

*Supporting Information for*

**Identification of Chalcone Analogues as Anti-  
Inflammatory Agents through Regulation of NF- $\kappa$ B  
and JNK Activation**

Die Zhang<sup>1,‡</sup>, Wenping Wang<sup>1,‡</sup>, Huiping Ou<sup>1, 2‡</sup>, Jinhua Ning<sup>1</sup>, Yingxun Zhou<sup>1</sup>, Jin Ke<sup>1</sup>, Anguo Hou<sup>1</sup>, Linyun Chen<sup>1</sup>, Peng Li<sup>2, 3\*</sup>, Yunshu Ma<sup>1\*</sup> and Wen Bin Jin<sup>1, 3\*</sup>

1 Key Laboratory of External Drug Delivery System and Preparation Technology in Universities of Yunnan and Faculty of Chinese Materia Medica, Yunnan University of Chinese Medicine, Kunming, Yunnan, China

2 School of Food and Drug, Shenzhen Polytechnic University, Shenzhen, Guangdong, China

3 State Key Laboratory of Chemical Biology and Drug Discovery and Department of Applied Biology and Chemical Technology, The Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong SAR, China

‡These authors contributed equally.

\*Corresponding authors: Yunshu Ma, Peng Li and Wenbin Jin

For Y. S. M., email: [yunshuma2@126.com](mailto:yunshuma2@126.com)

For L. P., email: [lipengwd@szpt.edu.cn](mailto:lipengwd@szpt.edu.cn)

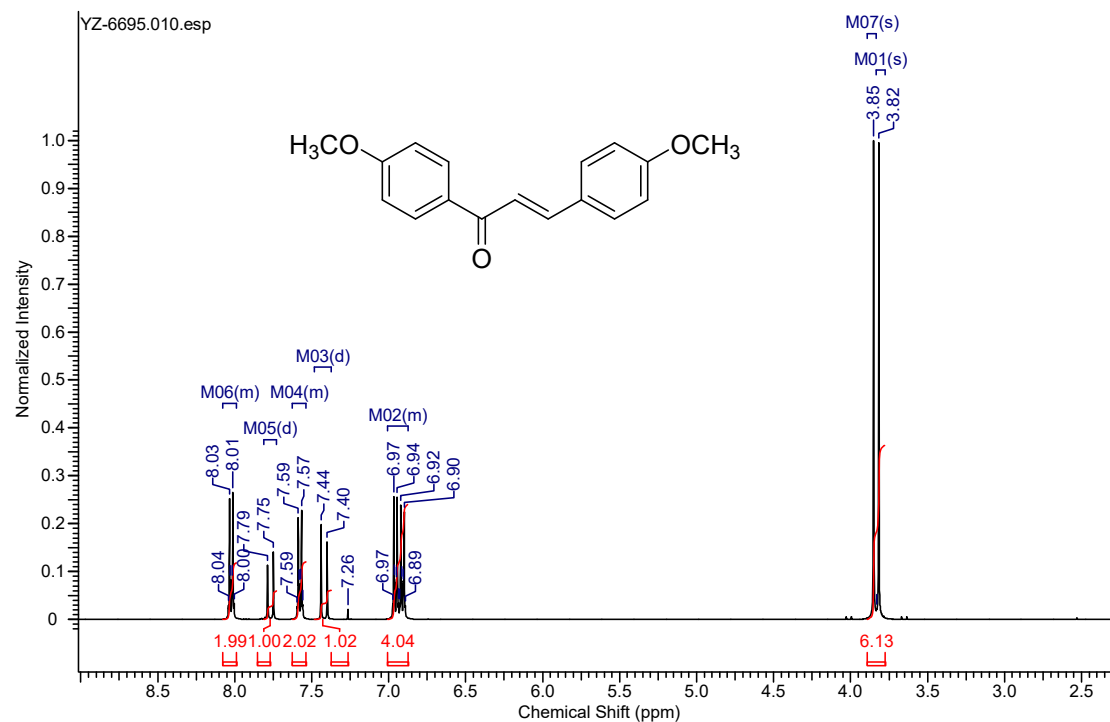
For W. B. J., email: [14900326r@connect.polyu.hk](mailto:14900326r@connect.polyu.hk)

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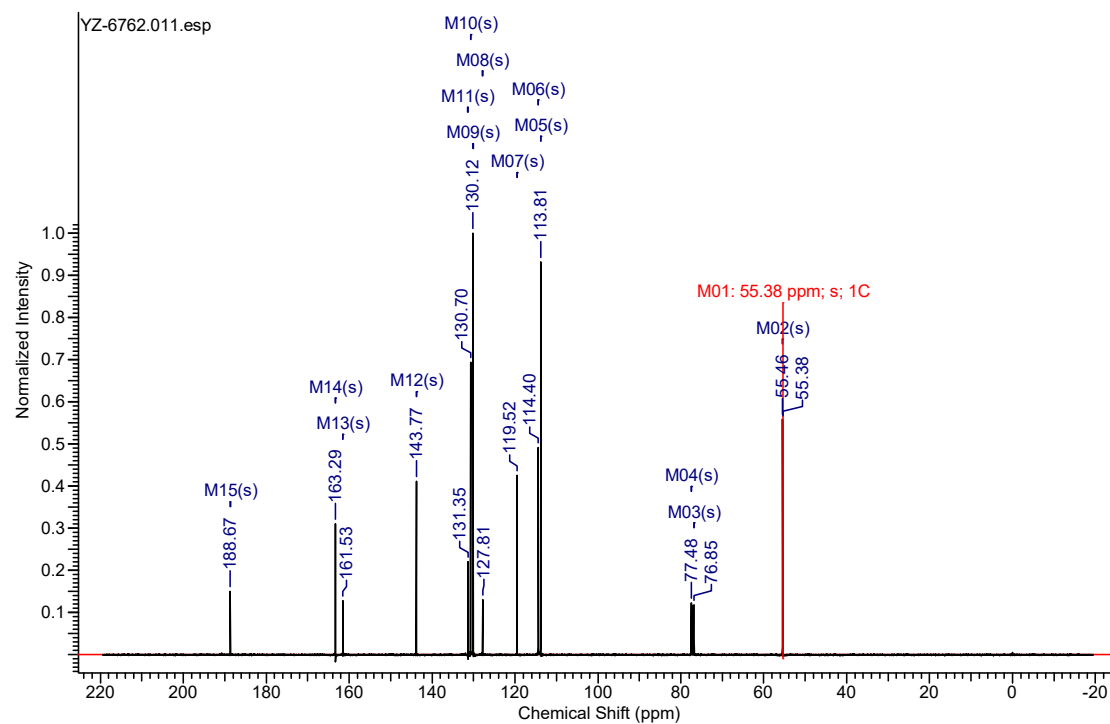
- Figure S1-S28**  $^1\text{H}$  and  $^{13}\text{C}$  spectra of compounds **3a-3n**, and **4a-4n**.  
**Figure S29-S56** HPLC-purity spectra of compounds **3a-3n**, and **4a-4n**.  
**Figure S57-S64** FT-IR spectra of compounds **3e**, **3j**, **4d**, **4e**, **4i**, **4j**, **4m**, and **4n**

