

Supporting Information

For

(*E*)-1-(Furan-2-yl)-(substituted phenyl)prop-2-en-1 one derivatives as tyrosinase inhibitors

and melanogenesis inhibition: An *in vitro* and *in silico* study

Hee Jin Jung¹, Sang Gyun Noh¹, Il Young Ryu¹, Chaeun Park¹, Ji Young Lee¹, Pusoon Chun²,
Hyung Ryong Moon^{1,*}, Hae Young Chung^{1,*}

¹*College of Pharmacy, Pusan National University, Busan 46241, Republic of Korea.* ²*College of Pharmacy and Inje Institute of Pharmaceutical Sciences and Research, Inje University, Gimhae, Gyeongnam 50834, South Korea*

Contents

Fig. S1. ^1H NMR spectrum of compound 1	4
Fig. S2. ^{13}C NMR spectrum of compound 1	4
Fig. S3. ESI-MS spectrum of compound 1	5
Fig. S4. ^1H NMR spectrum of compound 2	6
Fig. S5. ^{13}C NMR spectrum of compound 2	6
Fig. S6. ESI-MS spectrum of compound 2	7
Fig. S7. ^1H NMR spectrum of compound 3	8
Fig. S8. ^{13}C NMR spectrum of compound 3	8
Fig. S9. ESI-MS spectrum of compound 3	9
Fig. S10. ^1H NMR spectrum of compound 4	10
Fig. S11. ^{13}C NMR spectrum of compound 4	10
Fig. S12. ESI-MS spectrum of compound 4	11
Fig. S13. ^1H NMR spectrum of compound 5	12
Fig. S14. ^{13}C NMR spectrum of compound 5	12
Fig. S15. ESI-MS spectrum of compound 5	13
Fig. S16. ^1H NMR spectrum of compound 6	14
Fig. S17. ^{13}C NMR spectrum of compound 6	14
Fig. S18. ESI-MS spectrum of compound 6	15
Fig. S19. ^1H NMR spectrum of compound 7	16
Fig. S20. ^{13}C NMR spectrum of compound 7	16
Fig. S21. ESI-MS spectrum of compound 7	17
Fig. S22. ^1H NMR spectrum of compound 8	18
Fig. S23. ^{13}C NMR spectrum of compound 8	18
Fig. S24. ESI-MS spectrum of compound 8	19

Fig. S25. ^1H NMR spectrum of compound **9**.....20

Fig. S26. ^{13}C NMR spectrum of compound **9**.....20

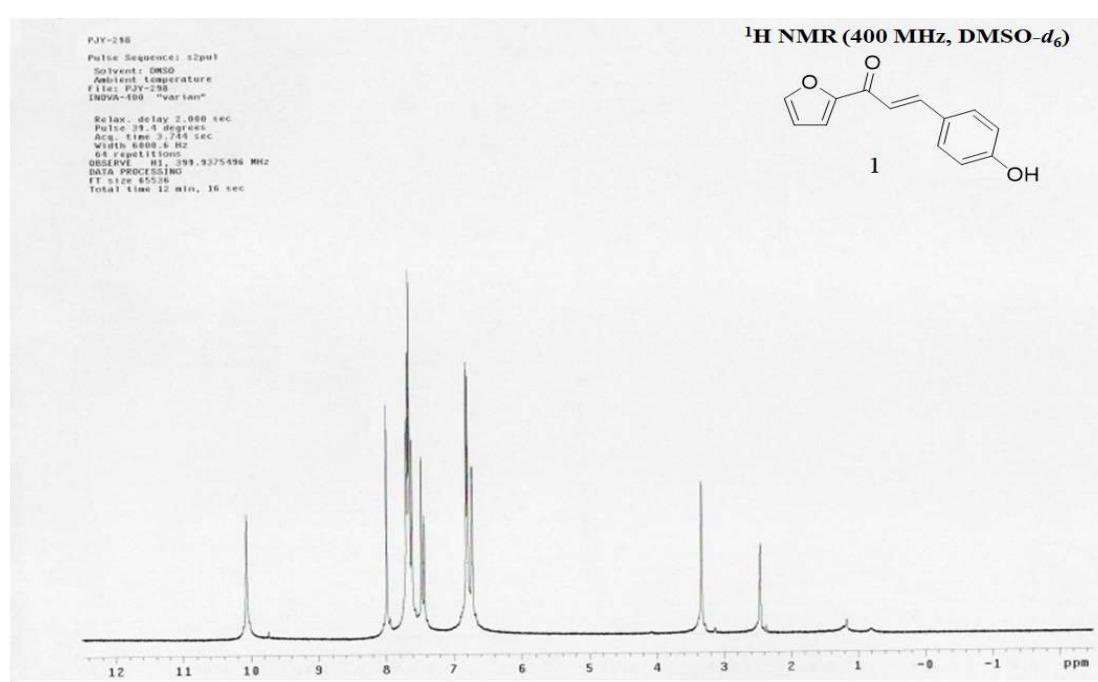


Fig. S1. ^1H -NMR spectrum of **1**.

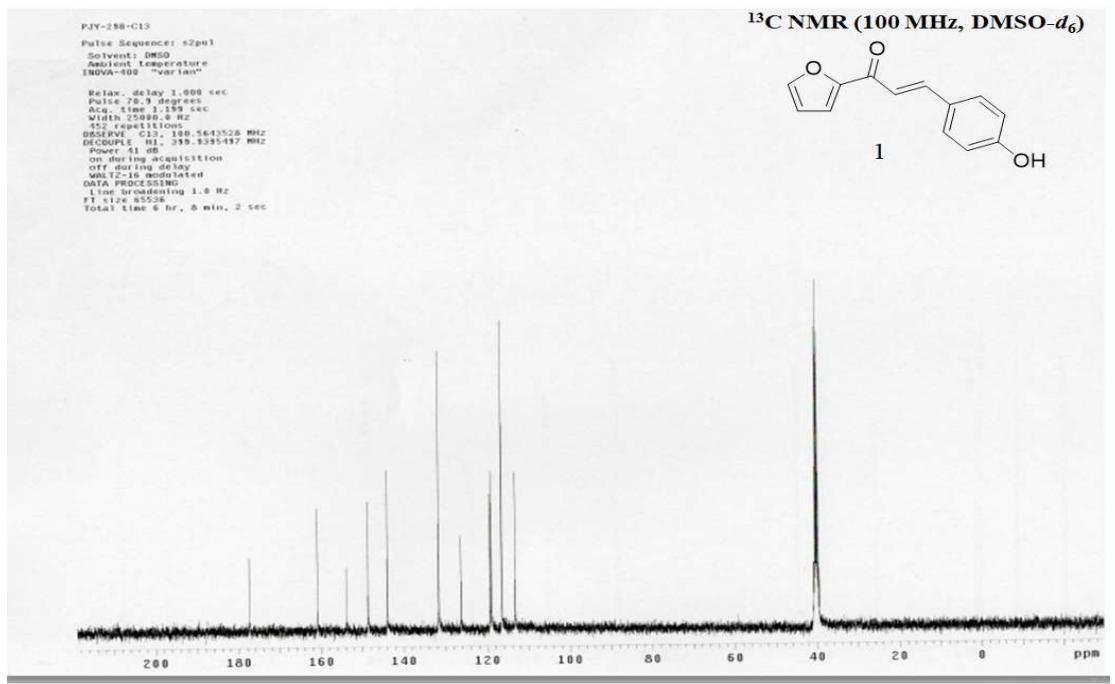


Fig. S2. ¹³C-NMR spectrum of **1**.

HRMS (ESI+) m/z C₁₃H₁₁O₃ (M+H)⁺ calcd 215.0703, obsd 215.0701.

