

Supplementary Materials

Synthesis of Fused-Ring Systems and Diarylmethane Flavonoids *via Ortho*-Quinone Methide Intermediates

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NMR Spectra

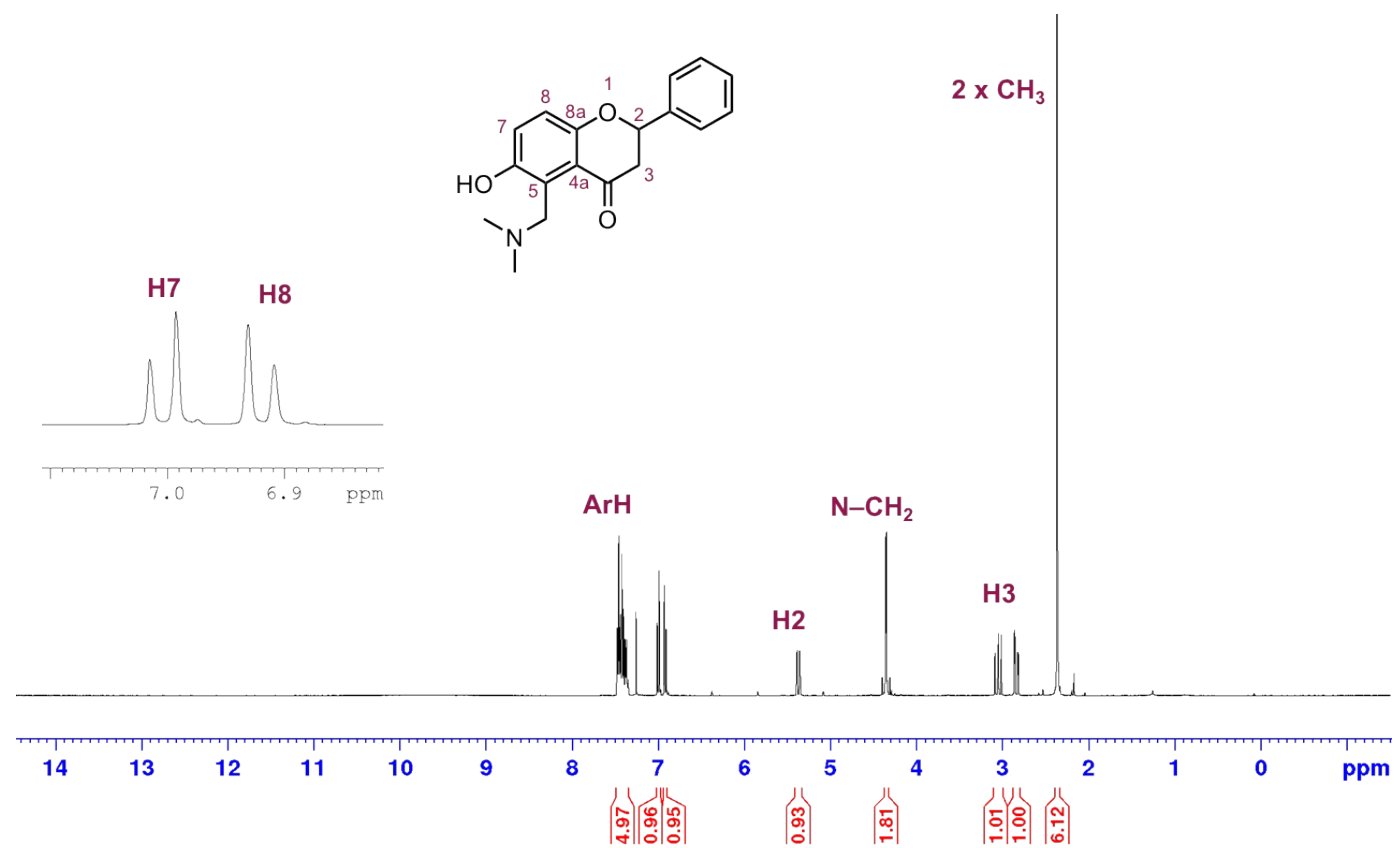


Figure S1. ¹H NMR (400 MHz, CDCl₃) spectrum of 5-((Dimethylamino)methyl)-6-hydroxy-2-phenylchroman-4-one (9)

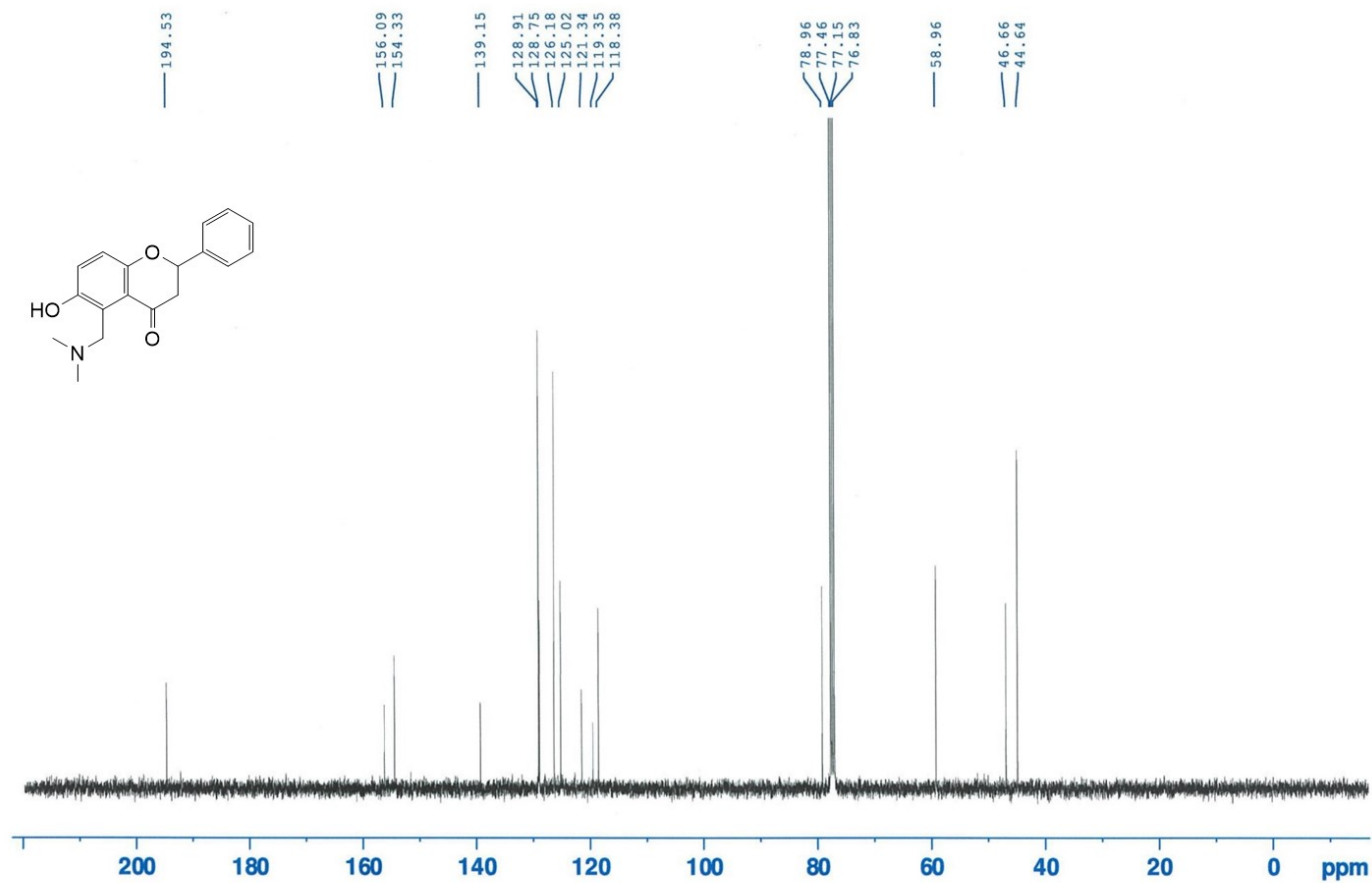


Figure S2. ¹³C NMR (100 MHz, CDCl₃) spectrum of 5-((Dimethylamino)methyl)-6-hydroxy-2-phenylchroman-4-one (9)

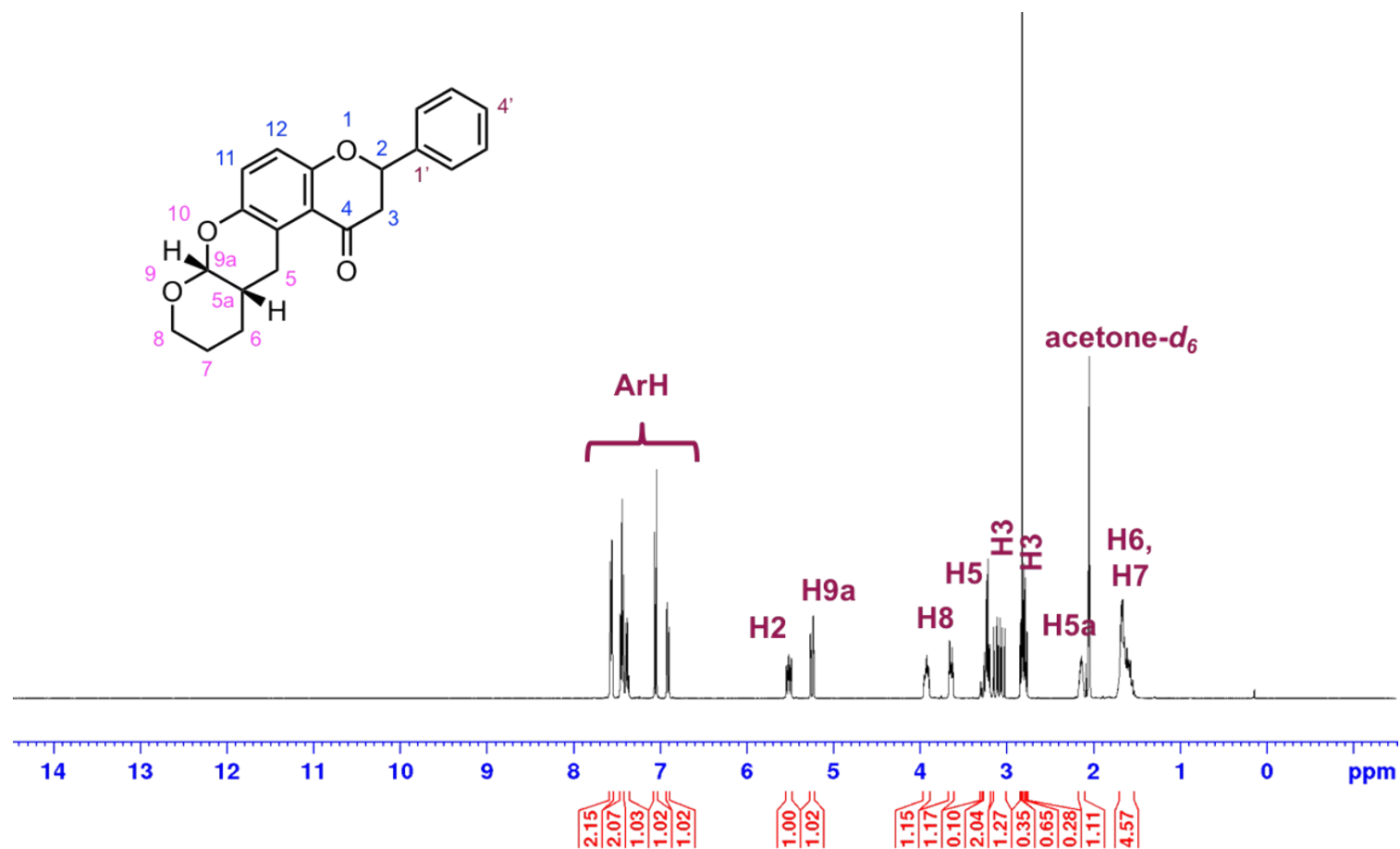


Figure S3. ^1H NMR (400 MHz, $\text{acetone-}d_6$) spectrum of 2-Phenyl-2,3,10,11,11a,12-hexahydro-9H-dipyrano[2,3-b:3',2'-f]chromen-1(7aH)-one (13a)

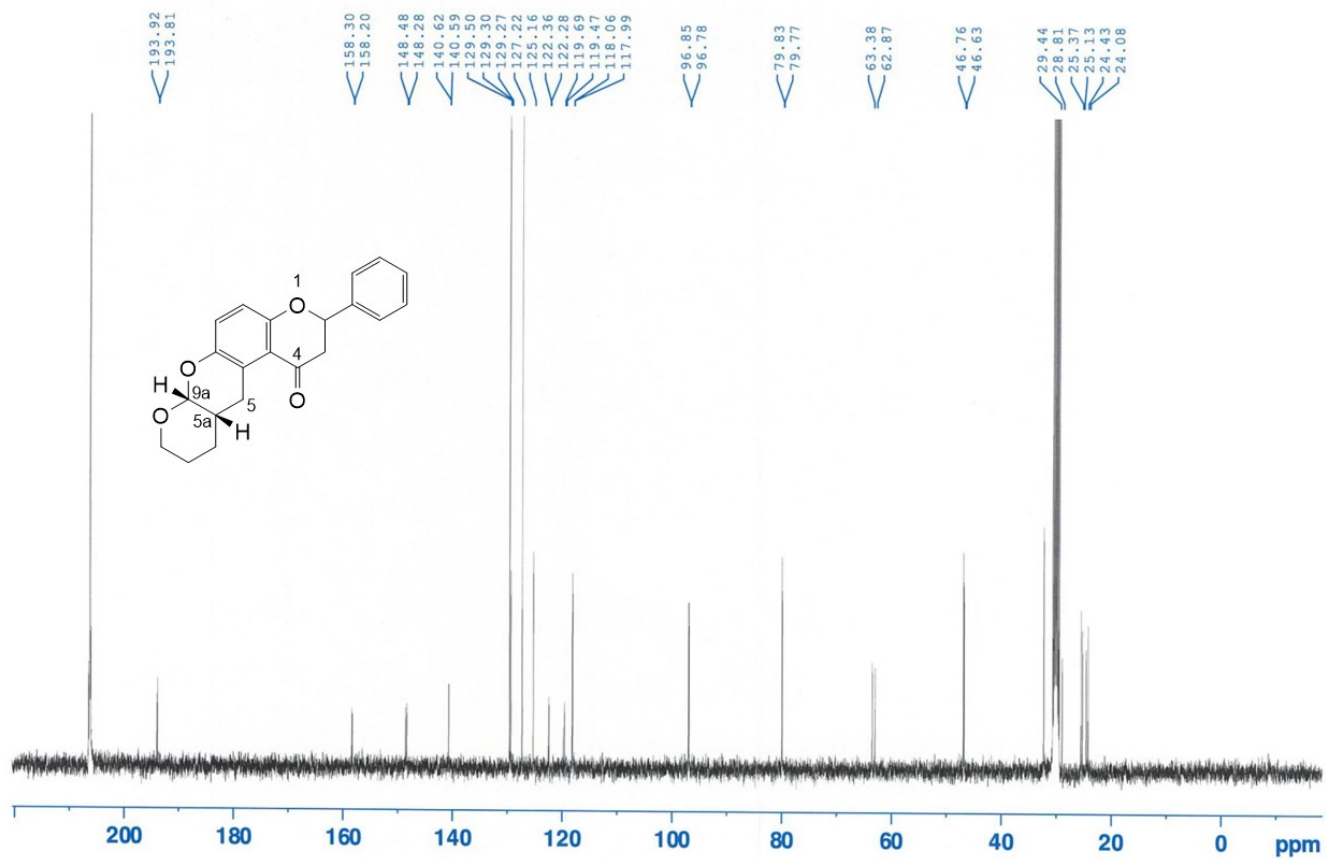


Figure S4. ^{13}C NMR (100 MHz, acetone- d_6) spectrum of 2-Phenyl-2,3,10,11,11a,12-hexahydro-9H-dipyrano[2,3-b:3',2'-f]chromen-1(7aH)-one (**13a**)

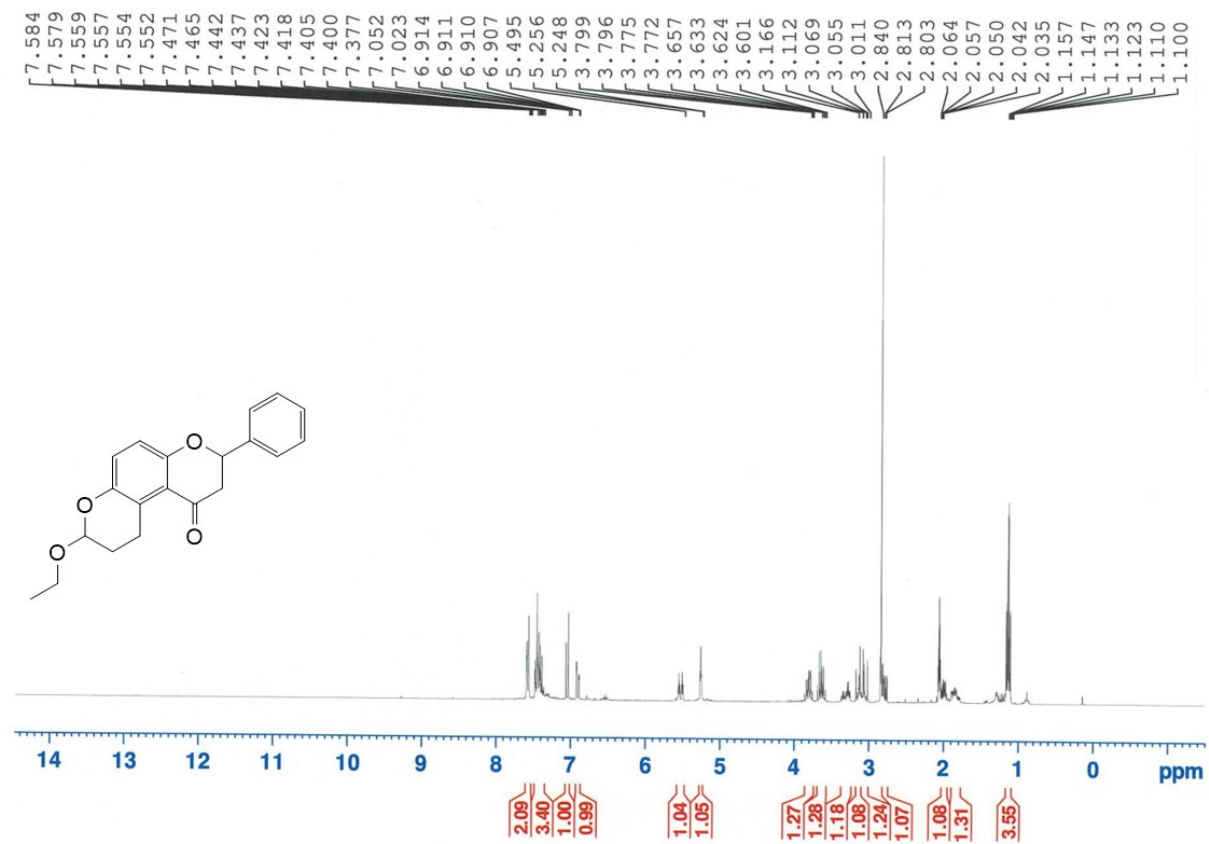


Figure S5. ¹H NMR (300 MHz, acetone-*d*₆) spectrum of 7-Ethoxy-2-phenyl-2,3,9,10-tetrahydropyrano[3,2-f]chromen-1(8H)-one (13b)

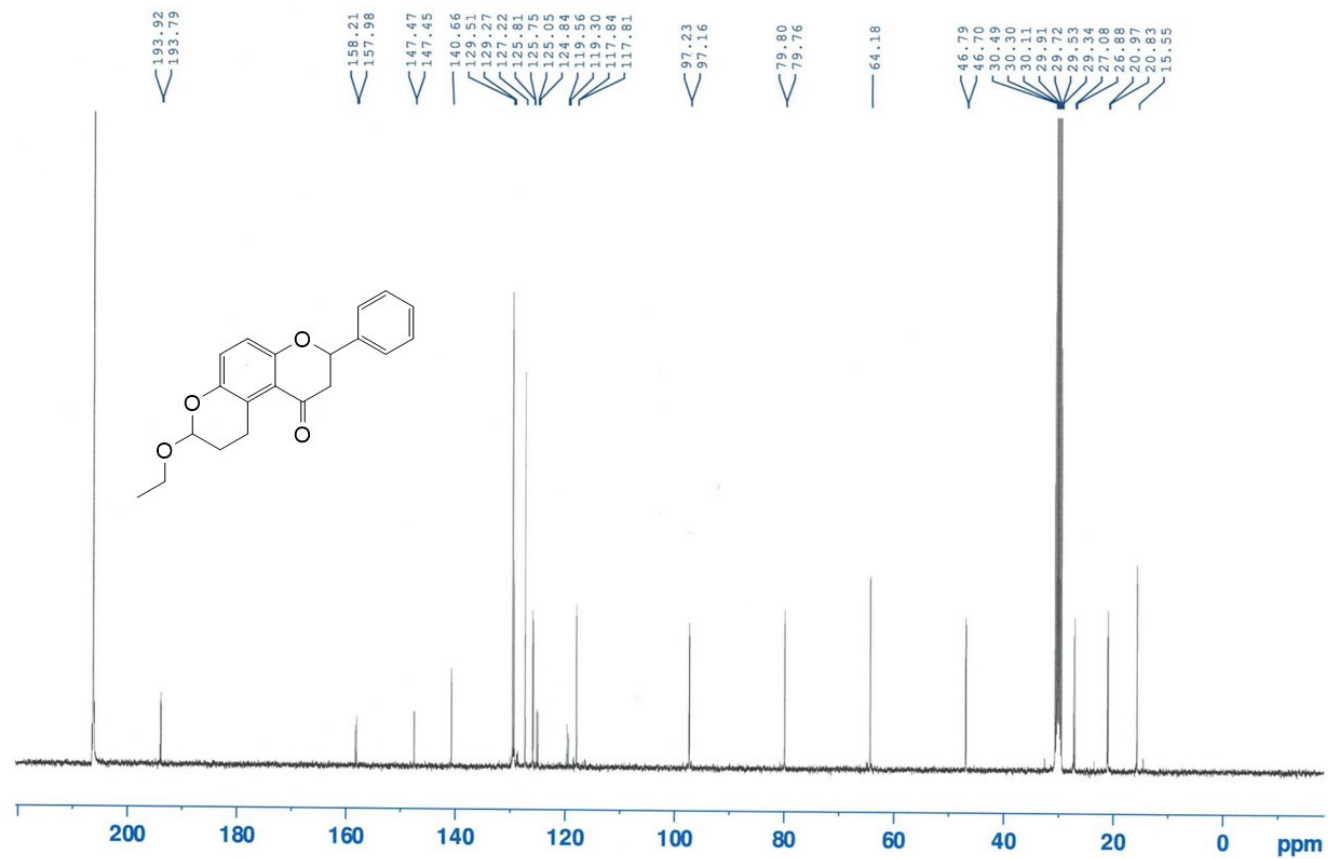


Figure S6. ¹³C NMR (100 MHz, acetone-*d*₆) spectrum of 7-Ethoxy-2-phenyl-2,3,9,10-tetrahydropyrano[3,2-f]chromen-1(8H)-one (13b)

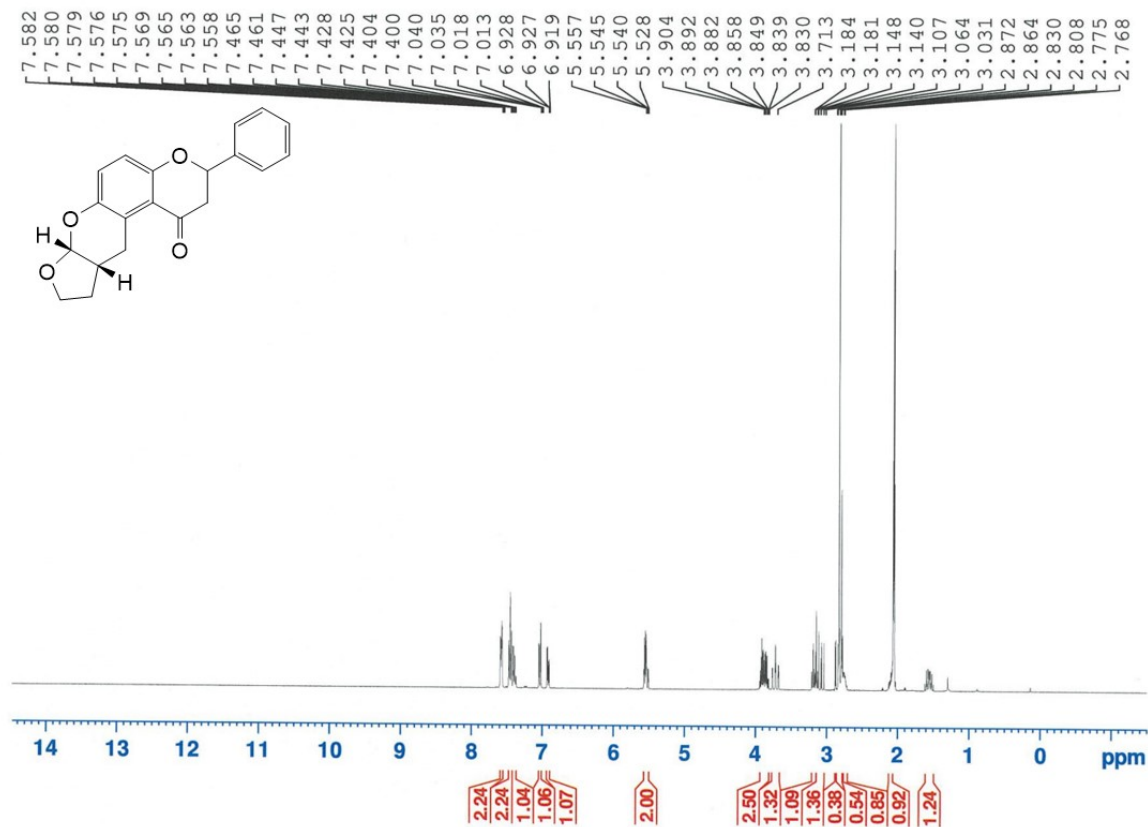


Figure S7. ¹H NMR (400 MHz, acetone-*d*₆) spectrum of 2-Phenyl-2,3,9,10,10a,11-hexahydrofuro[2,3-b]pyrano[3,2-f]chromen-1(7aH)-one (13c)

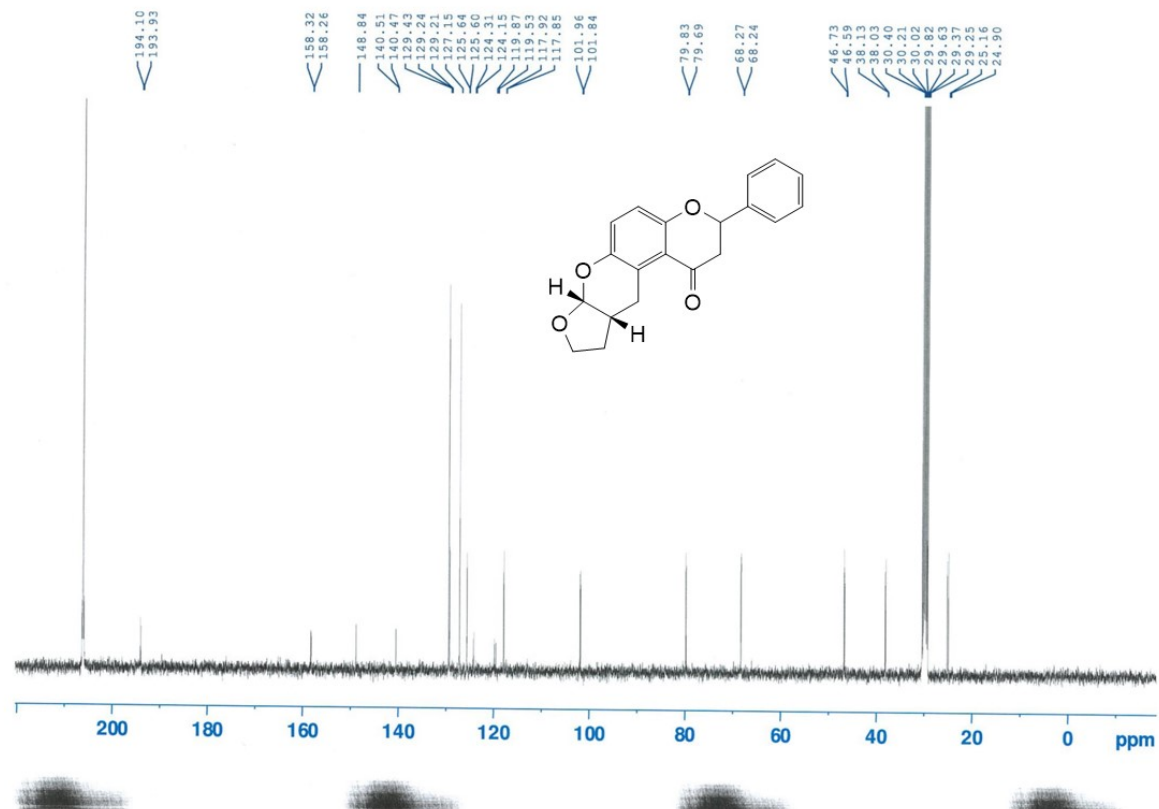


Figure S8. ¹³C NMR (100 MHz, acetone-*d*₆) spectrum of 2-Phenyl-2,3,9,10,10a,11-hexahydrofuro[2,3-b]pyrano[3,2-f]chromen-1(7aH)-one (13c)