**Figure S1.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **(E)-1,3-bis(4-methoxyphenyl)prop-2-en-1-one(3a)**<sup>1</sup>

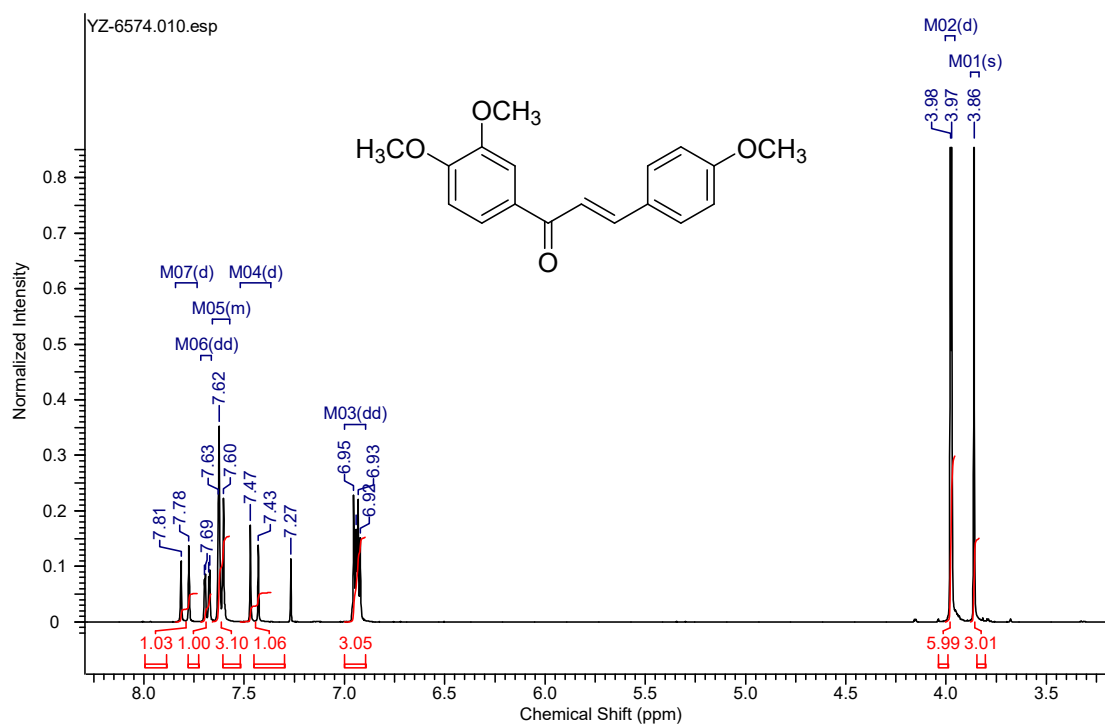
$^1\text{H}$  NMR (400 MHz, CHLOROFORM-*d*)  $\delta$  ppm 3.85 (s, 3 H) 3.82 (s, 3 H) 6.88 - 7.01 (m, 4 H) 7.42 (d,  $J=15.65$  Hz, 1 H) 7.54 - 7.63 (m, 2 H) 7.77 (d,  $J=15.65$  Hz, 1 H) 7.99 - 8.08 (m, 2 H)



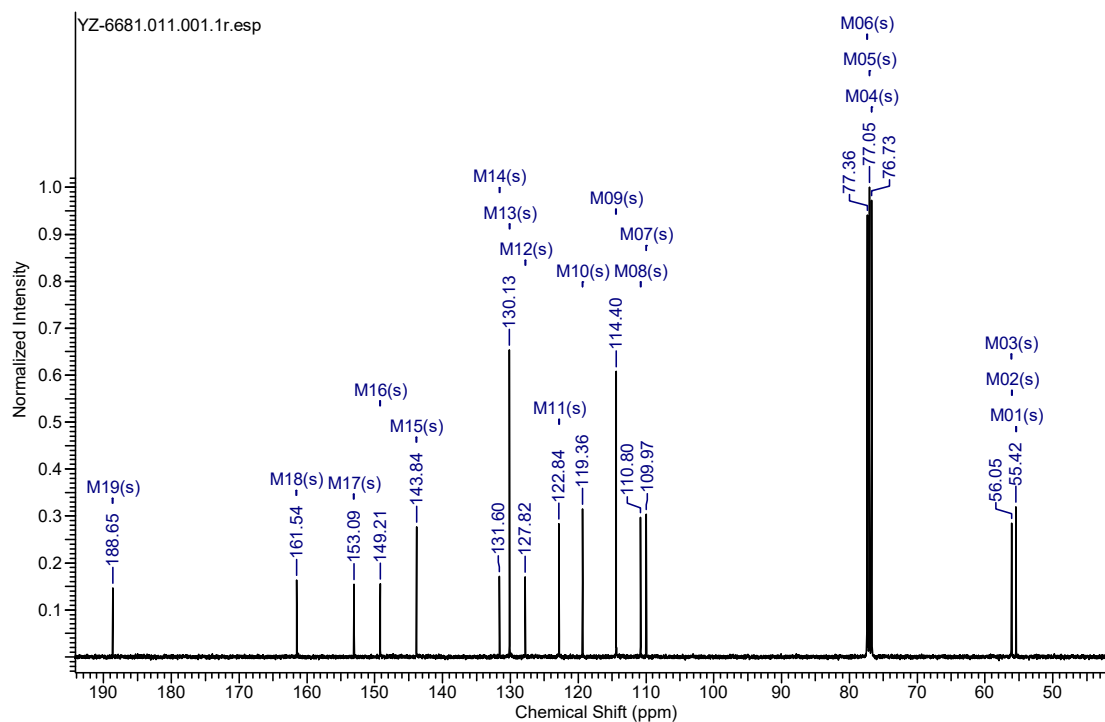
$^{13}\text{C}$  NMR (101 MHz, CHLOROFORM-*d*)  $\delta$  188.7, 163.3, 161.5, 143.8, 131.3, 130.7, 130.1, 127.8, 119.5, 114.4, 113.8, 77.5, 76.8, 55.5, 55.4