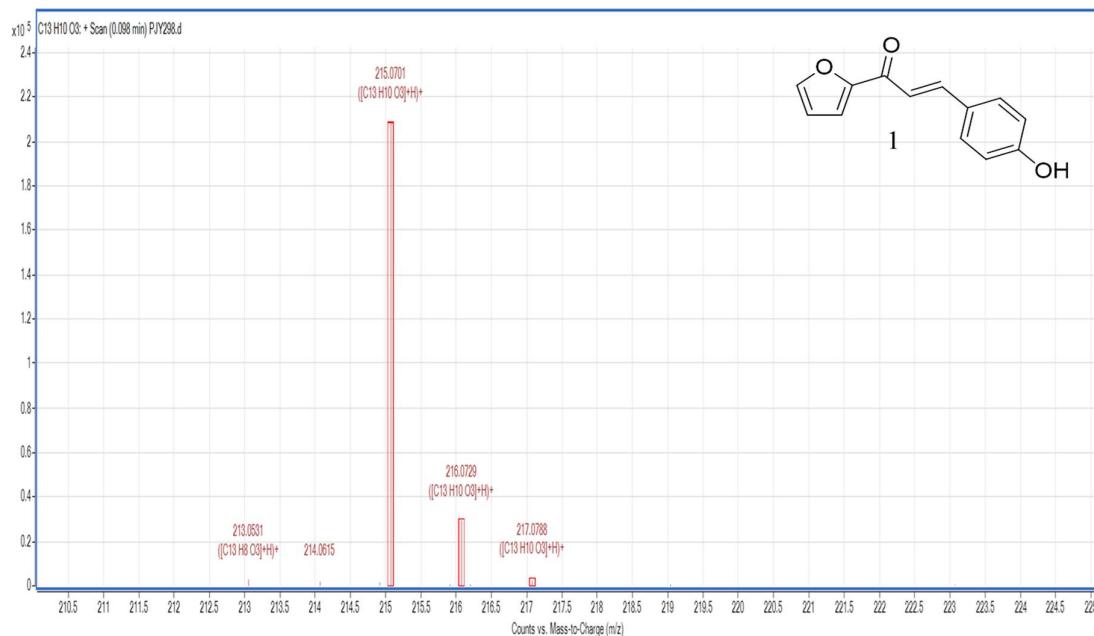


Fig. S3. ESI-MS spectrum of **1**.

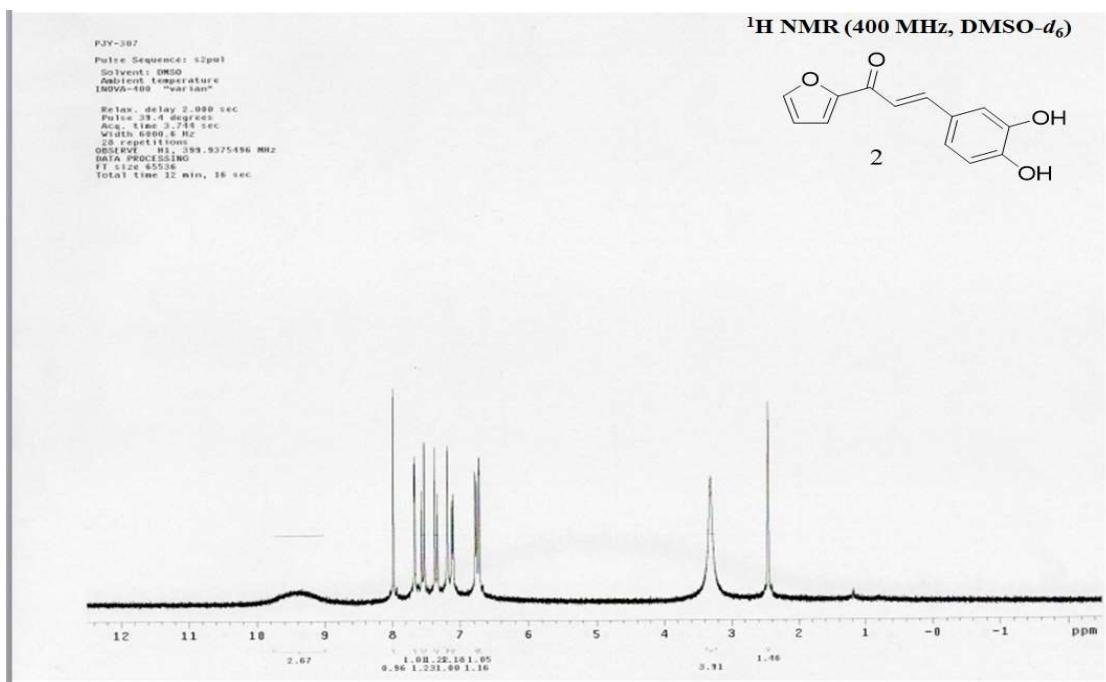


Fig. S4. ¹H-NMR spectrum of 2.

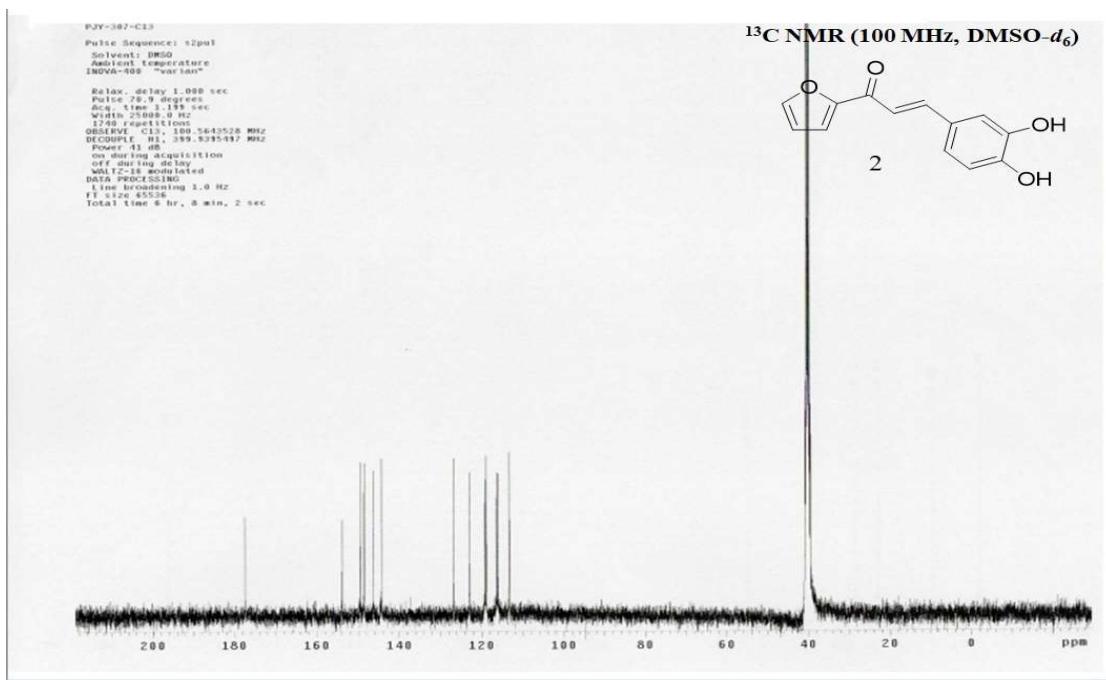


Fig. S5. ¹³C-NMR spectrum of 2.

HRMS (ESI+) m/z C₁₃H₁₁O₄ (M+H)⁺ calcd 231.0652, obsd 231.0643.

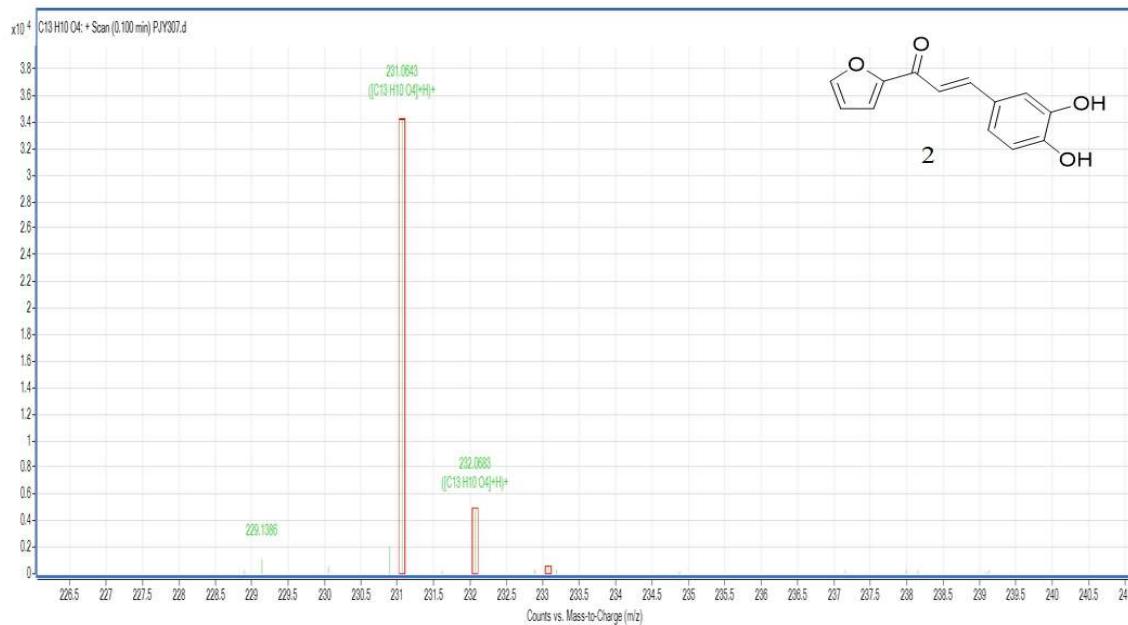


Fig. S6. ESI-MS spectrum of **2**.