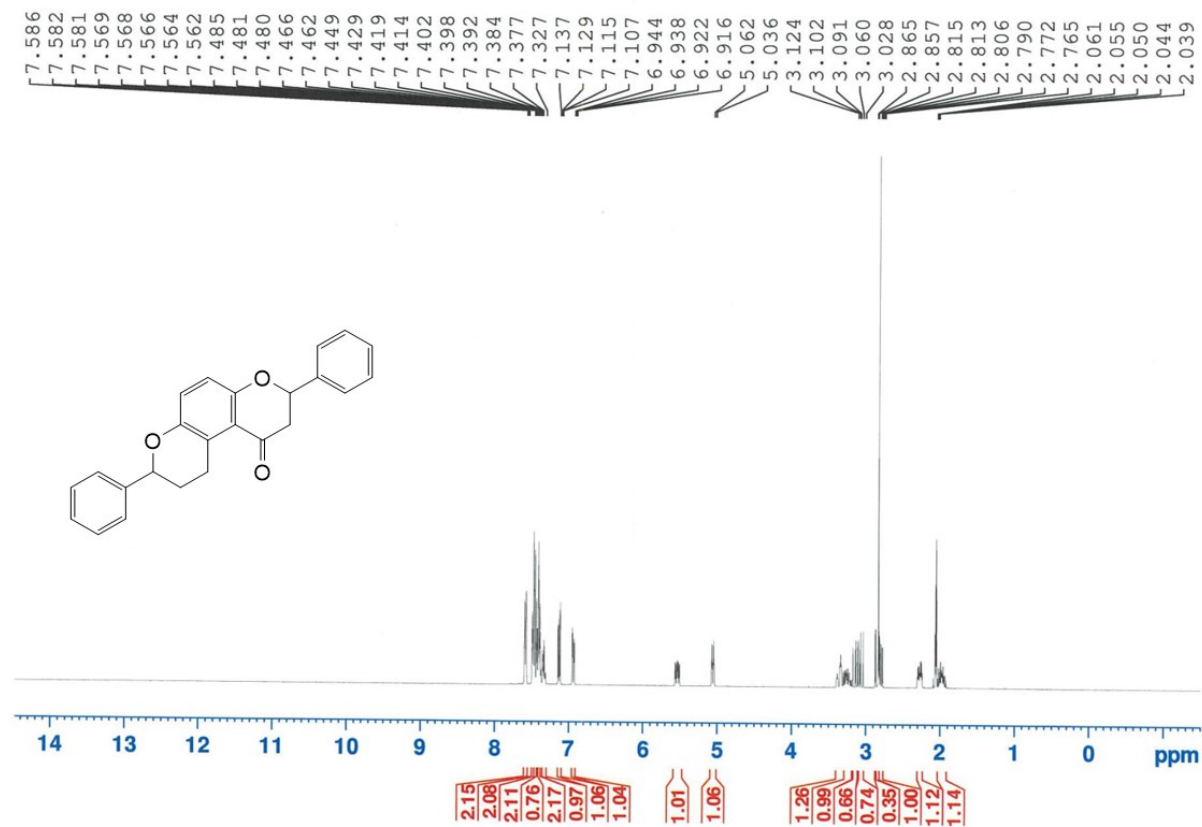


Figure S9. ¹H NMR (400 MHz, acetone-*d*₆) spectrum of 2,7-Diphenyl-2,3,9,10-tetrahydropyrano[3,2-f]chromen-1(8H)-one (13d)

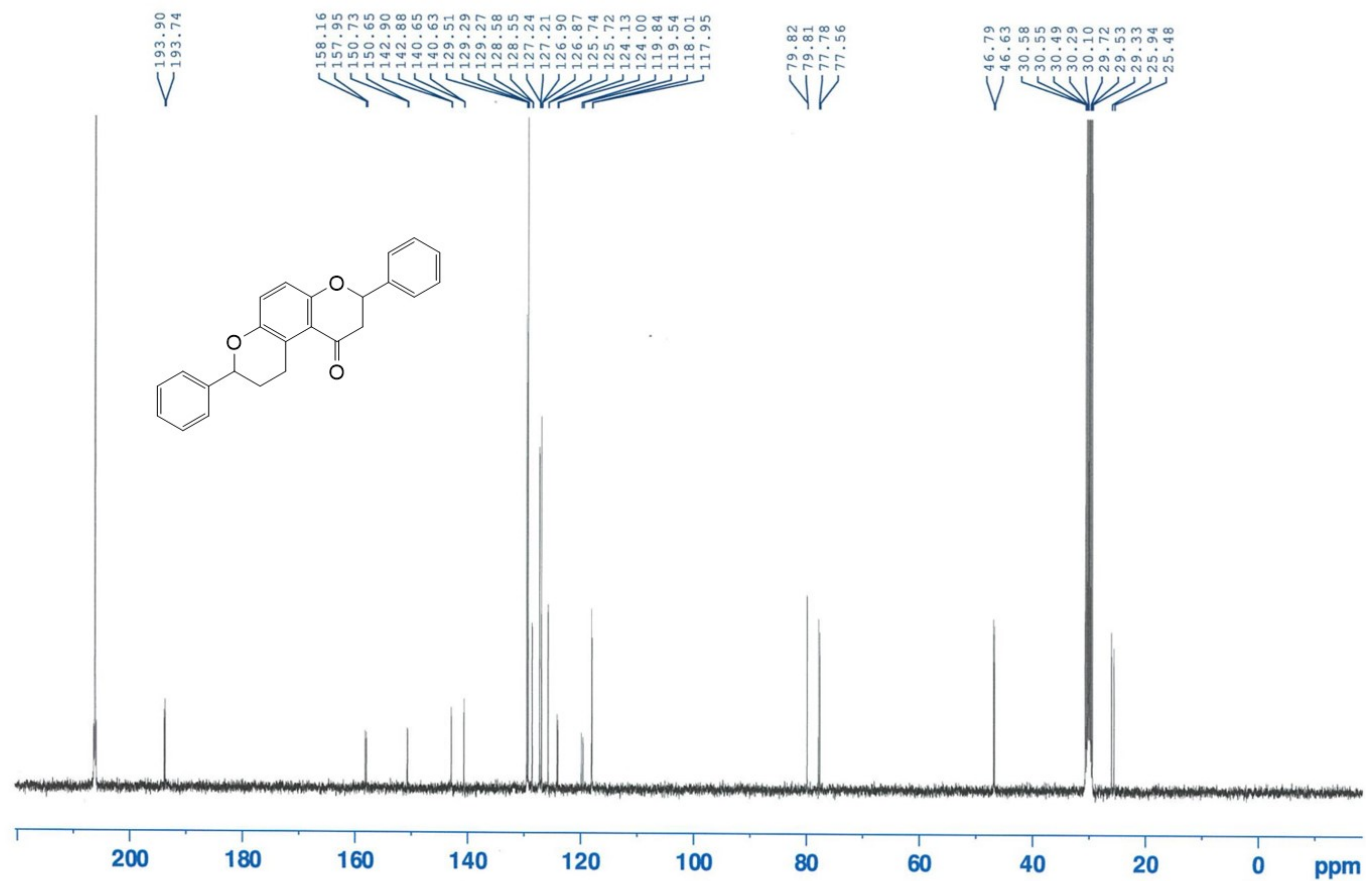


Figure S10. ¹³C NMR (100 MHz, acetone-*d*₆) spectrum of 2,7-Diphenyl-2,3,9,10-tetrahydropyrano[3,2-f]chromen-1(8H)-one (13d)

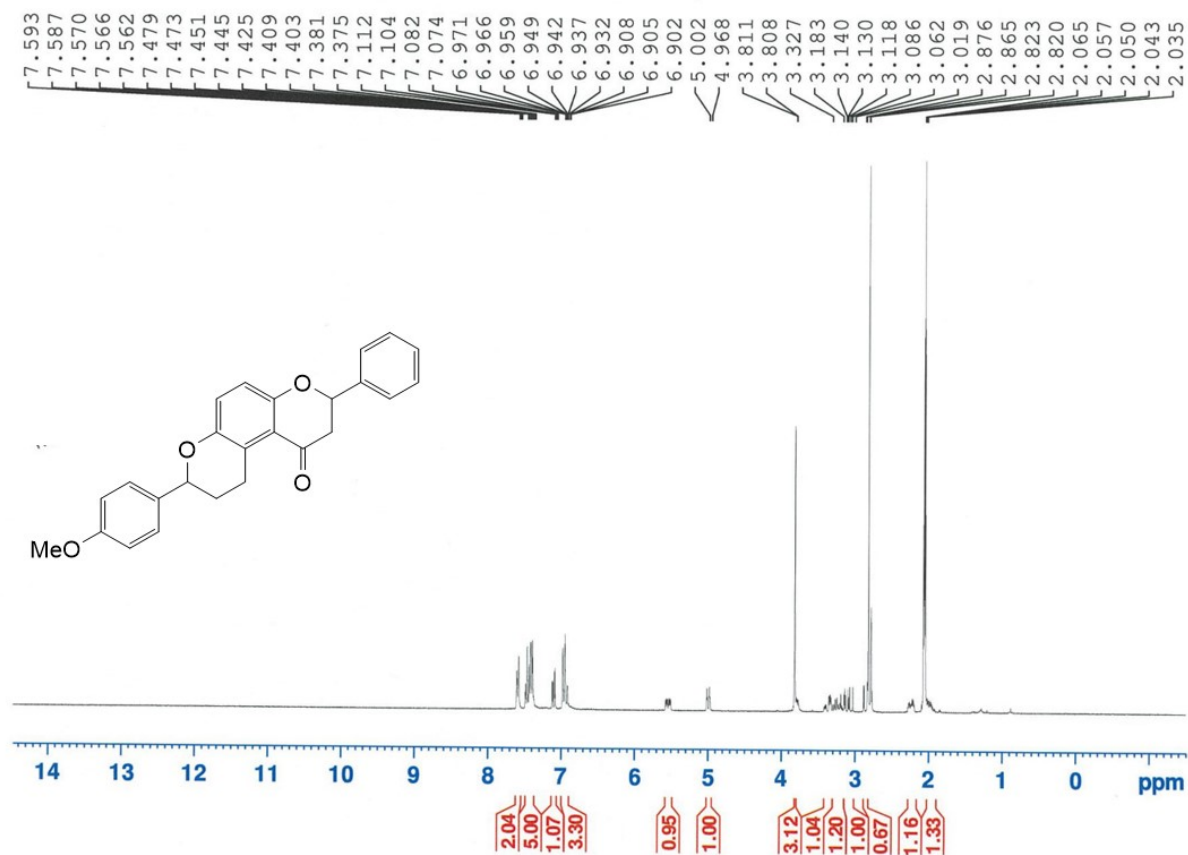


Figure S11. ¹H NMR (400 MHz, acetone-*d*₆) spectrum of 7-(4-Methoxyphenyl)-2-phenyl-2,3,9,10-tetrahydropyrano[3,2-f]chromen-1(8H)-one (13e)

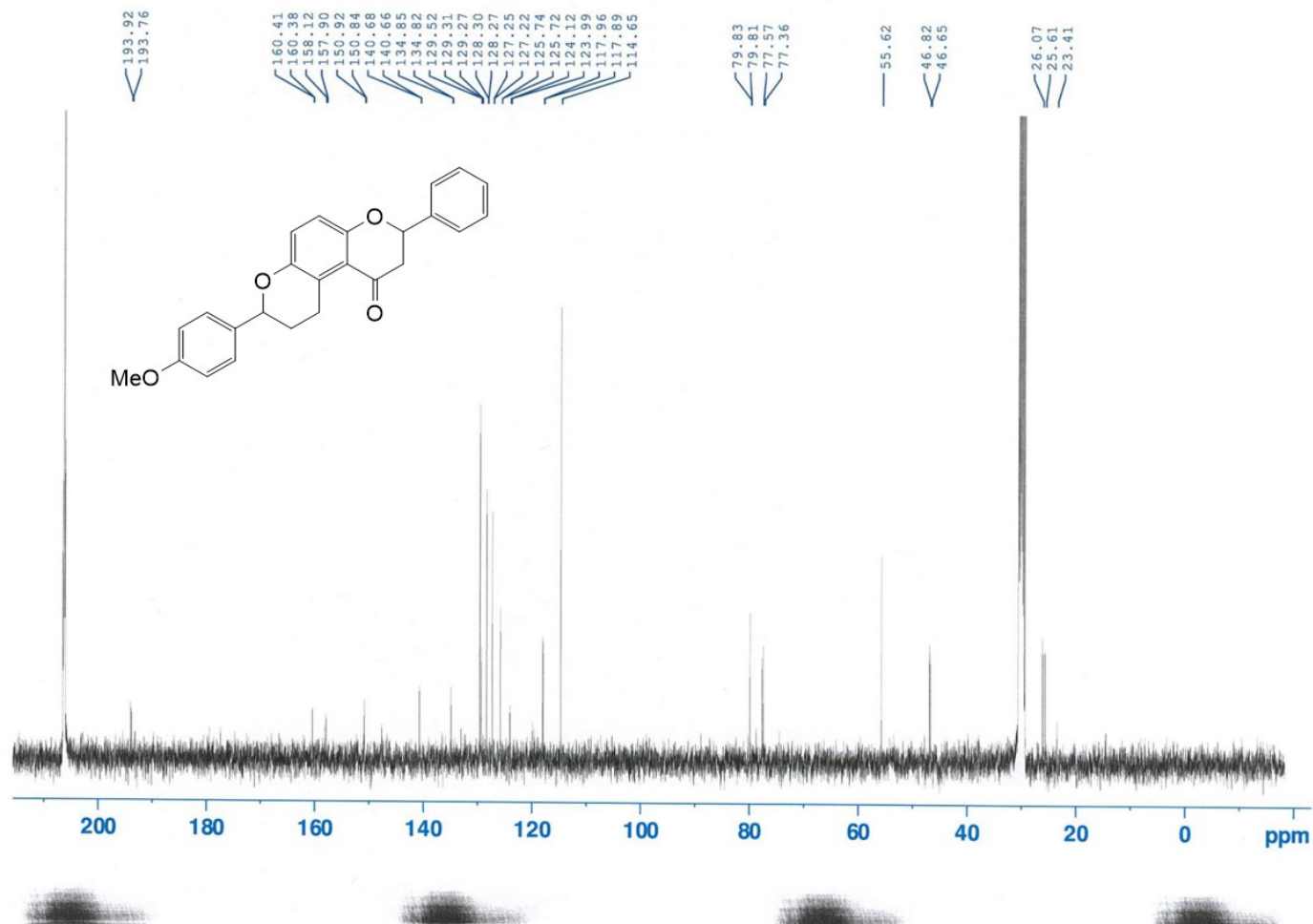


Figure S12. ¹³C NMR (100 MHz, acetone-*d*₆) spectrum of 7-(4-Methoxyphenyl)-2-phenyl-2,3,9,10-tetrahydropyrano[3,2-f]chromen-1(8*H*)-one (**13e**)

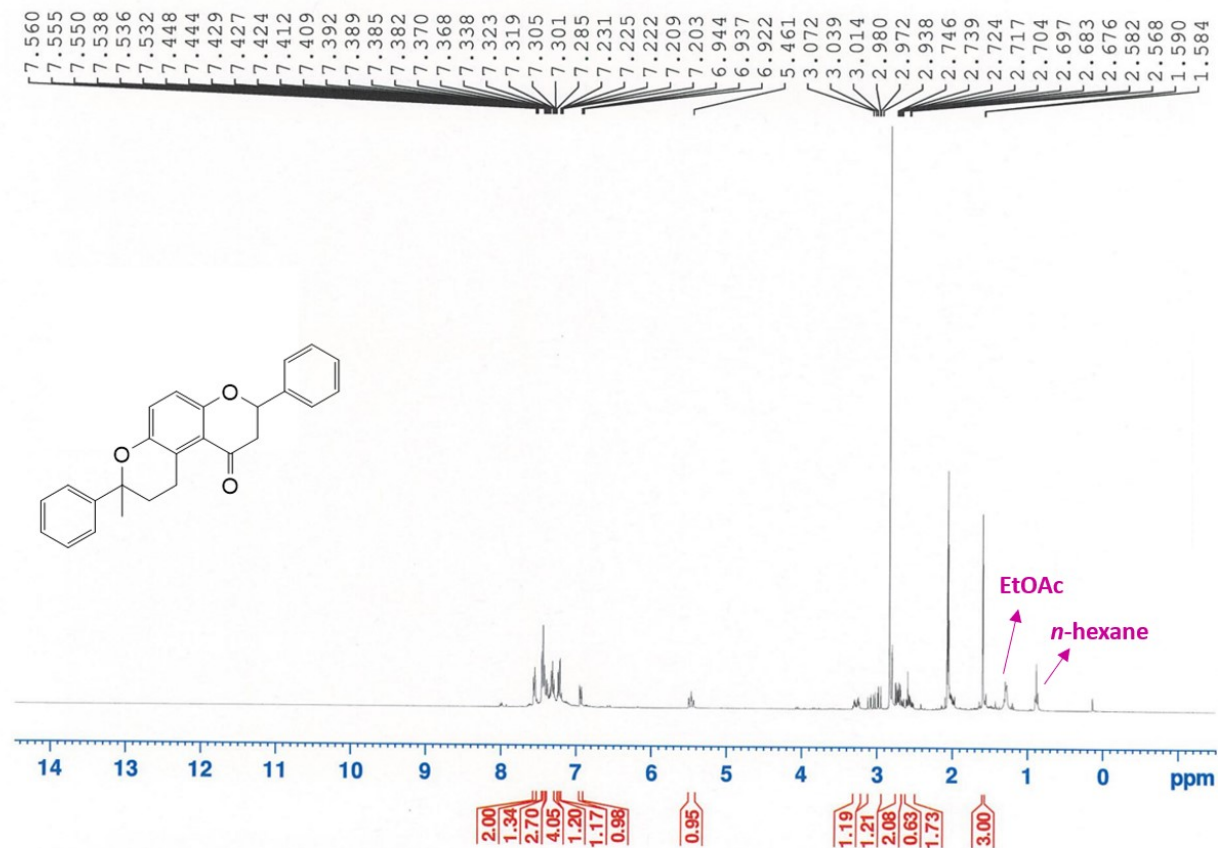


Figure S13. ¹H NMR (400 MHz, acetone-*d*₆) spectrum of 7-Methyl-2,7-diphenyl-2,3,9,10-tetrahydropyrano[3,2-f]chromen-1(8H)-one (**13f**)

Ethyl acetate and *n*-hexane are the solvents used for purification of **13f** using column chromatography.

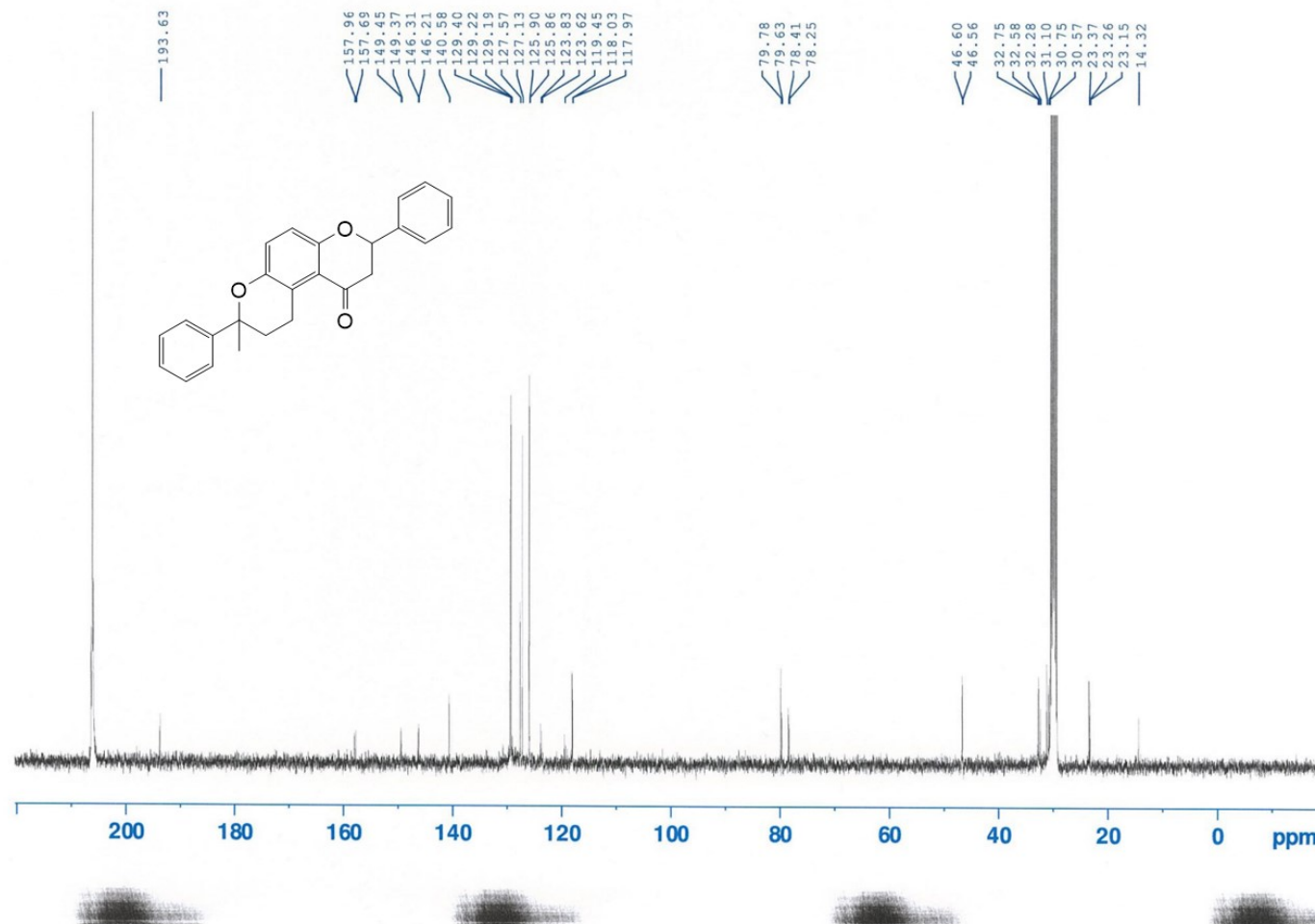


Figure S14. ¹³C NMR (100 MHz, acetone-*d*₆) spectrum of 7-Methyl-2,7-diphenyl-2,3,9,10-tetrahydropyrano[3,2-f]chromen-1(8H)-one (13f)

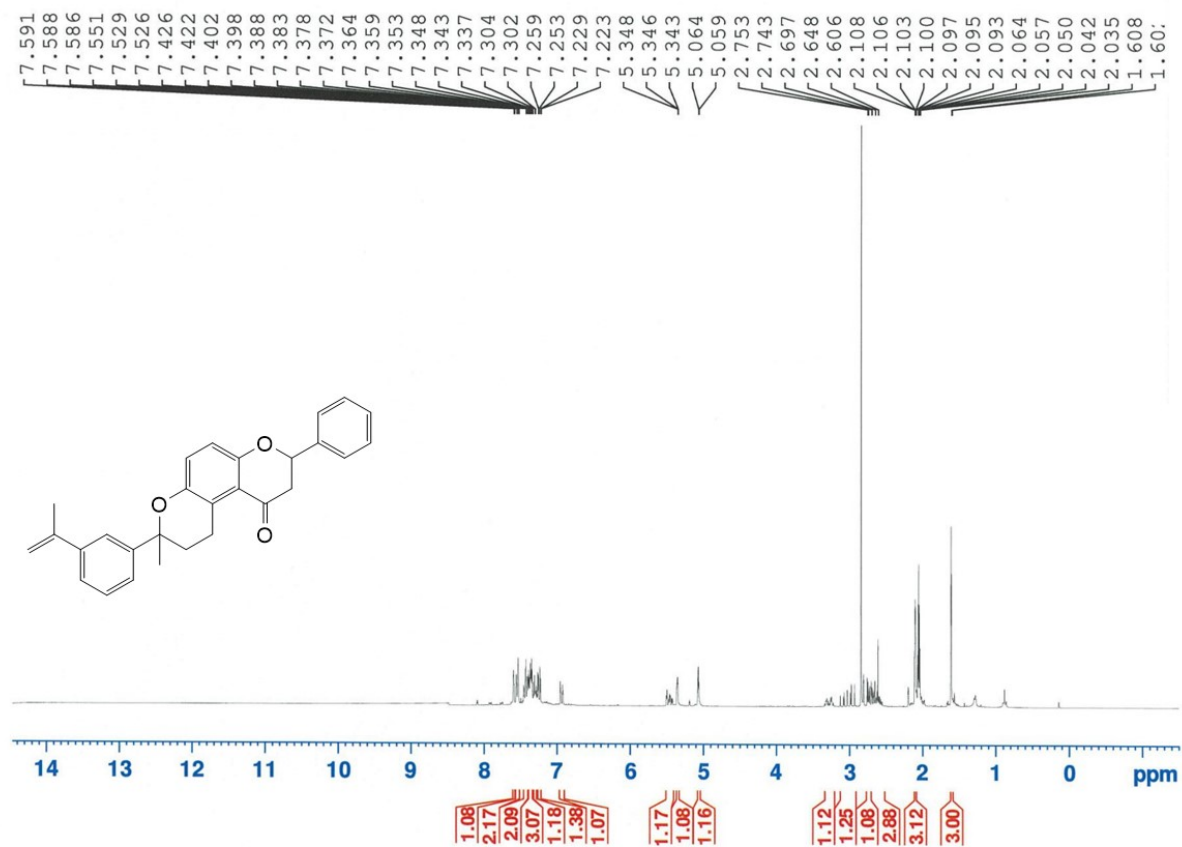


Figure S15. ¹H NMR (400 MHz, acetone-*d*₆) spectrum of 7-Methyl-2-phenyl-7-(3-(prop-1-en-2-yl)phenyl)-2,3,9,10-tetrahydropyrano[3,2-f]chromen-1(8H)-one (13g)

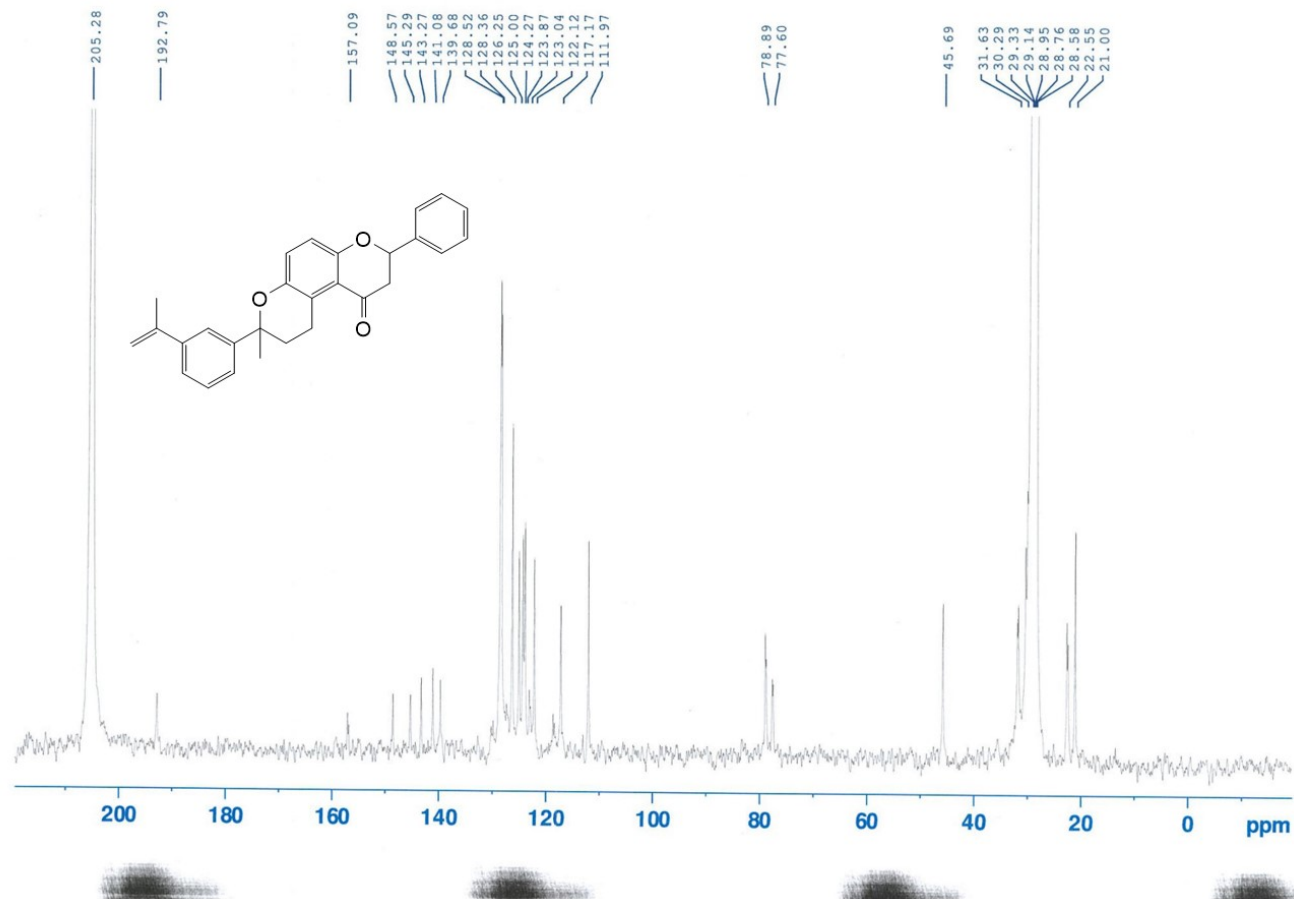


Figure S16. ¹³C NMR (100 MHz, acetone-*d*₆) spectrum of 7-Methyl-2-phenyl-7-(3-(prop-1-en-2-yl)phenyl)-2,3,9,10-tetrahydropyrano[3,2-f]chromen-1(8H)-one (13g)

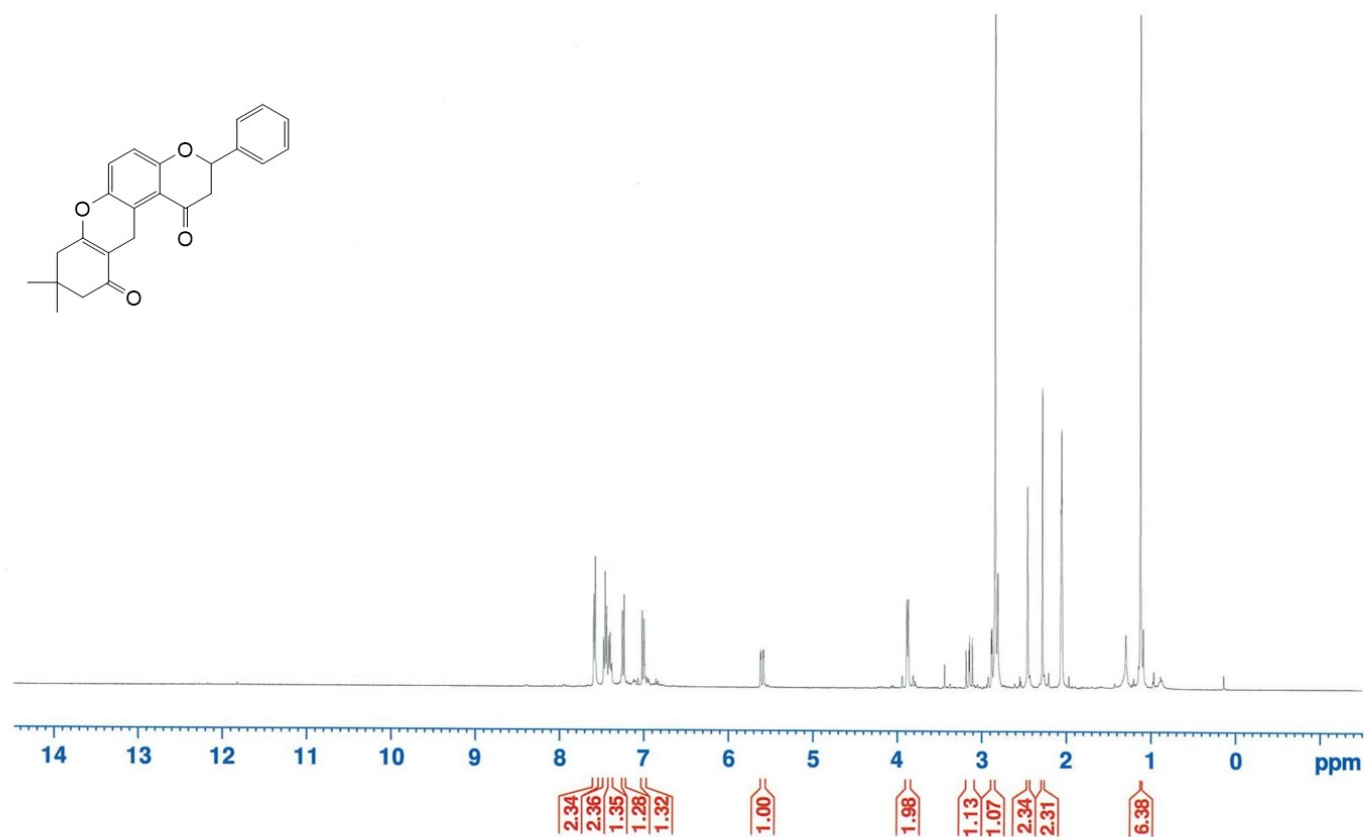


Figure S17. ¹H NMR (400 MHz, acetone-*d*₆) spectrum of 8,8-Dimethyl-2-phenyl-2,3,8,9,10,12-hexahydropyrano[3,2-a]xanthene-1,11-dione (**13h**)

