Electronic Supplementary Material (ESI) for RSC Advances.
This journal is © The Royal Society of Chemistry 2019

Synthesis, structural studies and biological properties of some phosphono-perfluorophenylalanine derivatives formed by S_NAr reactions

Joanna Kwiczak-Yiğitbaşı[a,b], Jean-Luc Pirat[b], David Virieux[b], Jean-Noël Volle[b,*], Agnieszka Janiak[a], Marcin Hoffmann[a], Jakub Mrzygłód[a], Dariusz Wawrzyniak[c], Jan Barciszewski[c,d] and Donata Pluskota-Karwatka[a,*]

[a] *Adam Mickiewicz University in Poznań, Faculty of Chemistry, Umultowska 89b, 61-614 Poznań, Poland*

[b] *AM2N, UMR 5253, ICGM, ENSCM, 8 rue de l'Ecole Normale, 34296 Montpellier Cedex 5, France*

[c] *Institute of Bioorganic Chemistry, Polish Academy of Sciences, Noskowskiego 12/14, 61-704 Poznań, Poland*

[d] *NanoBioMedical Center of Adam Mickiewicz University, Umultowska 85, 61-614, Poznań, Poland*

Supplementary Information

NMR spectra and HRMS data of compounds 2a-2s

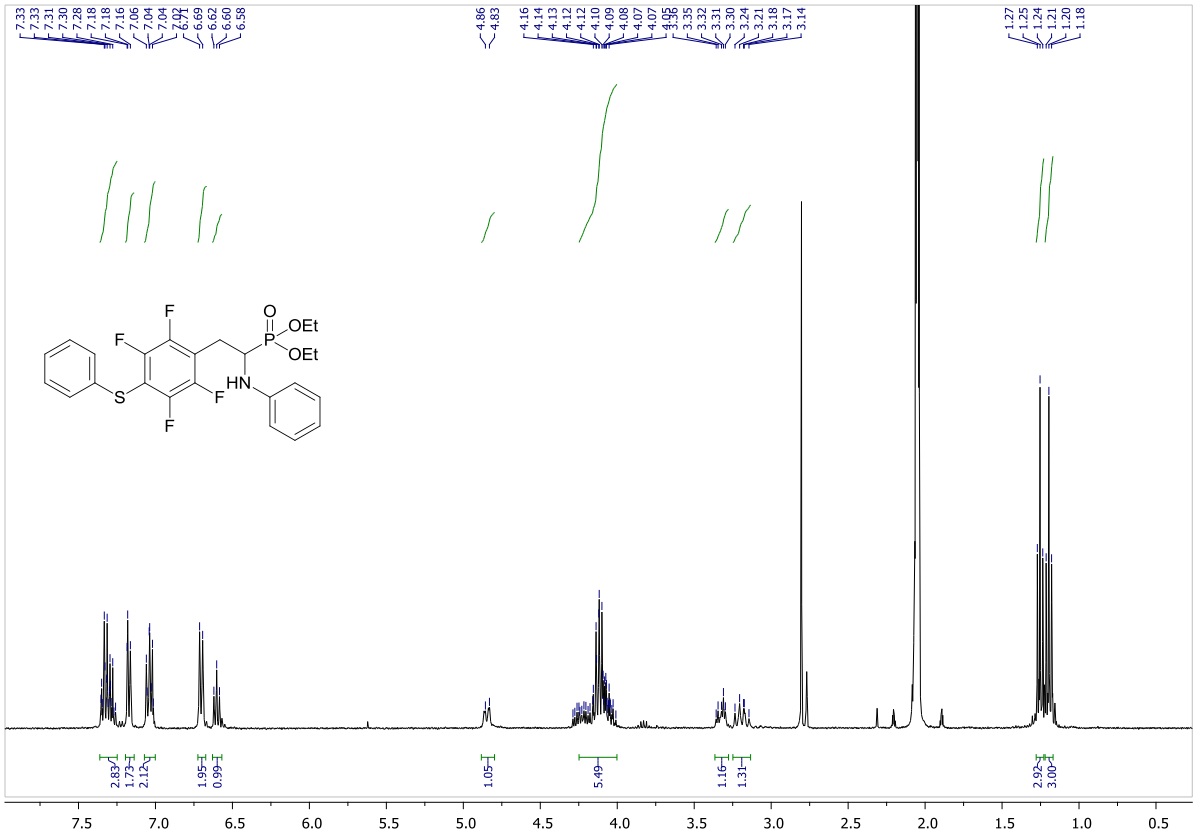

Fig. S1. ^{1}H NMR spectrum of 2a (Acetone-d6)

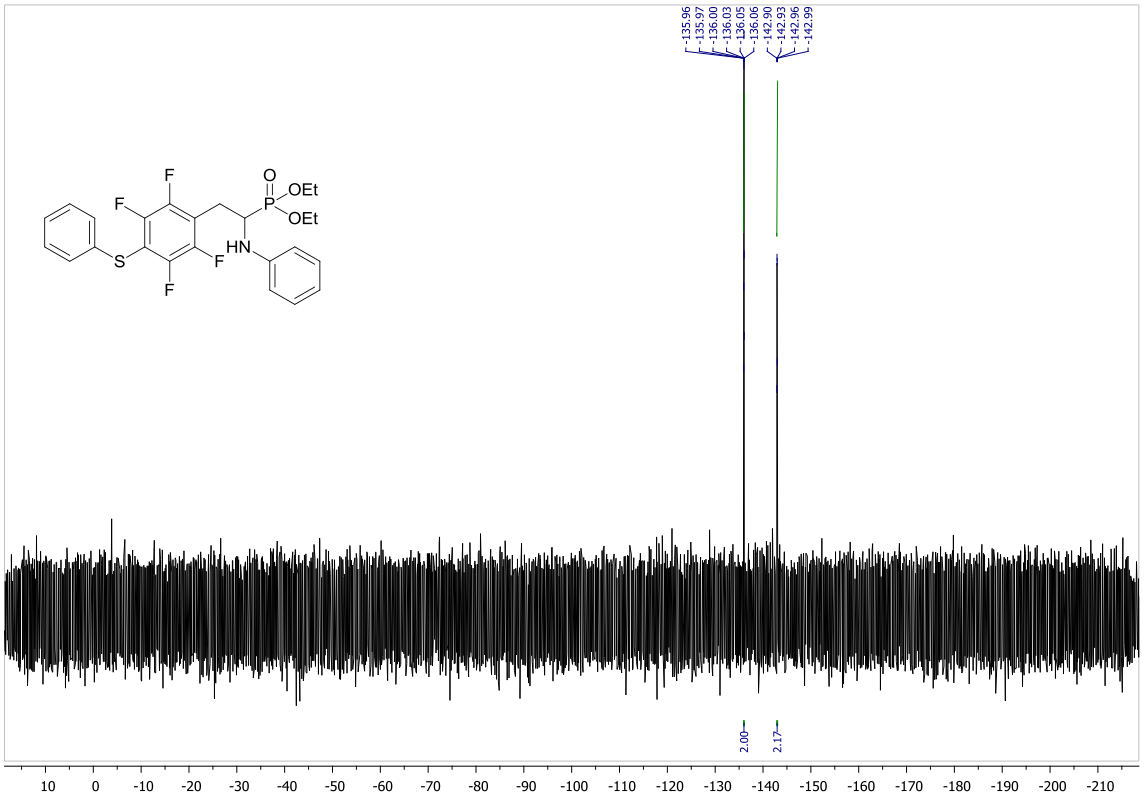

Fig. S2. ^{19}F NMR spectrum of 2a (Acetone-d6)

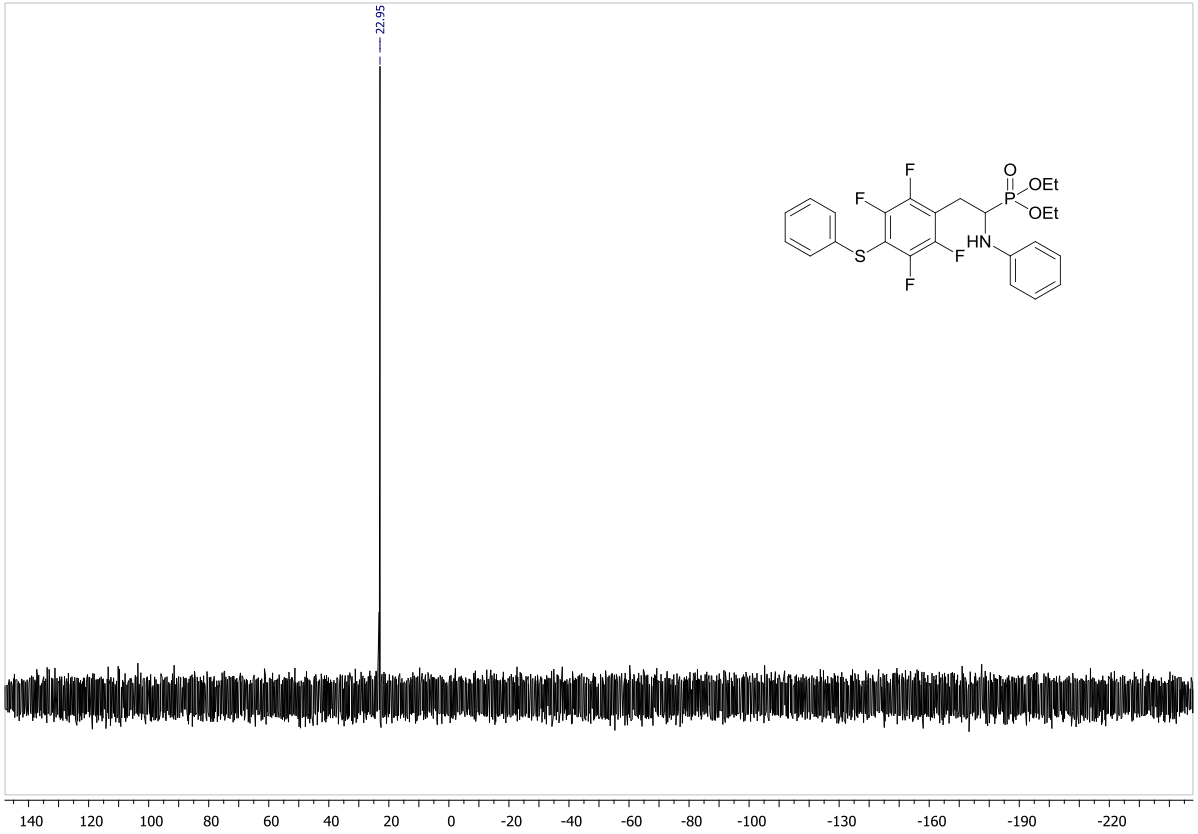

Fig. S3. ^{31}P NMR spectrum of 2a (Acetone-d6)

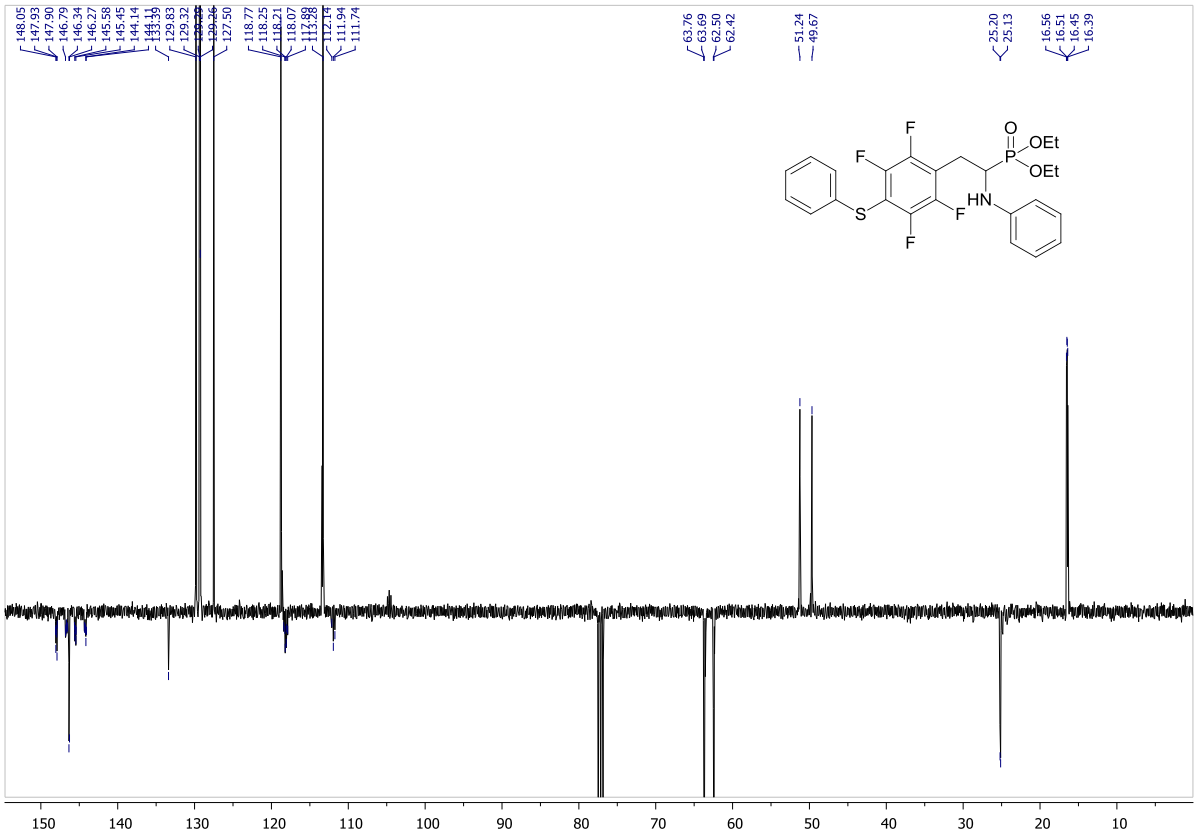

Fig. S4. ^{13}C NMR spectrum of 2a ($CDCl_3$)

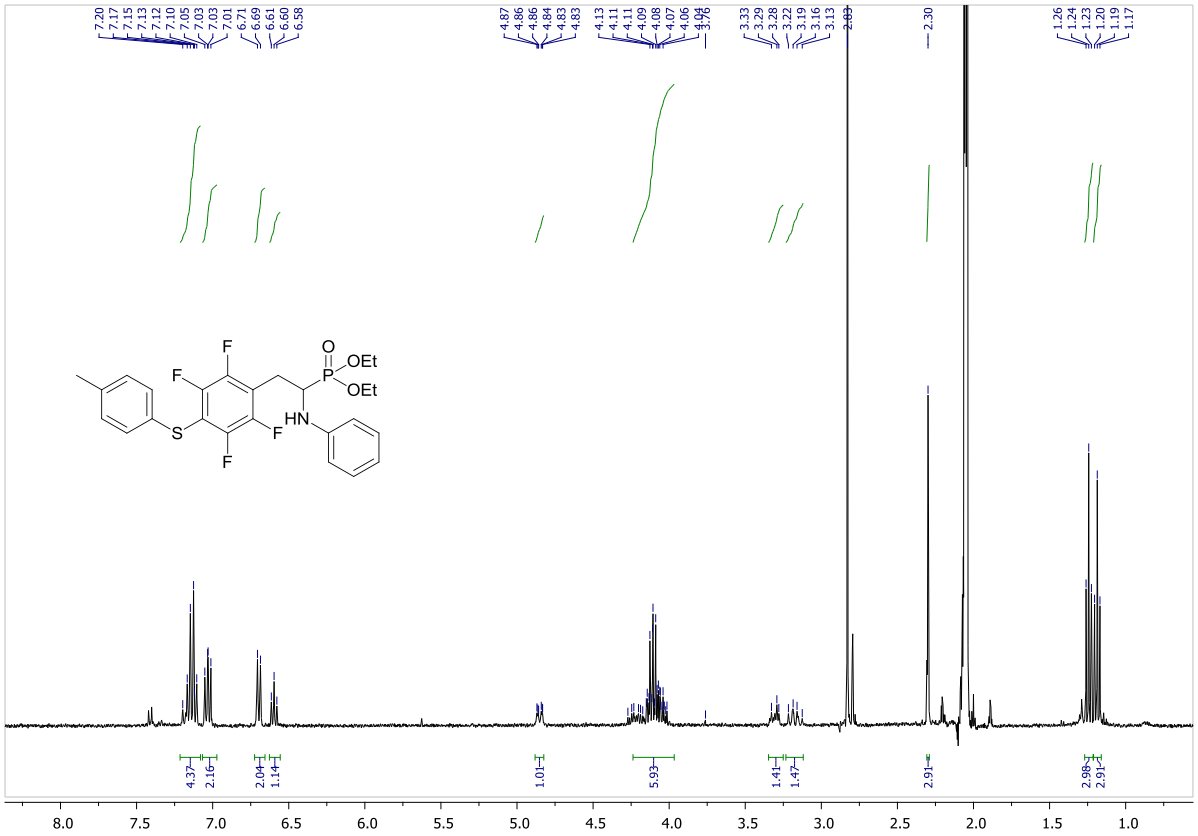

Fig. S5. ^{1}H NMR spectrum of 2b (Acetone-d6)

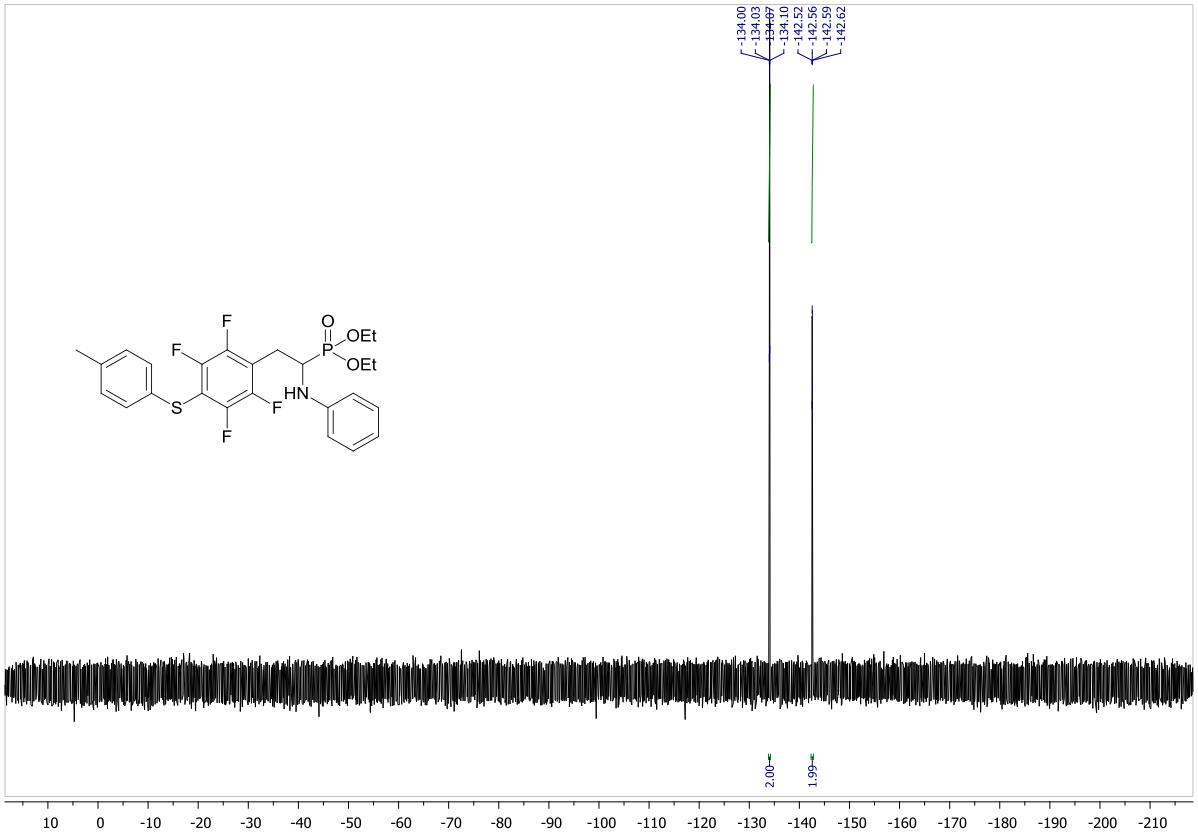

Fig. S6. ^{19}F NMR spectrum of 2b ($CDCl_3$)

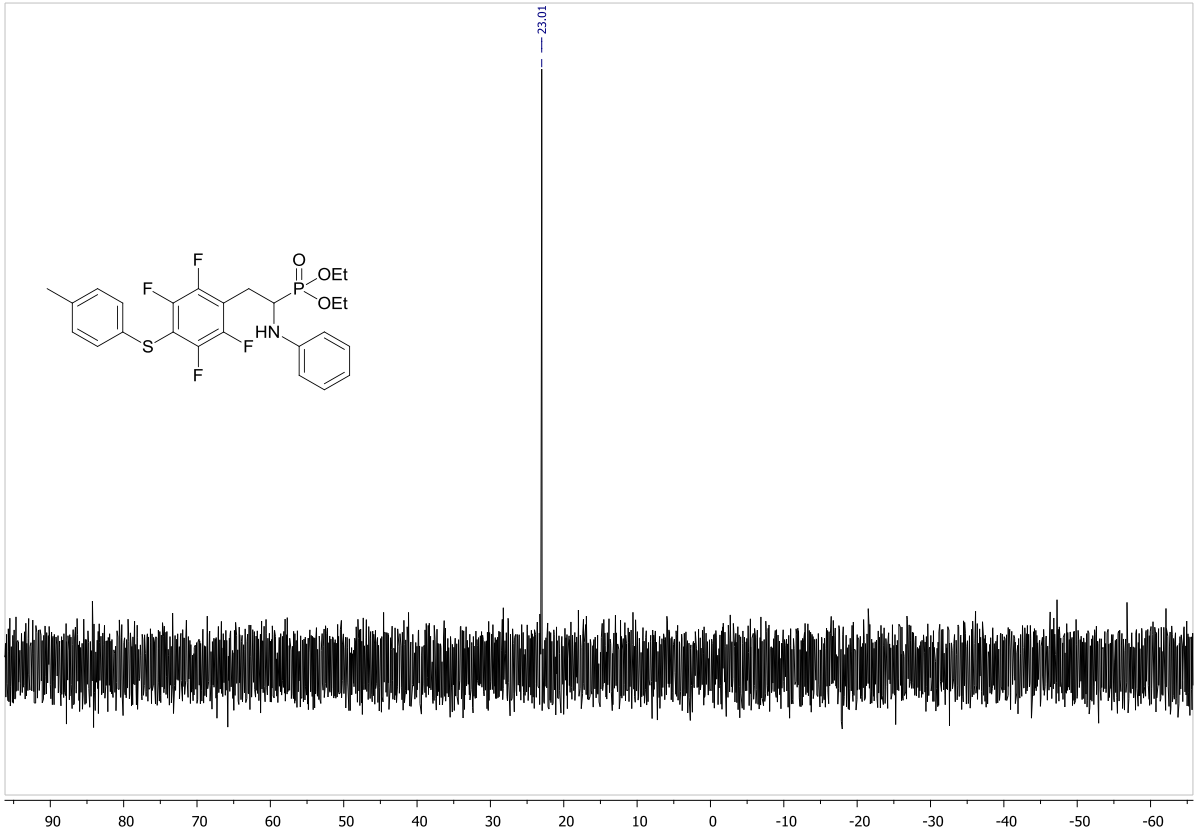

Fig. S7. ^{31}P NMR spectrum of 2b (Acetone-d6)

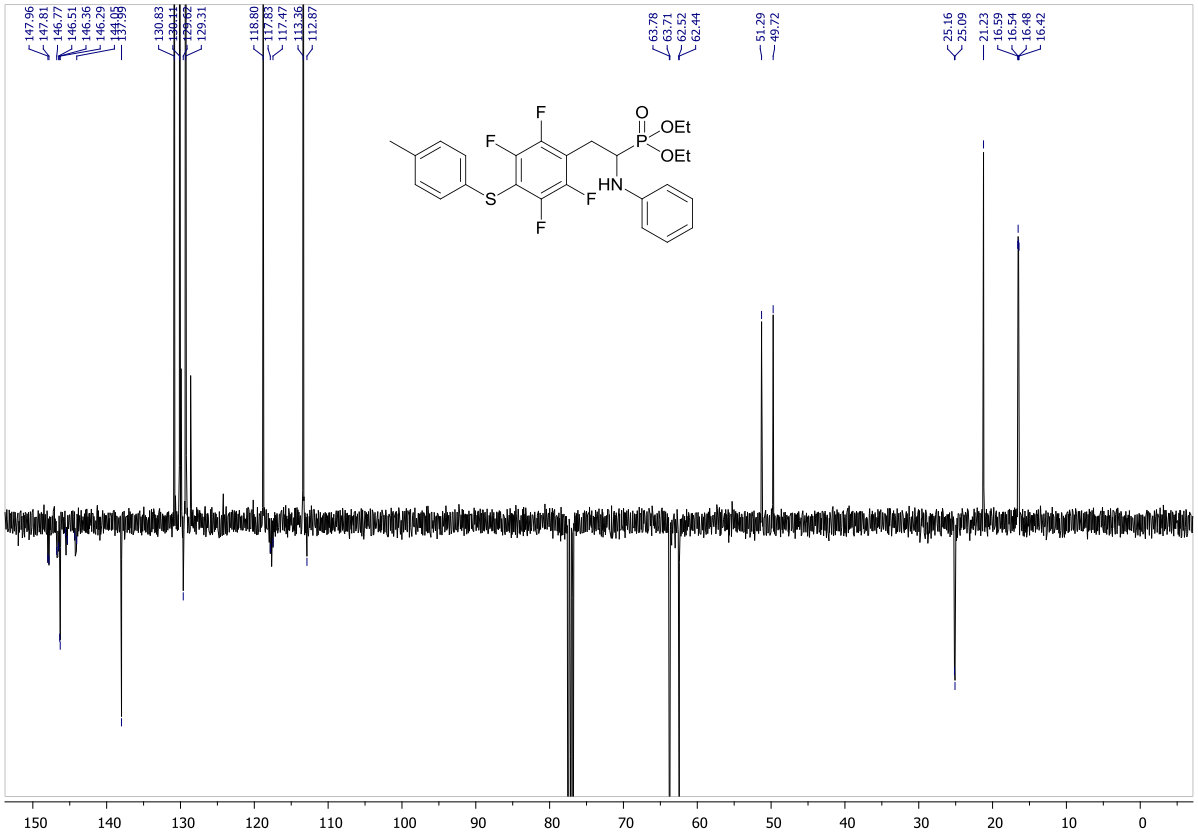

Fig. S8. ^{13}C NMR spectrum of 2b ($CDCl_3$)

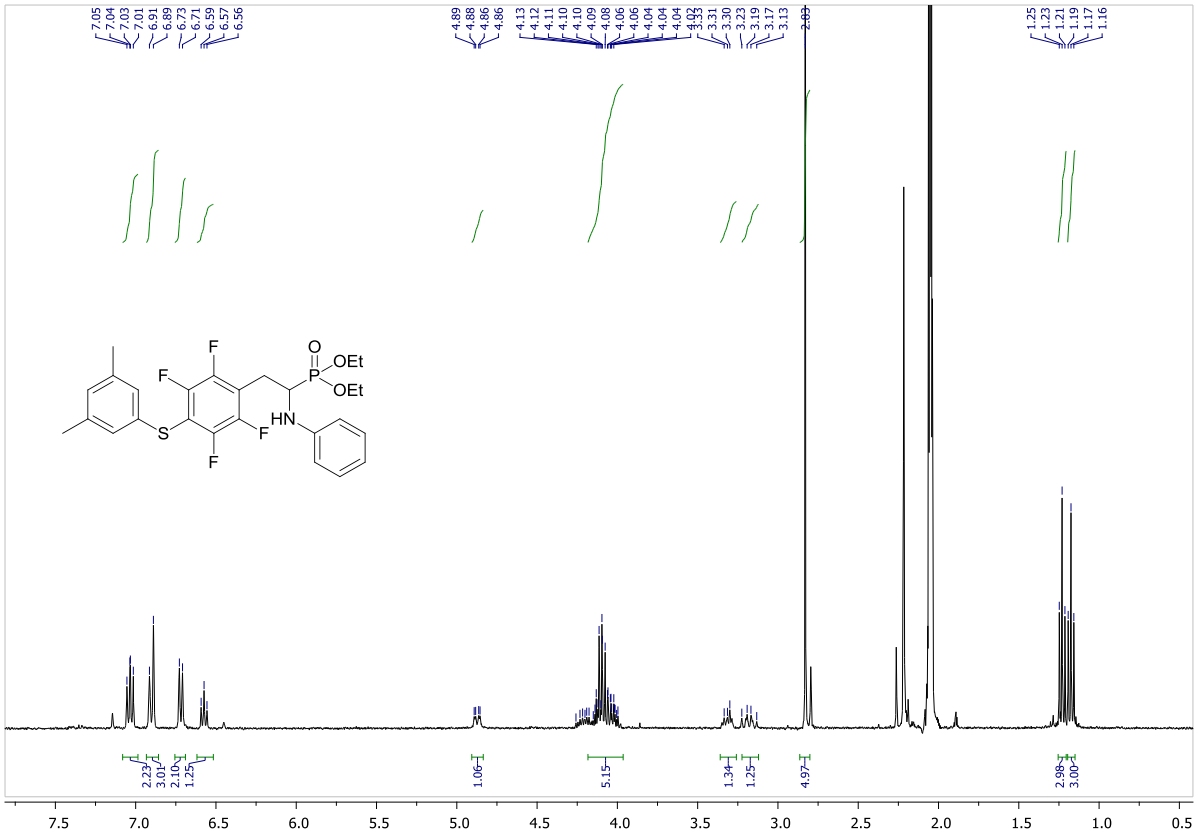

Fig. S9. ^{1}H NMR spectrum of 2c (Acetone-d6)