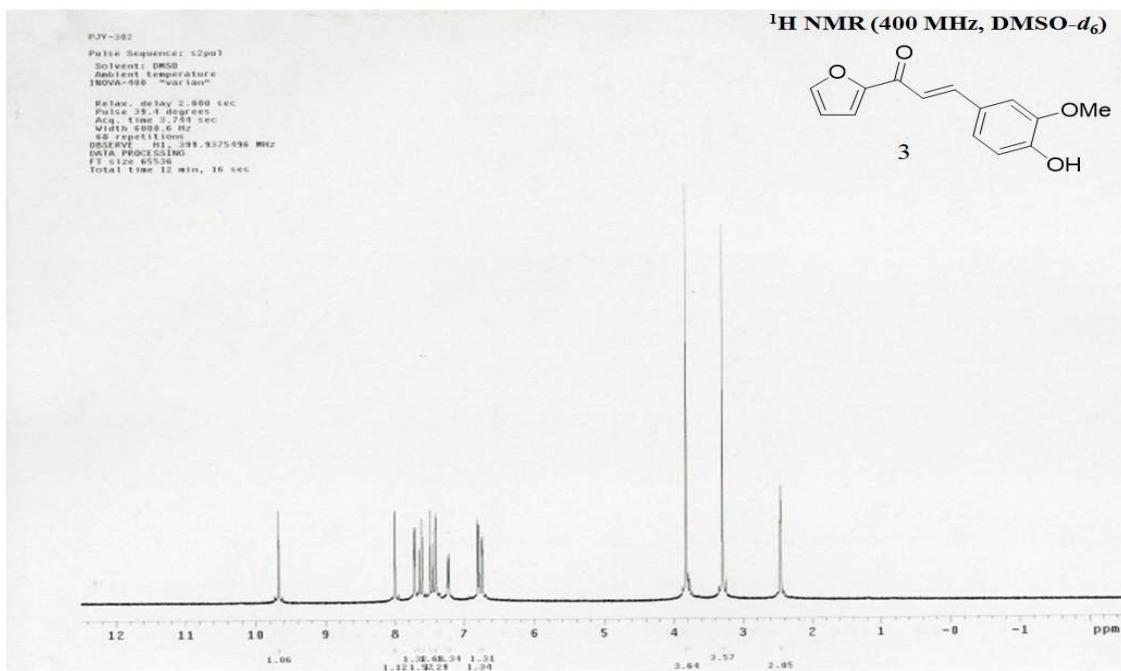


Fig. S7. ^1H -NMR spectrum of 3.

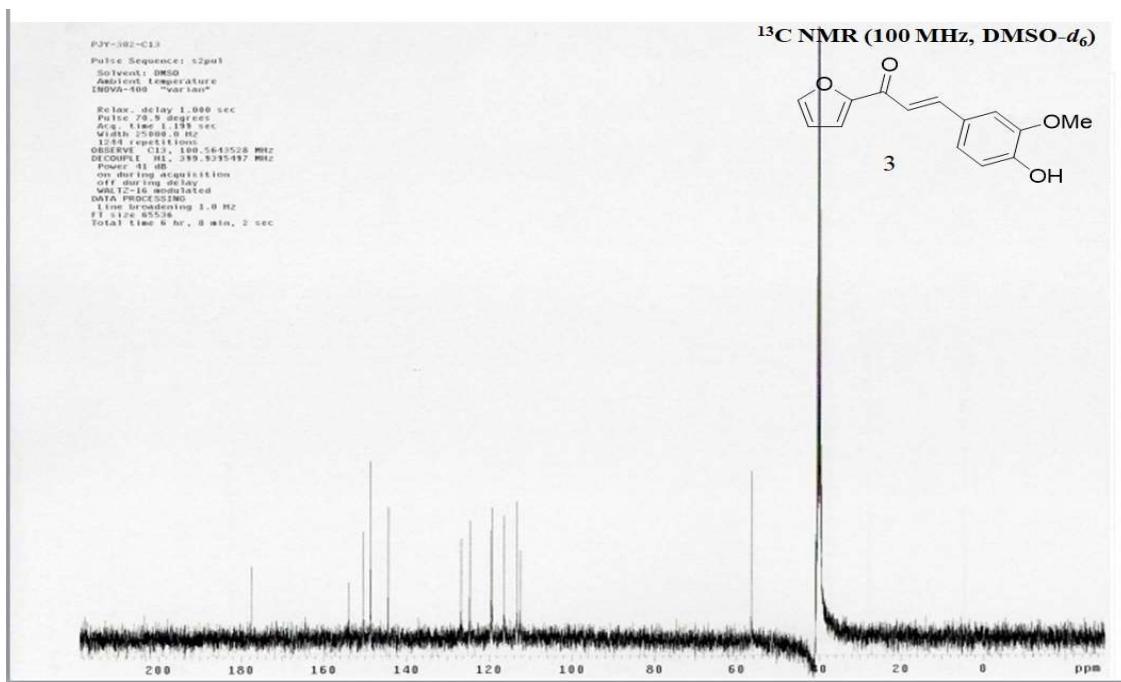


Fig. S8. ^{13}C -NMR spectrum of 3.

HRMS (ESI+) m/z C₁₄H₁₃O₄ (M+H)⁺ calcd 245.0808, obsd 245.0806.

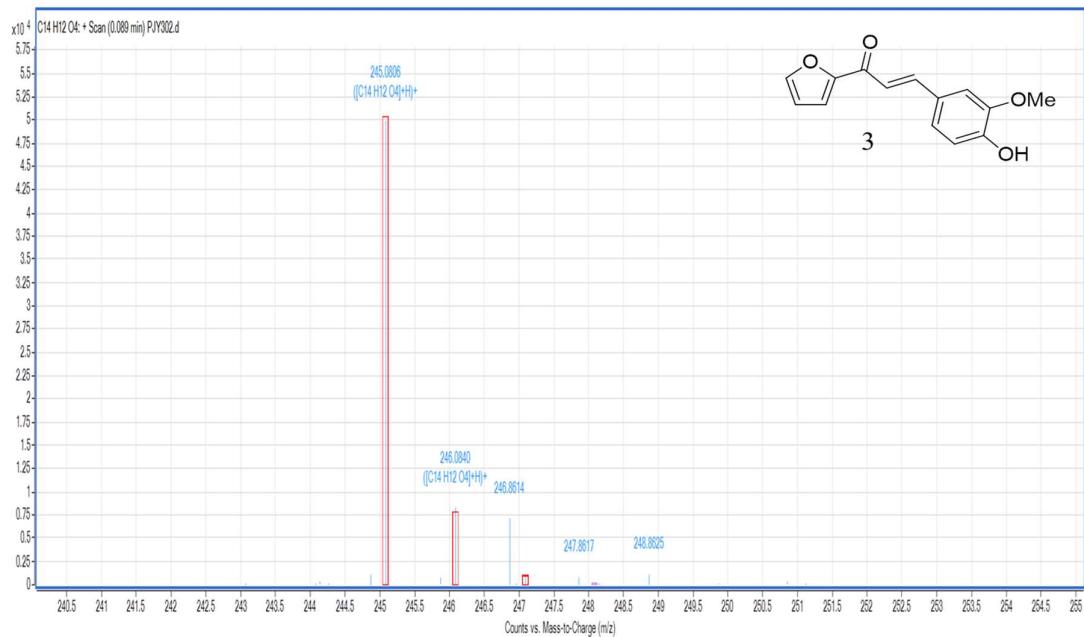


Fig. S9. ESI-MS spectrum of 3.

