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Supporting information

Highly functionalised (*γ*-azido/*γ*-fluoro-*β*-iodo)vinyl derivatives from phosphorus based allenes or allenoates: I•••O halogen bonding interactions

Mandala Anitha and K. C. Kumara Swamy*

School of Chemistry, University of Hyderabad,

Hyderabad -500046, Telangana, India.

E-mail: kckssc@uohyd.ac.in, kckssc@yahoo.com

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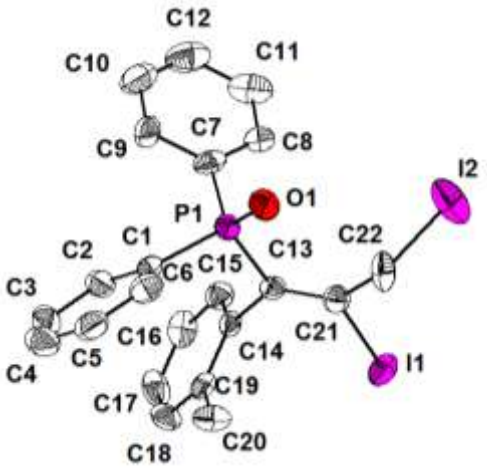

Figure S1. ORTEP diagram of compound **6** (probability ellipsoid at 30%). CCDC 1905975.

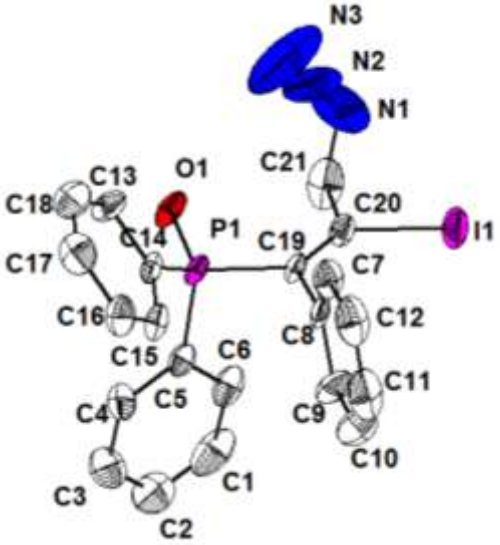

Figure S2. ORTEP diagram of compound **17** (probability ellipsoid at 30%). Hydrogen atoms are omitted for clarity. CCDC 1905976.

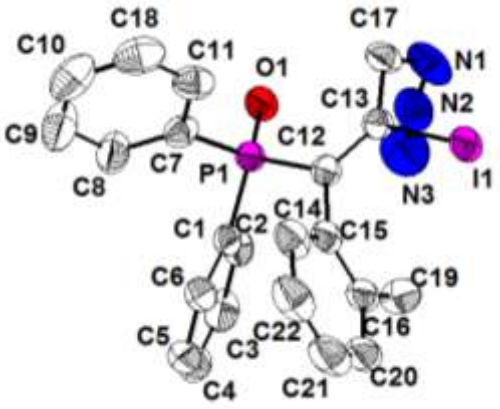

Figure S3. ORTEP diagram of compound **18** (probability ellipsoid at 30%). Hydrogen atoms are omitted for clarity. CCDC 1905977.

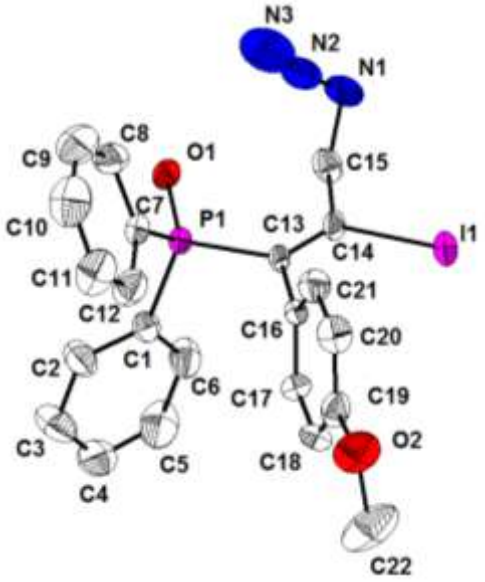

Figure S4. ORTEP diagram of compound **19** (probability ellipsoid at 30%). Hydrogen atoms are omitted for clarity. Selected bond lengths [Å] with esds are given in parentheses: Compound **16** P1-C13 1.844(6), C13-C14 1.329(8), C14-C15 1.516(9), N1-C15 1.485(10), N1-N2 1.244(11), N2-N3 1.119(12), I1-C14 2.112(5), C13-C16 1.488(8). CCDC 1905978.

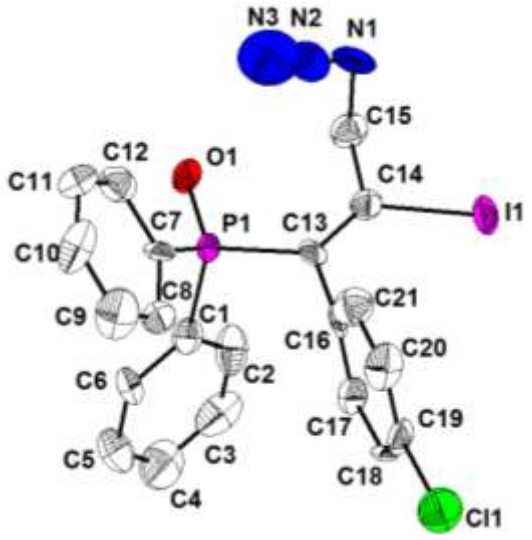

Figure S5: ORTEP diagram of compound **20** (probability ellipsoid at 30%). Hydrogen atoms are omitted for clarity. Selected bond lengths [Å] with esds are given in parentheses: P1-C13 1.822(13), I1-C14 2.102(12), C13-C14 1.315(18), N1-C15 1.50(2), N1-N2 1.23(2), N2-N3 1.12(2), C16-C13 1.521(19). CCDC 1905979.

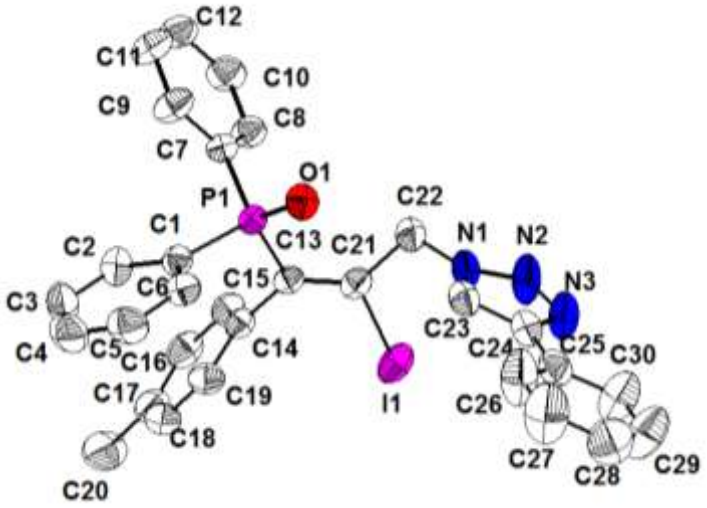

Figure S6: ORTEP diagram of compound **25** (probability ellipsoid at 30%). Hydrogen atoms are omitted for clarity. CCDC 1905980.

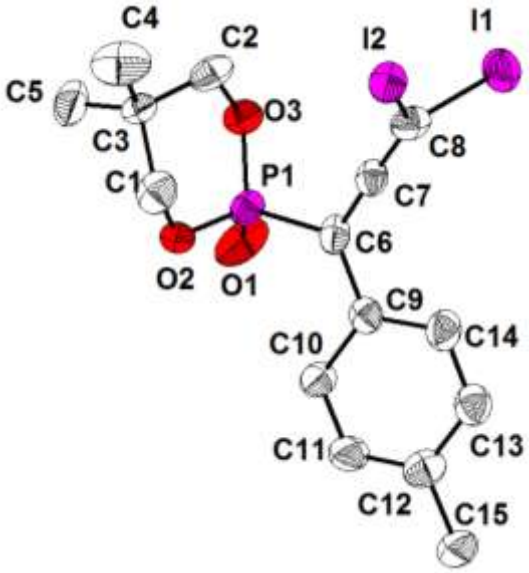

Figure S7: ORTEP diagram of compound **27** (probability ellipsoid at 30%). Hydrogen atoms are omitted for clarity. CCDC 1905981.

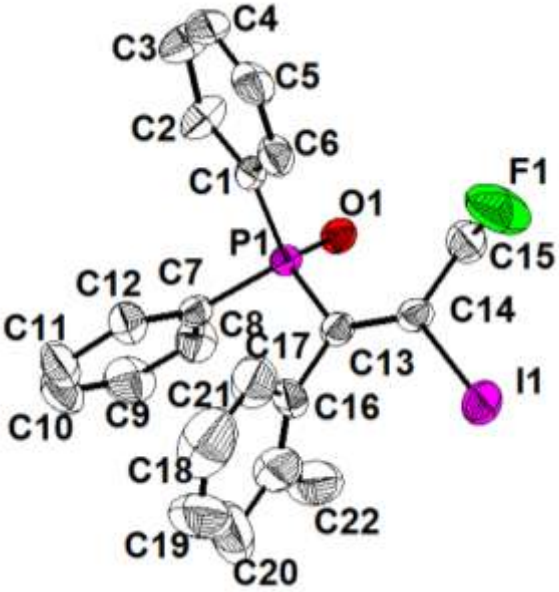

Figure S8: ORTEP diagram of compound **29** (probability ellipsoid at 30%). Hydrogen atoms are omitted for clarity. CCDC 1905982.

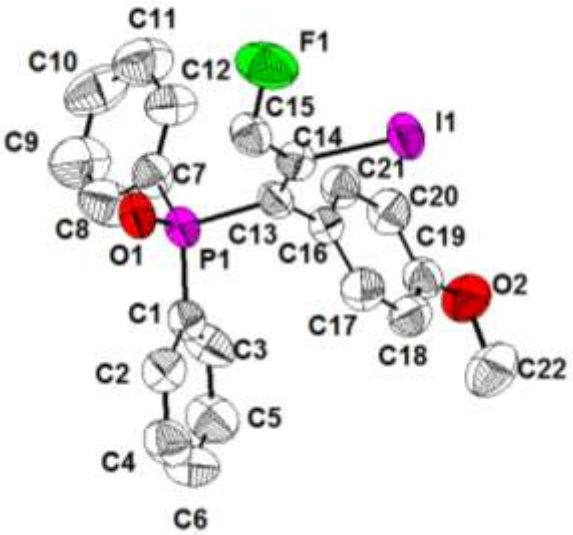

Figure S9: ORTEP diagram of compound **30** (probability ellipsoid at 30%). Hydrogen atoms are omitted for clarity. CCDC 1905983.

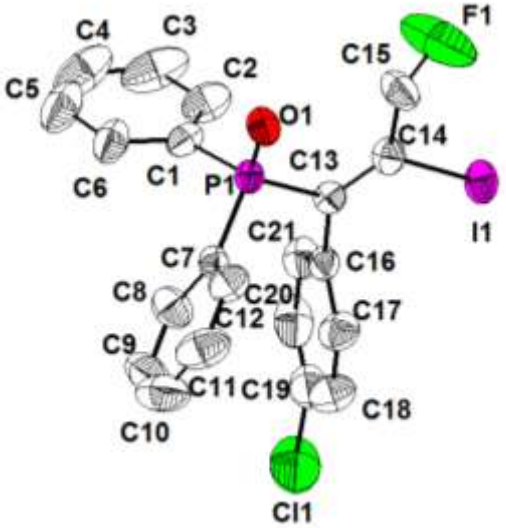

Figure S10: ORTEP diagram of compound **31** (probability ellipsoid at 30%). Hydrogen atoms are omitted for clarity. CCDC 1905984.

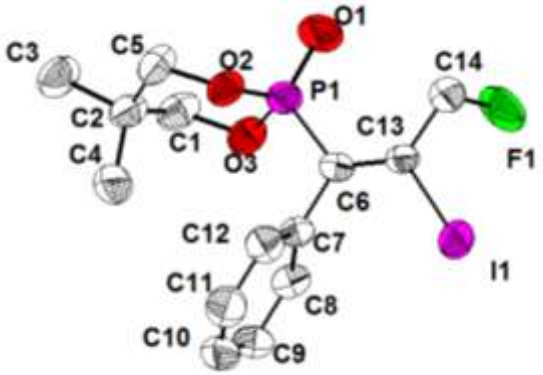

Figure S11: ORTEP diagram of compound **32** (probability ellipsoid at 30%). Hydrogen atoms are omitted for clarity. CCDC 1905985.

X-ray data:

Crystallographic data were collected on a Bruker APX-II-SMART using Mo-K_α radiation (λ = 0.71073 Å) and have been deposited at the Cambridge Crystallographic Data Center (CCDC). Copies of the information may be obtained free of charge from The Director, CCDC, 12 Union Road, Cambridge CB2 1 EZ, UK (Fax: +44-1223-336033; email: deposit@ccdc.cam.ac.uk or www.ccdc.can.ac.uk).

Compound 6: $C_{22}H_{19}I_2OP$, *M* = 584.14**,** Orthorhombic, Space group *p_n_a_21, a* = 19.5490(16), *b* = 9.8719(8), *c* = 10.8488(8) Å, *V*= 2093.7(3) Å^3, *α* = 90, *β* = 90, *γ* = 90, *Z* = 4, *μ* = 3.089 mm^{-1}, data/restraints/parameters: 3647/1/237, R indices (I > 2σ(I)) R1 = 0.0347, *w*R2 (all data) = 0.1021. CCDC No. 1905975.

Compound 17: $C_{21}H_{17}IN_3OP$, *M* = 485.25**,** Monoclinic, Space group *P 1 21/c 1, a* = 9.1543(3), *b* = 10.0610(4), *c* = 22.0753(9) Å, *V*= 2032.48(13) Å^3, *β* = 91.464(3), *Z* = 4, *μ* = 13.245 mm^{-1}, data/restraints/parameters: 3907/0/244, R indices (I > 2σ(I)) R1 = 0.0726, *w*R2 (all data) = 0.1985. CCDC No. 1905976.

Compound 18: $C_{22}H_{19}IN_3OP$, *M* = 499.27**,** Monoclinic, Space group *P2(1)/c, a* = 8.209(3), *b* = 16.624(7), *c* = 15.715(6) Å, *V*= 2142.9(14) Å^3, *β* = 92.215(6), *Z* = 4, *μ* = 1.586 mm^{-1},

data/restraints/parameters: 3686/0/254, R indices (I > 2σ(I)) R1 = 0.0268, *w*R2 (all data) = 0.0698. CCDC No. 1905977.

Compound 19: $C_{22}H_{19}IN_3O_2P$, *M* = 515.27**,** Orthorhombic, Space group *P 21 21 21, α* = 8.3026(2), *b* = 8.5630(2), *c* = 30.1250(8) Å, *V*= 2141.75(10) Å^3, *α* = 90, *β* = 90, *γ* = 90, *Z* = 4, *μ* = 12.643 mm^{-1}, data/restraints/parameters: 3737 /0/263, R indices (I > 2σ(I)) R1 = 0.0476, *w*R2 (all data) = 0.1264. CCDC No. 1905978.

Compound 20: $C_{21}H_{16}ClIN_3OP$, *M* = 519.69**,** Orthorhombic, Space group *P_21_21_21, α* = 29.548(4), *b* = 8.3033(8), *c* = 8.5609(11) Å, *V*= 2100.4(4) Å^3, *α* = 90, *β* = 90, *γ* = 90, *Z* = 4, *μ* = 1.745 mm^{-1}, data/restraints/parameters: 3693/0/253, R indices (I > 2σ(I)) R1 = 0.0780, *w*R2 (all data) = 0.2136. CCDC No. 1905979.

Compound 25: $C_{30}H_{25}IN_3OP$, *M* = 601.40**,** Triclinic, Space group *P-1, α* = 8.9643(4), *b* = 11.6596(6), *c* = 14.2643(7) Å, *V*= 1324.64(11) Å^3, *α* = 69.832(2), *β* = 71.872(2), *γ* = 79.193(2), *Z* = 2, *μ* = 1.297mm^{-1}, data/restraints/parameters: 6145/0/327, R indices (I > 2σ(I)) R1 = 0.0293, *w*R2 (all data) = 0.0875. CCDC No. 1905980.

Compound 27: $C_{15}H_{17}I_2O_3P$, *M* = 530.06**,** Monoclinic, Space group *P 21/n, α* = 9.1150(7), *b* = 10.3990(10), *c* = 19.1186(18) Å, *V*= 1810.7(3) Å^3, *β* = 92.325(4), *Z* = 4, *μ* = 3.568 mm^{-1}, data/restraints/parameters: 3140/0/194, R indices (I > 2σ(I)) R1 = 0.0869, *w*R2 (all data) = 0.2603. CCDC No. 1905981.

Compound 29: $C_{22}H_{19}FIOP$, *M* = 476.24**,** Monoclinic, Space group *P2(1), α* = 9.6921(13), *b* = 9.8549(12), *c* = 11.1815(15) Å, *V*= 1015.7(2) Å^3, *β* = 107.996(4), *Z* = 2, *μ* = 1.671 mm^{-1}, data/restraints/parameters: 3554/1/235, R indices (I > 2σ(I)) R1 = 0.0308, *w*R2 (all data) = 0.0944. CCDC No. 1905982.

Compound 30: $C_{22}H_{19}FIO_2P$, *M* = 492.24**,** Monoclinic, Space group *Pn, α* = 8.2948(19), *b* = 26.144(6), *c* = 14.533(3) Å, *V*= 3142.3(12) Å^3, *β* = 94.408(4), *Z* = 6, *μ* = 1.627 mm^{-1}, data/restraints/parameters: 11020/2/733, R indices (I > 2σ(I)) R1 = 0.0724, *w*R2 (all data) = 0.1884. CCDC No. 1905983.

Compound 31: $C_{21}H_{16}ClFIOP$, *M* = 496.66**,** Monoclinic, Space group *P2(1)/c, α* = 8.2639(11), *b* = 8.5040(13), *c* = 29.114(5) Å, *V*= 2030.9(5) Å^3, *β* = 96.974(5), *Z* = 4, *μ* = 1.803 mm^{-1},

data/restraints/parameters: 4277/0/235, R indices (I > 2σ(I)) R1 = 0.0516, *w*R2 (all data) = 0.1046. CCDC No. 1905984.

Compound 32: $C_{14}H_{17}FIO_3P$, *M* = 410.15**,** Monoclinic, Space group *P2(1)/c, a* = 16.7231(17), *b* = 7.8520(8), *c* = 12.4005(17) Å, *V*= 1582.0(3) $Å^3$, *β* = 103.700(13), *Z* = 4, *μ* = 2.139 mm^{-1}, data/restraints/parameters: 2789/0/183, R indices (I > 2σ(I)) R1 = 0.0536, *w*R2 (all data) = 0.1714. CCDC No. 1905985.

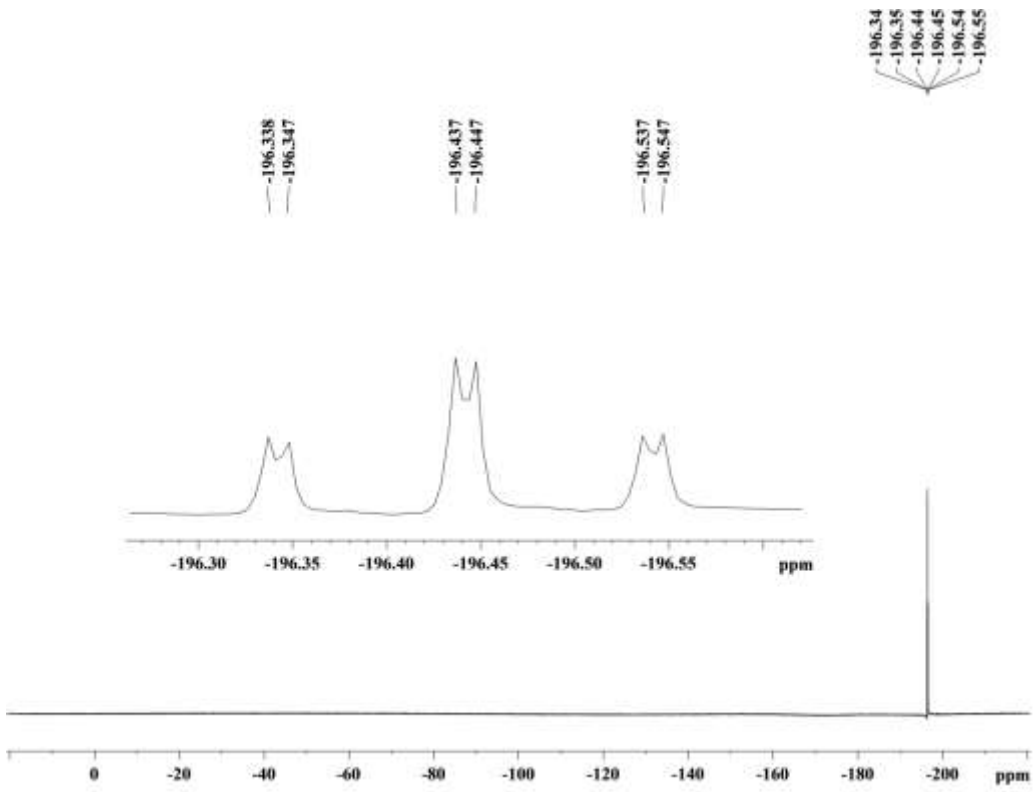

Figure S12. H-coupled ^{19}F NMR spectrum of compound **28** showing triplet of doublet

