

Supplementary Materials

for

Design, Synthesis, In Vitro, and In Silico Insights of 5-(Substituted benzylidene)-2-phenylthiazol-4(5H)-one Derivatives: A Novel Class of Anti-Melanogenic Compounds

Dahye Yoon^{1,†}, Min Kyung Kang^{1,†}, Hee Jin Jung^{2,†}, Sultan Ullah³, Jieun Lee¹, Yeongmu Jeong¹, Sang Gyun Noh², Dongwan Kang⁴, Yujin Park⁴, Pusoon Chun⁵, Hae Young Chung² and Hyung Ryong Moon^{1,*}

¹ Department of Manufacturing Pharmacy, College of Pharmacy, Pusan National University, Busan 46241, Republic of Korea; dahae0528@pusan.ac.kr (D.Y.); kmk87106@pusan.ac.kr (M.K.K.); yijiun@pusan.ac.kr (J.L.); dassabn@pusan.ac.kr (Y.J.)

² Department of Pharmacy, College of Pharmacy, Pusan National University, Busan 46241, Republic of Korea; hjjung2046@pusan.ac.kr (H.J.J.); rskrsk92@pusan.ac.kr (S.G.N.); hyjung@pusan.ac.kr (H.Y.C.)

³ Department of Molecular Medicine, The Herbert Wertheim UF Scripps Institute for Biomedical Innovation & Technology, Jupiter, FL 33458, USA; sultanullahf@ufl.edu

⁴ Department of Medicinal Chemistry, New Drug Development Center, Daegu-Gyeongbuk Medical Innovation Foundation, Daegu 41061, Republic of Korea; kdw4106@kmedihub.re.kr (D.K.); pyj1016@kmedihub.re.kr (Y.P.)

⁵ College of Pharmacy and Inje Institute of Pharmaceutical Sciences and Research, Inje University, Gimhae 50834, Republic of Korea; pusoon@inje.ac.kr

* Correspondence: mhr108@pusan.ac.kr; Tel.: +82 51 510 2815; Fax: +82 51 513 6754

† These authors contributed equally to this work.

Contents

Figure S1. ^1H NMR spectrum of compound 1	4
Figure S2. ^{13}C NMR spectrum of compound 1	5
Figure S3. LRMS spectrum of compound 1	6
Figure S4. ^1H NMR spectrum of compound 2	7
Figure S5. ^{13}C NMR spectrum of compound 2	8
Figure S6. Proton-coupled ^{13}C NMR spectrum of compound 2	9
Figure S7. LRMS spectrum of compound 2	10
Figure S8. ^1H NMR spectrum of compound 3	11
Figure S9. ^{13}C NMR spectrum of compound 3	12
Figure S10. LRMS spectrum of compound 3	13
Figure S11. ^1H NMR spectrum of compound 4	14
Figure S12. ^{13}C NMR spectrum of compound 4	15
Figure S13. LRMS spectrum of compound 4	16
Figure S14. ^1H NMR spectrum of compound 5	17
Figure S15. ^{13}C NMR spectrum of compound 5	18
Figure S16. LRMS spectrum of compound 5	19
Figure S17. ^1H NMR spectrum of compound 6	20
Figure S18. ^{13}C NMR spectrum of compound 6	21
Figure S19. LRMS spectrum of compound 6	22
Figure S20. ^1H NMR spectrum of compound 7	23
Figure S21. ^{13}C NMR spectrum of compound 7	24
Figure S22. LRMS spectrum of compound 7	25
Figure S23. ^1H NMR spectrum of compound 8 (in $\text{DMSO}-d_6$).....	26

Figure S24. ^{13}C NMR spectrum of compound 8 (in $\text{DMSO}-d_6$).....	27
Figure S25. LRMS spectrum of compound 8	28
Figure S26. ^1H NMR spectrum of compound 9	29
Figure S27. ^{13}C NMR spectrum of compound 9	30
Figure S28. LRMS spectrum of compound 9	31
Figure S29. ^1H NMR spectrum of compound 10	32
Figure S30. ^{13}C NMR spectrum of compound 10	33
Figure S31. LRMS spectrum of compound 10	34
Figure S32. ^1H NMR spectrum of compound 11	35
Figure S33. ^{13}C NMR spectrum of compound 11	36
Figure S34. LRMS spectrum of compound 11	37
Figure S35. ^1H NMR spectrum of compound 12	38
Figure S36. ^{13}C NMR spectrum of compound 12	39
Figure S37. LRMS spectrum of compound 12	40
Figure S38. ^1H NMR spectrum of compound 13	41
Figure S39. ^{13}C NMR spectrum of compound 13	42
Figure S40. LRMS spectrum of compound 13	43
Figure S41. ^1H NMR spectrum of compound 14	44
Figure S42. ^{13}C NMR spectrum of compound 14	45
Figure S43. LRMS spectrum of compound 14	46
Figure S44. ^1H NMR spectrum of compound 8 (in CDCl_3) reported in other article.....	47
Figure S45. ^{13}C NMR spectrum of compound 8 (in CDCl_3) reported in other article	48
Figure S46. ^1H NMR spectrum of compound 8 in CDCl_3	49
Figure S47. ^{13}C NMR spectrum of compound 8 in CDCl_3	50

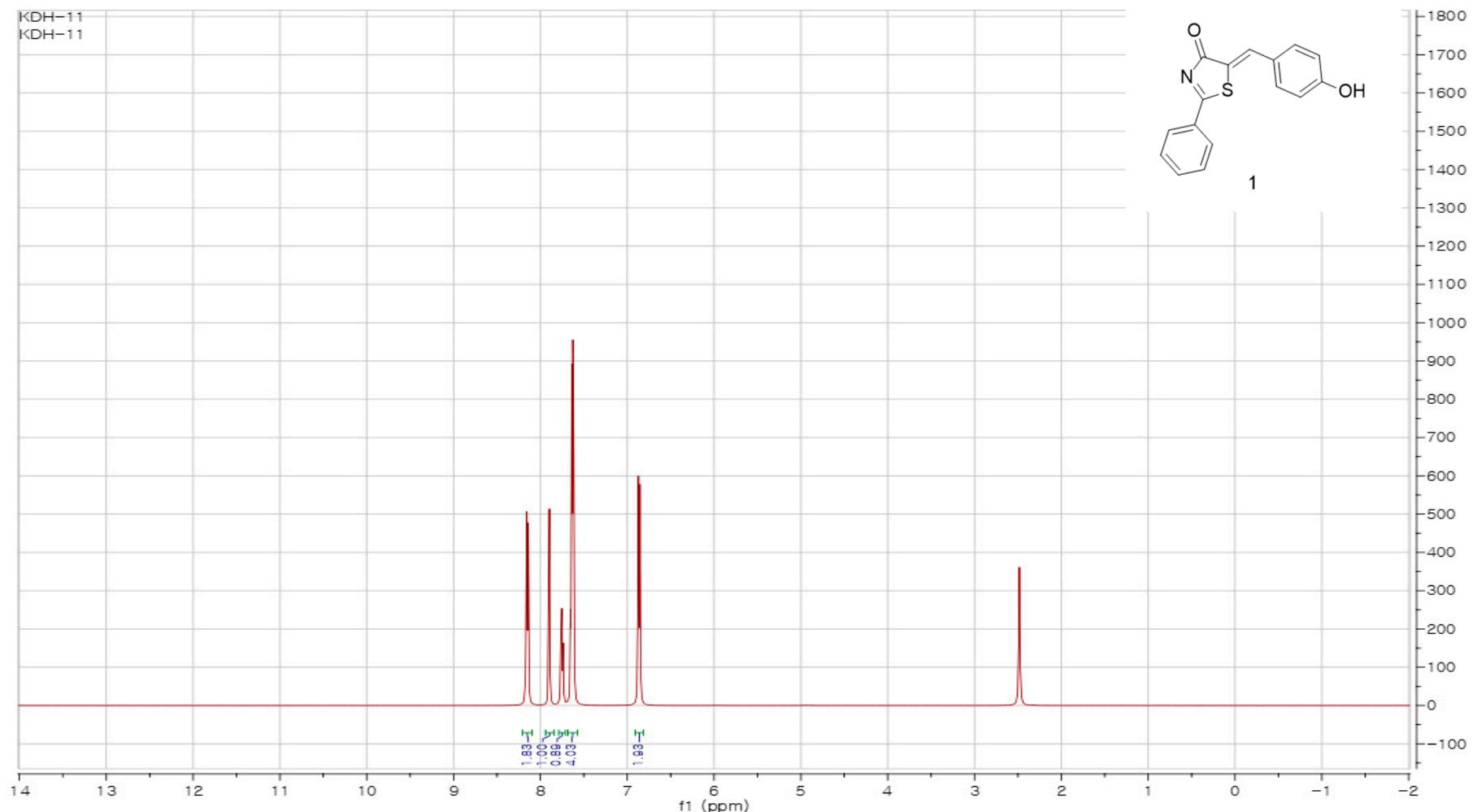
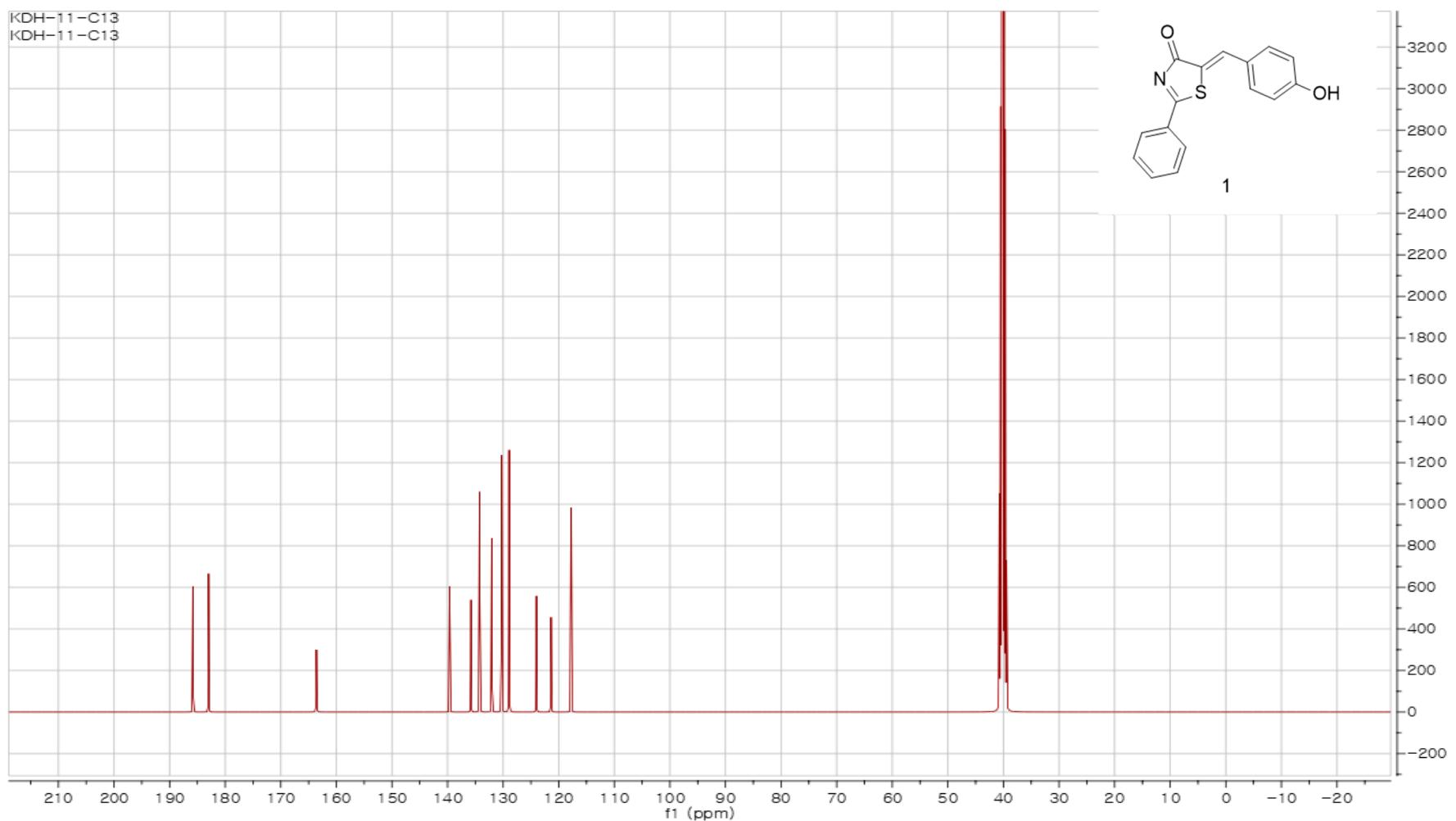


Figure S1. ^1H NMR spectrum of compound 1.



Intensity
Spectrum RT 2.05 (1 scans)- Background Subtracted 0.68 - 1.22
KDH-11.dat; 2015.11.02 13:05:42;
ESI - Max: 6.3E7

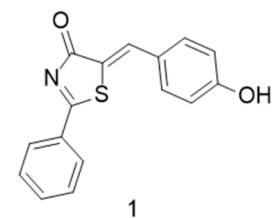
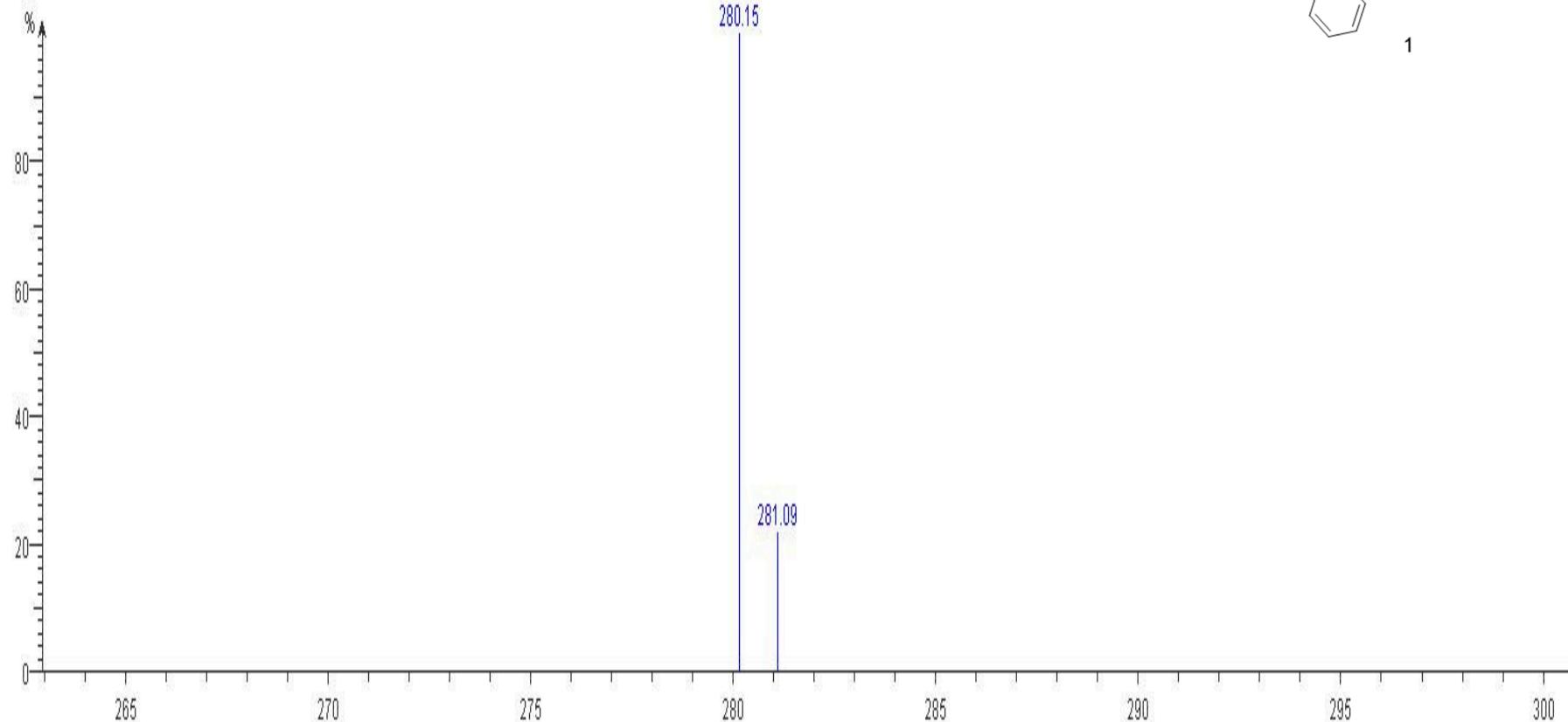


Figure S3. LRMS spectrum of compound **1**.

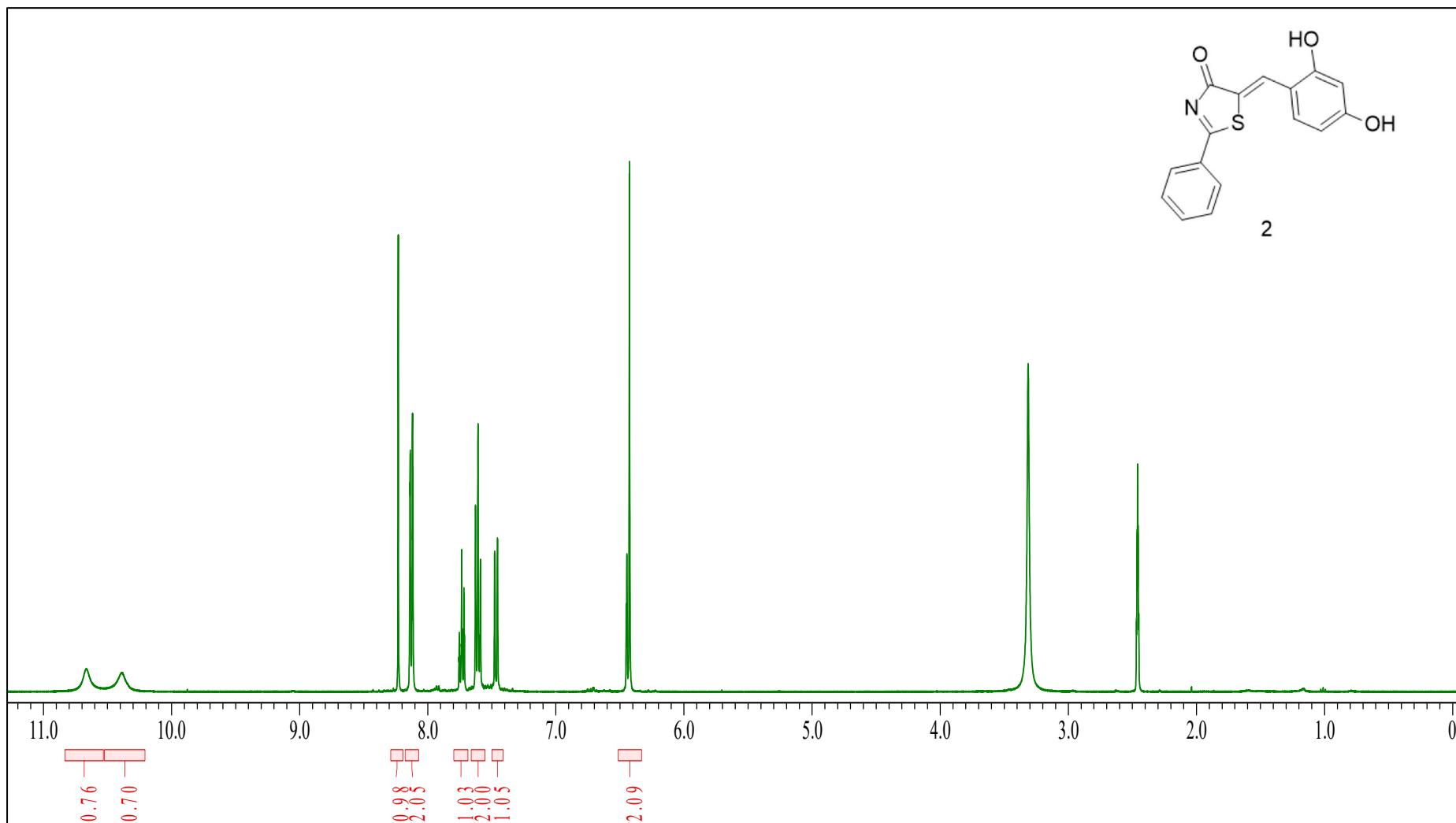


Figure S4. ^1H NMR spectrum of compound 2.