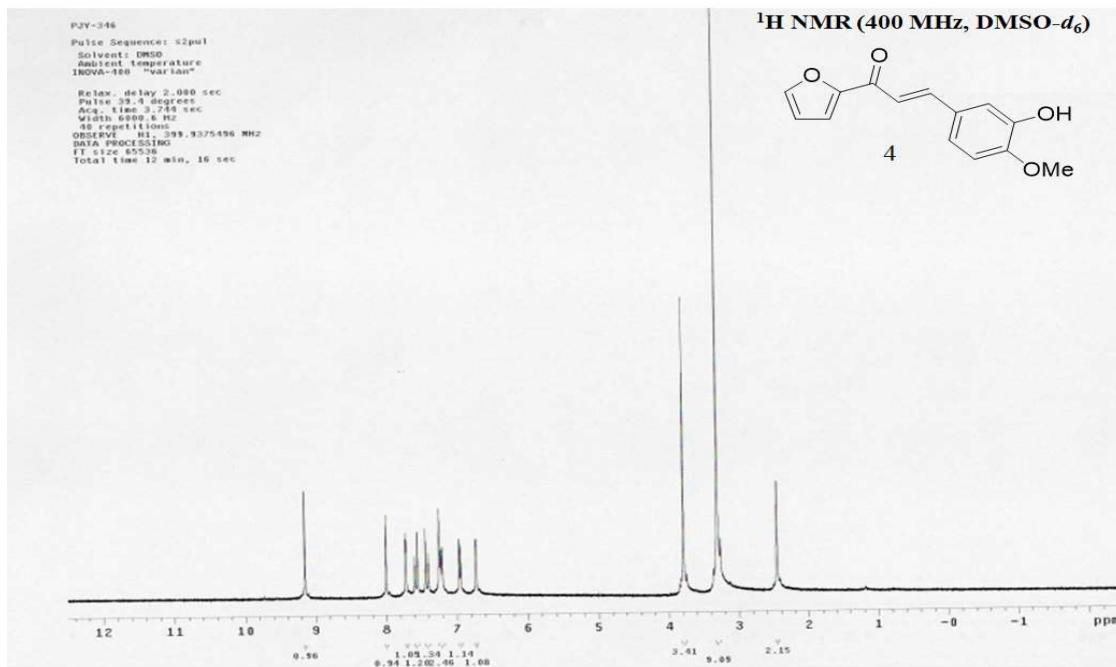


Fig. S10. ¹H-NMR spectrum of 4.

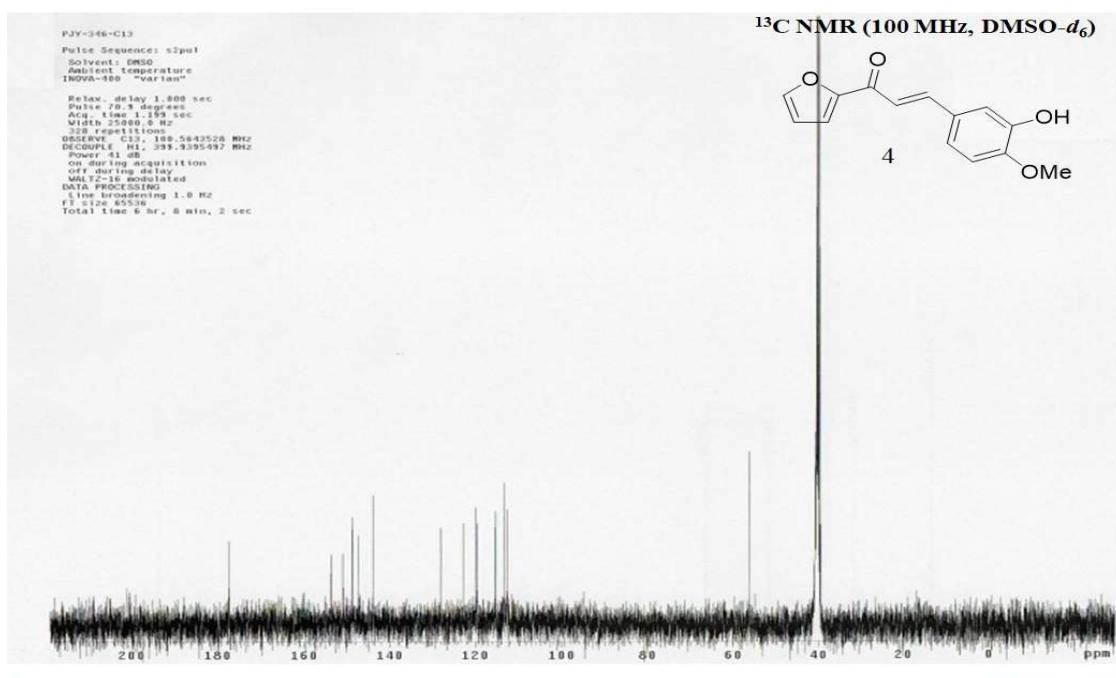


Fig. S11. ¹³C-NMR spectrum of 4.

HRMS (ESI+) m/z C₁₄H₁₃O₄ (M+H)⁺ calcd 245.0808, obsd 245.0802.

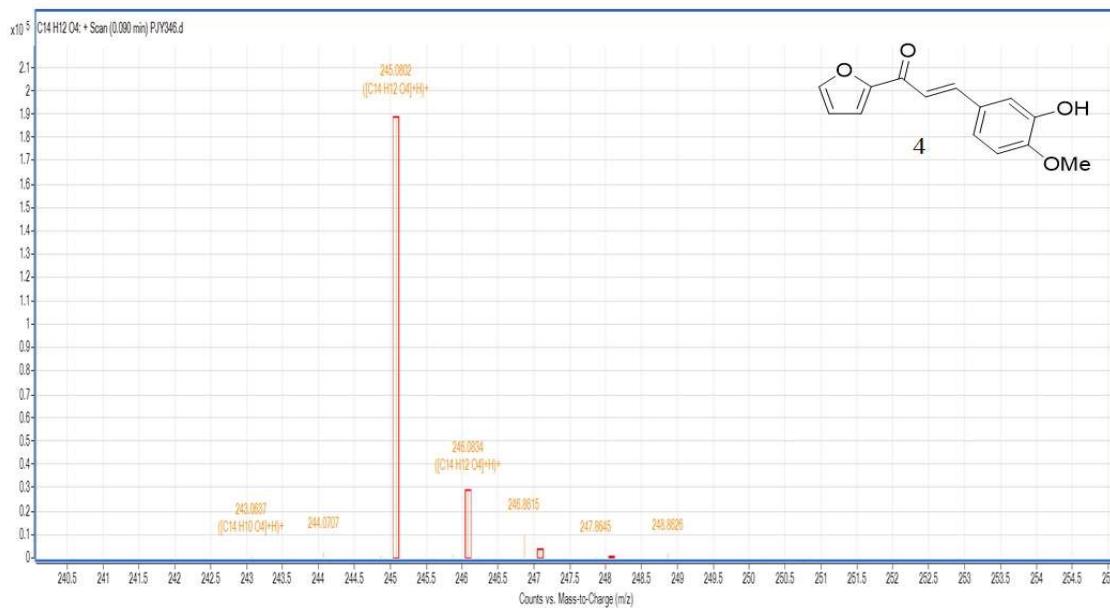


Fig. S12. ESI-MS spectrum of 4.

