

Utilizing Estra-1,3,5,16-tetraene Scaffold: Design and Synthesis of Nitric Oxide Donors as Chemotherapeutic Resistance Combating Agents in Liver Cancer

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1 Spectral data

1.1 Compound 7

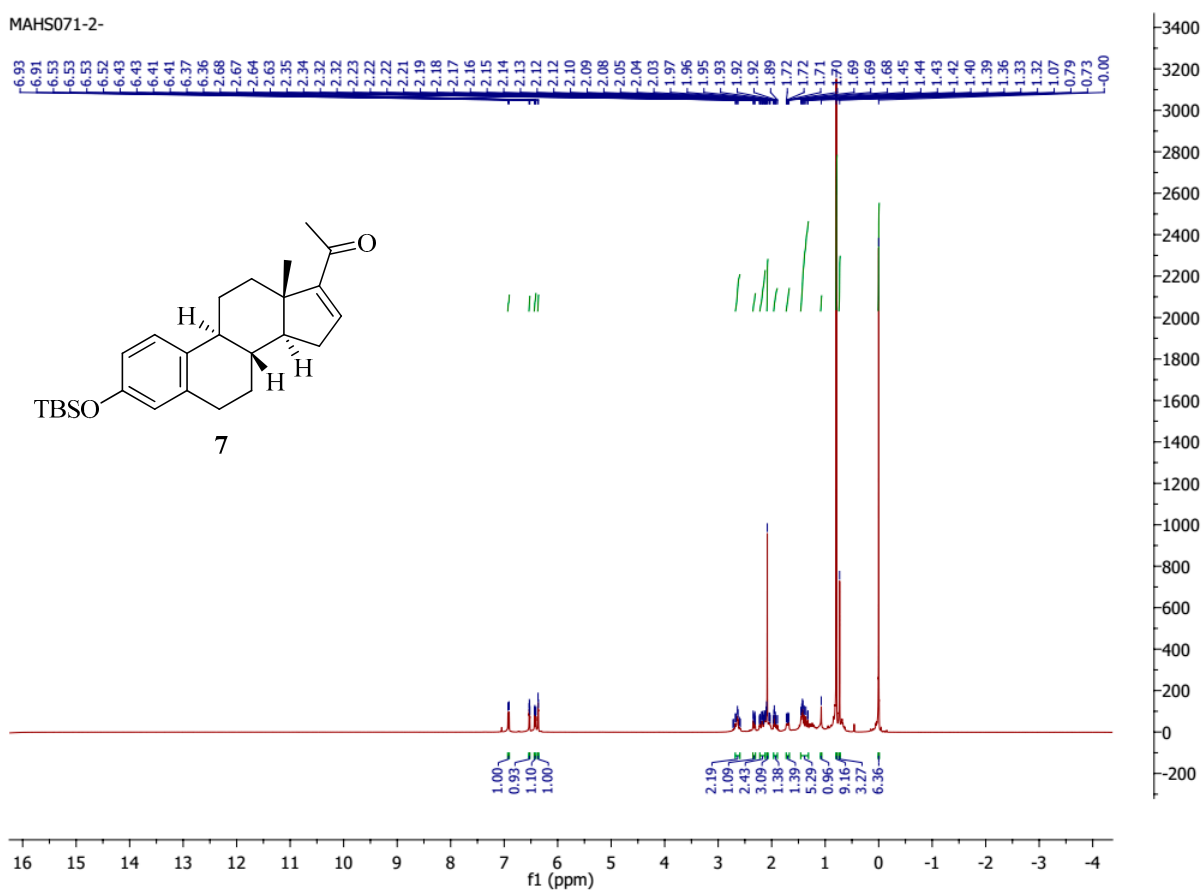


Figure S 1. ¹H NMR of compound 7.

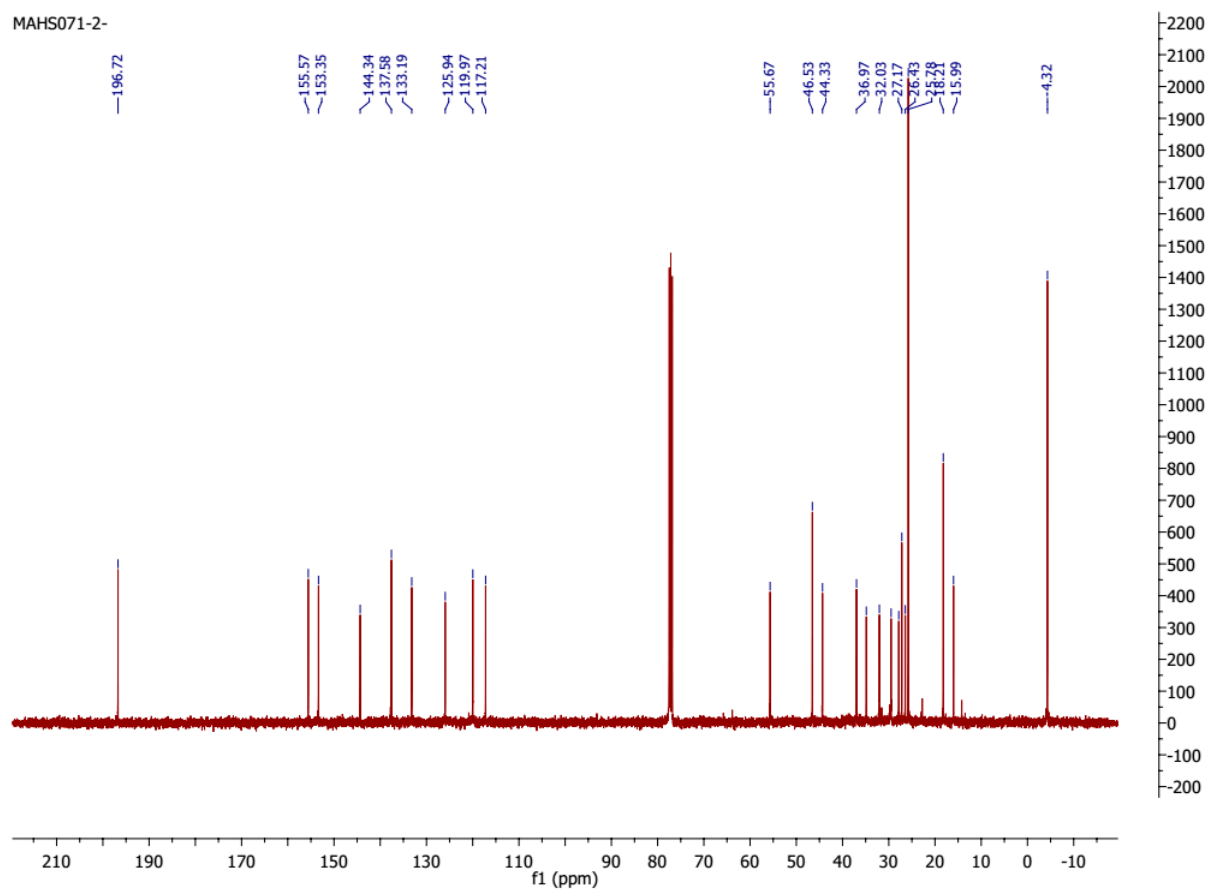


Figure S 2. ^{13}C NMR of compound **7**.

1.2 Compound 8

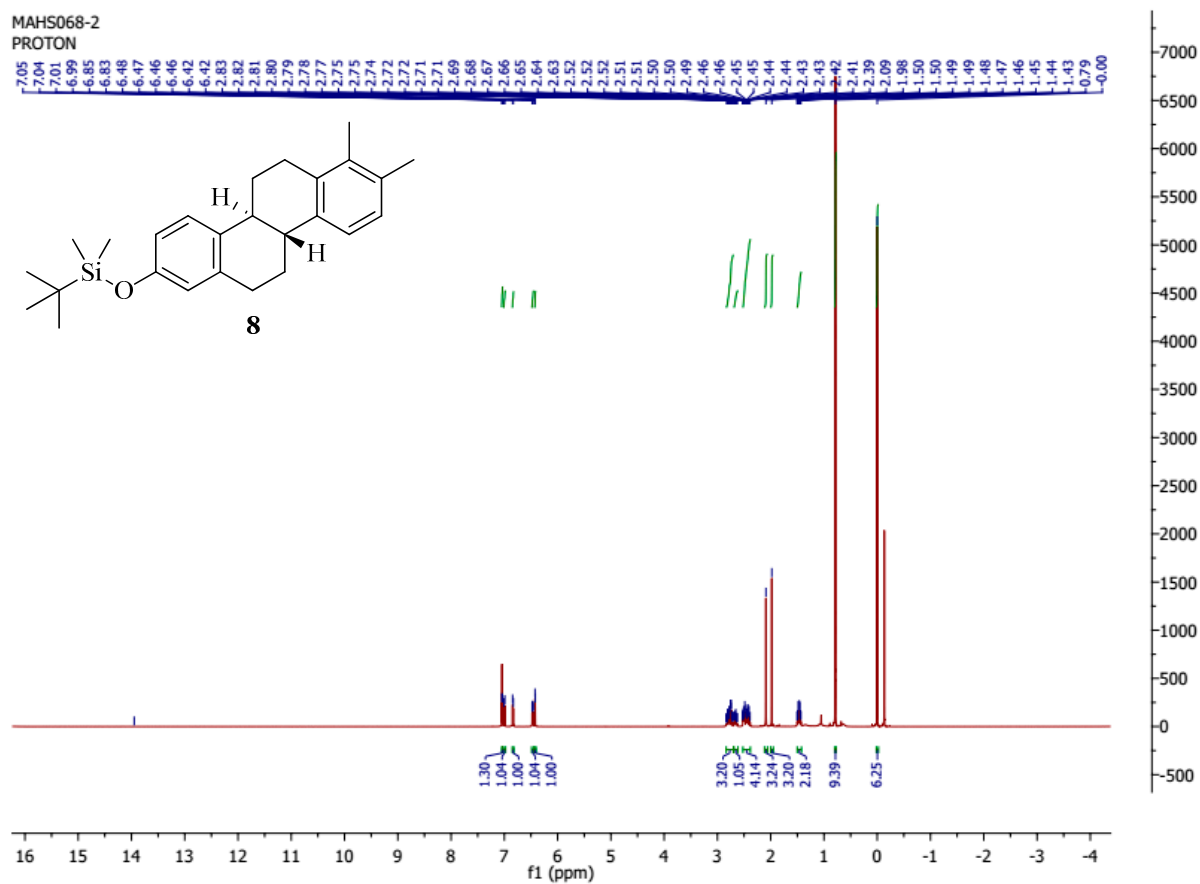


Figure S 3. ^1H NMR of compound 8.

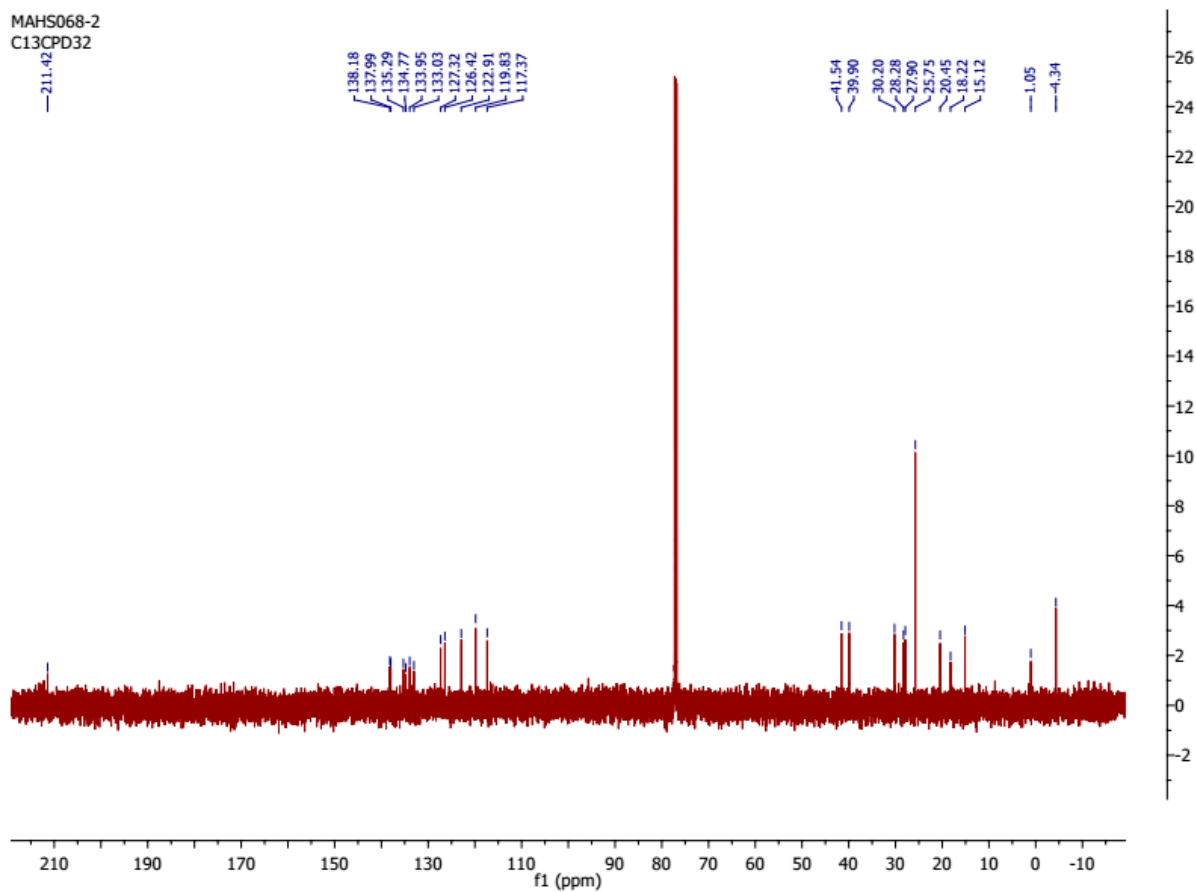


Figure S 4. ^{13}C NMR of compound **8**.

MAHS068-2
C13DEPT135

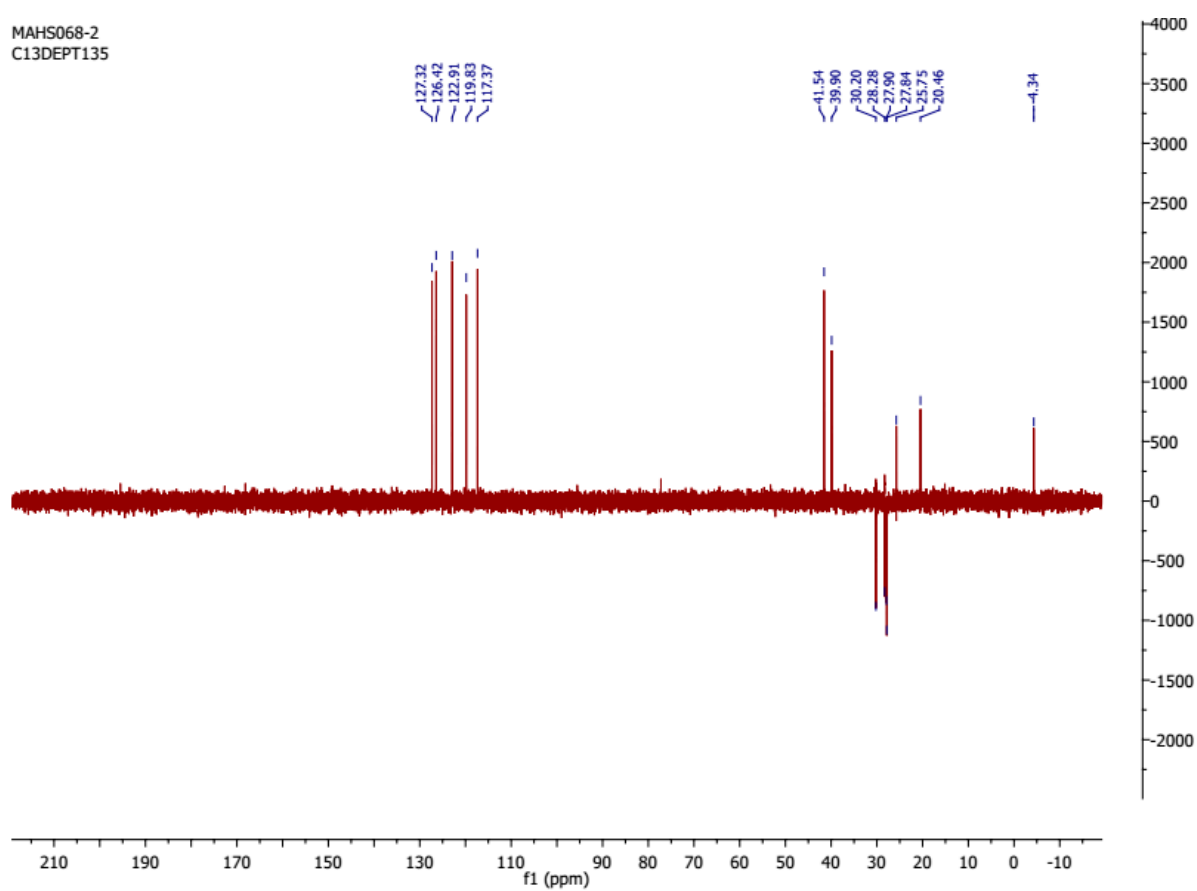


Figure S 5. DEPT135 ^{13}C NMR of compound **8**.

1.3 Compound 9

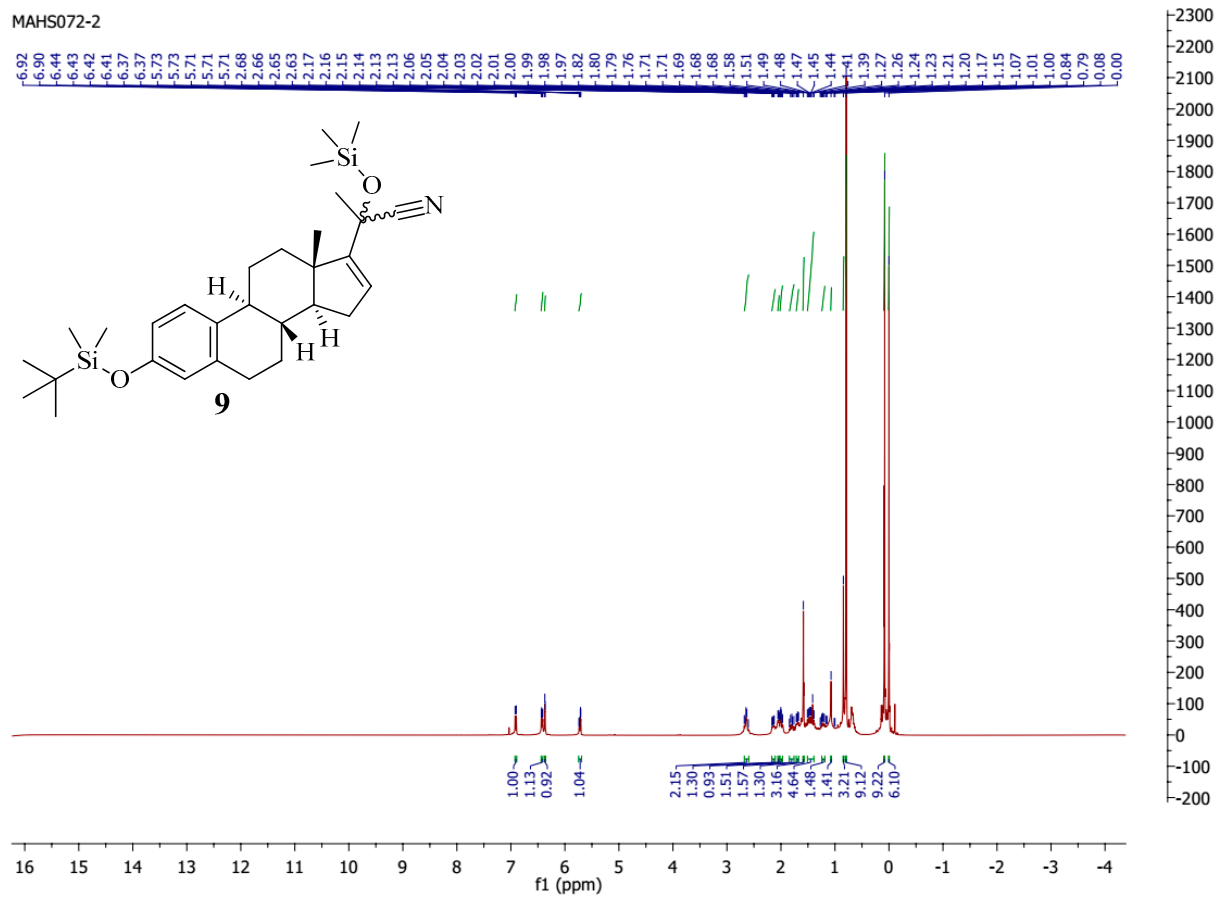


Figure S 6. ^1H NMR of compound 9.

MAHS072-2

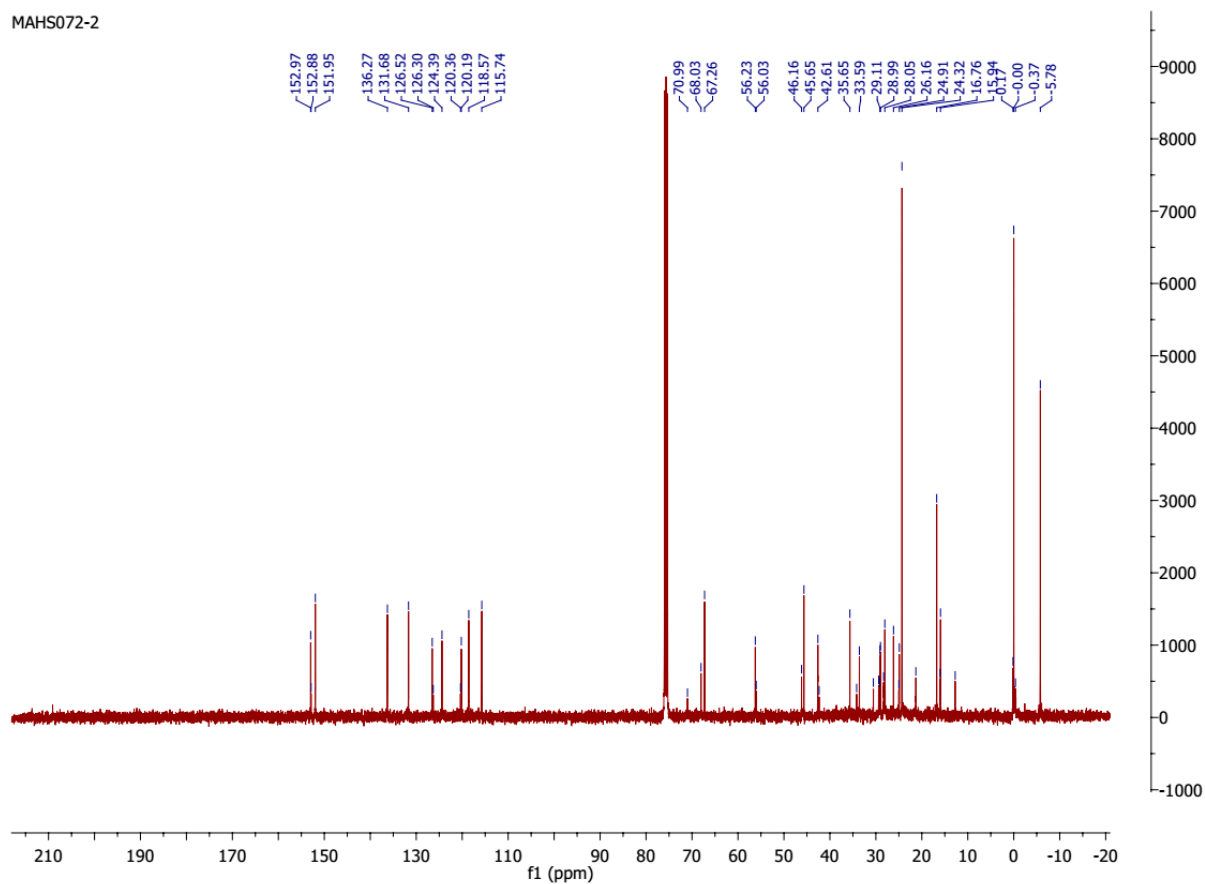


Figure S 7. ^{13}C NMR of compound **9**.

1.4 Compound 10

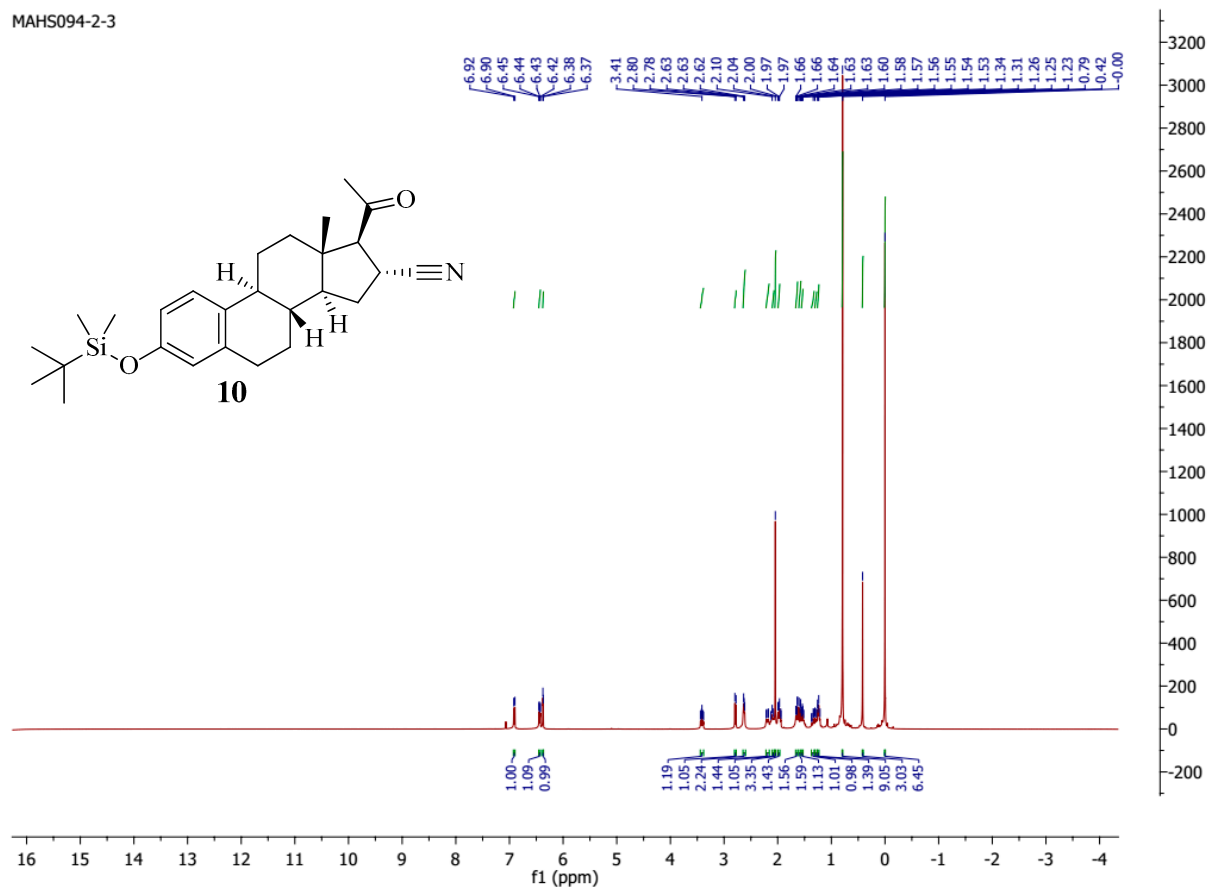


Figure S 8. ^1H NMR of compound 10.

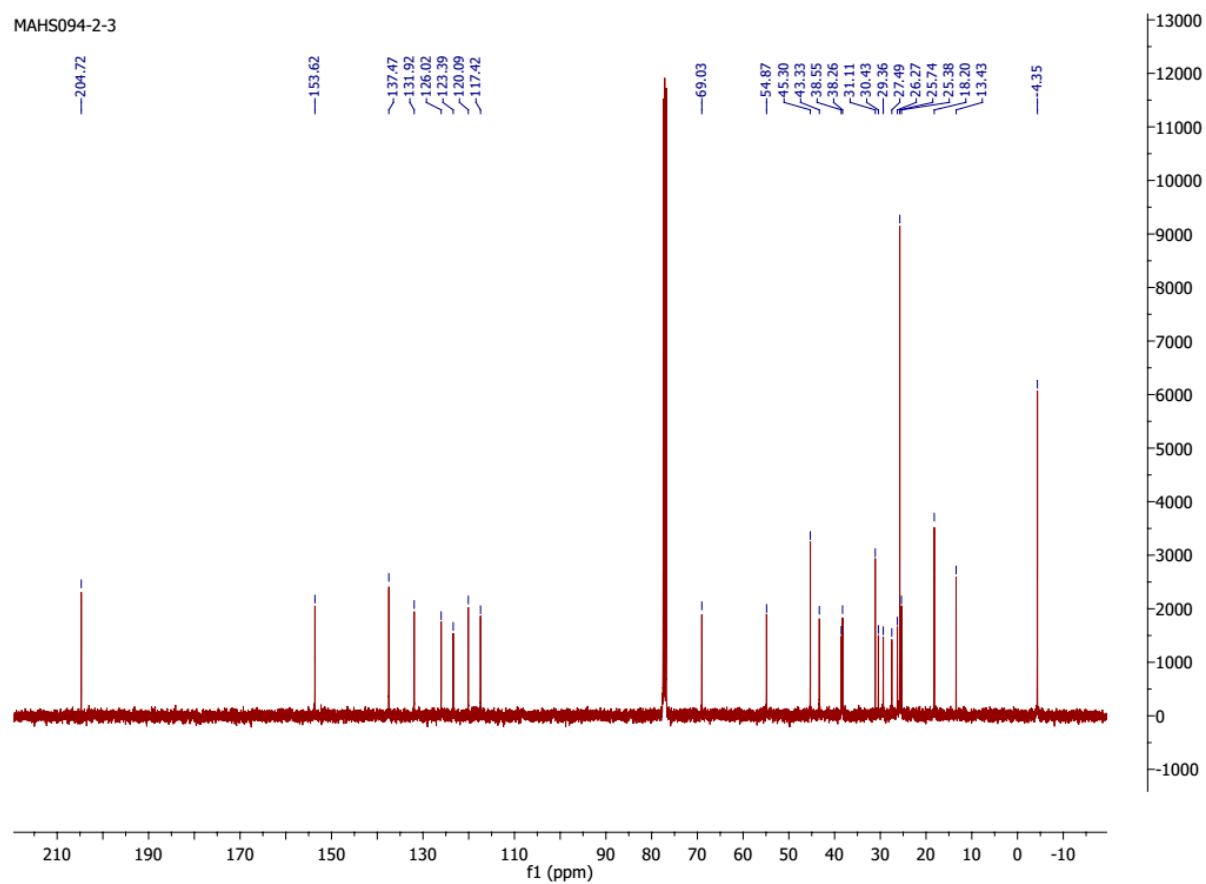


Figure S 9. ^{13}C NMR of compound **10**.

1.5 Compound 11a

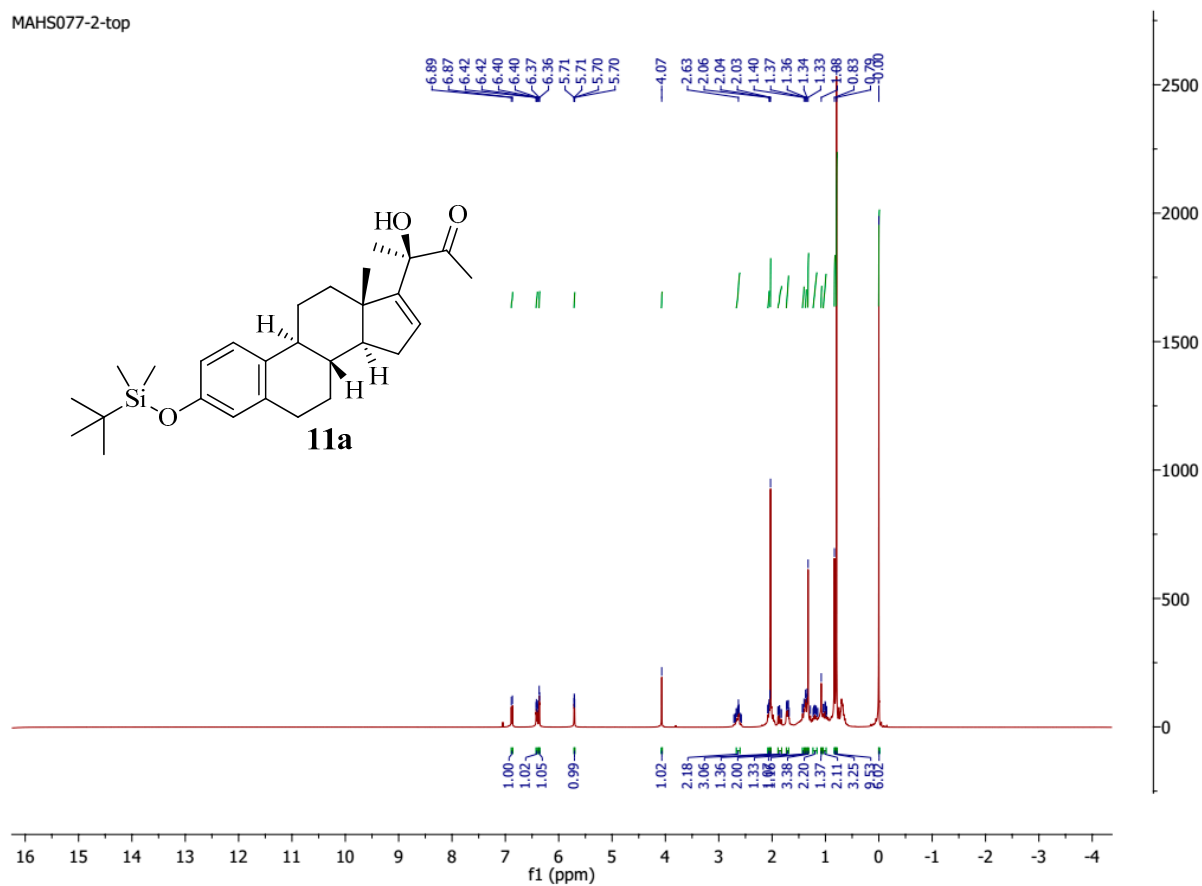


Figure S 10. ^1H NMR of compound **11a**.

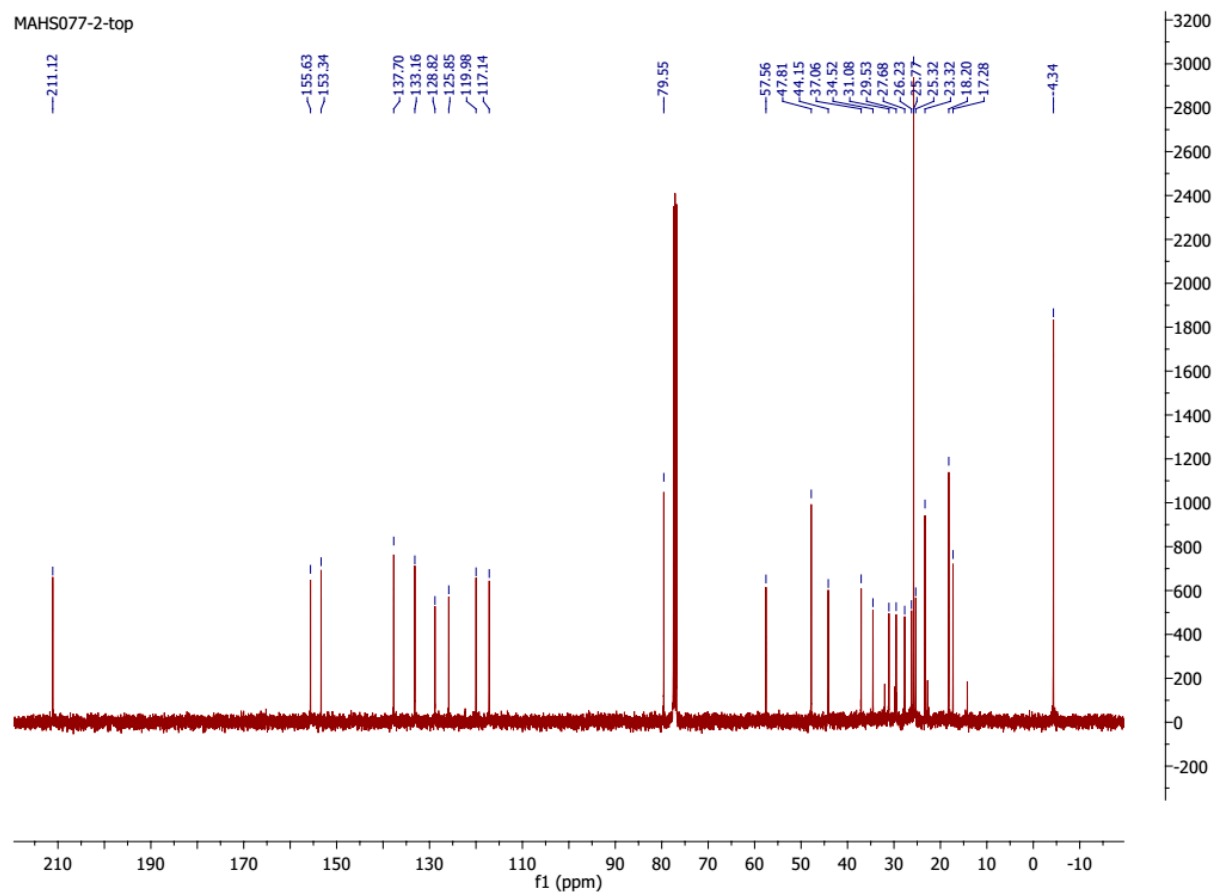


Figure S 11. ^{13}C NMR of compound **11a**.

1.6 Compound 11b

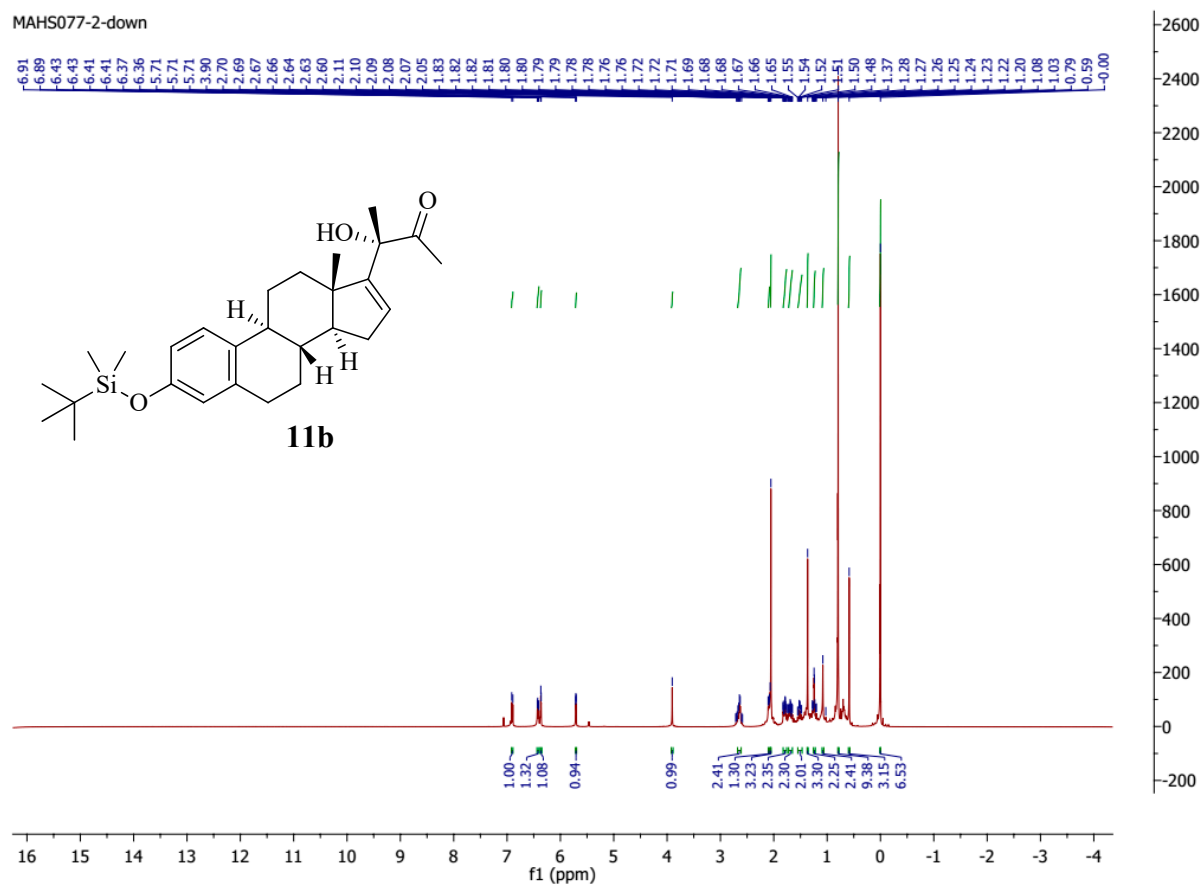


Figure S 12. ^1H NMR of compound **11b**.