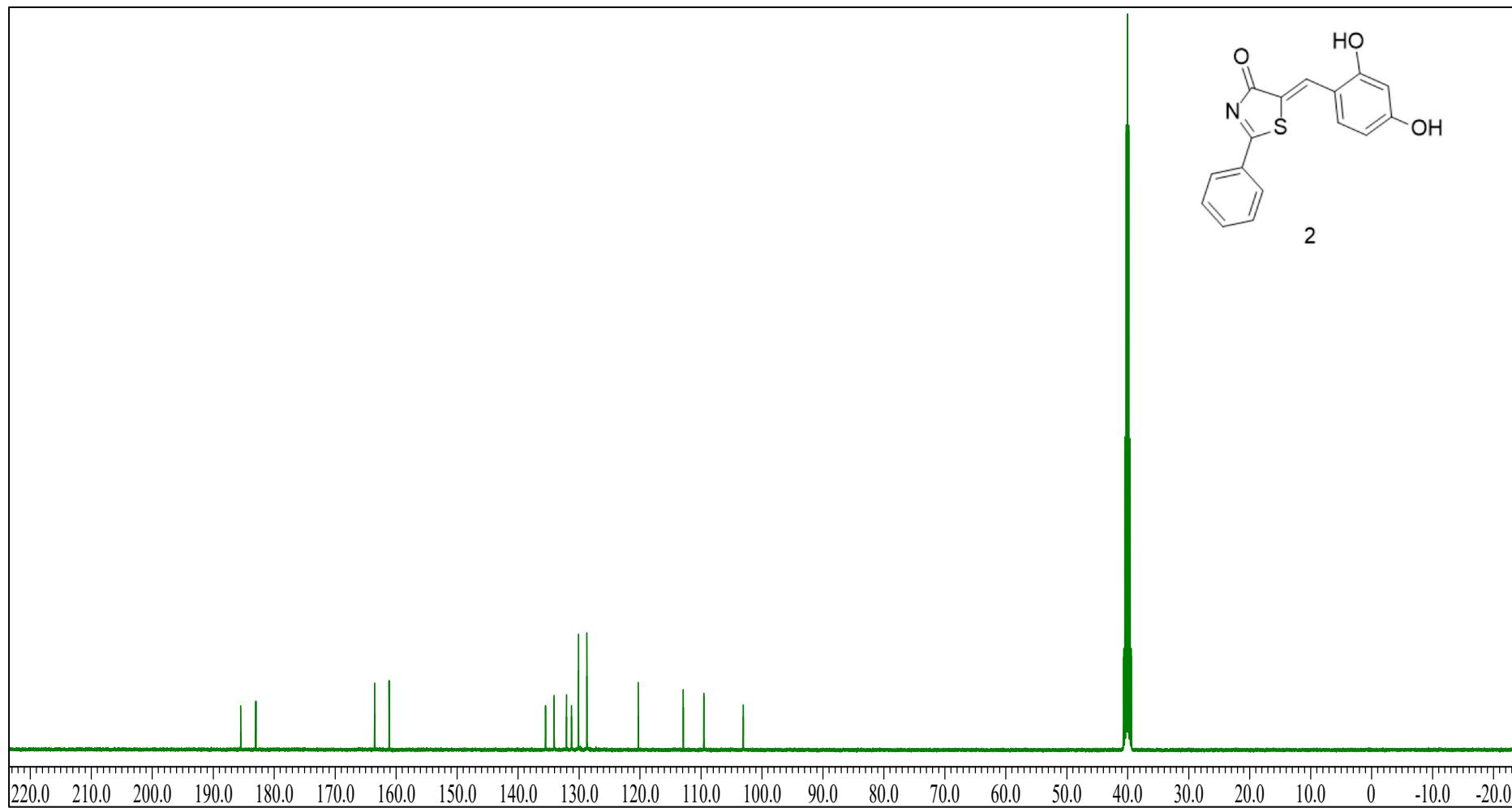


Figure S5. ^{13}C NMR spectrum of compound 2.

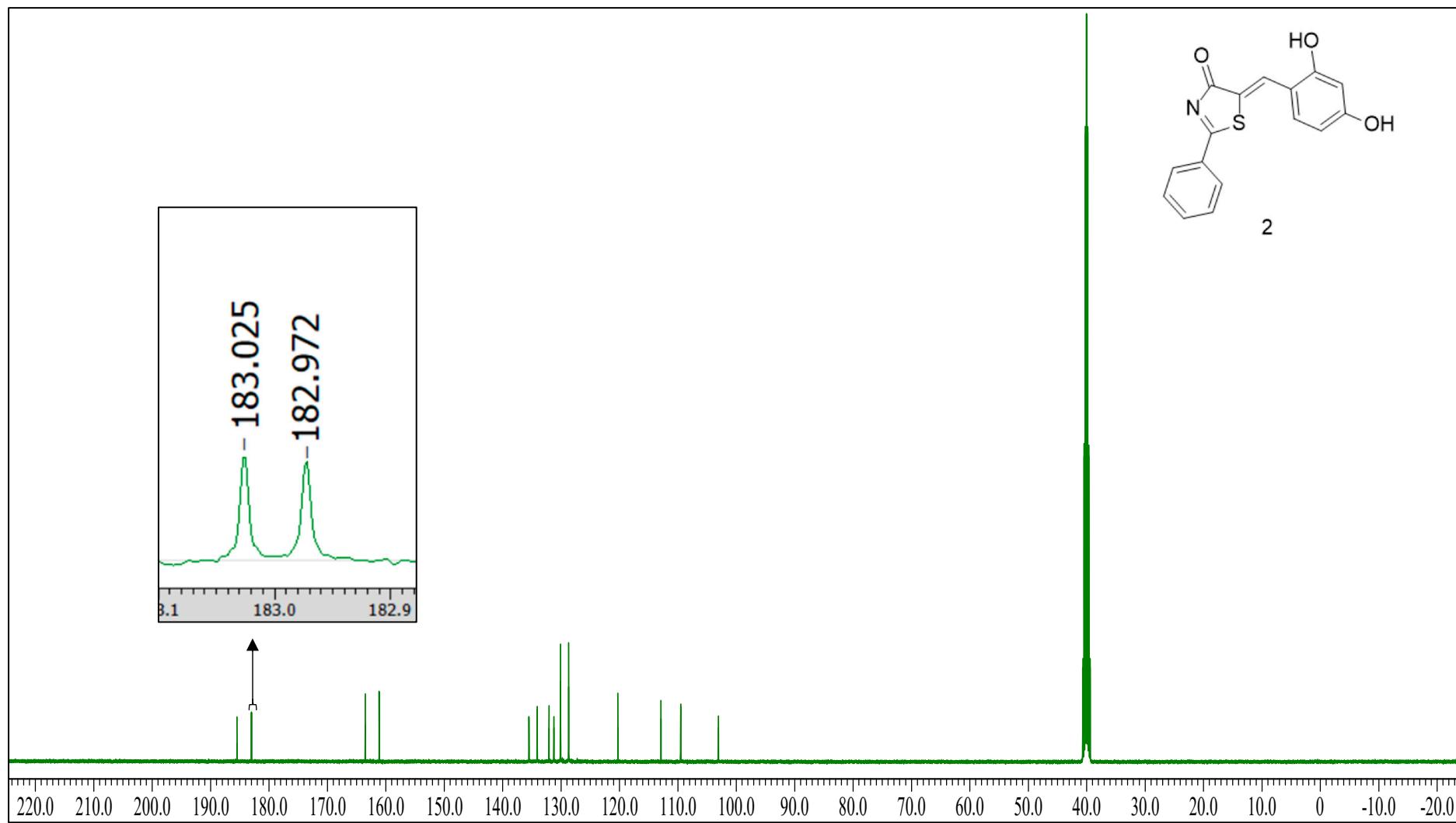


Figure S6. Proton-coupled ^{13}C NMR spectrum of compound 2.

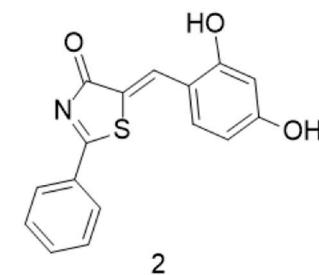
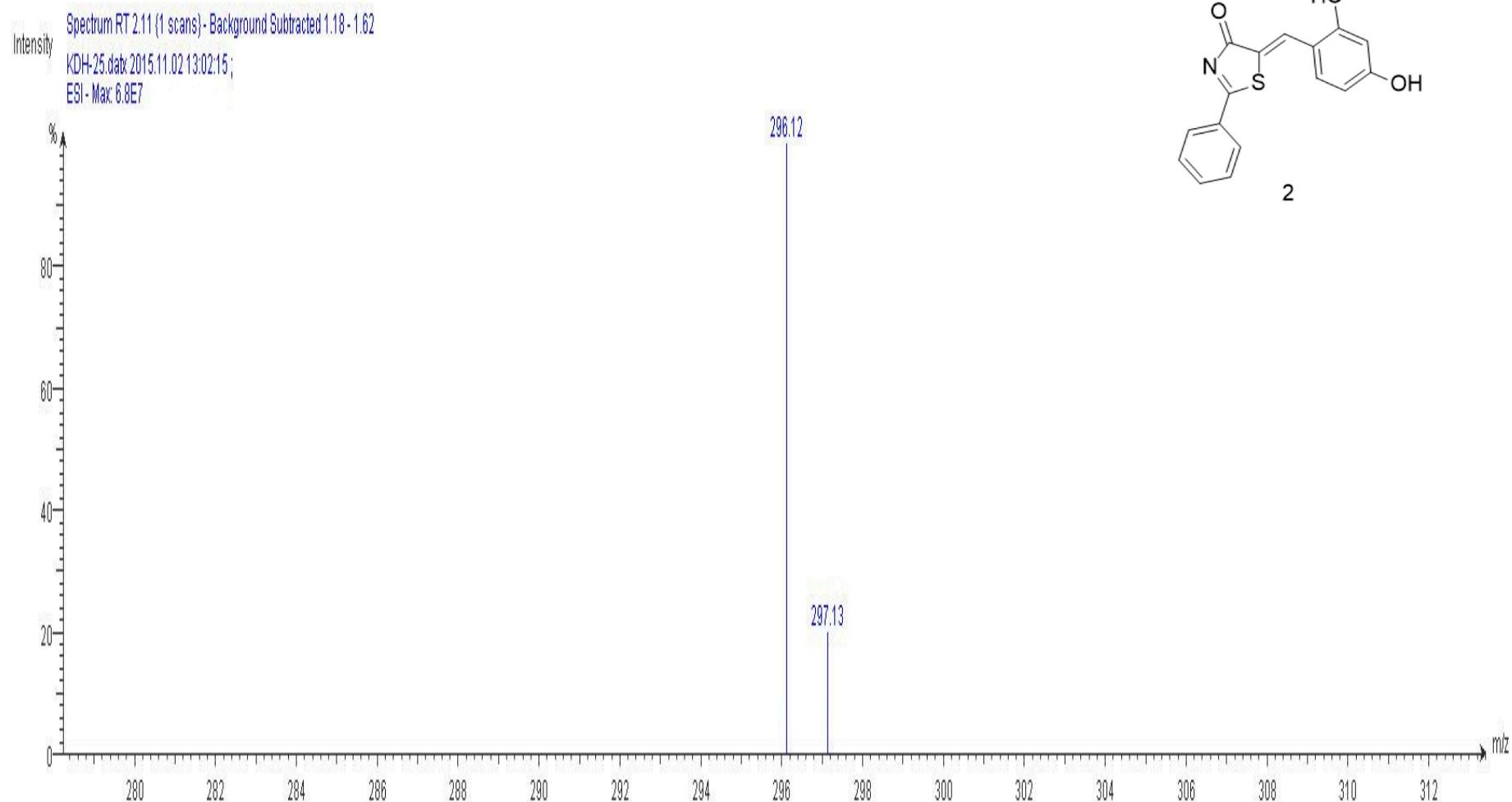


Figure S7. LRMS spectrum of compound 2.

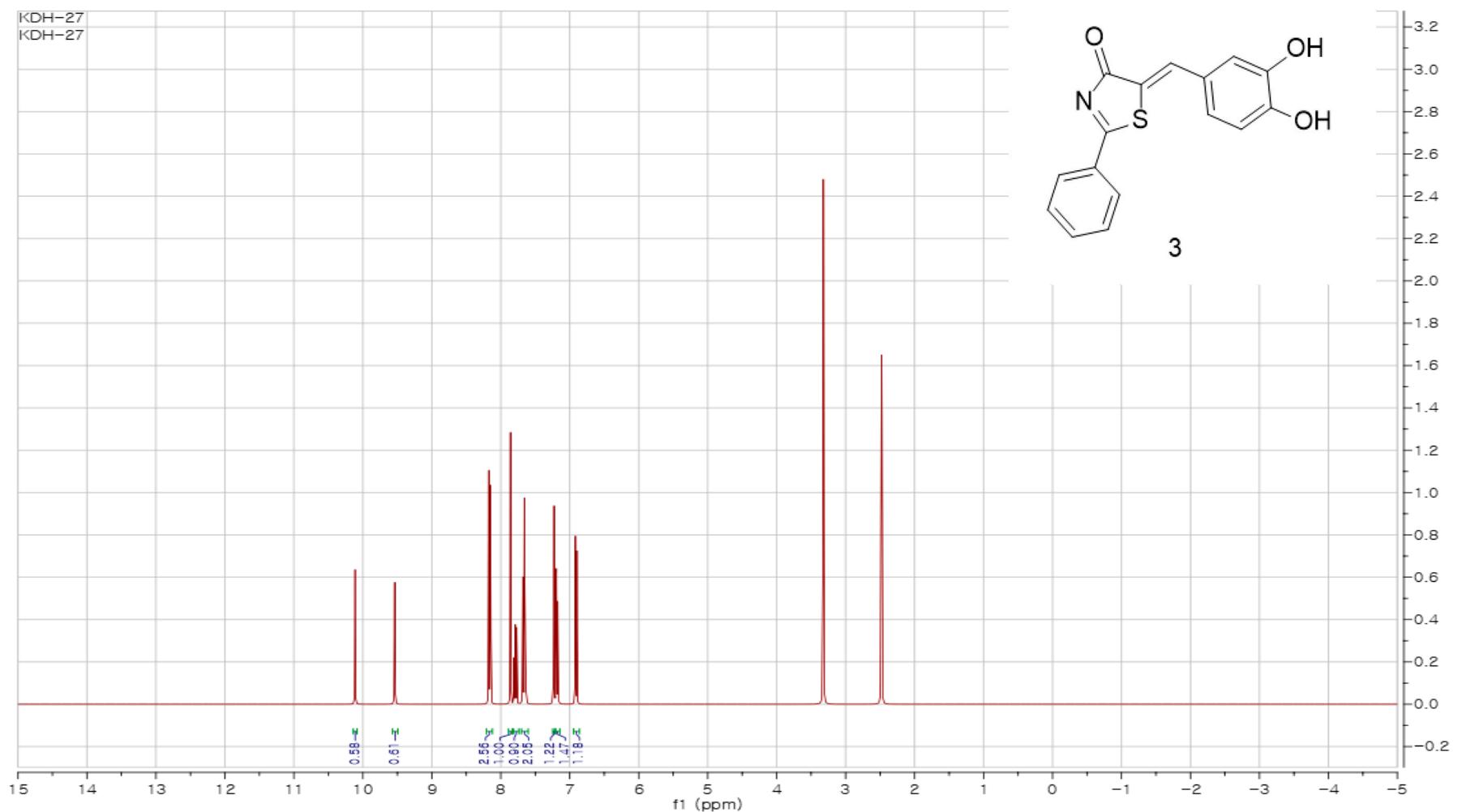


Figure S8. ^1H NMR spectrum of compound 3.

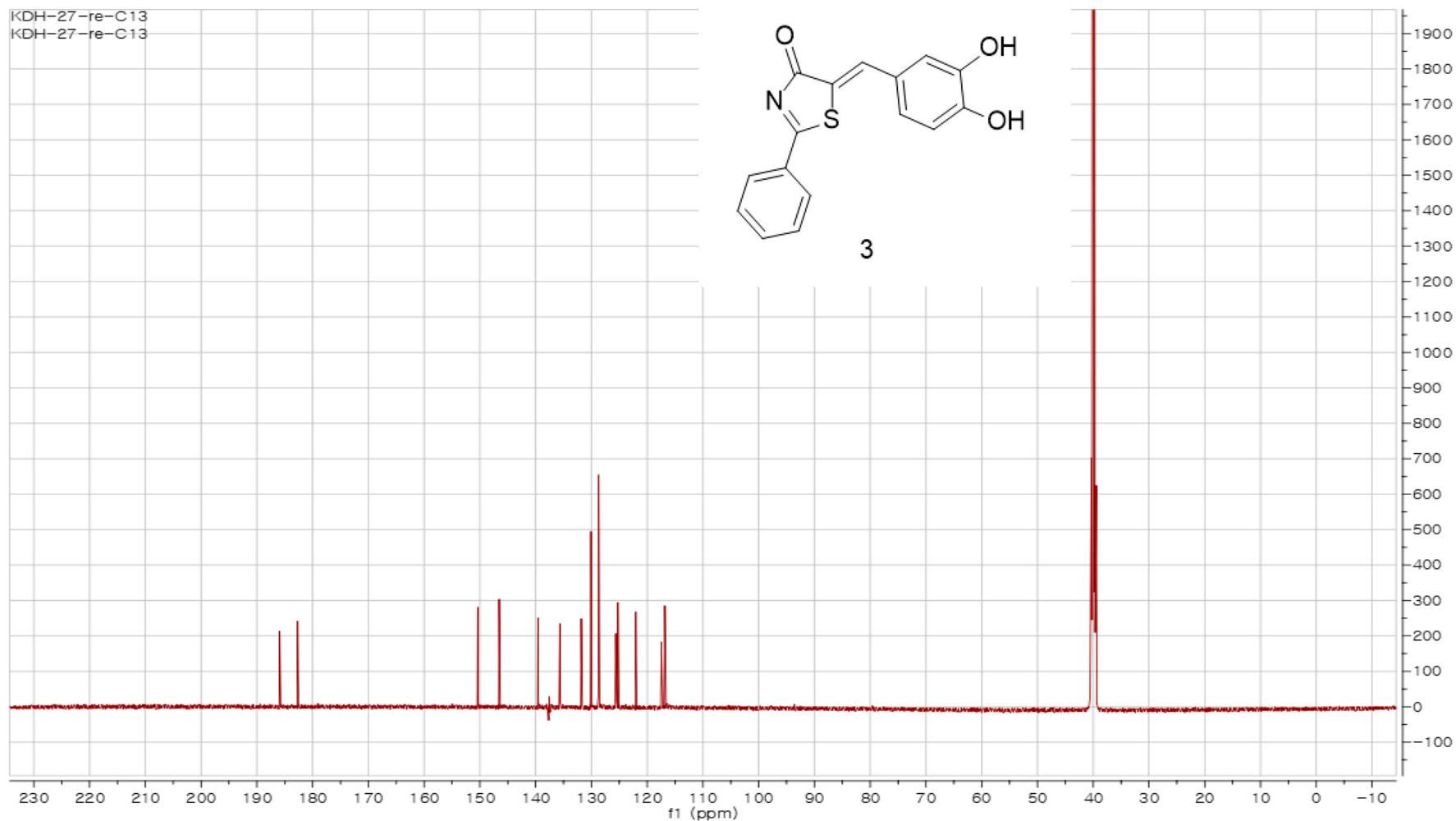


Figure S9. ¹³C NMR spectrum of compound 3.

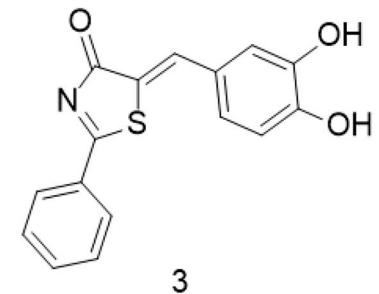
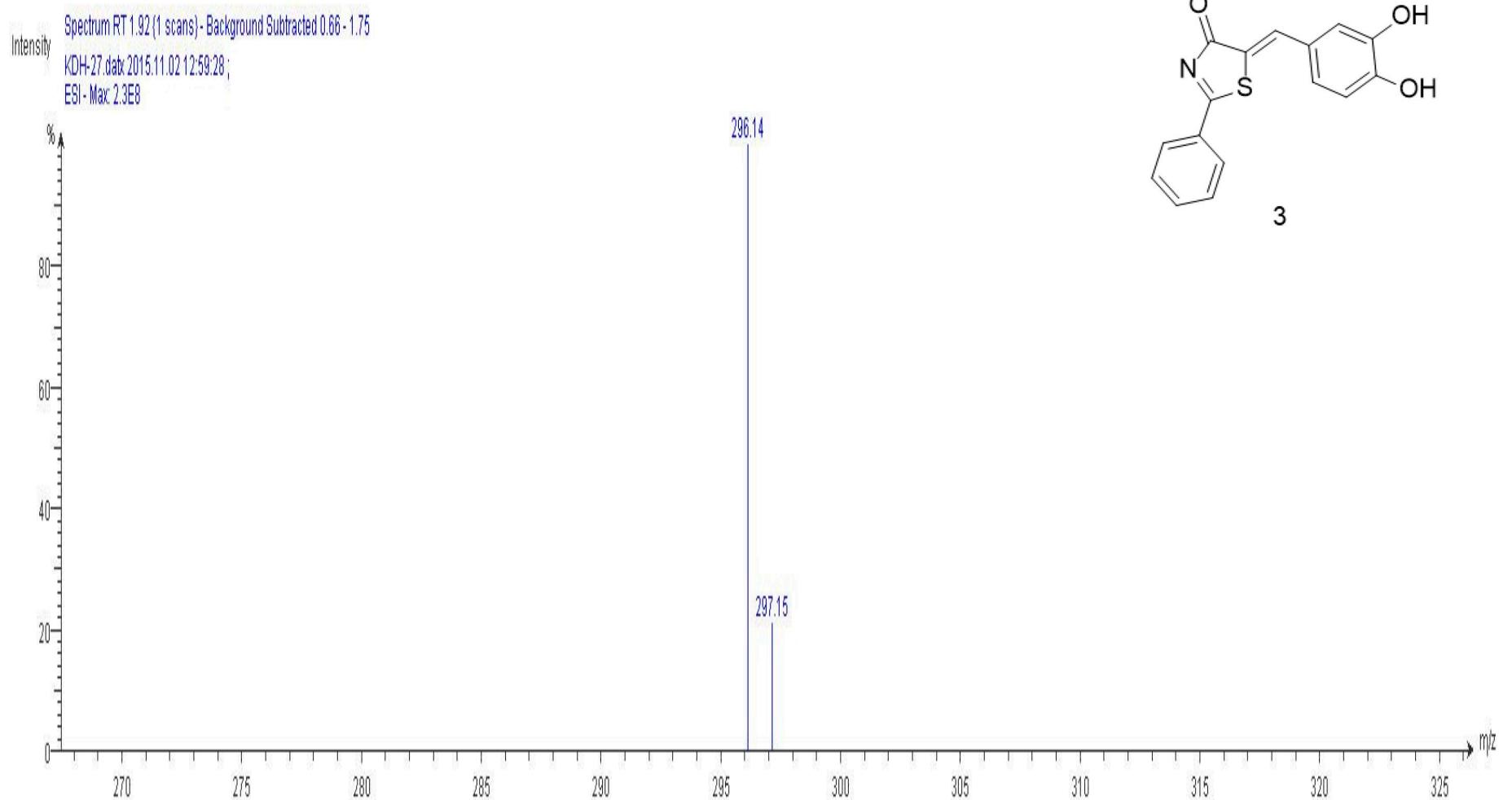


Figure S10. LRMS spectrum of compound 3.