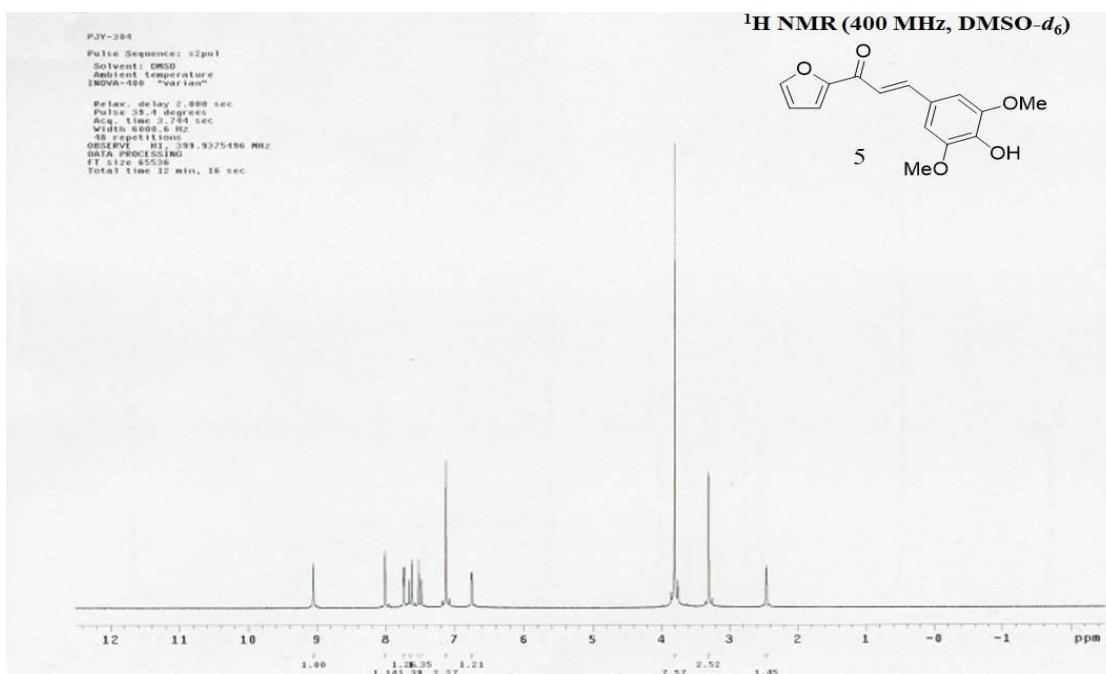


Fig. S13. ¹H-NMR spectrum of 5.

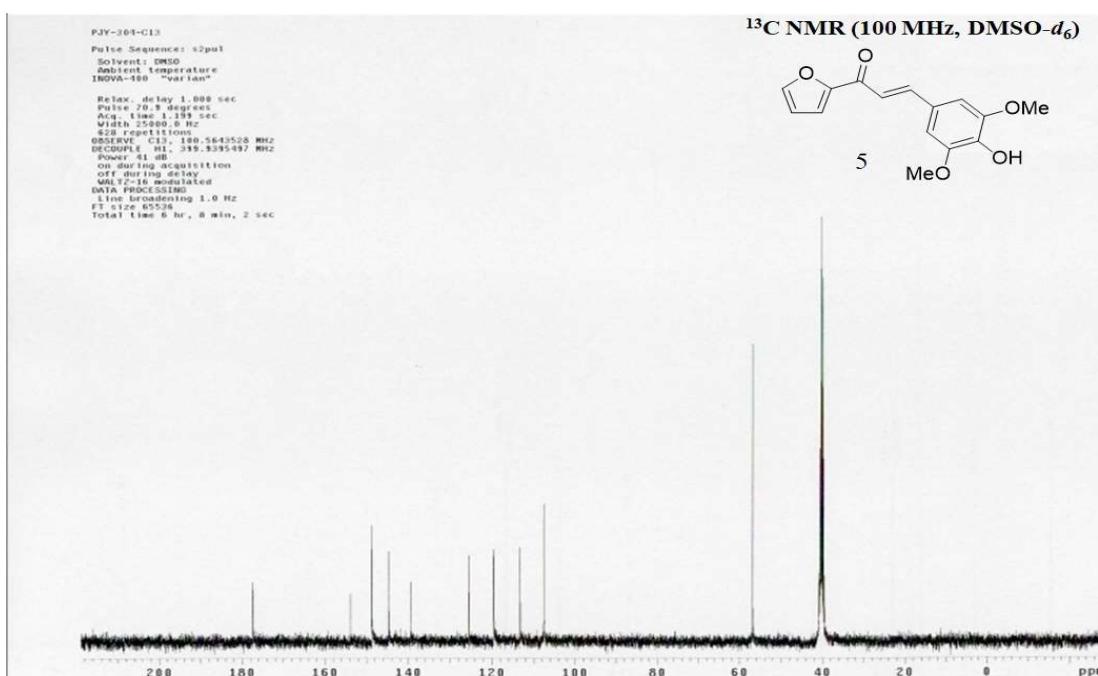


Fig. S14. ¹³C-NMR spectrum of 5.

HRMS (ESI+) m/z C₁₅H₁₅O₅ (M+H)⁺ calcd 275.0914, obsd 275.0906.

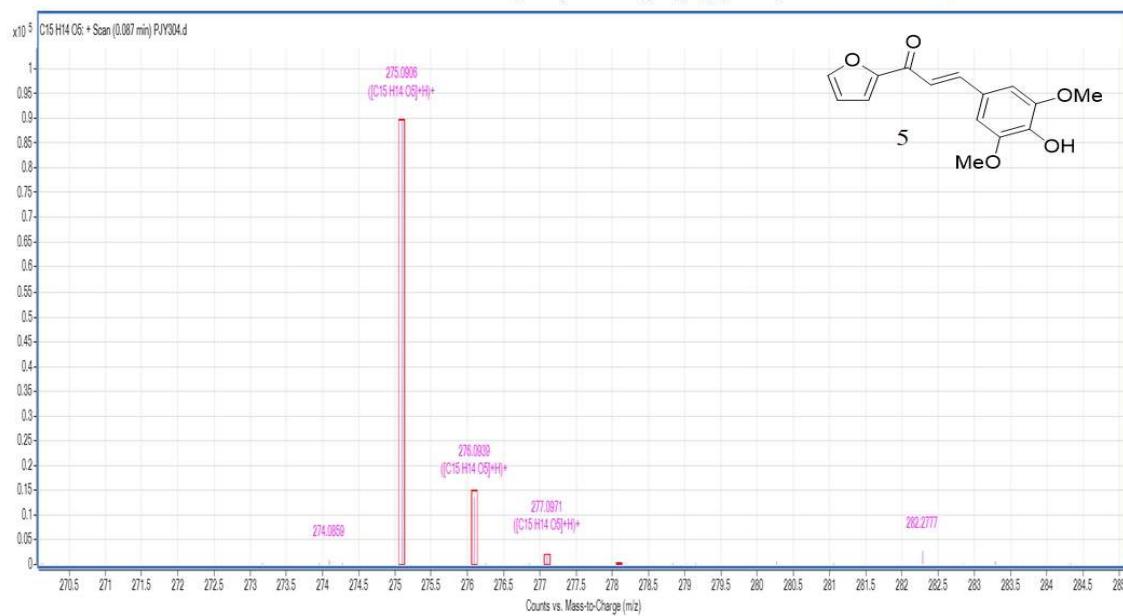


Fig. S15. ESI-MS spectrum of **5**.

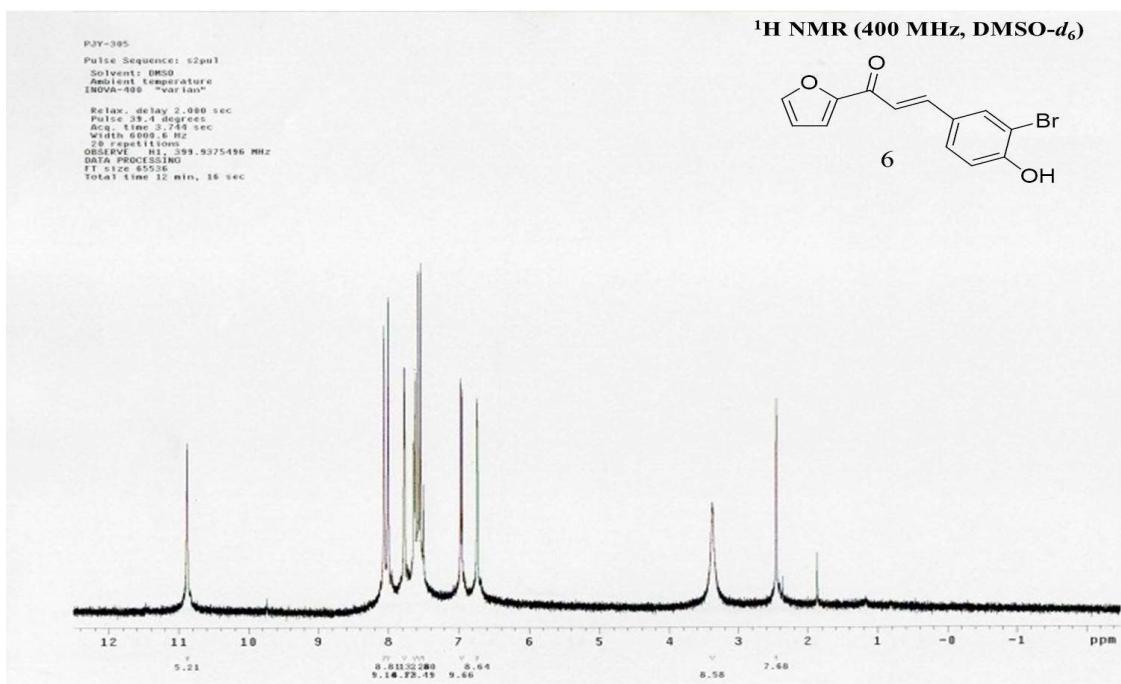


Fig. S16. ¹H-NMR spectrum of 6.