**Figure S2.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **(E)-1-(3,4-dimethoxyphenyl)-3-(4-methoxyphenyl)prop-2-en-1-one(3b)**<sup>1</sup>

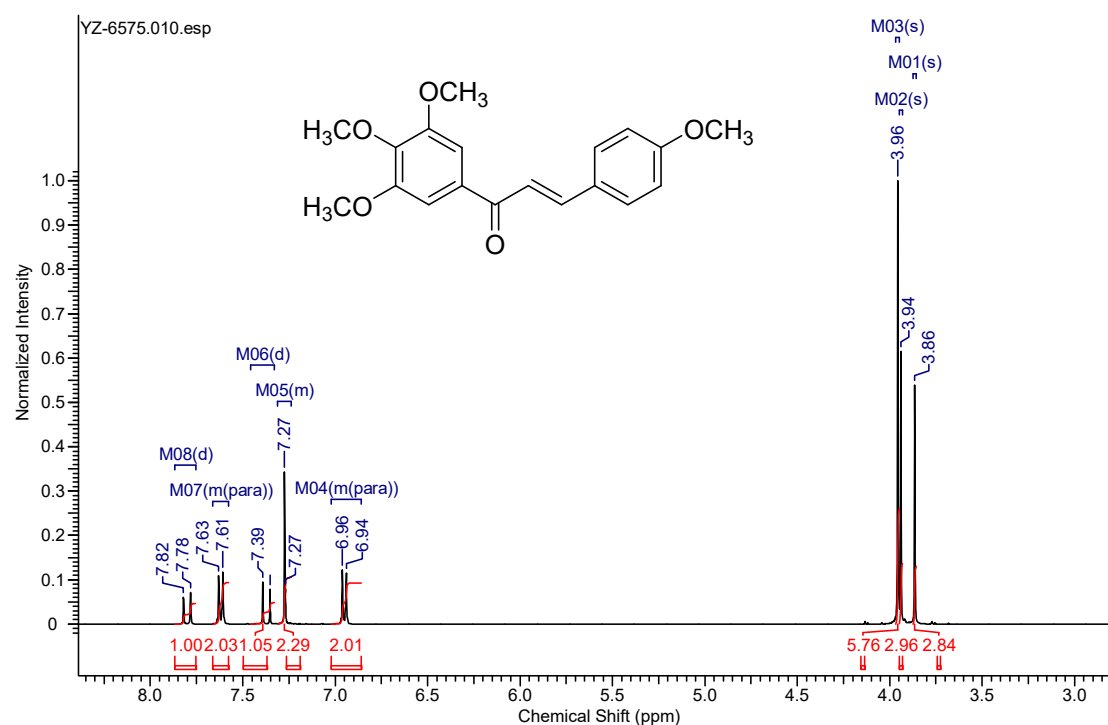


$^1\text{H}$  NMR (400 MHz, CHLOROFORM- $d$ )  $\delta$  7.80 (d,  $J = 15.41$  Hz, 1H), 7.68 (dd,  $J = 1.83, 8.44$  Hz, 1H), 7.57 - 7.66 (m, 3H), 7.45 (d,  $J = 15.65$  Hz, 1H), 6.94 (dd,  $J = 4.40, 8.56$  Hz, 3H), 3.97 (d,  $J = 2.69$  Hz, 6H), 3.86 (s, 3H)