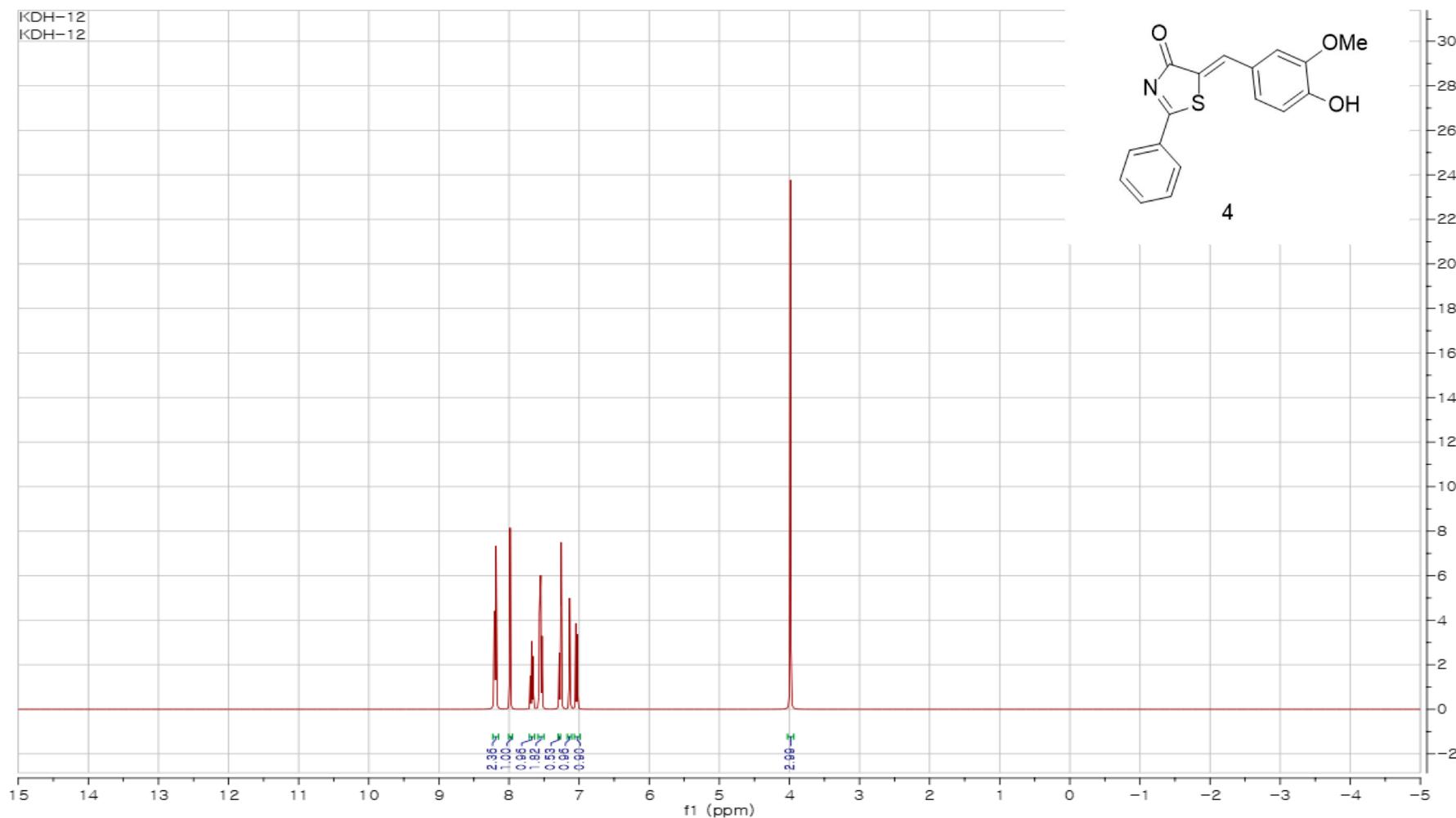


Figure S11. ^1H NMR spectrum of compound 4.

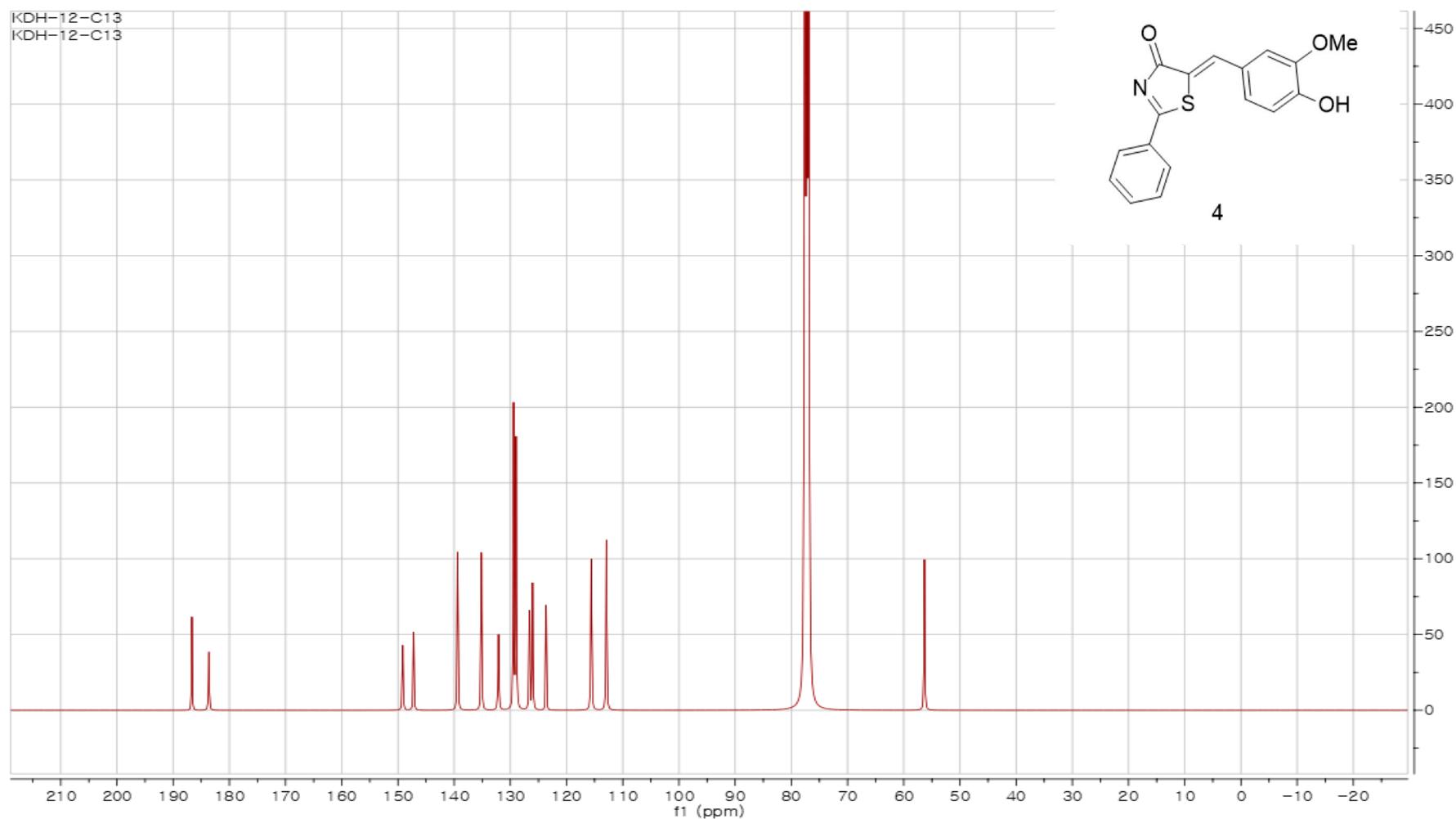


Figure S12. ¹³C NMR spectrum of compound 4.

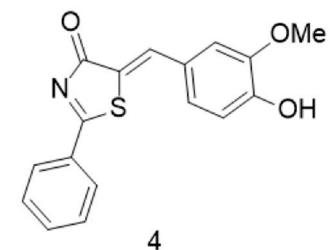
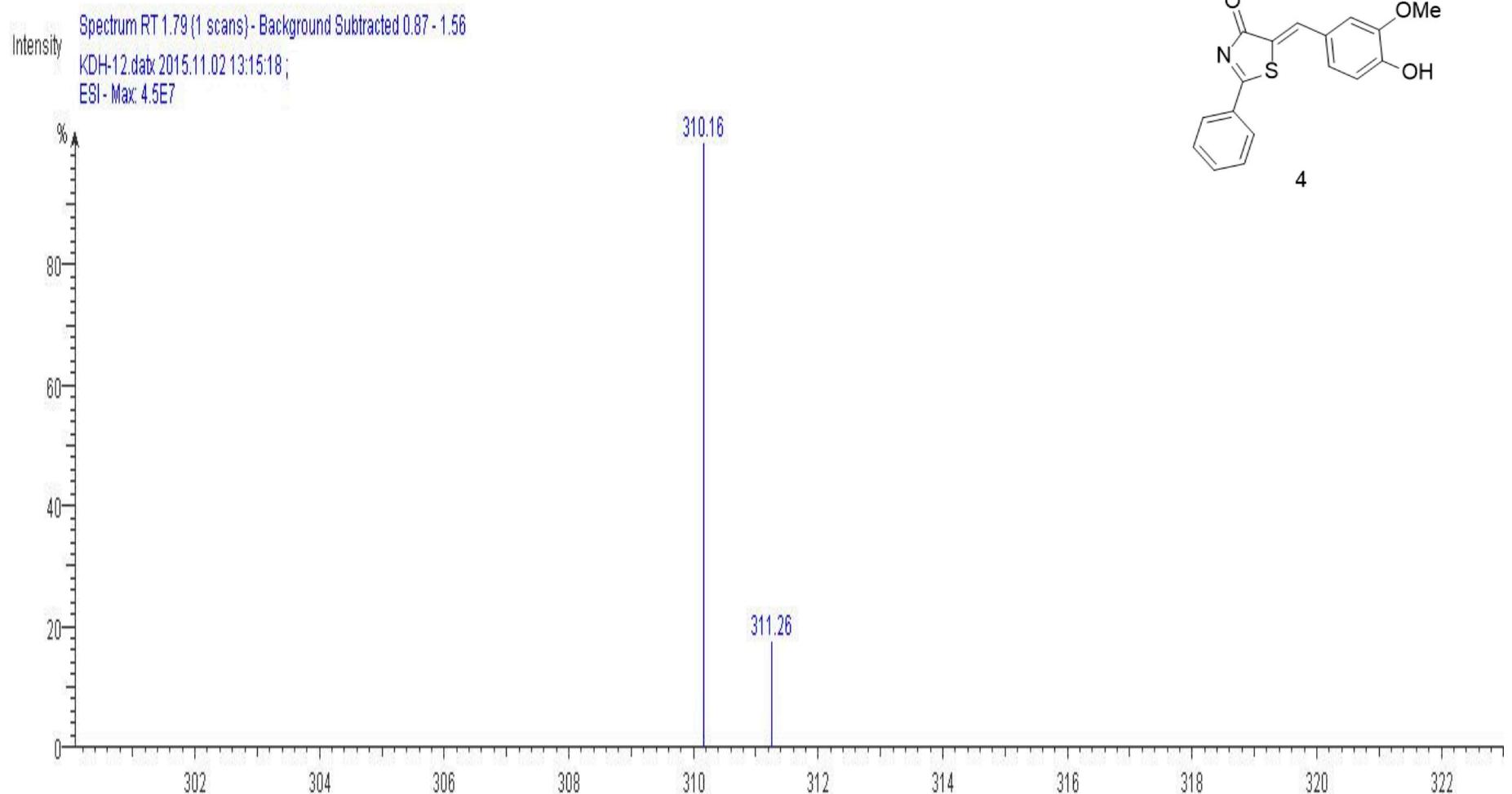


Figure S13. LRMS spectrum of compound 4.

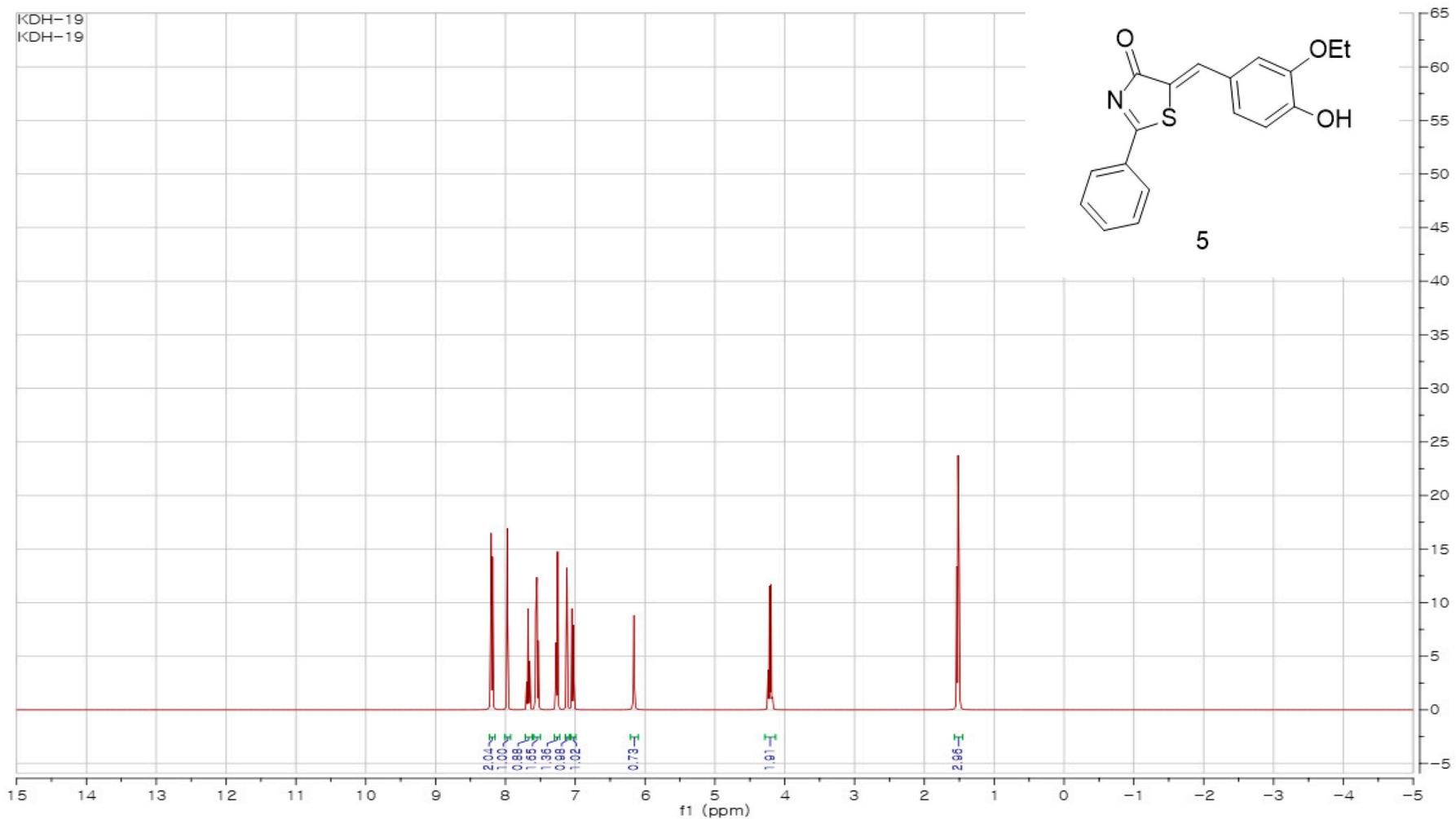


Figure S14. ^1H NMR spectrum of compound 5.

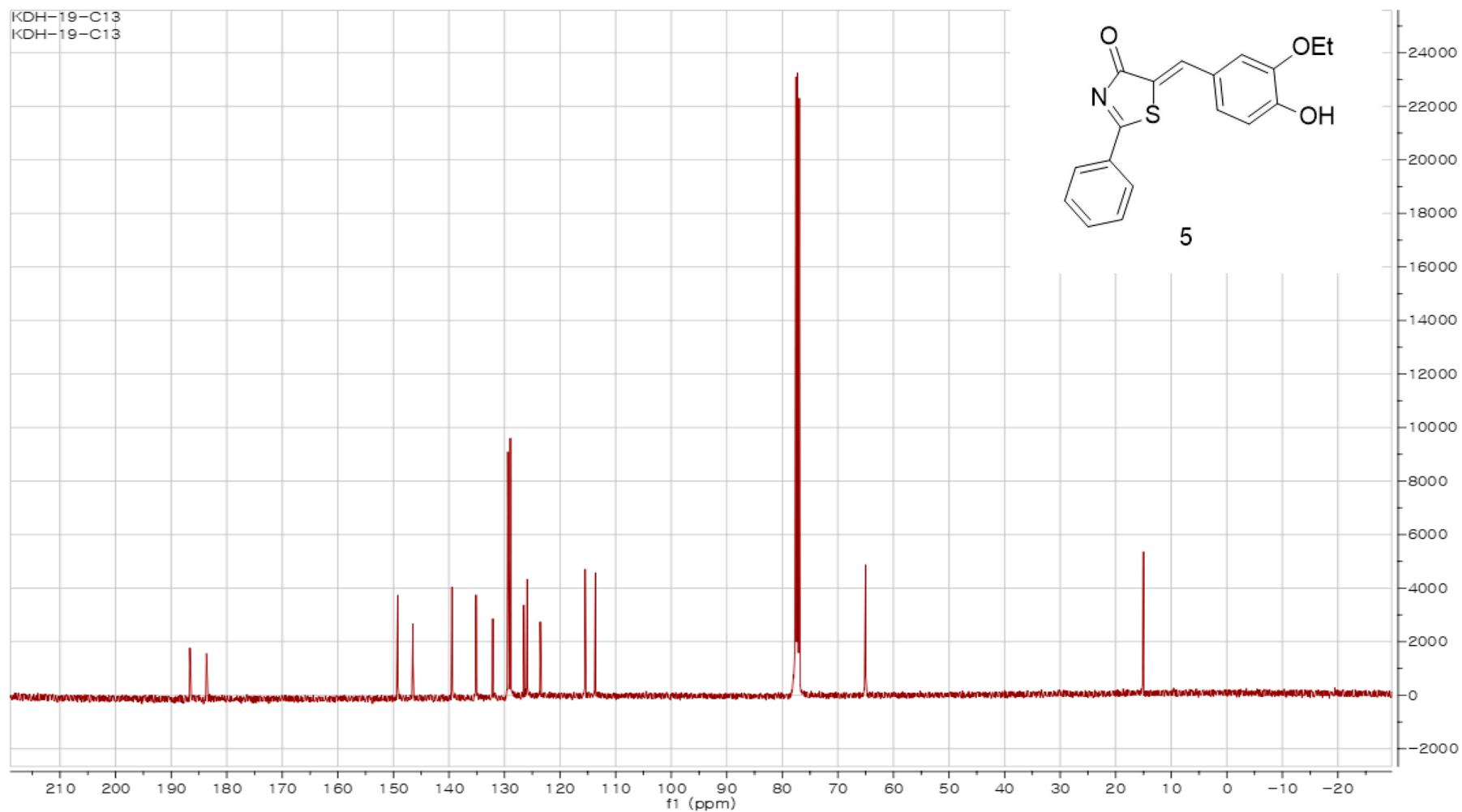


Figure S15. ¹³C NMR spectrum of compound 5.

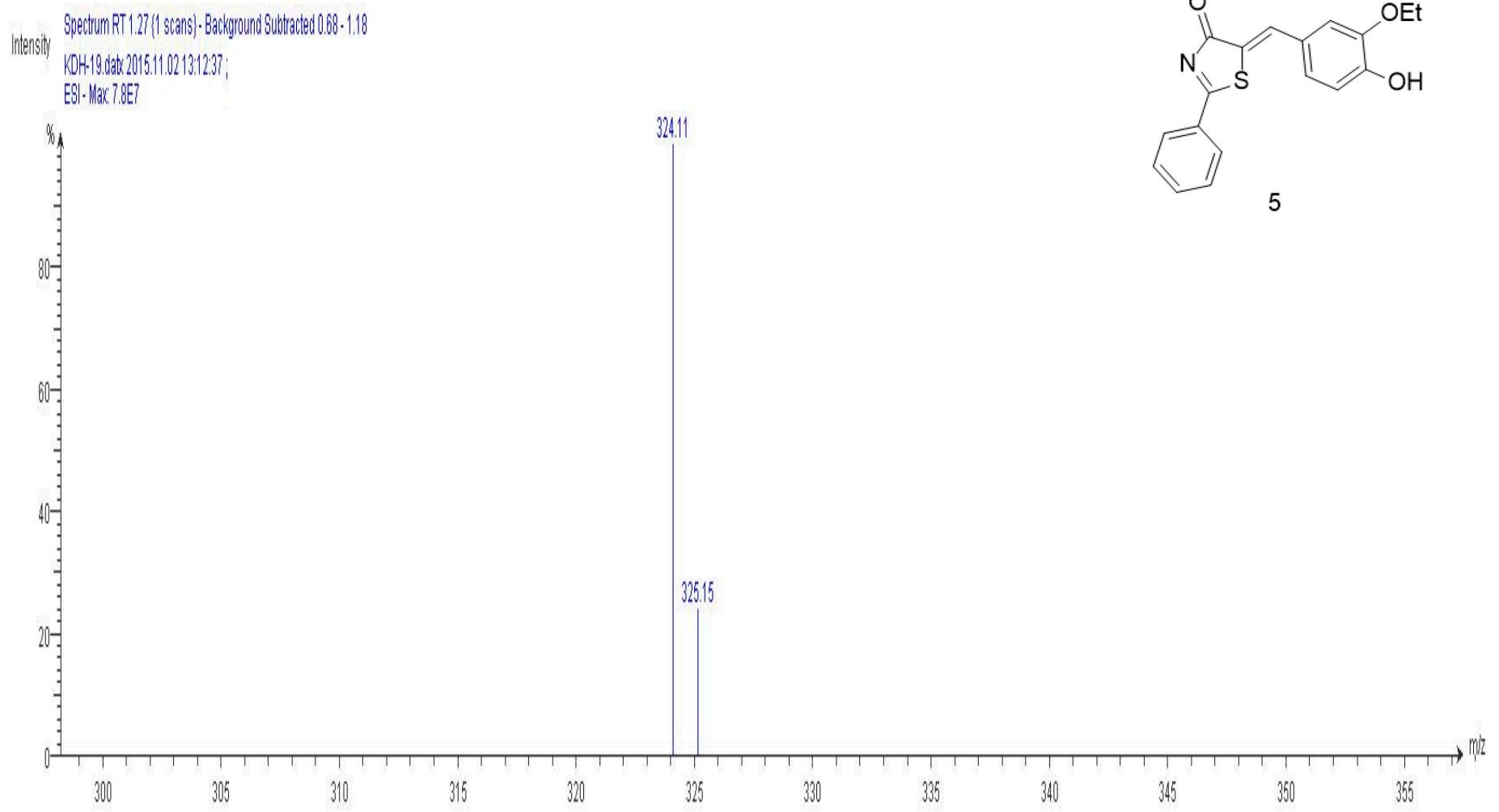


Figure S16. LRMS spectrum of compound 5.

