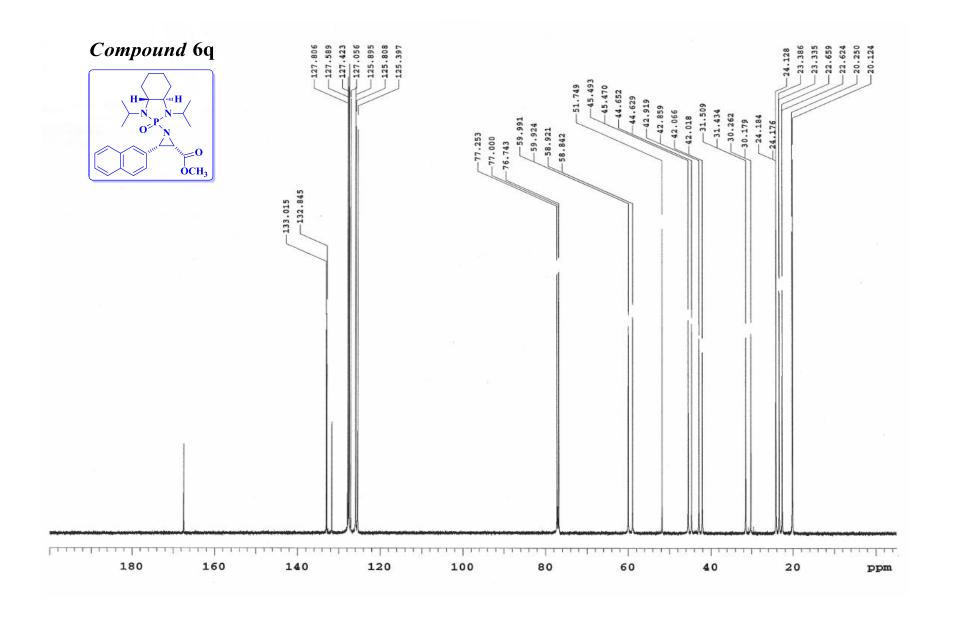


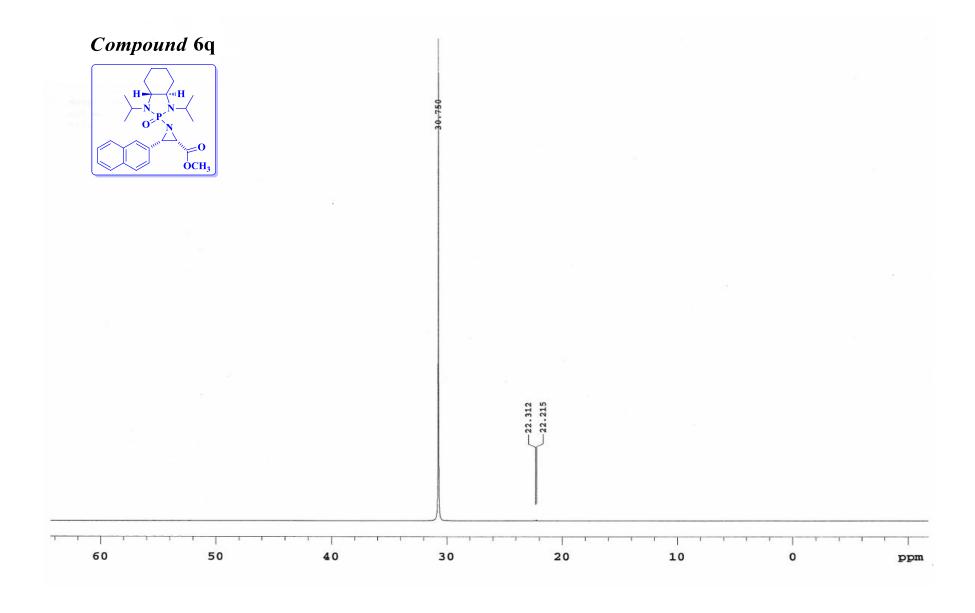


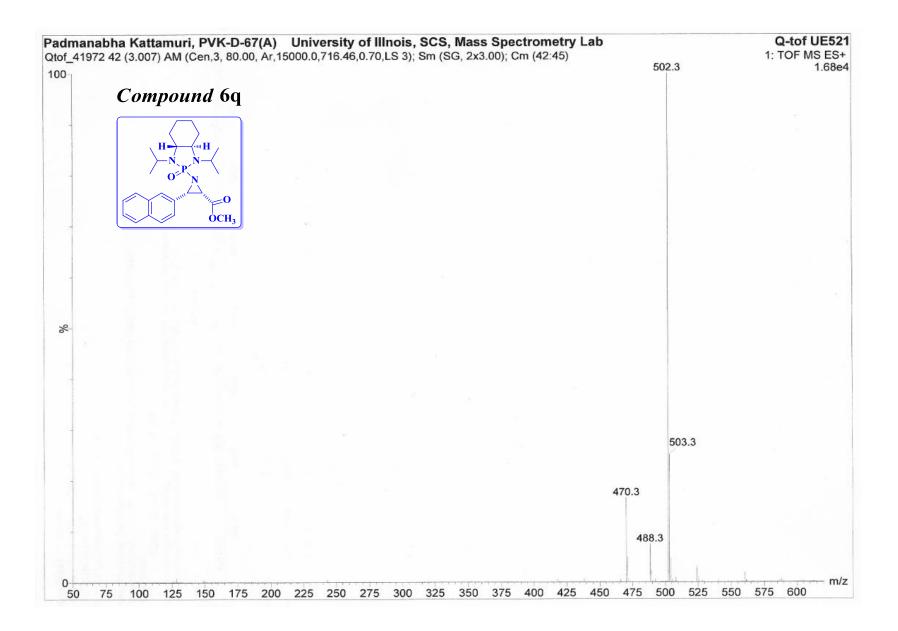
Elemental	Compositi	on Re	port									Page 1
Tolerance = Element pre		/ DB8		.5, max = 6	00.0							
103 formula(e Elements Use C: 0-150 H Padmanabha H Qtof_41968 54	: Mass, Even E e) evaluated w ed: H: 0-250 N: Kattamuri, PVK- I (3.864) AM (Ce	ith 1 re 2-4 D-53(B)	sults within O: 2-4 F	7: 0-1 Univers	sity of Illnois, S	SCS, Mass Spe	15 12				1: TO	-tof UE521 F MS ES+ 4.97e+002
100 % 456.246	9 458,2278 4	58.9178	462.3057	463.4429 46	4.2430 465.8	536 468,2393	0.00	471.2594 47	2.2650	476.2681	477.7593	478.8593
456.0	458.0	460.0	462.0	464.0	466.0	468.0	470.0		474.0	476.0	478.0	⊬∏ m/z
Minimum: Maximum:			5.0	10.0	-1.5 600.0							
Mass	Calc. Mas	S	mDa	PPM	DBE	i-FIT	For	mula				