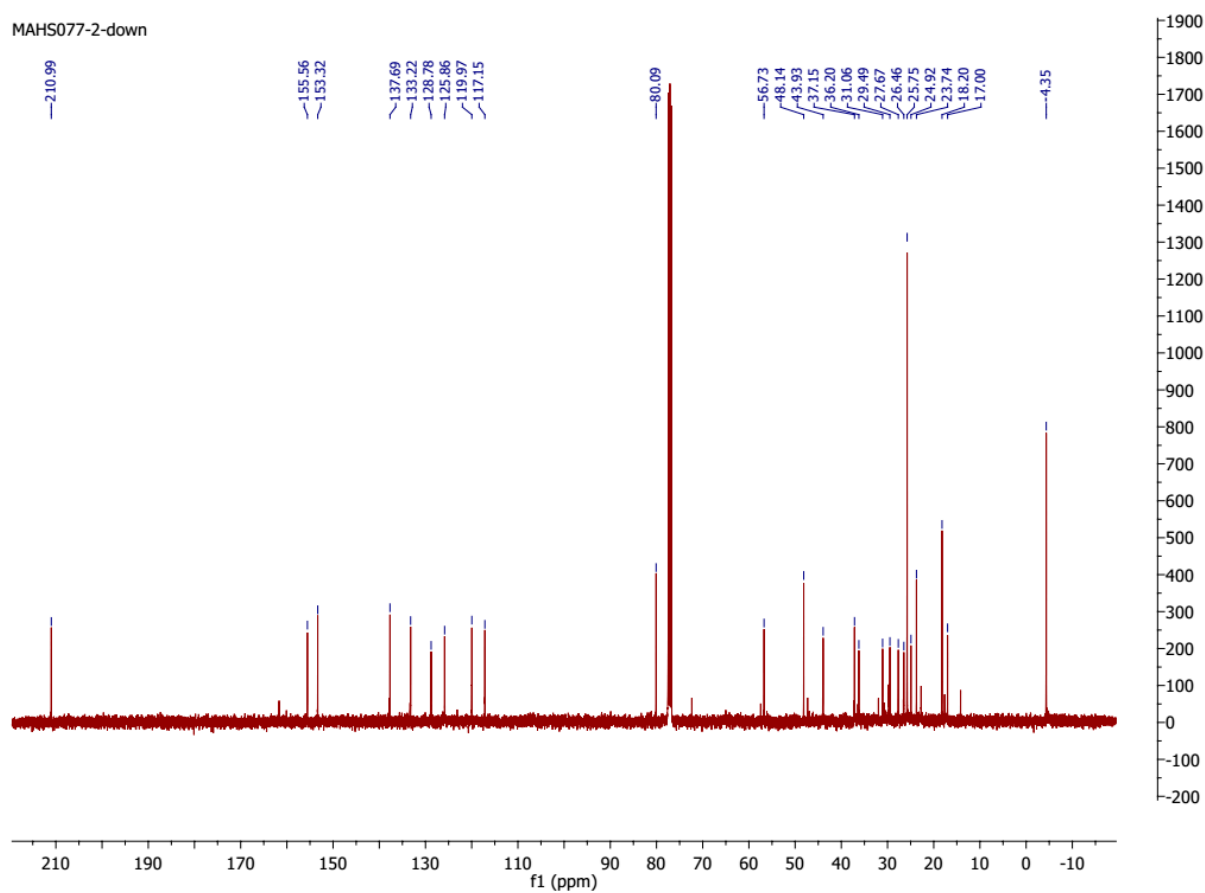


Figure S 13. ^{13}C NMR of compound **11b**.

1.7 Compound 12a

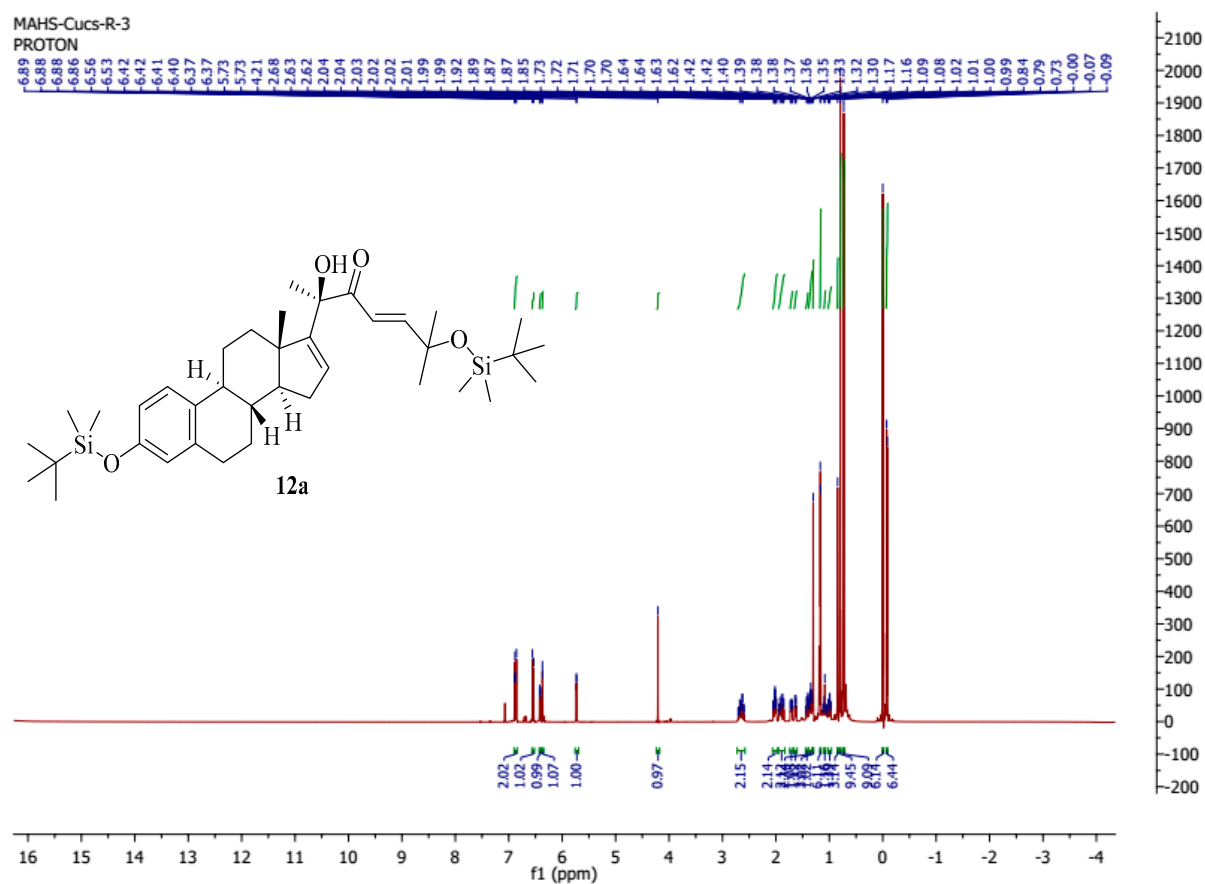


Figure S 14. ^1H NMR of compound 12a.

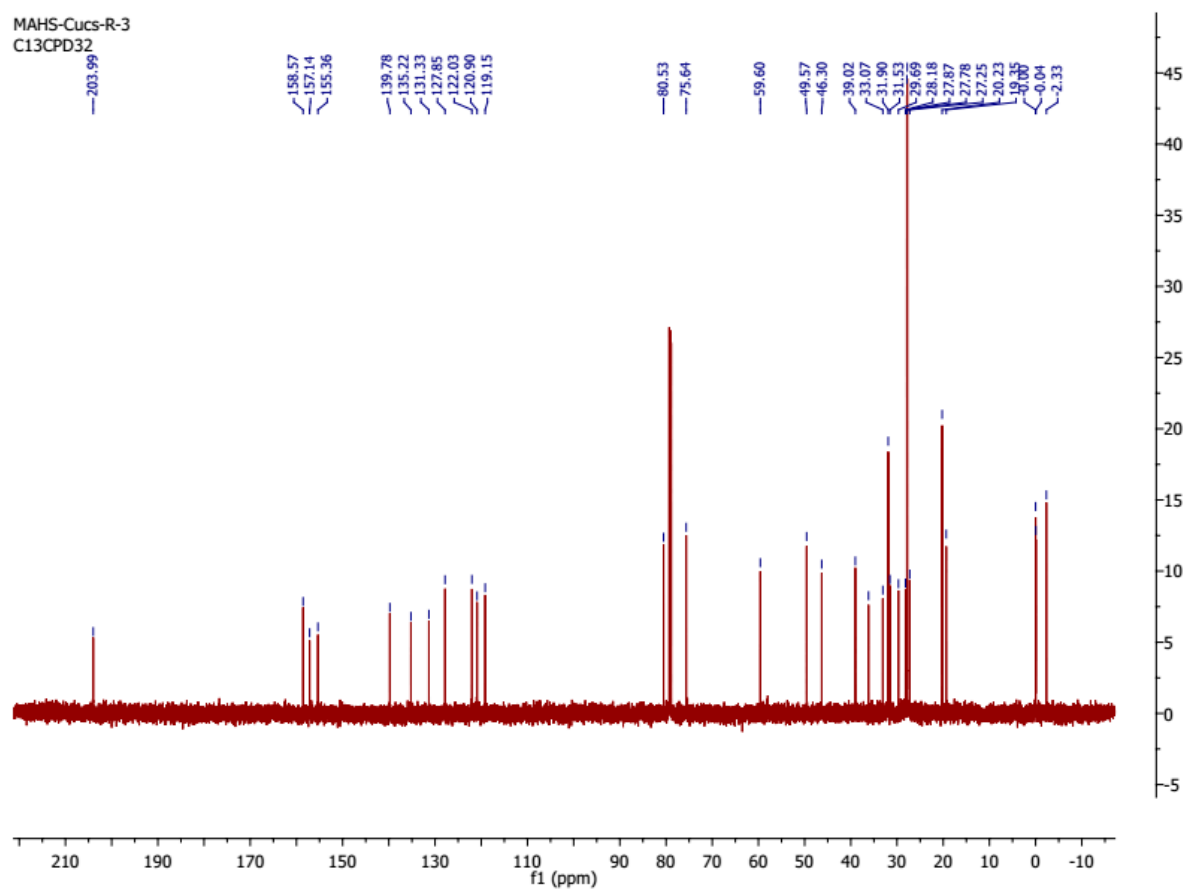


Figure S 15. ^{13}C NMR of compound **12a**.

1.8 Compound 12b

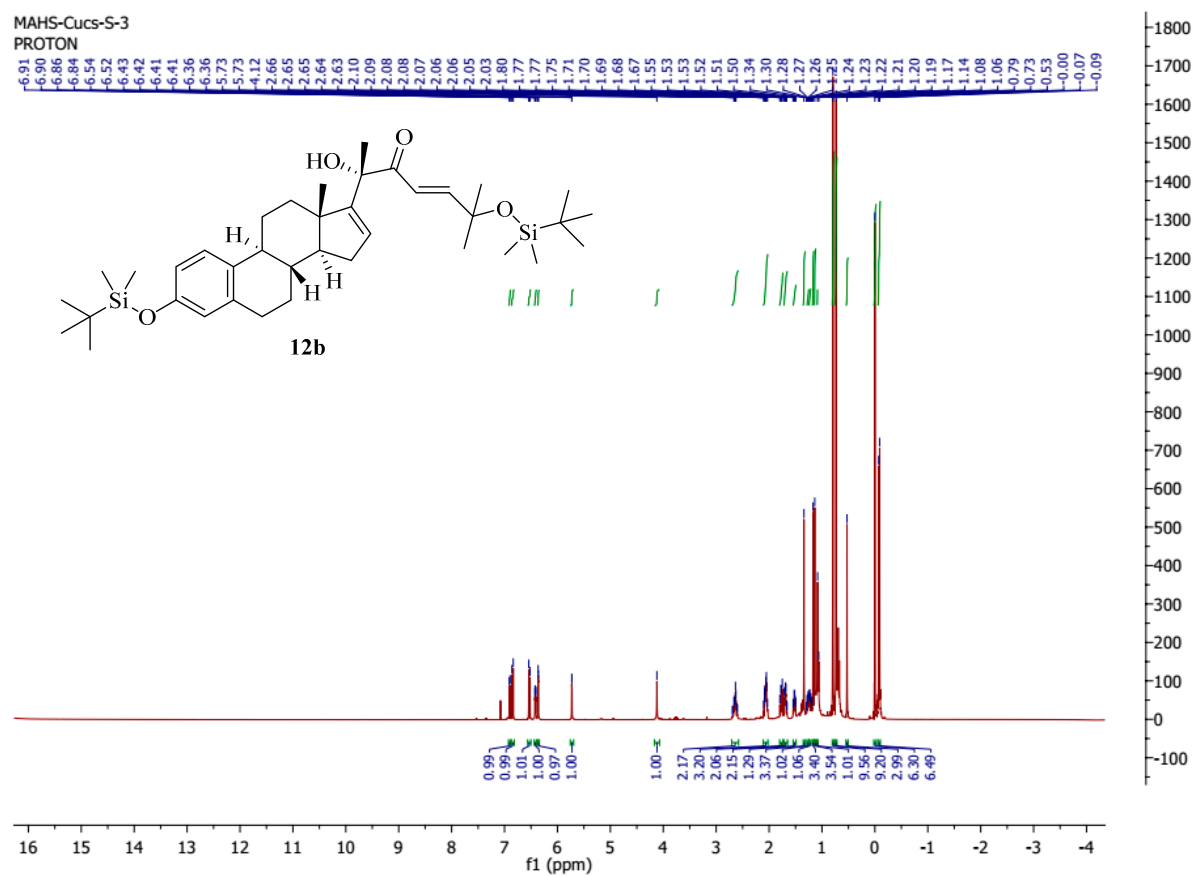


Figure S 16. ^1H NMR of compound 12b.

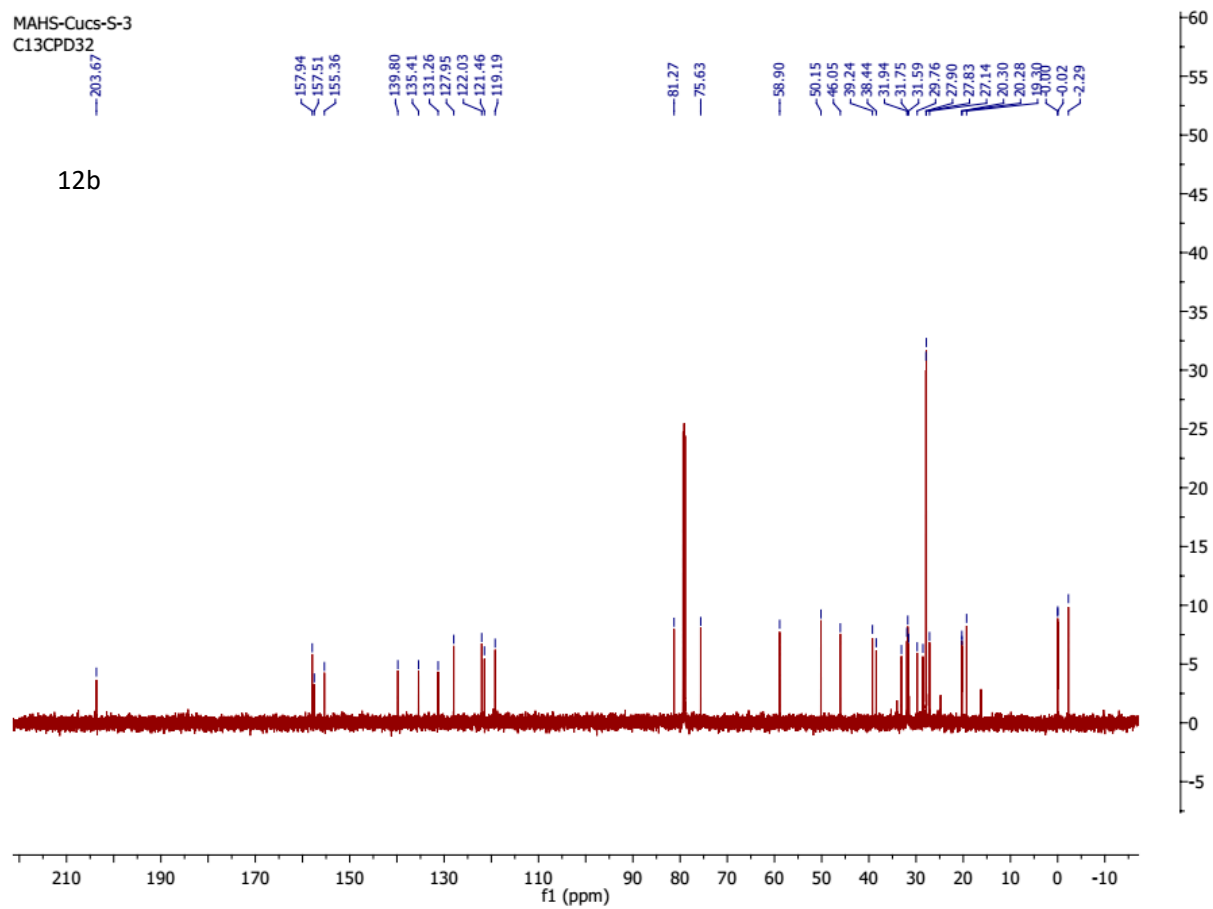


Figure S 17. ^{13}C NMR of compound **12b**.

1.9 Compound 13a

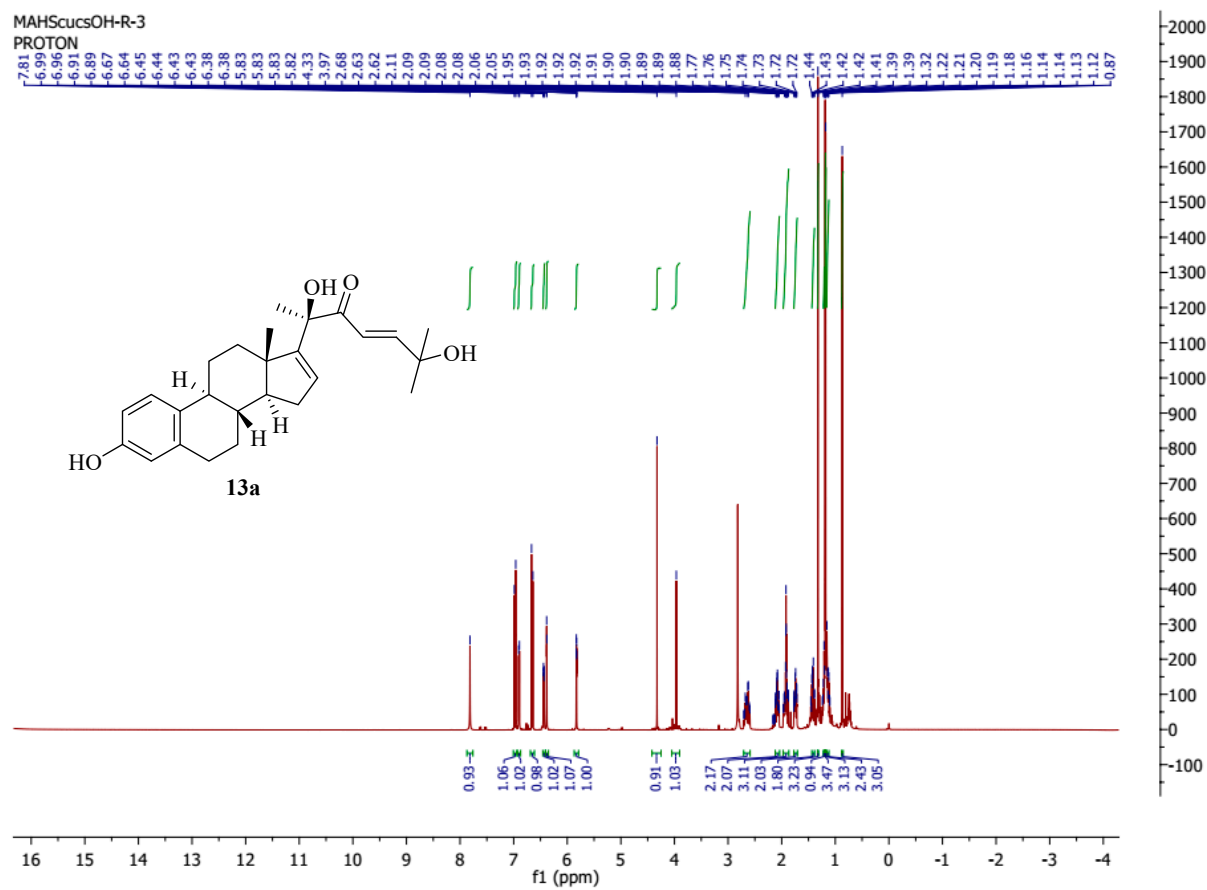


Figure S 18. ^1H NMR of compound **13a**.

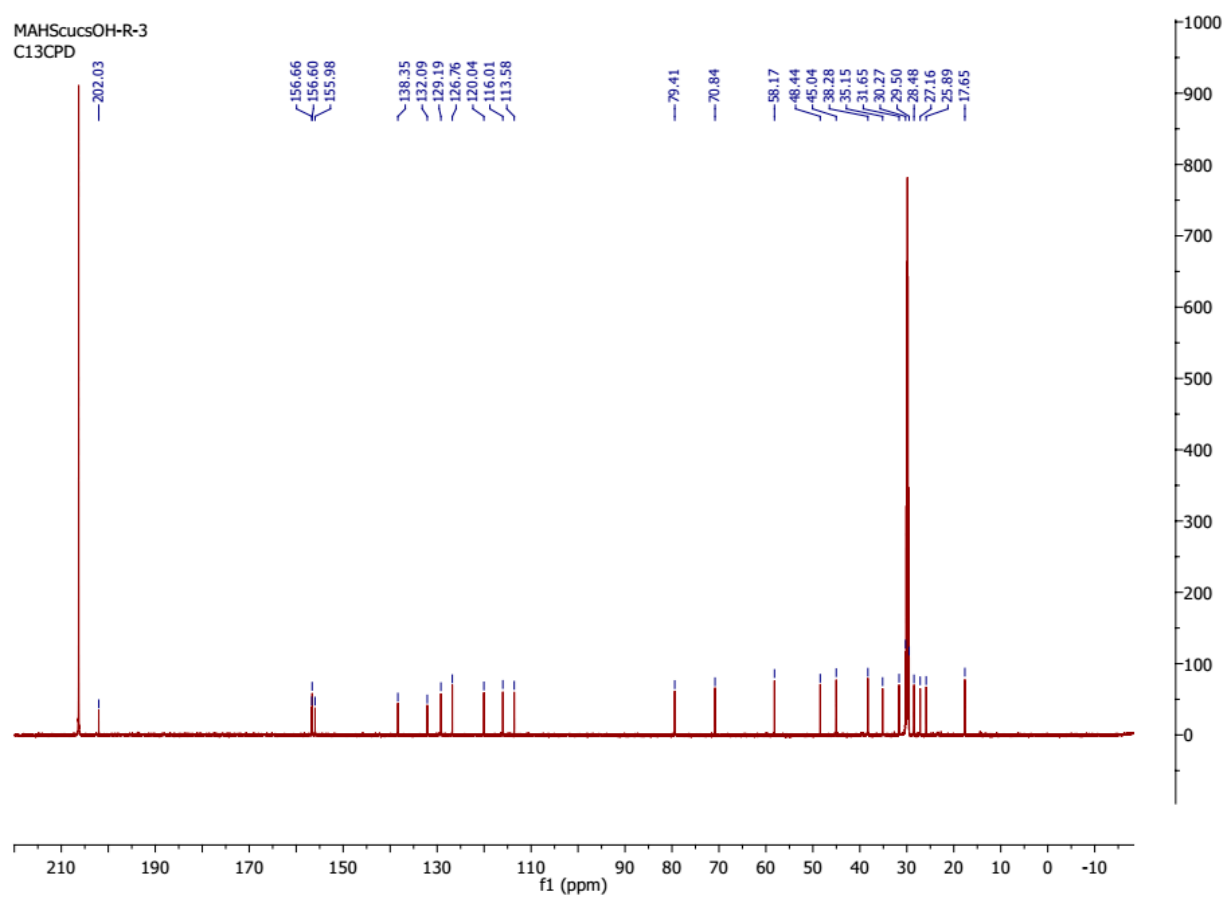
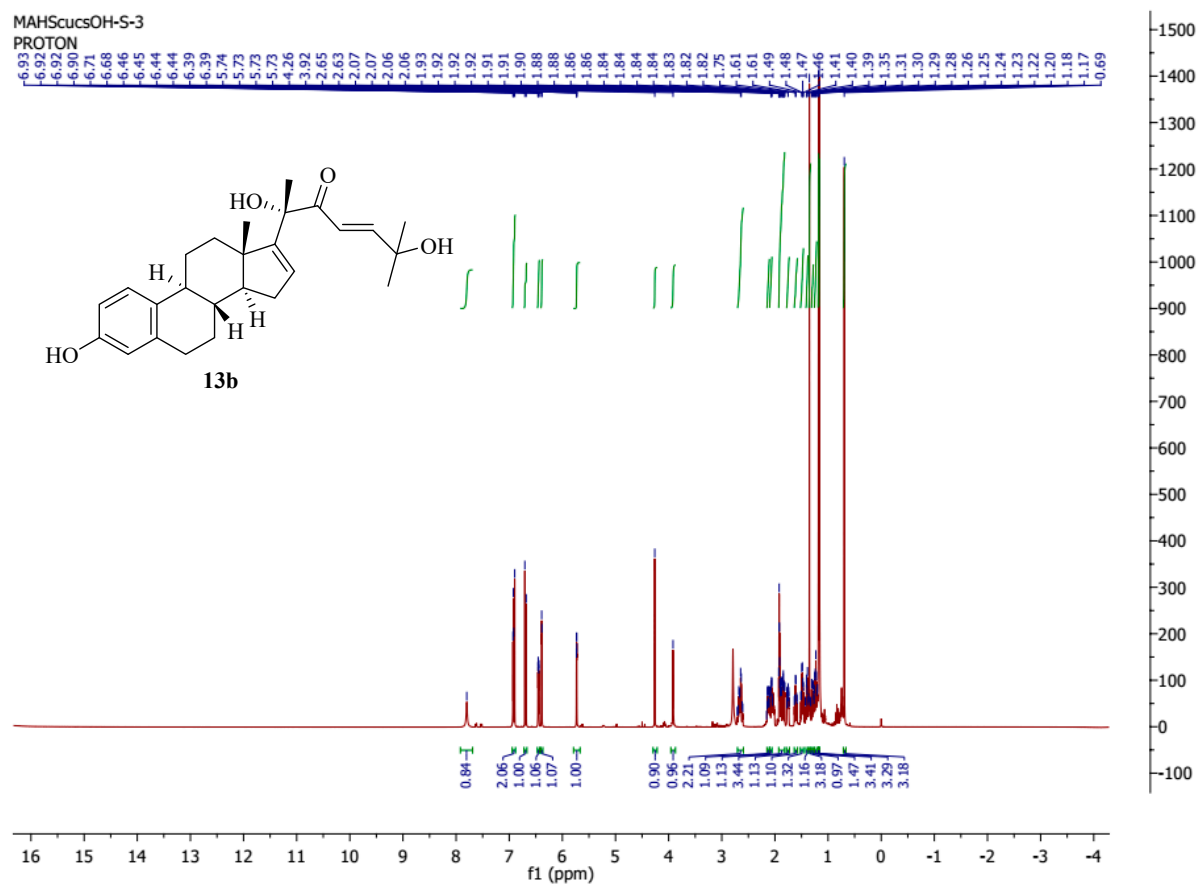


Figure S 19. ^{13}C NMR of compound **13a**.

Figure S 20. ^1H NMR of compound **13b**.



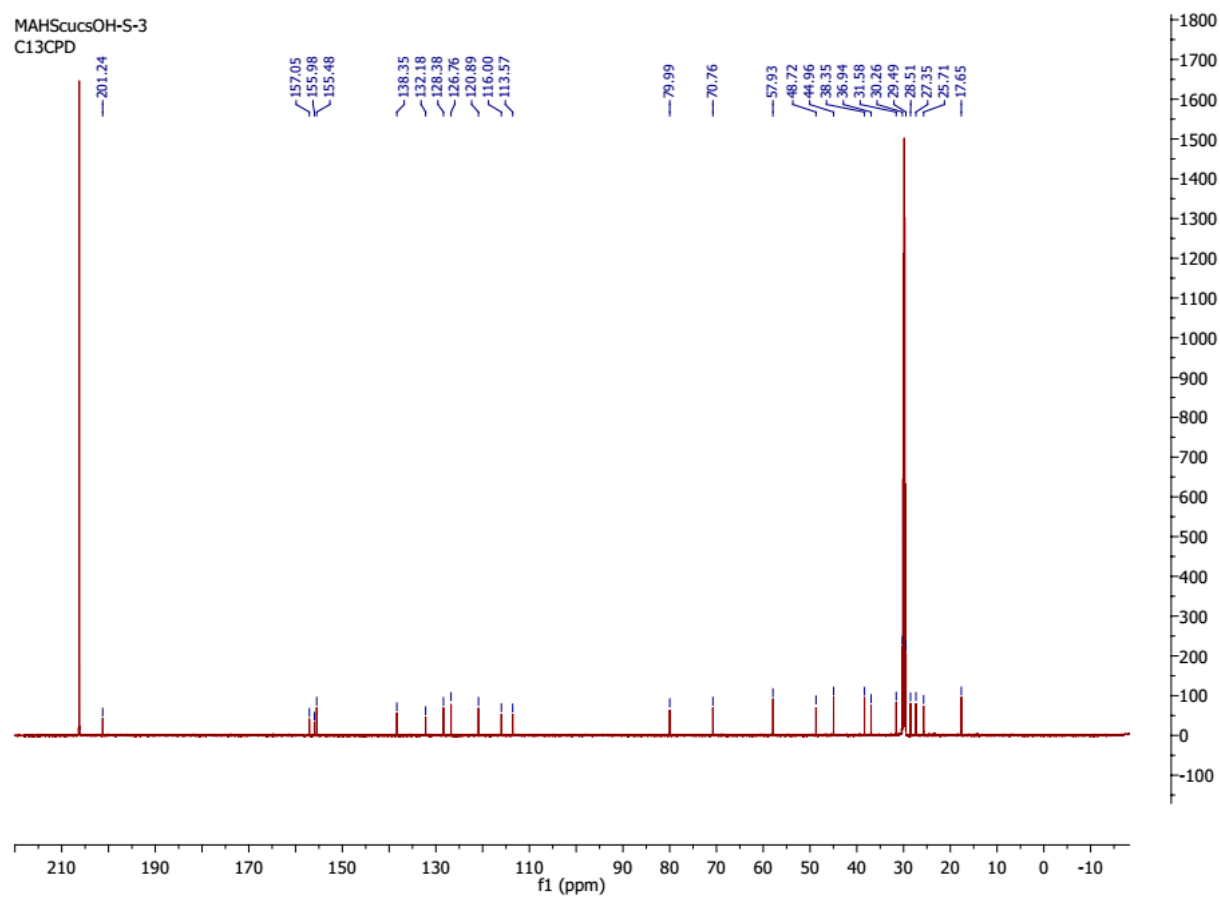


Figure S 21. ^{13}C NMR of compound **13b**.

1.11 Compound 14a

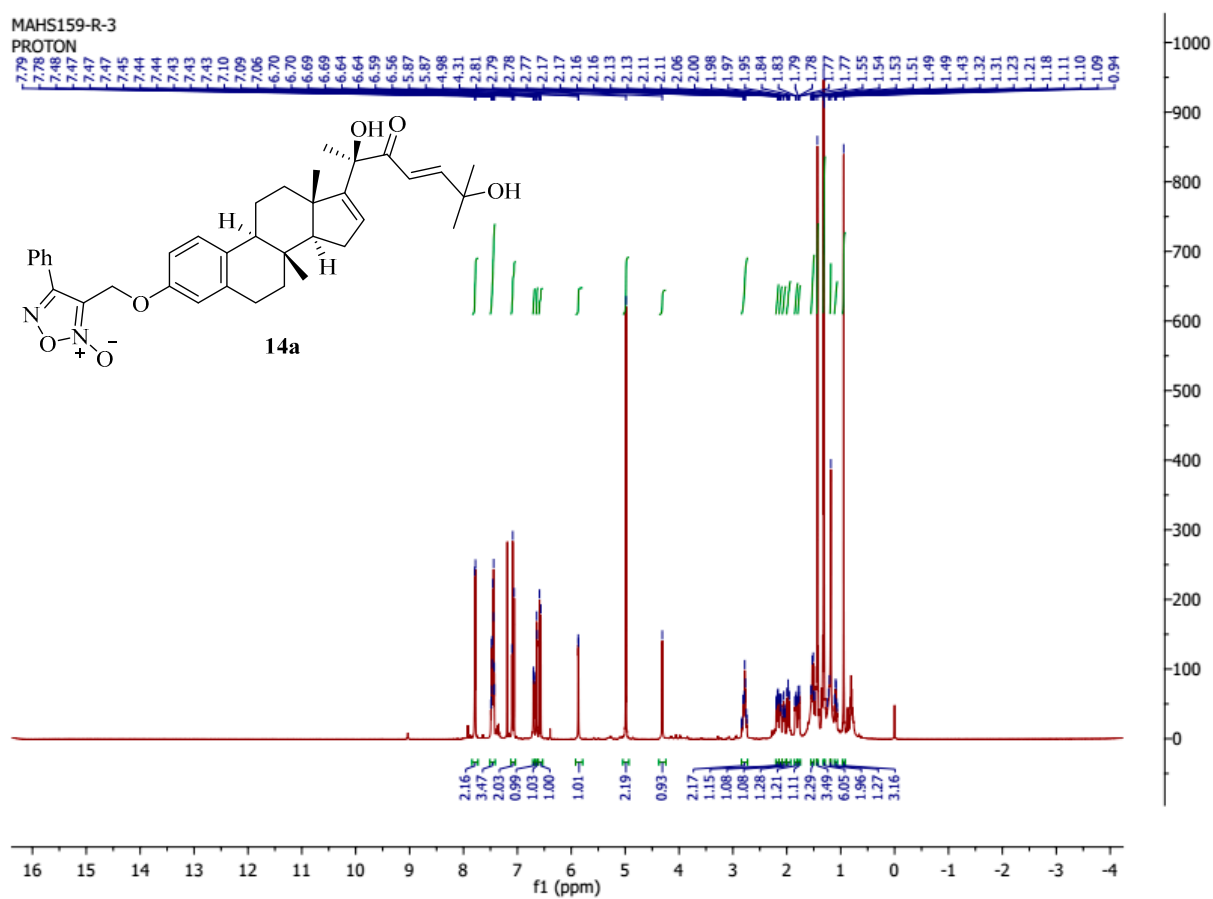


Figure S 22. ^1H NMR of compound 14a.

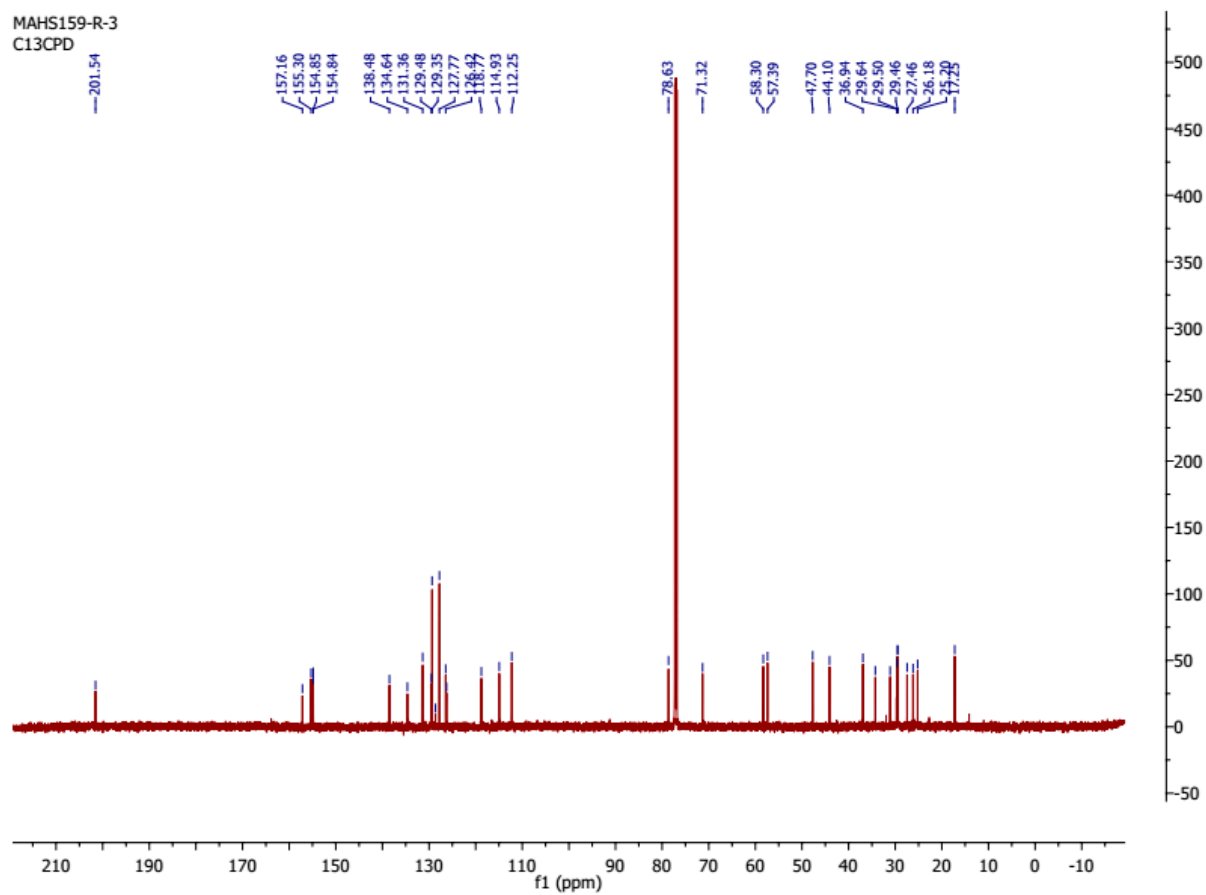


Figure S 23. ^{13}C NMR of compound **14a**.

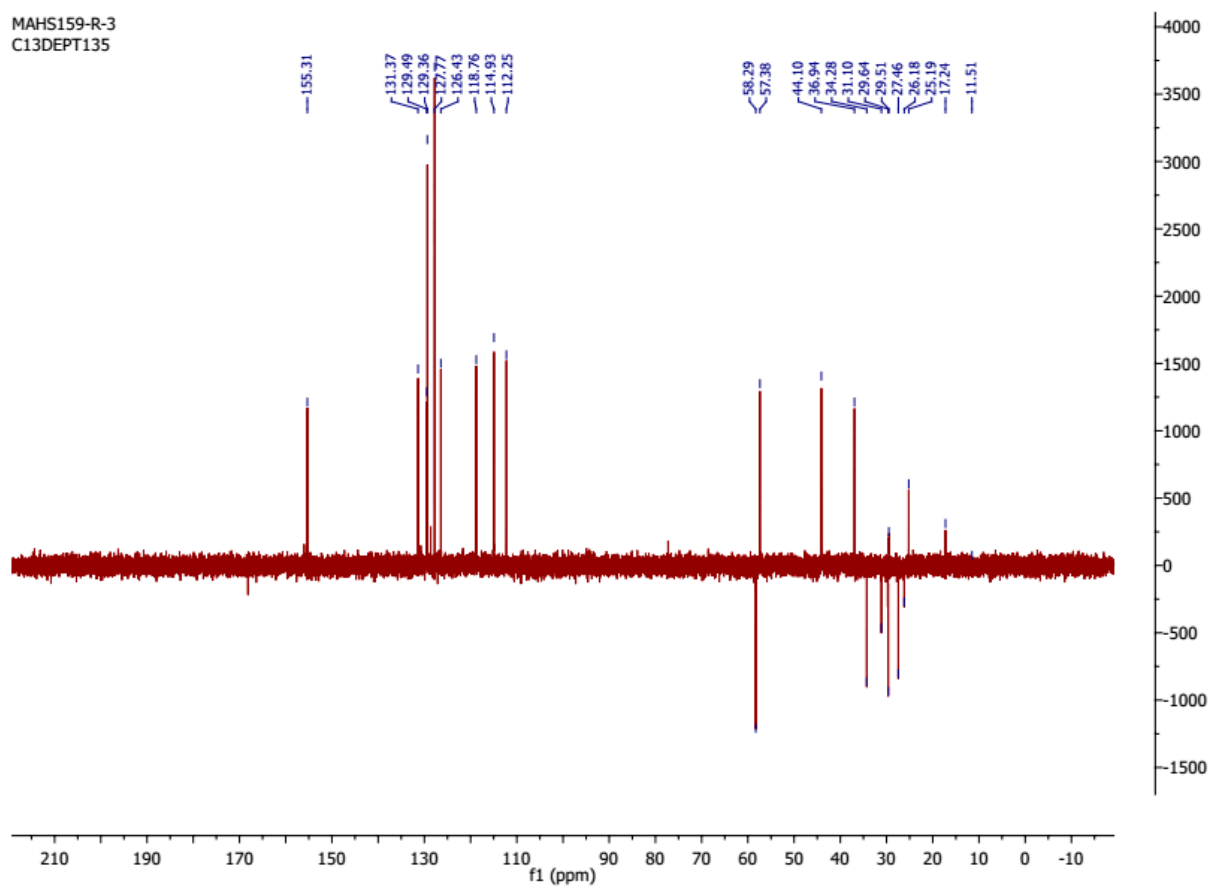


Figure S 24. DEPT135 ^{13}C NMR of compound **14a**.

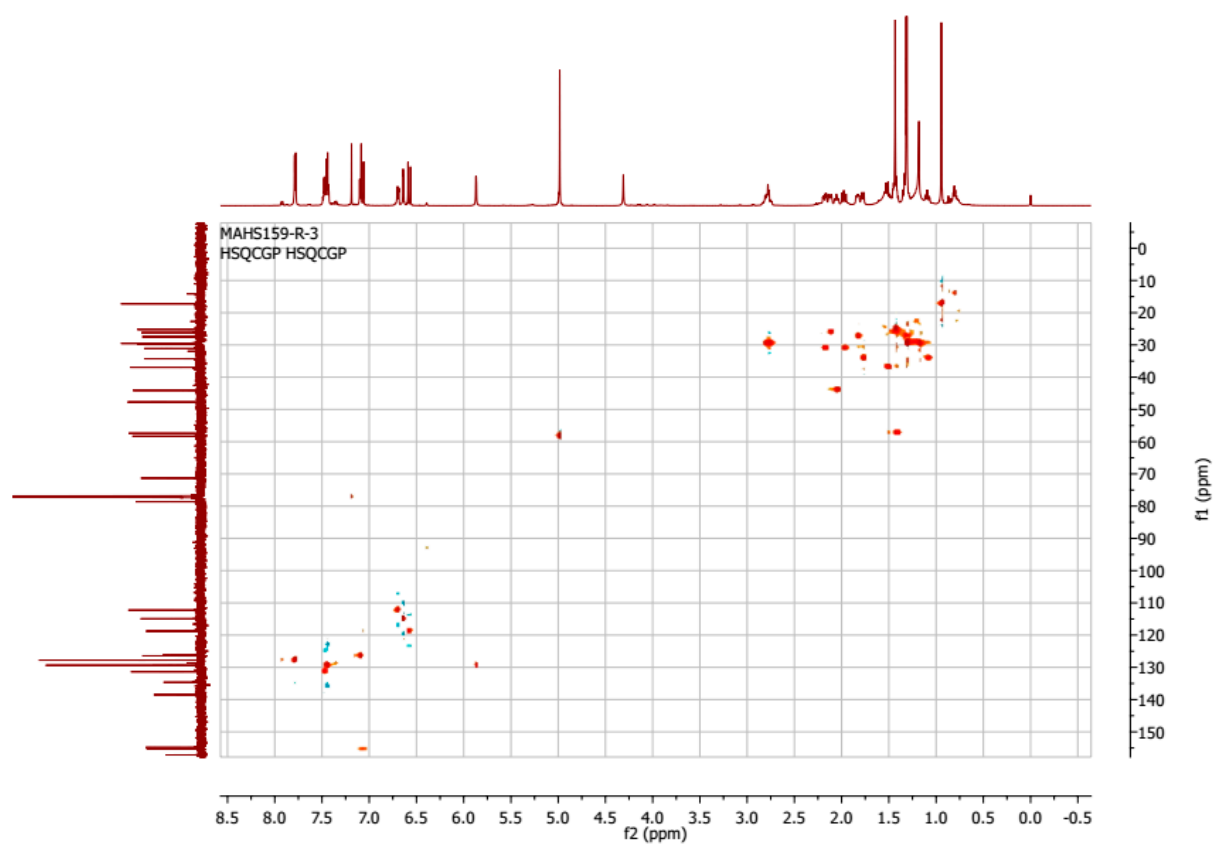


Figure S 25. HSQC GP of compound **14a**.