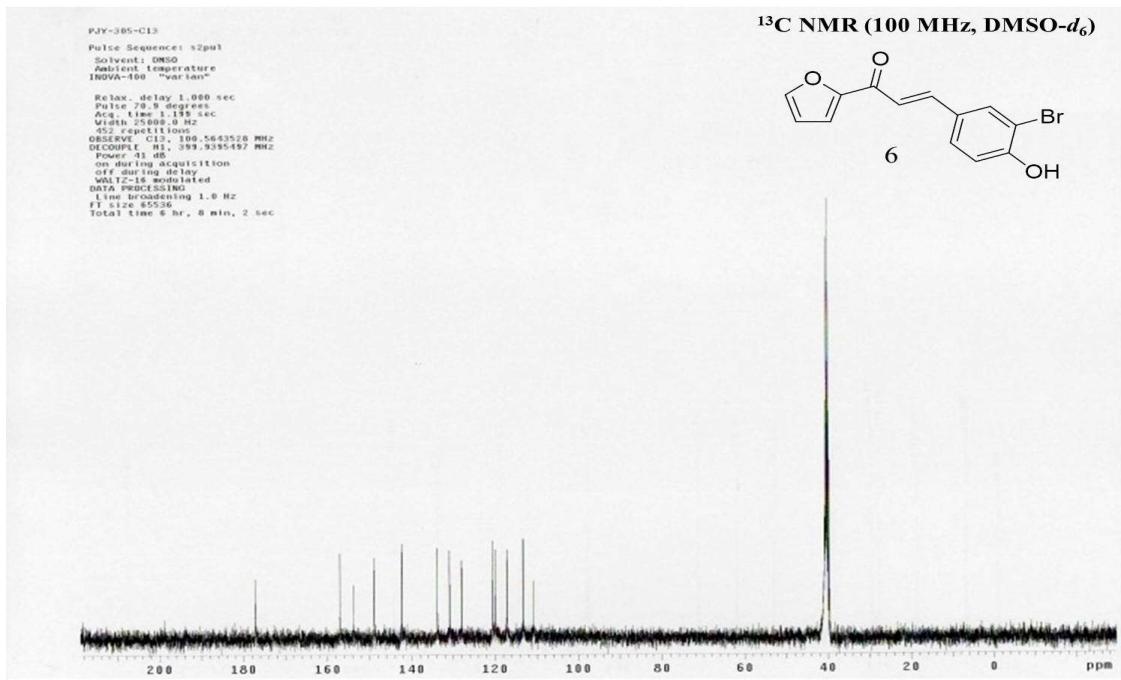


Fig. S17. ¹³C-NMR spectrum of 6.

HRMS (ESI+) m/z C₁₃H₁₀BrO₃ (M+H)⁺ calcd 292.9808, obsd 292.9802, C₁₃H₁₀BrO₃ (M+2+H)⁺ calcd 294.9789, obsd 294.9787.

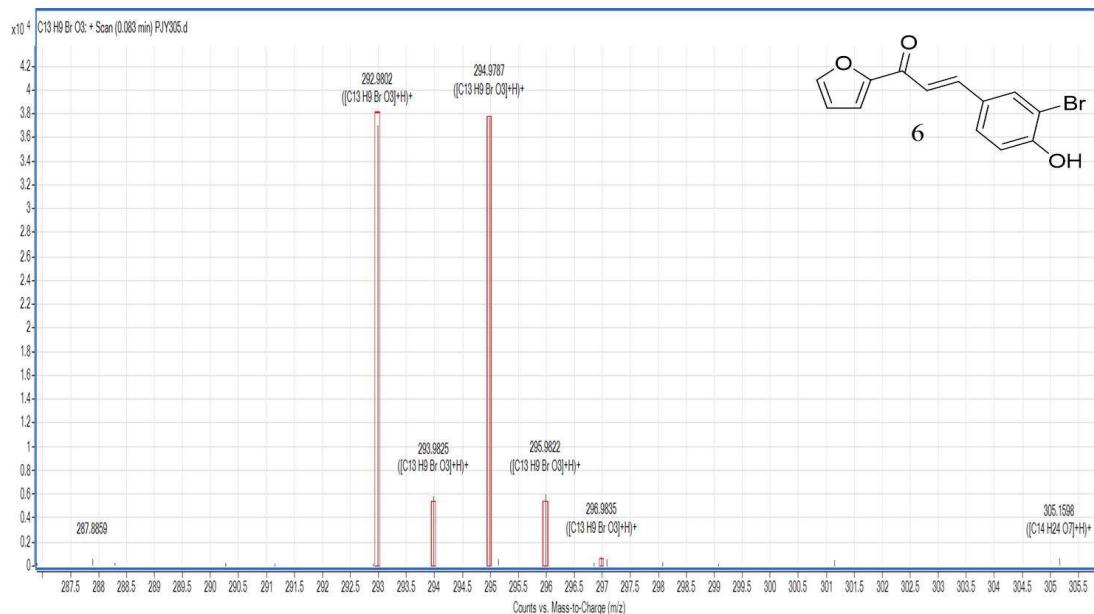


Fig. S18. ESI-MS spectrum of **6**.

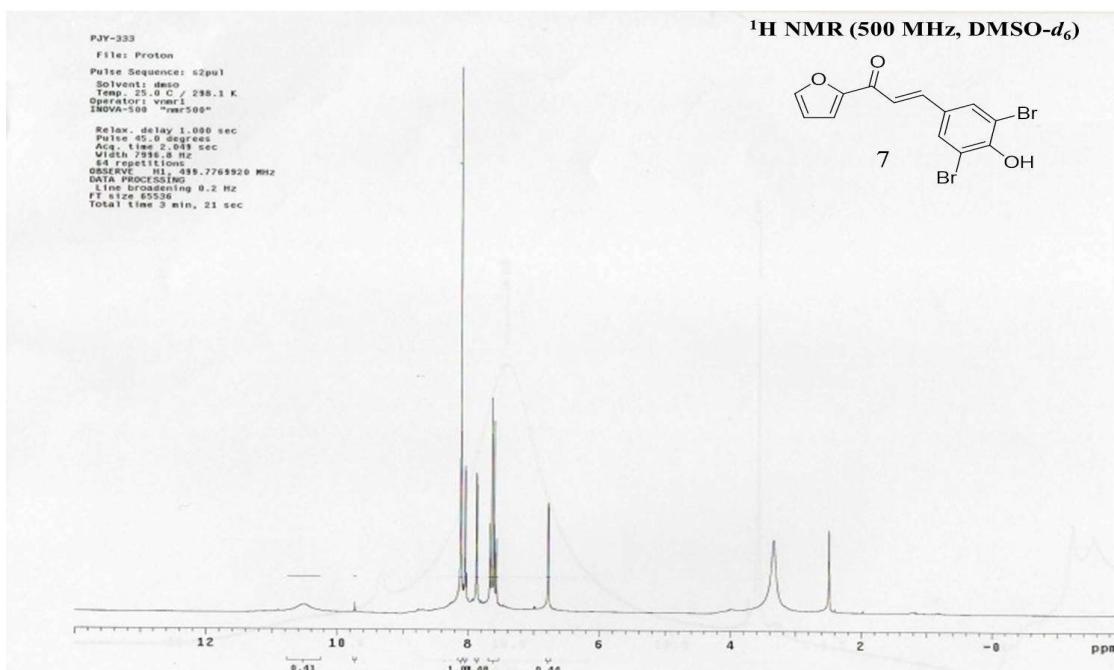


Fig. S19. ¹H-NMR spectrum of 7.