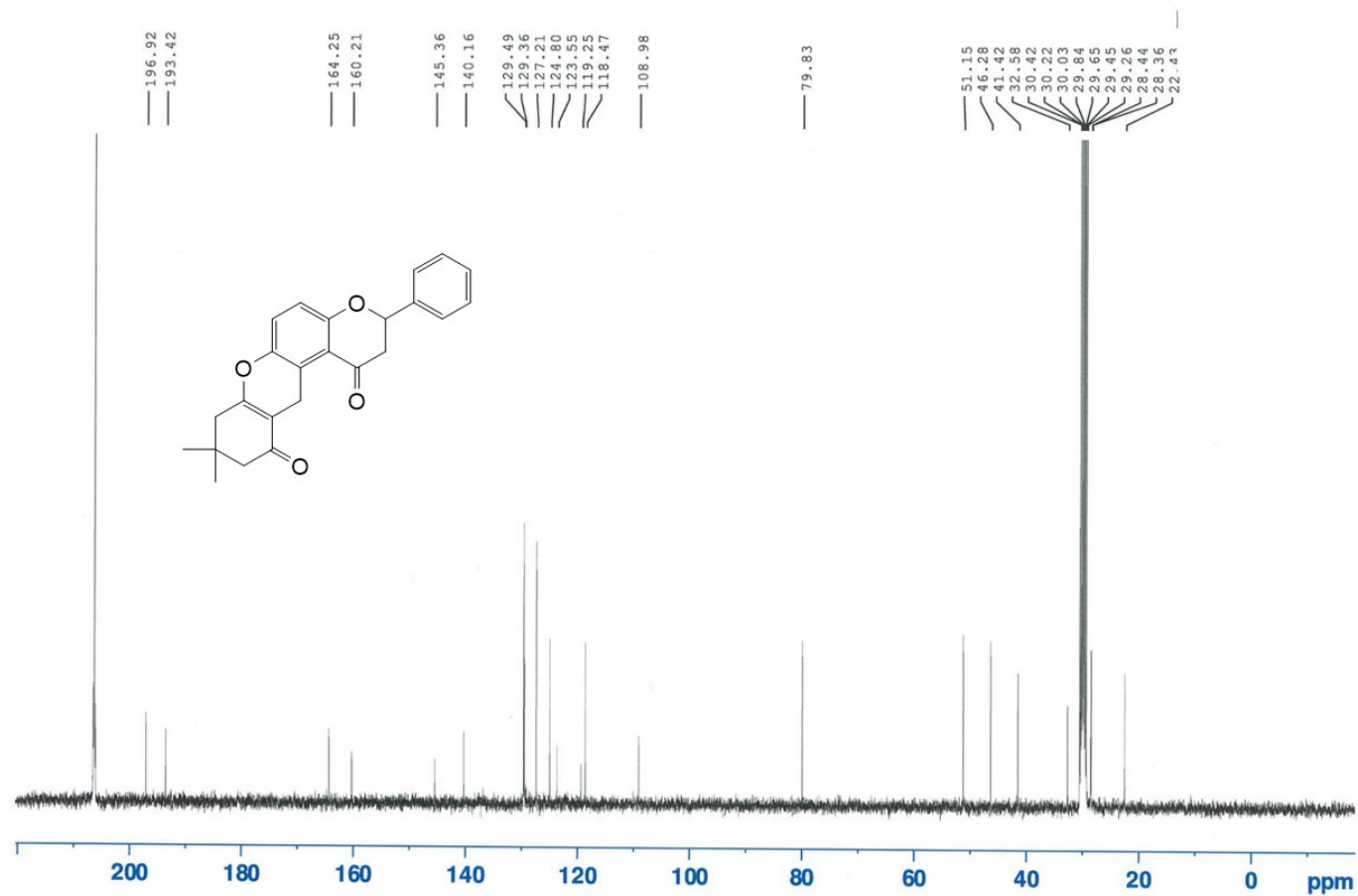


Figure S18. ¹³C NMR (100 MHz, acetone-*d*₆) spectrum of 8,8-Dimethyl-2-phenyl-2,3,8,9,10,12-hexahydropyrano[3,2-a]xanthene-1,11-dione (**13h**)

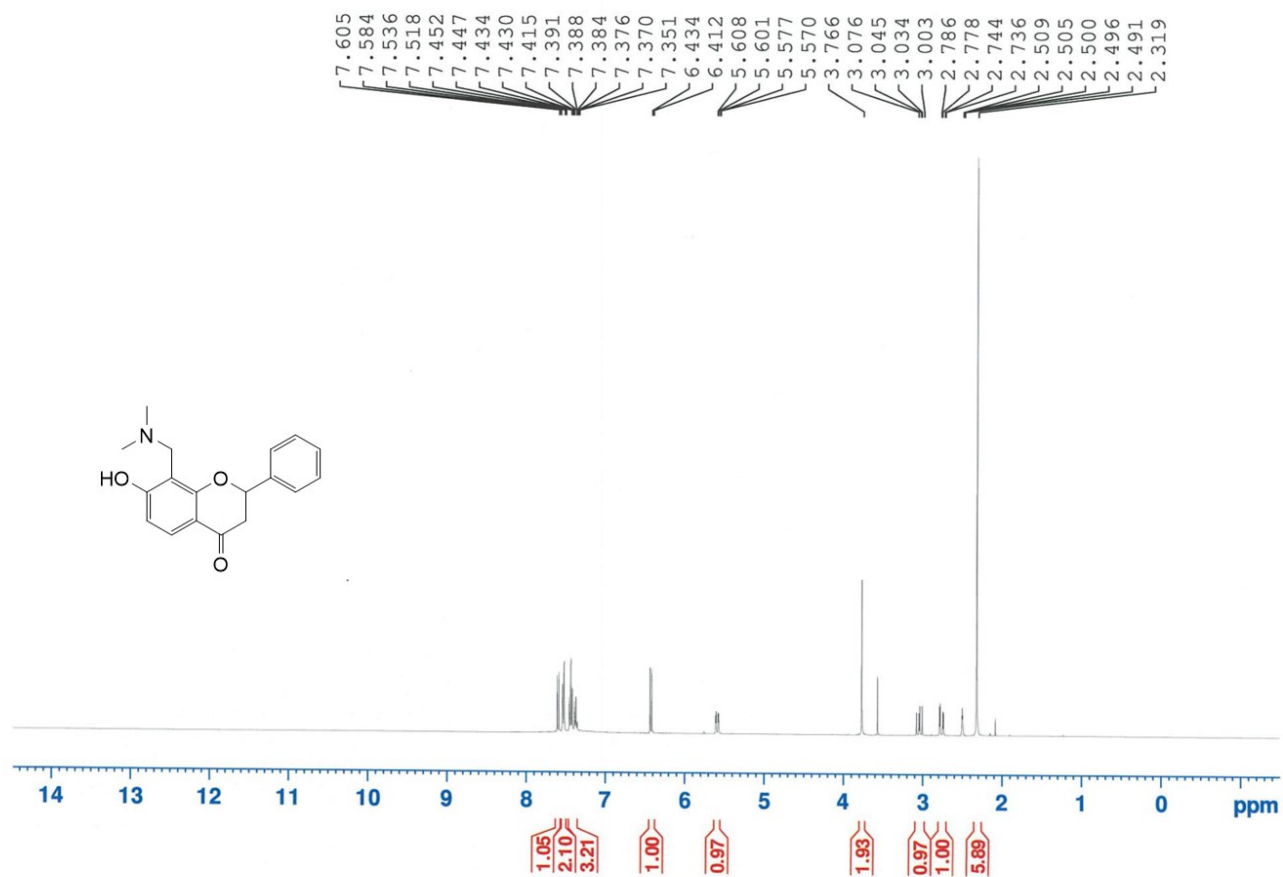


Figure S19. ¹H NMR (400 MHz, DMSO-*d*₆) spectrum of 8-((Dimethylamino)methyl)-7-hydroxy-2-phenylchroman-4-one (10)

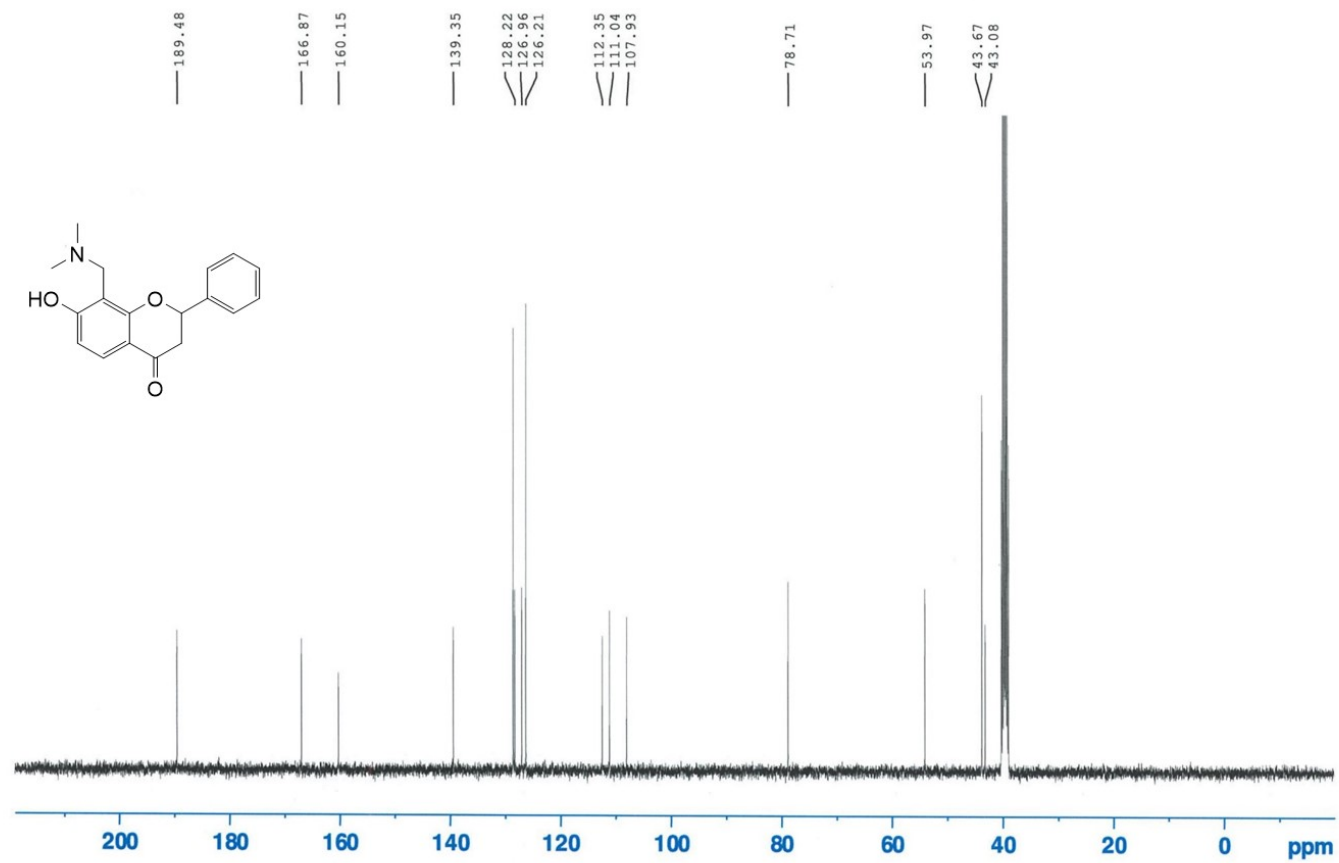


Figure S20. ¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of 8-((Dimethylamino)methyl)-7-hydroxy-2-phenylchroman-4-one (10)

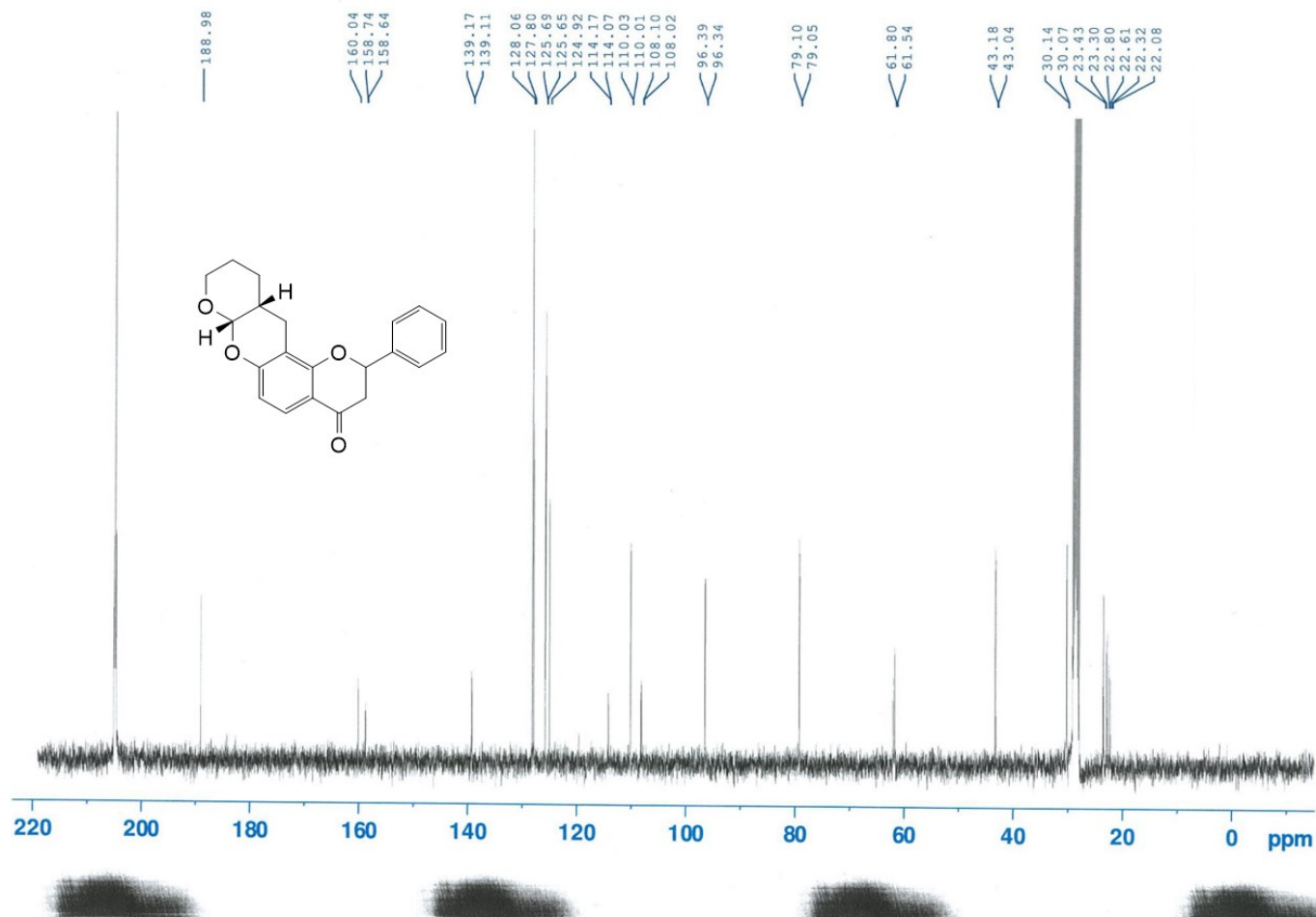


Figure S22. ¹³C NMR (100 MHz, acetone-*d*₆) spectrum of 2-Phenyl-7-((tetrahydro-2H-pyran-2-yl)oxy)chroman-4-one (15a)

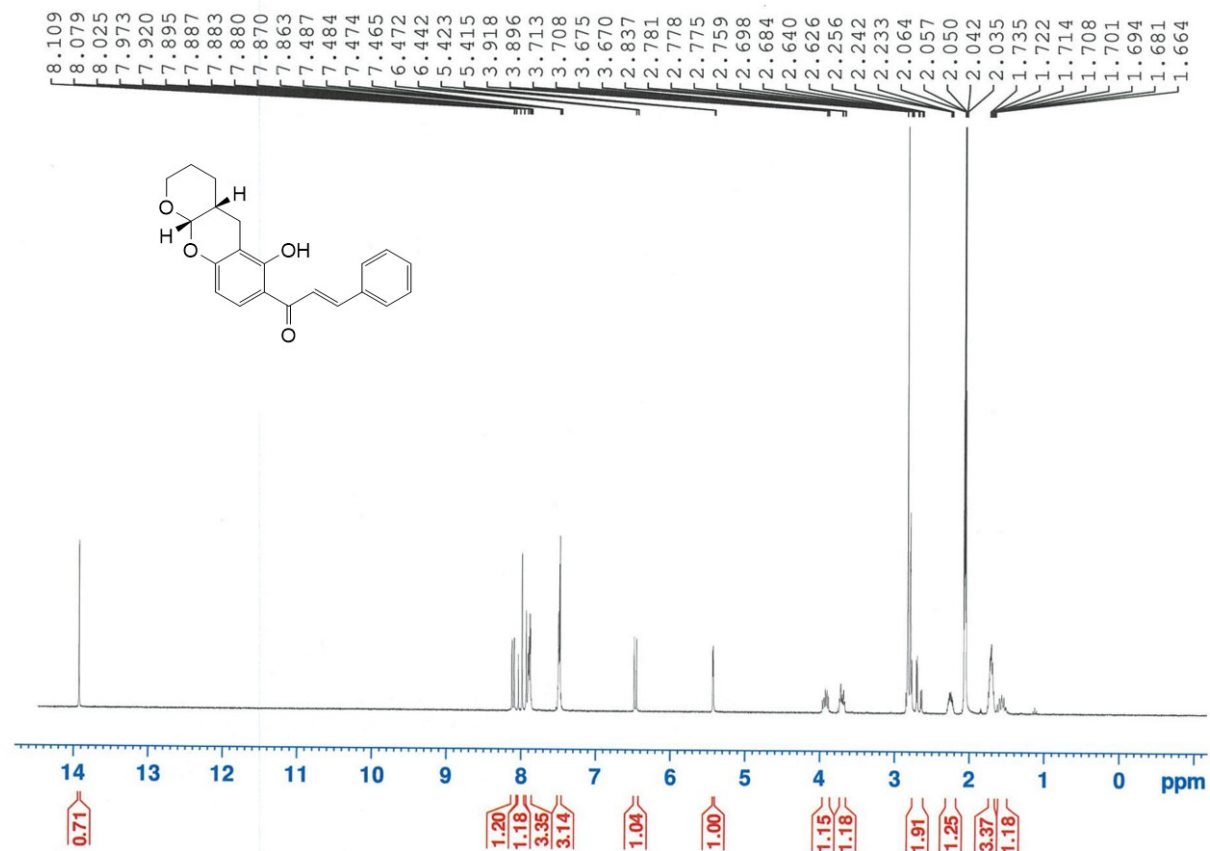


Figure S23. ¹H NMR (300 MHz, acetone-*d*₆) spectrum of (E)-1-(6-Hydroxy-3,4,4a,10a-tetrahydro-2H,5H-pyrano[2,3-b]chromen-7-yl)-3-phenylprop-2-en-1-one (16a)

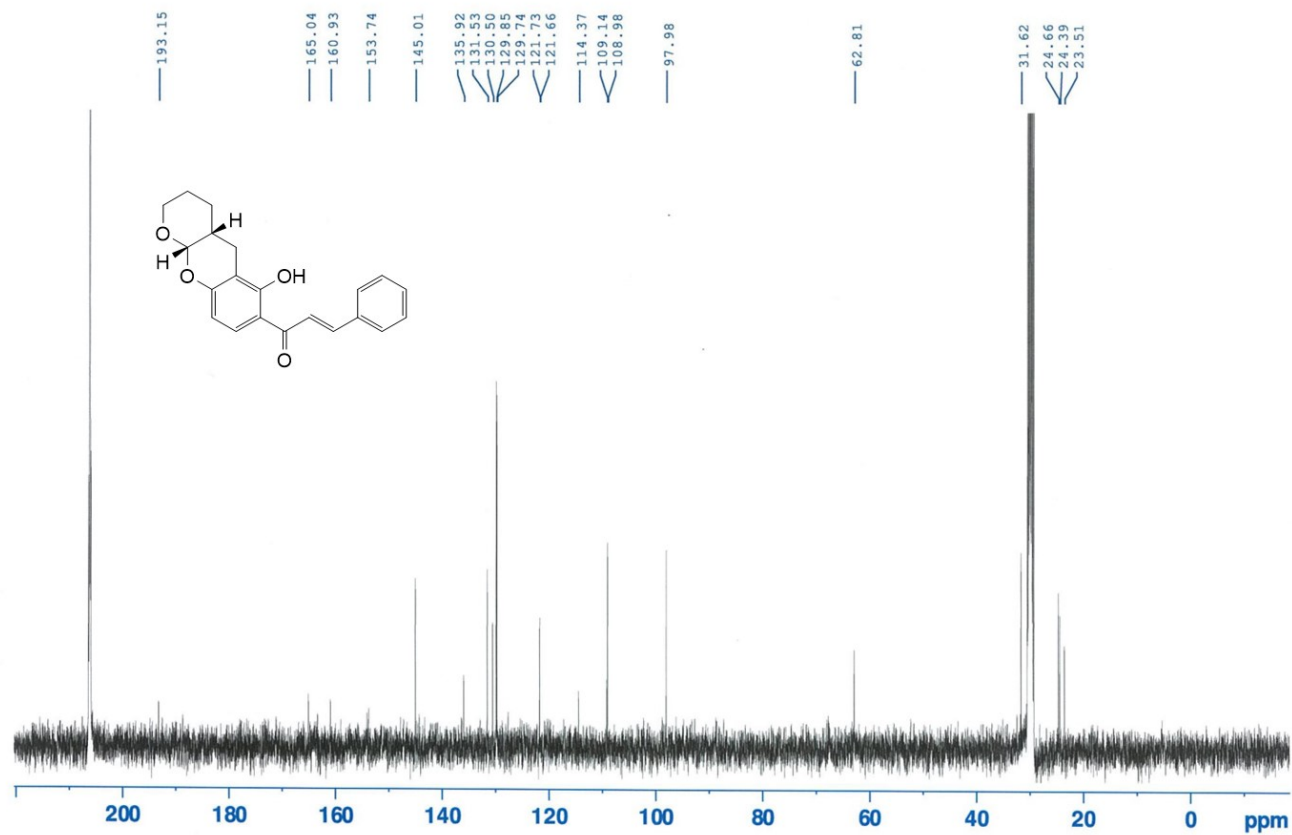


Figure S24. ¹³C NMR (100 MHz, acetone-*d*₆) spectrum of (*E*)-1-(6-Hydroxy-3,4,4a,10a-tetrahydro-2*H*,5*H*-pyrano[2,3-*b*]chromen-7-yl)-3-phenylprop-2-en-1-one (16a)

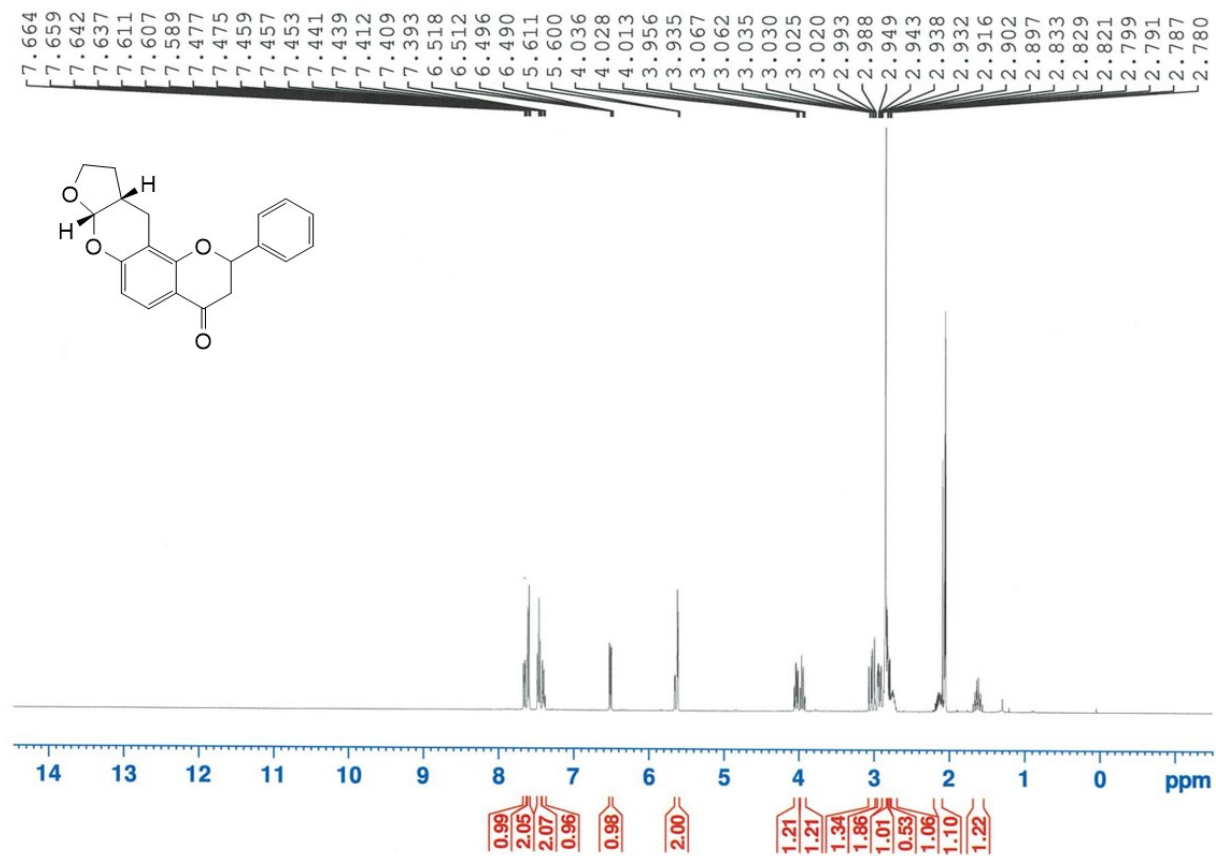


Figure S25. ¹H NMR (400 MHz, acetone-*d*₆) spectrum of 2-Phenyl-2,3,7a,9,10,10a-hexahydro-4*H*,11*H*-furo[2,3-*b*]pyrano[2,3-*f*]chromen-4-one (15b)

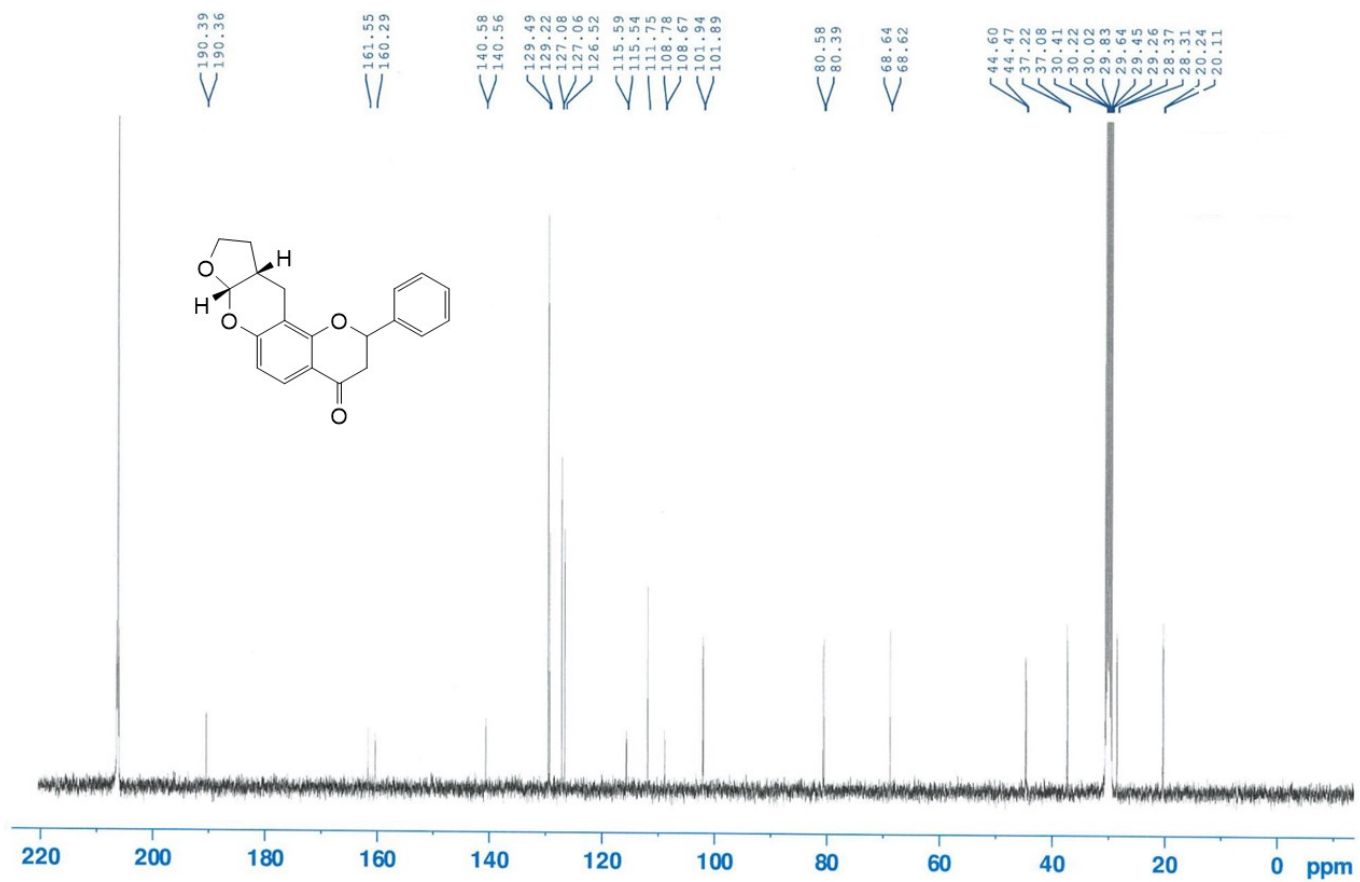


Figure S26. ¹³C NMR (100 MHz, acetone-*d*₆) spectrum of 2-Phenyl-2,3,7a,9,10,10a-hexahydro-4*H*,11*H*-furo[2,3-*b*]pyrano[2,3-*f*]chromen-4-one (**15b**)

