Electronic Supplementary Information

For

Palladium-Catalyzed Cascade Difluoroalkylation and Phosphinoylation of 2-Vinyloxy Arylalkynes: Selective Synthesis of Difluoroalkyl-Containing Tetrasubstituted Alkenylphosphine Oxides

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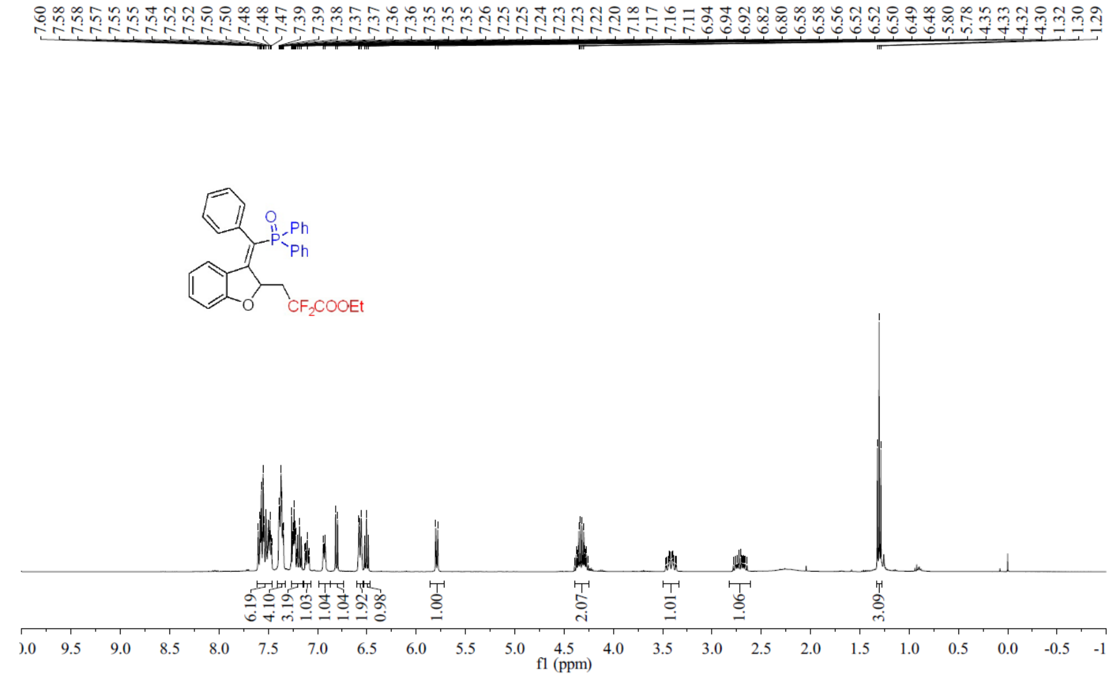
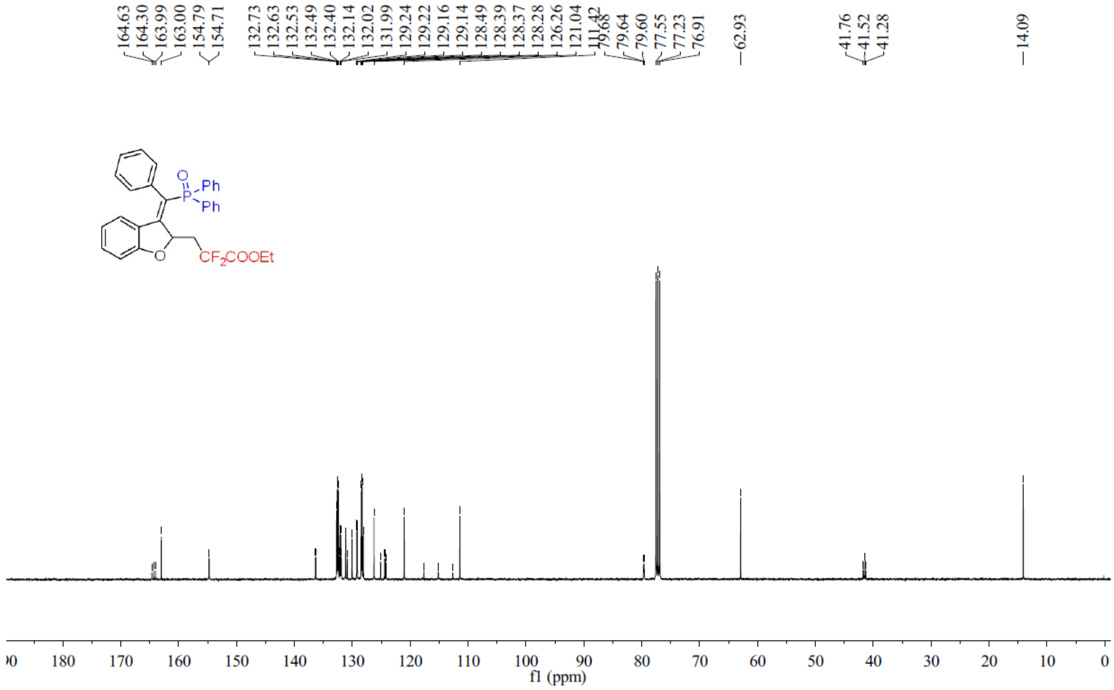
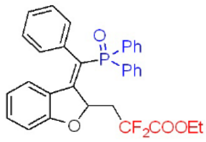
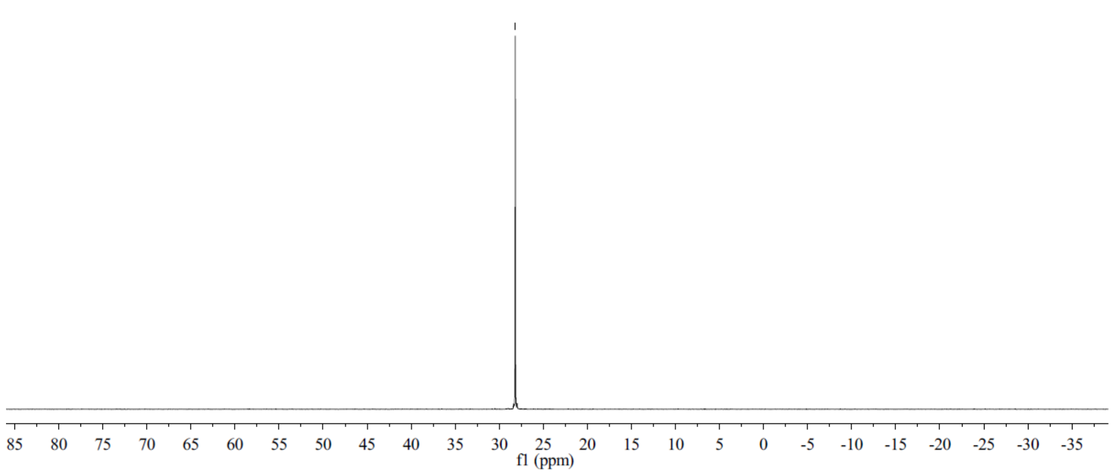


$^{13}C\{^{1}H\}$ NMR (100 MHz) Spectrum of **3a** in $CDCl_3$

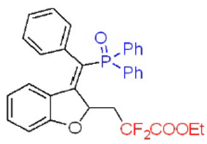


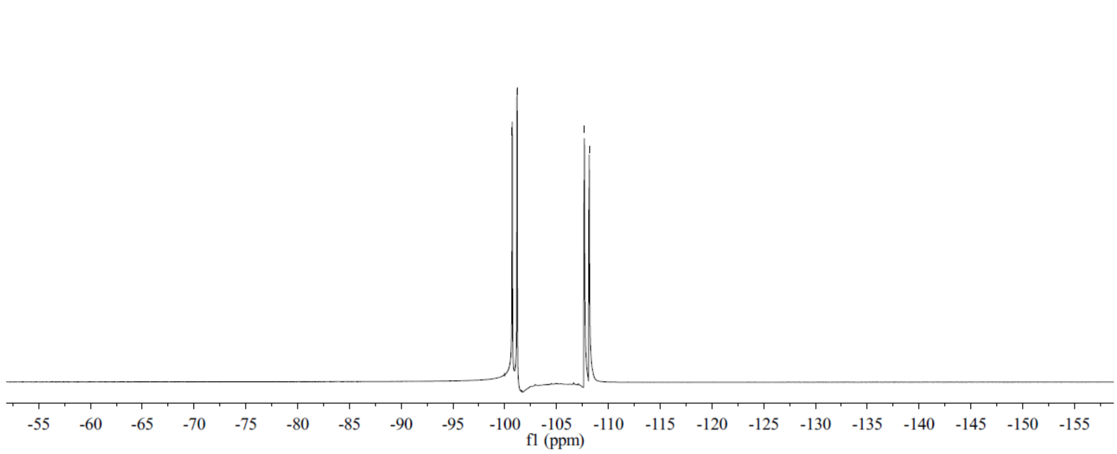
$^{31}P\{^1H\}$ NMR (243 MHz) Spectrum of **3a** in $CDCl_3$





$^{19}F\{^1H\}$ NMR (565 MHz) Spectrum of **3a** in $CDCl_3$





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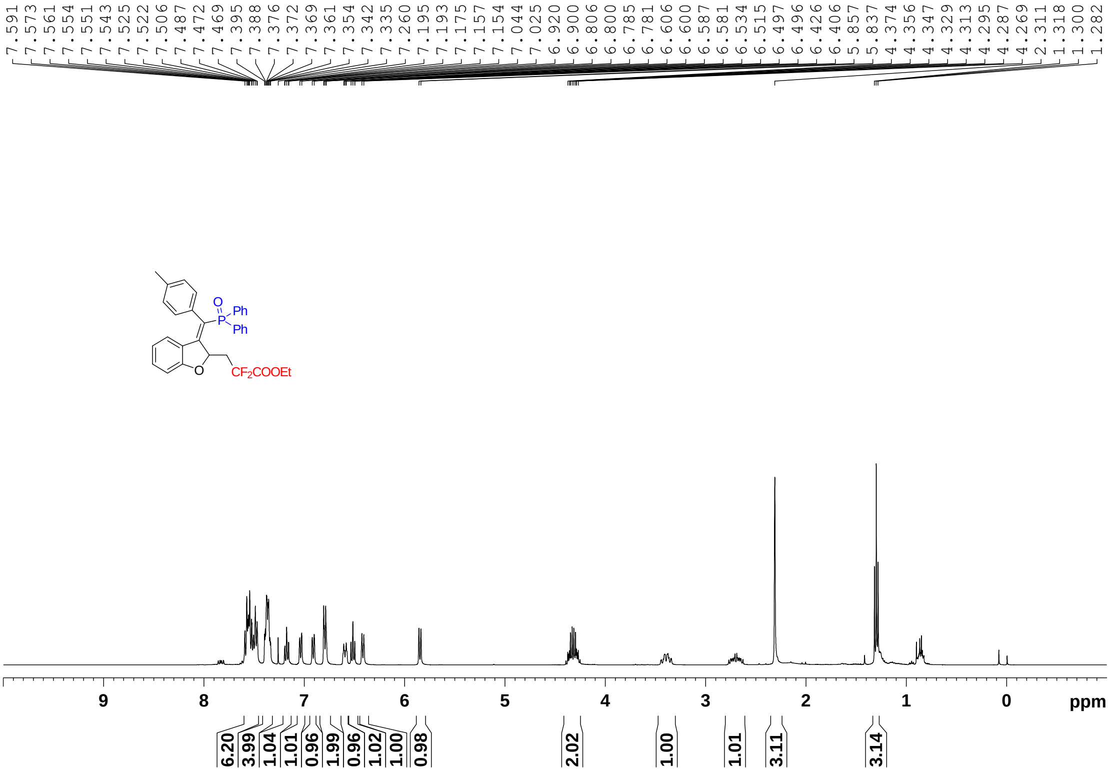

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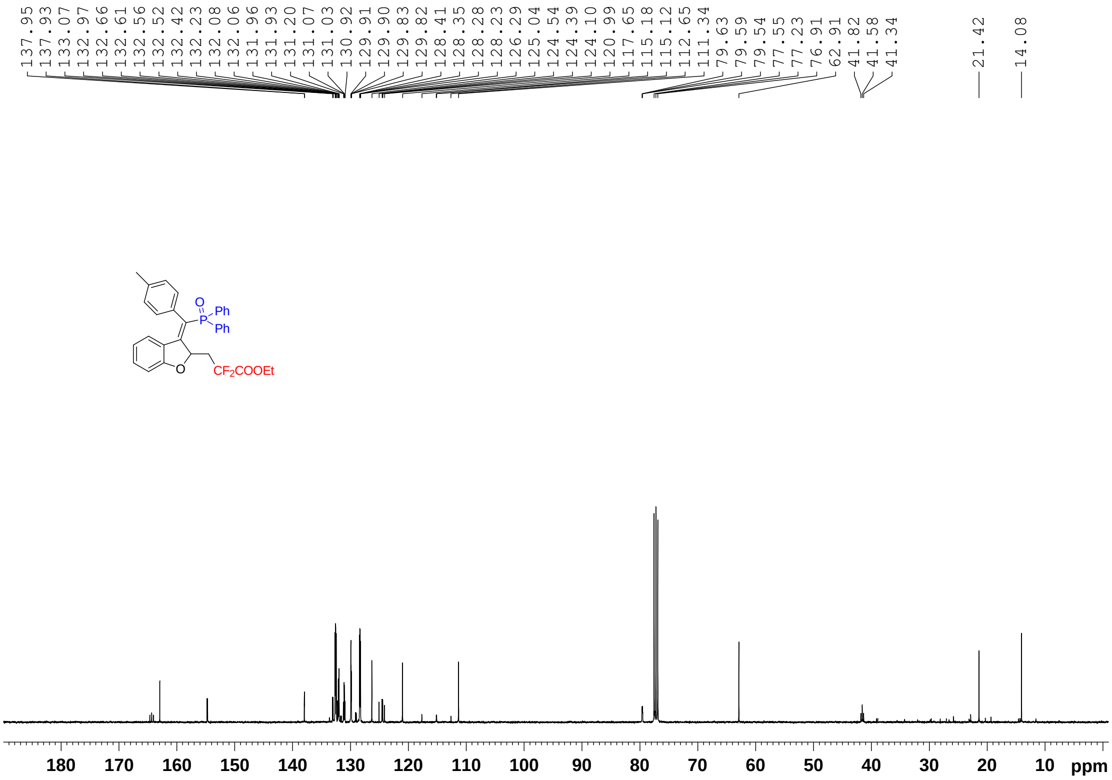
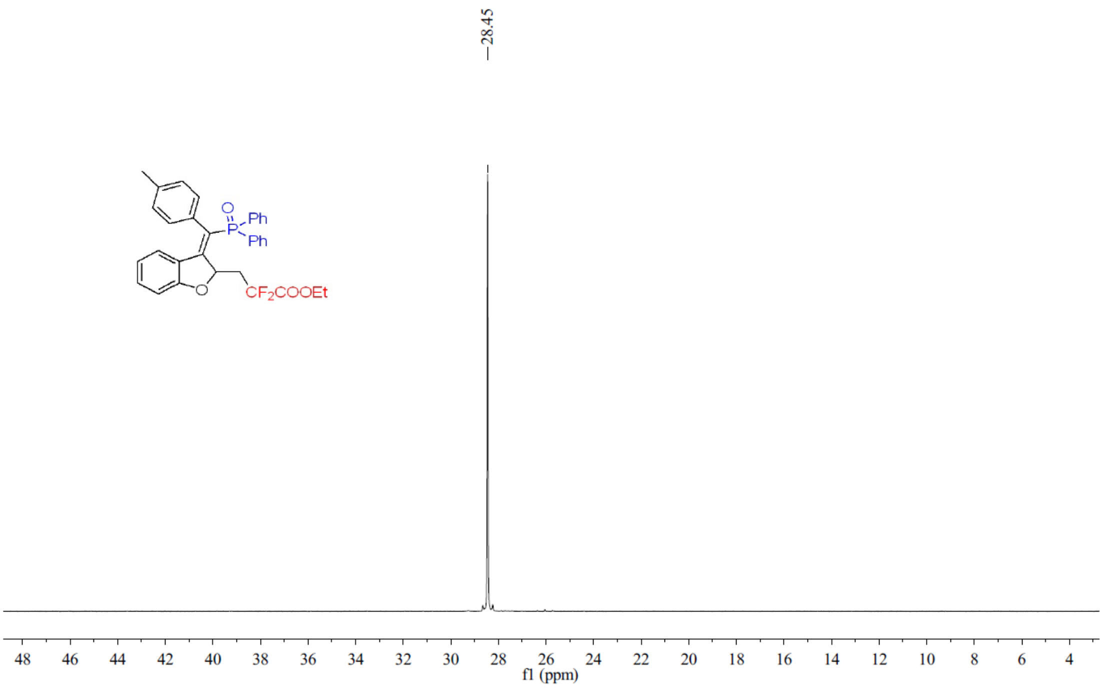


$^{31}P\{^1H\}$ NMR (243 MHz) Spectrum of **3b** in $CDCl_3$



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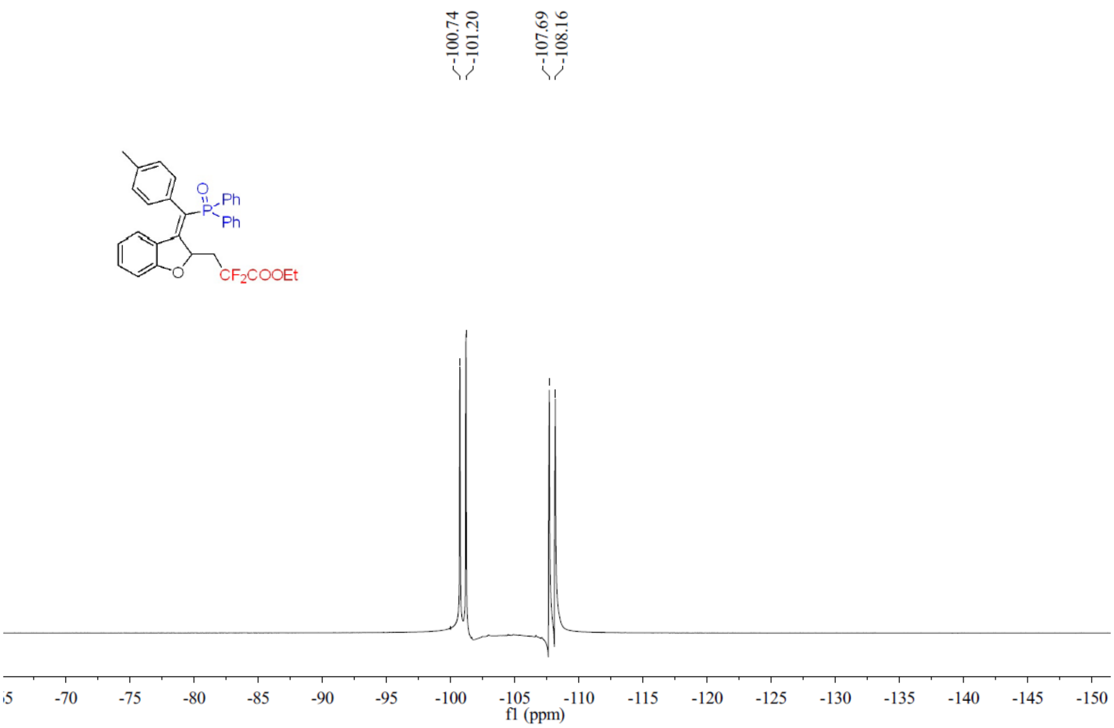

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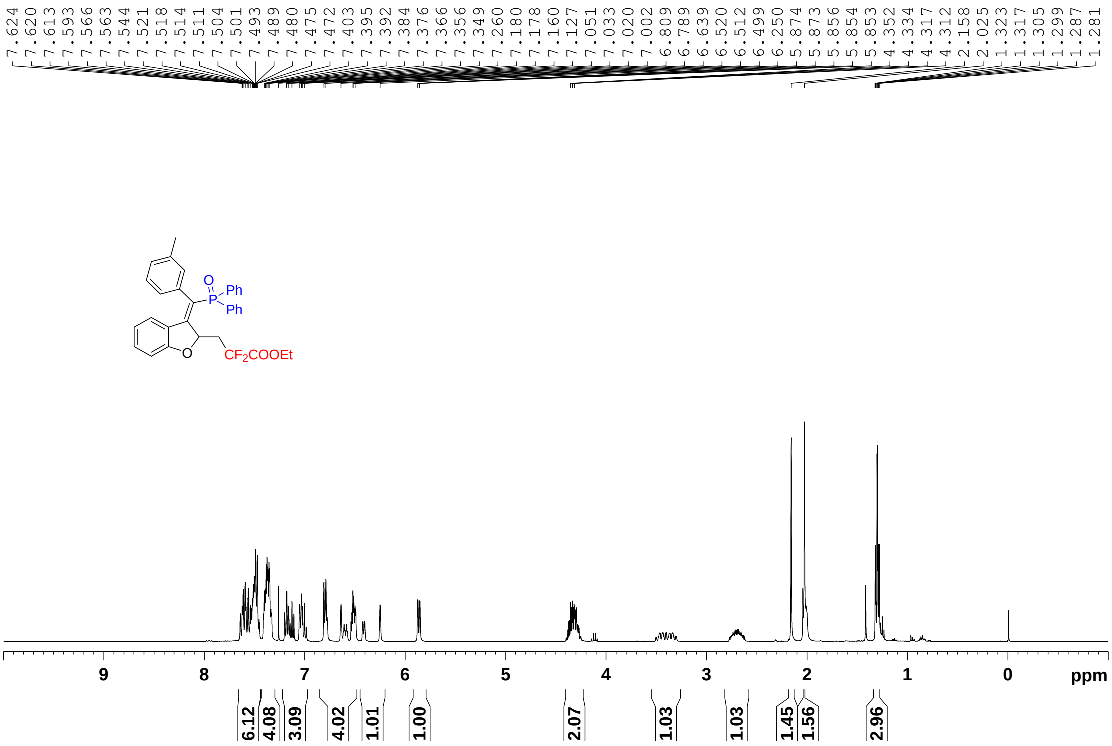
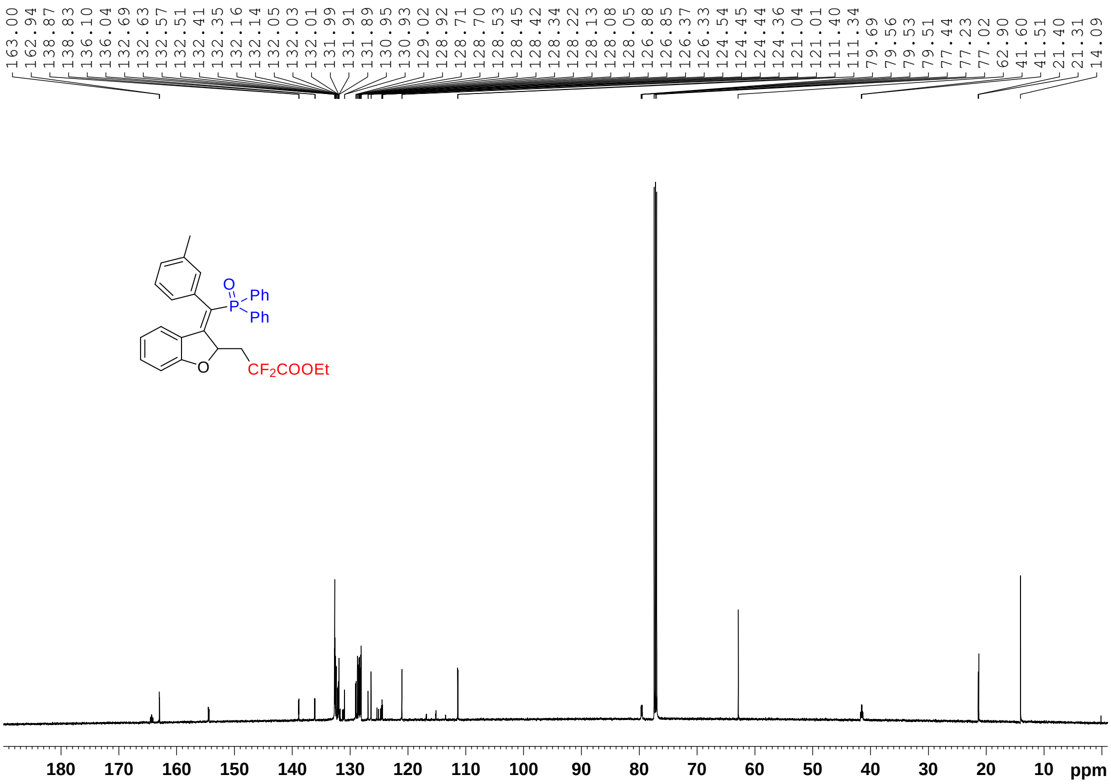


$^{13}C\{^{1}H\}$NMR (100 MHz) Spectrum of **3c** in $CDCl_3$



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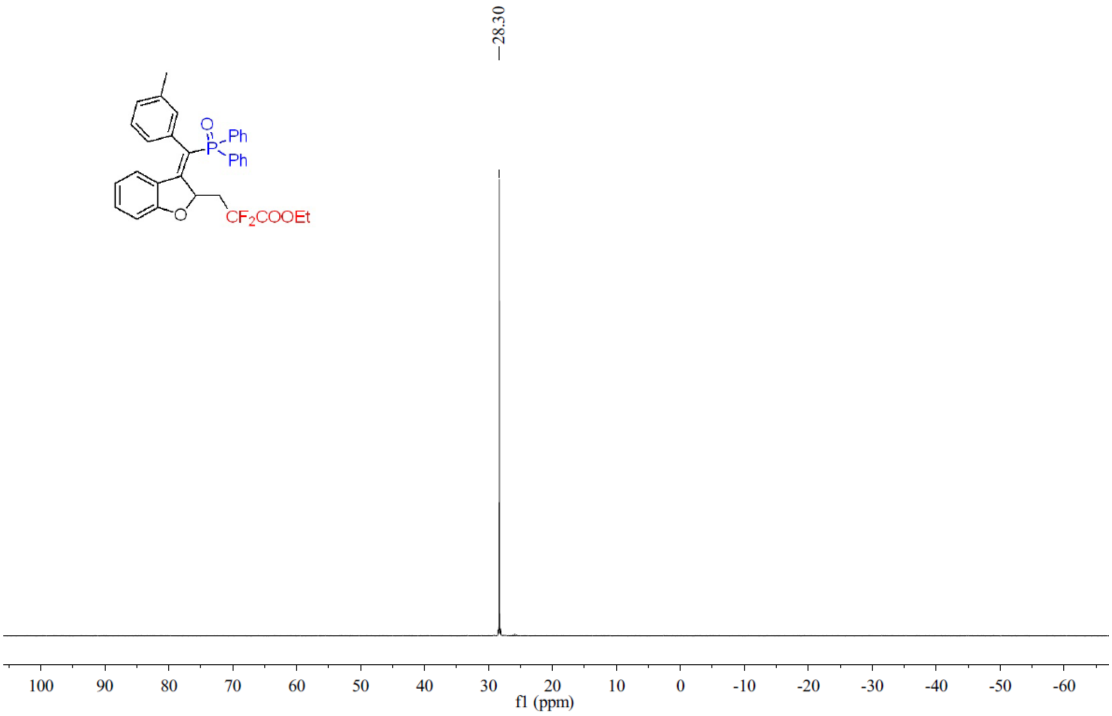
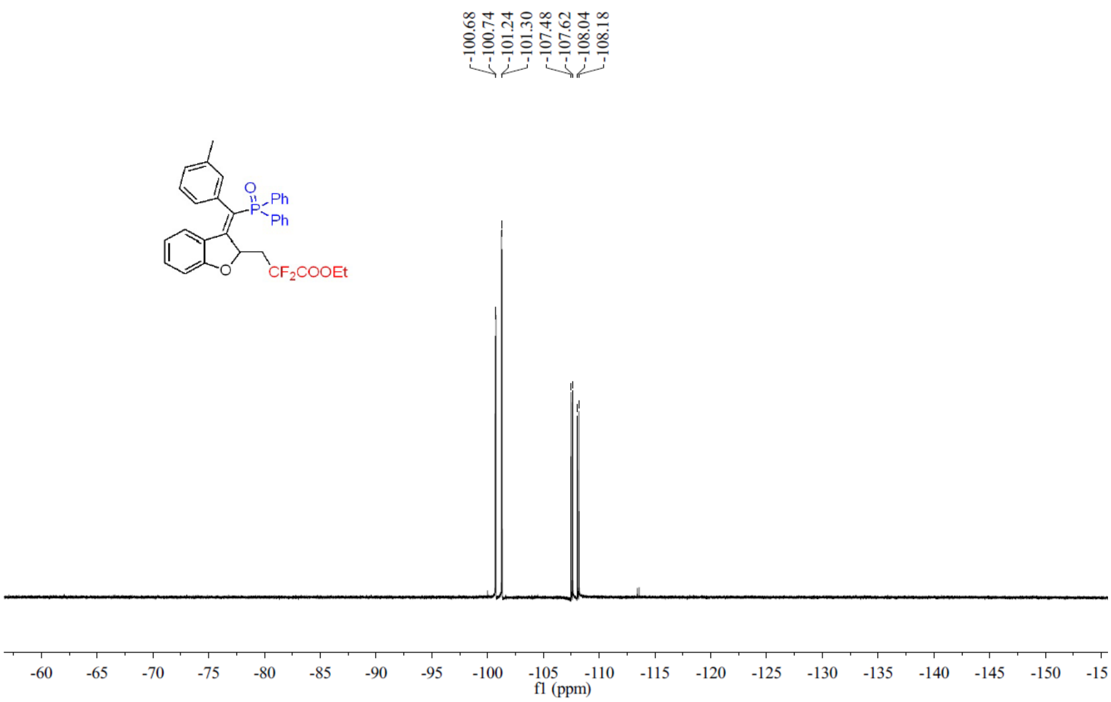


$^{19}F\{^{1}H\}$ NMR (471 MHz) Spectrum of **3c** in $CDCl_3$



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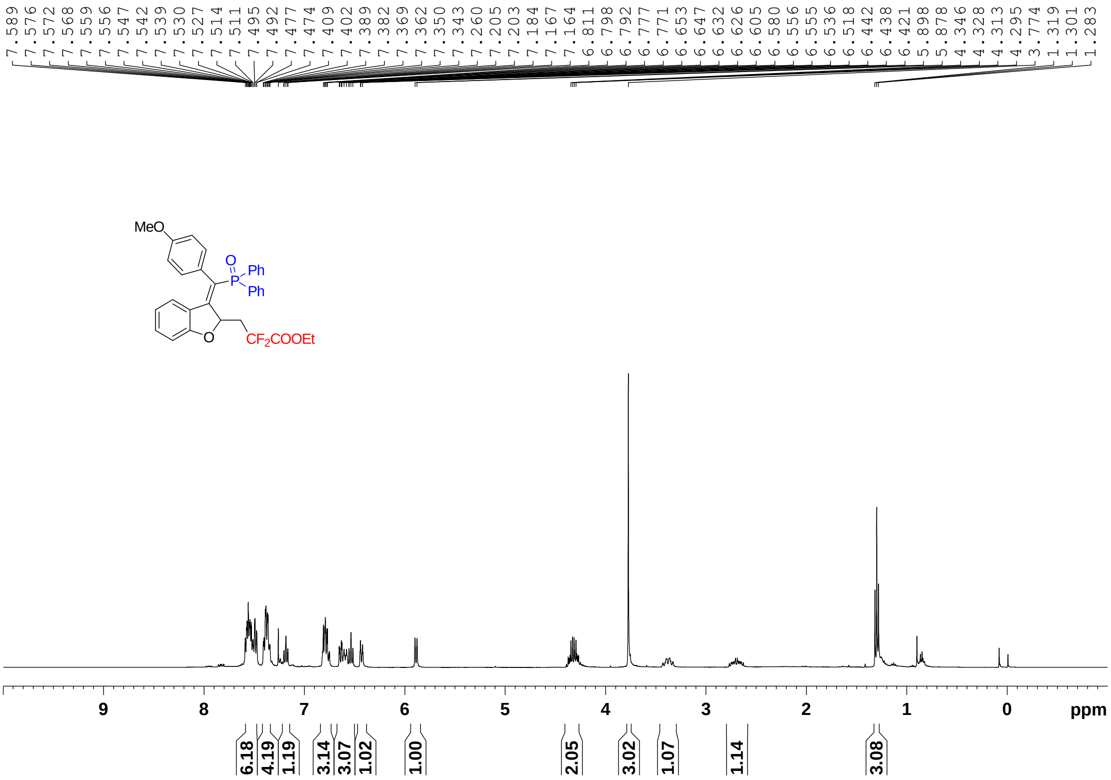
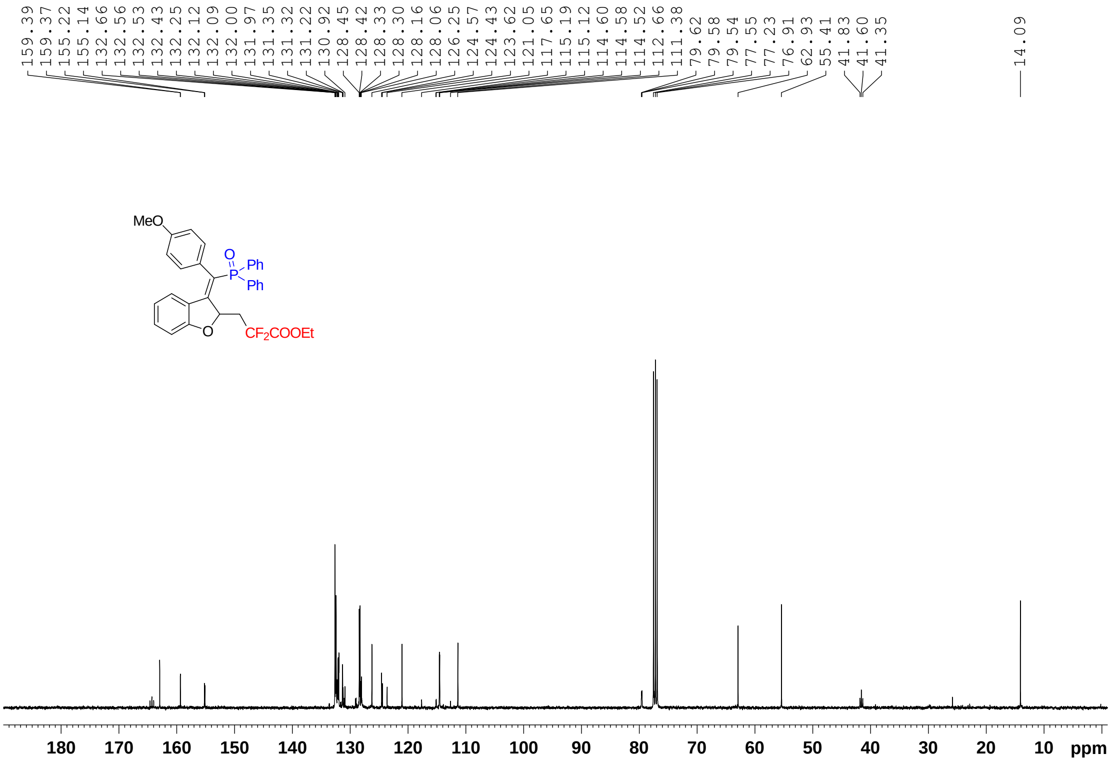
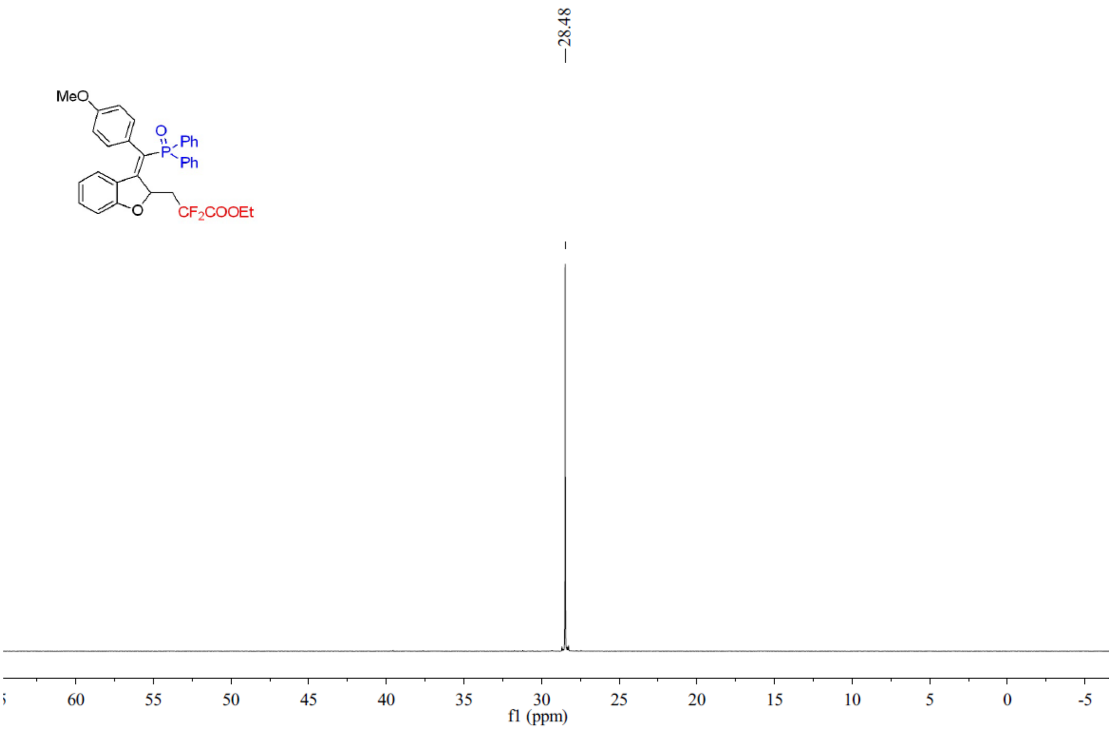


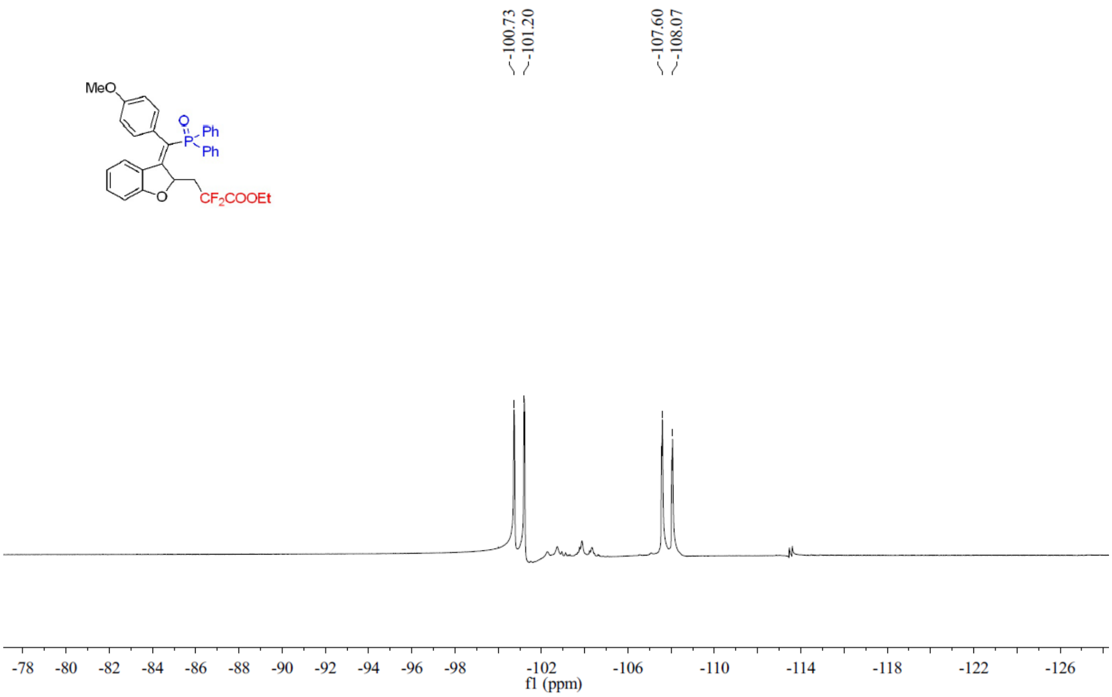
^{13}C{^{1}H}NMR (100 MHz) Spectrum of **3d** in $CDCl_3$



$^{31}P\{^{1}H\}$ NMR (243 MHz) Spectrum of **3d** in $CDCl_3$



$^{19}F\{^{1}H\}$ NMR (565 MHz) Spectrum of **3d** in $CDCl_3$



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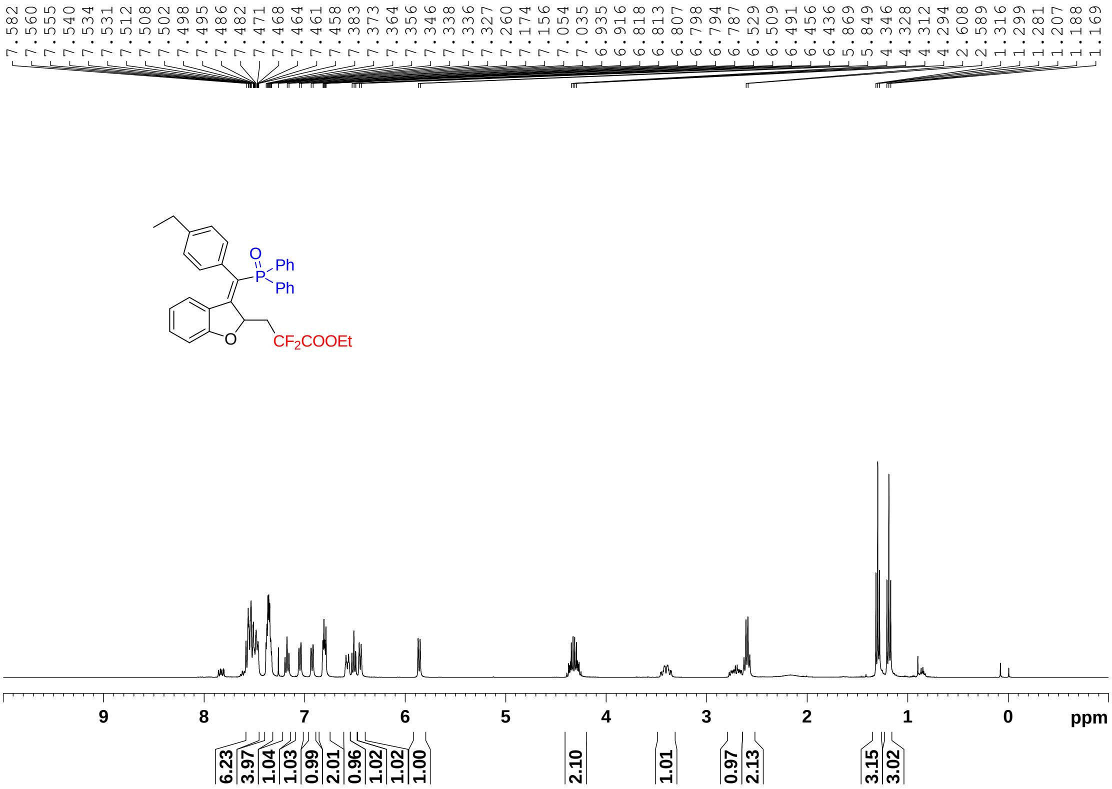

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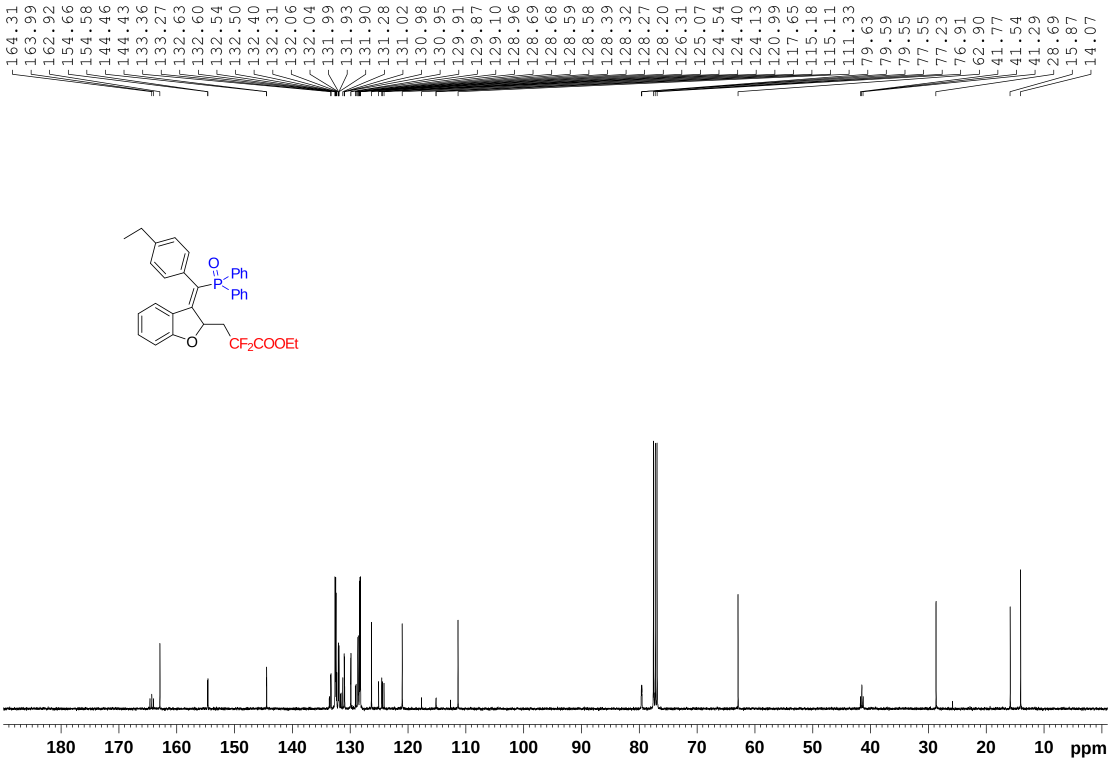