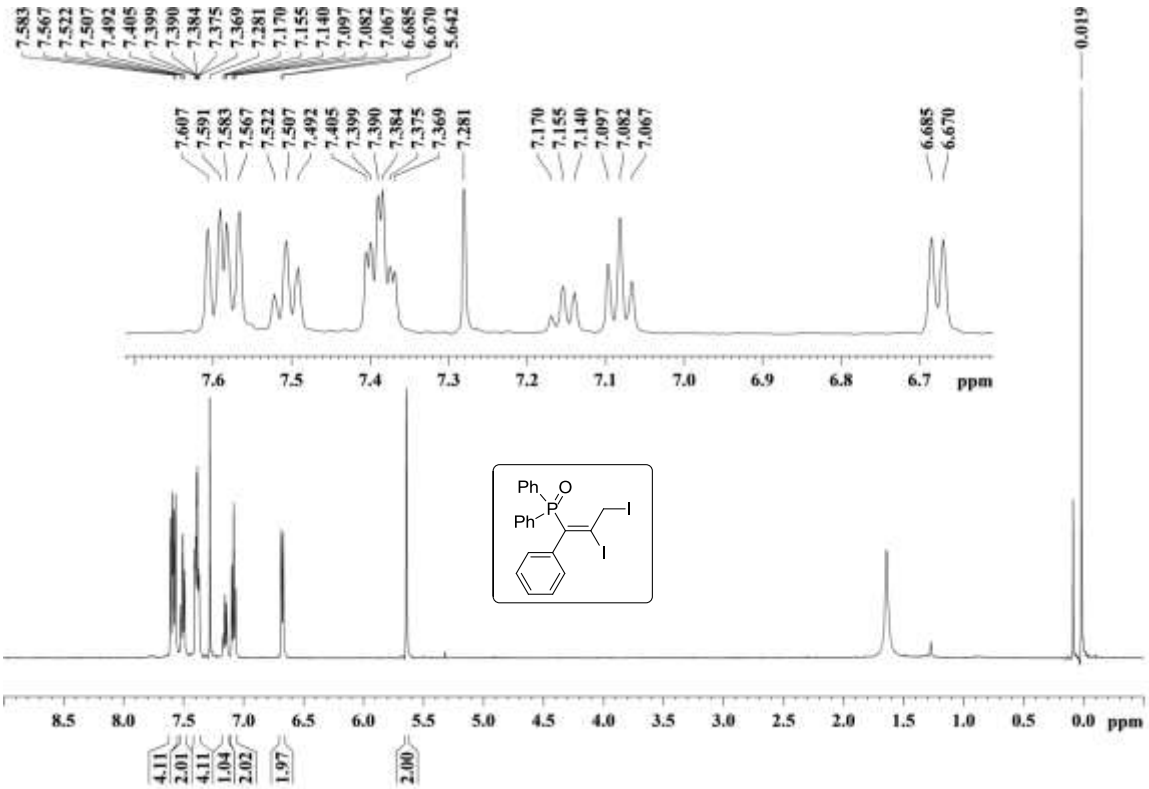

Figure S13. ^{1}H NMR spectrum of compound **5**

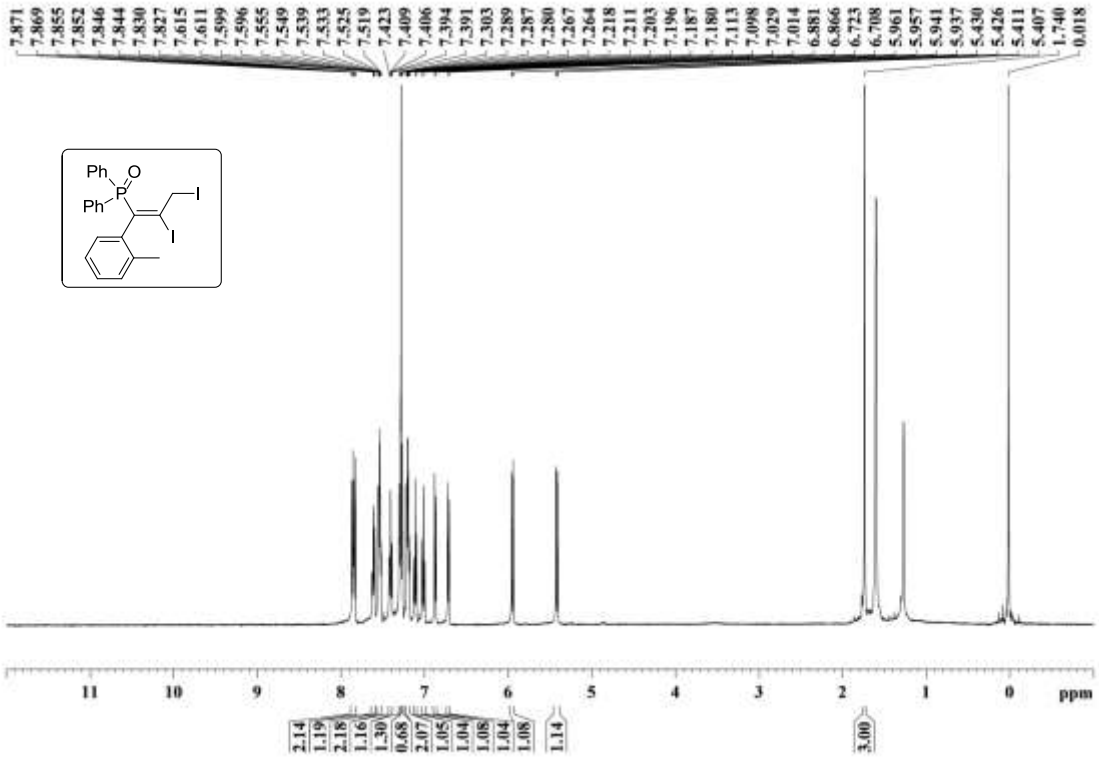

Figure S14. ^{1}H NMR spectrum of compound **6**

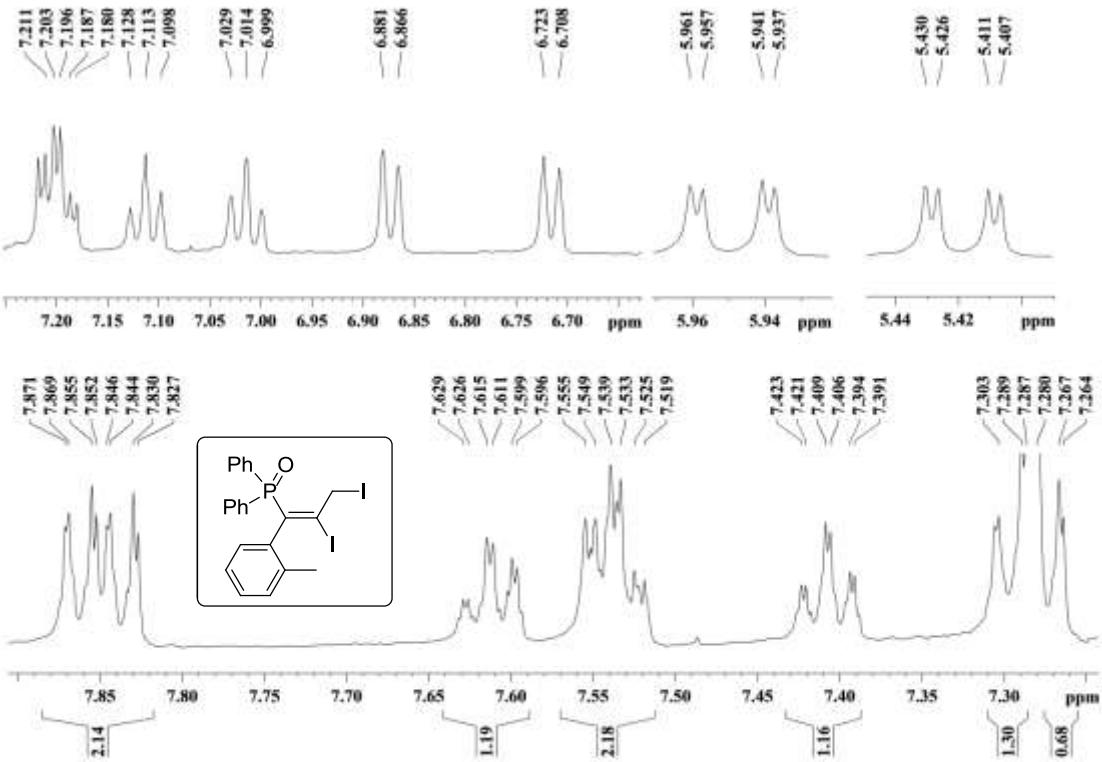

Figure S15. ^{1}H NMR spectrum Expansion of compound **6**

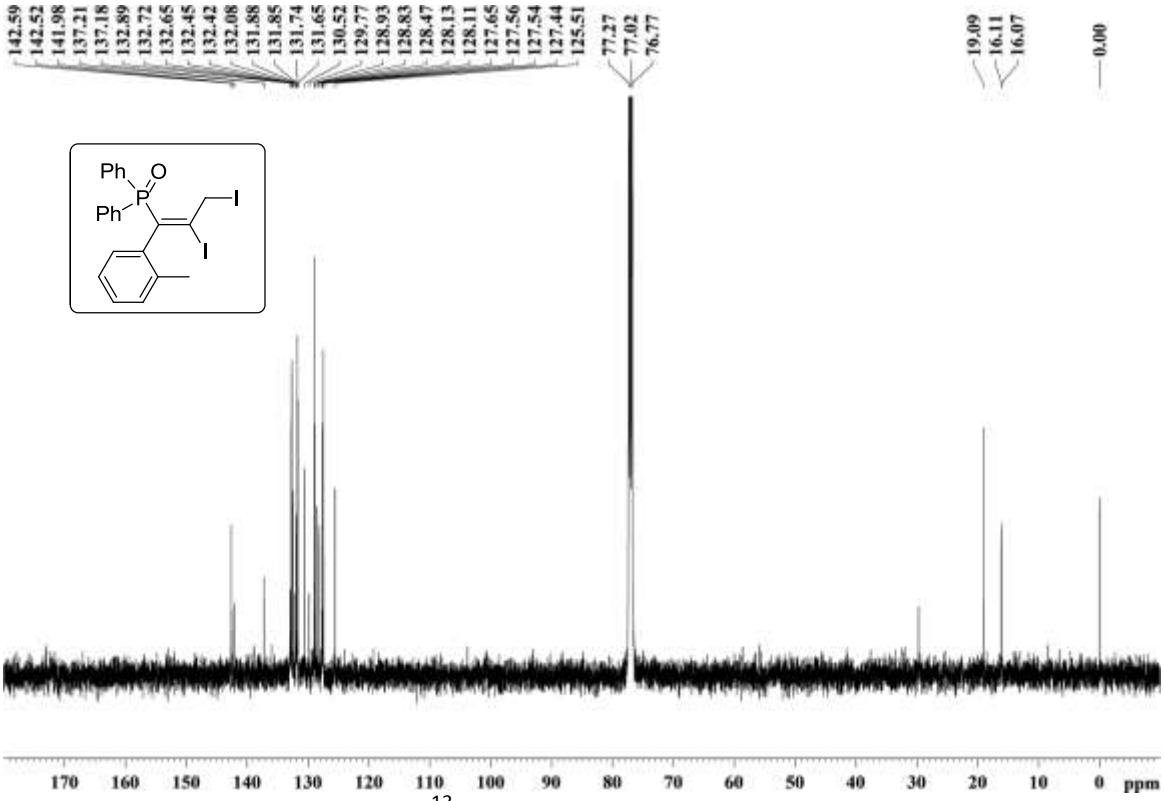

Figure S16. ^{13}C NMR spectrum of compound **6**

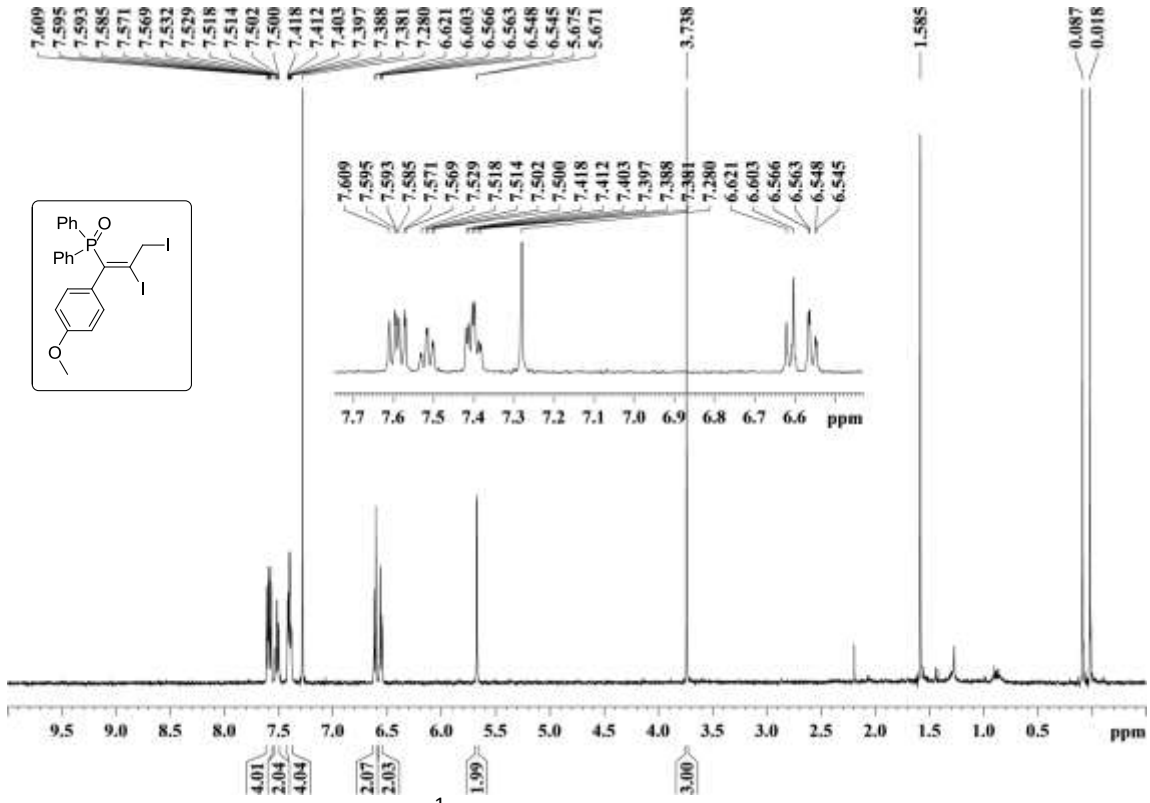

Figure S17. ^{1}H NMR spectrum of compound **7**

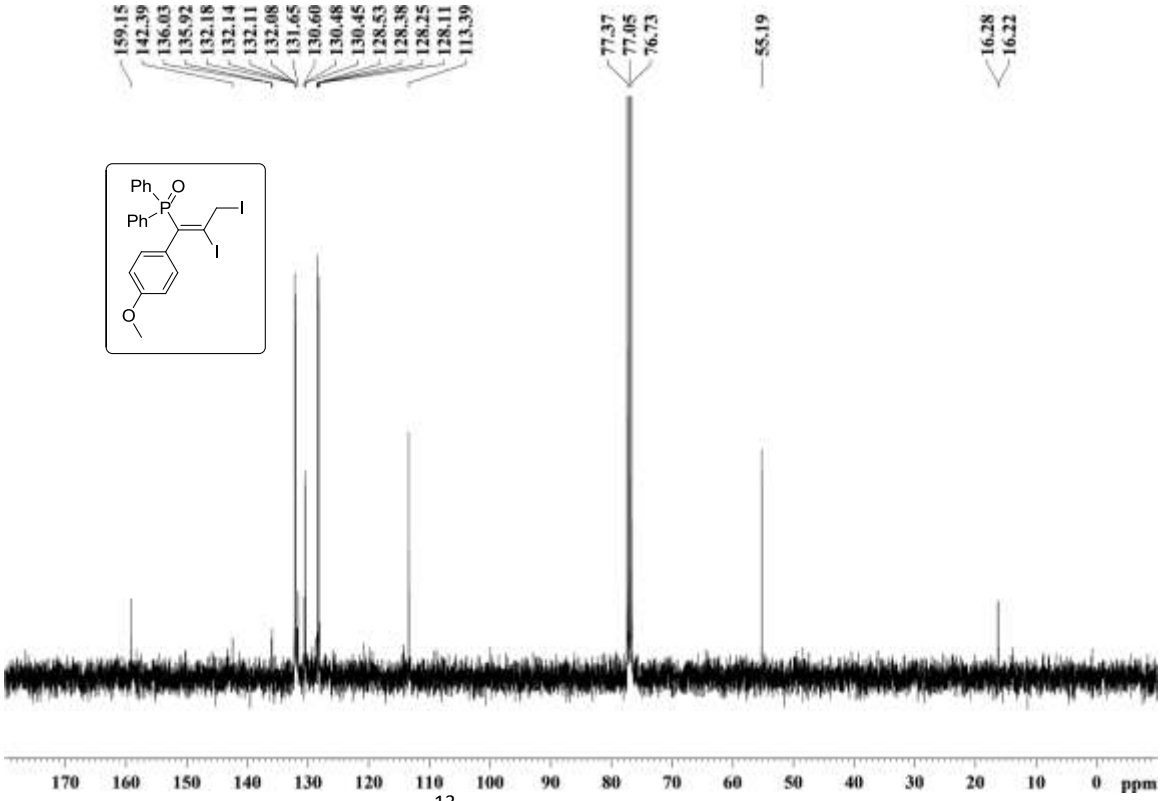

Figure S18. ^{13}C NMR spectrum of compound **7**

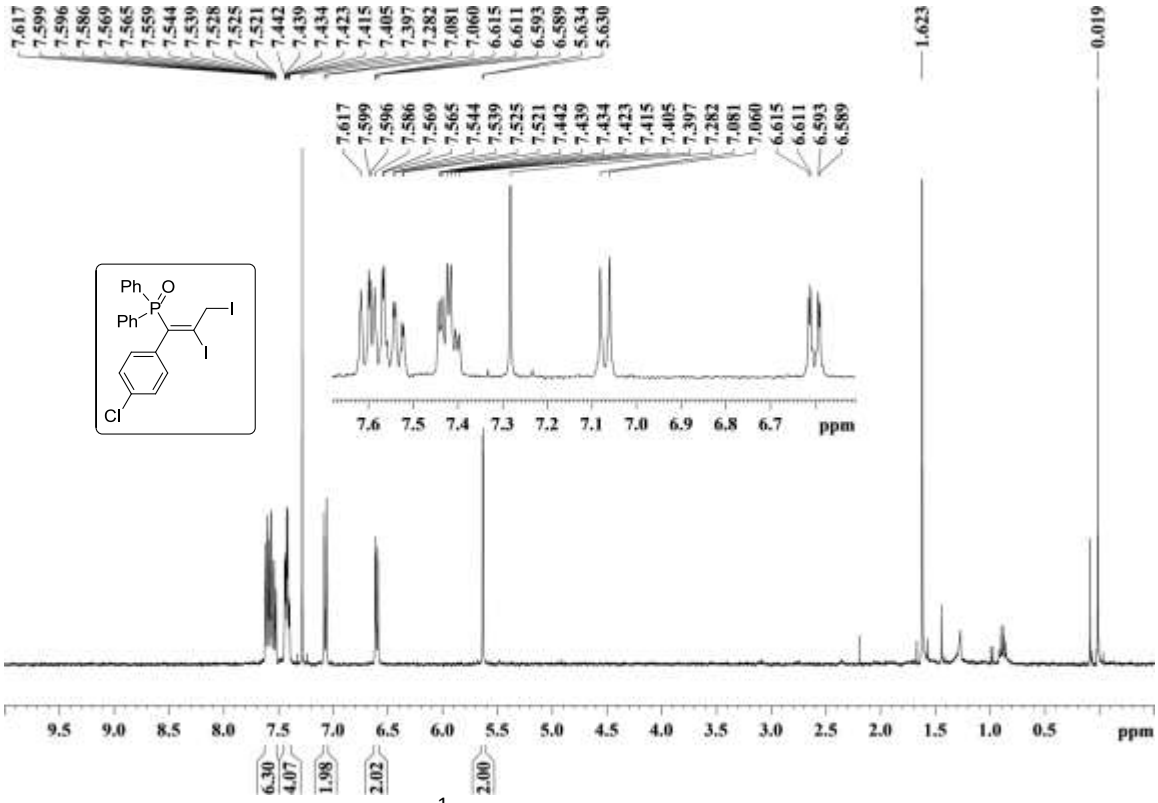

Figure S19. ^{1}H NMR spectrum of compound **8**

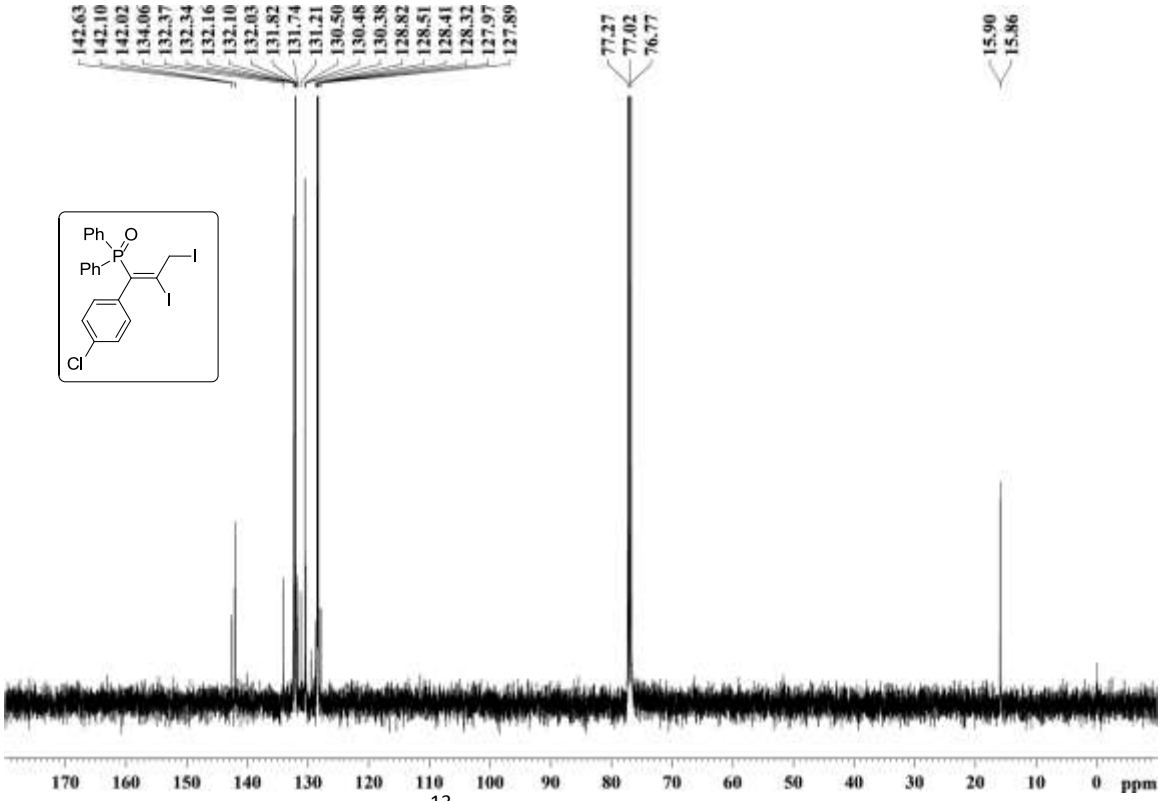

Figure S20. ^{13}C NMR spectrum of compound **8**

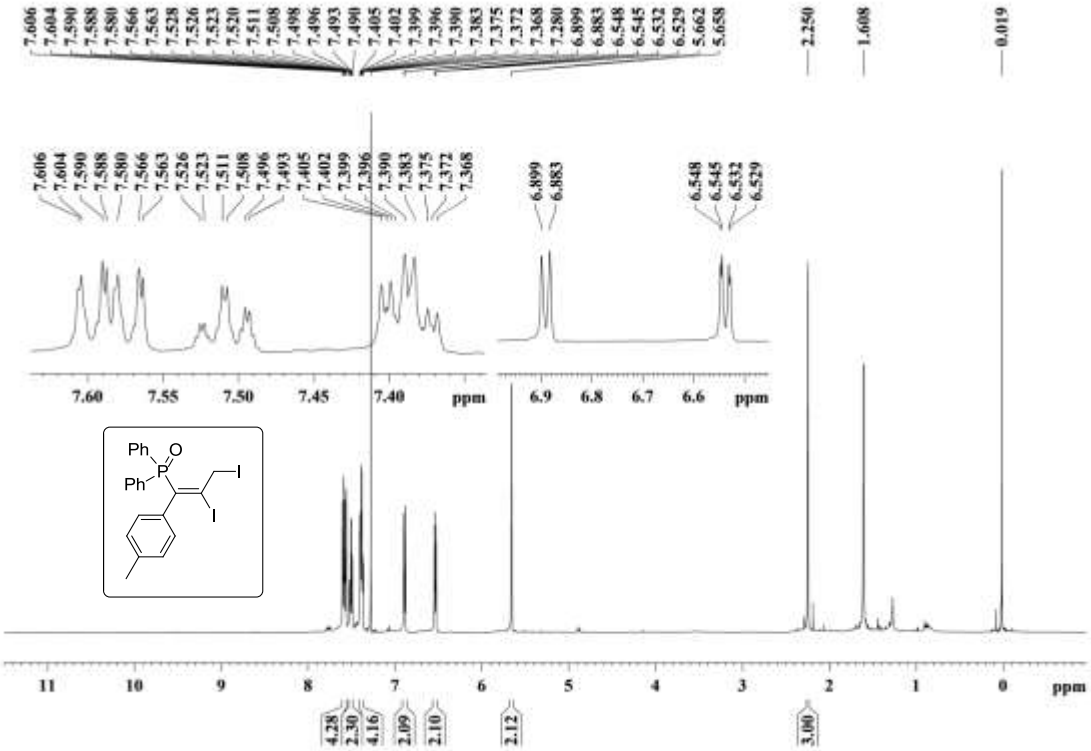

Figure S21. ^{1}H NMR spectrum of compound **9**

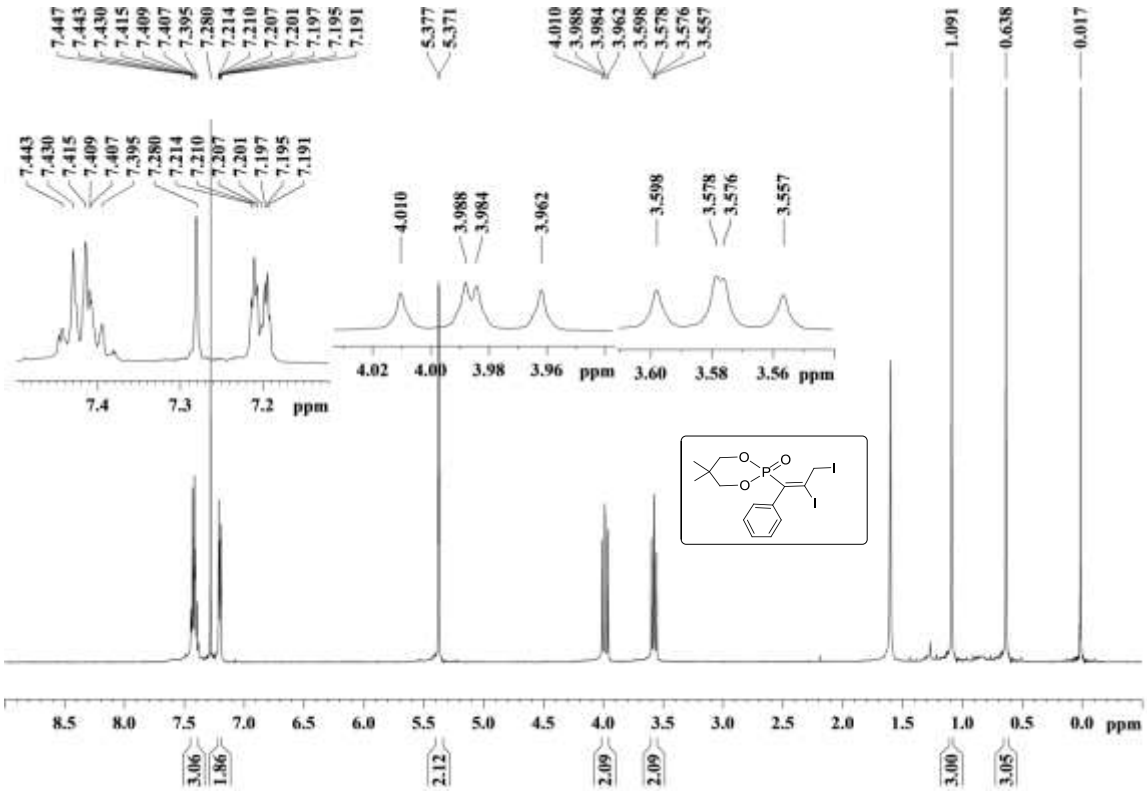

Figure S22. ^{1}H NMR spectrum of compound **10**

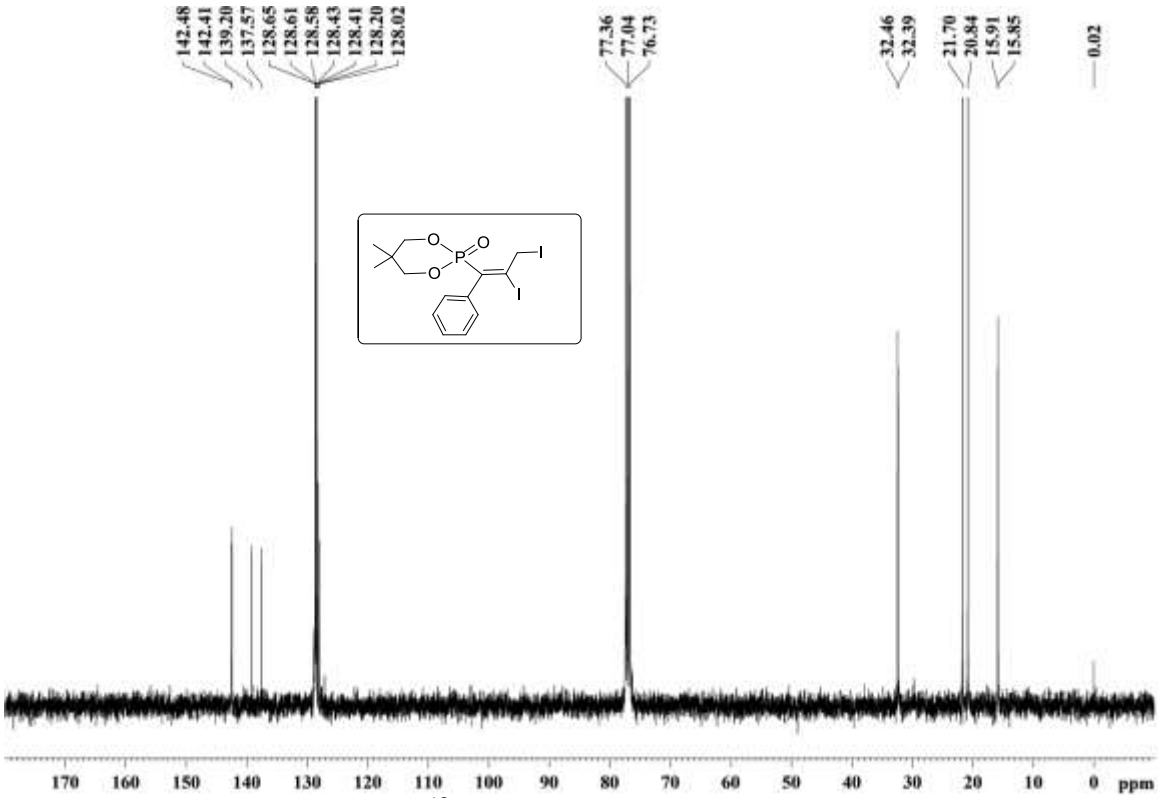