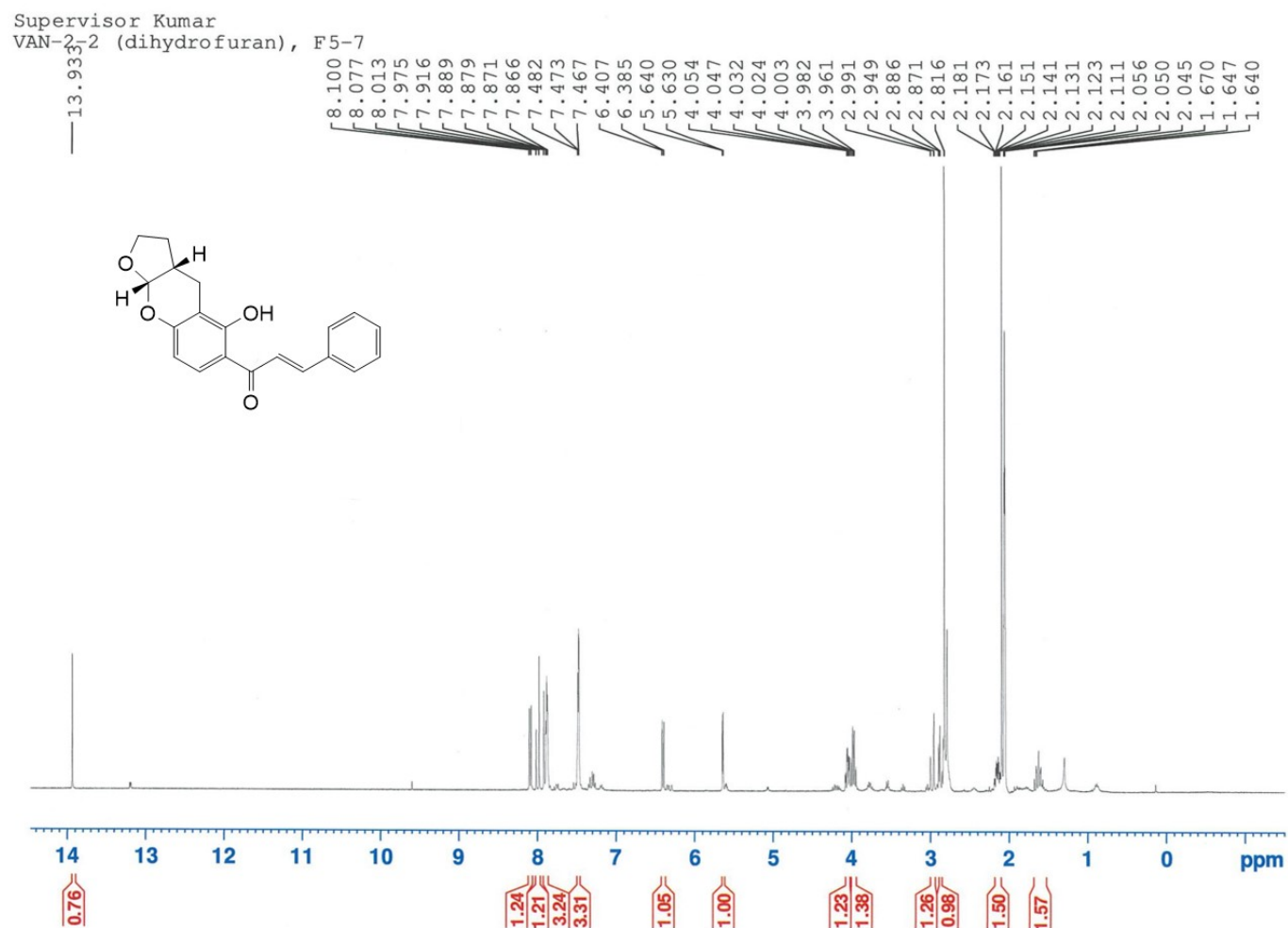


Figure S27. ¹H NMR (400 MHz, acetone-*d*₆) spectrum of (E)-1-(5-Hydroxy-2,3,3a,9a-tetrahydro-4H-furo[2,3-b]chromen-6-yl)-3-phenylprop-2-en-1-one (16b)

Supervisor Kumar
 VAN-2-2 (dihydrofuran), F5-7

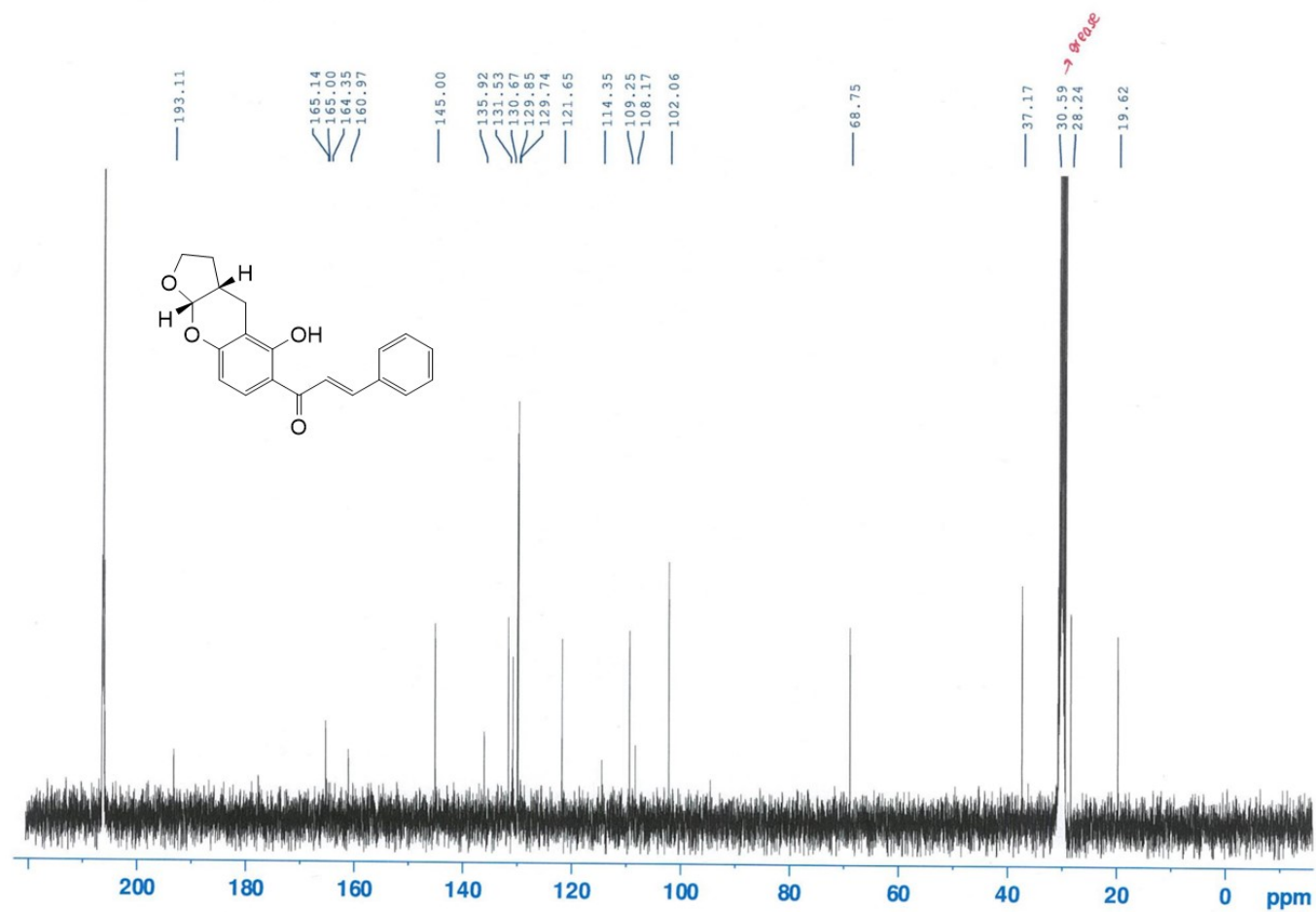


Figure S28. ¹³C NMR (100 MHz, acetone-*d*₆) of (*E*)-1-(5-Hydroxy-2,3,3a,9a-tetrahydro-4*H*-furo[2,3-*b*]chromen-6-yl)-3-phenylprop-2-en-1-one (**16b**)

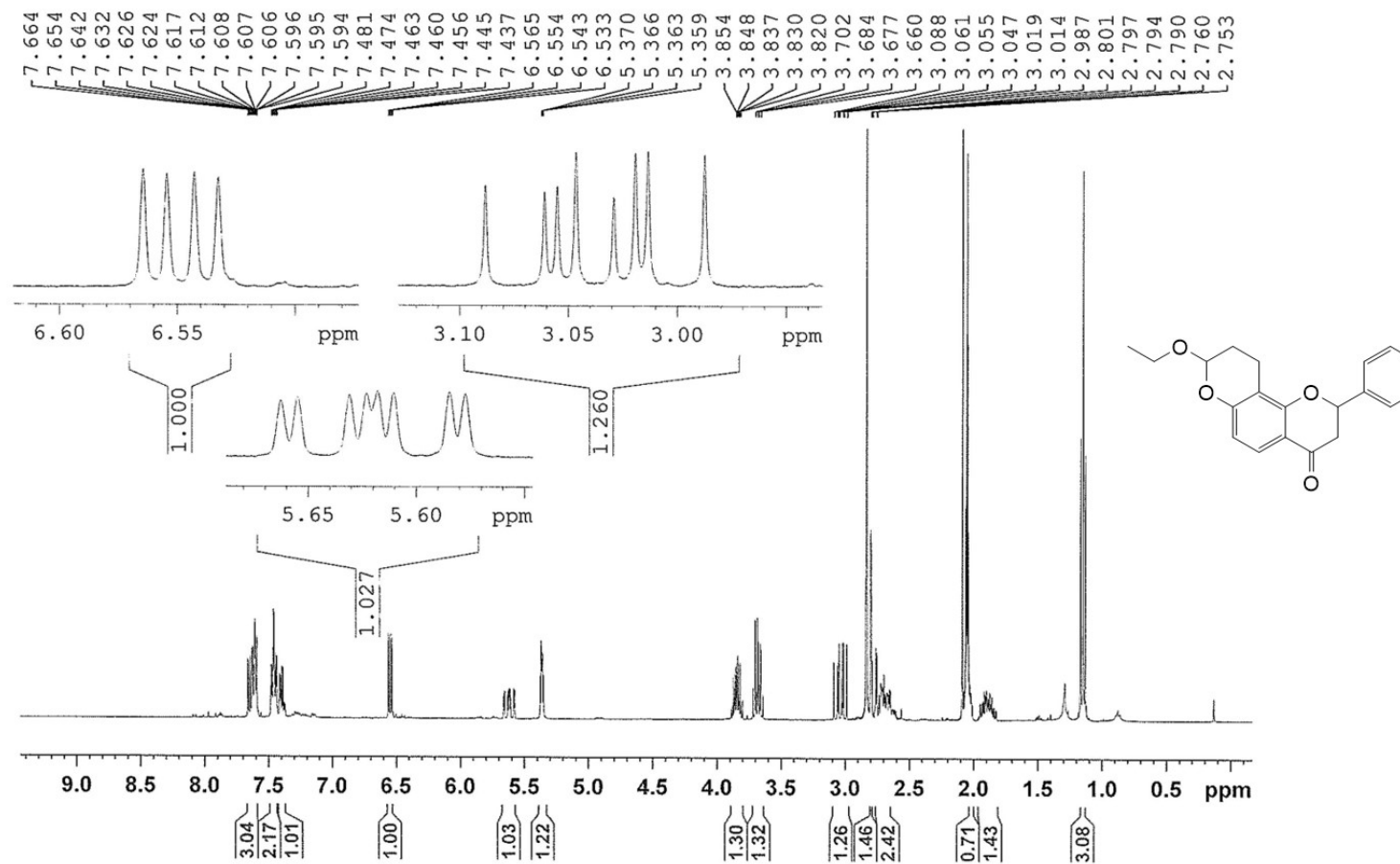


Figure S29. ¹H NMR (400 MHz, acetone-*d*₆) spectrum of 8-Ethoxy-2-phenyl-2,3,9,10-tetrahydro-4*H*,8*H*-pyrano[2,3-*f*]chromen-4-one (**15c**)

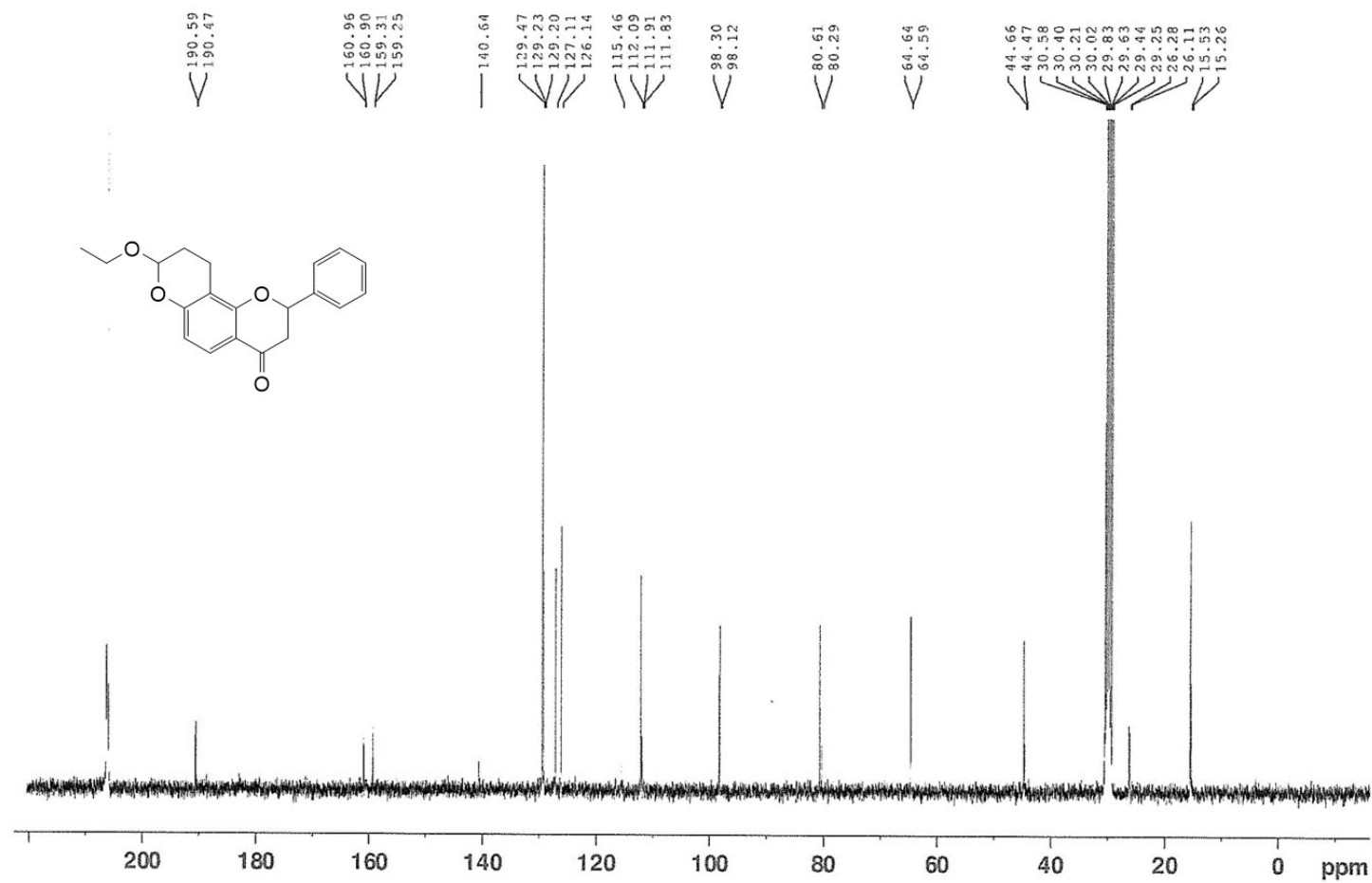


Figure S30. ¹³C NMR (100 MHz, acetone-*d*₆) spectrum of 8-Ethoxy-2-phenyl-2,3,9,10-tetrahydro-4H,8H-pyrano[2,3-f]chromen-4-one (15c)

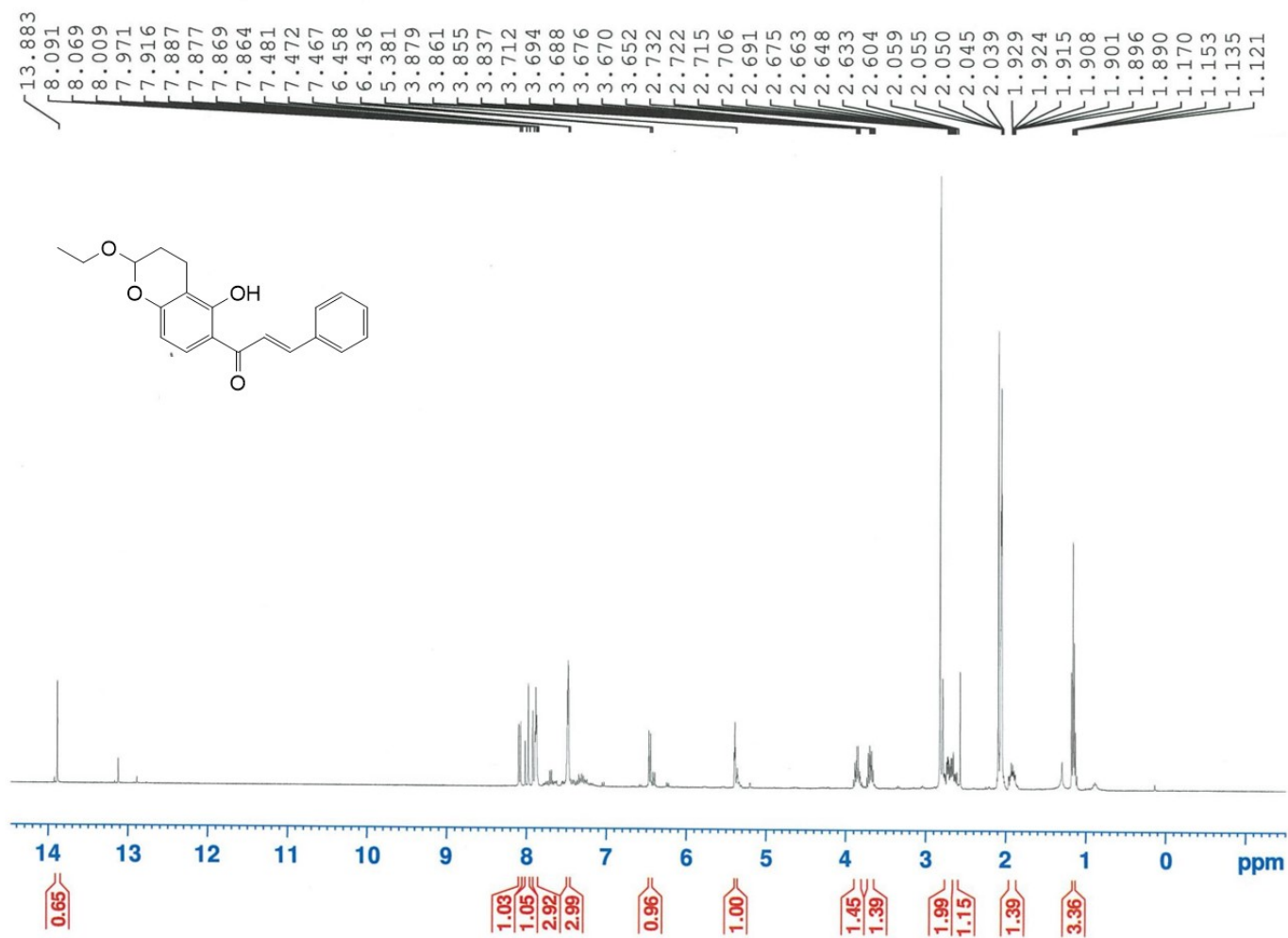


Figure S31. ¹H NMR (400 MHz, acetone-*d*₆) spectrum of (E)-1-(2-Ethoxy-5-hydroxychroman-6-yl)-3-phenylprop-2-en-1-one (16c)

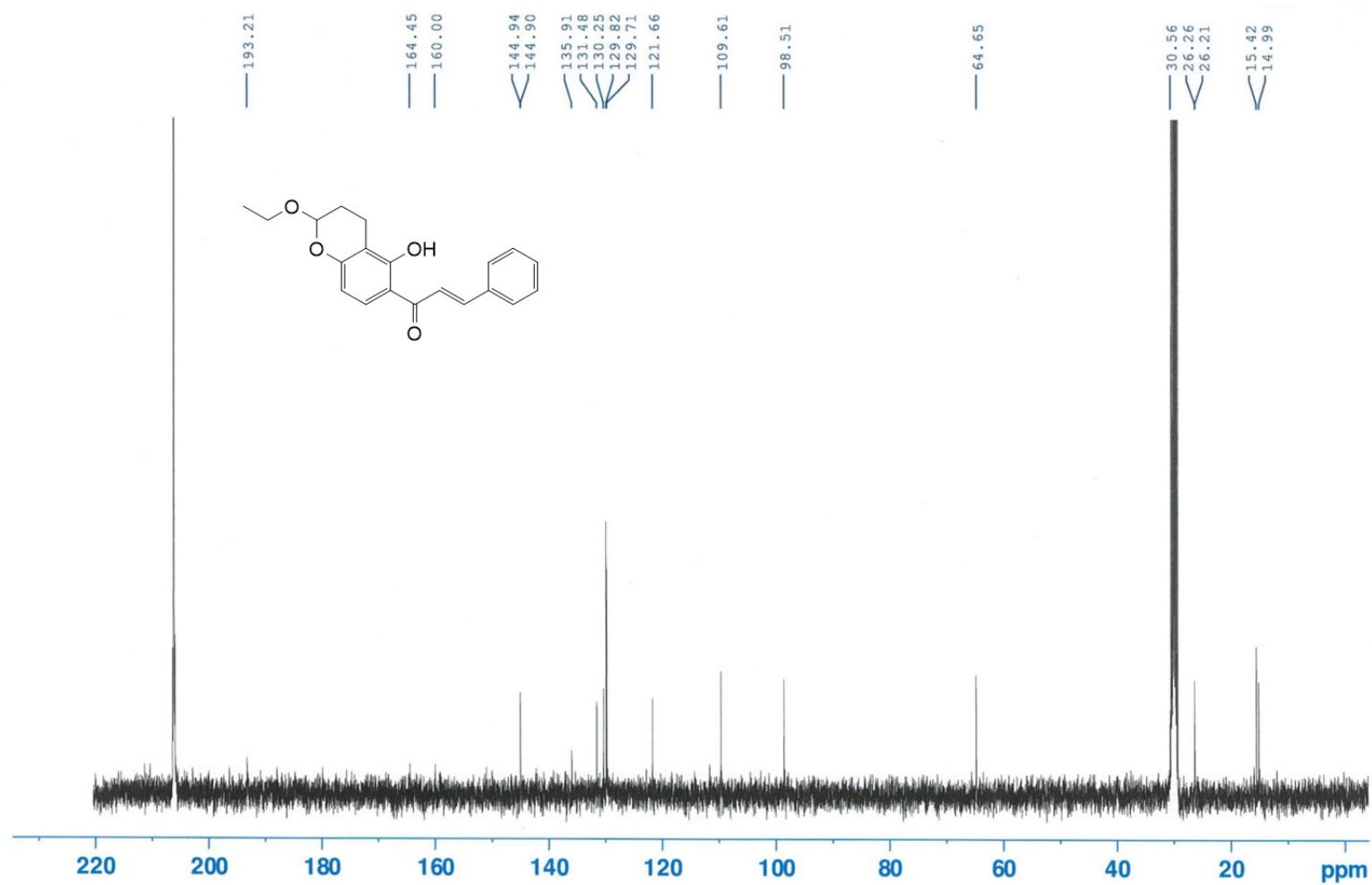


Figure S32. ¹³C NMR (100 MHz, acetone-*d*₆) spectrum of (E)-1-(2-Ethoxy-5-hydroxychroman-6-yl)-3-phenylprop-2-en-1-one (16c)

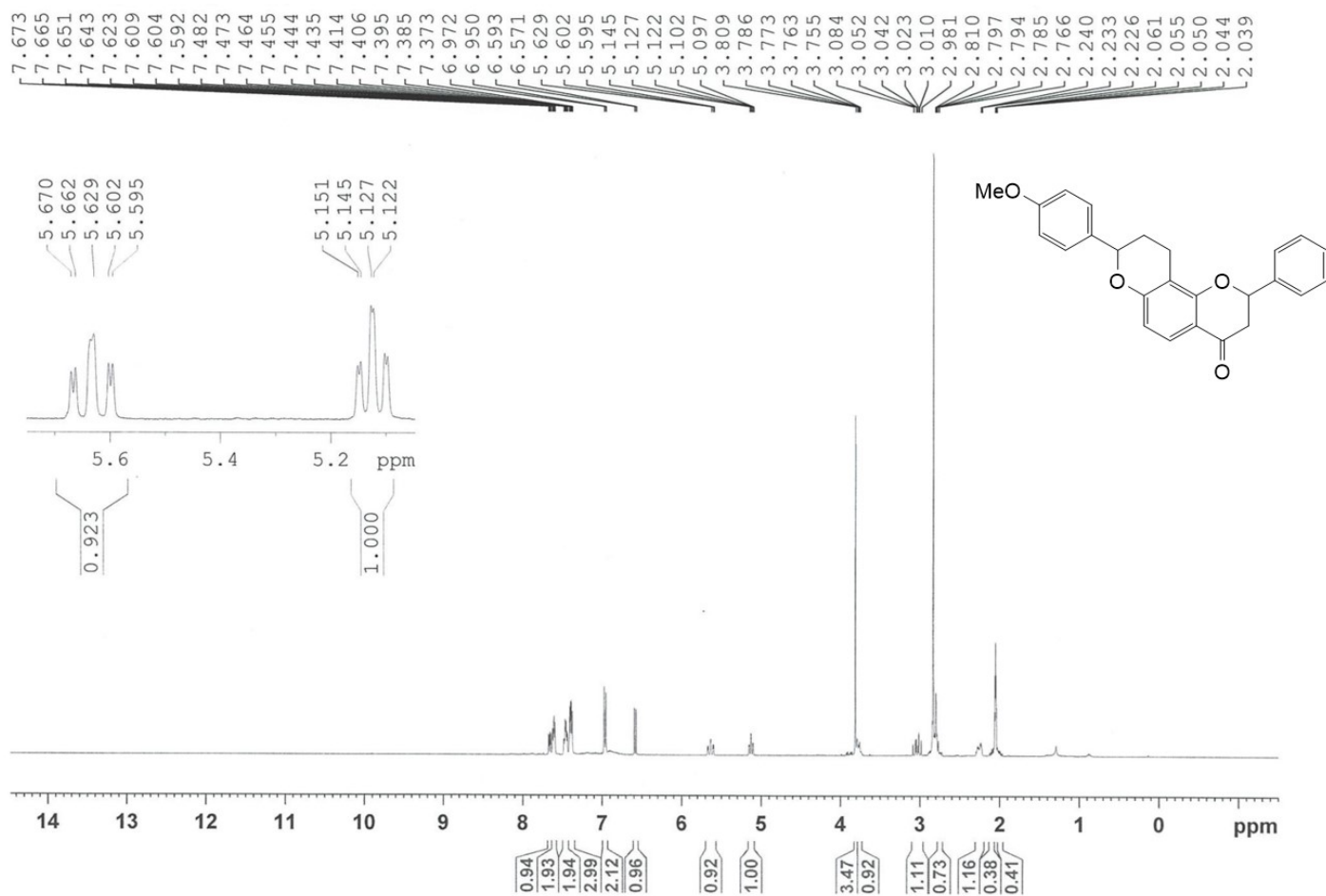


Figure S33. ¹H NMR (400 MHz, acetone-*d*₆) spectrum of 8-(4-Methoxyphenyl)-2-phenyl-2,3,9,10-tetrahydro-4H,8H-pyrano[2,3-f]chromen-4-one (**15d**)

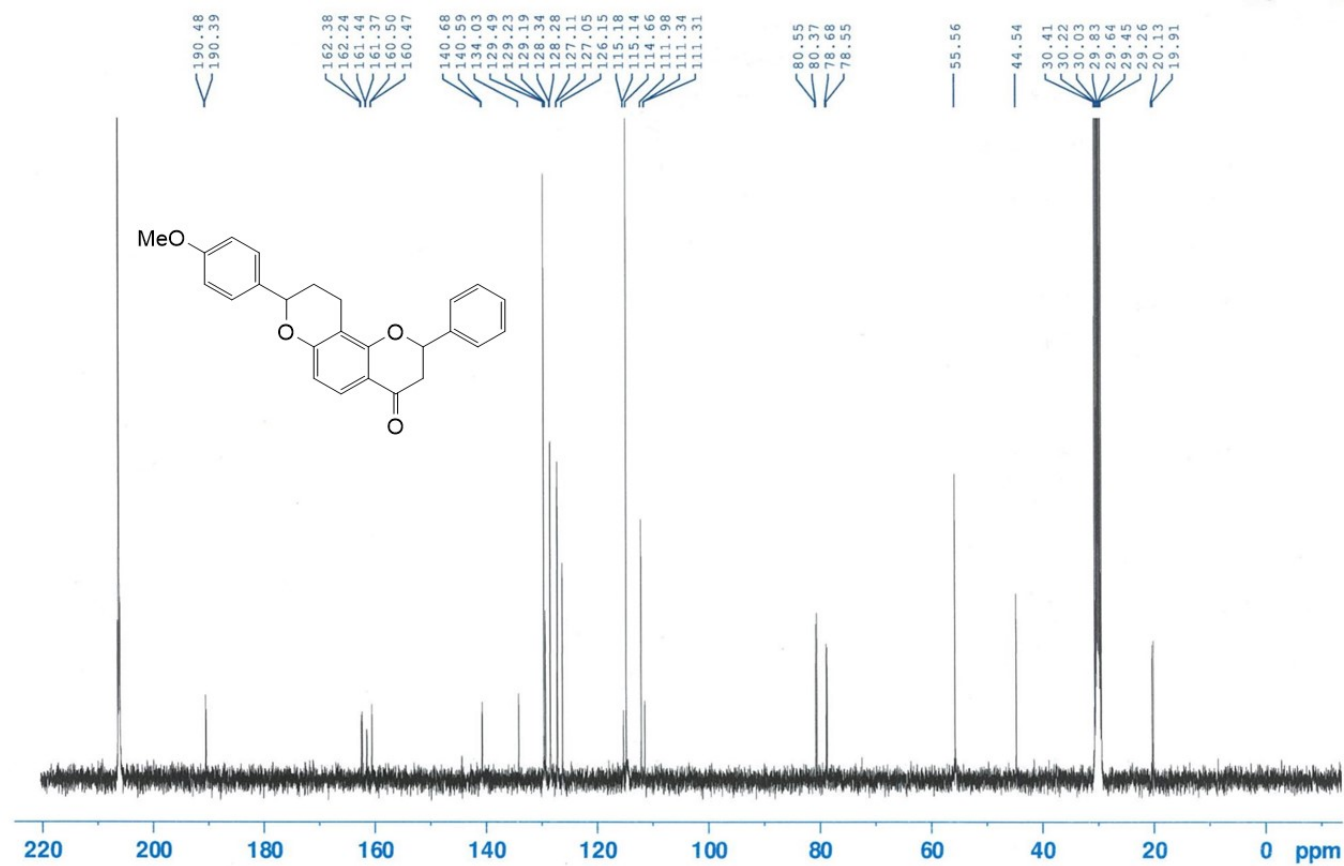


Figure S34. ¹³C NMR (100 MHz, acetone-*d*₆) spectrum of 8-(4-Methoxyphenyl)-2-phenyl-2,3,9,10-tetrahydro-4*H*,8*H*-pyrano[2,3-*f*]chromen-4-one (**15d**)