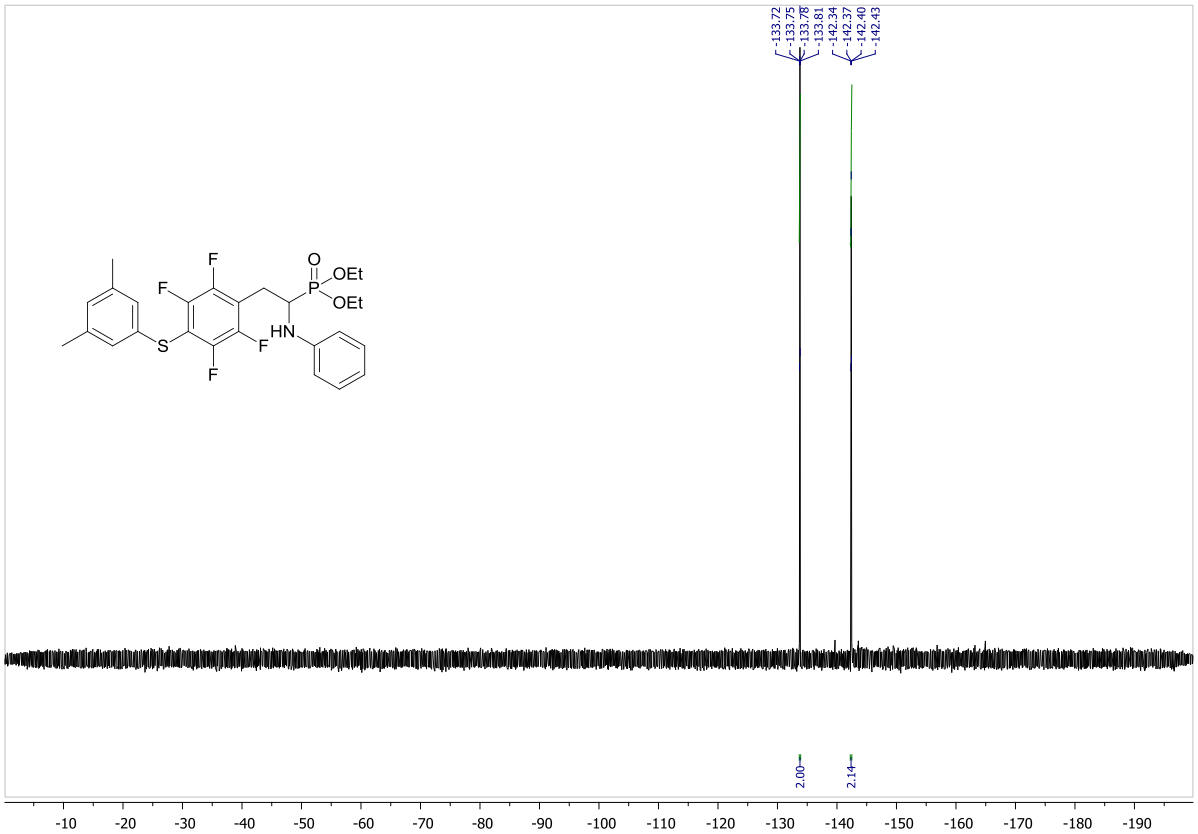

Fig. S10. ^{19}F NMR spectrum of 2c ($CDCl_3$)

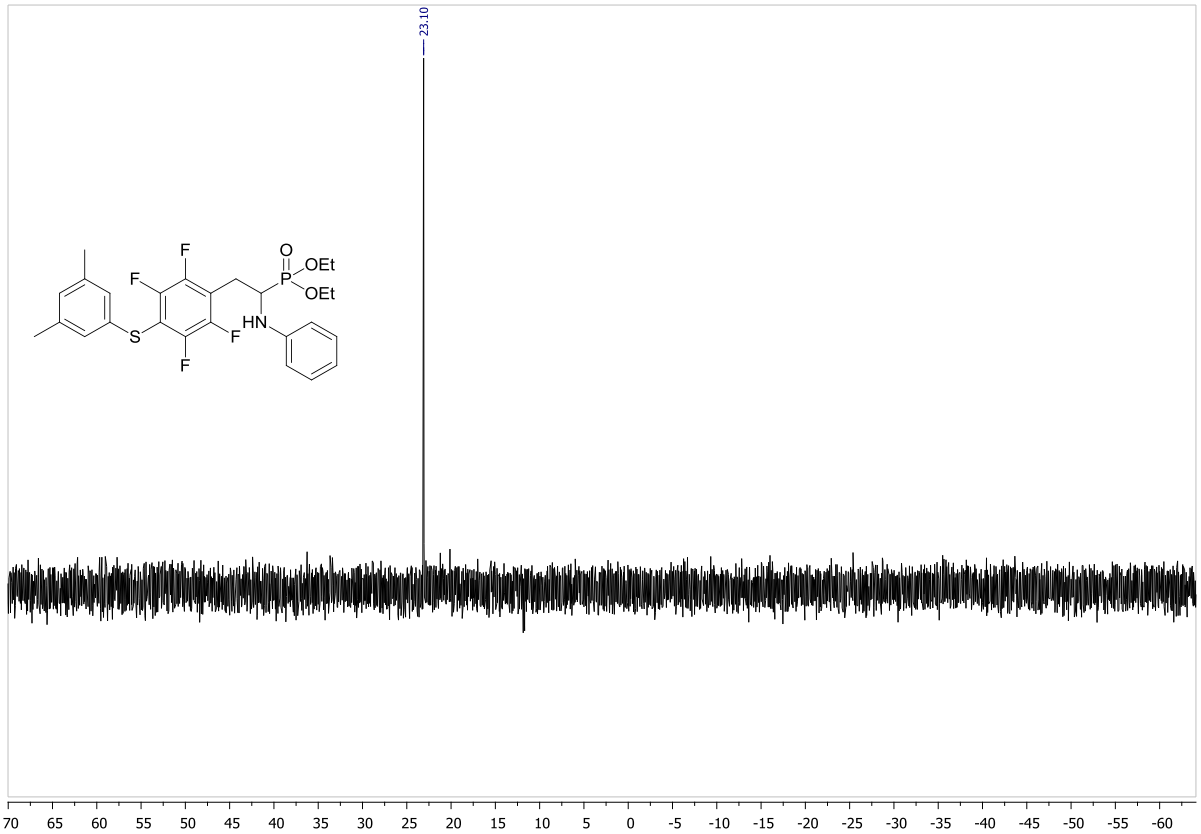

Fig. S11. ^{31}P NMR spectrum of 2c (Acetone-d6)

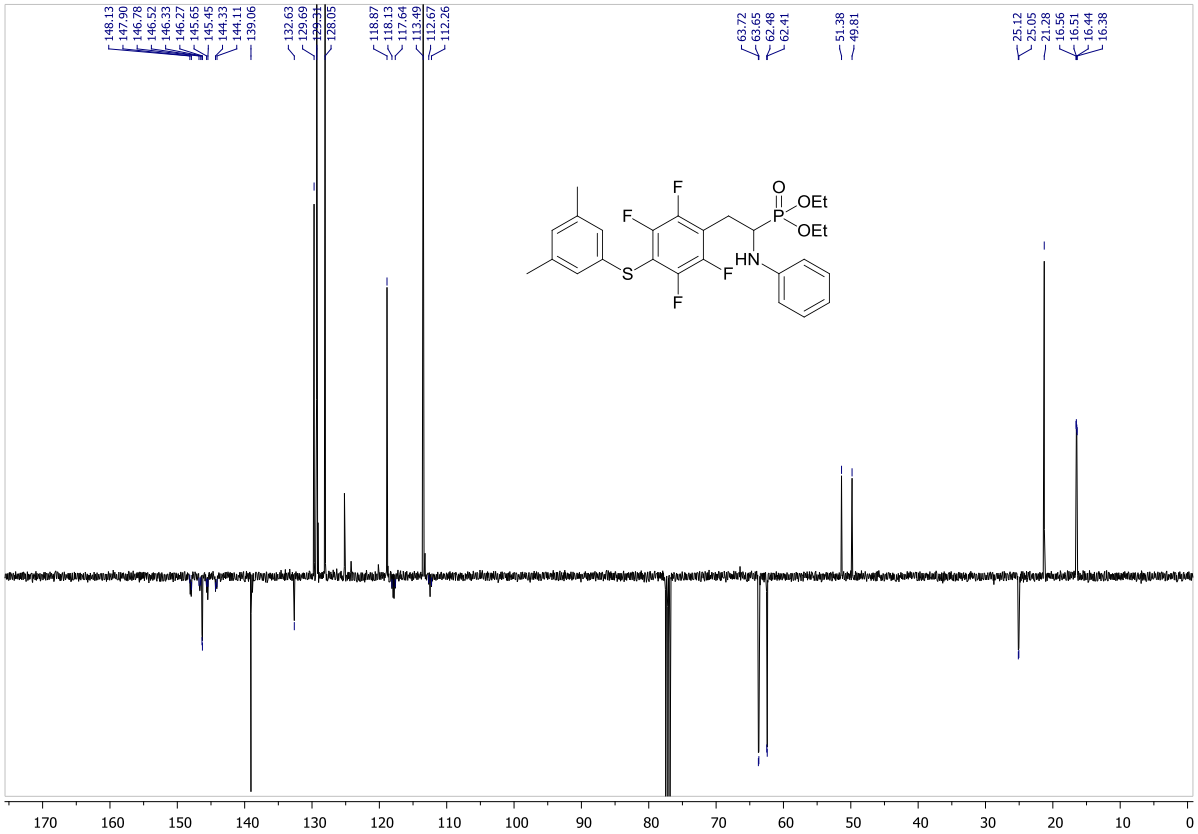

Fig. S12. ^{13}C NMR spectrum of 2c ($CDCl_3$)

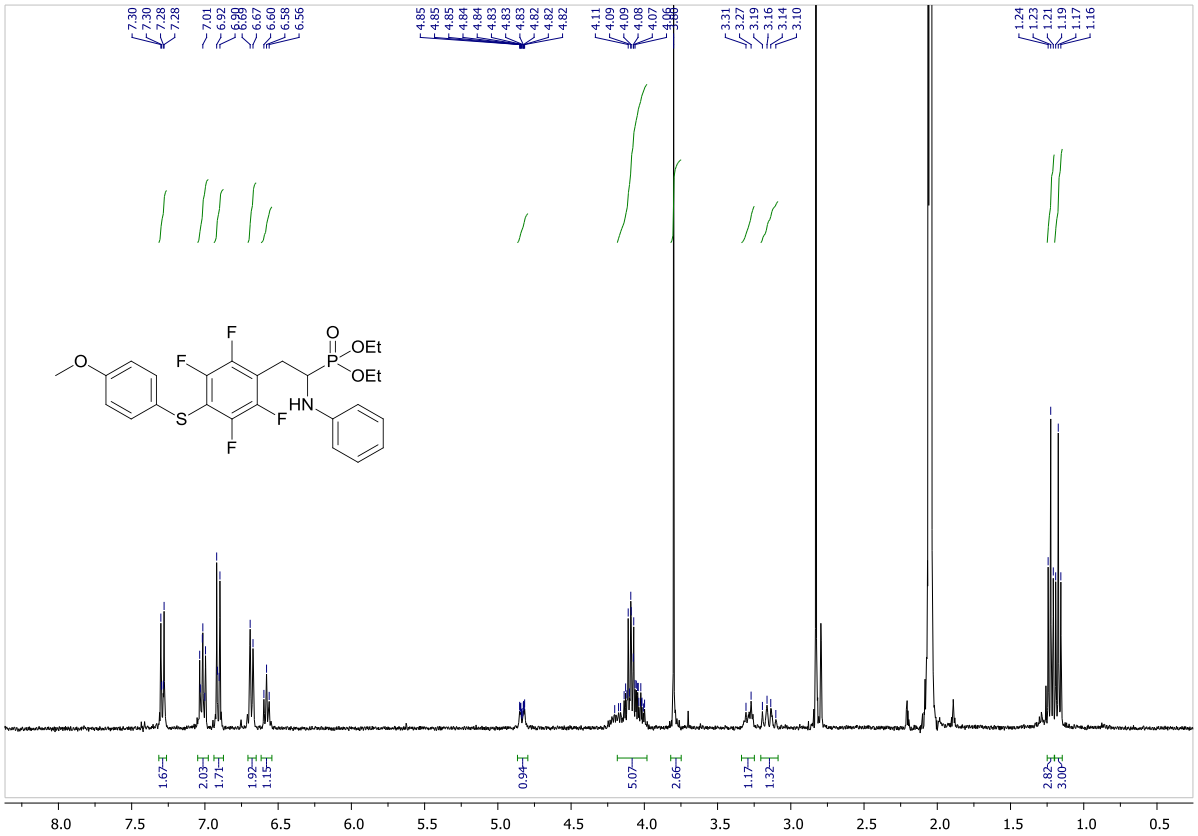

Fig. S13. ^{1}H NMR spectrum of 2d (Acetone-d6)

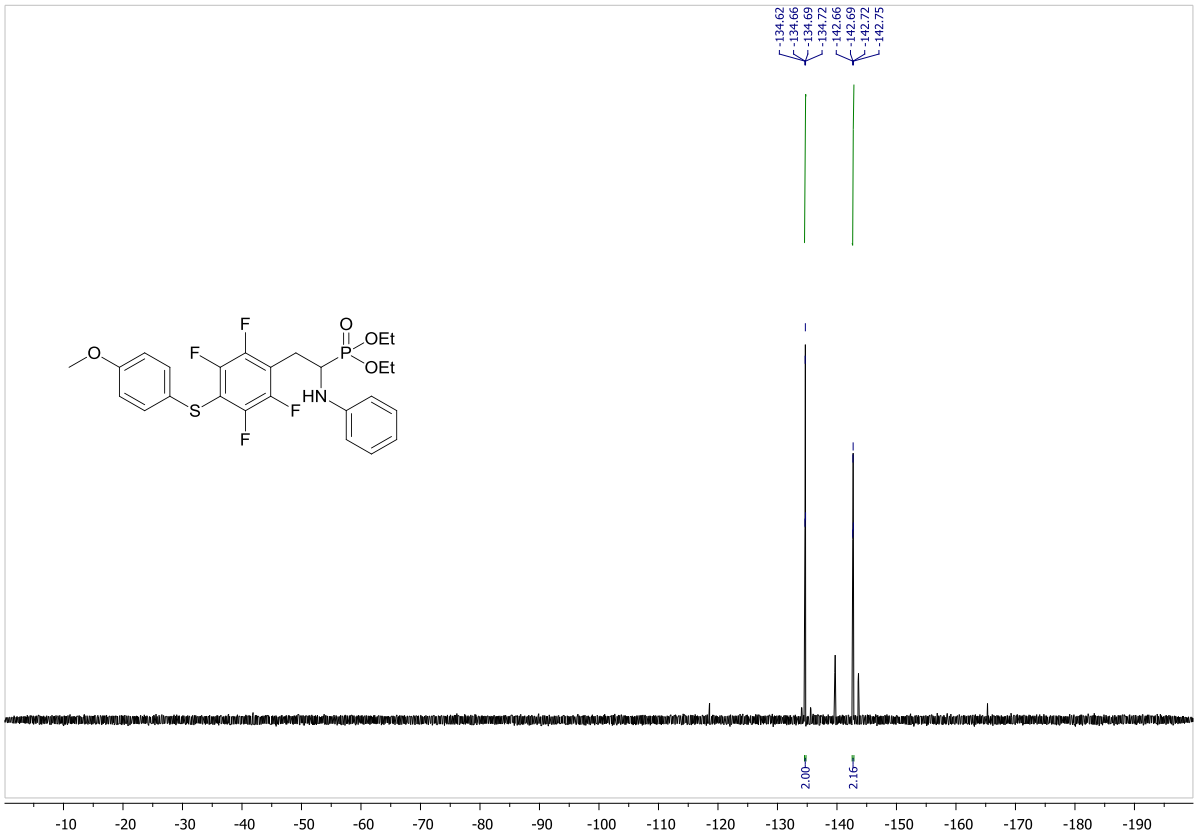

Fig. S14. ^{19}F NMR spectrum of 2d ($CDCl_3$)

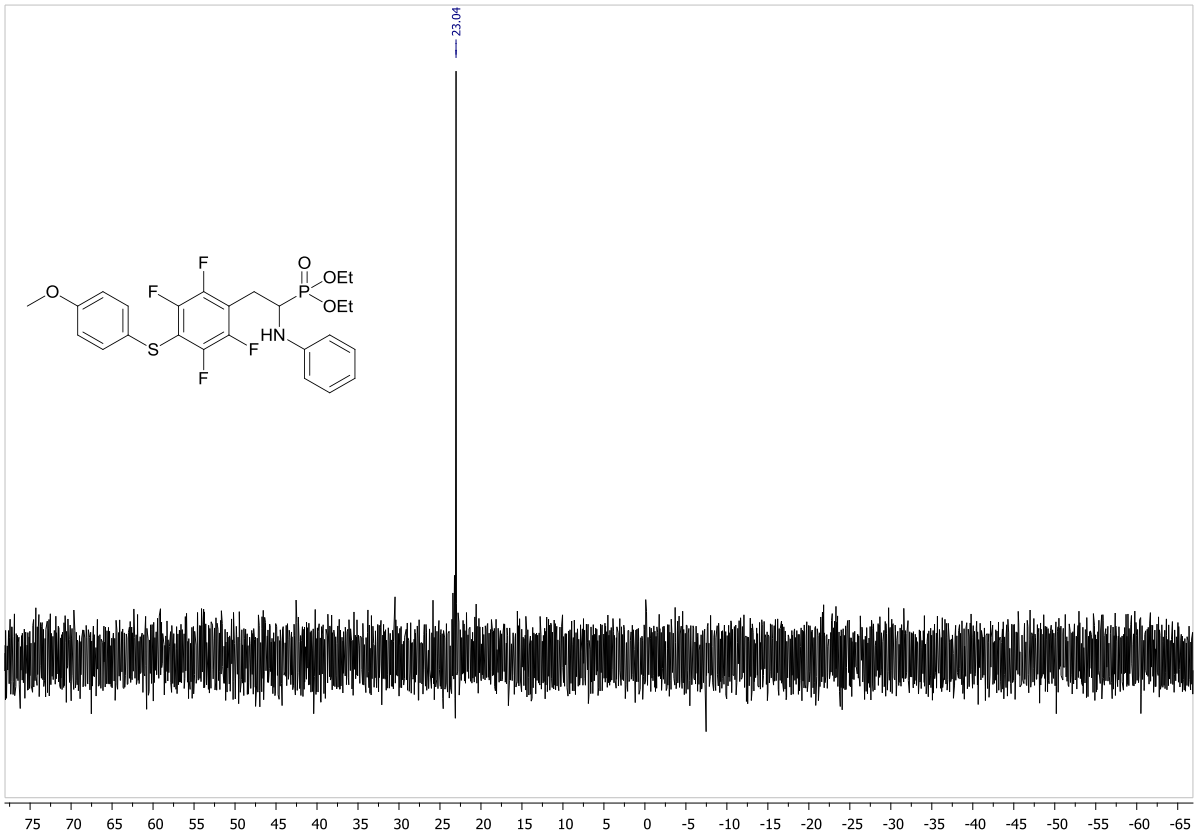

Fig. S15. ^{31}P NMR spectrum of 2d (Acetone-d6)

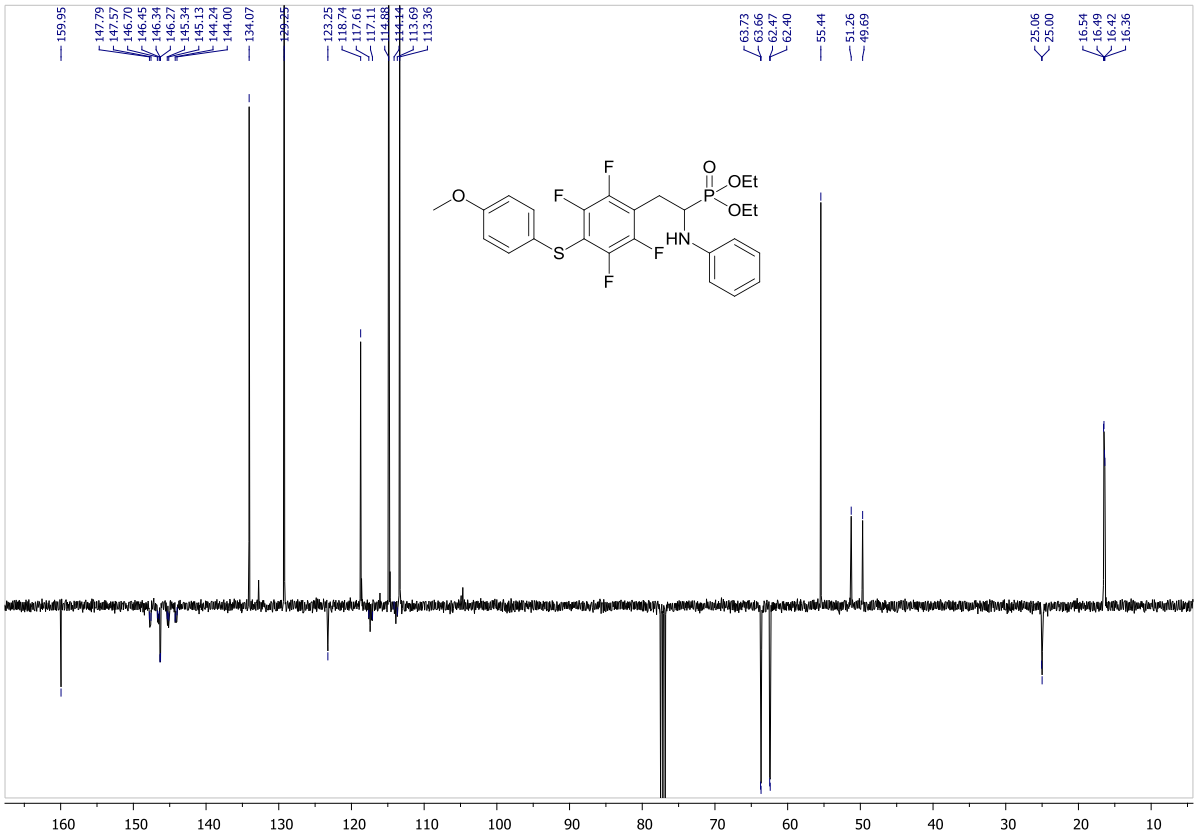

Fig. S16. ^{13}C NMR spectrum of 2d ($CDCl_3$)

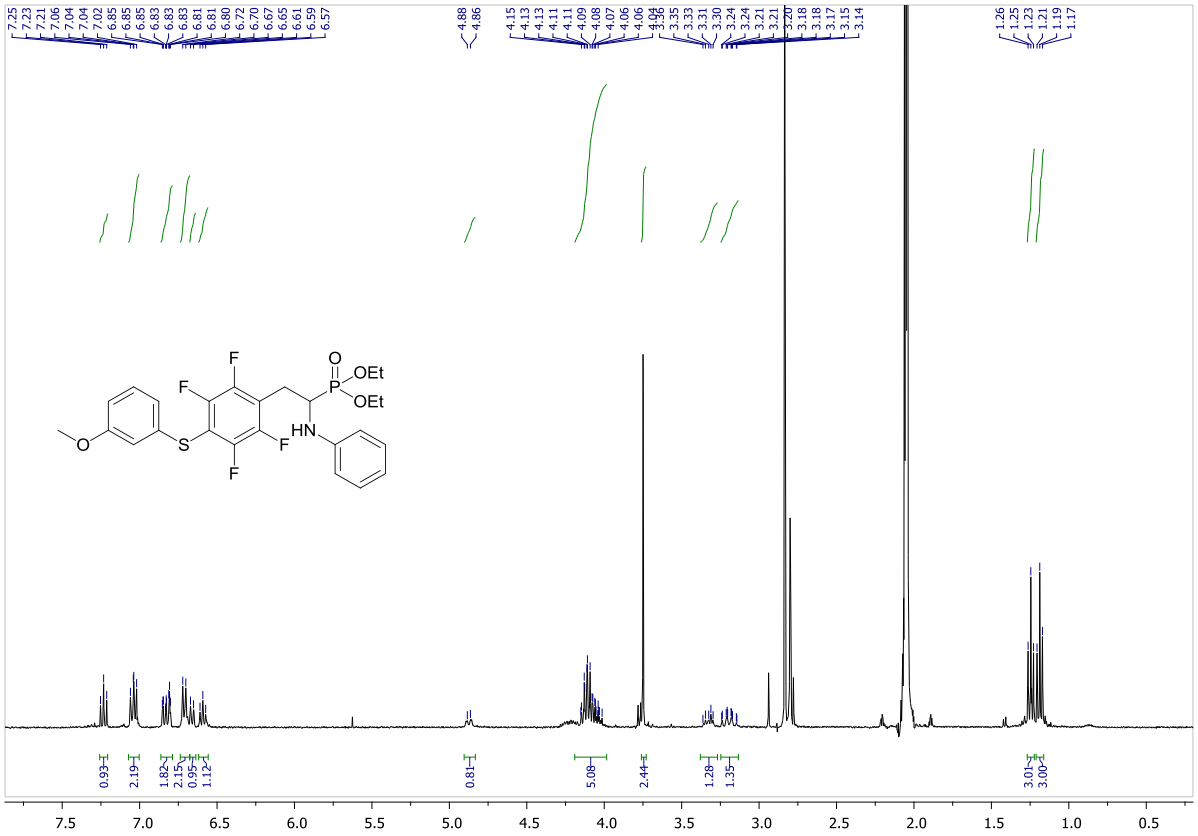

Fig. S17. ^{1}H NMR spectrum of 2e (Acetone-d6)

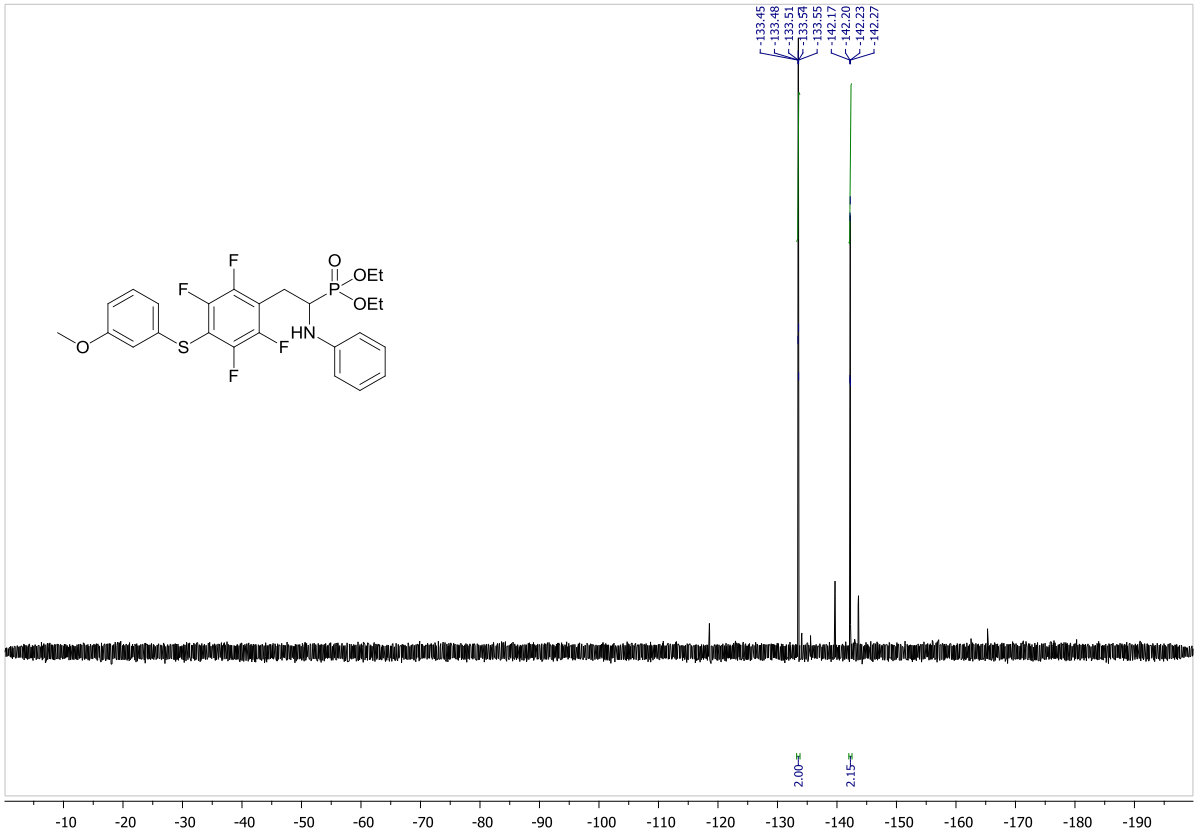

Fig. S18. ^{19}F NMR spectrum of 2e ($CDCl_3$)

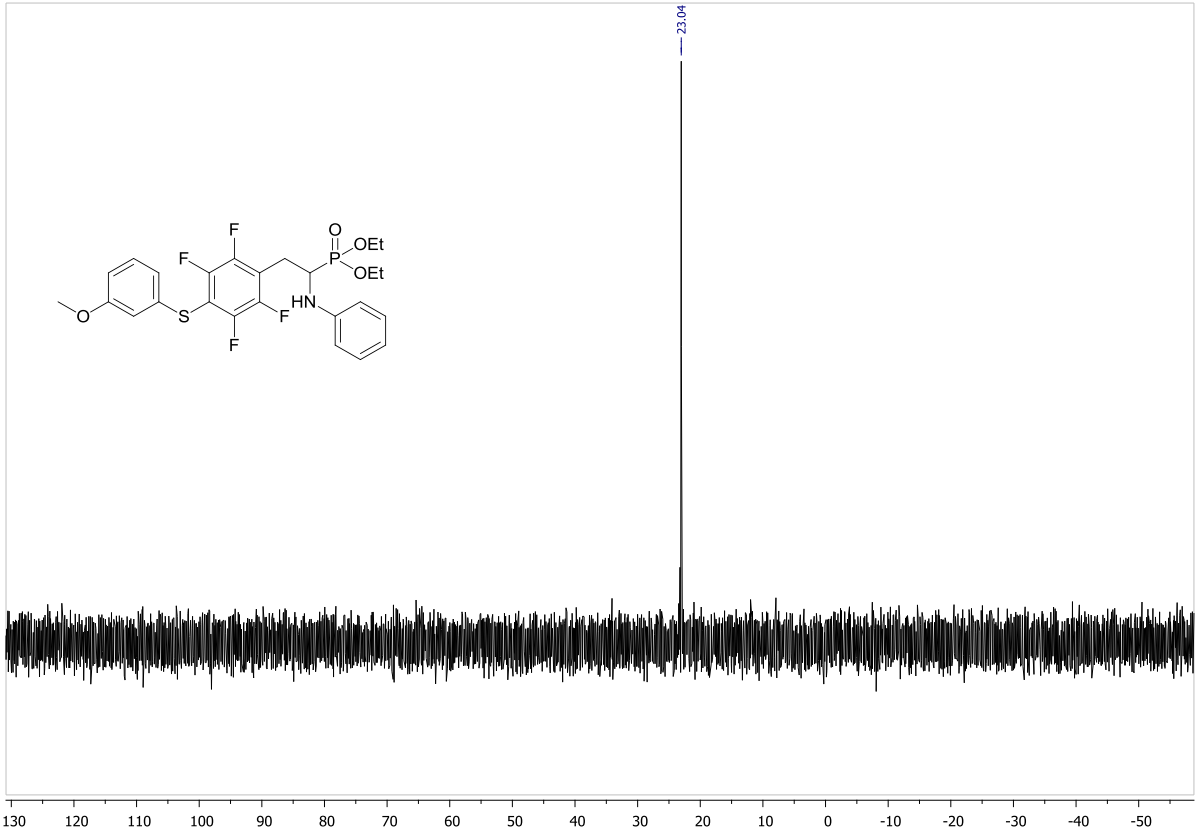

Fig. S19. ^{31}P NMR spectrum of 2e (Acetone-d6)