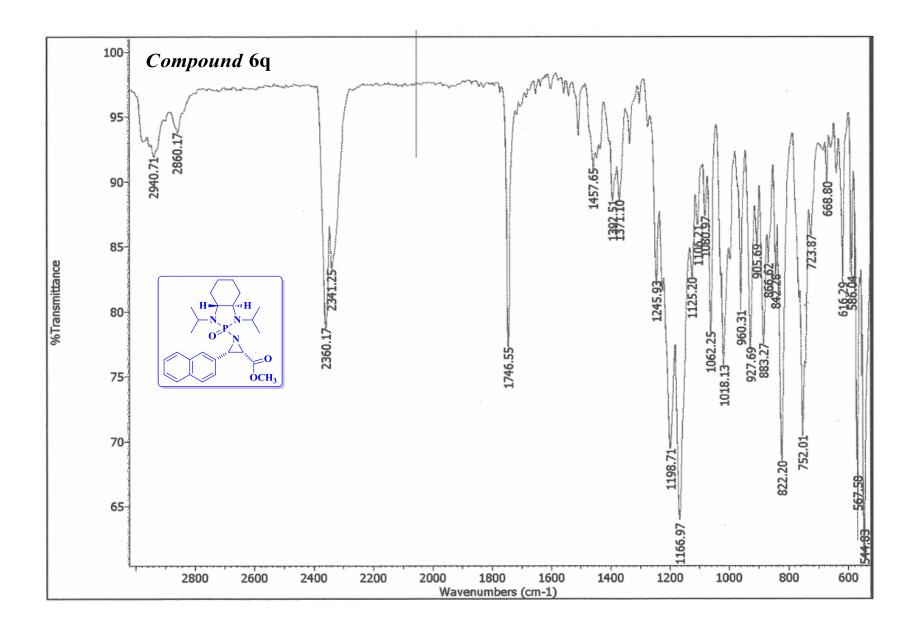


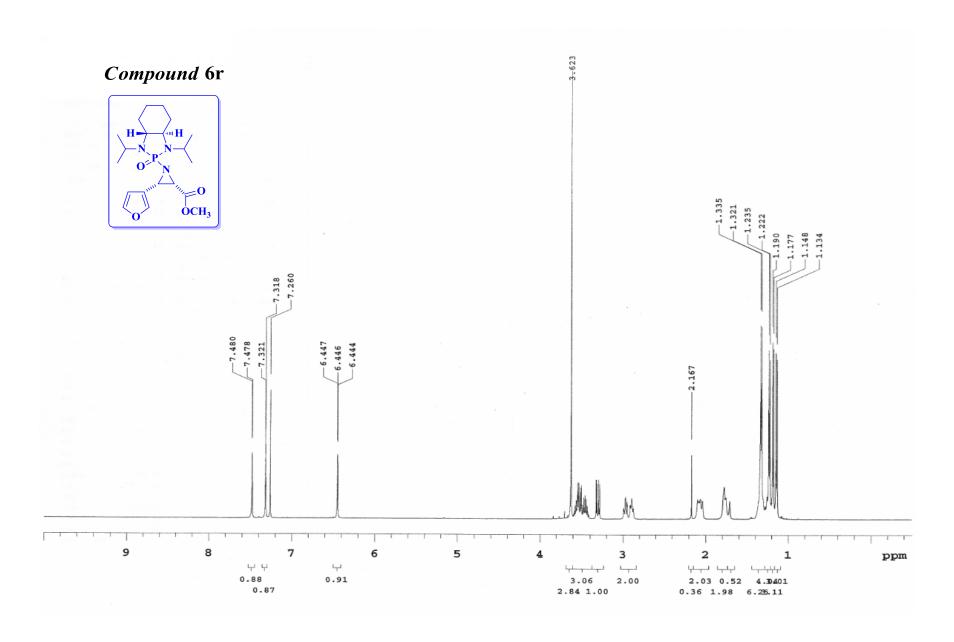


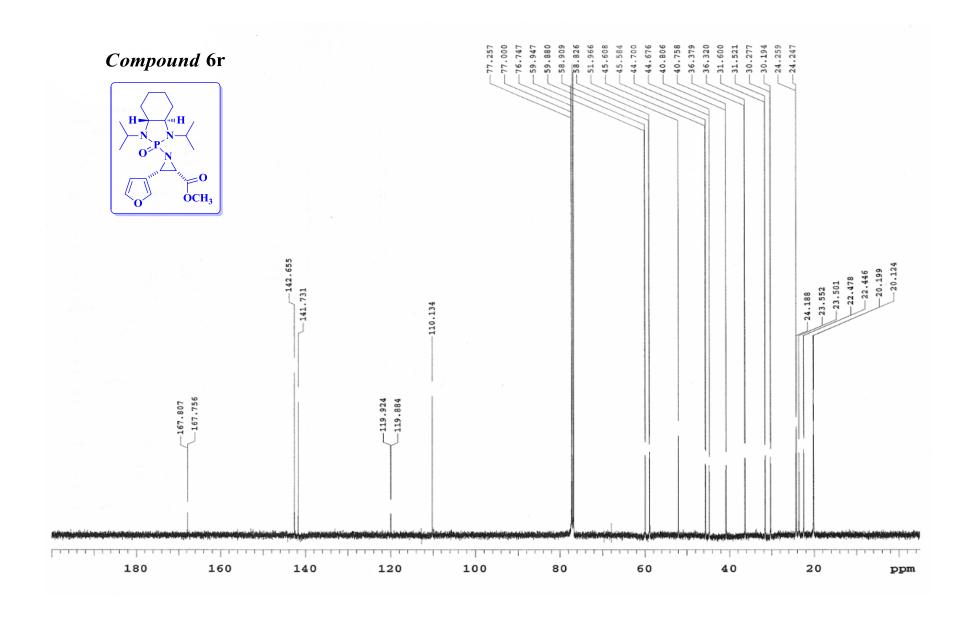


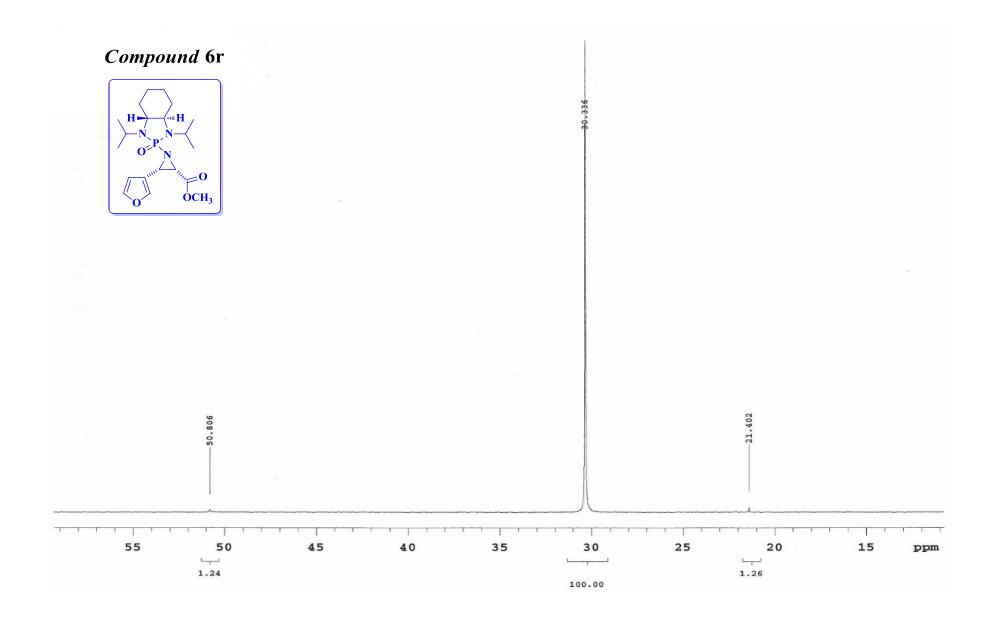


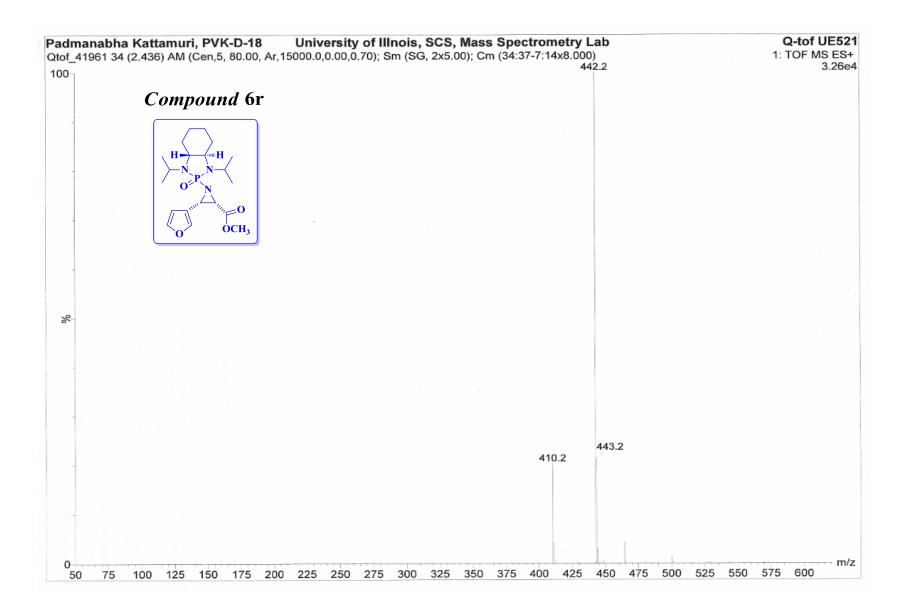
Elemental Composition Report Page 1 Single Mass Analysis Tolerance = 10.0 PPM / DBE: min = -1.5, max = 600.0 Element prediction: Off Number of isotope peaks used for i-FIT = 3 Monoisotopic Mass, Even Electron Ions 103 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each 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 Illnois, 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+003 470.2565 100 %-471.2595 472.2654 473.2691 474.2636 475.2575 476.2600 477.2681 465.2532466.2288467.2327468.2250 469.3543 0-466.0 468.0 474.0 470.0 472.0 476.0 464.0 Minimum: -1.55.0 10.0 600.0 Maximum: Mass Calc. Mass mDa PPM DBE i-FIT Formula -0.8 C26 H37 N3 O3 P 470.2565 470.2573 -1.710.5 1.1