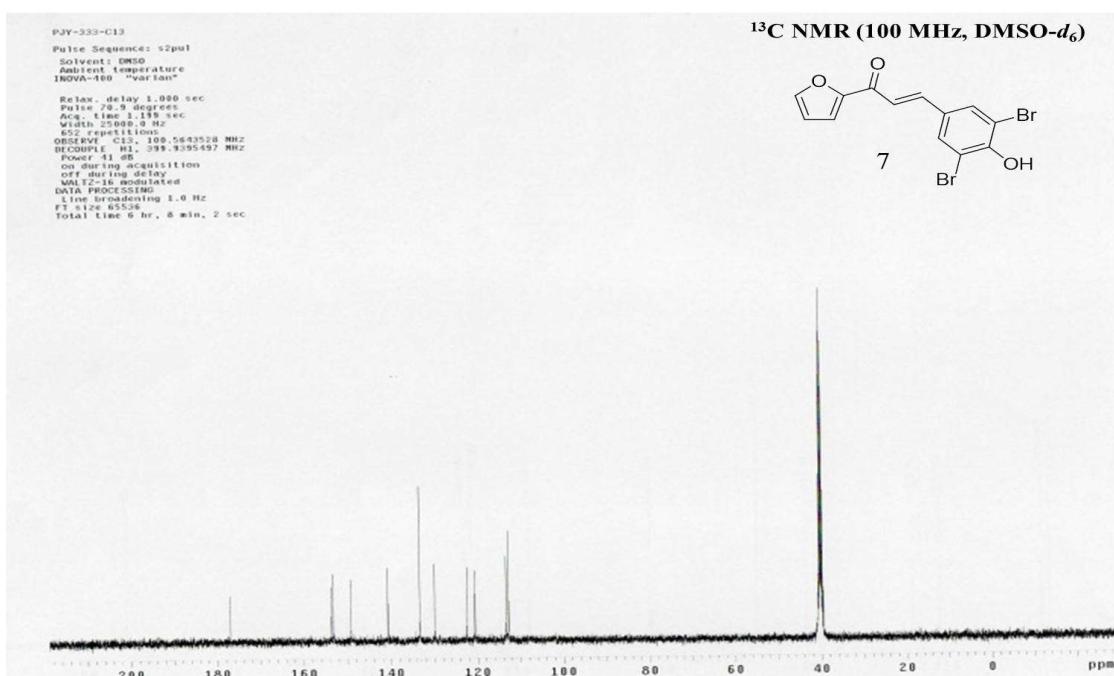


Fig. S20. ¹³C-NMR spectrum of 7.

HRMS (ESI+) m/z $C_{13}H_9Br_2O_3$ ($M+H$)⁺ calcd 370.8913, obsd 370.8900, $C_{13}H_9Br_2O_3$ ($M+2+H$)⁺ calcd 372.8893, obsd 372.8880, $C_{13}H_9Br_2O_3$ ($M+4+H$)⁺ calcd 374.8874, obsd 374.8861.

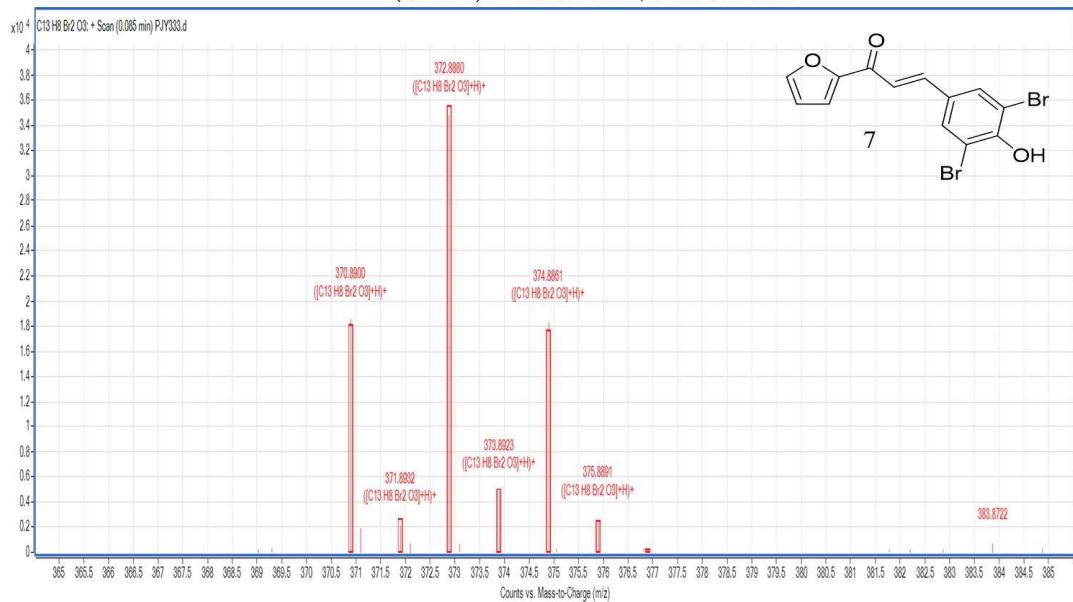


Fig. S21. ESI-MS spectrum of 7.

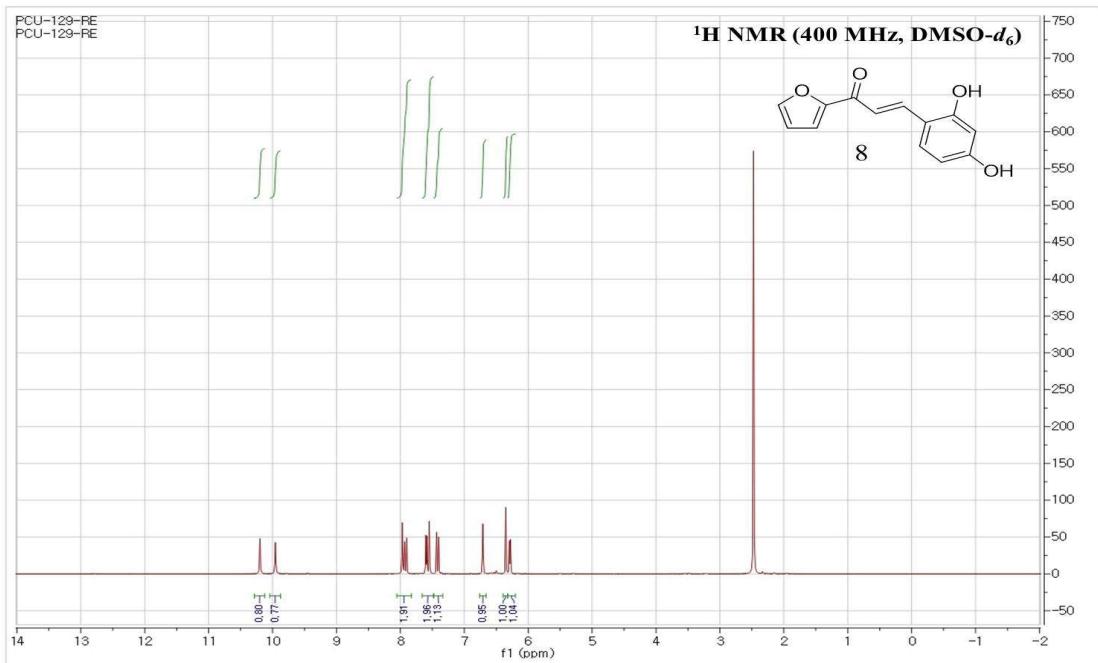


Fig. S22. ¹H-NMR spectrum of 8.

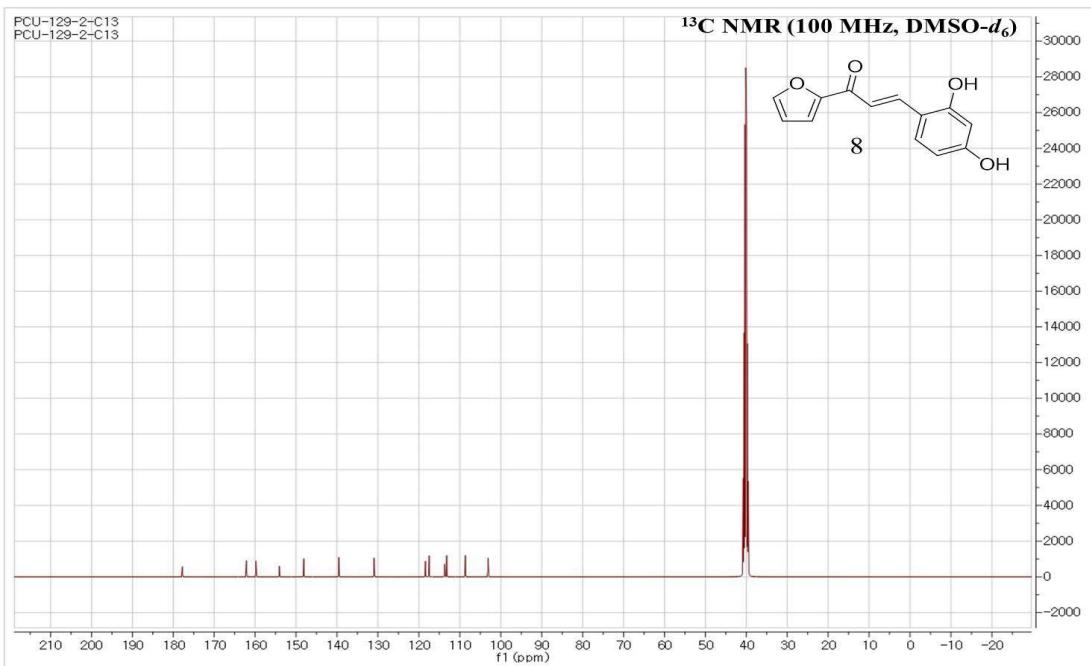


Fig. S23. ¹³C-NMR spectrum of 8.