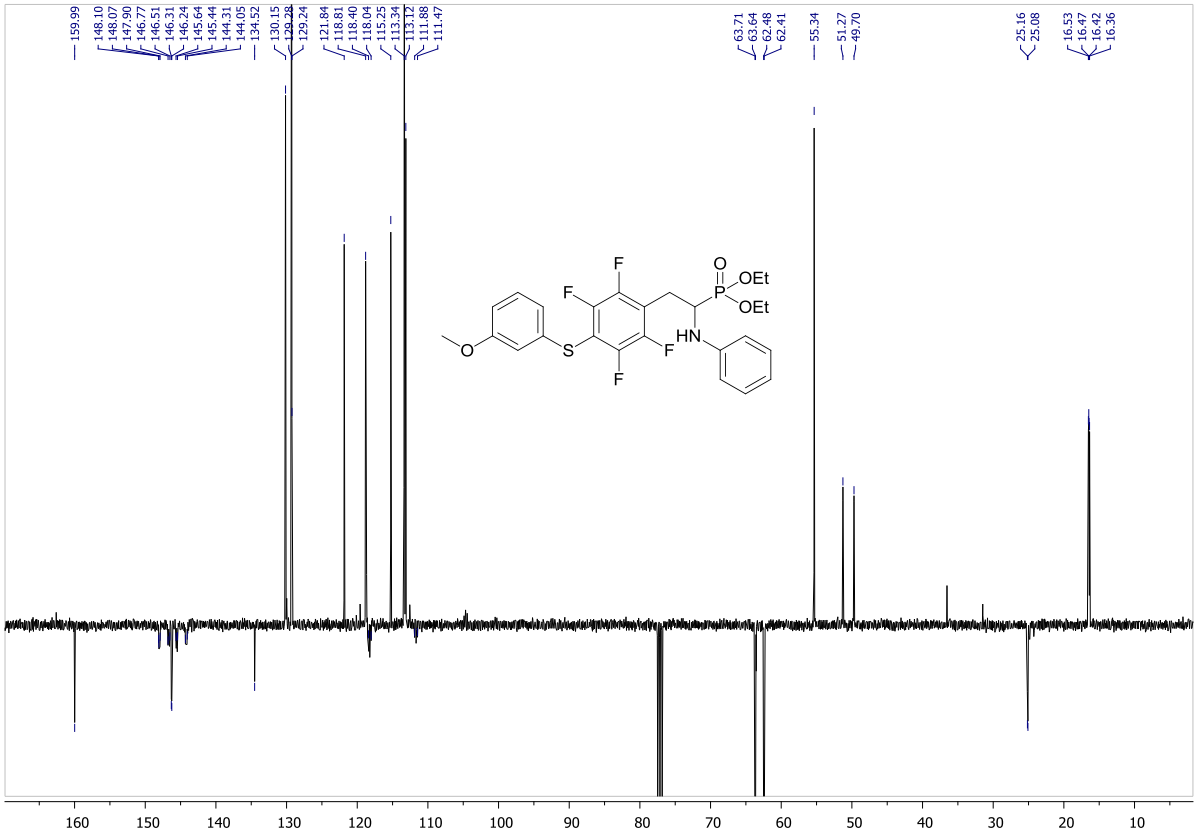

Fig. S20. ^{13}C NMR spectrum of 2e ($CDCl_3$)

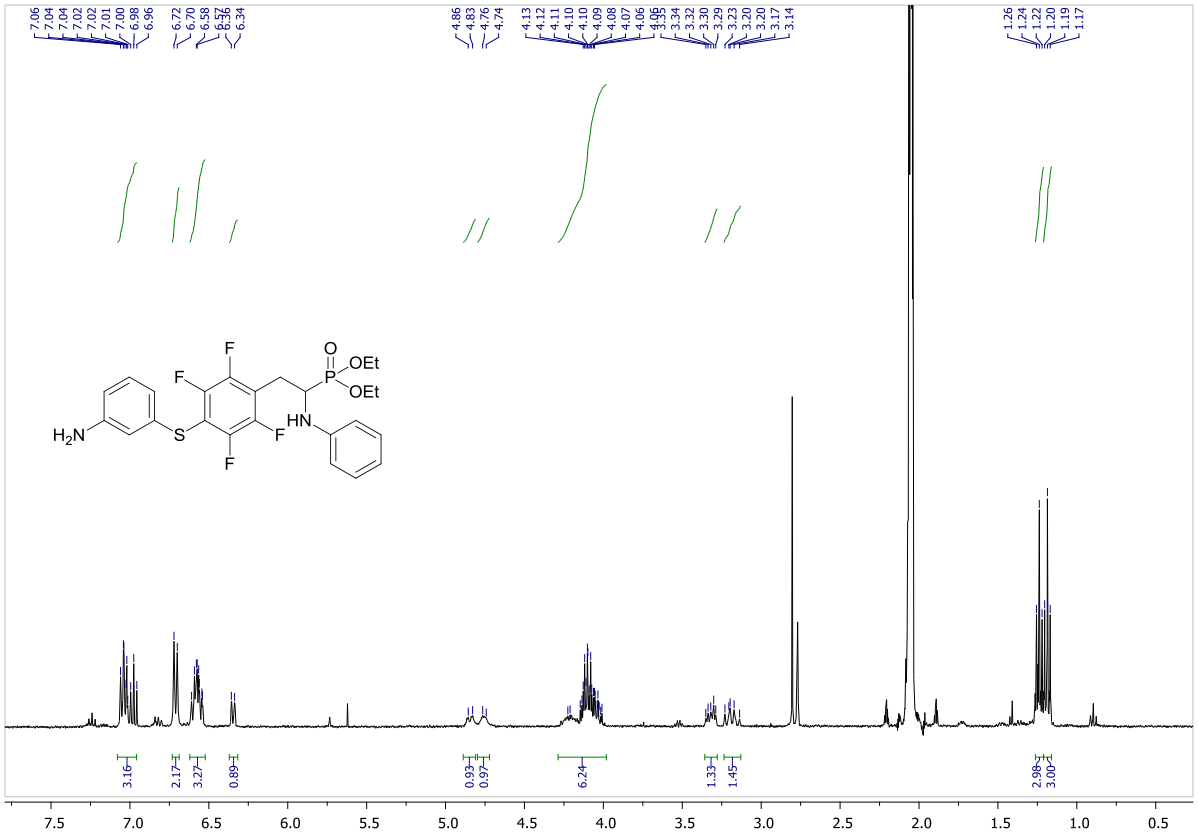

Fig. S21. ^{1}H NMR spectrum of 2f (Acetone-d6)

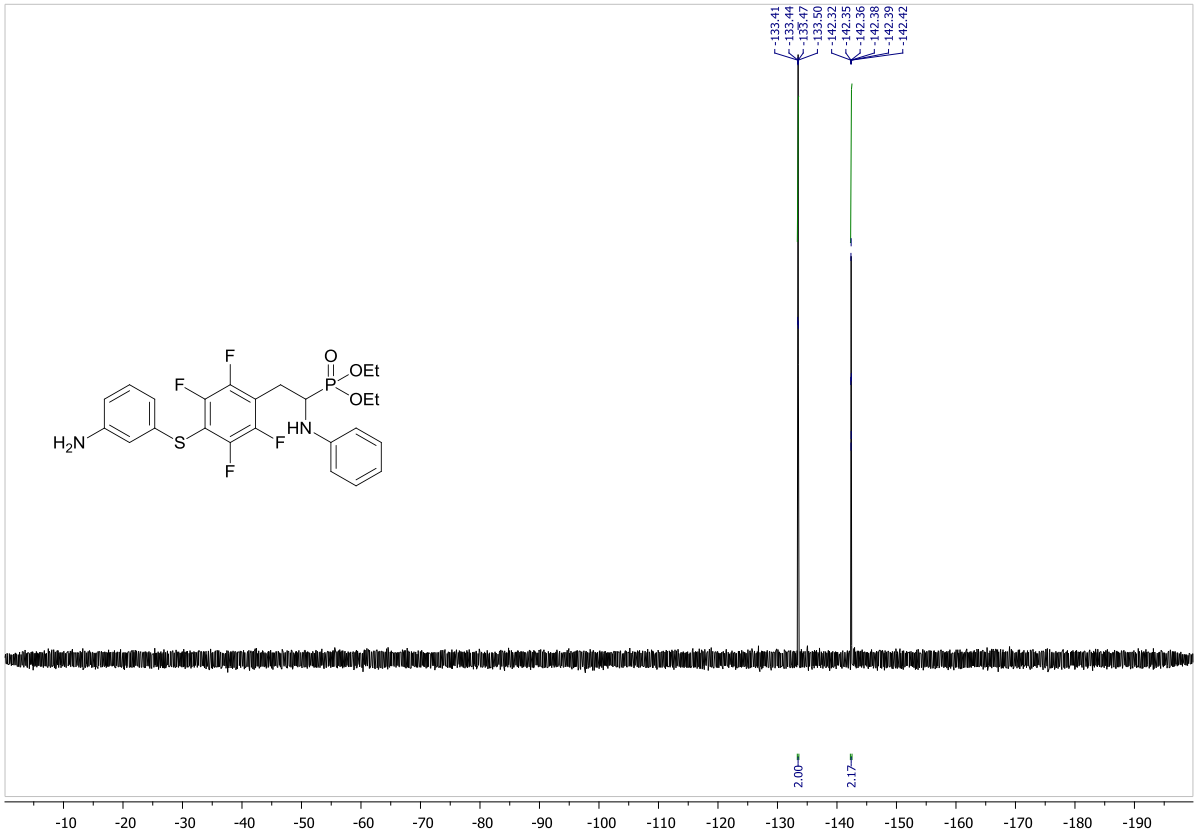

Fig. S22. ^{19}F NMR spectrum of 2f ($CDCl_3$)

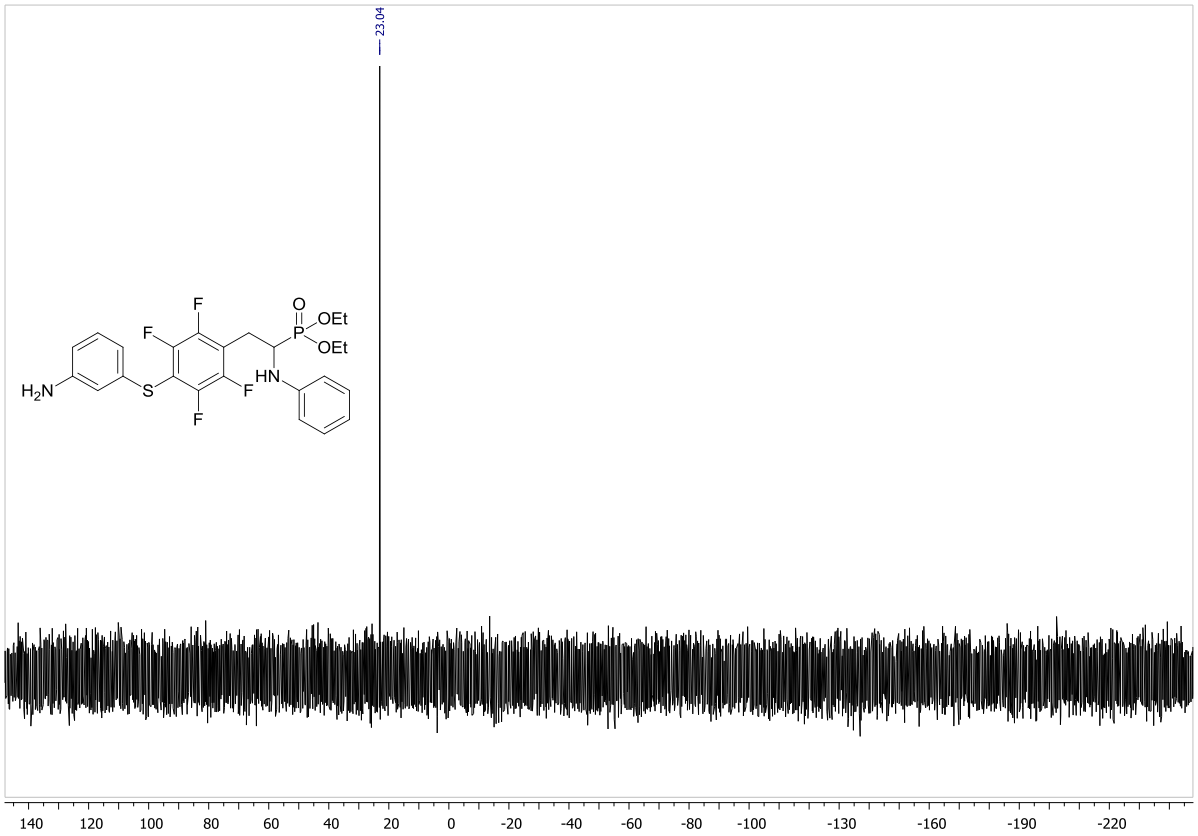

Fig. S23. ^{31}P NMR spectrum of 2f (Acetone-d6)

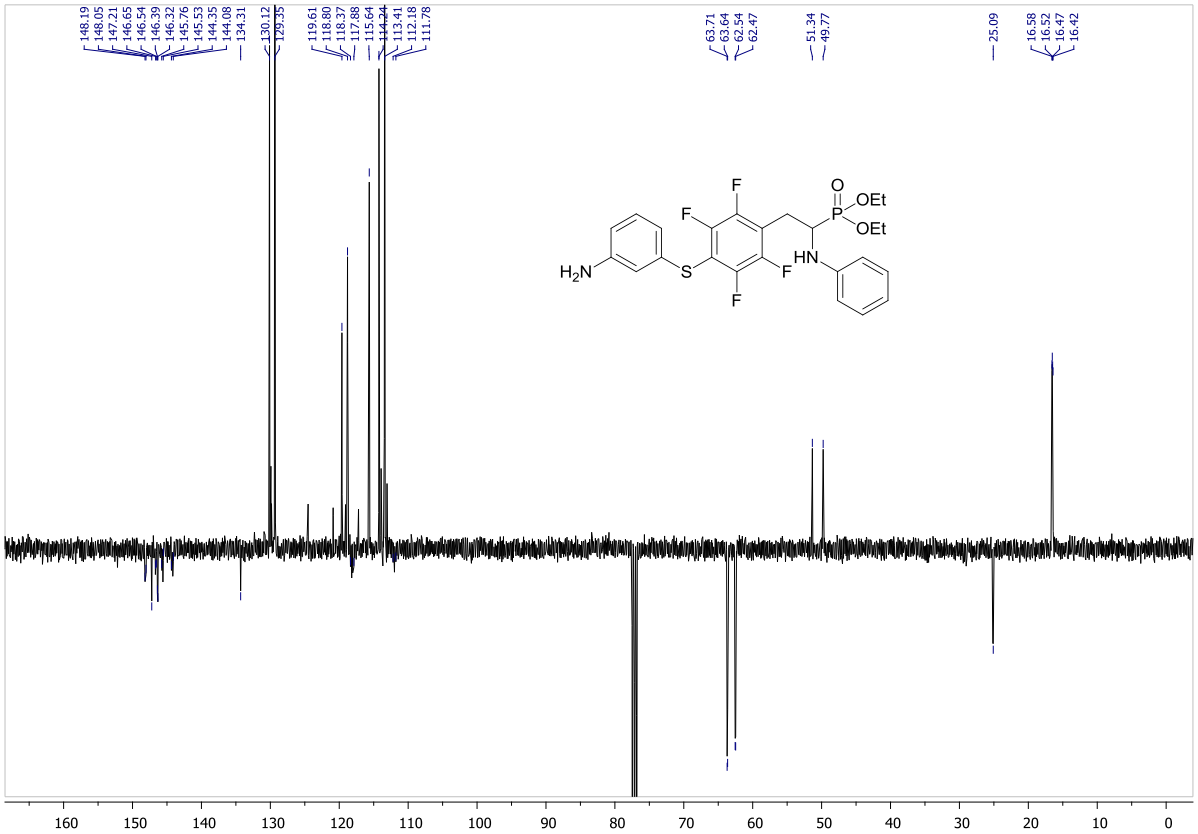

Fig. S24. ^{13}C NMR spectrum of 2f ($CDCl_3$)

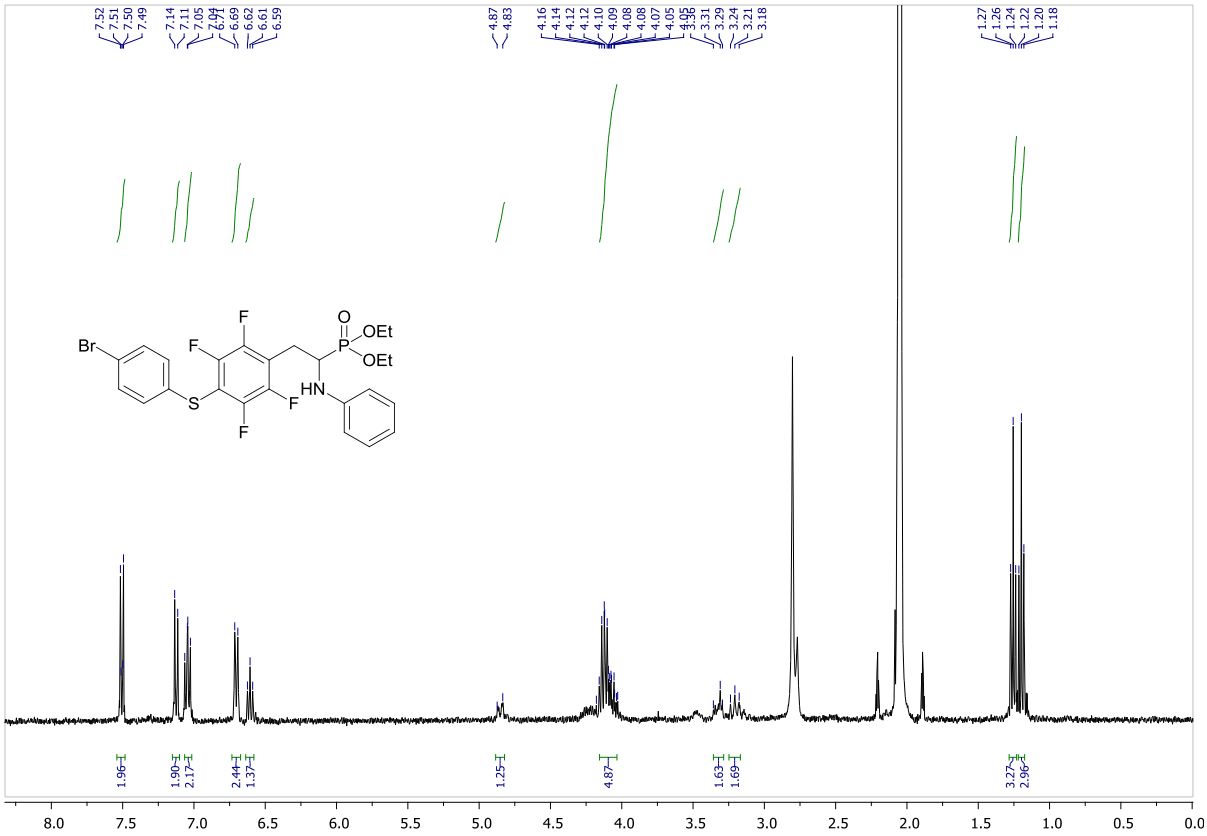

Fig. S25. ^{1}H NMR spectrum of 2g (Acetone-d6)

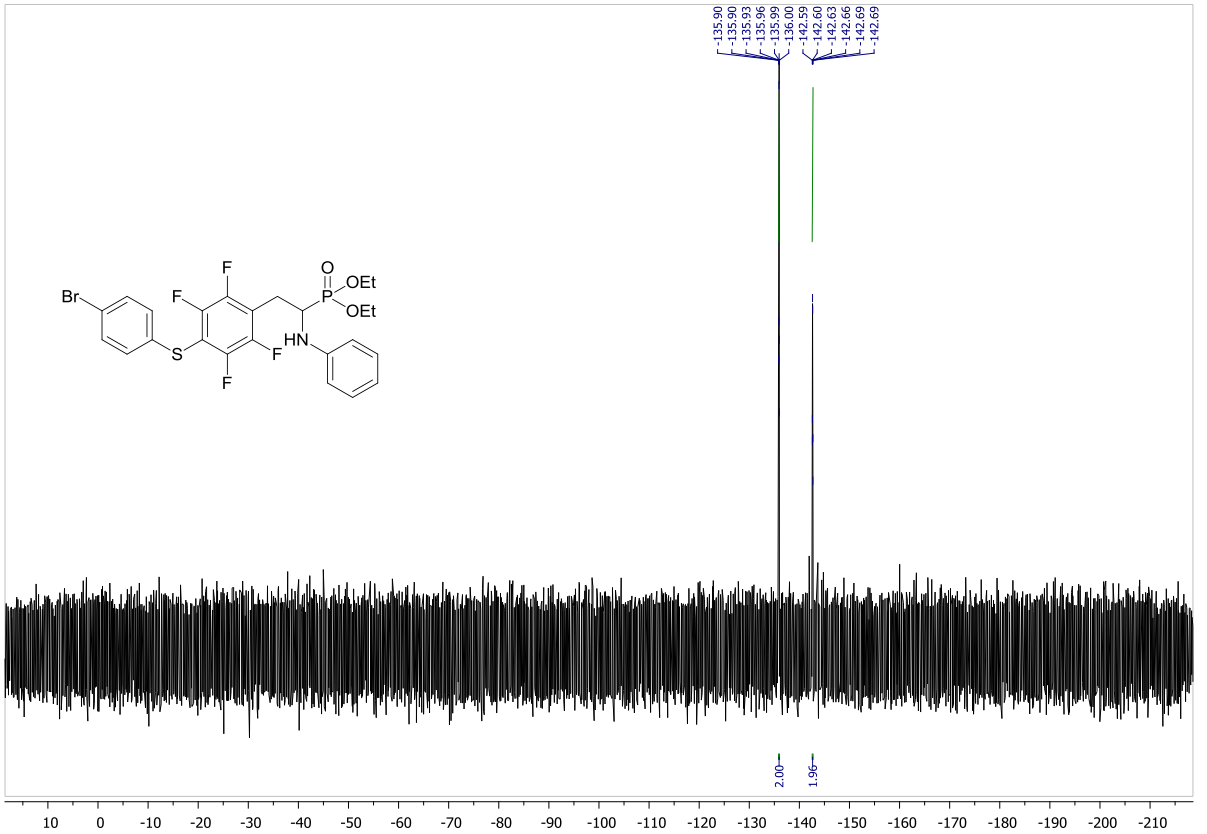

Fig. S26. ^{19}F NMR spectrum of 2g (Acetone-d6)

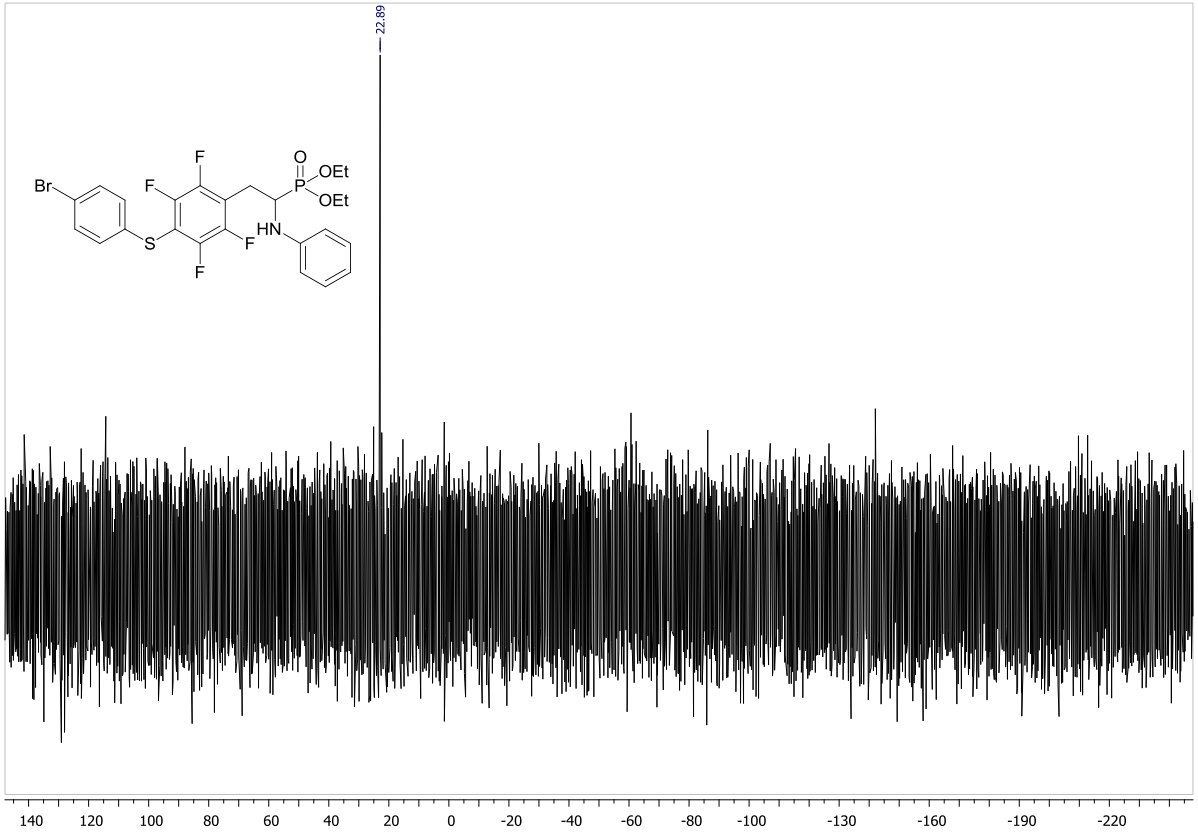

Fig. S27. ^{31}P NMR spectrum of 2g (Acetone-d6)

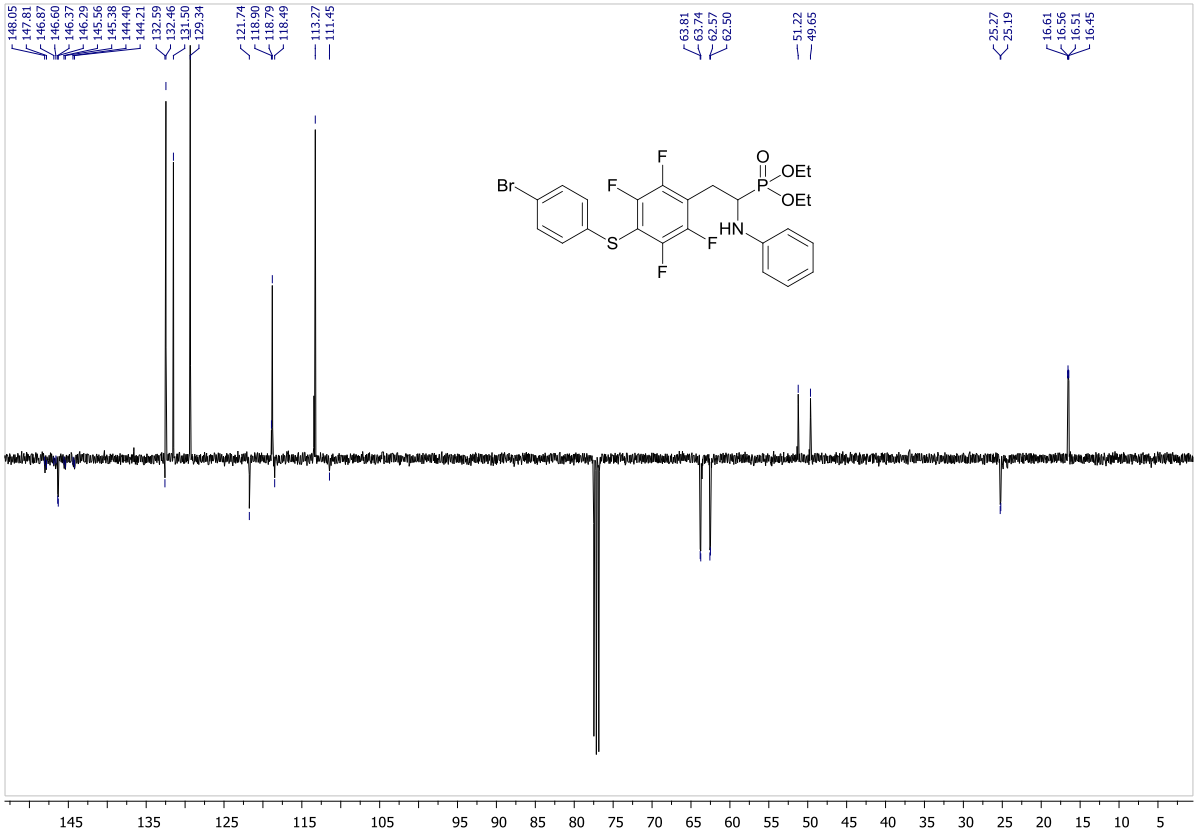

Fig. S28. ^{13}C NMR spectrum of 2g ($CDCl_3$)

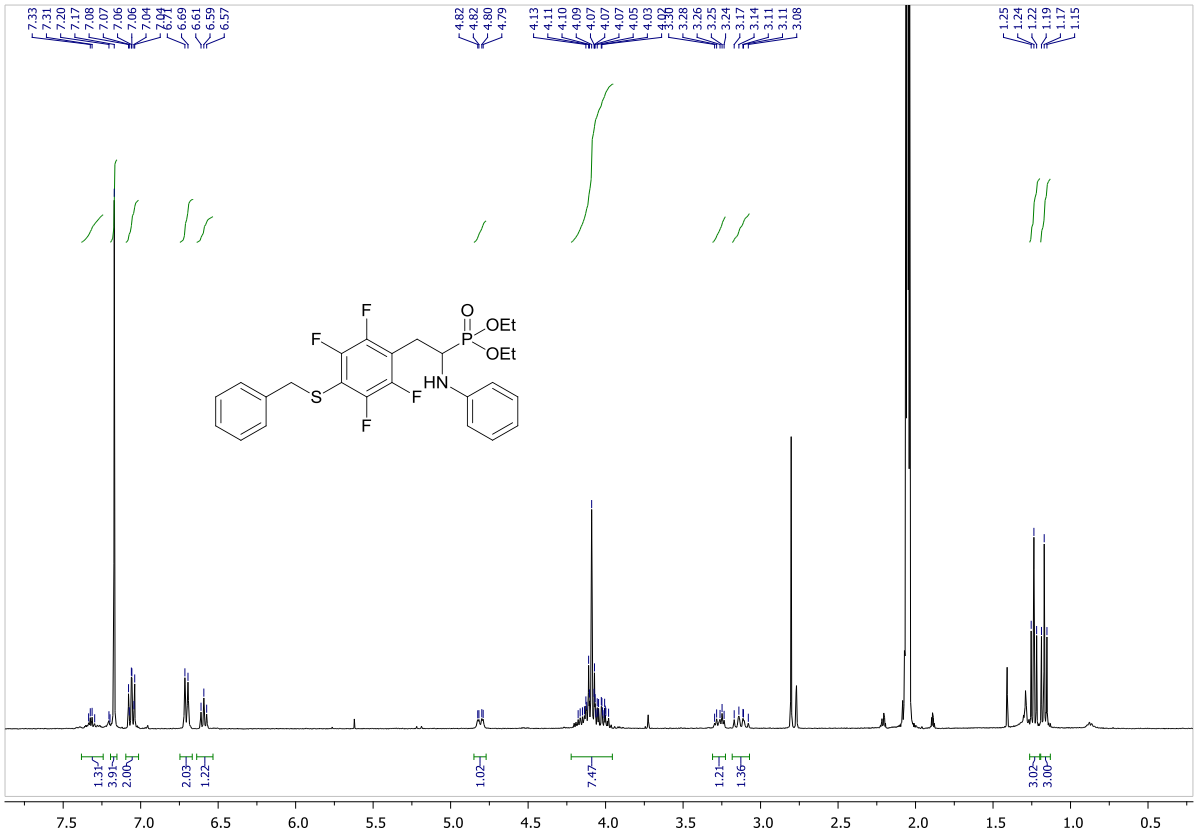

Fig. S29. ^{1}H NMR spectrum of 2h (Acetone-d6)