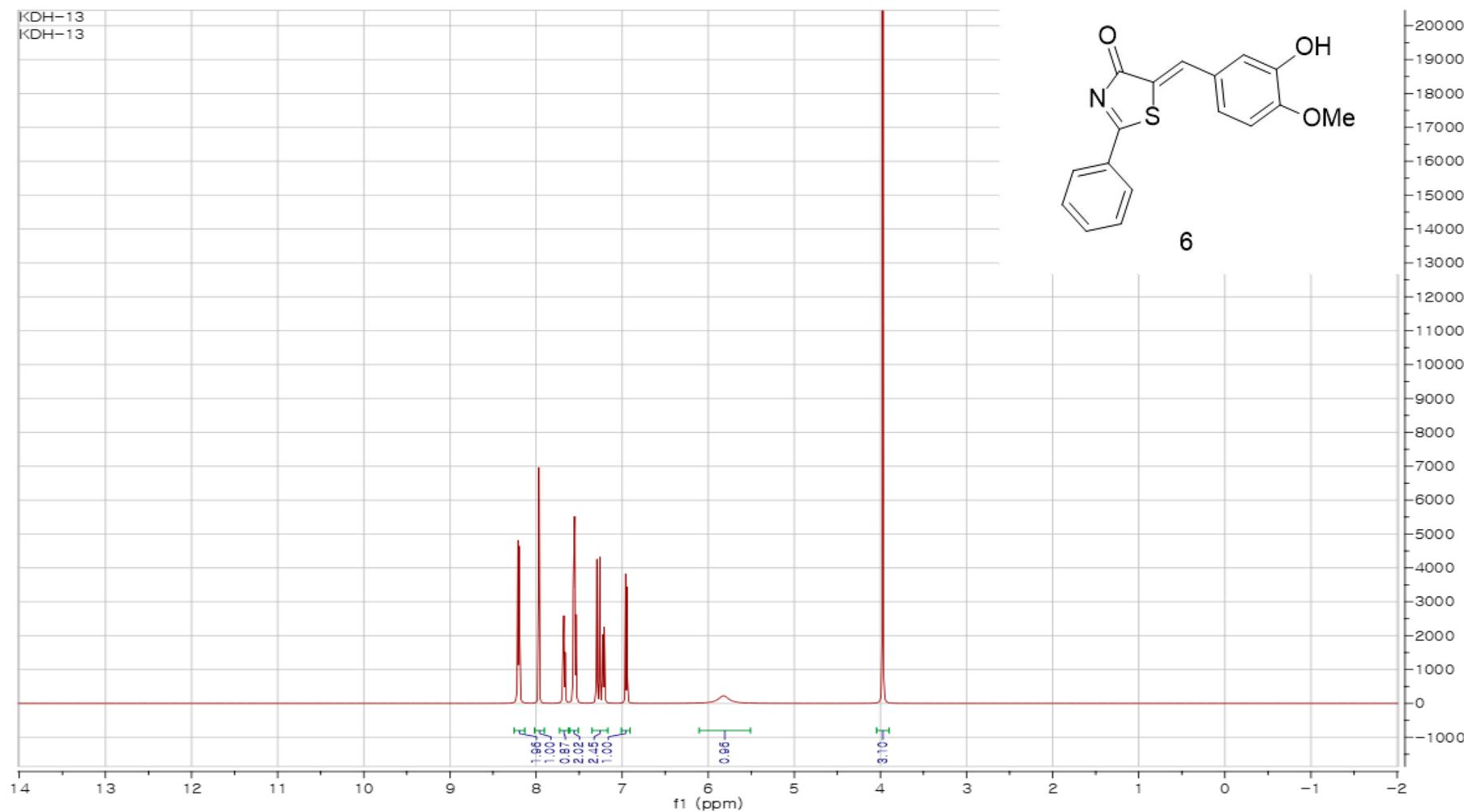


Figure S17. ^1H NMR spectrum of compound 6.

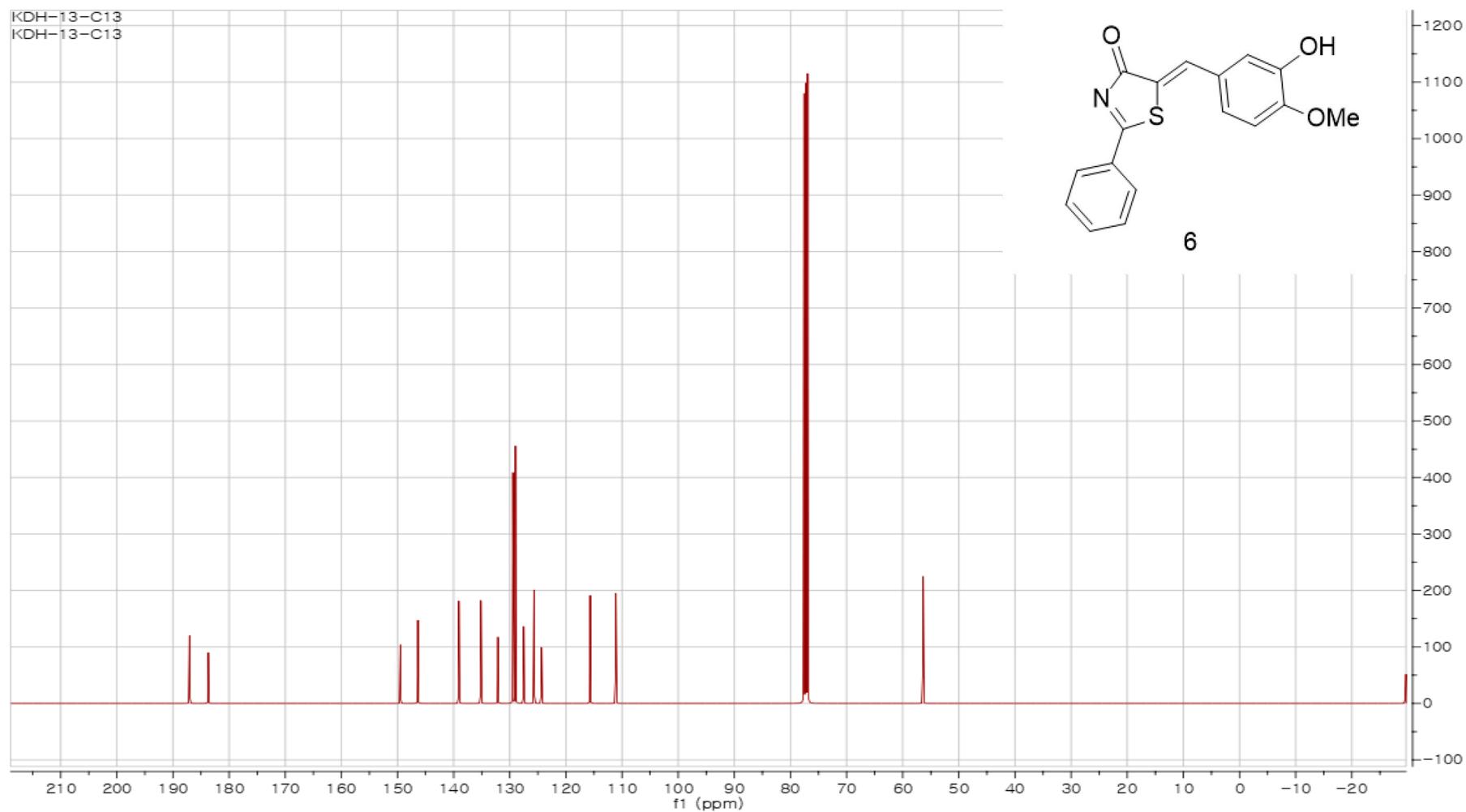


Figure S18. ¹³C NMR spectrum of compound 6.

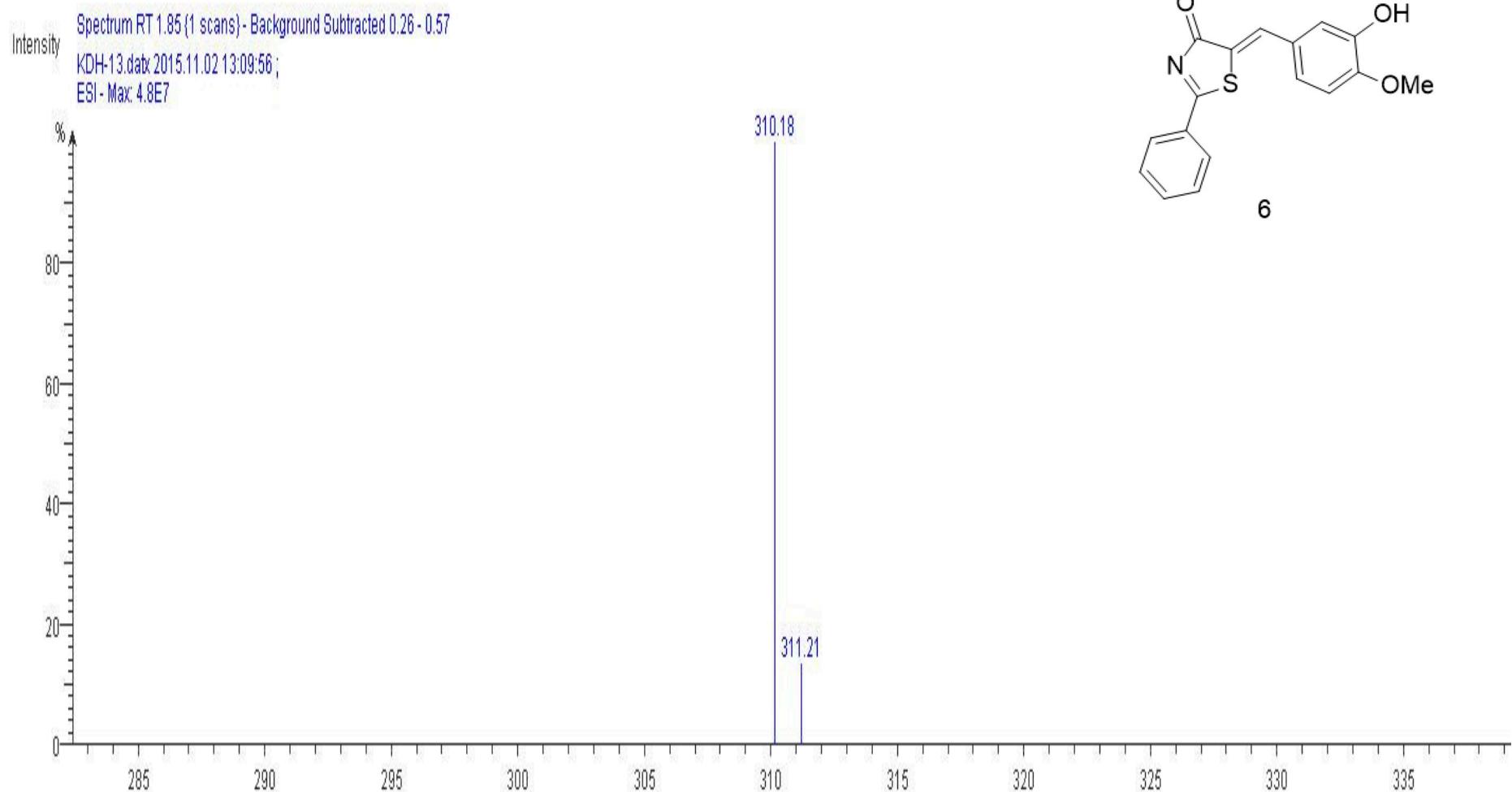


Figure S19. LRMS spectrum of compound 6.

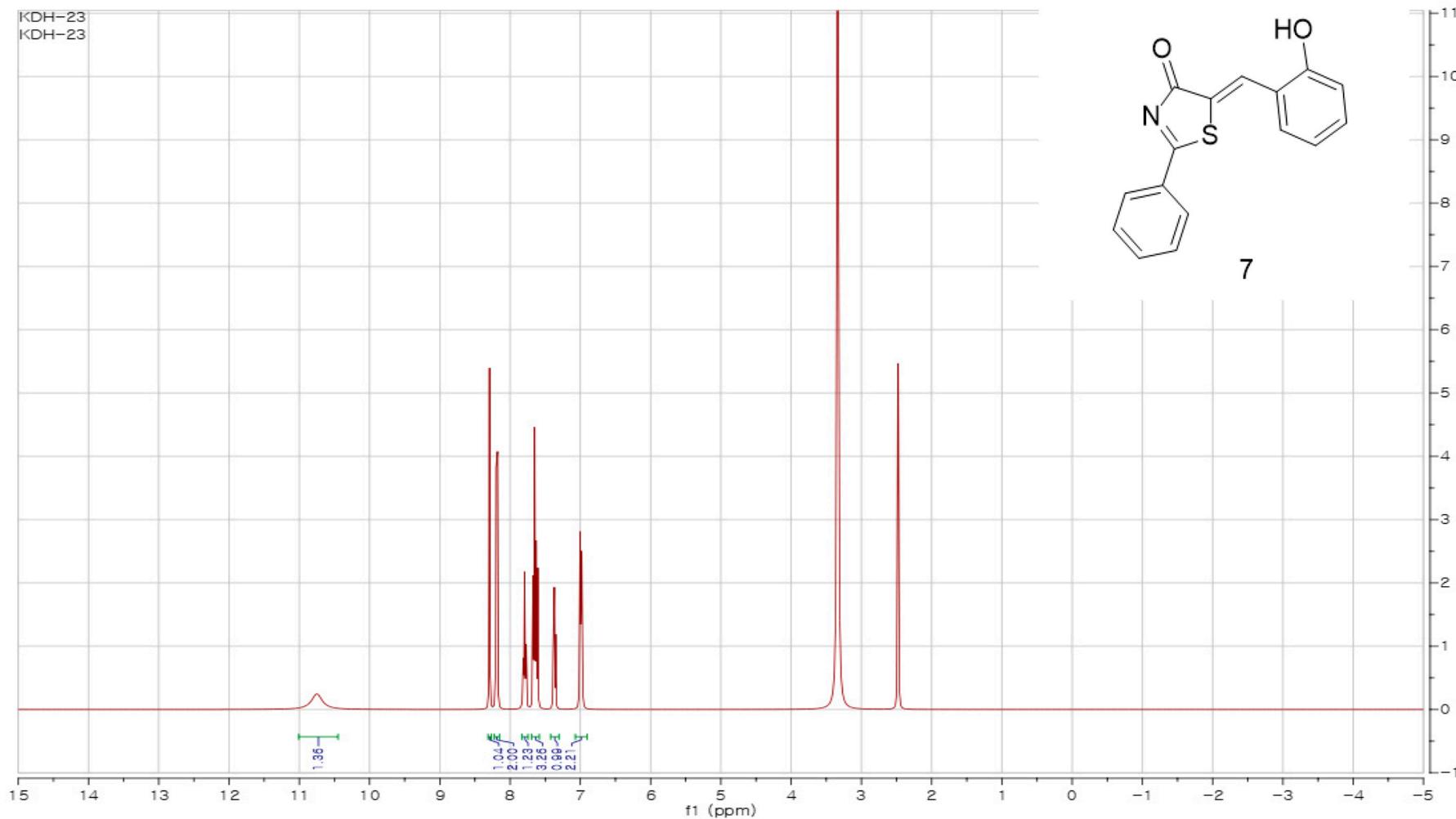


Figure S20. ^1H NMR spectrum of compound 7.

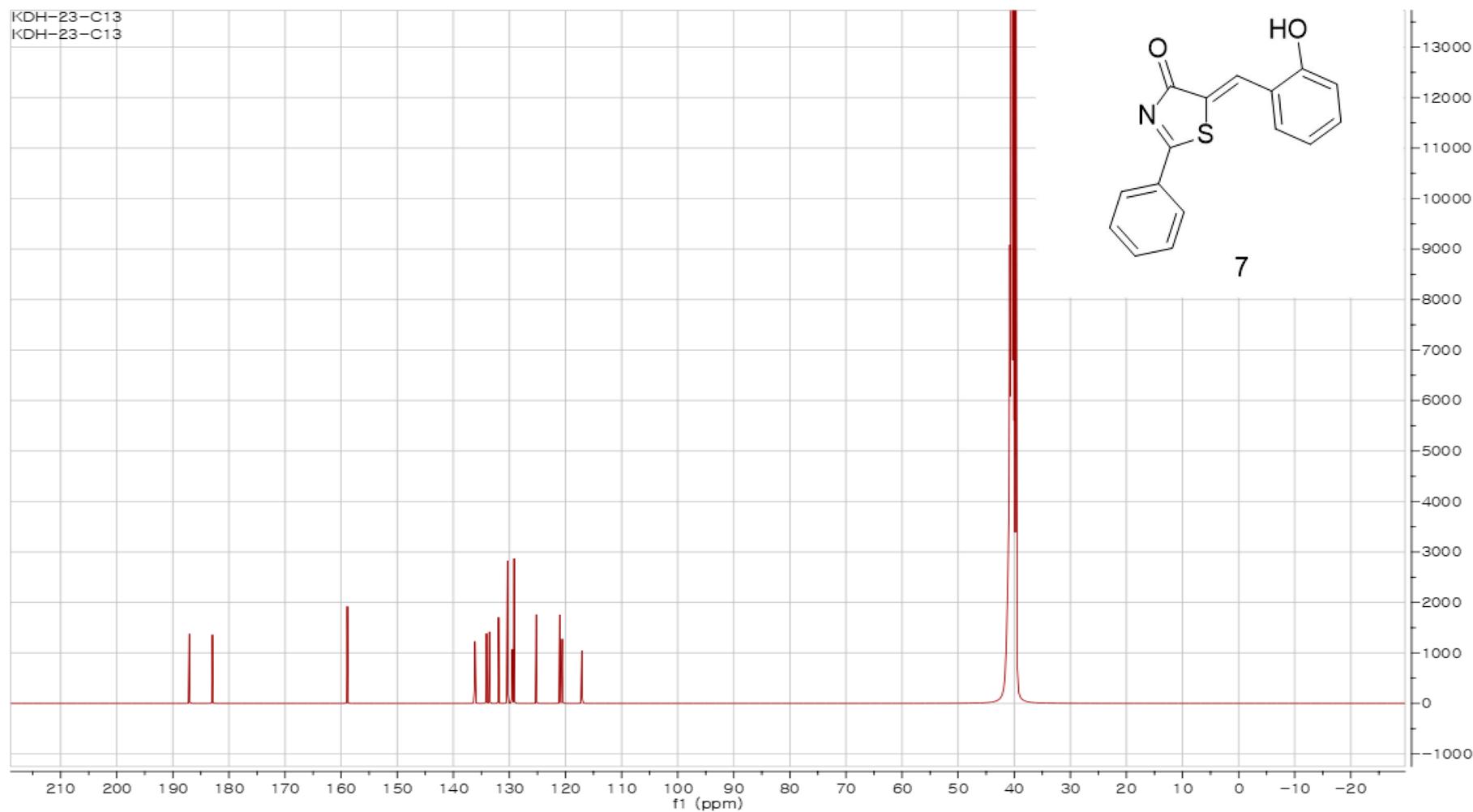


Figure S21. ¹³C NMR spectrum of compound 7.

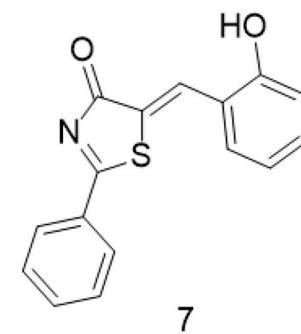
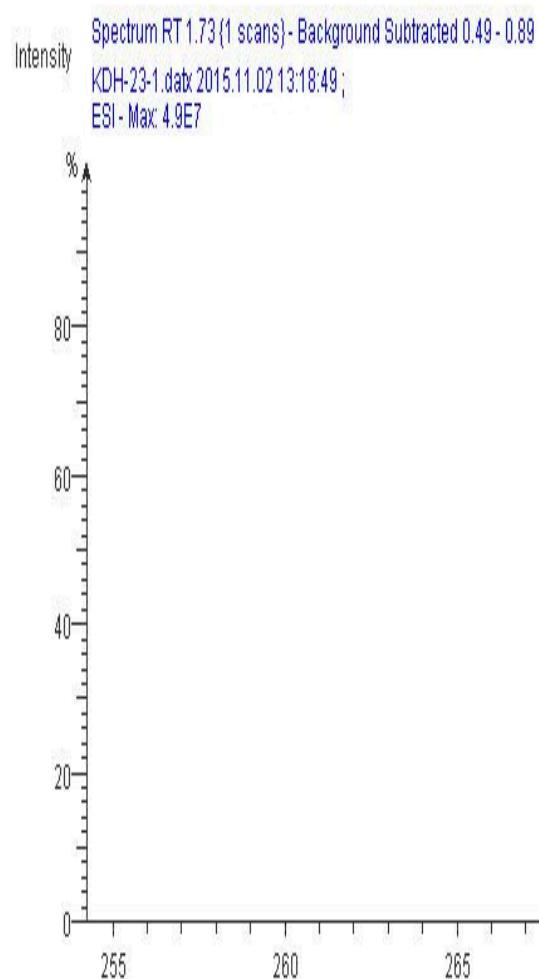


Figure S22. LRMS spectrum of compound 7.