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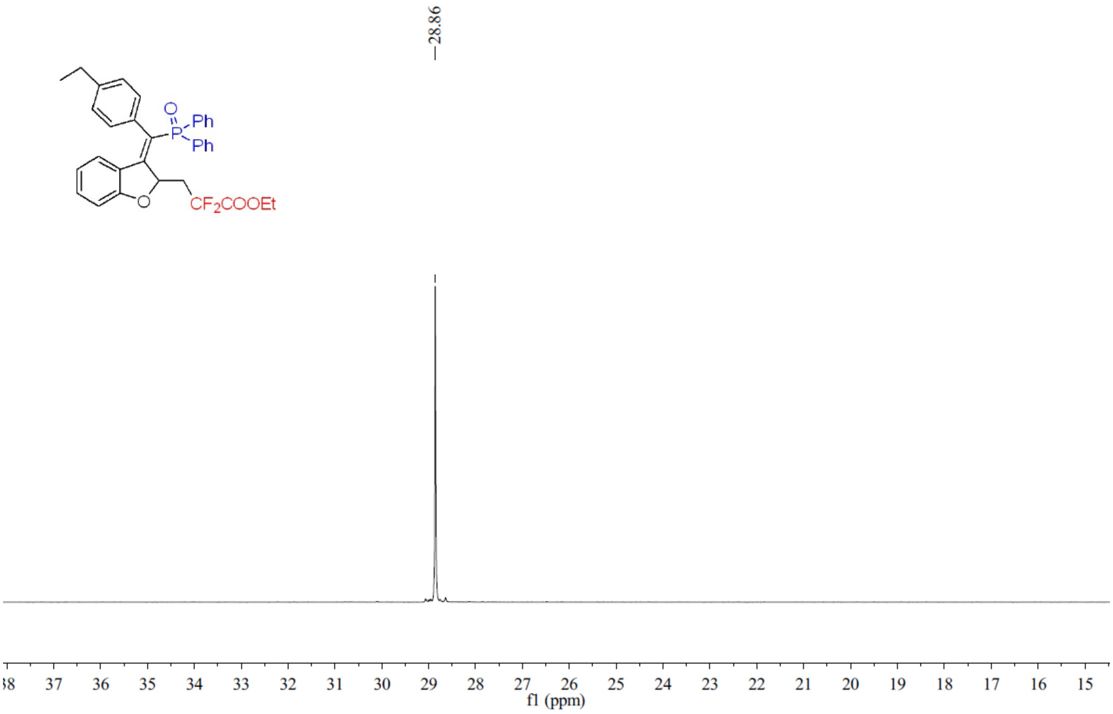
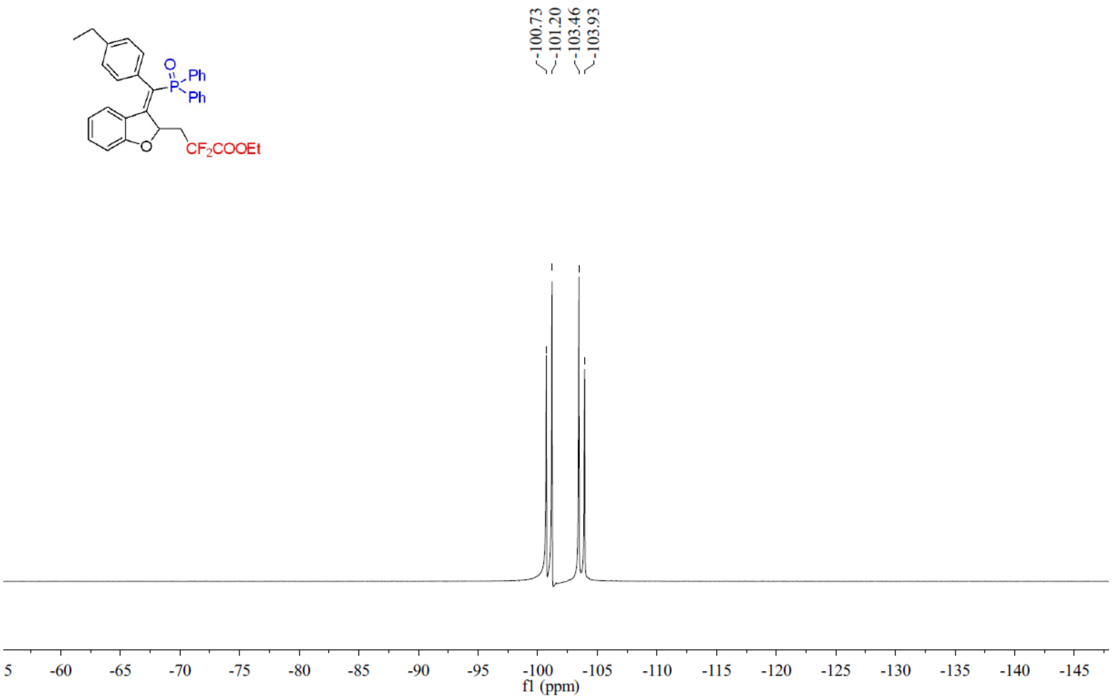
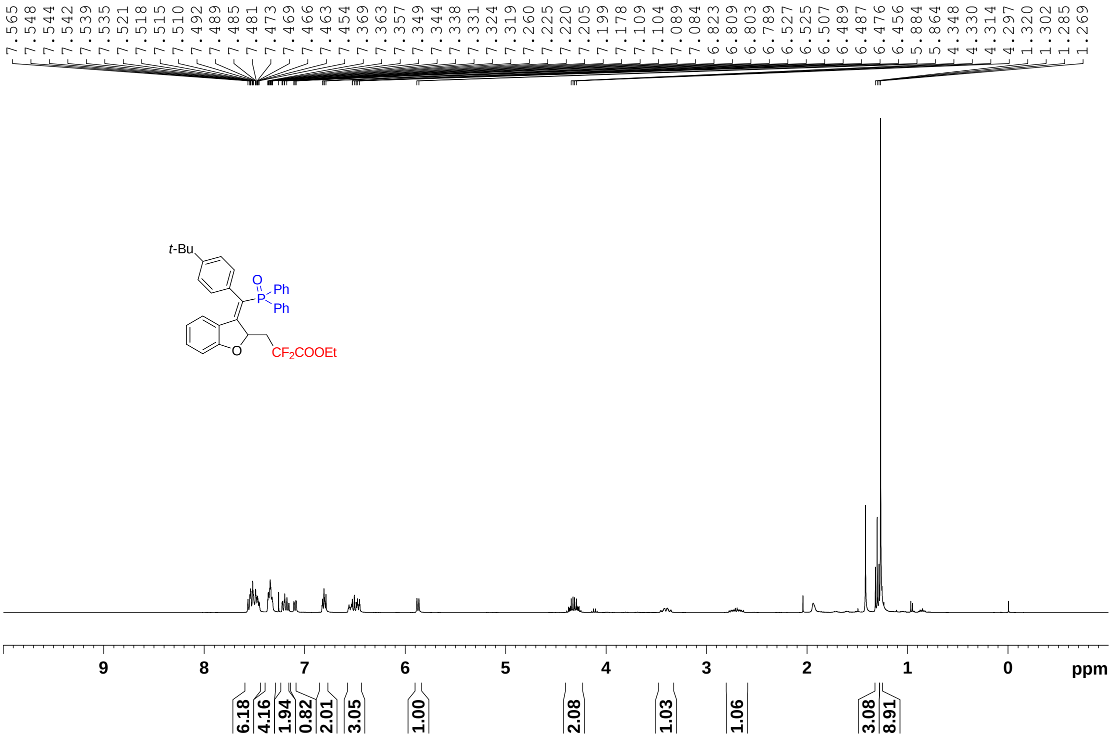


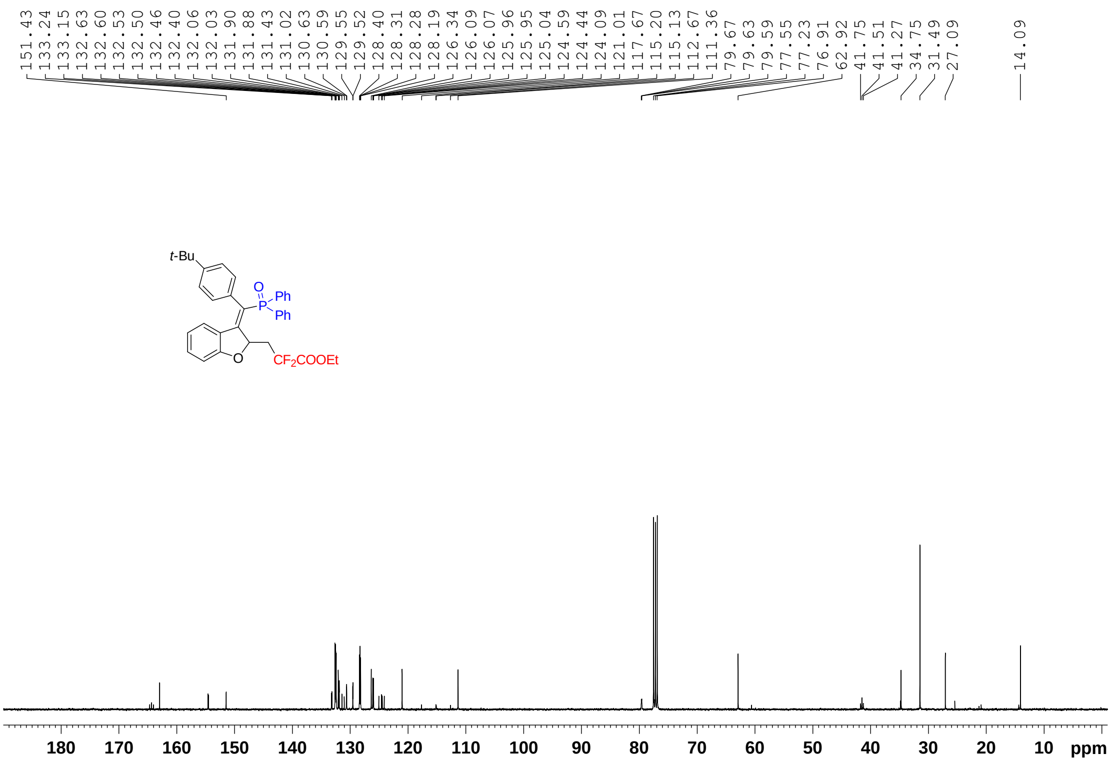
$^{19}F\{^{1}H\}$ NMR (565 MHz) Spectrum of **3e** in $CDCl_3$



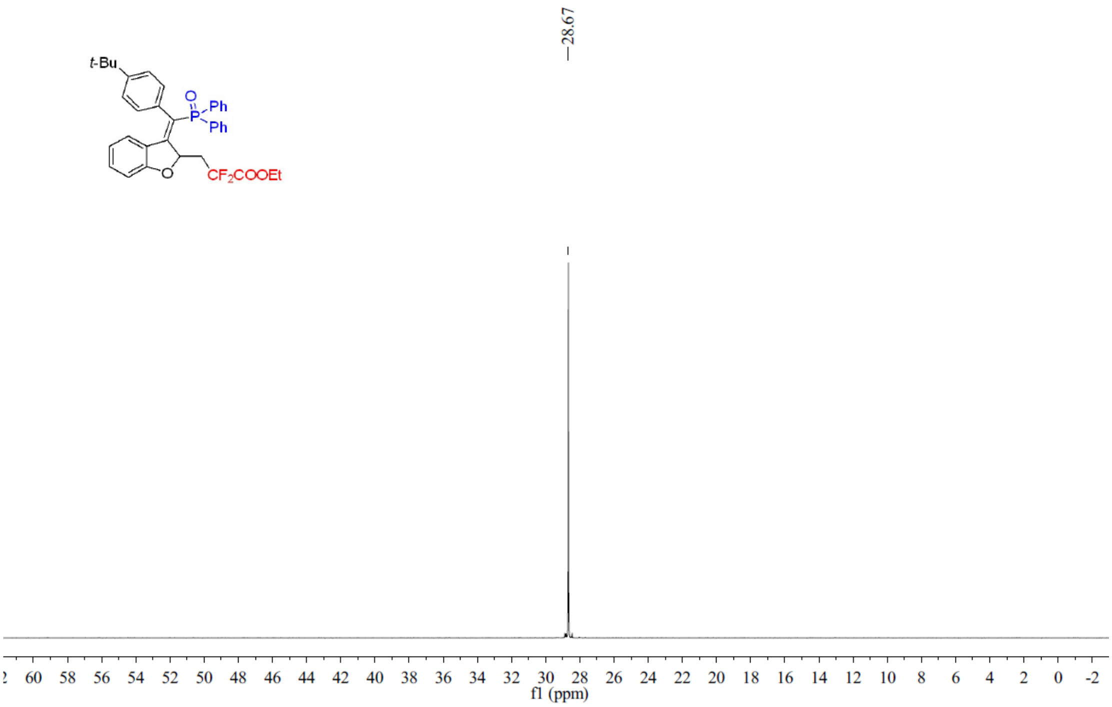
[1]H NMR (400 MHz) Spectrum of **3f** in $CDCl_3$



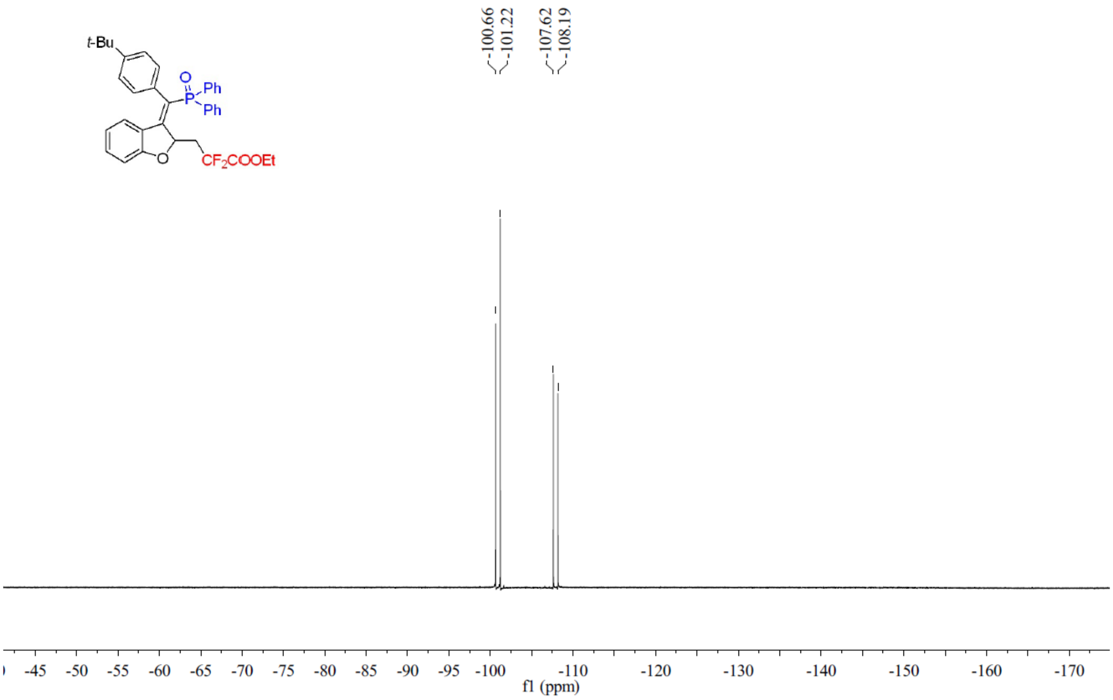
[13]C{[1]H}NMR (100 MHz) Spectrum of **3f** in $CDCl_3$



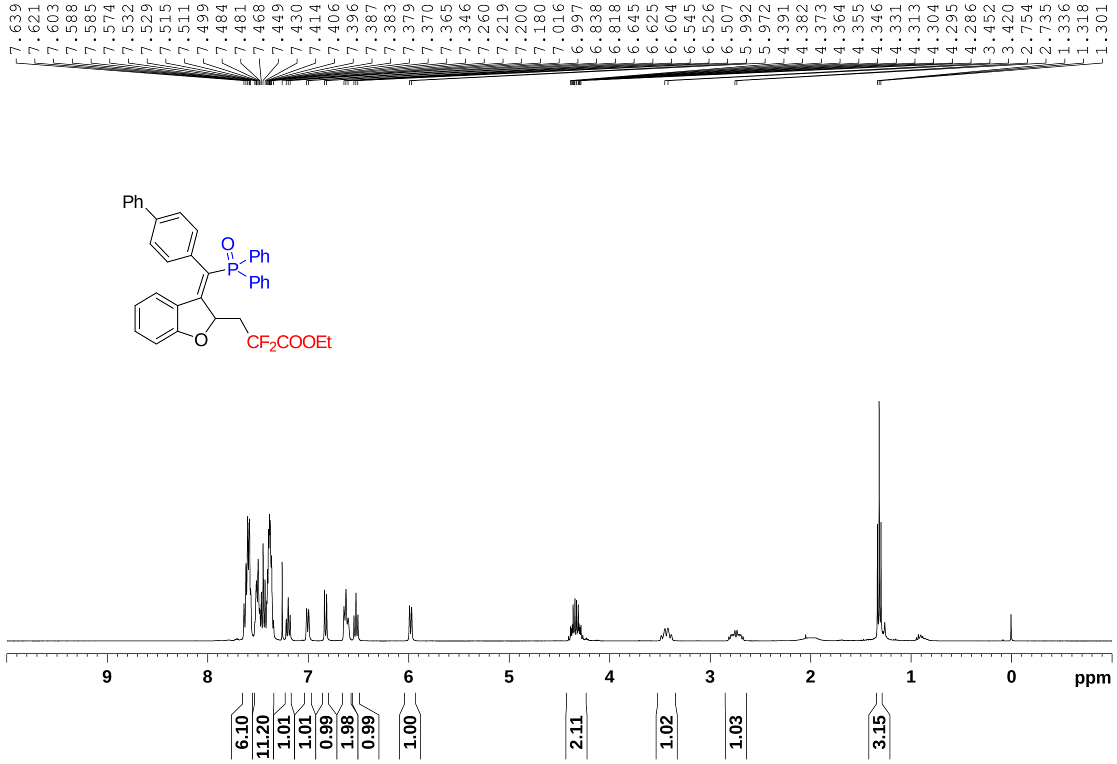
$^{31}P\{^1H\}$ NMR (243 MHz) Spectrum of **3f** in $CDCl_3$



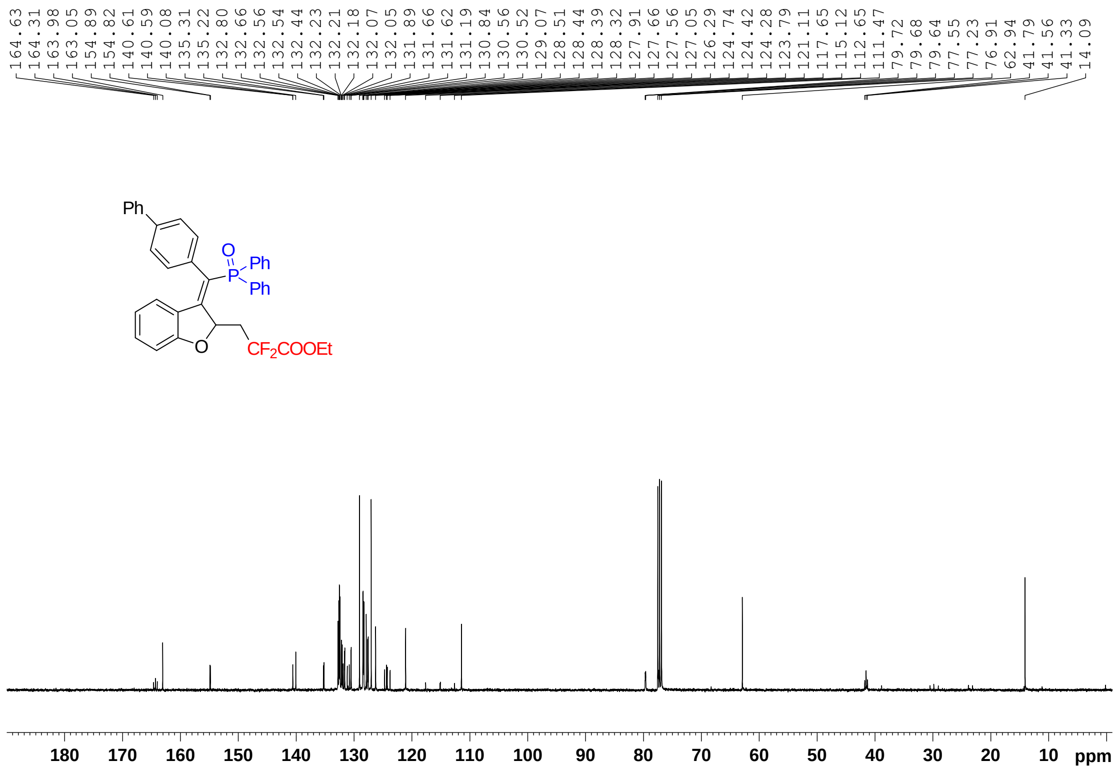
$^{19}F\{^1H\}$ NMR (471 MHz) Spectrum of **3f** in $CDCl_3$



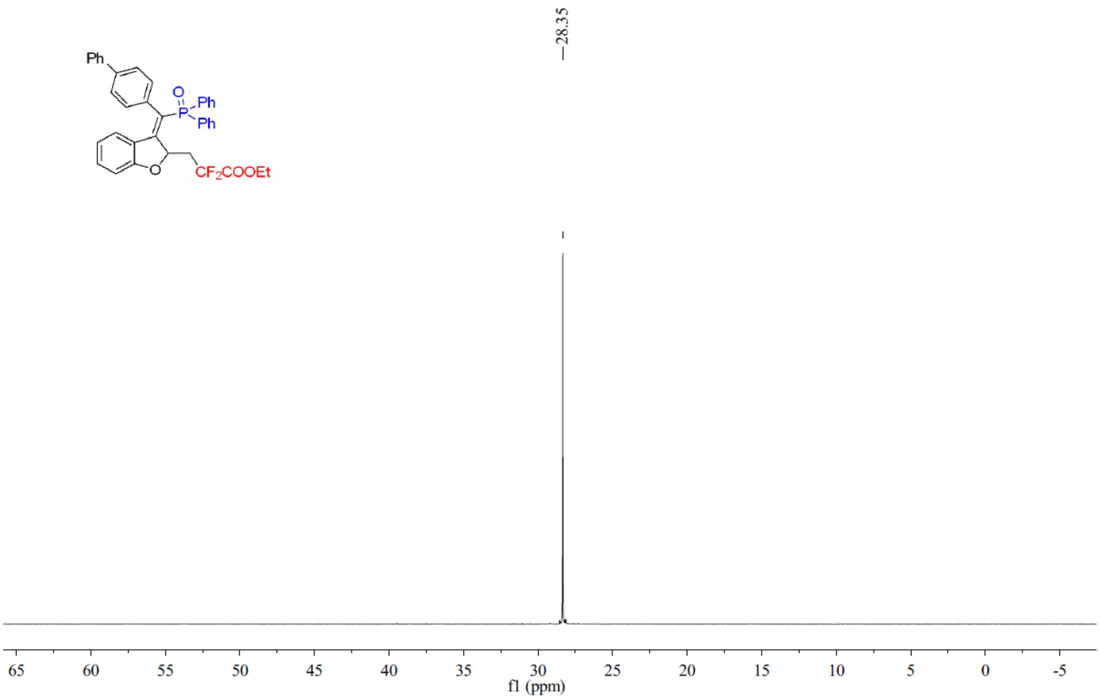
^{1}H NMR (400 MHz) Spectrum of **3g** in $CDCl_3$



$^{13}C\{^{1}H\}$NMR (100 MHz) Spectrum of **3g** in $CDCl_3$



$^{31}P\{^{1}H\}$ NMR (243 MHz) Spectrum of **3g** in $CDCl_3$



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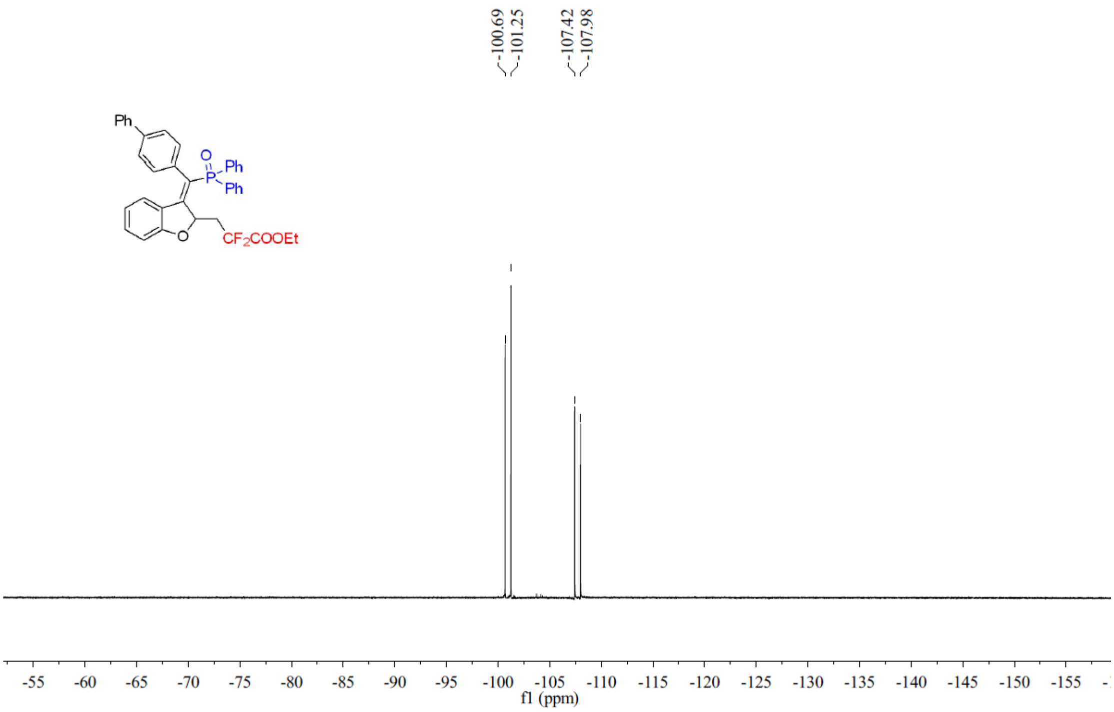
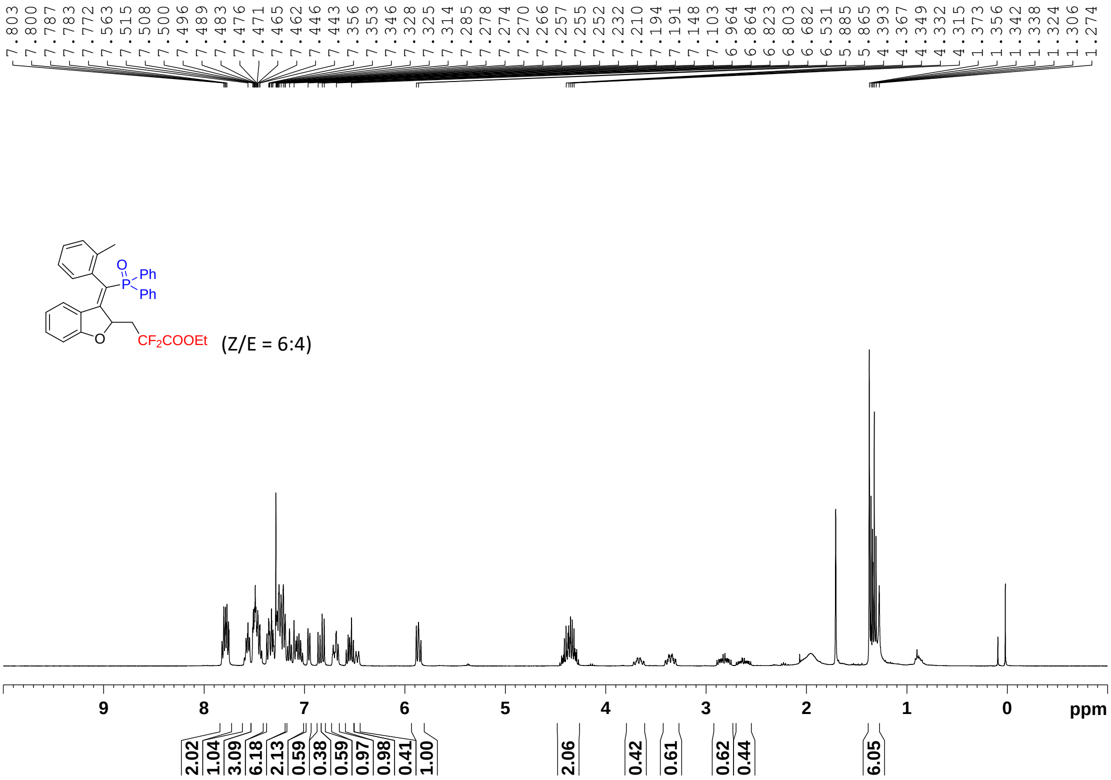
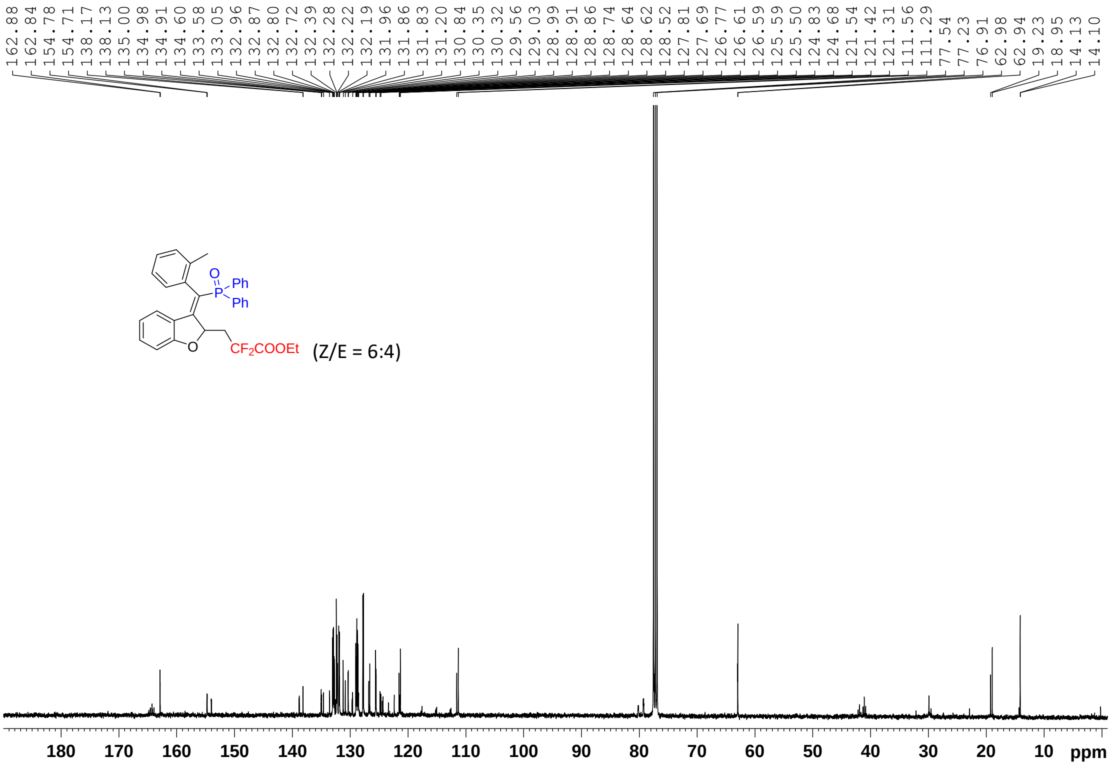


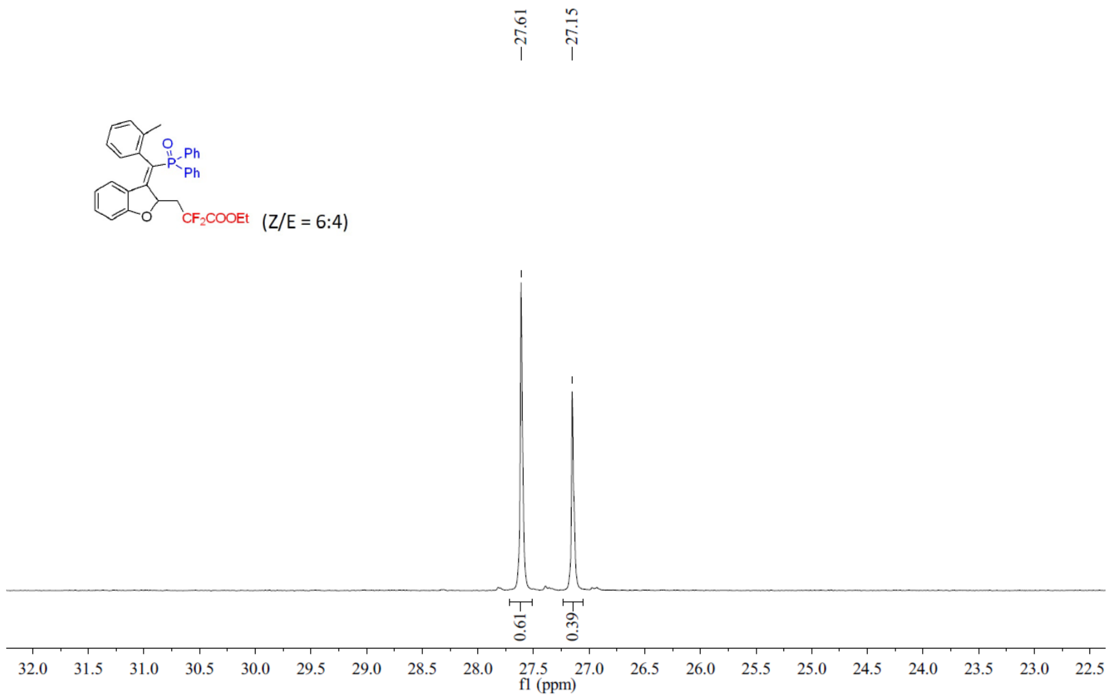
^{1}H NMR (400 MHz) Spectrum of **3h** in $CDCl_3$



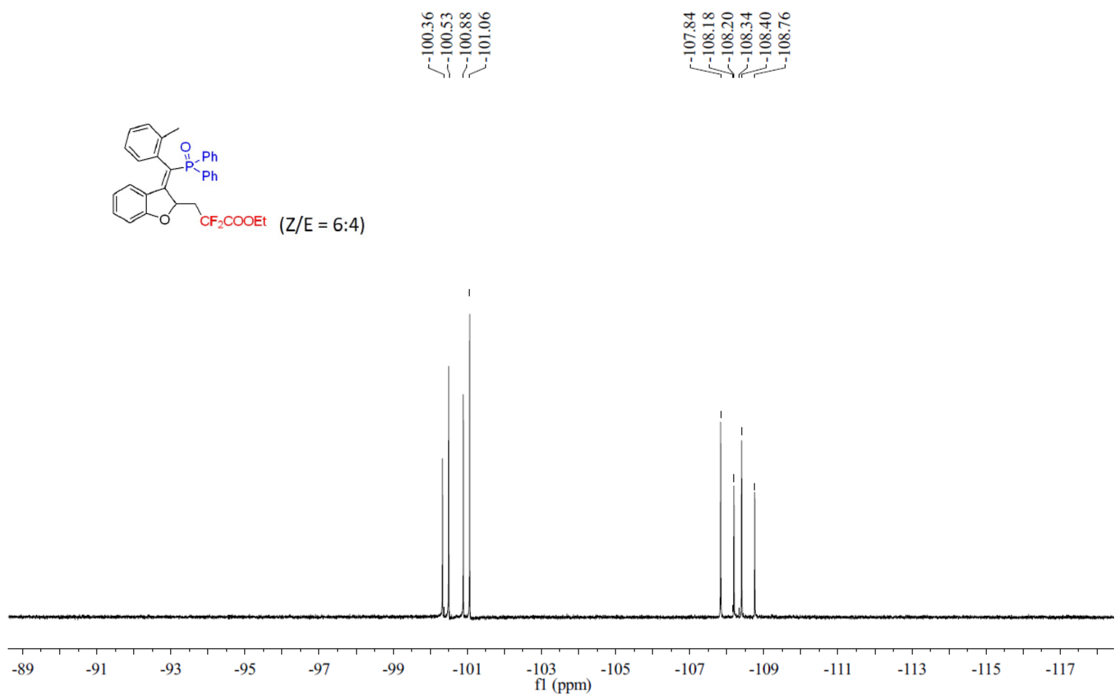
$^{13}C\{^{1}H\}$NMR (100 MHz) Spectrum of **3h** in $CDCl_3$



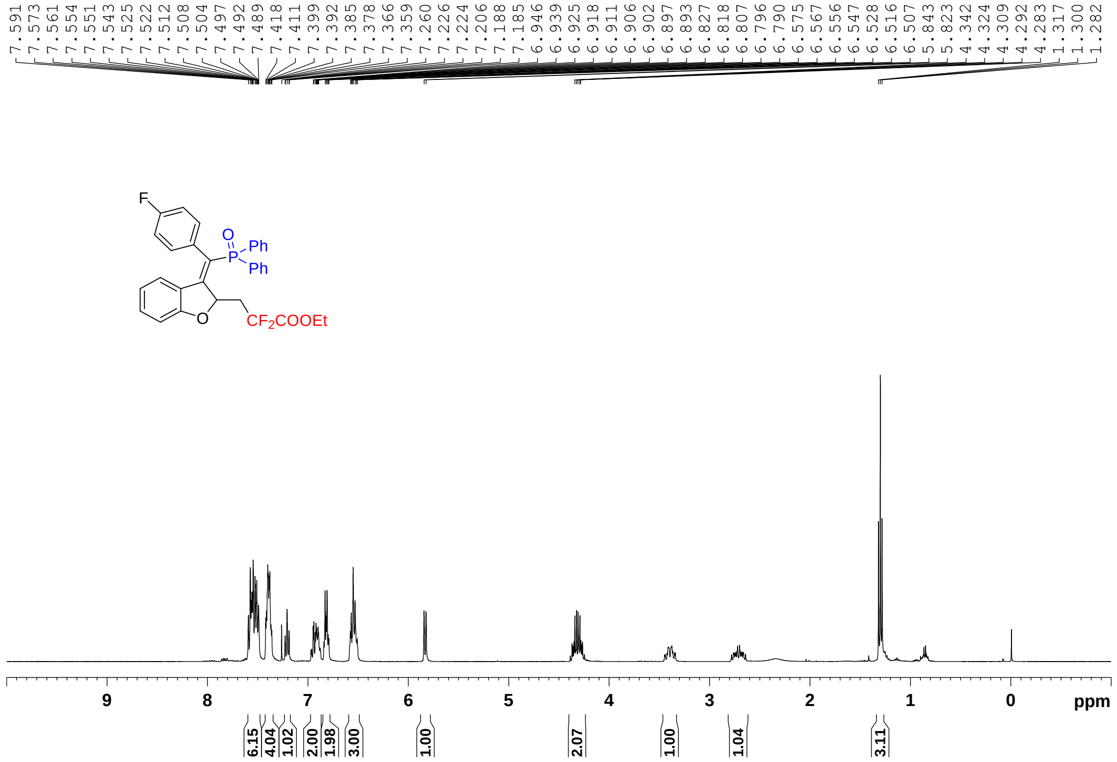
$^{31}P\{^{1}H\}$ NMR (243 MHz) Spectrum of **3h** in $CDCl_3$



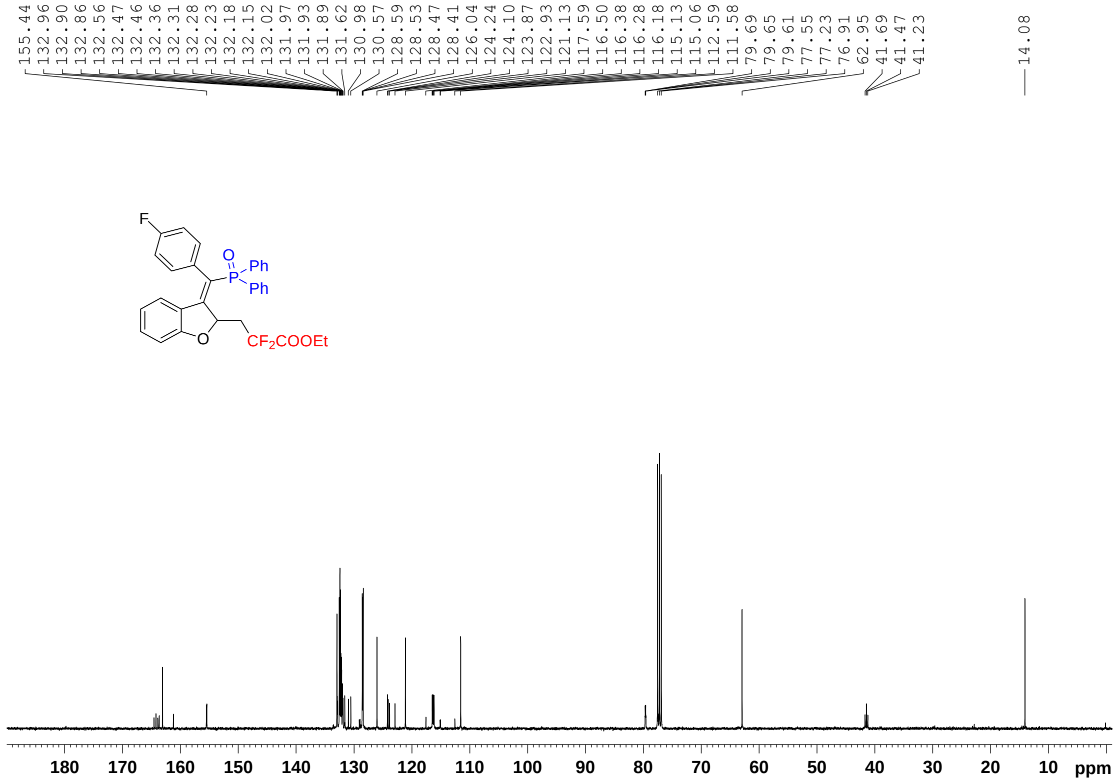
$^{19}F\{^{1}H\}$ NMR (471 MHz) Spectrum of **3h** in $CDCl_3$



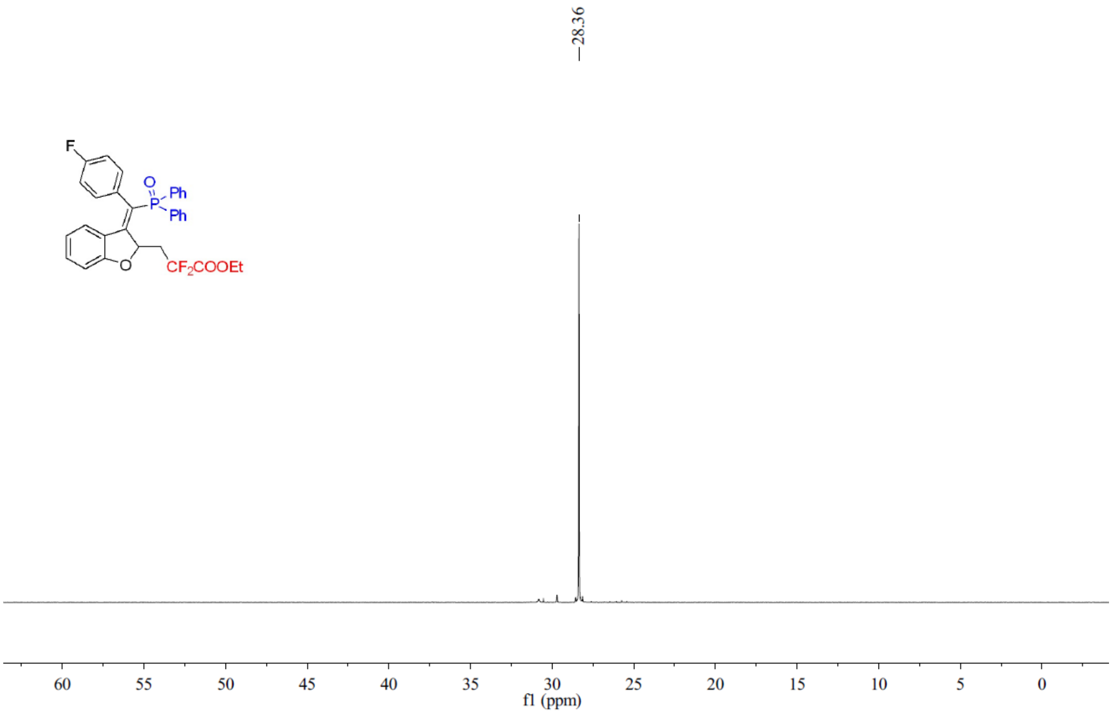
^{1}H NMR (400 MHz) Spectrum of **3i** in $CDCl_3$



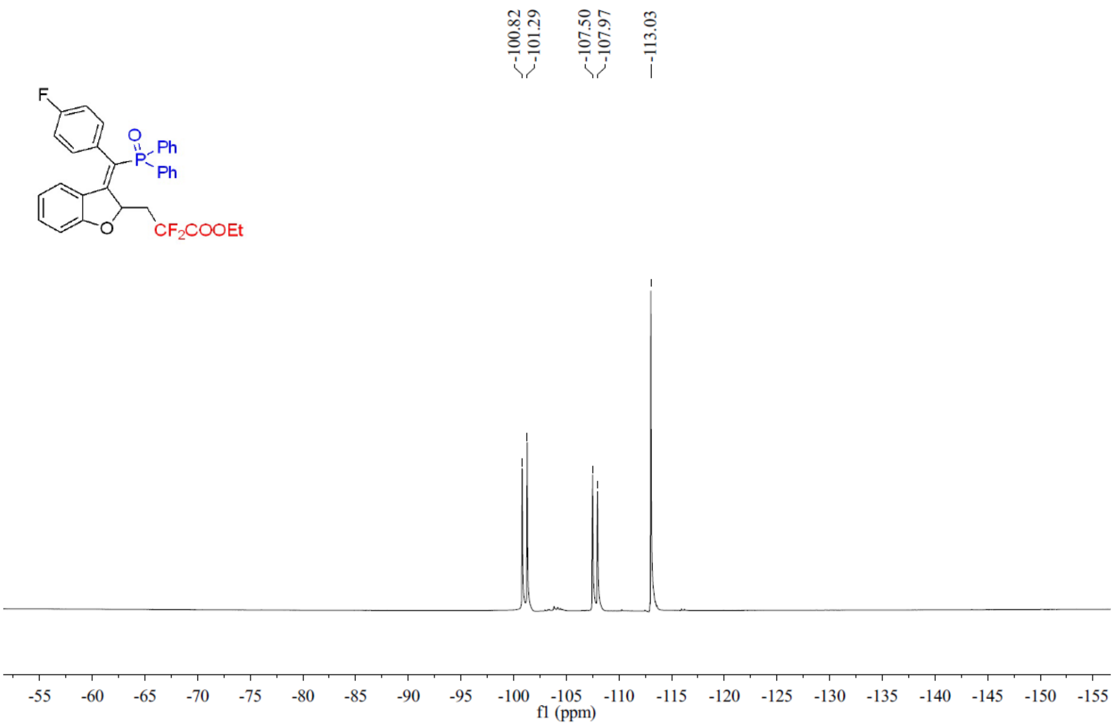
$^{13}C\{^{1}H\}$NMR (100 MHz) Spectrum of **3i** in $CDCl_3$



$^{31}P\{^1H\}$ NMR (243 MHz) Spectrum of **3i** in $CDCl_3$



$^{19}F\{^1H\}$ NMR (565 MHz) Spectrum of **3i** in $CDCl_3$



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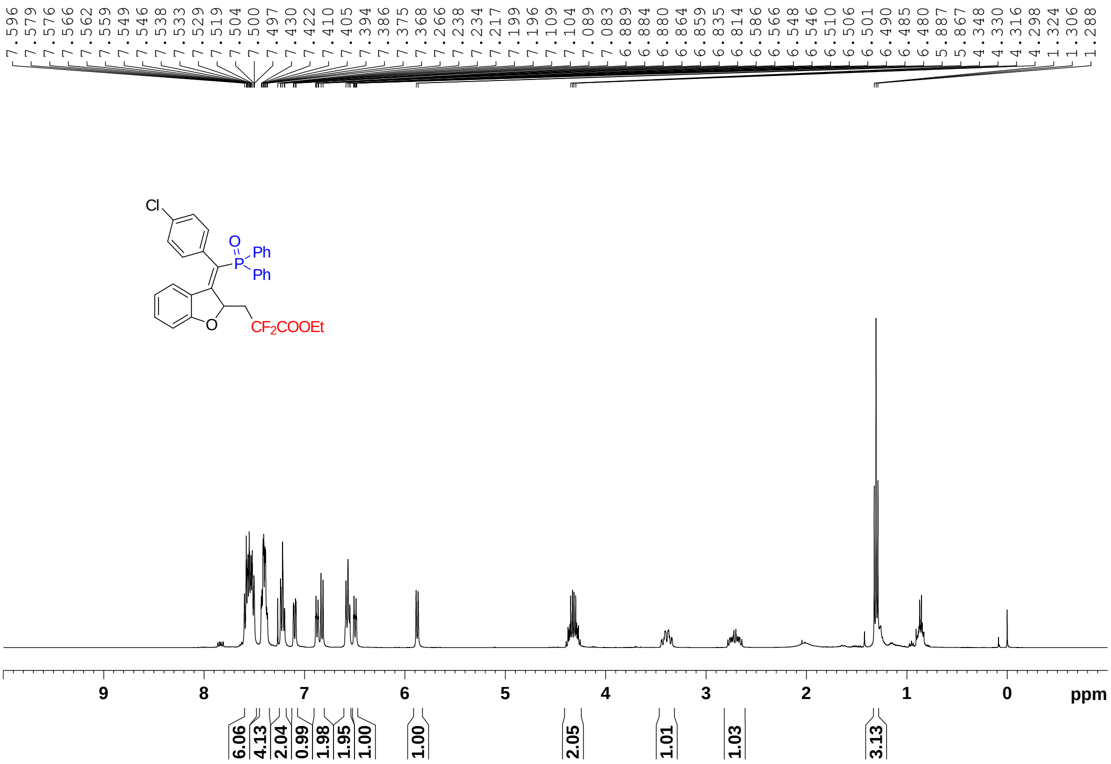