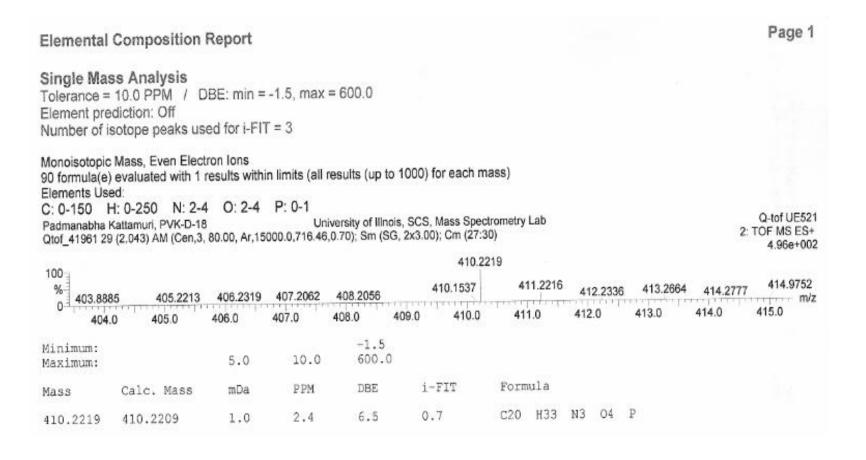


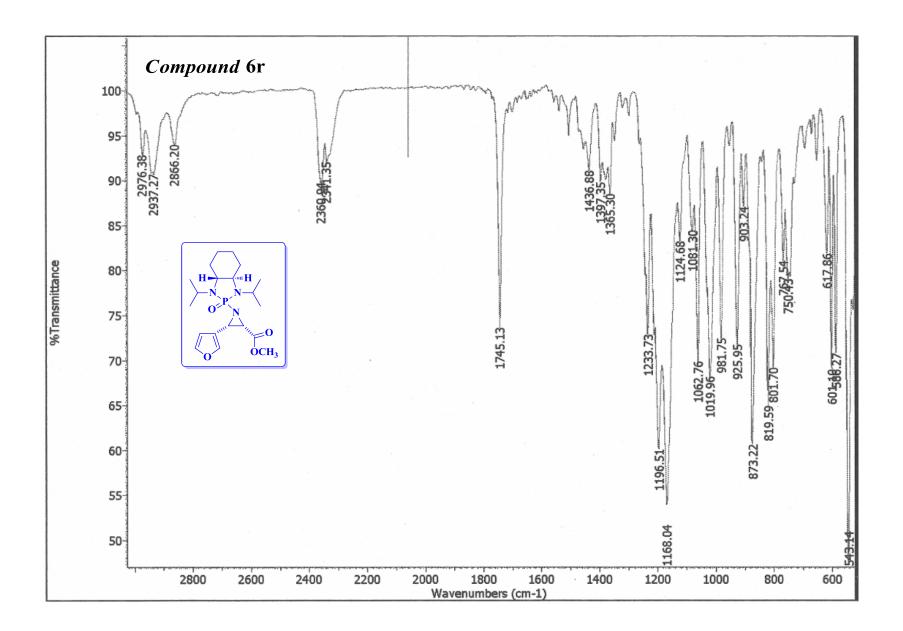


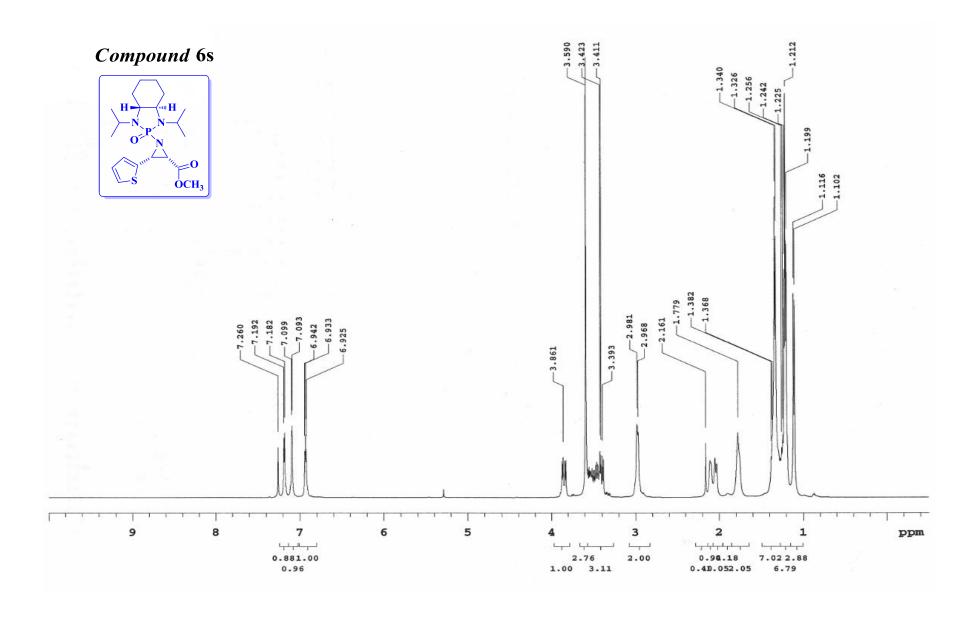


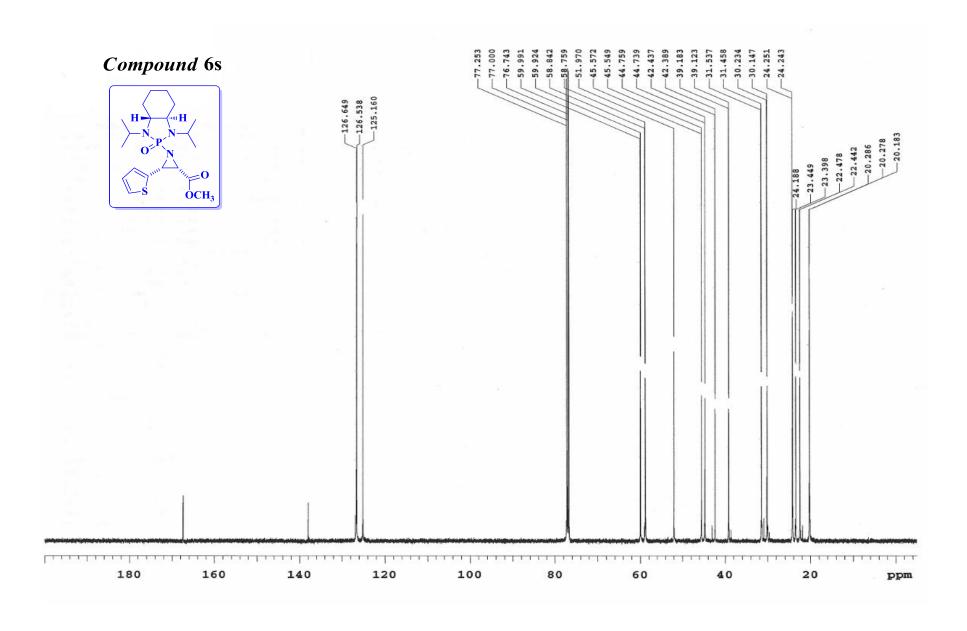


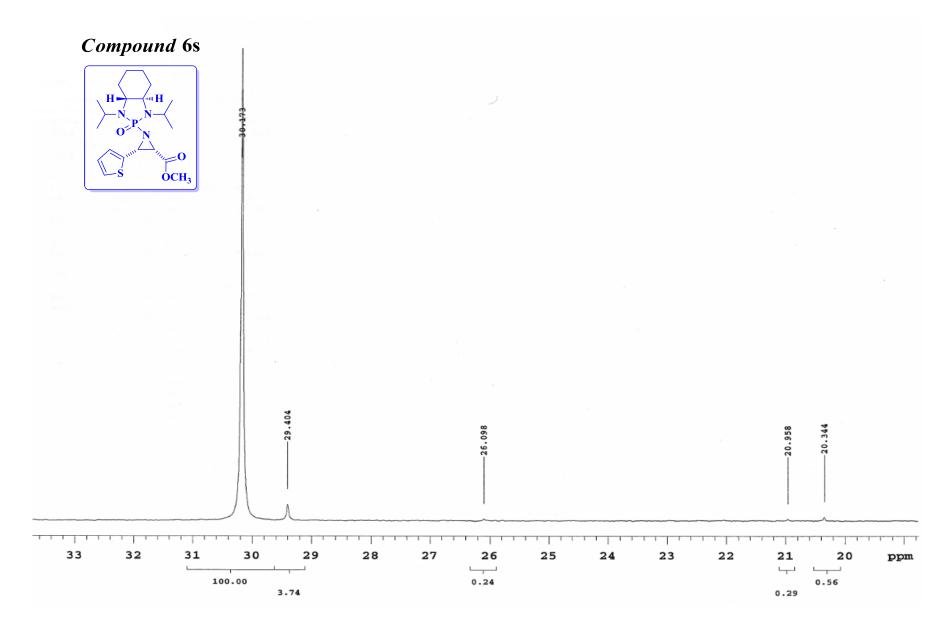


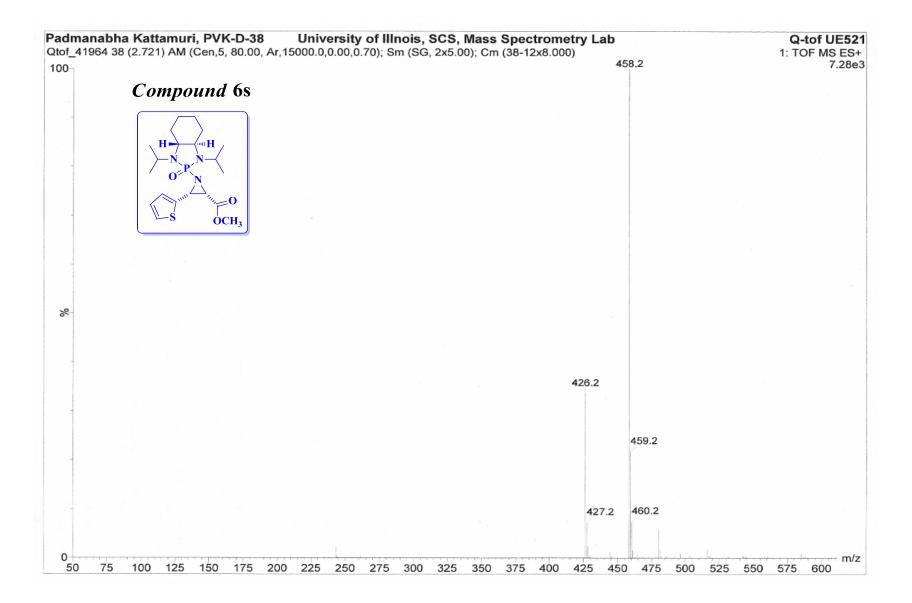






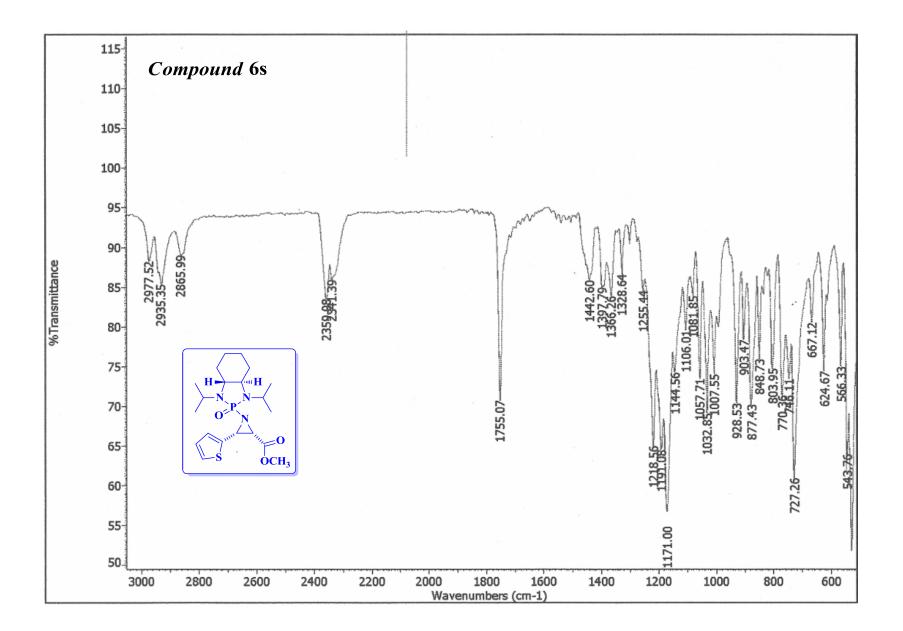


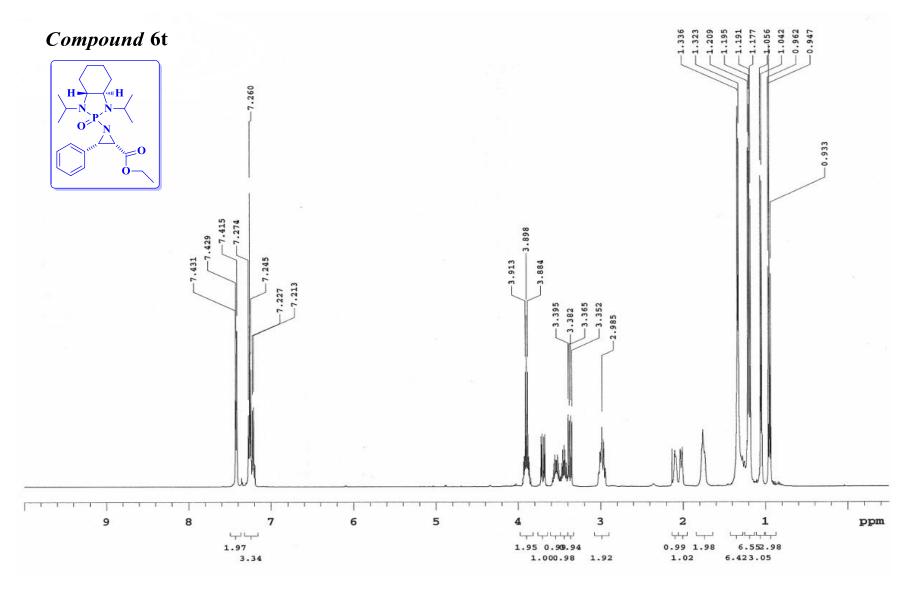


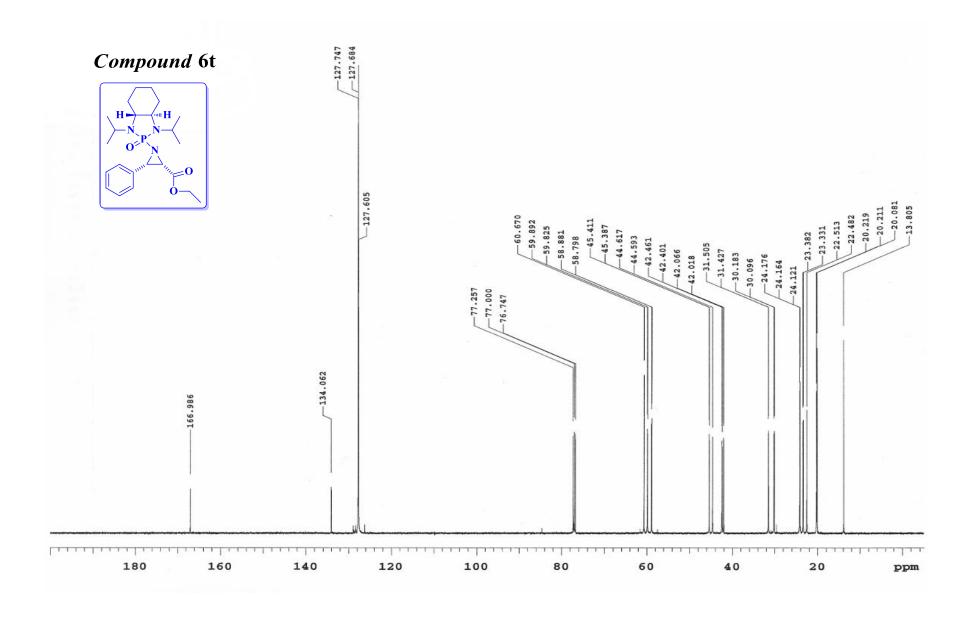


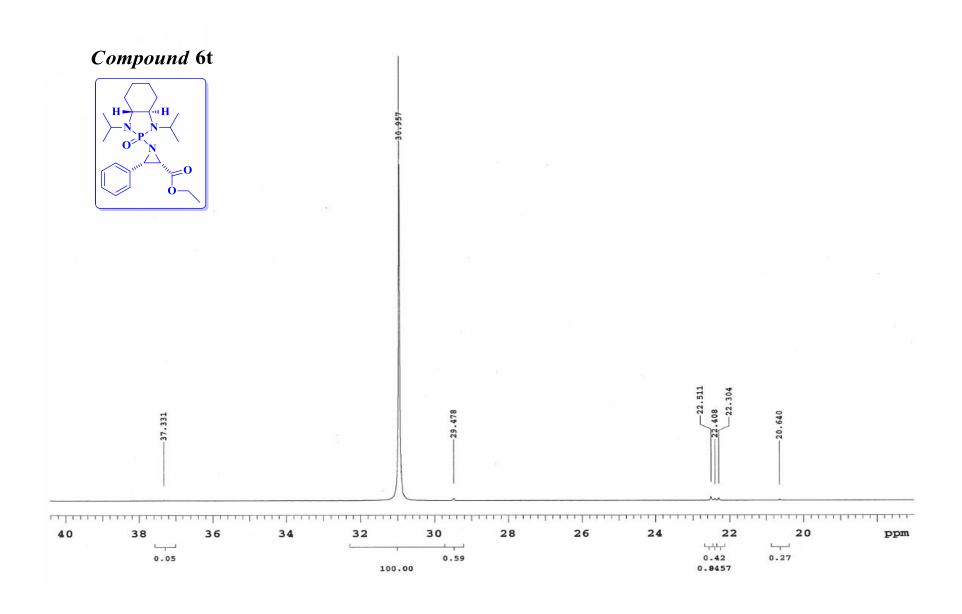