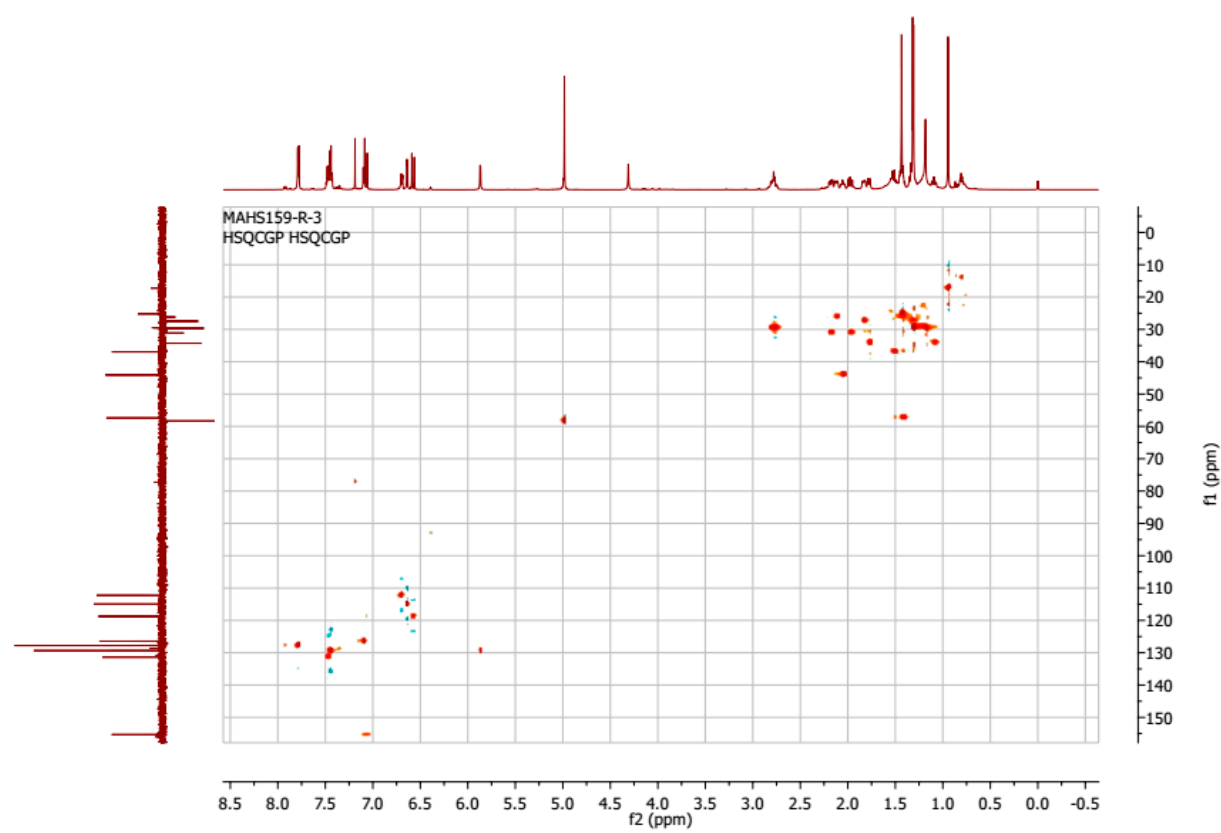


Figure S 26. HSQCGP of compound **14a**.

1.12 Compound 14b

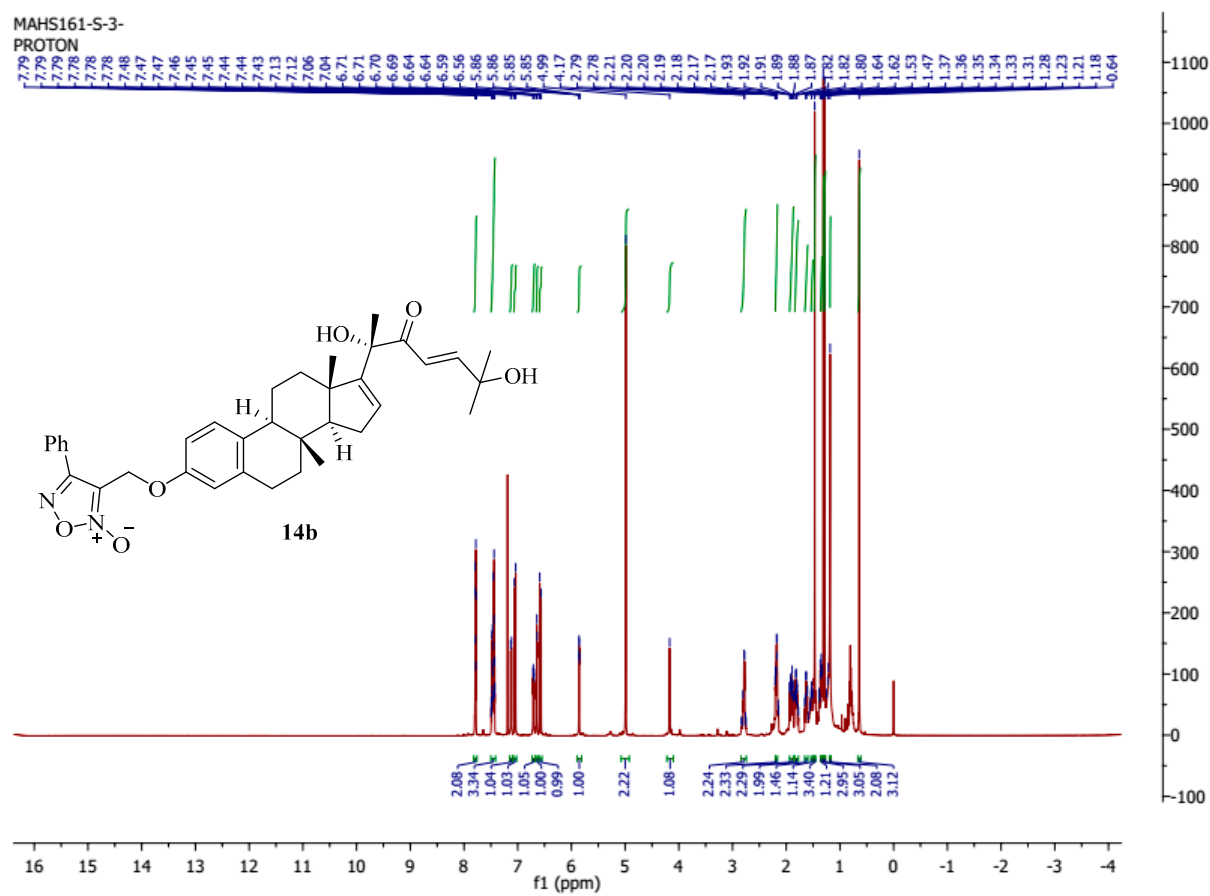


Figure S 27. ¹H NMR of compound 14b.

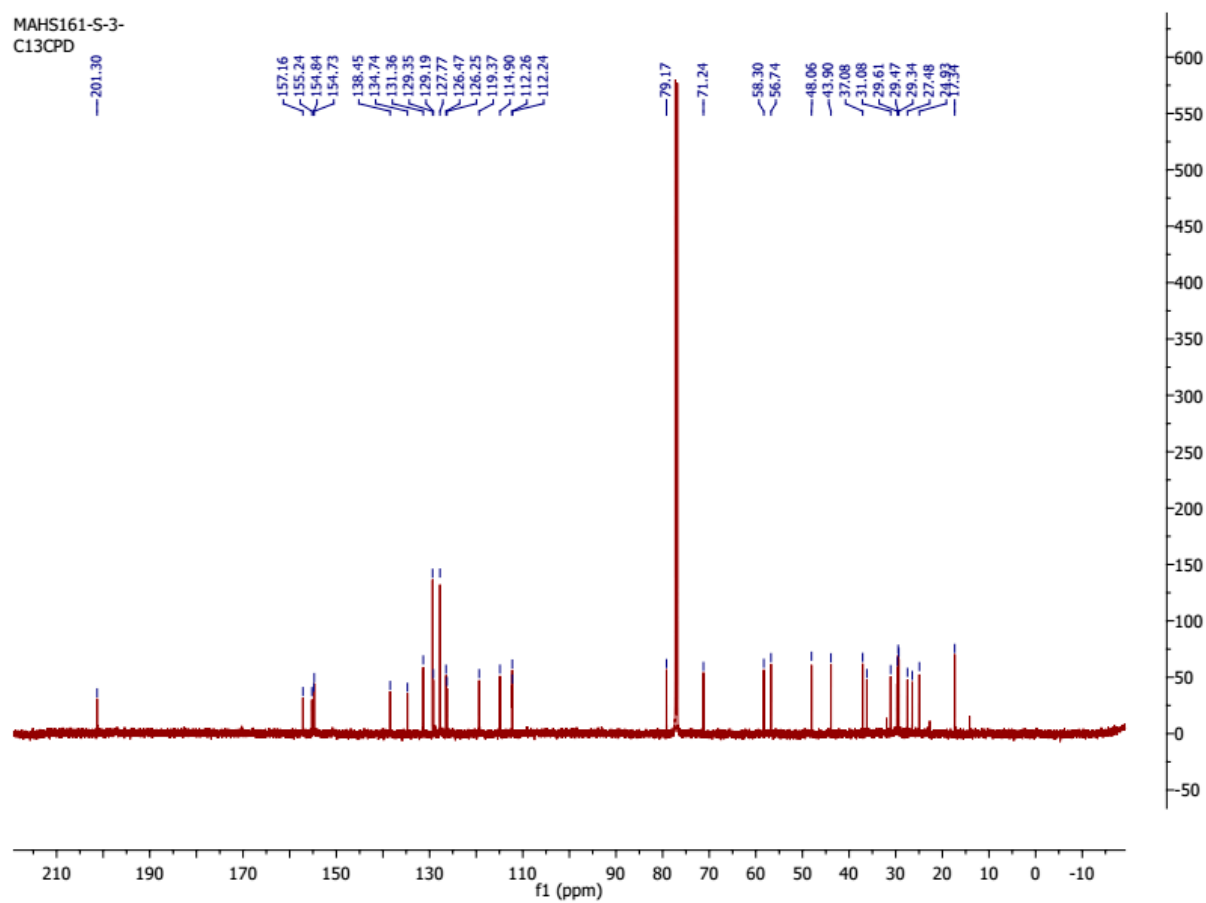


Figure S 28. ^{13}C NMR of compound **14b**.

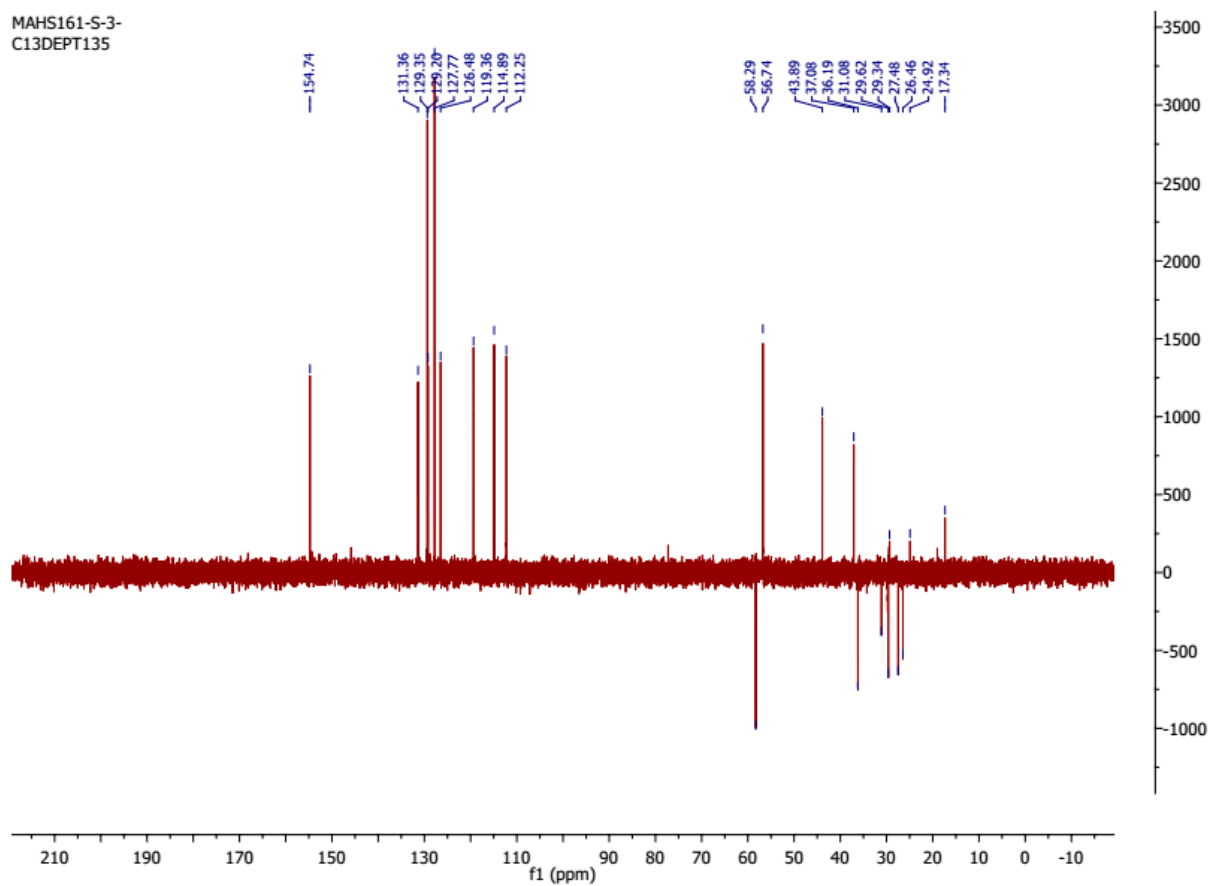


Figure S 29. DEPT135 ^{13}C NMR of compound **14b**.

1.13 Compound 15a

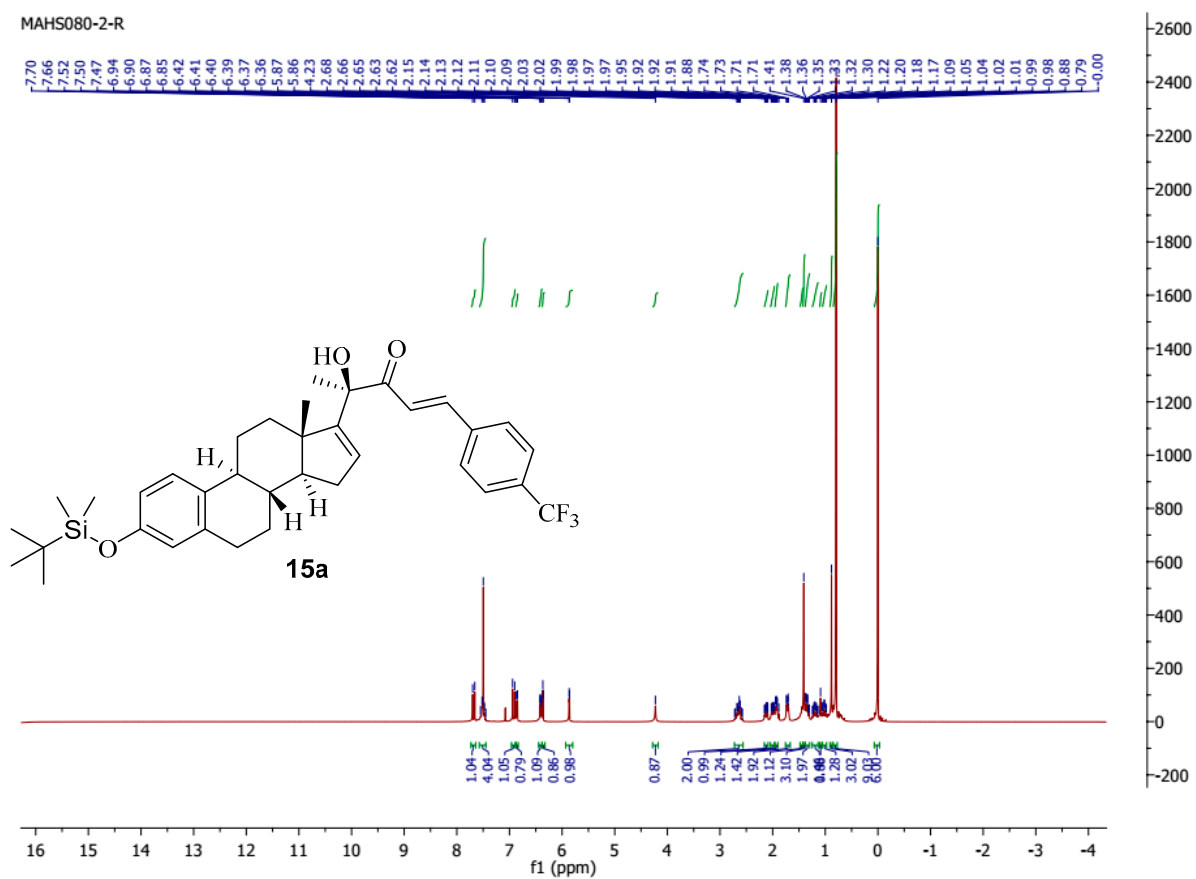


Figure S 30. ¹H NMR of compound **15a**.

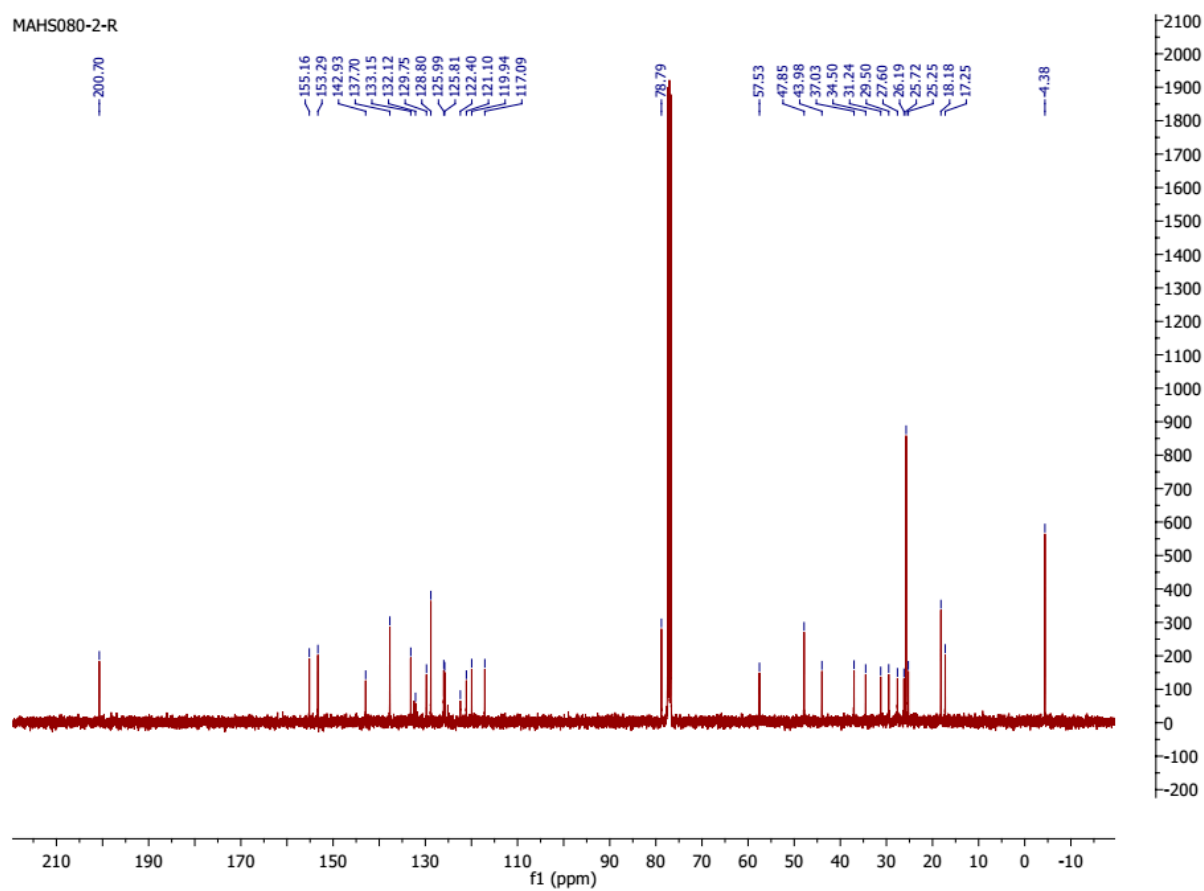


Figure S 31. ^{13}C NMR of compound **15a**.

1.14 Compound 15b

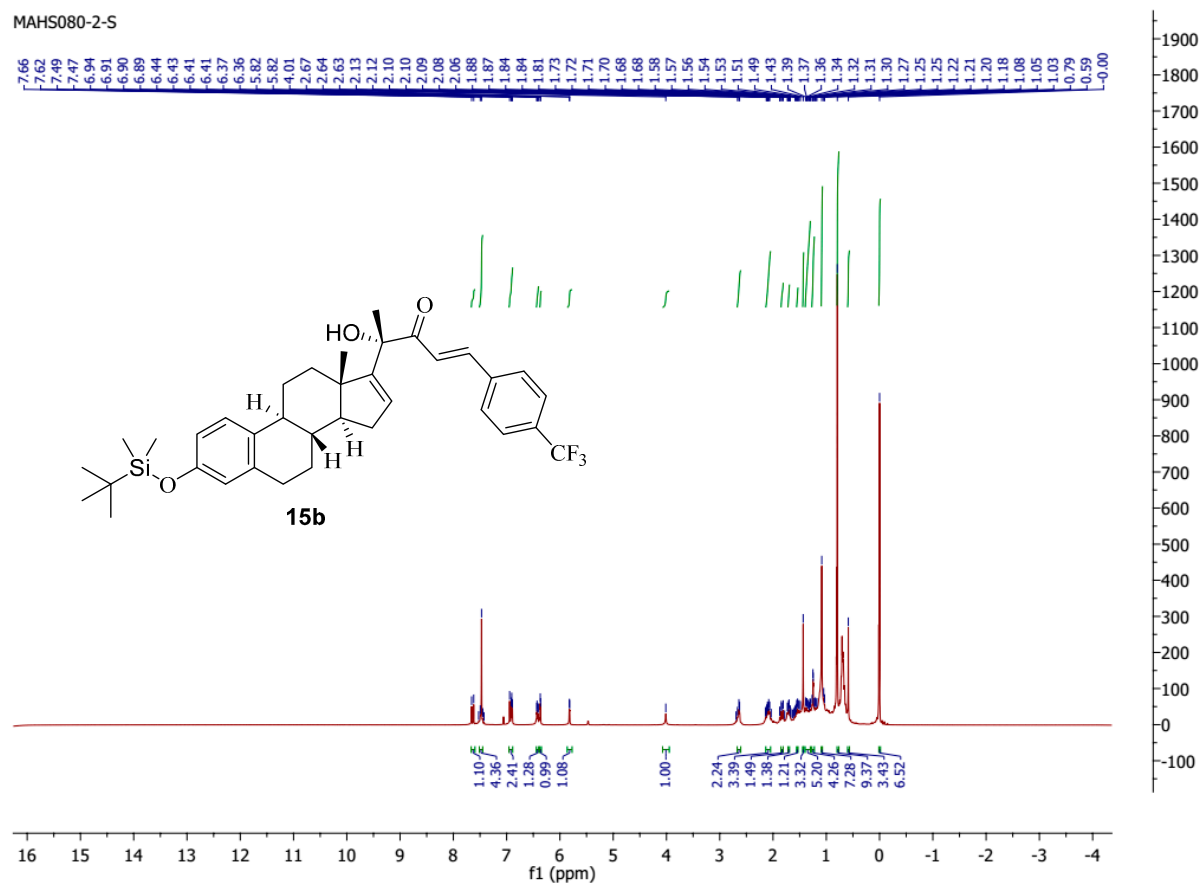


Figure S 32. ^1H NMR of compound **15b**.

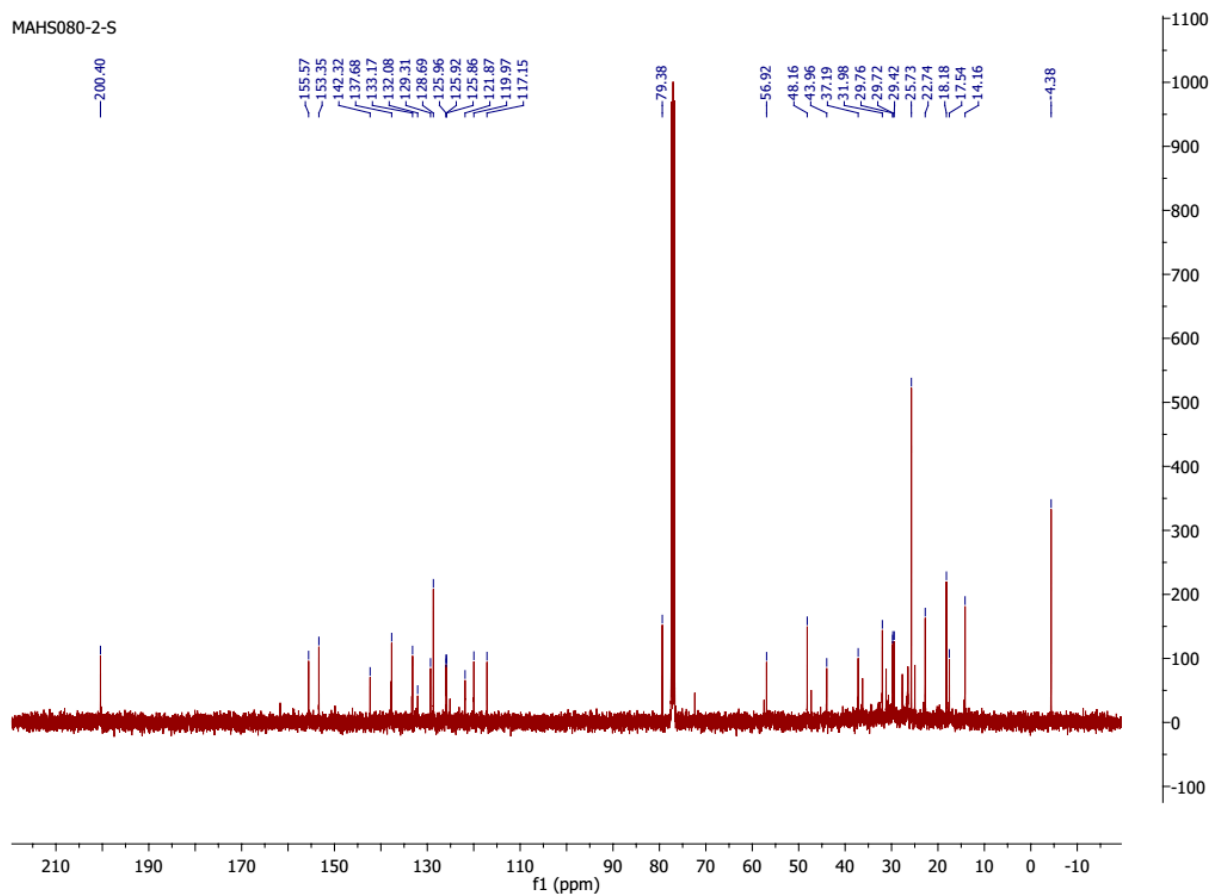


Figure S 33. ^{13}C NMR of compound **15b**.

1.15 Compound 15c

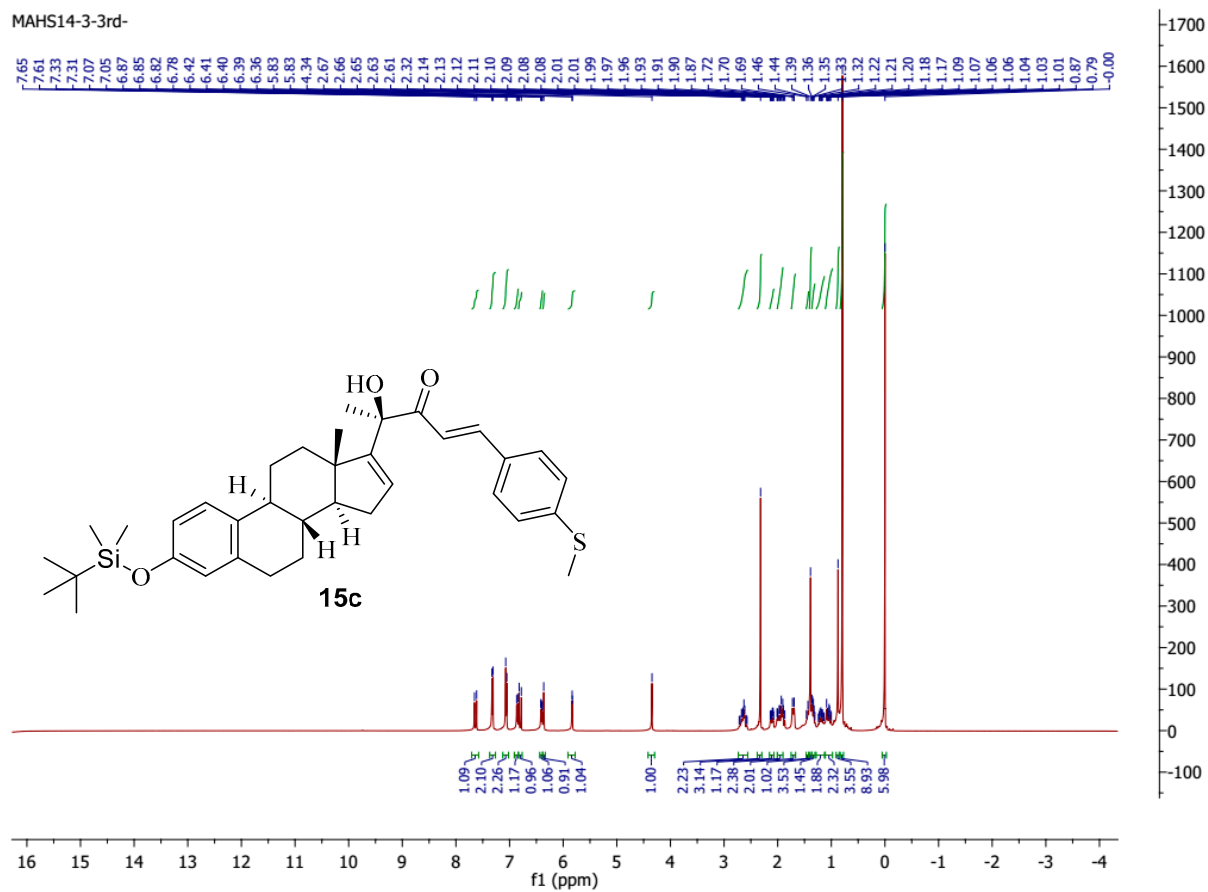


Figure S 34. ^1H NMR of compound **15c**.

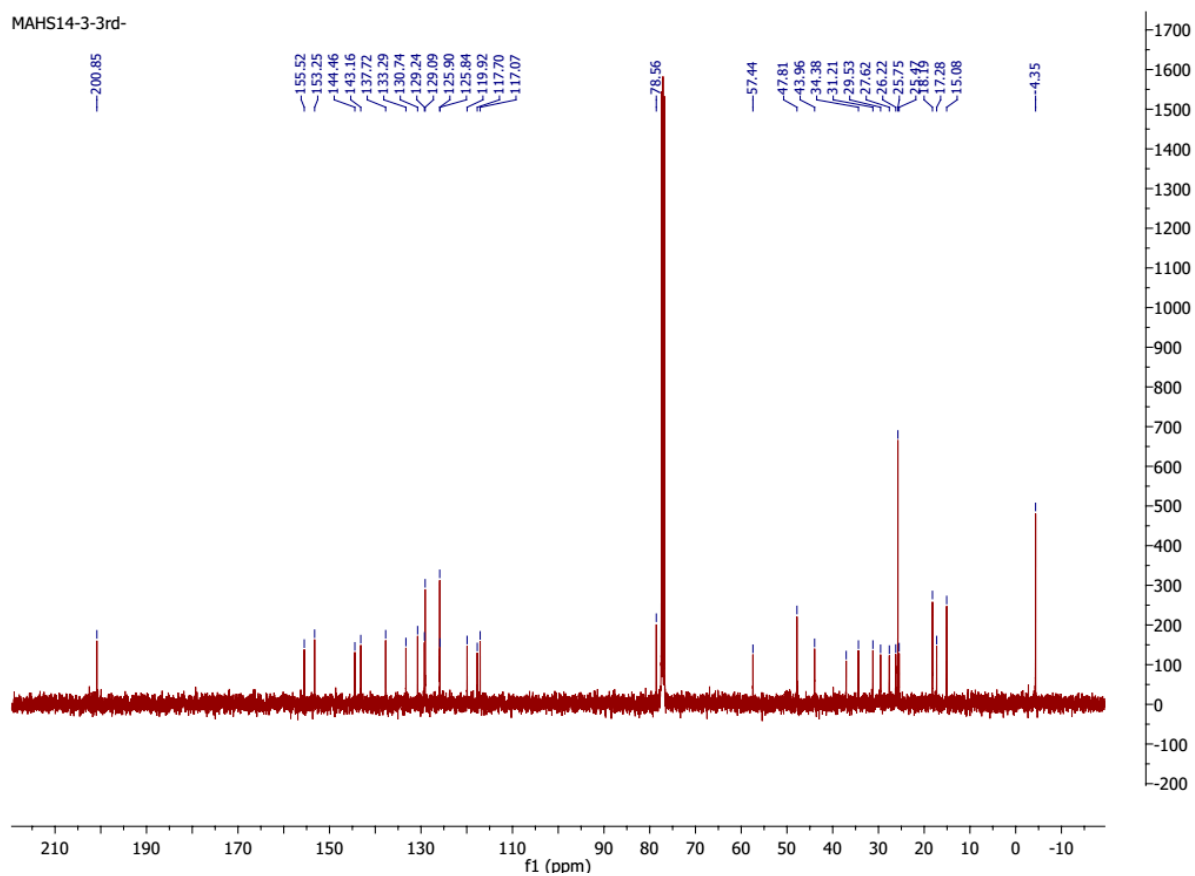


Figure S 35. ^{13}C NMR of compound **15c**.

1.16 Compound 15d

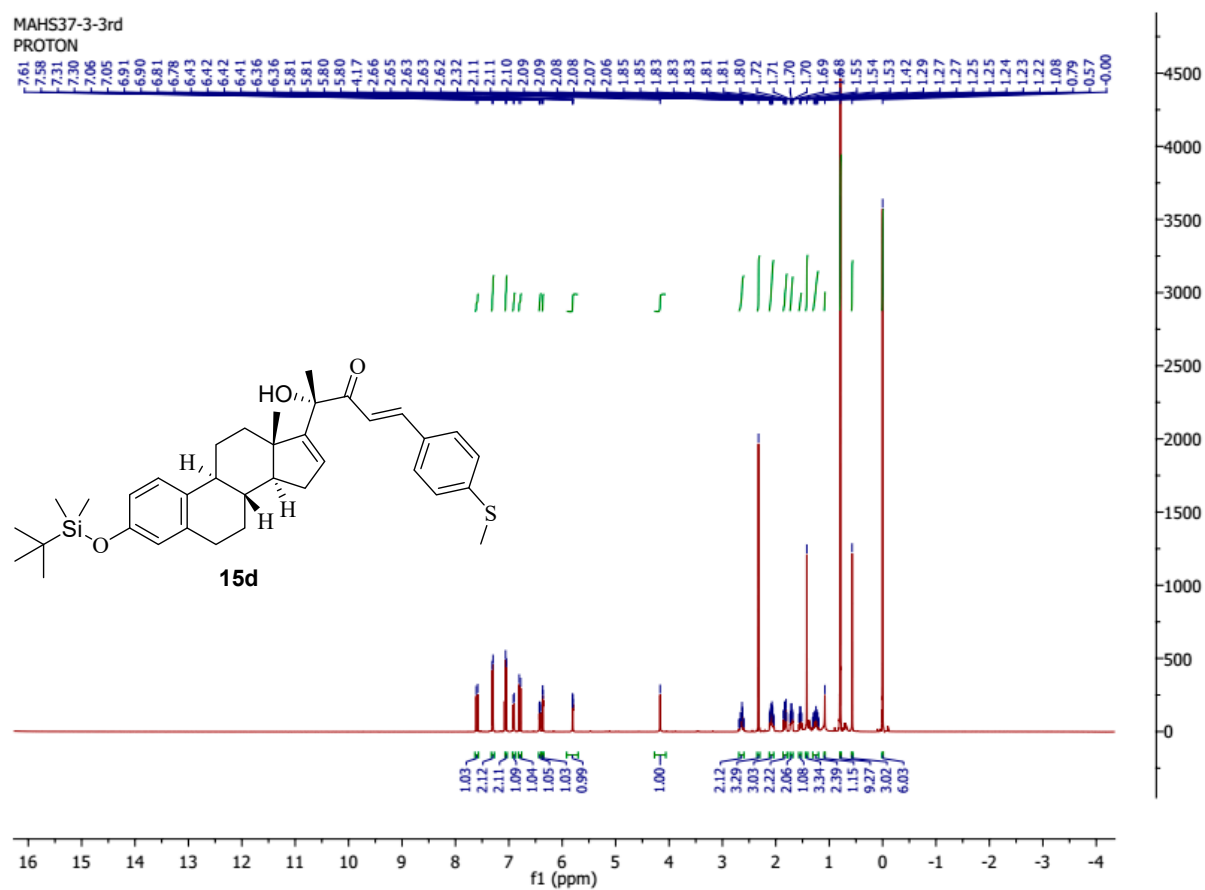


Figure S 36. ^1H NMR of compound **15d**.

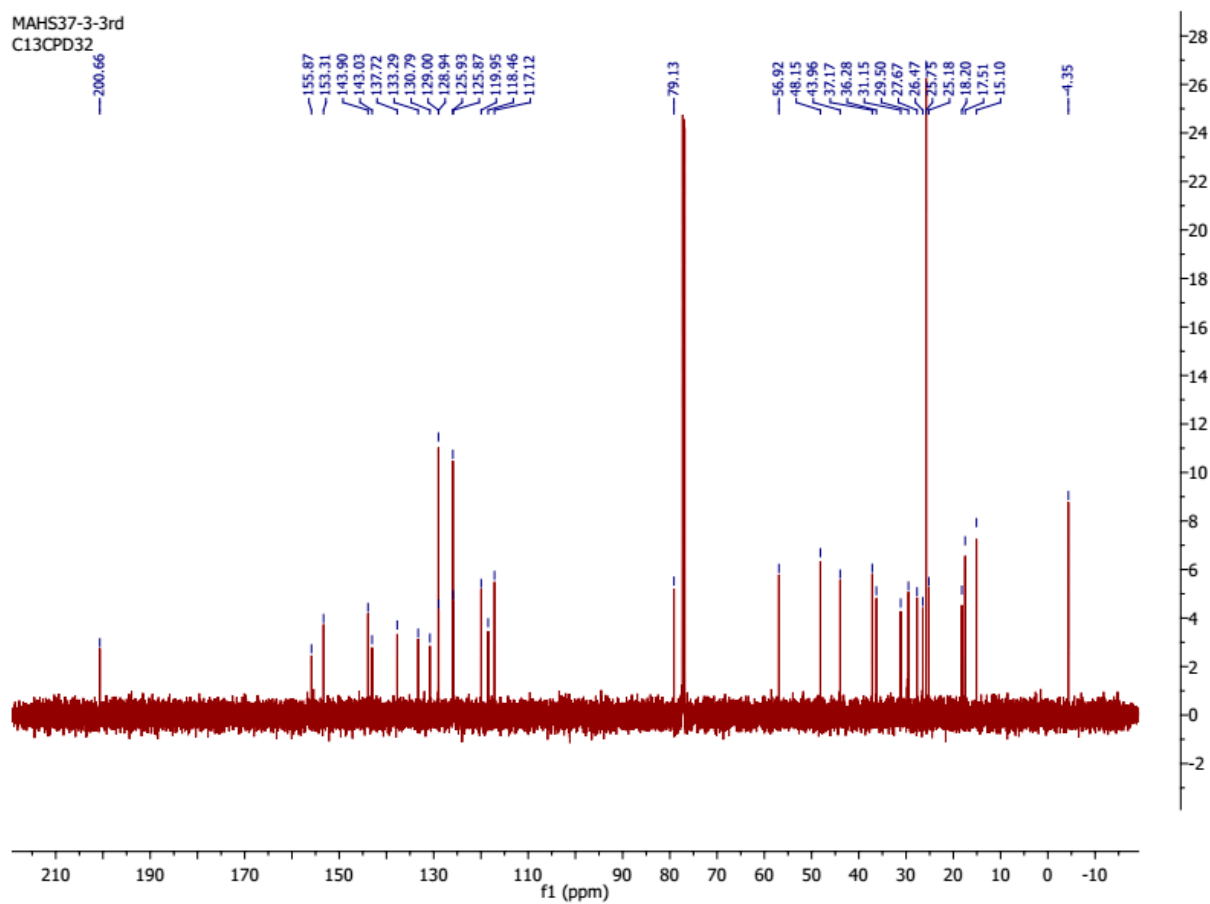


Figure S 37. ^{13}C NMR of compound **15d**.