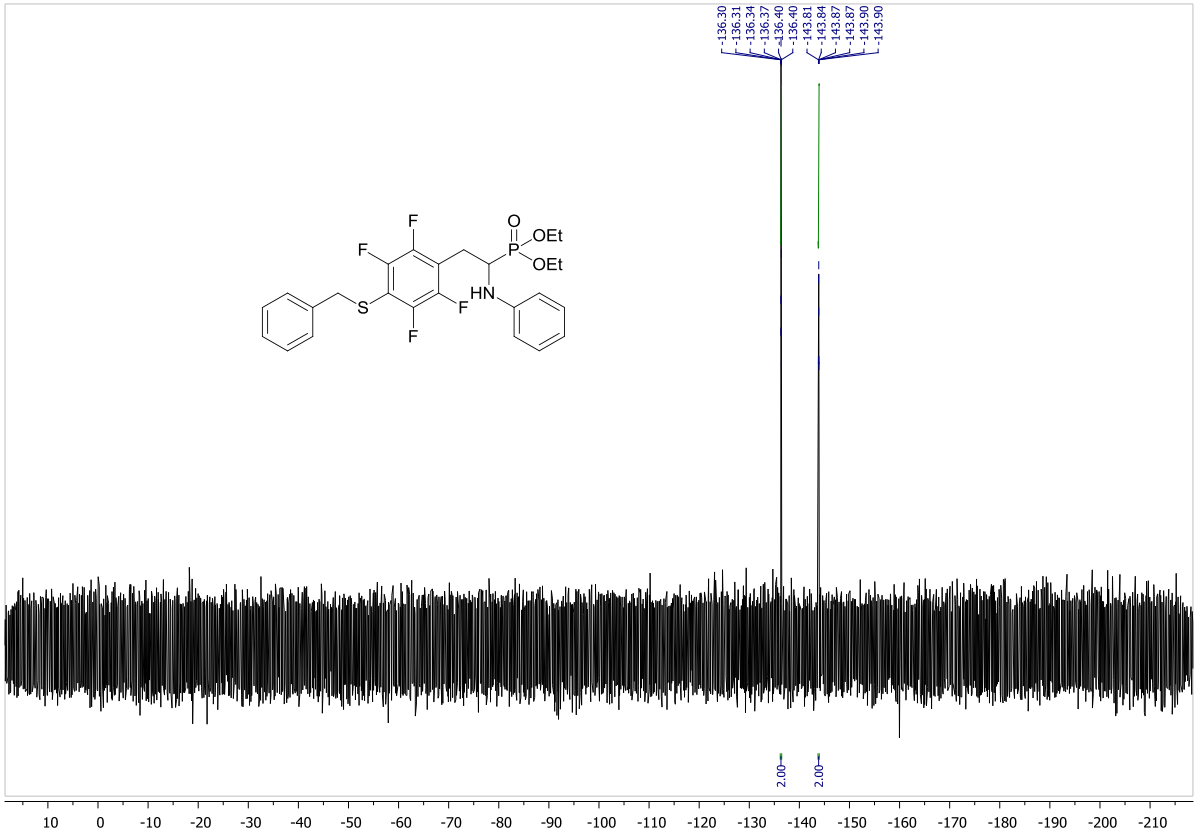

Fig. S30. ^{19}F NMR spectrum of 2h (Acetone-d6)

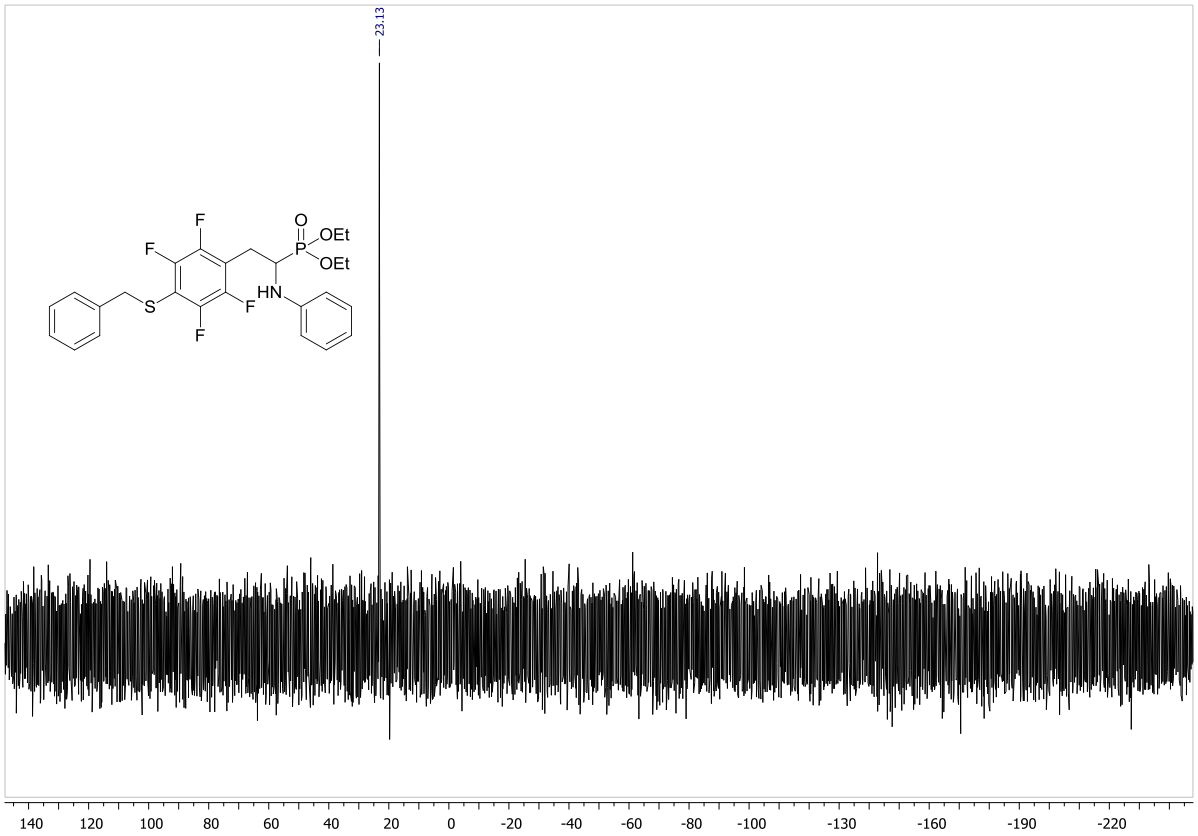

Fig. S31. ^{31}P NMR spectrum of 2h (Acetone-d6)

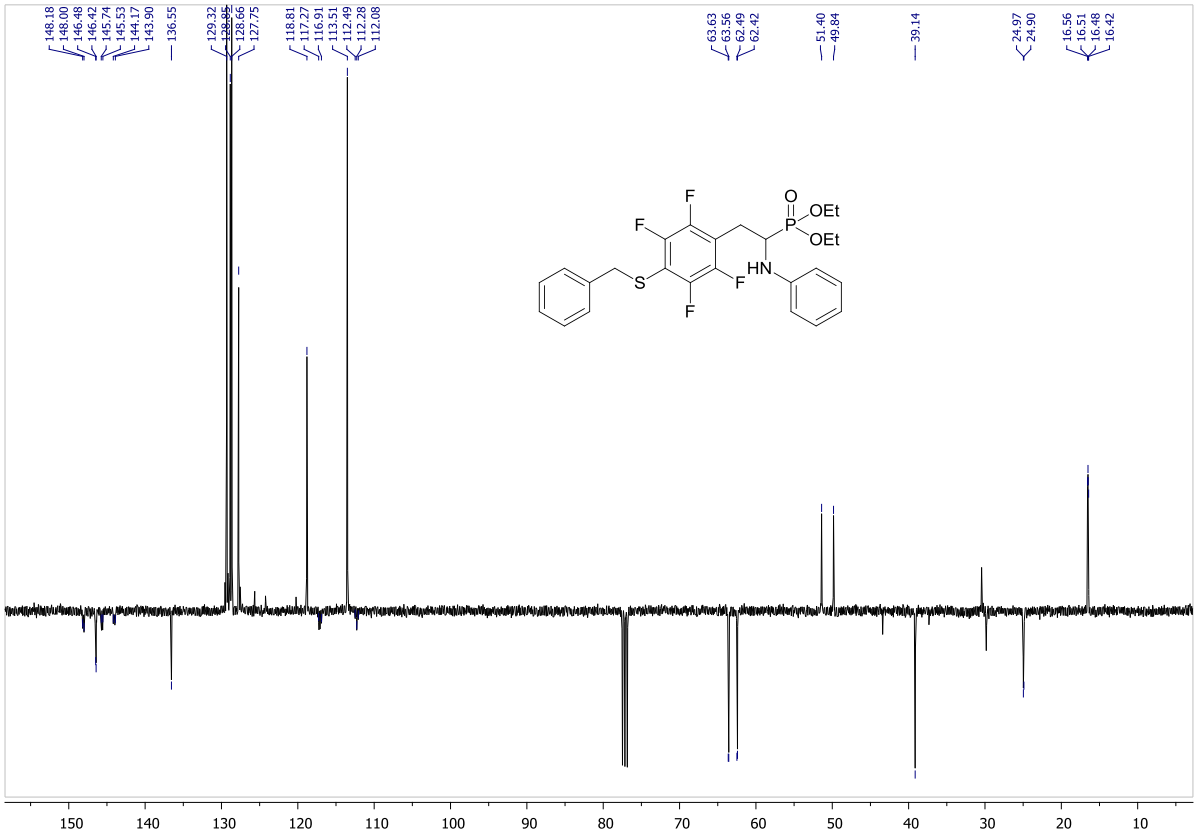

Fig. S32. ^{13}C NMR spectrum of 2h ($CDCl_3$)

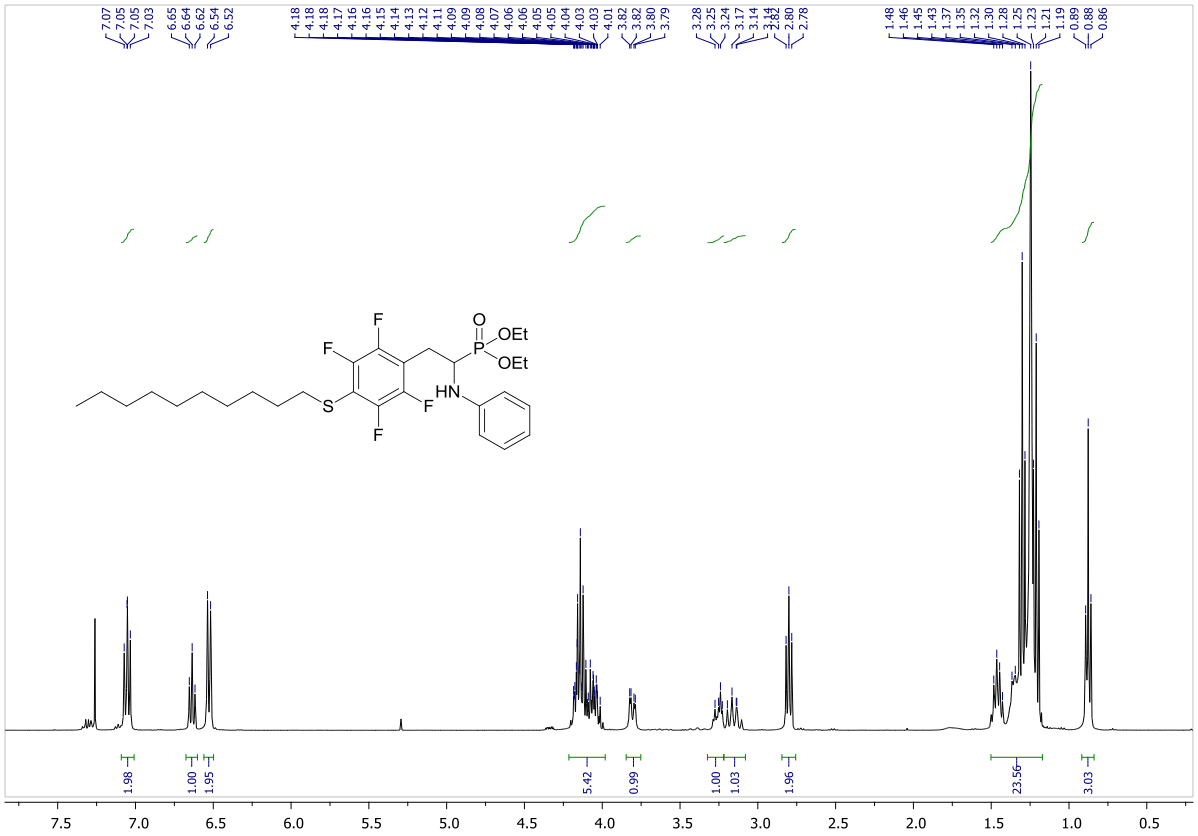

Fig. S33. ^{1}H NMR spectrum of 2i ($CDCl_3$)

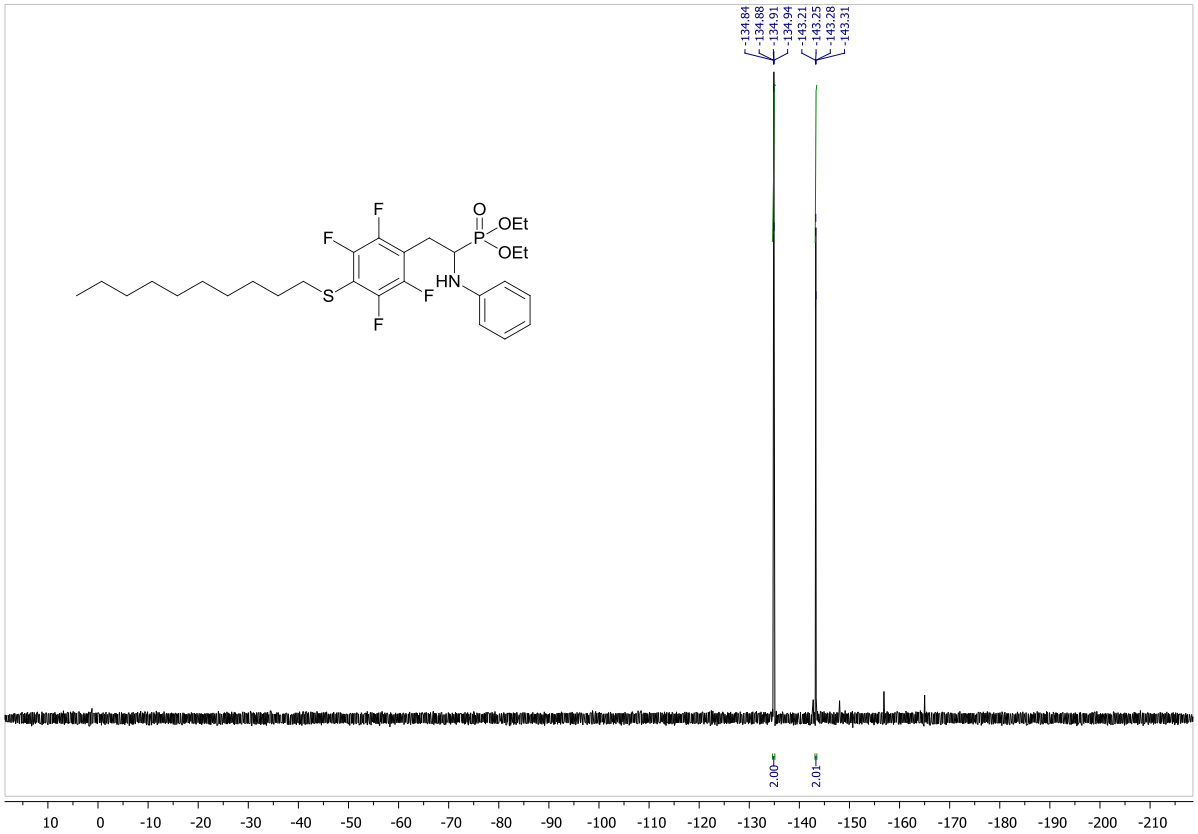

Fig. S34. ^{19}F NMR spectrum of 2i ($CDCl_3$)

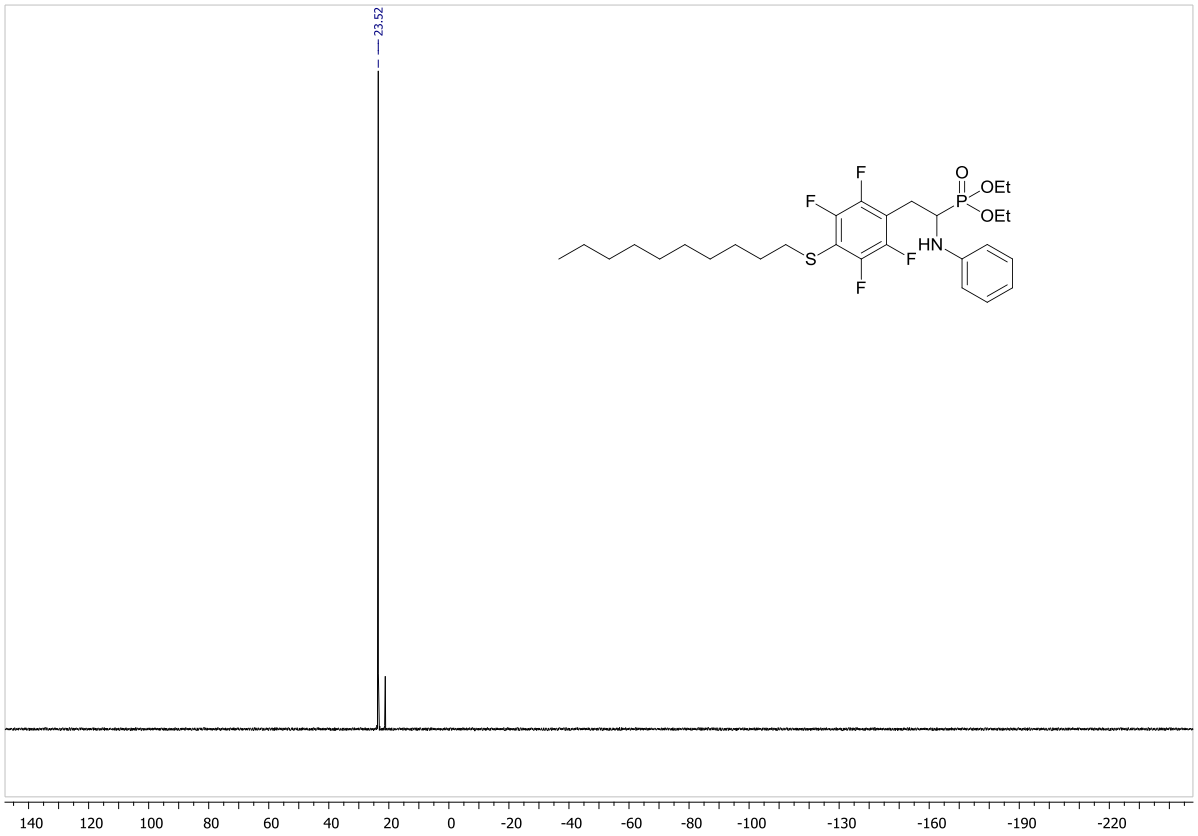

Fig. S35. ^{31}P NMR spectrum of 2i ($CDCl_3$)

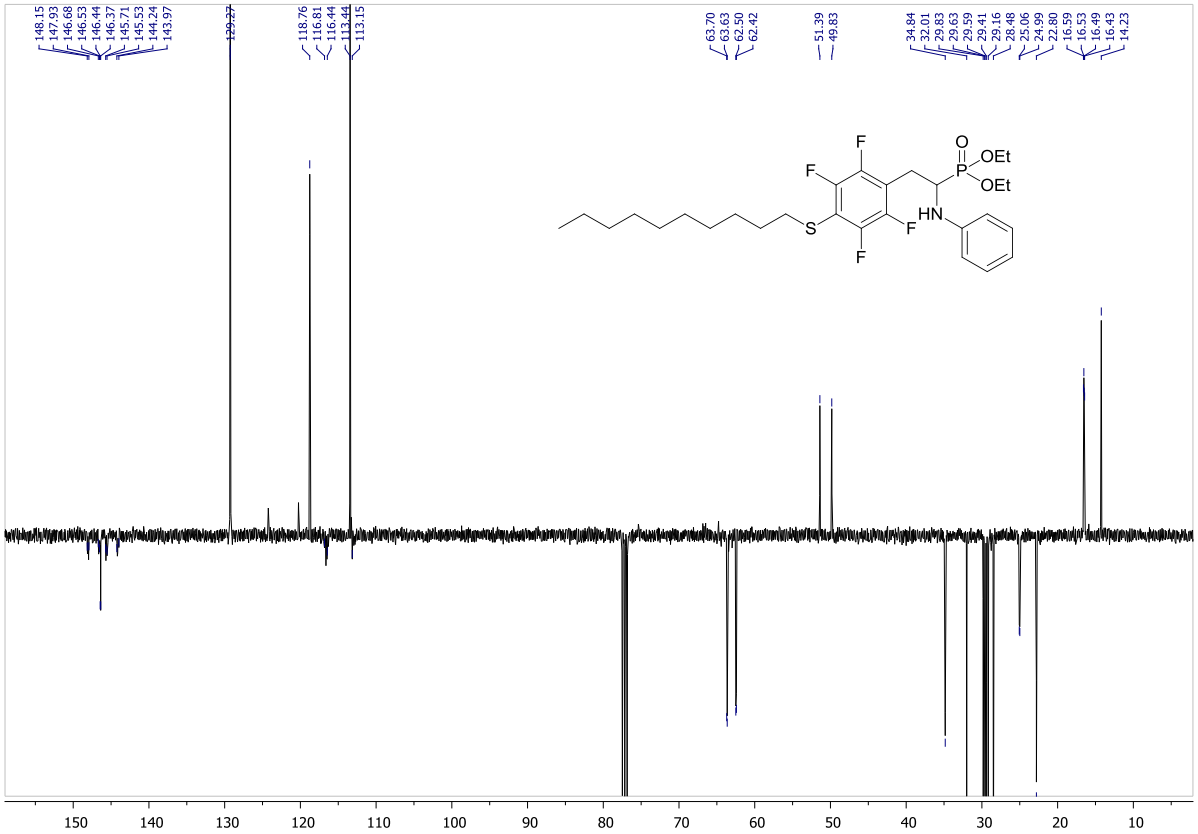

Fig. S36. ^{13}C NMR spectrum of 2i ($CDCl_3$)

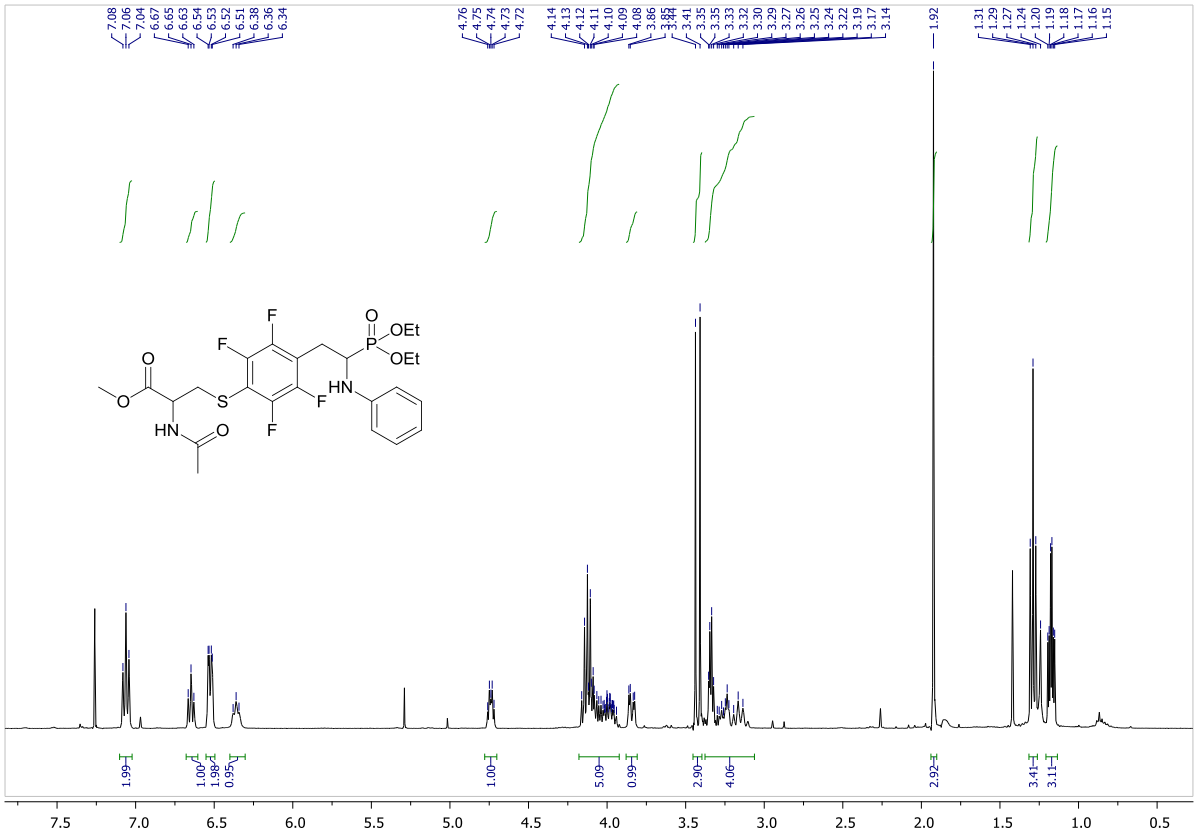

Fig. S37. ^{1}H NMR spectrum of 2j ($CDCl_3$)

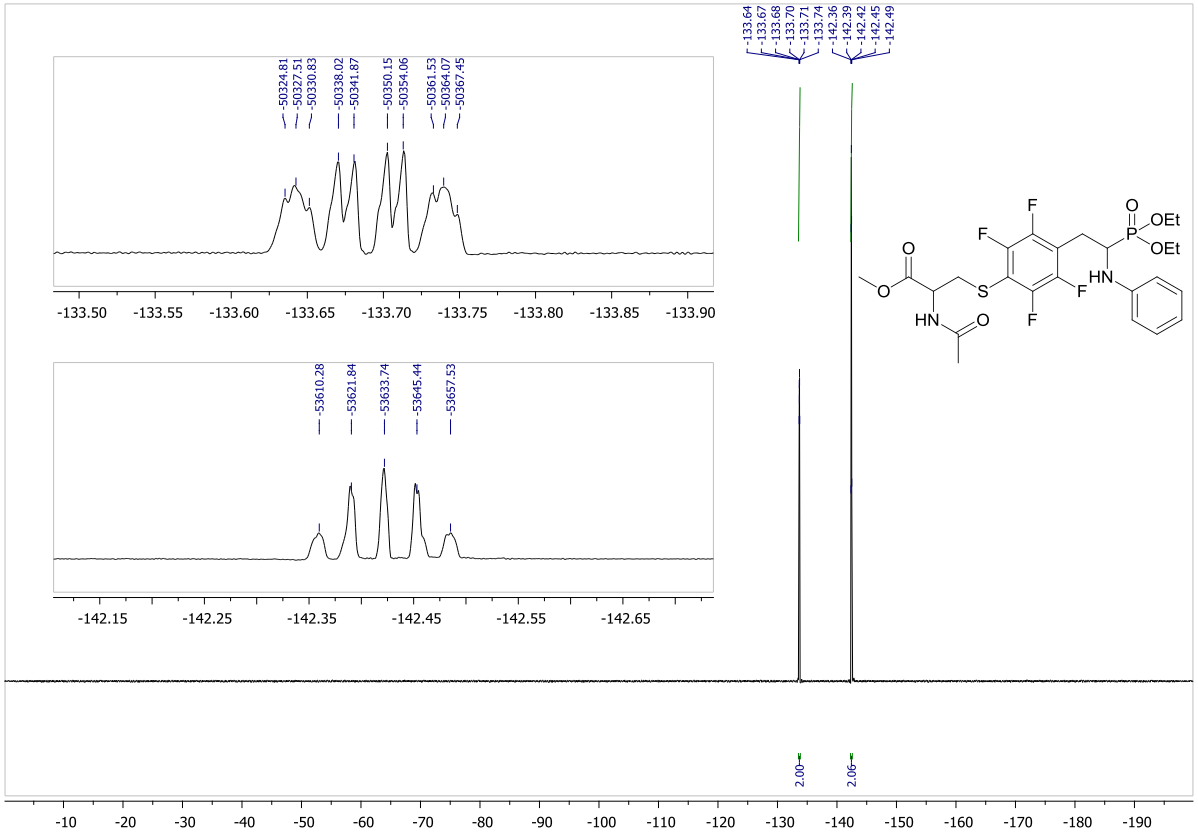

Fig. S38. ^{19}F NMR spectrum of 2j ($CDCl_3$)

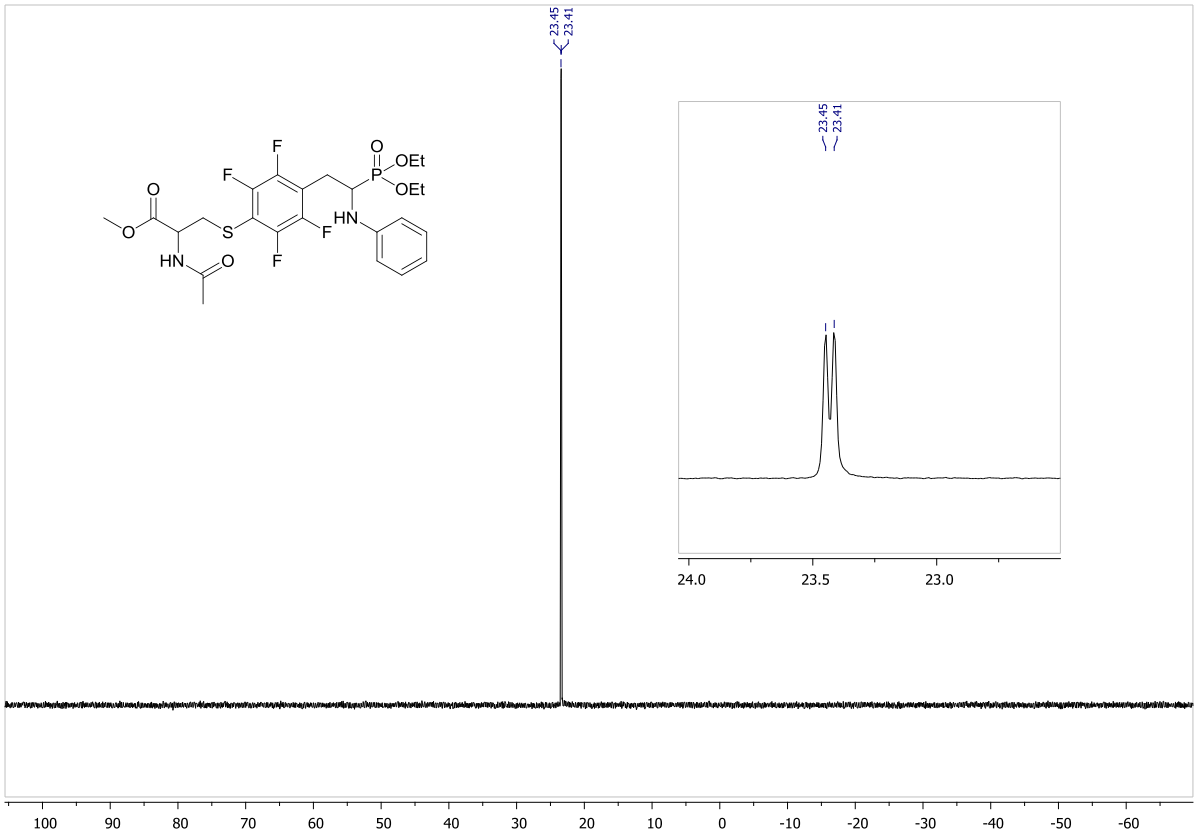

Fig. S39. ^{31}P NMR spectrum of 2j ($CDCl_3$)