Figure S23. ^{13}C NMR spectrum of compound **10**

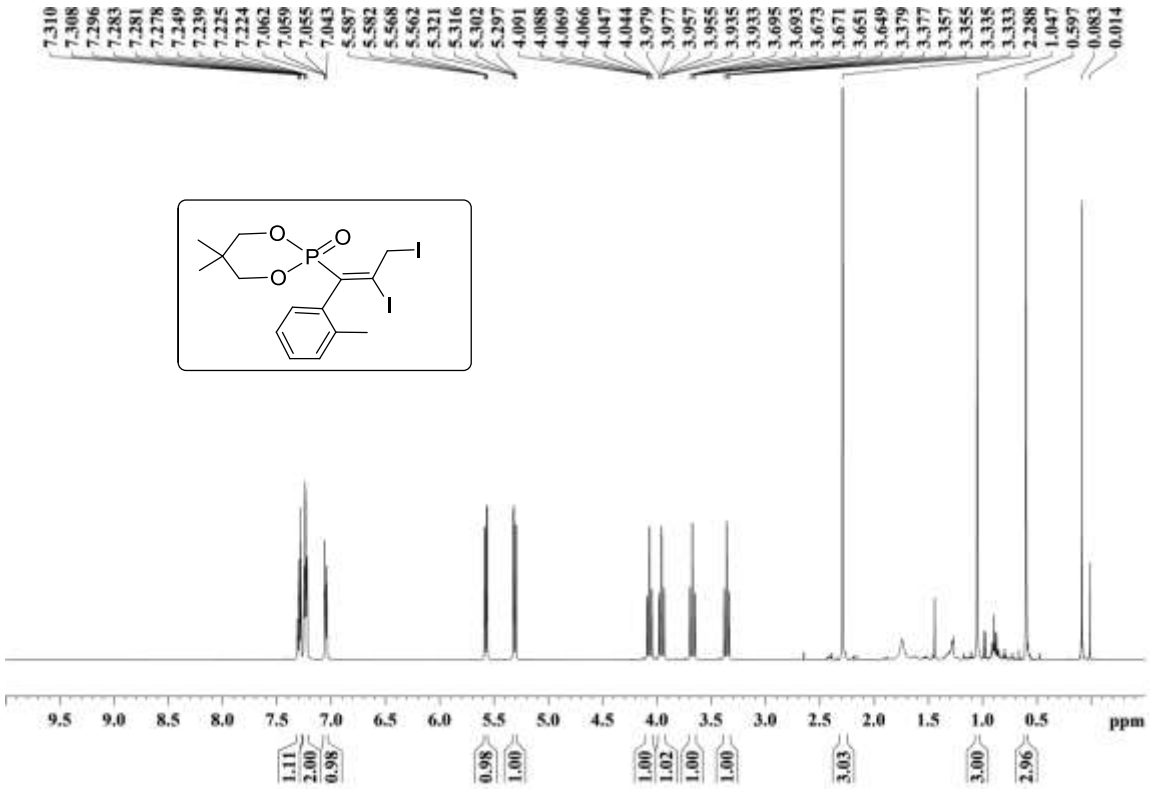

Figure S24. ^{1}H NMR spectrum of compound **11**

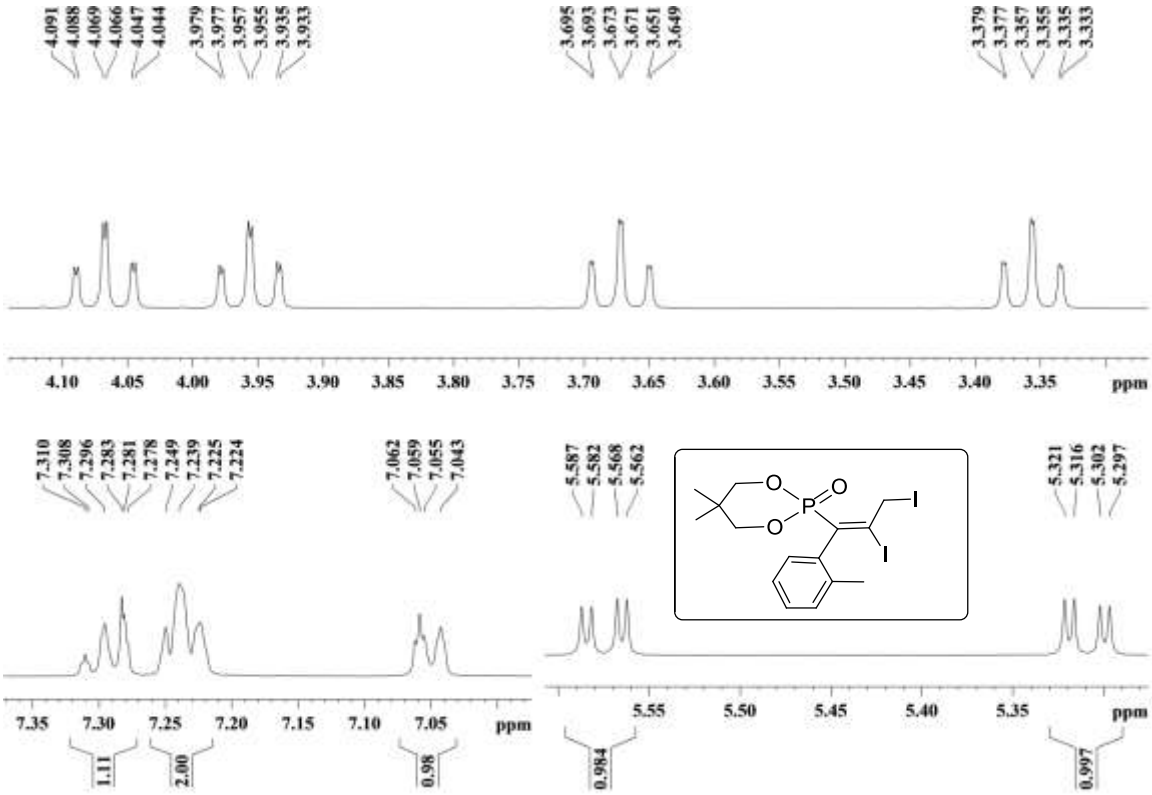

Figure S25. ^{1}H NMR spectrum of compound **11**

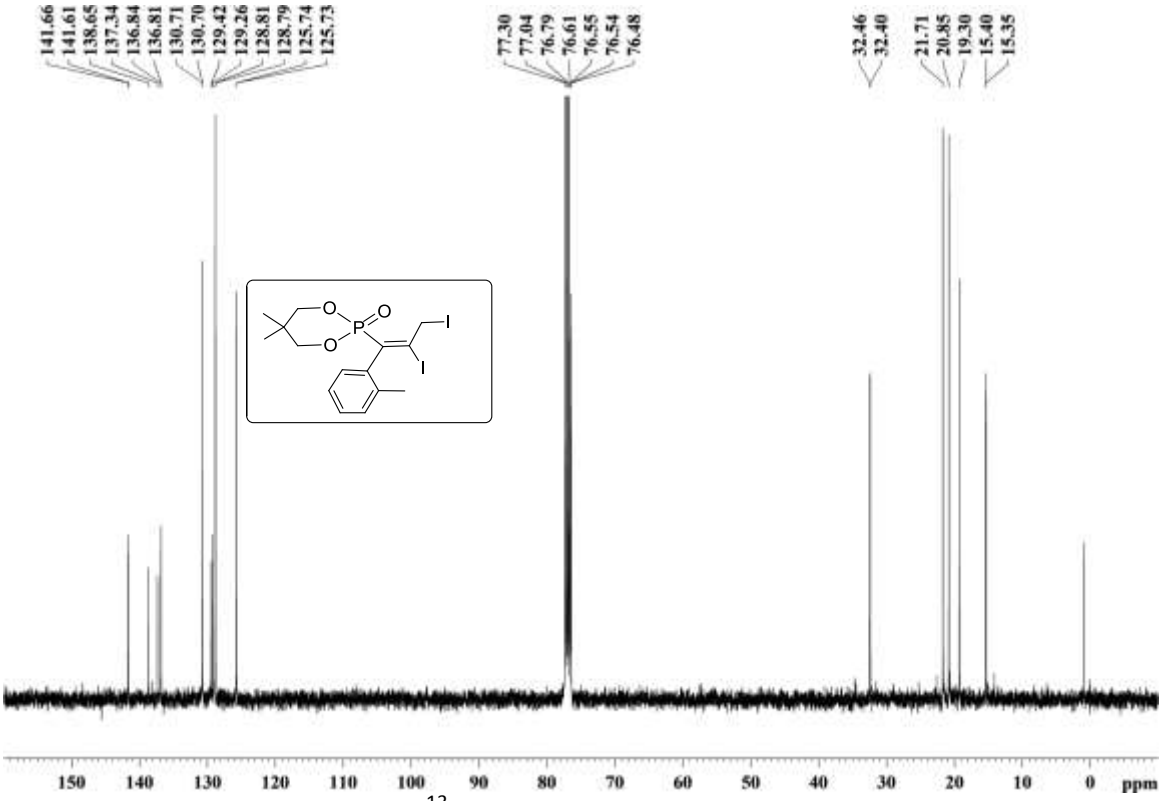

Figure S26. ^{13}C NMR spectrum of compound **11**

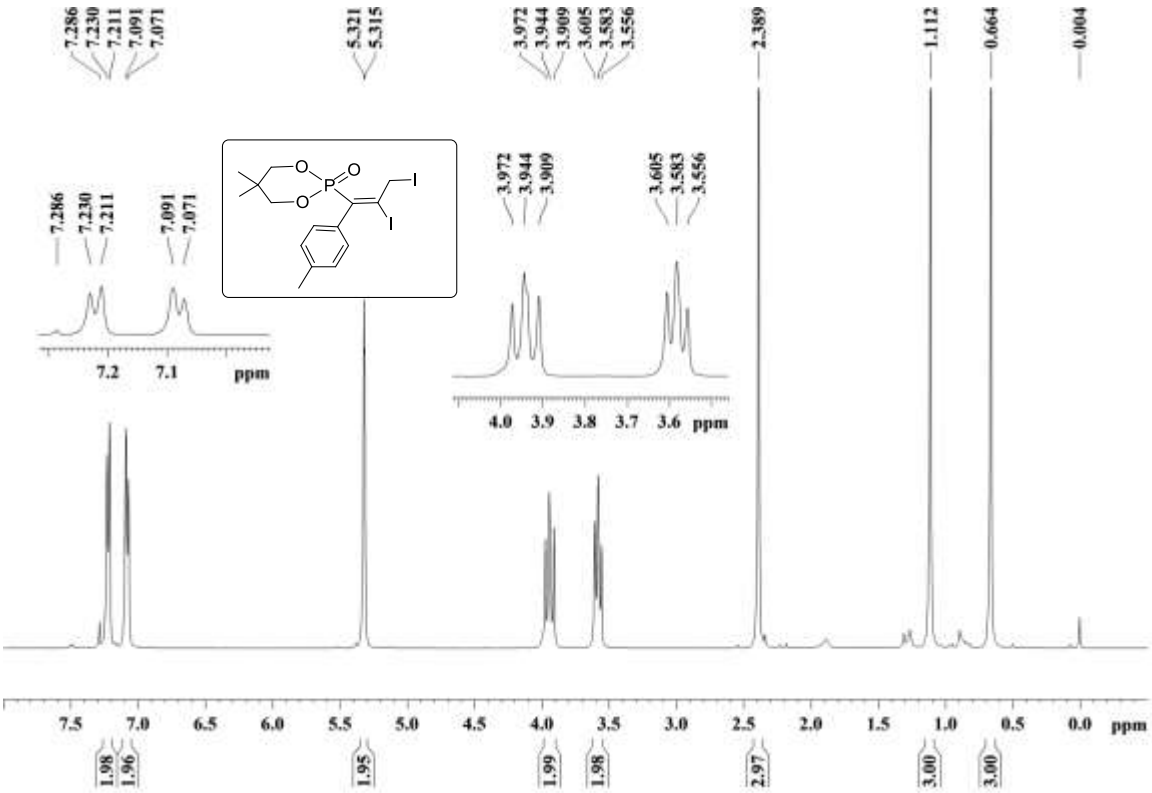

Figure S27. ^{1}H NMR spectrum of compound **12**

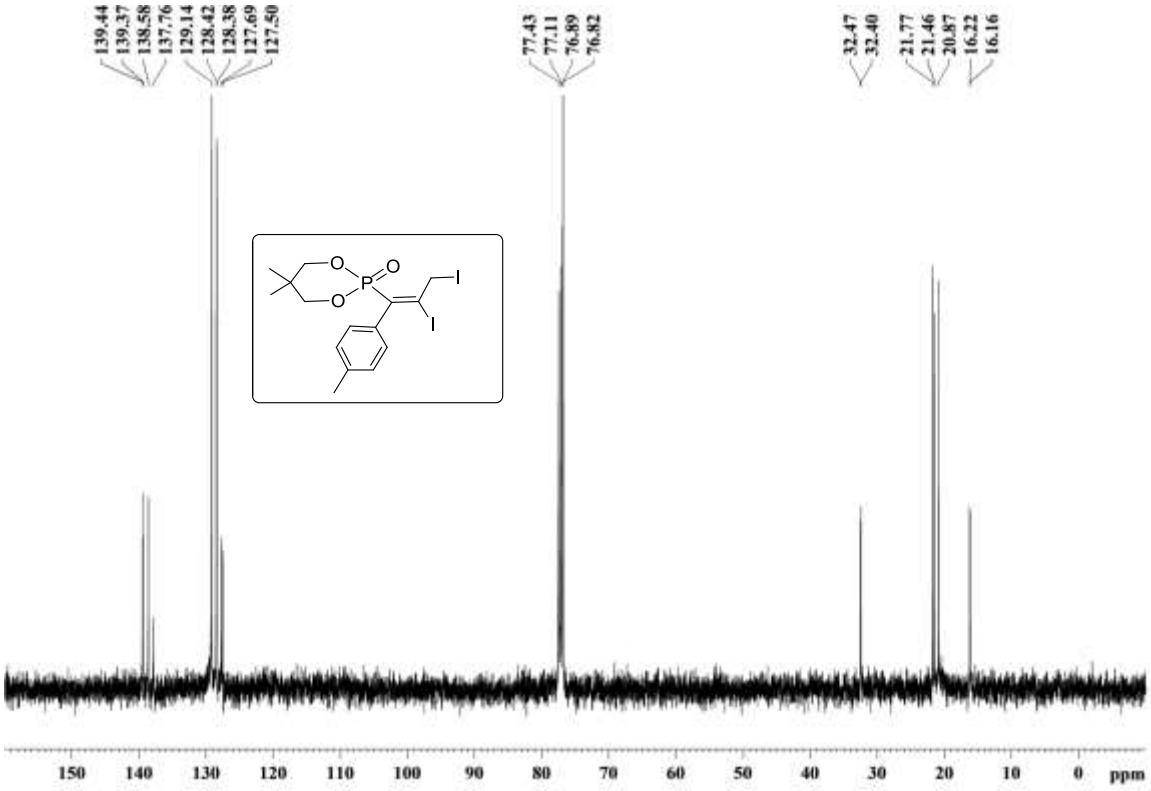

Figure S28. ^{13}C NMR spectrum of compound **12**

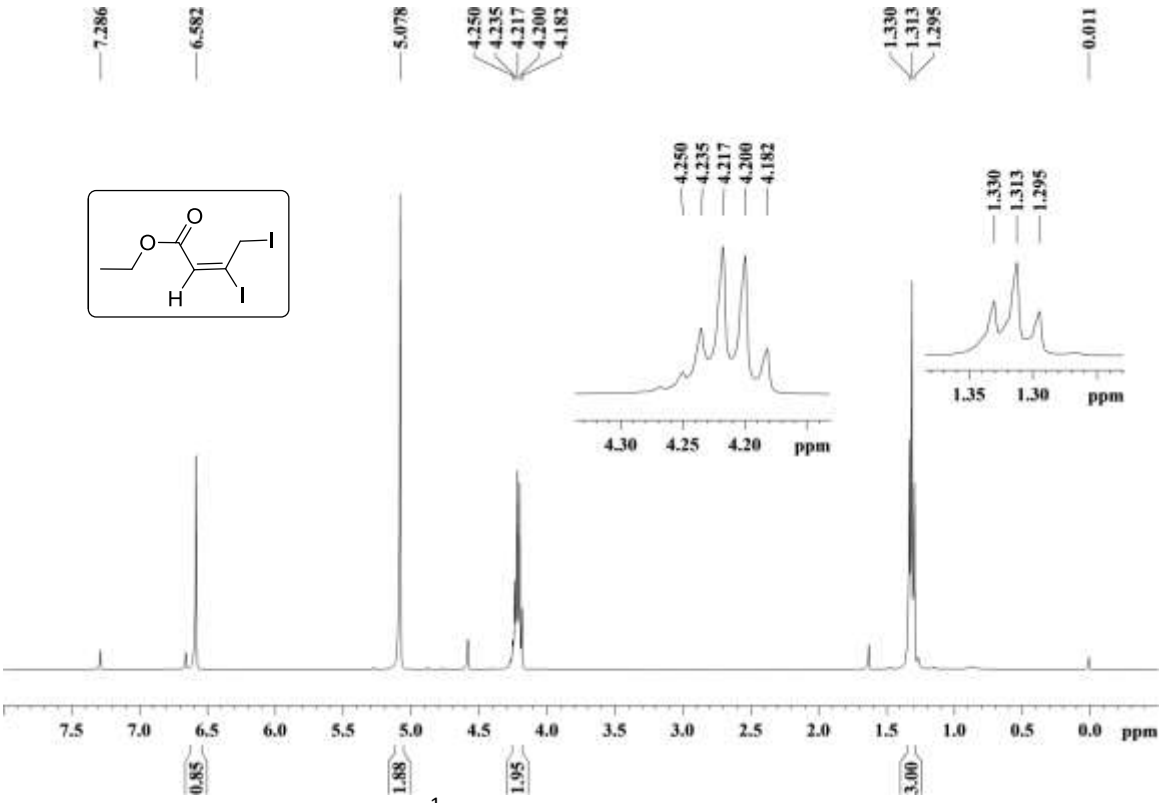

Figure S29. ^{1}H NMR spectrum of compound **13**

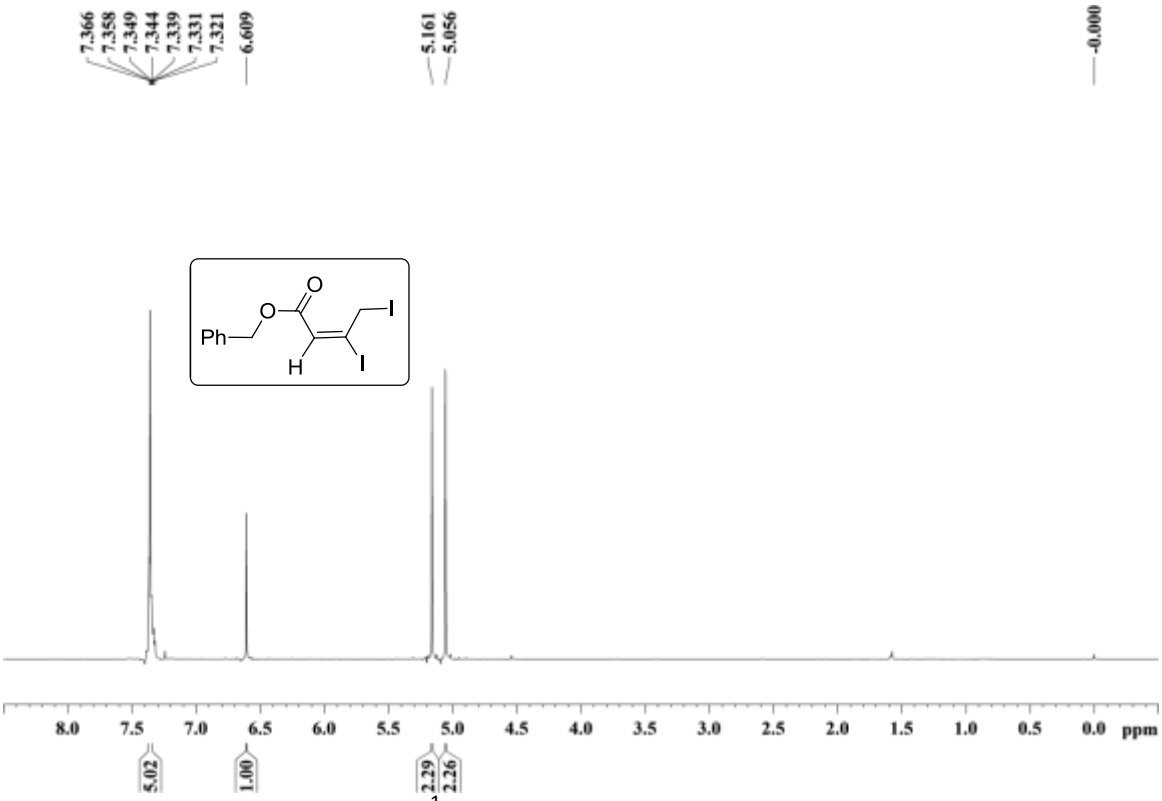

Figure S30. ^{1}H NMR spectrum of compound **14**

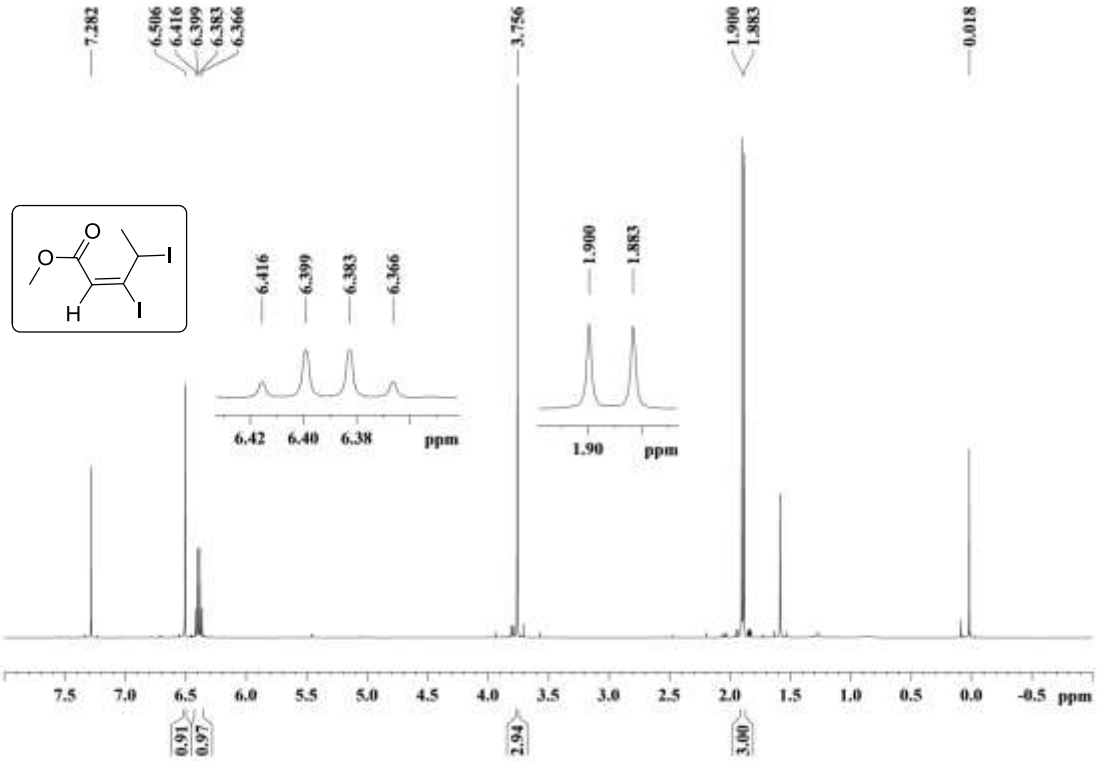

Figure S31. ^{1}H NMR spectrum of compound **15**

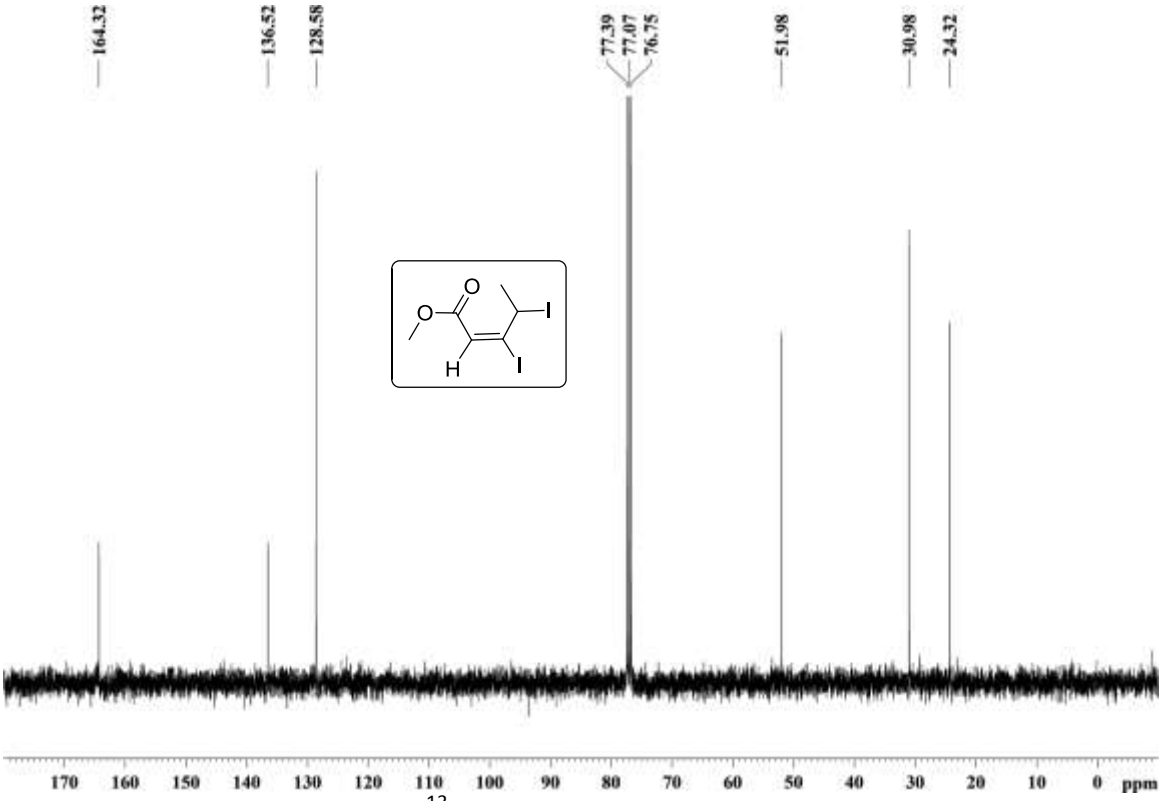

Figure S32. ^{13}C NMR spectrum of compound **15**

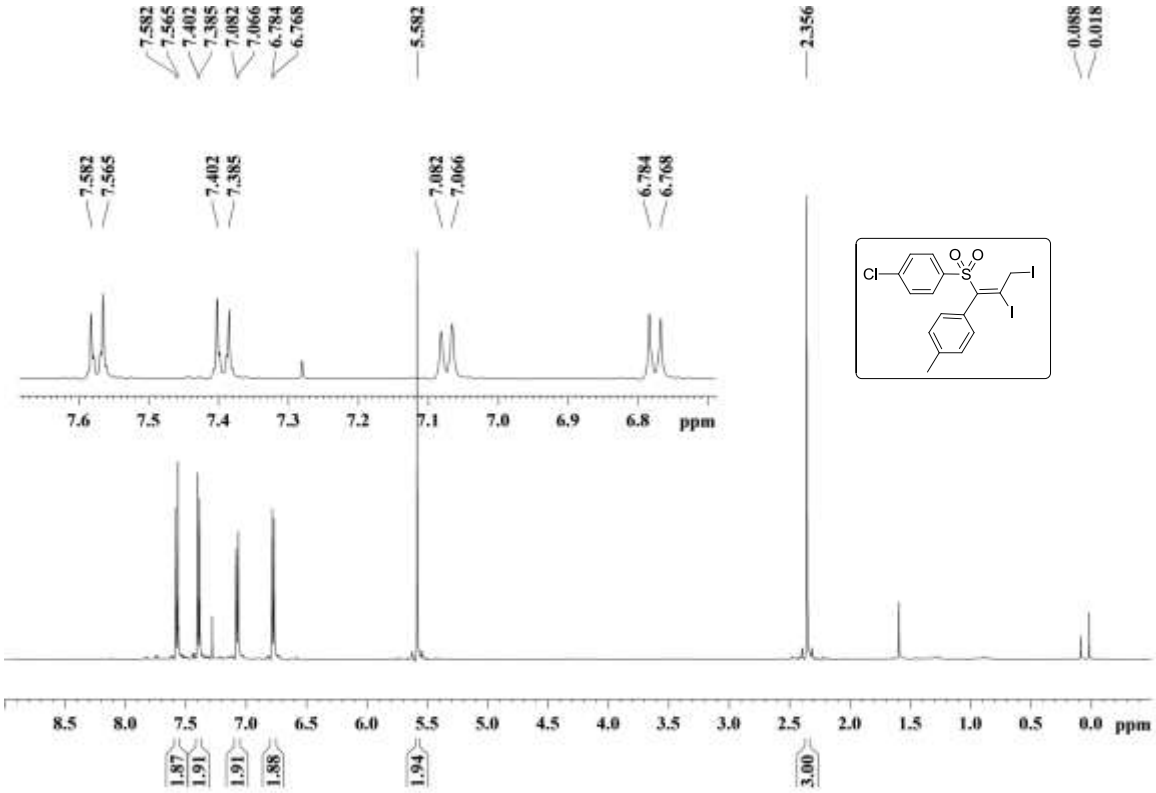

Figure S33. ^{1}H NMR spectrum of compound **16**