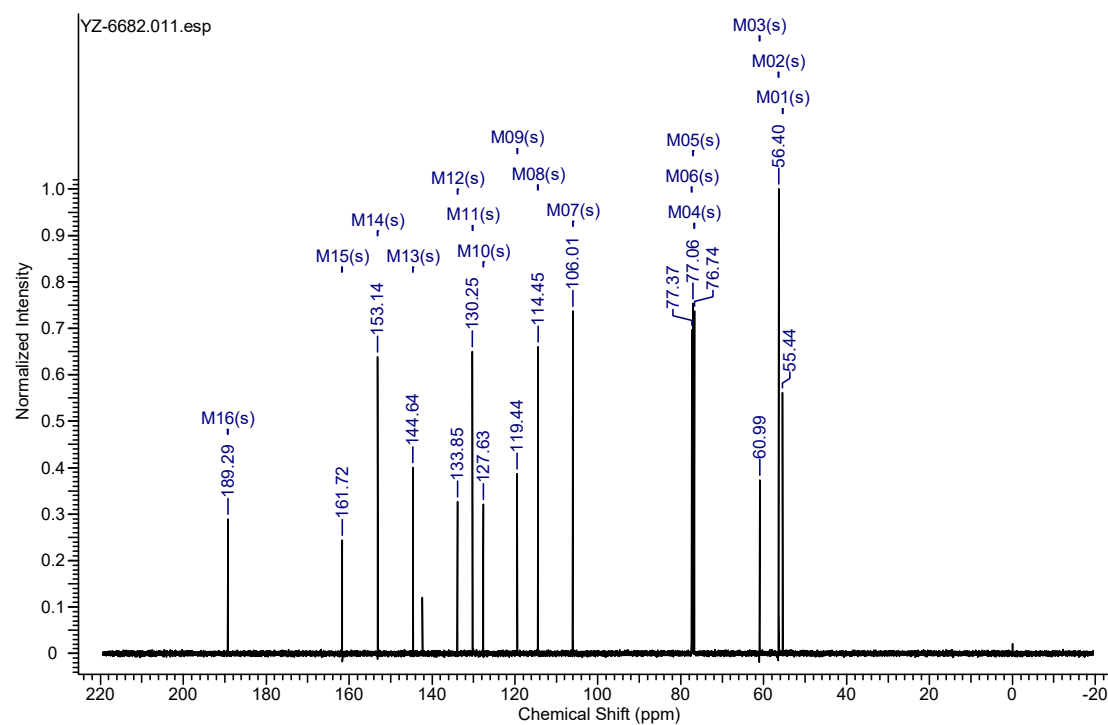


$^{13}\text{C}$  NMR (101 MHz, CHLOROFORM- $d$ )  $\delta$  188.6, 161.5, 153.1, 149.2, 143.8, 131.6, 130.1, 127.8, 122.8, 119.4, 114.4, 110.8, 110.0, 77.4, 77.0, 76.7, 56.1, 56.1, 55.4

**Figure S3.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of (E)-3-(4-methoxyphenyl)-1-(3,4,5-trimethoxyphenyl)prop-2-en-1-one(3c) $^2$

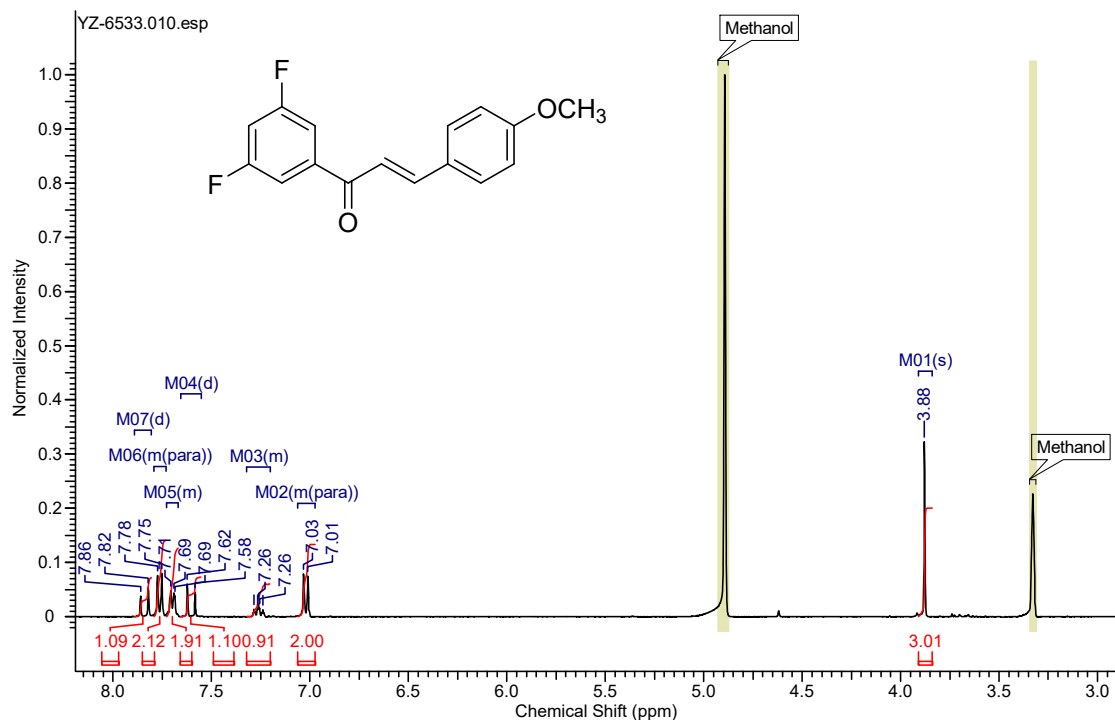


$^1\text{H}$  NMR (400 MHz, CHLOROFORM- $d$ )  $\delta$  7.80 (d,  $J = 15.41$  Hz, 1H), 7.58 - 7.66 (m,  $J = 8.80$  Hz, 2H), 7.37 (d,  $J = 15.65$  Hz, 1H), 7.24 - 7.31 (m, 2H), 6.86 - 7.02 (m,  $J = 8.80$  Hz, 2H), 3.96 (s, 6H), 3.94 (s, 3H), 3.86 (s, 3H)