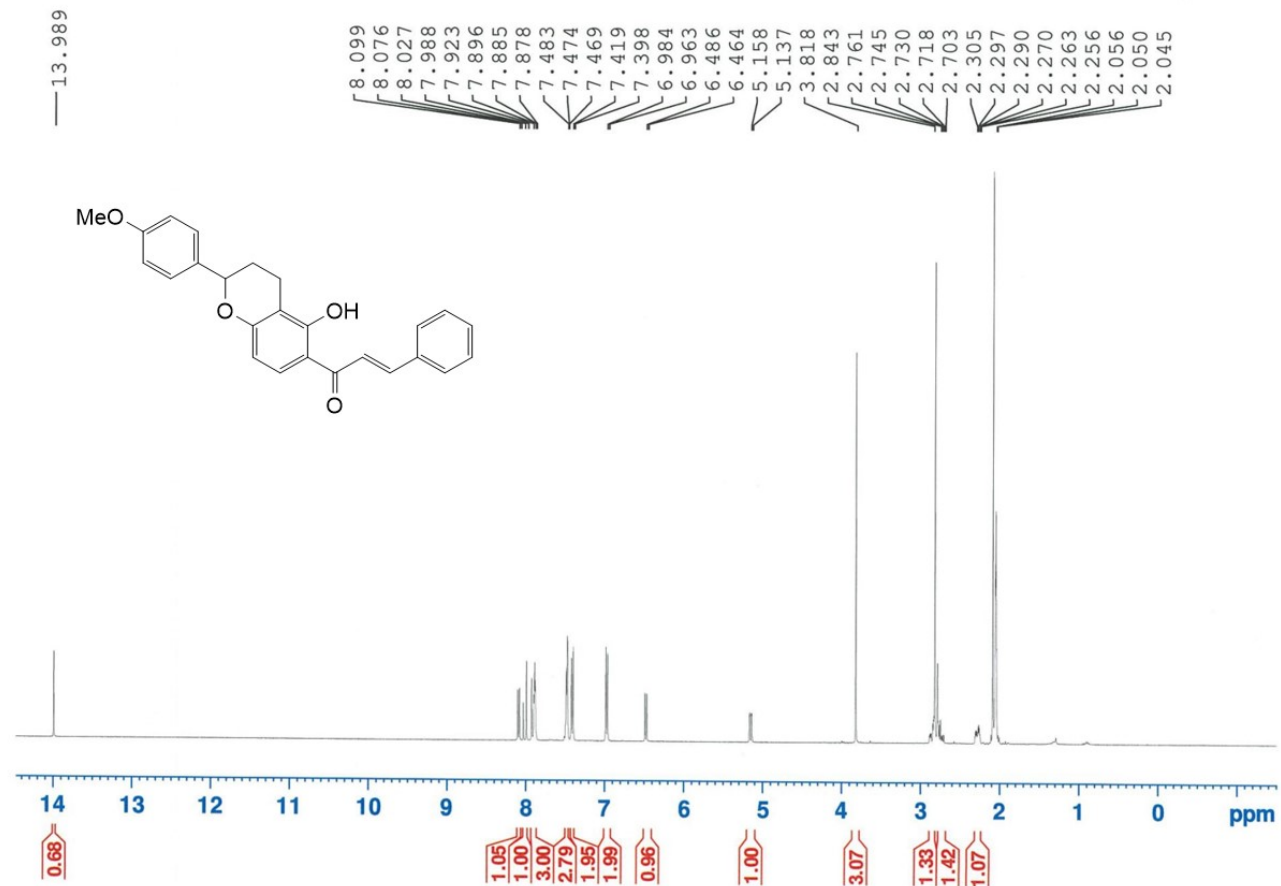


Figure S35. ¹H NMR (400 MHz, acetone-*d*₆) spectrum of (*E*)-1-(5-Hydroxy-2-(4-methoxyphenyl)chroman-6-yl)-3-phenylprop-2-en-1-one (16d)

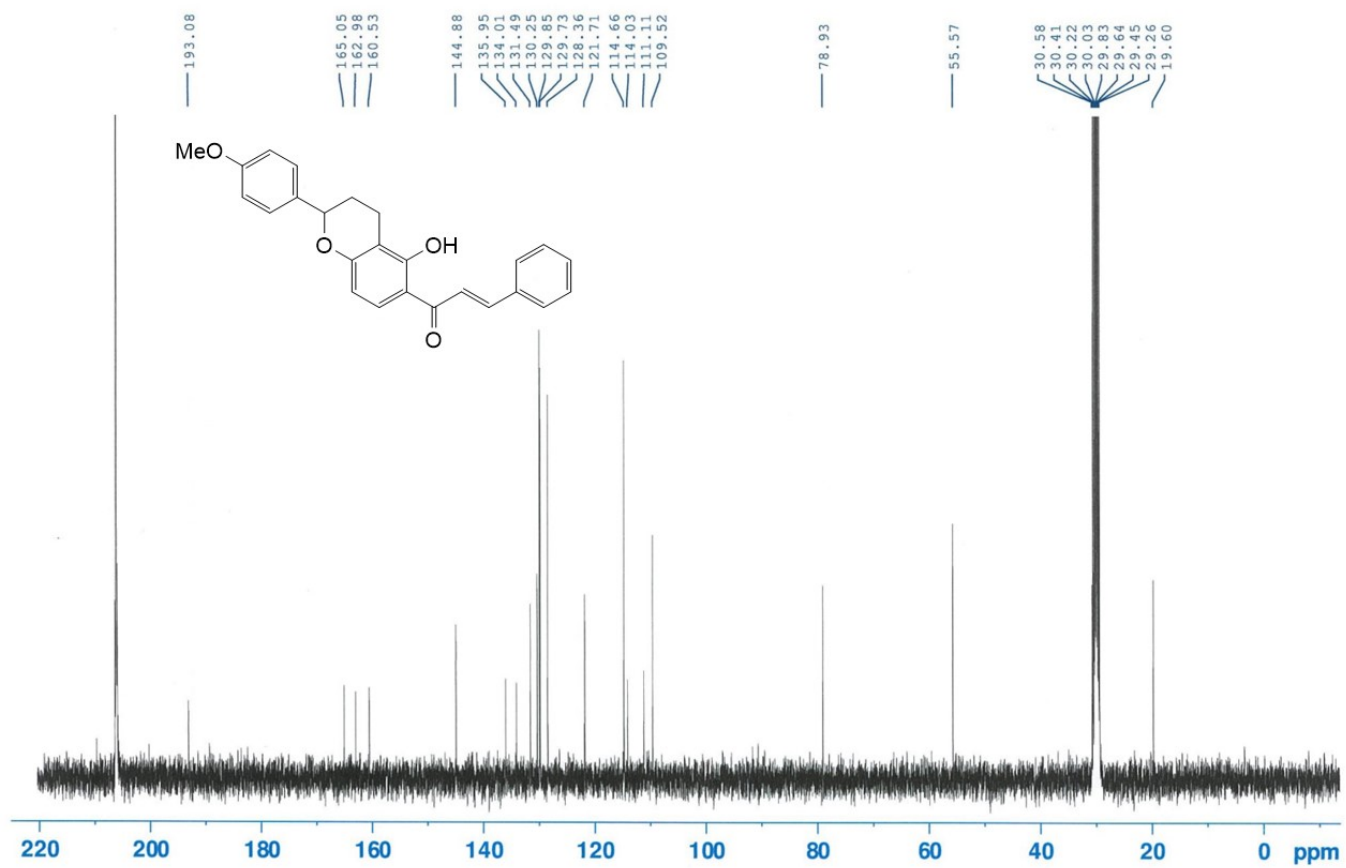


Figure S36. ¹³C NMR (100 MHz, acetone-*d*₆) spectrum of (*E*)-1-(5-Hydroxy-2-(4-methoxyphenyl)chroman-6-yl)-3-phenylprop-2-en-1-one (**16d**)

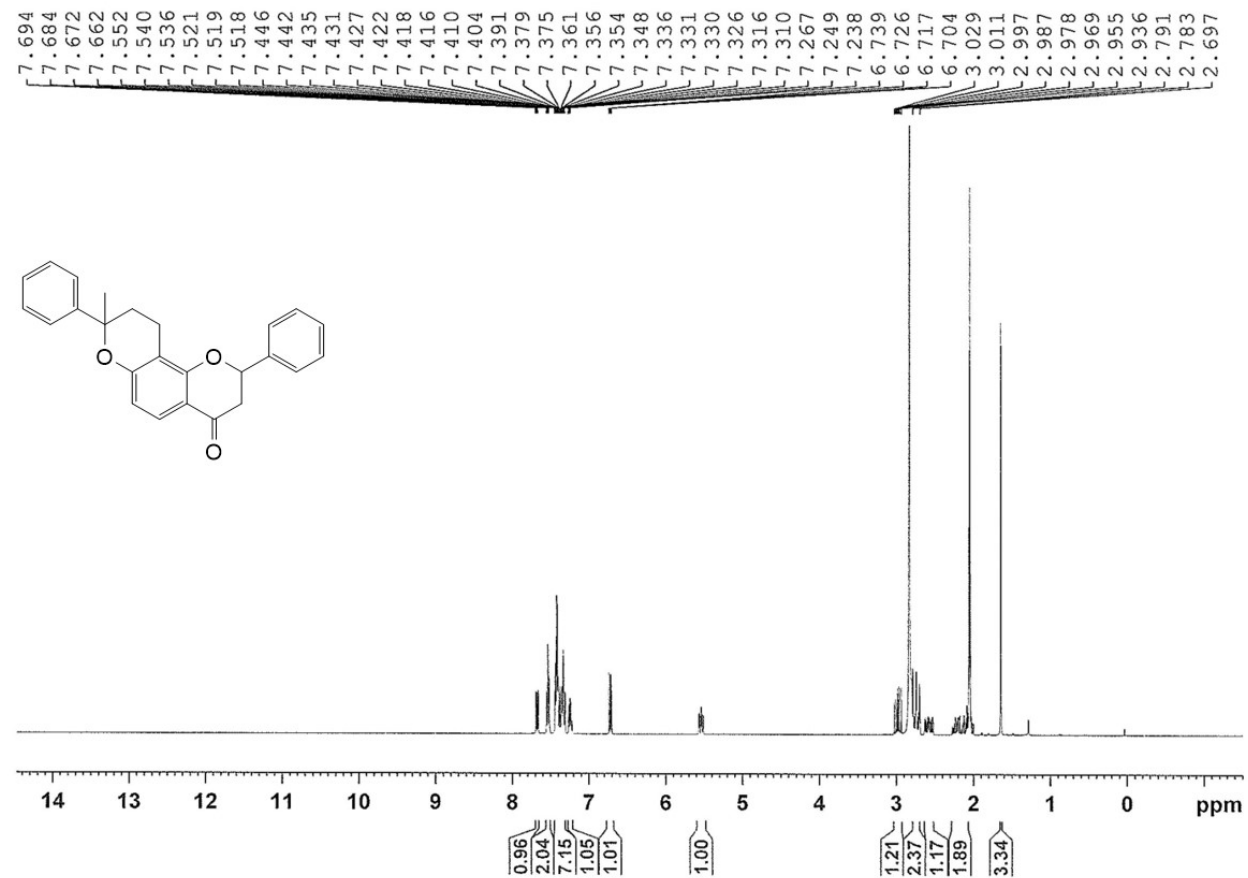


Figure S37. ¹H NMR (400 MHz, acetone-*d*₆) spectrum of 8-Methyl-2,8-diphenyl-2,3,9,10-tetrahydro-4*H*,8*H*-pyrano[2,3-*f*]chromen-4-one (15e)

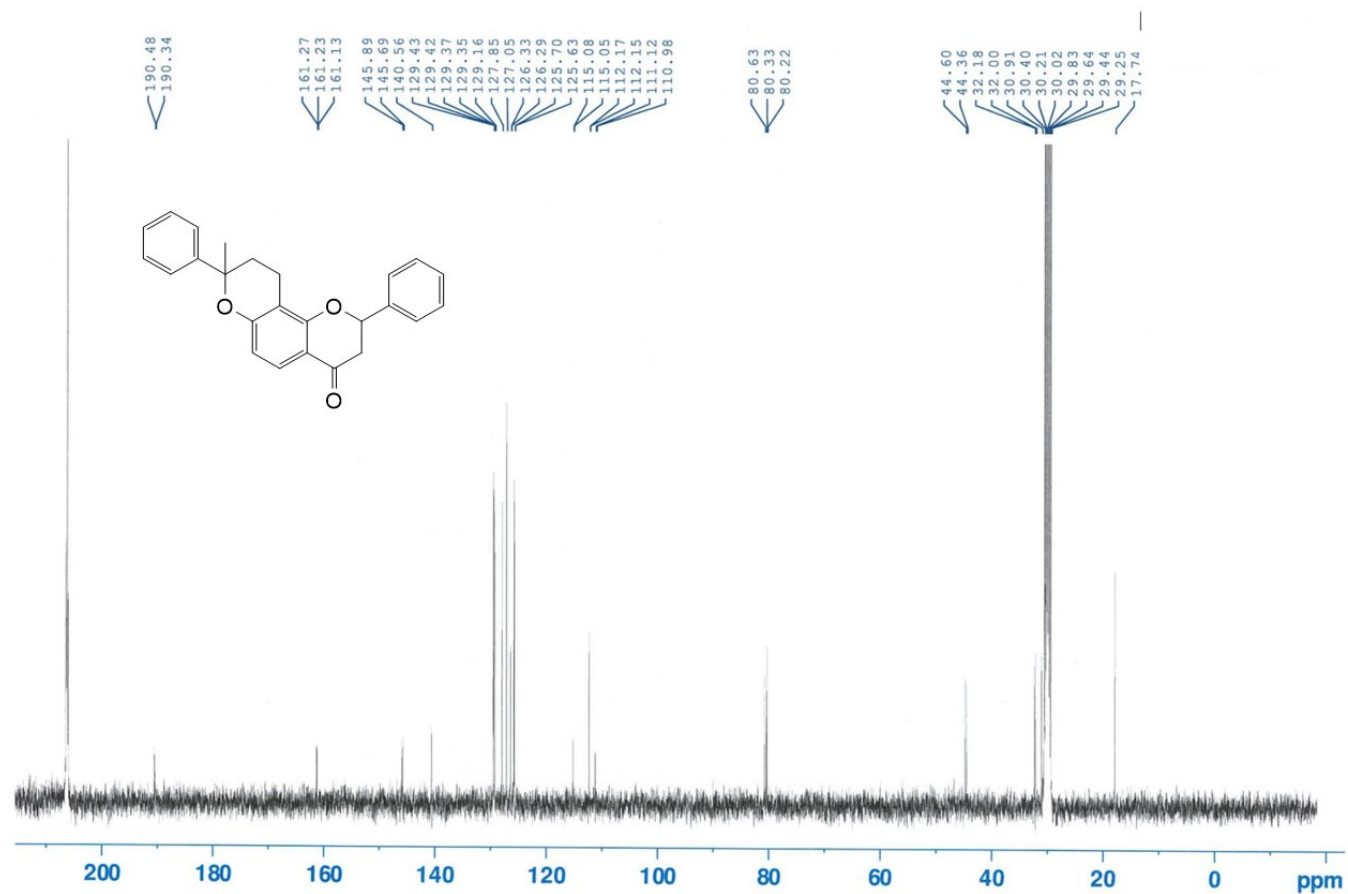


Figure S38. ¹³C NMR (100 MHz, acetone-*d*₆) spectrum of 8-Methyl-2,8-diphenyl-2,3,9,10-tetrahydro-4H,8H-pyrano[2,3-f]chromen-4-one (15e)

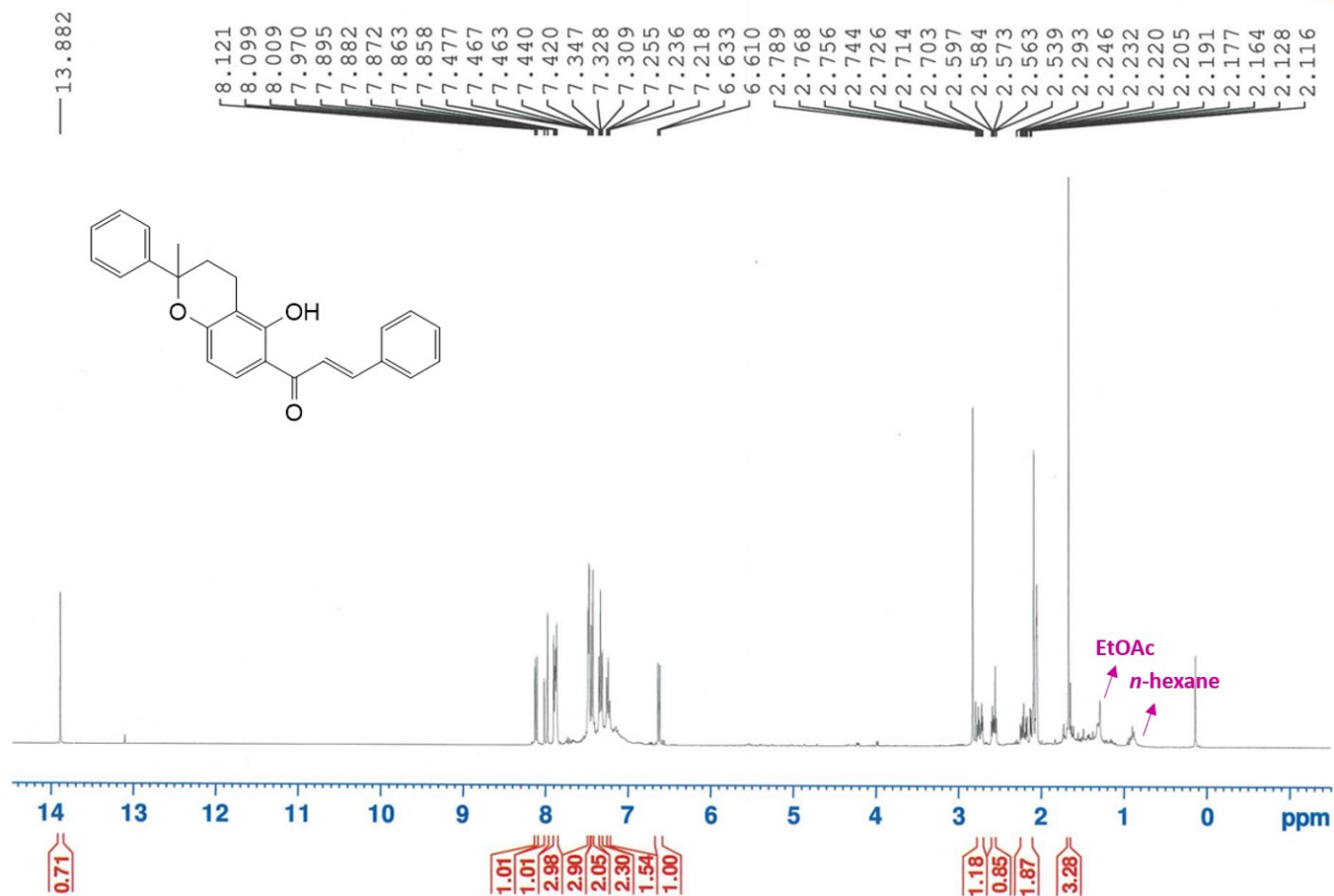


Figure S39. ¹H NMR (400 MHz, acetone-*d*₆) spectrum of (*E*)-1-(5-Hydroxy-2-methyl-2-phenylchroman-6-yl)-3-phenylprop-2-en-1-one (**16e**)

Ethyl acetate and *n*-hexane are the solvents used for purification of **16e** using column chromatography

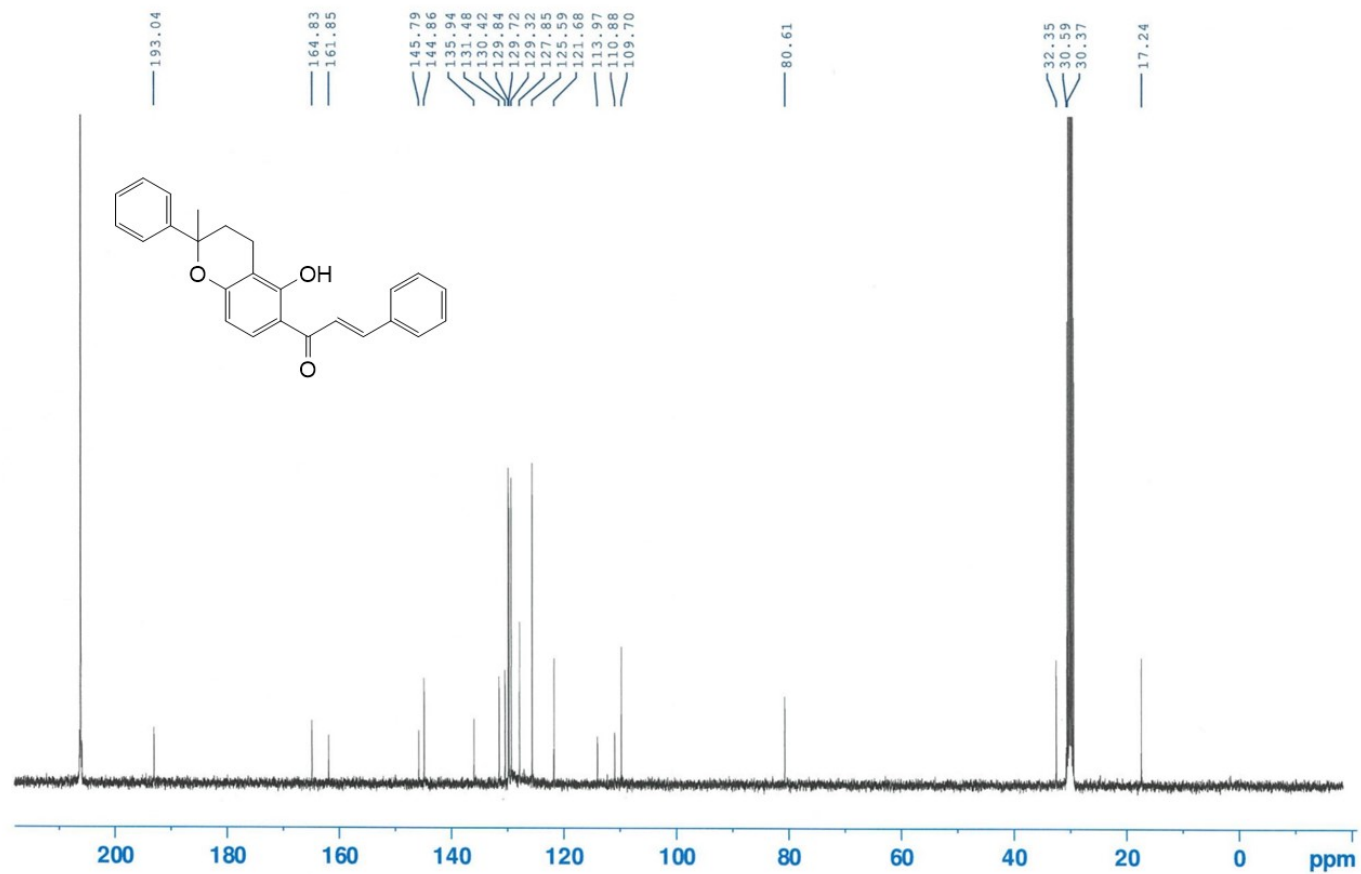


Figure S40. ¹³C NMR (100 MHz, acetone-*d*₆) spectrum of (*E*)-1-(5-Hydroxy-2-methyl-2-phenylchroman-6-yl)-3-phenylprop-2-en-1-one (**16e**)

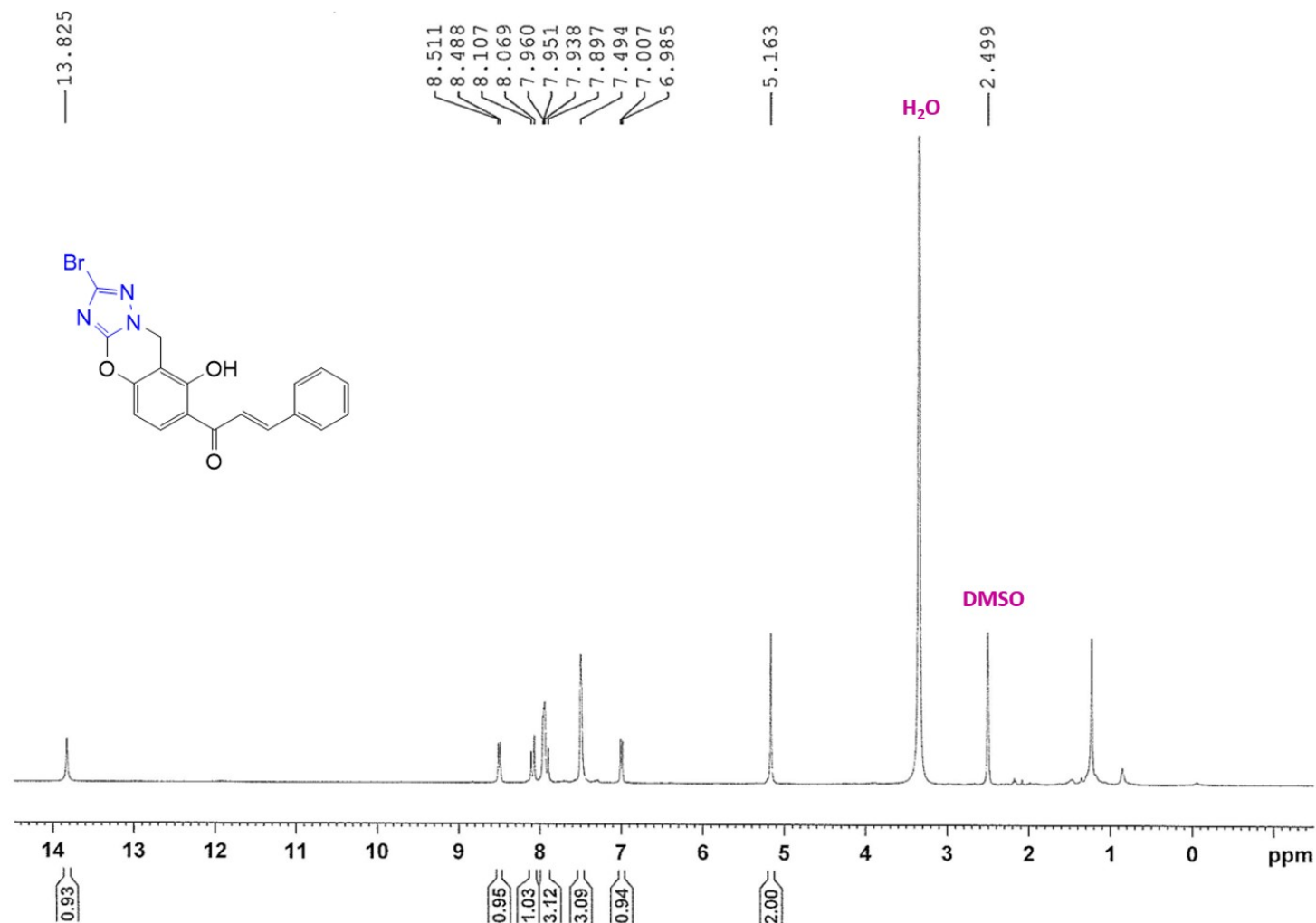


Figure S41. ¹H NMR (400 MHz, DMSO-*d*₆) spectrum of (*E*)-1-(2-Bromo-8-hydroxy-9H-benzo[e][1,2,4]triazolo[5,1-b][1,3]oxazin-7-yl)-3-phenylprop-2-en-1-one (18)