Elemental Composition Report	Page 1
Single Mass Analysis Tolerance = 10.0 PPM / DBE: min = -1.5, max = 600.0 Element prediction: Off Number of isotope peaks used for i-FIT = 3	
Monoisotopic Mass, Even Electron Ions 178 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass) Elements Used: C: 0-150 H: 0-250 N: 2-4 O: 2-4 P: 0-1 S: 0-1	0.4405604
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

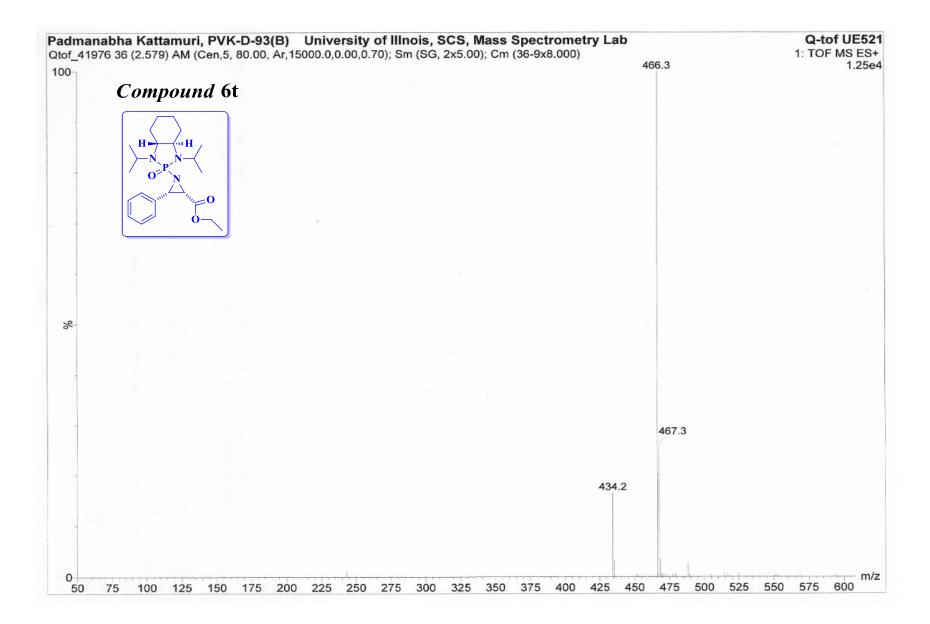
400		426.1974										
100 % 0 401.2	4	13.2707 4	16.0173 418	3.0095419.01454	427.2015 432.2048			101111000	436.2692	m/z		
400.0	405.0	410.0		415.0	420.0	425.0		430	.0	435.0		440.0
Minimum: Maximum:		5.0	10.0	-1.5 600.0								
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula						
426.1974	426.1980 426.1947	-0.6 2.7	-1.4 6.3	6.5 11.5	6.2 26.8	C20 H33		03 03	P P	S		