1.17 Compound 15e

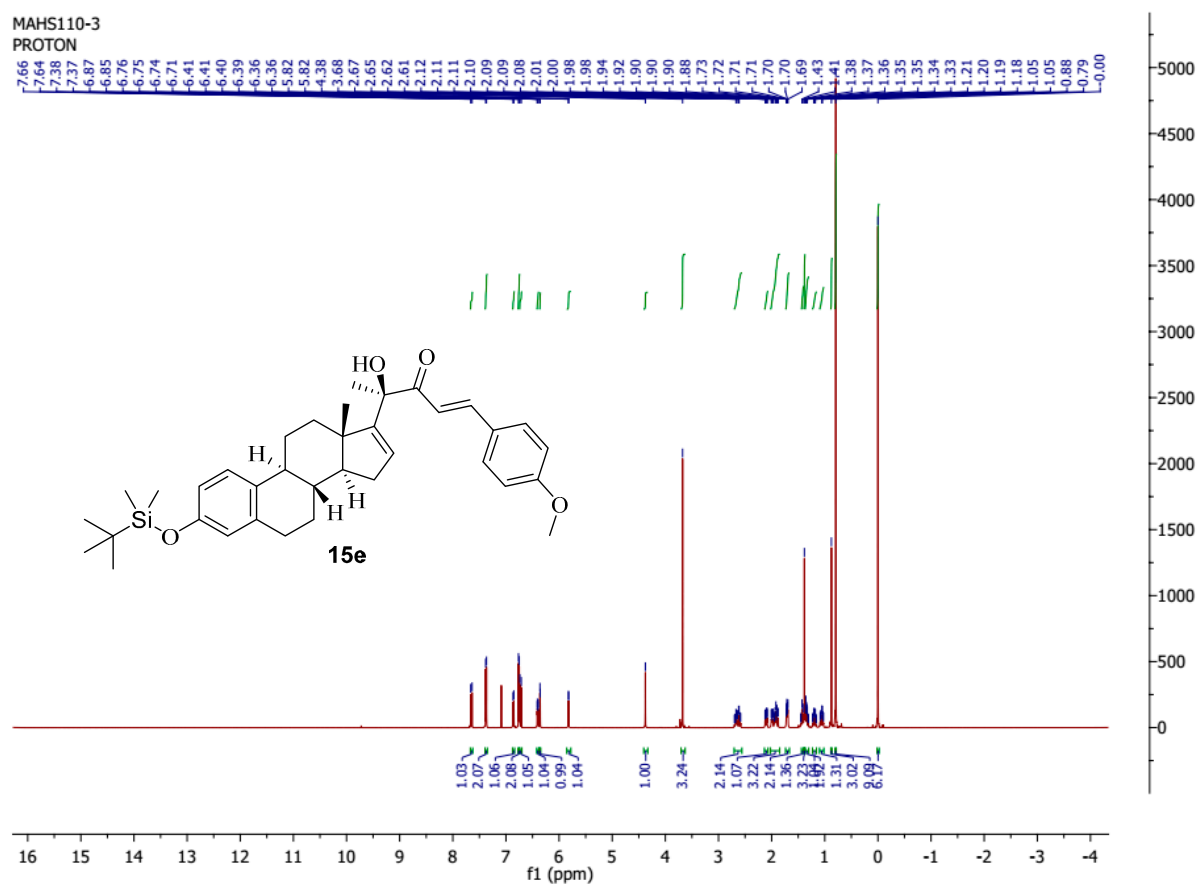


Figure S 38. ^1H NMR of compound **15e**.

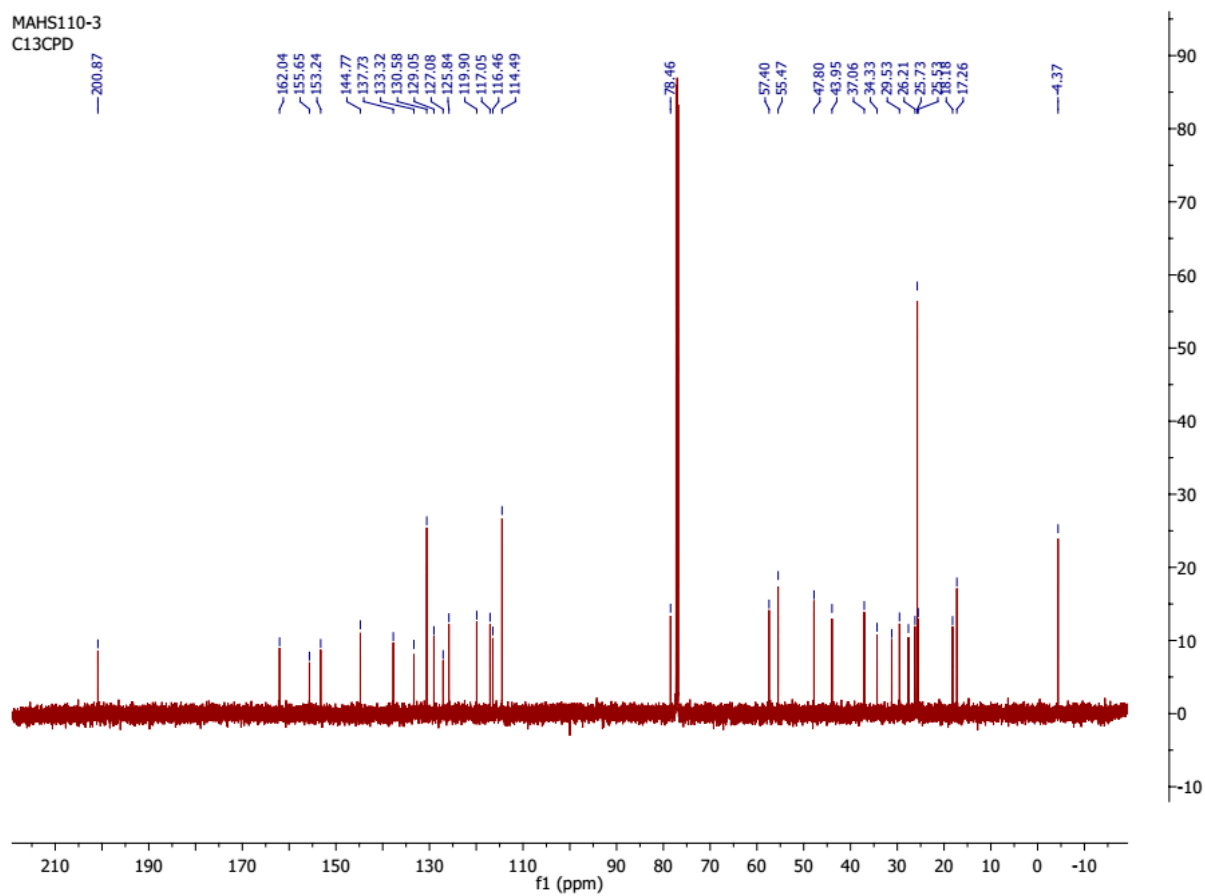


Figure S 39. ^{13}C NMR of compound **15e**.

1.18 Compound 15f

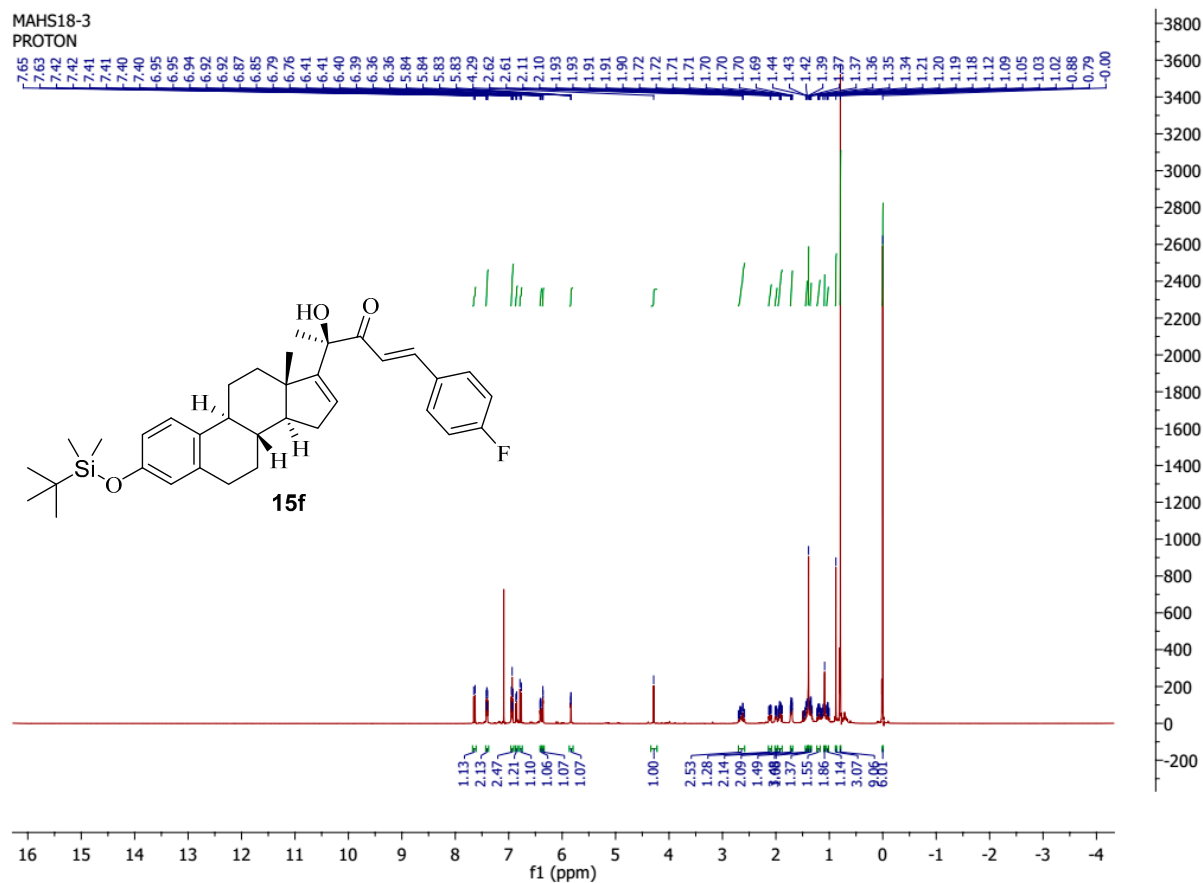


Figure S 40. ^1H NMR of compound **15f**.

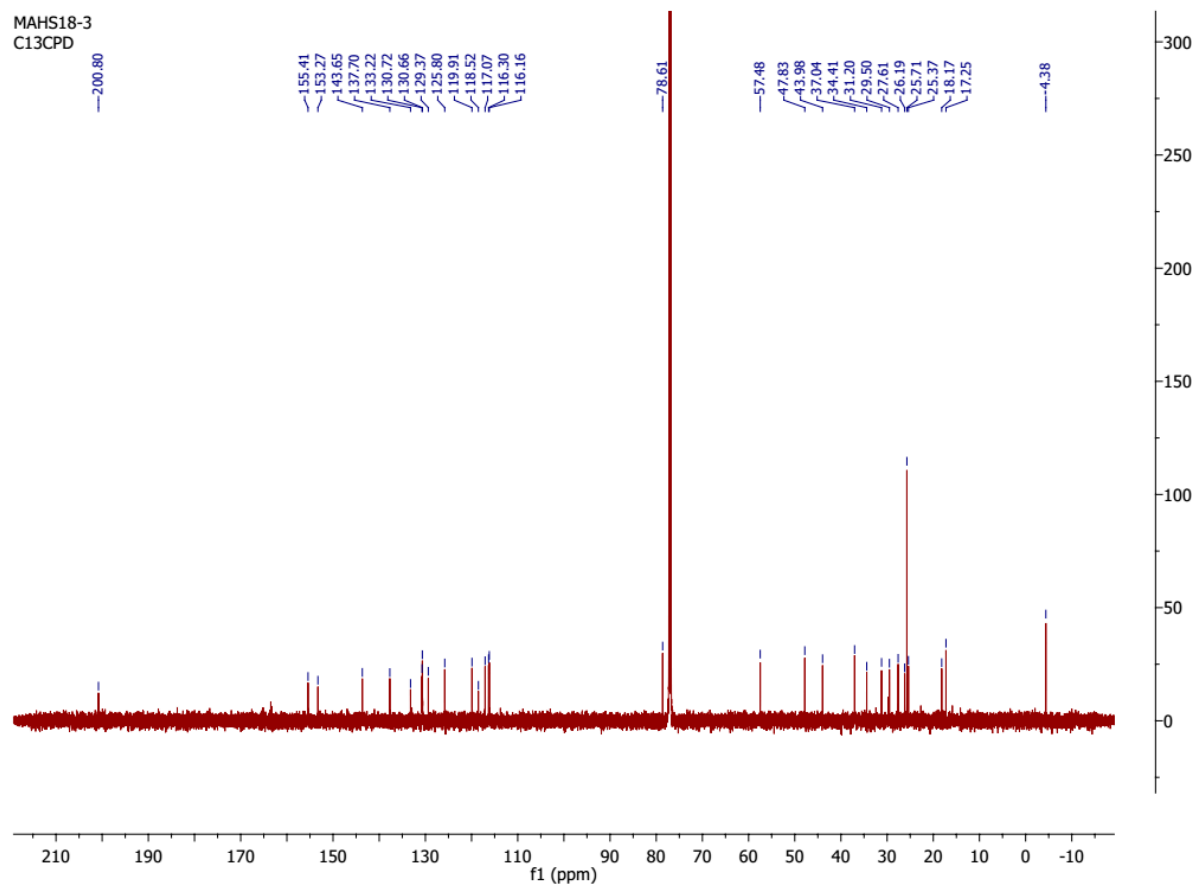


Figure S 41. ^{13}C NMR of compound **15f**.

1.19 Compound 15g

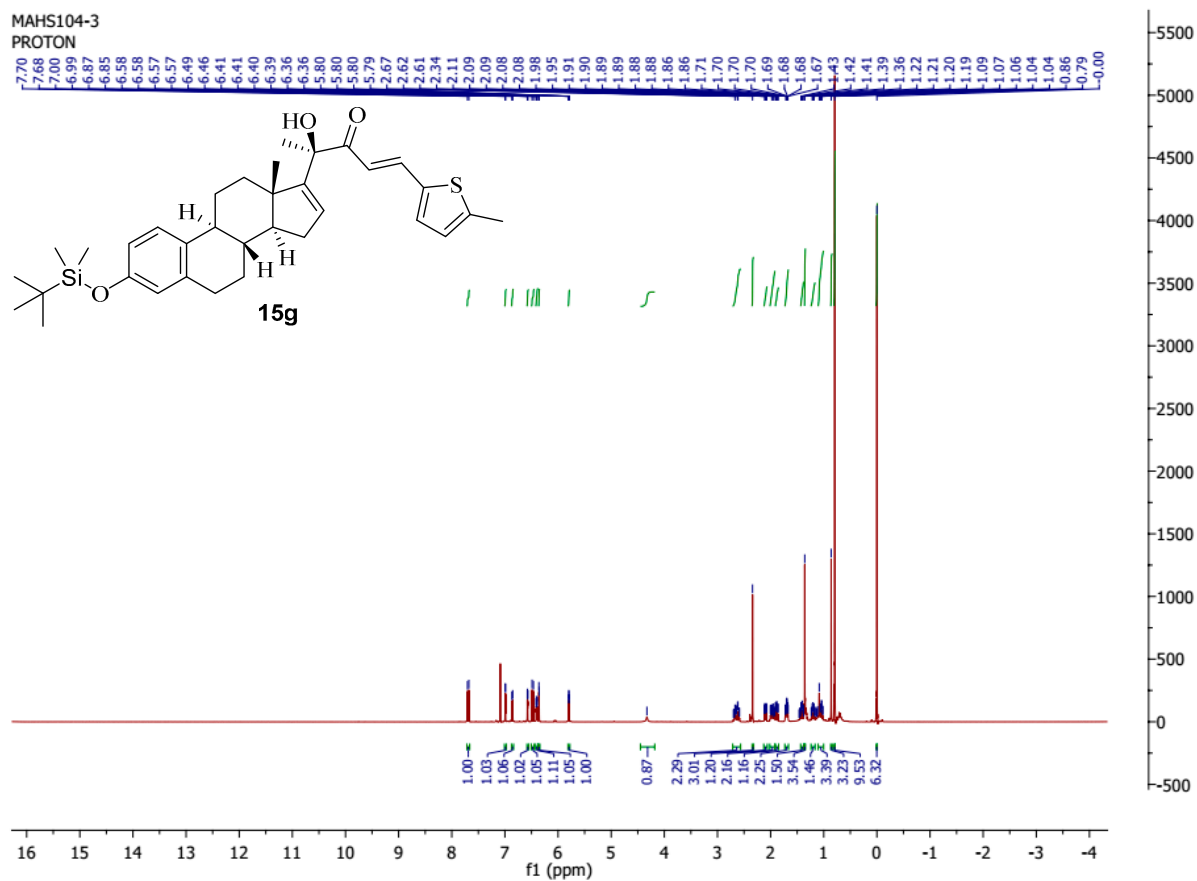


Figure S 42. ^1H NMR of compound **15g**.

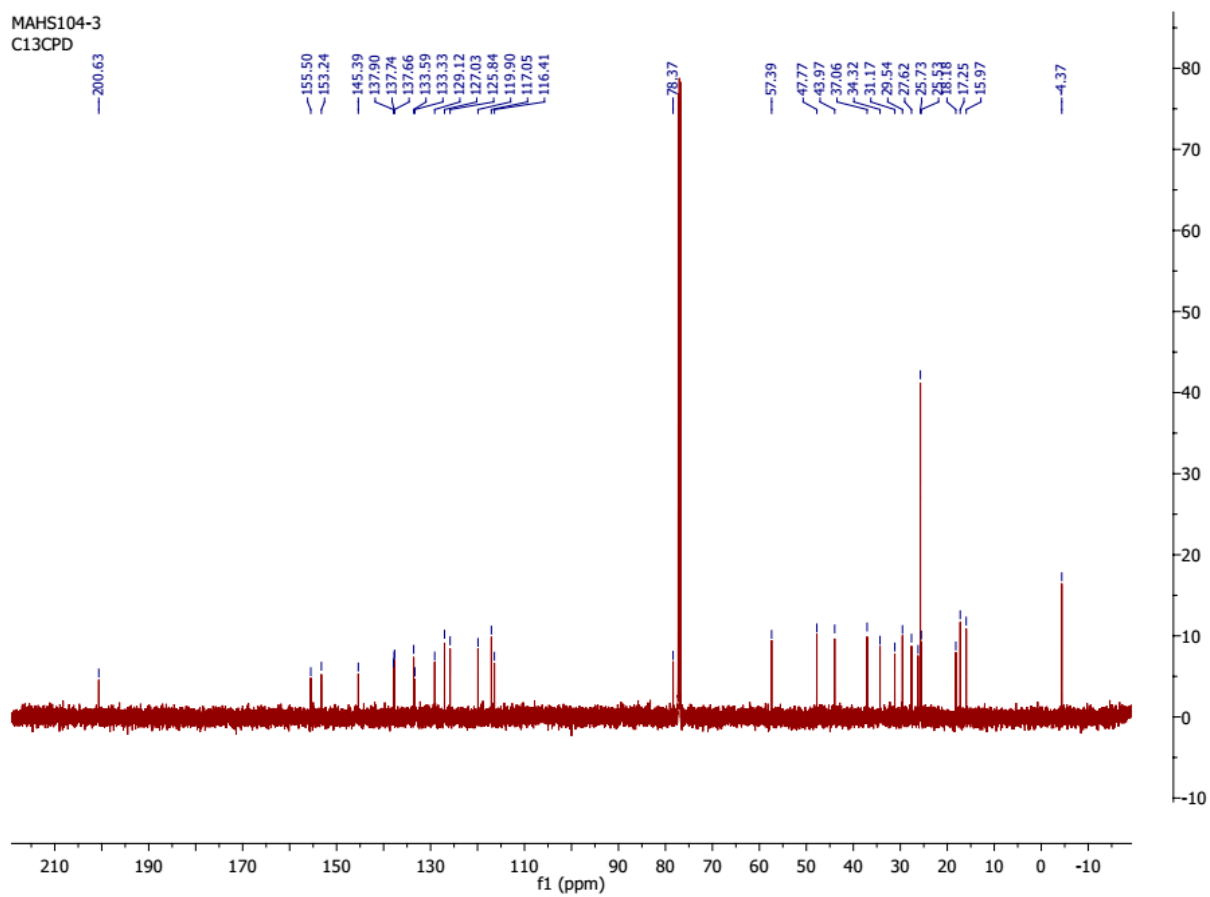


Figure S 43. ^{13}C NMR of compound **15g**.

1.20 Compound 15h

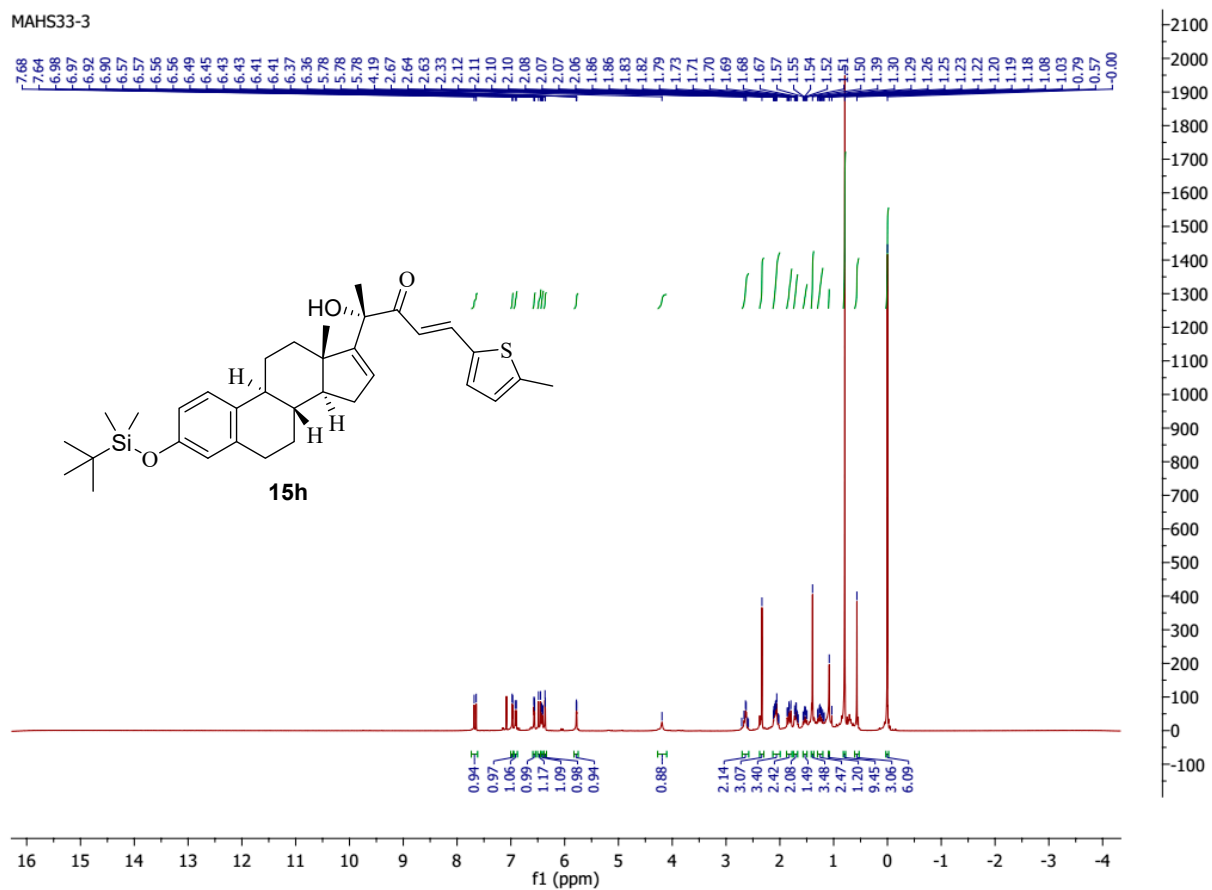


Figure S 44. ^1H NMR of compound 15h.

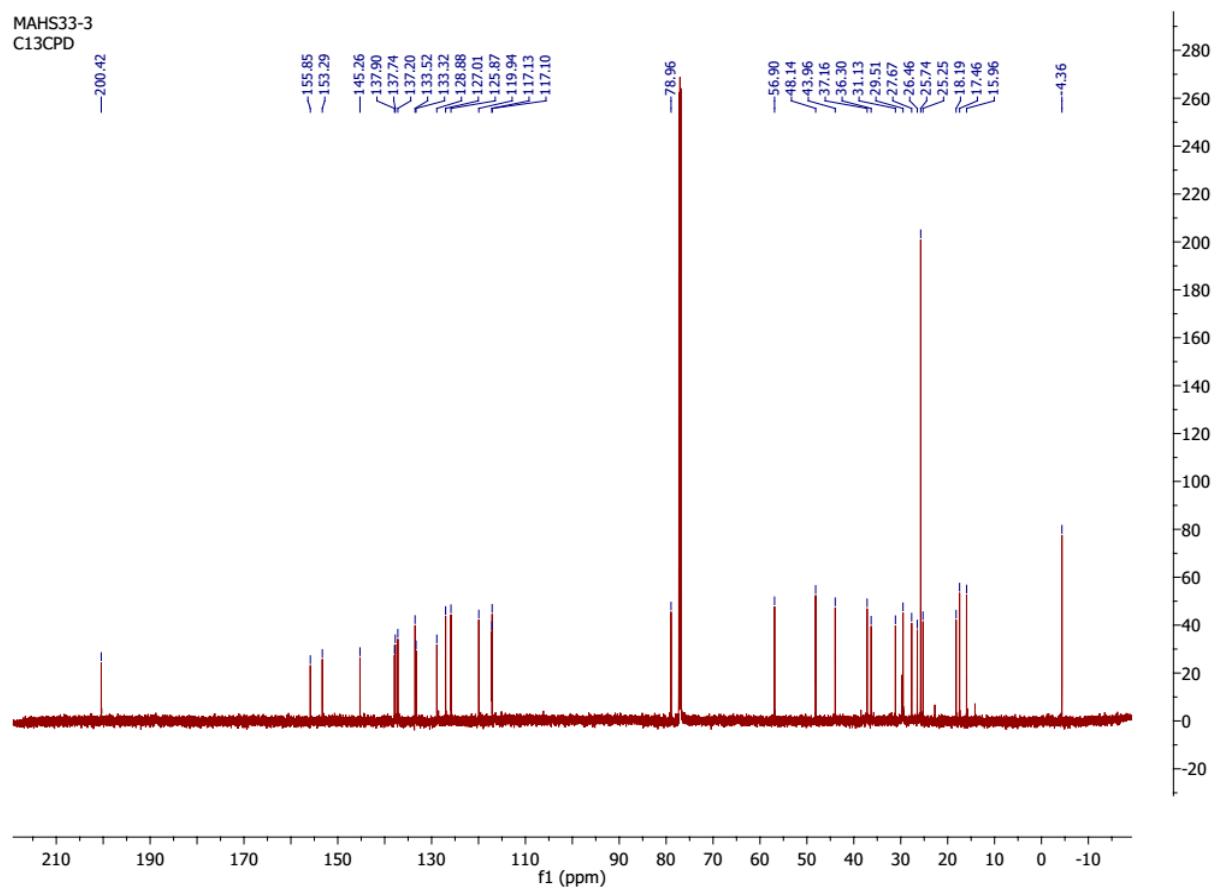


Figure S 45. ^{13}C NMR of compound **15h**.

1.21 Compound 15i

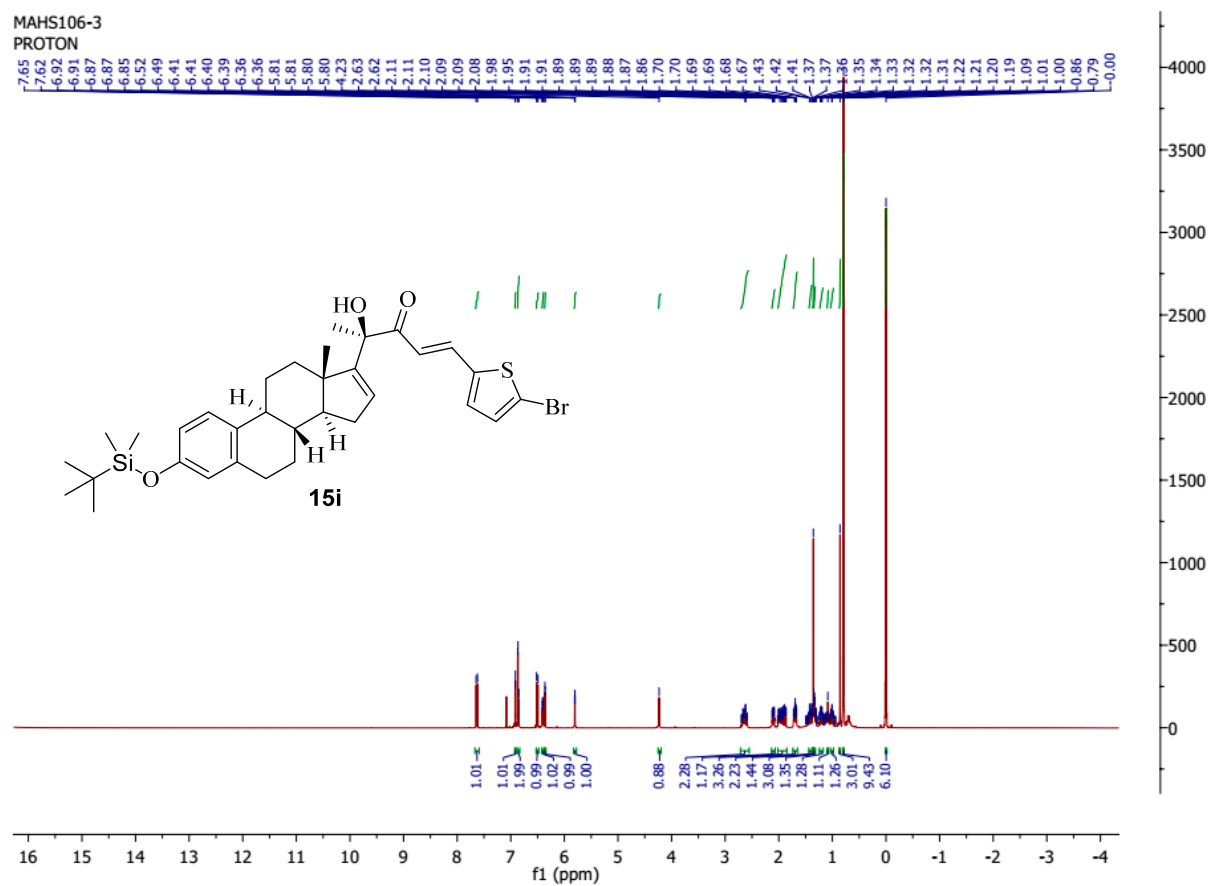


Figure S 46. ^1H NMR of compound **15i**.

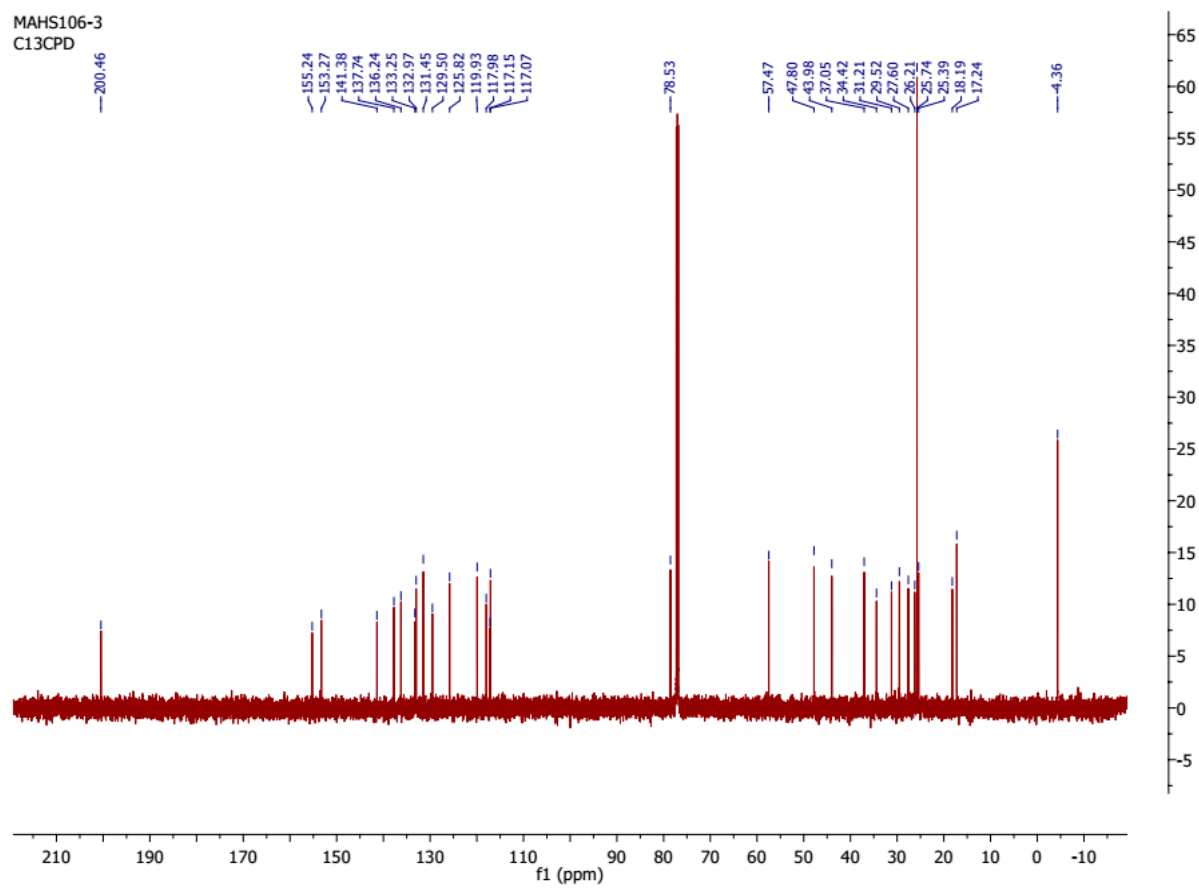


Figure S 47. ^{13}C NMR of compound **15i**.

1.22 Compound 15j

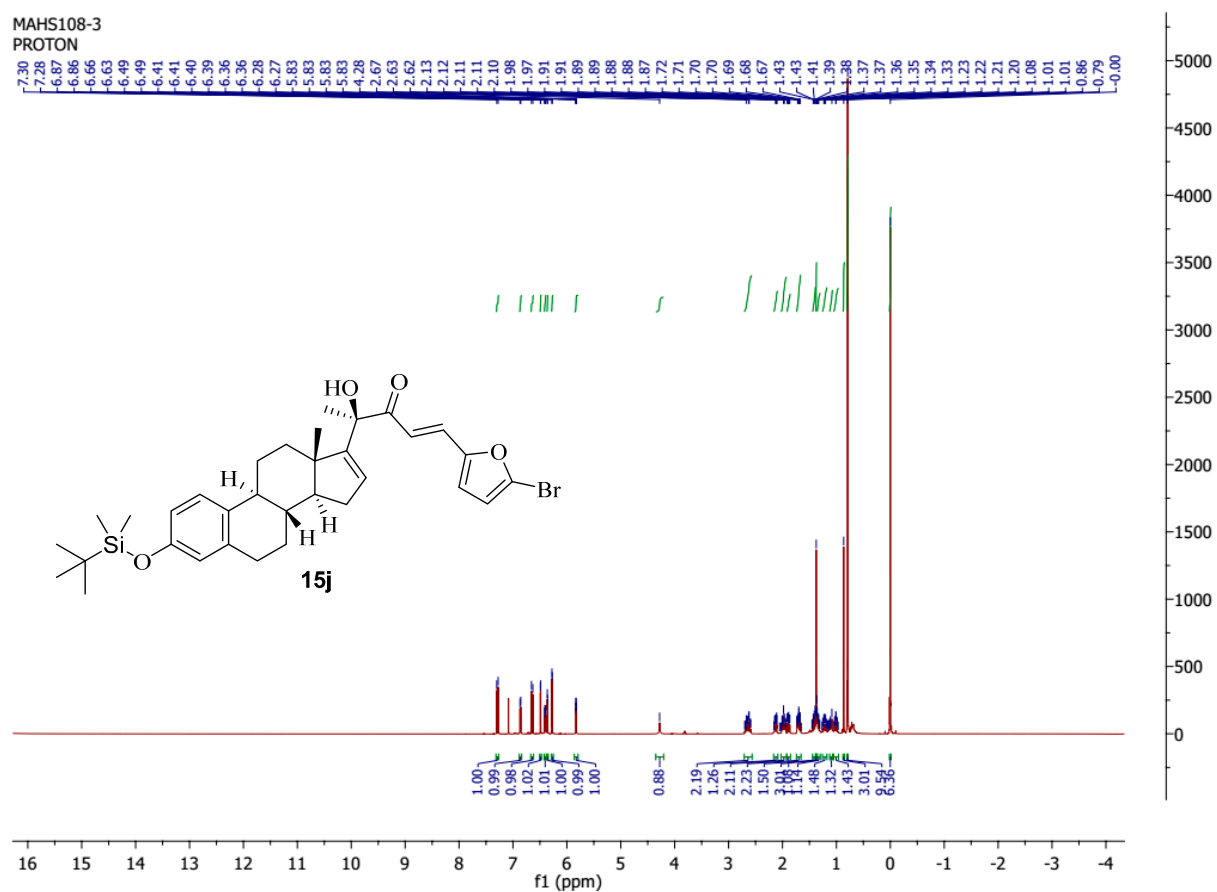


Figure S 48. ^1H NMR of compound **15j**.

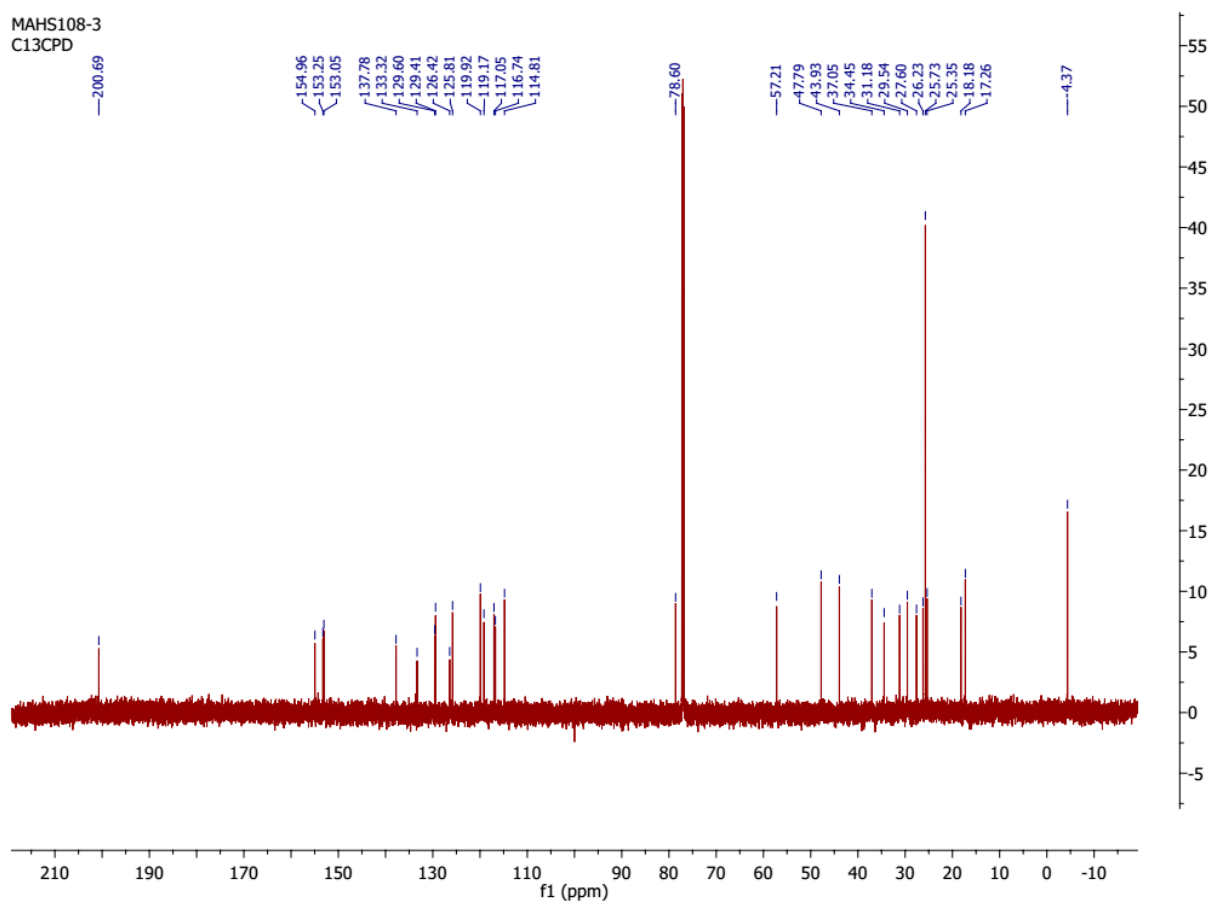


Figure S 49. ^{13}C NMR of compound **15j**.

1.23 Compound 16a

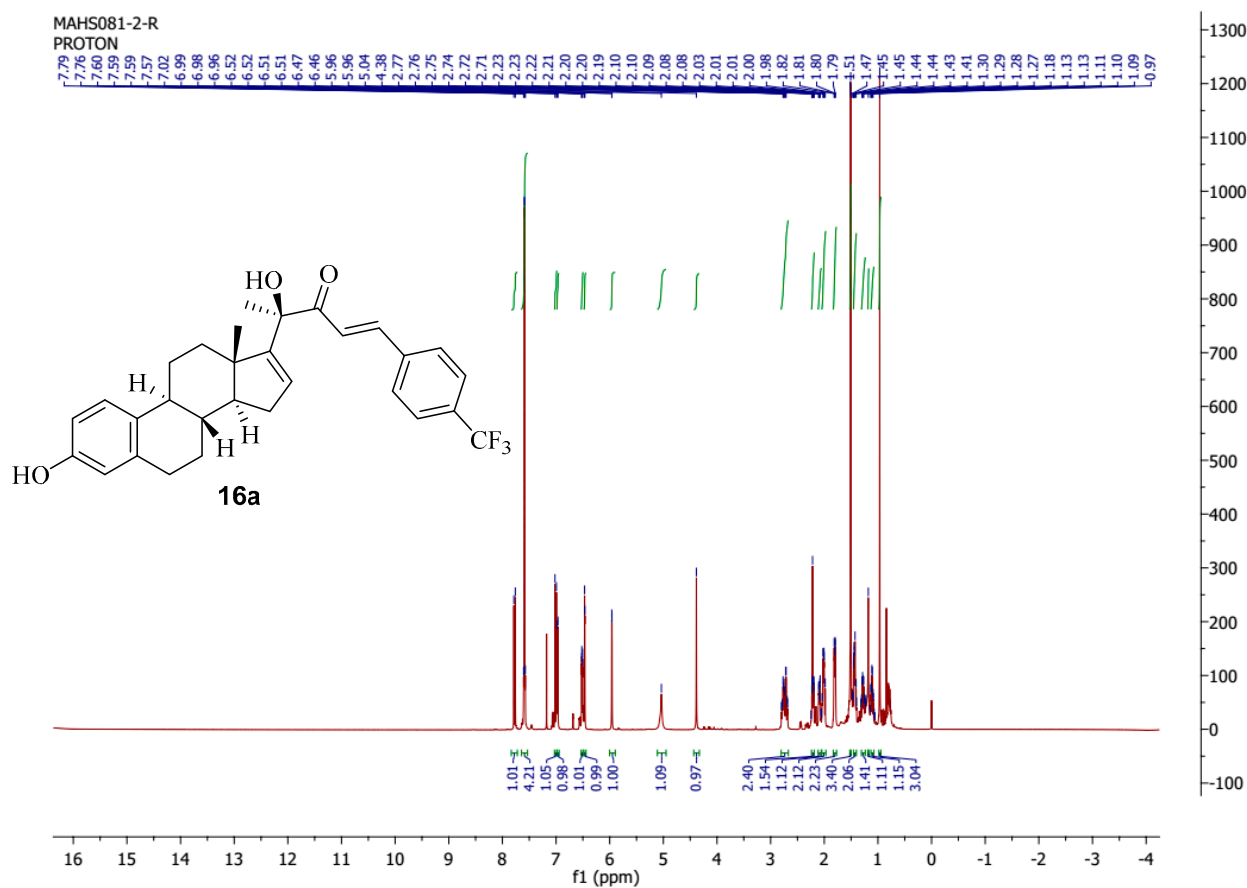


Figure S 50. ^1H NMR of compound **16a**.