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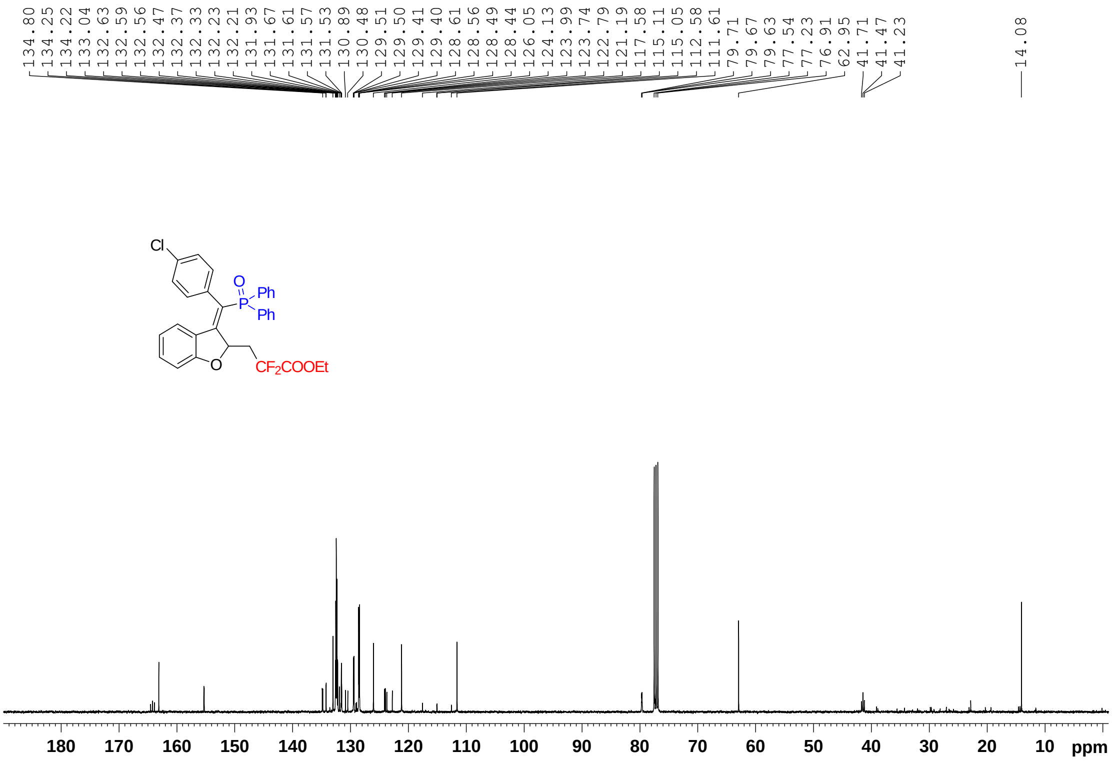

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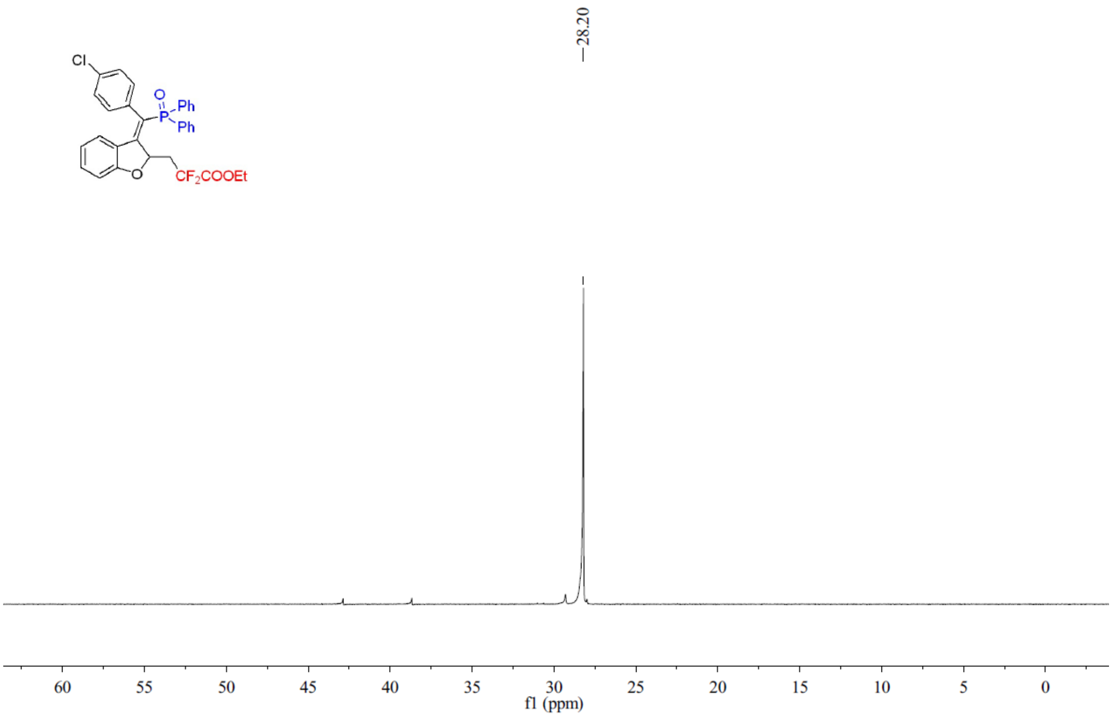
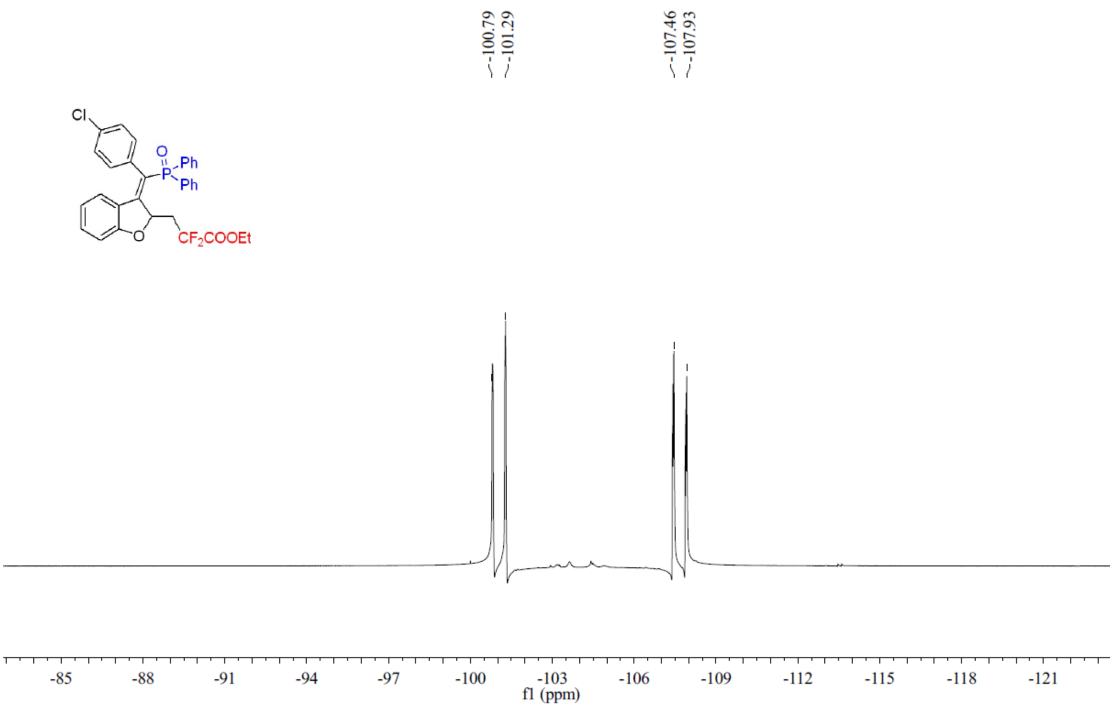


$^{19}F\{^{1}H\}$ NMR (565 MHz) Spectrum of **3j** in $CDCl_3$



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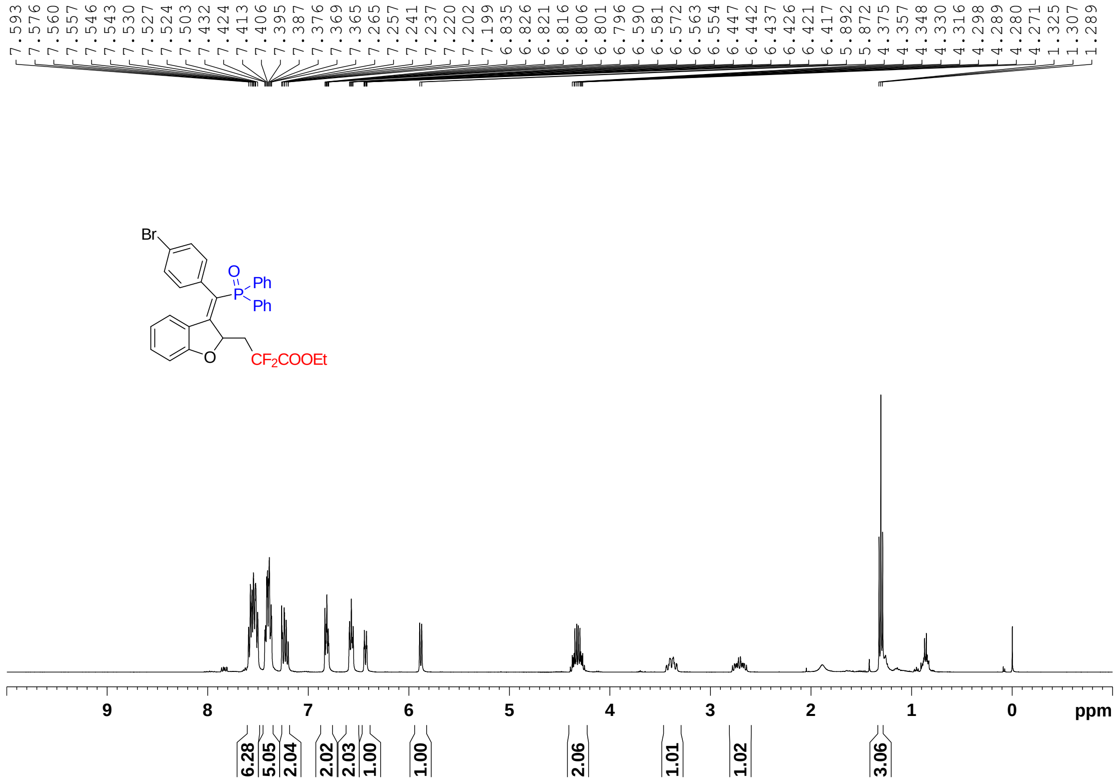
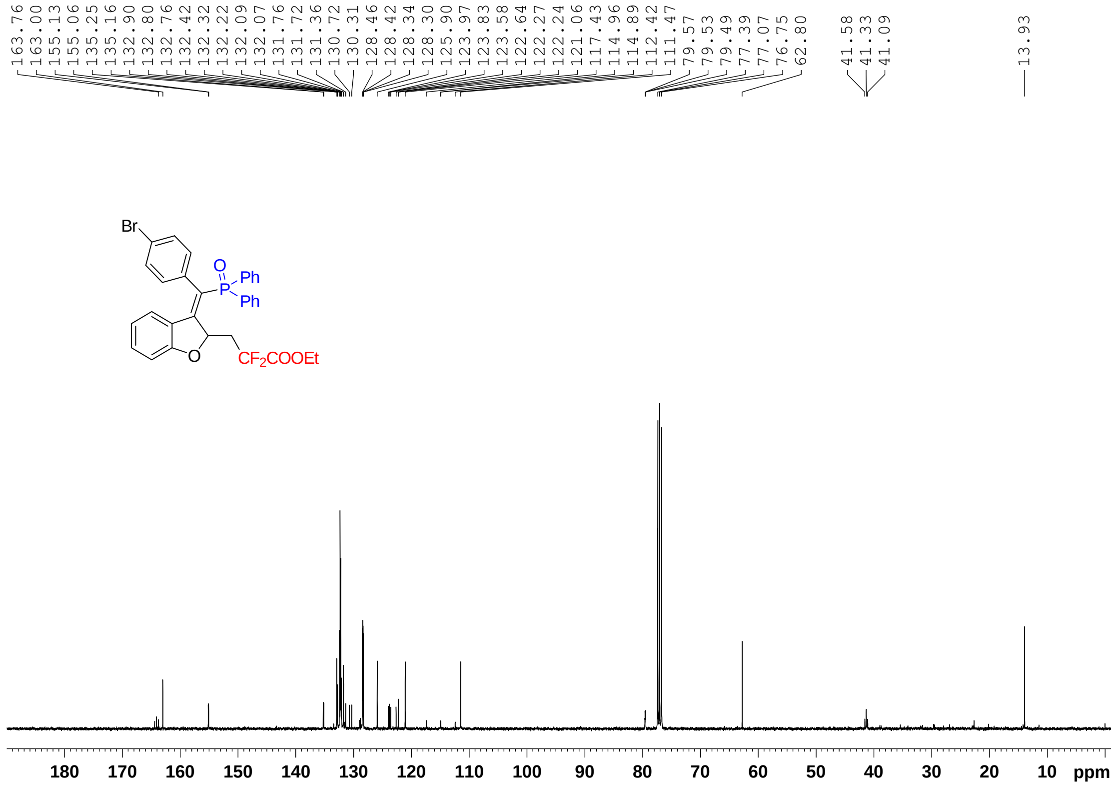
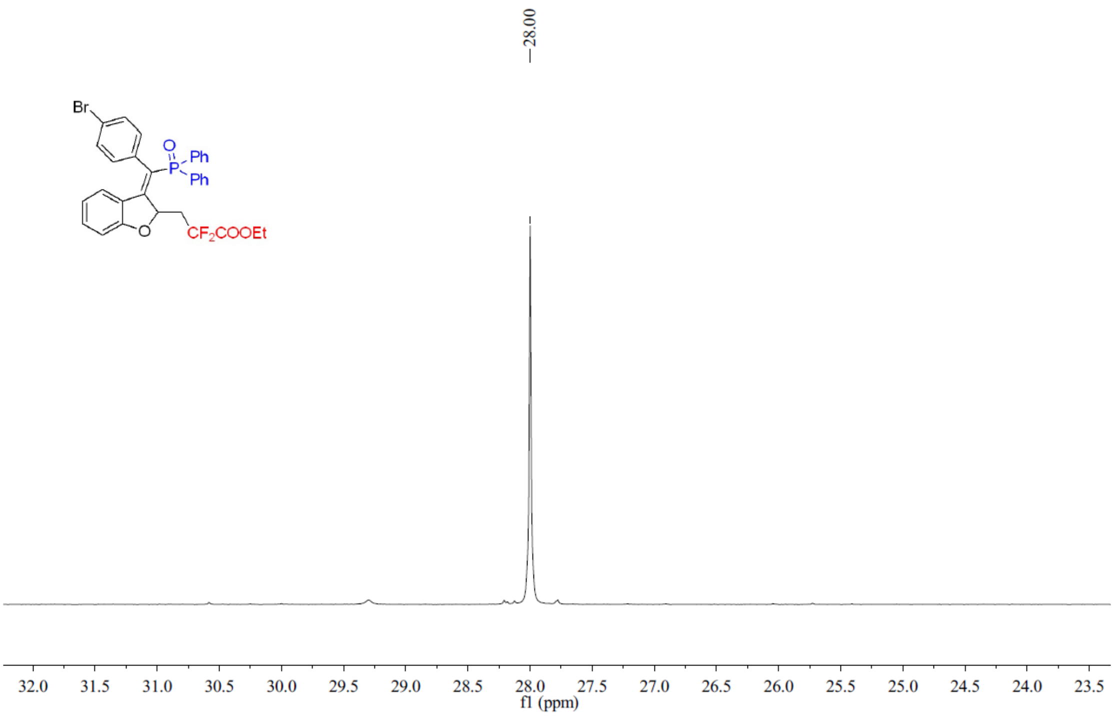


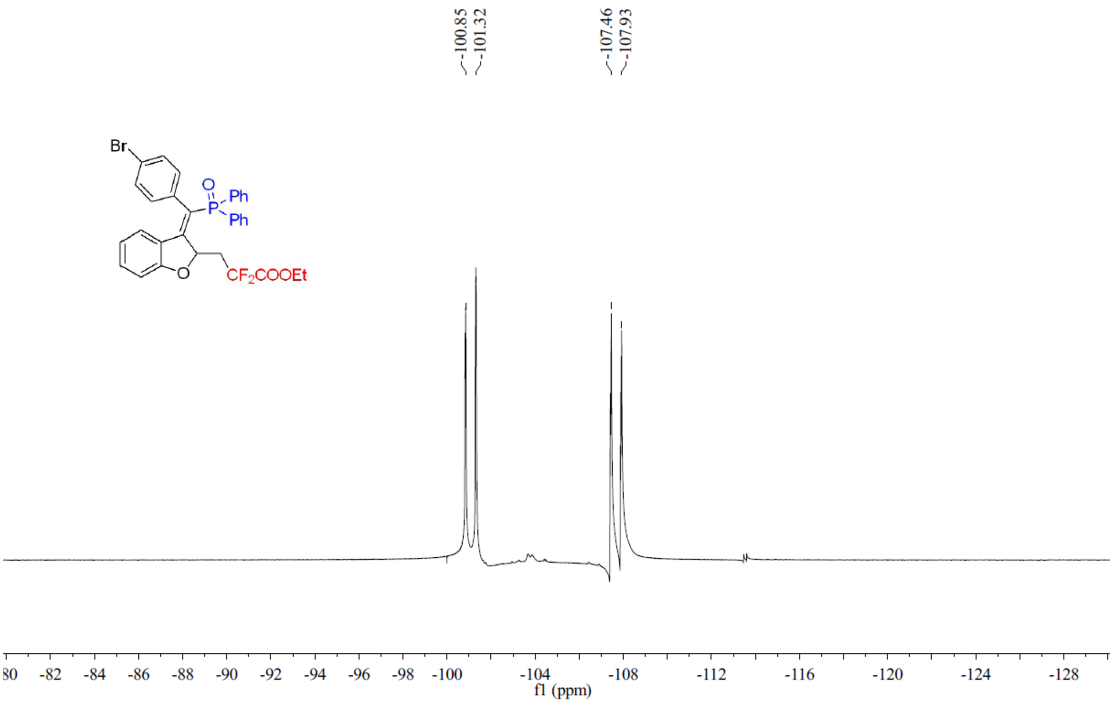
^{13}C{^{1}H}NMR (100 MHz) Spectrum of **3k** in $CDCl_3$



$^{31}P\{^{1}H\}$ NMR (243 MHz) Spectrum of **3k** in $CDCl_3$



$^{19}F\{^{1}H\}$ NMR (565 MHz) Spectrum of **3k** in $CDCl_3$



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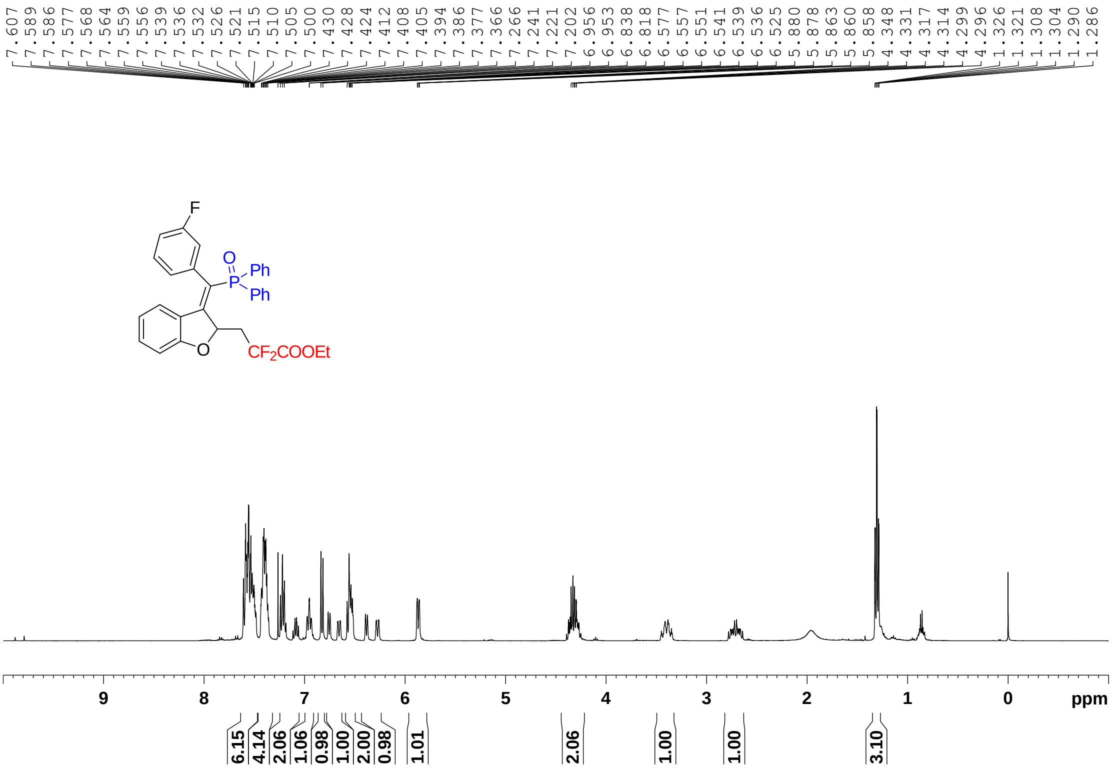
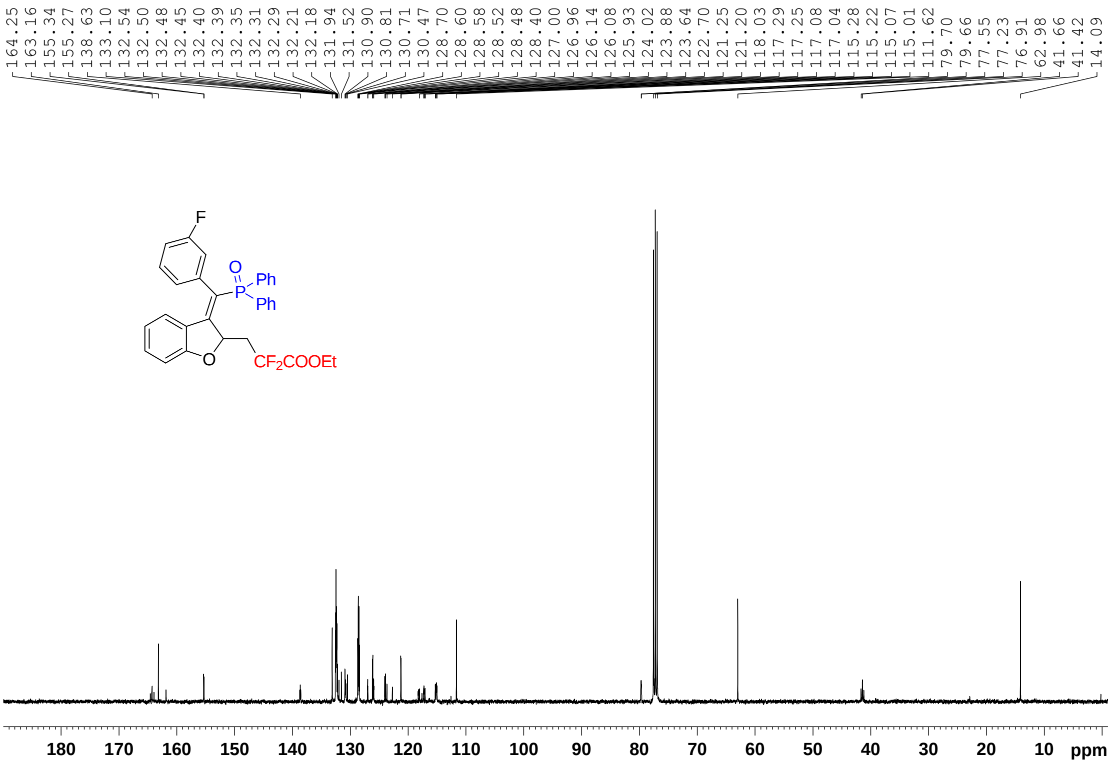
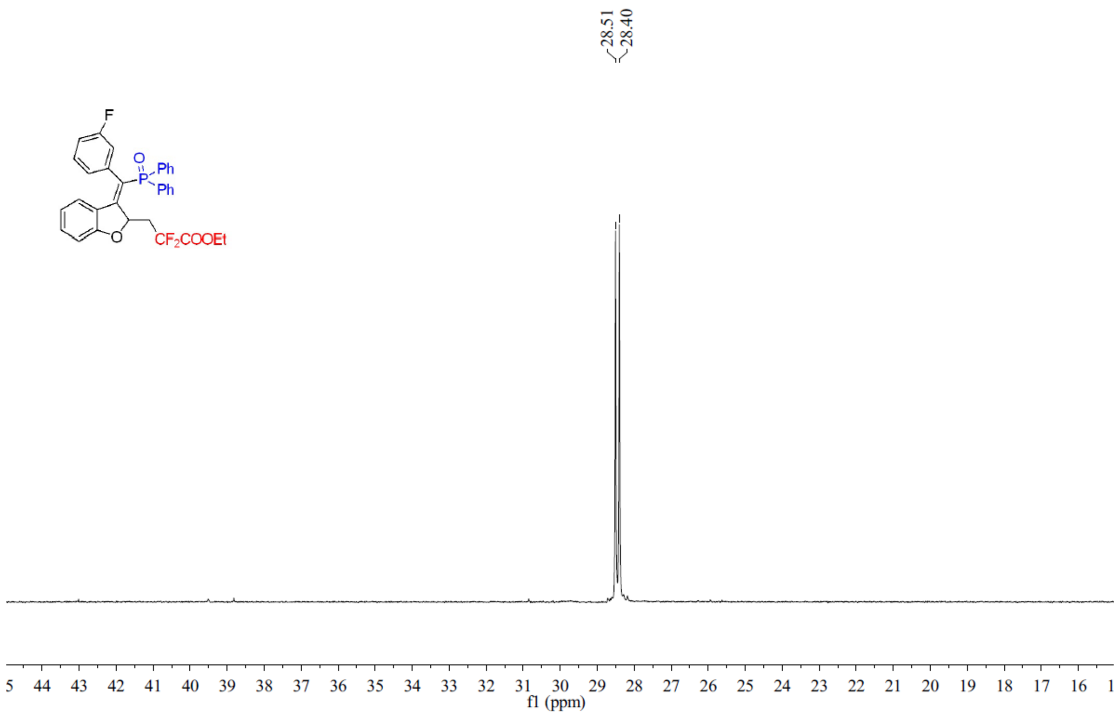


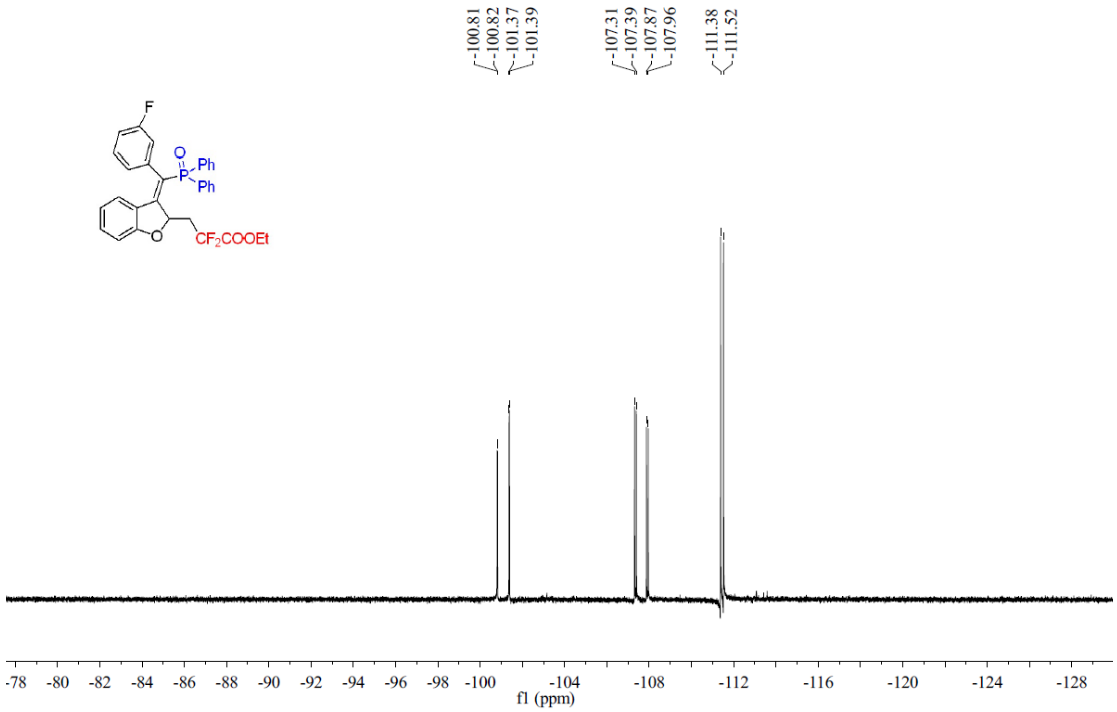
[13]C{[1]H}NMR (100 MHz) Spectrum of **3l** in $CDCl_3$



$^{31}P\{^{1}H\}$ NMR (243 MHz) Spectrum of **3l** in $CDCl_3$



$^{19}F\{^{1}H\}$ NMR (471 MHz) Spectrum of **3l** in $CDCl_3$



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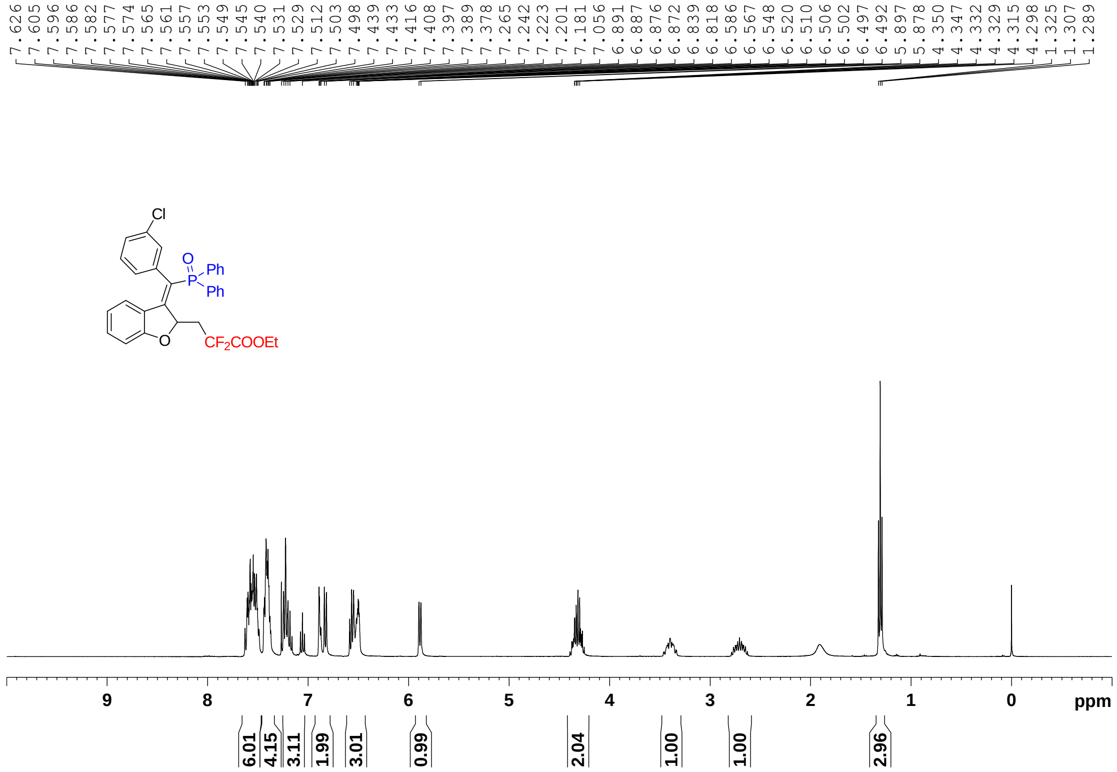
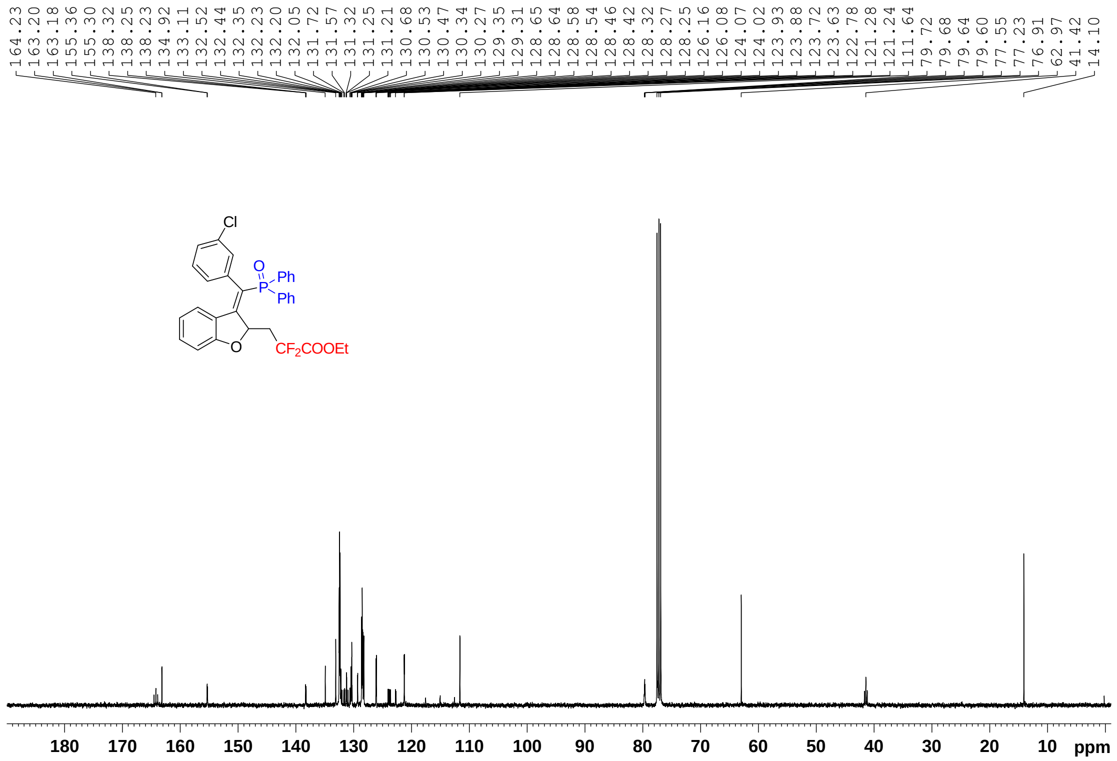
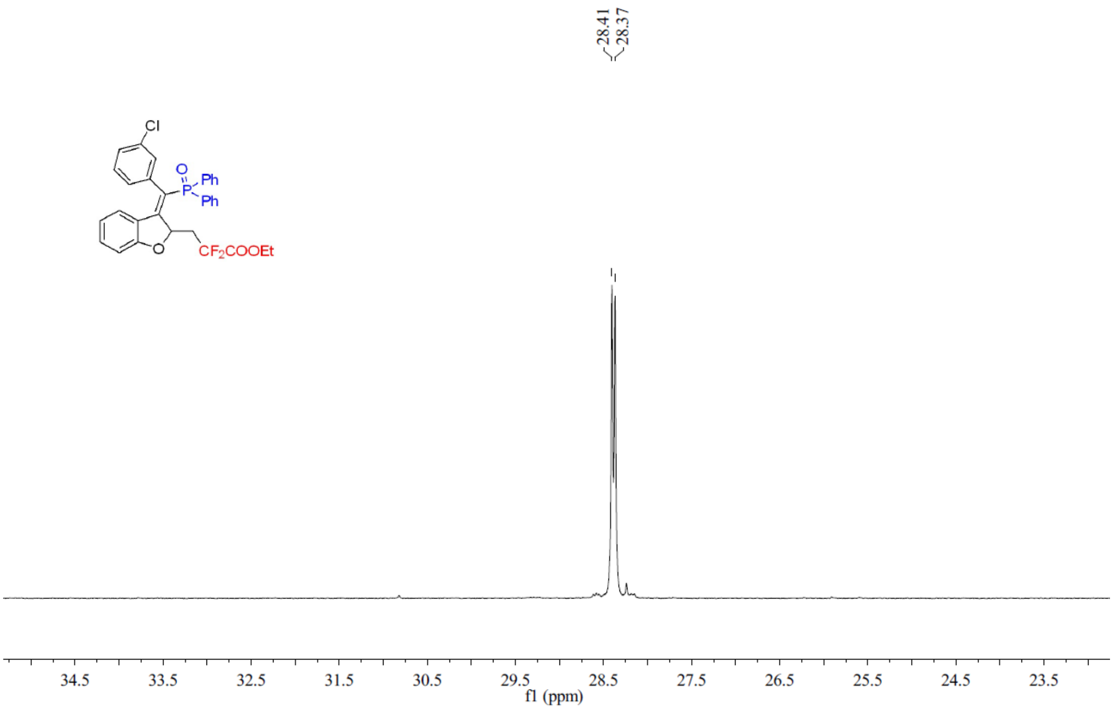


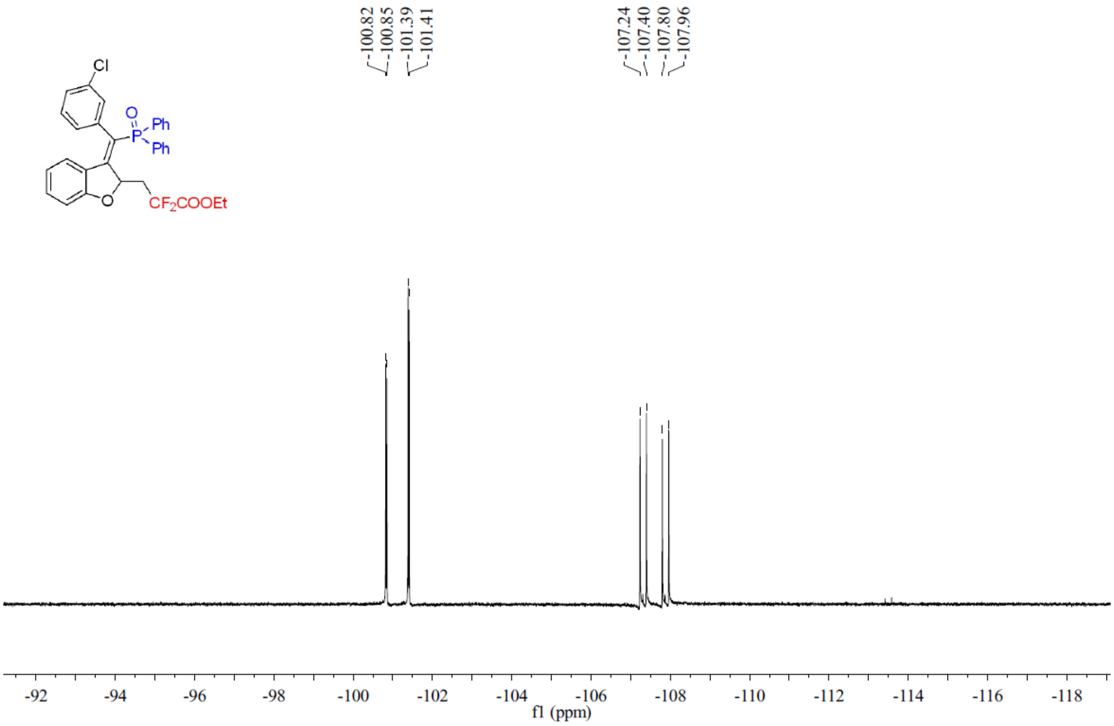
^{13}C{^{1}H}NMR (100 MHz) Spectrum of **3m** in $CDCl_3$



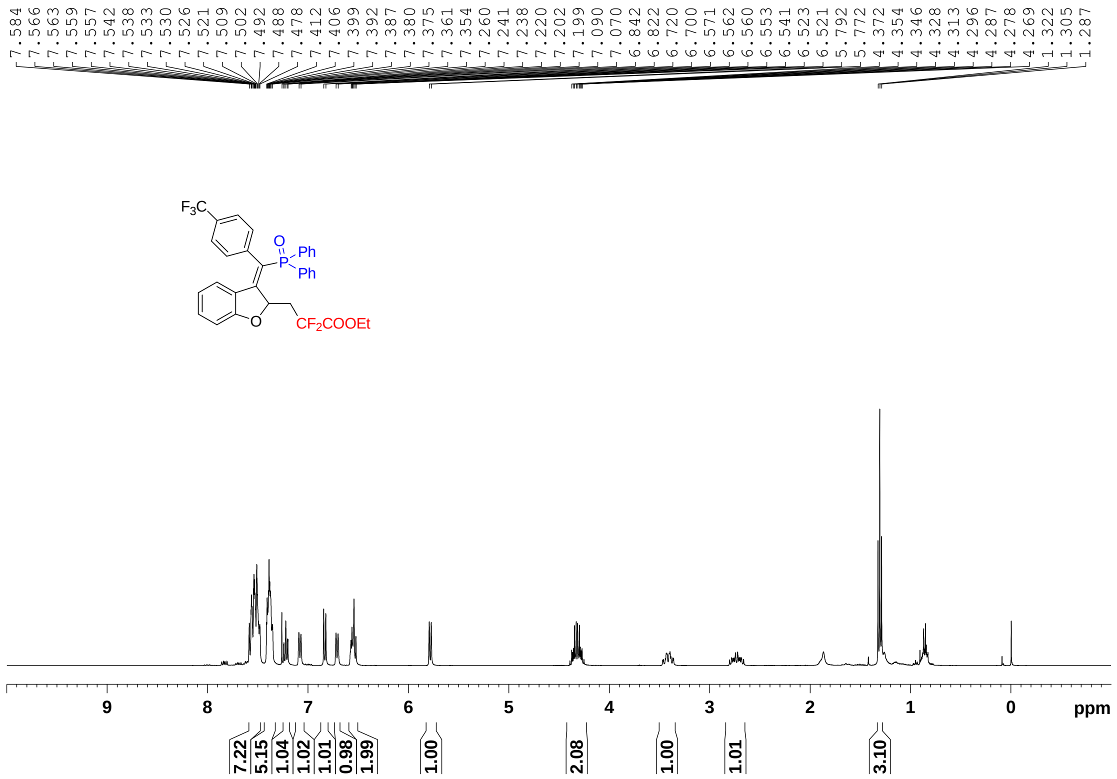
$^{31}P\{^{1}H\}$ NMR (243 MHz) Spectrum of **3m** in $CDCl_3$



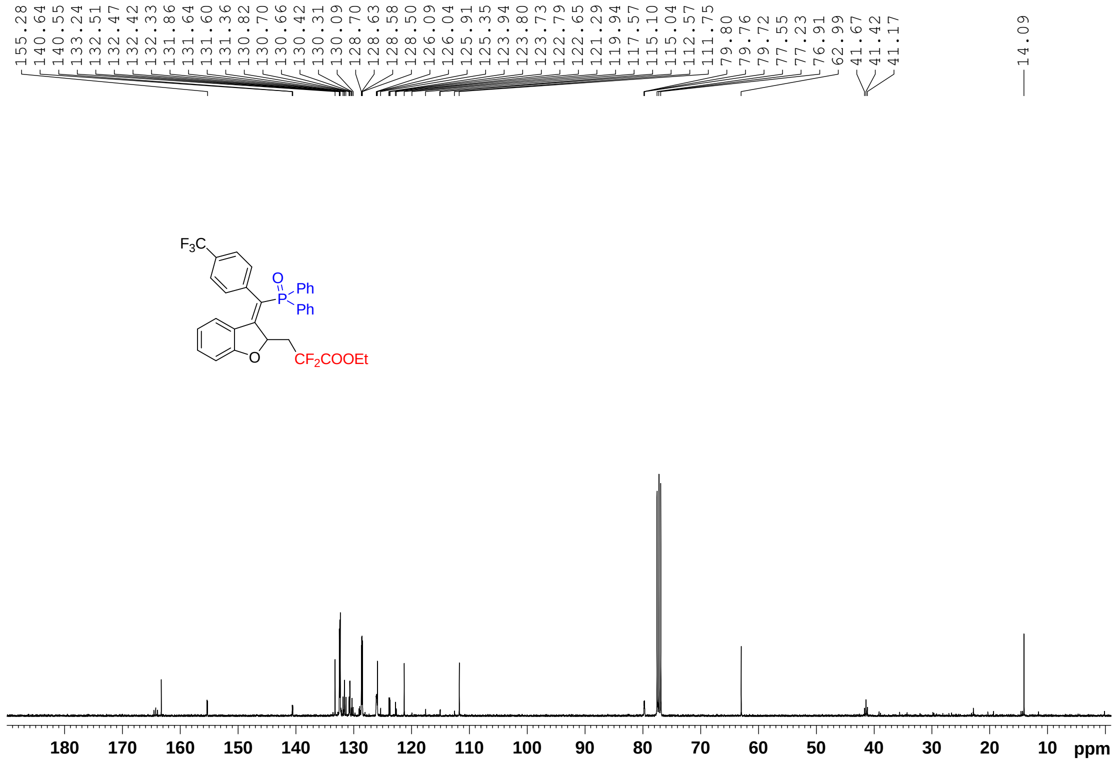
$^{19}F\{^{1}H\}$ NMR (471 MHz) Spectrum of **3m** in $CDCl_3$



[1]H NMR (400 MHz) Spectrum of **3n** in $CDCl_3$



[13]C{[1]H}NMR (100 MHz) Spectrum of **3n** in $CDCl_3$



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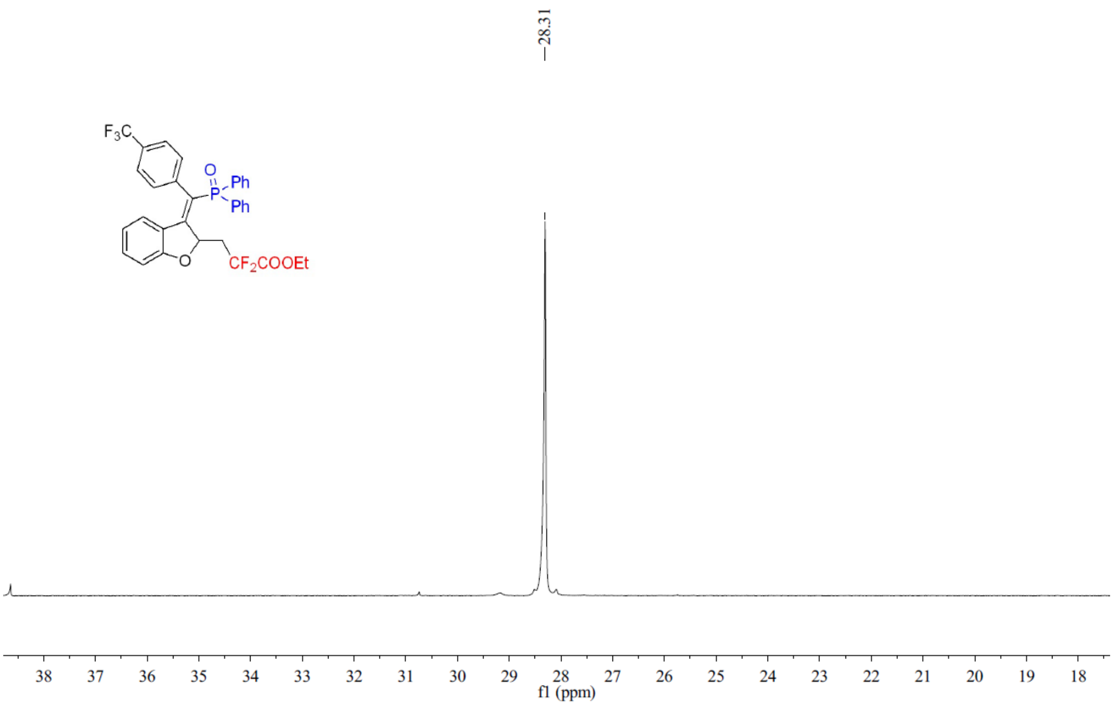
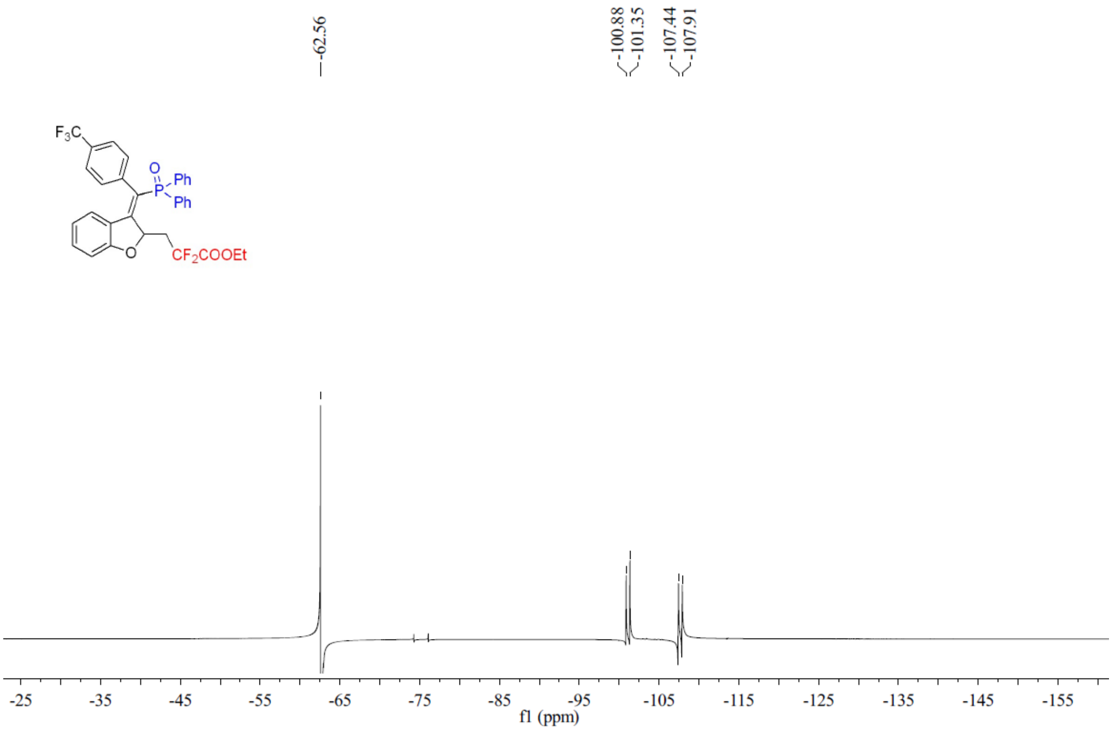