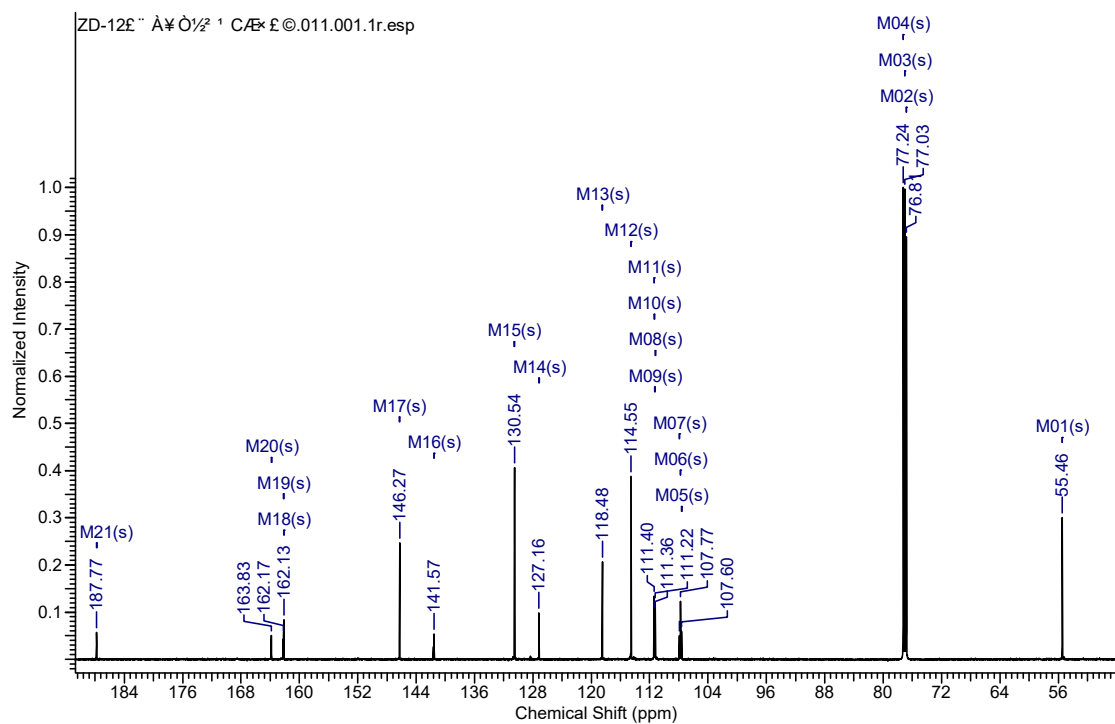


$^{13}\text{C}$  NMR (101 MHz, CHLOROFORM- $d$ )  $\delta$  189.3, 161.7, 153.1, 144.6, 133.9, 130.3, 127.6, 119.4, 114.5, 106.0, 77.4, 77.1, 76.7, 61.0, 56.4, 55.4

**Figure S4.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of (*E*)-1-(3,5-difluorophenyl)-3-(4-methoxyphenyl)prop-2-en-1-one(3d)<sup>3</sup>

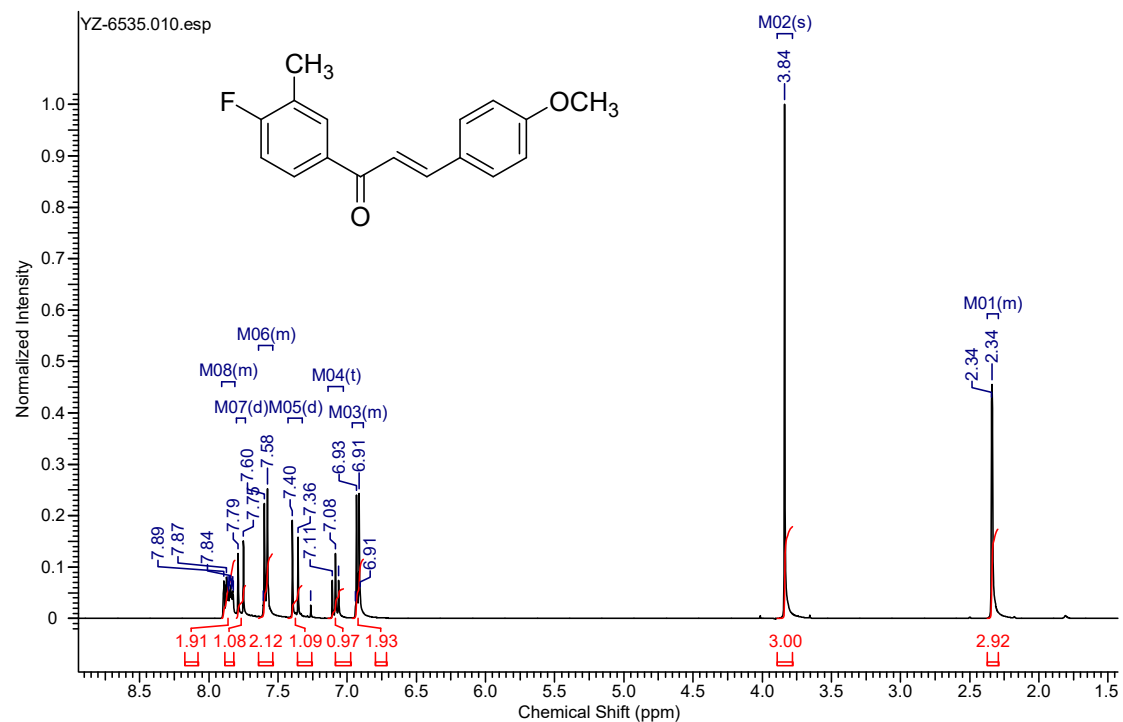


$^1\text{H}$  NMR (400 MHz, METHANOL- $d_4$ )  $\delta$  7.84 (d,  $J$  = 15.41 Hz, 1H), 7.73 - 7.79 (m,  $J$  = 8.80 Hz, 2H), 7.67 - 7.73 (m, 2H), 7.60 (d,  $J$  = 15.65 Hz, 1H), 7.20 - 7.32 (m, 1H), 6.97 - 7.06 (m,  $J$  = 8.80 Hz, 2H), 3.88 (s, 3H)