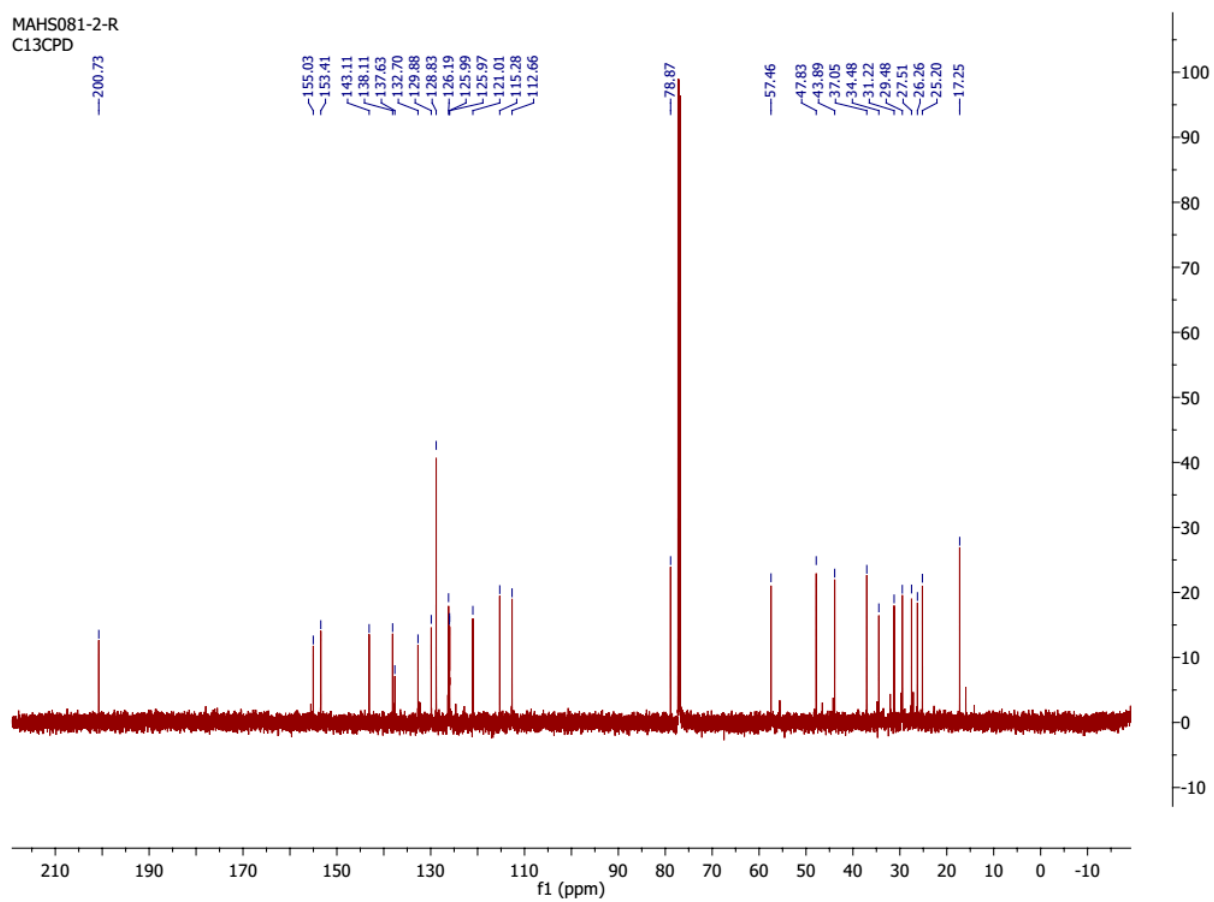


Figure S 51. ^{13}C NMR of compound **16a**.

1.24 Compound 16b

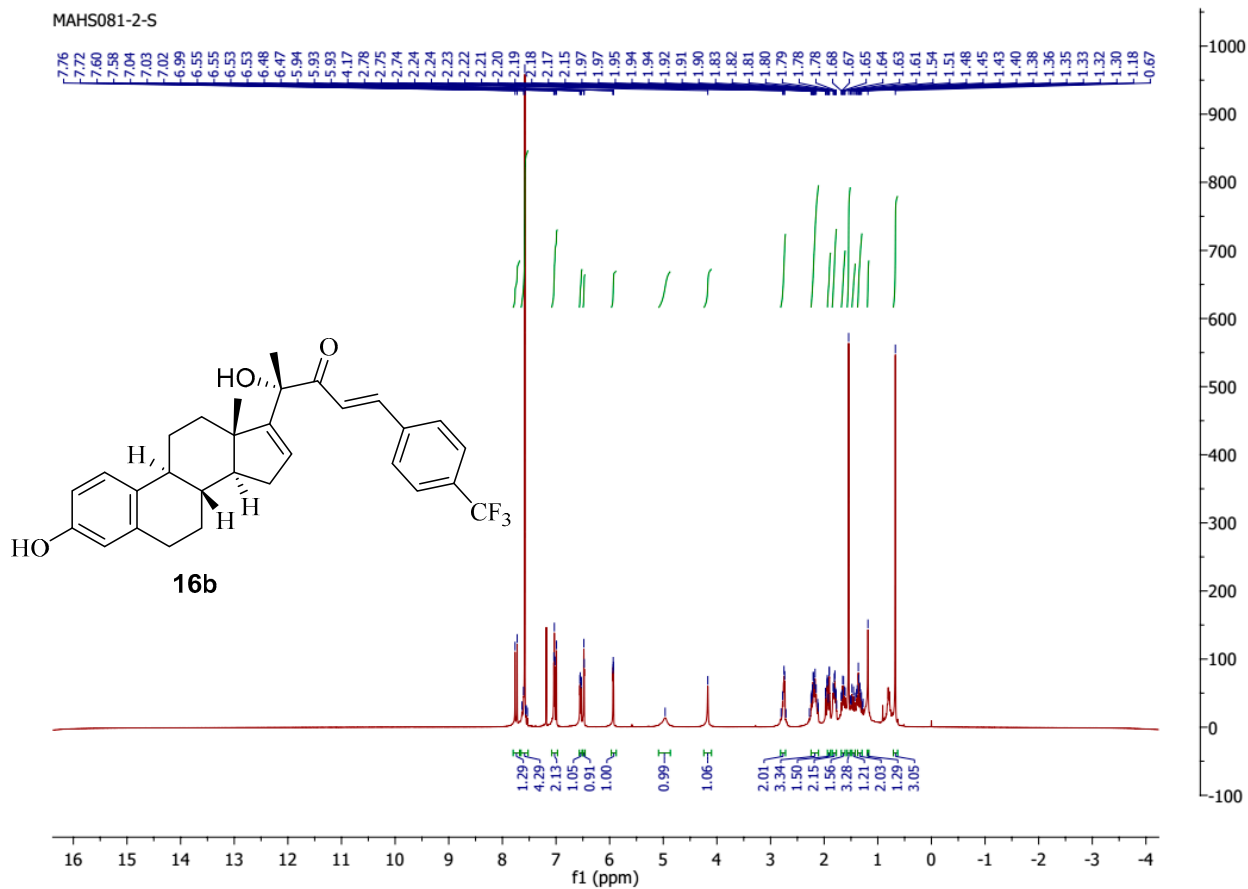


Figure S 52. ^1H NMR of compound 16b.

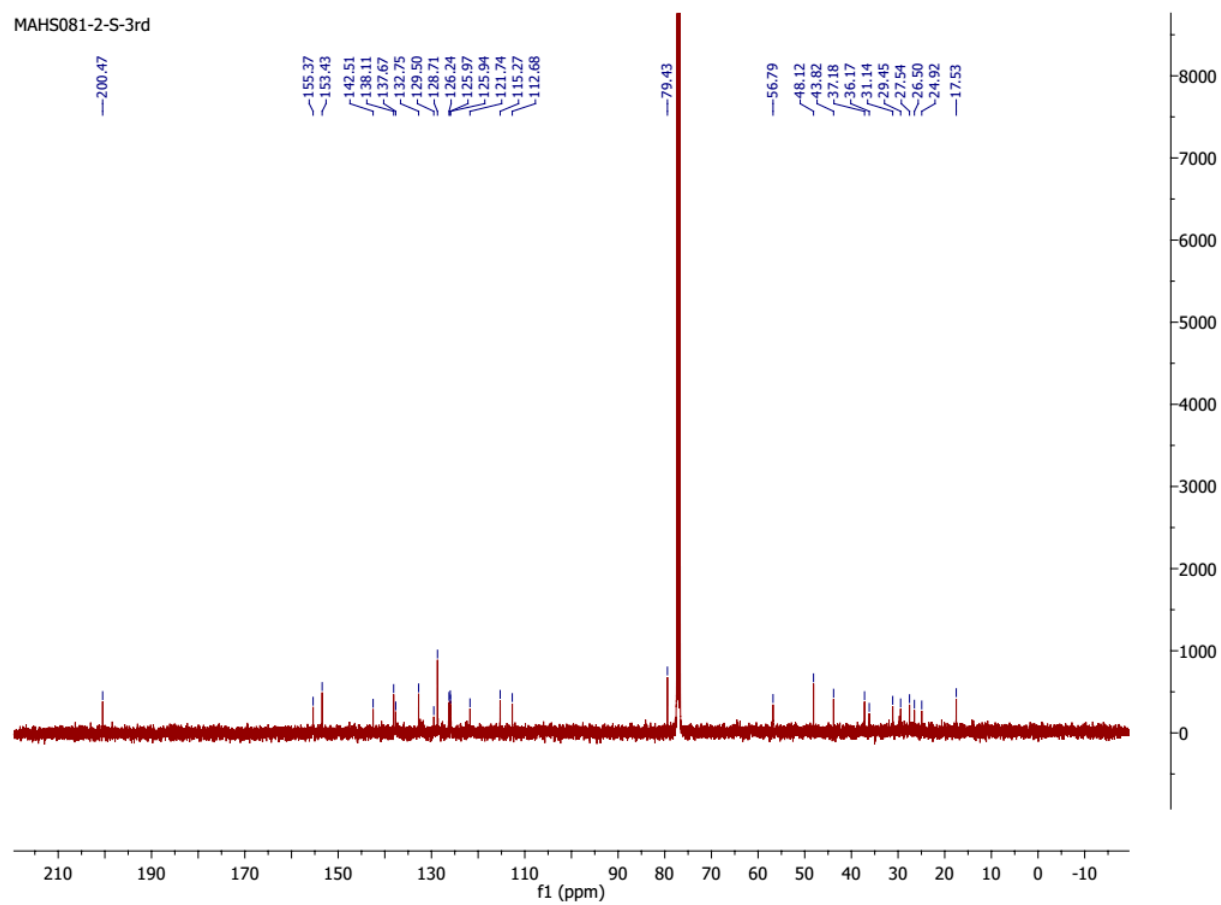


Figure S 53. ^{13}C NMR of compound **16b**.

1.25 Compound 16c

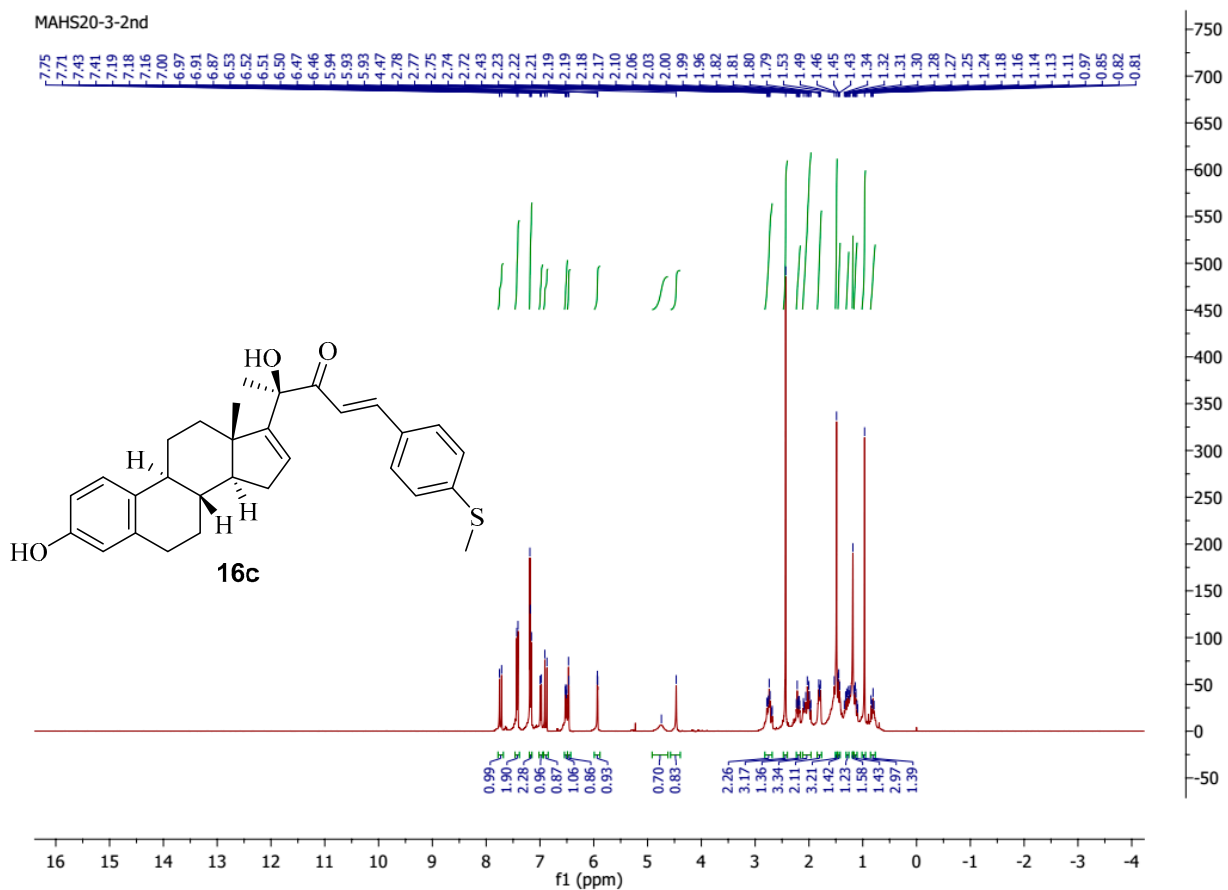


Figure S 54. ¹H NMR of compound **16c**.

1.26 Compound 16d

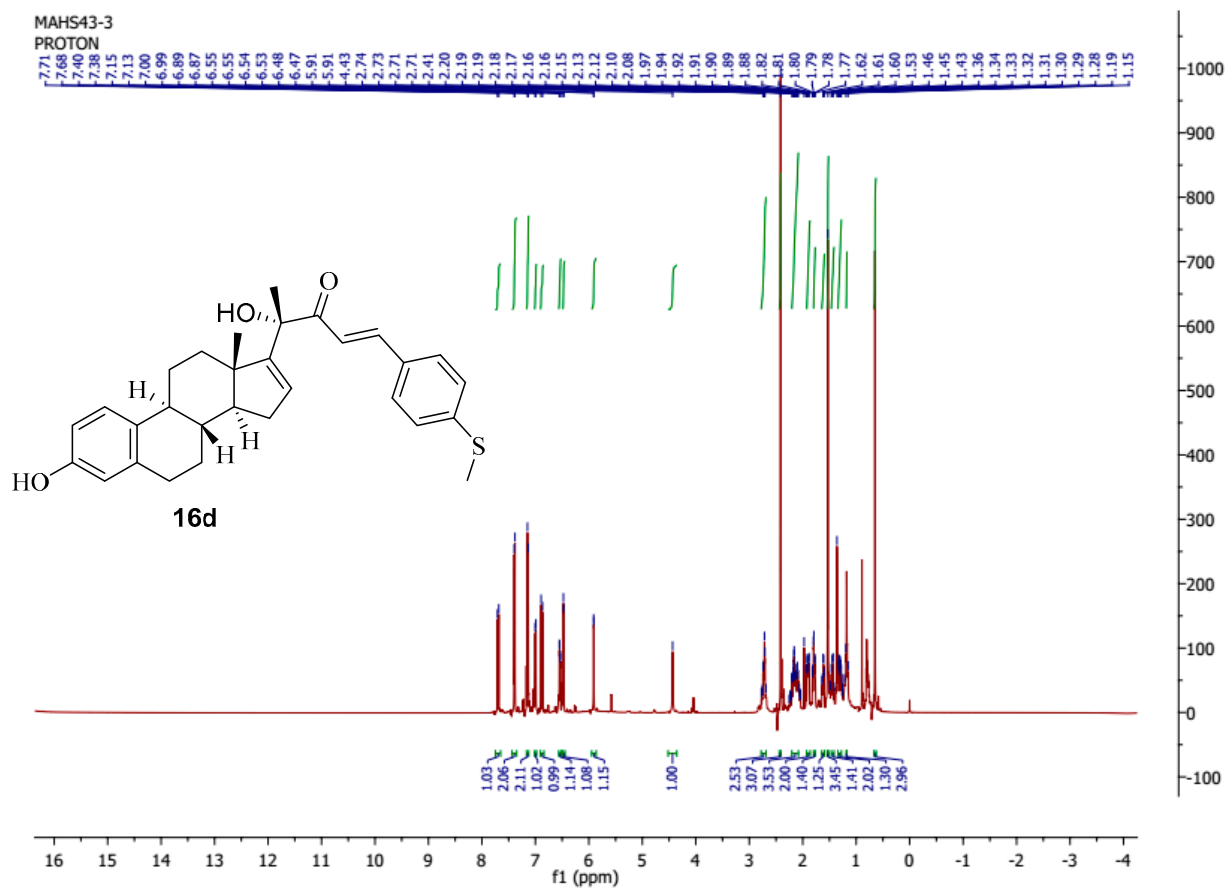


Figure S 55. ^1H NMR of compound **16d**.

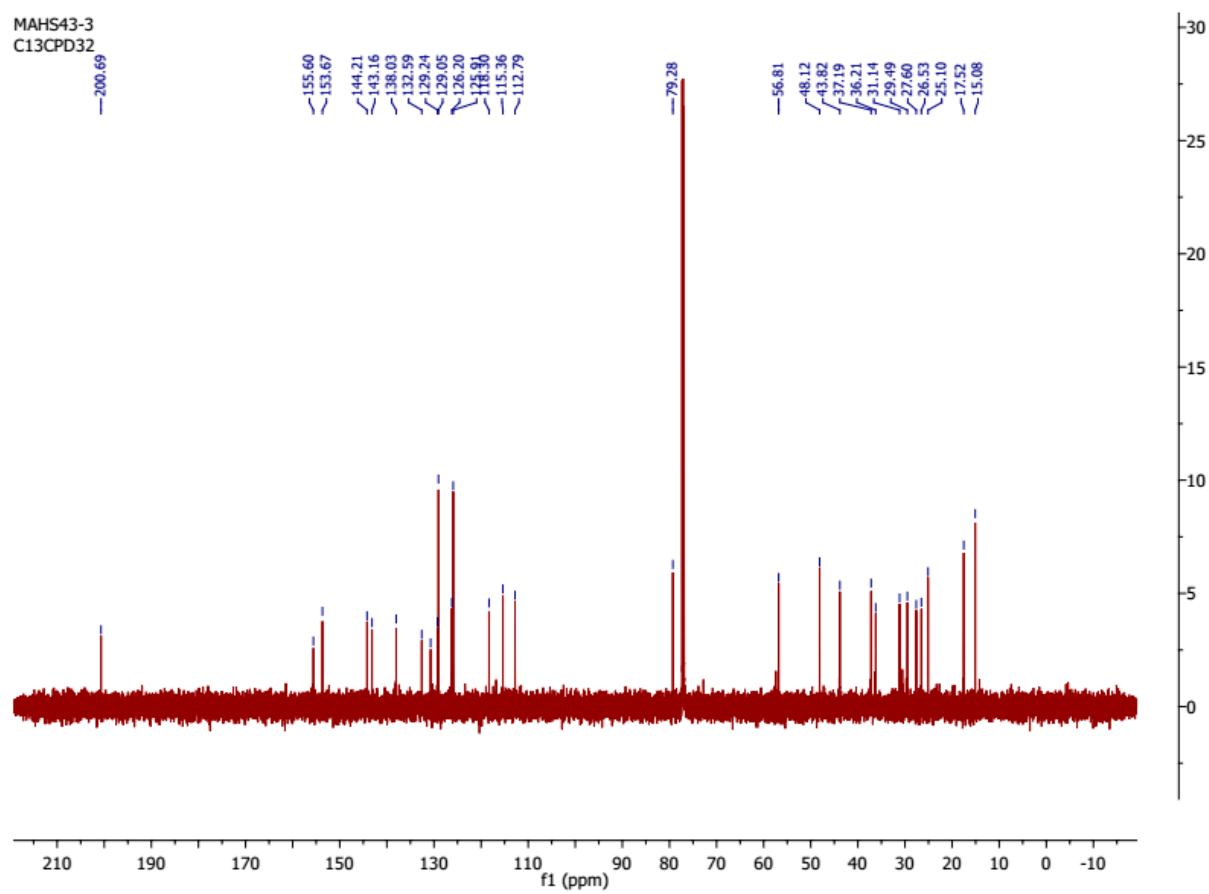


Figure S 56. ^{13}C NMR of compound **16d**.

1.27 Compound 16e

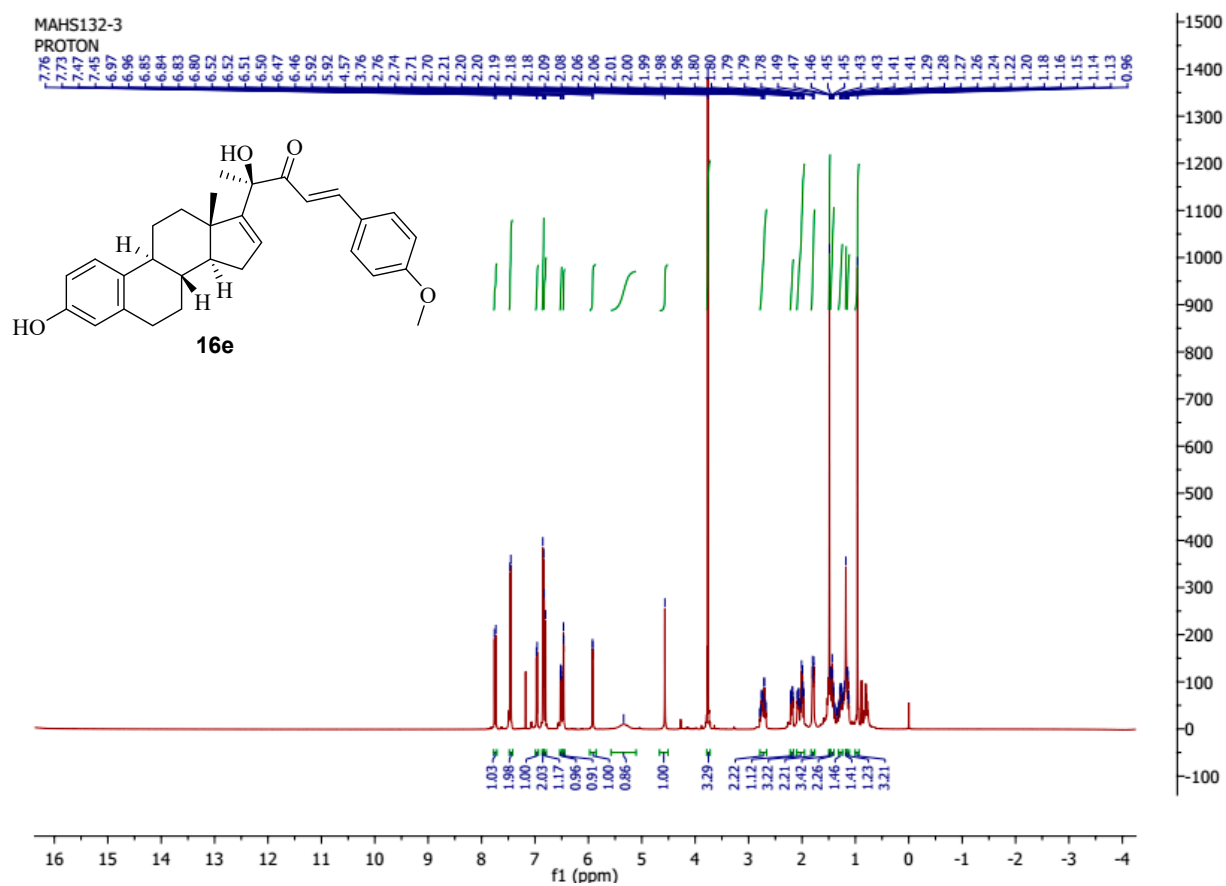


Figure S 57. ^1H NMR of compound **16e**.

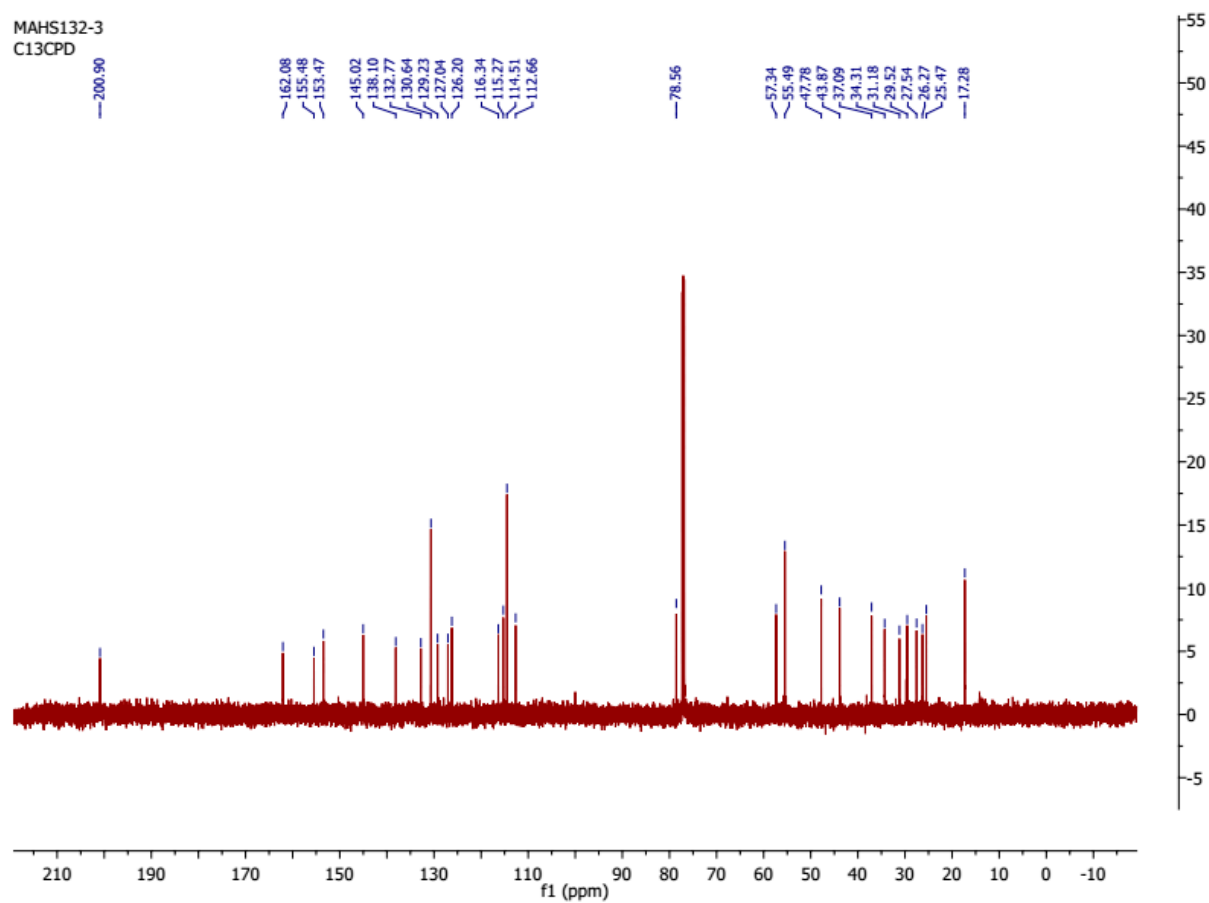


Figure S 58. ^{13}C NMR of compound **16e**.

1.28 Compound 16f

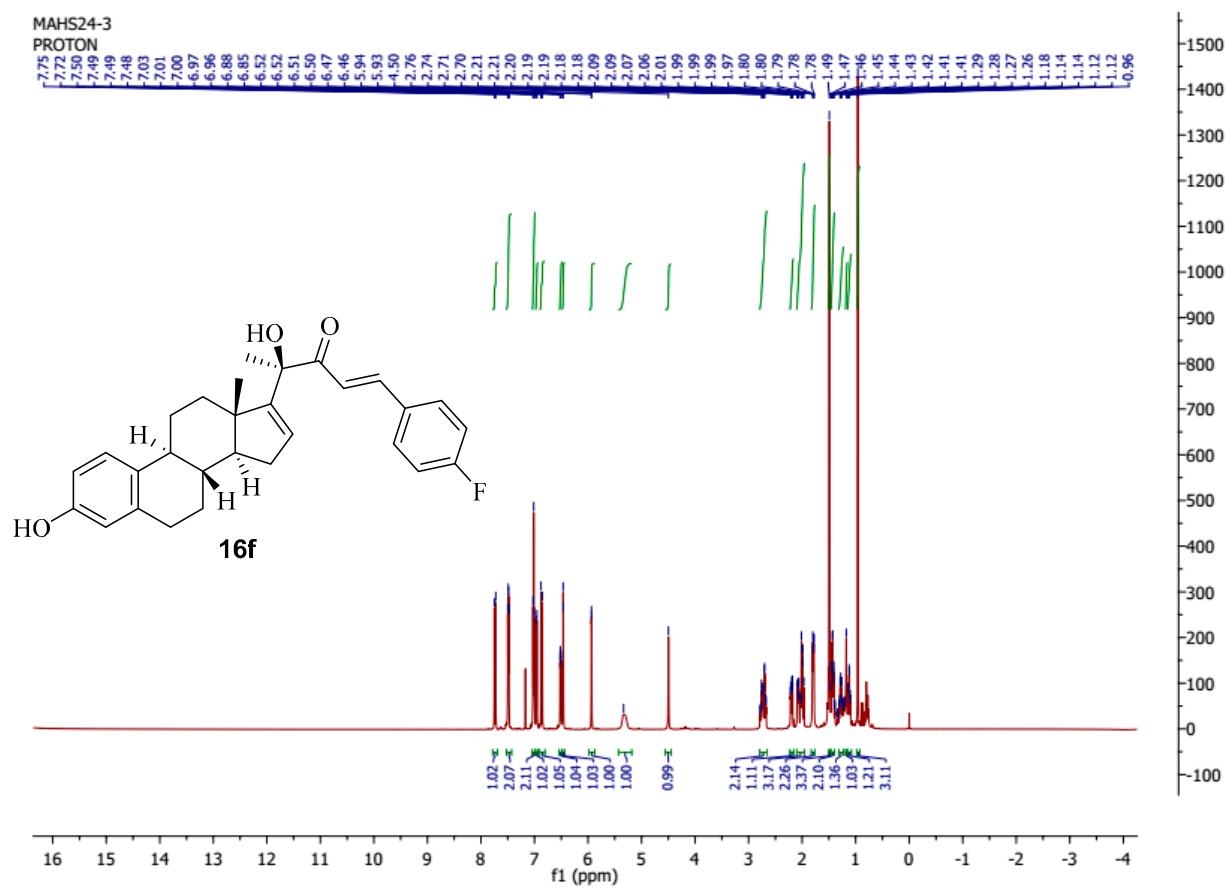


Figure S 59. ^1H NMR of compound **16f**.

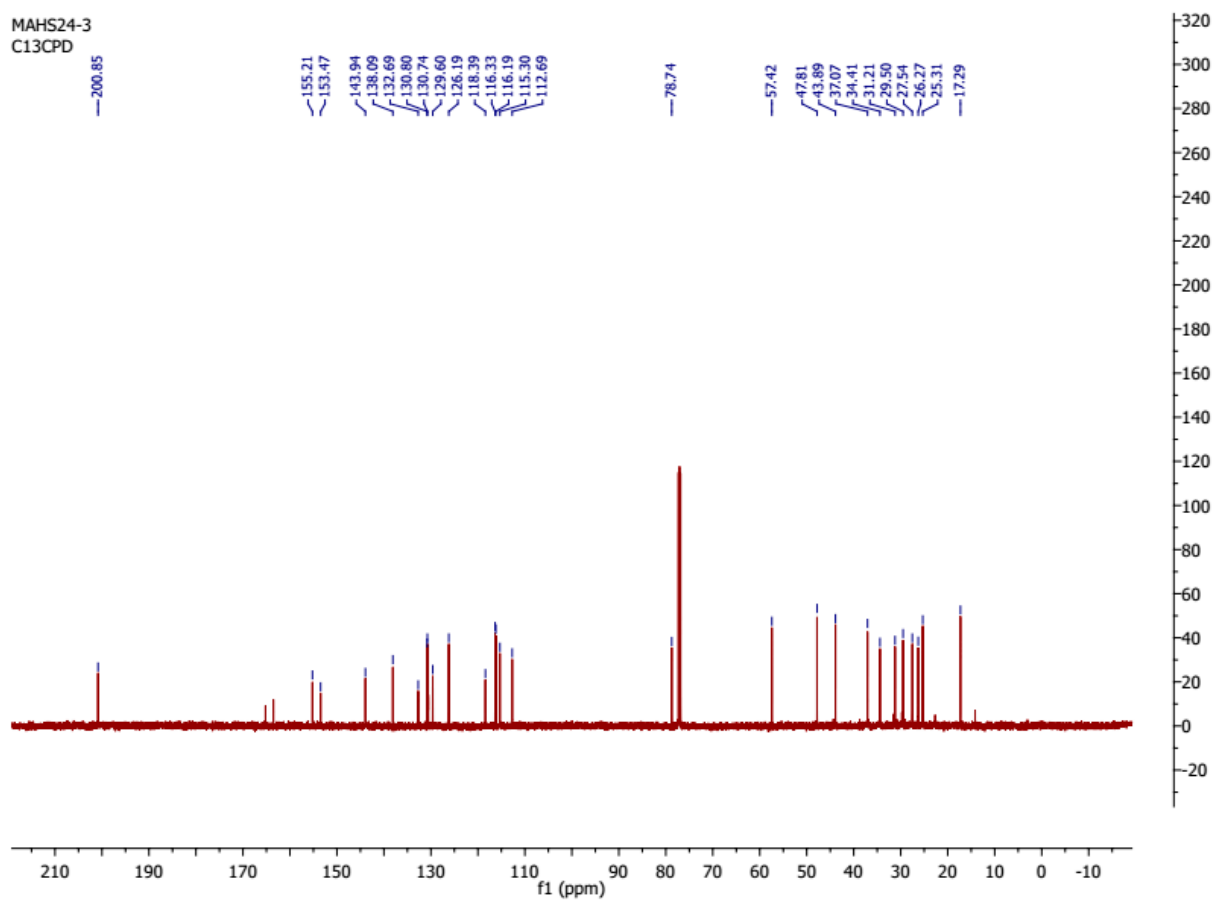


Figure S 60. ^{13}C NMR of compound **16f**.

1.29 Compound 16g

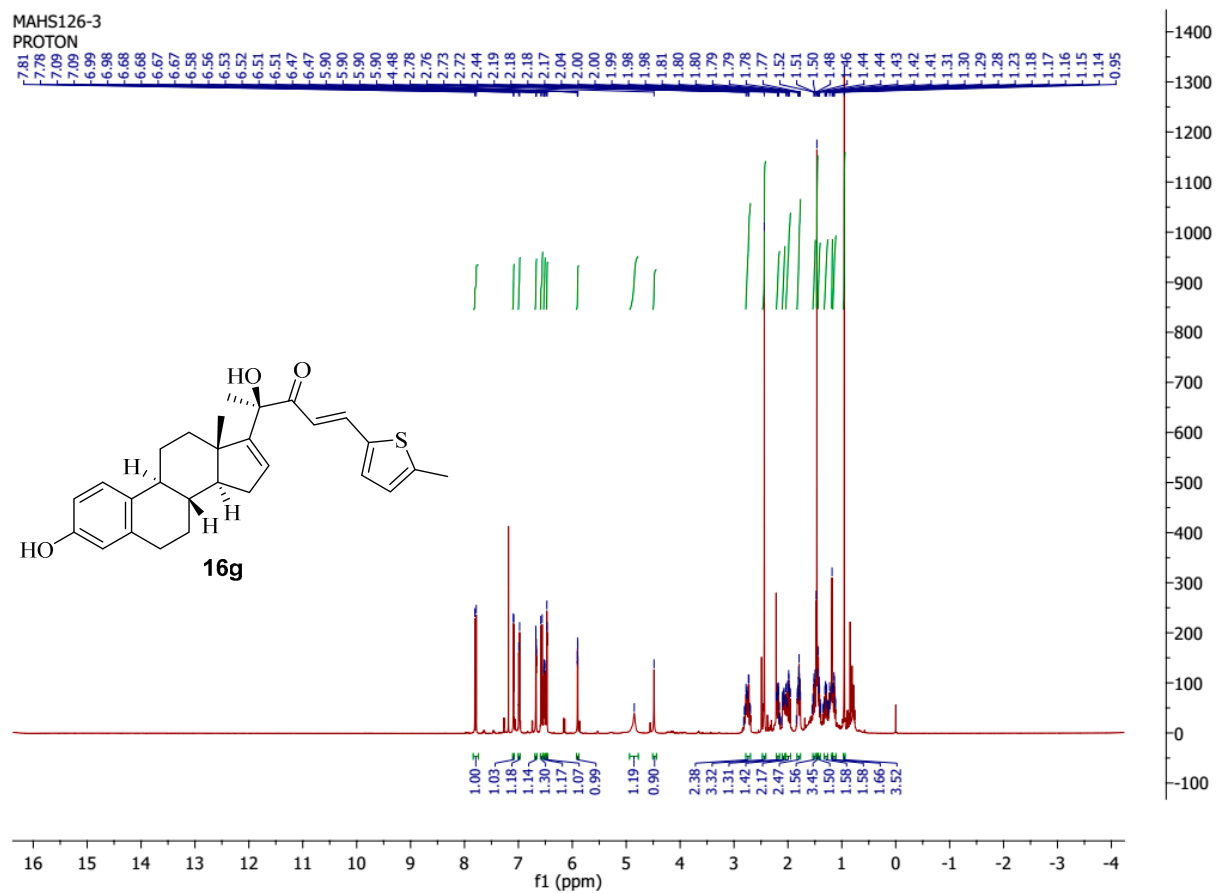


Figure S 61. ^1H NMR of compound **16g**.

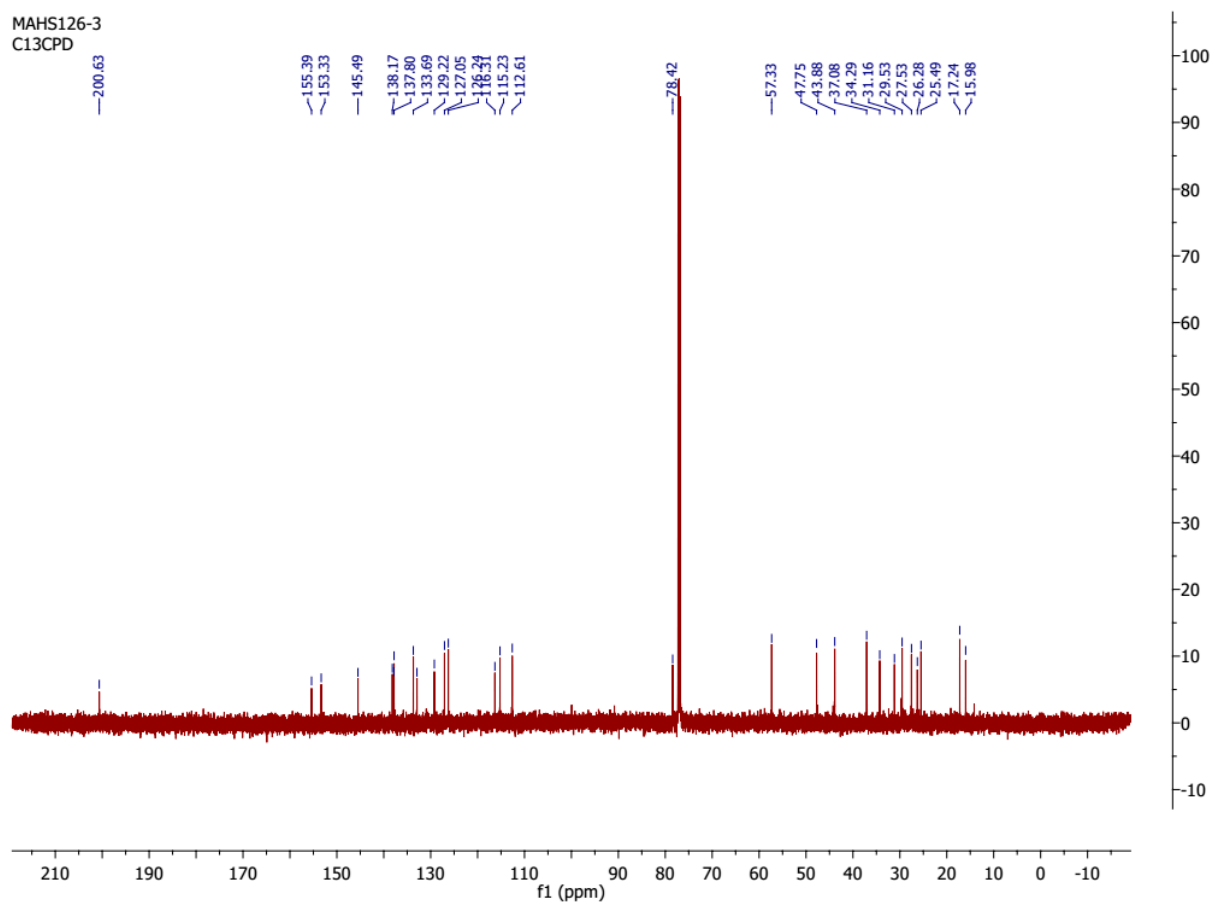


Figure S 62. ^{13}C NMR of compound **16g**.