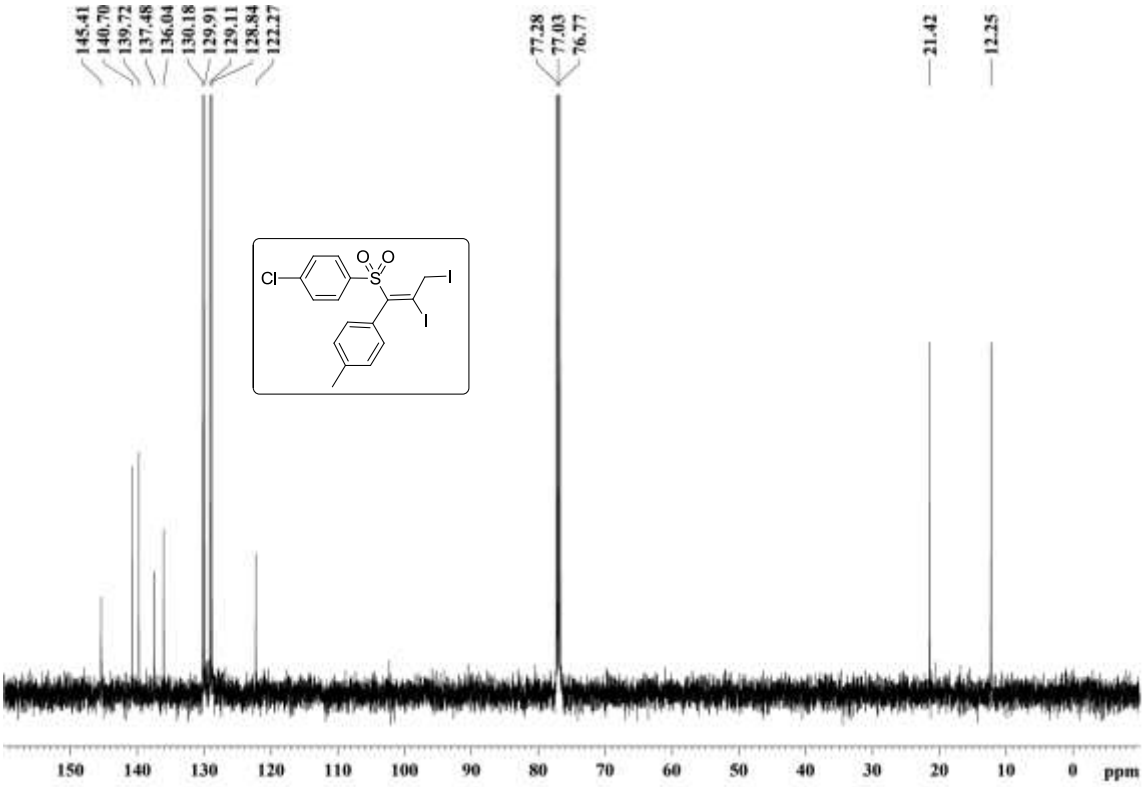

Figure S34. ^{13}C NMR spectrum of compound **16**

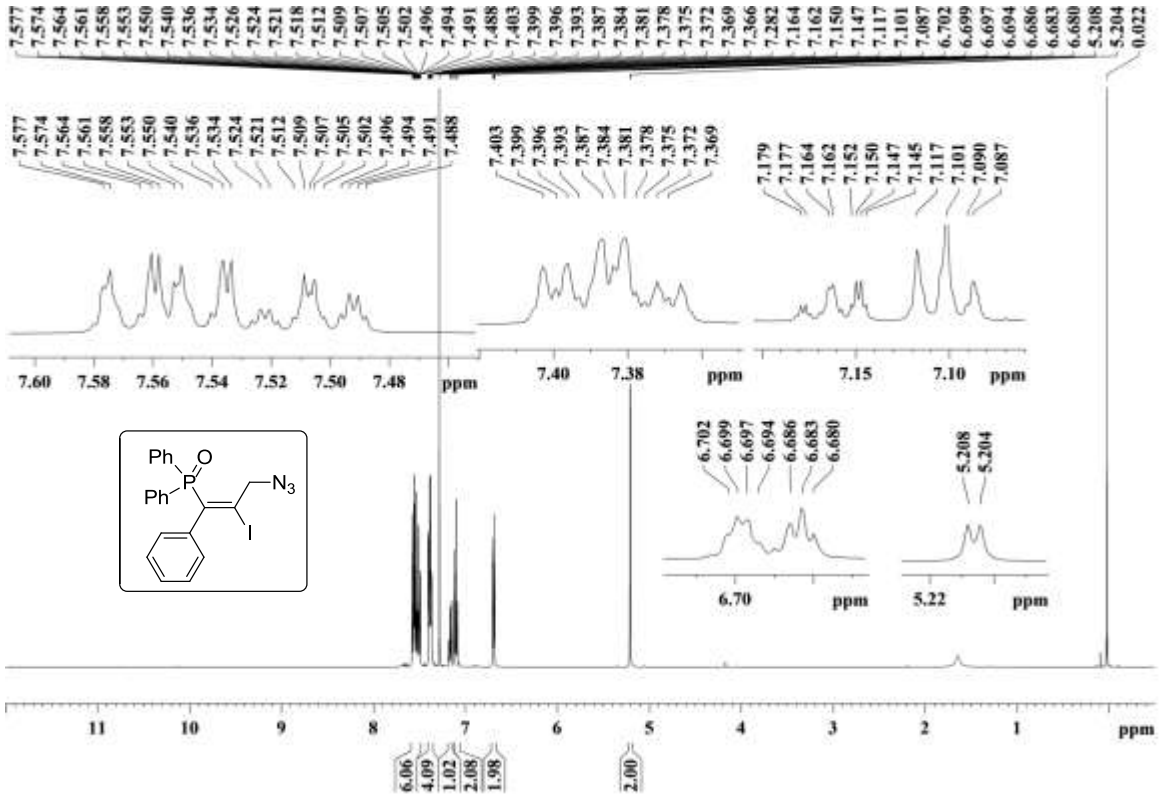

Figure S35. ^{1}H NMR spectrum of compound **17**

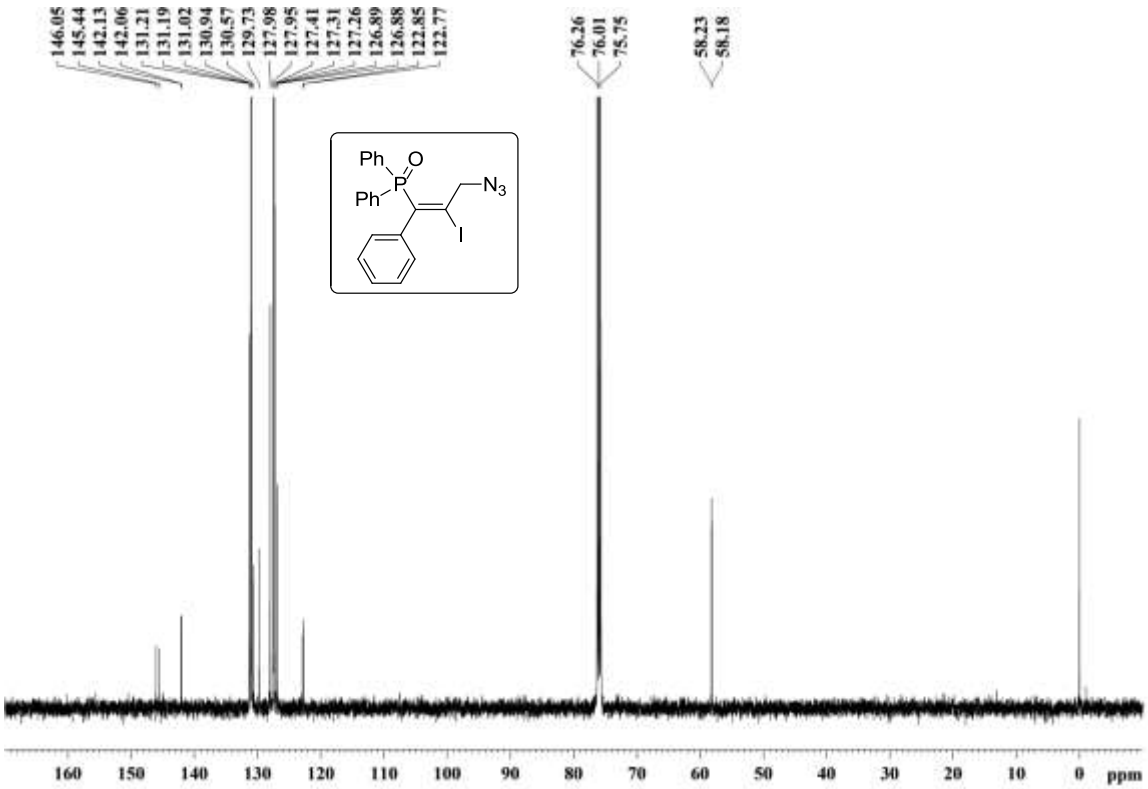

Figure S36. ^{13}C NMR spectrum of compound **17**

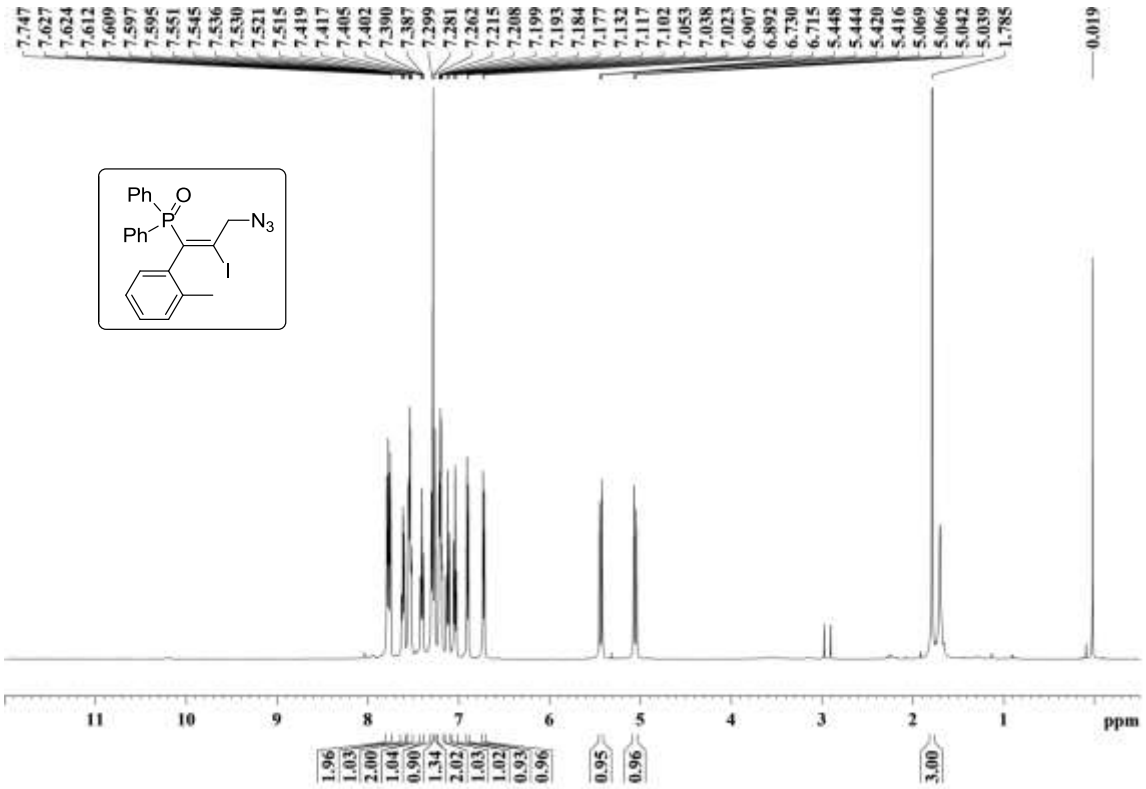

Figure S37. ^{1}H NMR spectrum of compound **18**

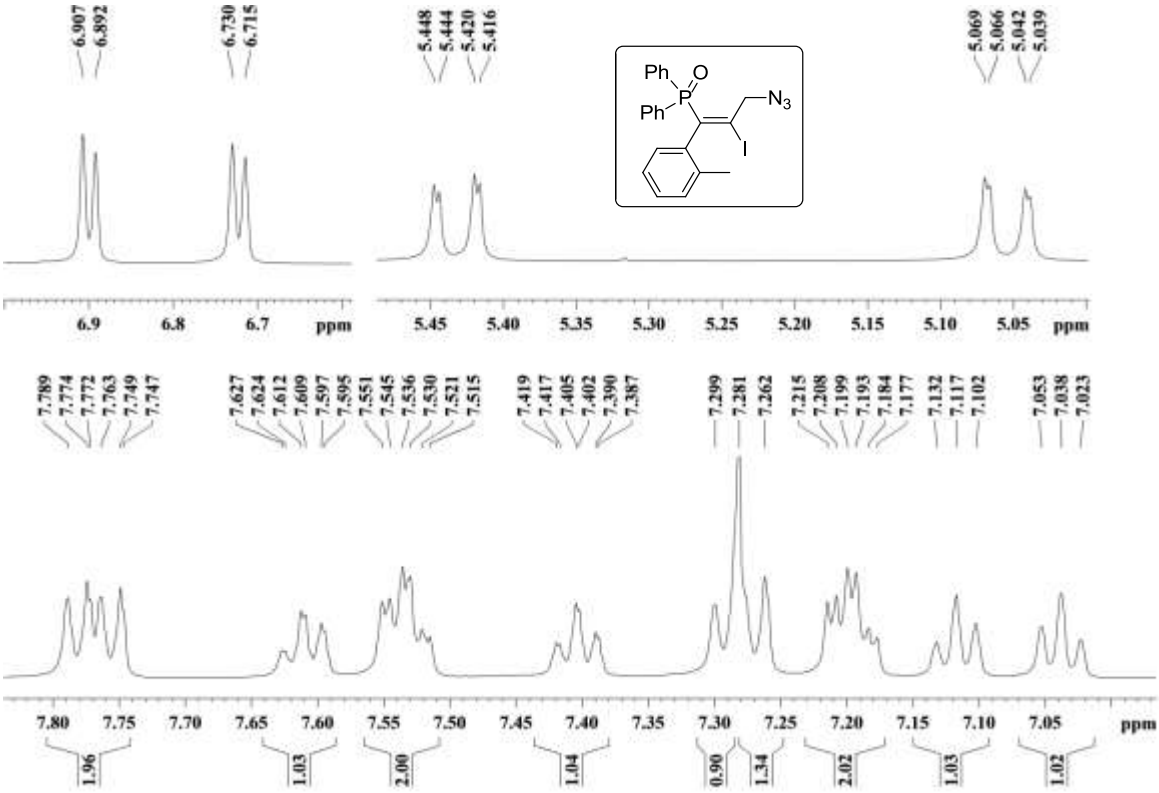

Figure S38. ^{1}H NMR spectrum Expansion of compound **18**

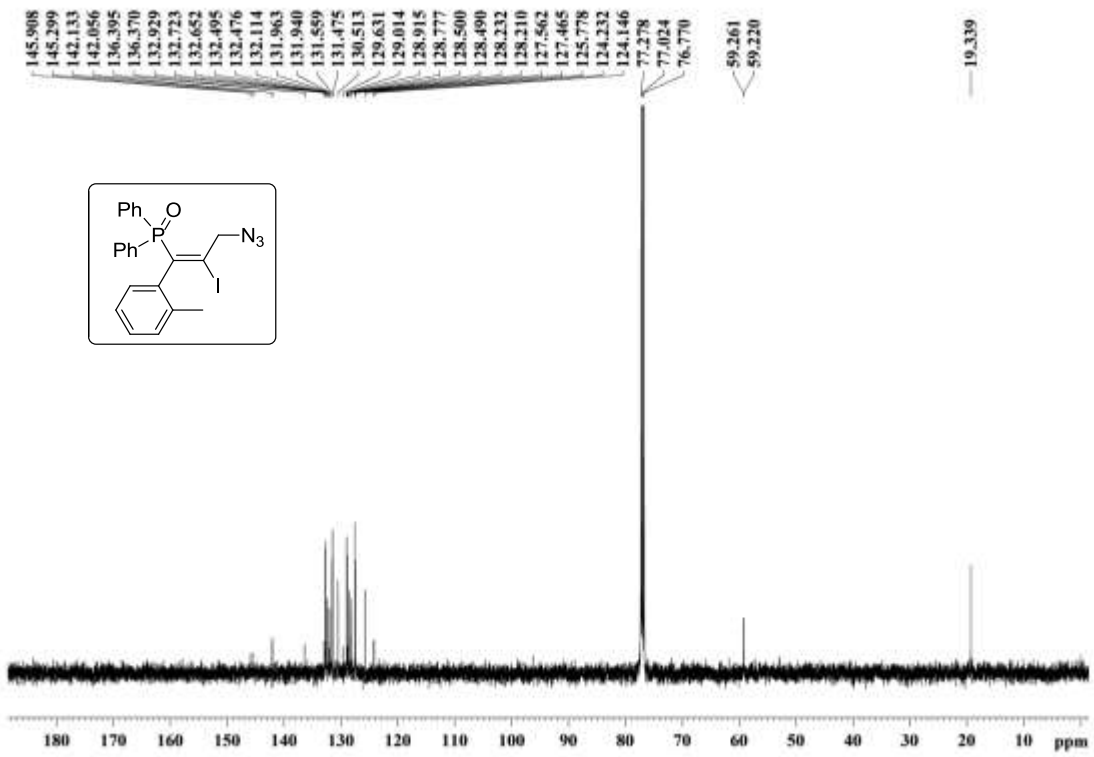

Figure S39. ^{13}C NMR spectrum of compound **18**

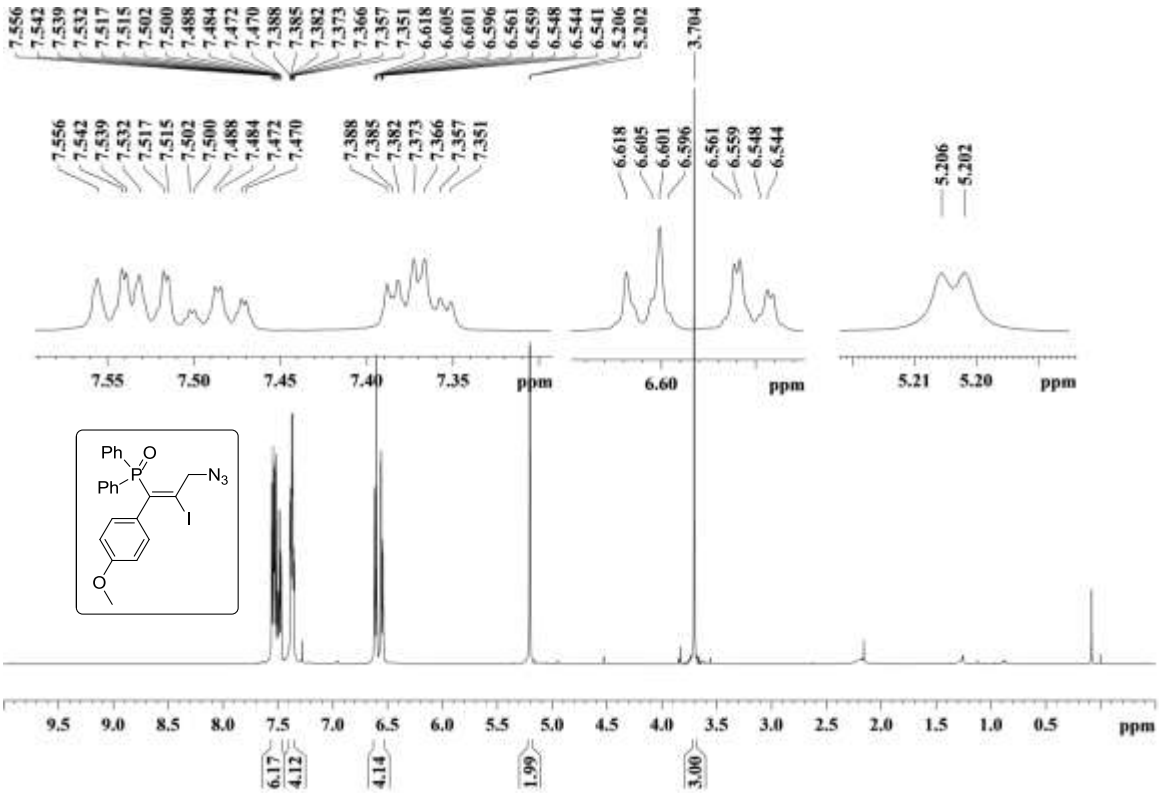

Figure S40. ^{1}H NMR spectrum of compound **19**

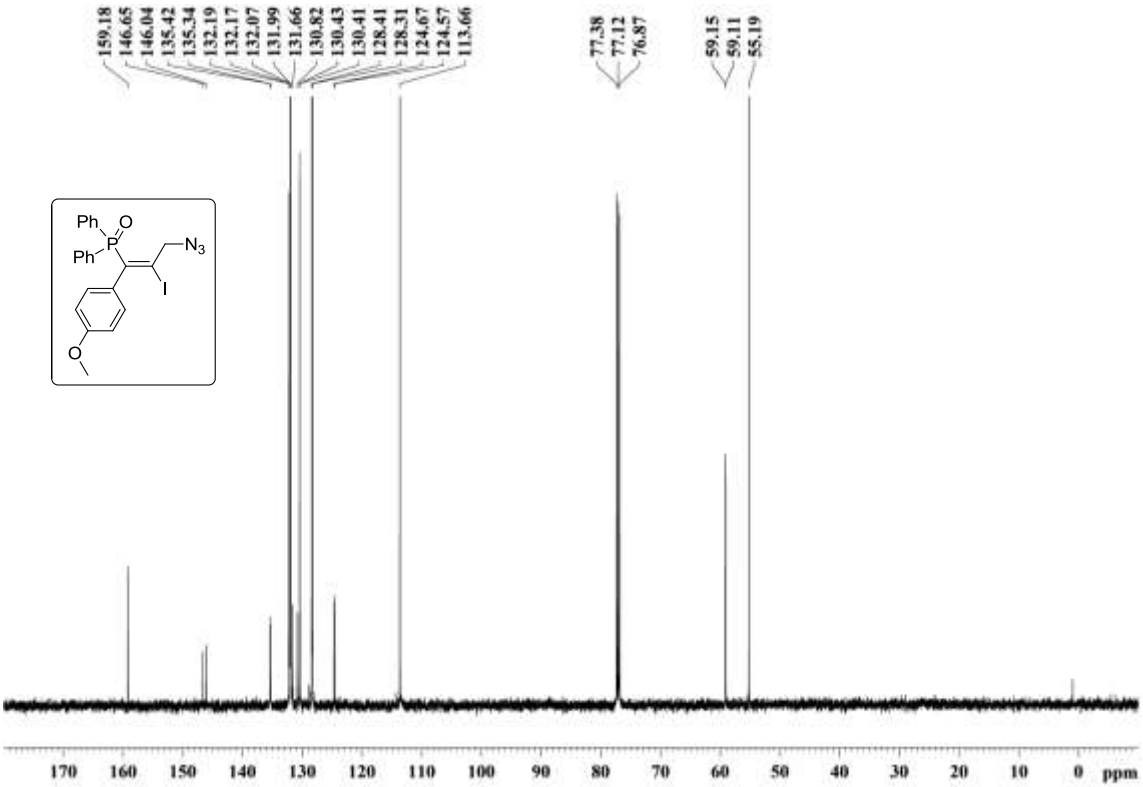

Figure S41. ^{13}C NMR spectrum of compound **19**

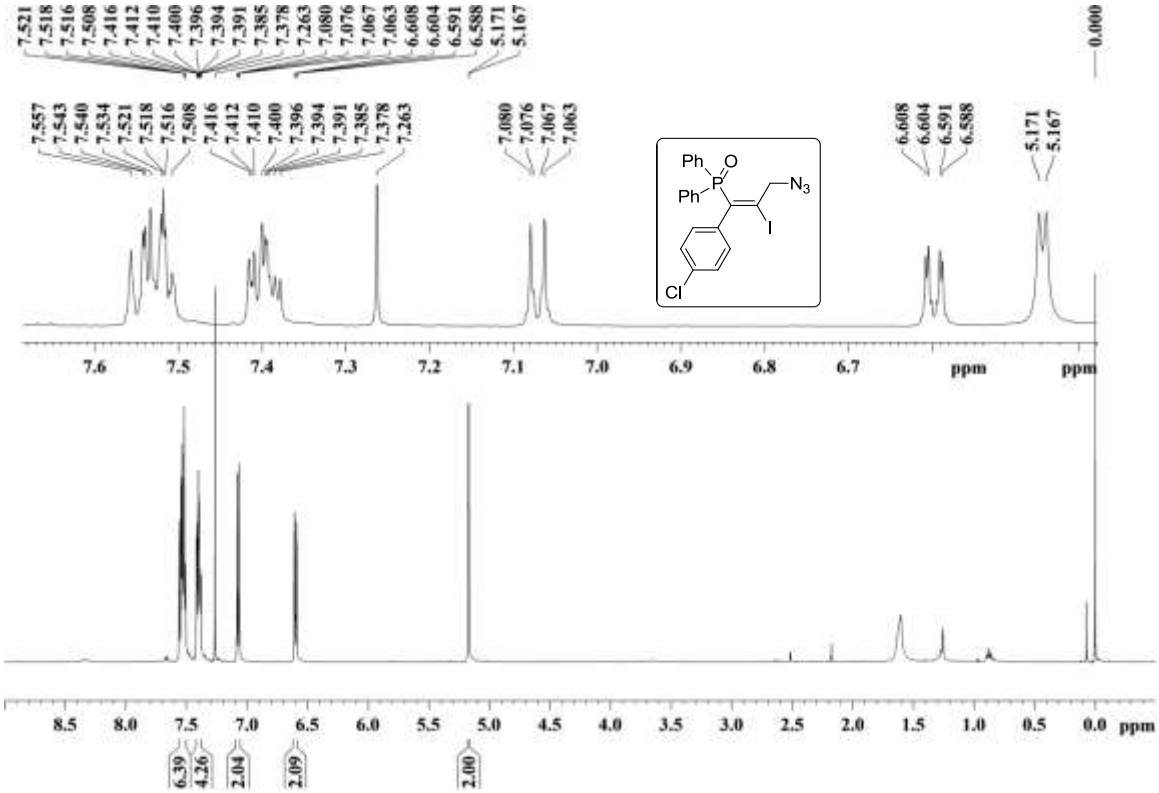

Figure S42. ^{1}H NMR spectrum of compound **20**

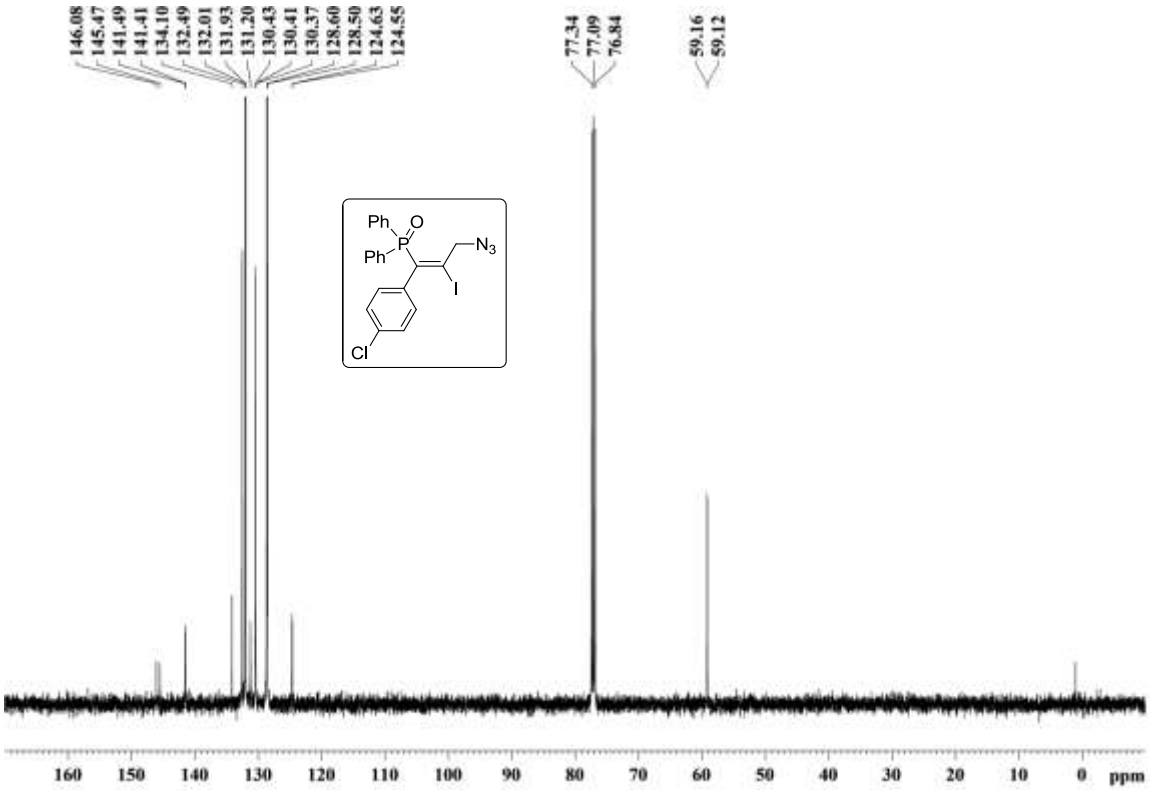

Figure S43. ^{13}C NMR spectrum of compound **20**