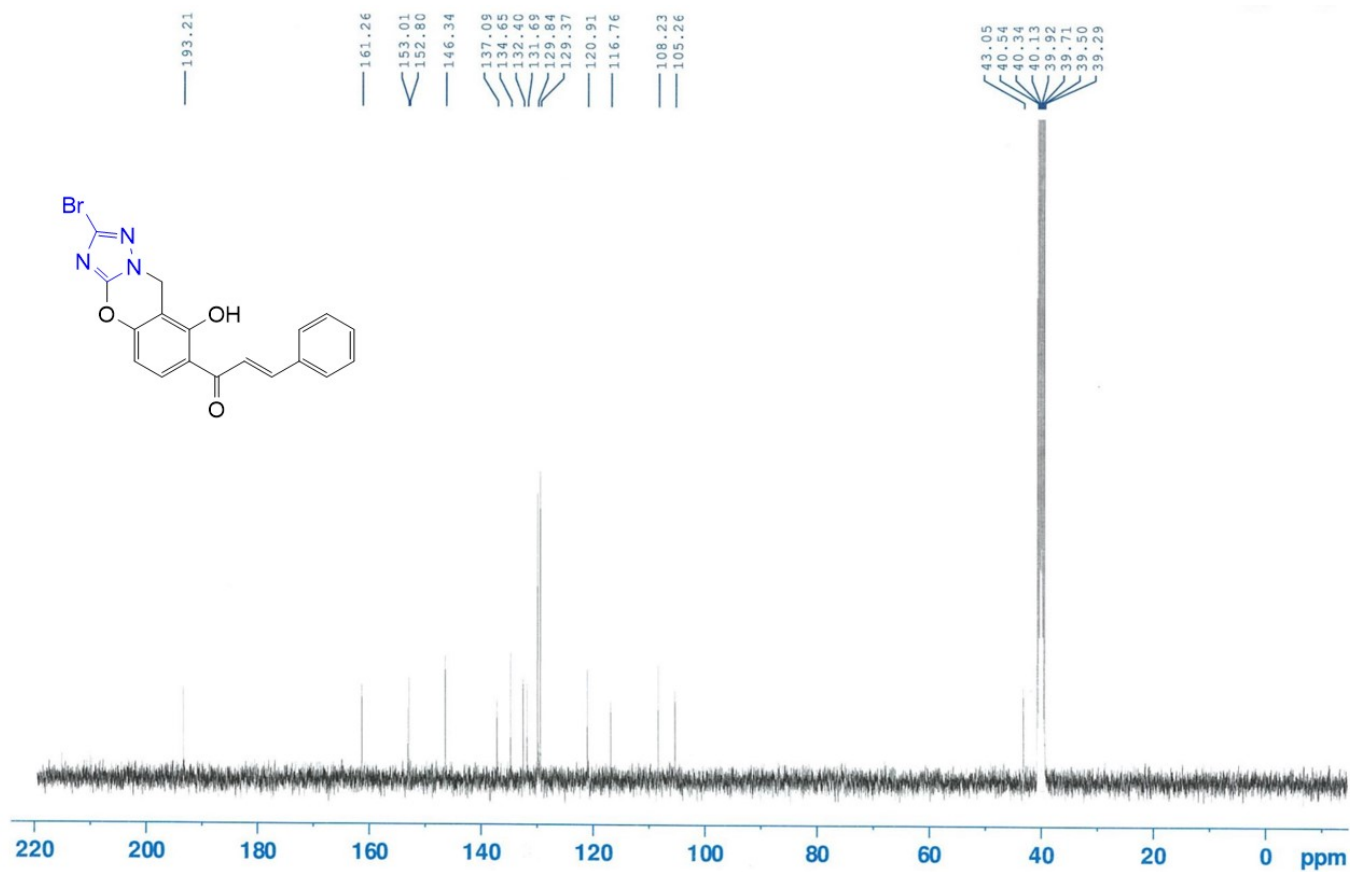


Figure S42. ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) spectrum of (E)-1-(2-Bromo-8-hydroxy-9H-benzo[e][1,2,4]triazolo[5,1-b][1,3]oxazin-7-yl)-3-phenylprop-2-en-1-one (18)

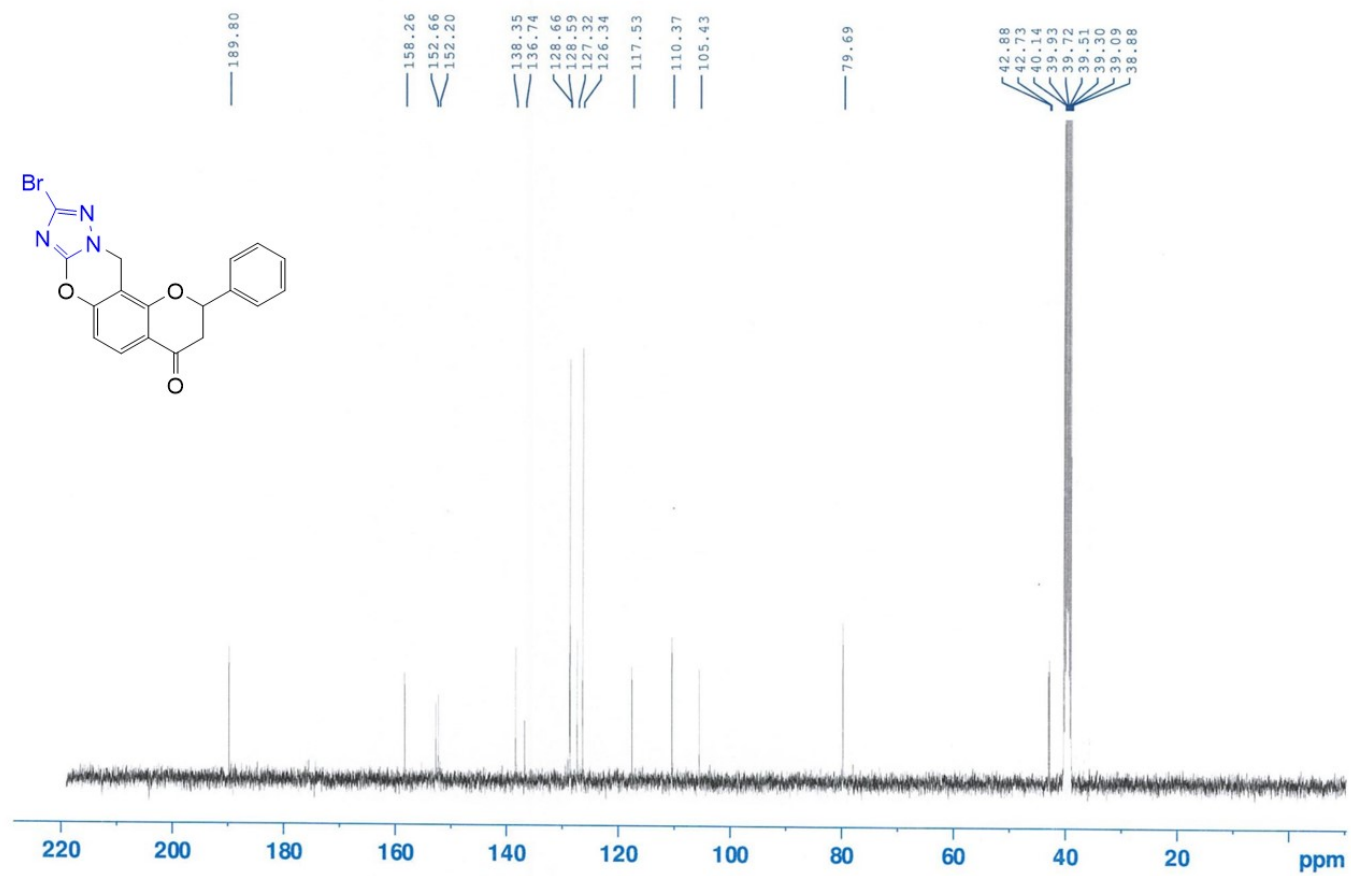


Figure S44. ¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of 9-Bromo-2-phenyl-2,3-dihydro-4H,12H-chromeno[8,7-e][1,2,4]triazolo[5,1-b][1,3]oxazin-4-one (19)

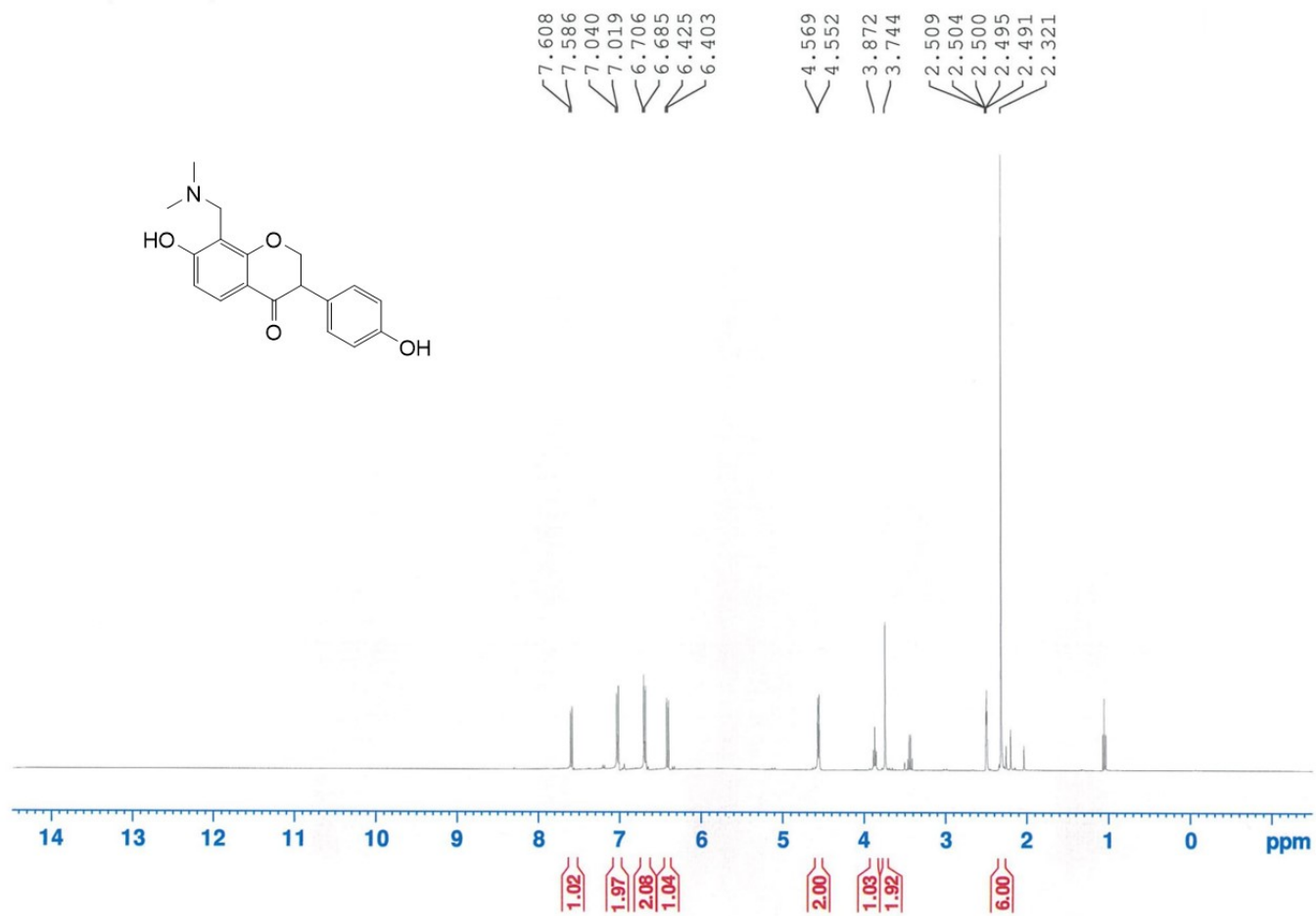


Figure S45. ¹H NMR (400 MHz, DMSO-*d*₆) spectrum of 8-((Dimethylamino)methyl)-7-hydroxy-3-(4-hydroxyphenyl)chroman-4-one (11)

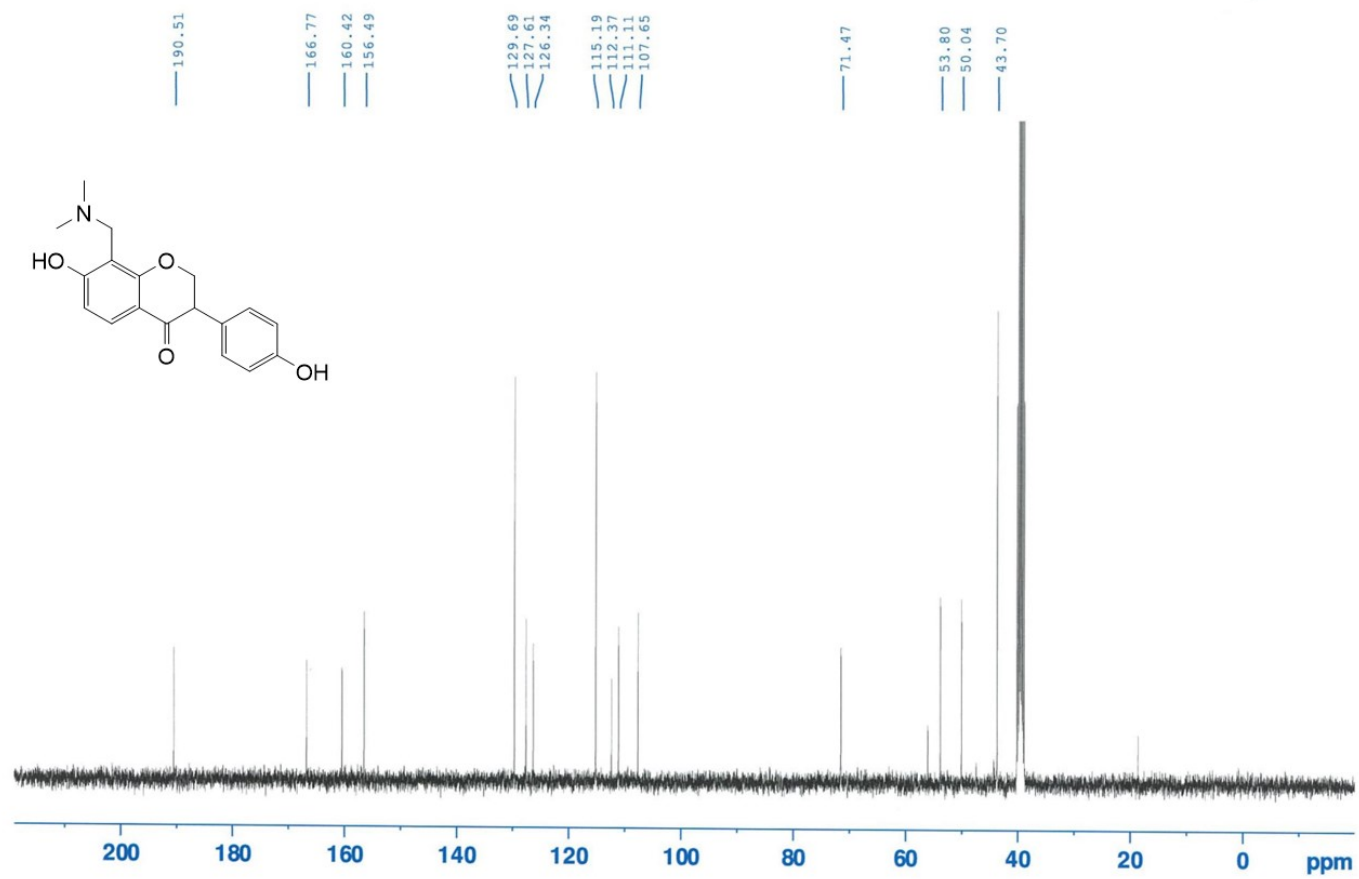


Figure S46. ¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of 8-((Dimethylamino)methyl)-7-hydroxy-3-(4-hydroxyphenyl)chroman-4-one (11)

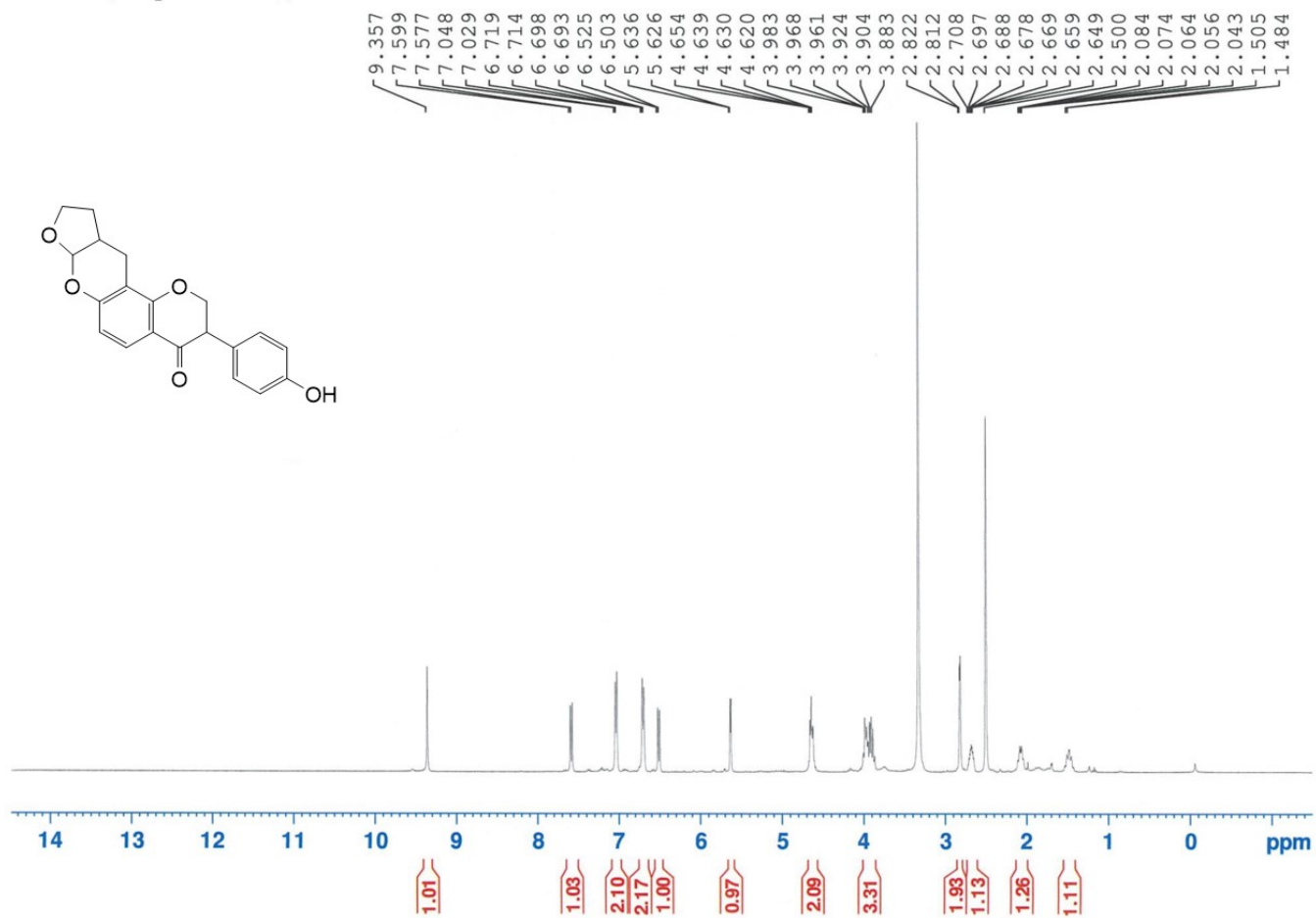


Figure S47. ¹H NMR (400 MHz, DMSO-*d*₆) spectrum of 3-(4-Hydroxyphenyl)-2,3,7a,9,10,10a-hexahydro-4H,11H-furo[2,3-b]pyrano[2,3-f]chromen-4-one (21a)

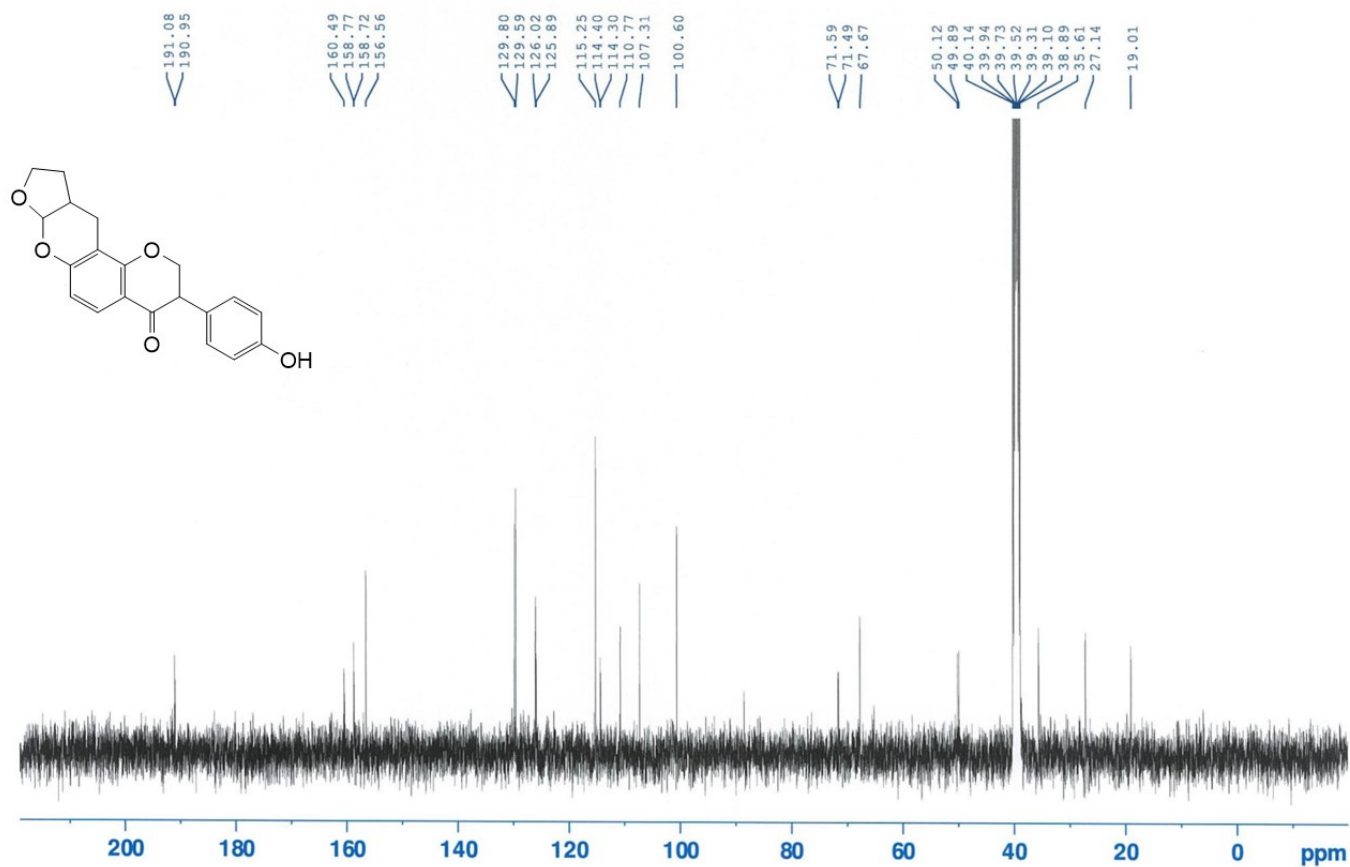


Figure S48. ¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of 3-(4-Hydroxyphenyl)-2,3,7a,9,10,10a-hexahydro-4H,11H-furo[2,3-b]pyrano[2,3-f]chromen-4-one (21a)

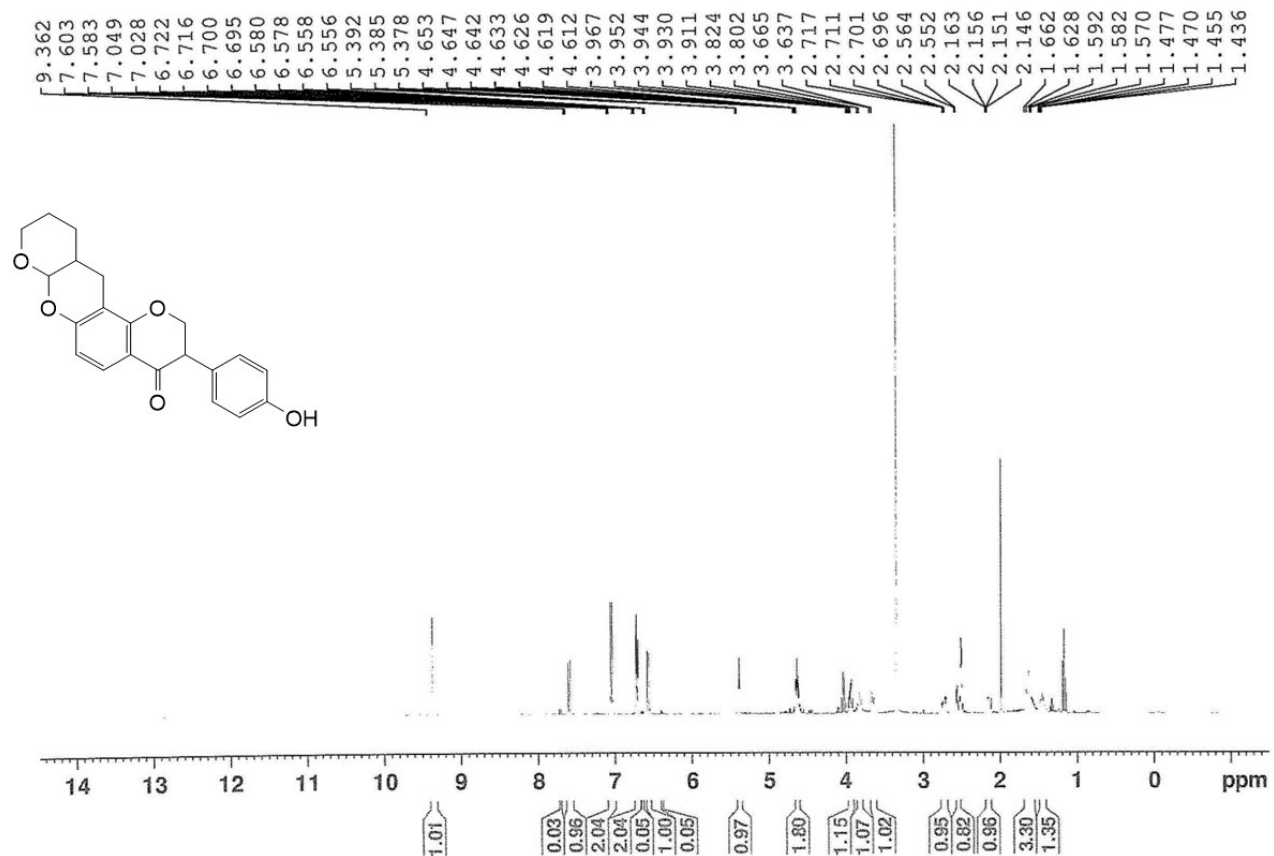


Figure S49. ¹H NMR (400 MHz, DMSO-*d*₆) spectrum of 3-(4-Hydroxyphenyl)-2,3,7a,10,11,11a-hexahydro-4H,9H,12H-dipyrano[2,3-b:2',3'-f]chromen-4-one (21b)

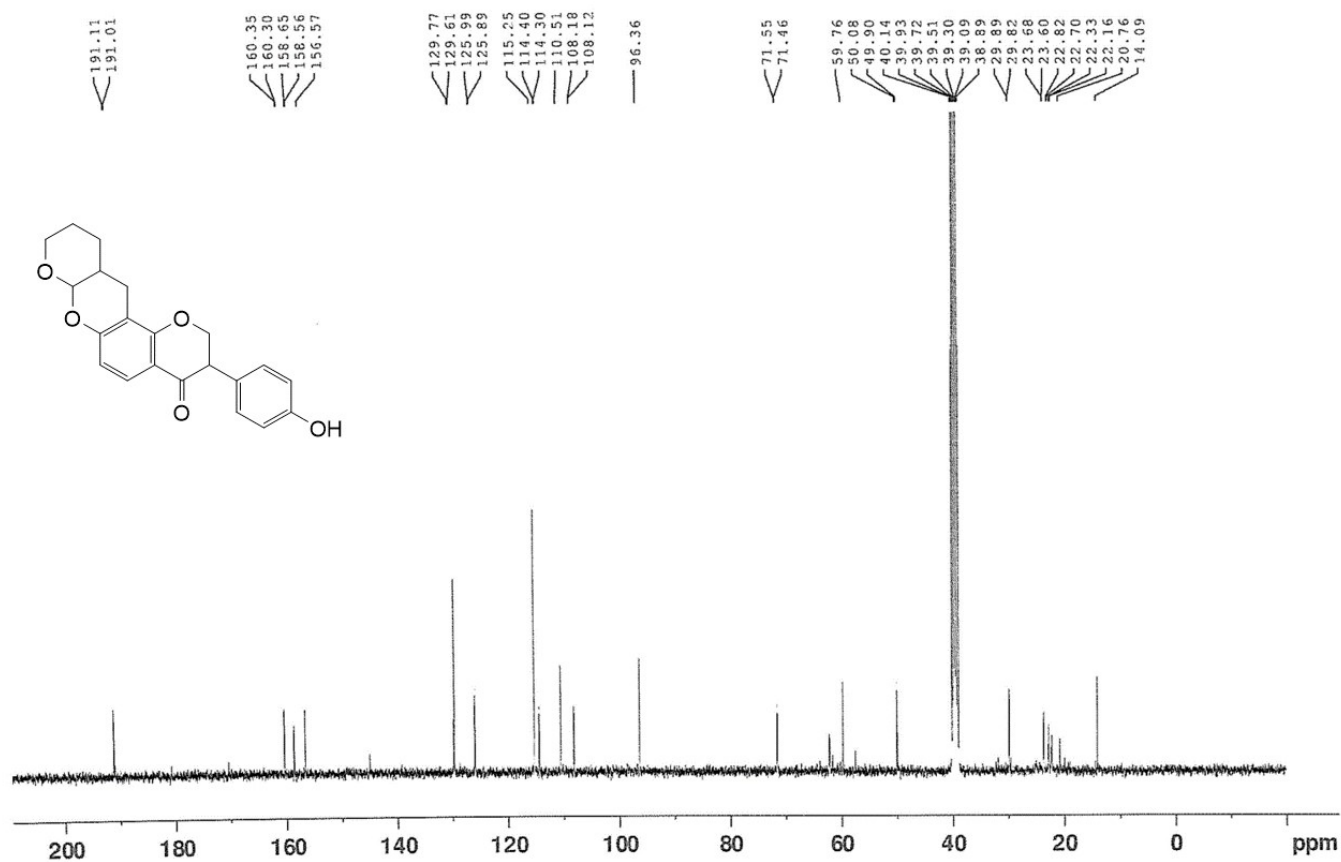


Figure S50. ¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of 3-(4-Hydroxyphenyl)-2,3,7a,10,11,11a-hexahydro-4*H*,9*H*,12*H*-dipyrano[2,3-*b*:2',3'-*f*]chromen-4-one (21b)