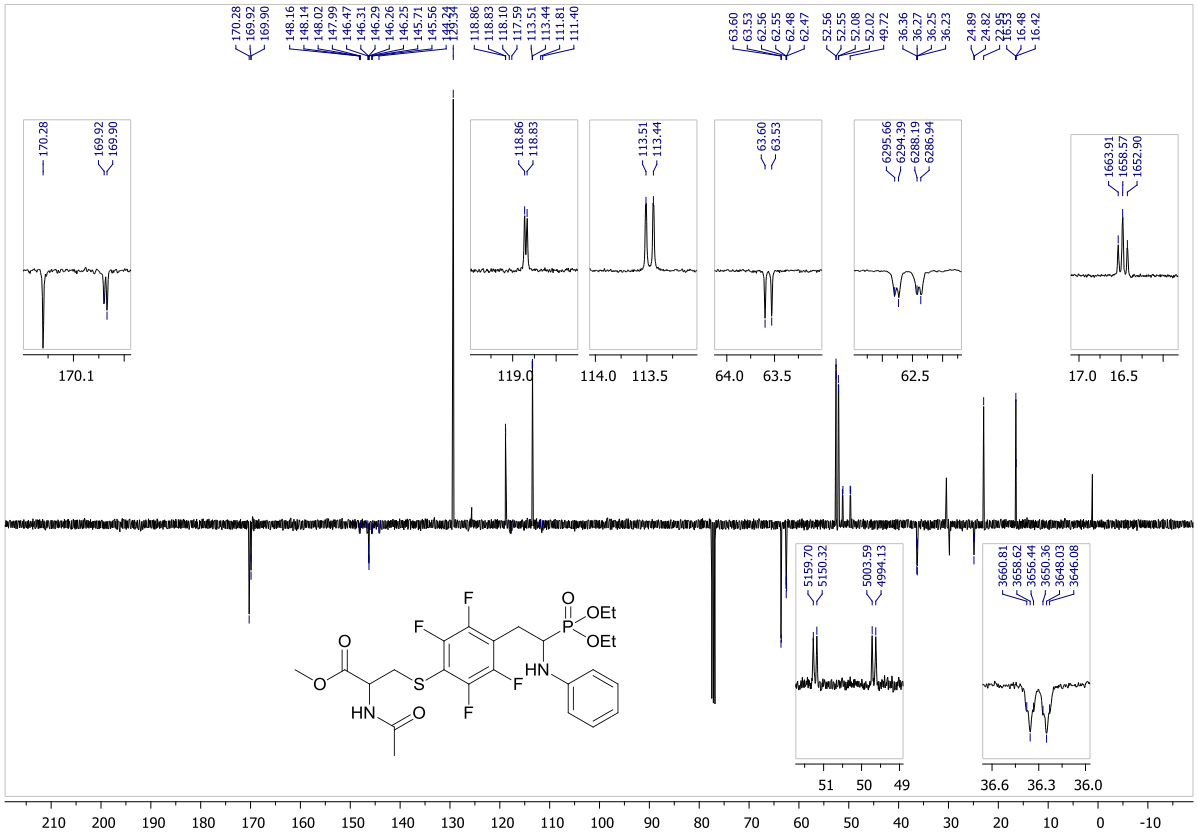

Fig. S40. ^{13}C NMR spectrum of 2j ($CDCl_3$)

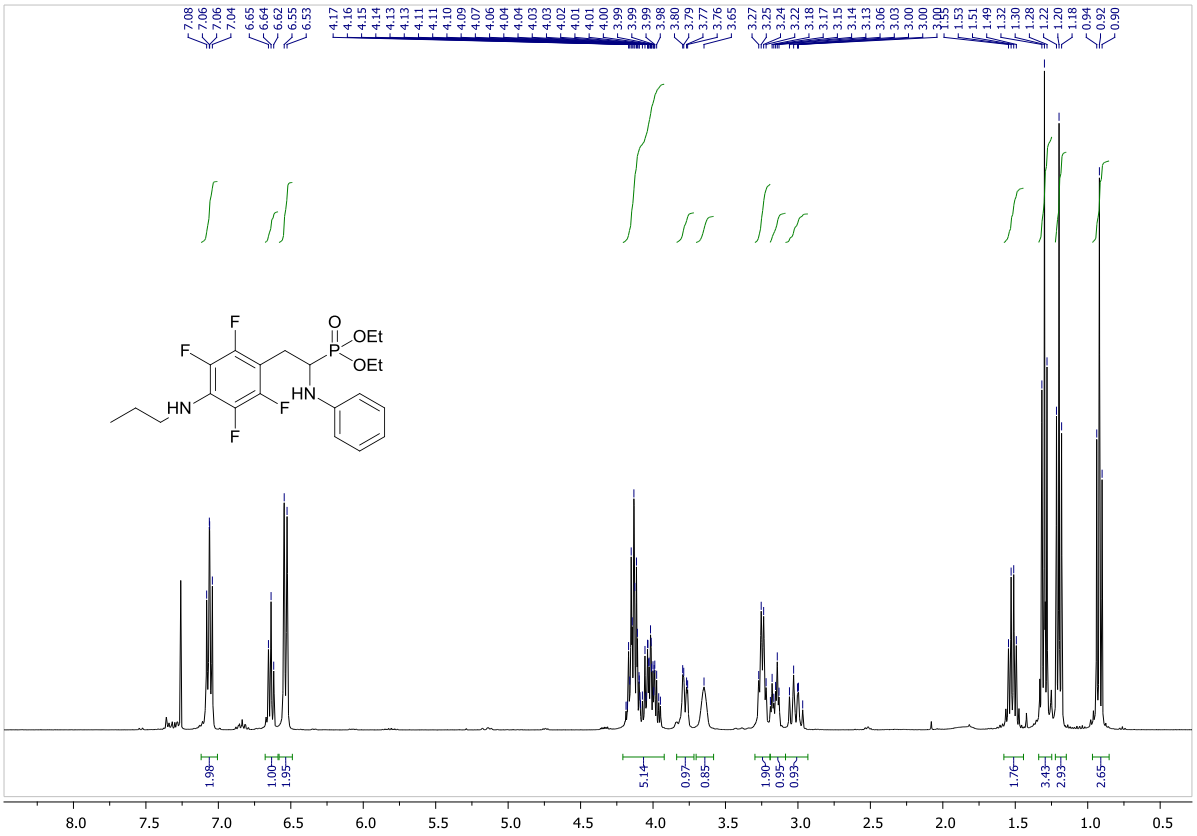

Fig. S41. ^{1}H NMR spectrum of 2l ($CDCl_3$)

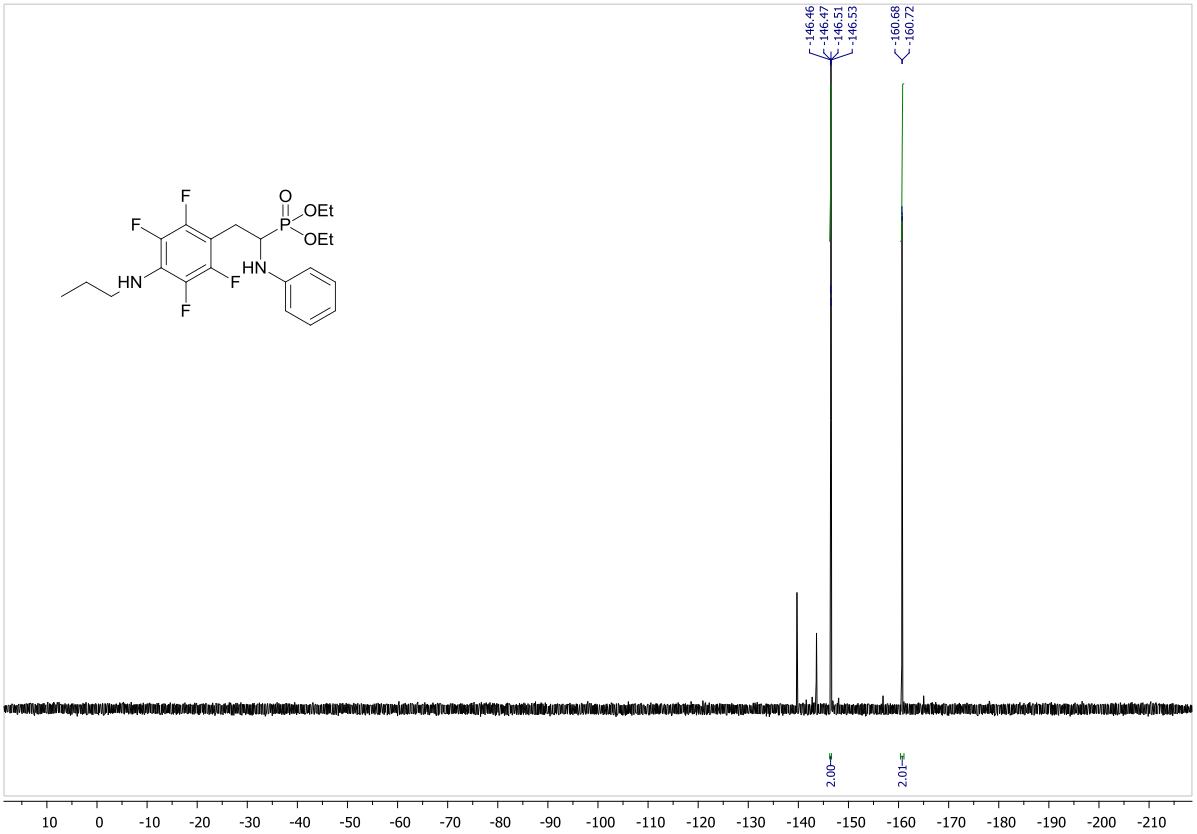

Fig. S42. ^{19}F NMR spectrum of 2l ($CDCl_3$)

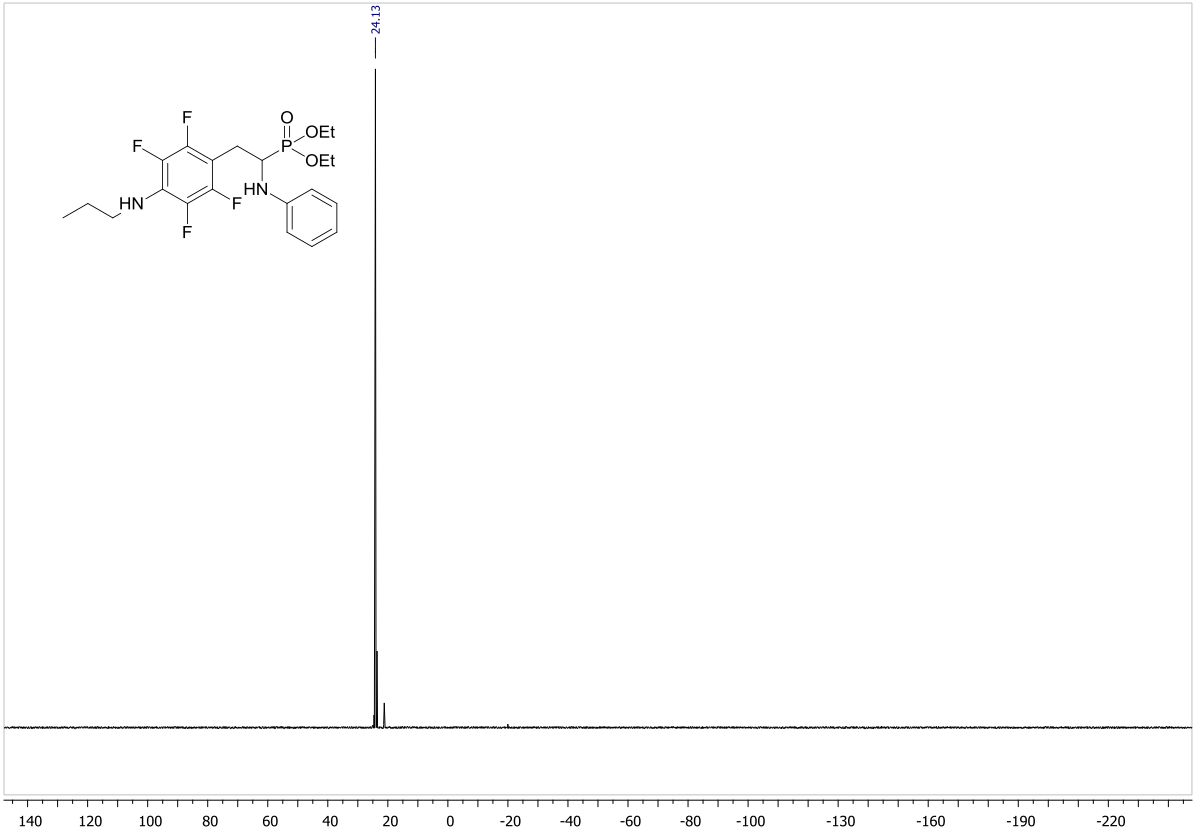

Fig. S43. ^{31}P NMR spectrum of 2l ($CDCl_3$)

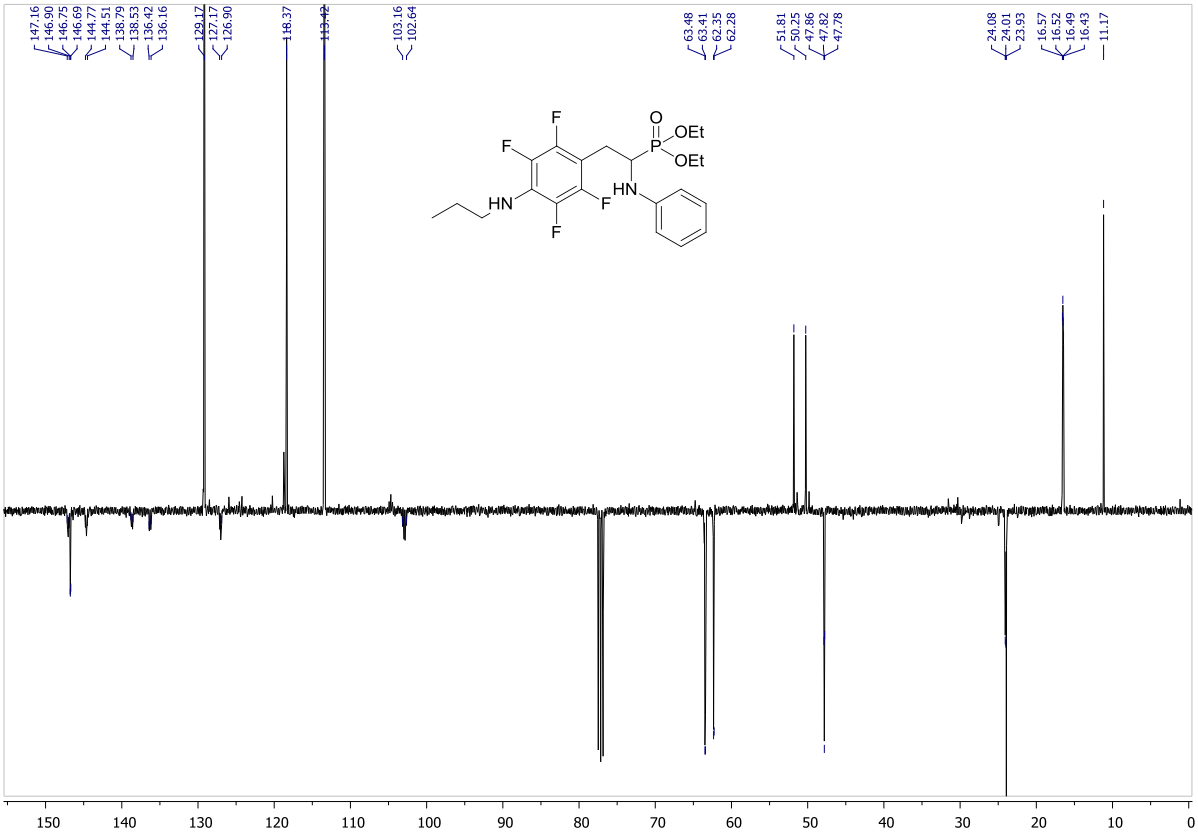

Fig. S44. ^{13}C NMR spectrum of 2l ($CDCl_3$)

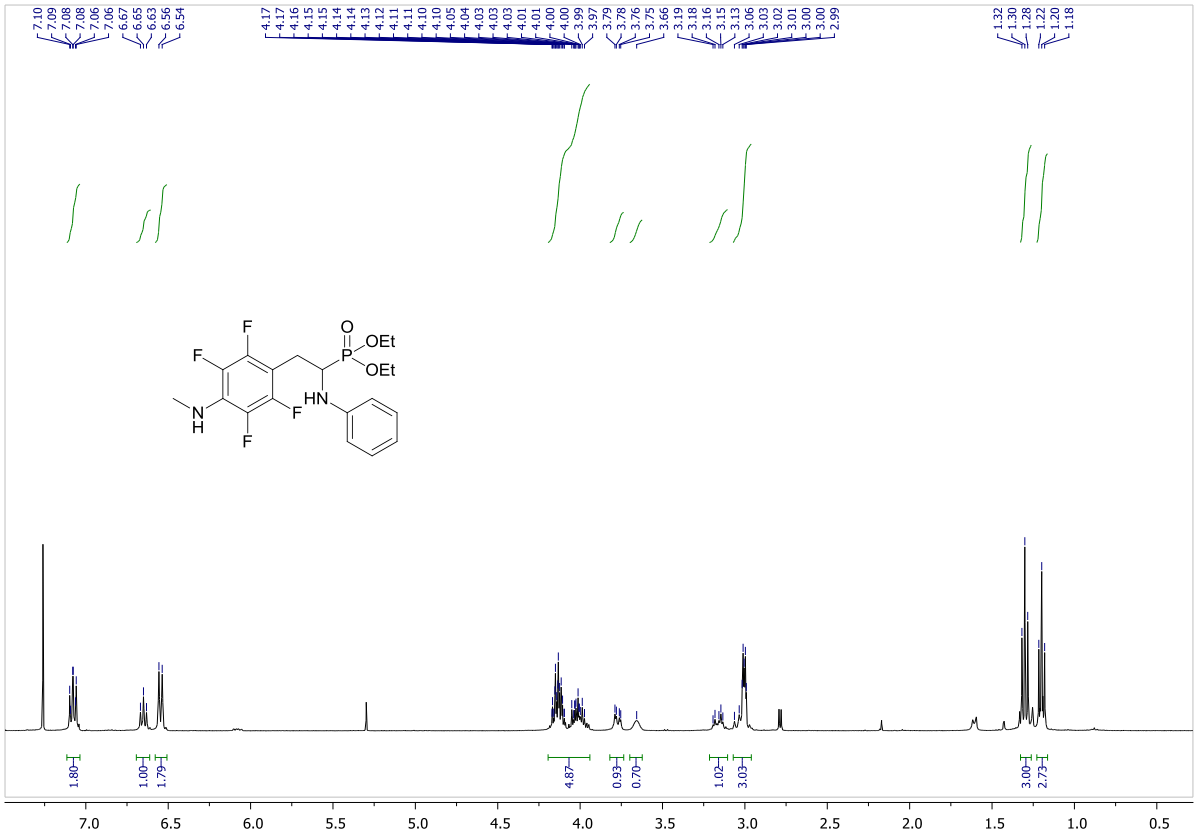

Fig. S45. ^{1}H NMR spectrum of 2k ($CDCl_3$)

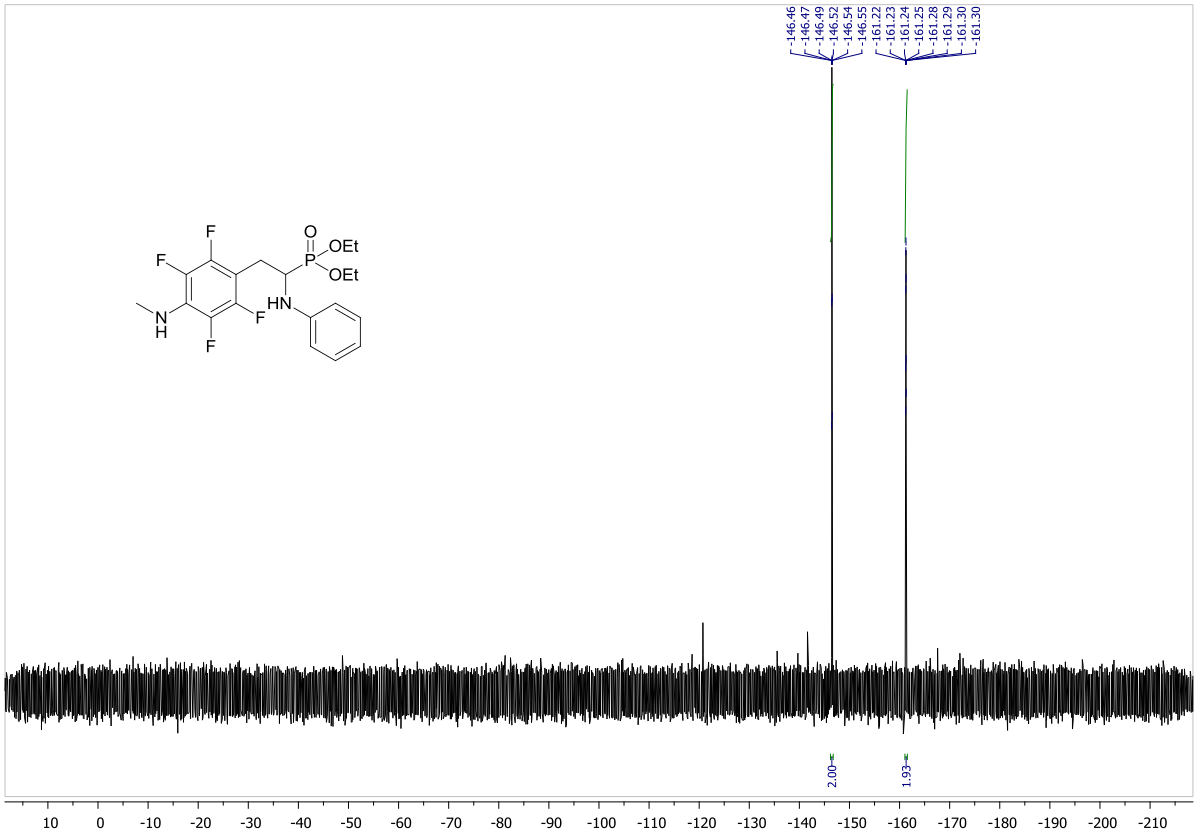

Fig. S46. ^{19}F NMR spectrum of 2k ($CDCl_3$)

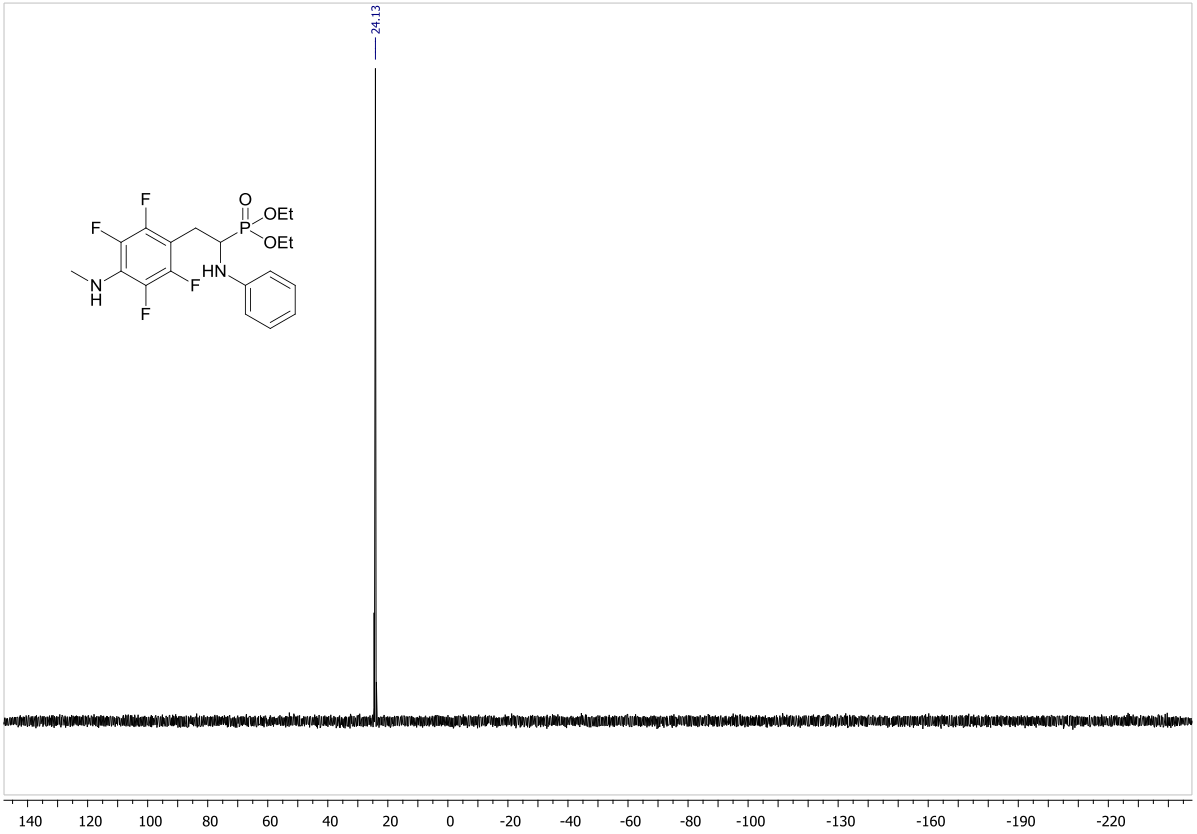

Fig. S47. ^{31}P NMR spectrum of 2k ($CDCl_3$)

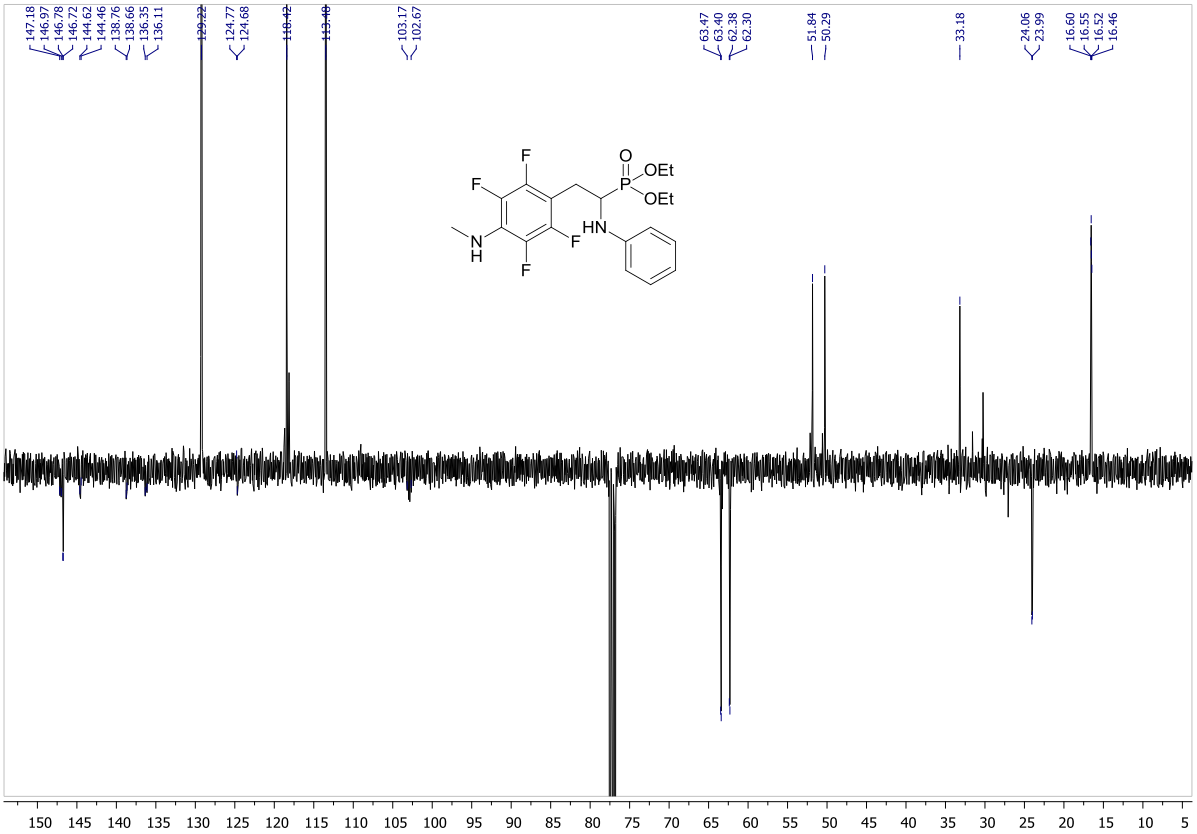

Fig. S48. ^{13}C NMR spectrum of 2k ($CDCl_3$)

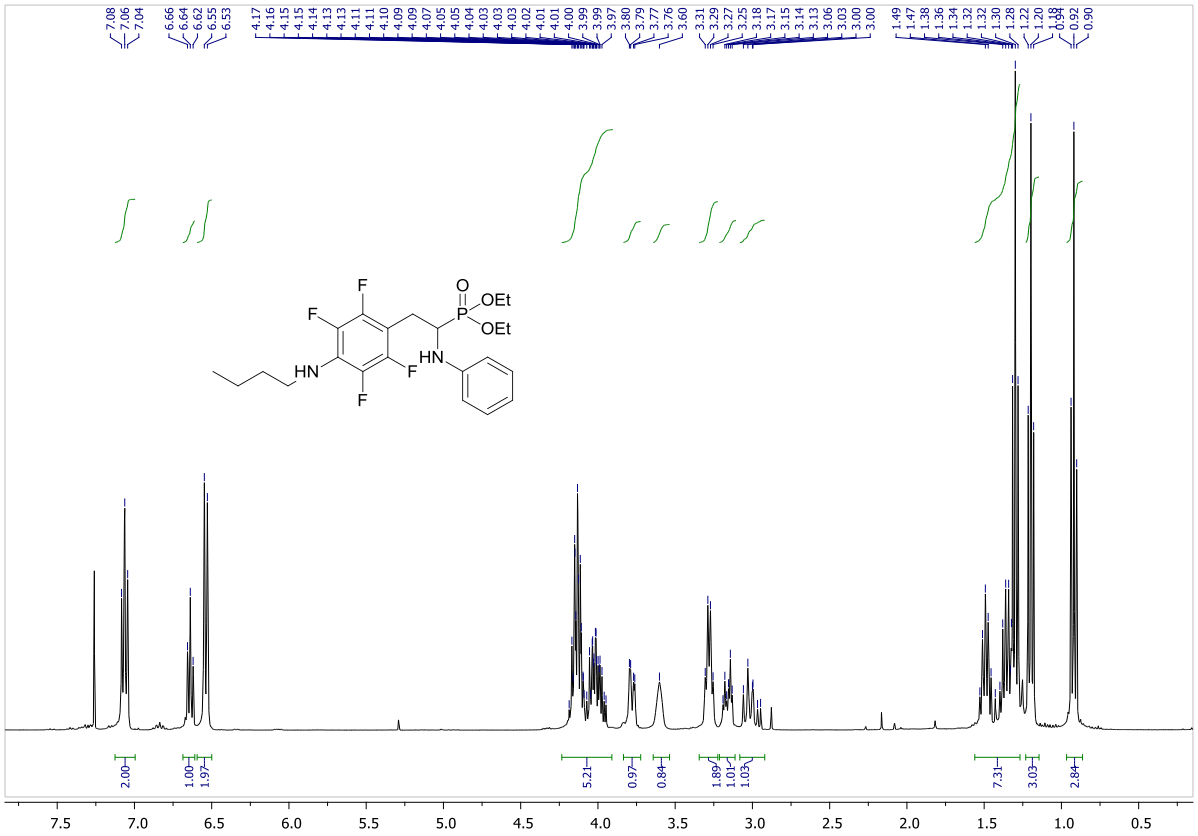

Fig. S49. ^{1}H NMR spectrum of 2m ($CDCl_3$)