$^{19}F\{^1H\}$ NMR (565 MHz) Spectrum of **3n** in $CDCl_3$



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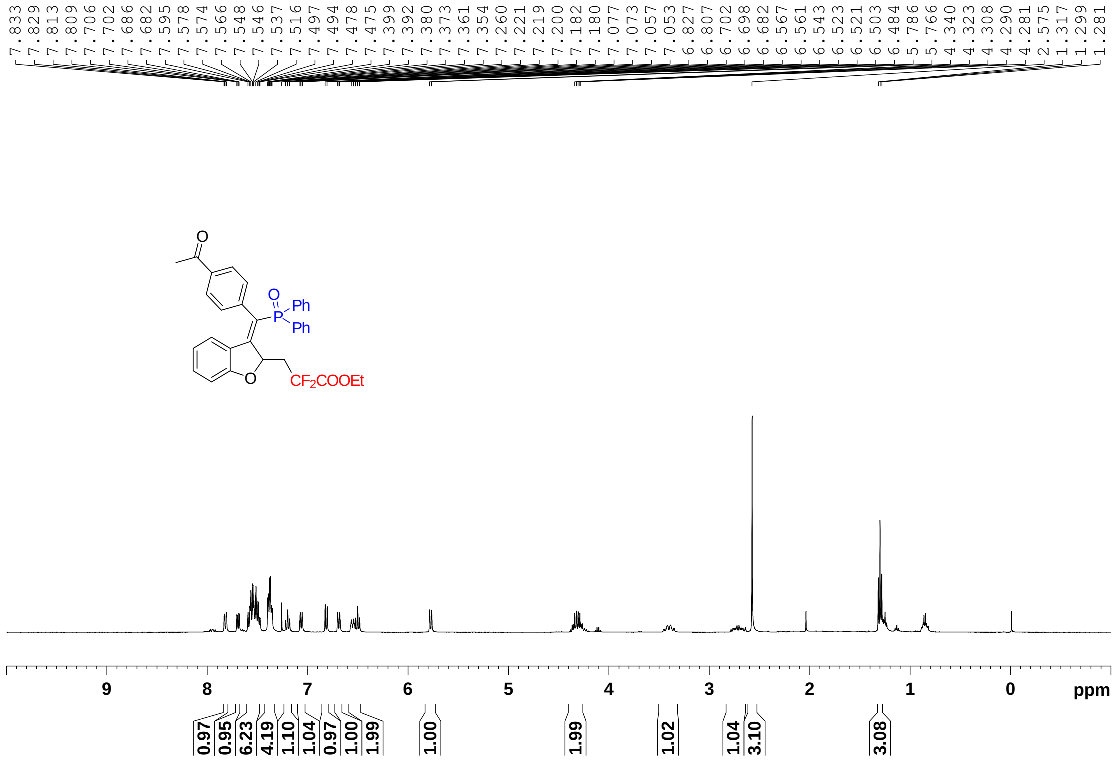
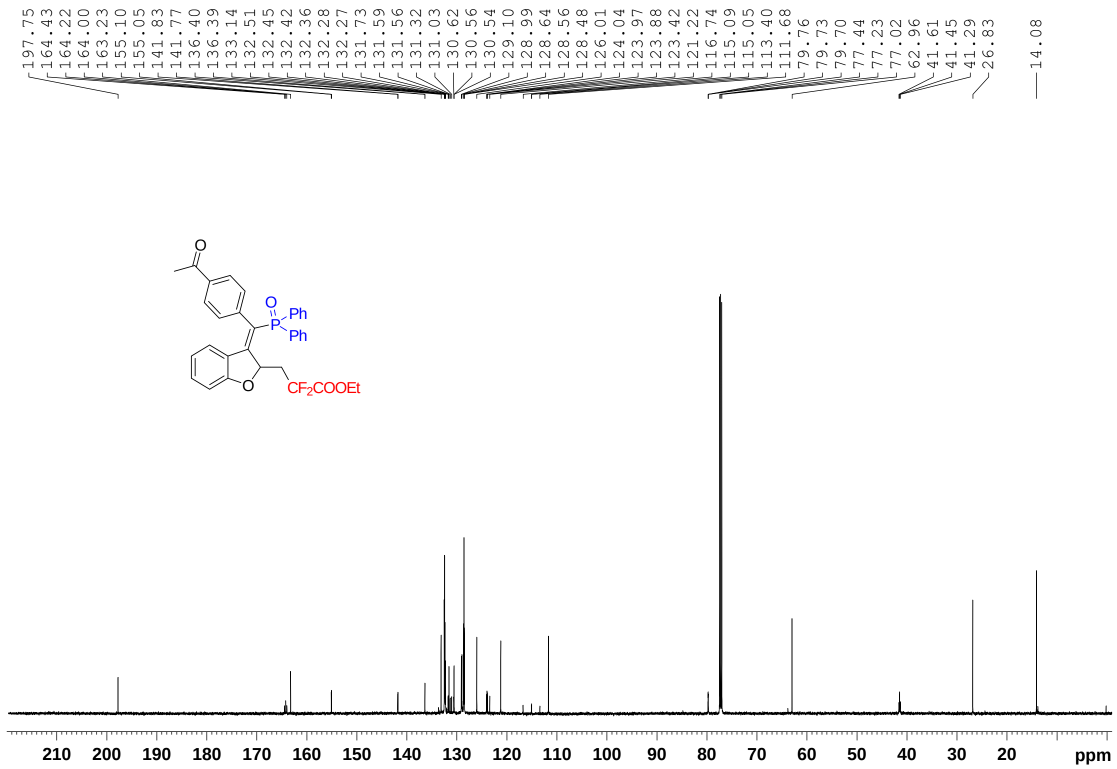
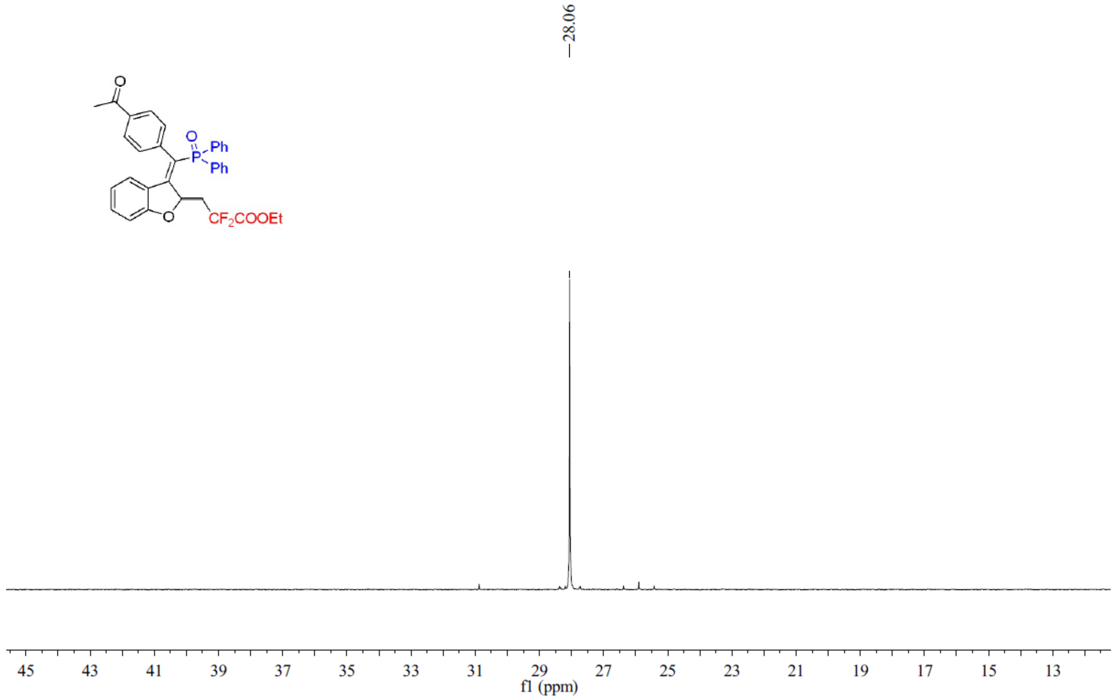


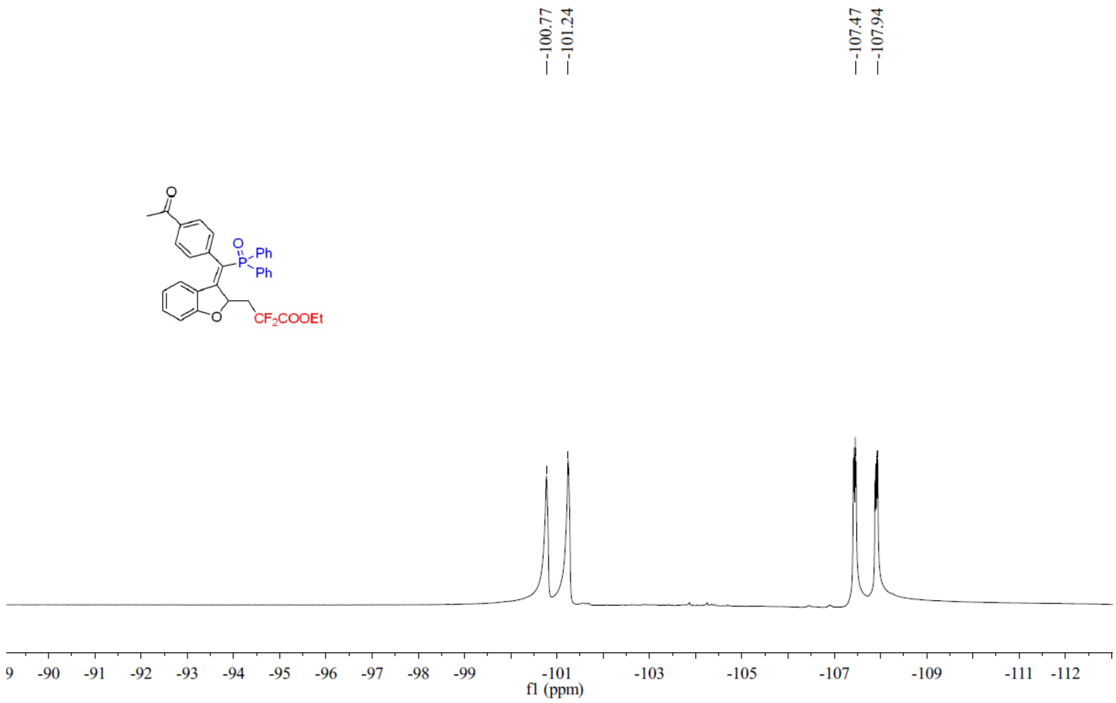
^{13}C{^{1}H}NMR (100 MHz) Spectrum of **3o** in $CDCl_3$



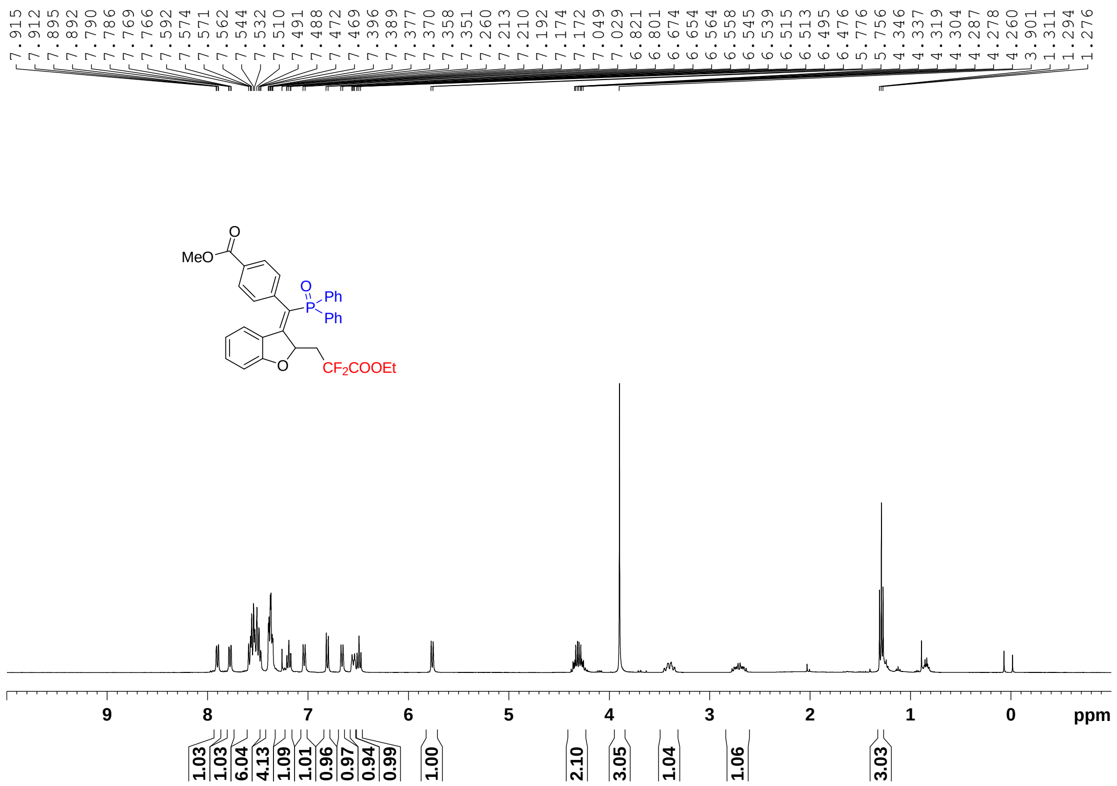
$^{31}P\{^{1}H\}$ NMR (243 MHz) Spectrum of **3o** in $CDCl_3$



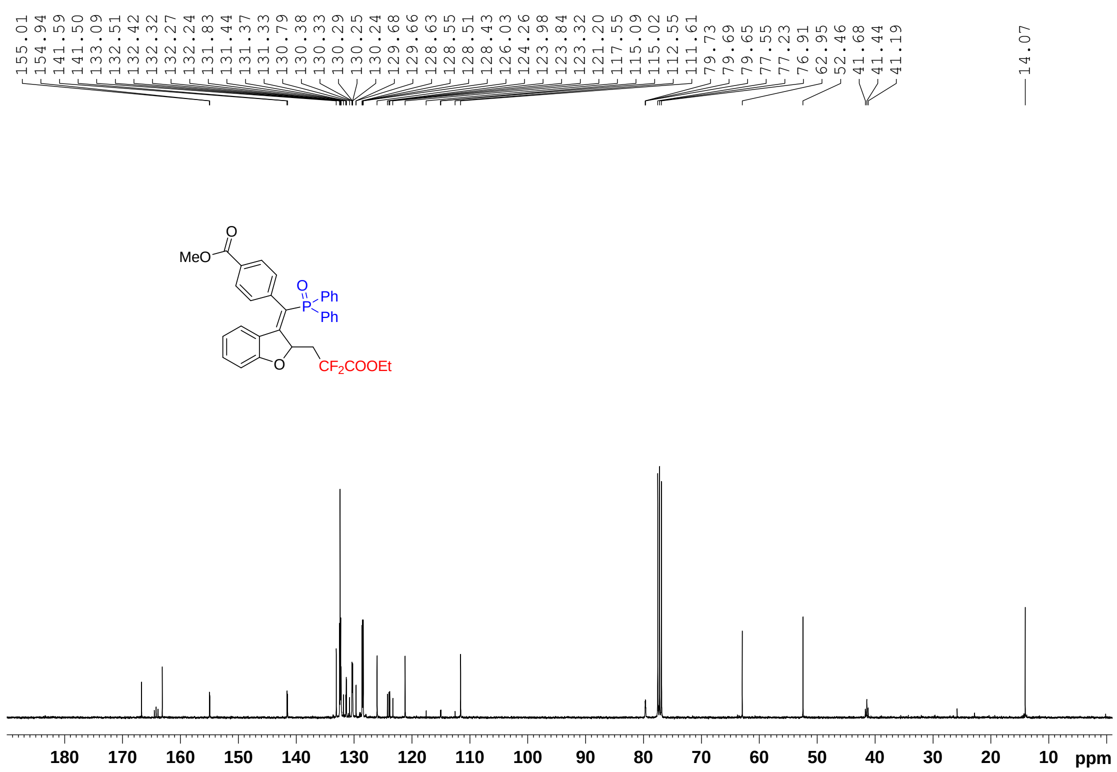
$^{19}F\{^{1}H\}$ NMR (565 MHz) Spectrum of **3o** in $CDCl_3$



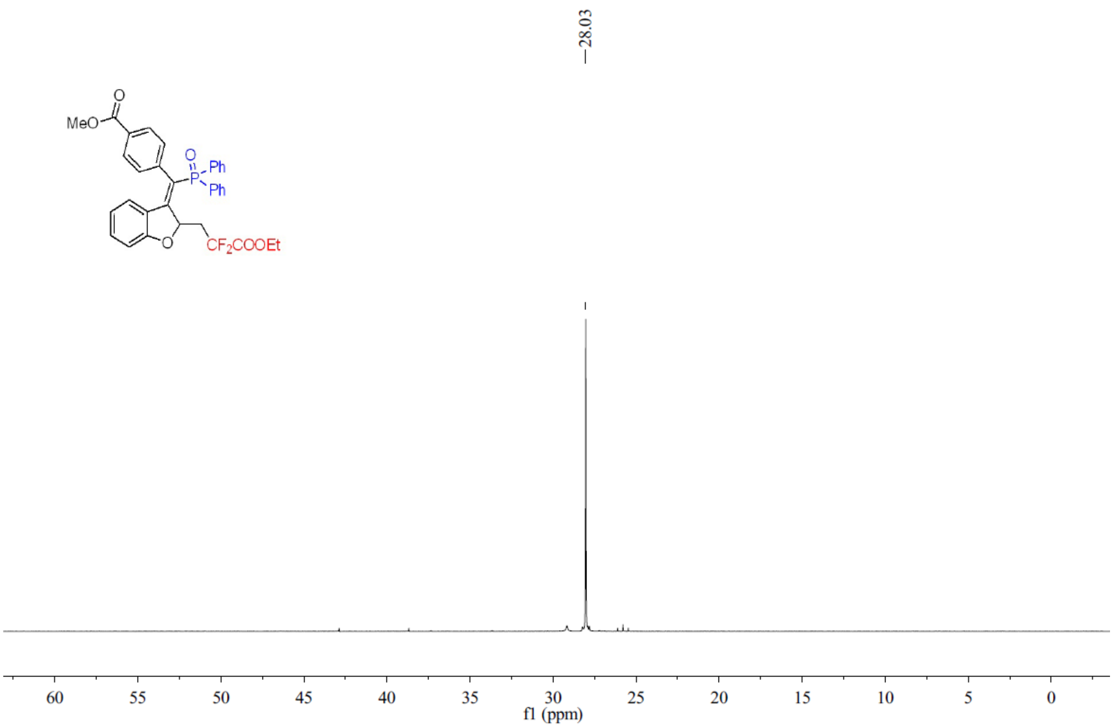
^{1}H NMR (400 MHz) Spectrum of **3p** in $CDCl_3$



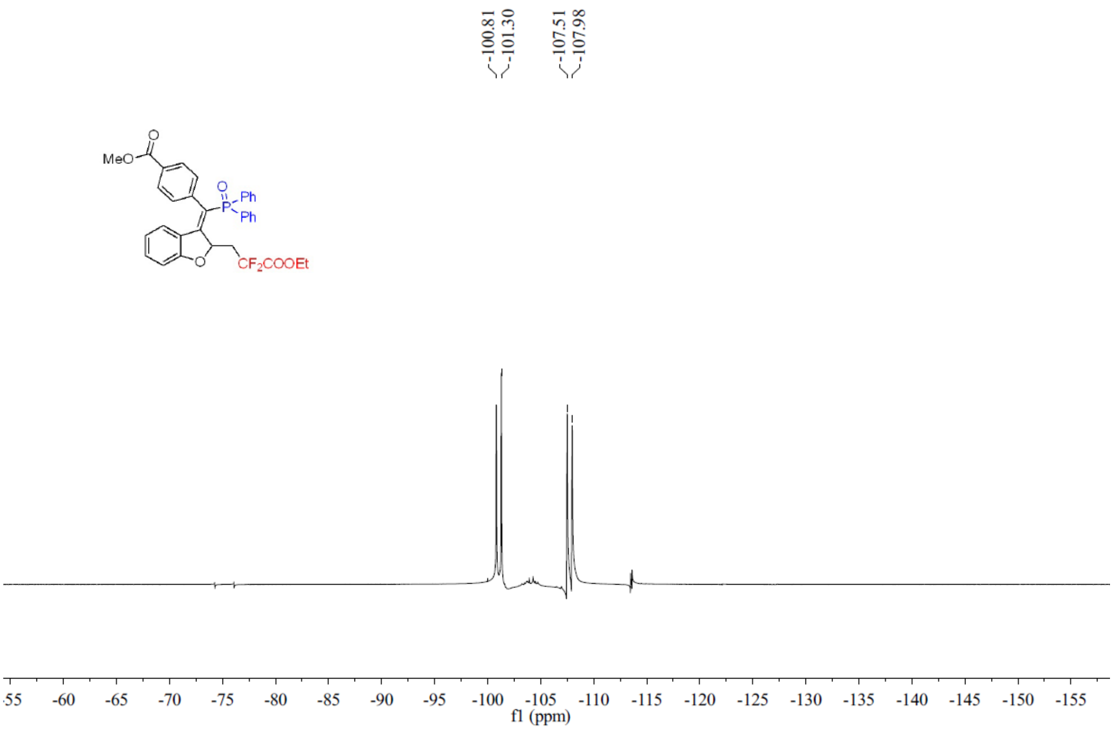
^{13}C{^{1}H}NMR (100 MHz) Spectrum of **3p** in $CDCl_3$



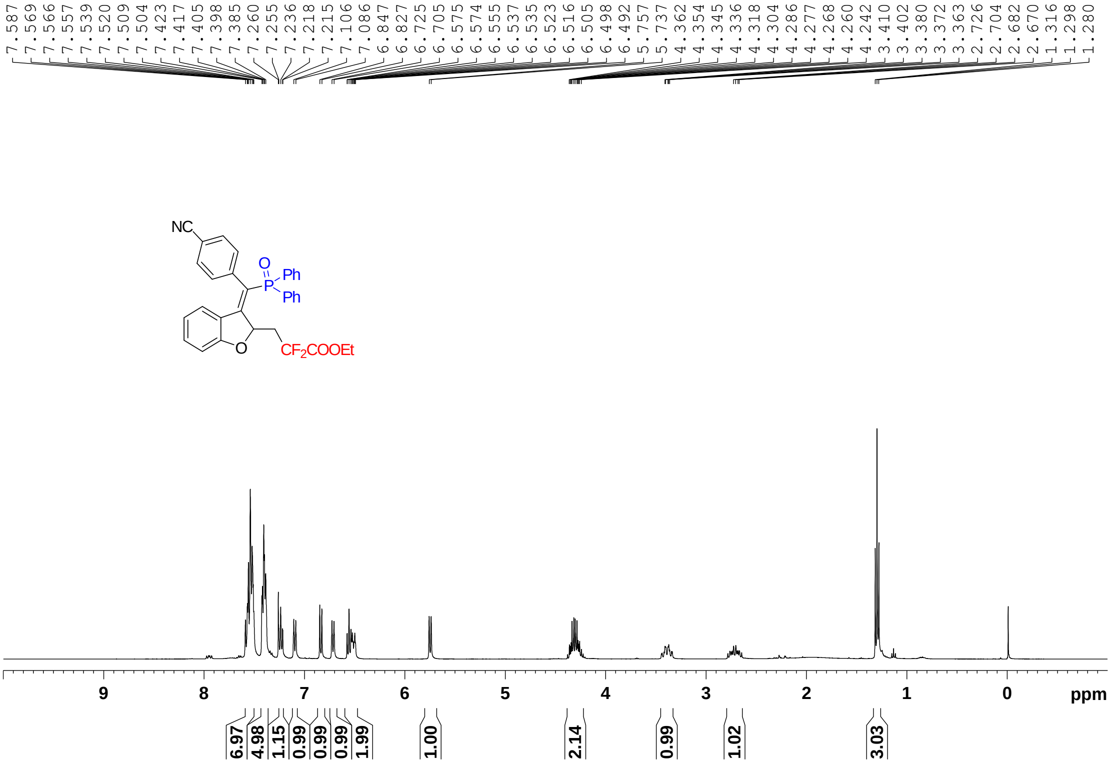
$^{31}P\{^{1}H\}$ NMR (243 MHz) Spectrum of **3p** in $CDCl_3$



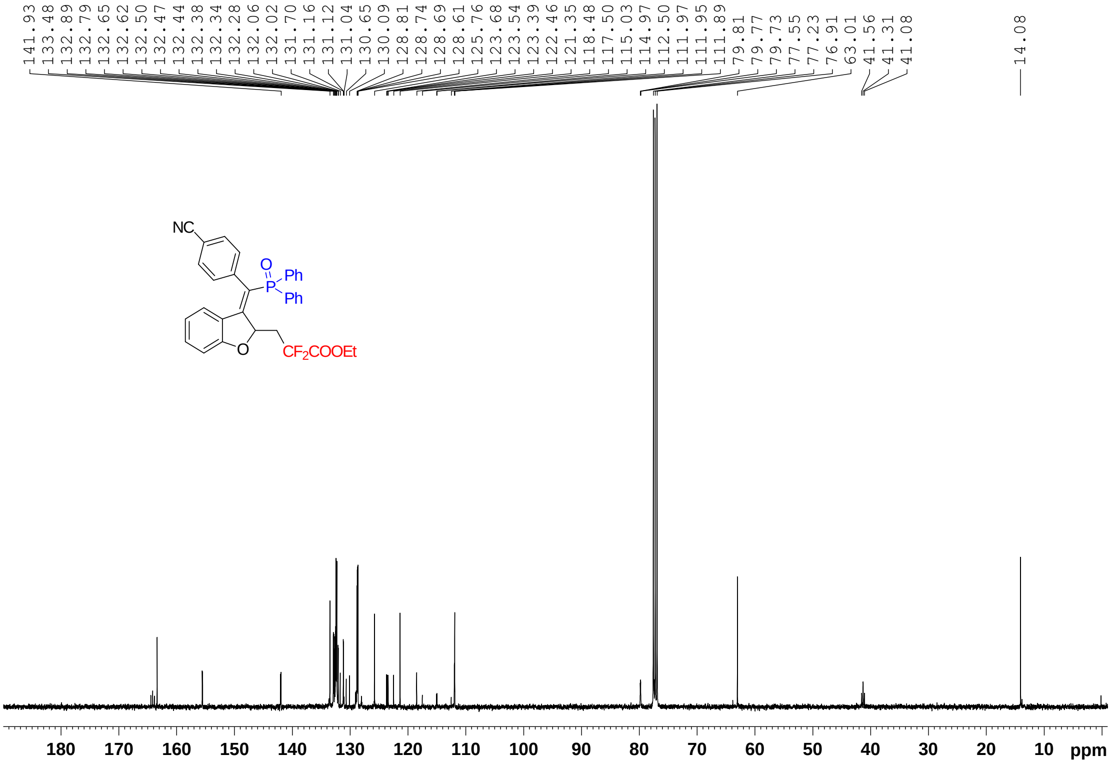
$^{19}F\{^{1}H\}$ NMR (565 MHz) Spectrum of **3p** in $CDCl_3$



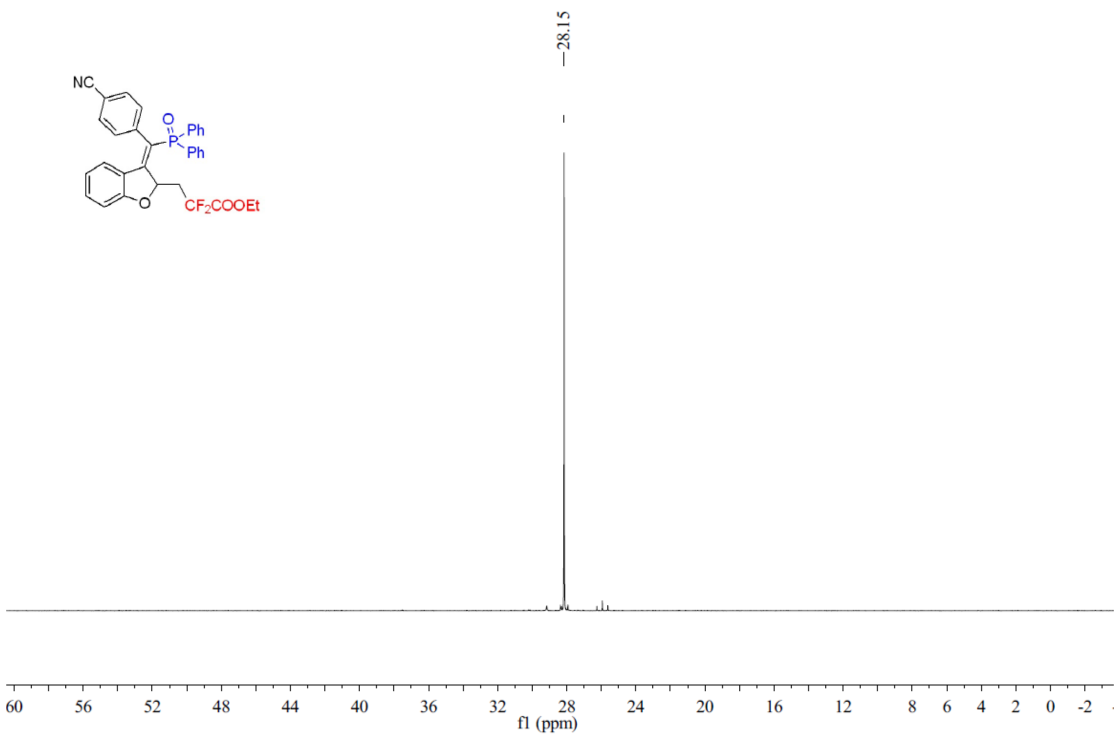
^{1}H NMR (400 MHz) Spectrum of **3q** in $CDCl_3$



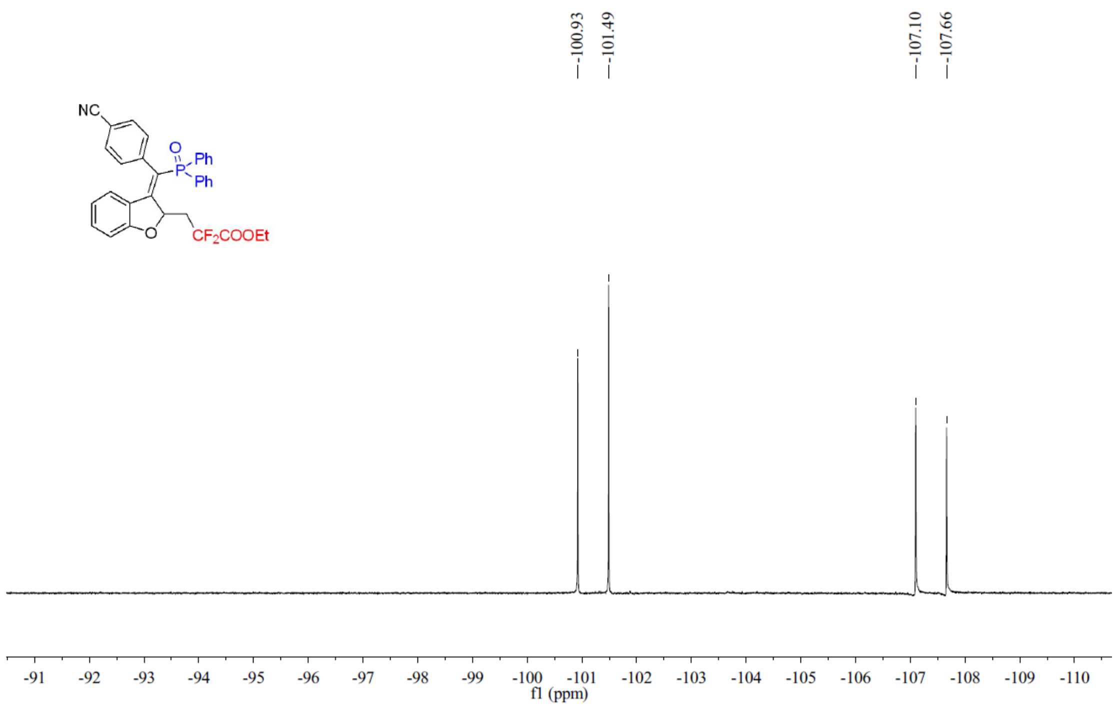
^{13}C{^{1}H}NMR (100 MHz) Spectrum of **3q** in $CDCl_3$



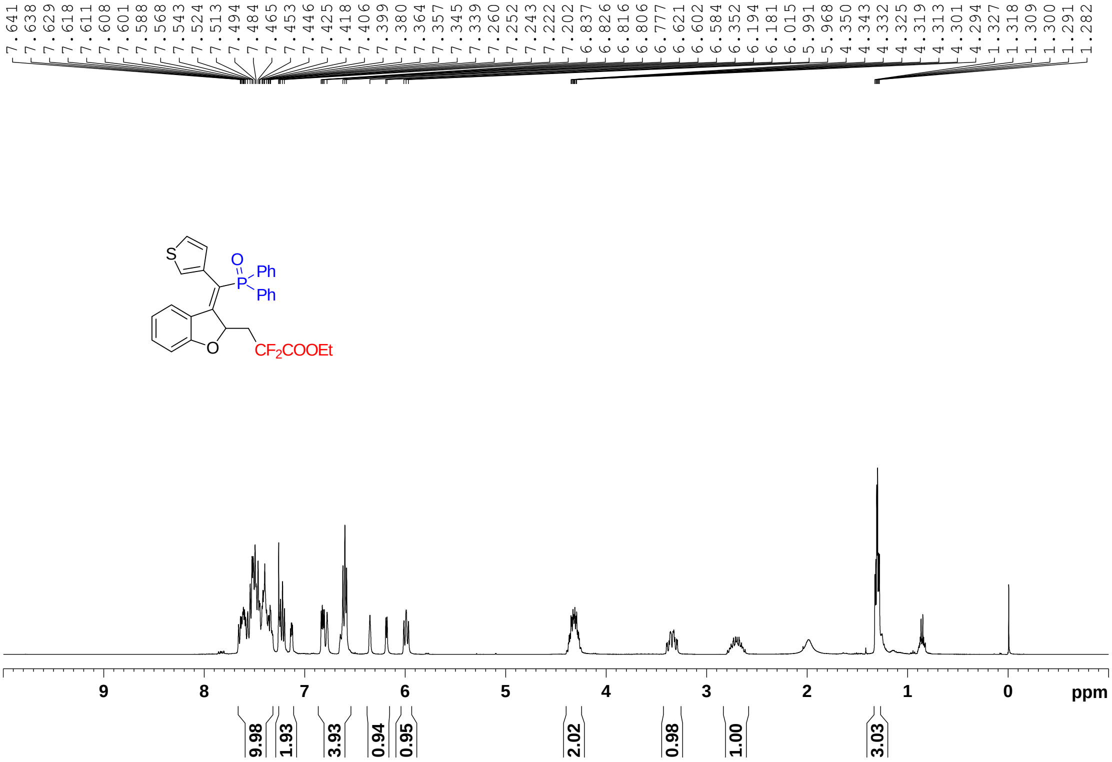
$^{31}P\{^{1}H\}$ NMR (243 MHz) Spectrum of **3q** in $CDCl_3$



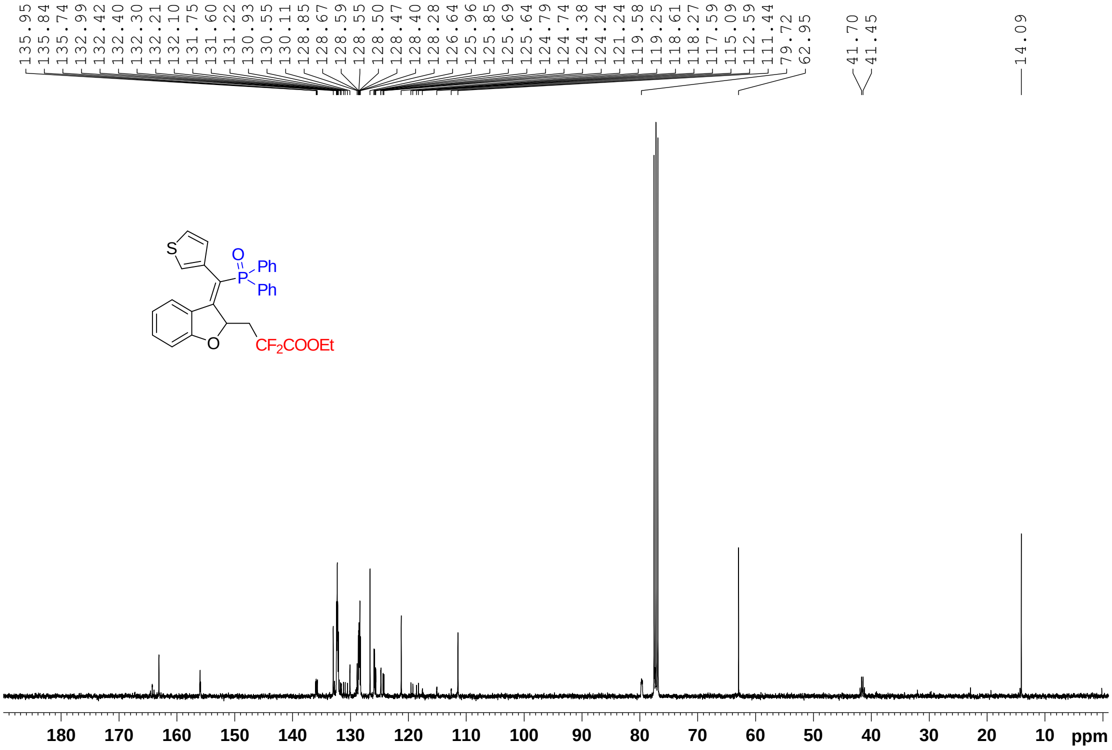
$^{19}F\{^{1}H\}$ NMR (471 MHz) Spectrum of **3q** in $CDCl_3$



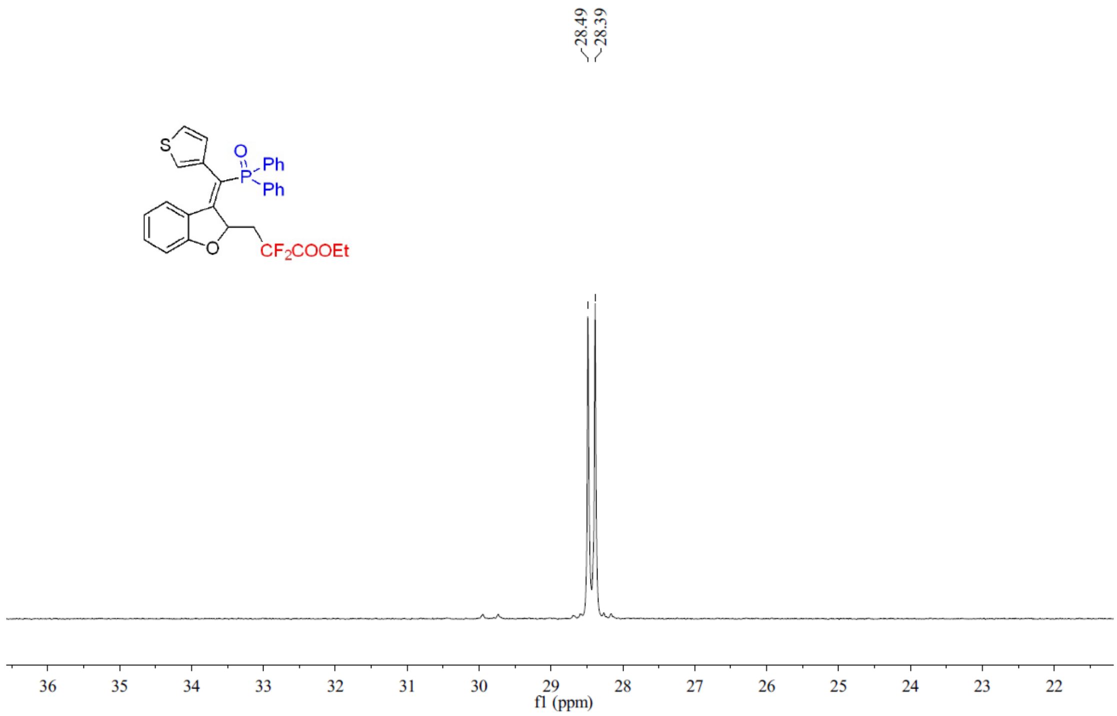
[1]H NMR (400 MHz) Spectrum of **3r** in $CDCl_3$



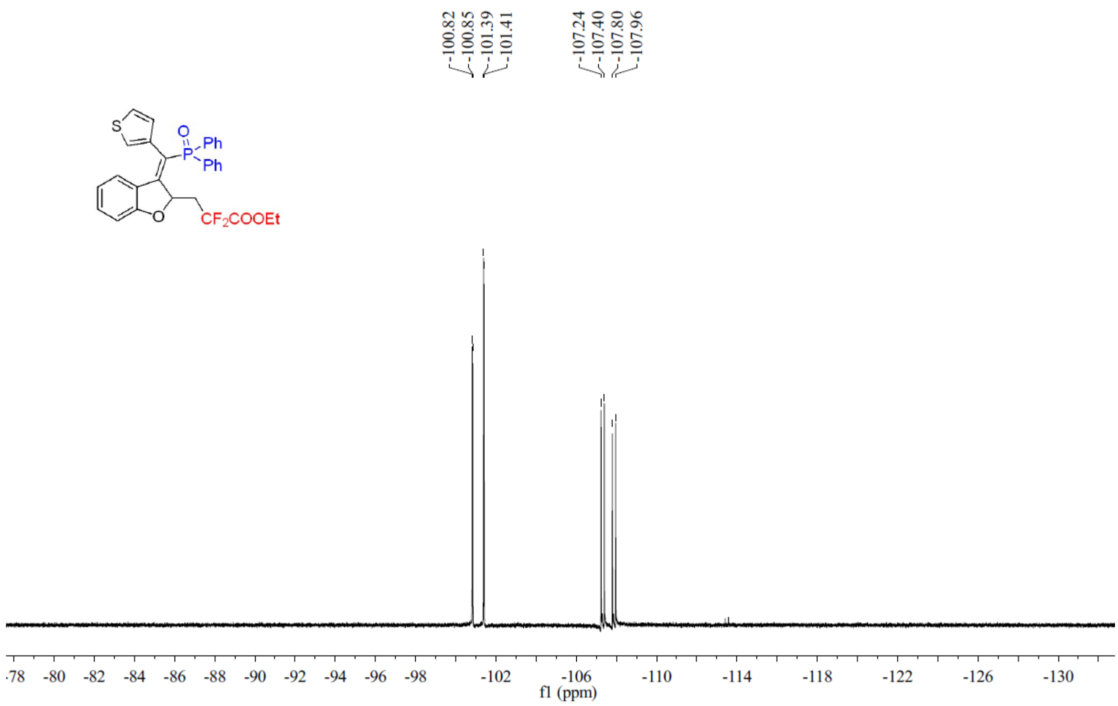
[13]C{[1]H}NMR (100 MHz) Spectrum of **3r** in $CDCl_3$



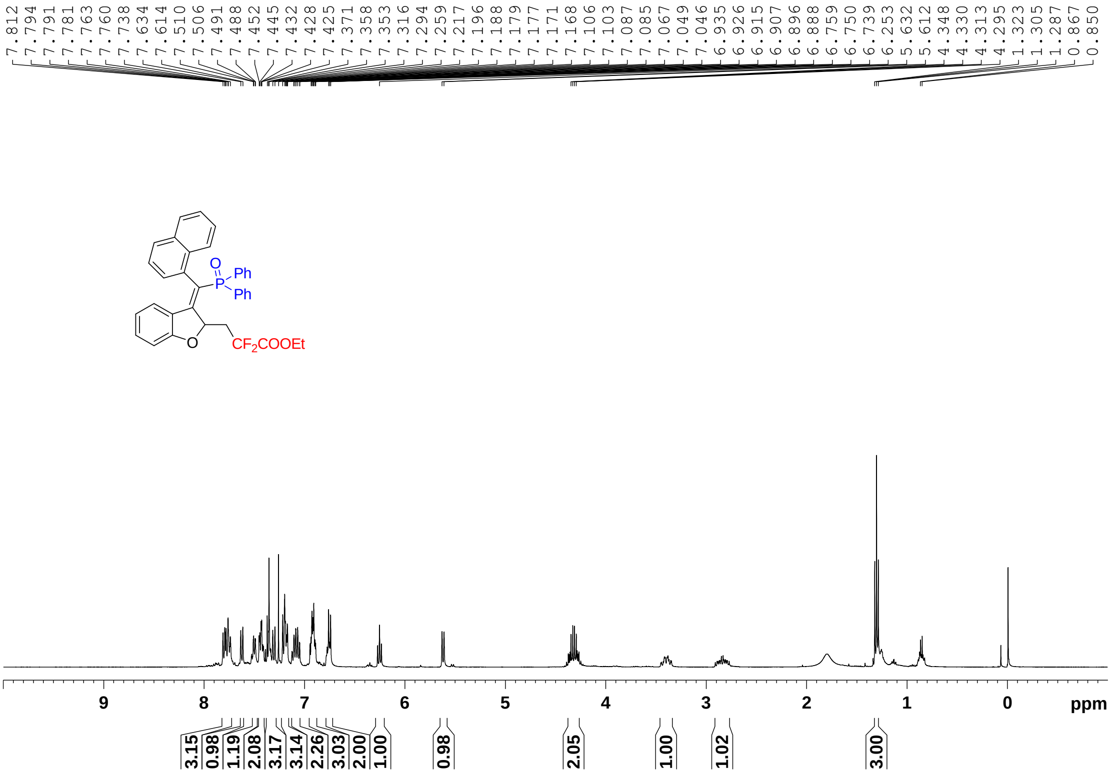
$^{31}P\{^{1}H\}$ NMR (243 MHz) Spectrum of **3r** in $CDCl_3$