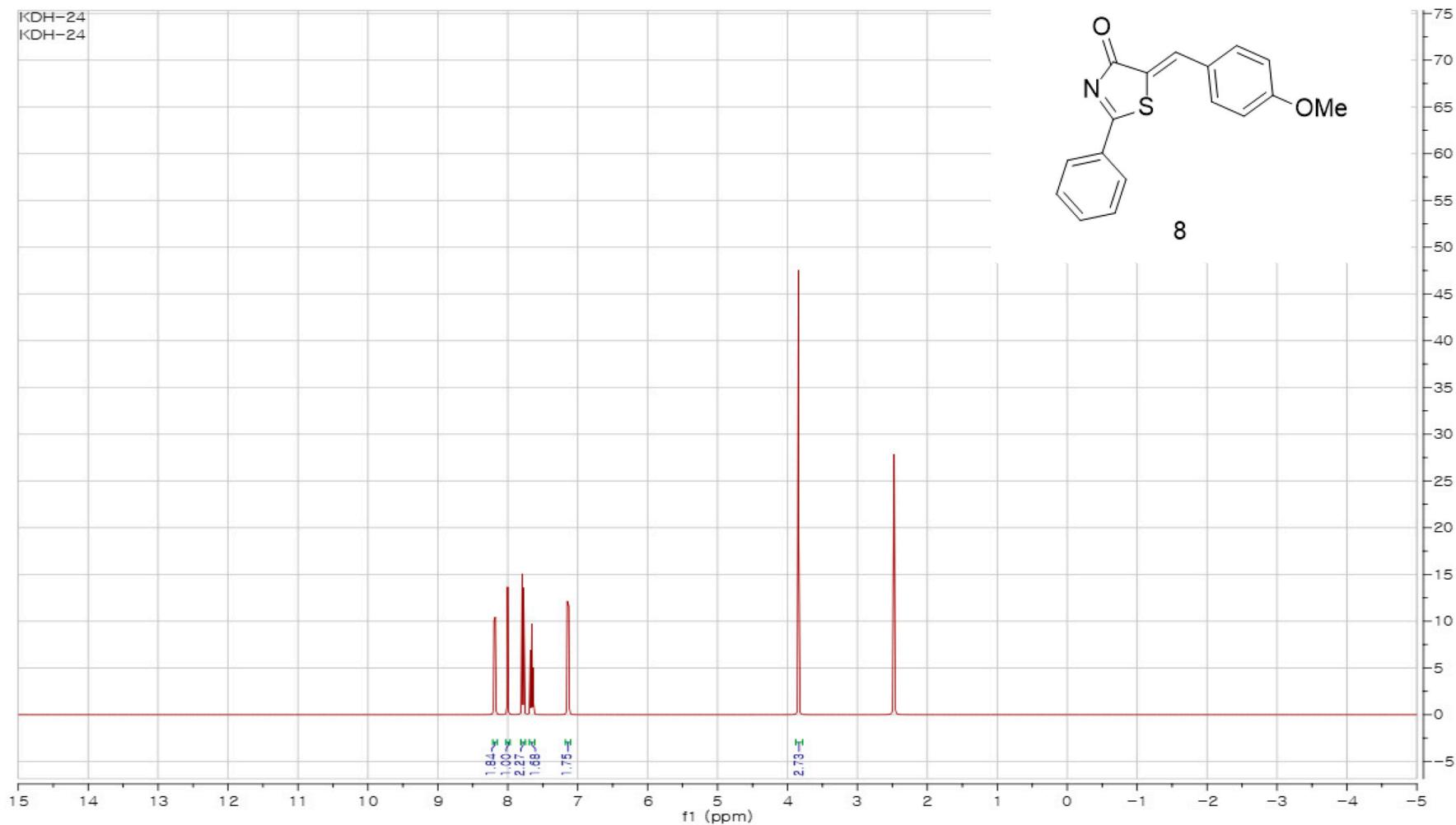


Figure S23. ¹H NMR spectrum of compound 8.

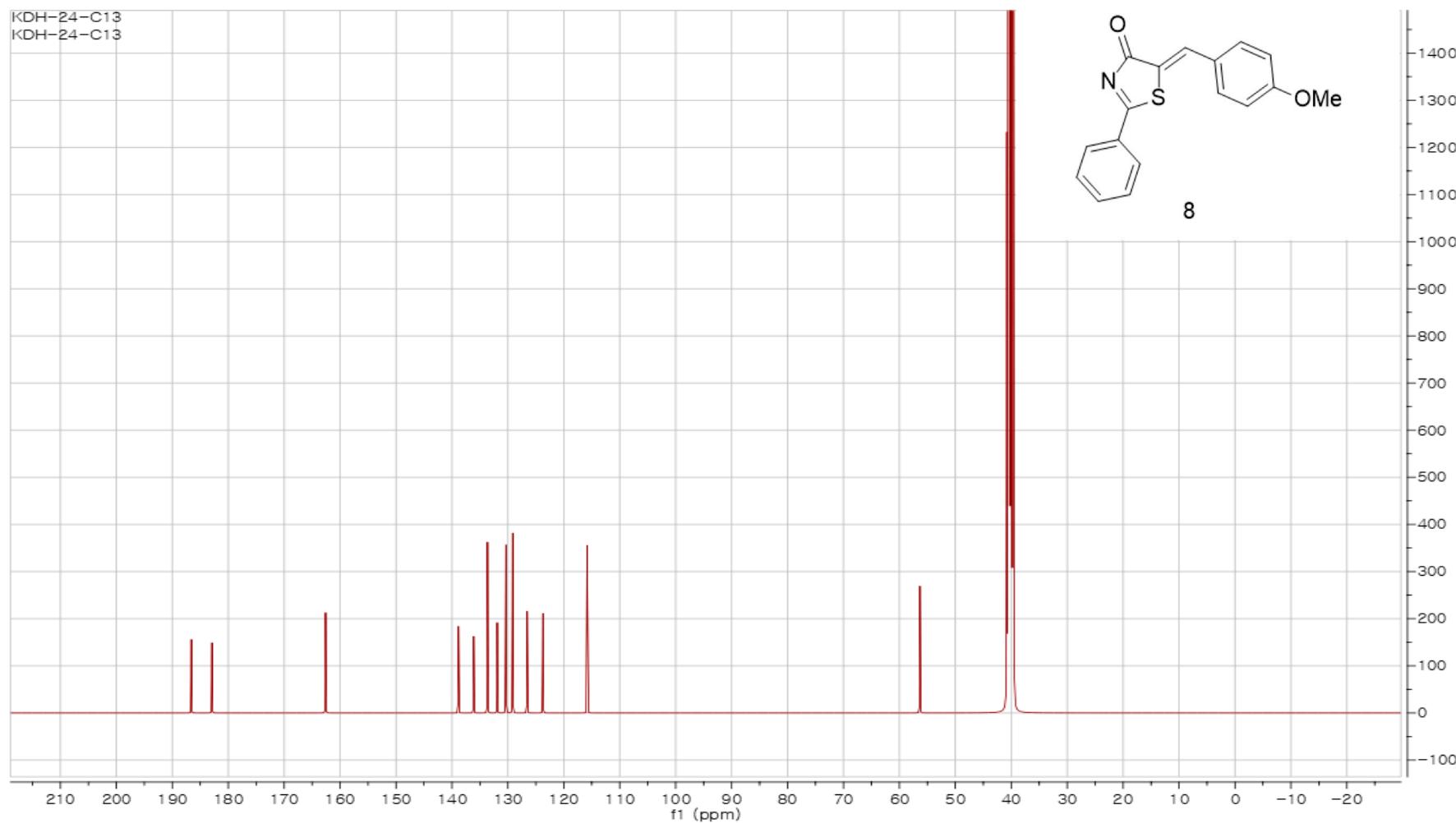


Figure S24. ¹³C NMR spectrum of compound 8.

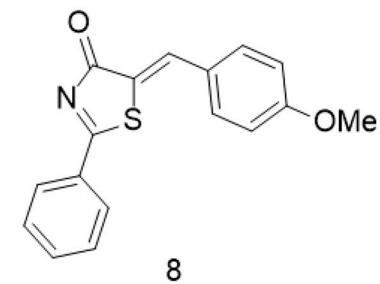
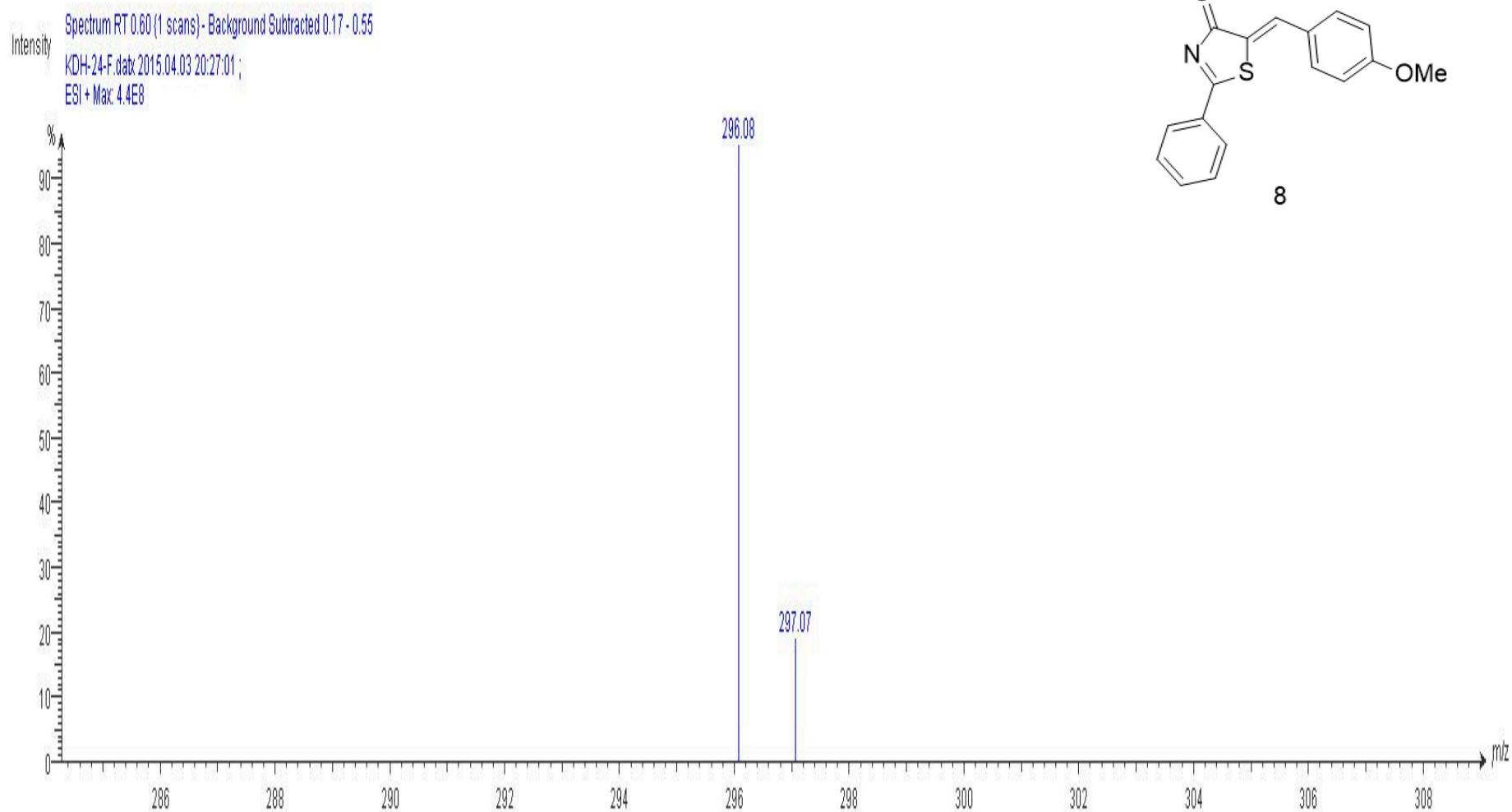


Figure S25. LRMS spectrum of compound 8.

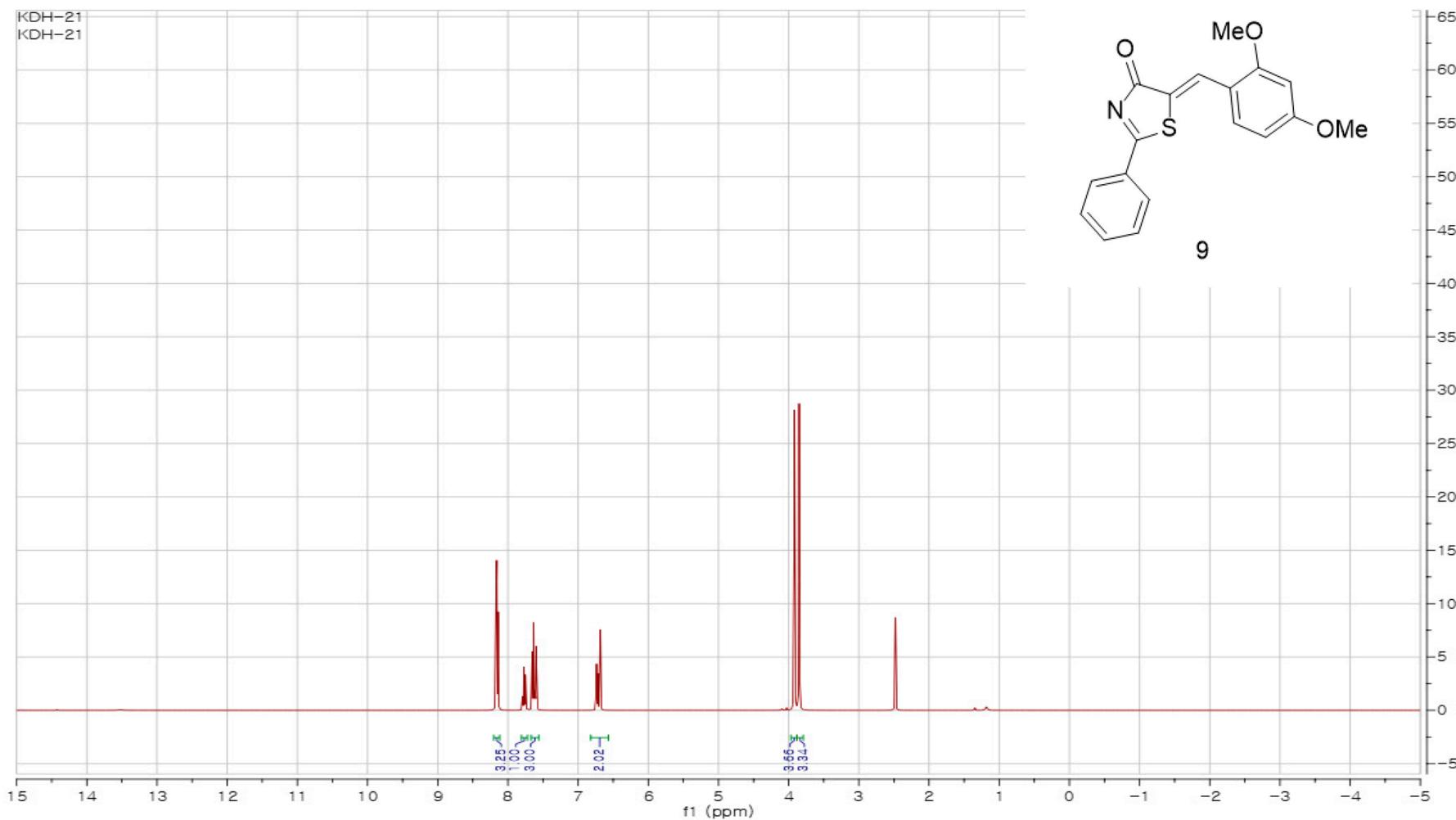


Figure S26. ¹H NMR spectrum of compound 9.

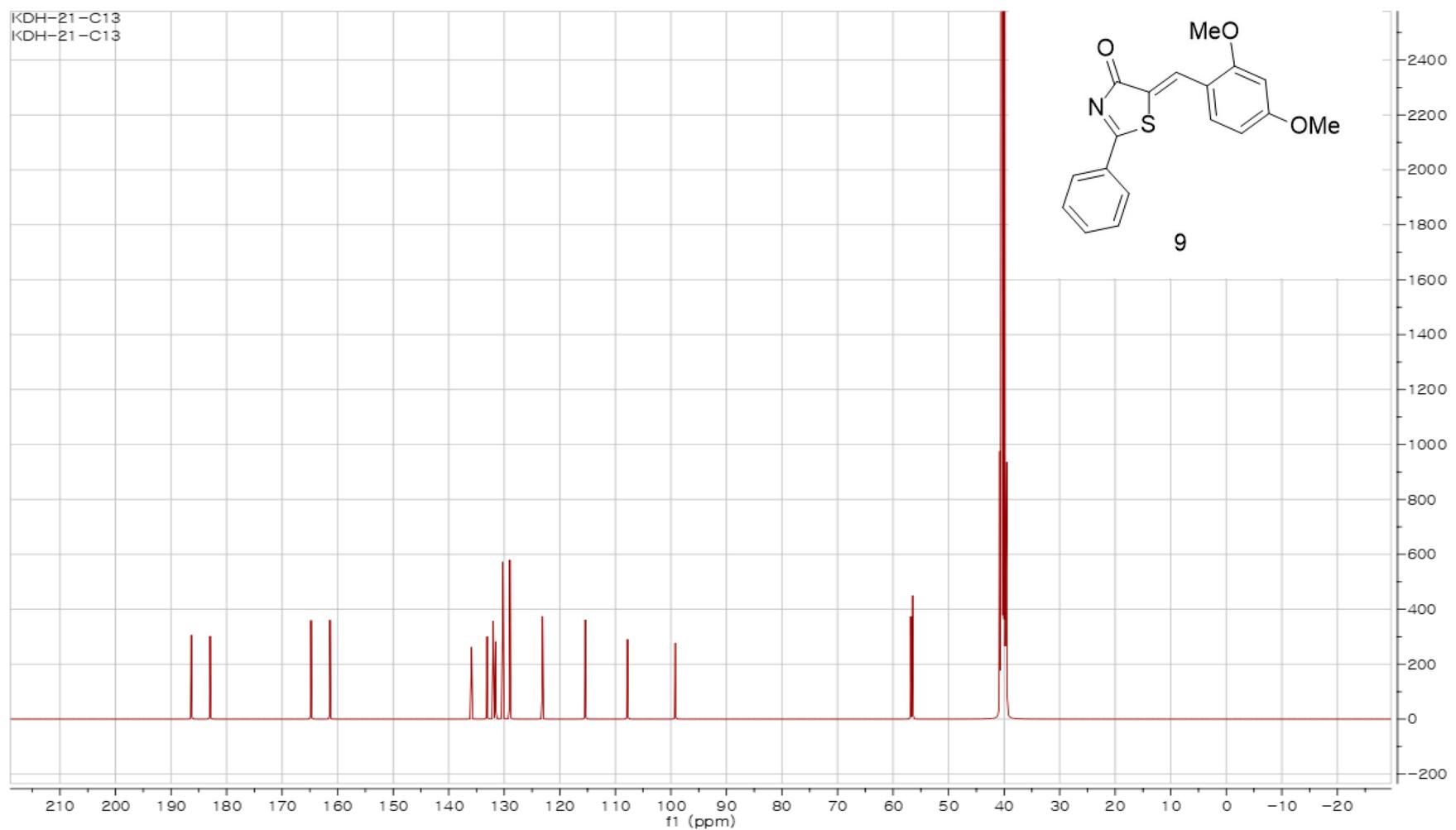


Figure S27. ¹³C NMR spectrum of compound 9.

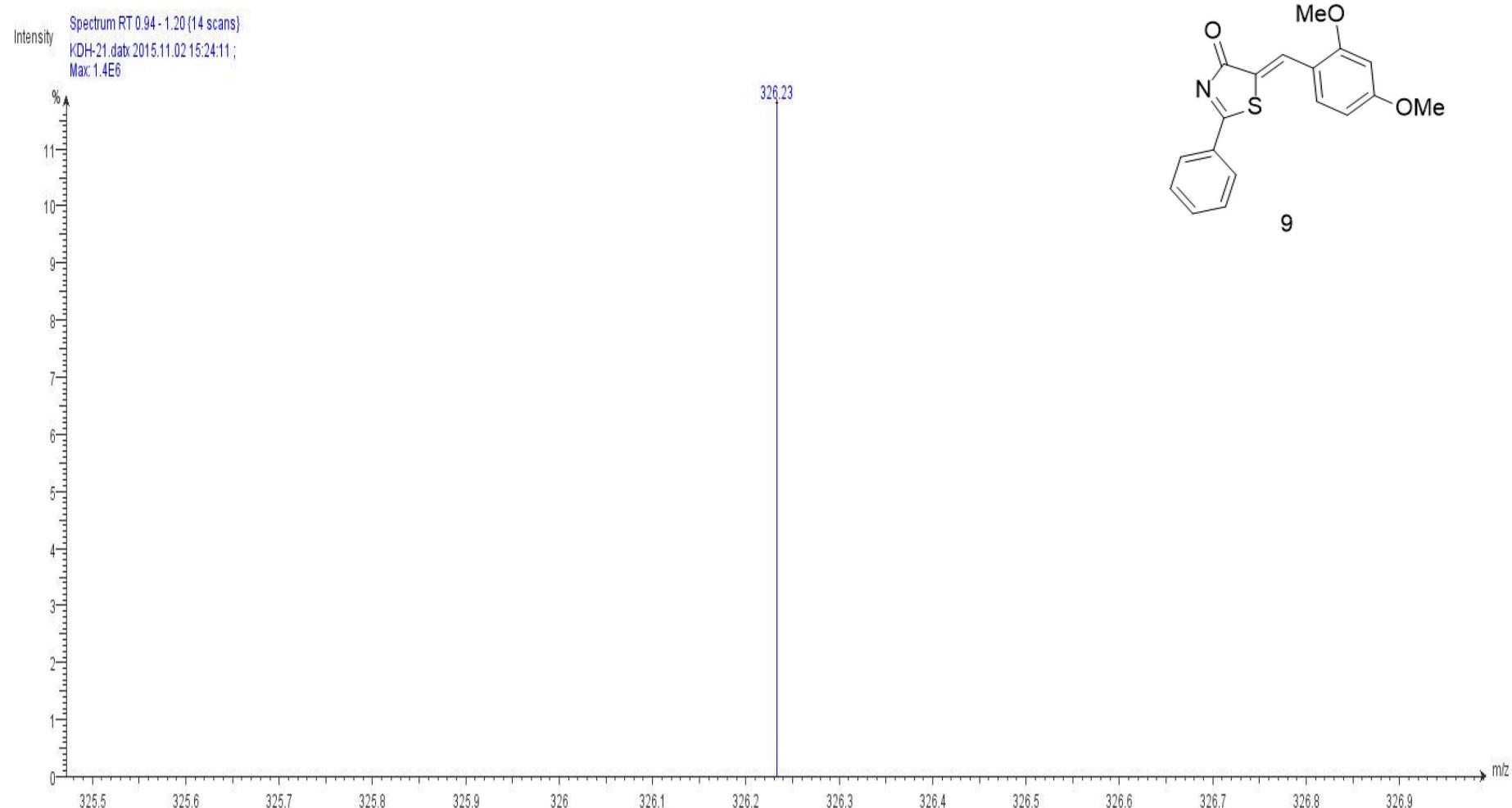


Figure S28. LRMS spectrum of compound 9.