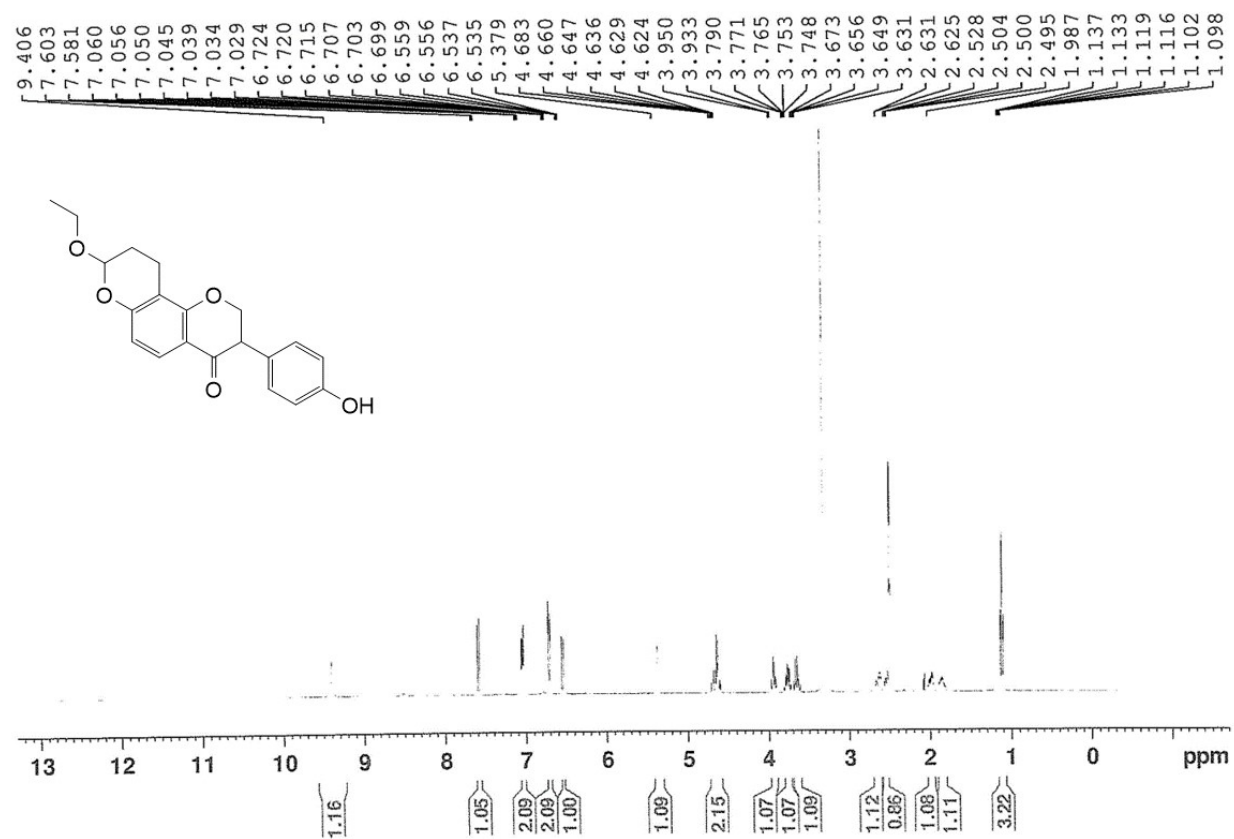


Figure S51. ¹H NMR (400 MHz, DMSO-*d*₆) of 8-Ethoxy-3-(4-hydroxyphenyl)-2,3,9,10-tetrahydro-4*H*,8*H*-pyrano[2,3-*f*]chromen-4-one (21c)

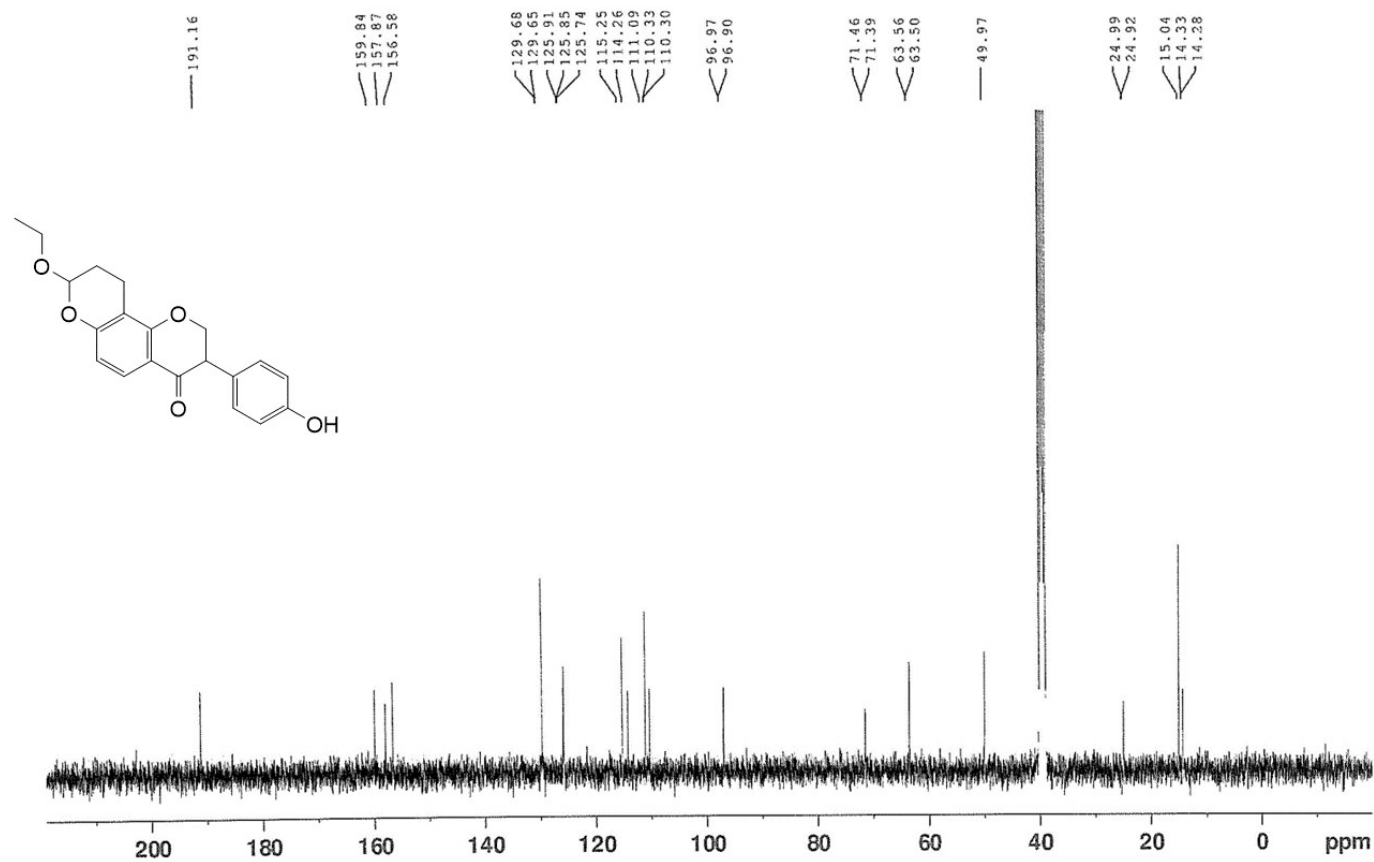


Figure S52. ¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of 8-Ethoxy-3-(4-hydroxyphenyl)-2,3,9,10-tetrahydro-4*H*,8*H*-pyrano[2,3-*f*]chromen-4-one (21c)

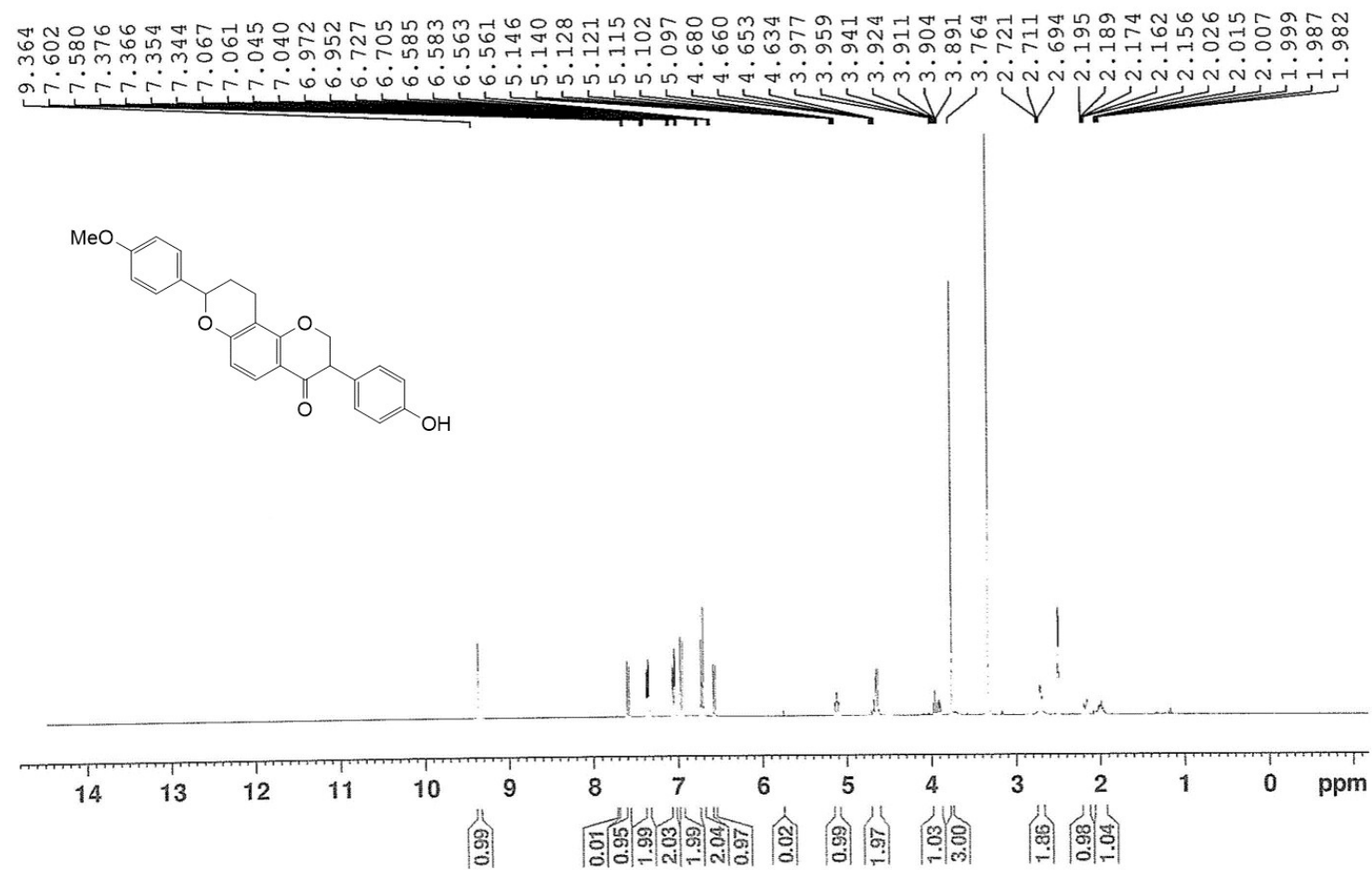


Figure S53. ¹H NMR (400 MHz, DMSO-*d*₆) spectrum of 3-(4-Hydroxyphenyl)-8-(4-methoxyphenyl)-2,3,9,10-tetrahydro-4H,8H-pyrano[2,3-f]chromen-4-one (21d)

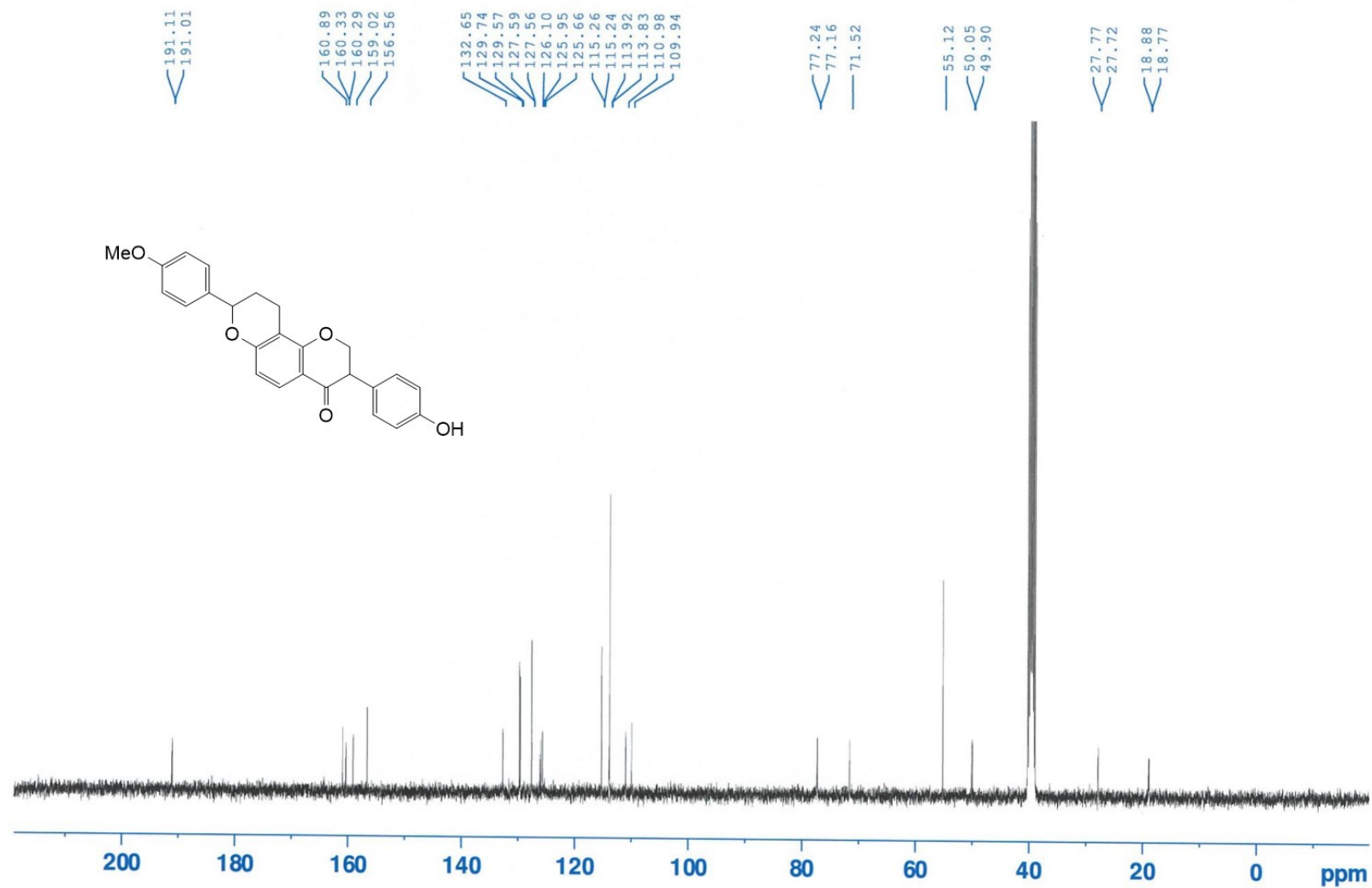


Figure S54. ¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of 3-(4-Hydroxyphenyl)-8-(4-methoxyphenyl)-2,3,9,10-tetrahydro-4H,8H-pyrano[2,3-f]chromen-4-one (21d)

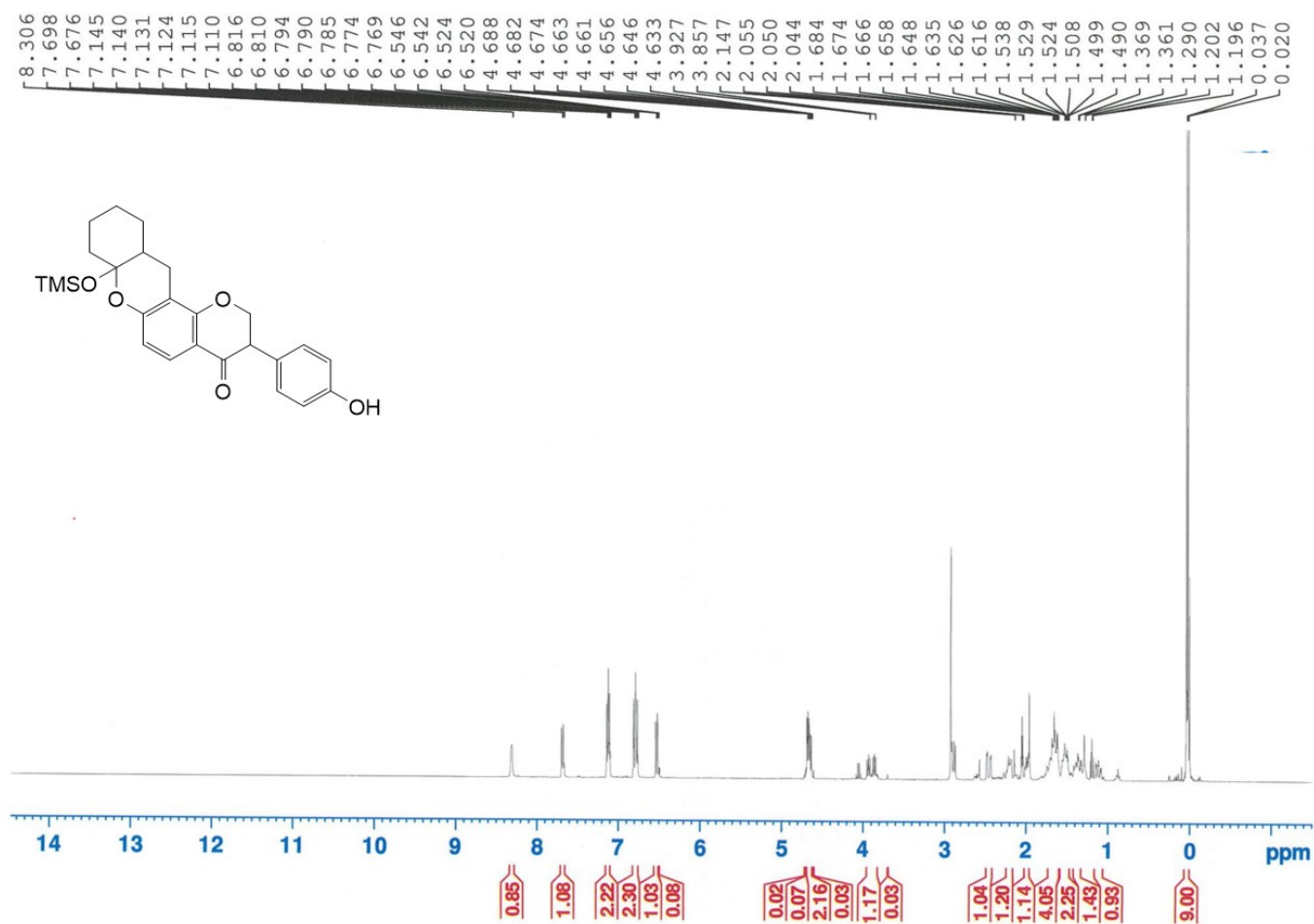


Figure S55. ¹H NMR (400 MHz, acetone-*d*₆) spectrum of 3-(4-Hydroxyphenyl)-7a-((trimethylsilyl)oxy)-2,3,7a,8,10,11,11a,12-octahydro-4H,9H-pyrano[2,3-a]xanthen-4-one (21e)

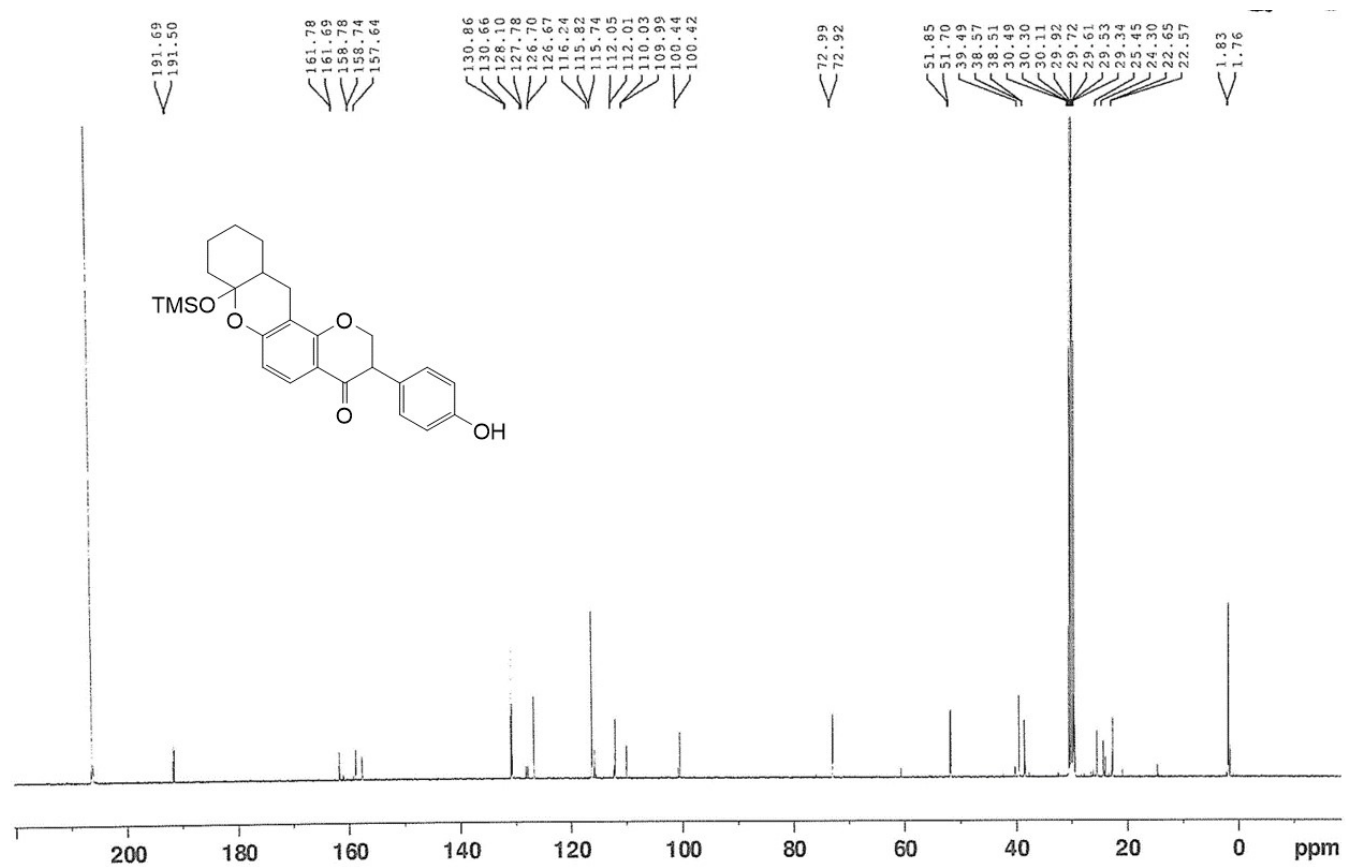


Figure S56. ¹³C NMR (100 MHz, acetone-*d*₆) spectrum of 3-(4-Hydroxyphenyl)-7a-((trimethylsilyl)oxy)-2,3,7a,8,10,11,11a,12-octahydro-4H,9H-pyrano[2,3-a]xanthen-4-one (**21e**)

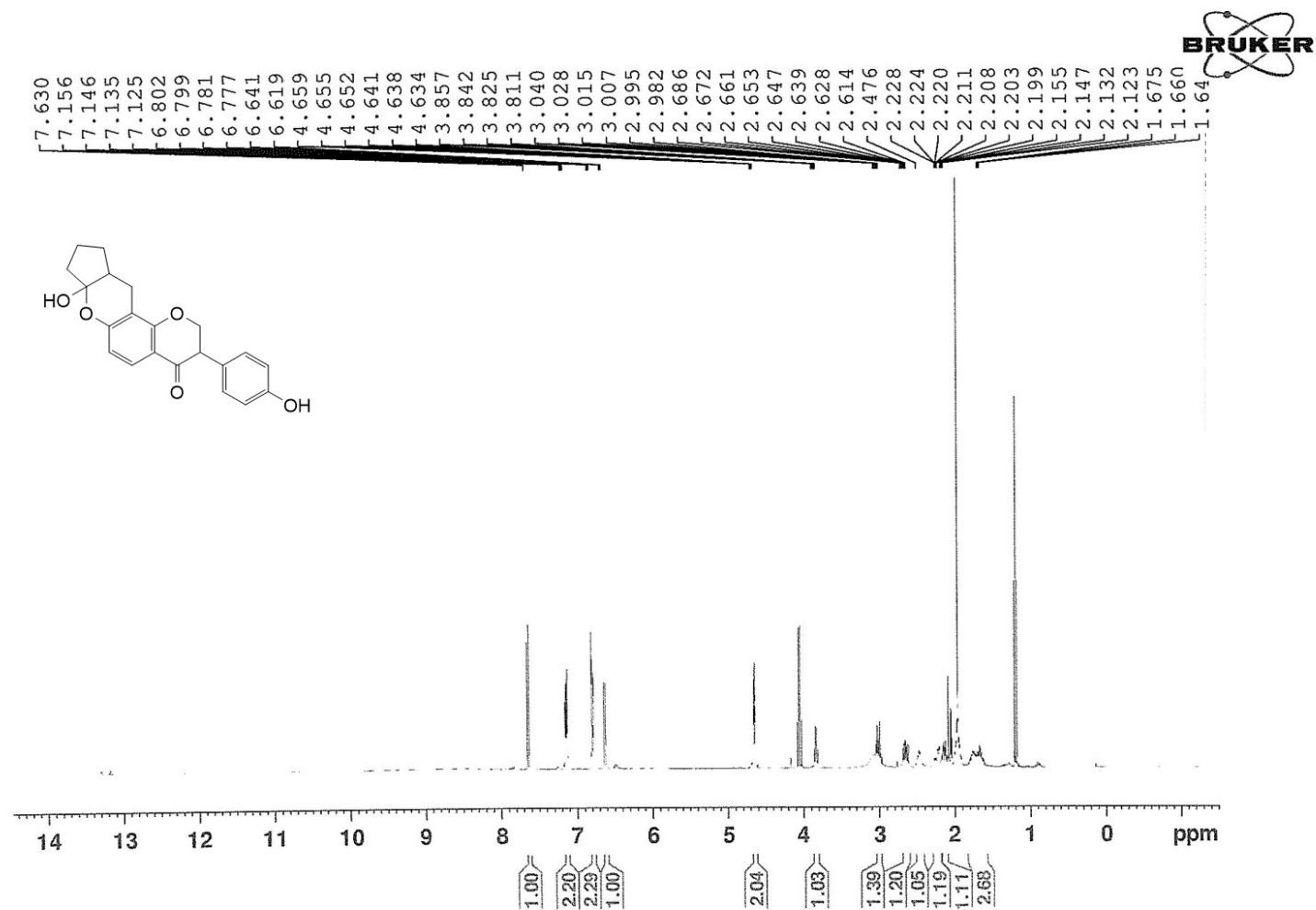


Figure S57. ¹H NMR (400 MHz, acetone-*d*₆) spectrum of 7a-hydroxy-3-(4-hydroxyphenyl)-2,3,7a,8,9,10,10a,11-octahydro-4H-cyclopenta[b]pyrano[2,3-f]chromen-4-one (21f)

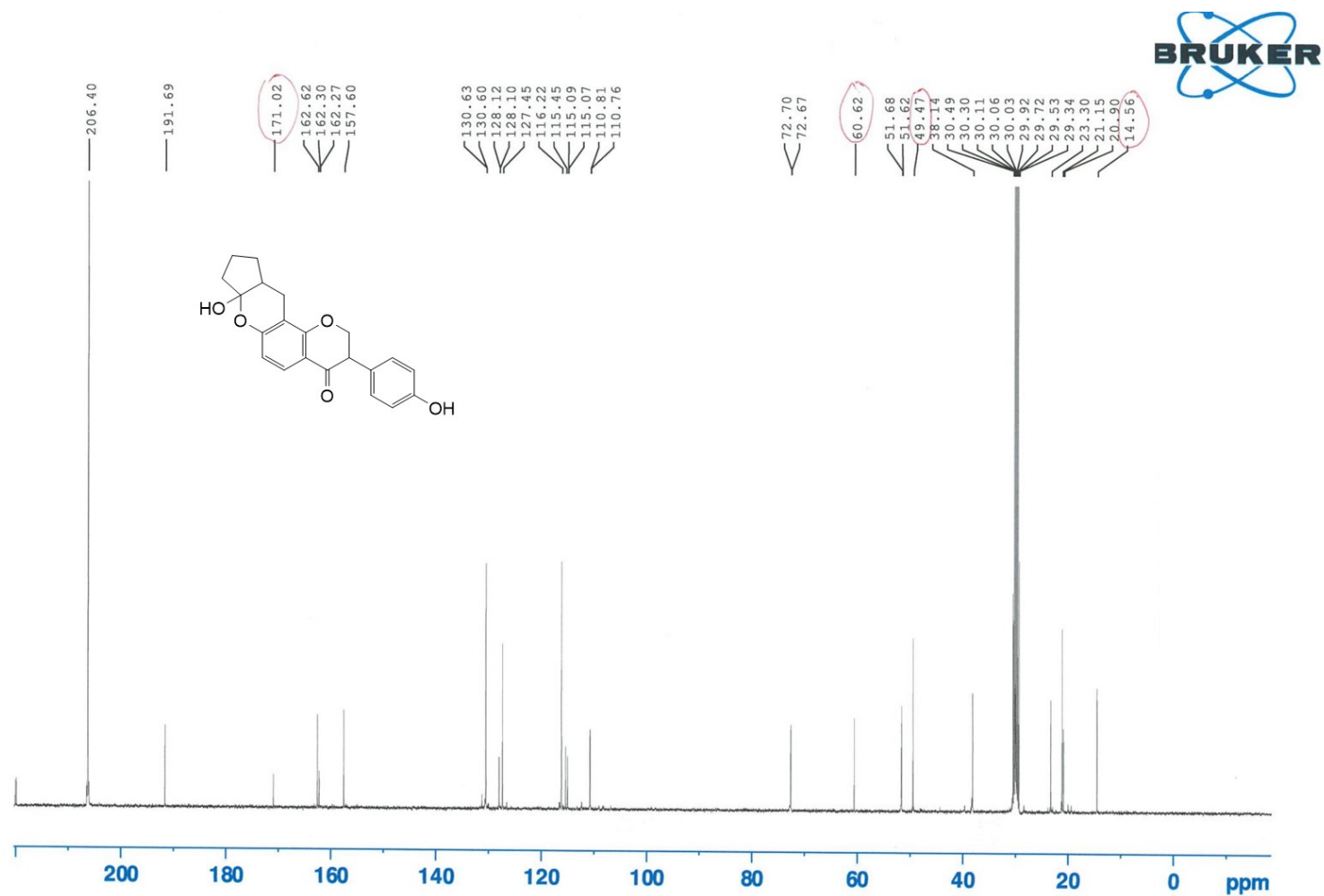


Figure S58. ¹³C NMR (100 MHz, acetone-*d*₆) spectrum of 7a-hydroxy-3-(4-hydroxyphenyl)-2,3,7a,8,9,10,10a,11-octahydro-4H-cyclopenta[b]pyrano[2,3-f]chromen-4-one (21f)