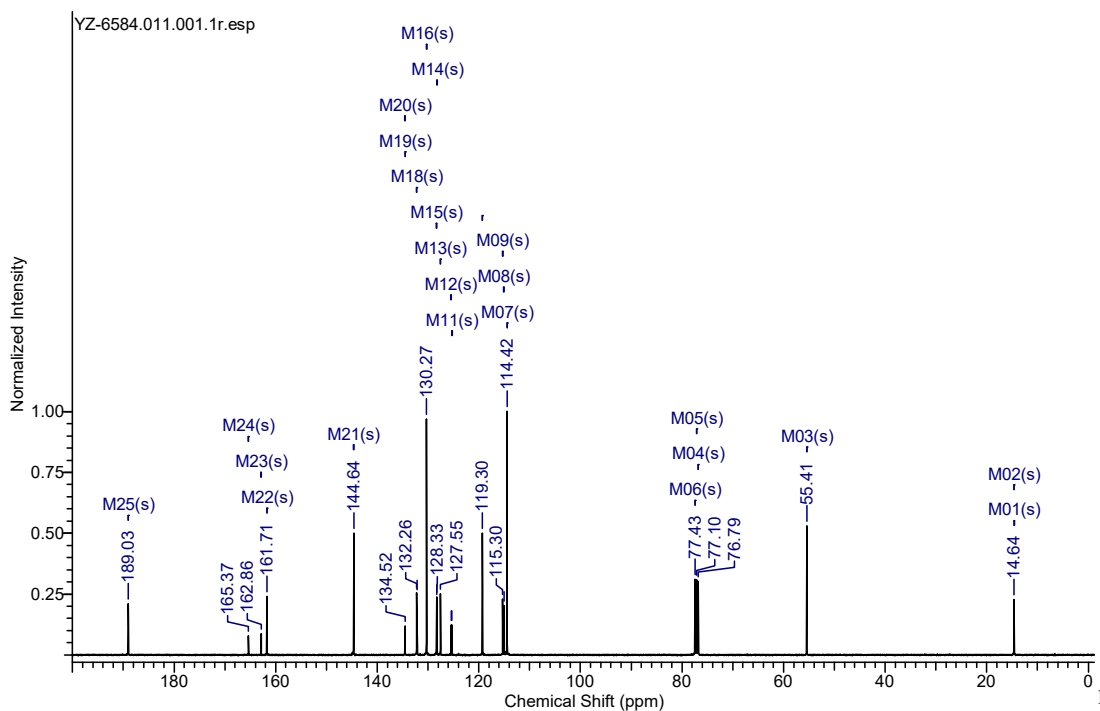


$^{13}\text{C}$  NMR (151 MHz, CHLOROFORM- $d$ )  $\delta$  187.8, 163.8, 162.2, 162.1, 146.3, 141.6, 130.5, 127.2, 118.5, 114.5, 111.4, 111.4, 111.3, 111.2, 107.9, 107.8, 107.6, 77.2, 77.0, 76.8, 55.5

**Figure S5.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **(E)-1-(4-fluoro-3-methylphenyl)-3-(4-methoxyphenyl)prop-2-en-1-one(3e)**

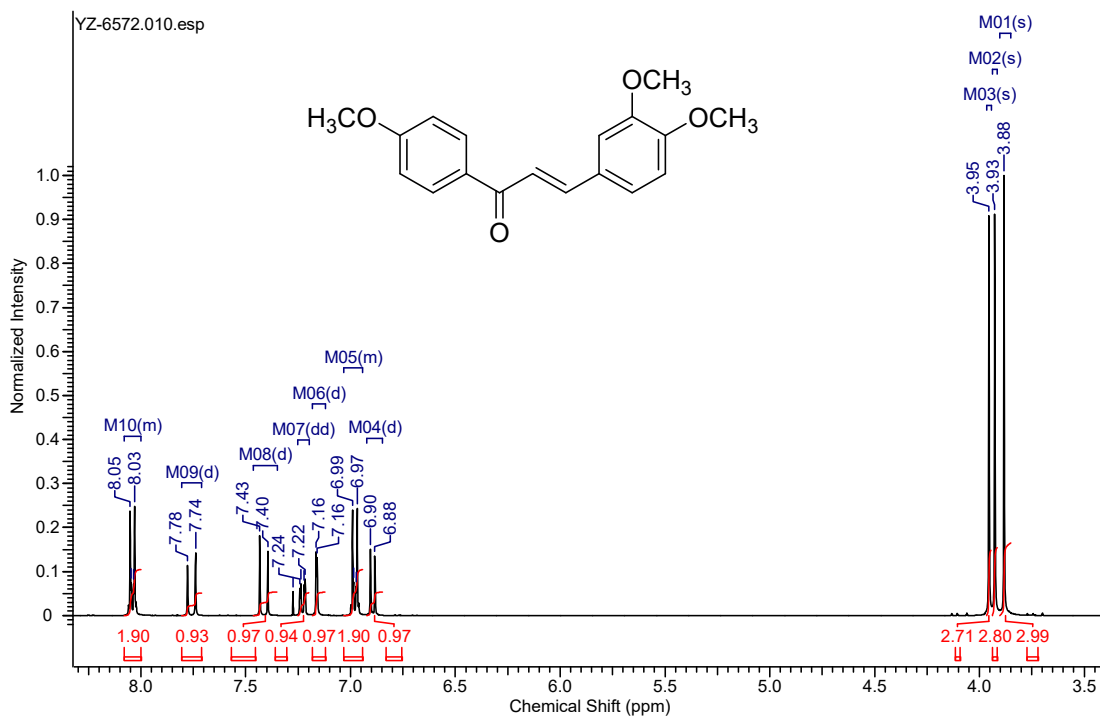


$^1\text{H}$  NMR (400 MHz, CHLOROFORM- $d$ )  $\delta$  7.81 - 7.91 (m, 2H), 7.77 (d,  $J = 15.65$  Hz, 1H), 7.54 - 7.64 (m, 2H), 7.38 (d,  $J = 15.65$  Hz, 1H), 7.08 (t,  $J = 8.80$  Hz, 1H), 6.88 - 6.96 (m, 2H), 3.84 (s, 3H), 2.29 - 2.37 (m, 3H)



$^{13}\text{C}$  NMR (101 MHz, CHLOROFORM- $d$ )  $\delta$  189.0, 165.4, 162.9, 161.7, 144.6, 134.5, 134.5, 132.3, 132.2, 130.3, 128.3, 128.2, 127.5, 125.5, 125.3, 119.3, 115.3, 115.1, 114.4, 77.4, 77.1, 76.8, 55.4, 14.6, 14.6