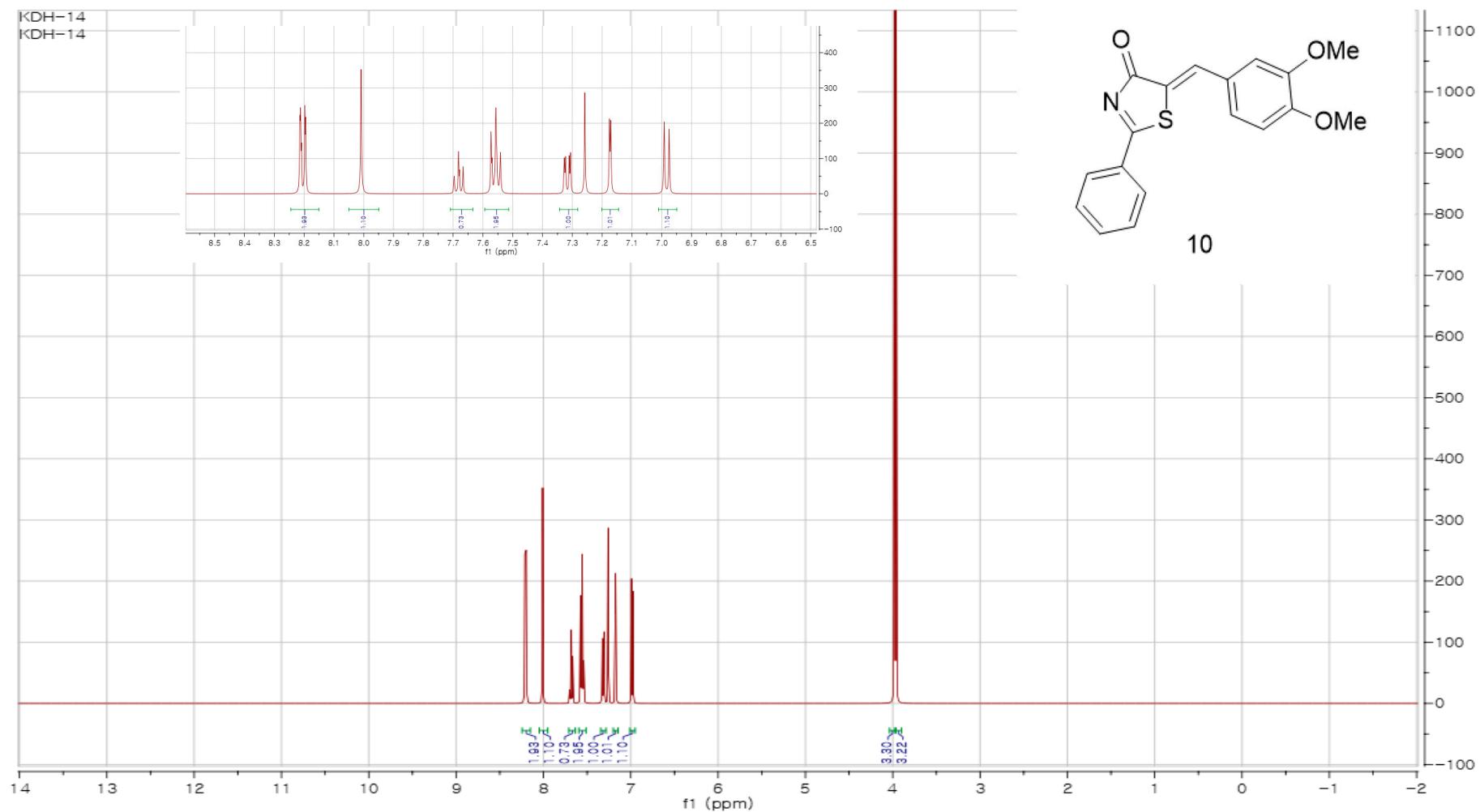


Figure S29. ^1H NMR spectrum of compound **10**.

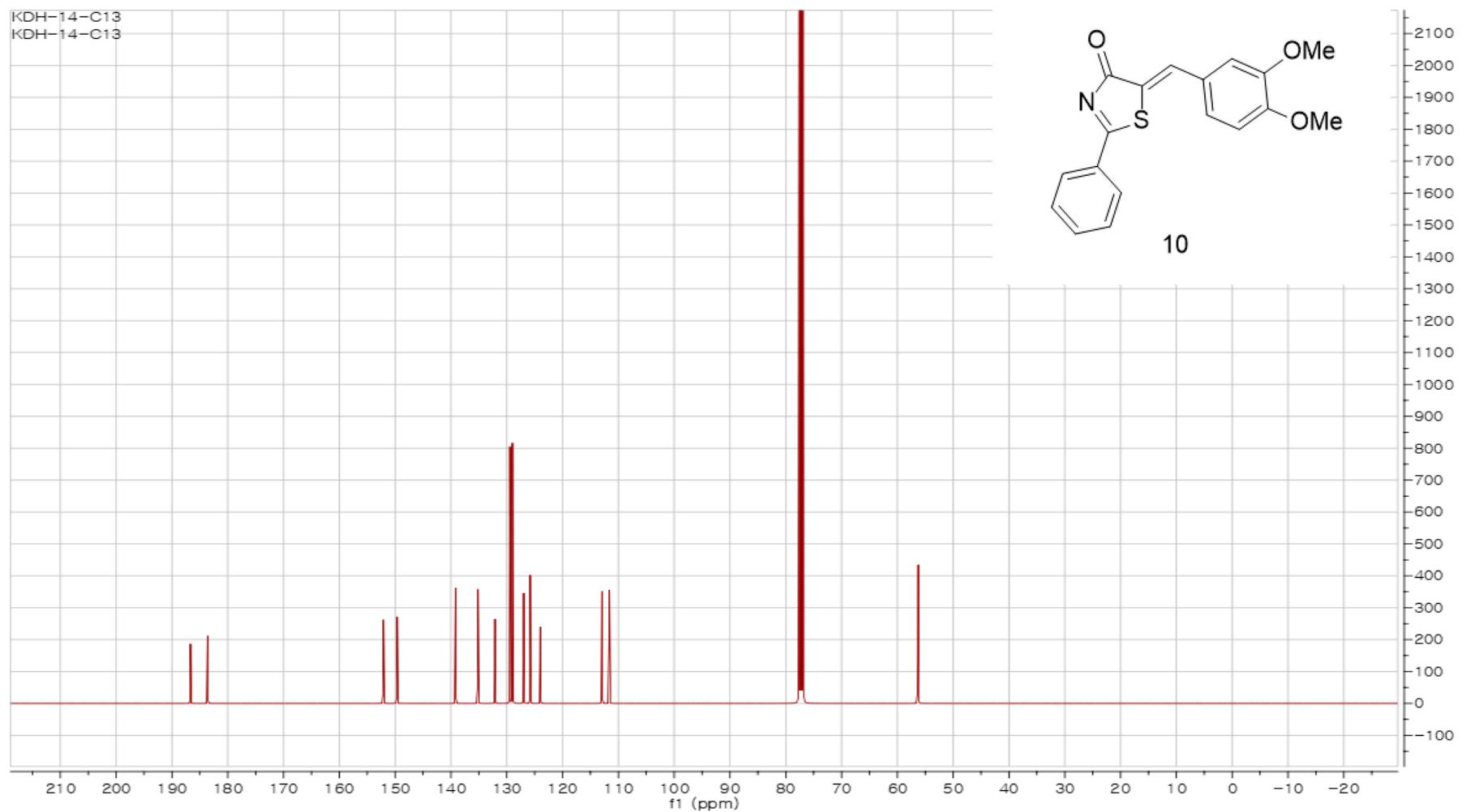


Figure S30. ^{13}C NMR spectrum of compound **10**.

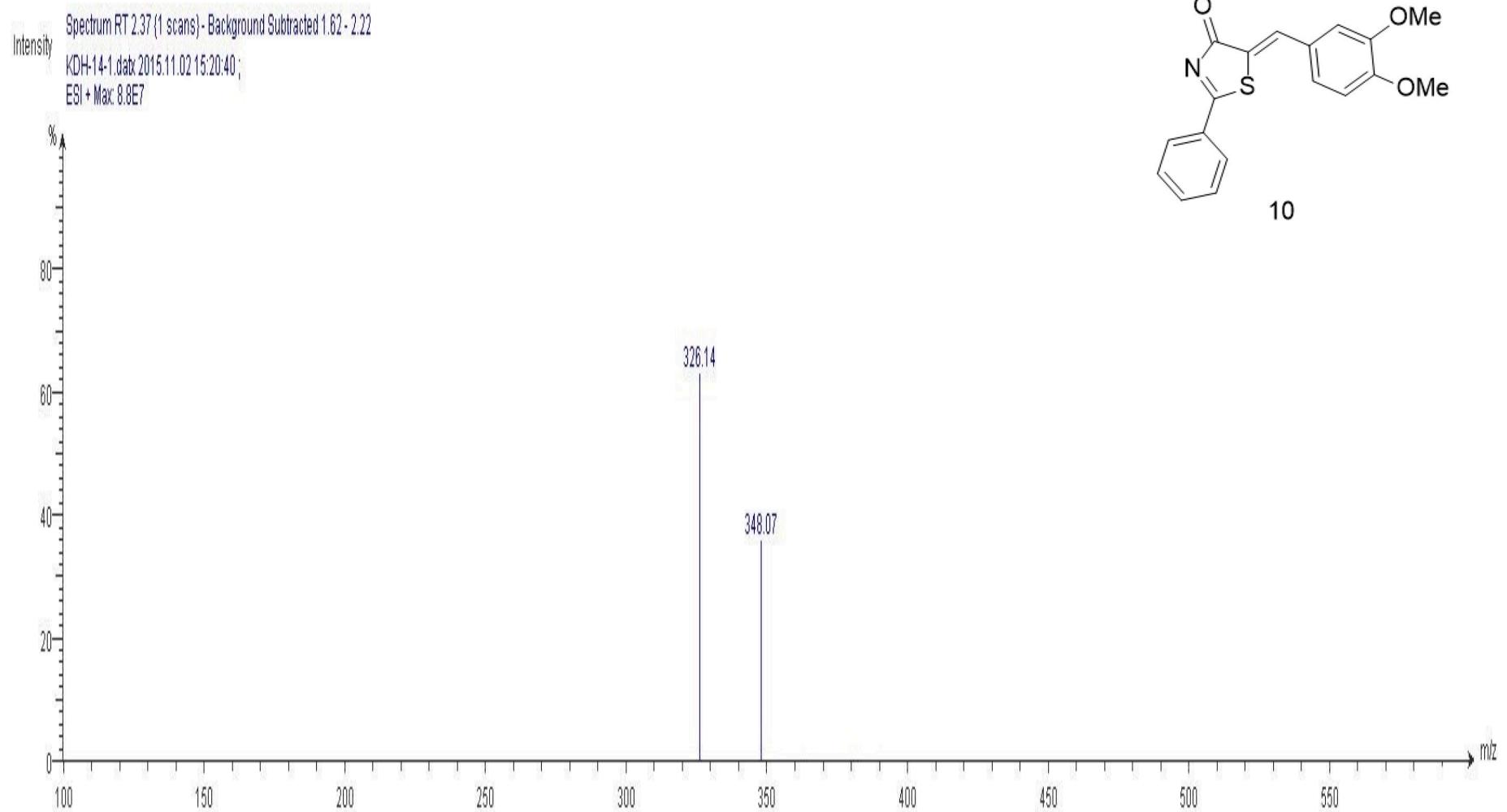


Figure S31. LRMS spectrum of compound **10**.

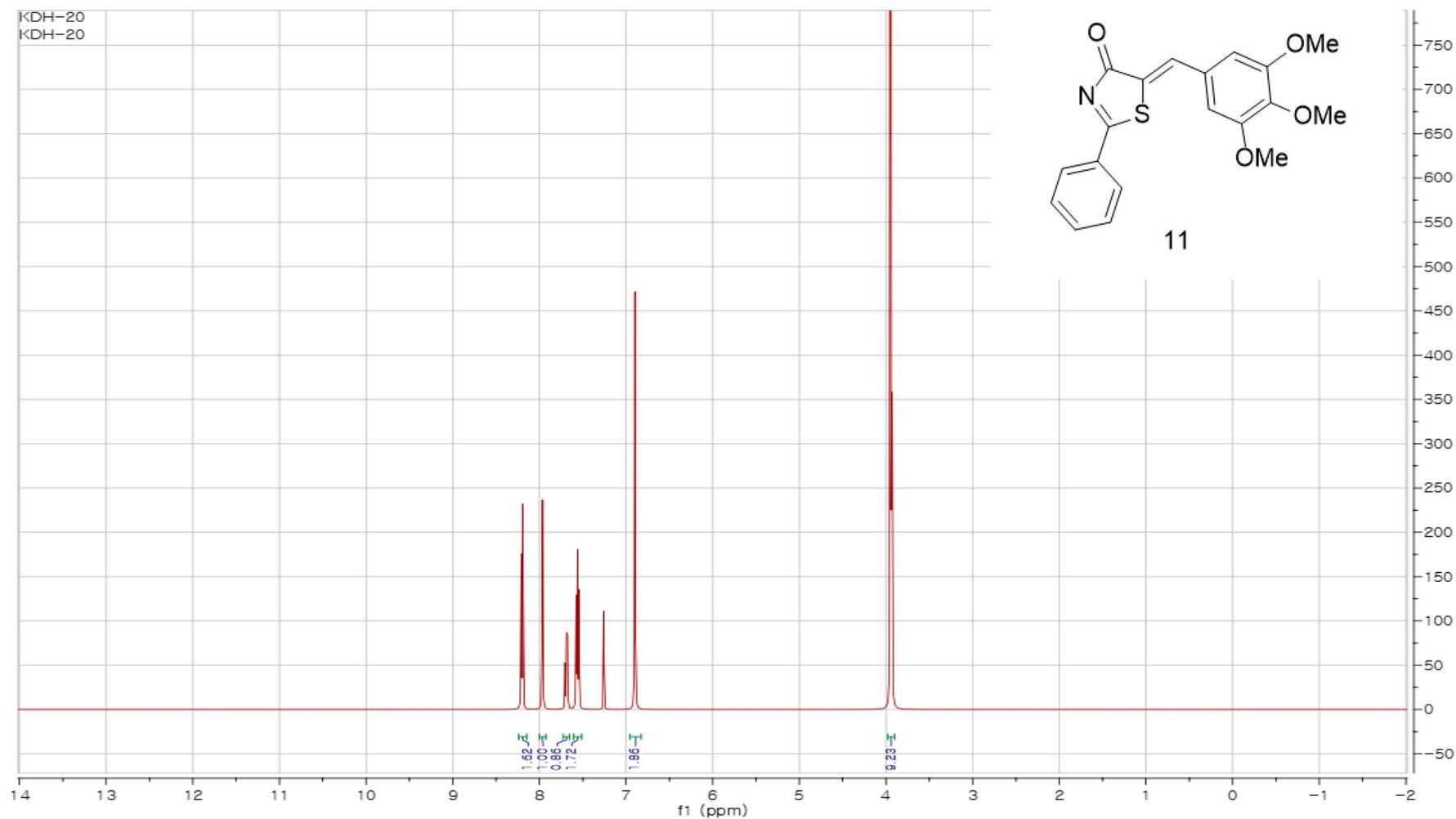


Figure S32. ^1H NMR spectrum of compound 11.

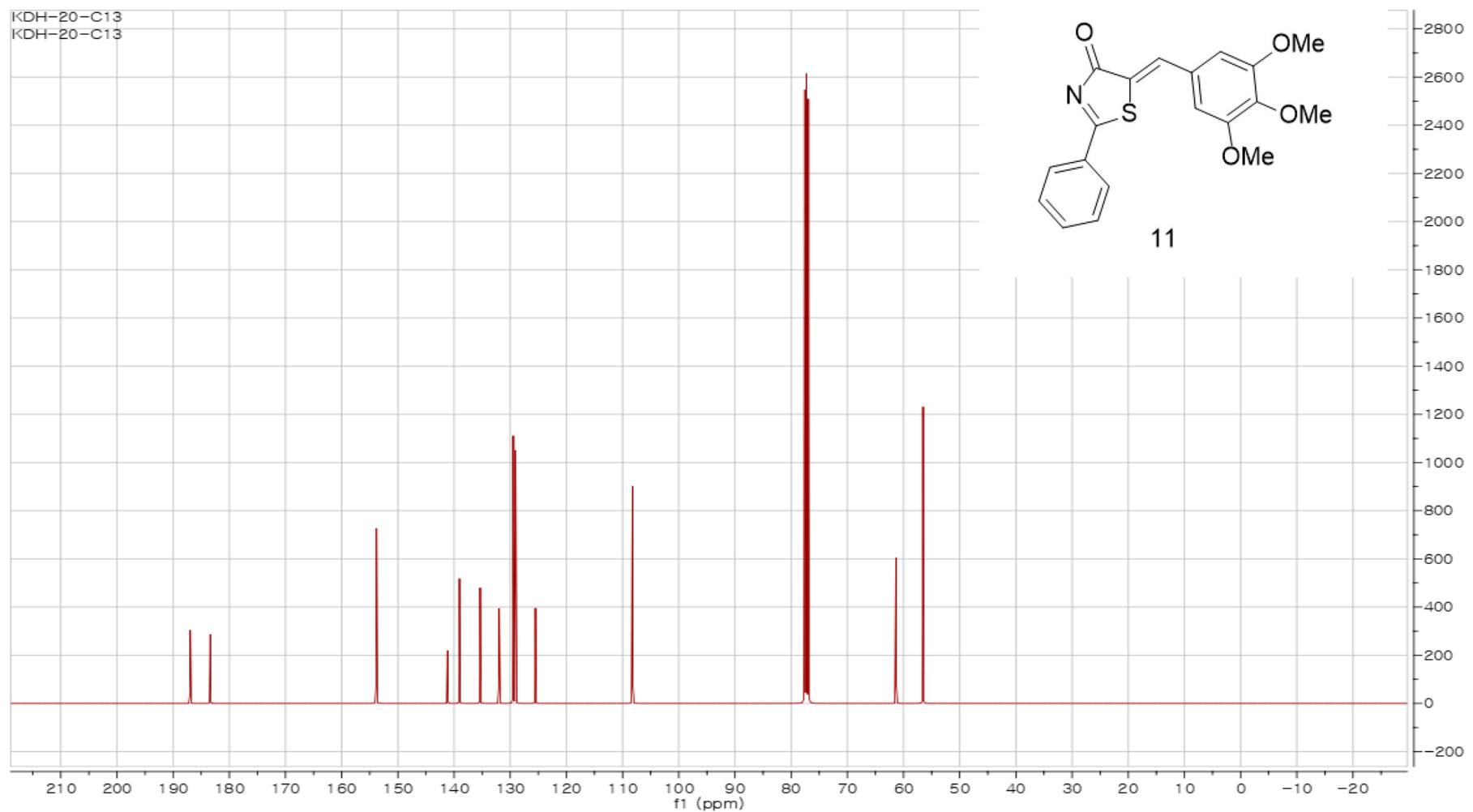


Figure S33. ¹³C NMR spectrum of compound 11.

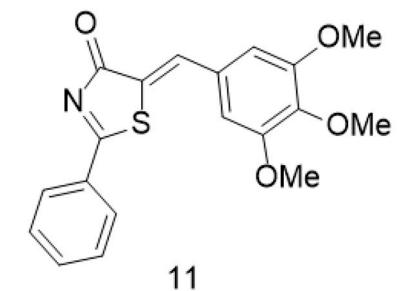
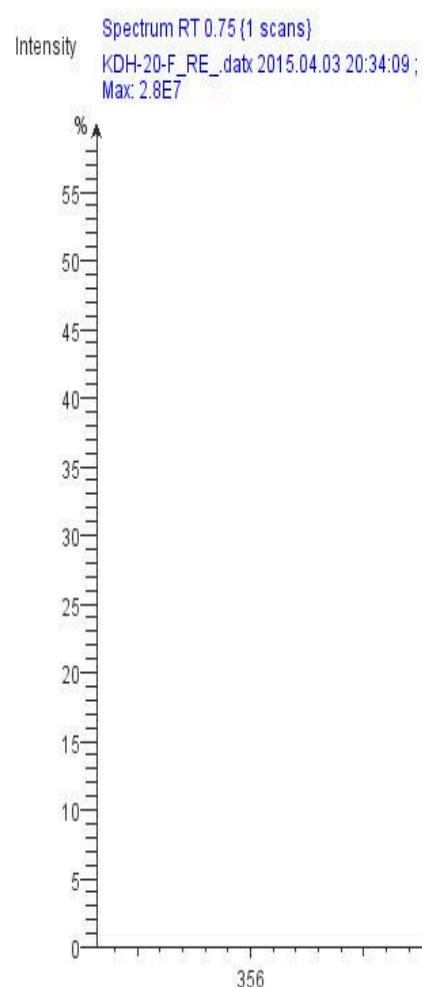


Figure S34. LRMS spectrum of compound **11**.