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

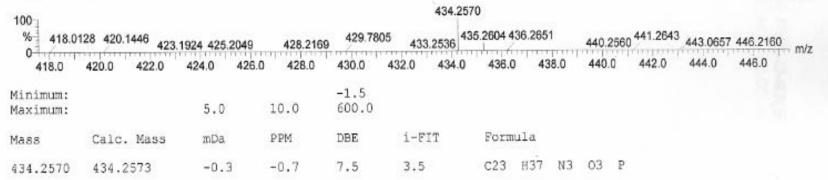
91 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

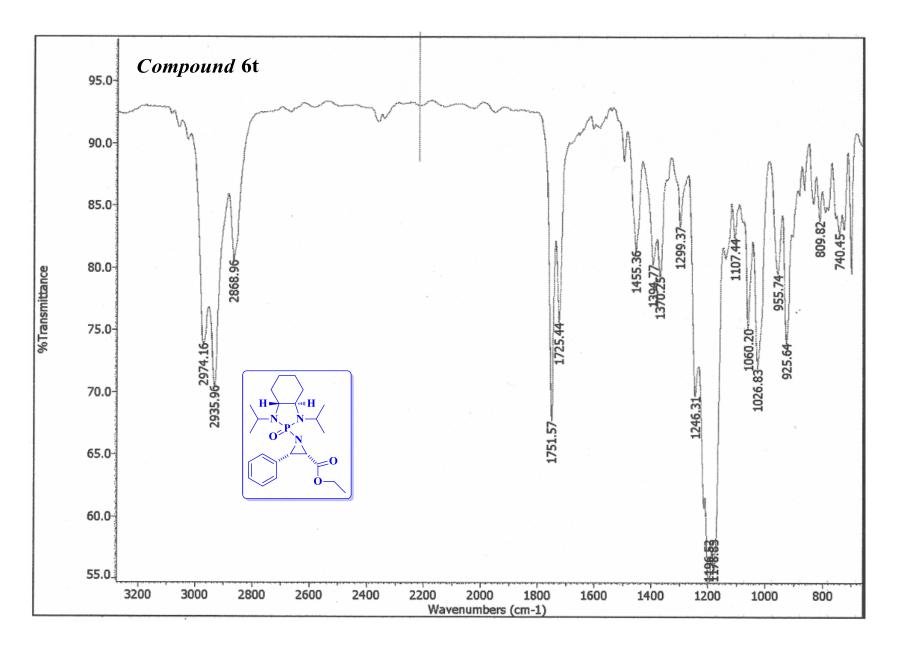
Elements Used:

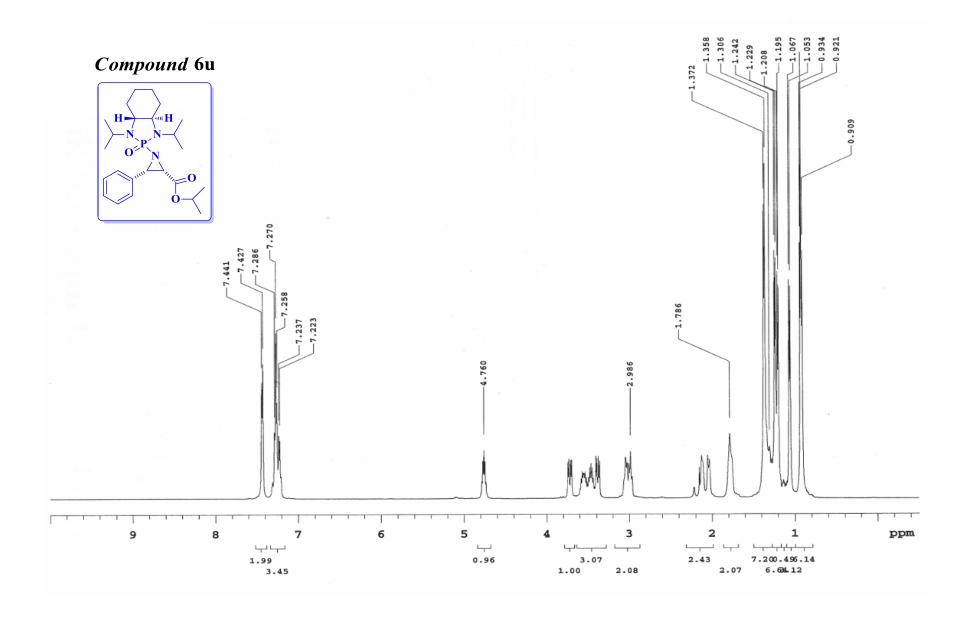
C: 0-150 H: 0-250 N: 2-4 O: 2-4 P: 0-1

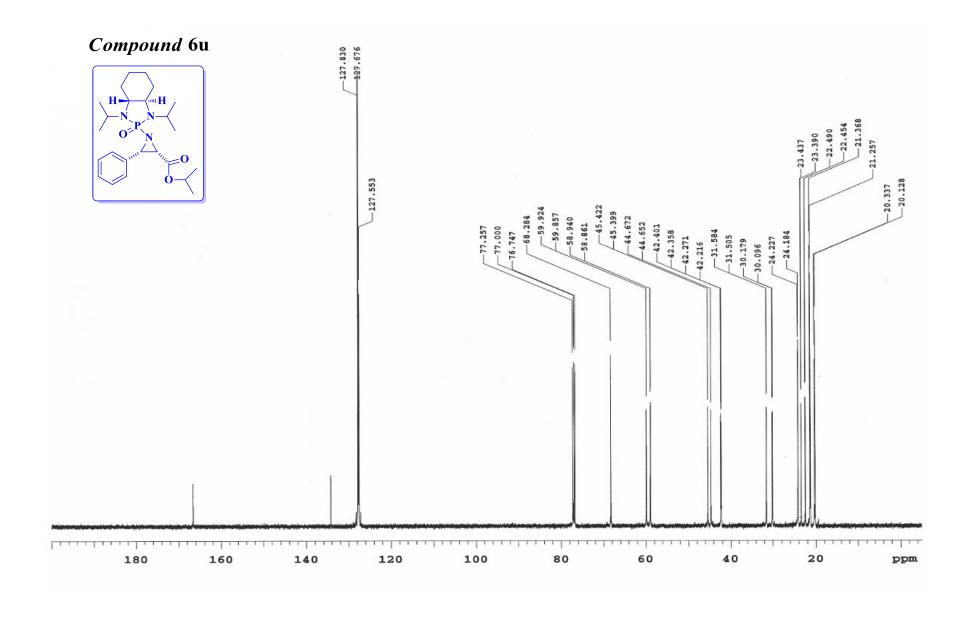
Padmanabha Kattamuri, PVK-D-93(B) University of Illnois, SCS, Mass Spectrometry Lab Qtof_41976 51 (3.650) AM (Cen.3, 80.00, Ar,15000.0,716.46,0.70,LS 3); Sm (SG, 2x3.00); Cm (51:52)