1.30 Compound 16h

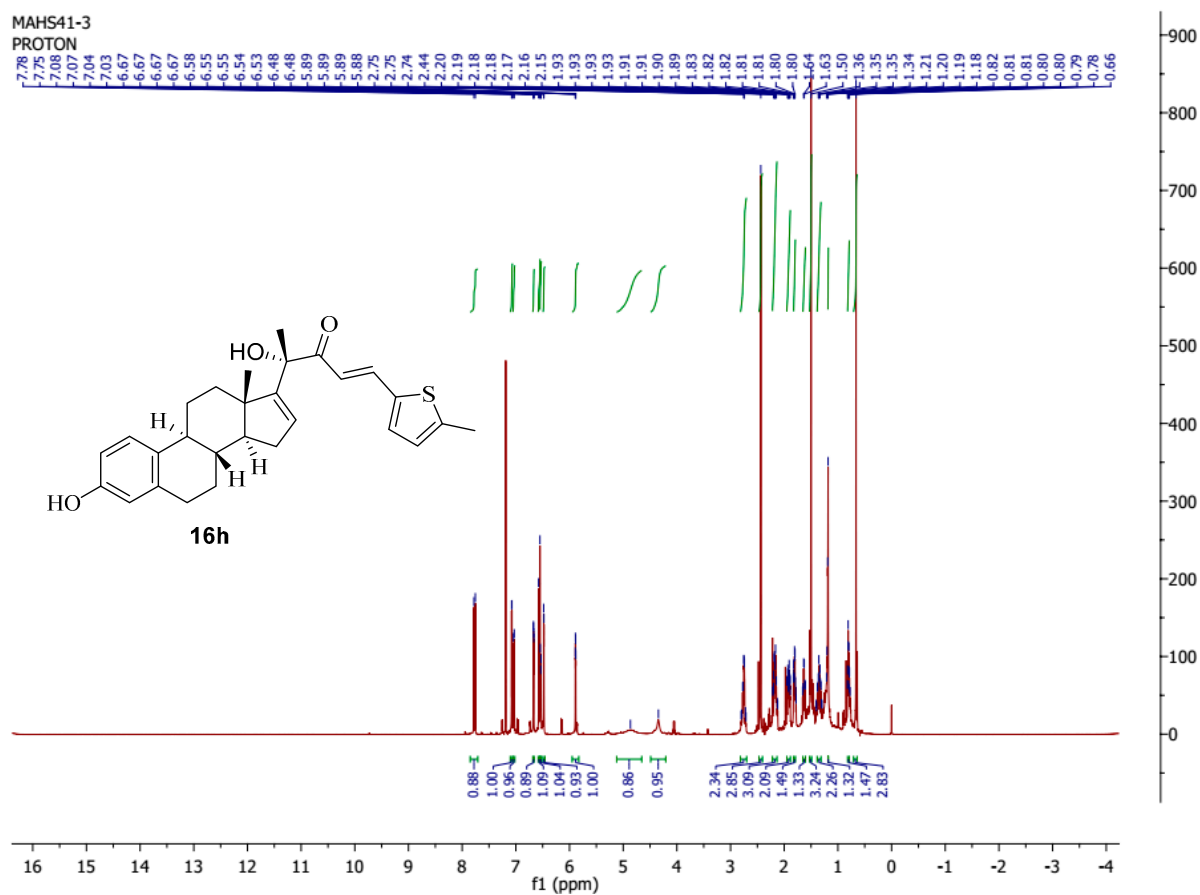


Figure S 63. ^1H NMR of compound **16h**.

1.31 Compound 16i

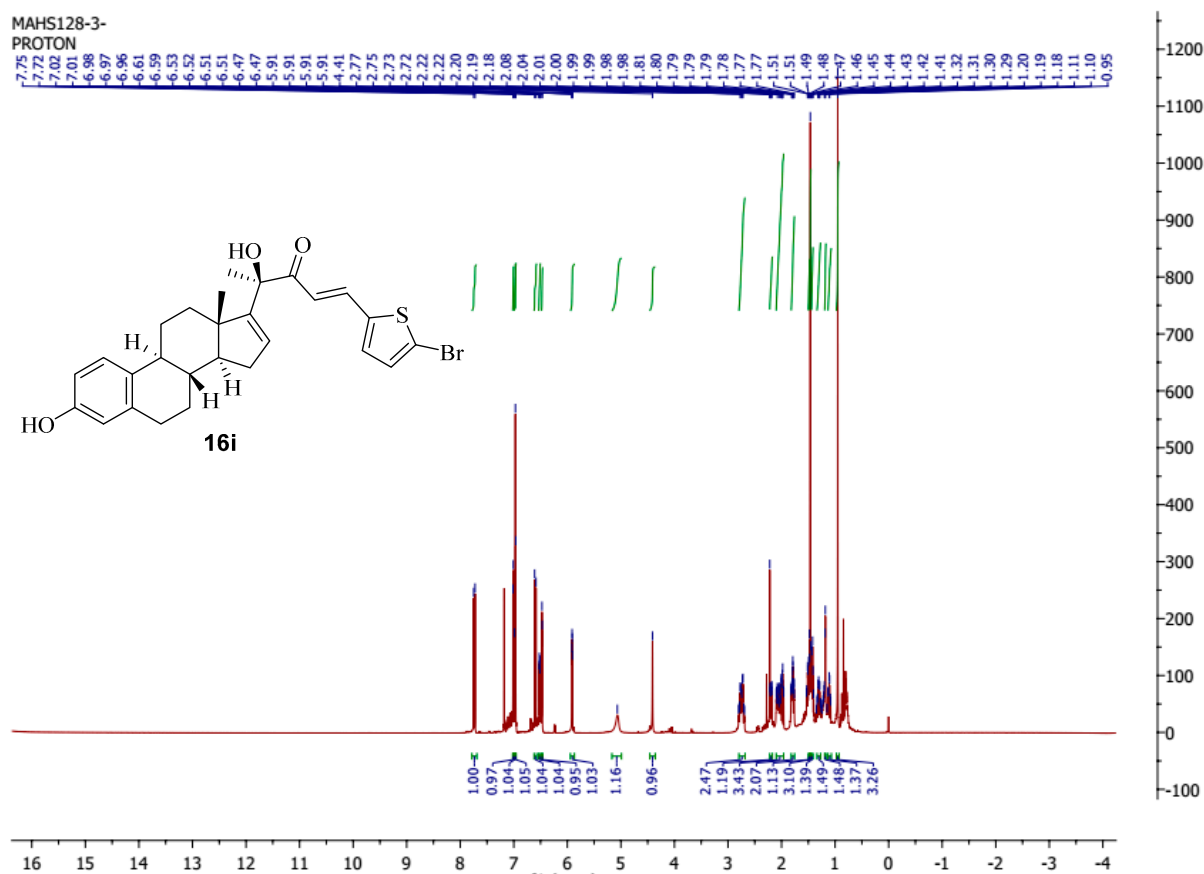


Figure S 64. ^1H NMR of compound **16i**.

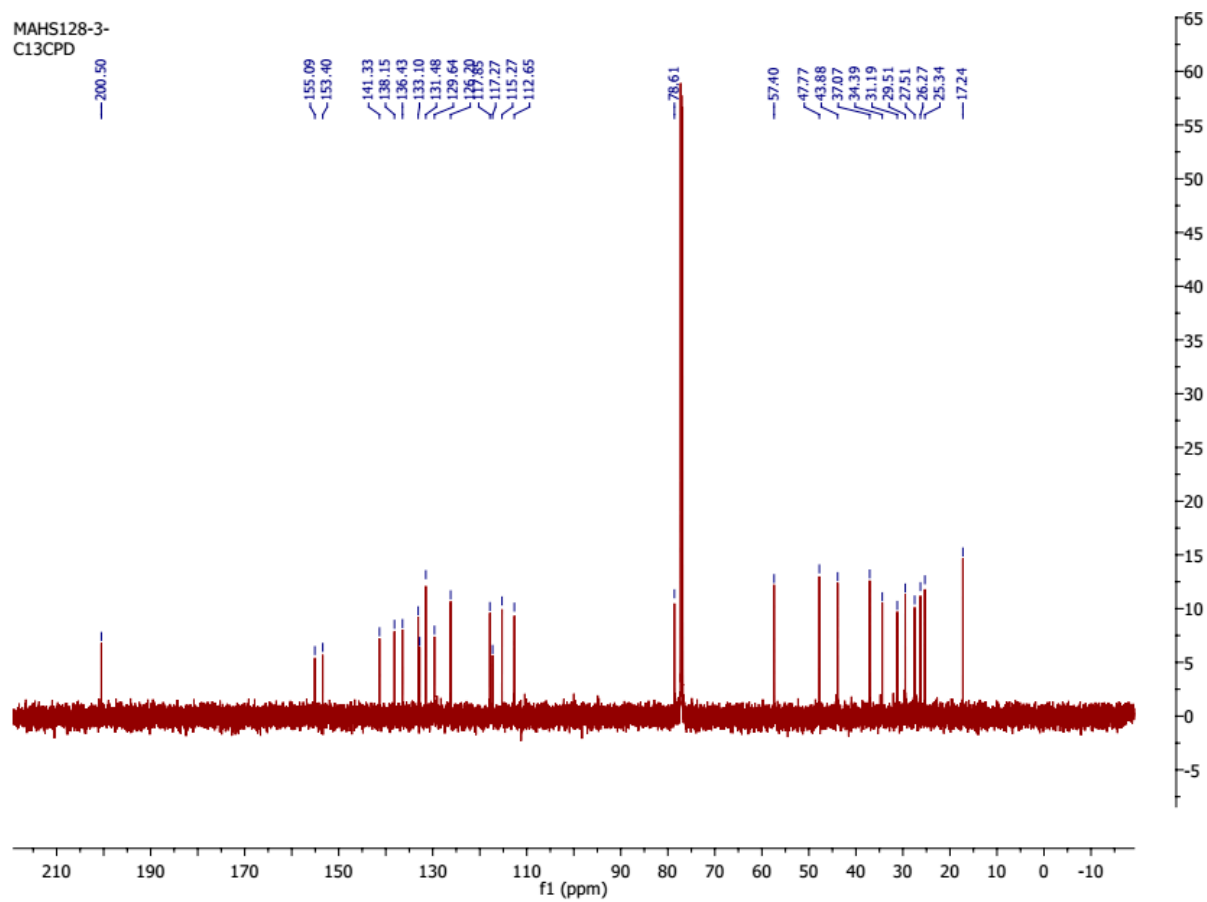


Figure S 65. ^{13}C NMR of compound **16i**.

1.32 Compound 16j

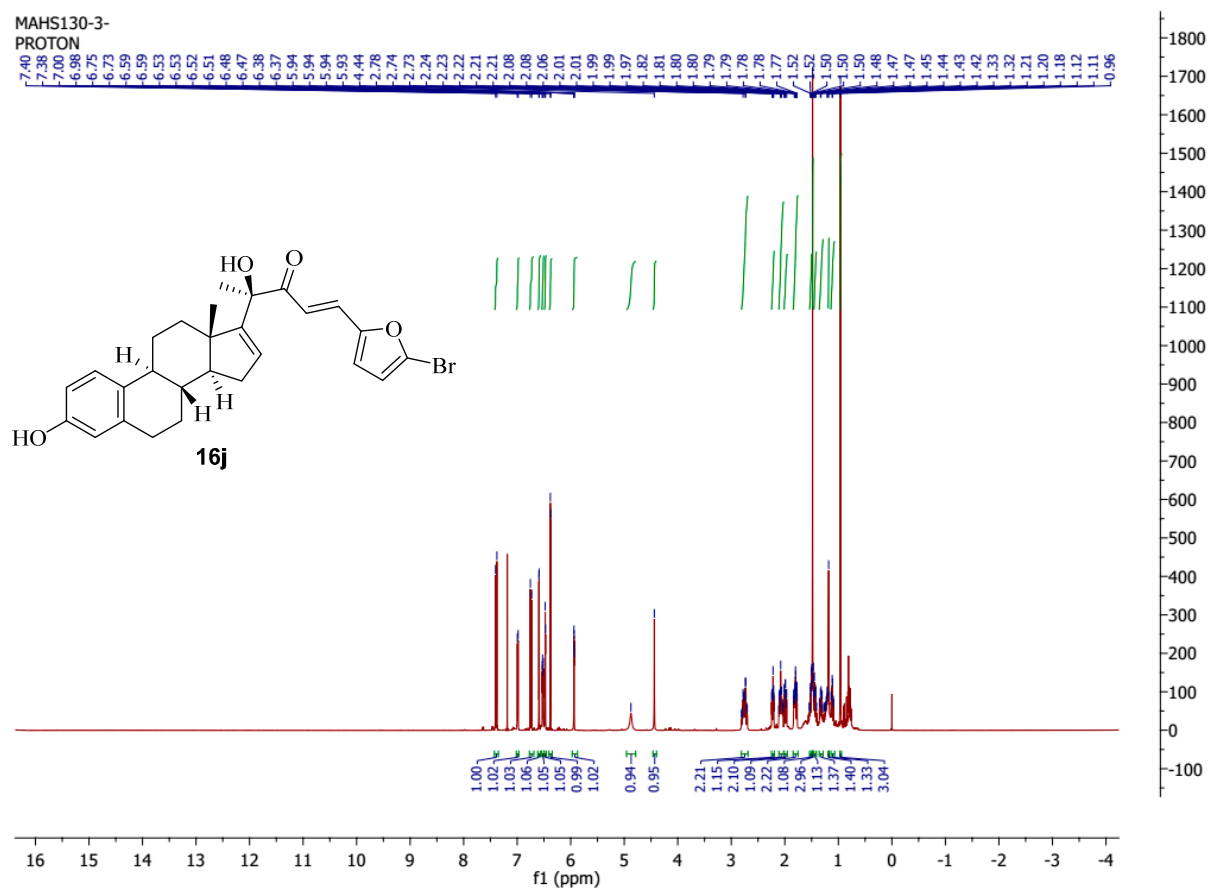


Figure S 66. ^1H NMR of compound **16j**.

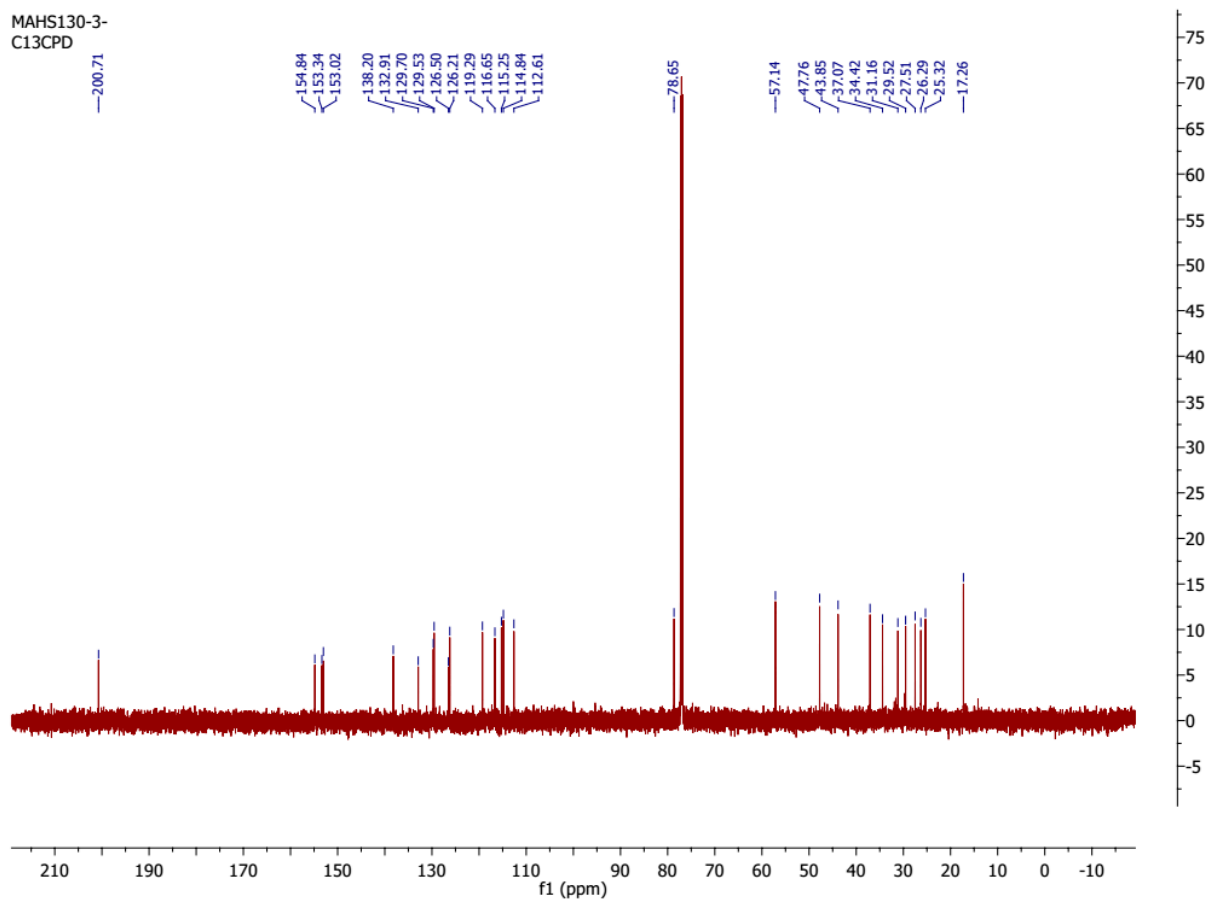


Figure S 67. ^{13}C NMR of compound 16j.

1.33 Compound 17a

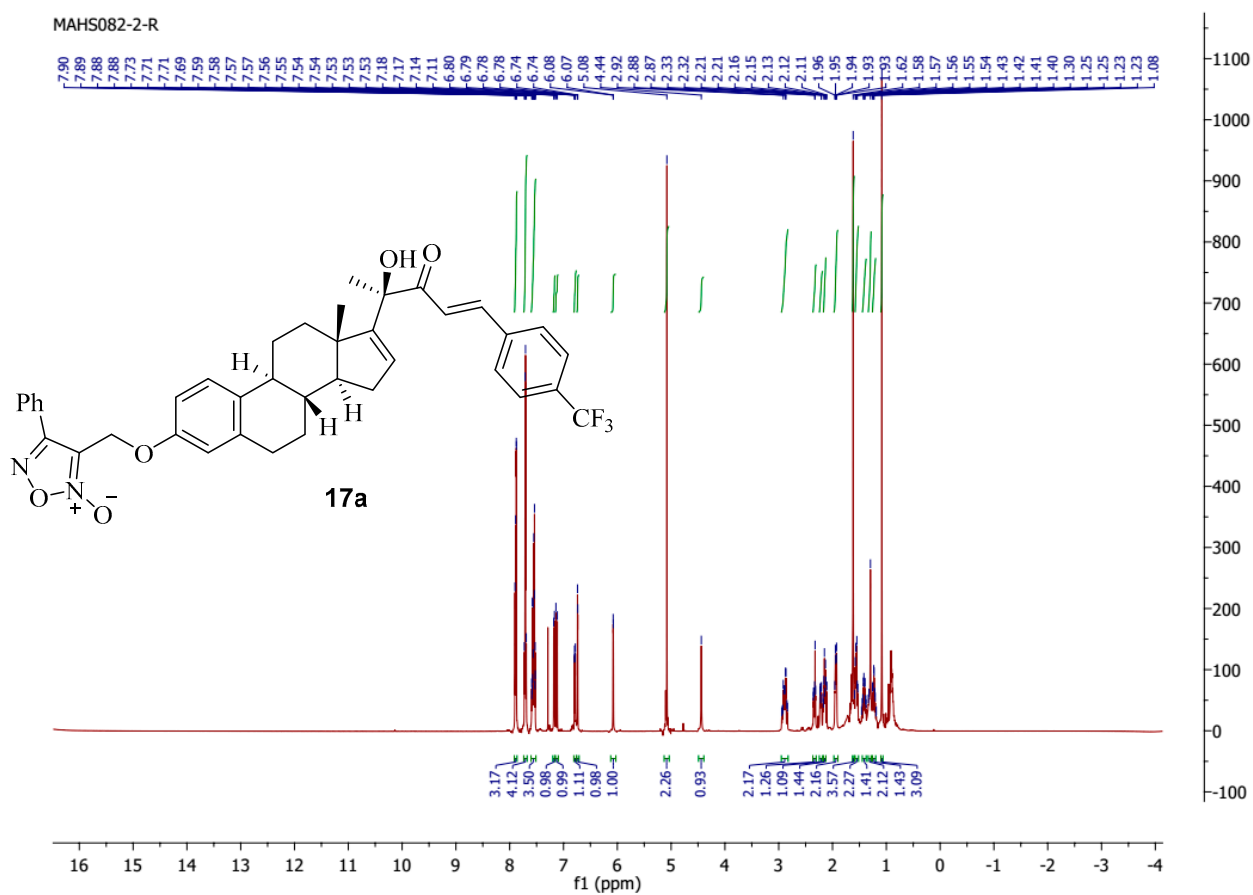


Figure S 68. ¹H NMR of compound **17a**.

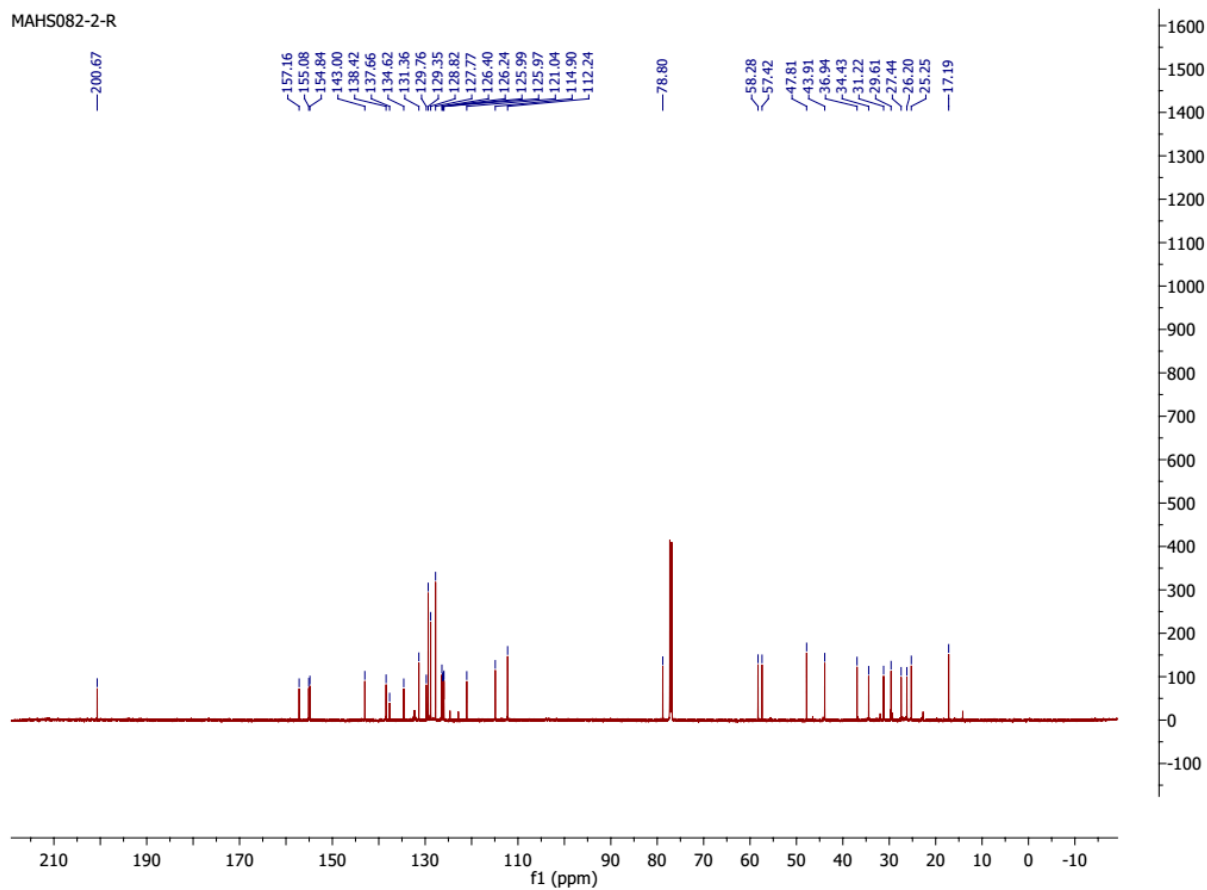


Figure S 69. ^{13}C NMR of compound **17a**.

1.34 Compound 17b

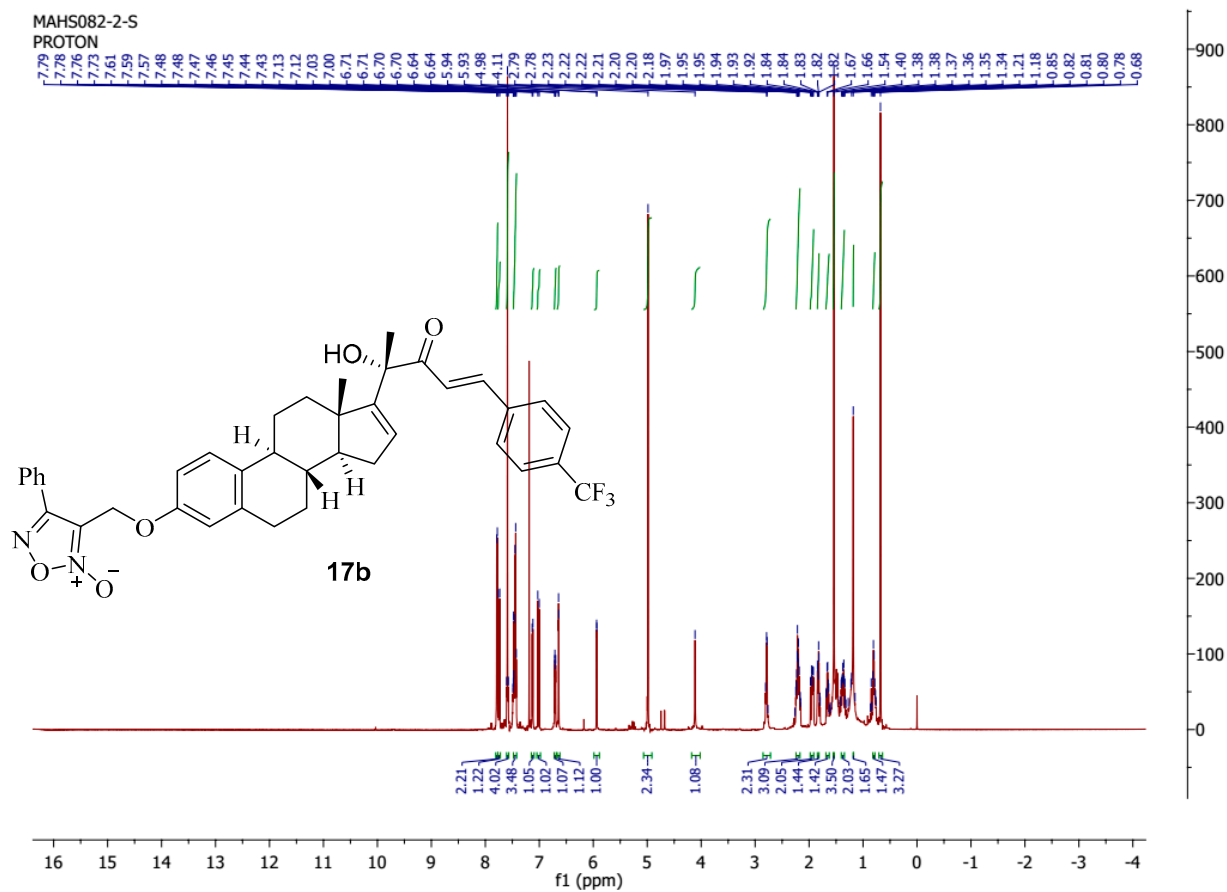


Figure S 70. ^1H NMR of compound **17b**.

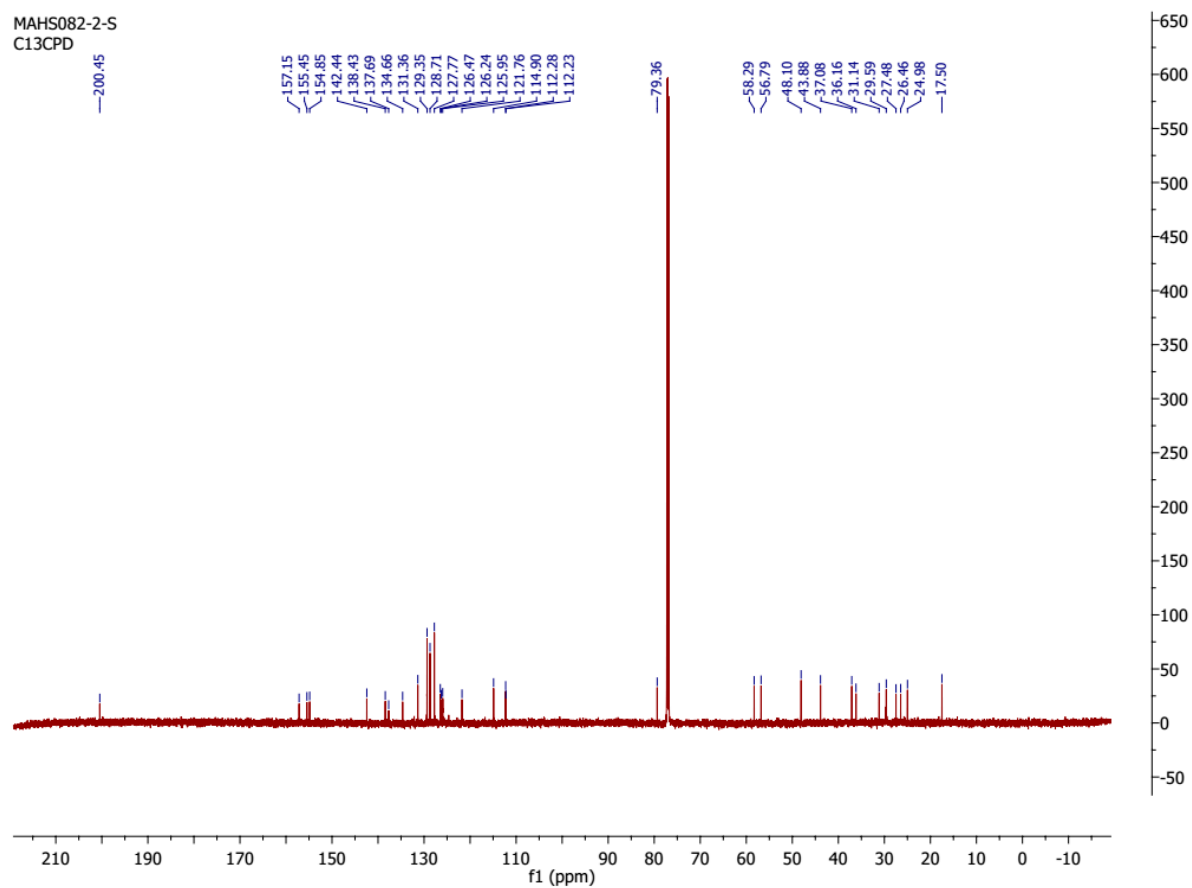


Figure S 71. ^{13}C NMR of compound **17b**.

1.35 Compound 17c

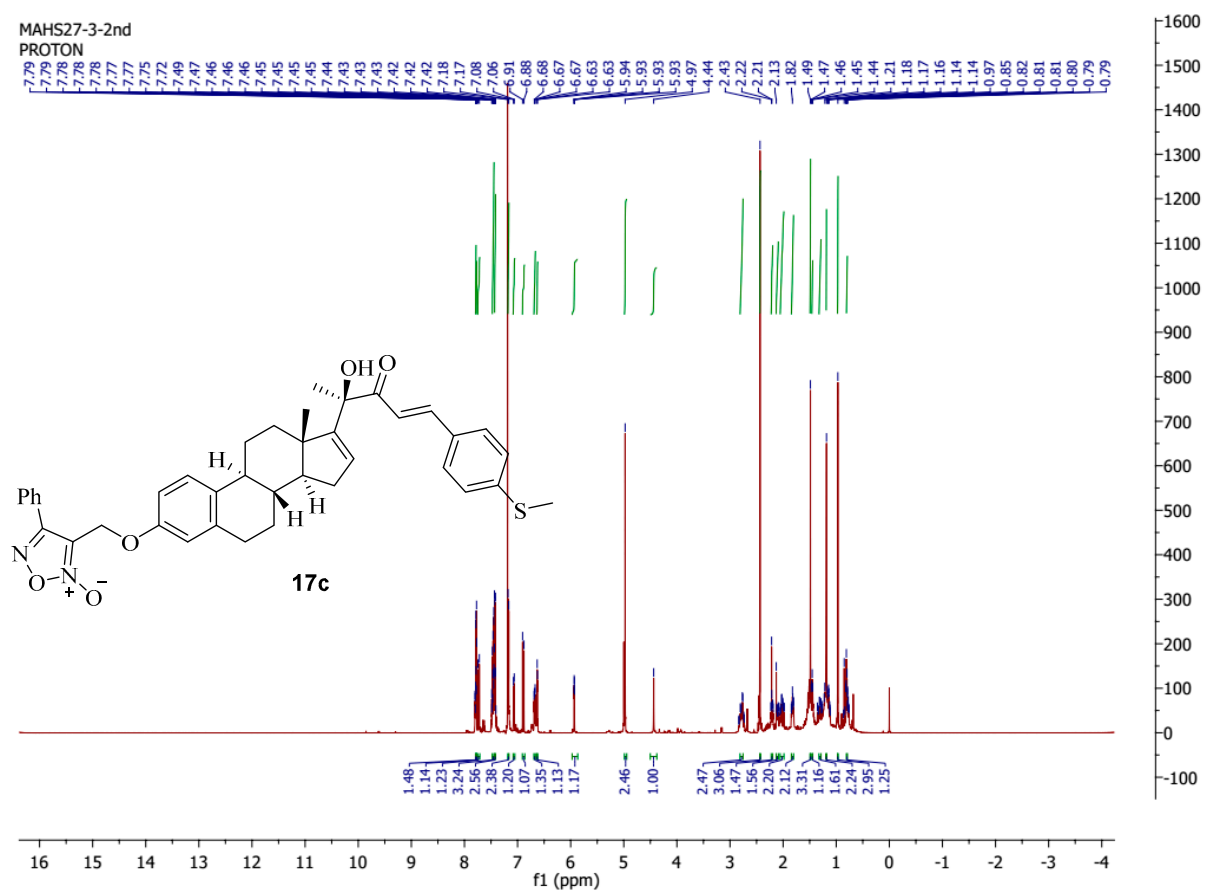


Figure S 72. ^1H NMR of compound **17c**.

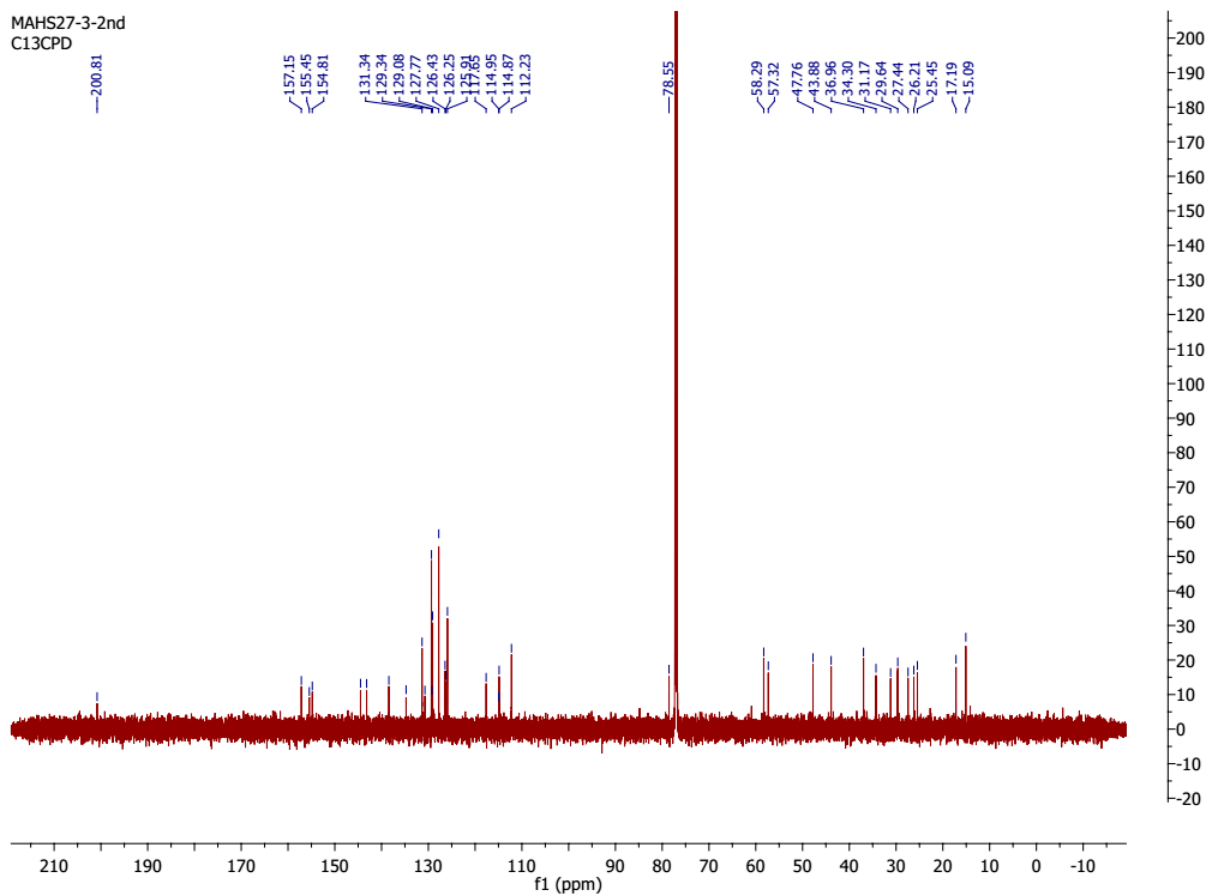


Figure S 73. ^{13}C NMR of compound **17c**.

1.36 Compound 17d

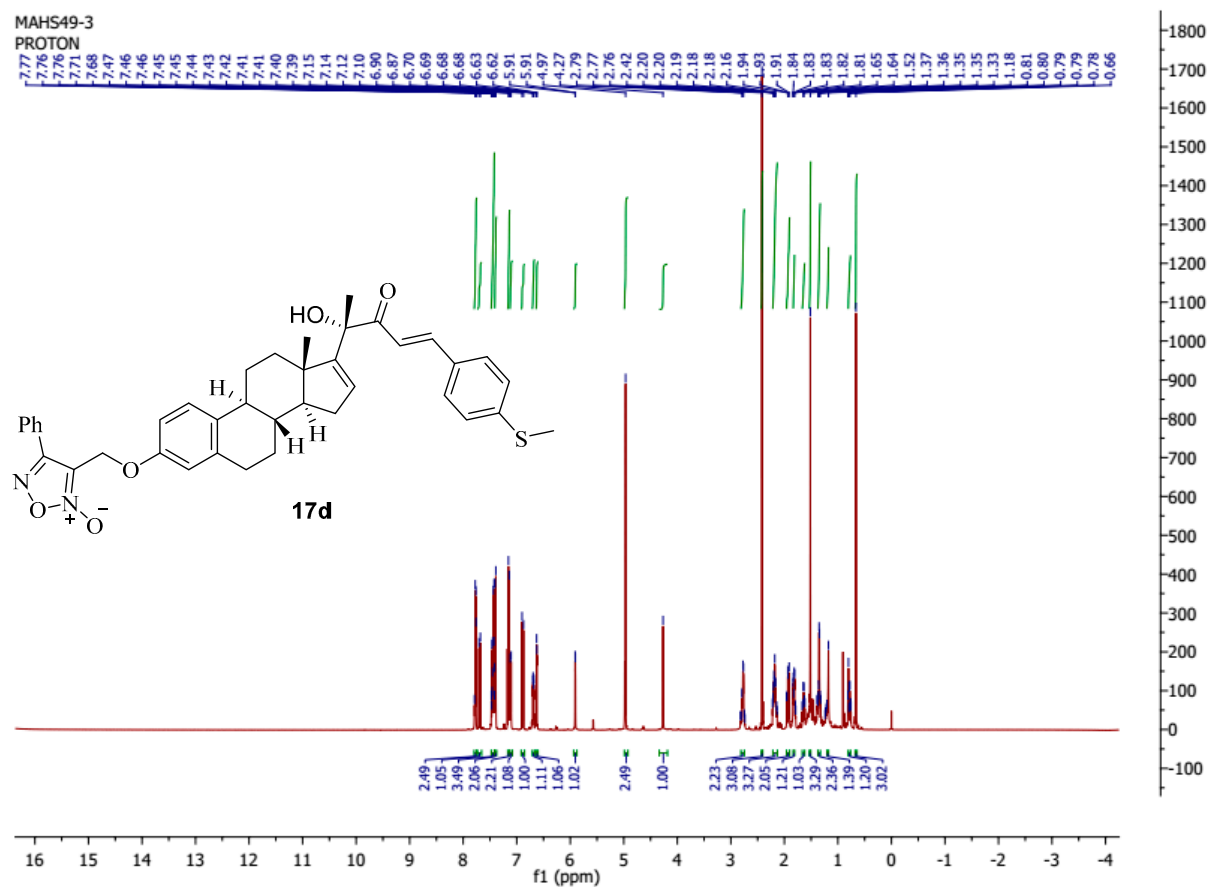


Figure S 74. ^1H NMR of compound **17d**.