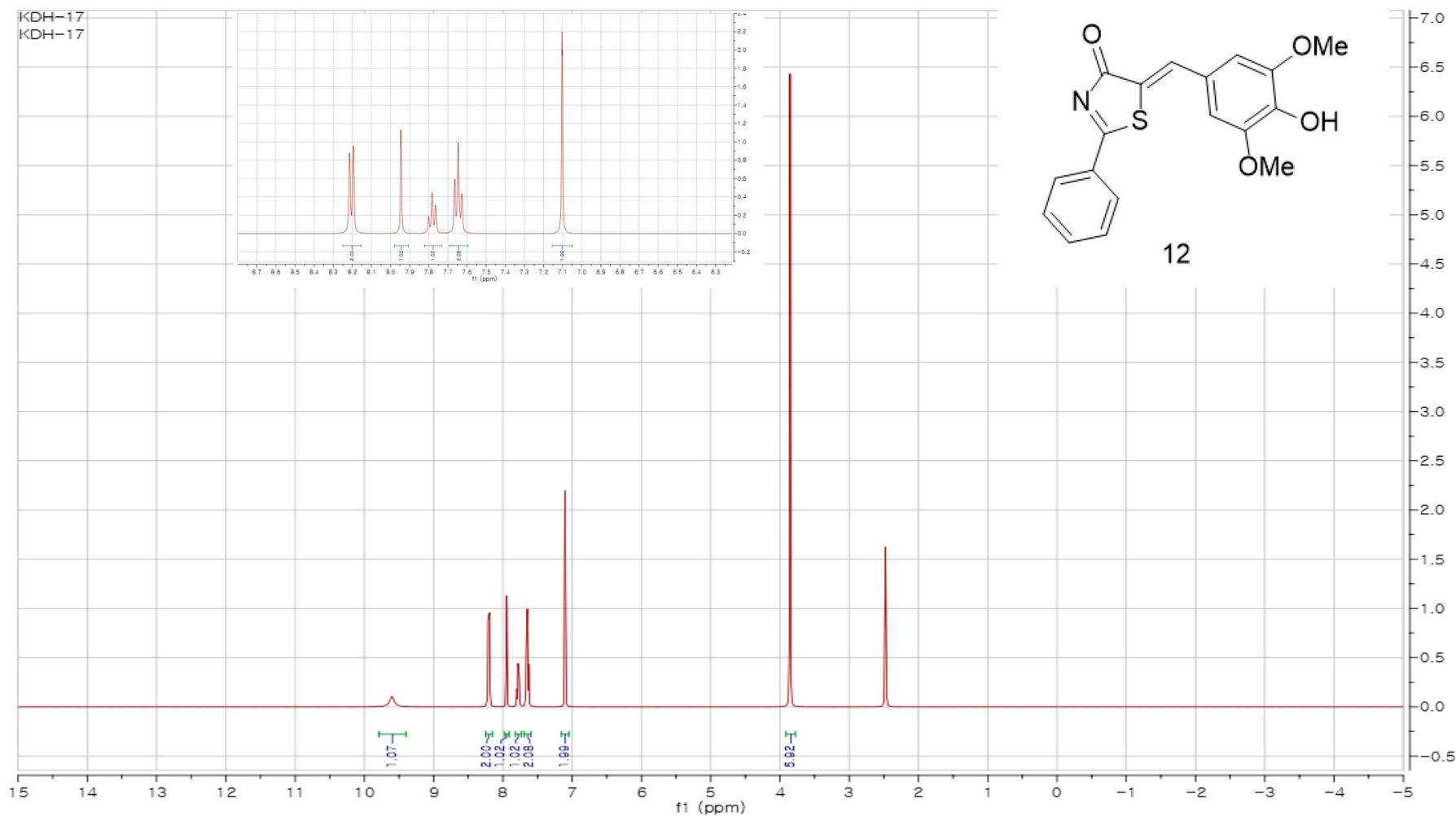


Figure S35. ^1H NMR spectrum of compound **12**.

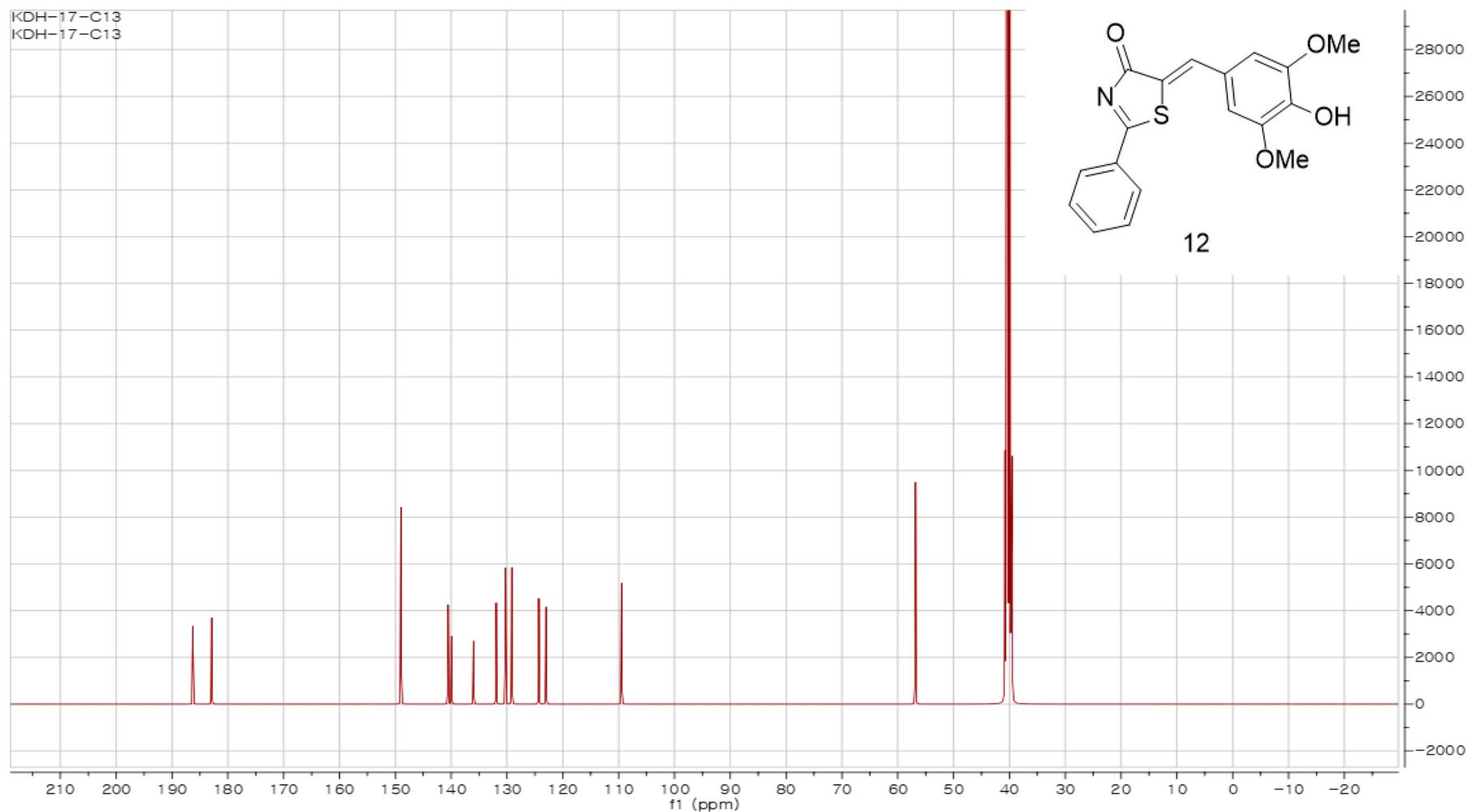


Figure S36. ¹³C NMR spectrum of compound 12.

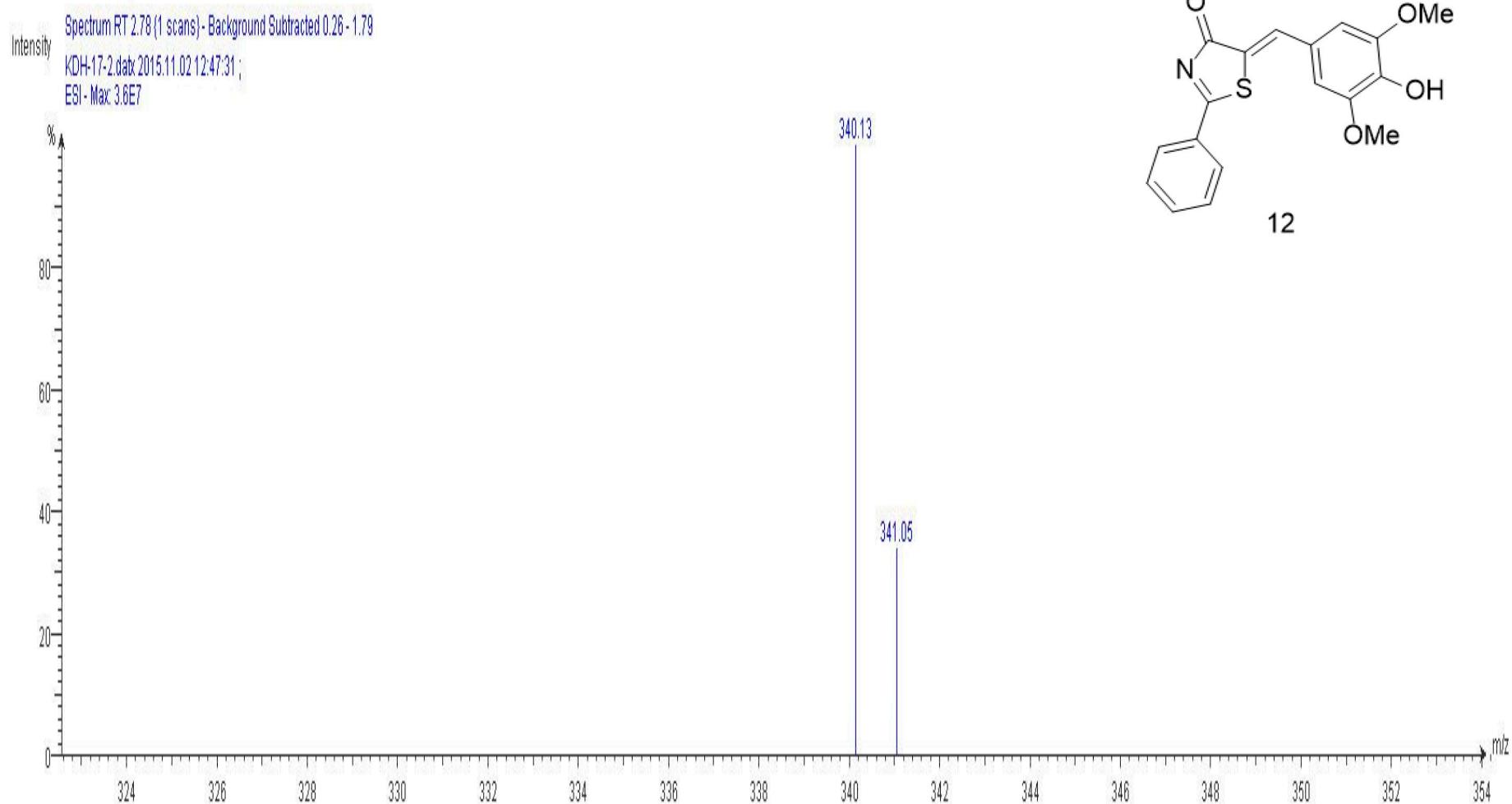


Figure S37. LRMS spectrum of compound **12**.

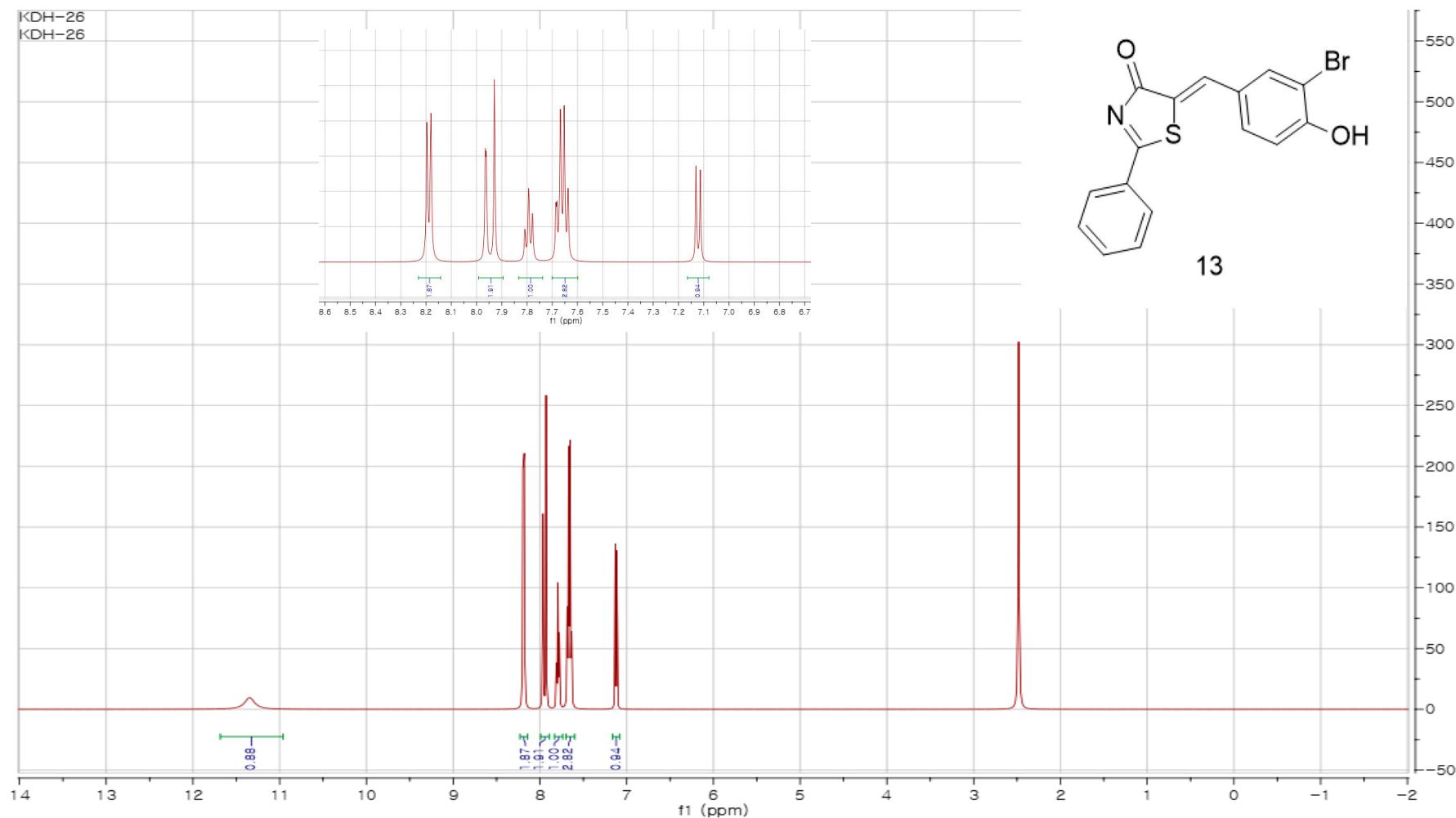


Figure S38. ^1H NMR spectrum of compound 13.

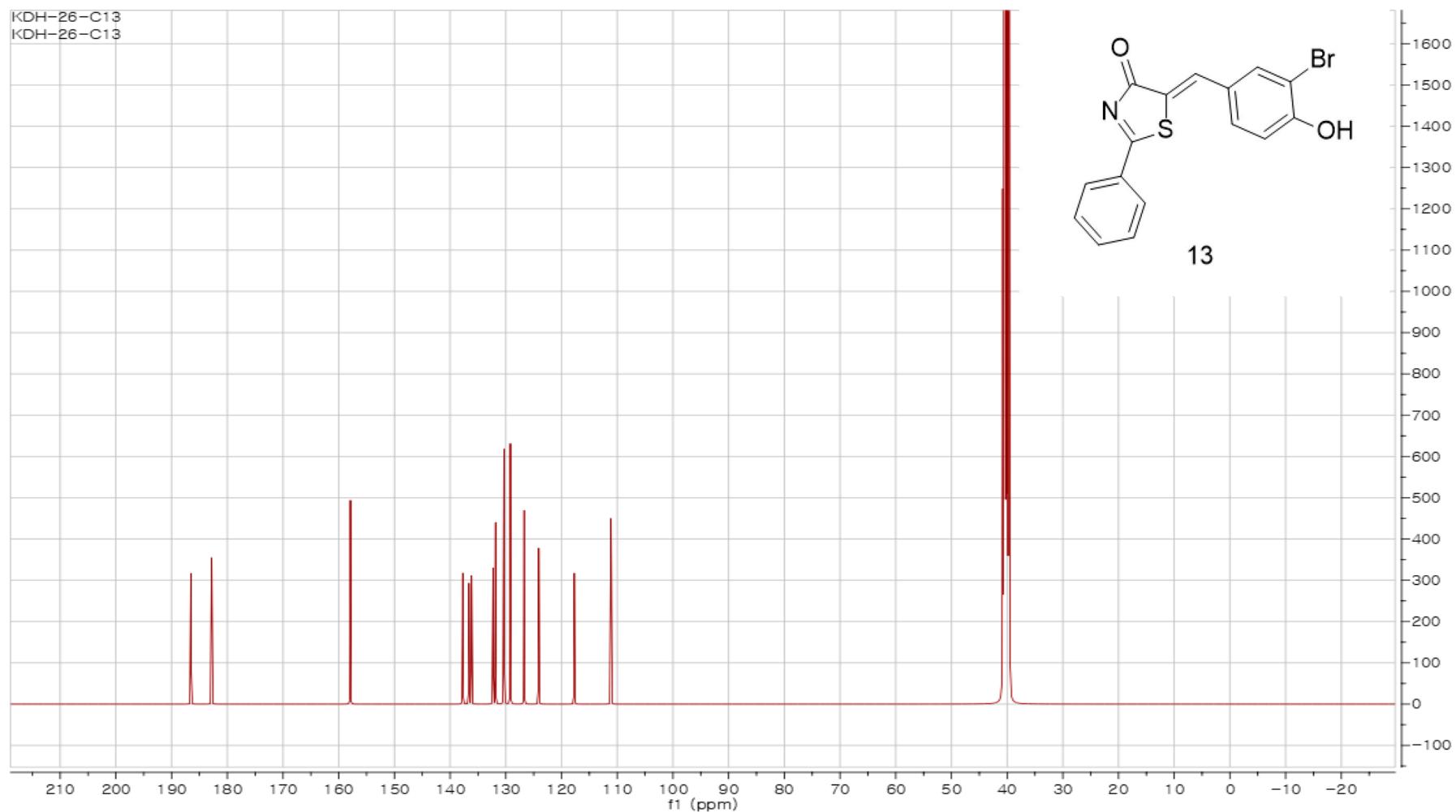


Figure S39. ¹³C NMR spectrum of compound 13.

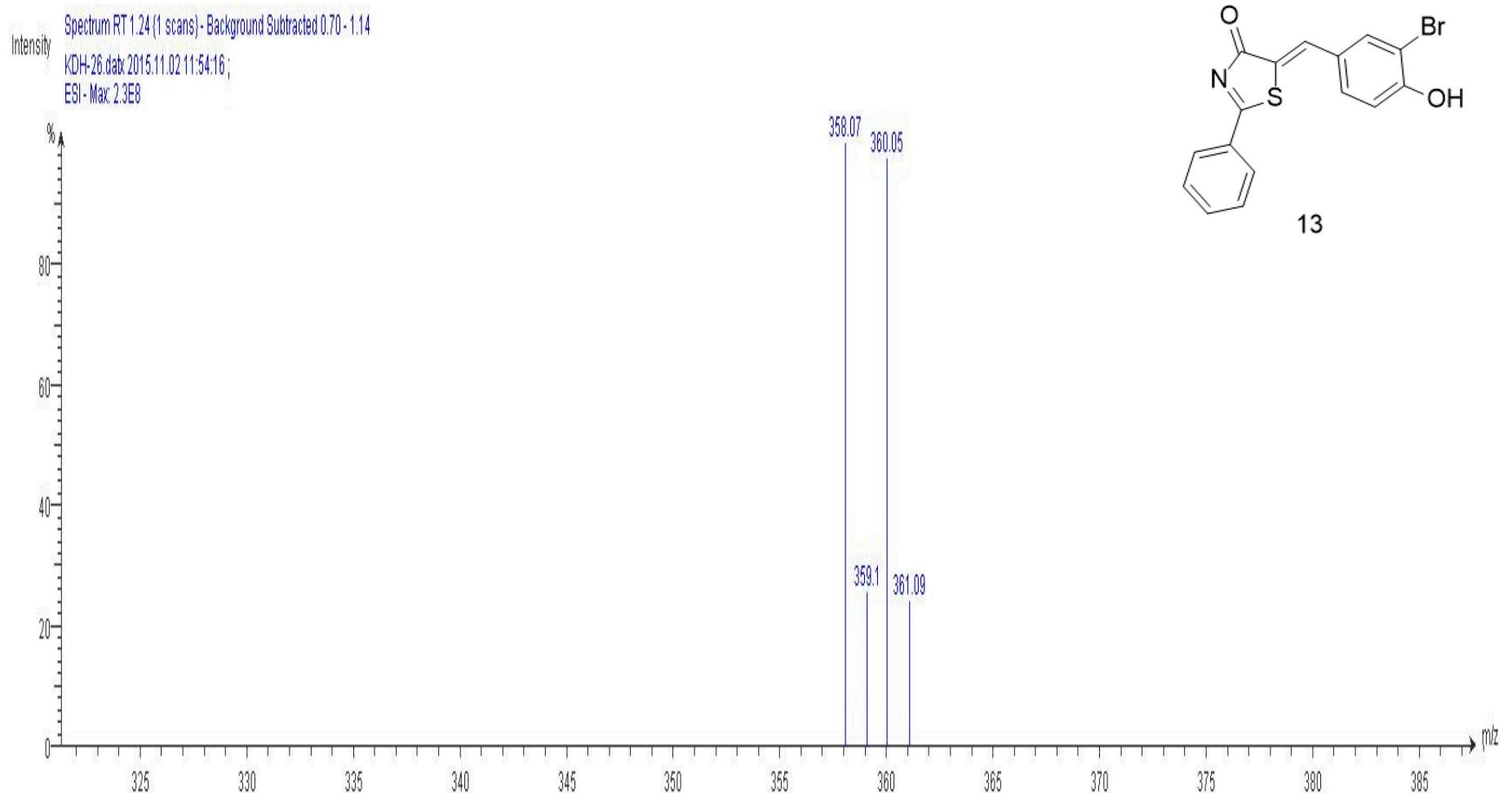


Figure S40. LRMS spectrum of compound **13**.