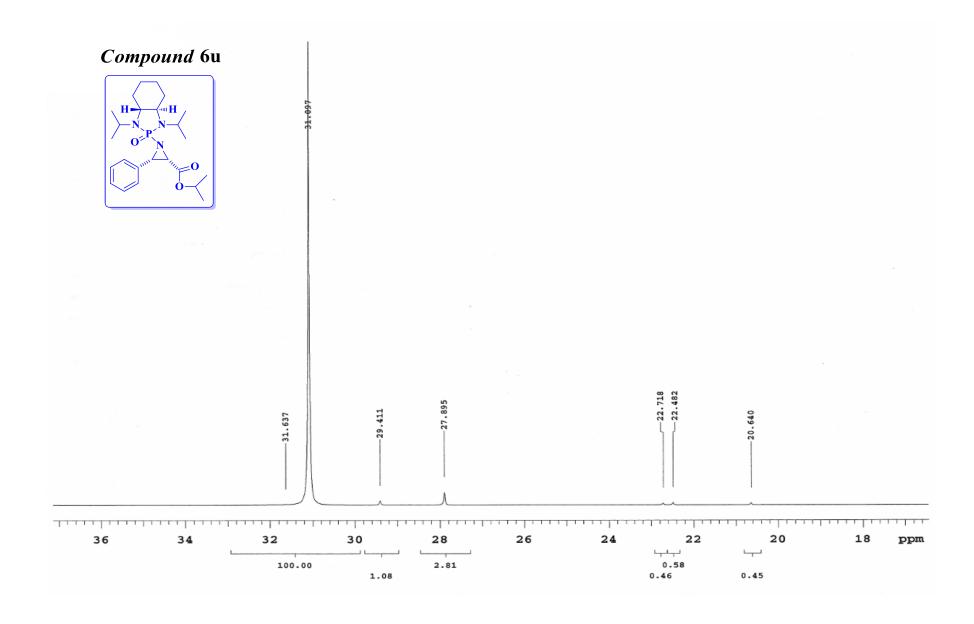
Q-tof UE521 1: TOF MS ES+ 1.89e+003

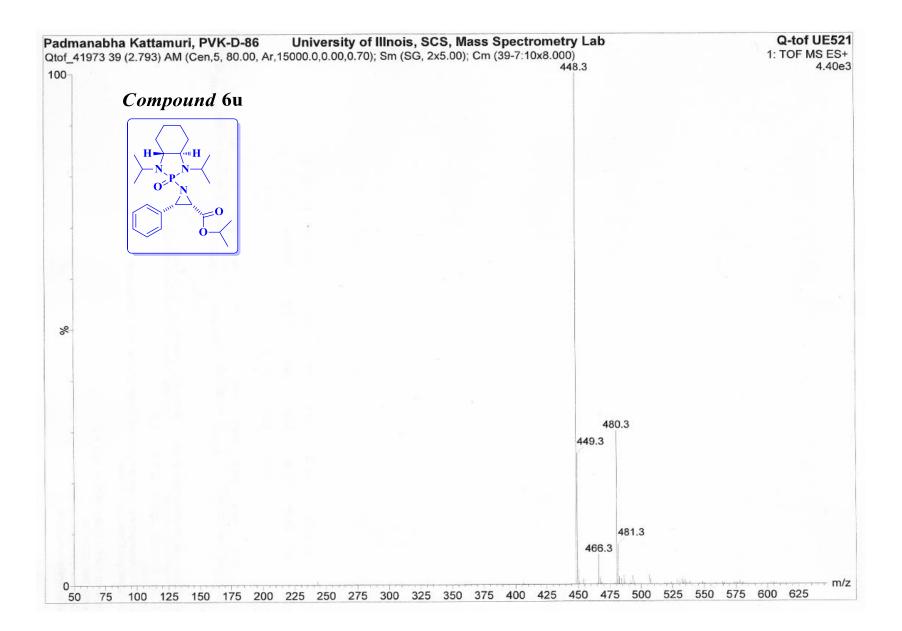


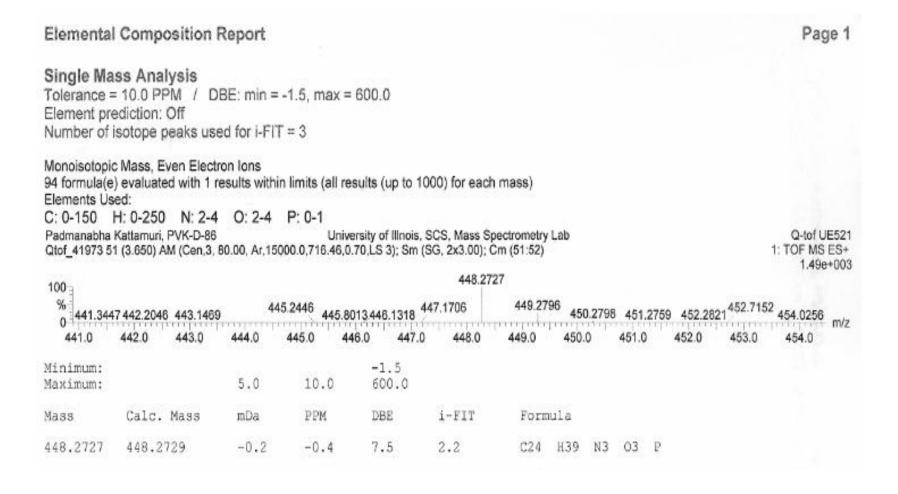


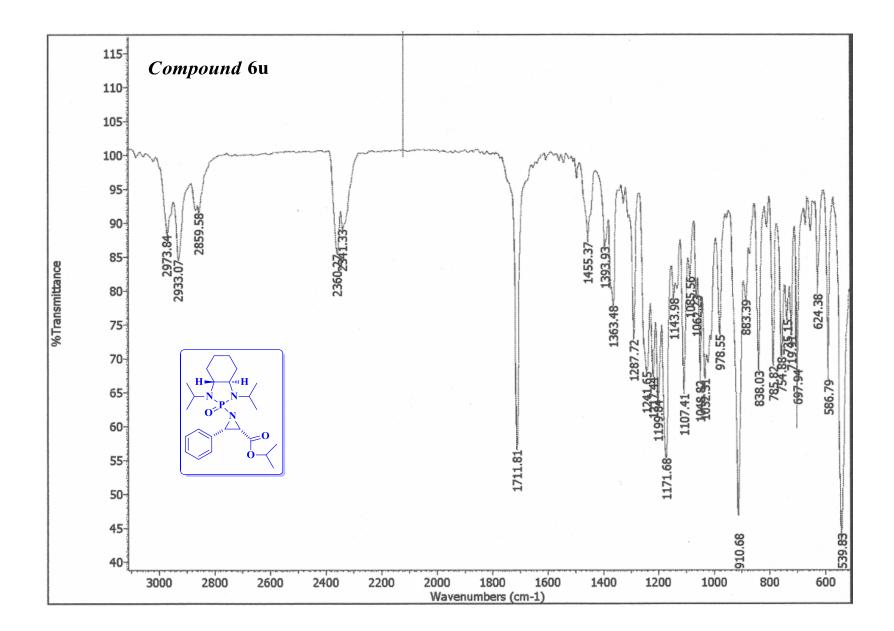


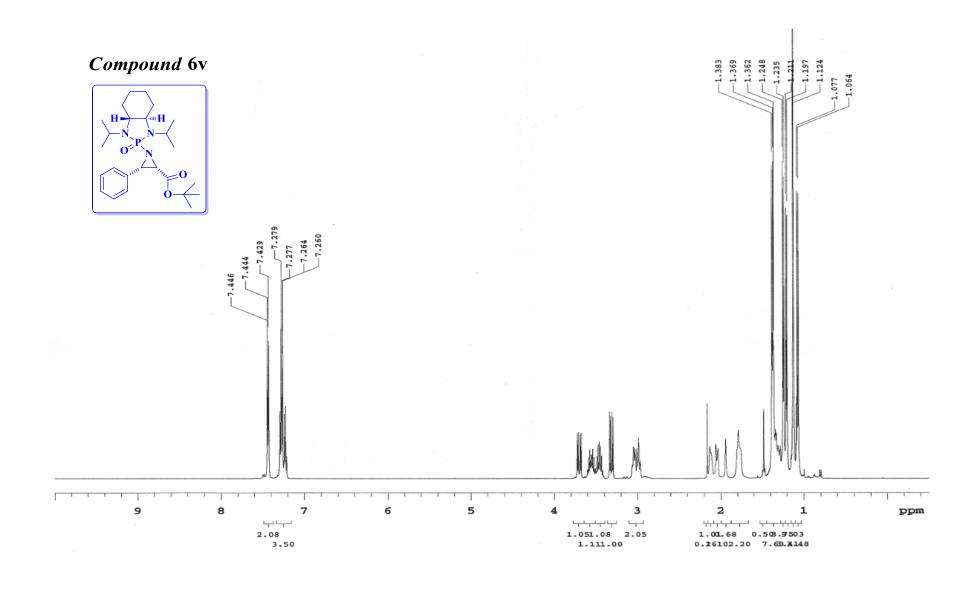


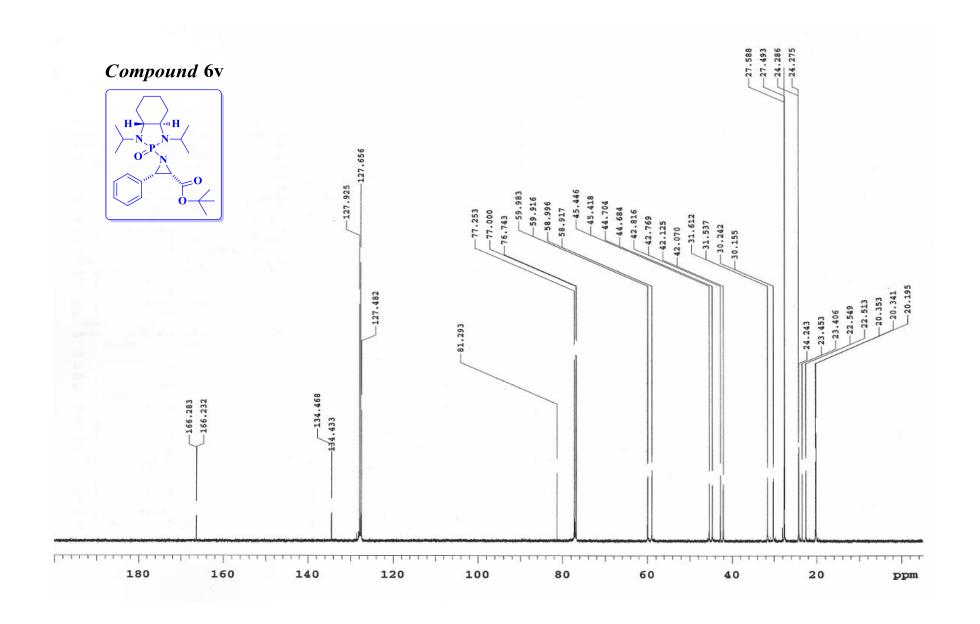


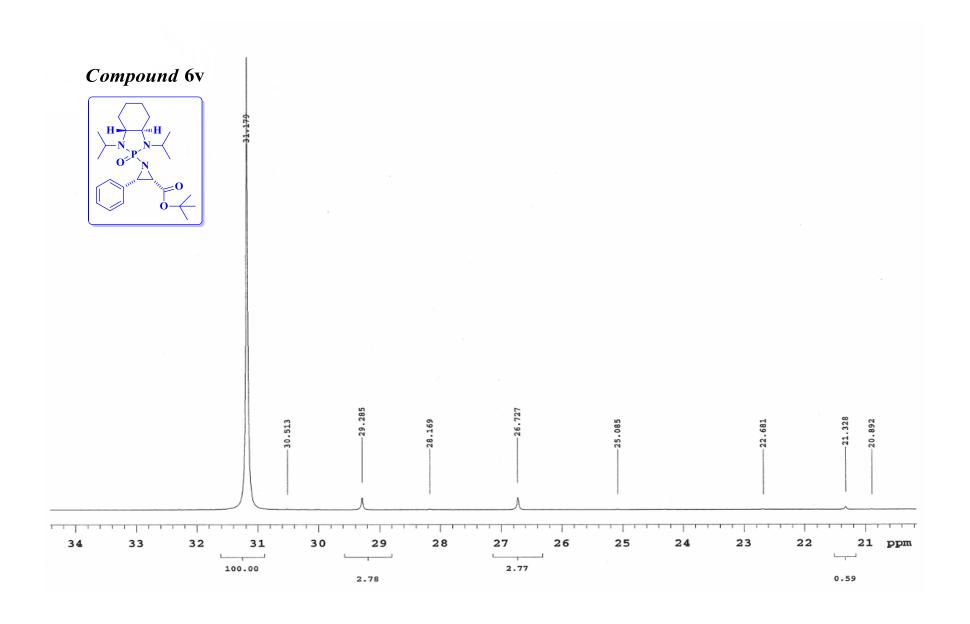


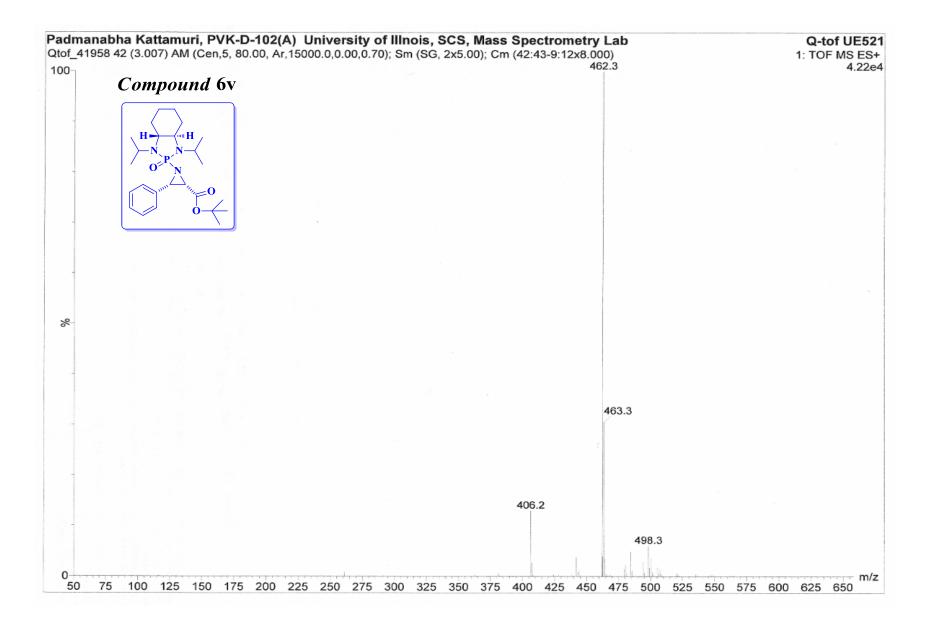












Page 1 **Elemental Composition Report** Single Mass Analysis Tolerance = 10.0 PPM / DBE: min = -1.5, max = 600.0 Element prediction: Off Number of isotope peaks used for i-FIT = 3 Monoisotopic Mass, Even Electron Ions 97 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass) Elements Used: C: 0-150 H: 0-250 N: 2-4 O: 2-4 P: 0-1 Q-tof UE521 Padmanabha Kattamuri, PVK-D-102(A) University of Illnois, SCS, Mass Spectrometry Lab 2: TOF MS ES+ Qtof_41958 39 (2.757) AM (Cen,3, 80.00, Ar,15000.0,716.46,0.70); Sm (SG, 2x3.00); Cm (39) 4.93e+002 462.2881 100 462.1599 463.2921 464.3008 447.0772 467.3126 469.4939 470.2680 473.1355 450.3868 451.1107 m/z 470.0 474.0 472.0 454.0 464.0 456.0 458.0 460.0 462.0 450.0 452.0 448.0 -1.5Minimum: 600.0 5.0 10.0 Maximum: PPM i-FIT Formula DBE mDa Calc. Mass Mass 0.5 H41 N3 O3 P -1.17.5 C25 -0.5462.2881 462.2886