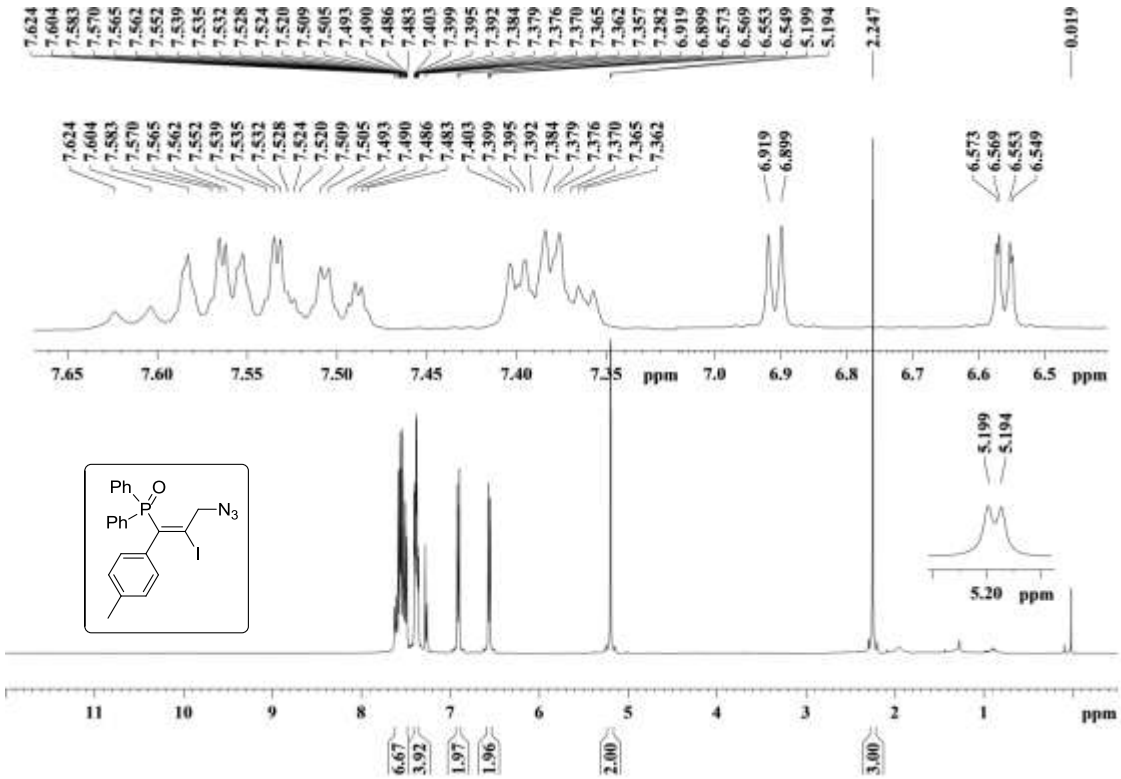

Figure S44. ^{1}H NMR spectrum of compound **21**

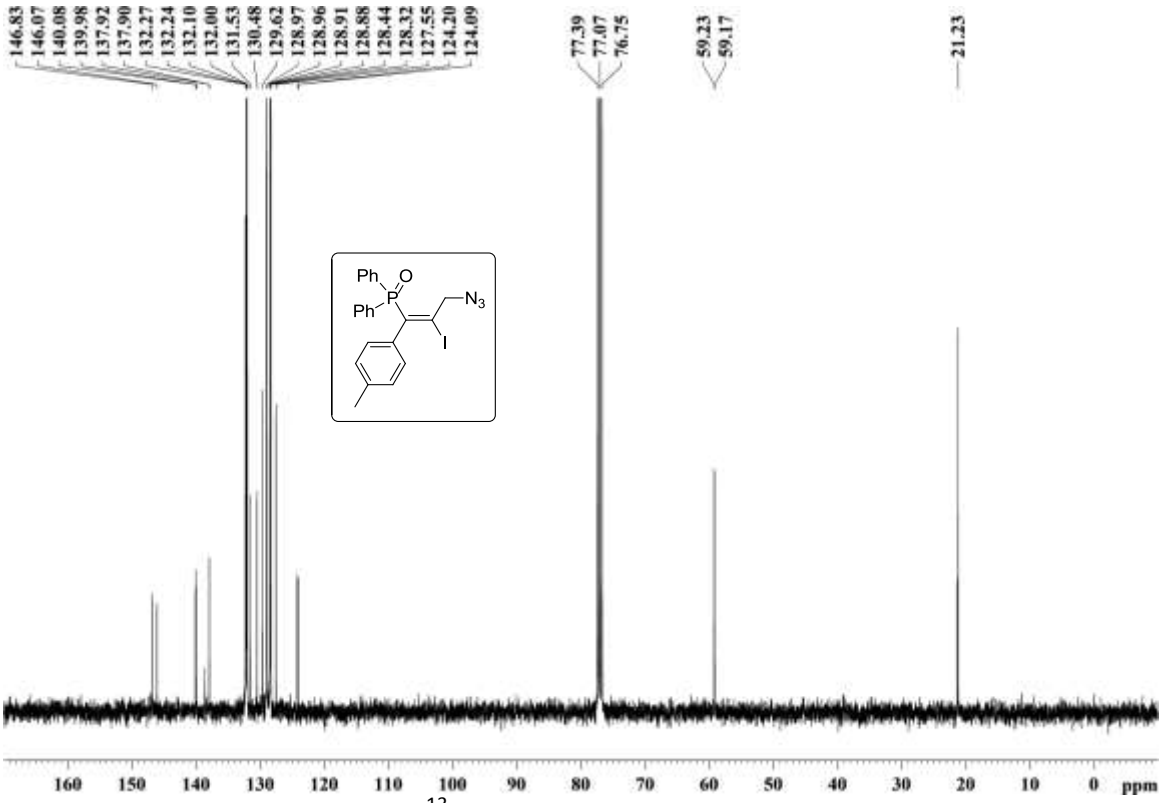

Figure S45. ^{13}C NMR spectrum of compound **21**

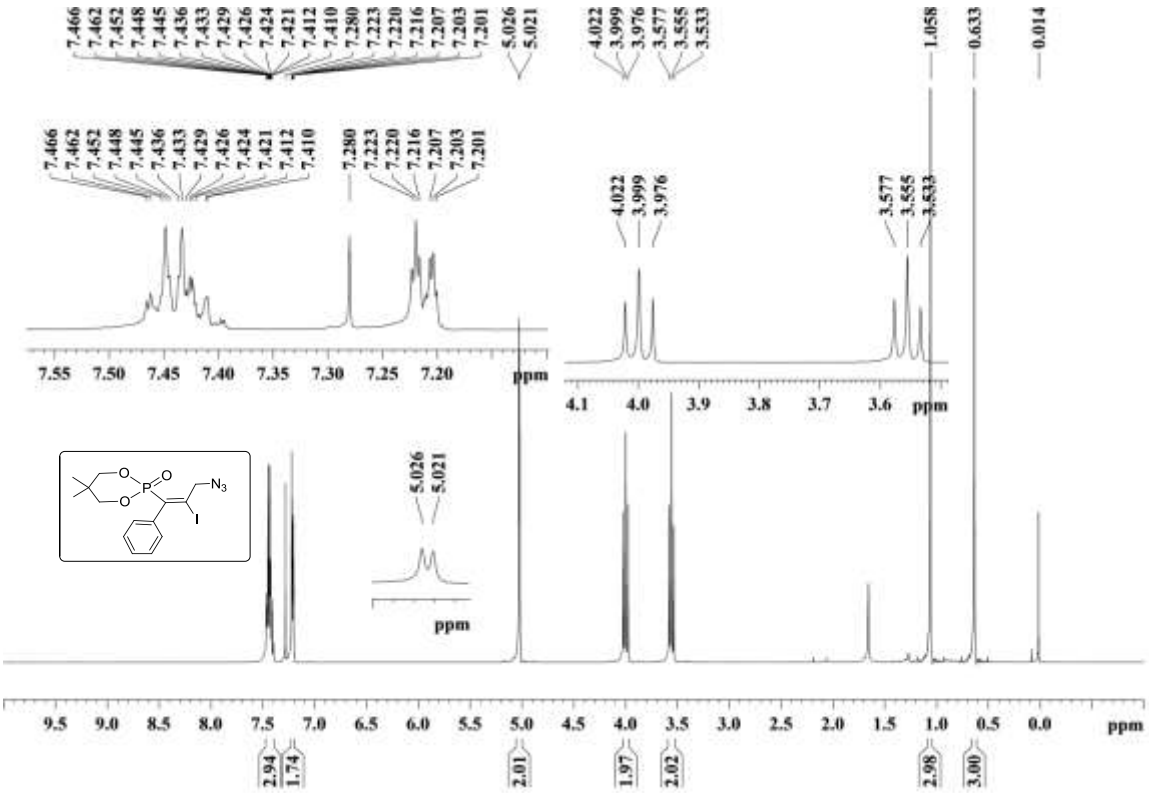

Figure S46. ^{1}H NMR spectrum of compound **22**

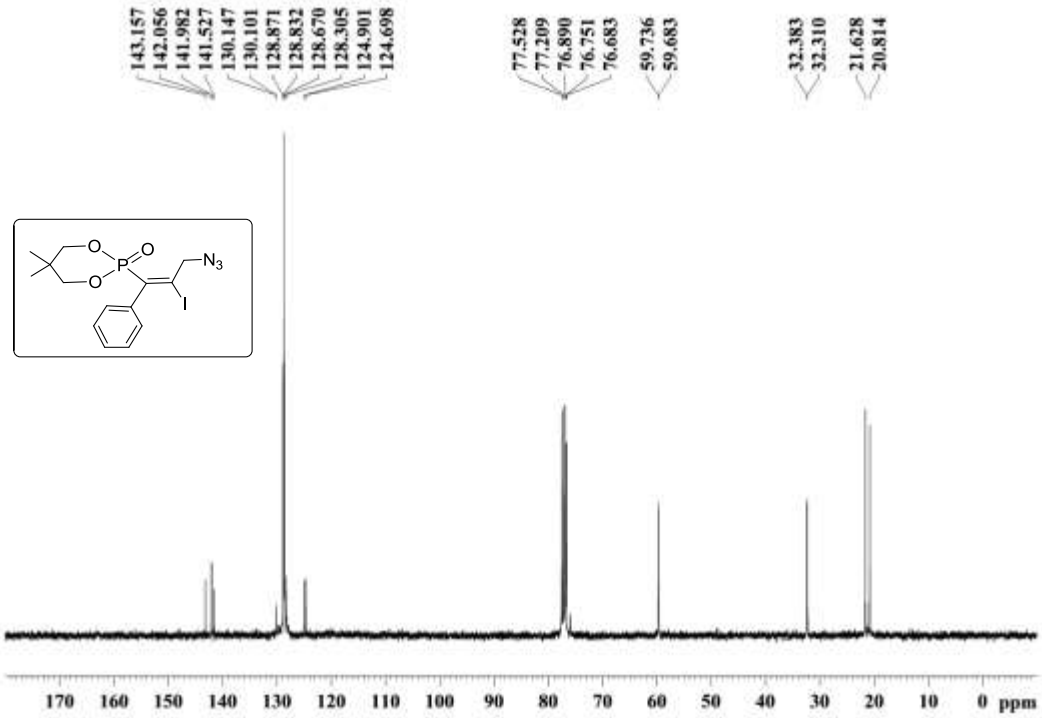

Figure S47. ^{13}C NMR spectrum of compound **22**

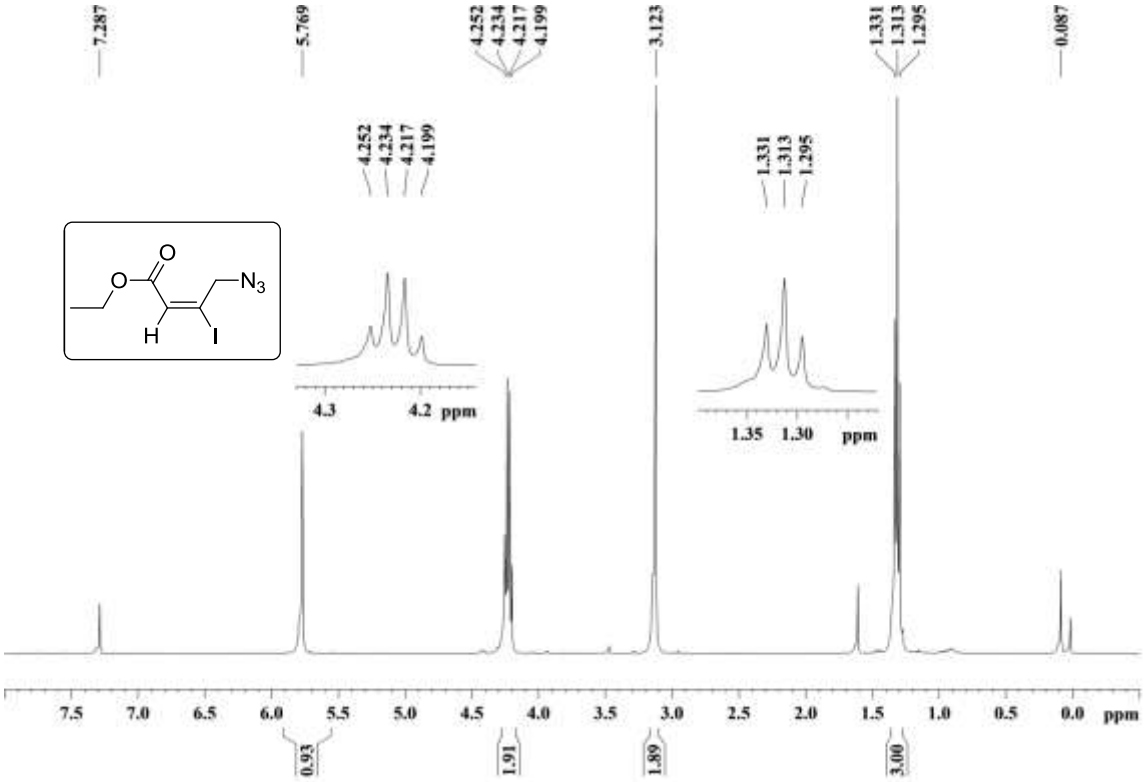

Figure S48. ^{1}H NMR spectrum of compound **23**

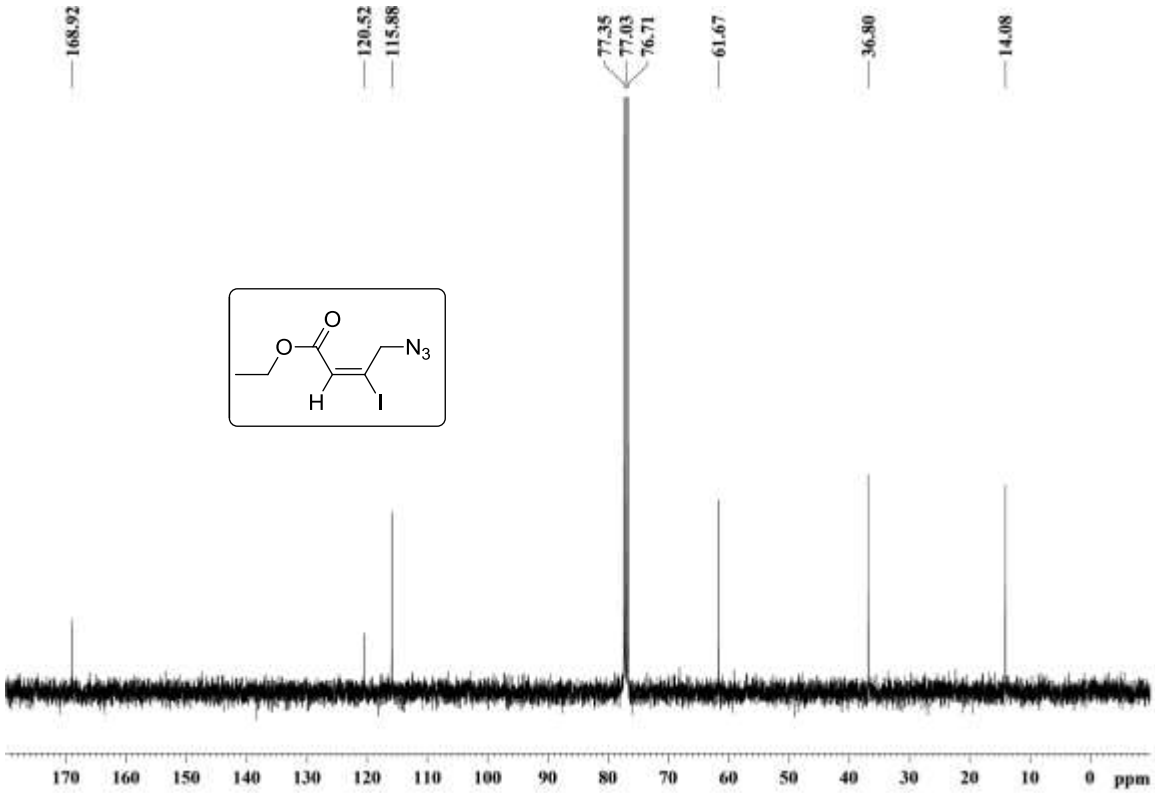

Figure S49. ^{13}C NMR spectrum of compound **23**

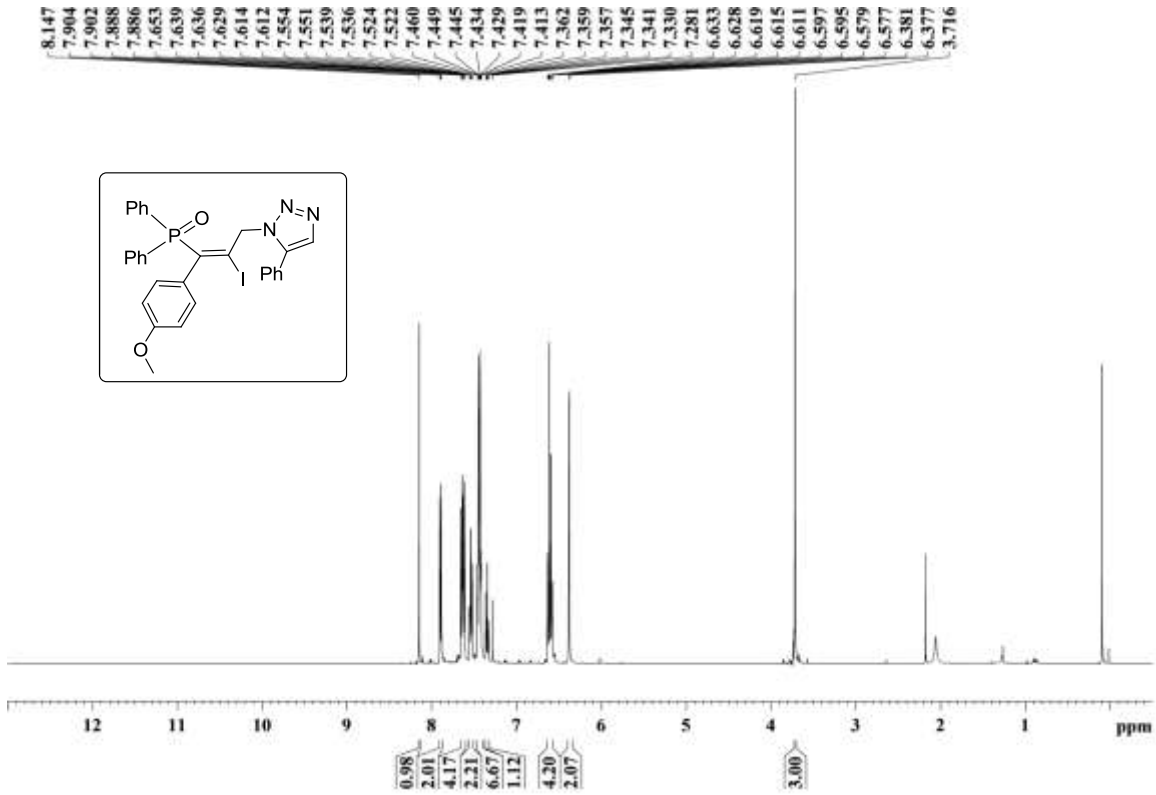

Figure S50. ^{1}H NMR spectrum of compound **24**

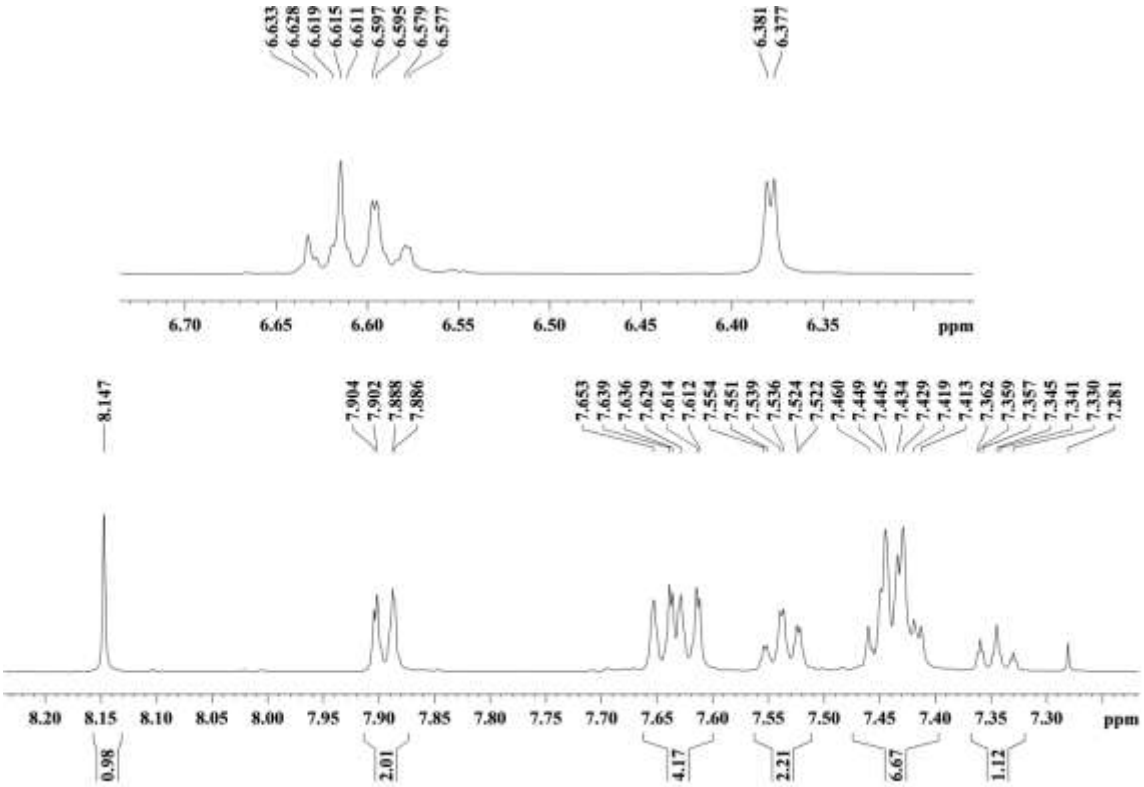

Figure S51. ^{1}H NMR spectrum expansion of compound **24**

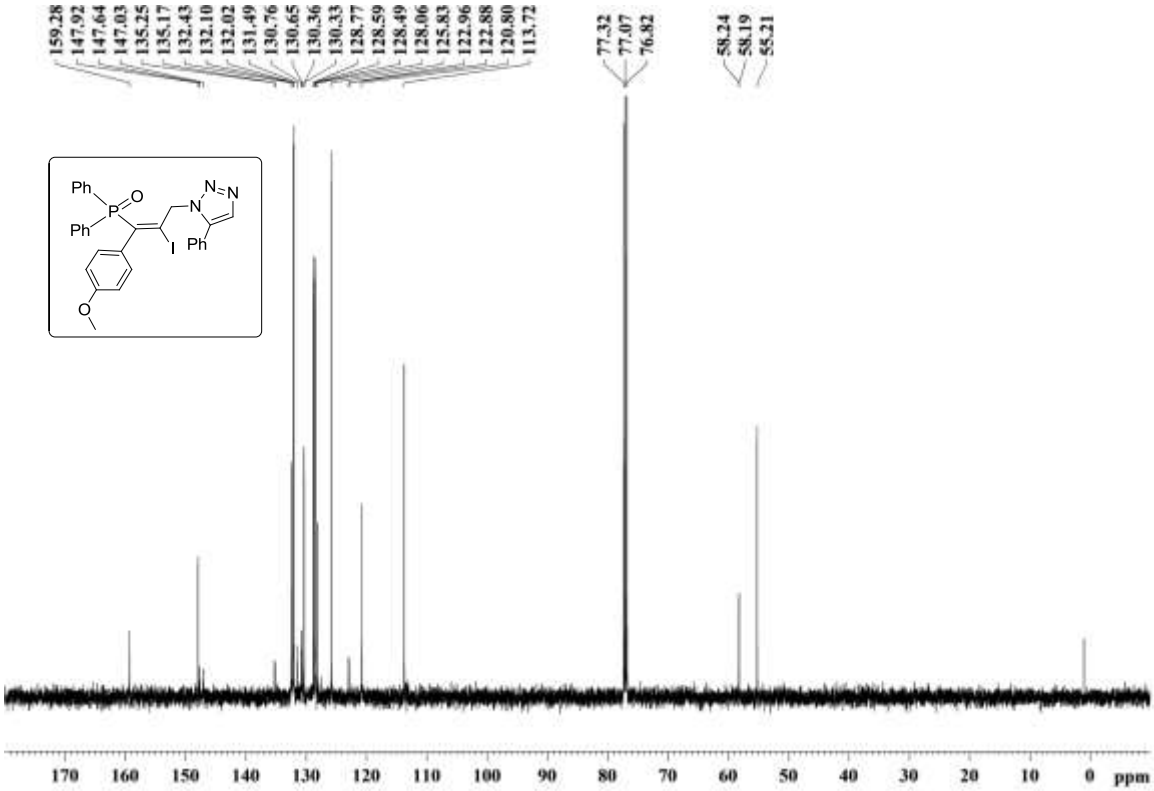

Figure S52. ^{13}C NMR spectrum of compound **24**

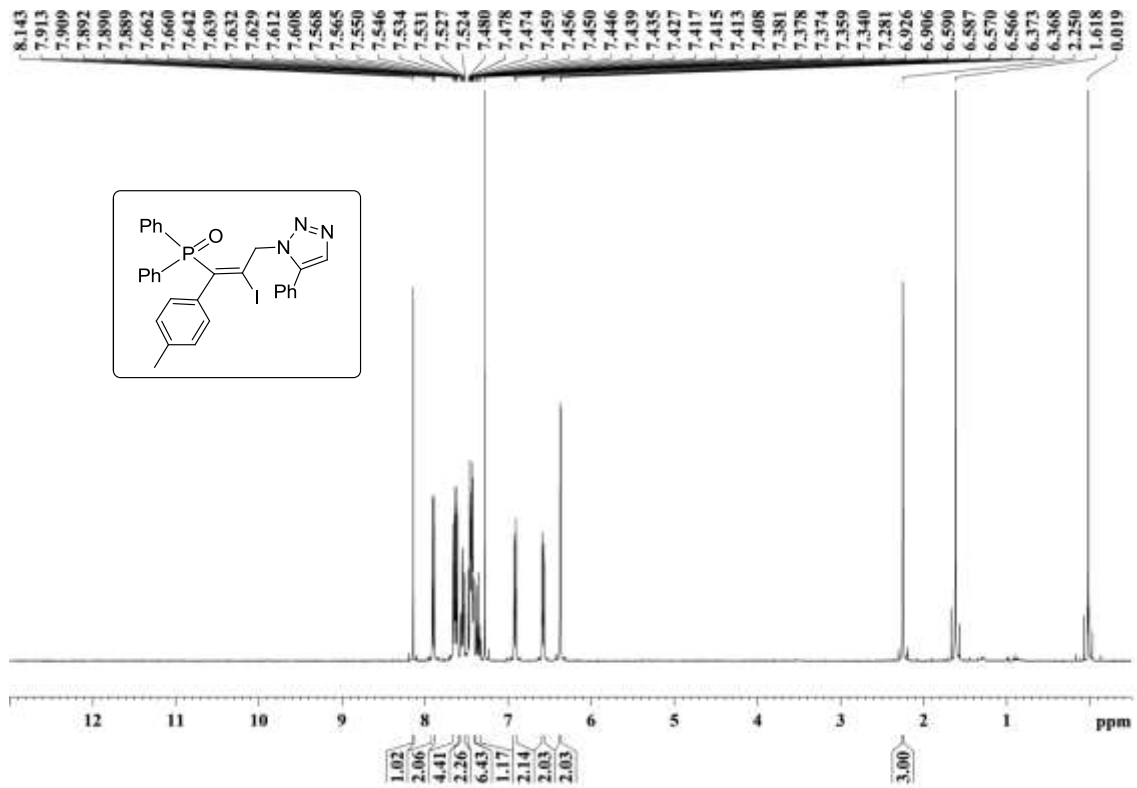

Figure S53. ^{1}H NMR spectrum of compound **25**

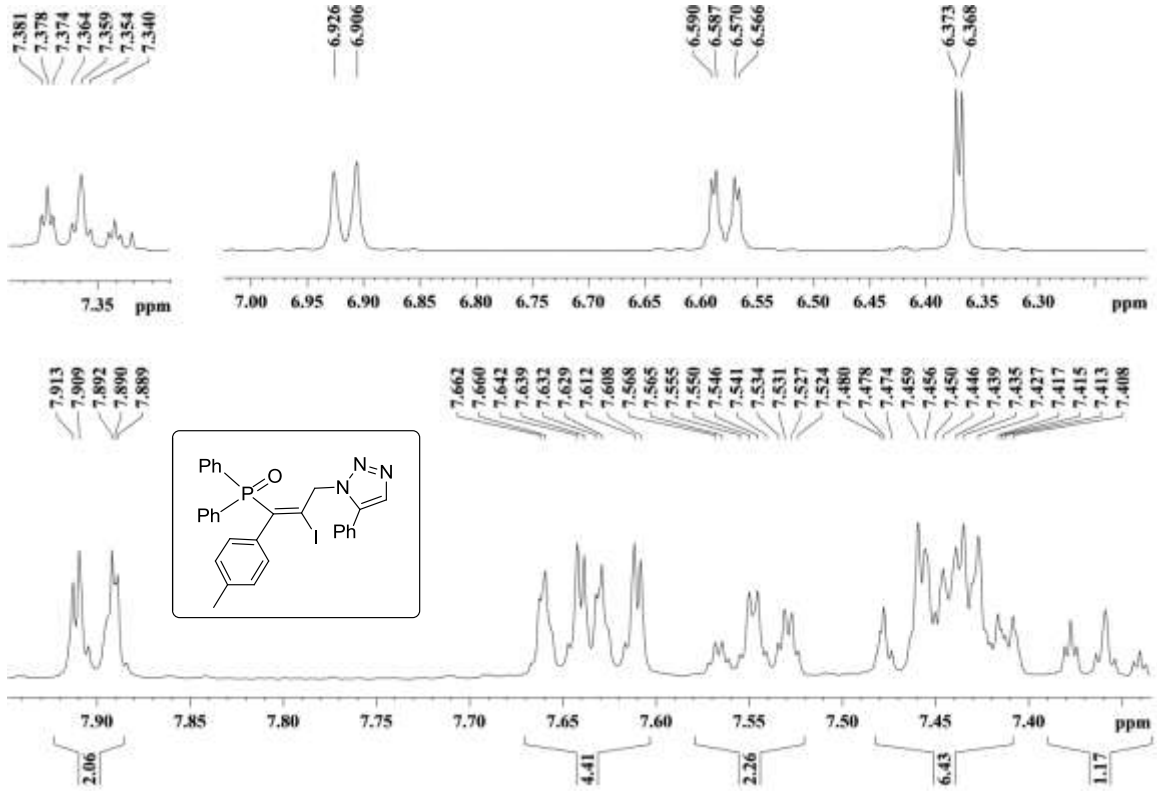