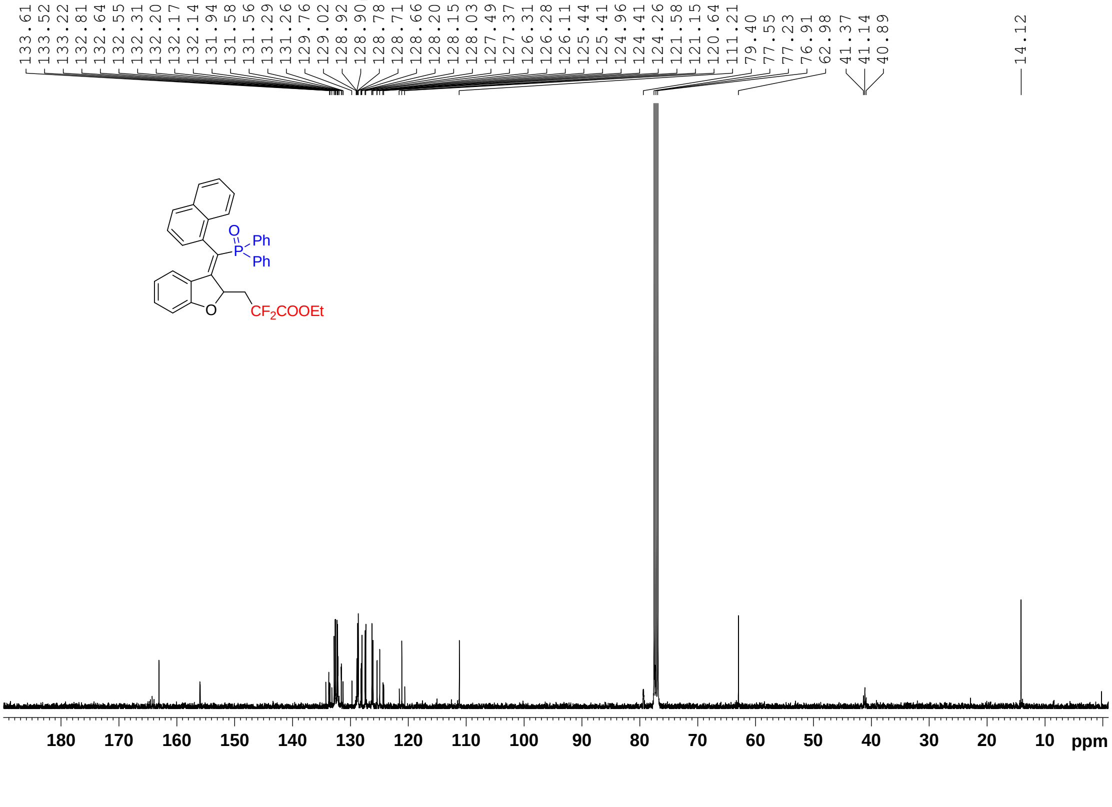
$^{19}F\{^{1}H\}$ NMR (471 MHz) Spectrum of **3r** in $CDCl_3$



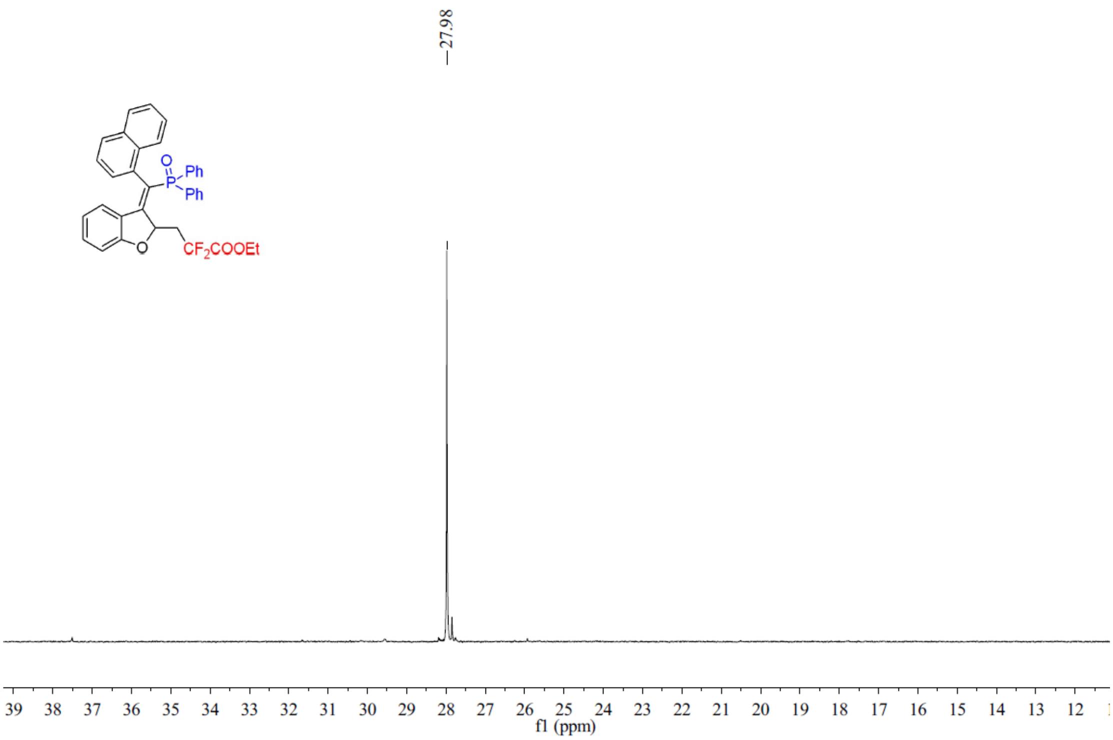
[1]H NMR (400 MHz) Spectrum of **3s** in $CDCl_3$



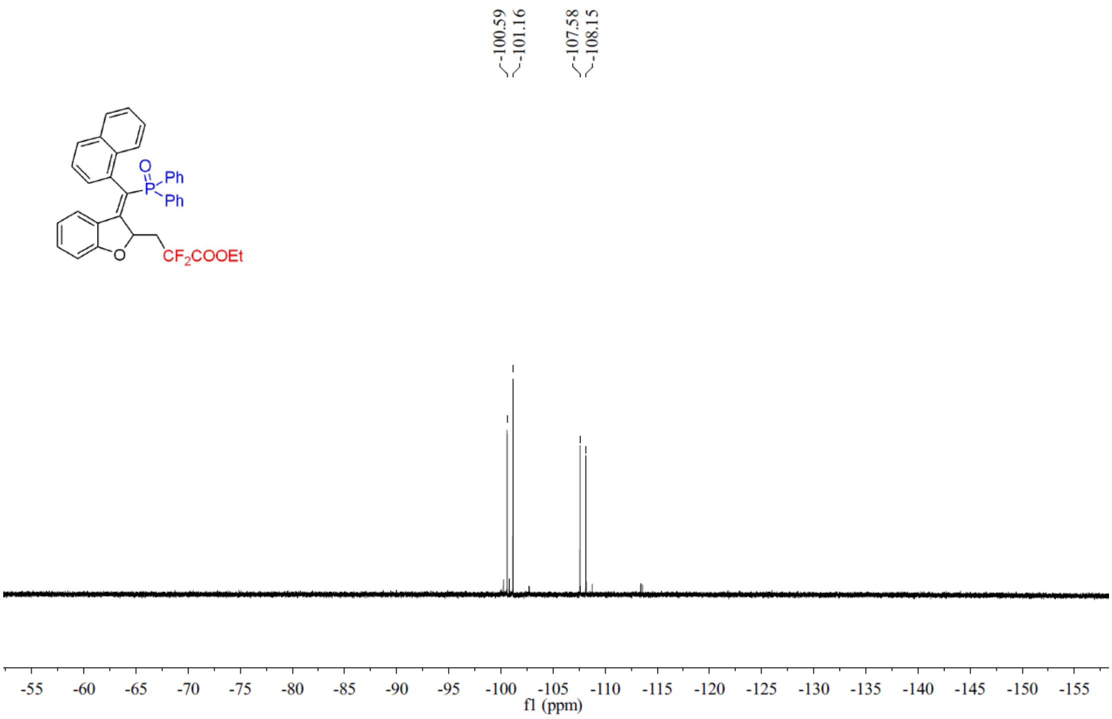
[13]C{[1]H}NMR (100 MHz) Spectrum of **3s** in $CDCl_3$



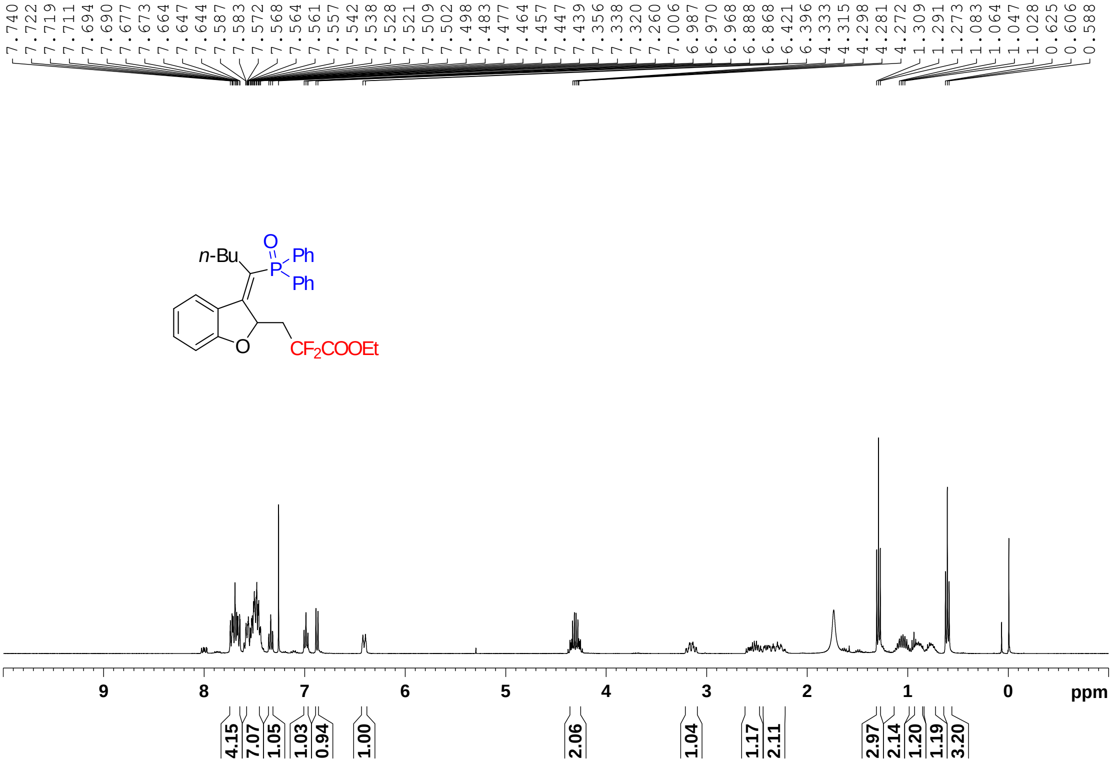
$^{31}P\{^{1}H\}$ NMR (243 MHz) Spectrum of **3s** in $CDCl_3$



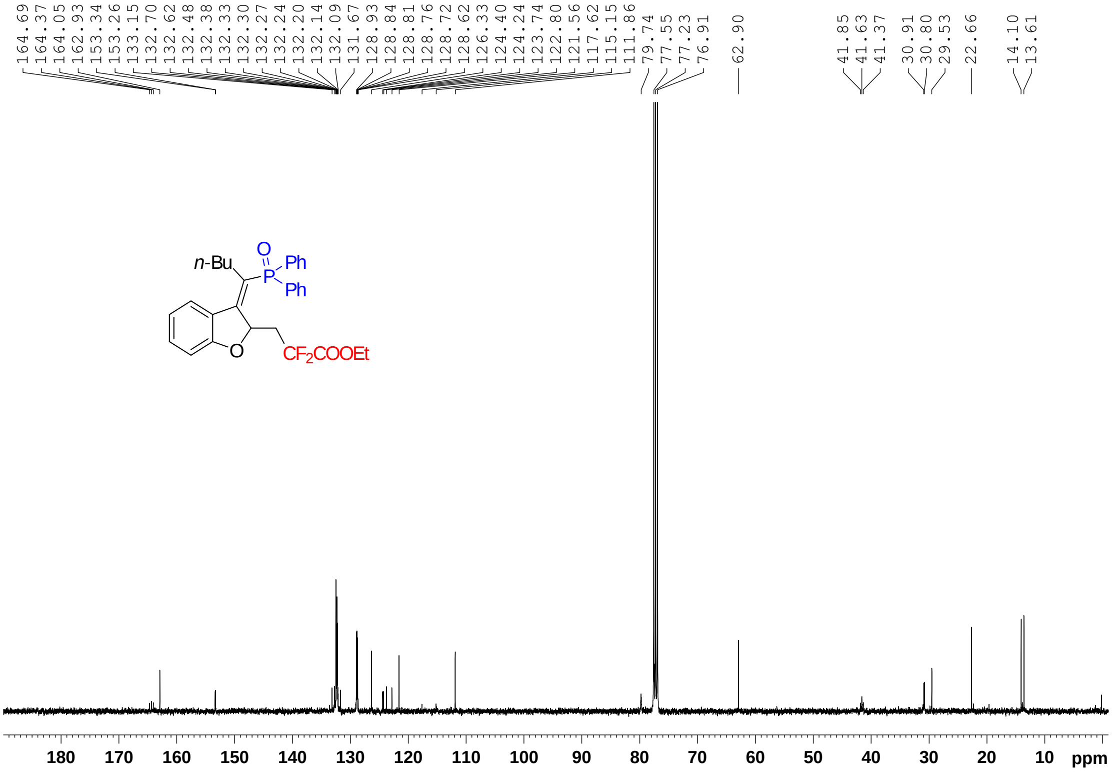
$^{19}F\{^{1}H\}$ NMR (471 MHz) Spectrum of **3s** in $CDCl_3$



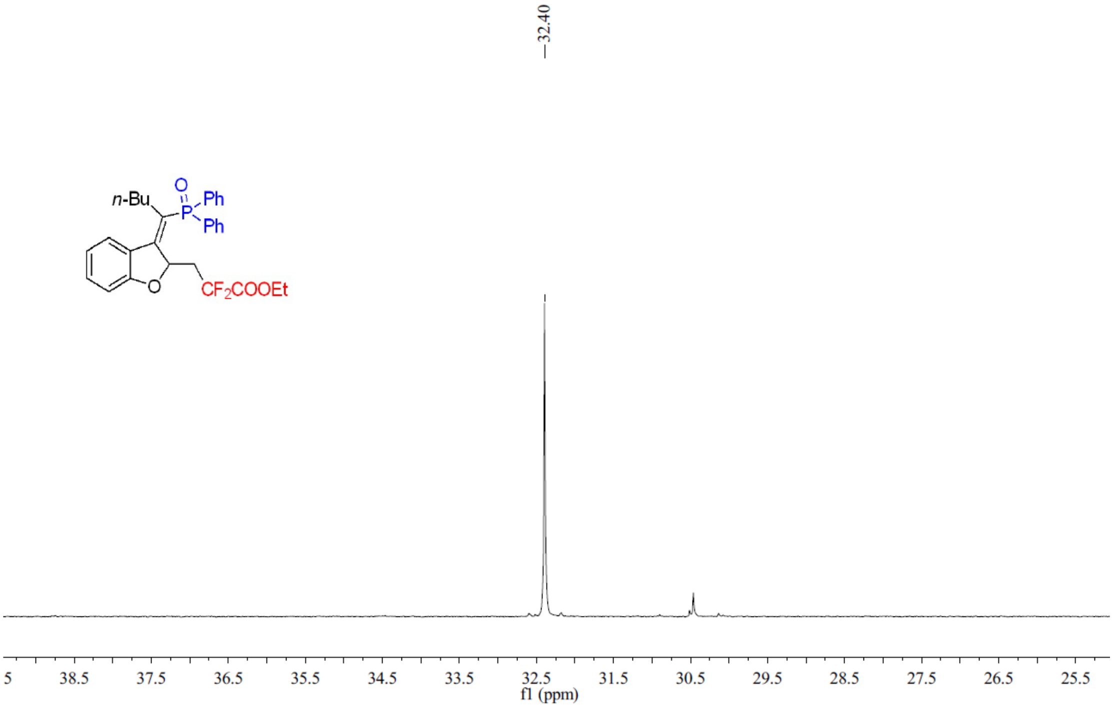
[1]H NMR (400 MHz) Spectrum of **3t** in $CDCl_3$



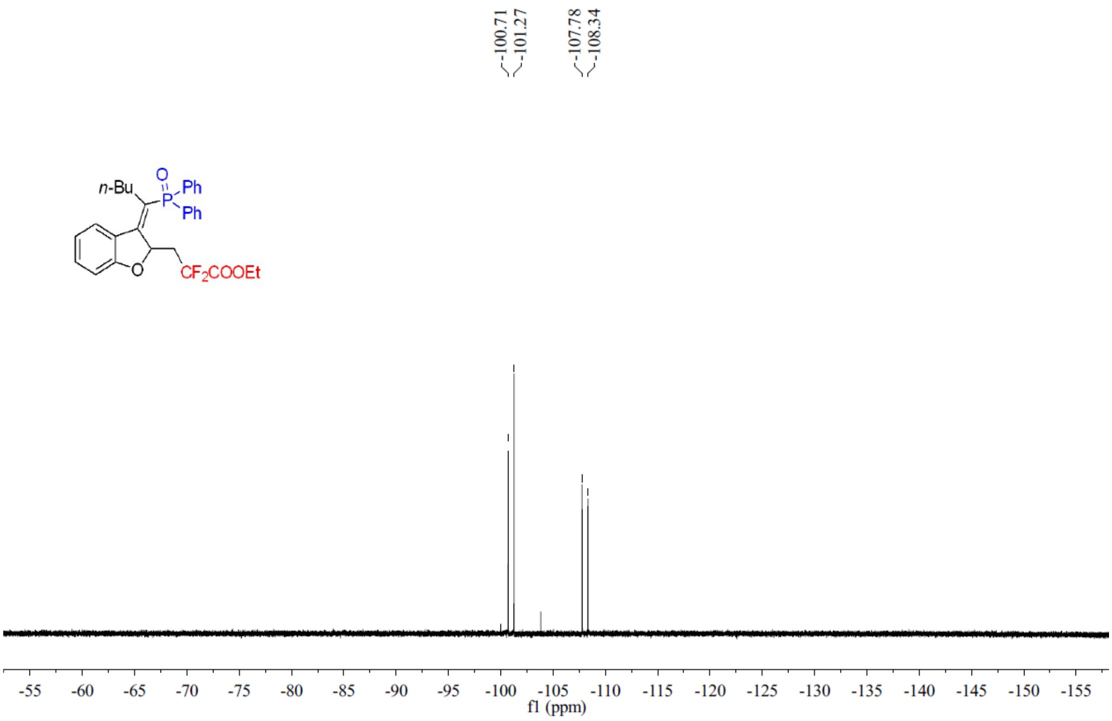
[13]C{[1]H}NMR (100 MHz) Spectrum of **3t** in $CDCl_3$



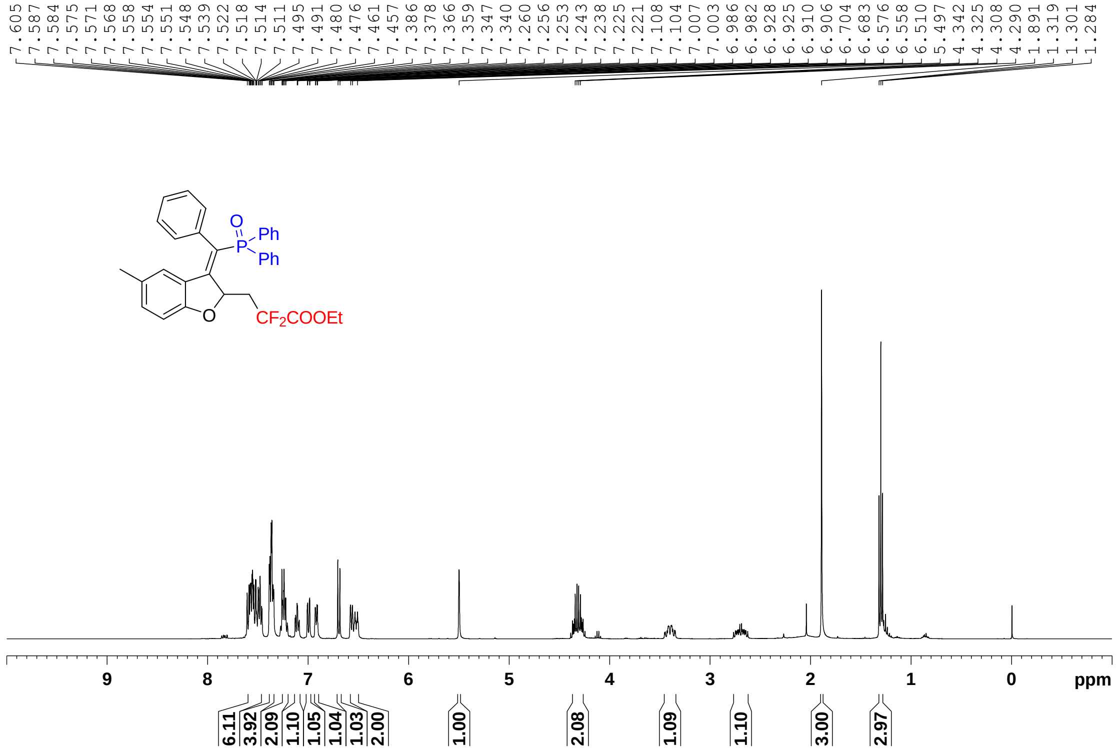
$^{31}P\{^1H\}$ NMR (243 MHz) Spectrum of **3t** in $CDCl_3$



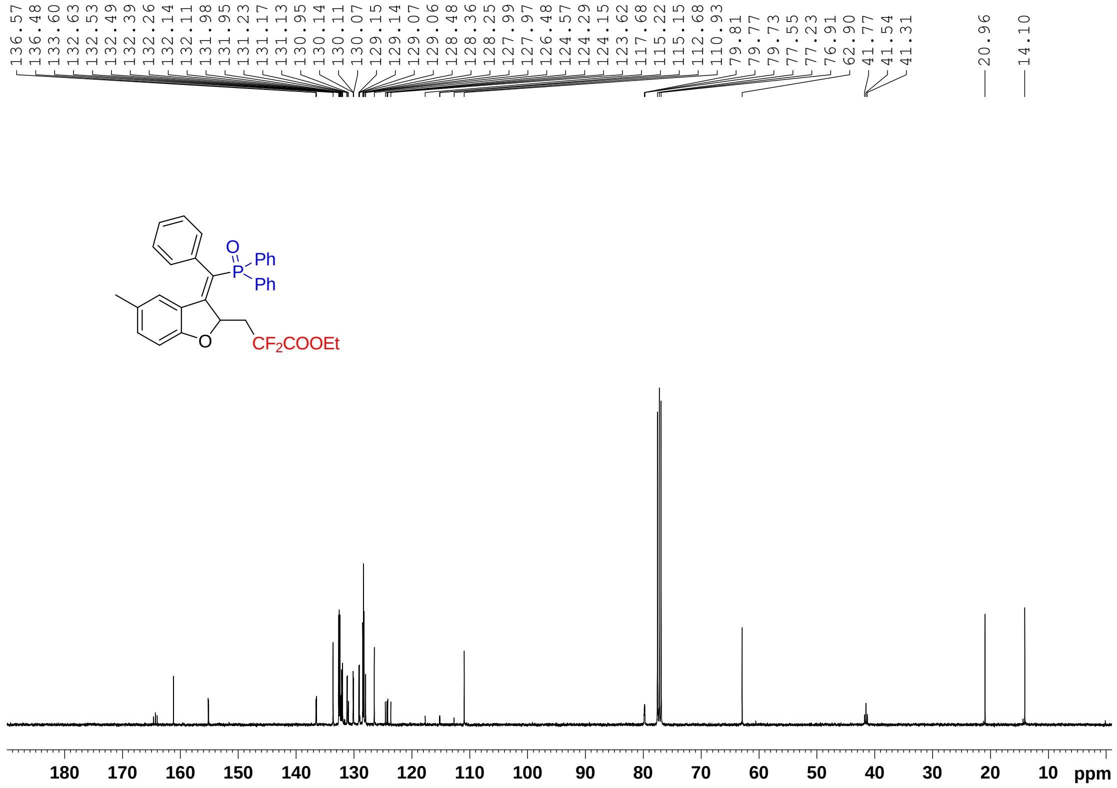
$^{19}F\{^1H\}$ NMR (471 MHz) Spectrum of **3t** in $CDCl_3$



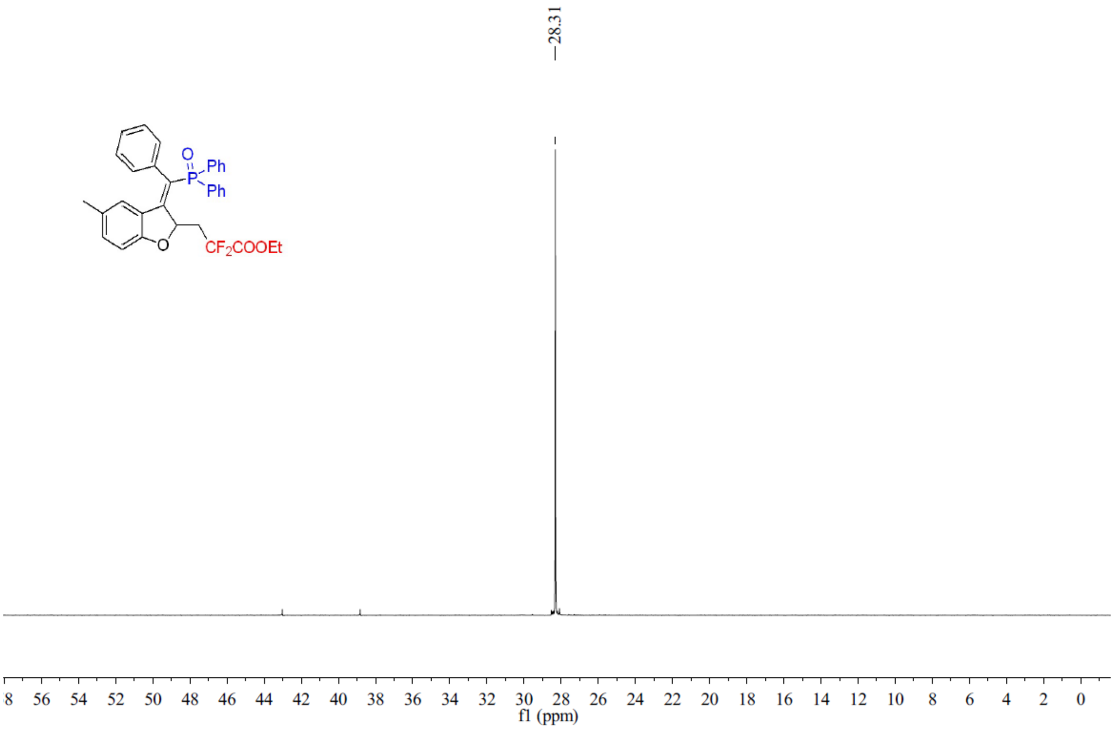
^{1}H NMR (400 MHz) Spectrum of **3u** in $CDCl_3$



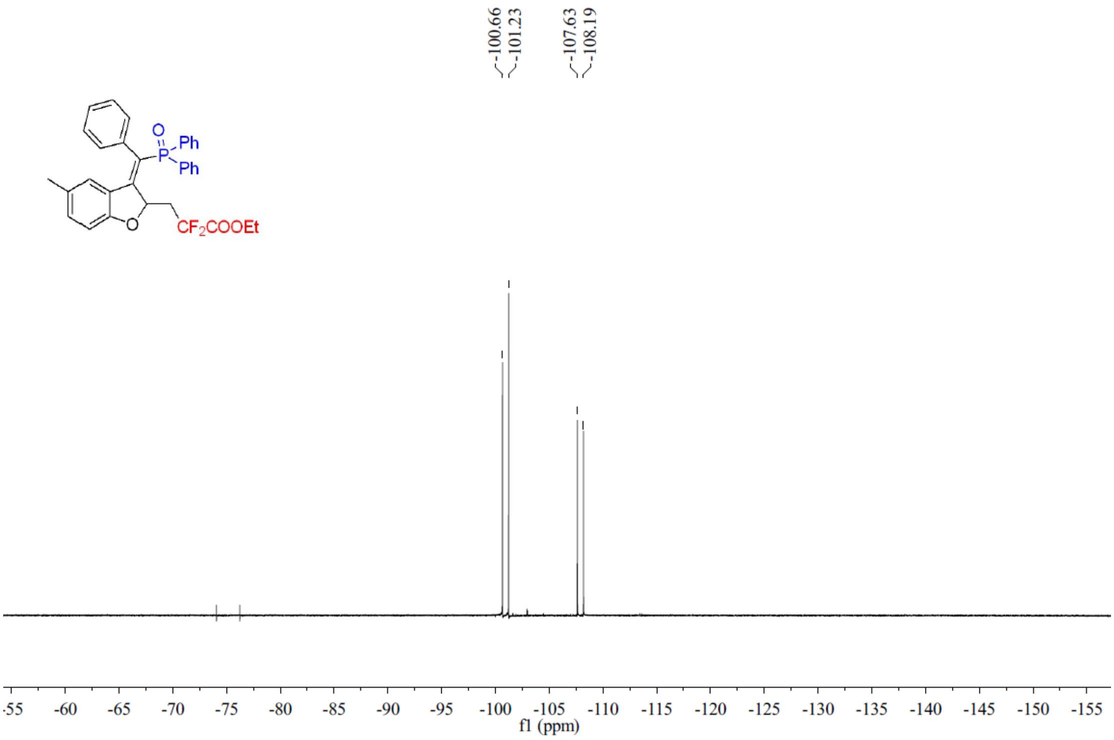
^{13}C{^{1}H}NMR (100 MHz) Spectrum of **3u** in $CDCl_3$



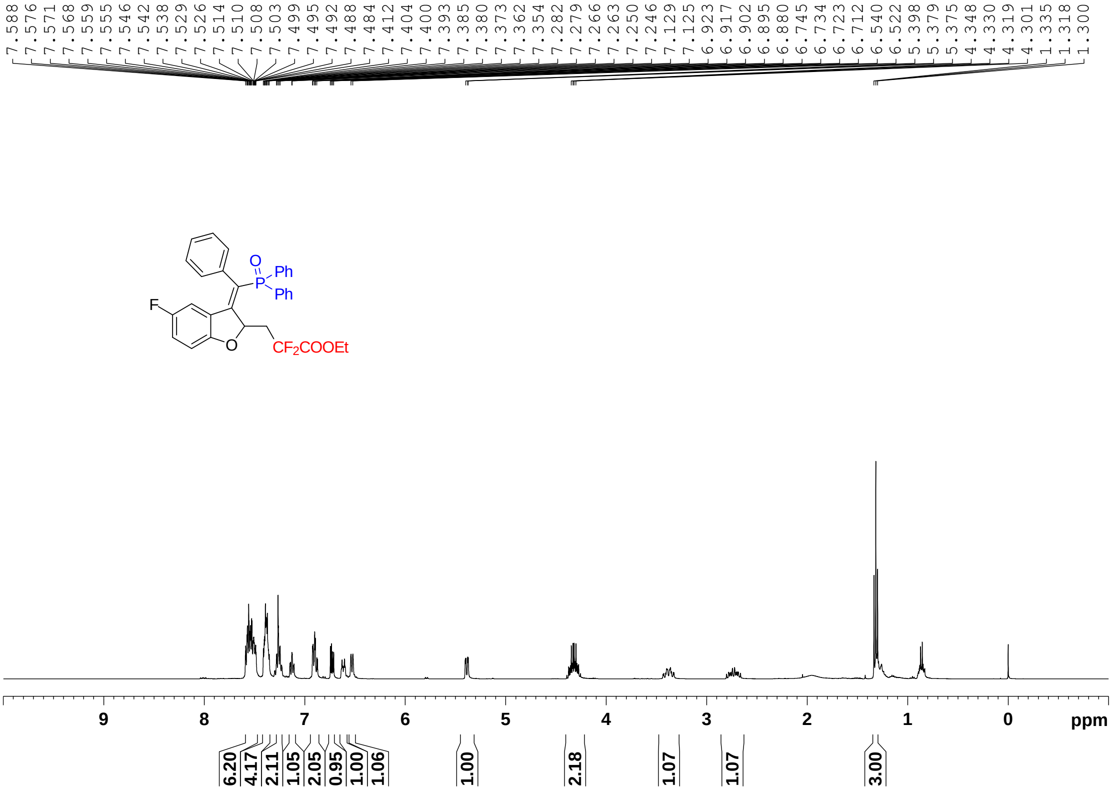
$^{31}P\{^{1}H\}$ NMR (243 MHz) Spectrum of **3u** in $CDCl_3$



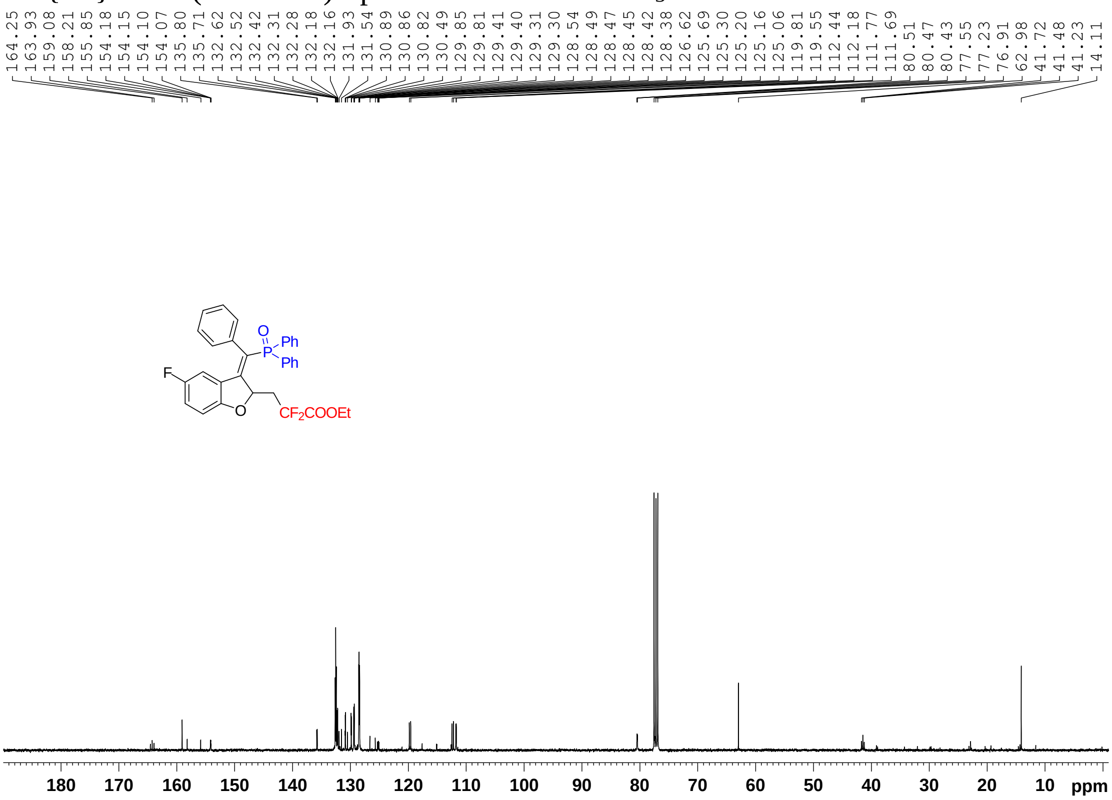
$^{19}F\{^{1}H\}$ NMR (471 MHz) Spectrum of **3u** in $CDCl_3$



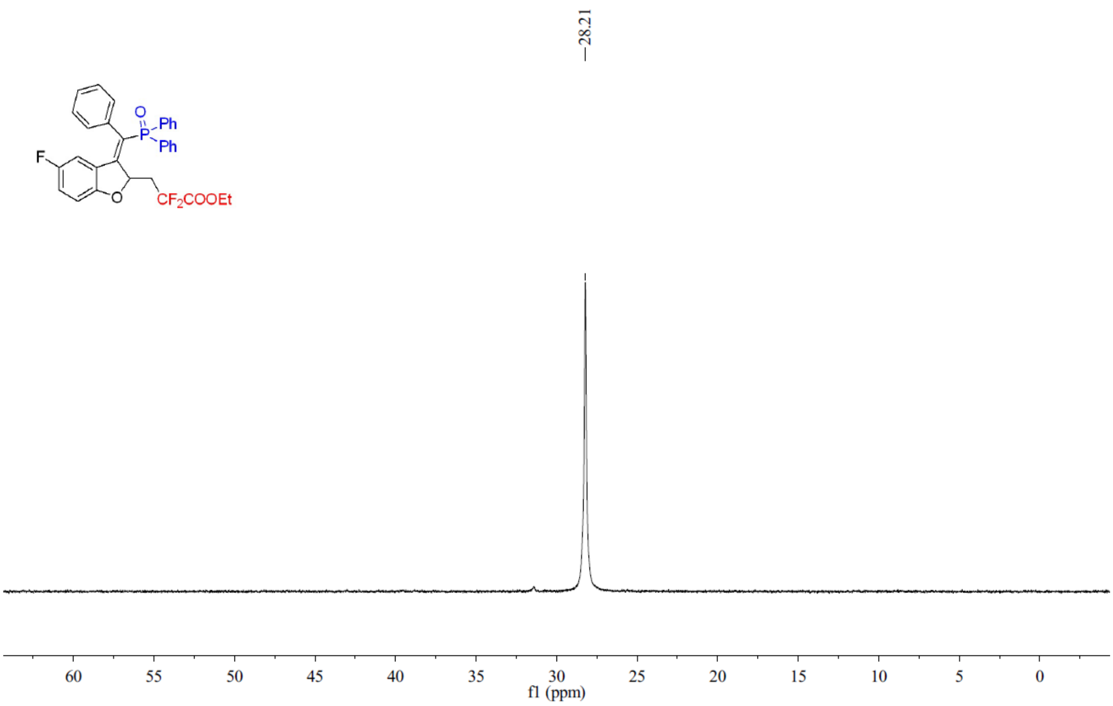
[1]H NMR (400 MHz) Spectrum of **3v** in $CDCl_3$



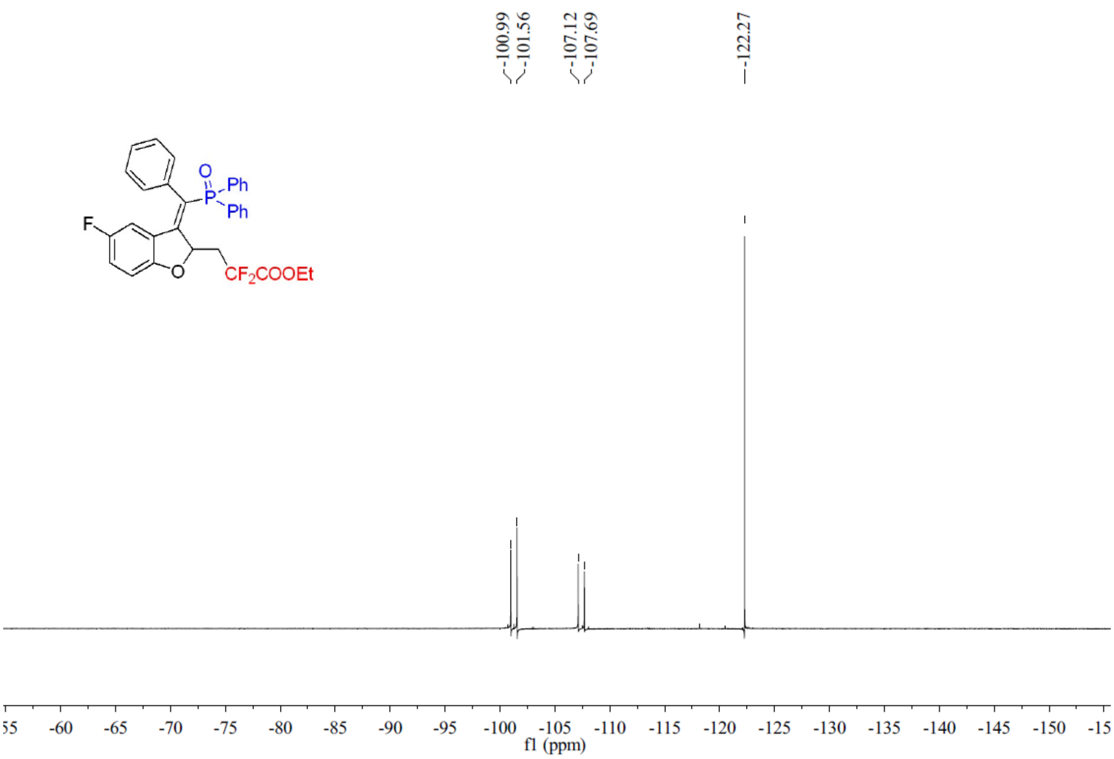
[13]C{[1]H}NMR (100 MHz) Spectrum of **3v** in $CDCl_3$



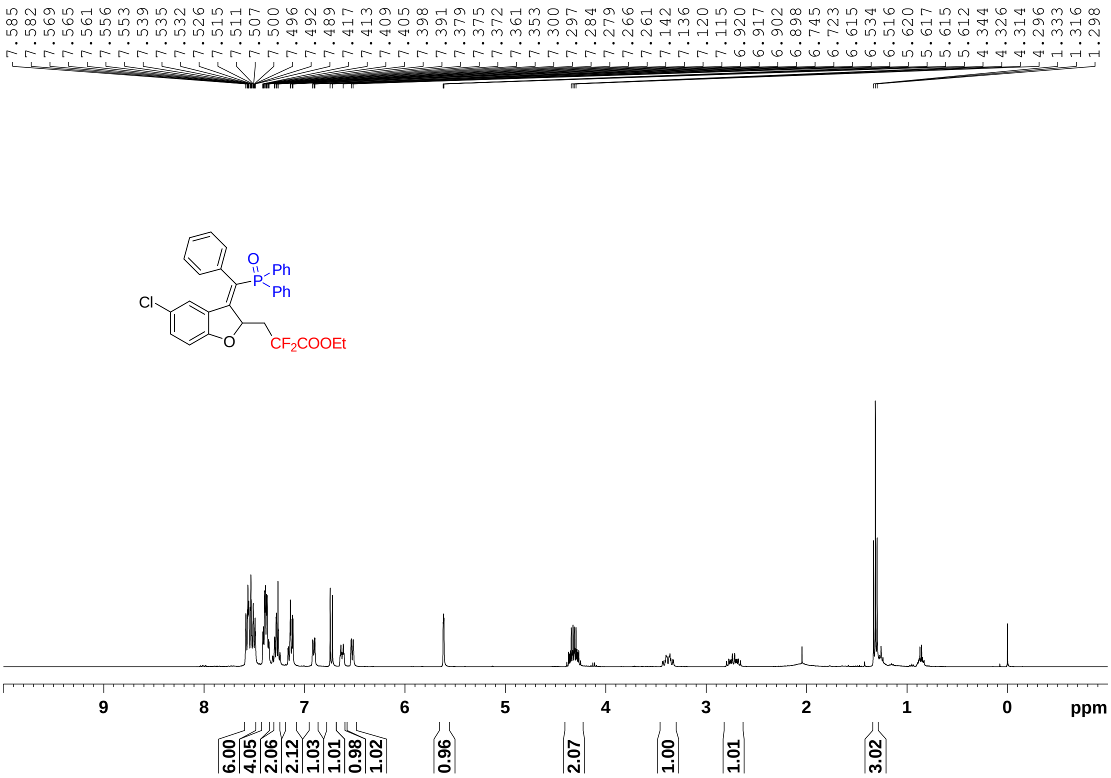
$^{31}P\{^1H\}$ NMR (243 MHz) Spectrum of **3v** in $CDCl_3$



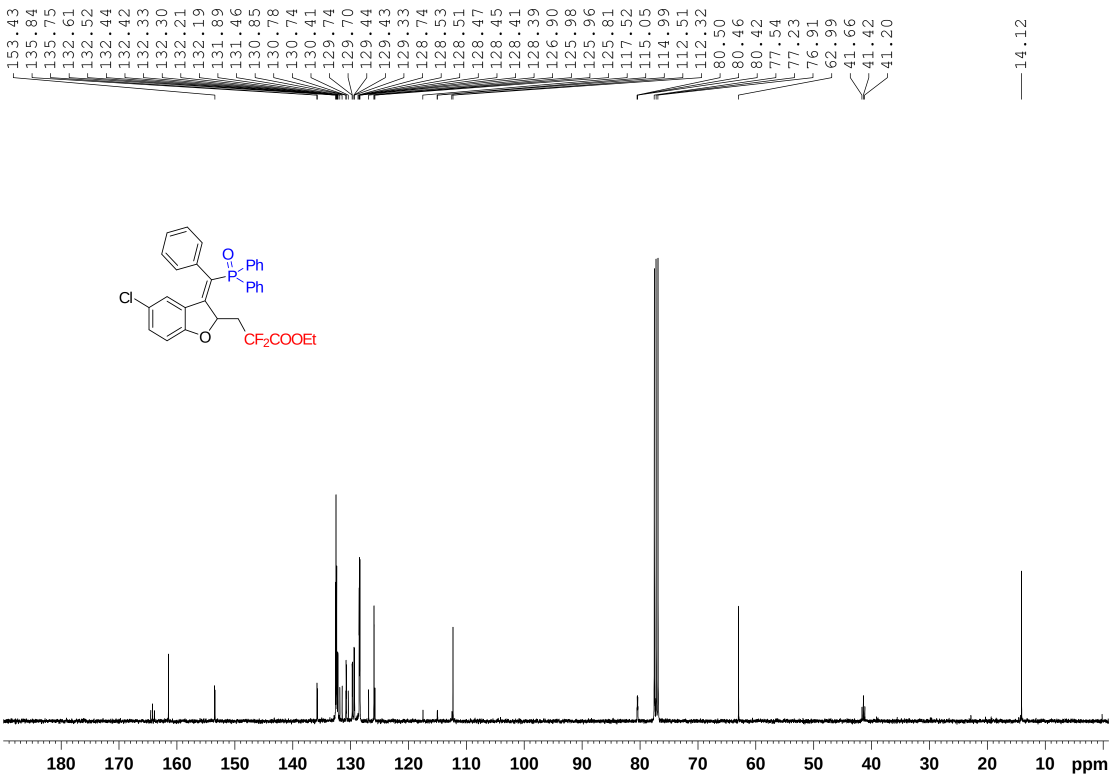
$^{19}F\{^1H\}$ NMR (471 MHz) Spectrum of **3v** in $CDCl_3$



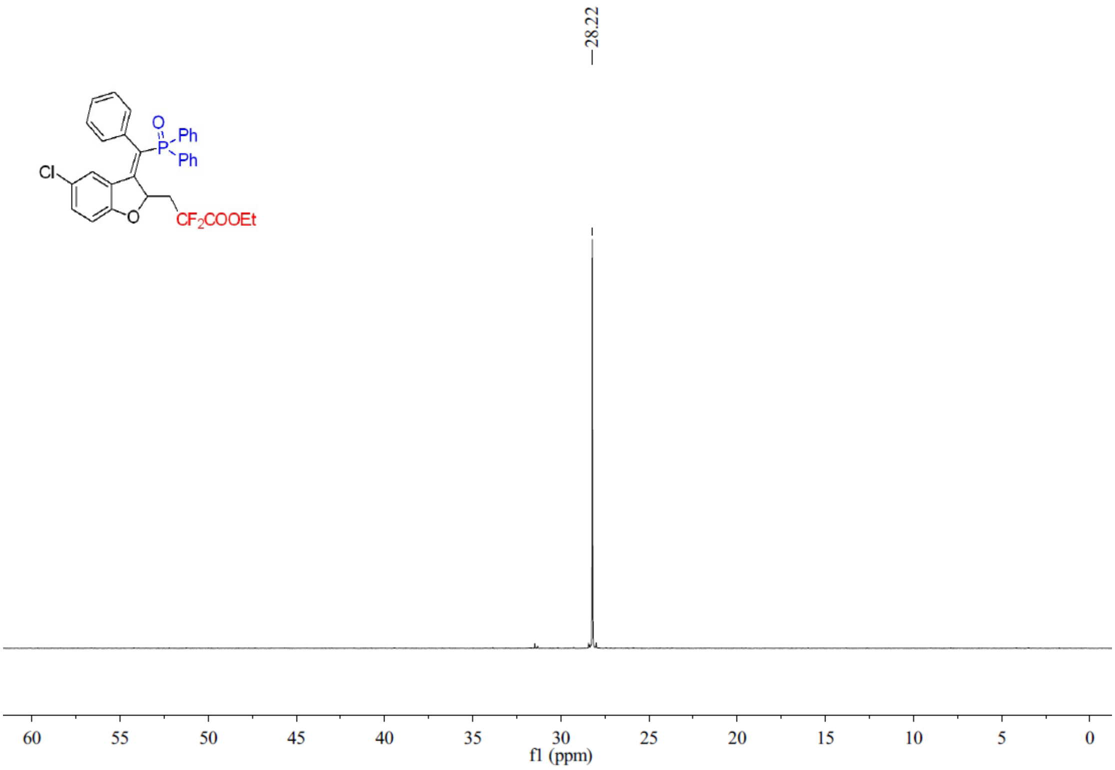
^{1}H NMR (400 MHz) Spectrum of **3w** in $CDCl_3$