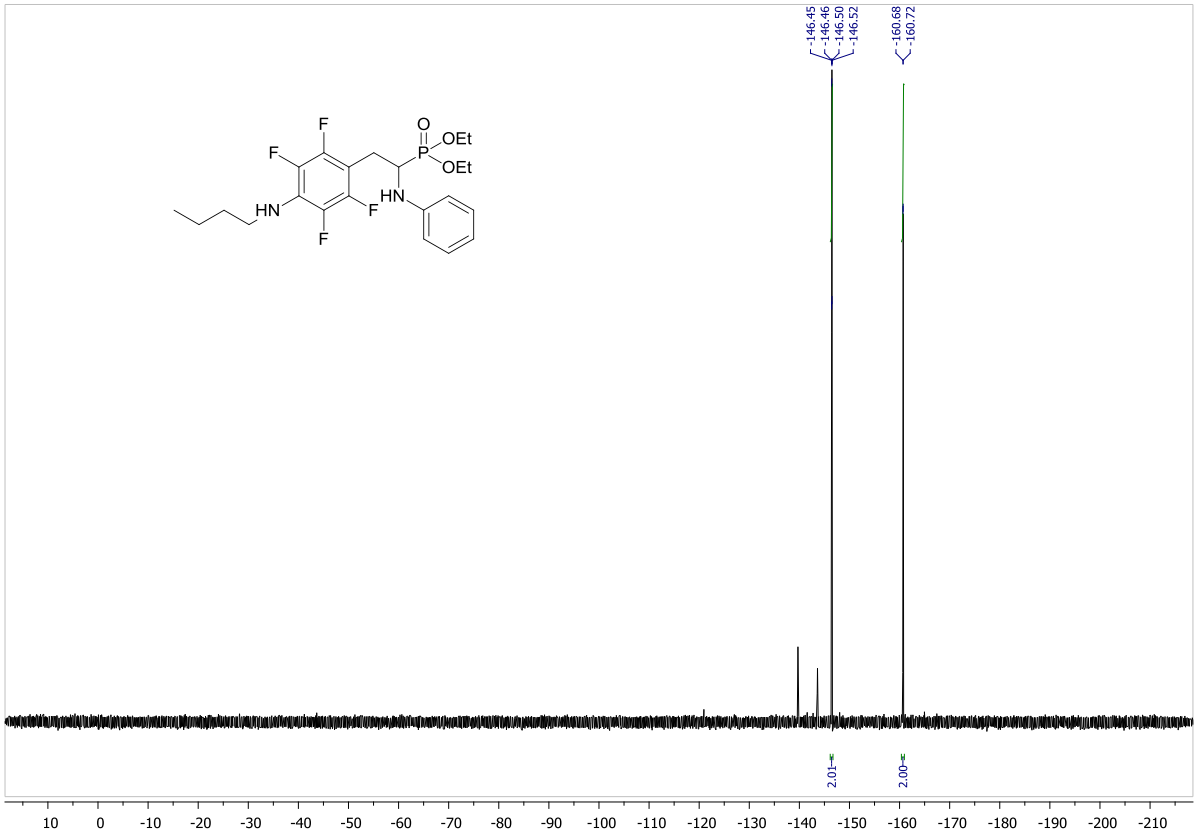

Fig. S50. ^{19}F NMR spectrum of 2m ($CDCl_3$)

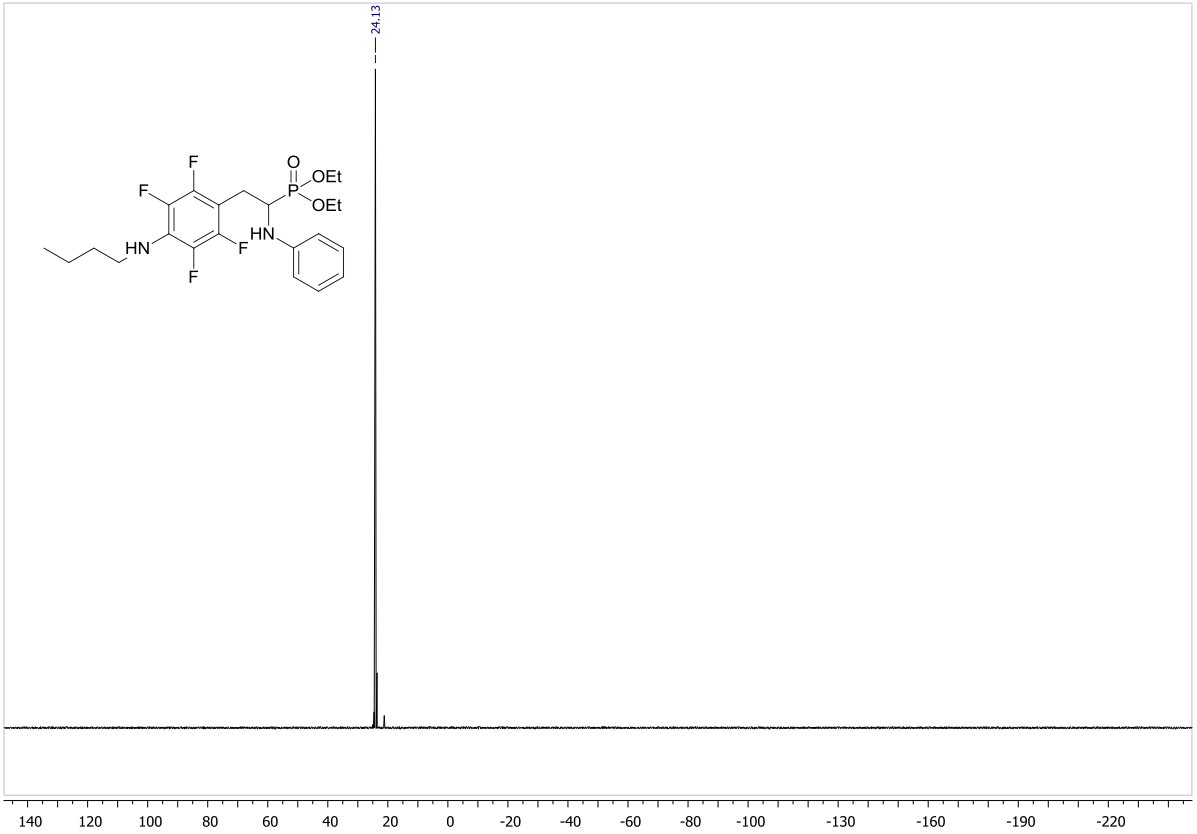

Fig. S51. ^{31}P NMR spectrum of 2m ($CDCl_3$)

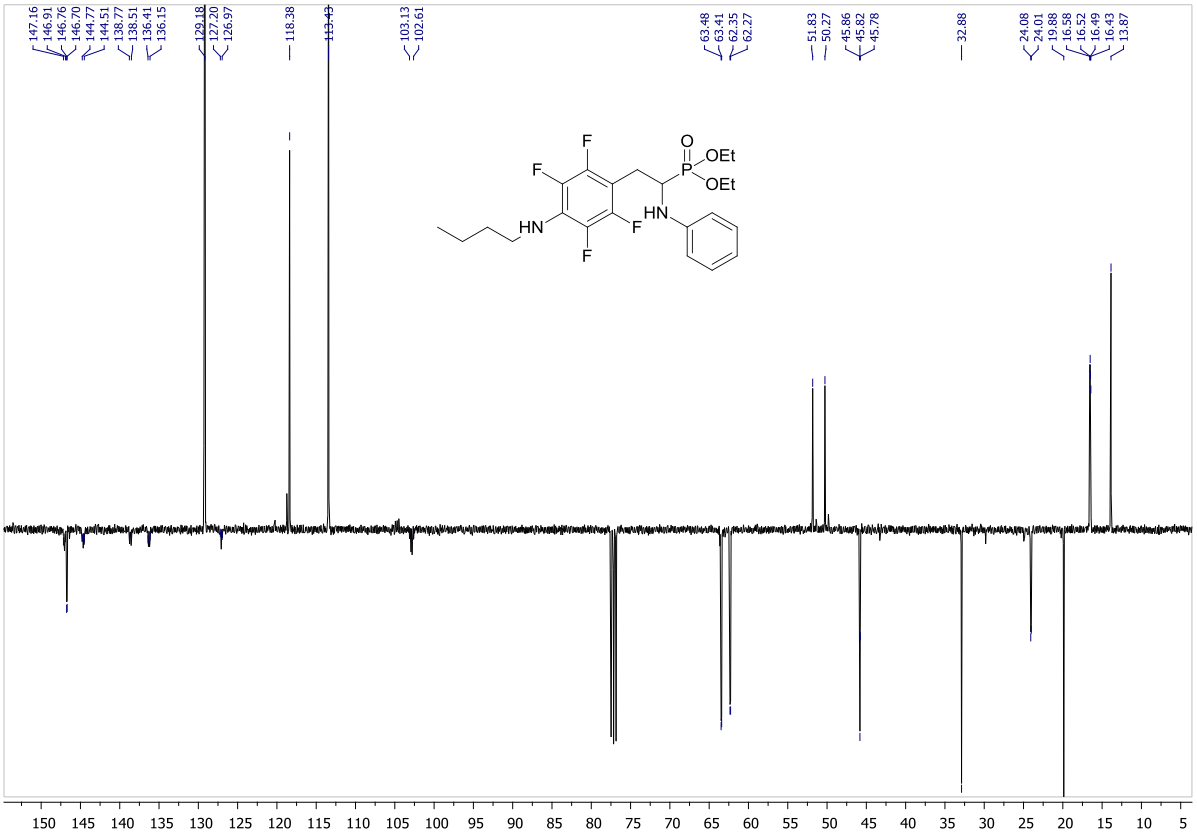

Fig. S52. ^{13}C NMR spectrum of 2m ($CDCl_3$)

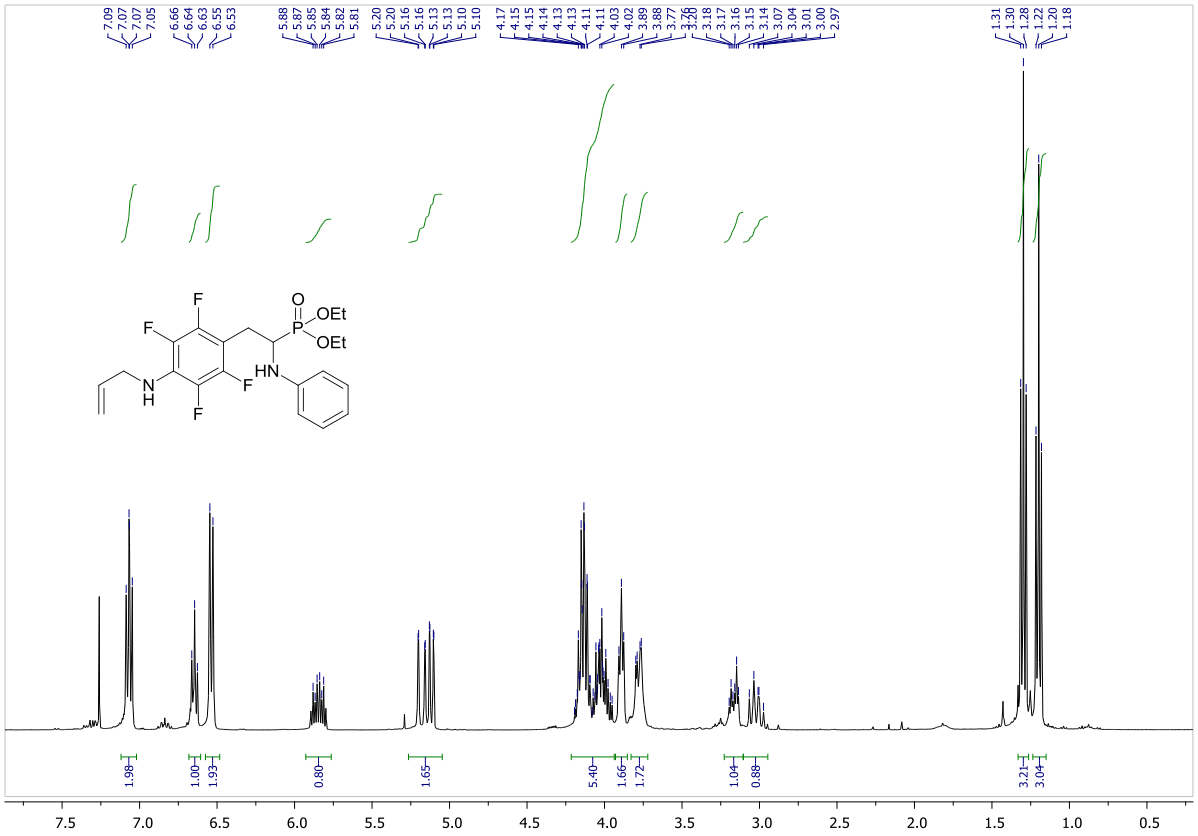

Fig. S53. ^{1}H NMR spectrum of 2n ($CDCl_3$)

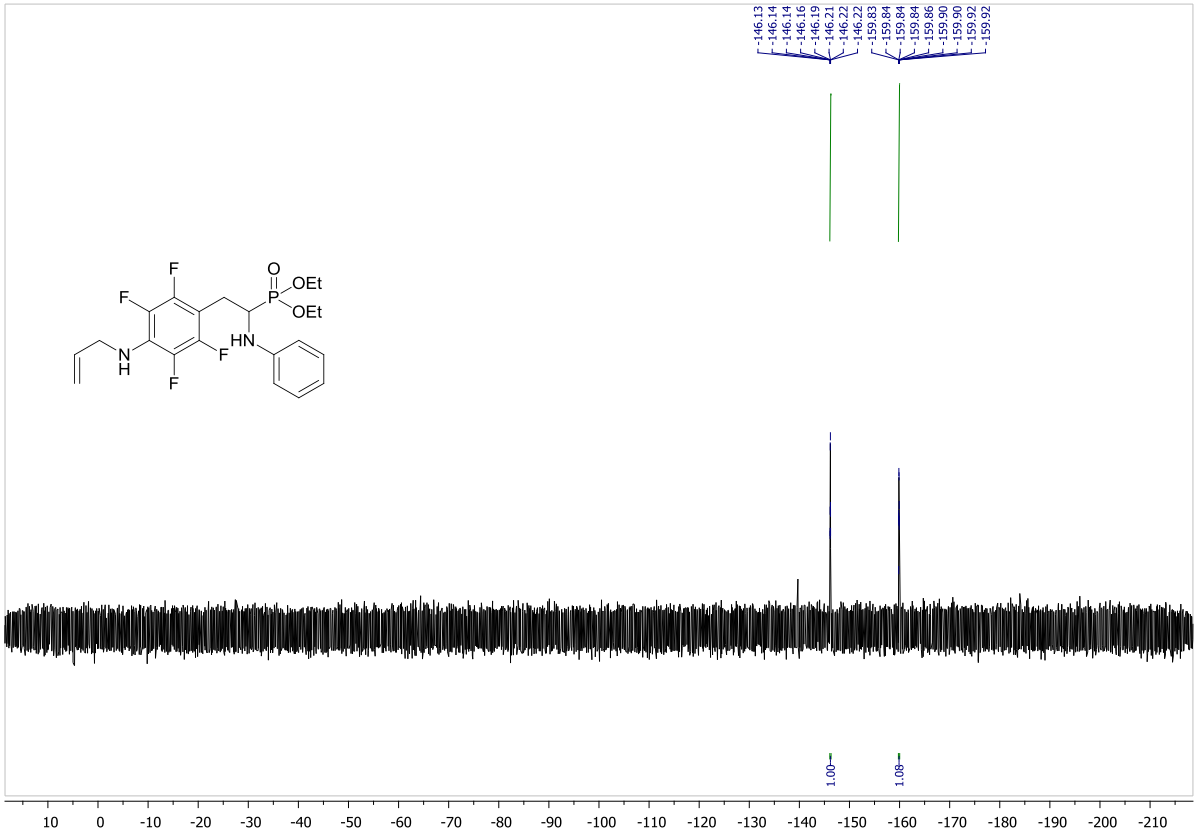

Fig. S54. ^{19}F NMR spectrum of 2n ($CDCl_3$)

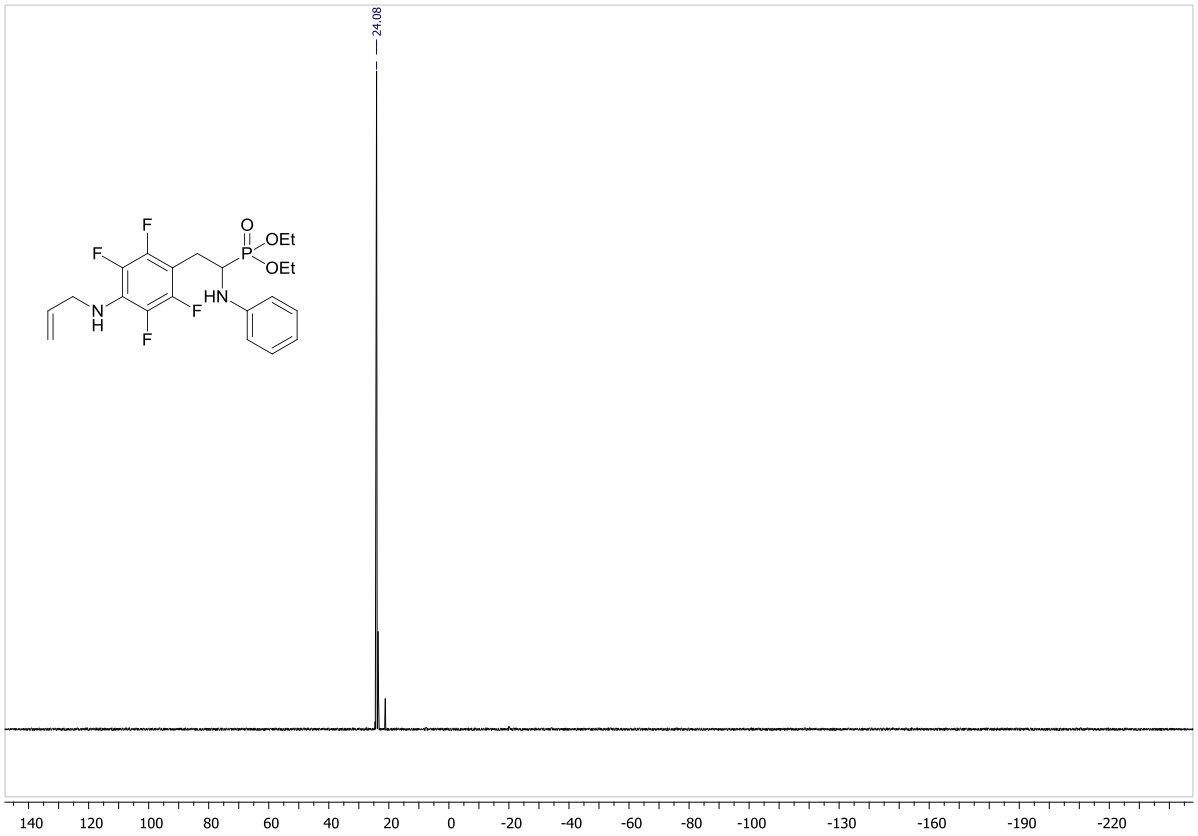

Fig. S55. ^{31}P NMR spectrum of 2n ($CDCl_3$)

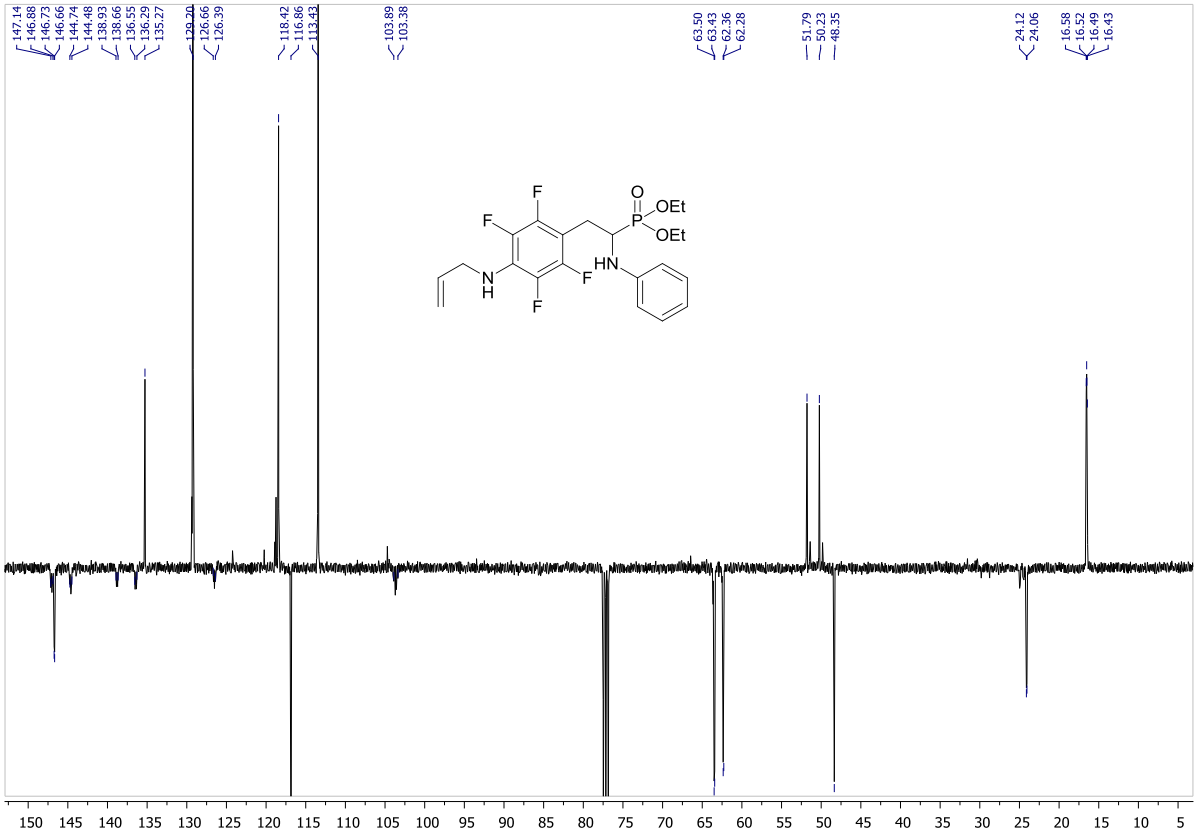

Fig. S56. ^{13}C NMR spectrum of 2n ($CDCl_3$)

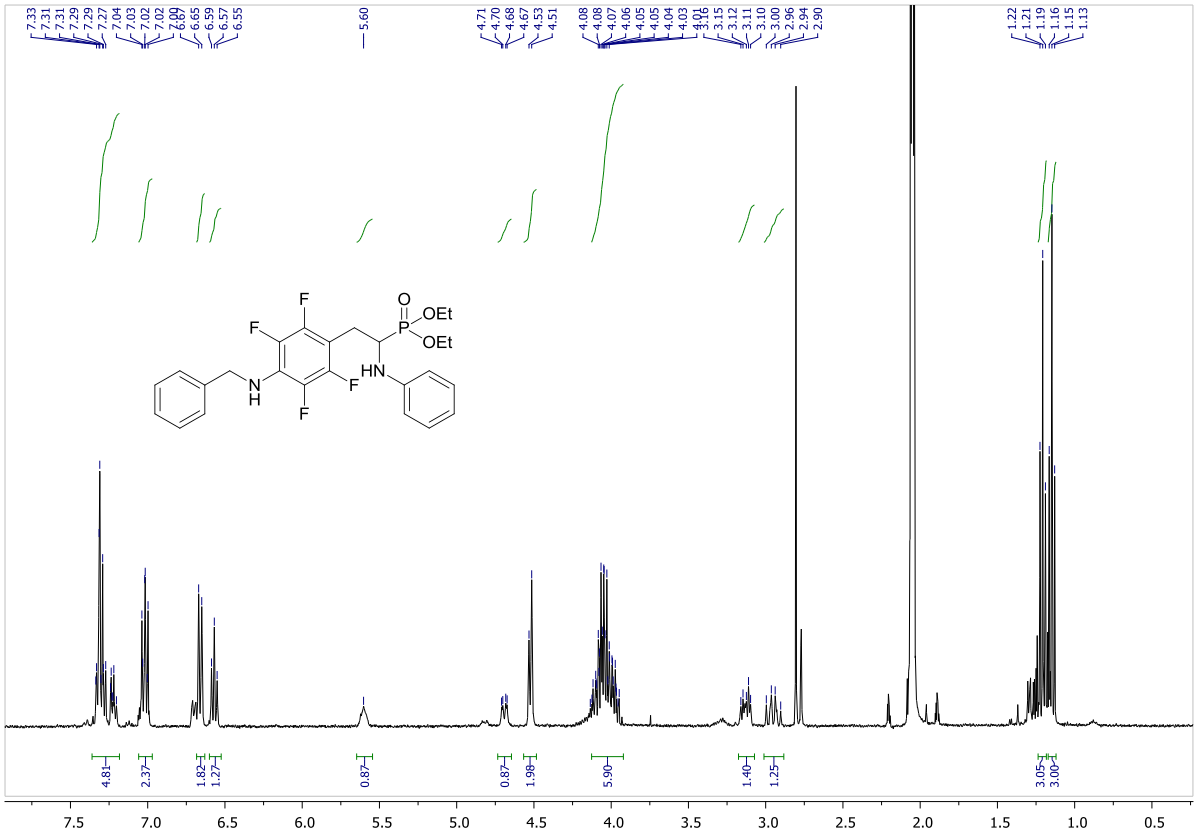

Fig. S57. ^{1}H NMR spectrum of 2o (Acetone-d6)

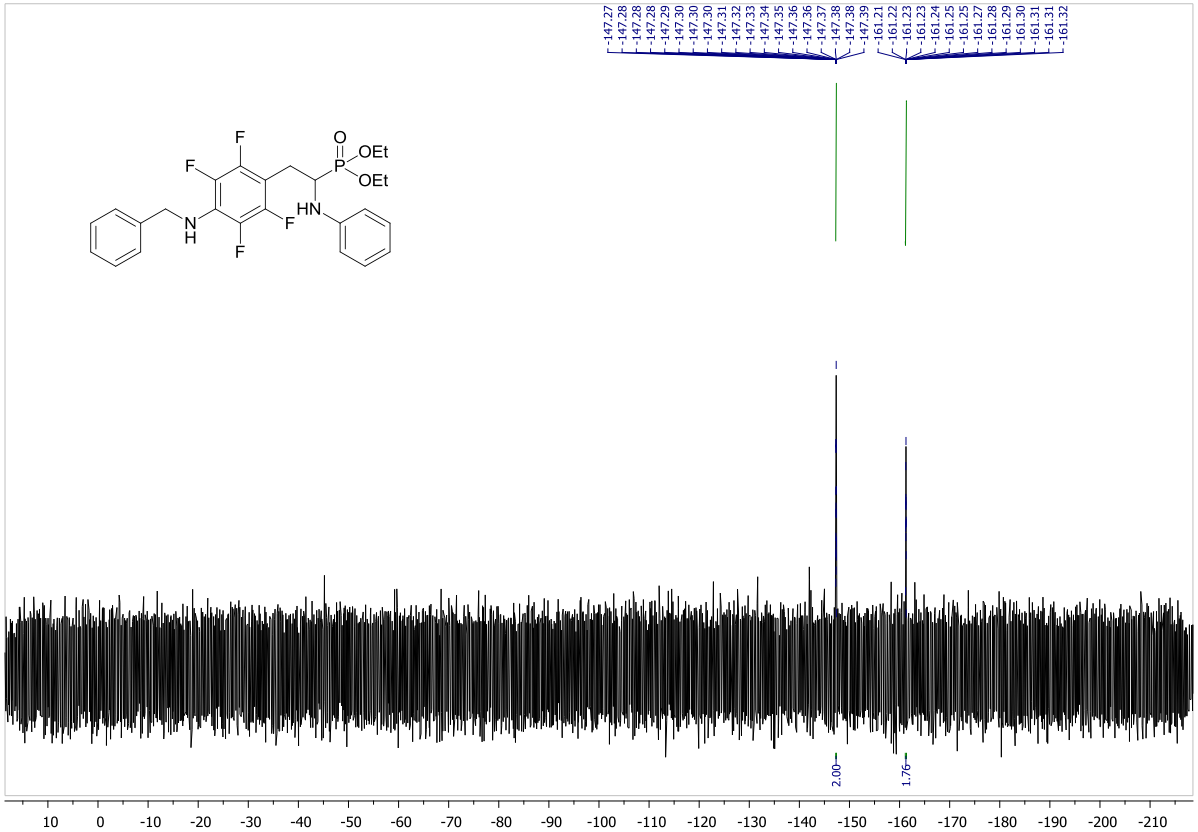

Fig. S58. ^{19}F NMR spectrum of 2o (Acetone-d6)