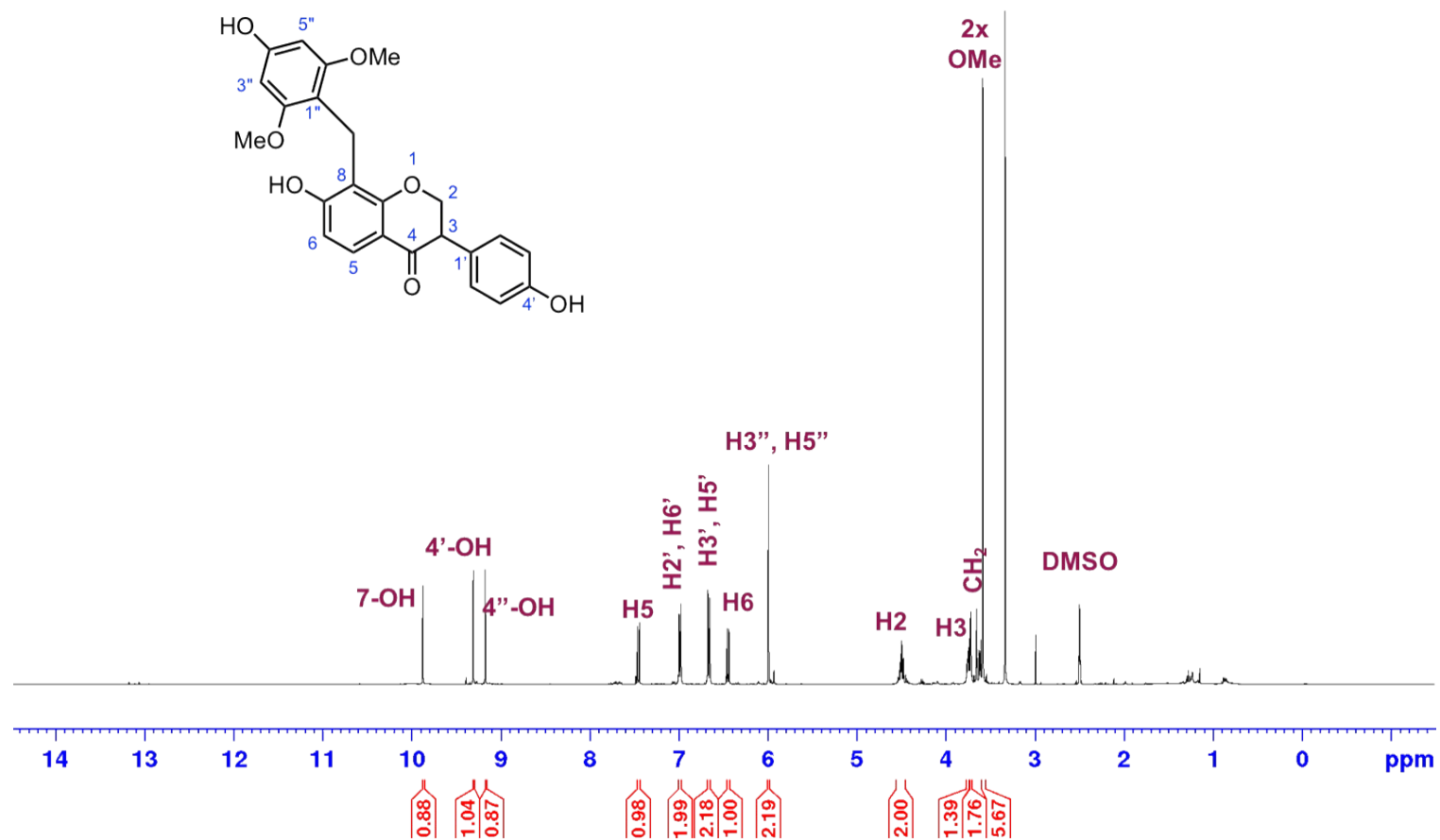


Figure S59. ^1H NMR (400 MHz, $\text{DMSO}-d_6$) spectrum of 7-Hydroxy-8-(4-hydroxy-2,6-dimethoxybenzyl)-3-(4-hydroxyphenyl)chroman-4-one (22a)

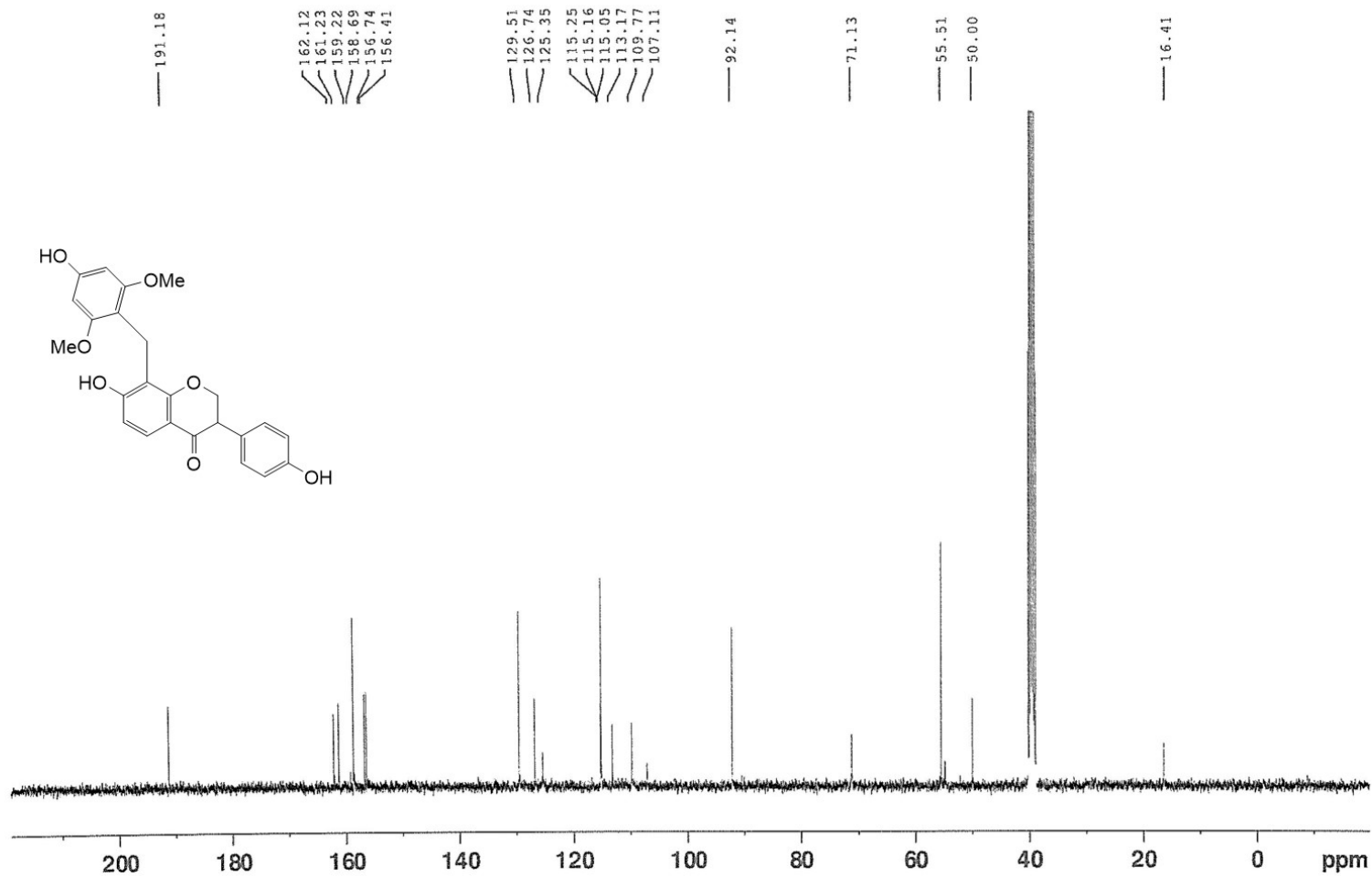


Figure S60. ¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of 7-Hydroxy-8-(4-hydroxy-2,6-dimethoxybenzyl)-3-(4-hydroxyphenyl)chroman-4-one (22a)

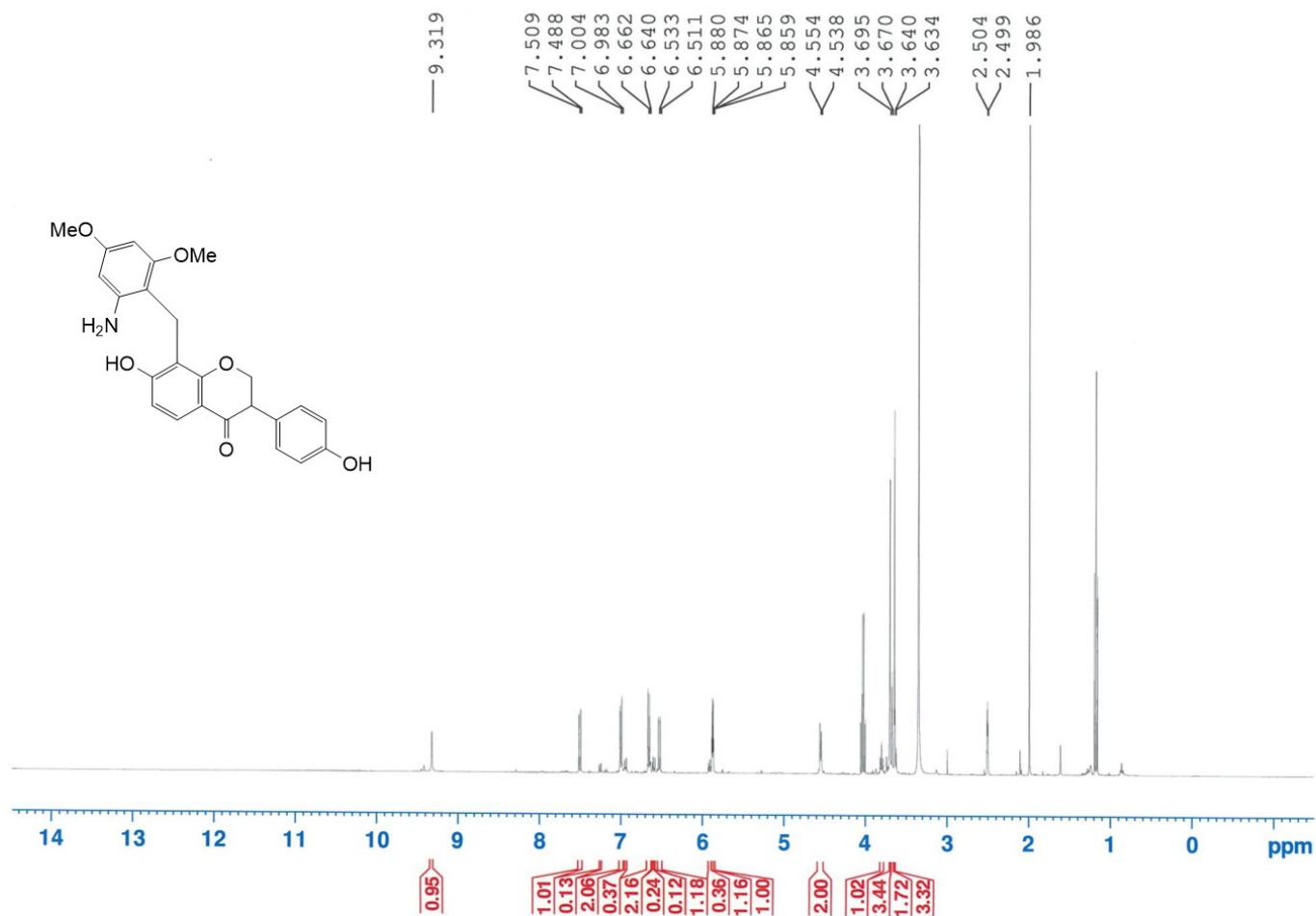


Figure S61. ¹H NMR (400 MHz, DMSO-*d*₆) spectrum of 8-(2-Amino-4,6-dimethoxybenzyl)-7-hydroxy-3-(4-hydroxyphenyl)chroman-4-one (22b)

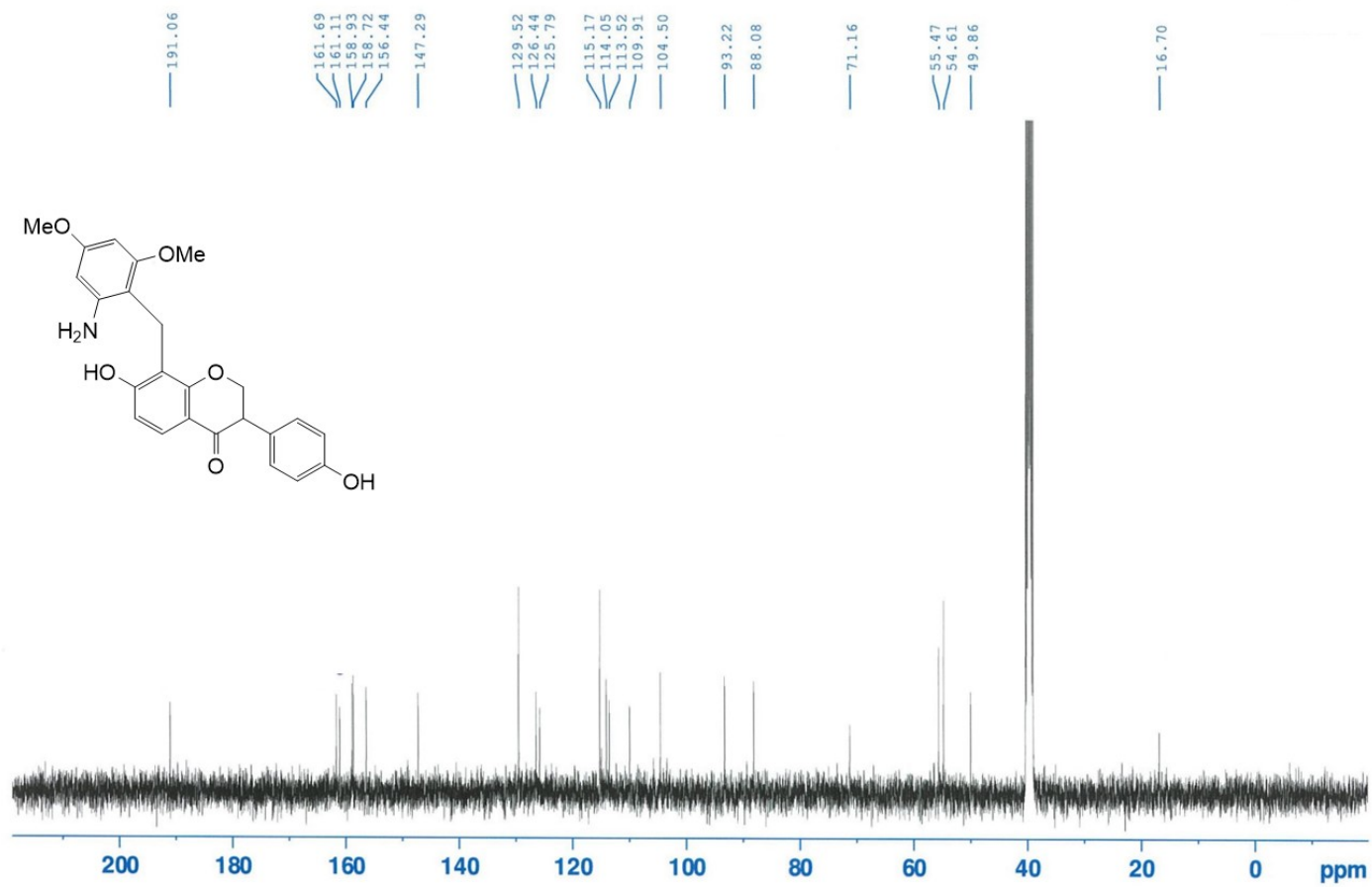


Figure S62. ¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of 8-(2-Amino-4,6-dimethoxybenzyl)-7-hydroxy-3-(4-hydroxyphenyl)chroman-4-one (**22b**)

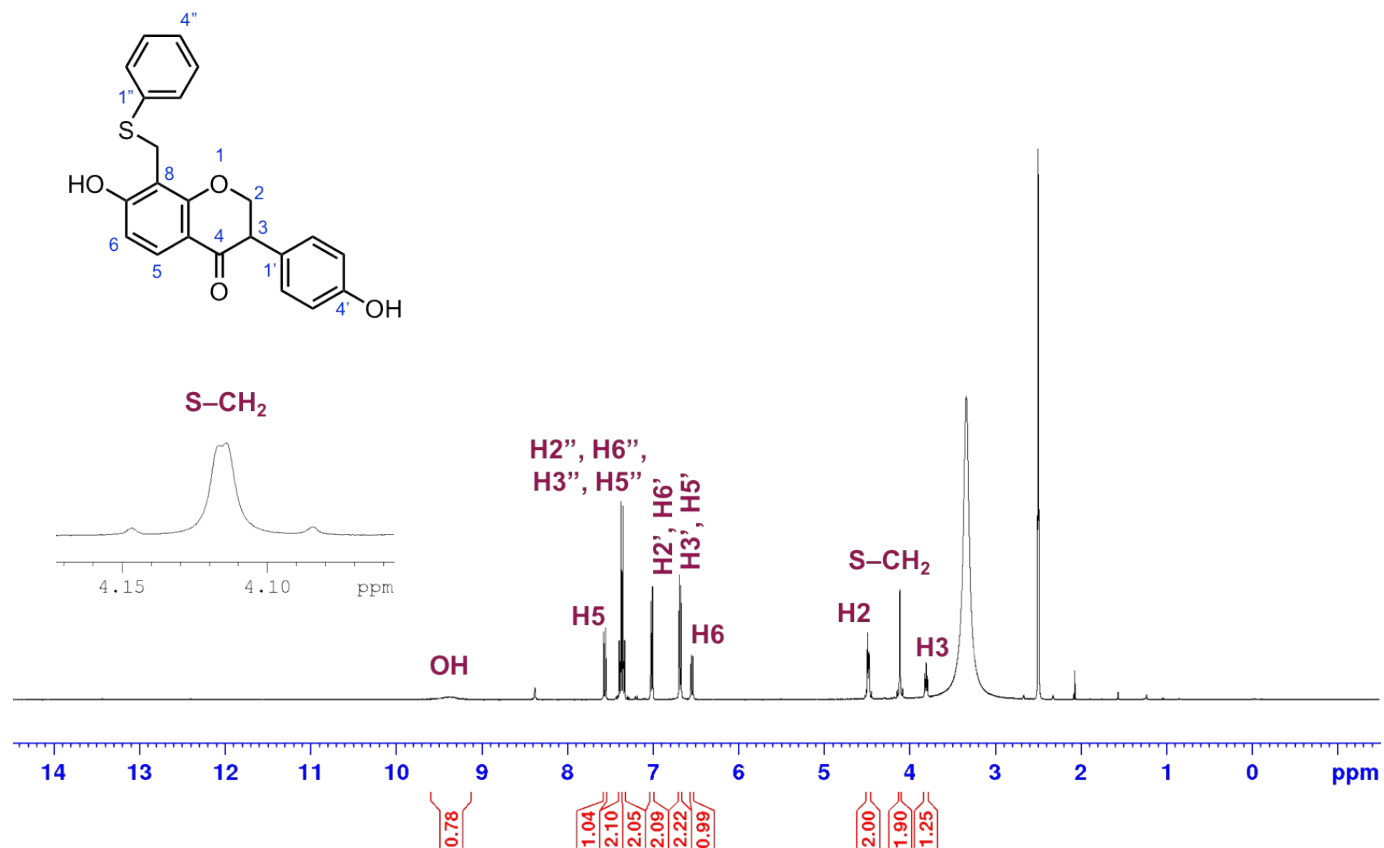


Figure S63. ¹H NMR (400 MHz, acetone-*d*₆) spectrum of 7-Hydroxy-3-(4-hydroxyphenyl)-8-((phenylthio)methyl)chroman-4-one (22c)

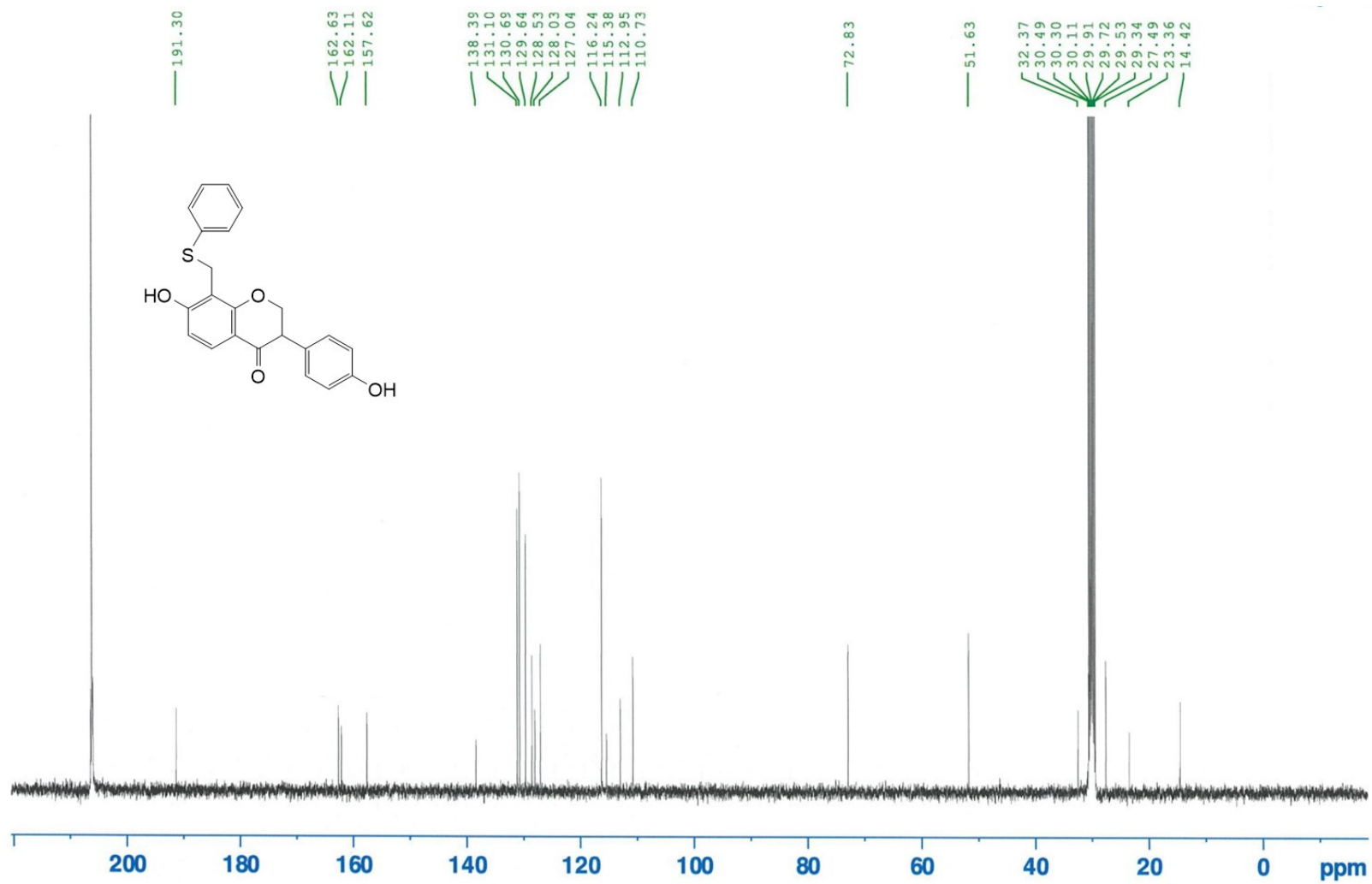


Figure S64. ¹³C NMR (100 MHz, acetone-*d*₆) spectrum of 7-Hydroxy-3-(4-hydroxyphenyl)-8-((phenylthio)methyl)chroman-4-one (22c)

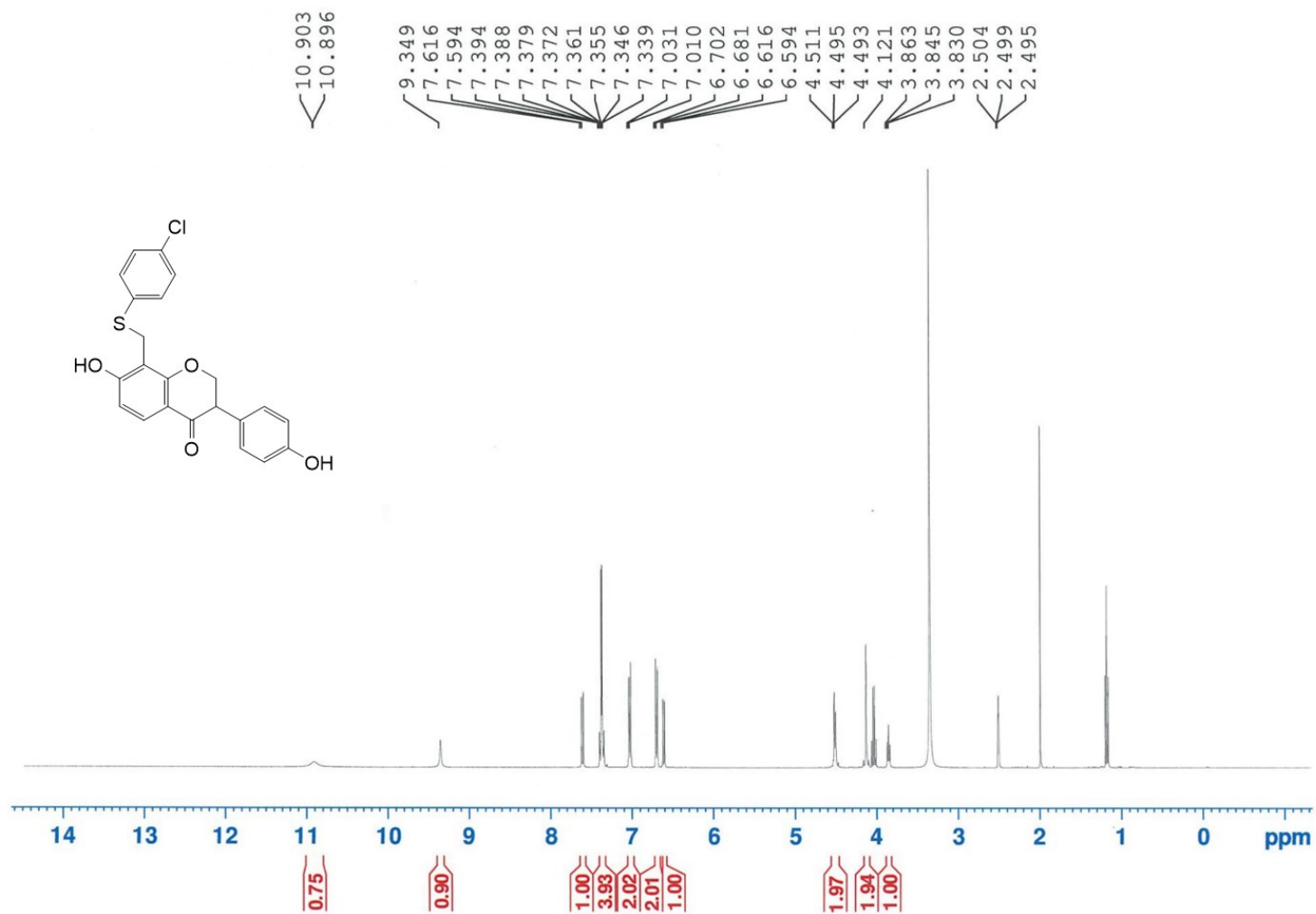


Figure S65. ¹H NMR (400 MHz, DMSO-*d*₆) spectrum of 8-(((4-Chlorophenyl)thio)methyl)-7-hydroxy-3-(4-hydroxyphenyl)chroman-4-one (22d)

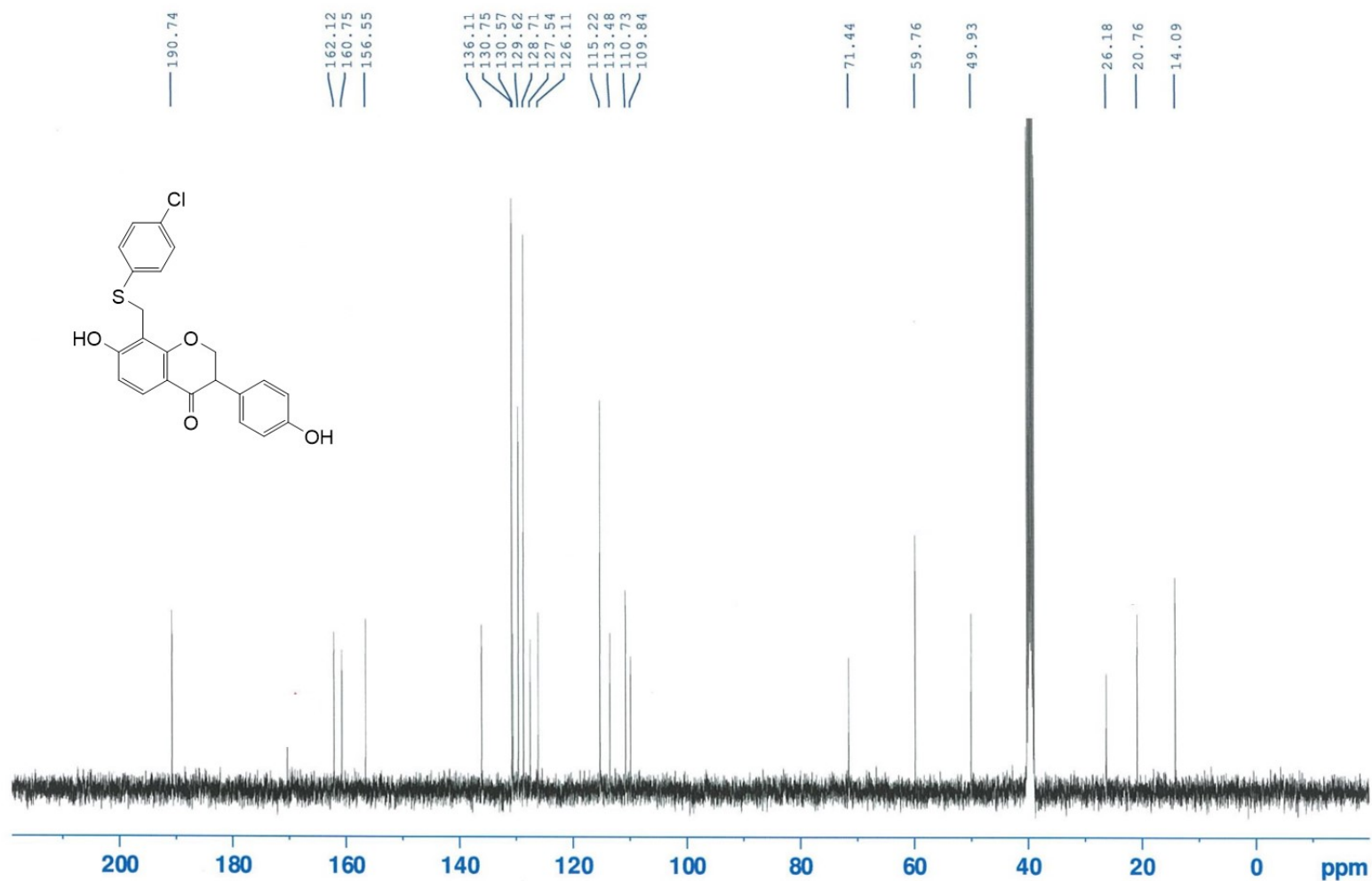


Figure S66. ¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of 8-(((4-chlorophenyl)thio)methyl)-7-hydroxy-3-(4-hydroxyphenyl)chroman-4-one (22d)