Figure S54. ^{1}H NMR spectrum expansion of compound **25**

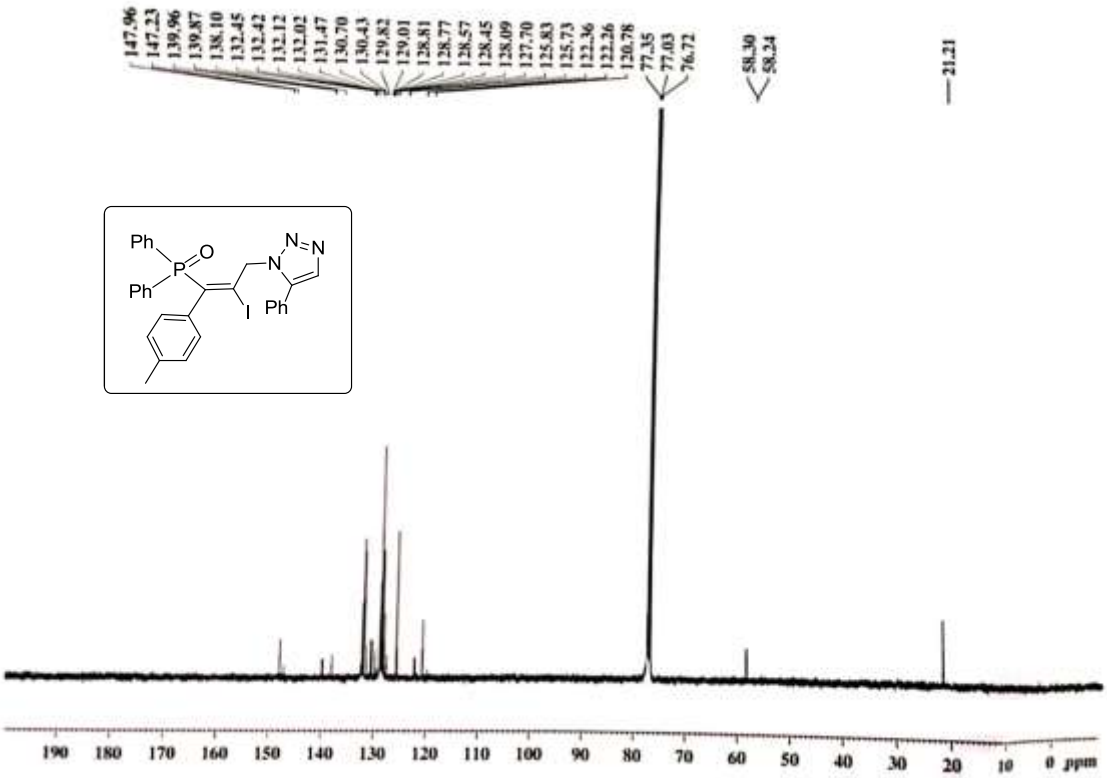

Figure S55. ^{13}C NMR spectrum of compound **25**

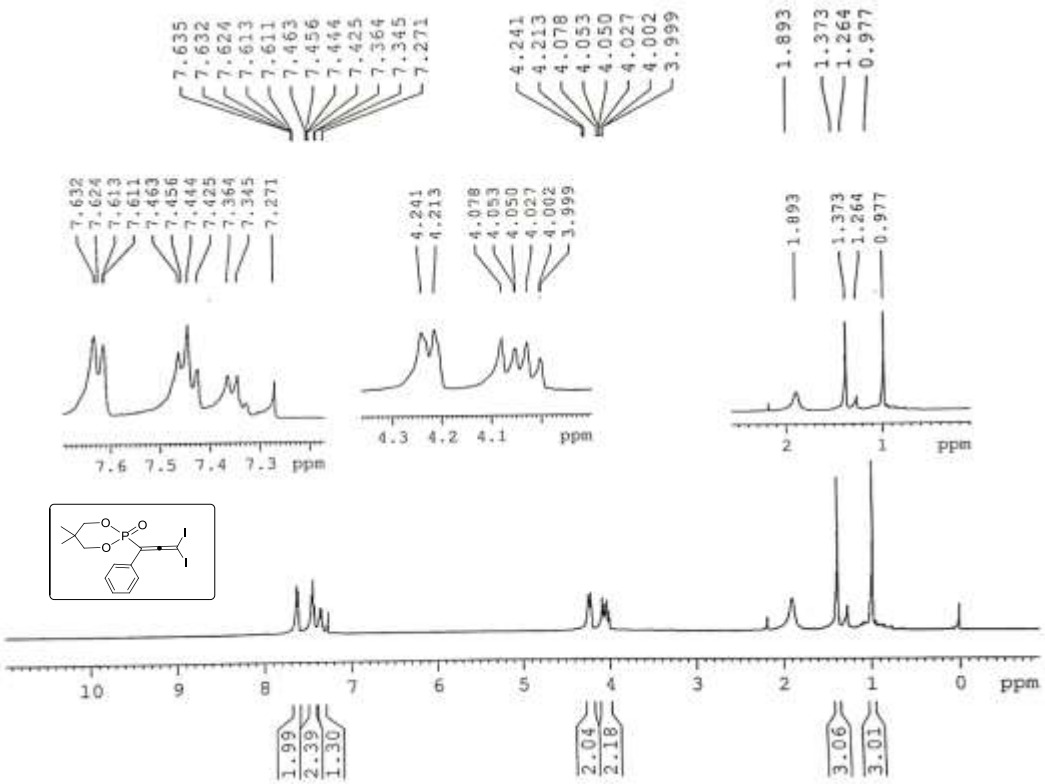

Figure S56. ^{1}H NMR spectrum of compound **26**

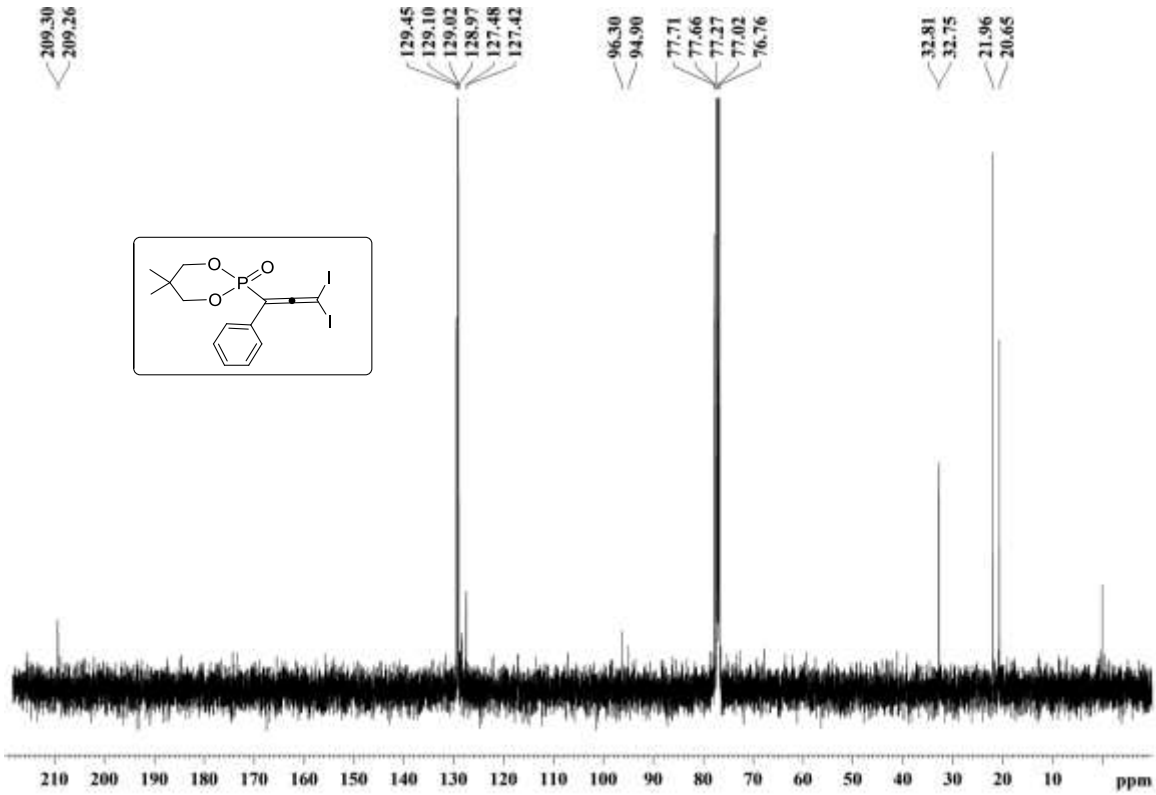

Figure S57. ^{13}C NMR spectrum of compound **26**

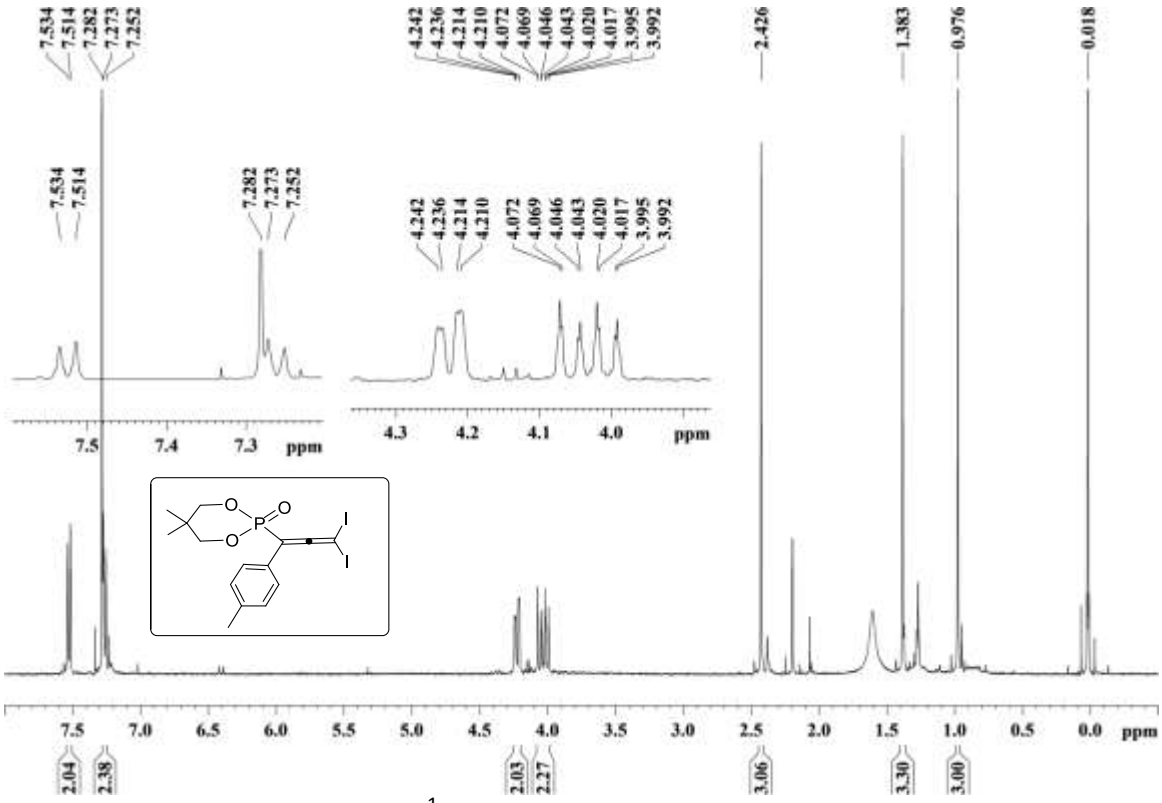

Figure S58. ^{1}H NMR spectrum of compound **27**

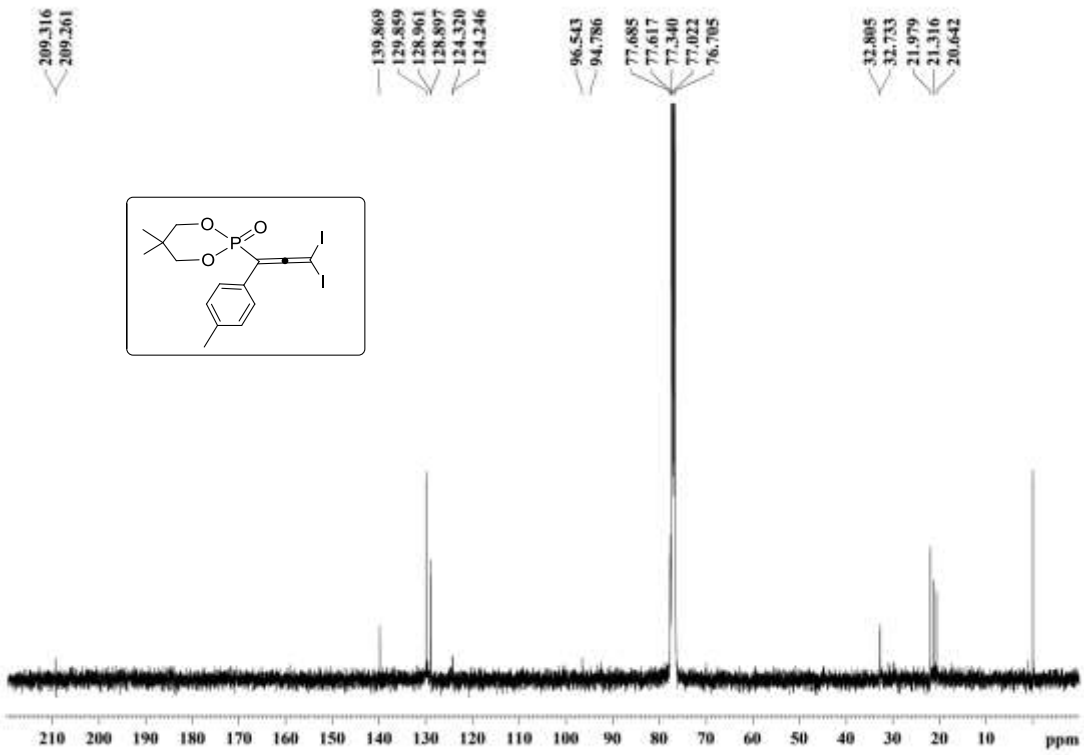

Figure S59. ^{13}C NMR spectrum of compound **27**

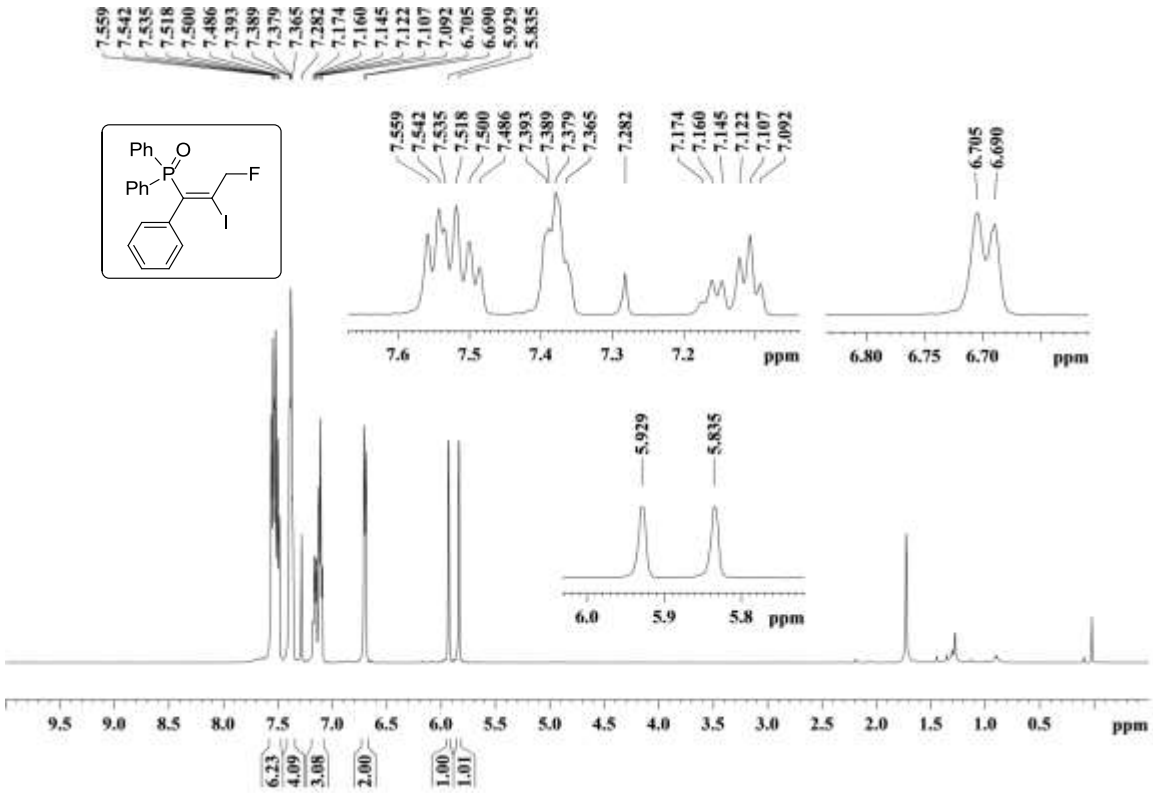

Figure S60. ^{1}H NMR spectrum of compound **28**

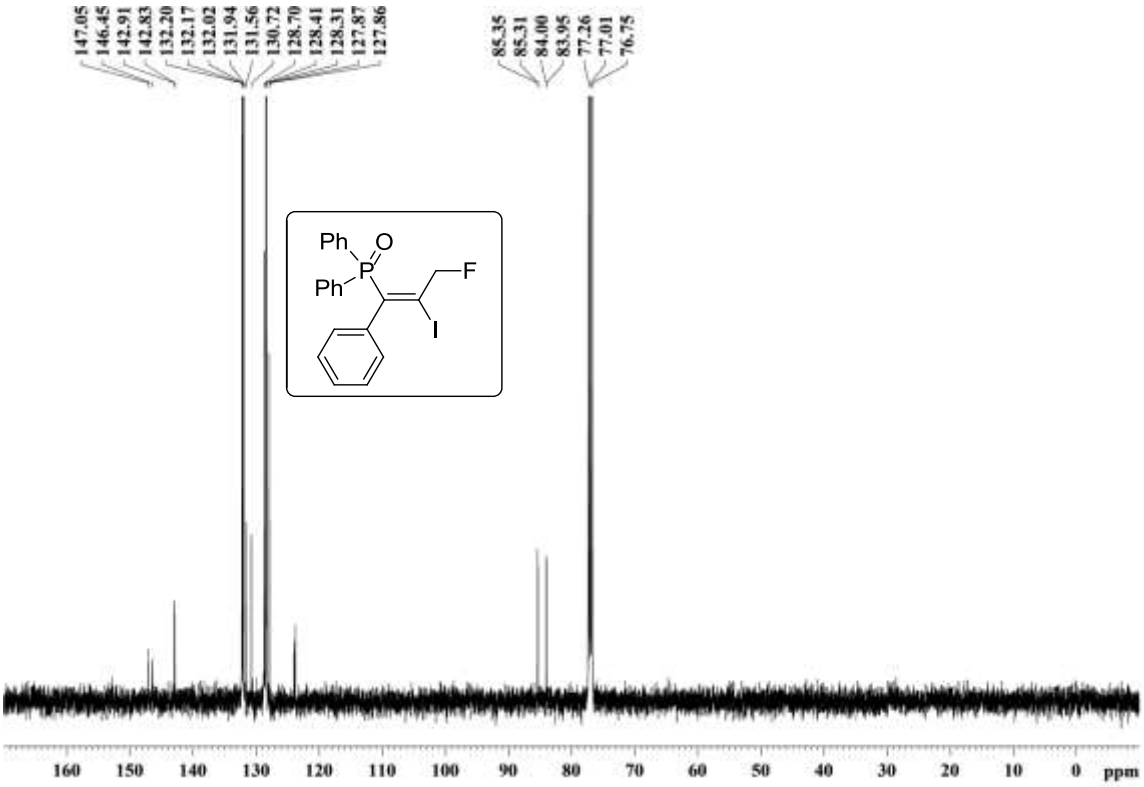

Figure S61. ^{13}C NMR spectrum of compound **28**

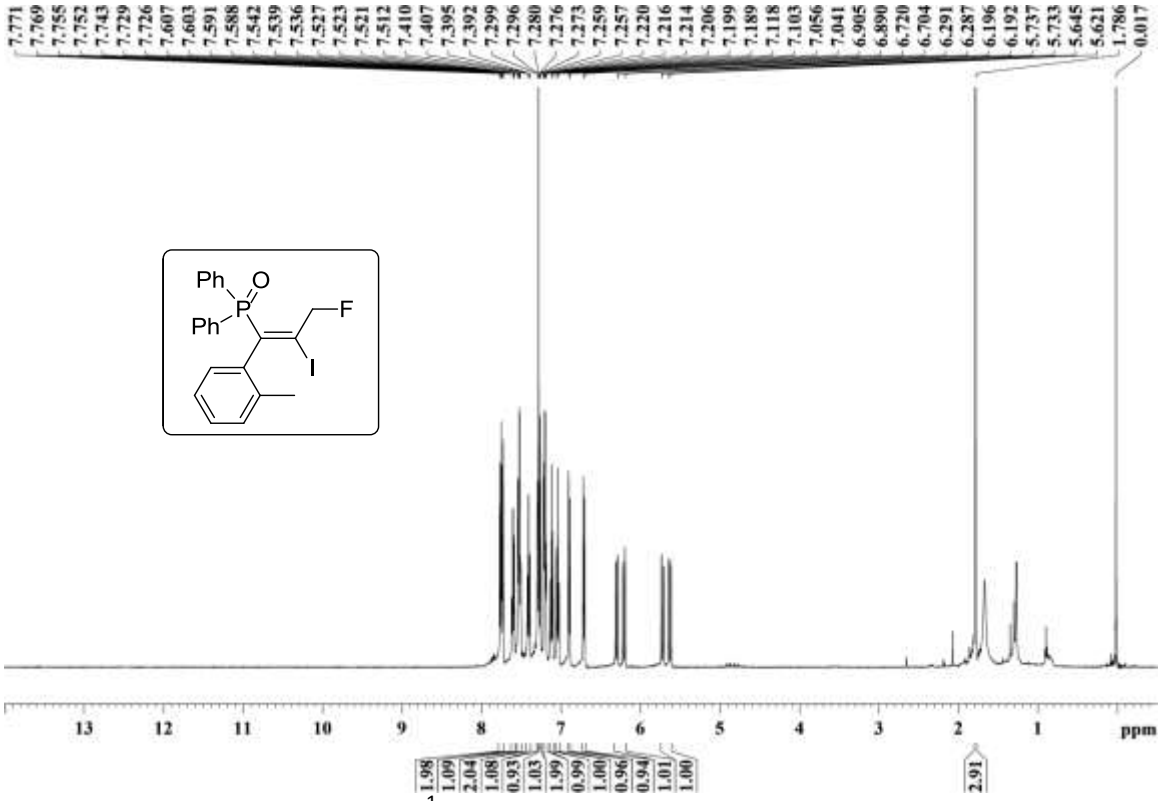

Figure S62. ^{1}H NMR spectrum of compound **29**

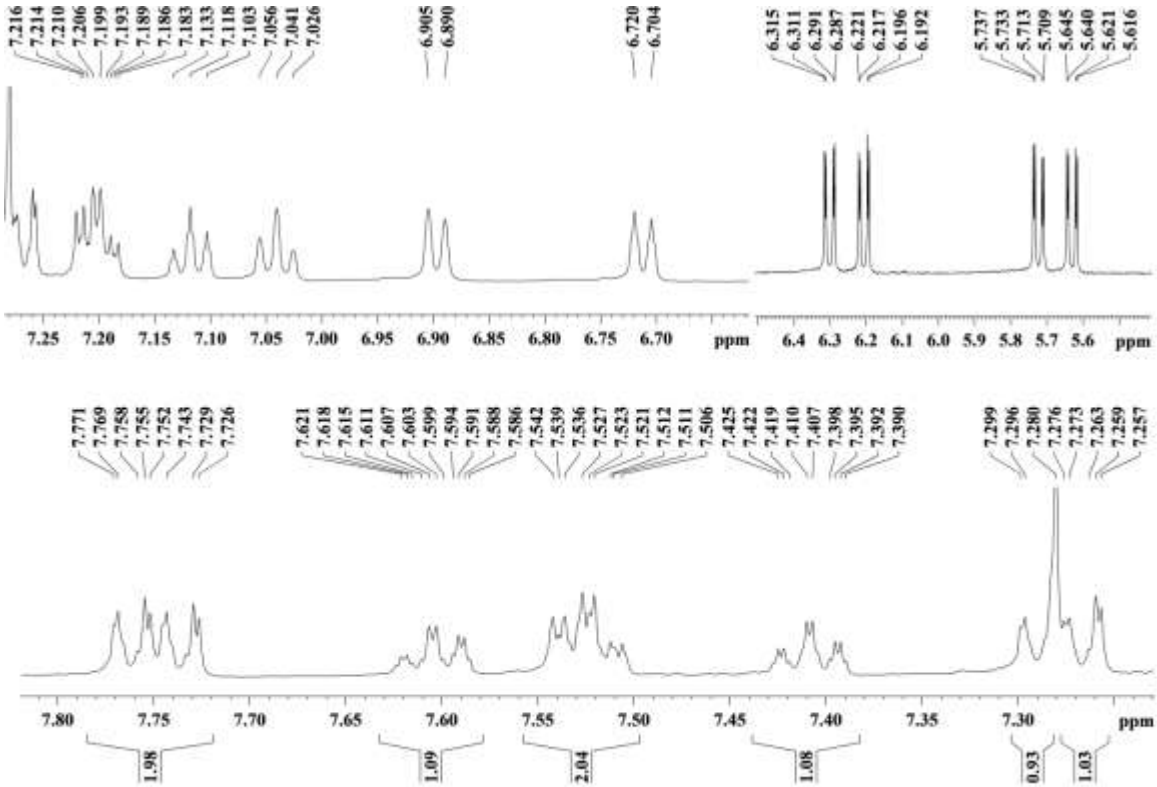

Figure S63. ^{1}H NMR spectrum expansion of compound **29**

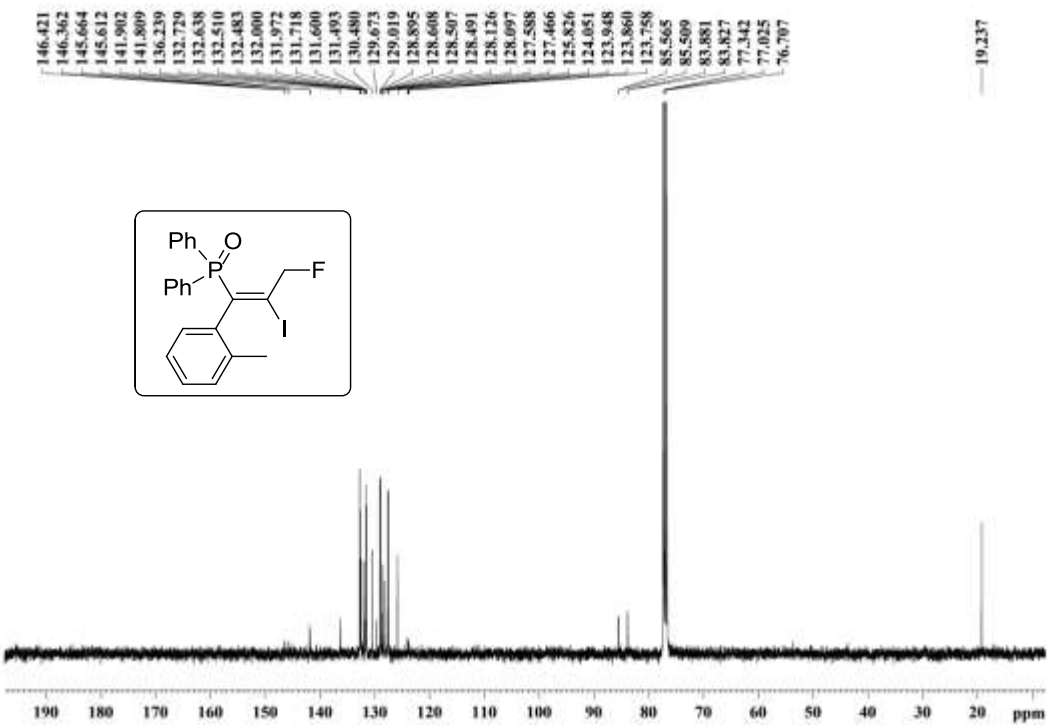