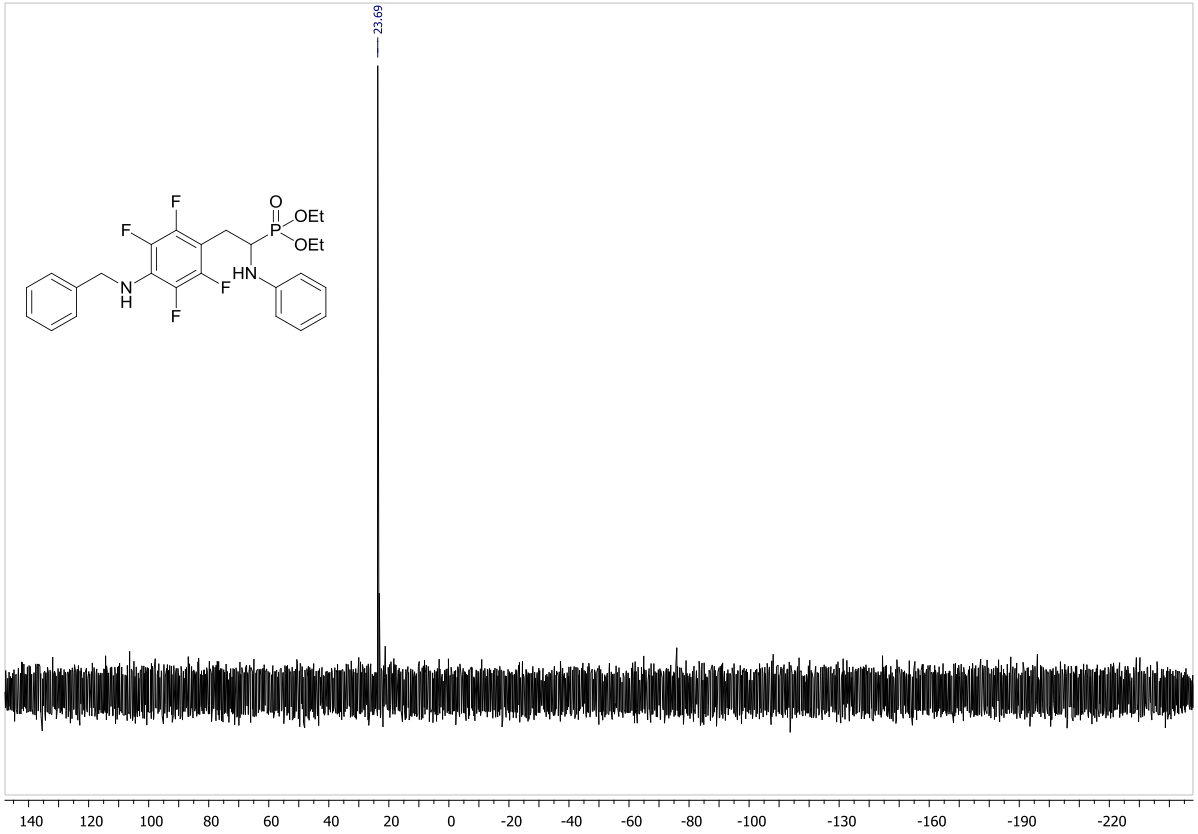

Fig. S59. ^{31}P NMR spectrum of 2o (Acetone-d6$_3$)

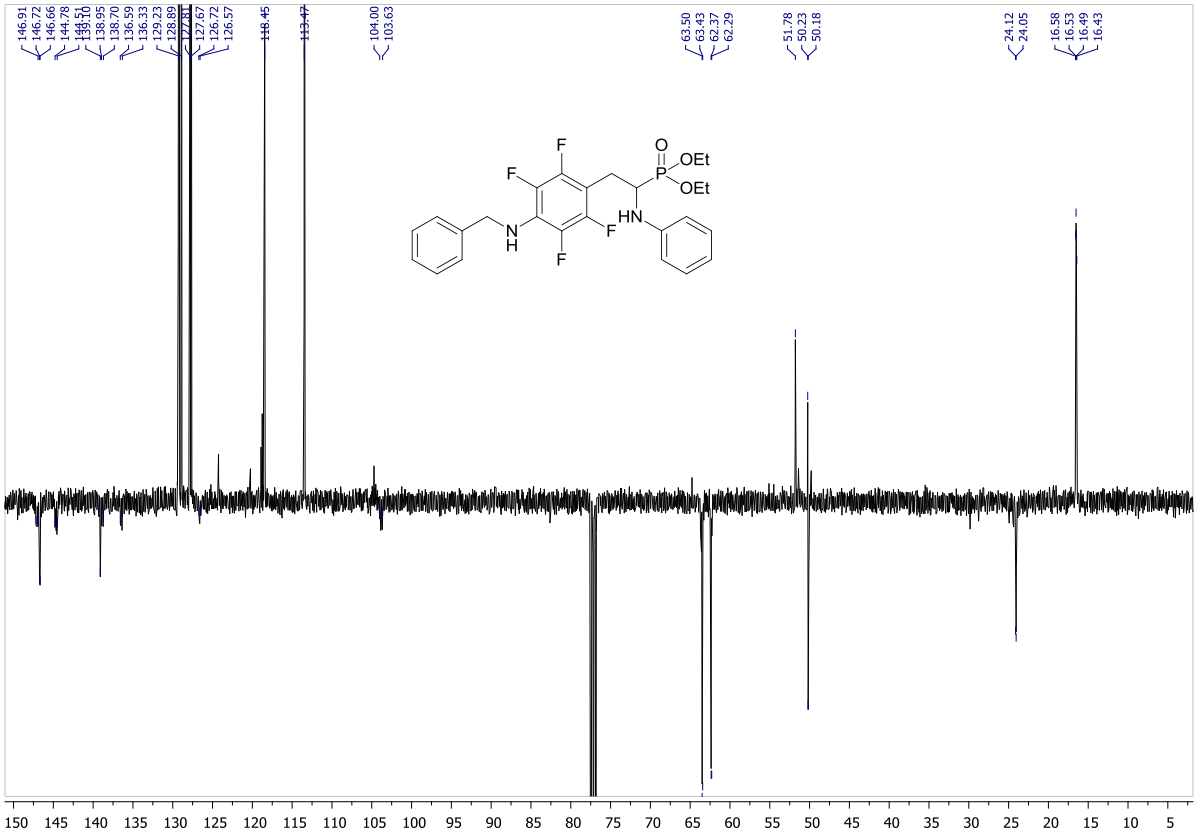

Fig. S60. ^{13}C NMR spectrum of 2o (CDCl$_3$)

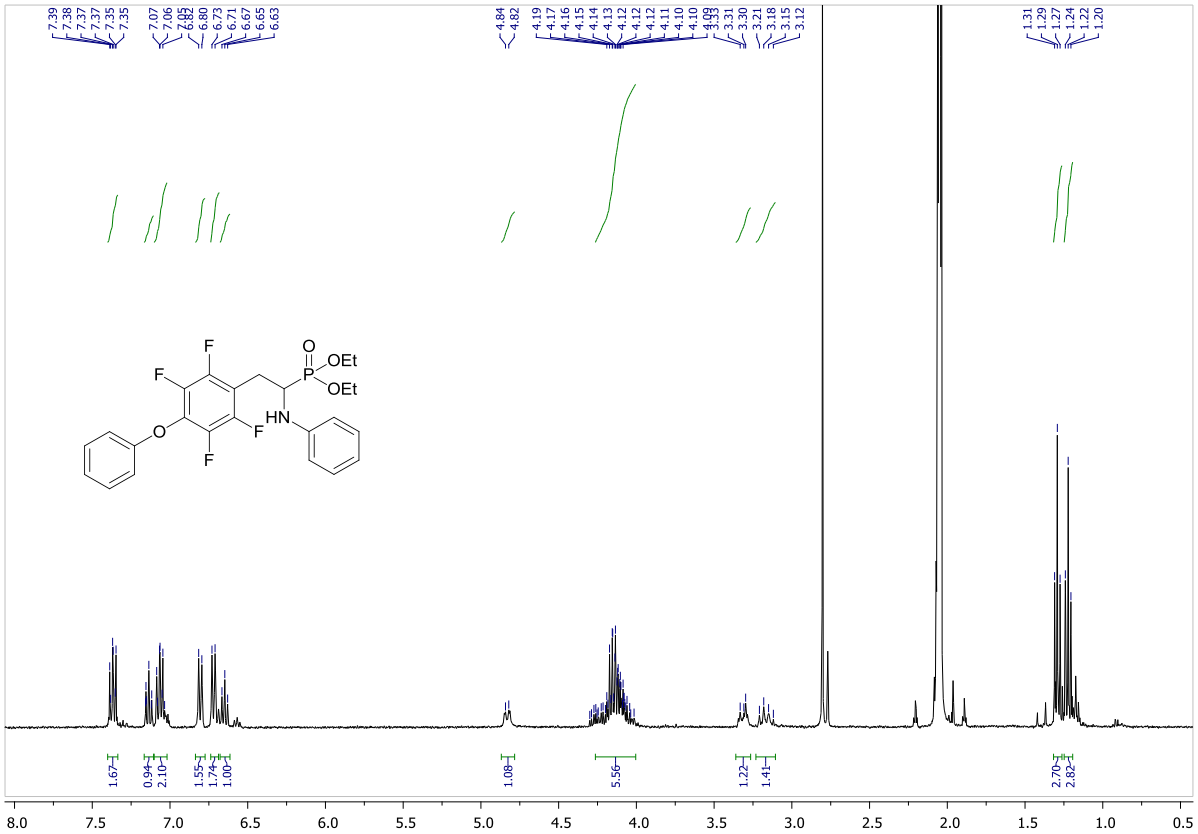

Fig. S61. ^{1}H NMR spectrum of 2p (Acetone-d6)

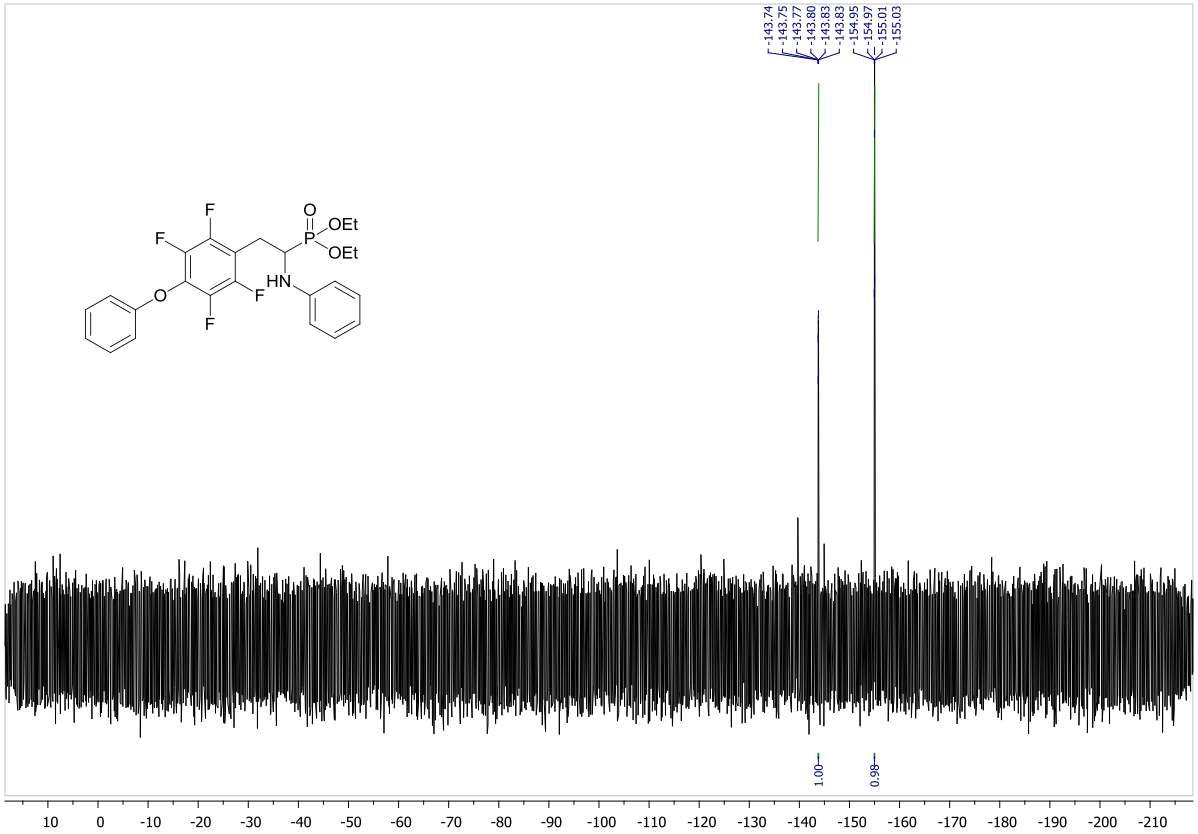

Fig. S62. ^{19}F NMR spectrum of 2p ($CDCl_3$)

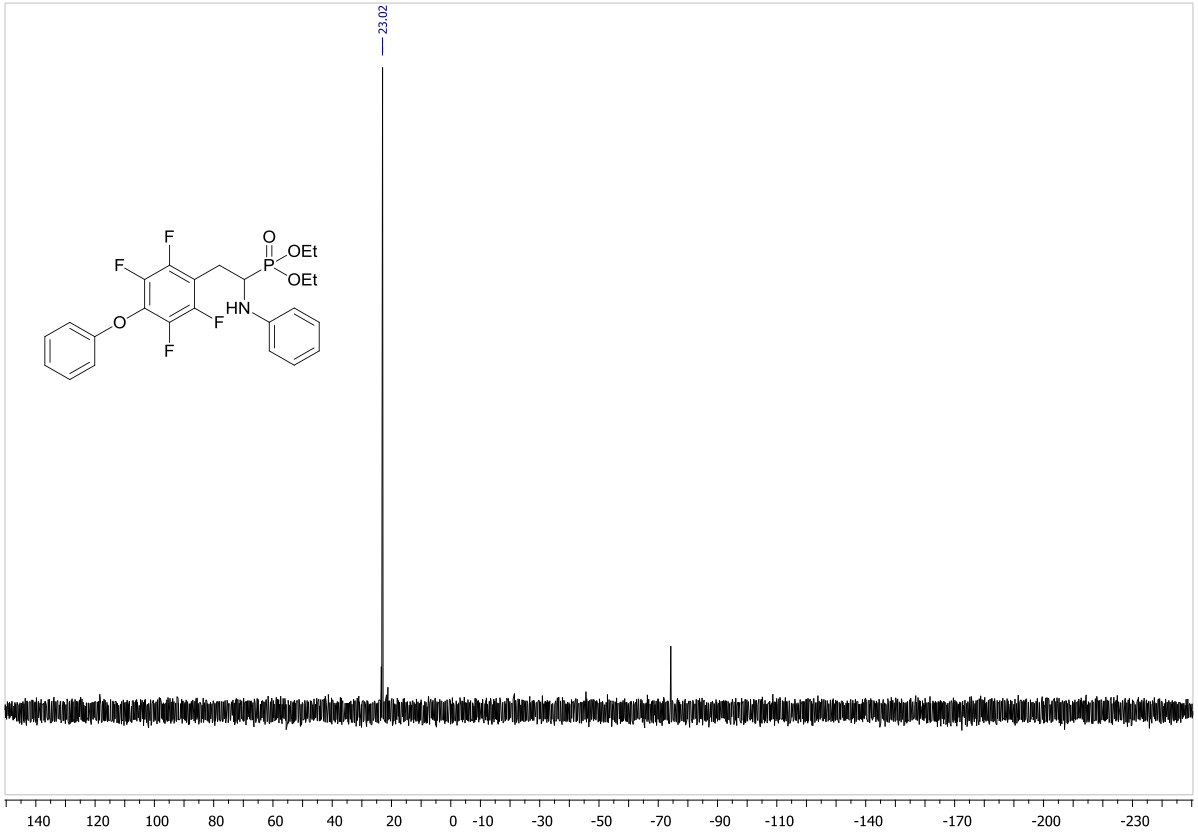

Fig. S63. ^{31}P NMR spectrum of 2p (Acetone-d6)

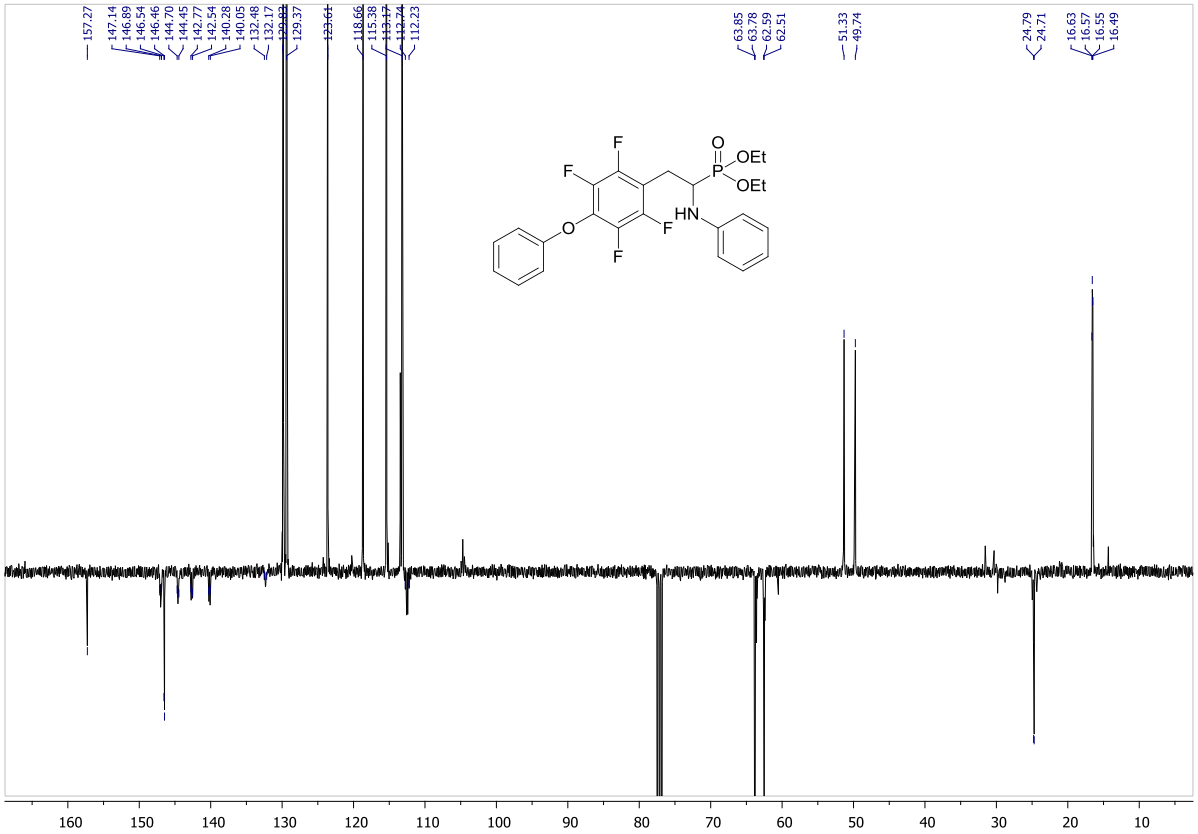

Fig. S64. ^{13}C NMR spectrum of 2p ($CDCl_3$)

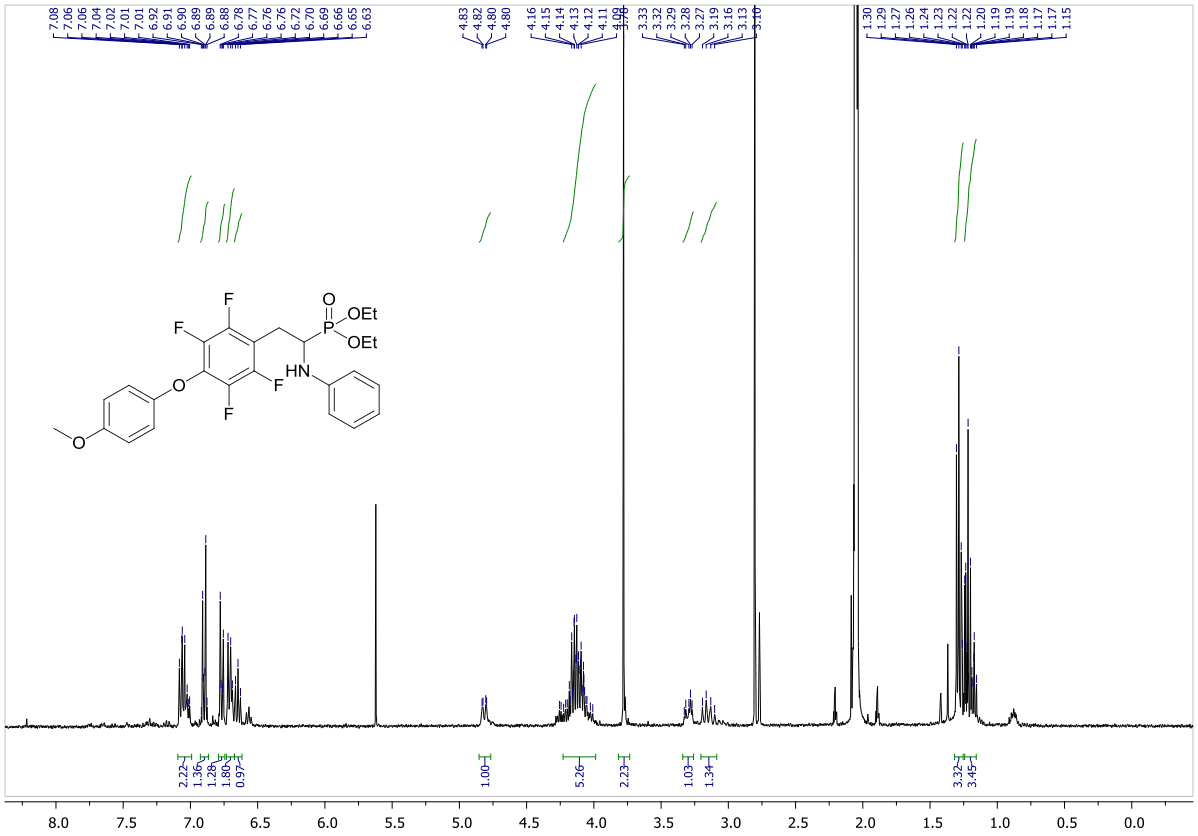

Fig. S65. ^{1}H NMR spectrum of 2q (Acetone-d6)

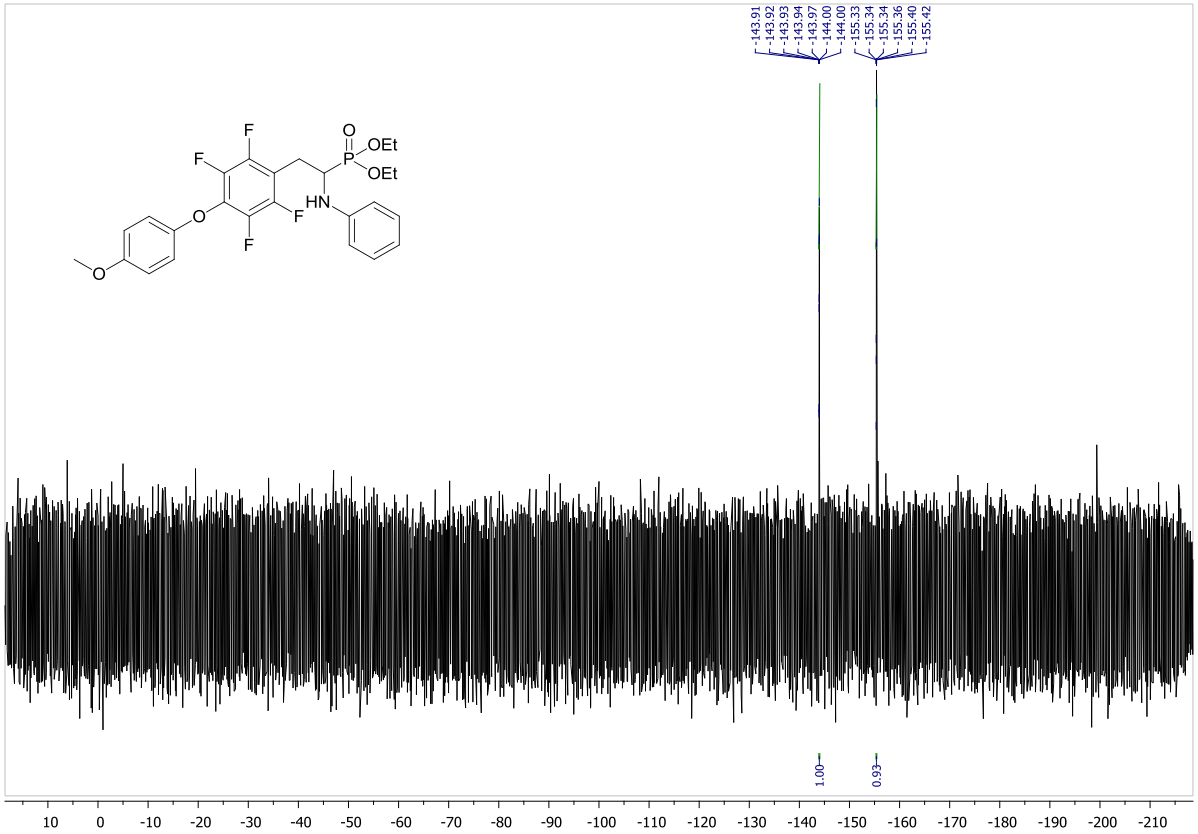

Fig. S66. ^{19}F NMR spectrum of 2q ($CDCl_3$)

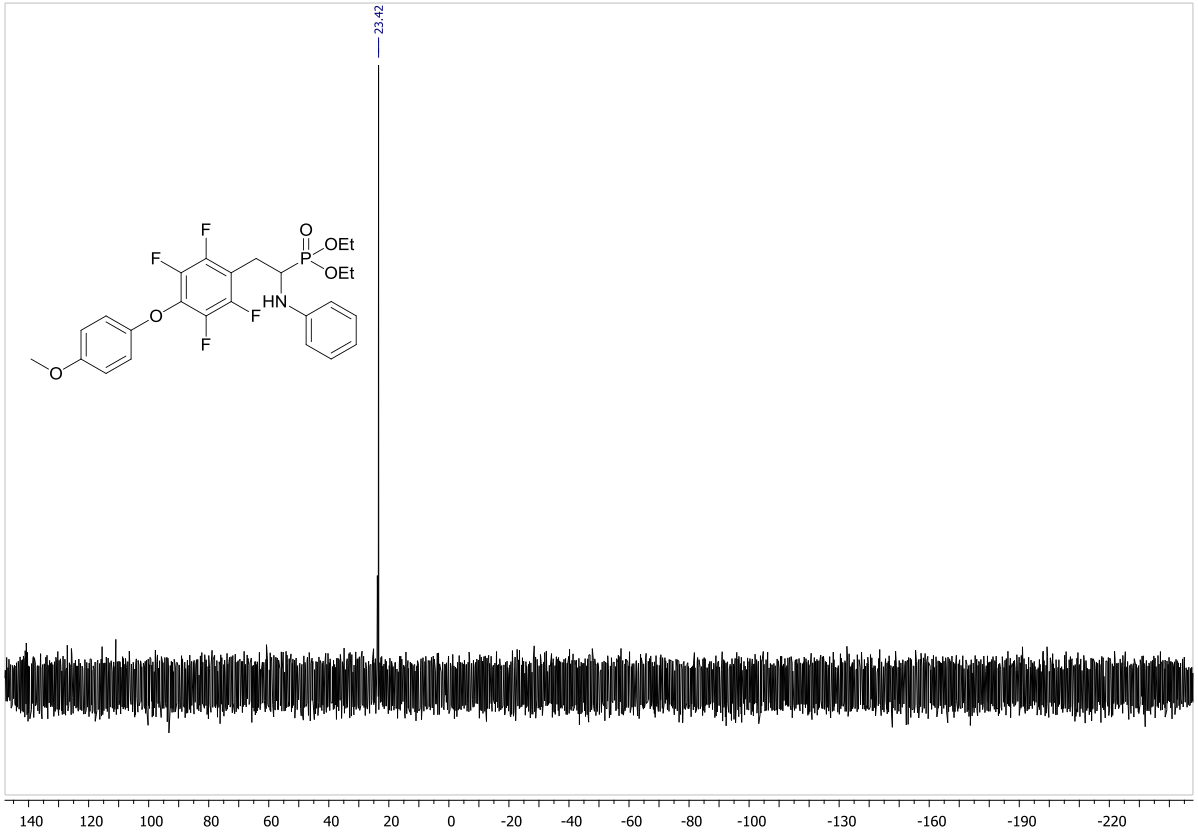

Fig. S67. ^{31}P NMR spectrum of 2q ($CDCl_3$)

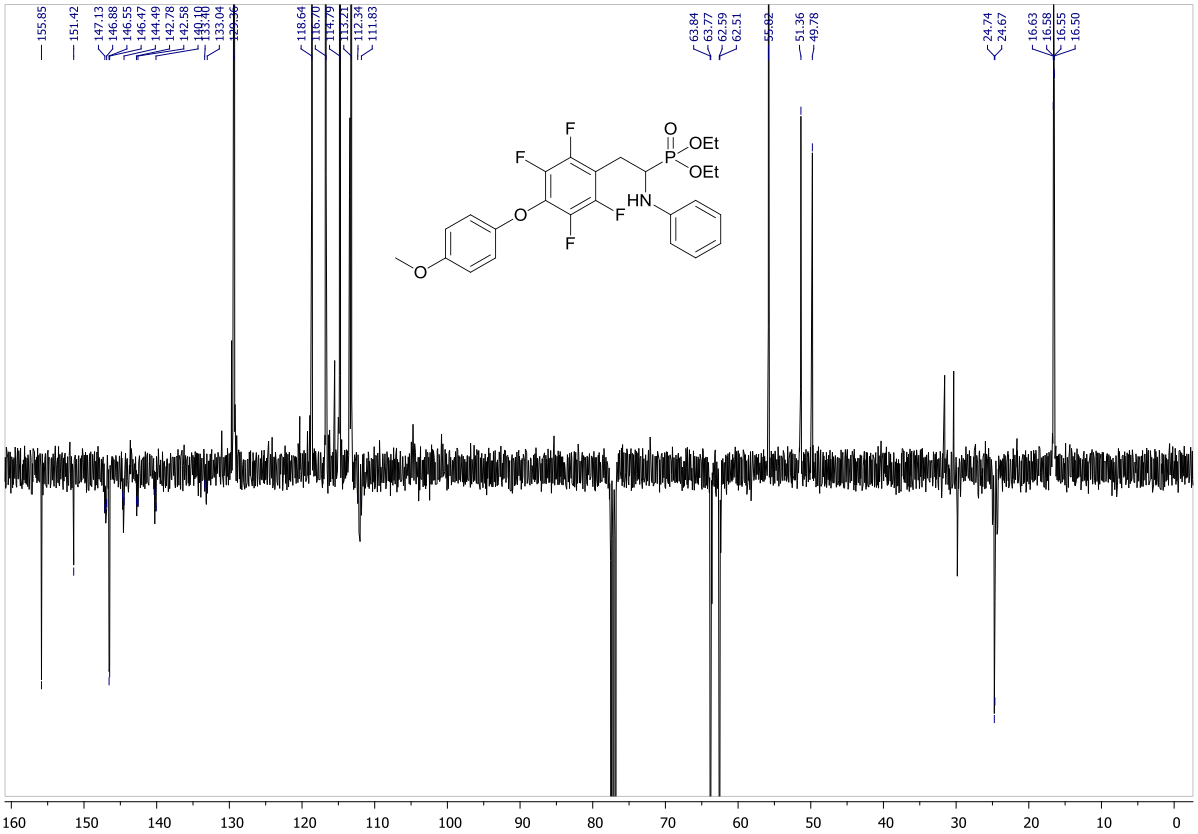

Fig. S68. ^{13}C NMR spectrum of 2q ($CDCl_3$)