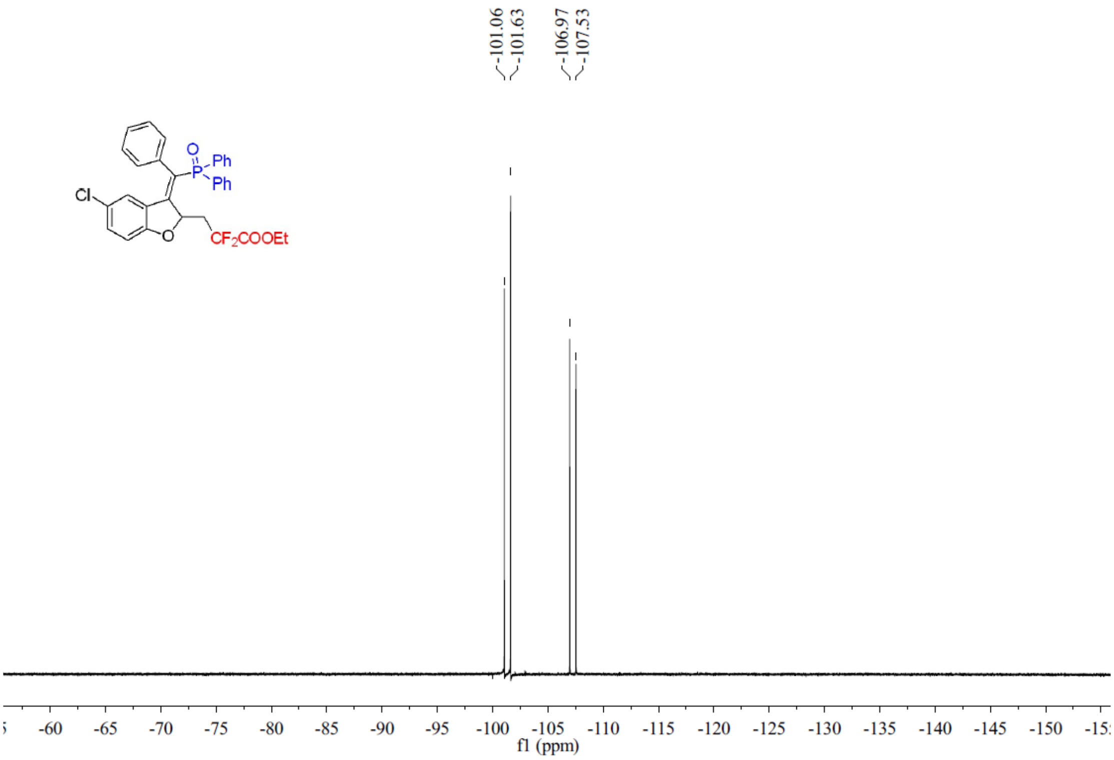
$^{13}C\{^{1}H\}$NMR (100 MHz) Spectrum of **3w** in $CDCl_3$



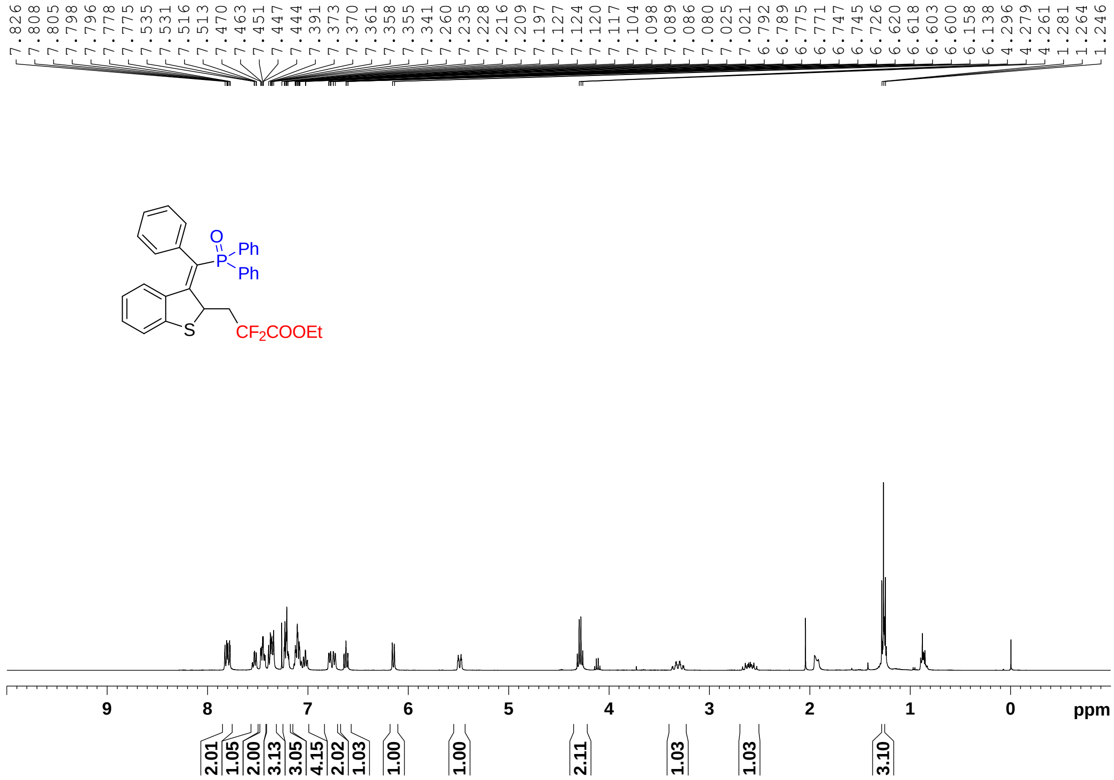
$^{31}P\{^1H\}$ NMR (243 MHz) Spectrum of **3w** in $CDCl_3$



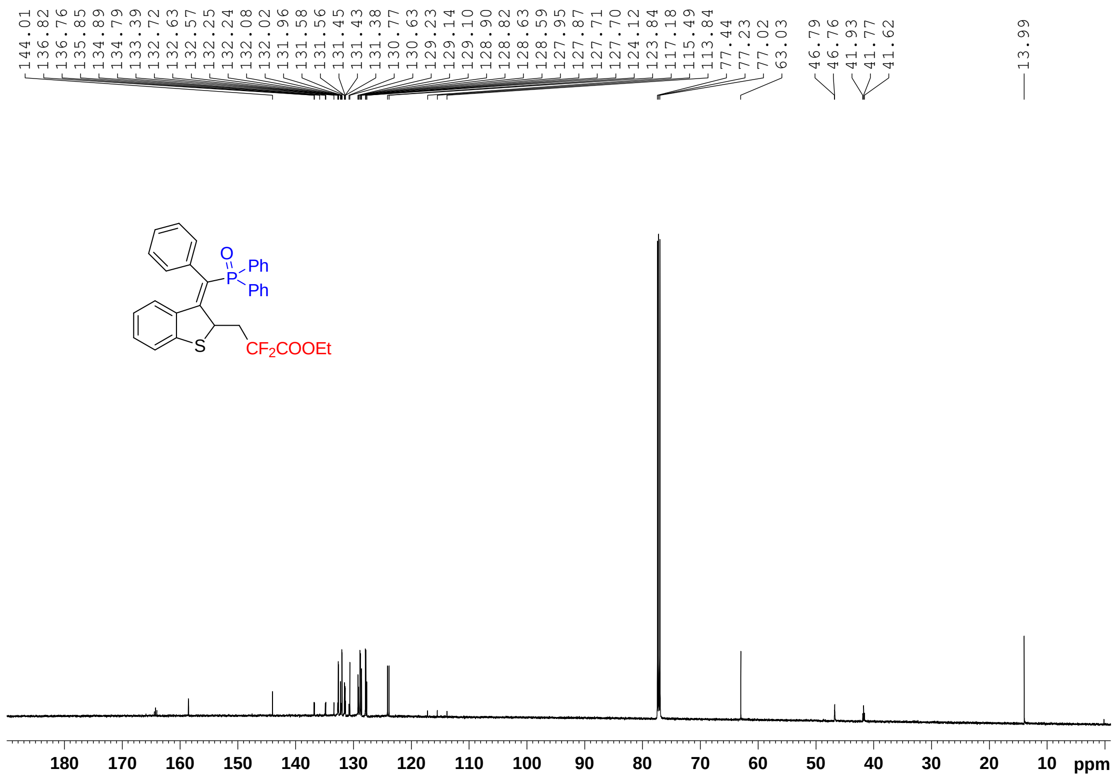
$^{19}F\{^1H\}$ NMR (471 MHz) Spectrum of **3w** in $CDCl_3$



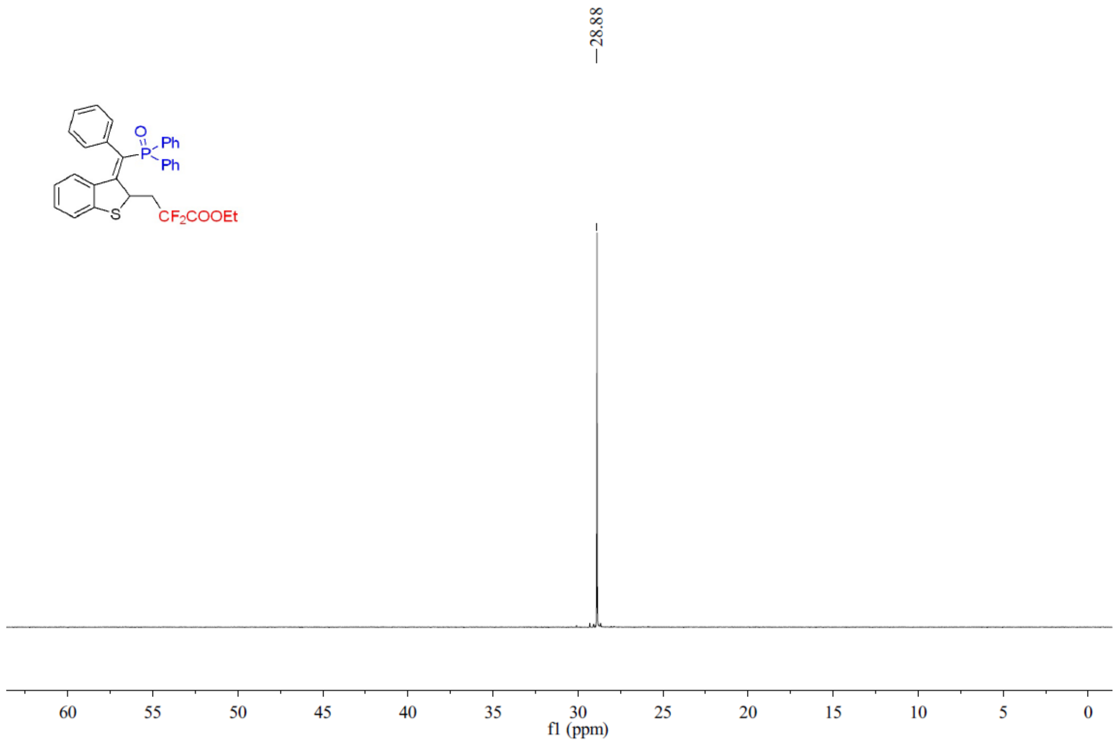
[1]H NMR (400 MHz) Spectrum of **3x** in $CDCl_3$



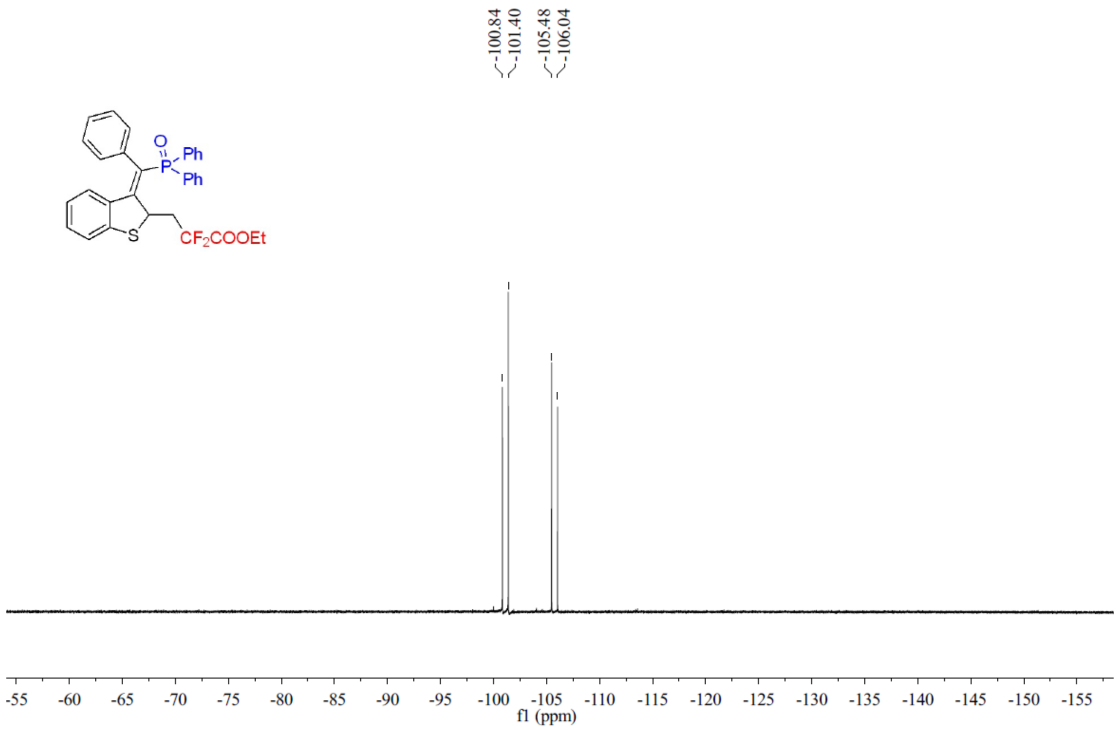
[13]C{[1]H}NMR (100 MHz) Spectrum of **3x** in $CDCl_3$



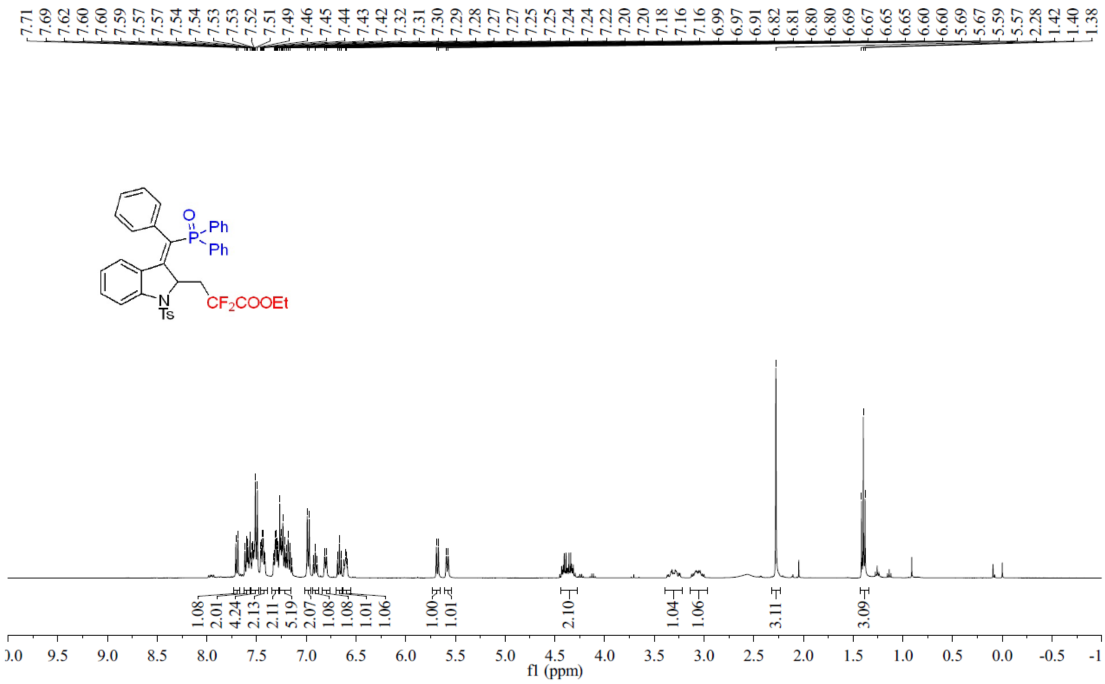
$^{31}P\{^{1}H\}$ NMR (243 MHz) Spectrum of **3x** in $CDCl_3$



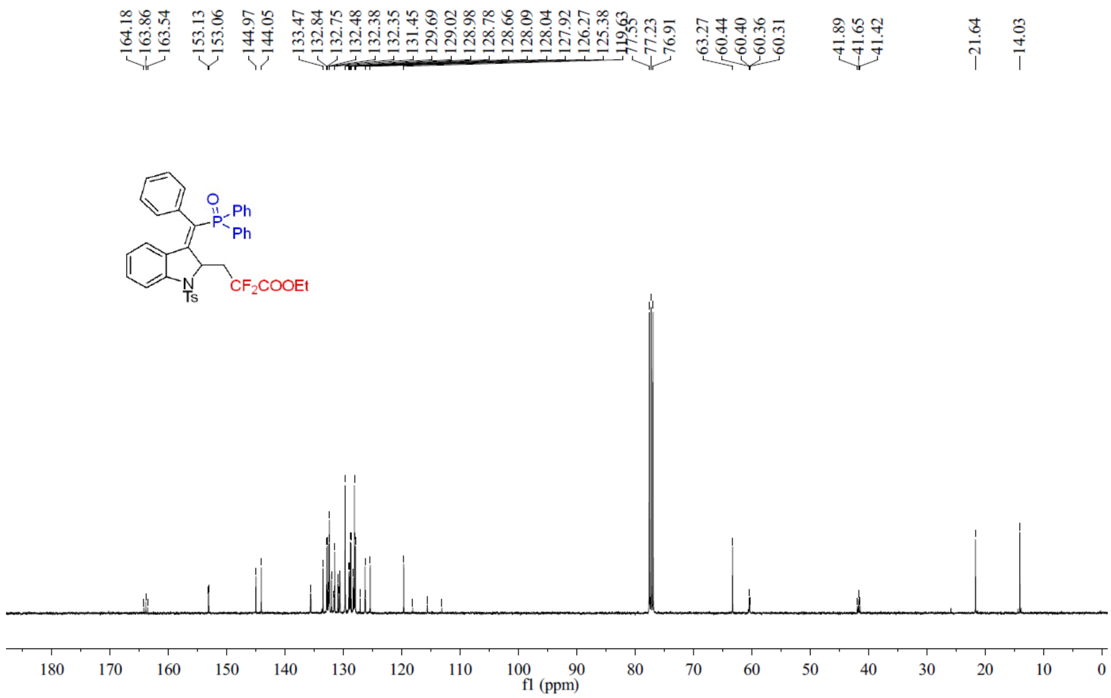
$^{19}F\{^{1}H\}$ NMR (471 MHz) Spectrum of **3x** in $CDCl_3$



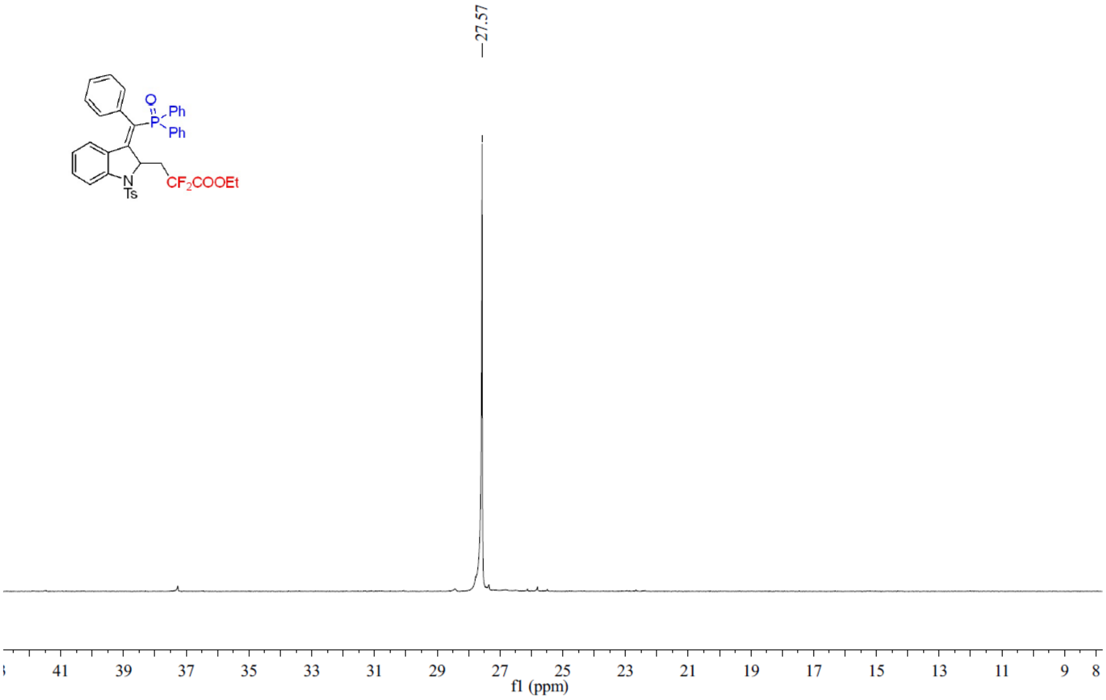
^{1}H NMR (400 MHz) Spectrum of **3y** in $CDCl_3$



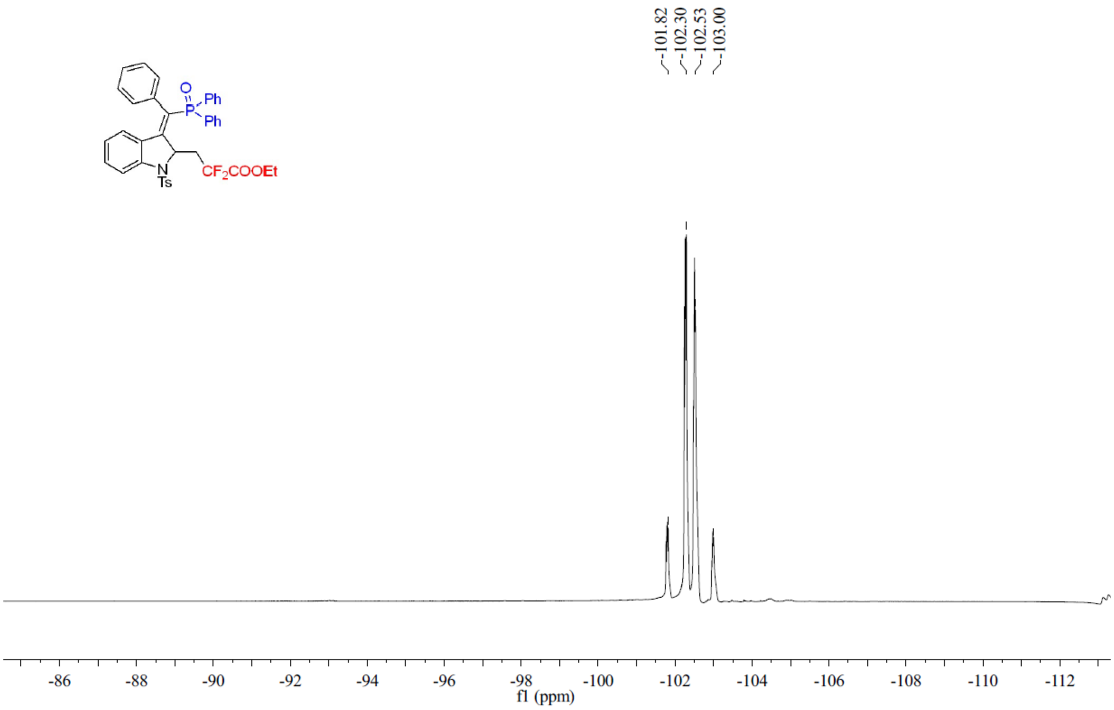
^{13}C{^{1}H}NMR (100 MHz) Spectrum of **3y** in $CDCl_3$



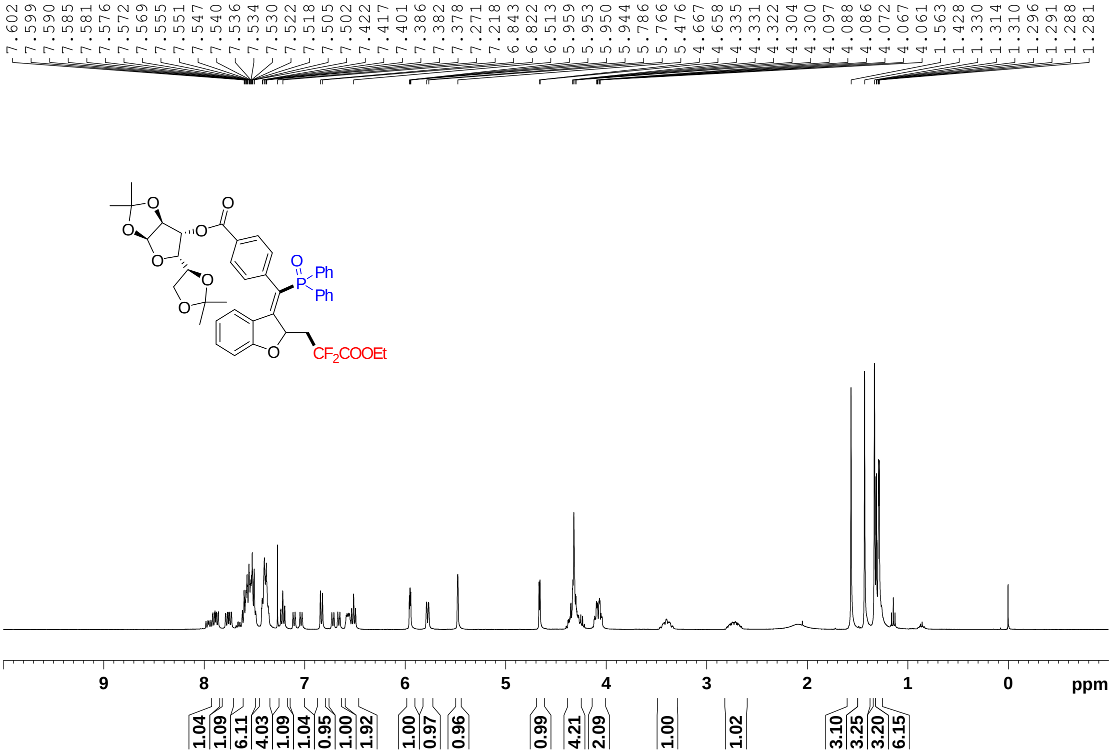
$^{31}P\{^1H\}$ NMR (243 MHz) Spectrum of **3y** in $CDCl_3$



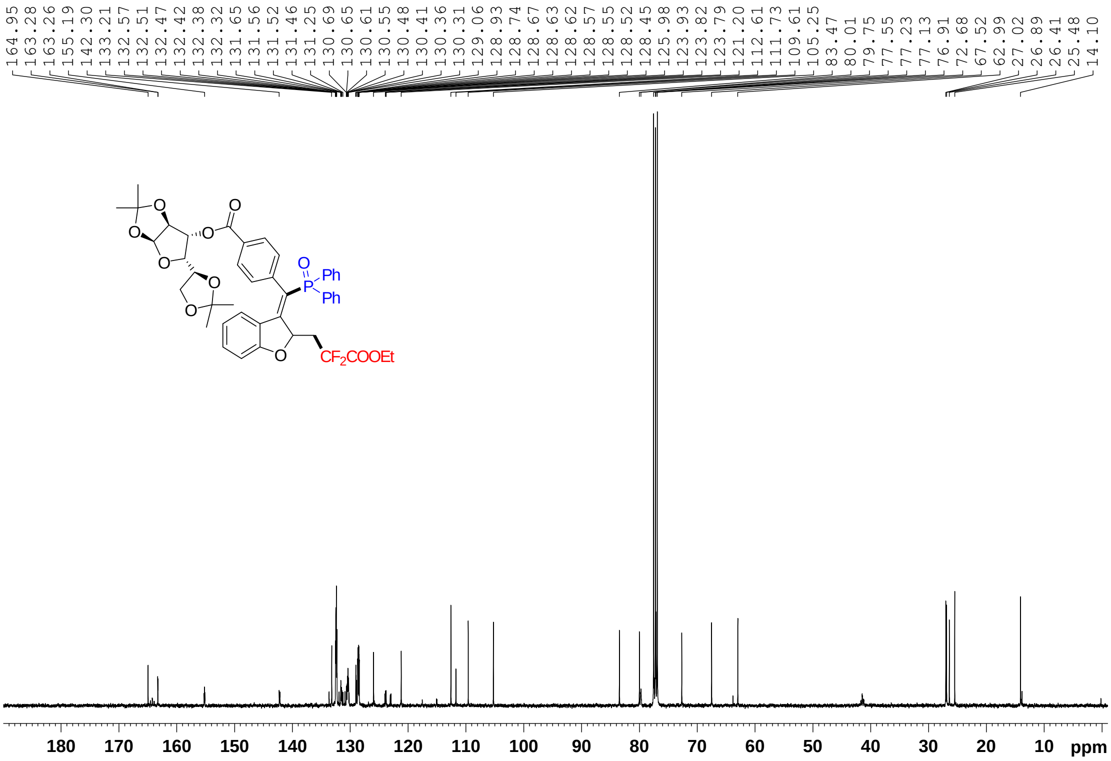
$^{19}F\{^1H\}$ NMR (565 MHz) Spectrum of **3y** in $CDCl_3$



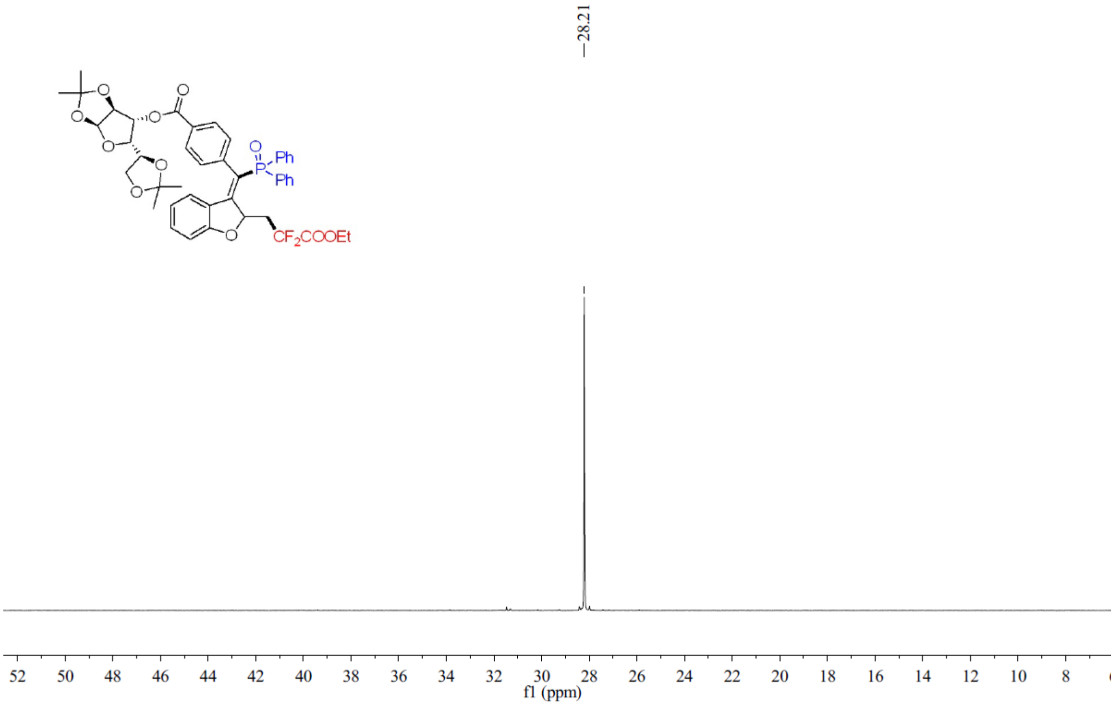
^{1}H NMR (400 MHz) Spectrum of **3z** in $CDCl_3$



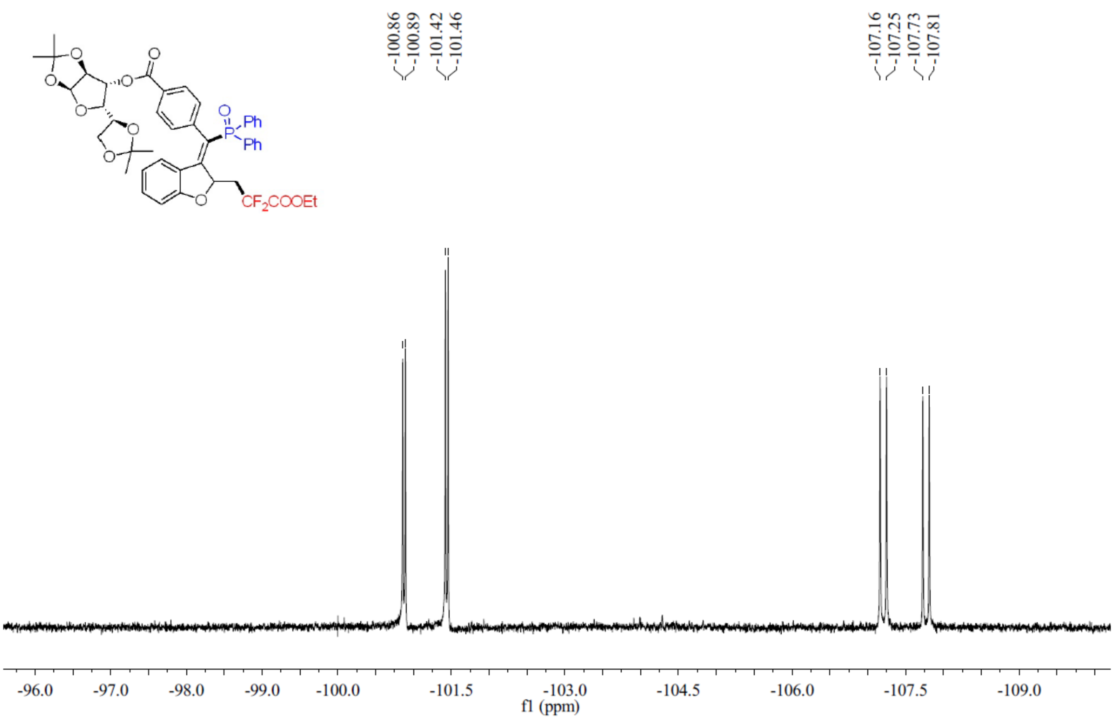
^{13}C{^{1}H}NMR (100 MHz) Spectrum of **3z** in $CDCl_3$



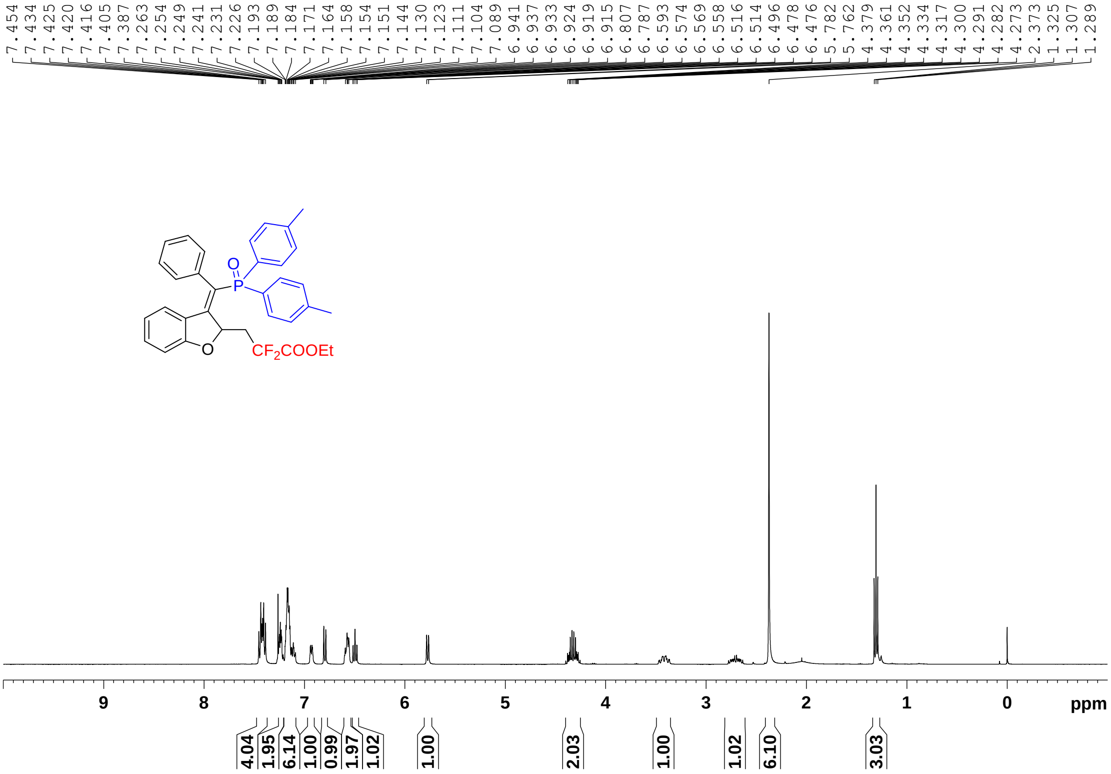
$^{31}P\{^1H\}$ NMR (243 MHz) Spectrum of **3z** in $CDCl_3$



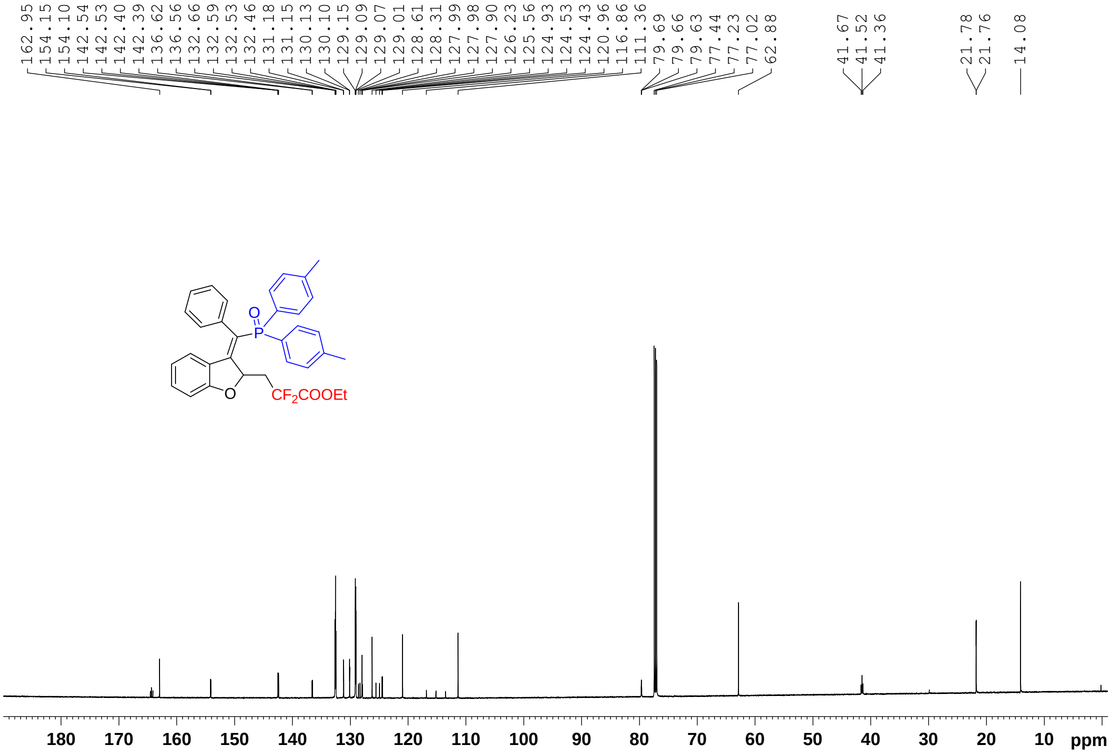
$^{19}F\{^1H\}$ NMR (471 MHz) Spectrum of **3z** in $CDCl_3$



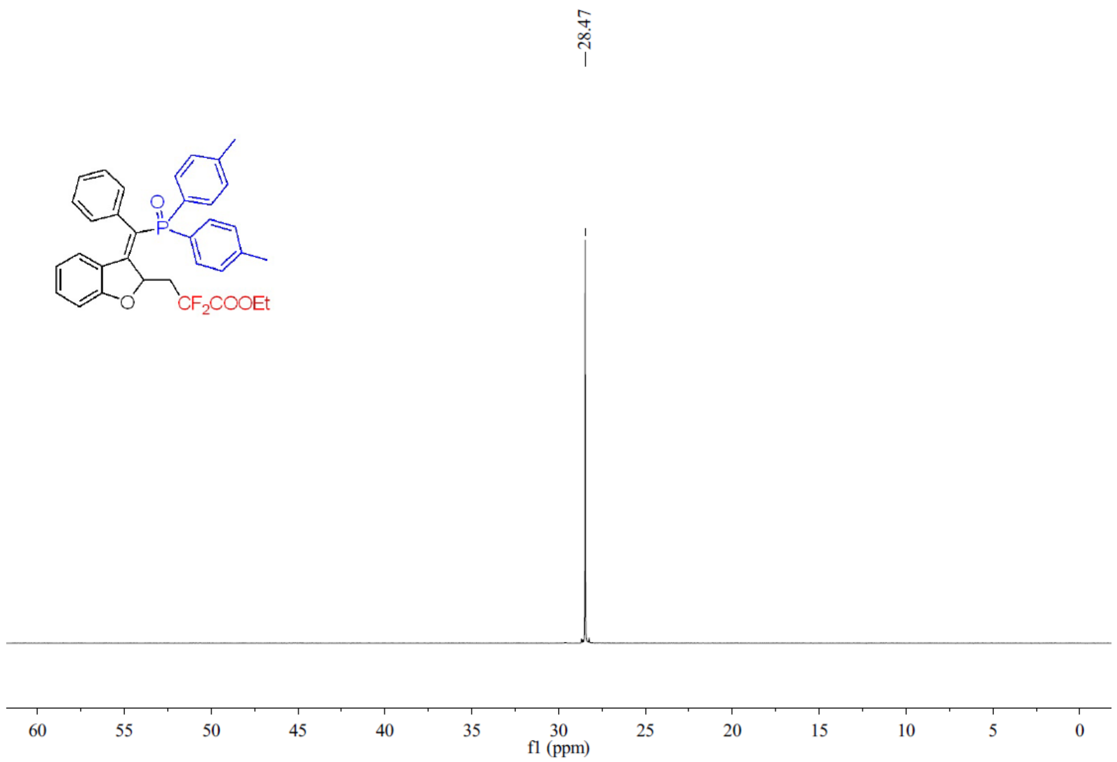
^{1}H NMR (400 MHz) Spectrum of **4a** in $CDCl_3$



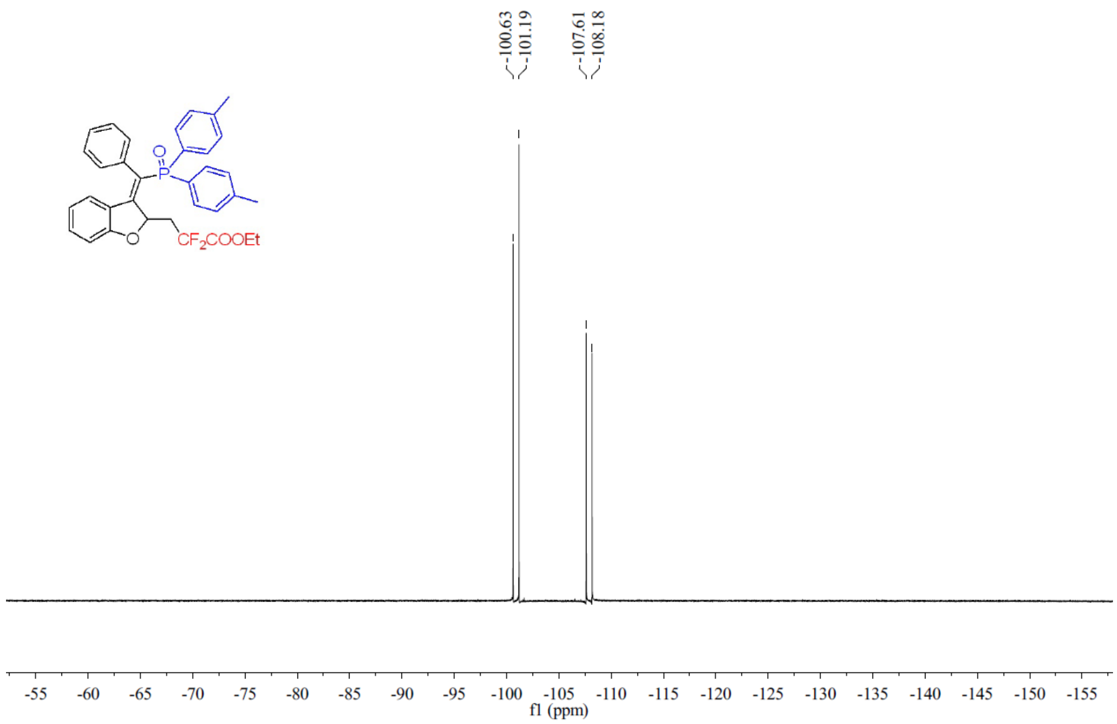
^{13}C{^{1}H}NMR (100 MHz) Spectrum of **4a** in $CDCl_3$



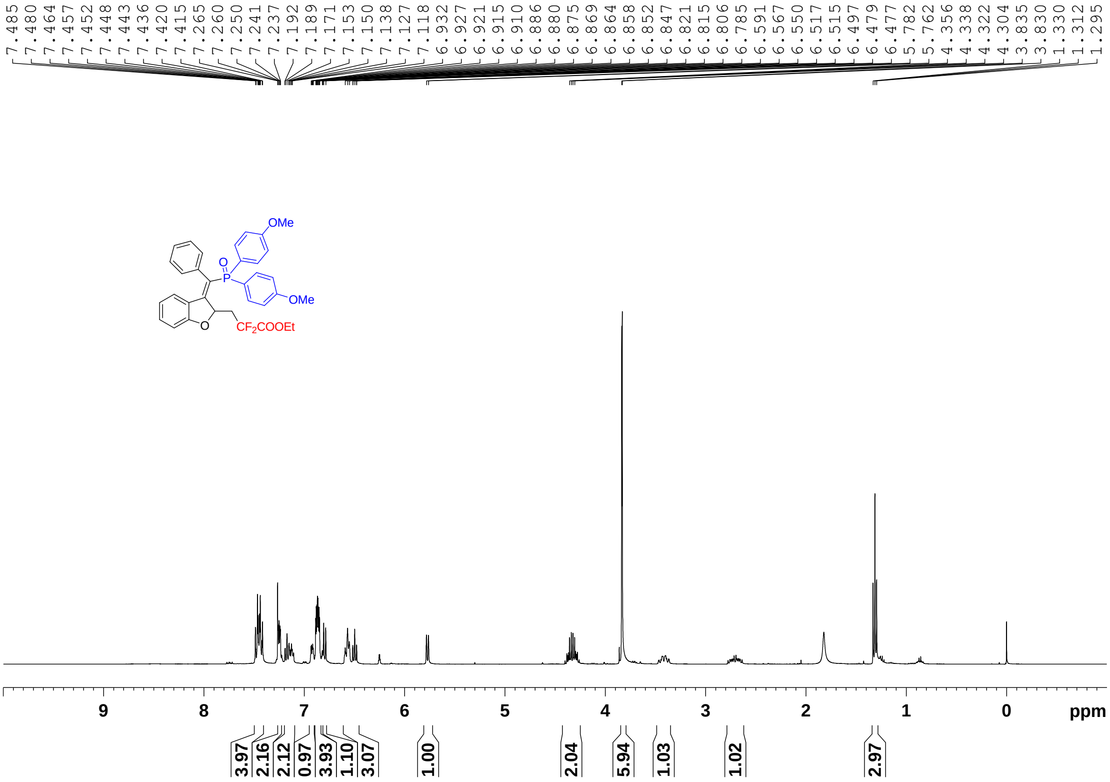
$^{31}P\{^1H\}$ NMR (243 MHz) Spectrum of **4a** in $CDCl_3$