Figure S64. ^{13}C NMR spectrum of compound **29**

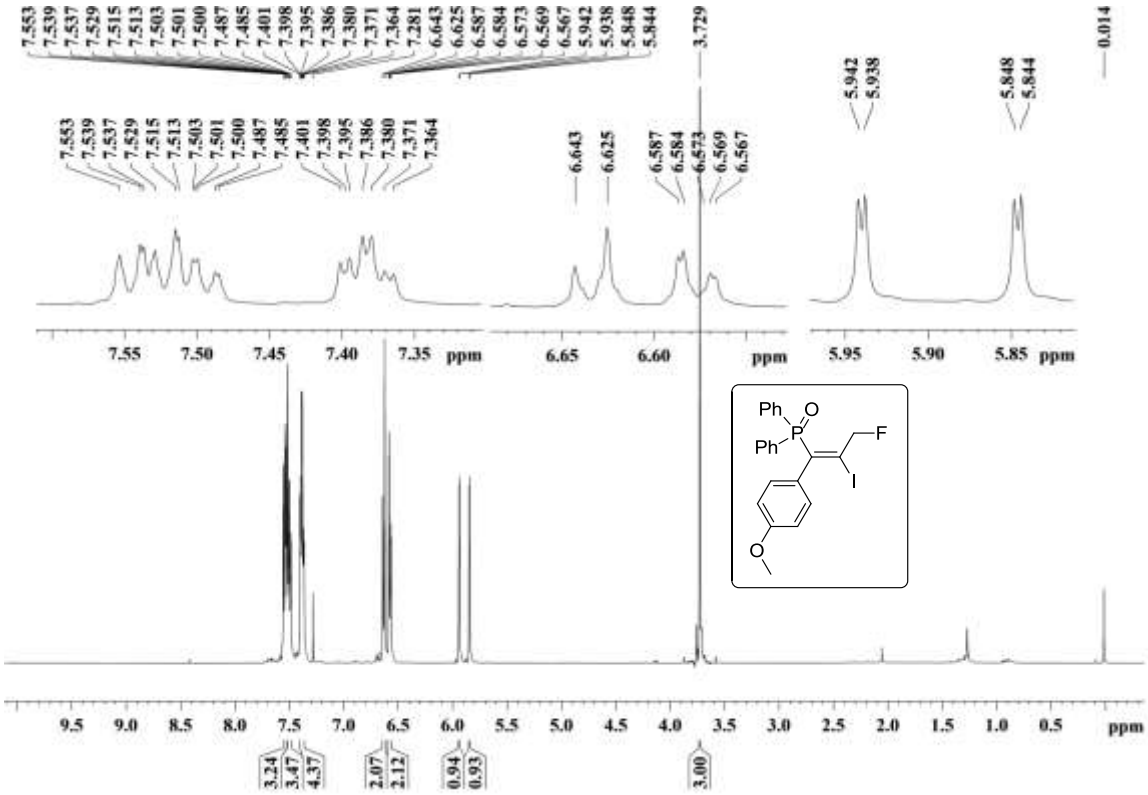

Figure S65. ^{1}H NMR spectrum of compound **30**

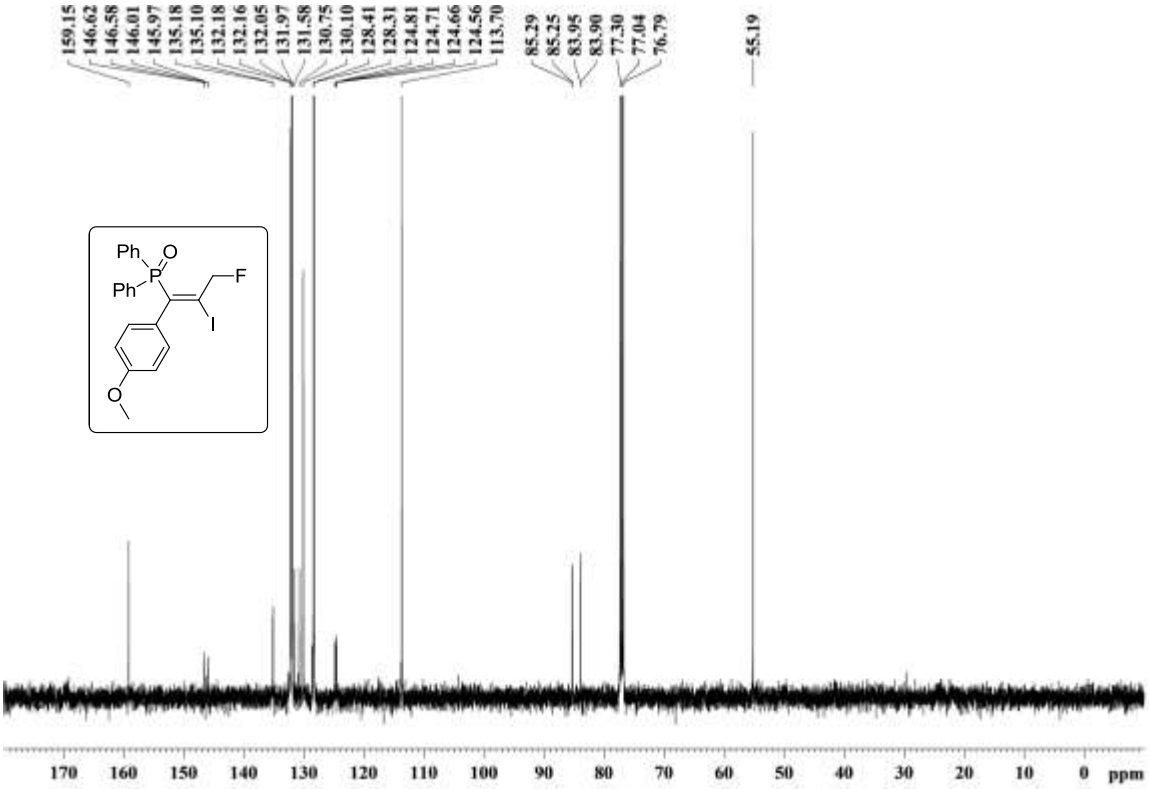

Figure S66. ^{13}C NMR spectrum of compound **30**

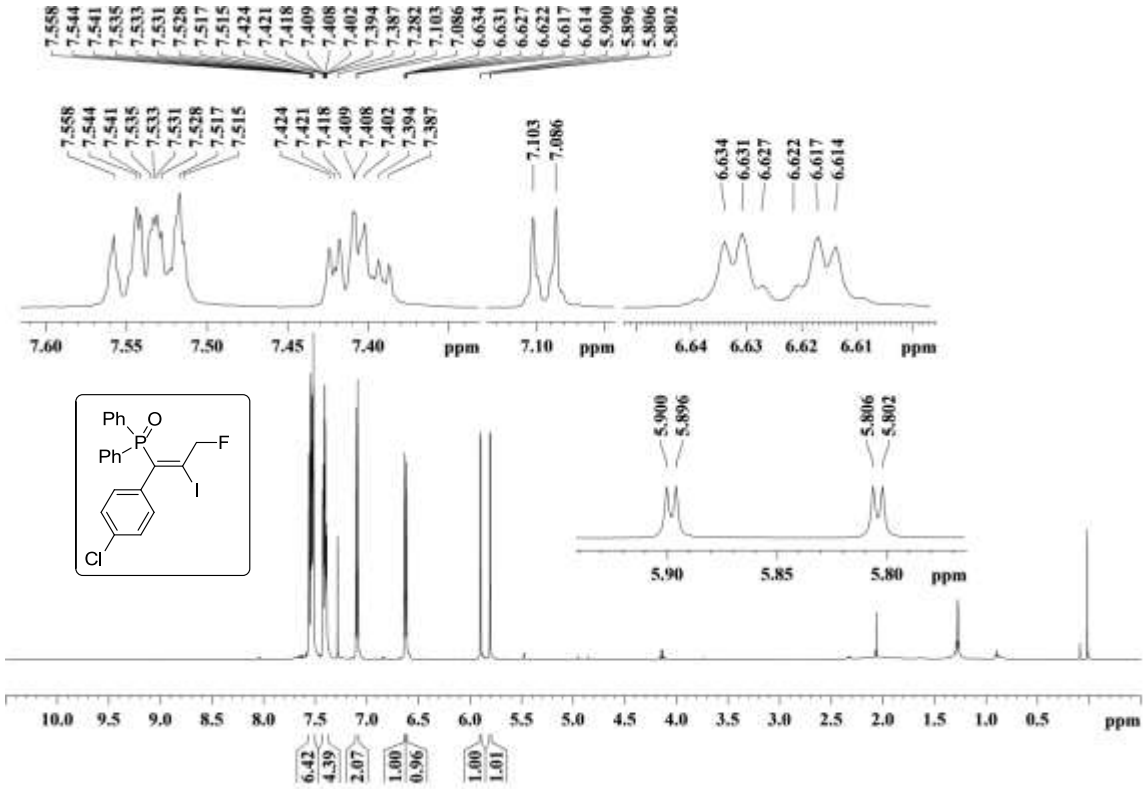

Figure S67. ^{1}H NMR spectrum of compound **31**

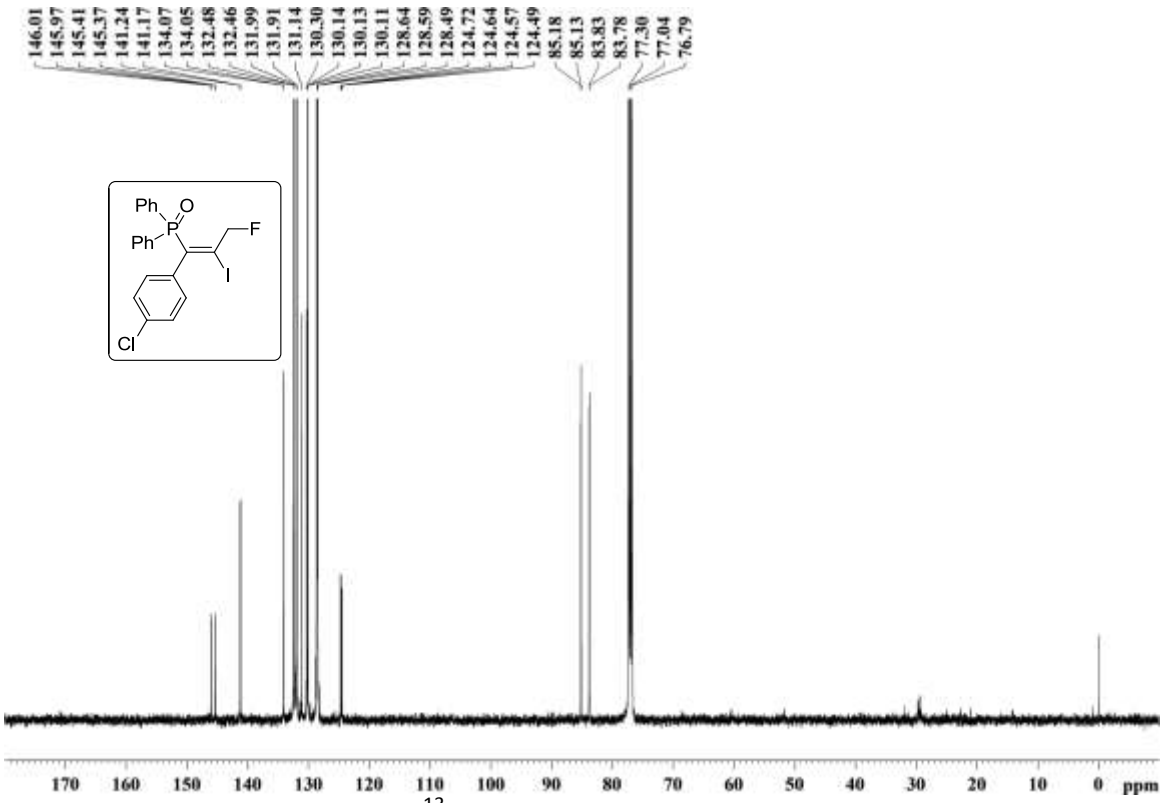

Figure S68. ^{13}C NMR spectrum of compound **31**

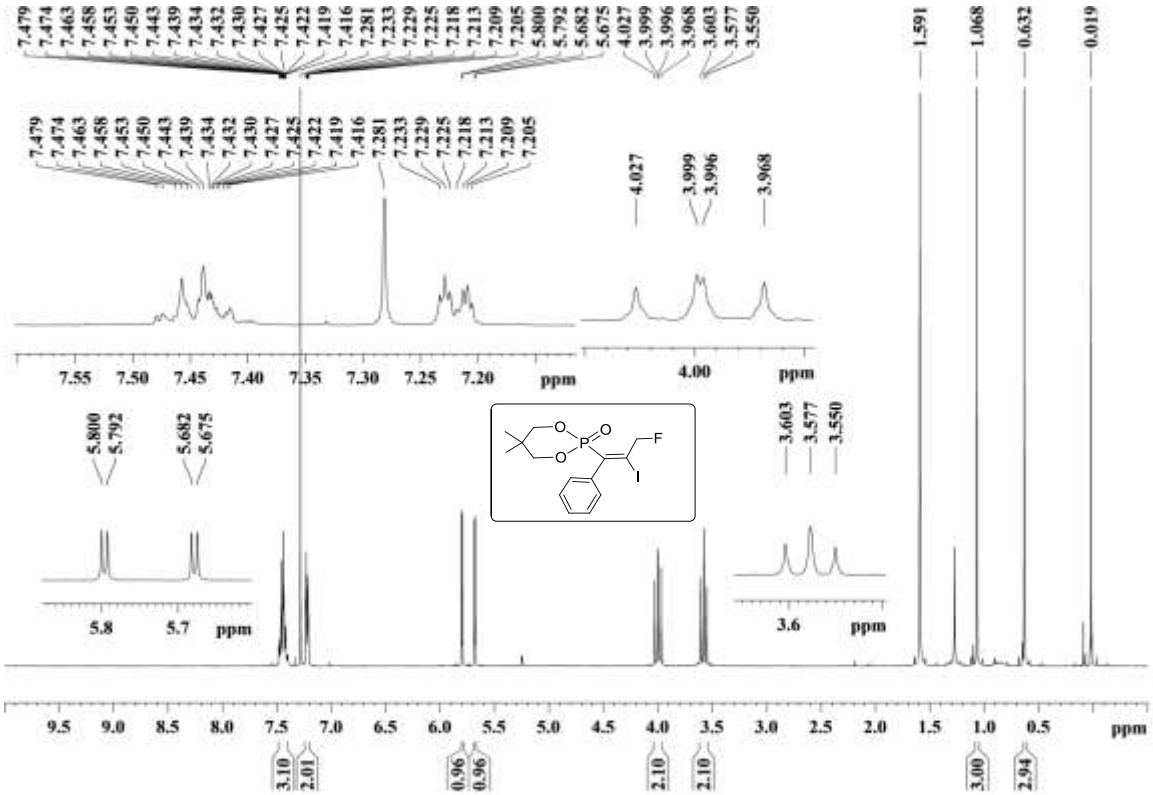

Figure S69. ^{1}H NMR spectrum of compound **32**

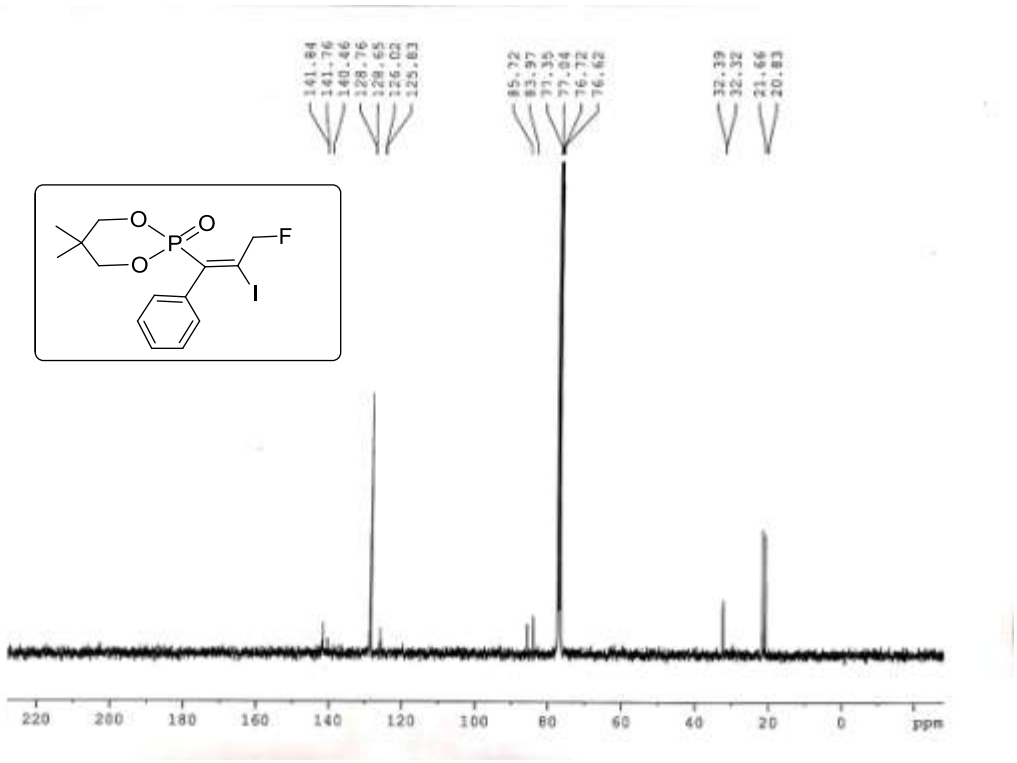

Figure S70. ^{13}C NMR spectrum of compound **32**

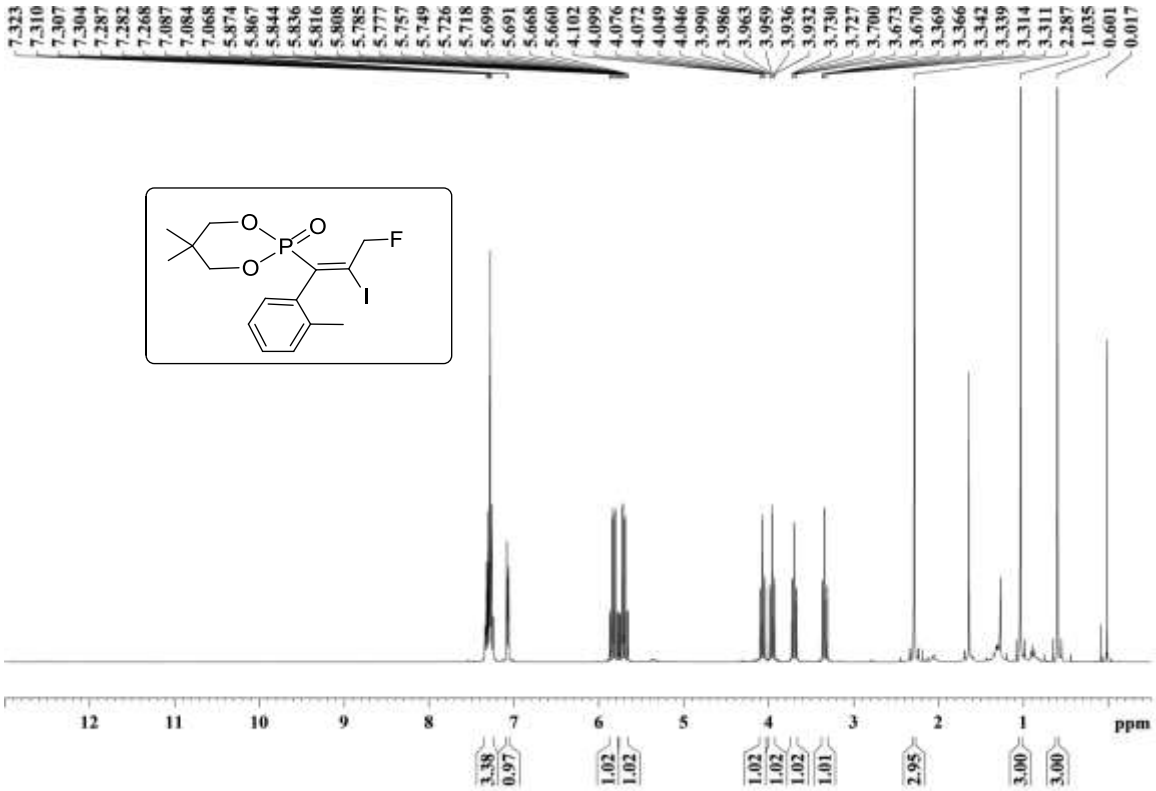

Figure S71. ^{1}H NMR spectrum of compound **33**

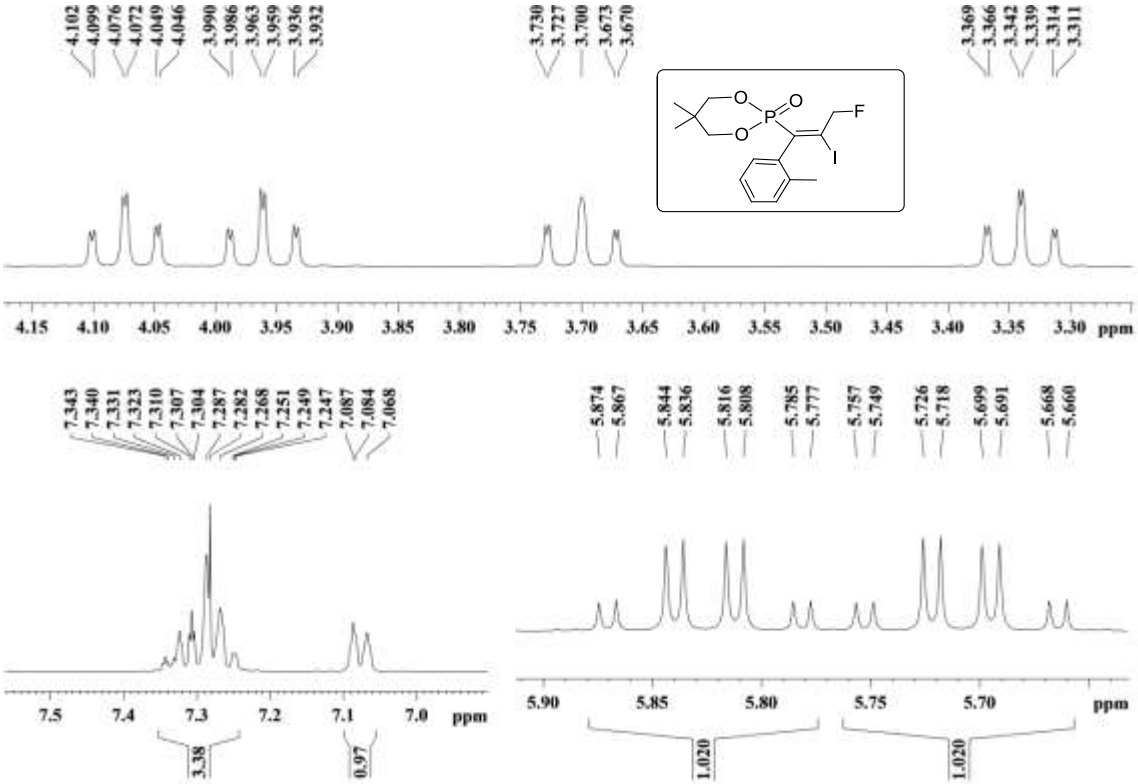

Figure S72. ^{1}H NMR spectrum expansion of compound **33**

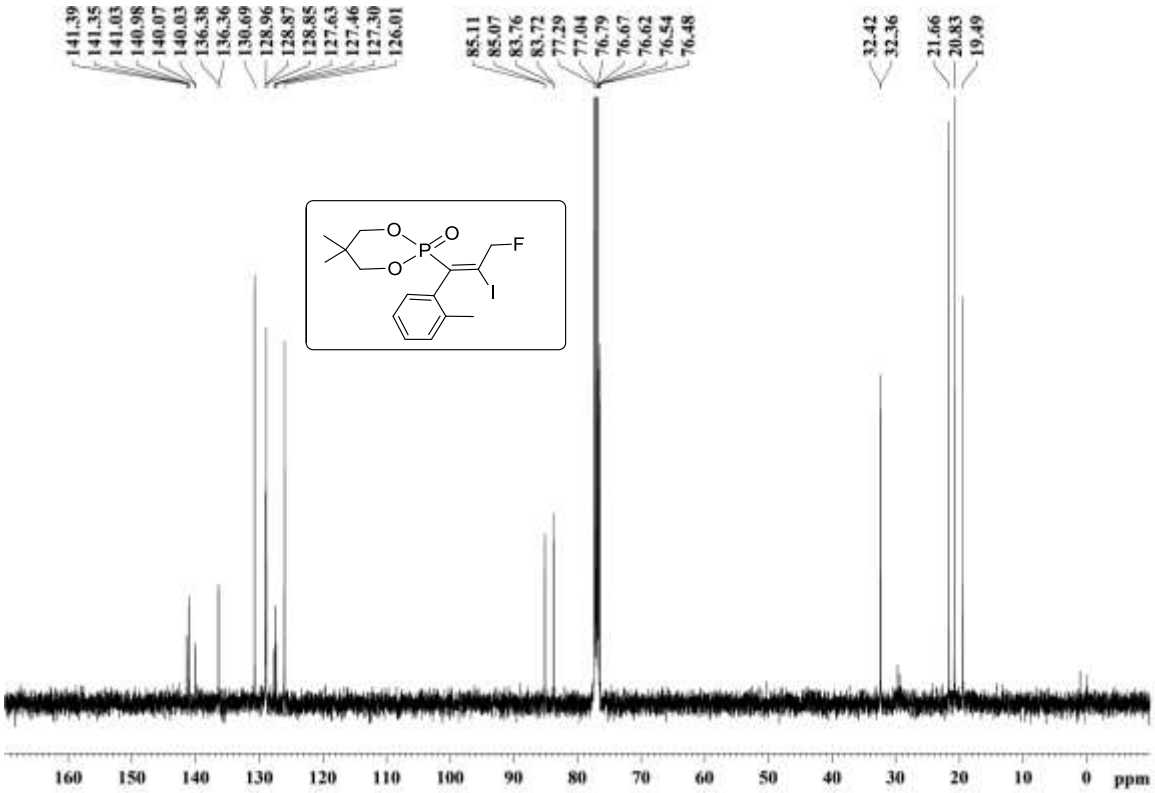

Figure S73. ^{13}C NMR spectrum of compound **33**

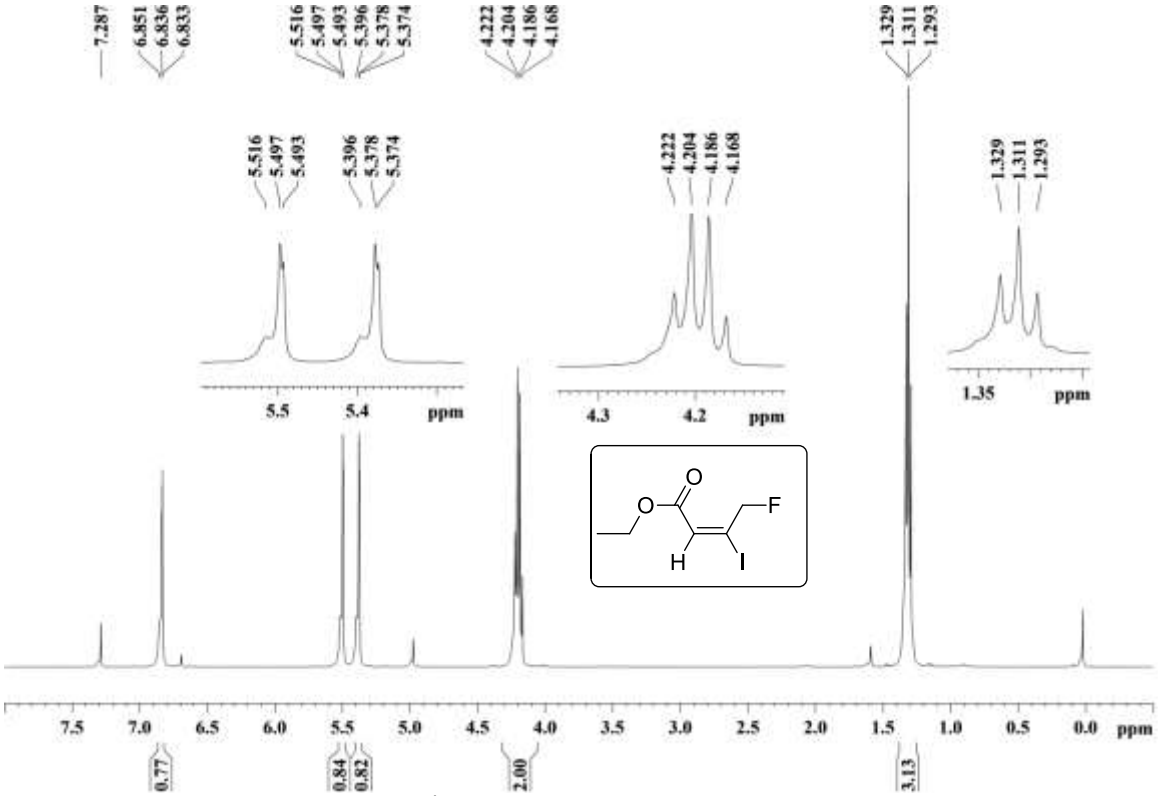