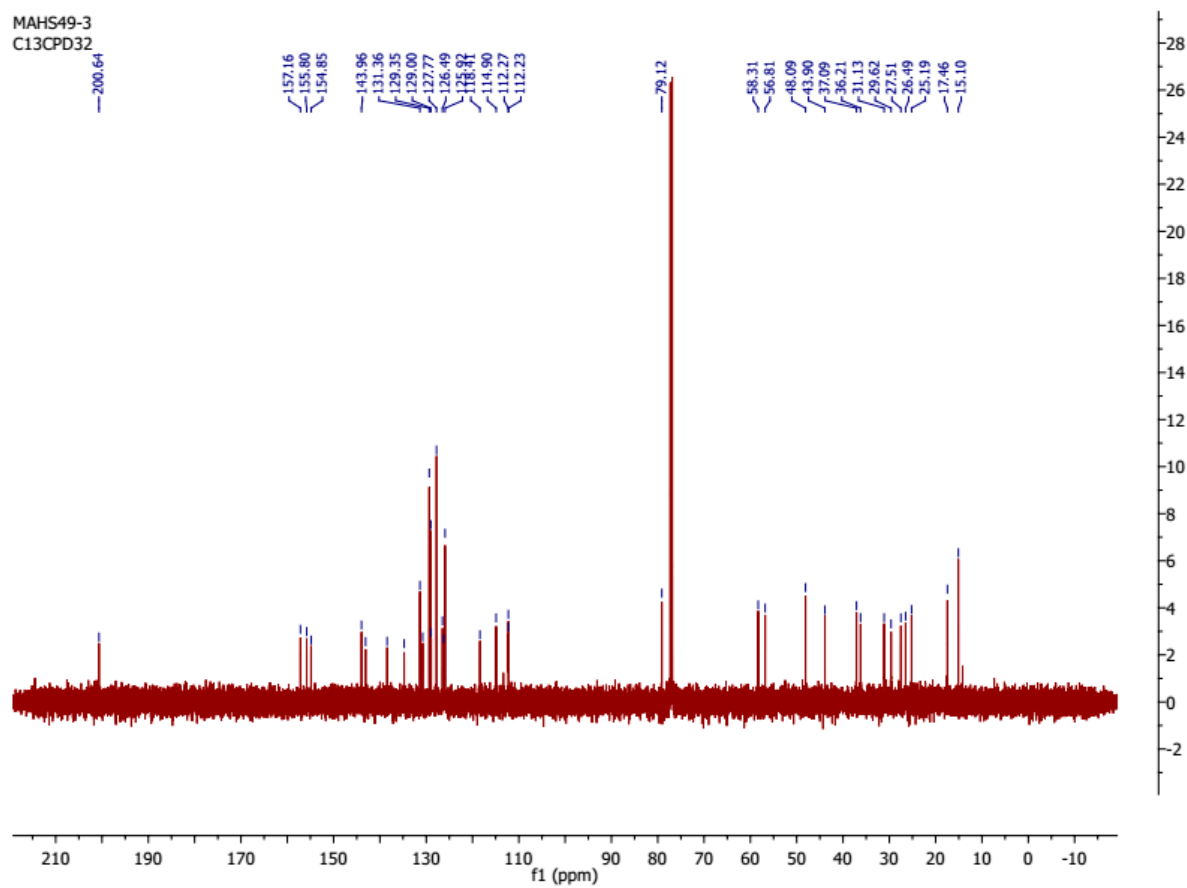


Figure S 75. ^{13}C NMR of compound **17d**.

1.37 Compound 17e

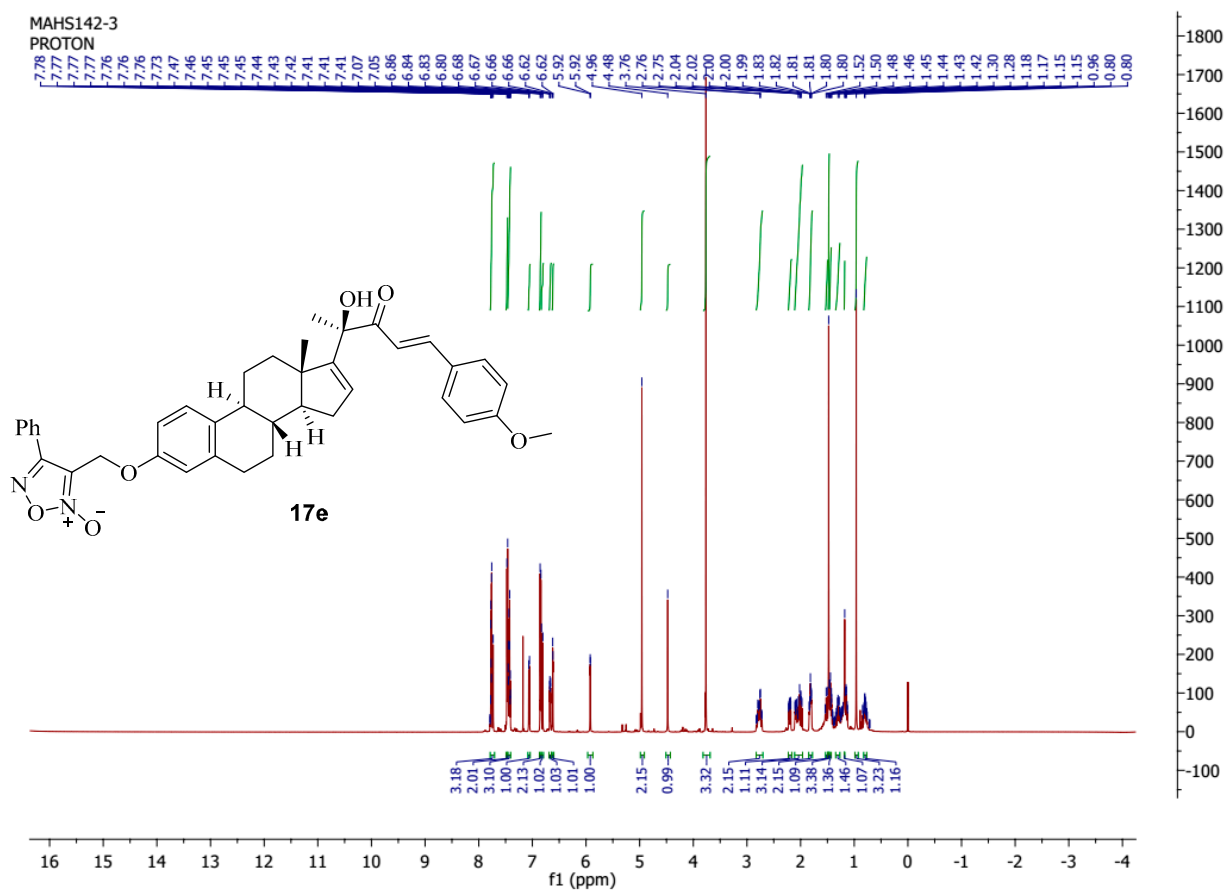


Figure S 76. ^1H NMR of compound **17e**.

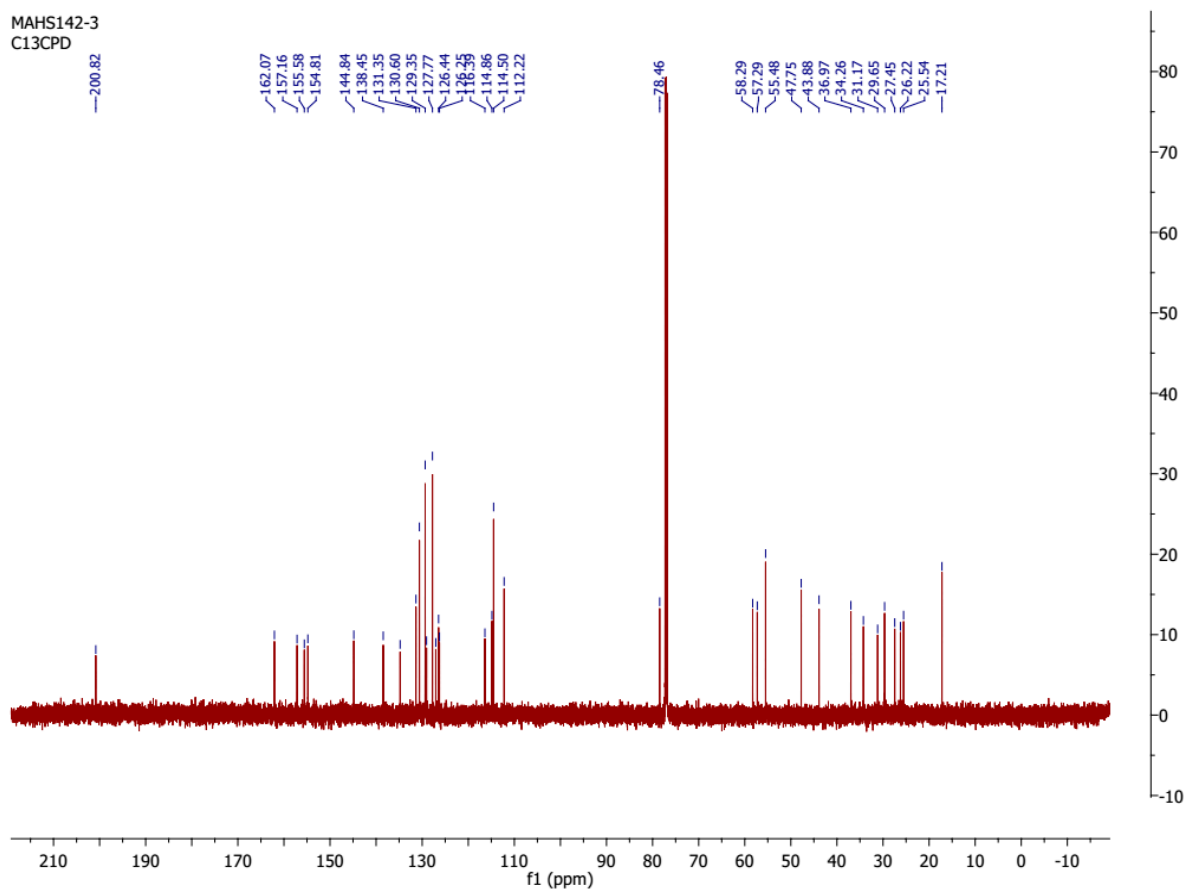


Figure S 77. ^{13}C NMR of compound **17e**.

1.38 Compound 17f

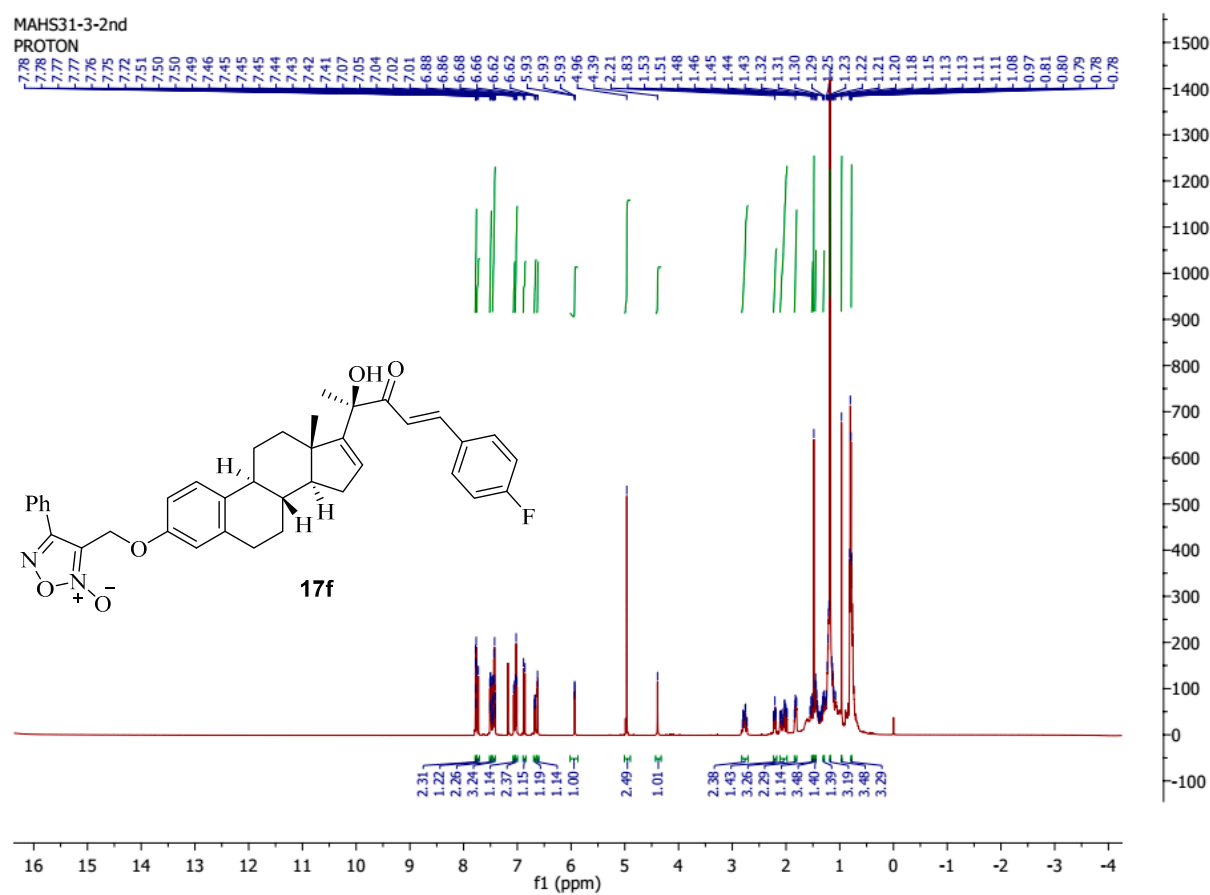


Figure S 78. ¹H NMR of compound 17f.

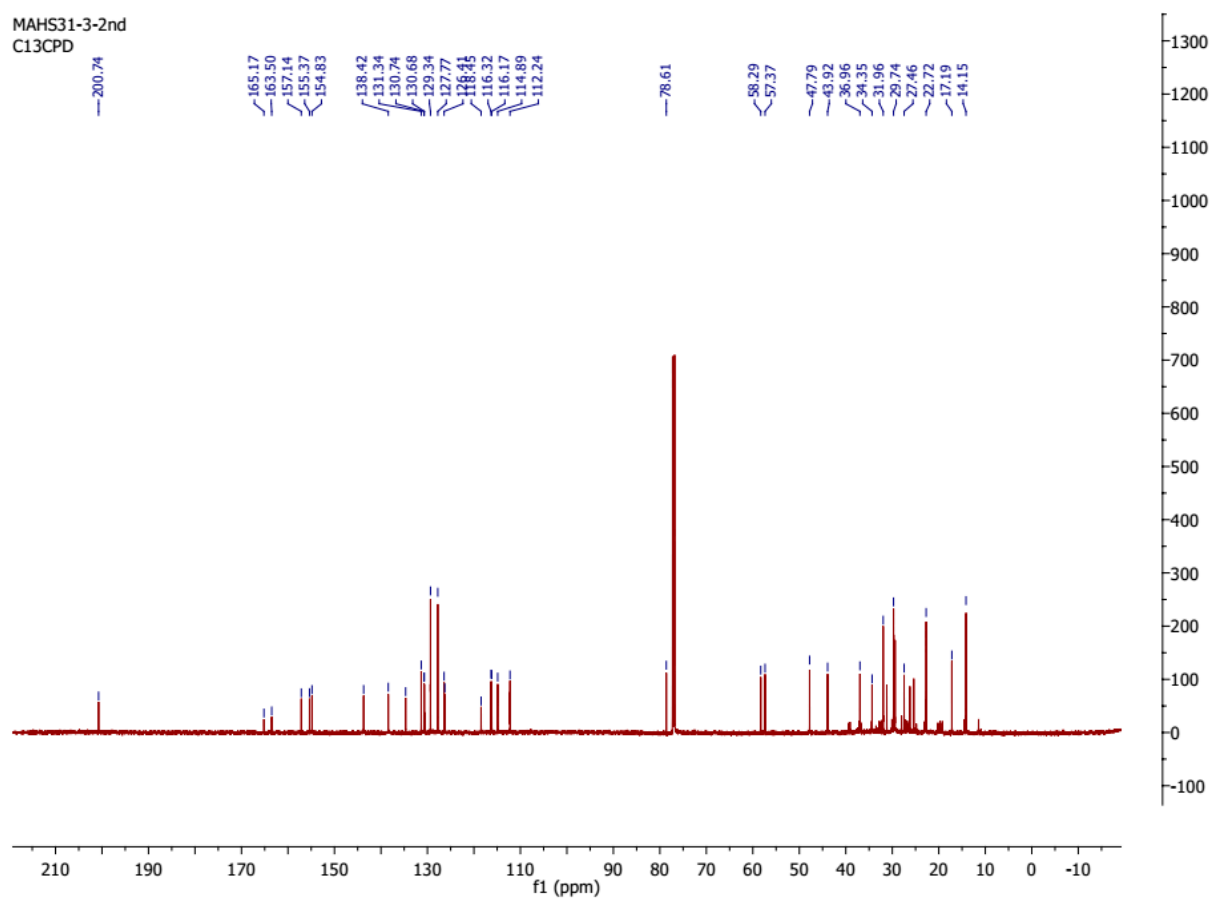


Figure S 79. ^{13}C NMR of compound **17f**.

1.39 Compound 17g

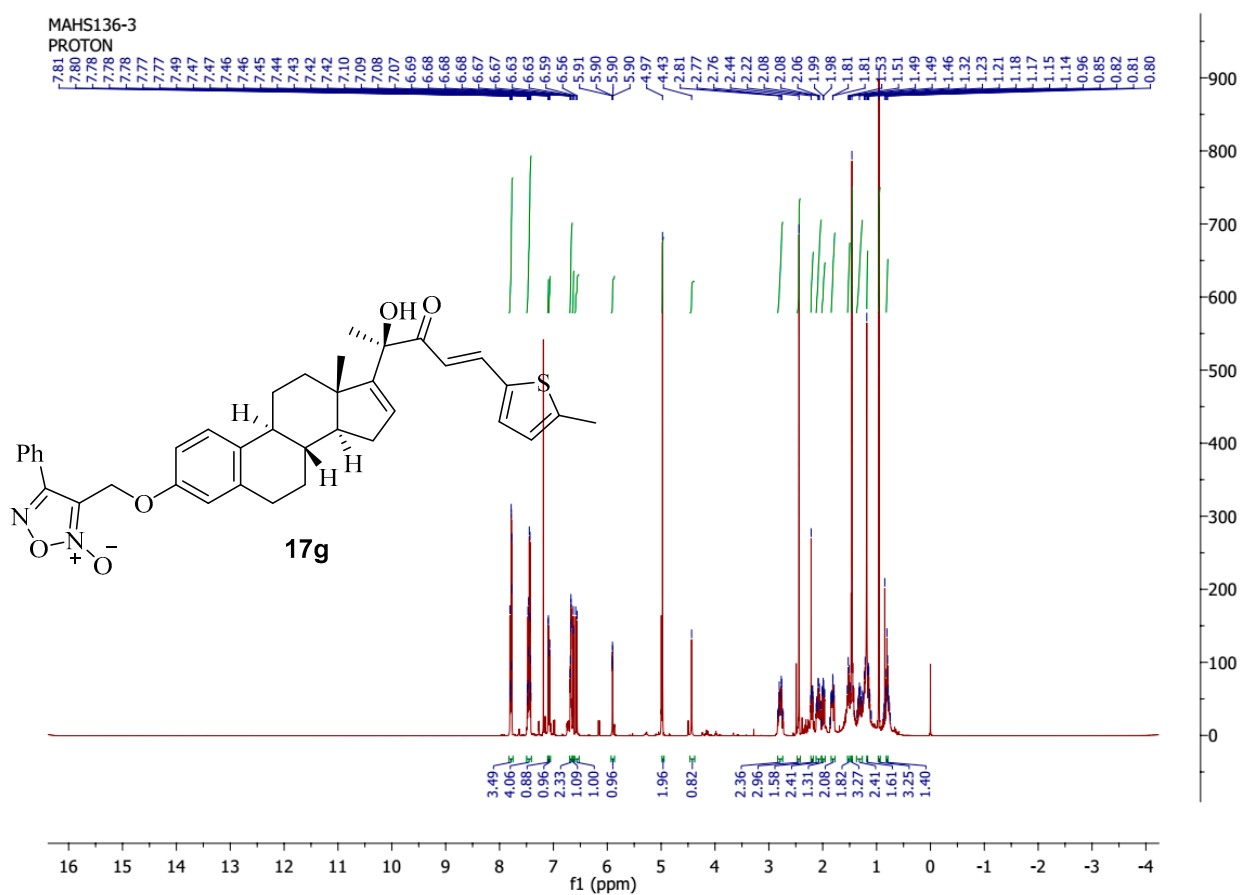


Figure S 80. ^1H NMR of compound **17g**.

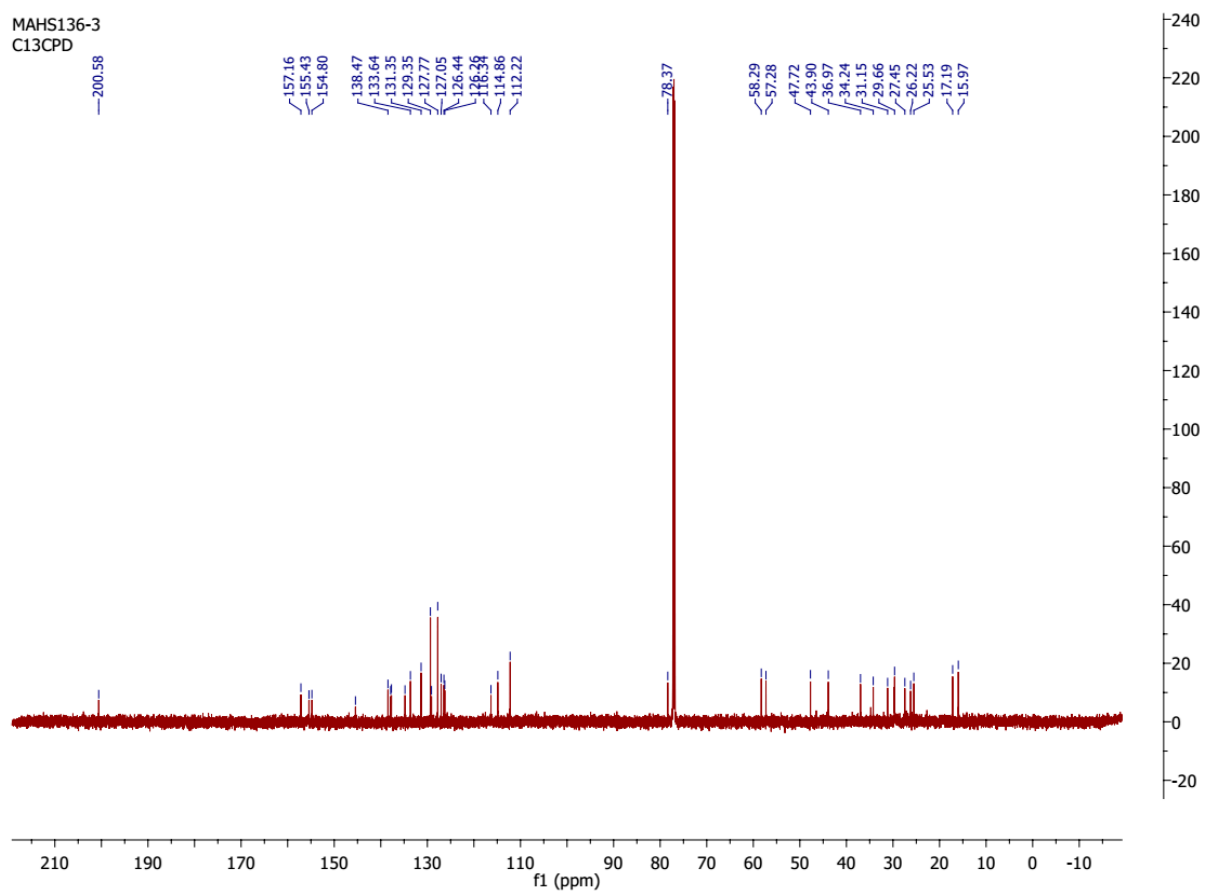


Figure S 81. ^{13}C NMR of compound **17g**.

1.40 Compound 17h

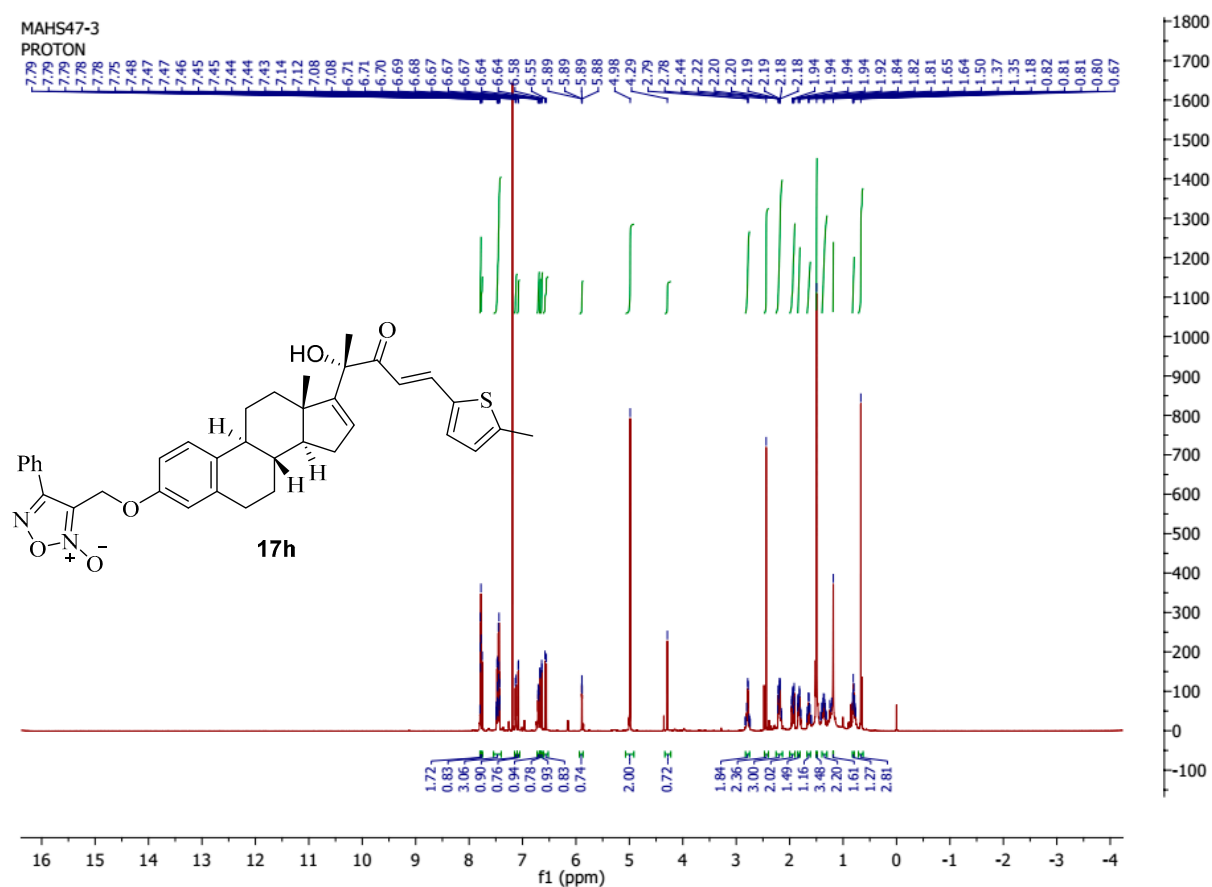


Figure S 82. ^1H NMR of compound **17h**.

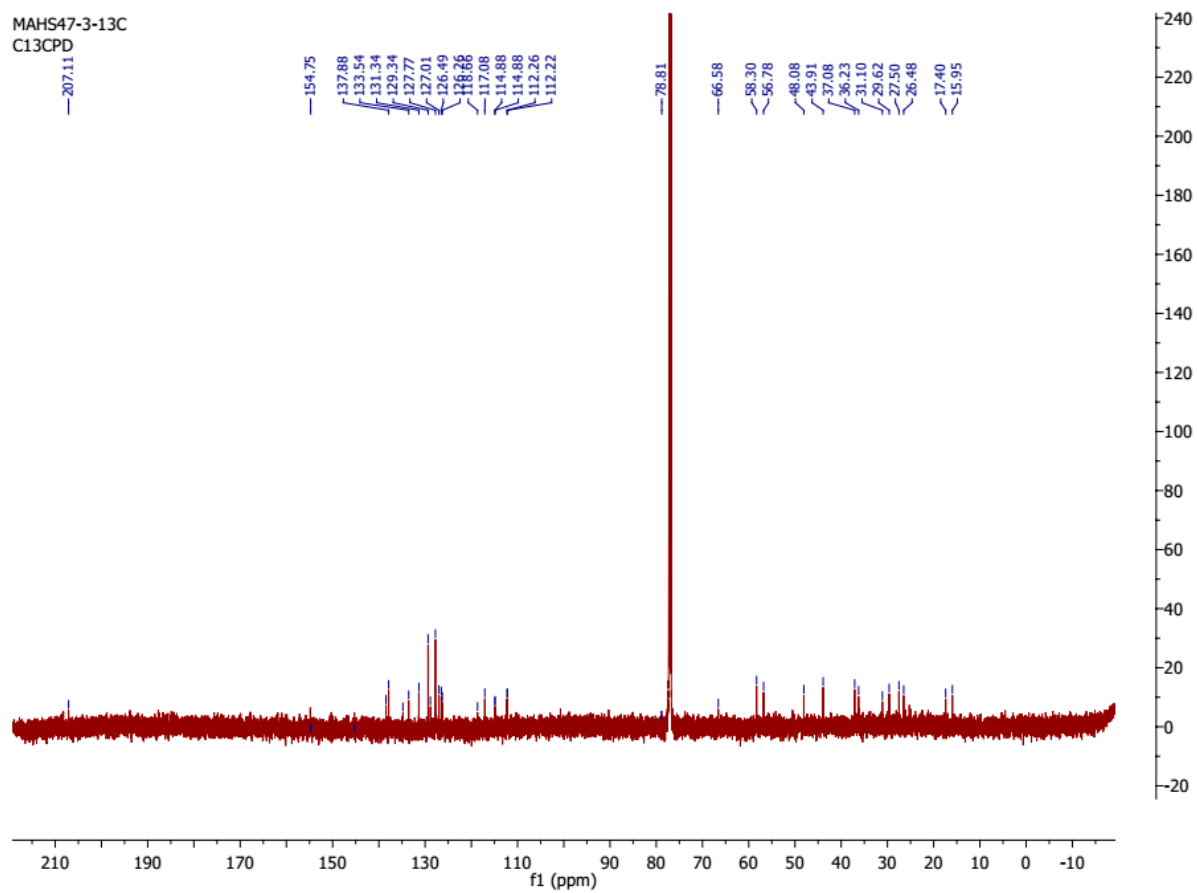


Figure S 83. ^{13}C NMR of compound **17h**.

1.41 Compound 17i

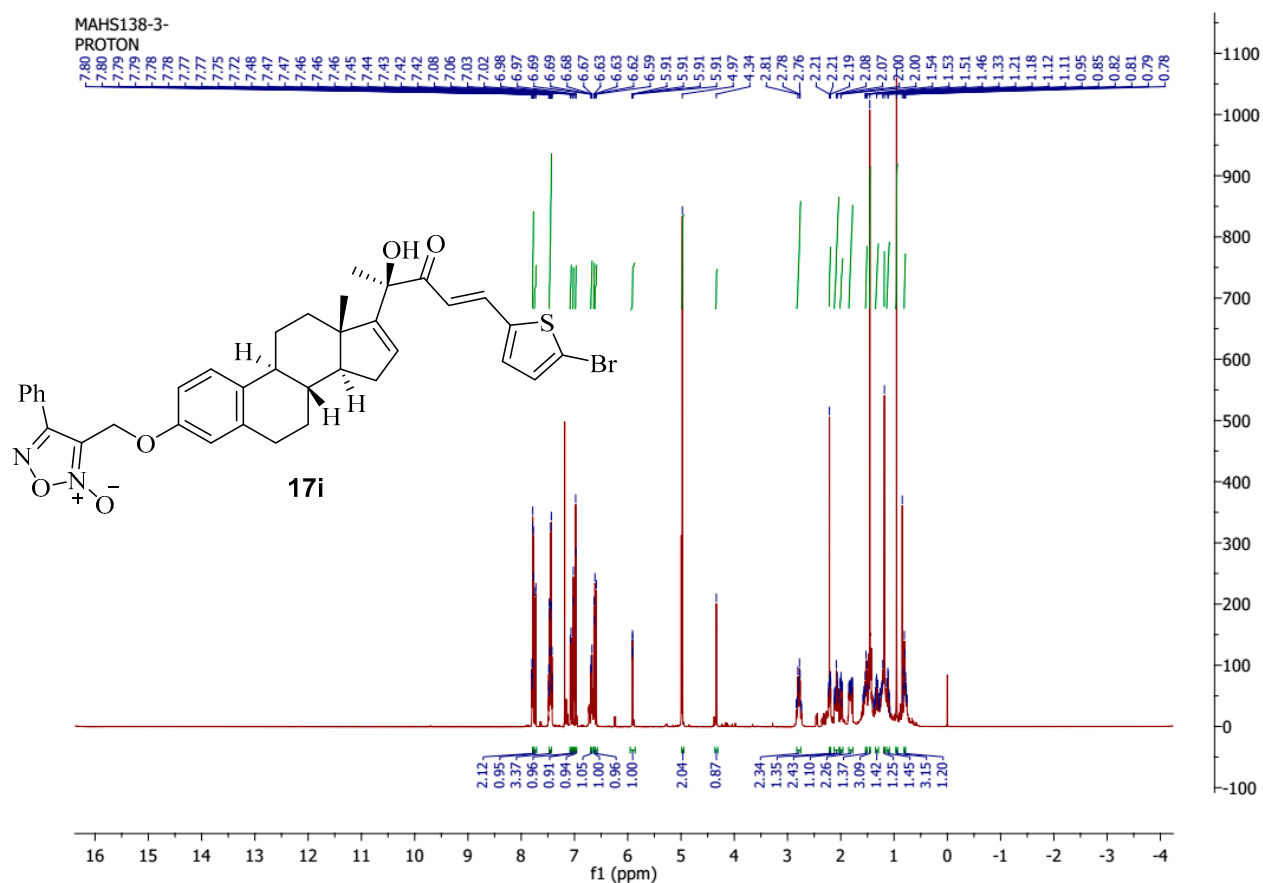


Figure S 84. ^1H NMR of compound **17i**.

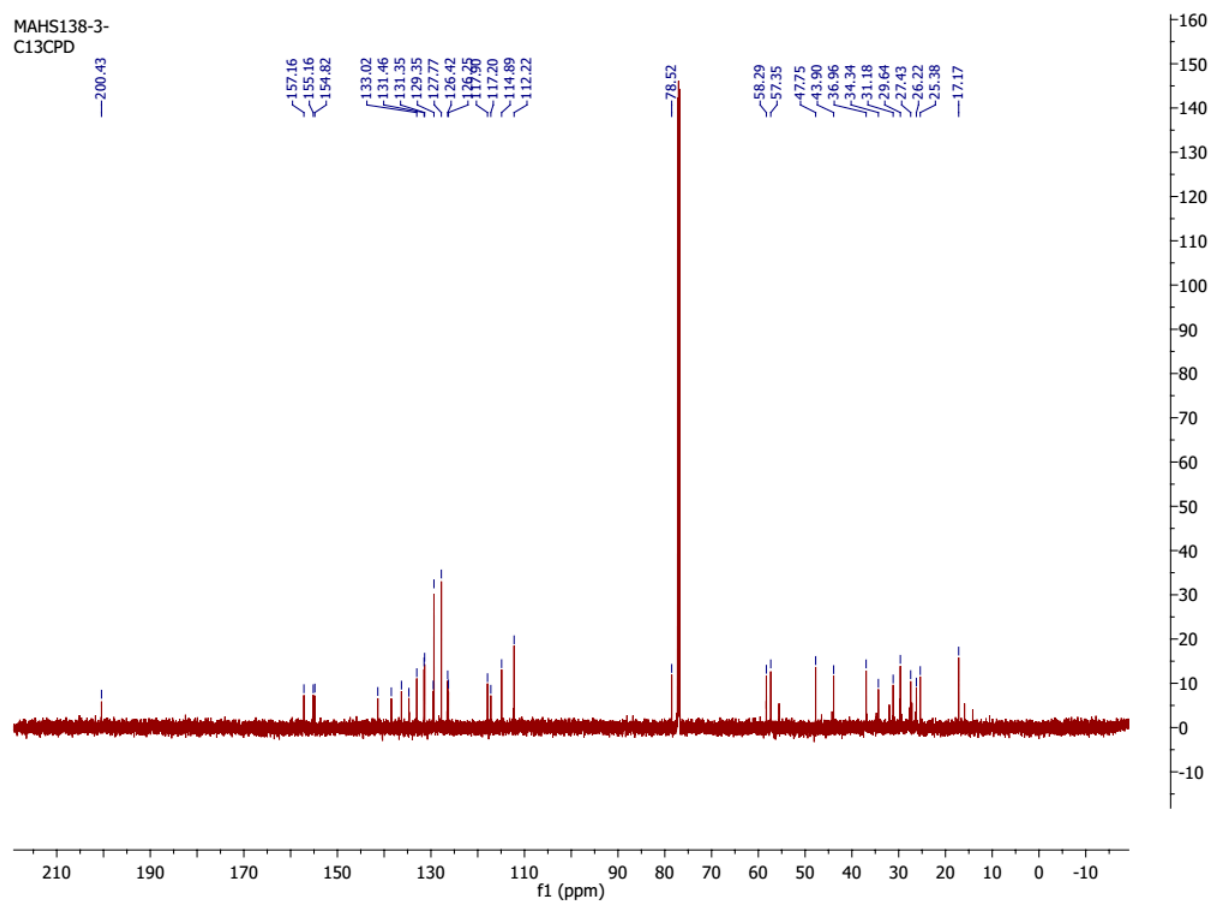


Figure S 85. ^{13}C NMR of compound **17i**.

1.42 Compound 17j

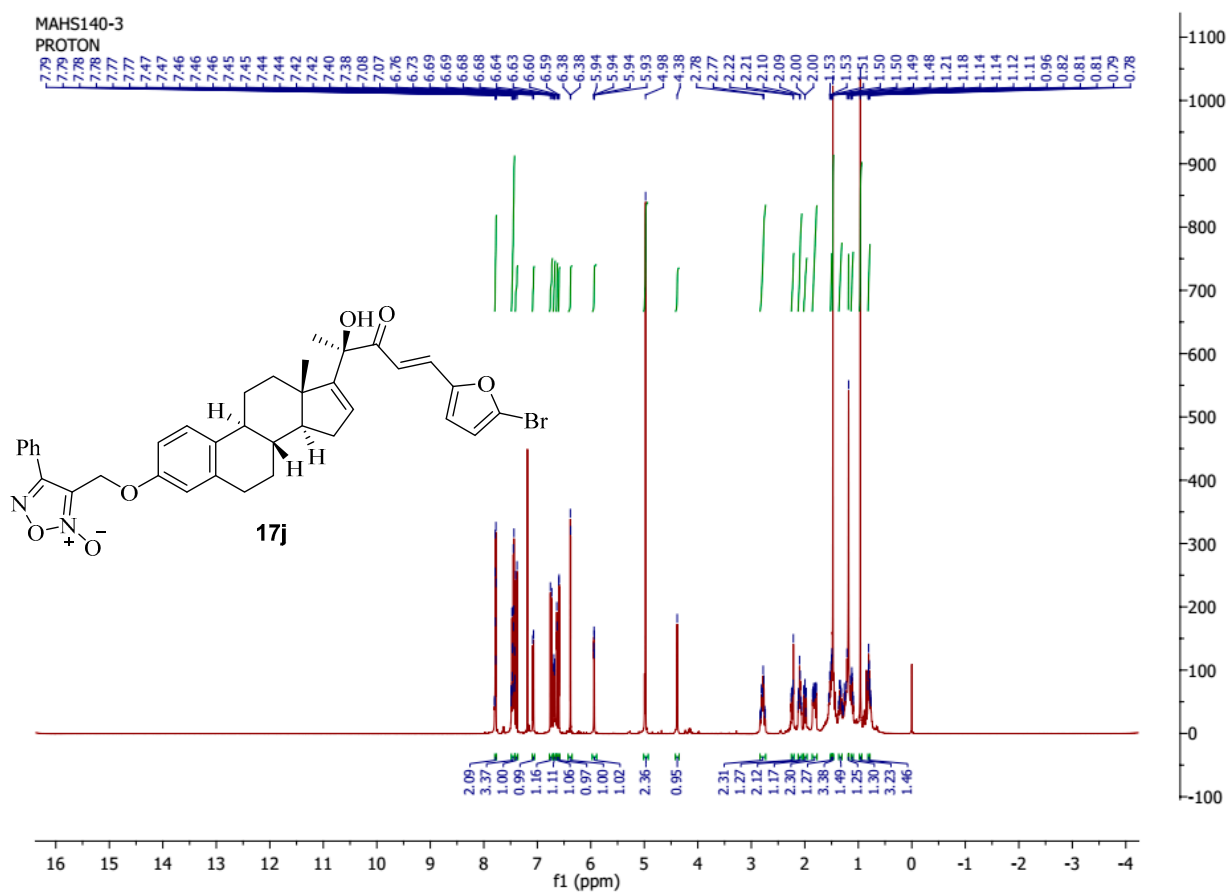


Figure S 86. ^1H NMR of compound 17j.

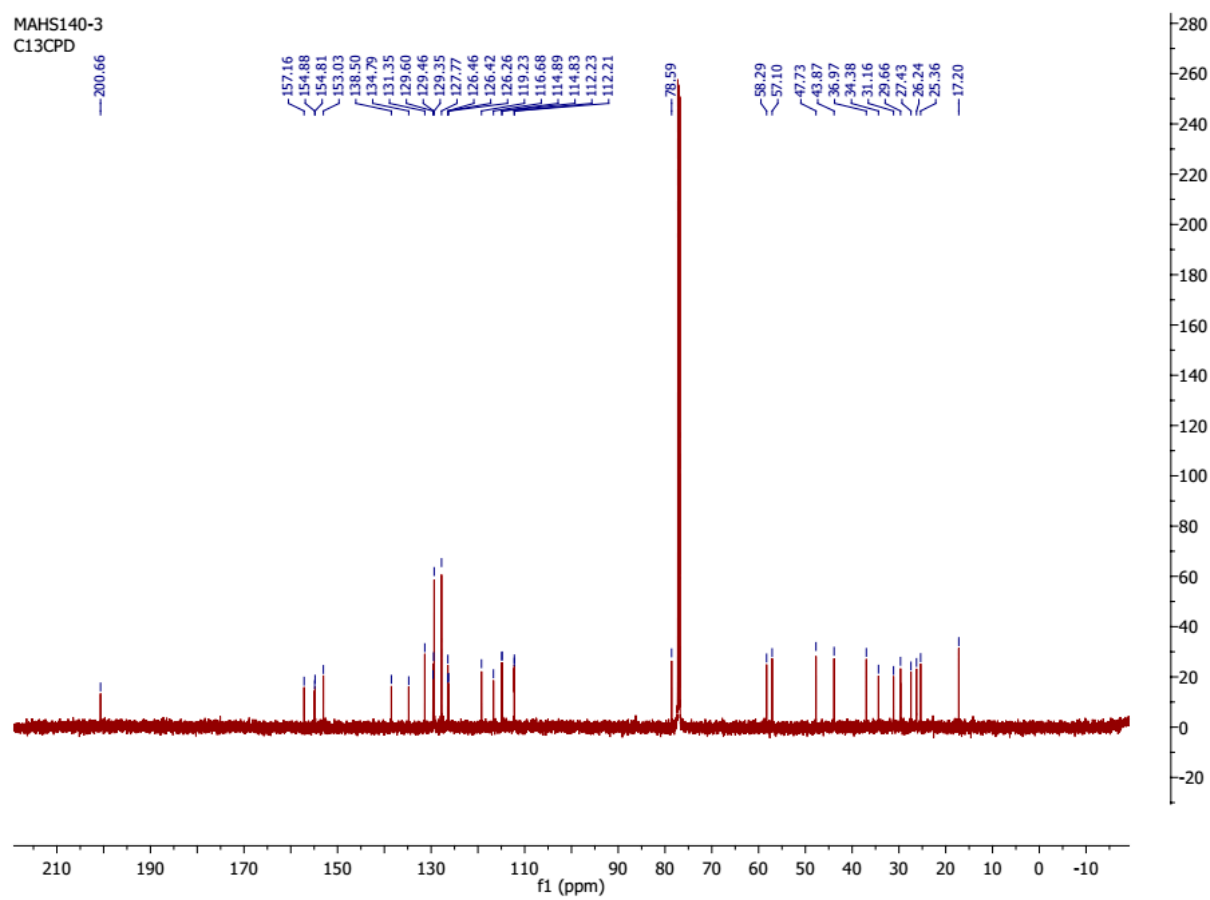


Figure S 87. ^{13}C NMR of compound **17j**.