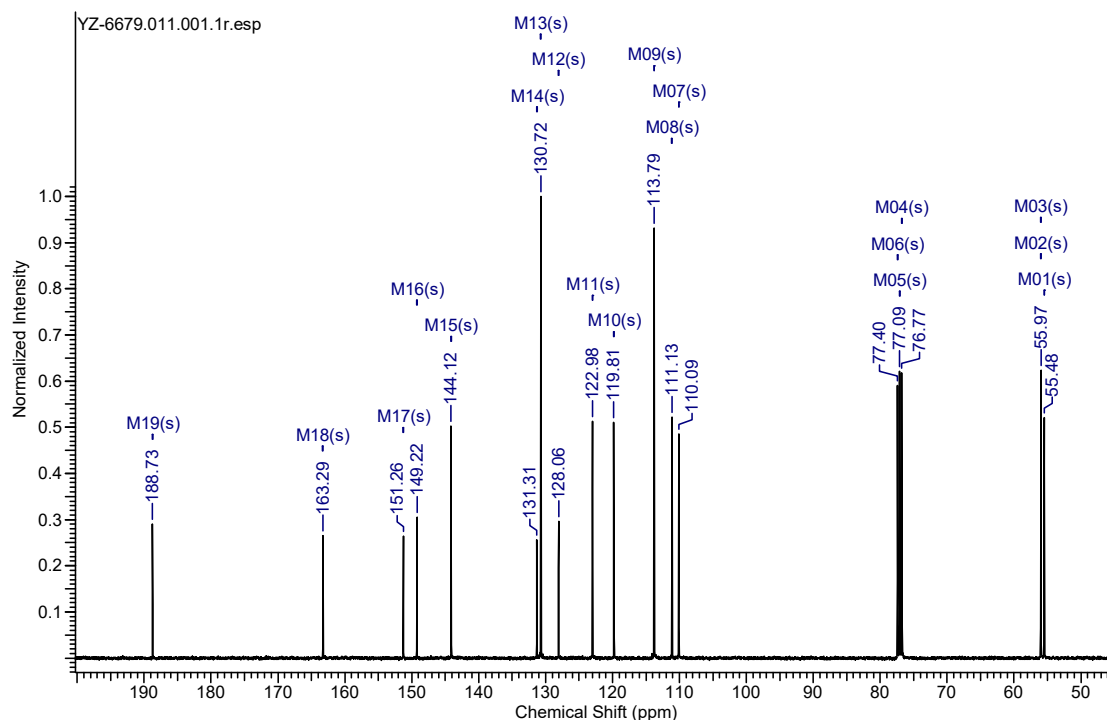
**Figure S6.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **(E)-3-(3,4-dimethoxyphenyl)-1-(4-methoxyphenyl)prop-2-en-1-one(3f)<sup>4</sup>**



$^1\text{H}$  NMR (400 MHz, CHLOROFORM- $d$ )  $\delta$  8.00 - 8.08 (m, 2H), 7.76 (d,  $J$  = 15.65 Hz, 1H), 7.41 (d,  $J$  = 15.41 Hz, 1H), 7.23 (dd,  $J$  = 1.96, 8.31 Hz, 1H), 7.16 (d,  $J$  = 1.96 Hz,



1H), 6.94 - 7.03 (m, 2H), 6.89 (d,  $J = 8.31$  Hz, 1H), 3.95 (s, 3H), 3.93 (s, 3H), 3.88 (s, 3H)

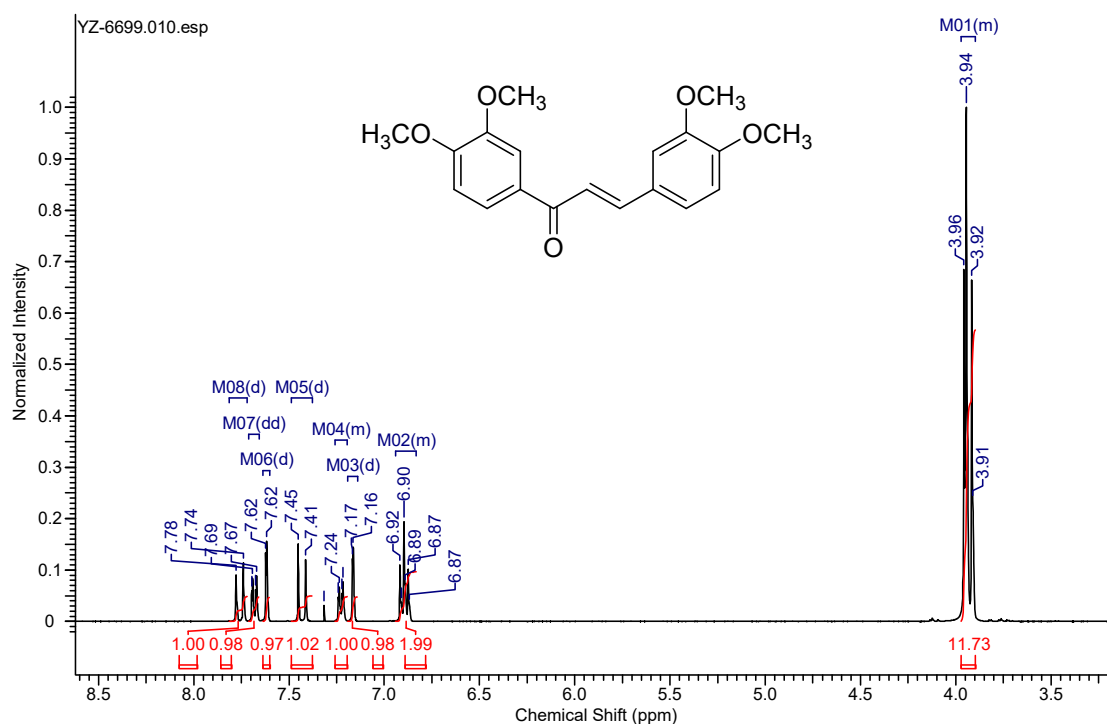


$^{13}\text{C}$  NMR (101 MHz, CHLOROFORM- $d$ )  $\delta$  188.7, 163.3, 151.3, 149.2, 144.1, 131.3, 130.7, 128.1, 123.0, 119.8, 113.8, 111.1, 110.1, 77.4, 77.1, 76.8, 56.0, 56.0, 55.5