LRMS (ESI-) m/z C₁₃H₁₀O₄ (M-H)⁻ calcd 230.06, obsd 299.08.

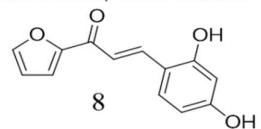
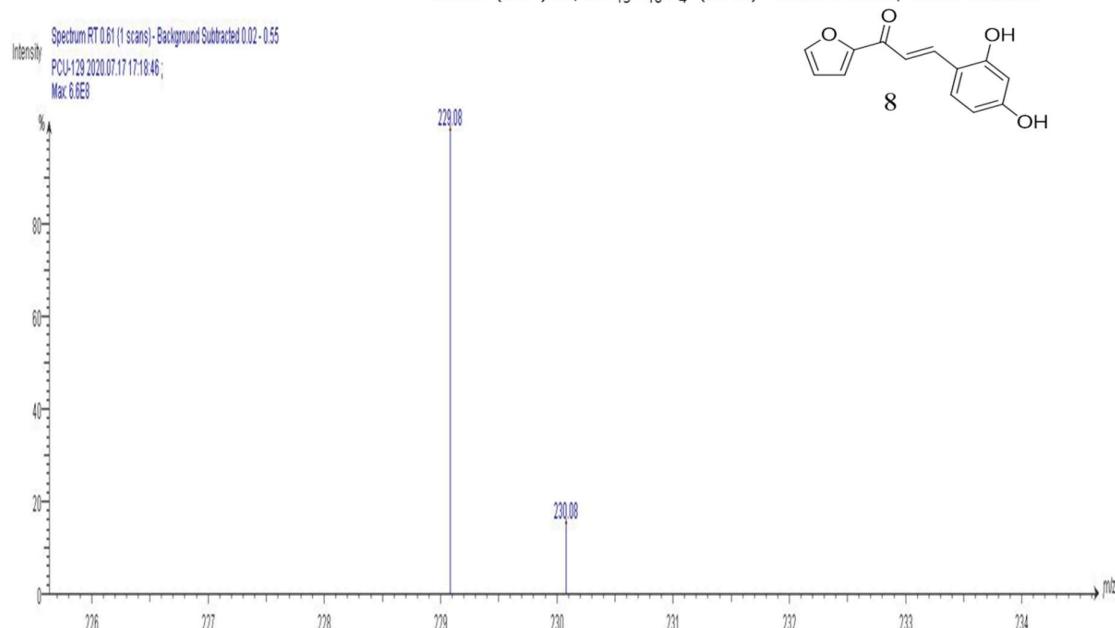


Fig. S24. ESI-MS spectrum of **8**

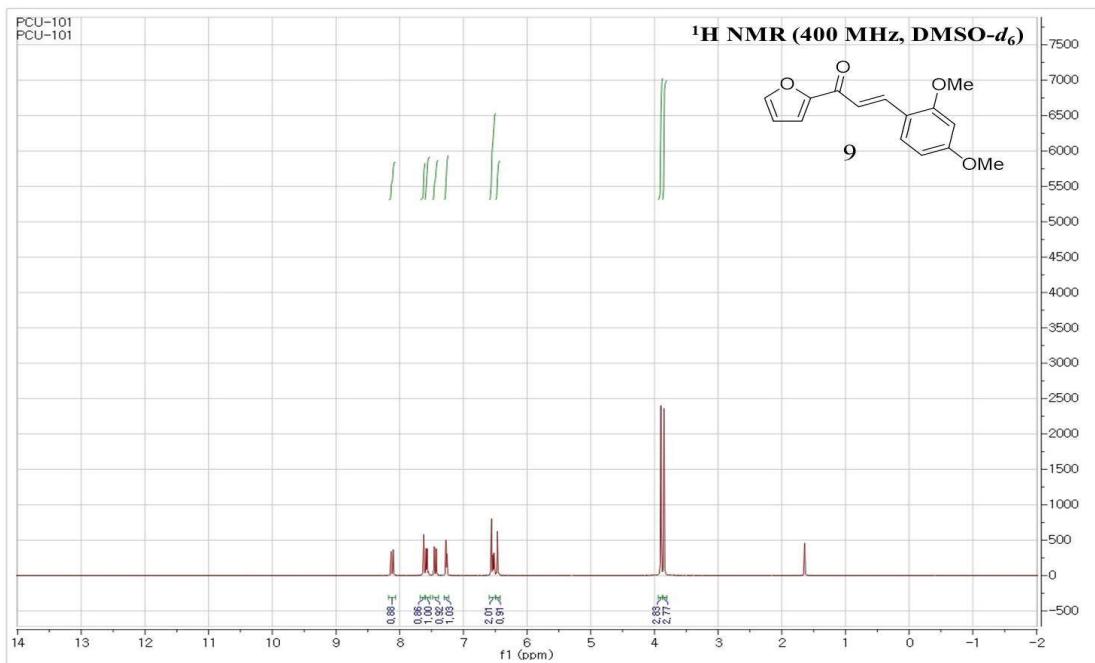


Fig. S25. ¹H-NMR spectrum of **9**.

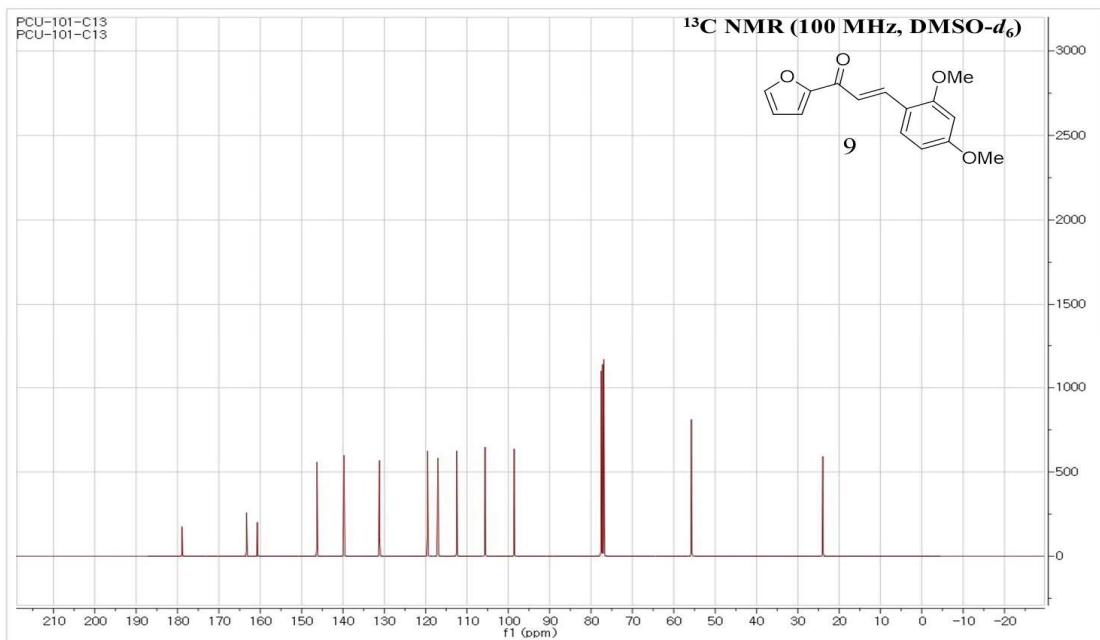


Fig. S26. ¹³C-NMR spectrum of **9**.