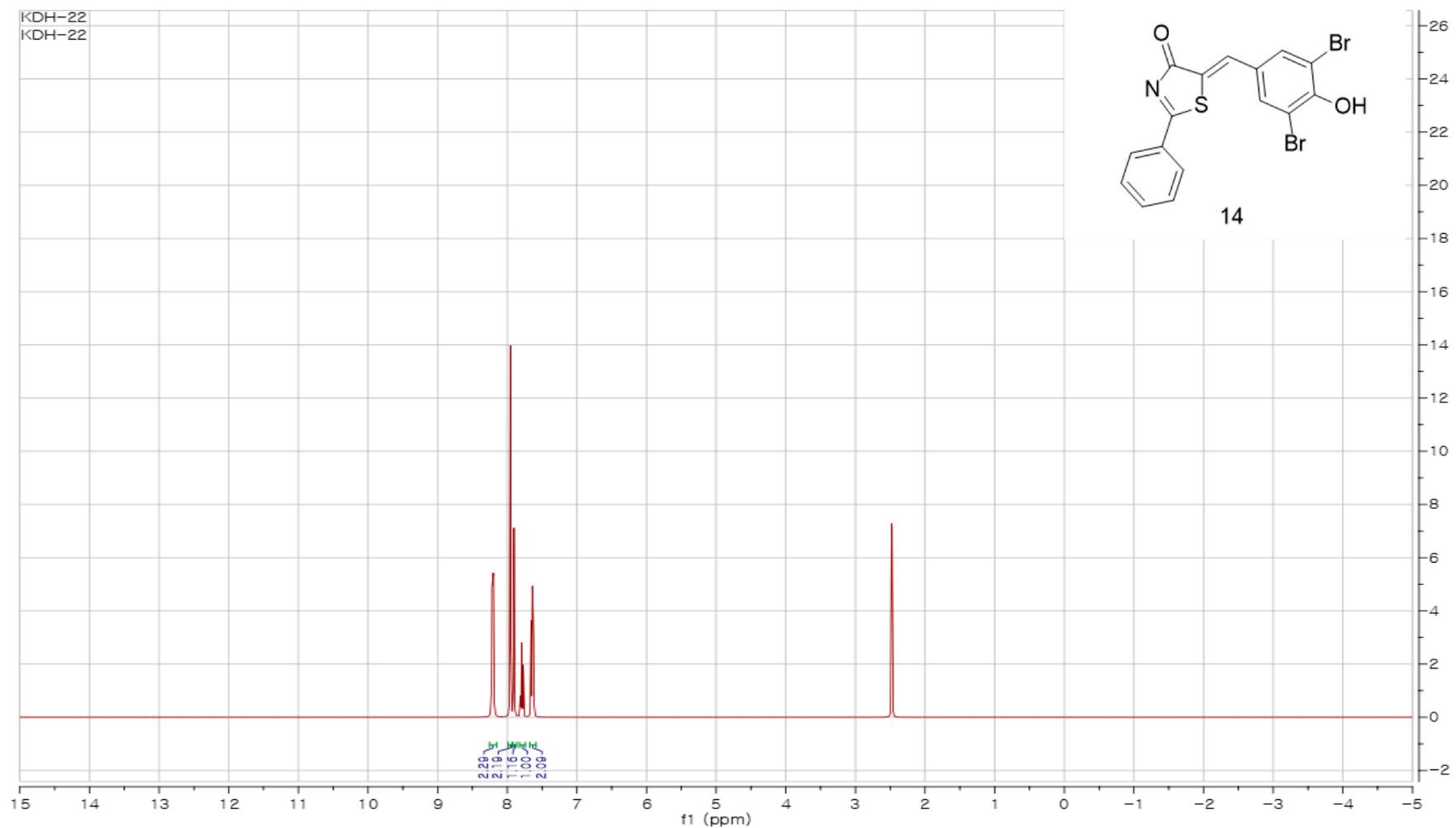


Figure S41. ¹H NMR spectrum of compound 14.

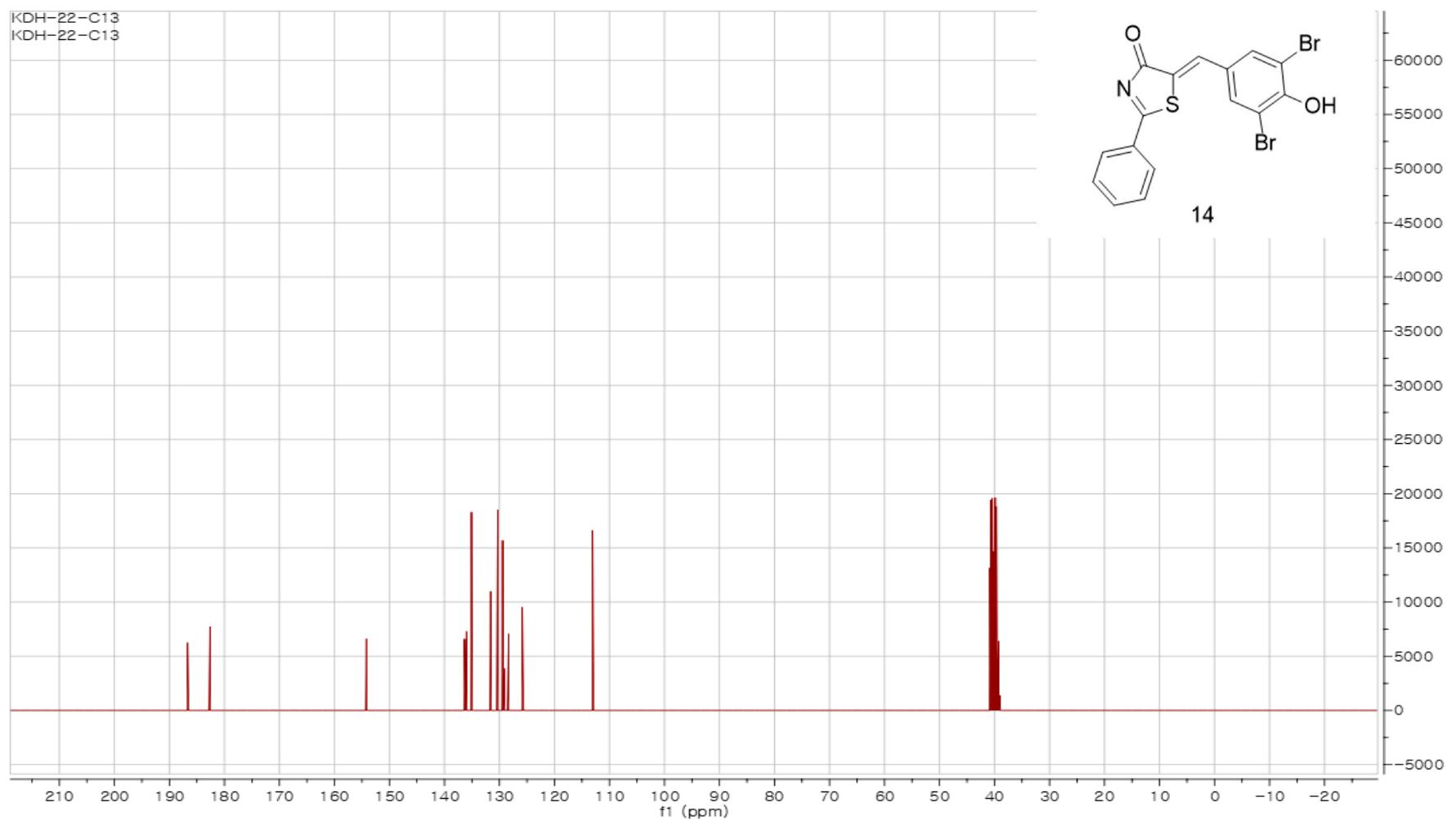


Figure S42. ^{13}C NMR spectrum of compound 14.

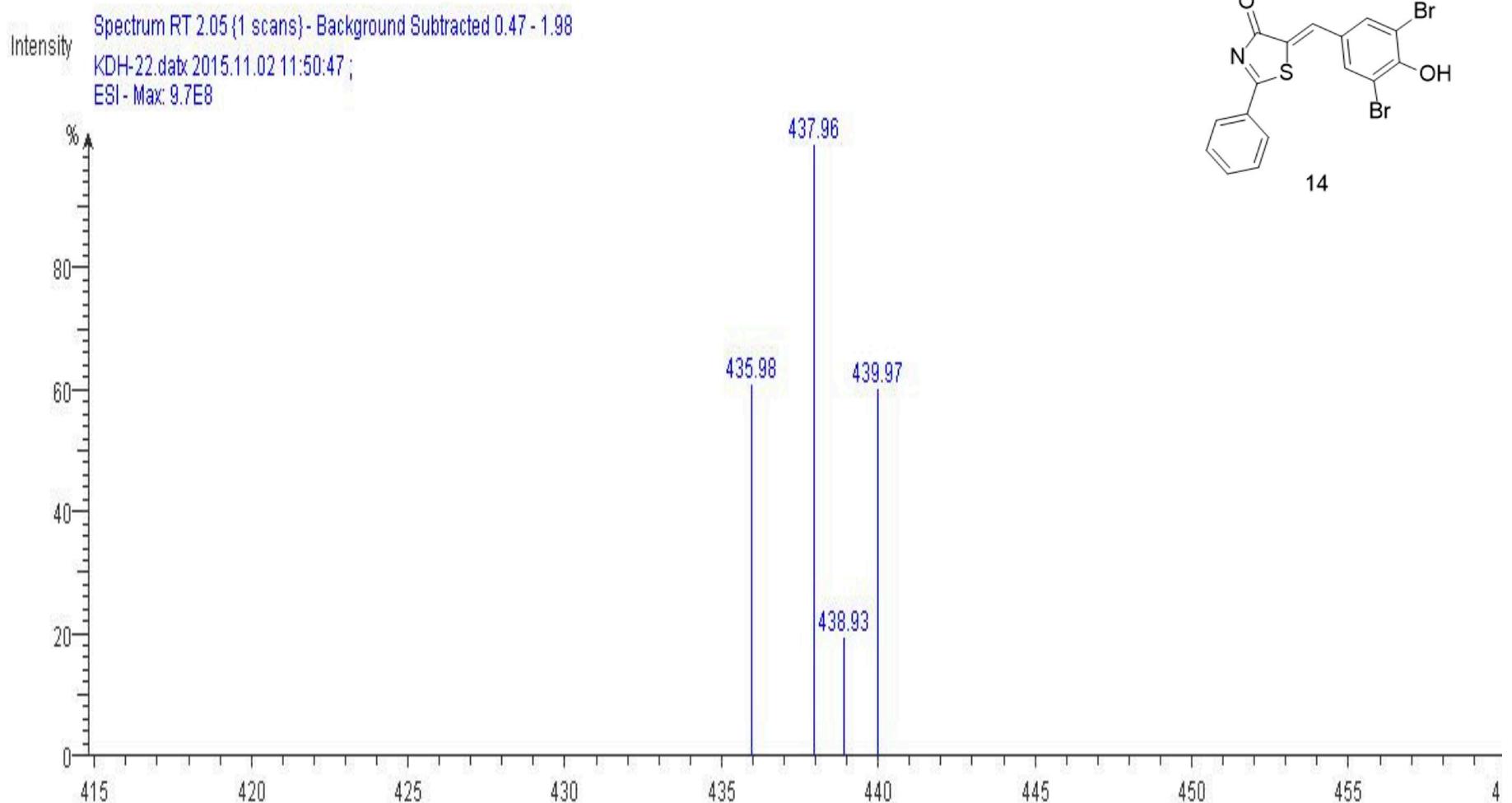
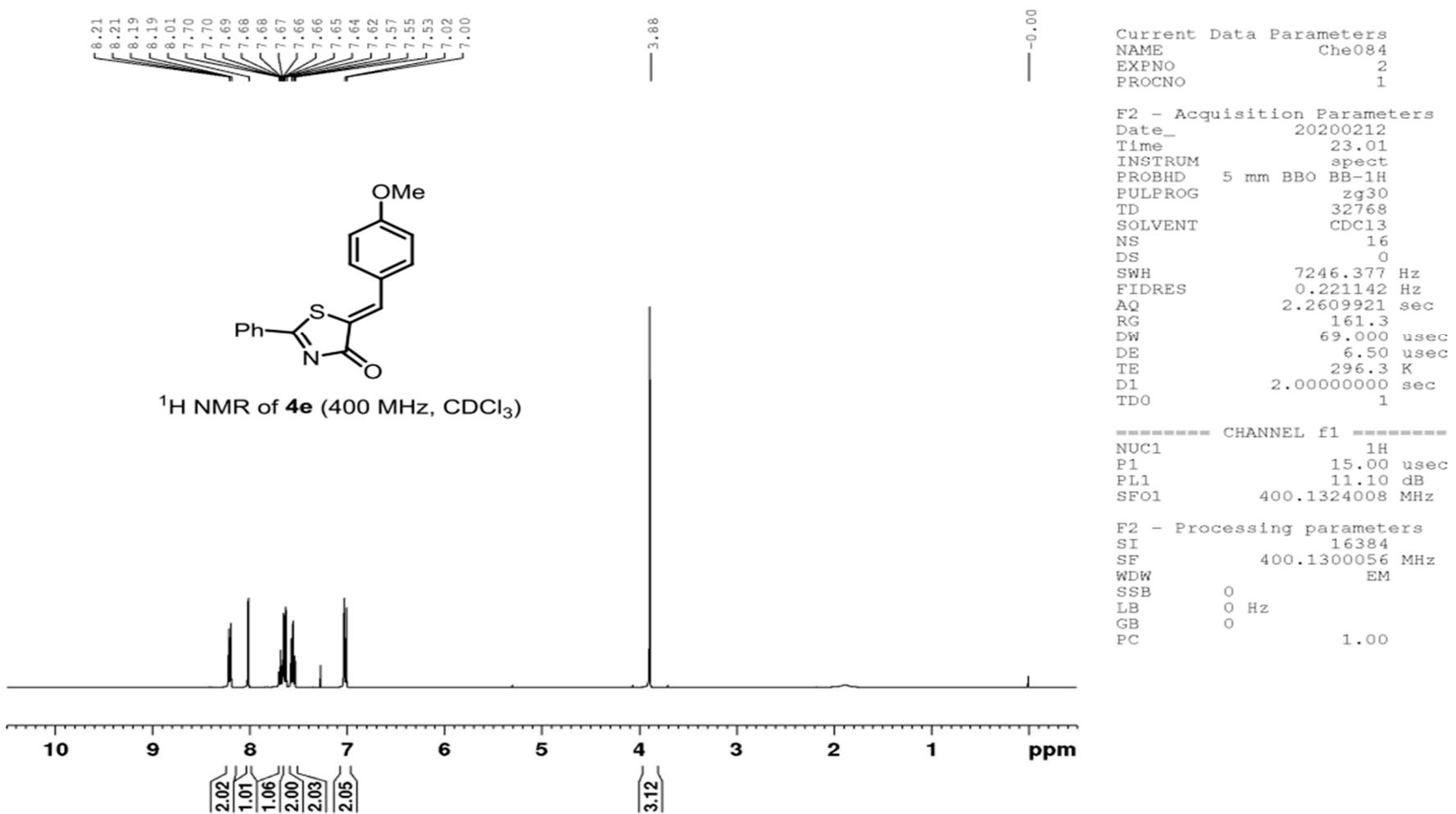


Figure S43. LRMS spectrum of compound **14**.



S149

Figure S44. ¹H NMR spectrum of compound **8** reported in other article (*Org. Lett.* 2020, 22, 17, 6868–6872).

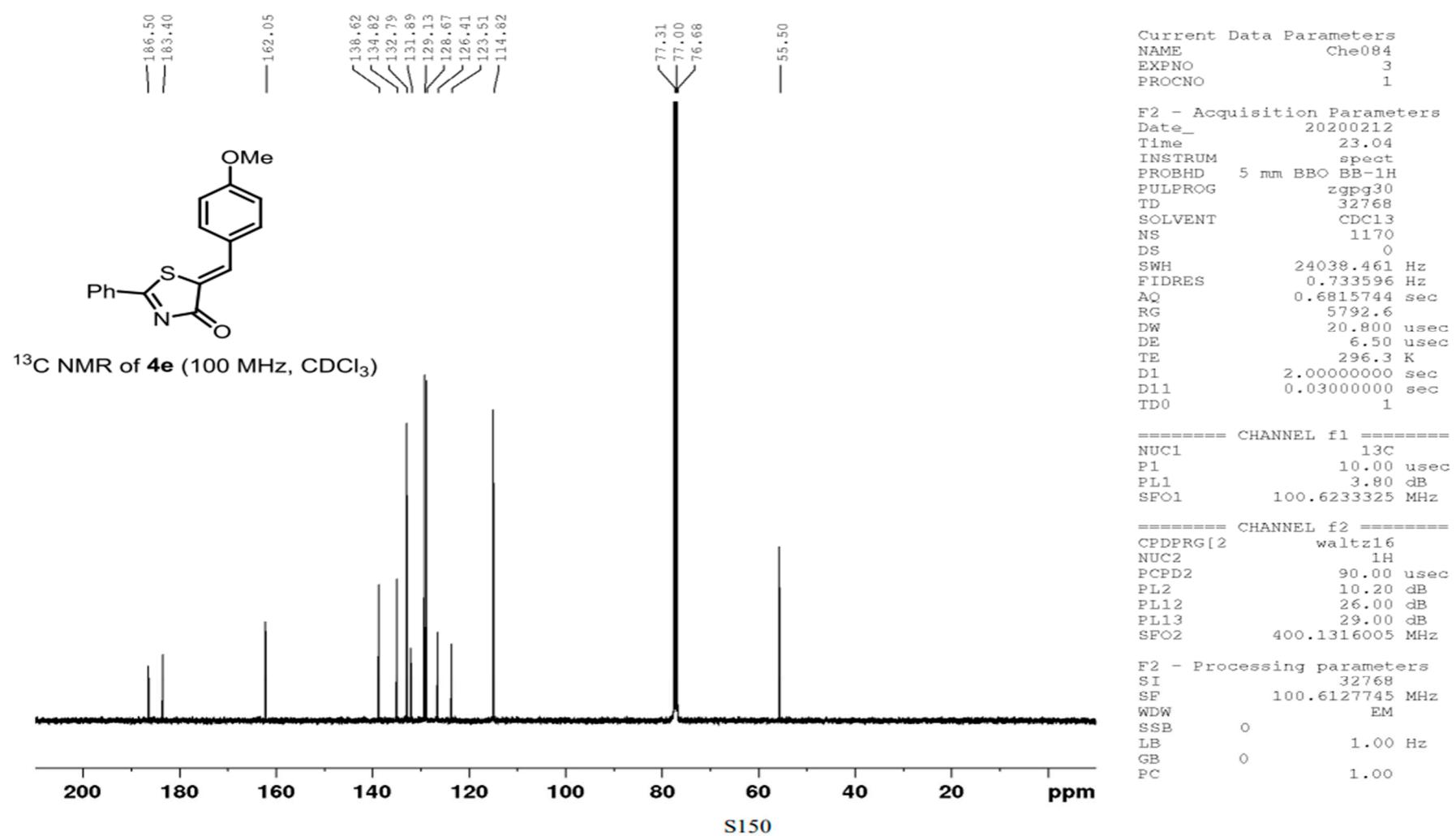


Figure S45. ¹³C NMR spectrum of compound **8** reported in other article (*Org. Lett.* 2020, 22, 17, 6868–6872).

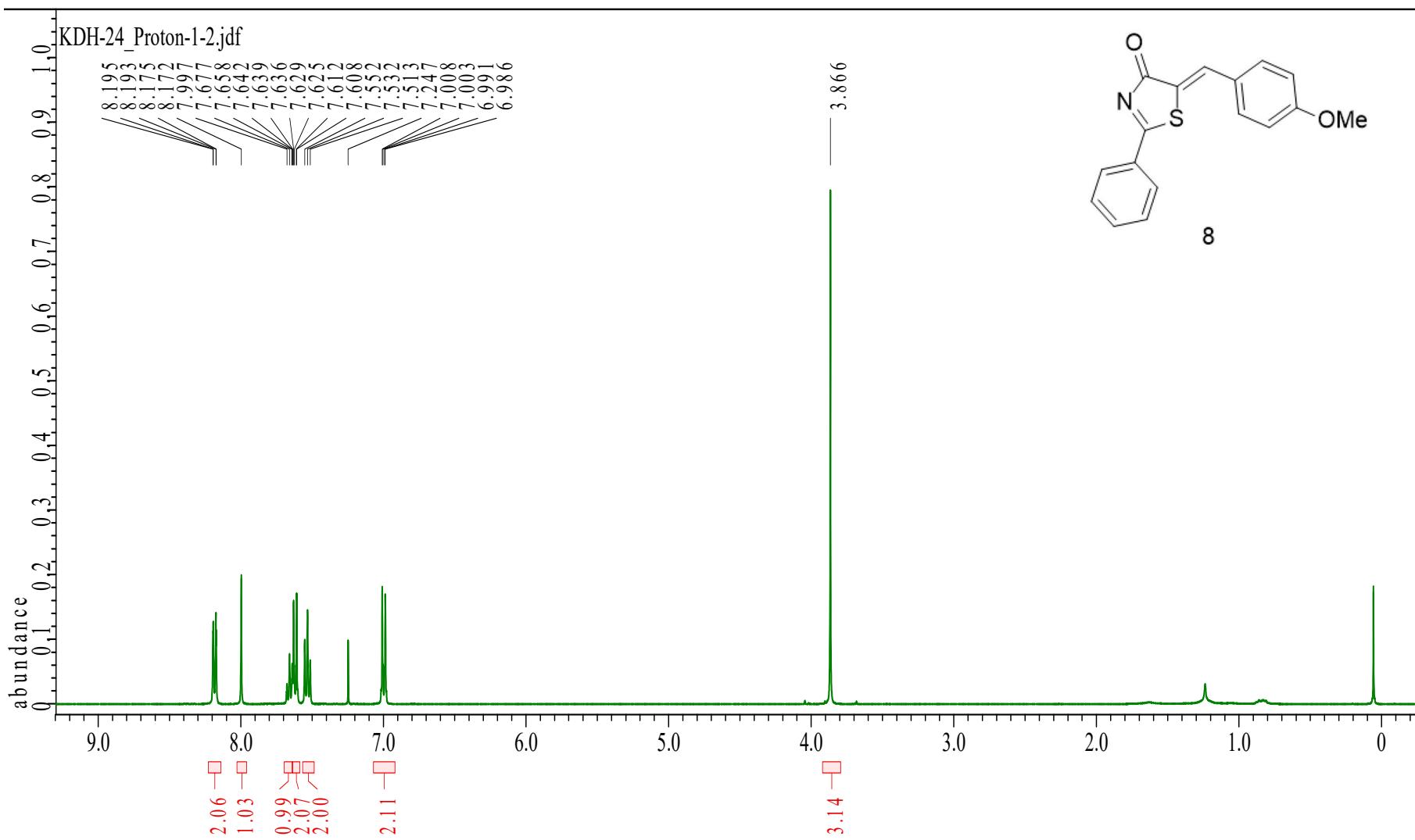


Figure S46. ¹H NMR spectrum of compound 8.