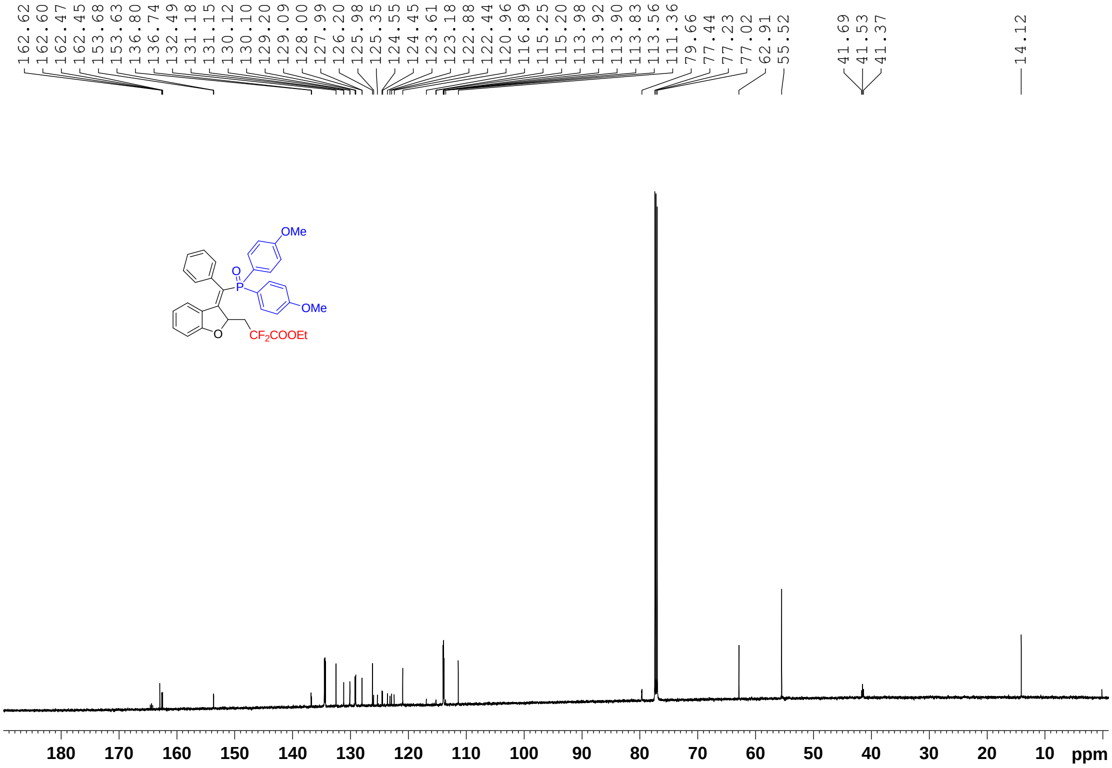
$^{19}F\{^1H\}$ NMR (471 MHz) Spectrum of **4a** in $CDCl_3$



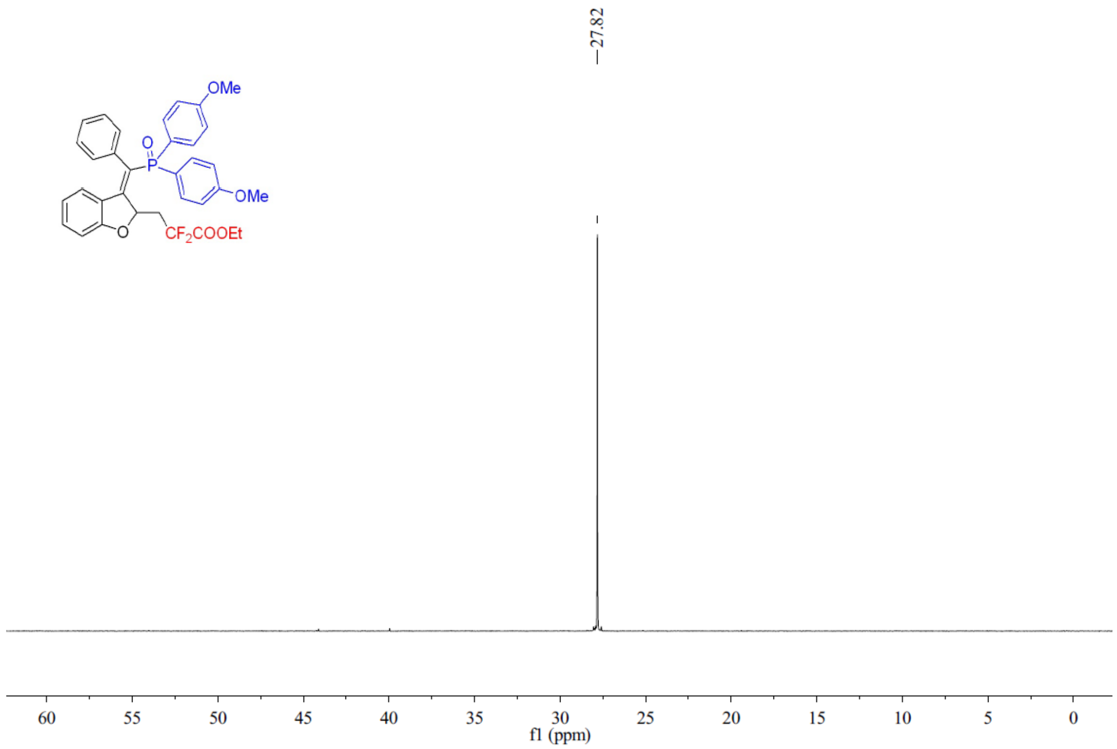
^{1}H NMR (400 MHz) Spectrum of **4b** in $CDCl_3$



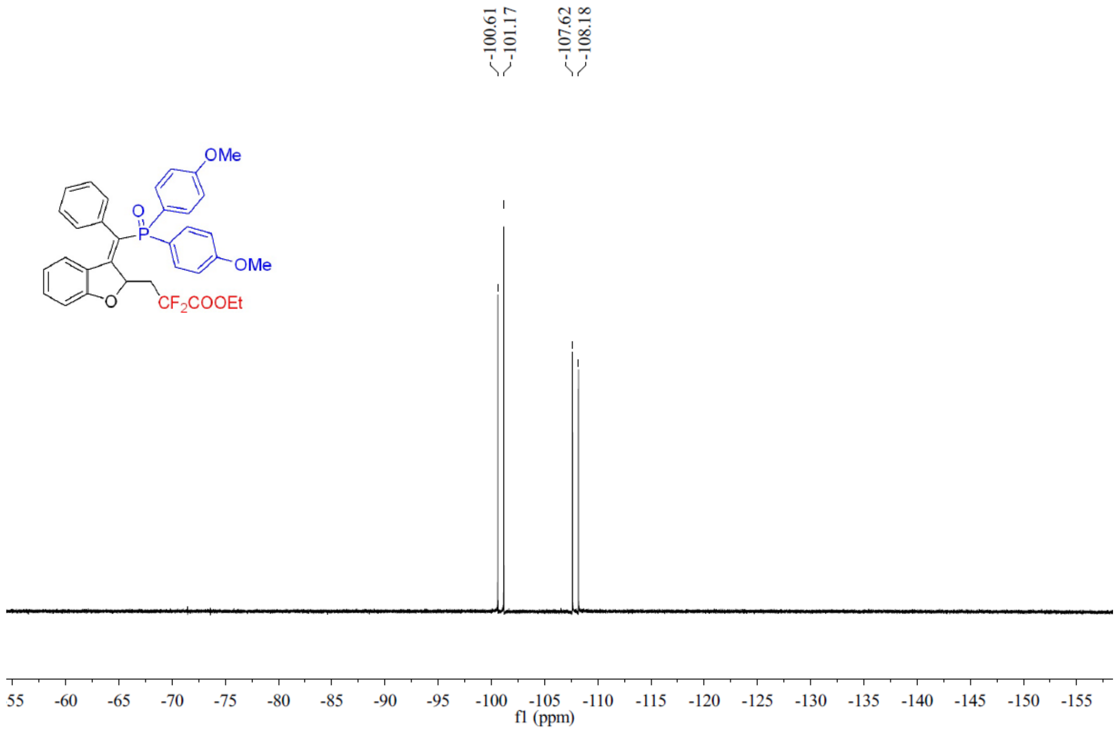
^{13}C{^{1}H}NMR (100 MHz) Spectrum of **4b** in $CDCl_3$



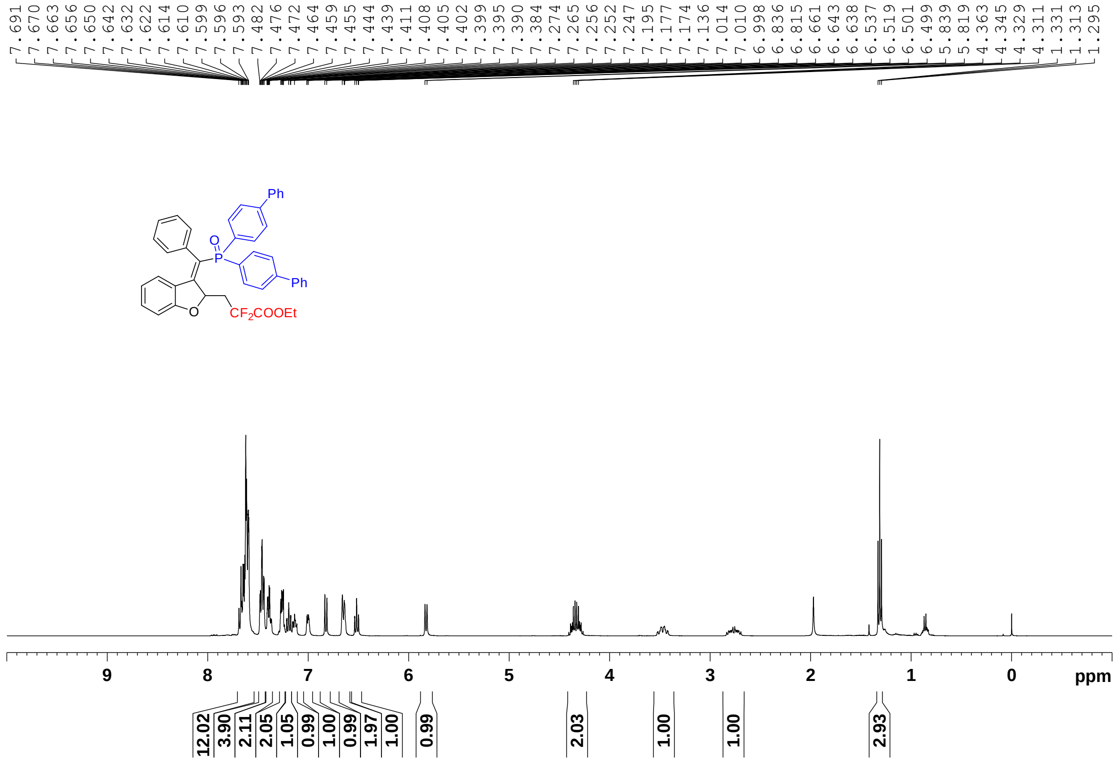
$^{31}P\{^{1}H\}$ NMR (243 MHz) Spectrum of **4b** in $CDCl_3$



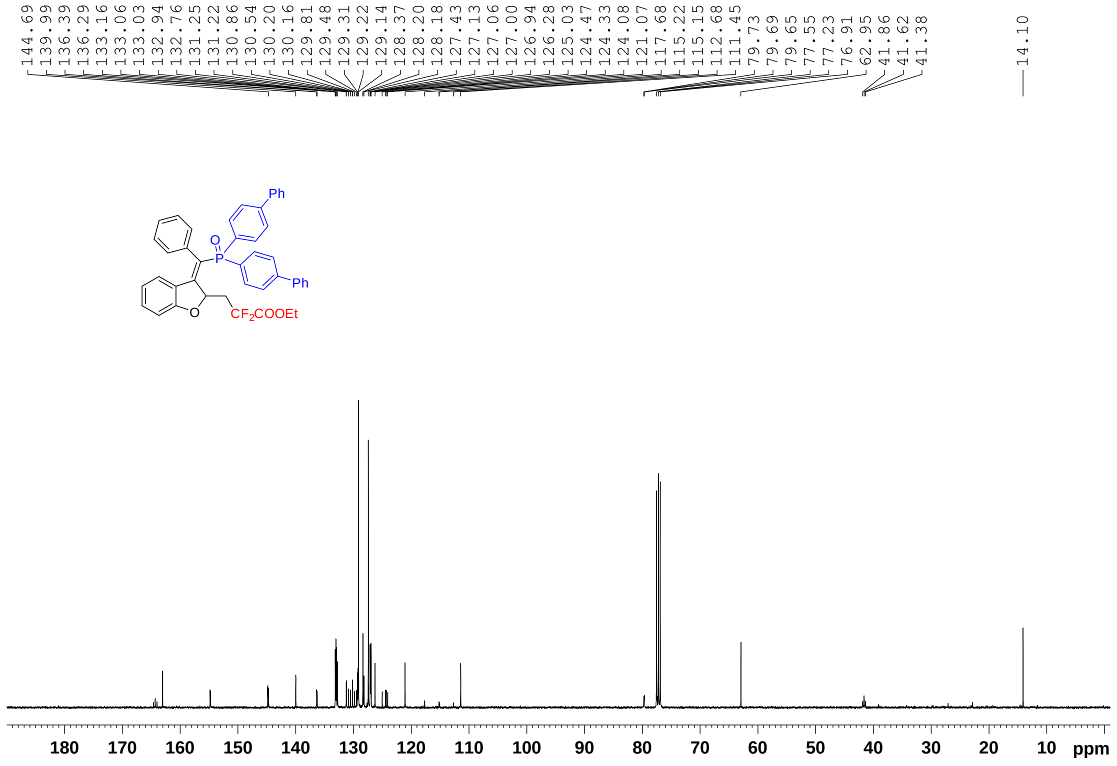
$^{19}F\{^{1}H\}$ NMR (471 MHz) Spectrum of **4b** in $CDCl_3$



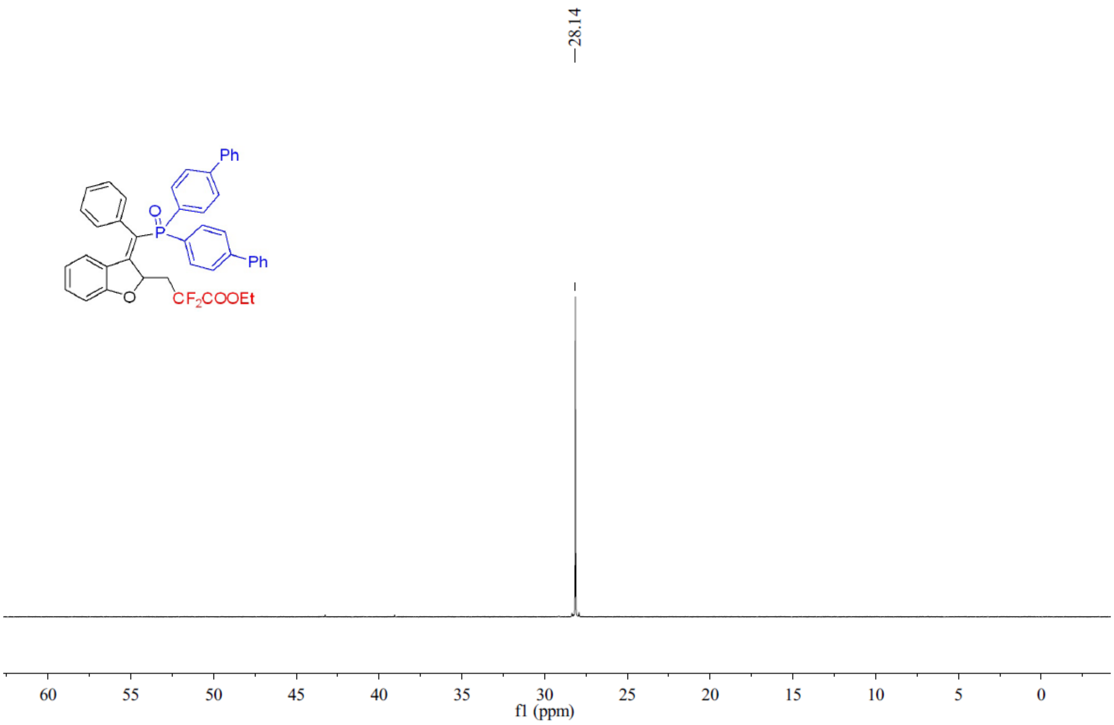
^{1}H NMR (400 MHz) Spectrum of **4c** in $CDCl_3$



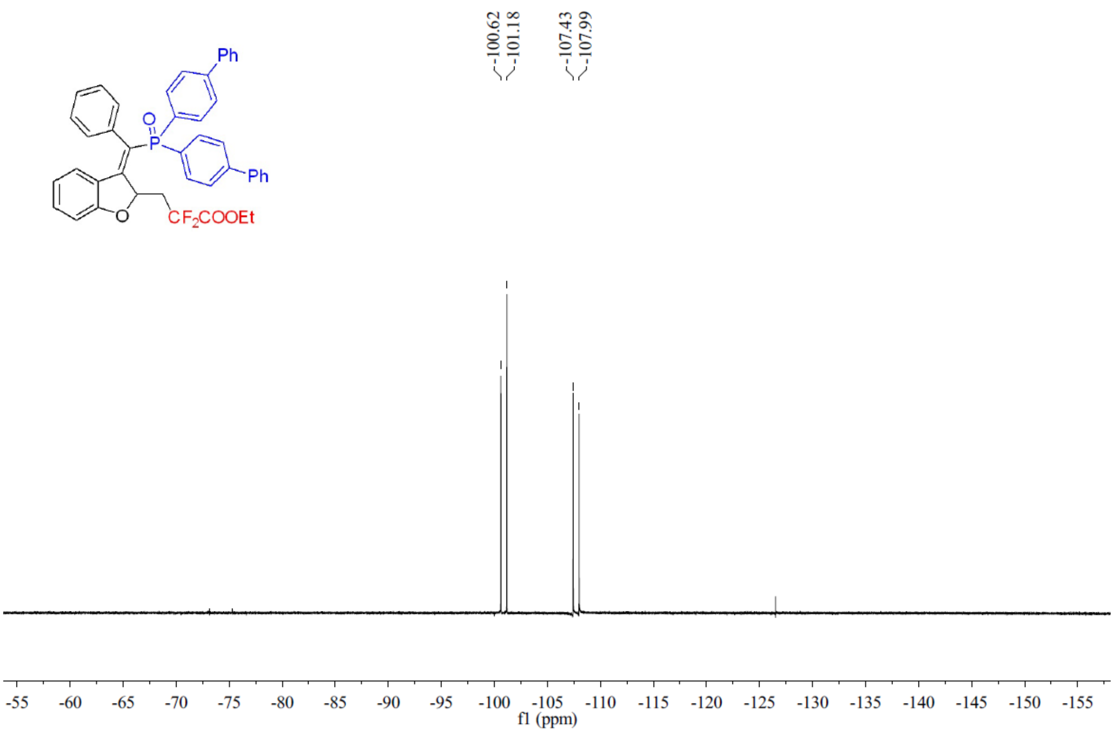
$^{13}C\{^{1}H\}$NMR (100 MHz) Spectrum of **4c** in $CDCl_3$



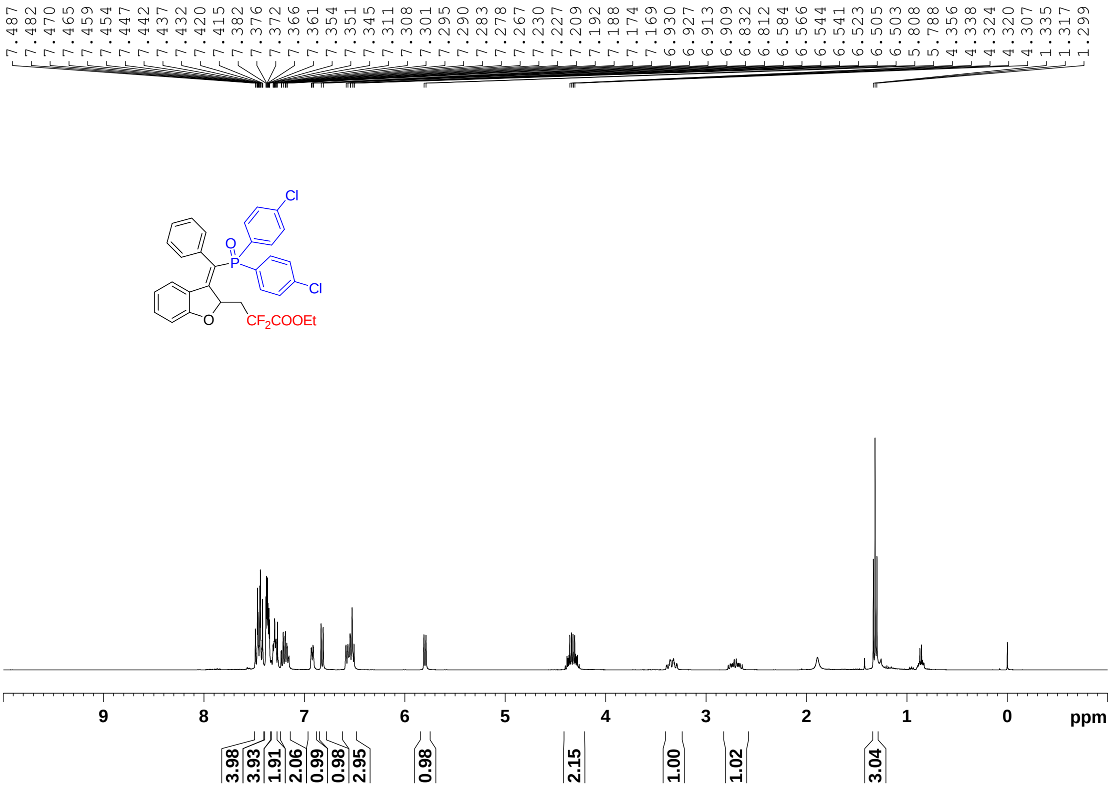
$^{31}P\{^{1}H\}$ NMR (243 MHz) Spectrum of **4c** in $CDCl_3$



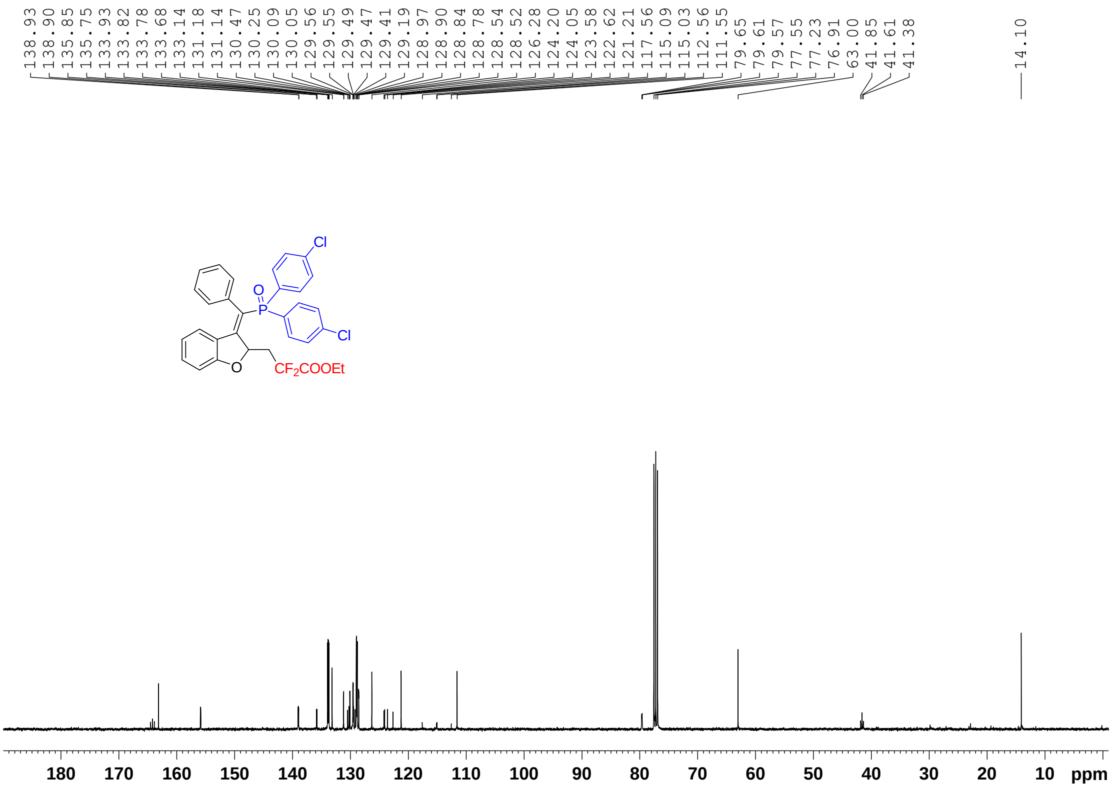
$^{19}F\{^{1}H\}$ NMR (471 MHz) Spectrum of **4c** in $CDCl_3$



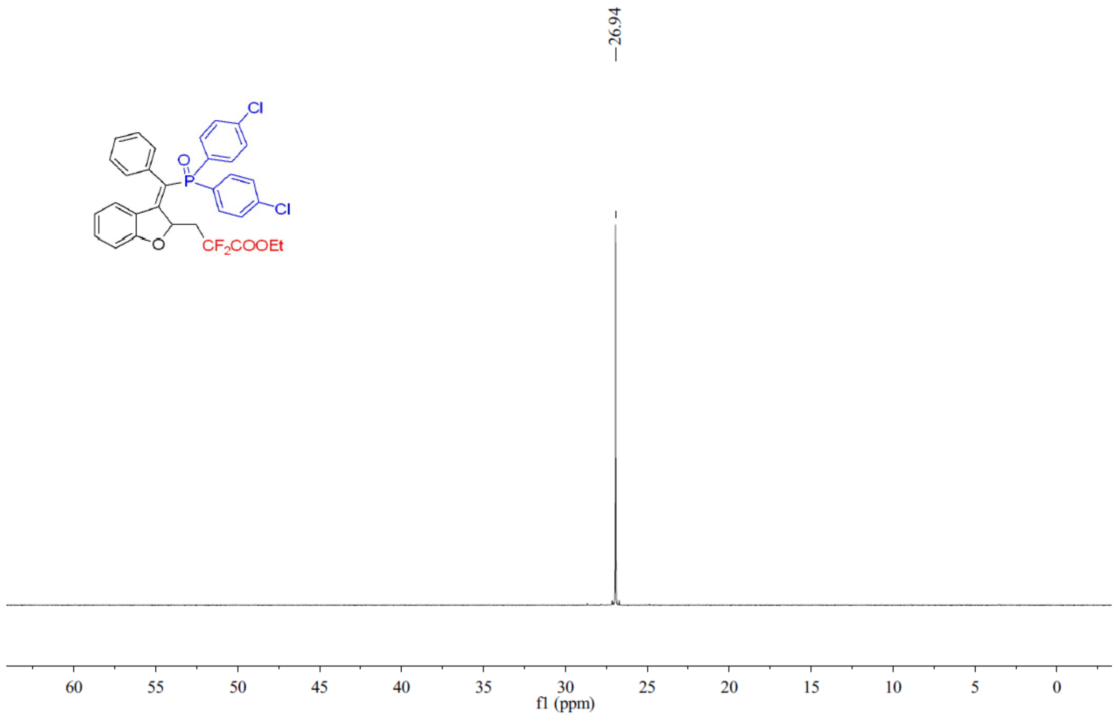
^{1}H NMR (400 MHz) Spectrum of **4d** in $CDCl_3$



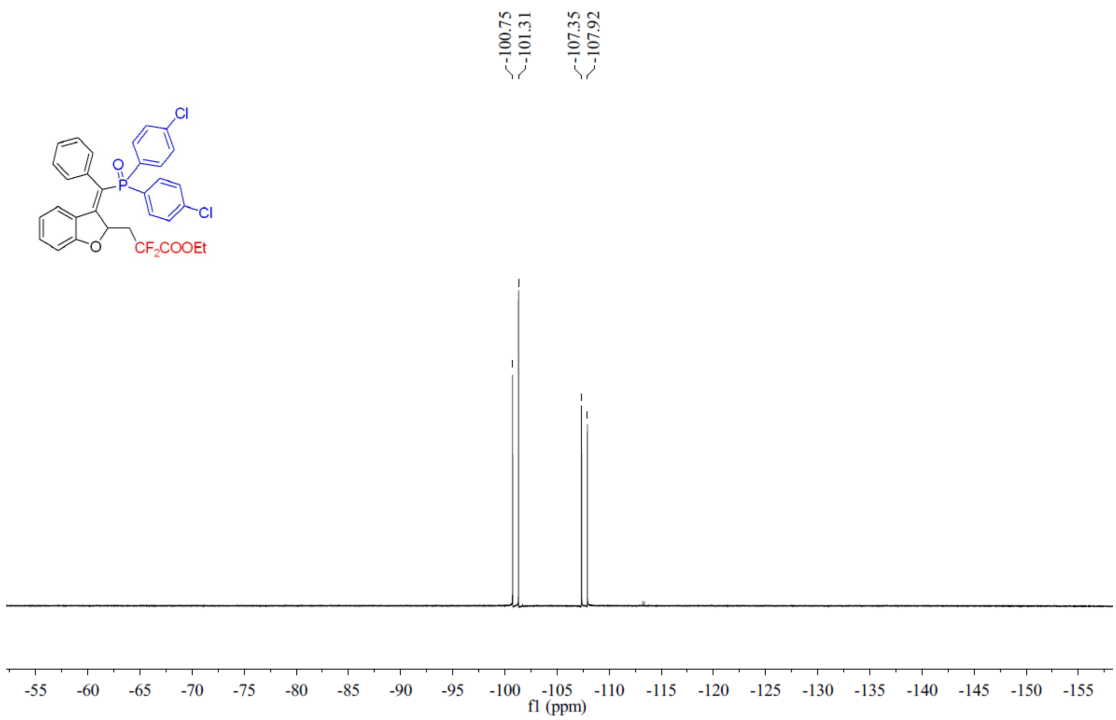
$^{13}C\{^{1}H\}$NMR (100 MHz) Spectrum of **4d** in $CDCl_3$



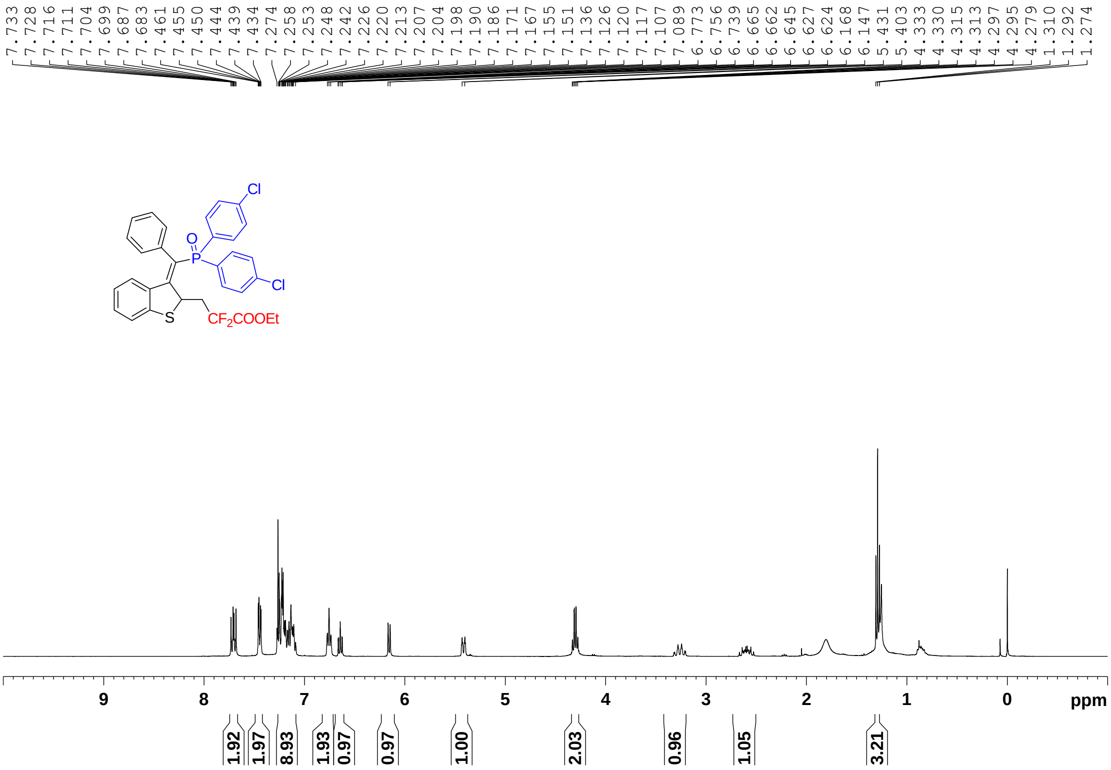
$^{31}P\{^{1}H\}$ NMR (243 MHz) Spectrum of **4d** in $CDCl_3$



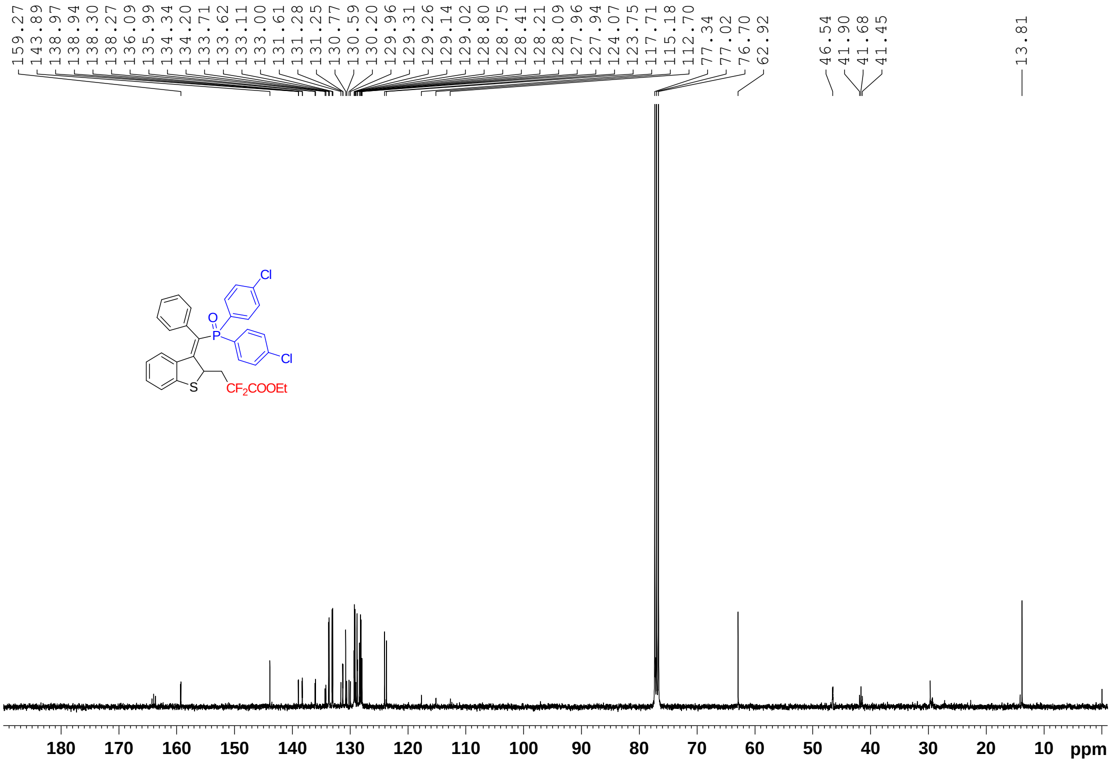
$^{19}F\{^{1}H\}$ NMR (471 MHz) Spectrum of **4d** in $CDCl_3$



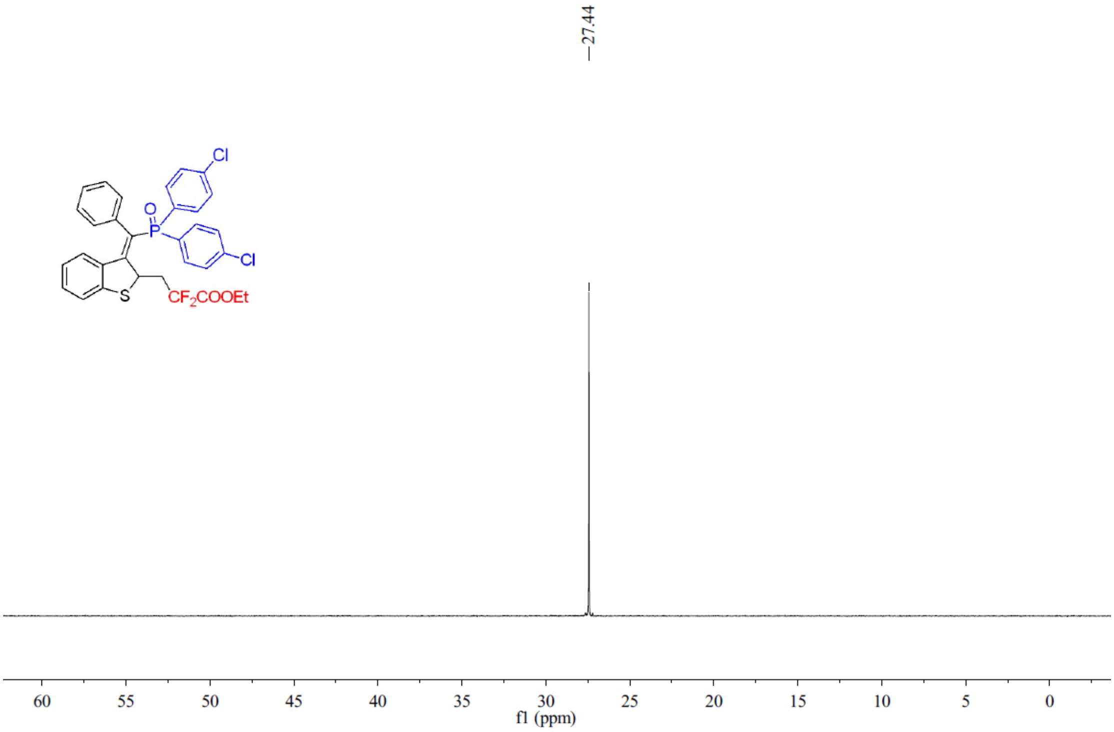
^1H NMR (400 MHz) Spectrum of **4e** in $CDCl_3$



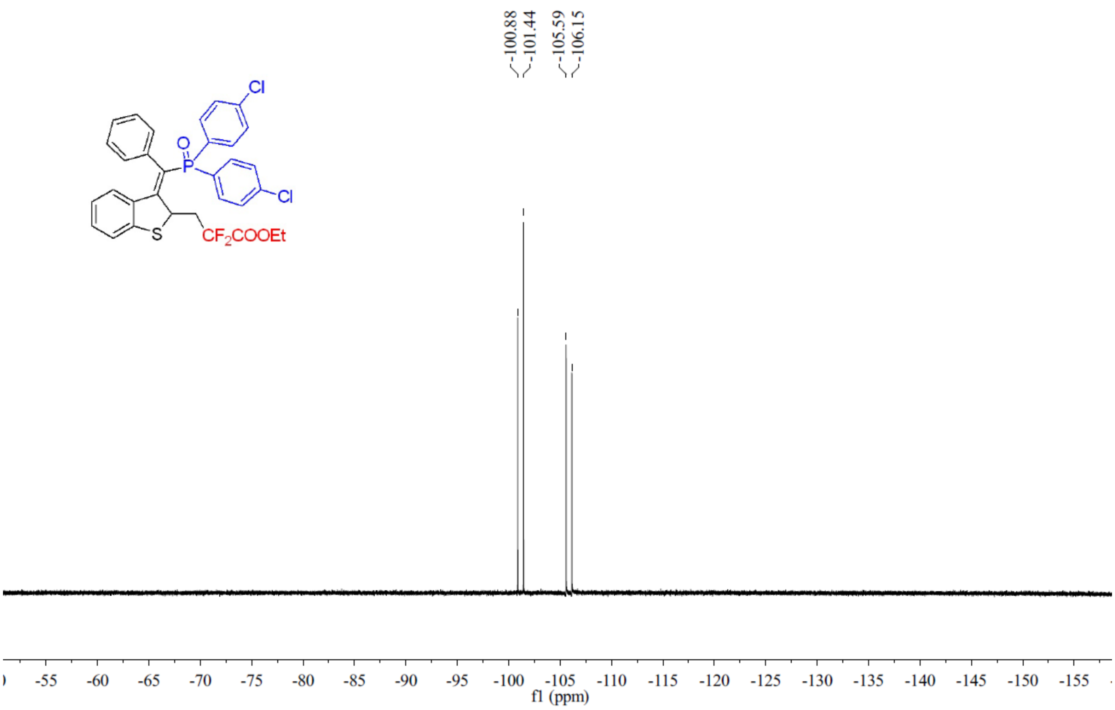
$^{13}C\{^1H\}$NMR (100 MHz) Spectrum of **4e** in $CDCl_3$



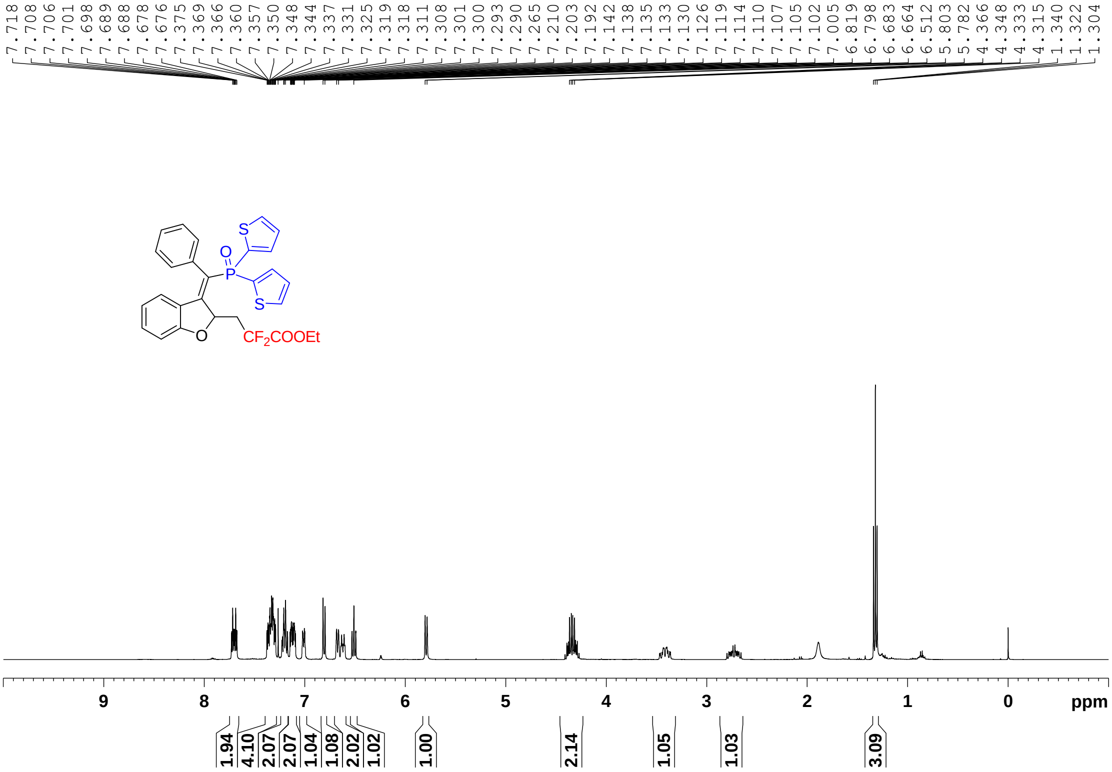
$^{31}P\{^1H\}$ NMR (243 MHz) Spectrum of **4e** in $CDCl_3$



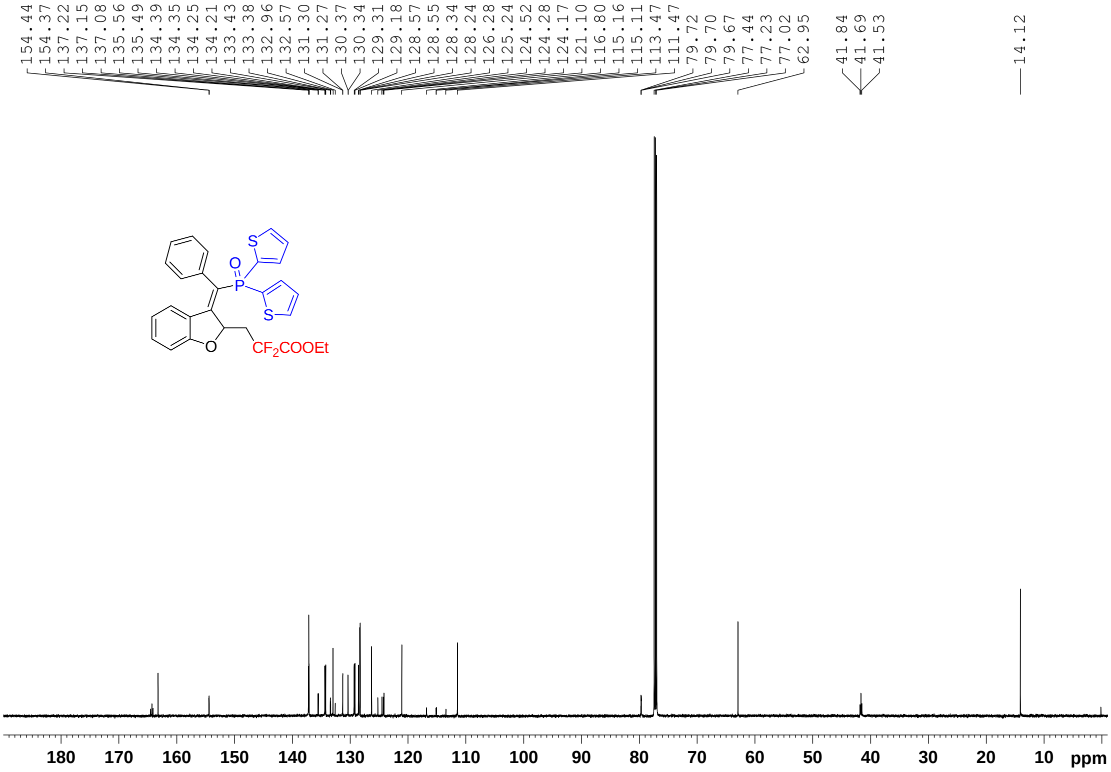
$^{19}F\{^1H\}$ NMR (471 MHz) Spectrum of **4e** in $CDCl_3$