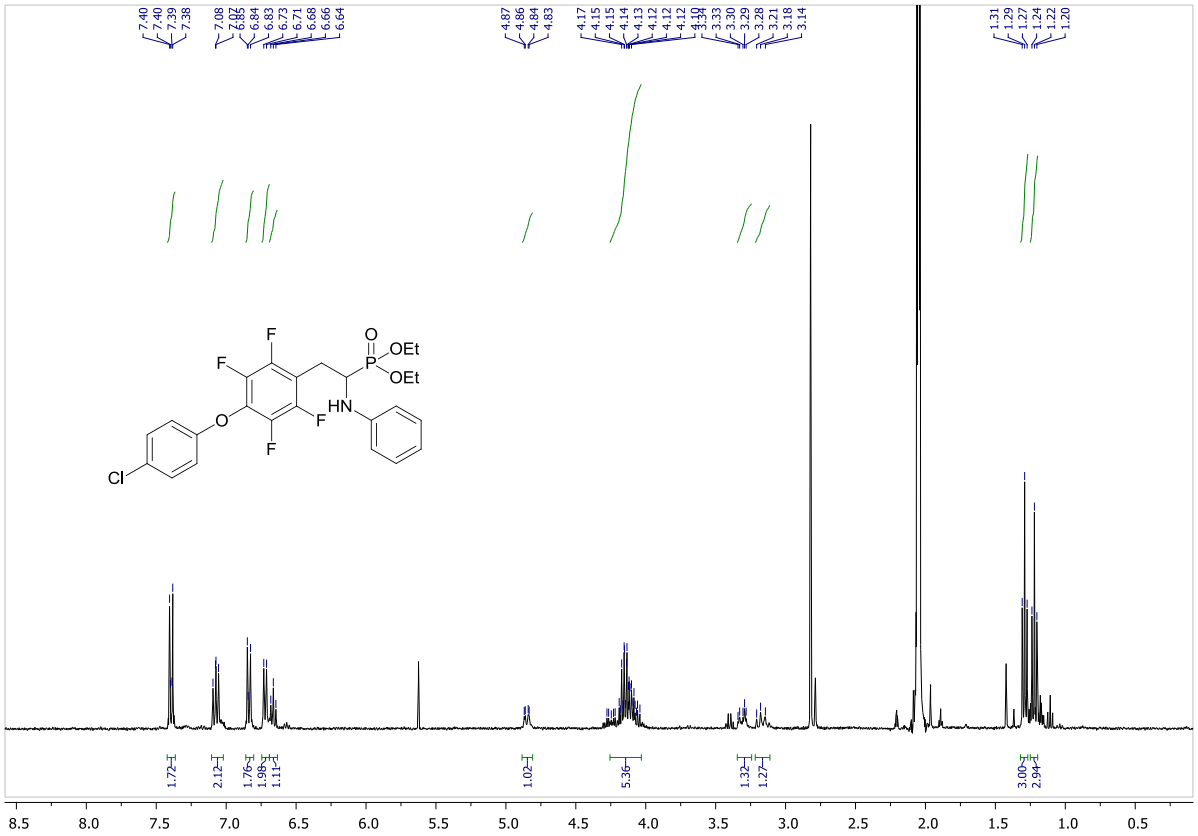

Fig. S69. ^{1}H NMR spectrum of 2r (Acetone-d6)

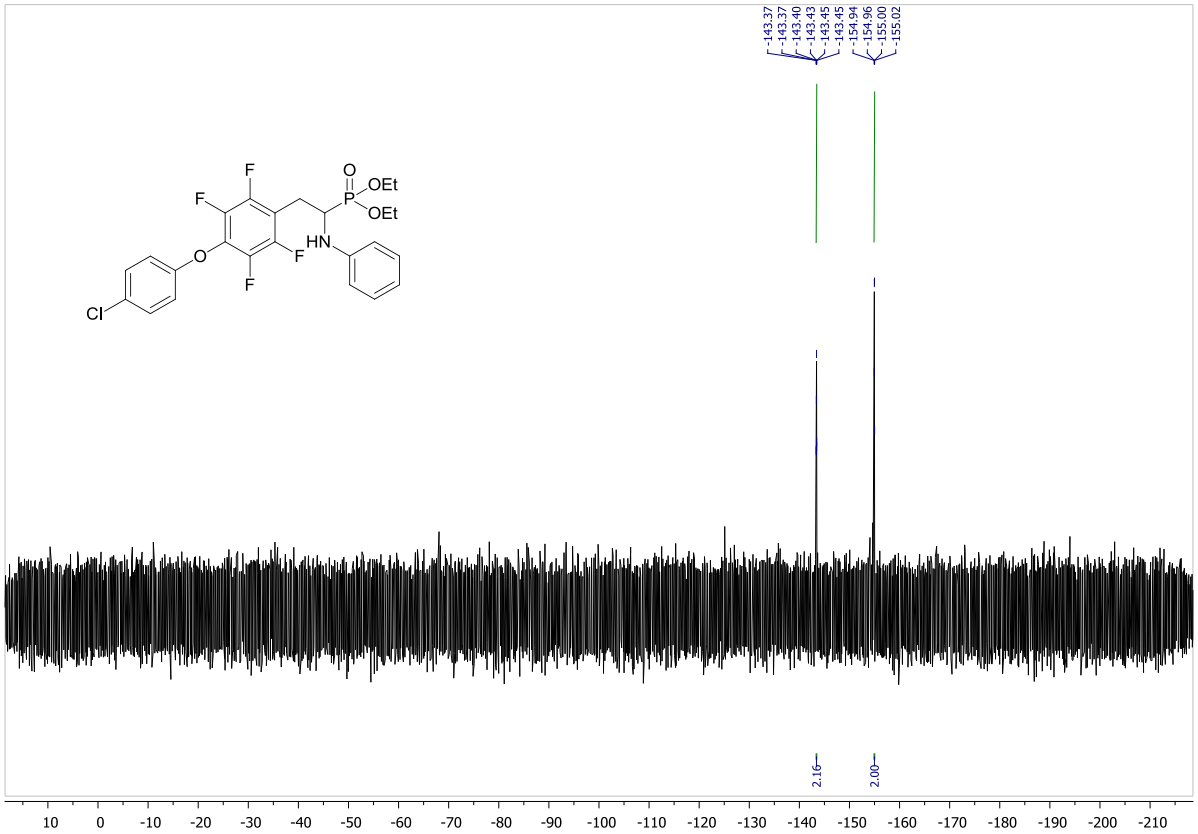

Fig. S70. ^{19}F NMR spectrum of 2r ($CDCl_3$)

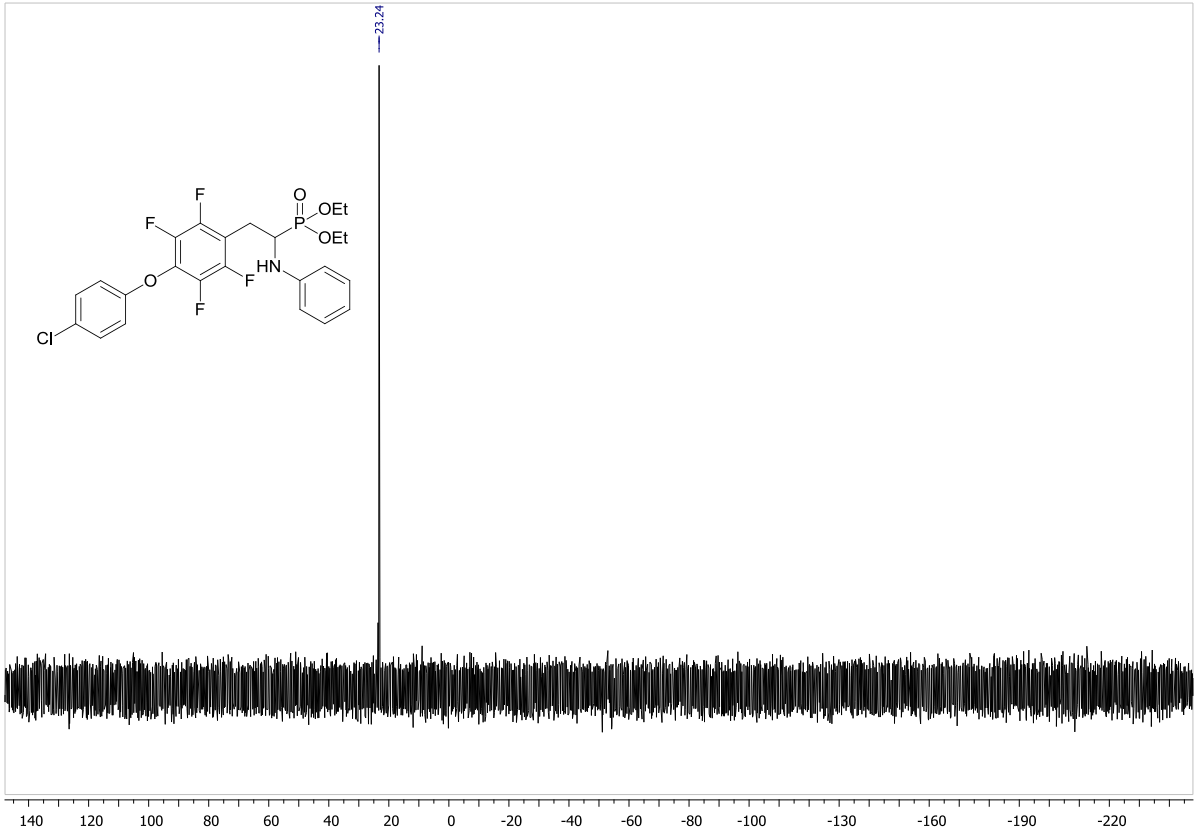

Fig. S71. ^{31}P NMR spectrum of 2r ($CDCl_3$)

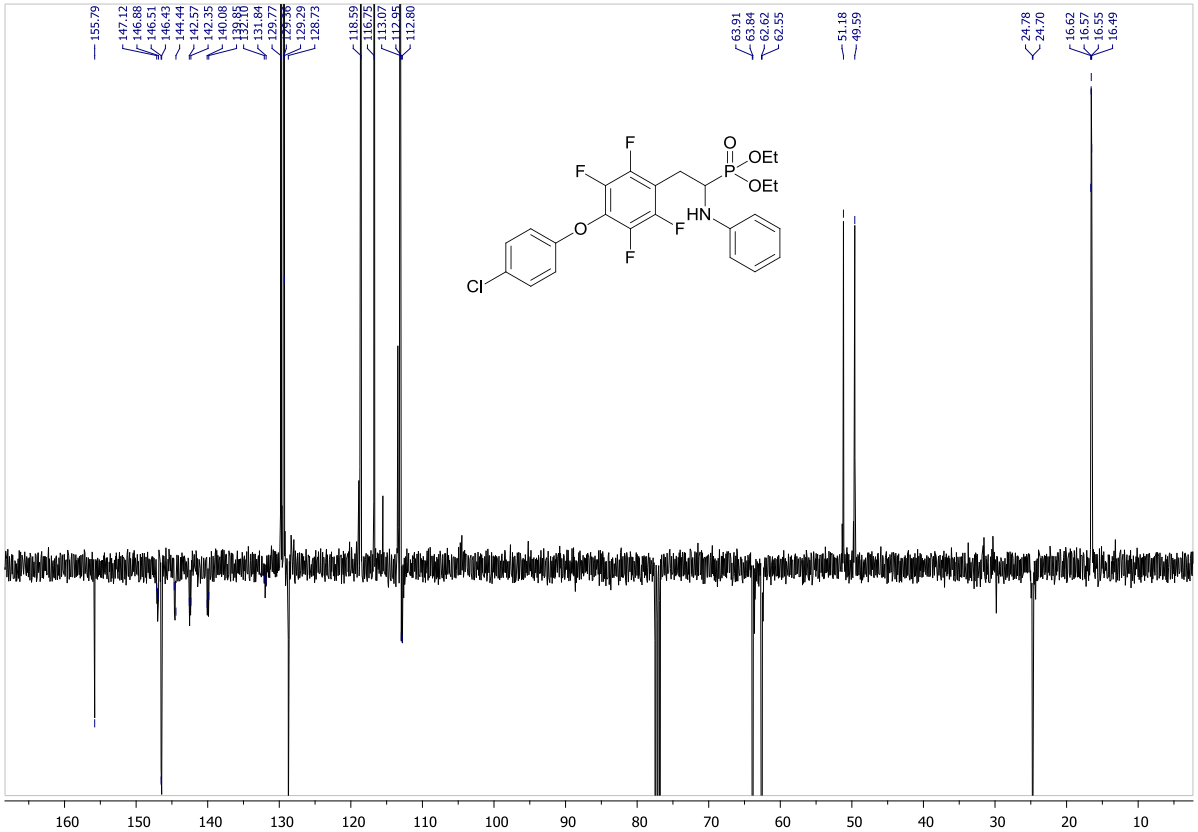

Fig. S72. ^{13}C NMR spectrum of 2r ($CDCl_3$)

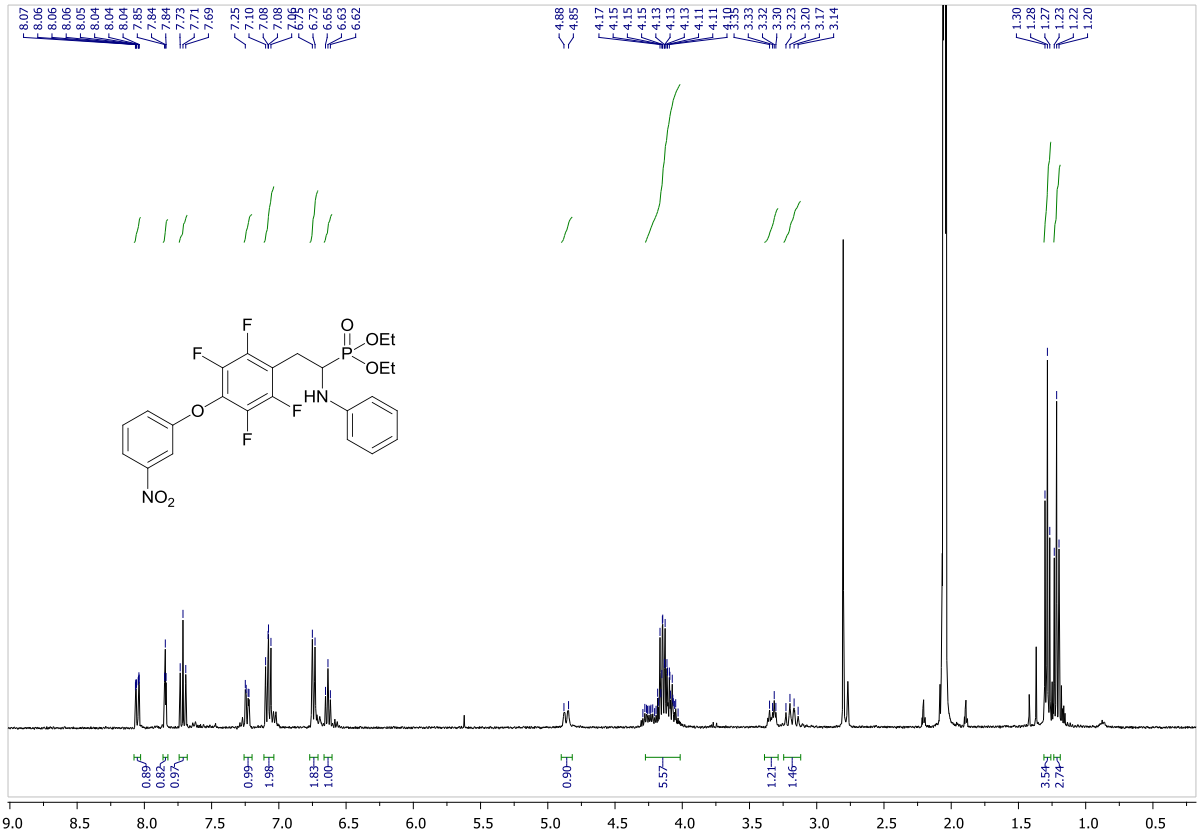

Fig. S73. ^{1}H NMR spectrum of 2s (Acetone-d6)

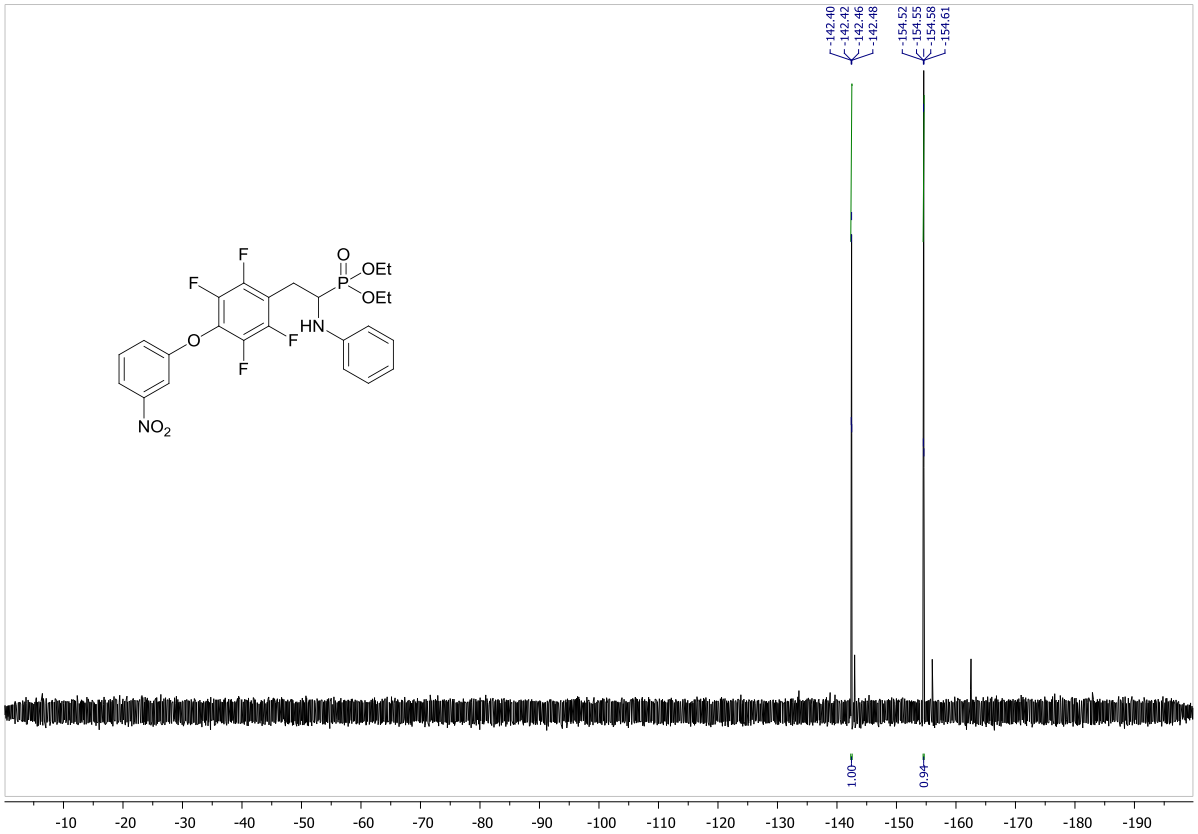

Fig. S74. ^{19}F NMR spectrum of 2s ($CDCl_3$)

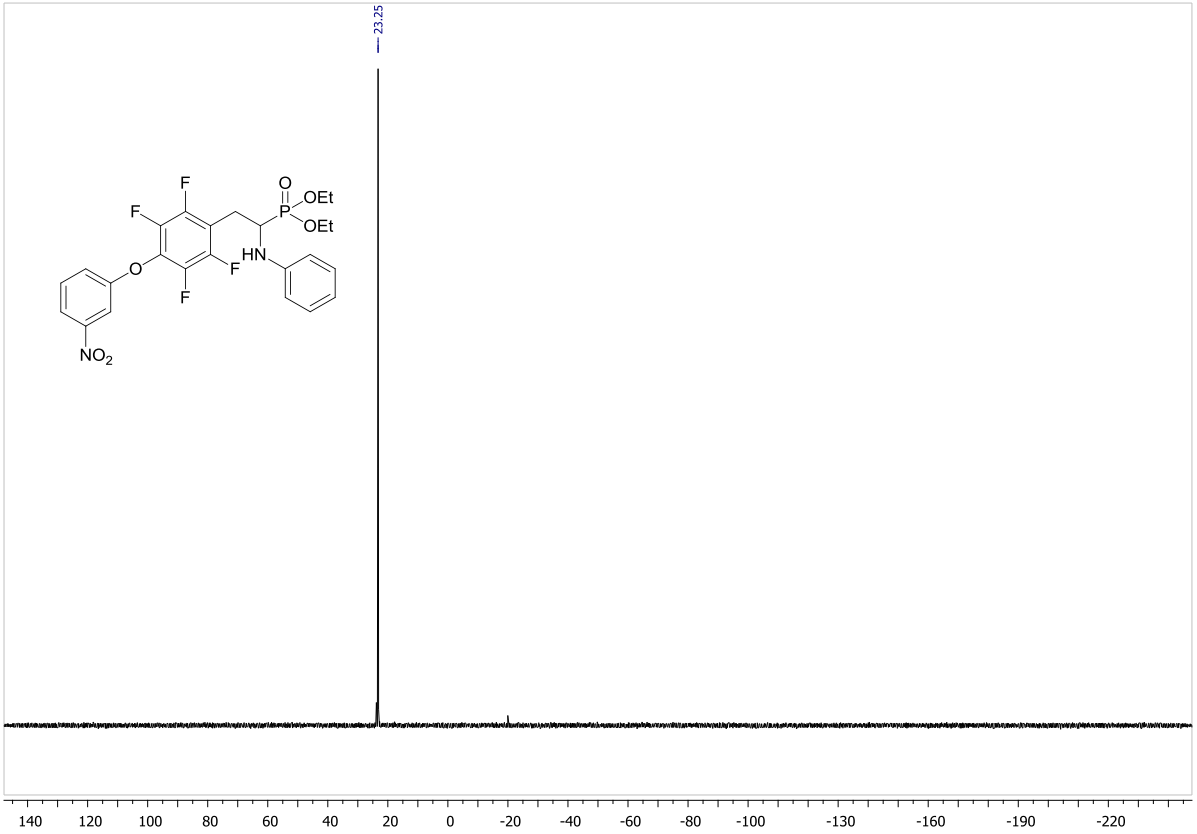

Fig. S75. ^{31}P NMR spectrum of 2s ($CDCl_3$)

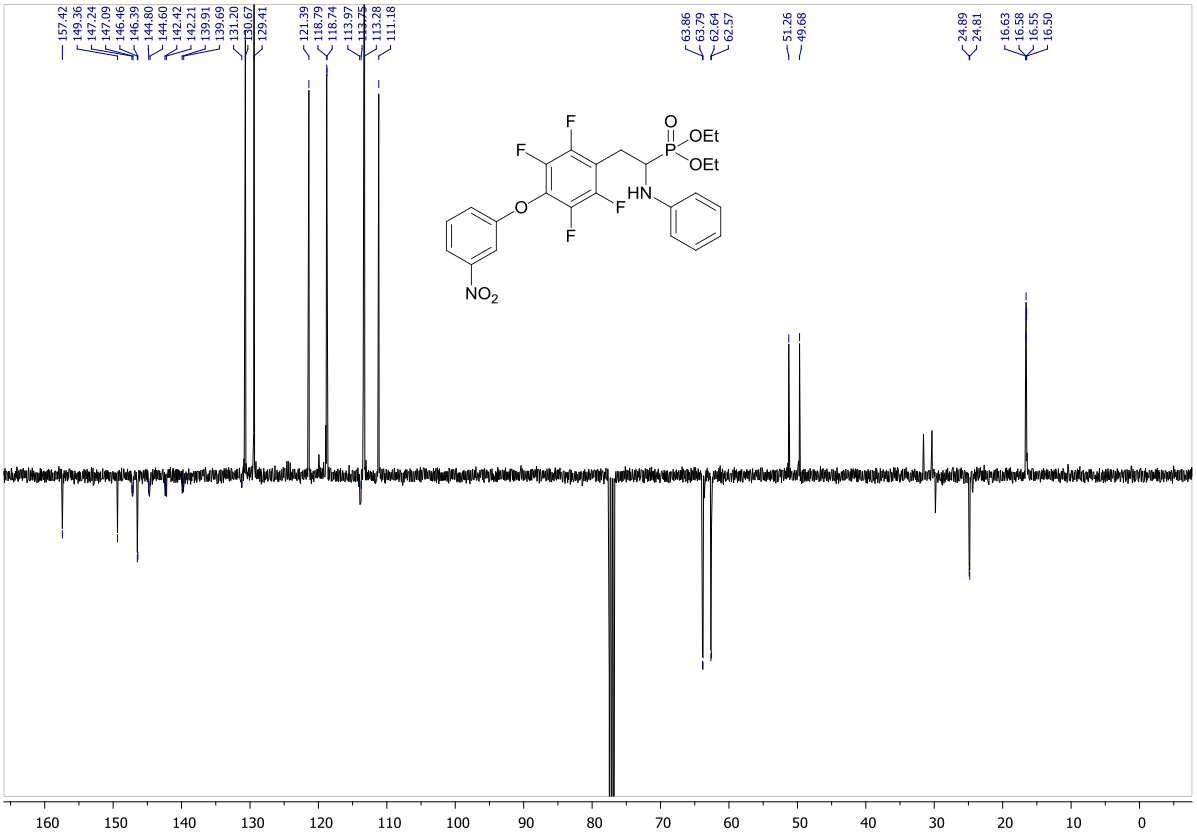

Fig. S76. ^{13}C NMR spectrum of 2s ($CDCl_3$)

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
514.1230	514.1229	0.1	0.2	11.5	1195.0	0.000	100.00	C24 H25 N O3 S P F4
	514.1234	-0.4	-0.8	4.5	1208.9	13.921	0.00	C9 H21 N13 O4 S P F4
	514.1221	0.9	1.8	-0.5	1210.0	15.058	0.00	C8 H25 N9 O8 S P F4

Fig. S77. HRMS of 2a

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
528.1387	528.1385	0.2	0.4	11.5	806.4	0.000	100.00	C25 H27 N O3 S P F4
	528.1390	-0.3	-0.6	4.5	817.7	11.299	0.00	C10 H23 N13 O4 S P F4
	528.1377	1.0	1.9	-0.5	818.7	12.316	0.00	C9 H27 N9 O8 S P F4

Fig. S78. HRMS of 2b

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
542.1542	542.1542	0.0	0.0	11.5	870.5	0.000	100.00	C26 H29 N O3 S P F4
	542.1547	-0.5	-0.9	4.5	883.7	13.124	0.00	C11 H25 N13 O4 S P F4
	542.1534	0.8	1.5	-0.5	885.1	14.526	0.00	C10 H29 N9 O8 S P F4

Fig. S79. HRMS of 2c

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
544.1339	544.1335	0.4	0.7	11.5	1238.4	0.021	97.94	C25 H27 N O4 S P F4
	544.1348	-0.9	-1.7	16.5	1242.3	3.883	2.06	C26 H23 N5 S P F4
	544.1340	-0.1	-0.2	4.5	1249.4	11.046	0.00	C10 H23 N13 O5 S P F4

Fig. S80. HRMS of 2d

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
544.1328	544.1335	-0.7	-1.3	11.5	1030.0	0.000	100.00	C25 H27 N O4 S P F4
	544.1326	0.2	0.4	-0.5	1039.9	9.924	0.00	C9 H27 N9 O9 S P F4

Fig. S81. HRMS of 2e

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
529.1335	529.1338	-0.3	-0.6	11.5	1186.3	0.000	100.00	C24 H26 N2 O3 S P F4
	529.1343	-0.8	-1.5	4.5	1199.4	13.093	0.00	C9 H22 N14 O4 S P F4
	529.1330	0.5	0.9	-0.5	1200.3	14.056	0.00	C8 H26 N10 O8 S P F4

Fig. S82. HRMS of 2f

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
592.0336	592.0334	0.2	0.3	11.5	1018.3	0.000	99.99	C24 H24 N O3 S Br P F4
	592.0339	-0.3	-0.5	4.5	1028.1	9.765	0.01	C9 H20 N13 O4 S Br P F4

Fig. S83. HRMS of 2g

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
528.1387	528.1385	0.2	0.4	11.5	1242.2	0.000	100.00	C25 H27 N O3 S P F4
	528.1390	-0.3	-0.6	4.5	1253.8	11.556	0.00	C10 H23 N13 O4 S P F4
	528.1377	1.0	1.9	-0.5	1255.0	12.819	0.00	C9 H27 N9 O8 S P F4

Fig. S84. HRMS of 2h

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
578.2477	578.2481	-0.4	-0.7	7.5	892.0	0.000	100.00	C28 H41 N O3 S P F4
	578.2486	-0.9	-1.6	0.5	905.7	13.678	0.00	C13 H37 N13 O4 S P F4

Fig. S85. HRMS of 2i

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
581.1503	581.1498	0.5	0.9	9.5	1256.7	0.053	94.80	C24 H30 N2 O6 S P F4
	581.1512	-0.9	-1.5	14.5	1259.6	2.956	5.20	C25 H26 N6 O2 S P F4
	581.1503	0.0	0.0	2.5	1267.9	11.301	0.00	C9 H26 N14 O7 S P F4

Fig. S86. HRMS of 2j

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
463.1773	463.1774	-0.1	-0.2	7.5	1496.4	n/a	n/a	C21 H28 N2 O3 F4 P

Fig. S87. HRMS of 2l

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
435.1465	435.1461	0.4	0.9	7.5	1402.8	0.000	100.00	C19 H24 N2 O3 F4 P
	435.1466	-0.1	-0.2	0.5	1422.0	19.215	0.00	C4 H20 N14 O4 F4 P

Fig. S88. HRMS of 2k

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
477.1932	477.1930	0.2	0.4	7.5	1626.9	0.000	100.00	C22 H30 N2 O3 F4 P
	477.1935	-0.3	-0.6	0.5	1640.7	13.792	0.00	C7 H26 N14 O4 F4 P

Fig. S89. HRMS of 2m

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
461.1616	461.1617	-0.1	-0.2	8.5	1595.0	n/a	n/a	C21 H26 N2 O3 F4 P

Fig. S90. HRMS of 2n

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
511.1774	511.1774	0.0	0.0	11.5	1541.3	0.000	100.00	C25 H28 N2 O3 F4 P
	511.1779	-0.5	-1.0	4.5	1552.5	11.176	0.00	C10 H24 N14 O4 F4 P

Fig. S91. HRMS of 2o

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
498.1459	498.1457	0.2	0.4	11.5	1594.7	0.000	100.00	C24 H25 N O4 F4 P
	498.1462	-0.3	-0.6	4.5	1606.2	11.464	0.00	C9 H21 N13 O5 F4 P

Fig. S92. HRMS of 2p

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
528.1567	528.1563	0.4	0.8	11.5	1428.7	0.000	100.00	C25 H27 N O5 F4 P
	528.1568	-0.1	-0.2	4.5	1442.4	13.692	0.00	C10 H23 N13 O6 F4 P

Fig. S93. HRMS of 2q

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
532.1066	532.1068	-0.2	-0.4	11.5	1483.7	n/a	n/a	C24 H24 N O4 F4 P Cl

Fig. S94. HRMS of 2r

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
543.1312	543.1308	0.4	0.7	12.5	1381.2	0.000	100.00	C24 H24 N2 O6 F4 P
	543.1313	-0.1	-0.2	5.5	1395.1	13.933	0.00	C9 H20 N14 O7 F4 P

Fig. S95. HRMS of 2s