1.43 Compound 18

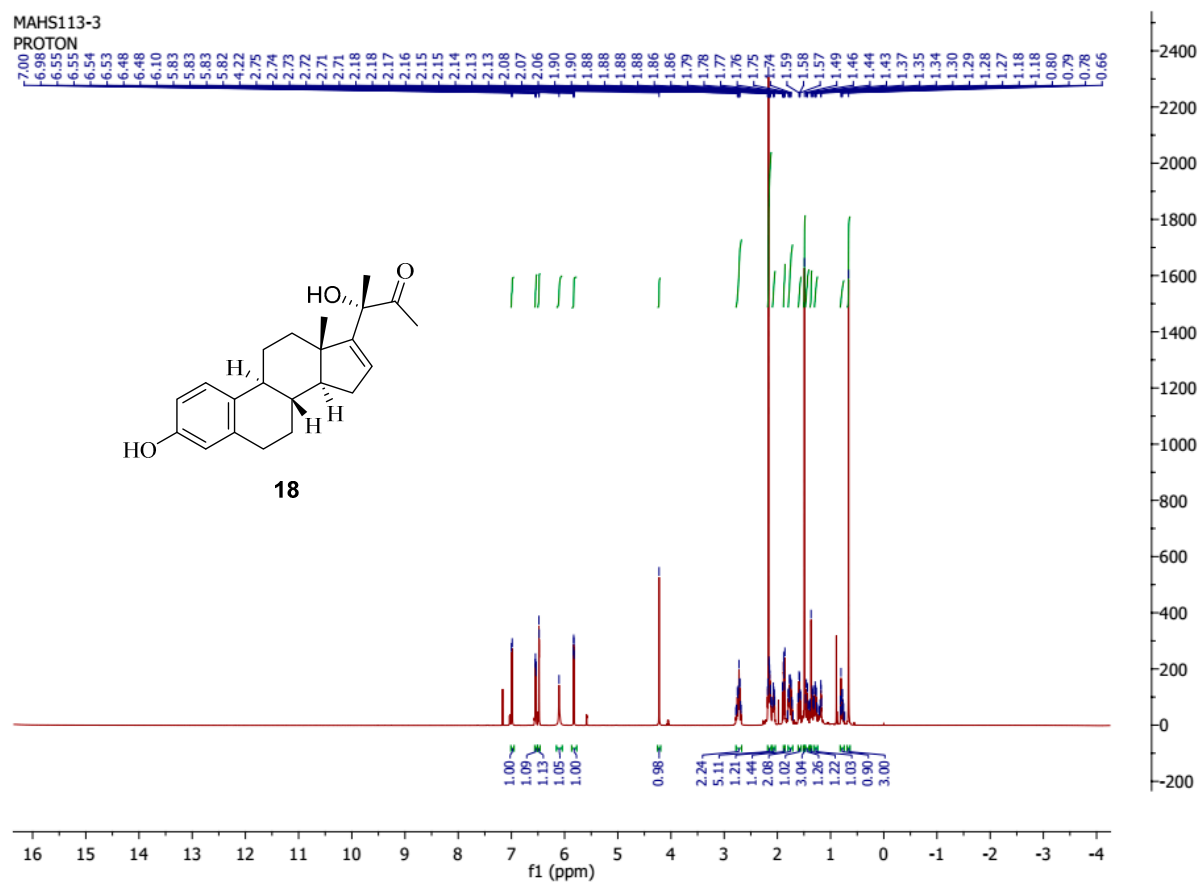


Figure S 88. ^1H NMR of compound 18.

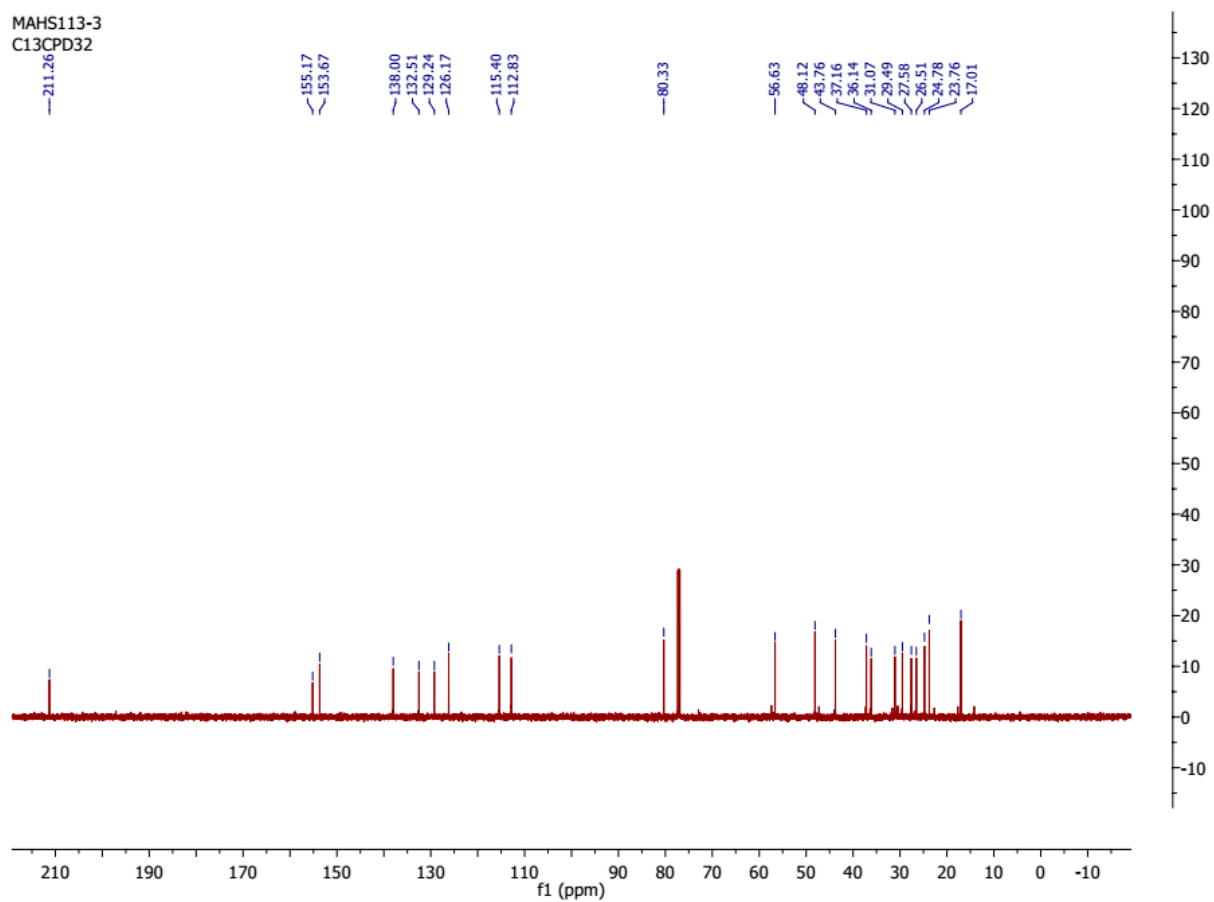


Figure S 89. ^{13}C NMR of compound **18**.

1.44 Compound 19

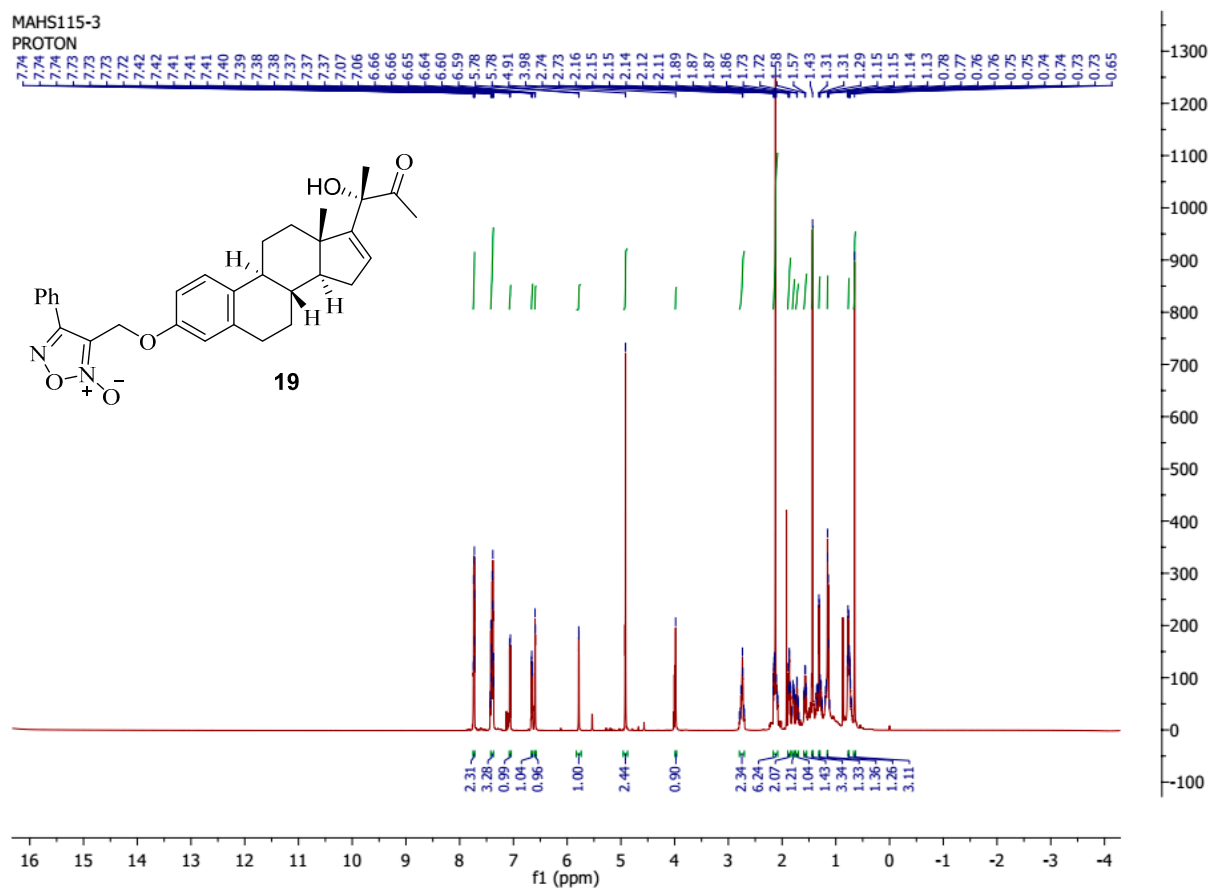


Figure S 90. ^1H NMR of compound 19.

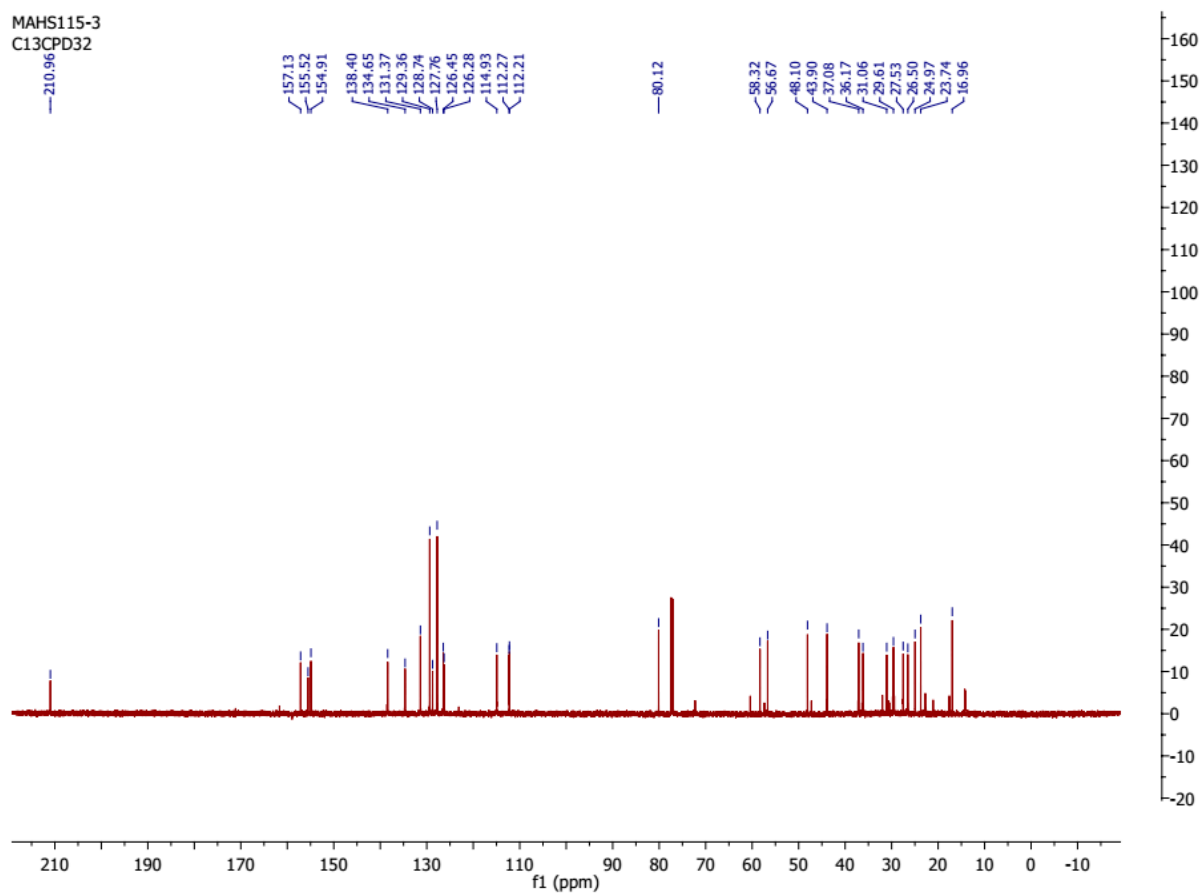


Figure S 91. ^{13}C NMR of compound **19**.

1.45 Compound 20a

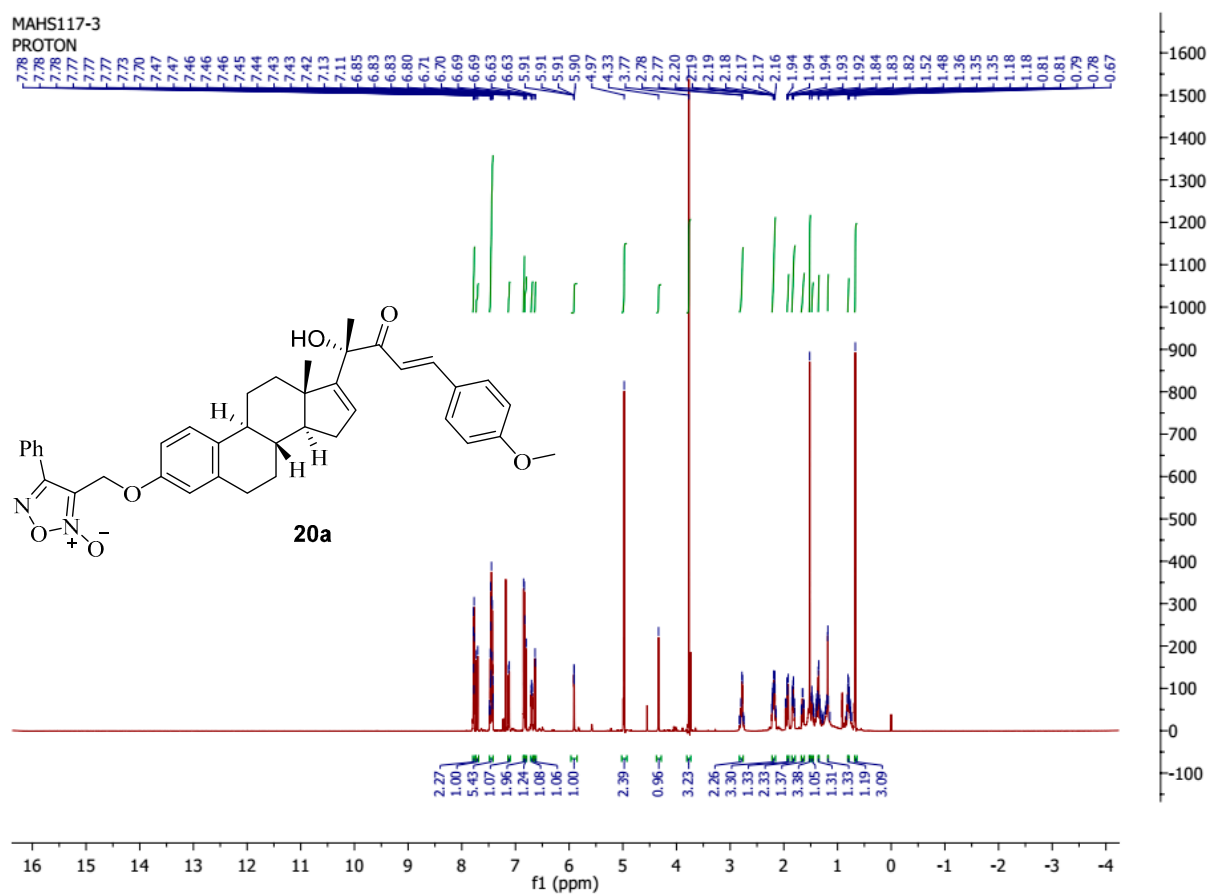


Figure S 92. ^1H NMR of compound **20a**.

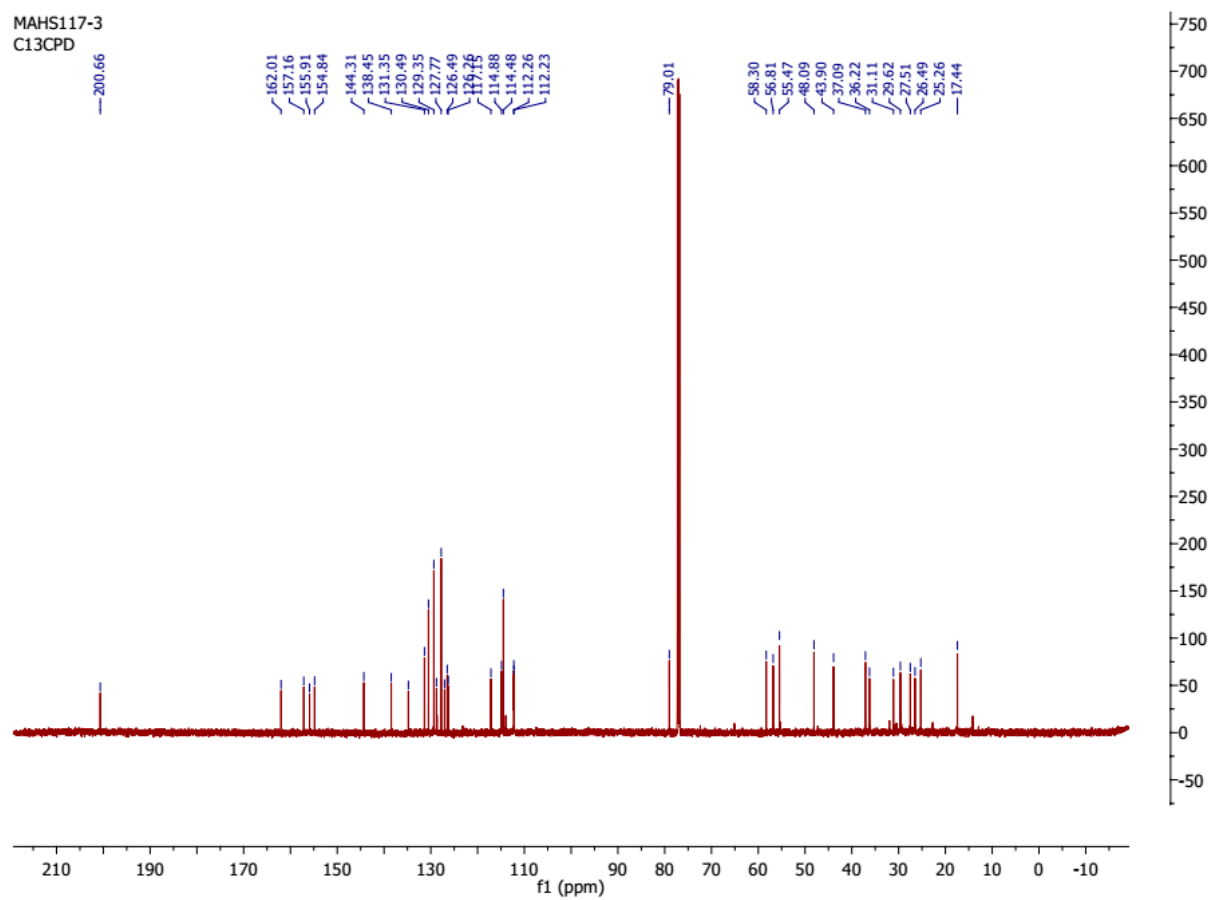


Figure S 93. ^{13}C NMR of compound **20a**.

1.46 Compound 20b

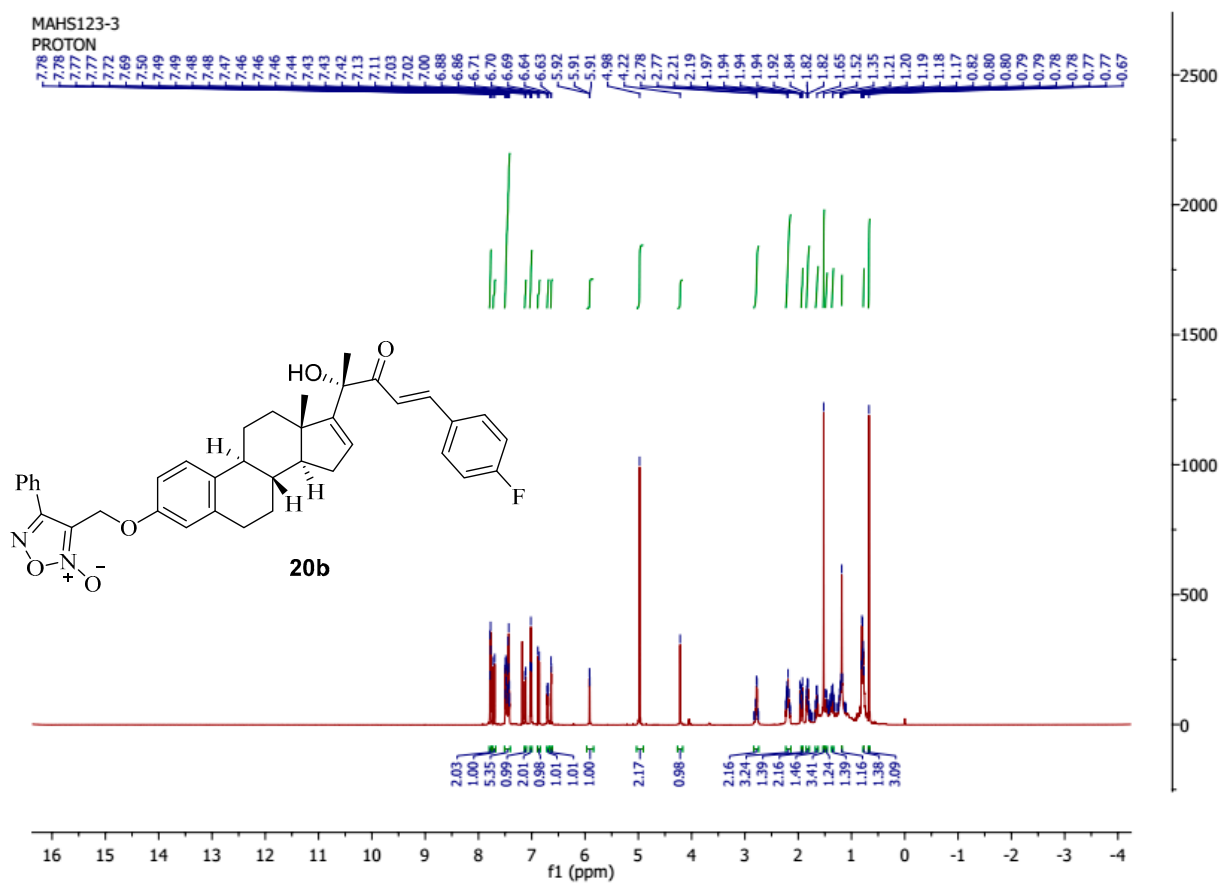


Figure S 94. ¹H NMR of compound **20b**.

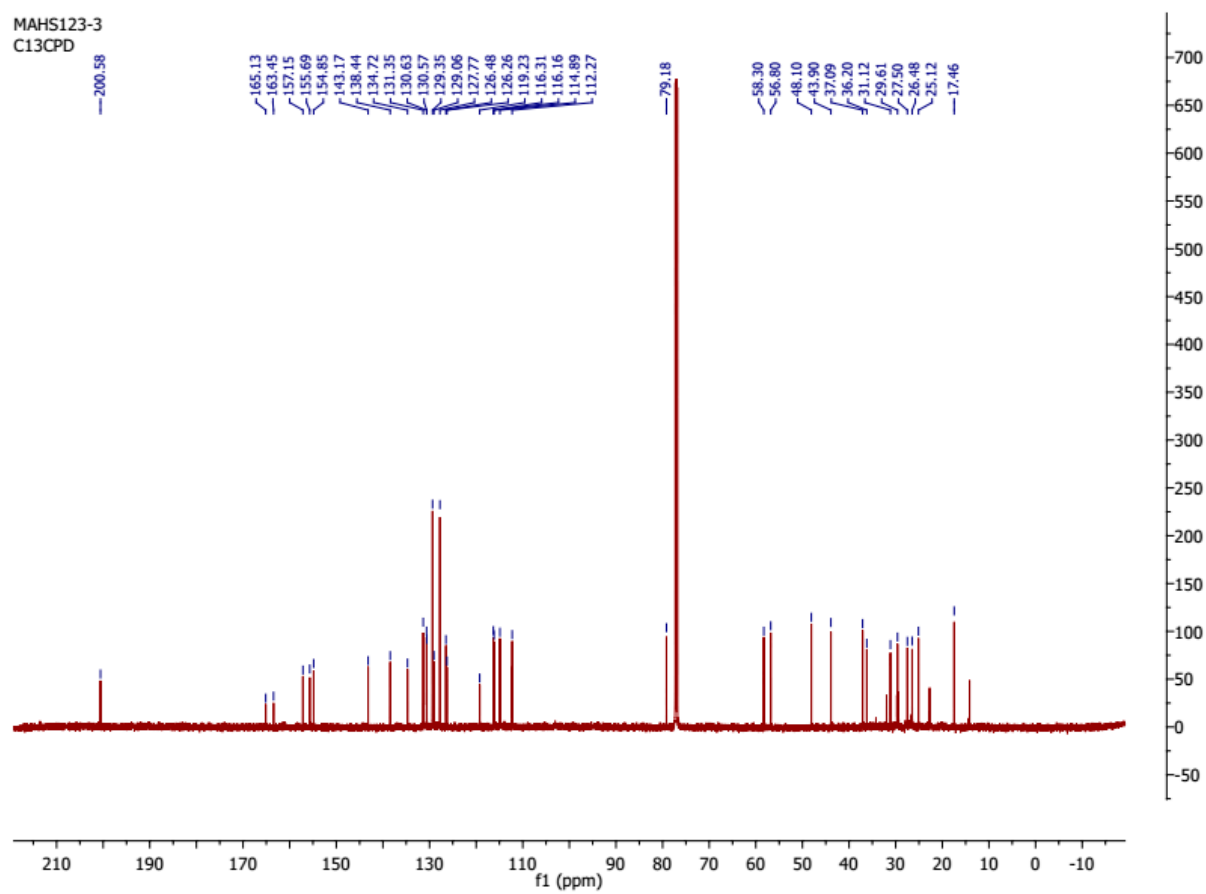


Figure S 95. ^{13}C NMR of compound **20b**.

1.47 Compound 20c

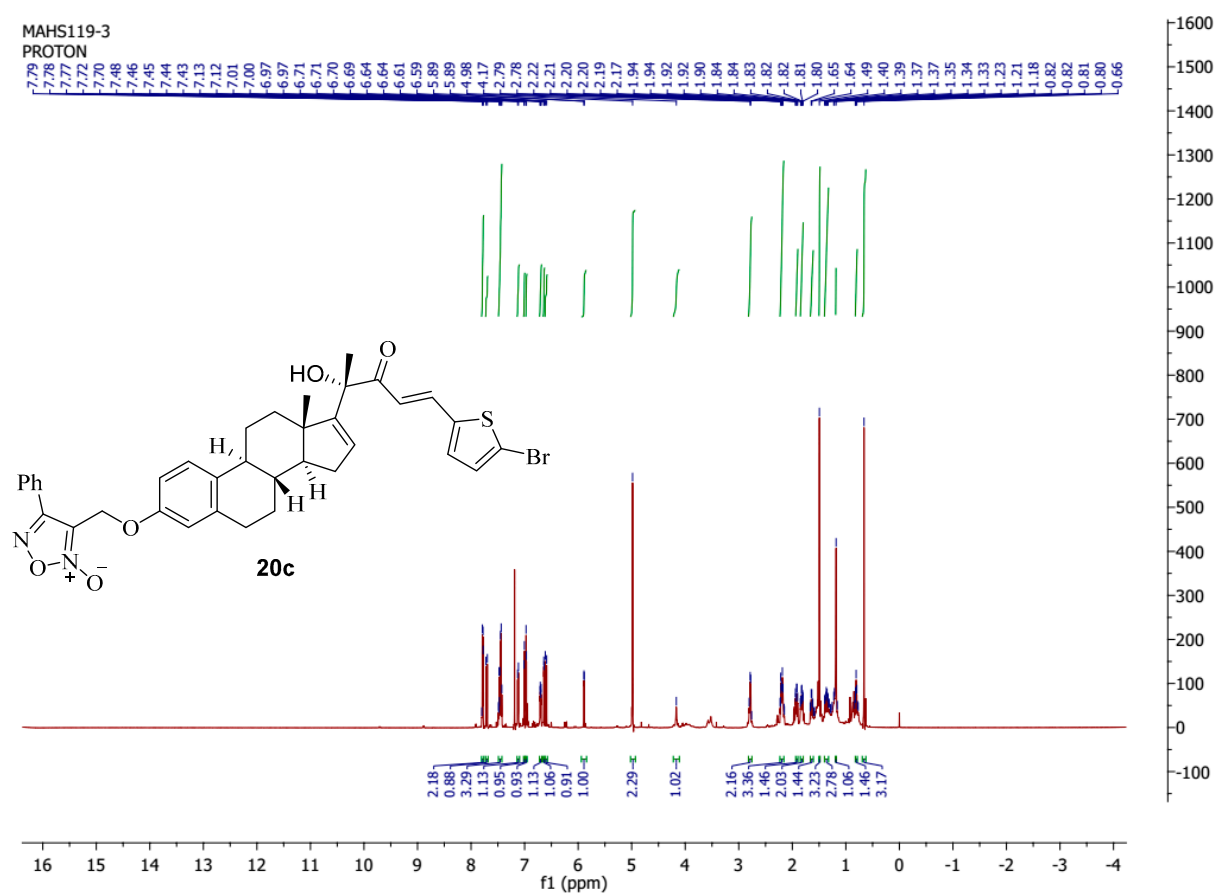


Figure S 96. ^1H NMR of compound **20c**.

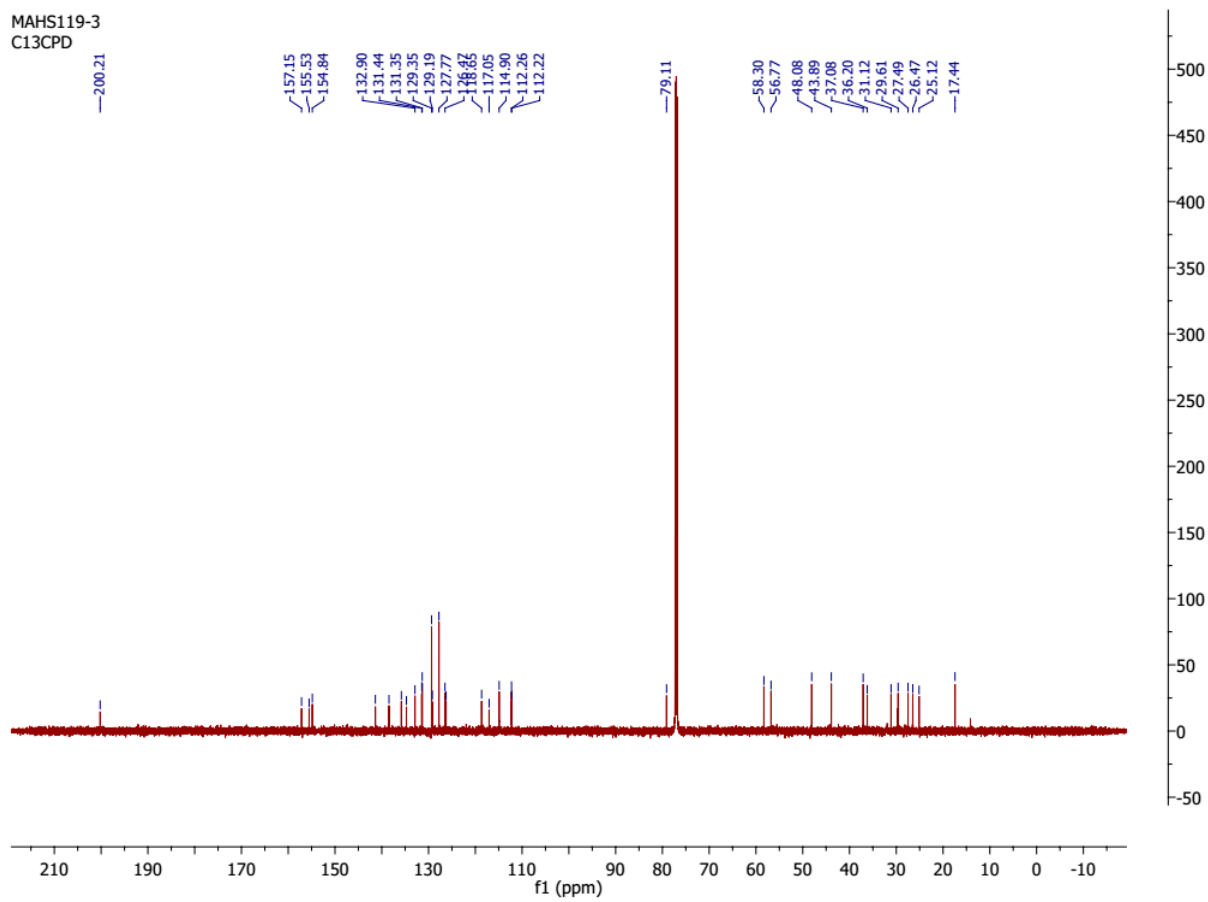


Figure S 97. ^{13}C NMR of compound **20c**.

1.48 Compound 20d

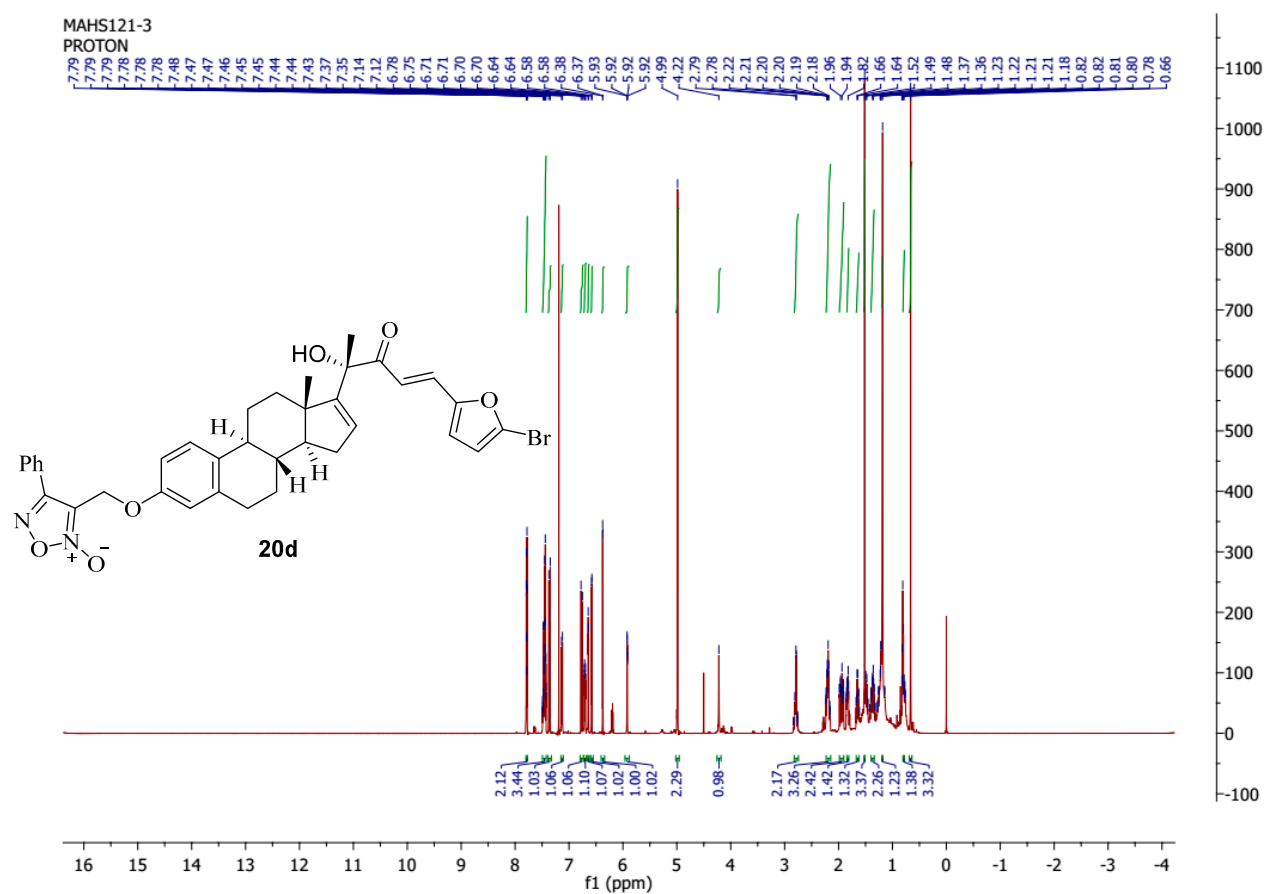


Figure S 98. ^1H NMR of compound **20d**.

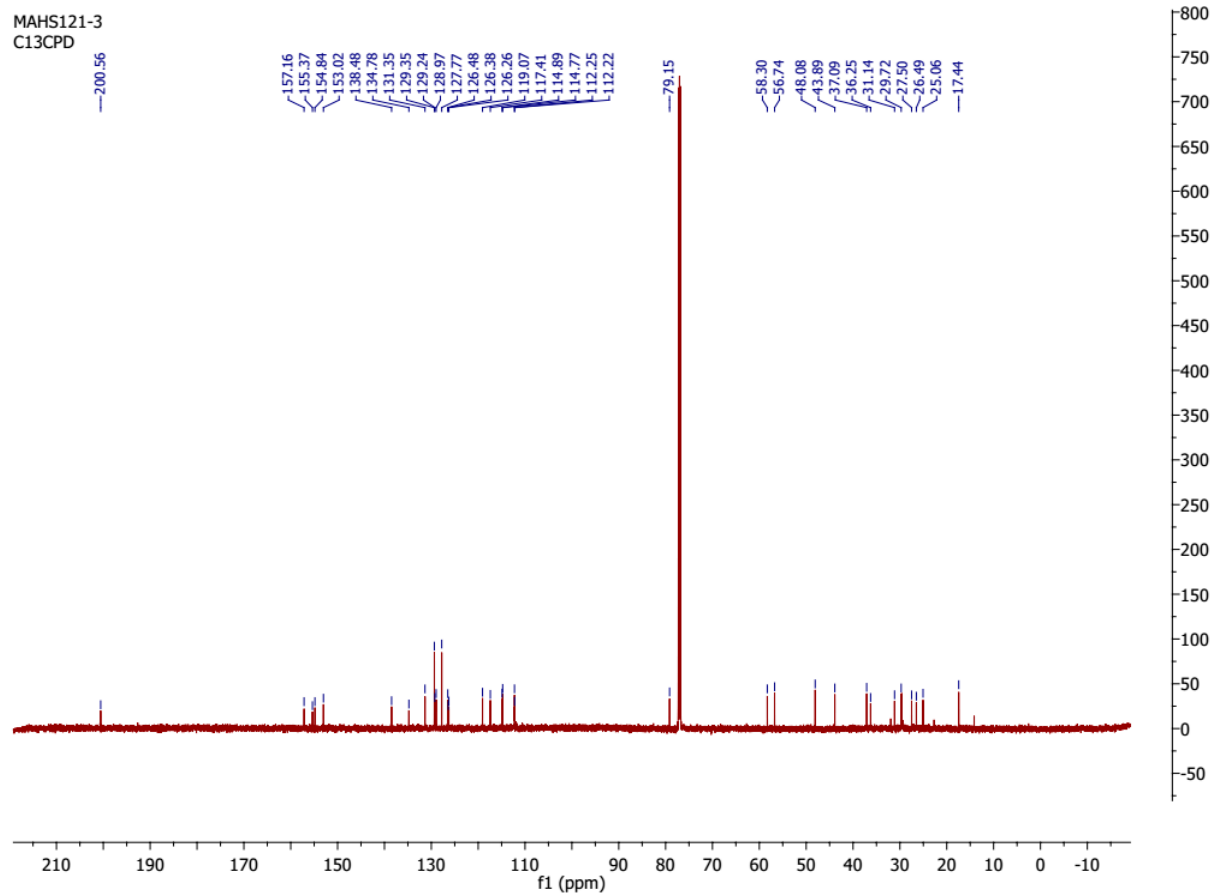


Figure S 99. ^{13}C NMR of compound **20d**.