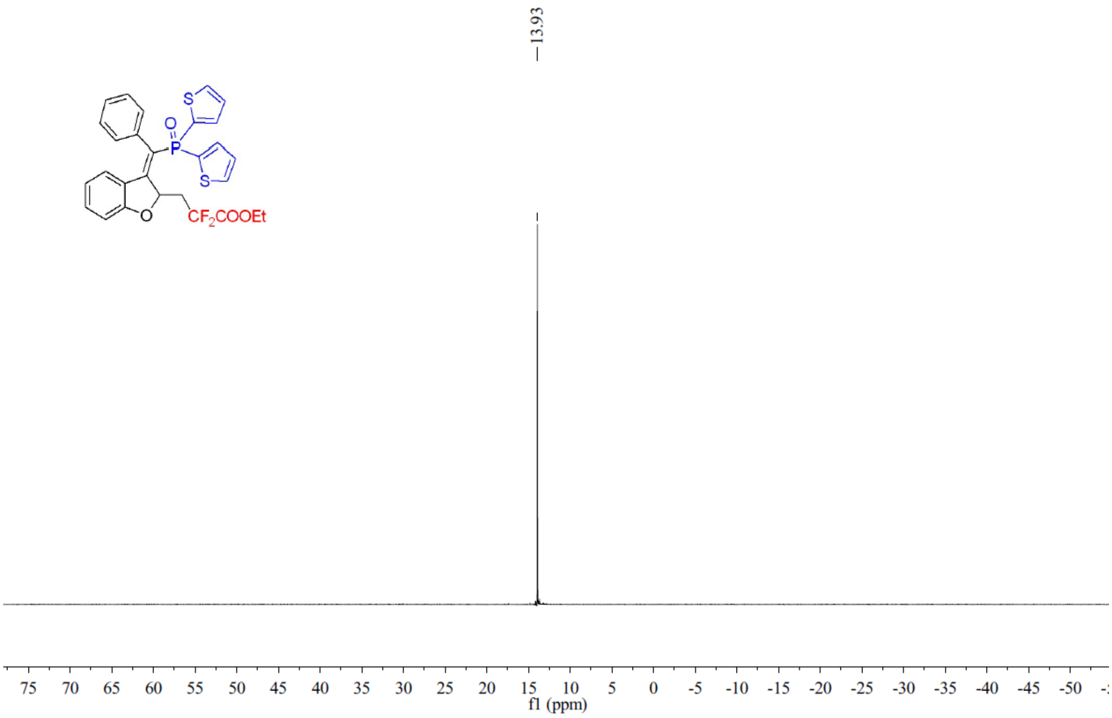
^{1}H NMR (400 MHz) Spectrum of **4f** in $CDCl_3$



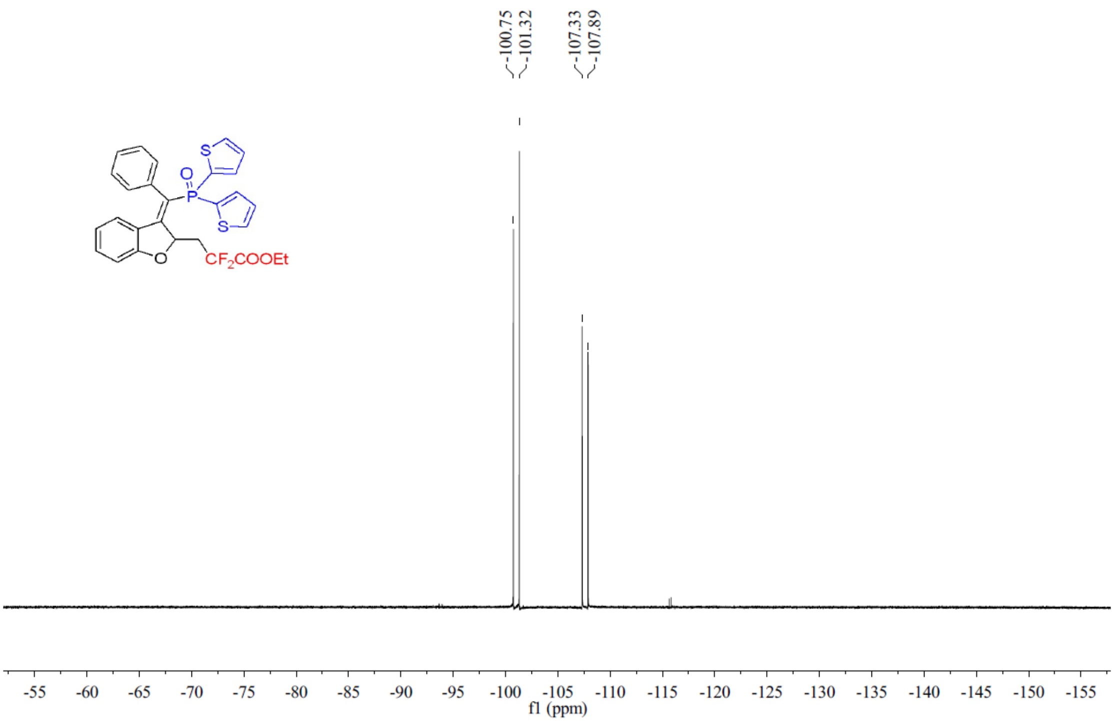
^{13}C{^{1}H}NMR (100 MHz) Spectrum of **4f** in $CDCl_3$



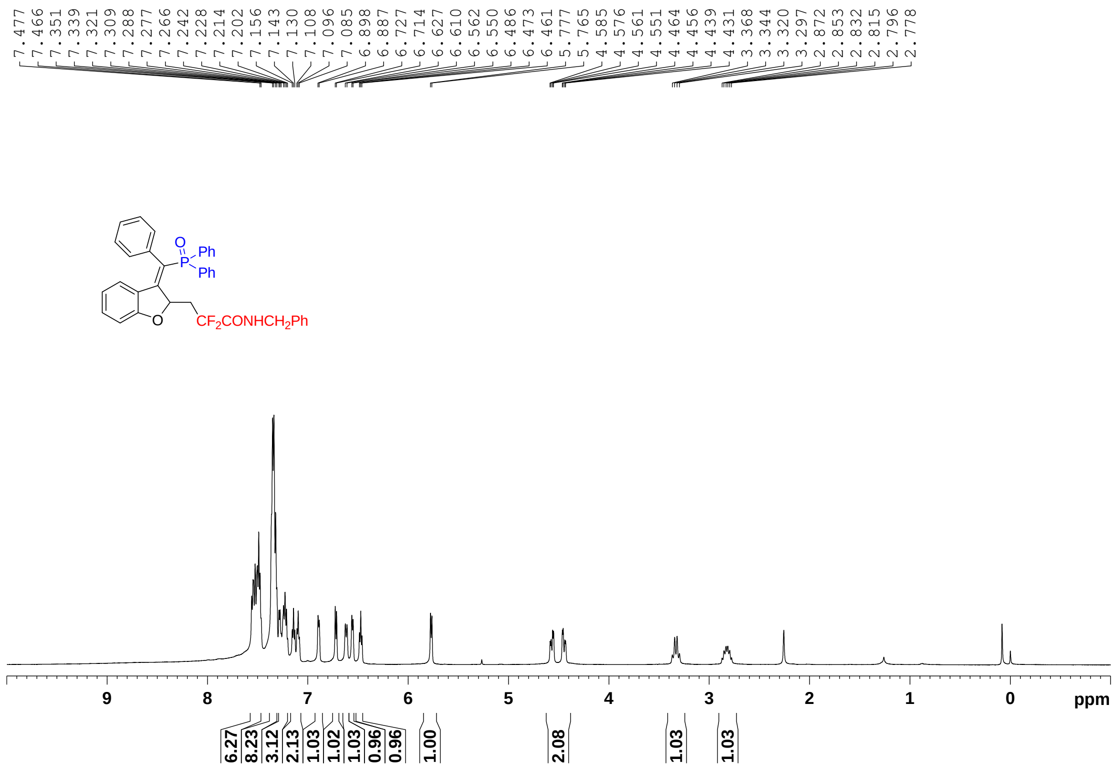
$^{31}P\{^{1}H\}$ NMR (243 MHz) Spectrum of **4f** in $CDCl_3$



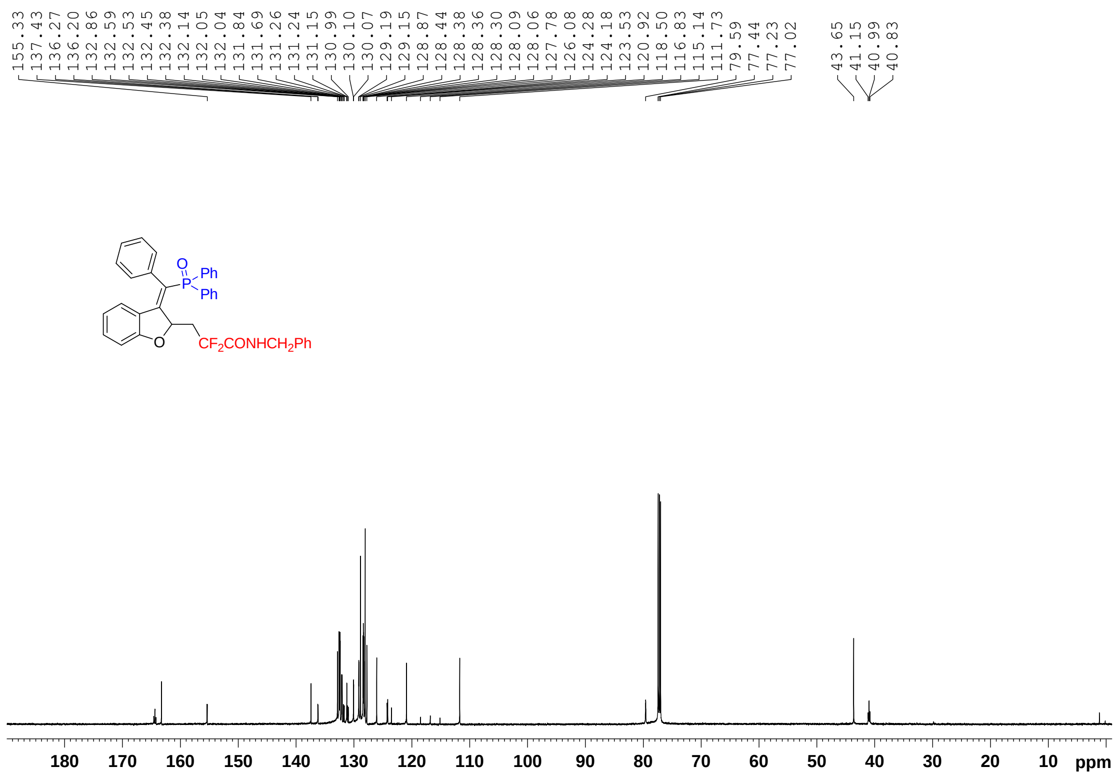
$^{19}F\{^{1}H\}$ NMR (471 MHz) Spectrum of **4f** in $CDCl_3$



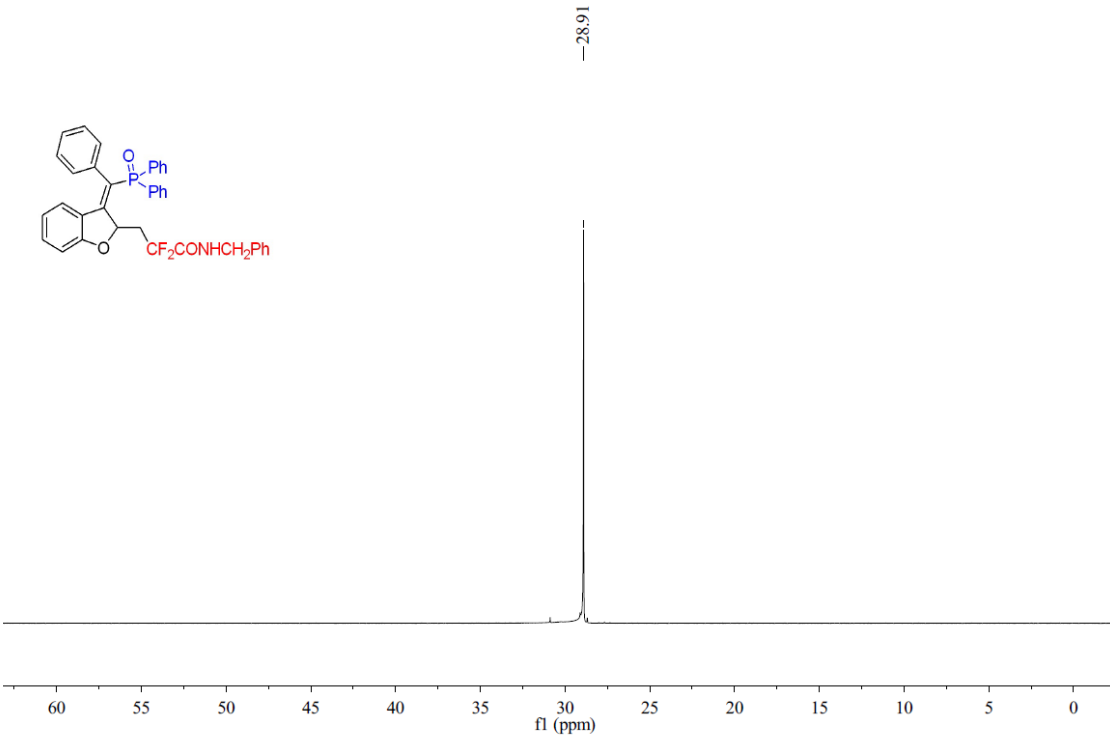
^{1}H NMR (400 MHz) Spectrum of **5** in $CDCl_3$



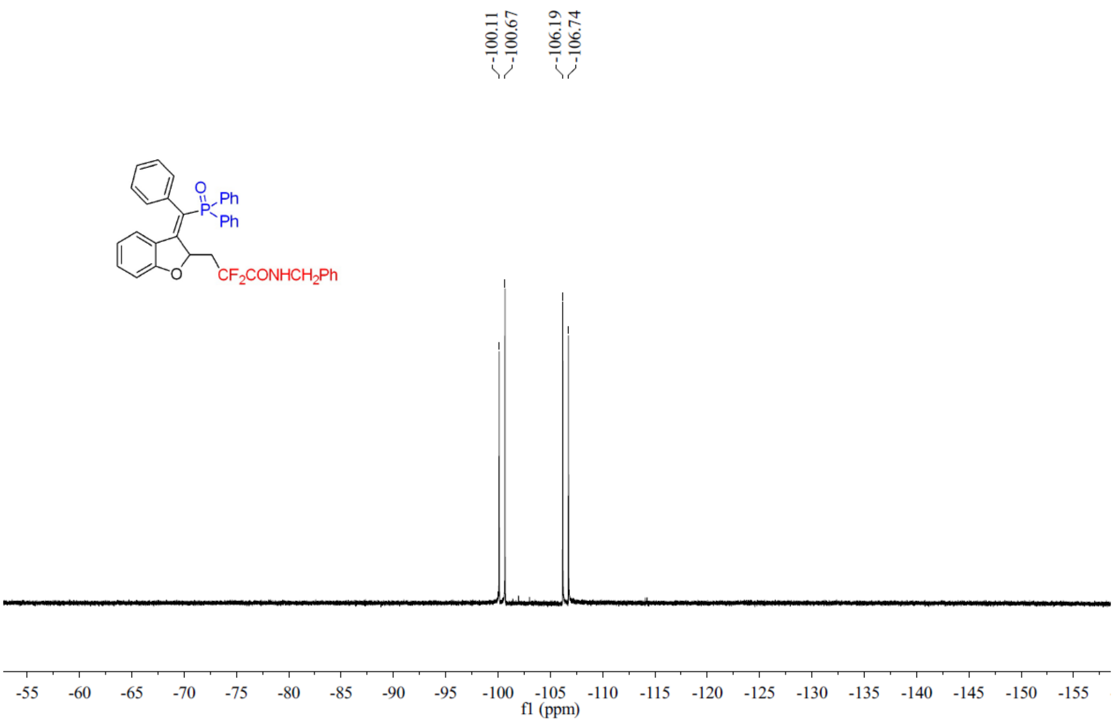
^{13}C{^{1}H}NMR (100 MHz) Spectrum of **5** in $CDCl_3$



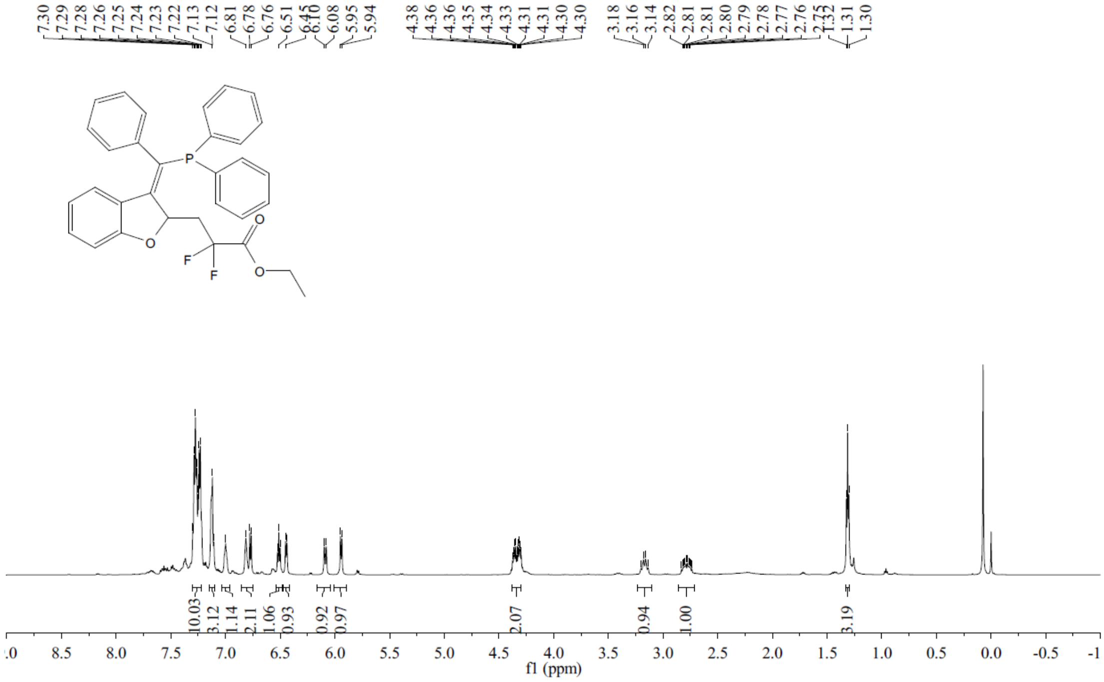
$^{31}P\{^1H\}$ NMR (243 MHz) Spectrum of **5** in $CDCl_3$



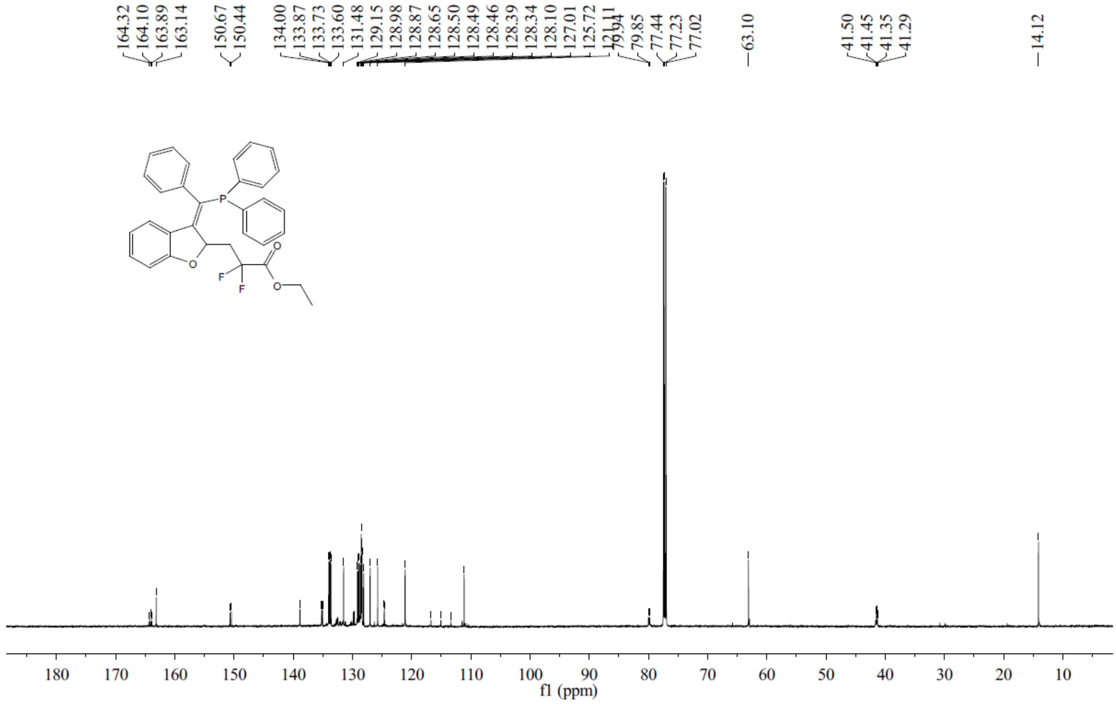
$^{19}F\{^1H\}$ NMR (471 MHz) Spectrum of **5** in $CDCl_3$



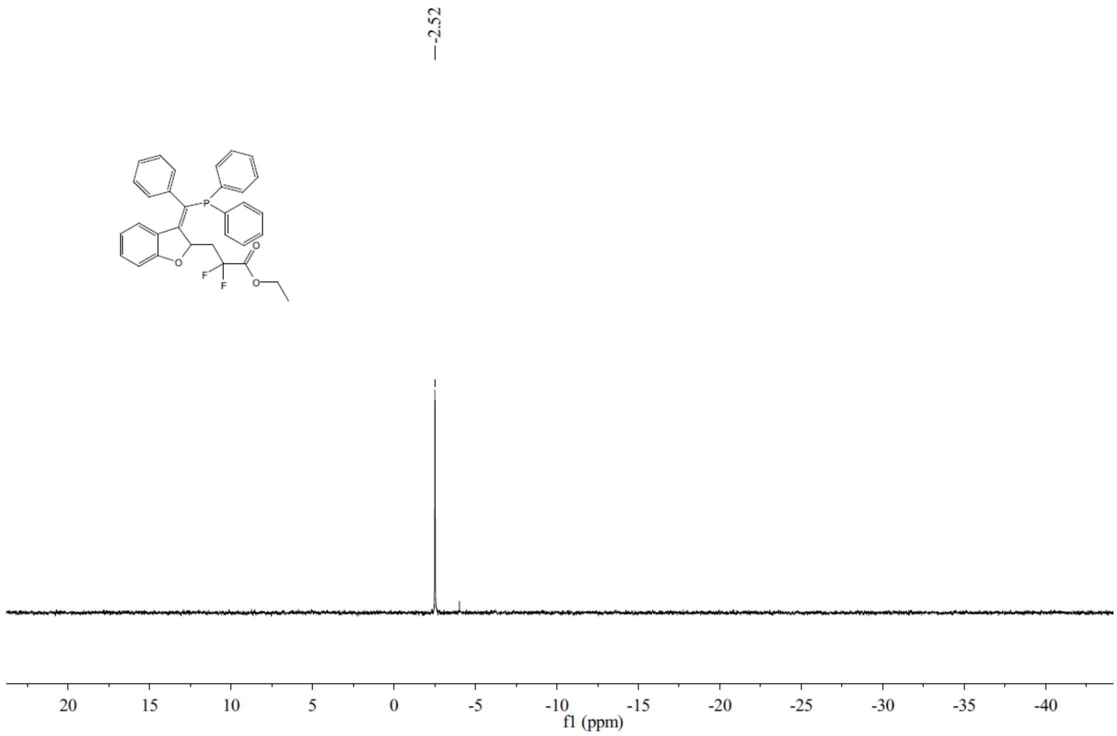
^{1}H NMR (400 MHz) Spectrum of **6** in $CDCl_3$



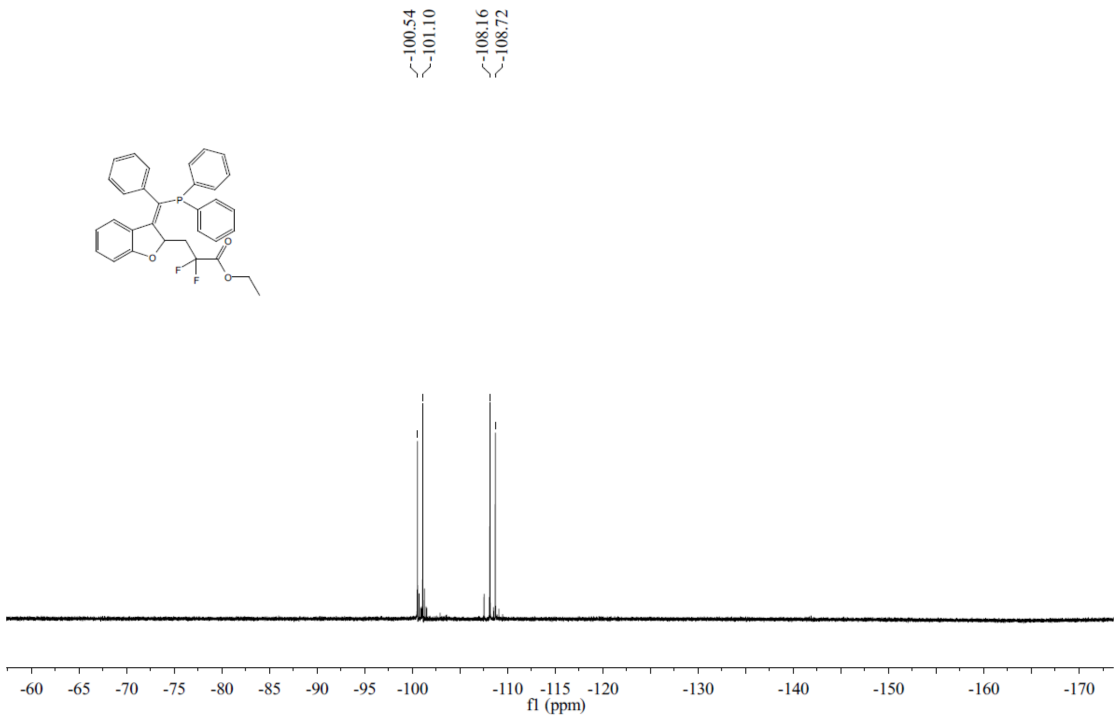
^{13}C{^{1}H}NMR (100 MHz) Spectrum of **6** in $CDCl_3$



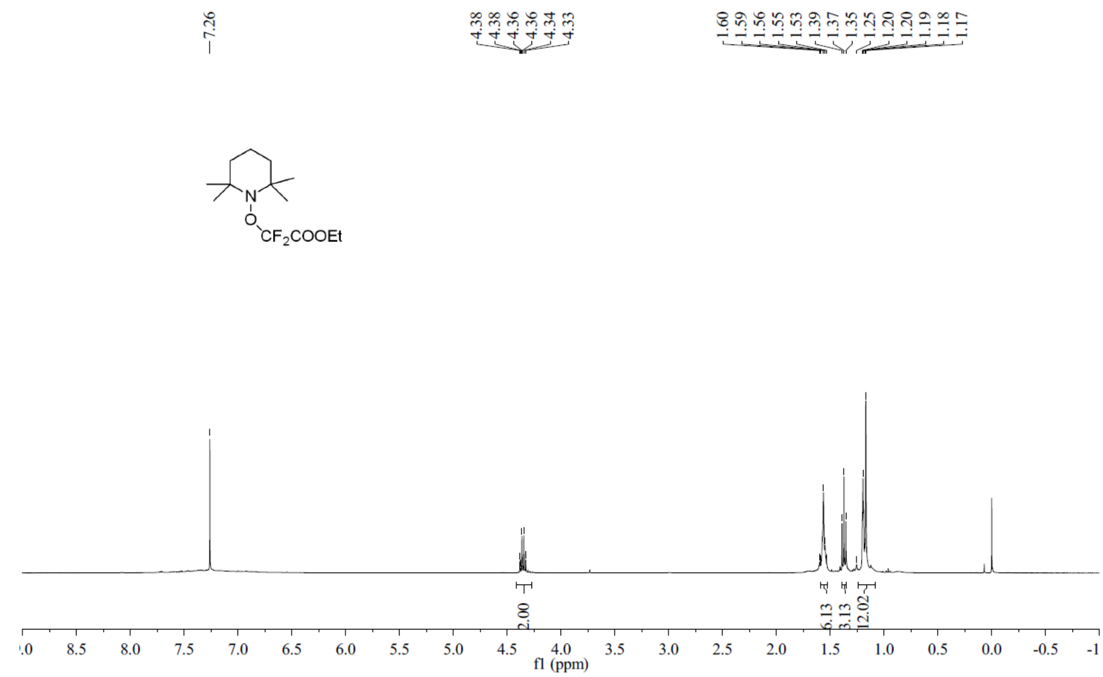
$^{31}P\{^1H\}$ NMR (243 MHz) Spectrum of **6** in $CDCl_3$



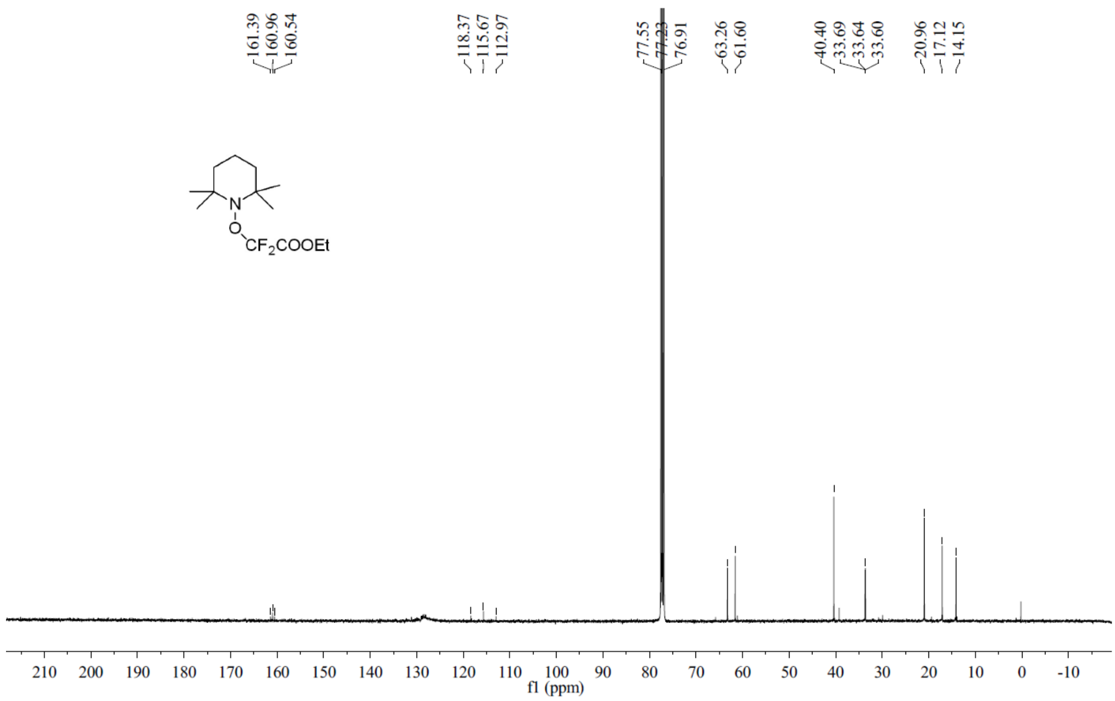
$^{19}F\{^1H\}$ NMR (471 MHz) Spectrum of **6** in $CDCl_3$



^{1}H NMR (400 MHz) Spectrum of **7** in $CDCl_3$



^{13}C{^{1}H}NMR (100 MHz) Spectrum of **7** in $CDCl_3$



$^{19}F\{^1H\}$ NMR (471 MHz) Spectrum of **7** in $CDCl_3$

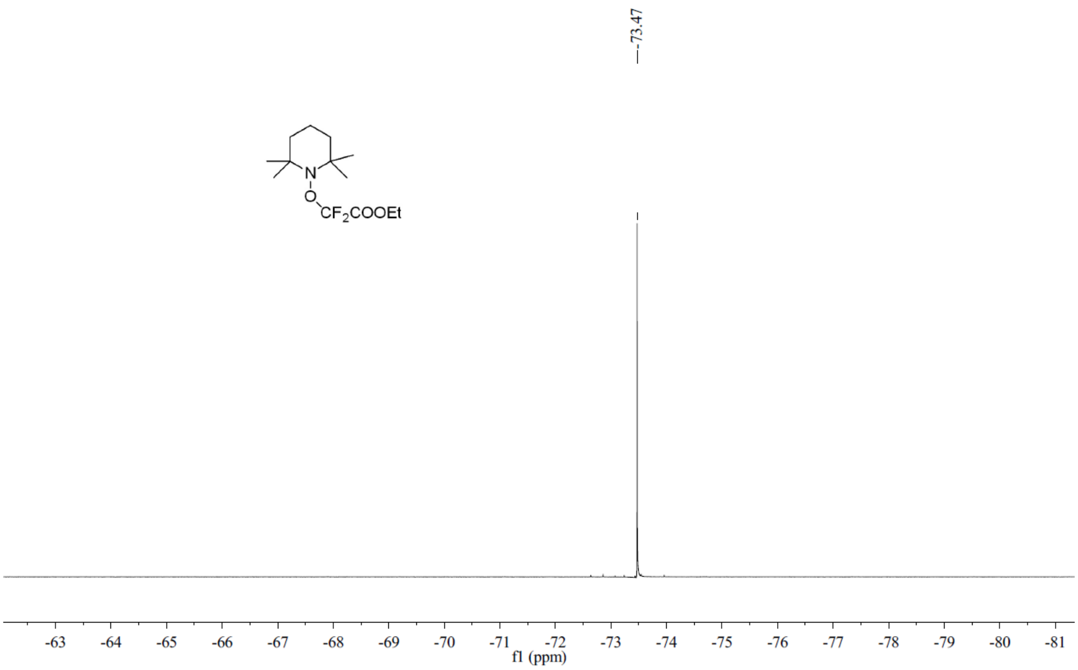
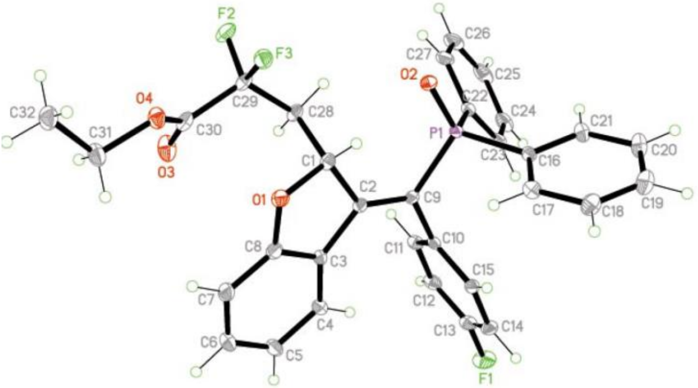


Figure S1. X-ray structure of **3i** (CCDC: 2050042)



The ellipsoid contour percent probability level is 30%.

Table S1. Crystal data and structure refinement for **3i**.

Identification code	zpb	
Empirical formula	C32 H26 F3 O4 P	
Formula weight	562.50	
Temperature	153(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 15.0975(2) Å	α= 90 °.
	b = 14.9246(2) Å	β= 110.397(2) °.
	c = 12.9734(2) Å	γ = 90 °.
Volume	2739.93(7) $Å^3$	
Z	4	
Density (calculated)	1.364 Mg/m^3	
Absorption coefficient	1.385 mm^{-1}	
F(000)	1168	
Crystal size	0.2 x 0.2 x 0.1 mm^3	
Theta range for data collection	3.12 to 74.29 °.	
Index ranges	-18<=h<=16, -14<=k<=18, -16<=l<=15	
Reflections collected	17797	
Independent reflections	5406 [R(int) = 0.0313]	
Completeness to theta = 74.29 °	96.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1 and 0.86833	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5406 / 0 / 361	
Goodness-of-fit on F^2	0.794	

Final R indices [I>2sigma(I)]	R1 = 0.0417, wR2 = 0.1654
R indices (all data)	R1 = 0.0446, wR2 = 0.1735
Largest diff. peak and hole	0.456 and -0.458 e.$Å^{-3}$

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)

for **3i**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
P(1)	1442(1)	4483(1)	3296(1)	20(1)
F(3)	3897(1)	4169(1)	7248(1)	30(1)
F(2)	4932(1)	3638(1)	6577(1)	36(1)
O(4)	5250(1)	5234(1)	8237(1)	30(1)
O(2)	1817(1)	3925(1)	4306(1)	28(1)
O(1)	3553(1)	6030(1)	6256(1)	26(1)
F(1)	1074(1)	7762(1)	-315(1)	43(1)
C(2)	2695(1)	5840(1)	4349(1)	20(1)
O(3)	5639(1)	5451(1)	6730(1)	40(1)
C(9)	2029(1)	5555(1)	3410(1)	19(1)
C(10)	1752(1)	6130(1)	2403(1)	18(1)
C(1)	3070(1)	5349(1)	5449(1)	21(1)
C(16)	204(1)	4735(1)	2966(1)	22(1)
C(15)	1007(1)	6738(1)	2180(1)	22(1)
C(4)	3291(1)	7403(1)	3883(1)	23(1)
C(12)	2044(1)	6641(1)	779(1)	28(1)
C(22)	1549(1)	3935(1)	2104(1)	24(1)
C(11)	2267(1)	6089(1)	1693(1)	23(1)
C(13)	1301(1)	7227(1)	590(1)	29(1)
C(23)	1133(1)	4260(1)	1027(1)	26(1)
C(18)	-989(1)	5496(1)	3489(2)	34(1)
C(29)	4425(1)	4388(1)	6616(1)	25(1)
C(17)	-44(1)	5349(1)	3627(1)	27(1)
C(3)	3214(1)	6695(1)	4555(1)	21(1)
C(30)	5169(1)	5105(1)	7204(1)	27(1)
C(21)	-505(1)	4251(1)	2177(1)	28(1)
C(28)	3806(1)	4637(1)	5464(1)	24(1)
C(5)	3867(1)	8129(1)	4365(1)	29(1)
C(31)	5963(1)	5884(1)	8849(1)	34(1)
C(8)	3704(1)	6749(1)	5685(1)	25(1)
C(27)	2079(1)	3146(1)	2281(2)	33(1)
C(14)	775(1)	7296(1)	1267(1)	27(1)

C(25)	1756(1)	3007(1)	336(2)	41(1)
C(6)	4359(1)	8151(1)	5499(2)	34(1)
C(19)	-1687(1)	5025(1)	2690(1)	36(1)
C(7)	4286(1)	7459(1)	6181(1)	33(1)
C(24)	1244(1)	3798(1)	151(2)	34(1)
C(20)	-1445(1)	4395(1)	2047(1)	35(1)
C(26)	2174(1)	2682(1)	1392(2)	41(1)
C(32)	6372(1)	5568(1)	10016(1)	36(1)

Table S3. Bond lengths [Å] and angles [°] for **3i**.

P(1)-O(2)	1.4876(10)
P(1)-C(22)	1.8067(15)
P(1)-C(16)	1.8064(14)
P(1)-C(9)	1.8101(14)
F(3)-C(29)	1.3668(18)
F(2)-C(29)	1.3661(18)
O(4)-C(30)	1.3166(19)
O(4)-C(31)	1.4604(19)
O(1)-C(8)	1.3670(19)
O(1)-C(1)	1.4599(17)
F(1)-C(13)	1.3611(17)
C(2)-C(9)	1.350(2)
C(2)-C(3)	1.472(2)
C(2)-C(1)	1.5273(18)
O(3)-C(30)	1.204(2)
C(9)-C(10)	1.4951(17)
C(10)-C(15)	1.395(2)
C(10)-C(11)	1.399(2)
C(1)-C(28)	1.531(2)
C(16)-C(17)	1.392(2)
C(16)-C(21)	1.397(2)
C(15)-C(14)	1.389(2)
C(4)-C(5)	1.394(2)
C(4)-C(3)	1.399(2)
C(12)-C(11)	1.386(2)
C(12)-C(13)	1.375(2)
C(22)-C(27)	1.397(2)
C(22)-C(23)	1.404(2)
C(13)-C(14)	1.378(2)
C(23)-C(24)	1.389(2)
C(18)-C(19)	1.385(3)
C(18)-C(17)	1.392(2)
C(29)-C(28)	1.5079(19)
C(29)-C(30)	1.547(2)
C(3)-C(8)	1.395(2)
C(21)-C(20)	1.386(2)

C(5)-C(6)	1.399(2)
C(31)-C(32)	1.498(2)
C(8)-C(7)	1.383(2)
C(27)-C(26)	1.394(3)
C(25)-C(24)	1.385(3)
C(25)-C(26)	1.382(3)
C(6)-C(7)	1.390(3)
C(19)-C(20)	1.387(3)

O(2)-P(1)-C(22)	112.33(7)
O(2)-P(1)-C(16)	111.69(6)
C(22)-P(1)-C(16)	106.57(7)
O(2)-P(1)-C(9)	113.47(6)
C(22)-P(1)-C(9)	106.44(6)
C(16)-P(1)-C(9)	105.84(6)
C(30)-O(4)-C(31)	116.08(12)
C(8)-O(1)-C(1)	107.10(10)
C(9)-C(2)-C(3)	128.24(13)
C(9)-C(2)-C(1)	127.49(13)
C(3)-C(2)-C(1)	104.26(11)
C(2)-C(9)-C(10)	120.07(12)
C(2)-C(9)-P(1)	122.79(11)
C(10)-C(9)-P(1)	117.13(10)
C(15)-C(10)-C(11)	118.98(13)
C(15)-C(10)-C(9)	120.98(12)
C(11)-C(10)-C(9)	119.99(12)
O(1)-C(1)-C(2)	105.37(11)
O(1)-C(1)-C(28)	107.17(11)
C(2)-C(1)-C(28)	112.10(11)
C(17)-C(16)-C(21)	119.36(13)
C(17)-C(16)-P(1)	117.97(11)
C(21)-C(16)-P(1)	122.11(12)
C(10)-C(15)-C(14)	120.86(13)
C(5)-C(4)-C(3)	118.83(14)
C(11)-C(12)-C(13)	118.07(14)
C(27)-C(22)-C(23)	119.17(14)
C(27)-C(22)-P(1)	117.29(13)
C(23)-C(22)-P(1)	123.54(11)

C(12)-C(11)-C(10)	120.84(14)
F(1)-C(13)-C(14)	118.55(15)
F(1)-C(13)-C(12)	118.13(14)
C(14)-C(13)-C(12)	123.31(14)
C(24)-C(23)-C(22)	120.17(15)
C(19)-C(18)-C(17)	119.62(15)
F(3)-C(29)-F(2)	106.13(12)
F(3)-C(29)-C(28)	111.30(12)
F(2)-C(29)-C(28)	109.11(12)
F(3)-C(29)-C(30)	110.18(12)
F(2)-C(29)-C(30)	105.39(12)
C(28)-C(29)-C(30)	114.24(13)
C(16)-C(17)-C(18)	120.53(15)
C(8)-C(3)-C(4)	118.82(13)
C(8)-C(3)-C(2)	107.12(12)
C(4)-C(3)-C(2)	134.06(13)
O(3)-C(30)-O(4)	126.50(15)
O(3)-C(30)-C(29)	120.02(14)
O(4)-C(30)-C(29)	113.37(13)
C(20)-C(21)-C(16)	119.92(15)
C(29)-C(28)-C(1)	112.38(12)
C(4)-C(5)-C(6)	120.61(15)
O(4)-C(31)-C(32)	107.83(13)
O(1)-C(8)-C(7)	123.19(13)
O(1)-C(8)-C(3)	113.37(13)
C(7)-C(8)-C(3)	123.44(14)
C(26)-C(27)-C(22)	120.04(17)
C(13)-C(14)-C(15)	117.94(14)
C(24)-C(25)-C(26)	120.32(16)
C(7)-C(6)-C(5)	121.42(15)
C(18)-C(19)-C(20)	120.19(15)
C(8)-C(7)-C(6)	116.86(14)
C(25)-C(24)-C(23)	120.08(18)
C(19)-C(20)-C(21)	120.34(15)
C(27)-C(26)-C(25)	120.20(16)

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2$x 10^3) for ZPB. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P(1)	20(1)	17(1)	19(1)	2(1)	3(1)	-1(1)
F(3)	29(1)	35(1)	24(1)	6(1)	6(1)	-3(1)
F(2)	36(1)	35(1)	29(1)	3(1)	3(1)	14(1)
O(4)	30(1)	37(1)	19(1)	0(1)	5(1)	-6(1)
O(2)	28(1)	23(1)	28(1)	9(1)	3(1)	-2(1)
O(1)	29(1)	27(1)	18(1)	-1(1)	3(1)	1(1)
F(1)	61(1)	37(1)	26(1)	17(1)	12(1)	3(1)
C(2)	19(1)	20(1)	19(1)	2(1)	5(1)	2(1)
O(3)	31(1)	62(1)	28(1)	-3(1)	12(1)	-12(1)
C(9)	20(1)	17(1)	17(1)	1(1)	4(1)	1(1)
C(10)	21(1)	16(1)	14(1)	-1(1)	2(1)	-4(1)
C(1)	22(1)	26(1)	14(1)	0(1)	4(1)	0(1)
C(16)	21(1)	21(1)	22(1)	4(1)	6(1)	-2(1)
C(15)	23(1)	22(1)	19(1)	0(1)	4(1)	-1(1)
C(4)	23(1)	22(1)	24(1)	-3(1)	8(1)	-3(1)
C(12)	39(1)	26(1)	21(1)	-2(1)	13(1)	-8(1)
C(22)	21(1)	19(1)	32(1)	-4(1)	8(1)	-5(1)
C(11)	28(1)	21(1)	22(1)	-2(1)	10(1)	-2(1)
C(13)	40(1)	24(1)	18(1)	7(1)	4(1)	-5(1)
C(23)	26(1)	23(1)	28(1)	-7(1)	8(1)	-4(1)
C(18)	36(1)	37(1)	32(1)	1(1)	16(1)	6(1)
C(29)	23(1)	30(1)	21(1)	5(1)	5(1)	5(1)
C(17)	29(1)	26(1)	25(1)	-2(1)	9(1)	-3(1)
C(3)	20(1)	21(1)	21(1)	-3(1)	4(1)	0(1)
C(30)	22(1)	35(1)	21(1)	3(1)	5(1)	7(1)
C(21)	27(1)	32(1)	24(1)	-3(1)	8(1)	-3(1)
C(28)	25(1)	26(1)	18(1)	2(1)	3(1)	3(1)
C(5)	27(1)	22(1)	36(1)	-3(1)	11(1)	-4(1)
C(31)	32(1)	37(1)	30(1)	-4(1)	8(1)	-10(1)
C(8)	25(1)	24(1)	22(1)	-2(1)	5(1)	3(1)
C(27)	30(1)	19(1)	51(1)	0(1)	17(1)	-1(1)
C(14)	30(1)	22(1)	24(1)	4(1)	2(1)	2(1)
C(25)	43(1)	34(1)	54(1)	-25(1)	30(1)	-15(1)

C(6)	29(1)	27(1)	38(1)	-11(1)	3(1)	-7(1)
C(19)	23(1)	56(1)	27(1)	6(1)	9(1)	5(1)
C(7)	31(1)	31(1)	28(1)	-7(1)	-1(1)	1(1)
C(24)	35(1)	36(1)	34(1)	-14(1)	16(1)	-12(1)
C(20)	25(1)	53(1)	24(1)	-3(1)	5(1)	-8(1)
C(26)	38(1)	21(1)	73(1)	-12(1)	30(1)	-3(1)
C(32)	34(1)	42(1)	28(1)	-2(1)	4(1)	-6(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **3i**.

	x	y	z	U(eq)
H(1A)	2550	5081	5630	26
H(15A)	661	6770	2648	27
H(4A)	2964	7389	3129	28
H(12A)	2387	6616	307	33
H(11A)	2765	5685	1835	28
H(23A)	782	4787	900	31
H(18A)	-1151	5908	3932	40
H(17A)	425	5664	4164	32
H(21A)	-347	3833	1739	33
H(28A)	3484	4105	5086	29
H(28B)	4199	4862	5068	29
H(5A)	3926	8603	3927	34
H(31A)	5677	6470	8820	40
H(31B)	6455	5929	8531	40
H(27A)	2368	2929	2992	39
H(14A)	280	7703	1117	33
H(25A)	1819	2694	-255	49
H(6A)	4743	8640	5803	40
H(19A)	-2320	5130	2585	43
H(7A)	4612	7472	6935	39
H(24A)	974	4020	-560	41
H(20A)	-1916	4069	1526	42
H(26A)	2520	2153	1511	50
H(32A)	6843	5985	10437	54
H(32B)	6655	4989	10035	54
H(32C)	5880	5526	10323	54