Figure S74. ^{1}H NMR spectrum of compound **34**

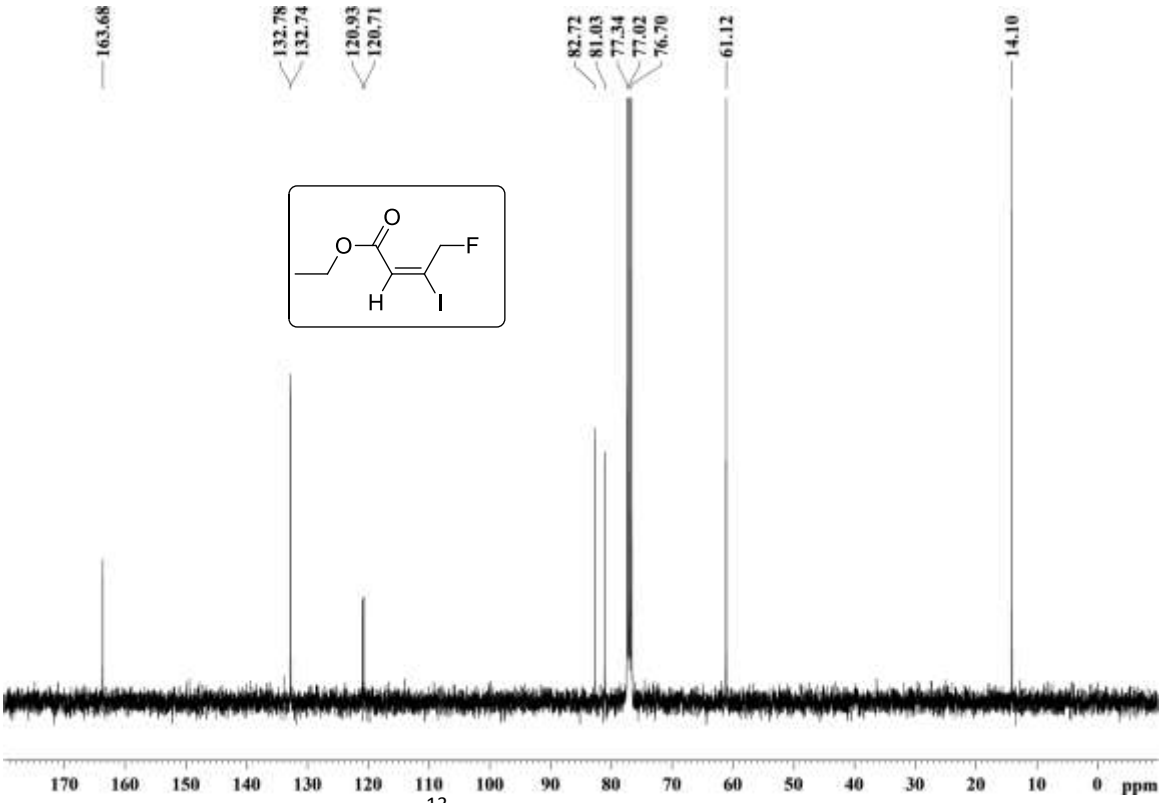

Figure S75. ^{13}C NMR spectrum of compound **34**

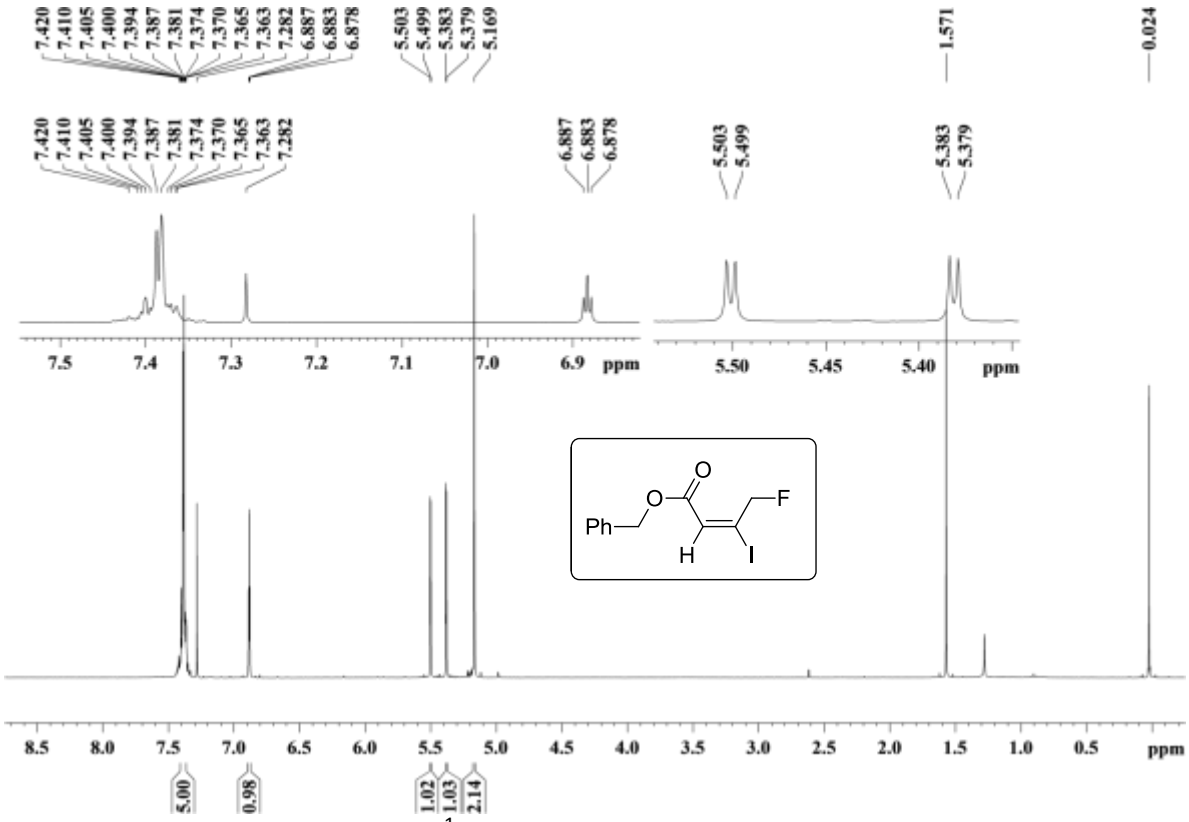

Figure S76. ^{1}H NMR spectrum of compound **35**

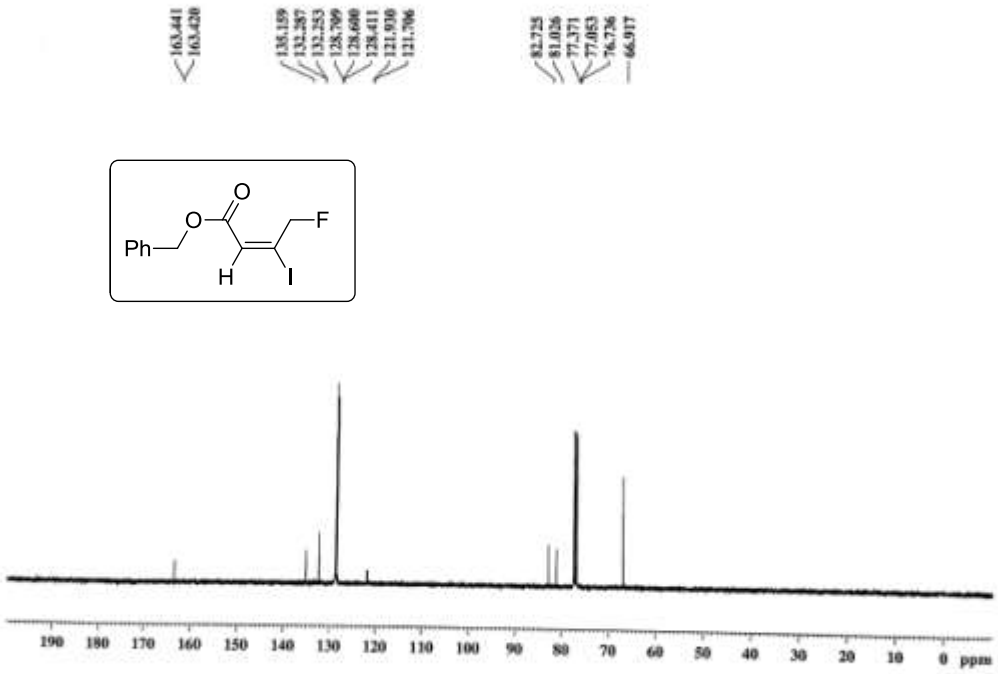

Figure S77. ^{13}C NMR spectrum of compound **35**

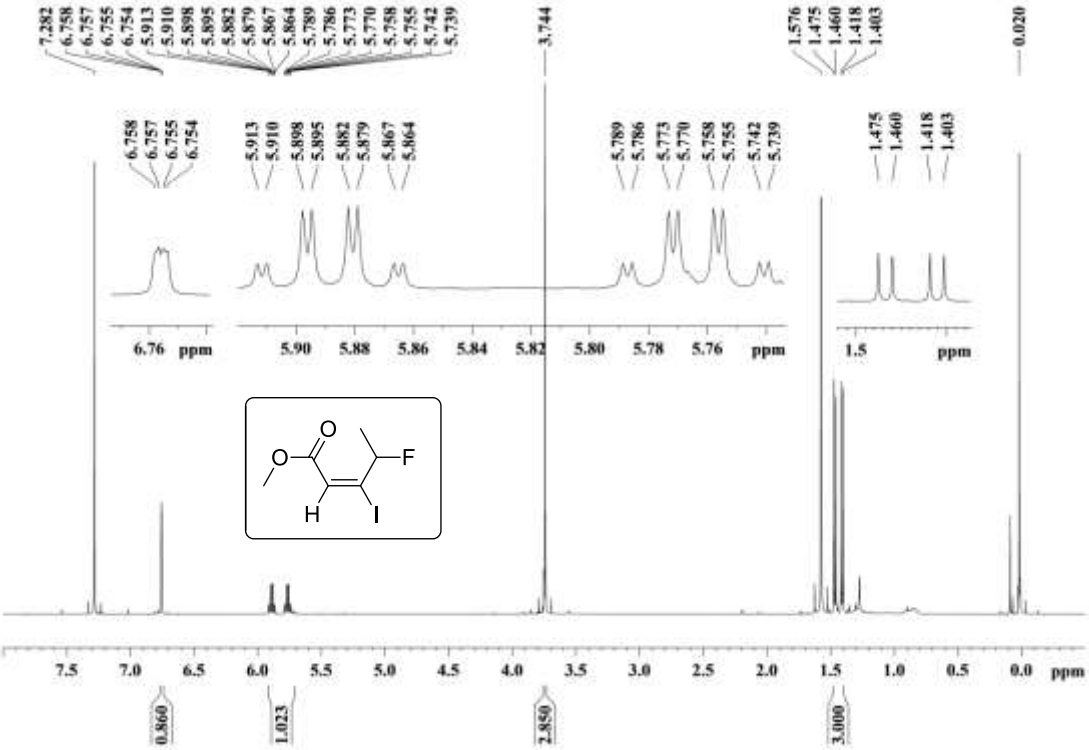

Figure S78. ^{1}H NMR spectrum of compound **36**

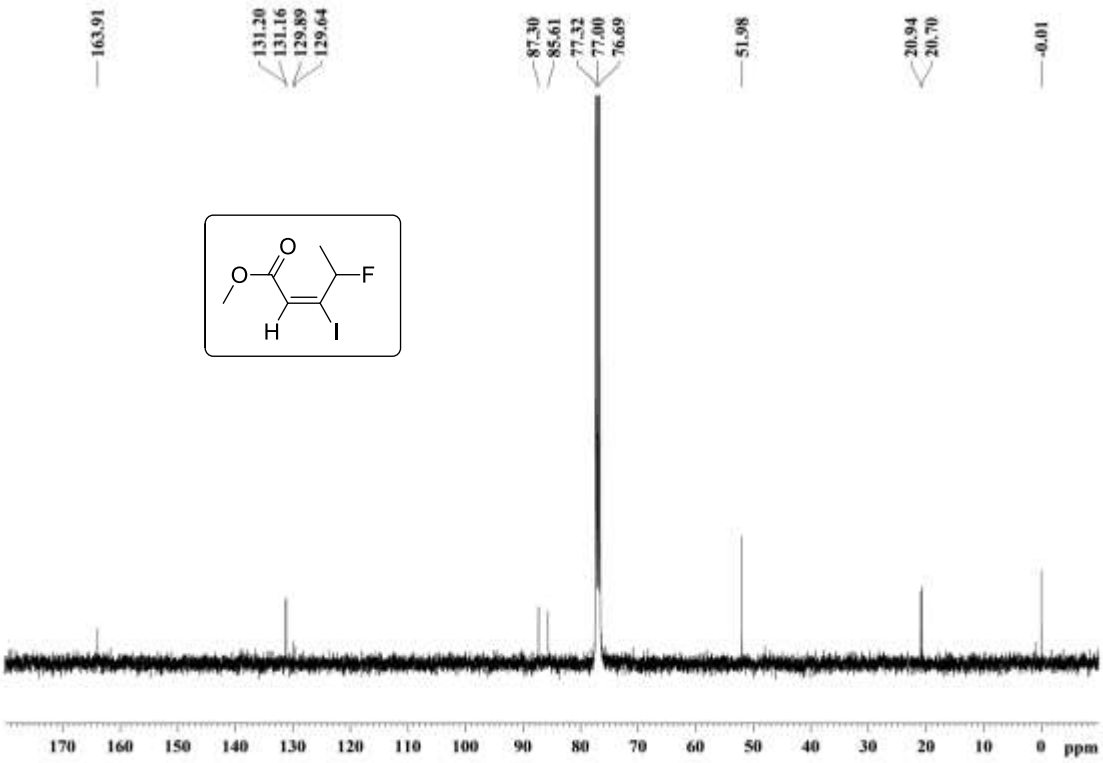

Figure S79. ^{13}C NMR spectrum of compound **36**

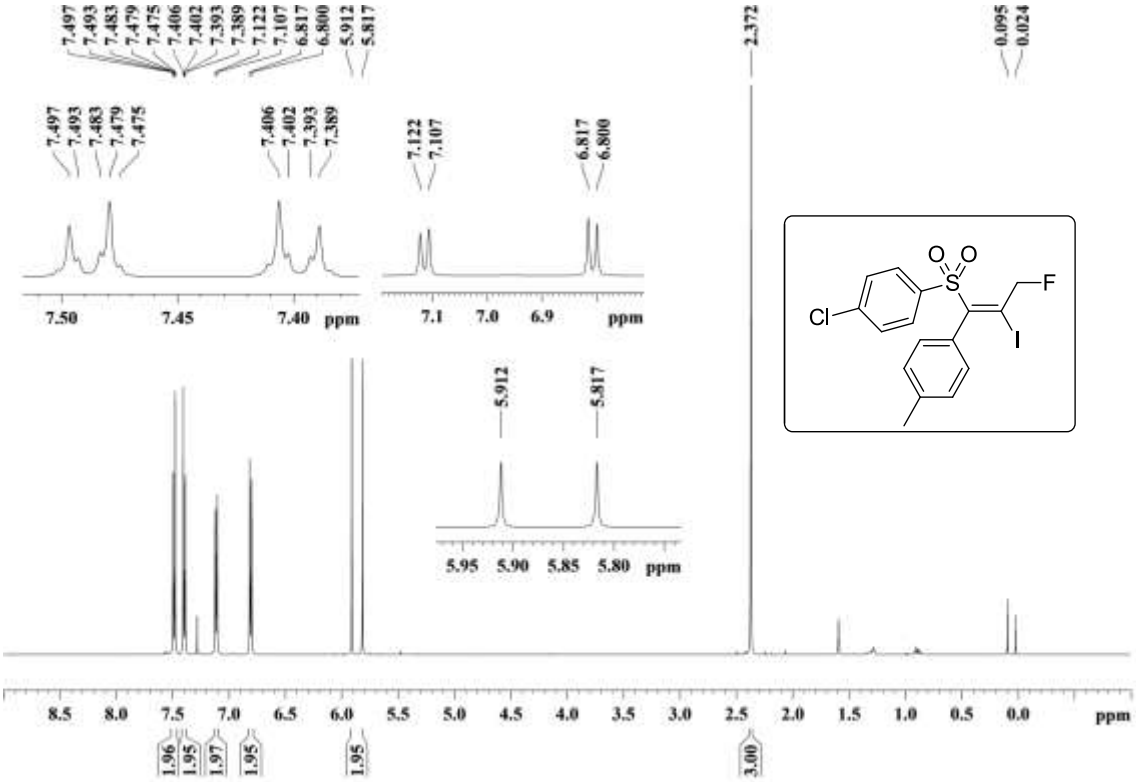

Figure S80. ^{1}H NMR spectrum of compound **37**

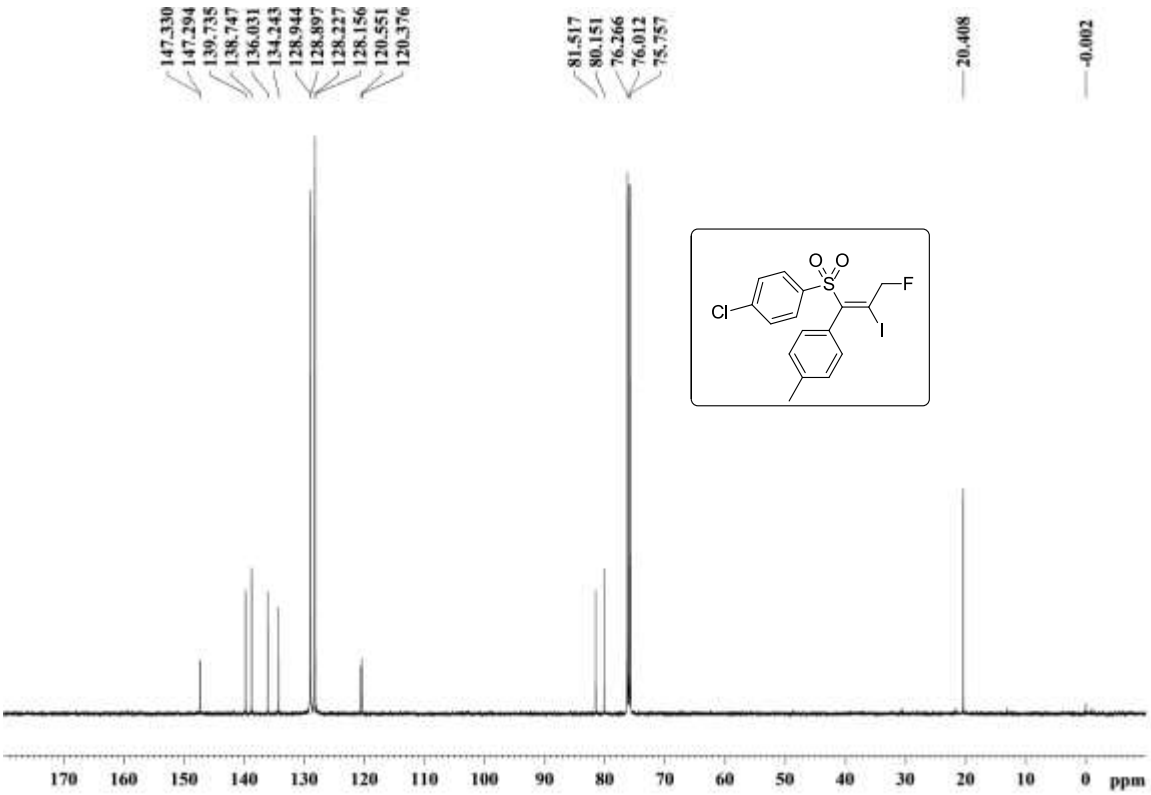

Figure S81. ^{13}C NMR spectrum of compound **37**

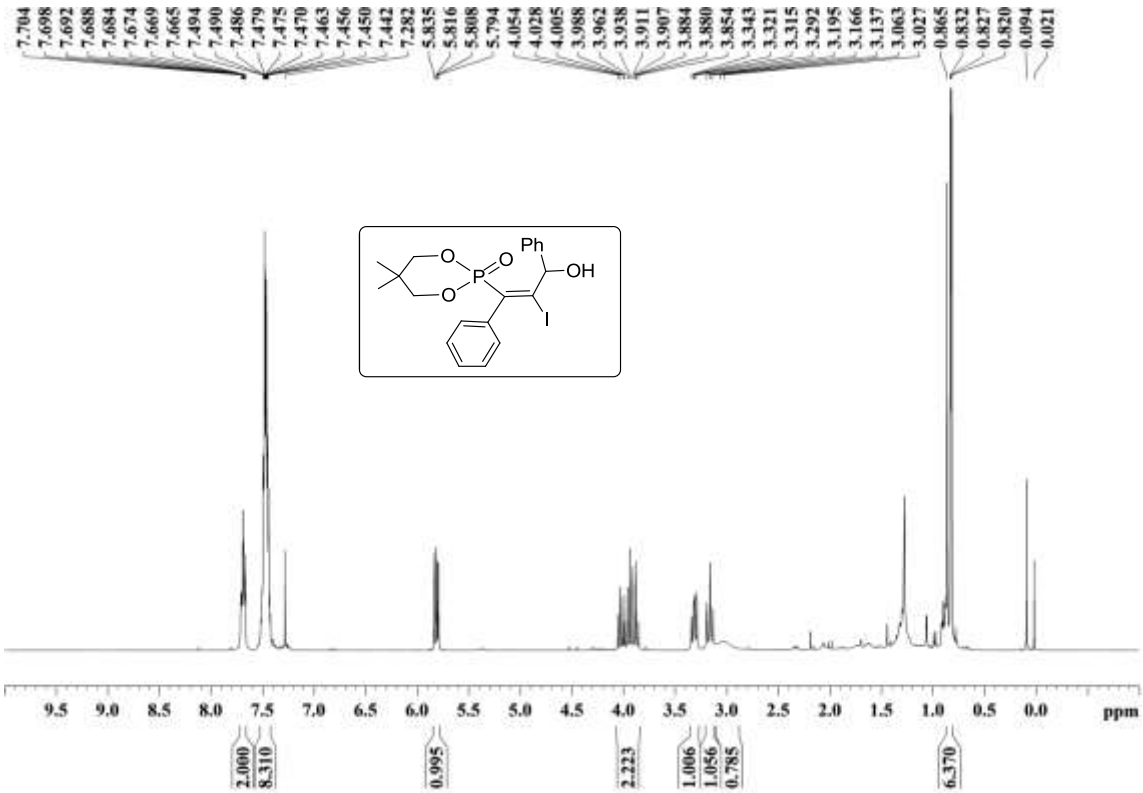

Figure S82. ^{1}H NMR spectrum of compound **38**

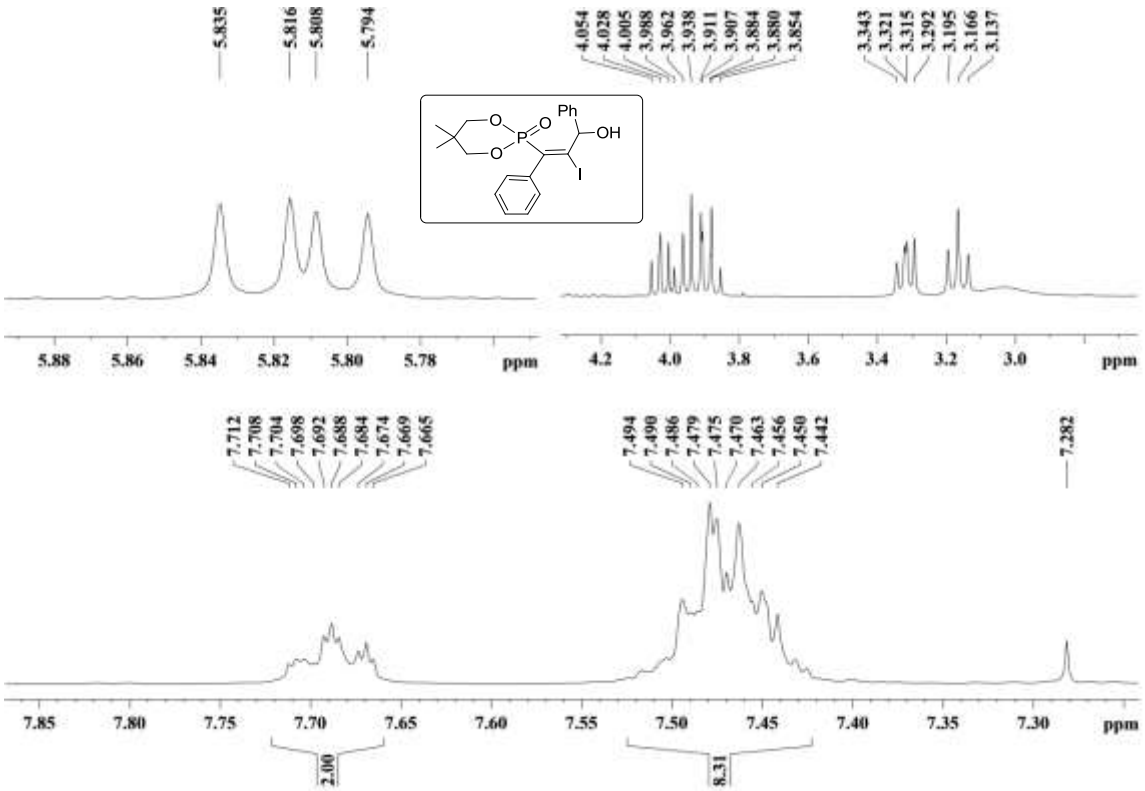

Figure S83. ^{1}H NMR spectrum expansion of compound **38**

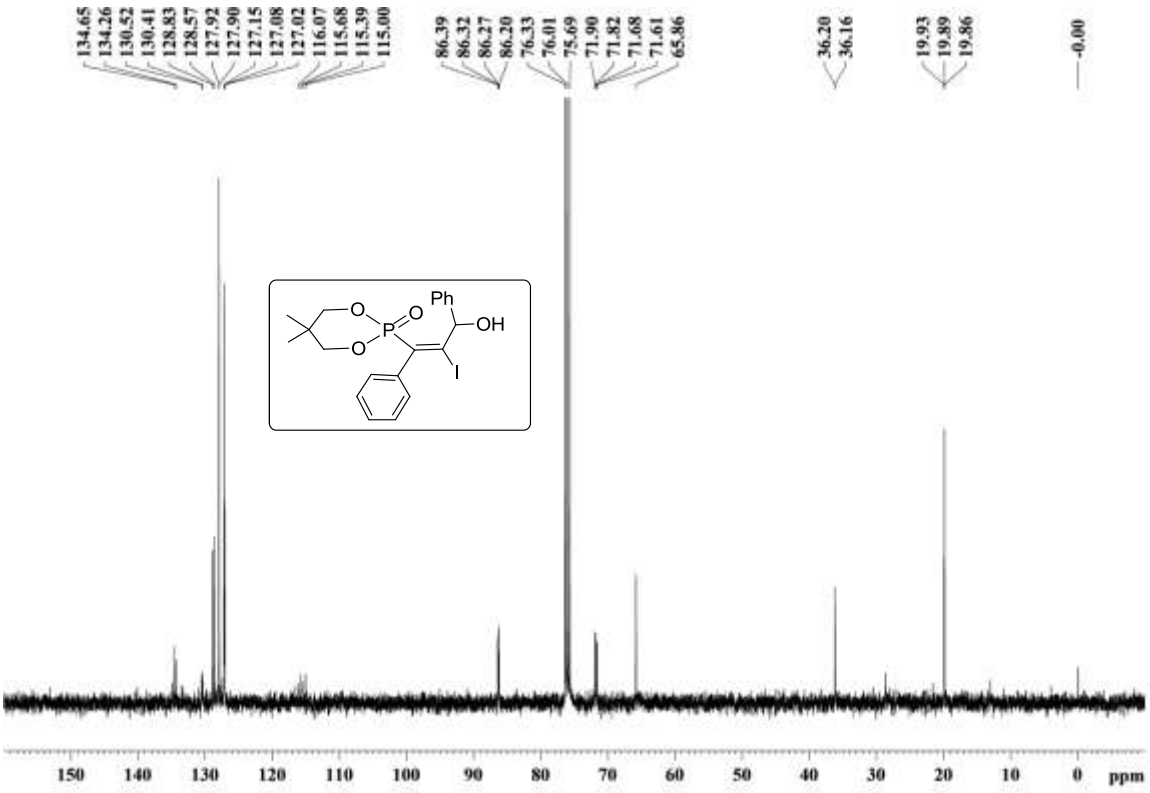

Figure S84. ^{13}C NMR spectrum of compound **38**