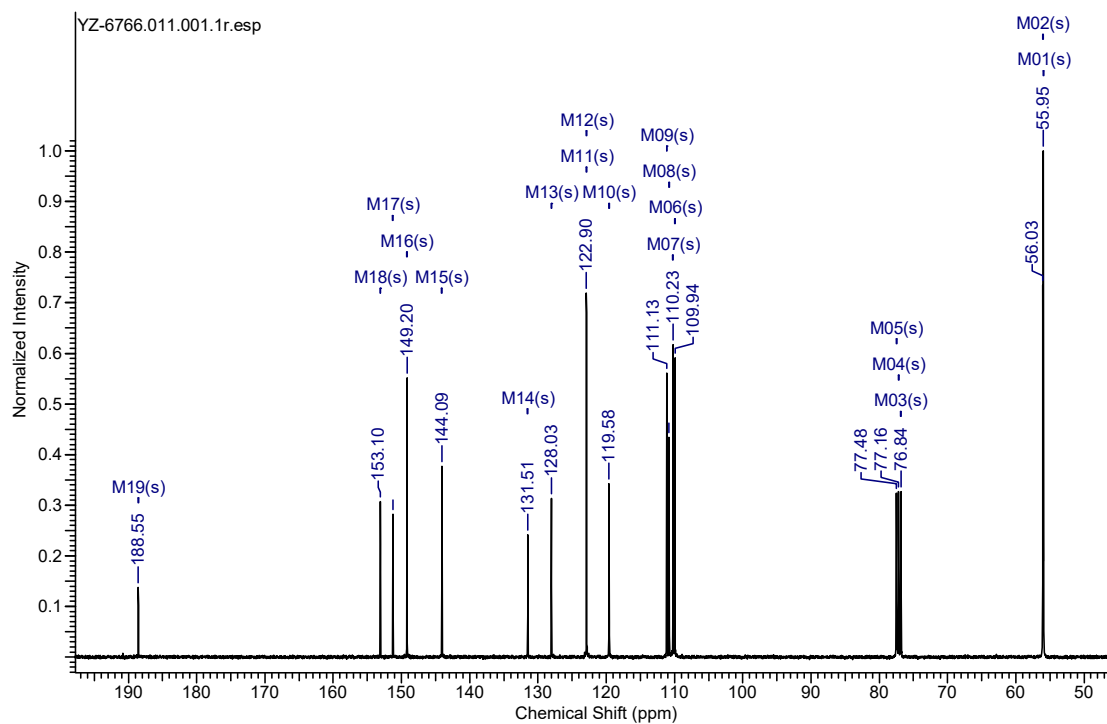
**Figure S7.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of

**(E)-1,3-bis(3,4-dimethoxyphenyl)prop-2-en-1-one(3g)<sup>1</sup>**

$^1\text{H}$  NMR (400 MHz, CHLOROFORM- $d$ )  $\delta$  ppm 3.90 - 3.97 (m, 12 H) 6.83 - 6.94 (m, 2 H) 7.17 (d,  $J=1.71$  Hz, 1 H) 7.20 - 7.26 (m, 1 H) 7.43 (d,  $J=15.65$  Hz, 1 H) 7.62 (d,  $J=1.96$  Hz, 1 H) 7.68 (dd,  $J=8.44, 2.08$  Hz, 1 H) 7.76 (d,  $J=15.65$  Hz, 1 H)

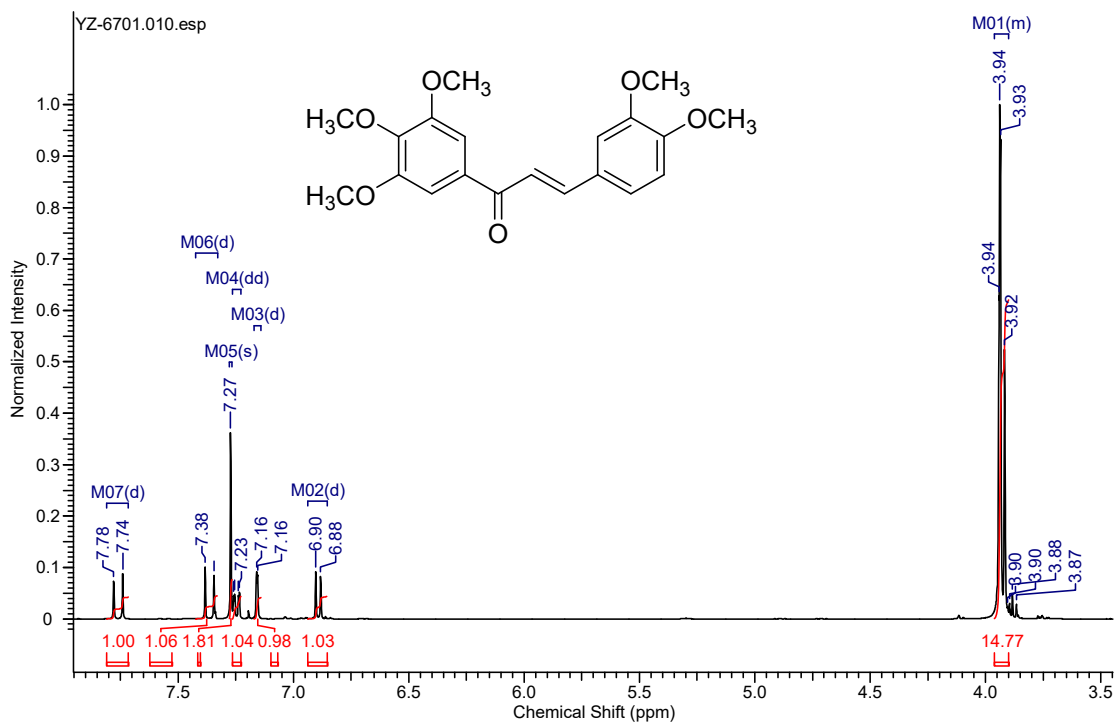


$^{13}\text{C}$  NMR (101 MHz, CHLOROFORM-*d*)  $\delta$  188.6, 153.1, 151.3, 149.2, 144.1, 131.5, 128.0, 122.9, 122.9, 119.6, 111.1, 110.8, 110.2, 109.9, 77.5, 77.2, 76.8, 56.0, 56.0

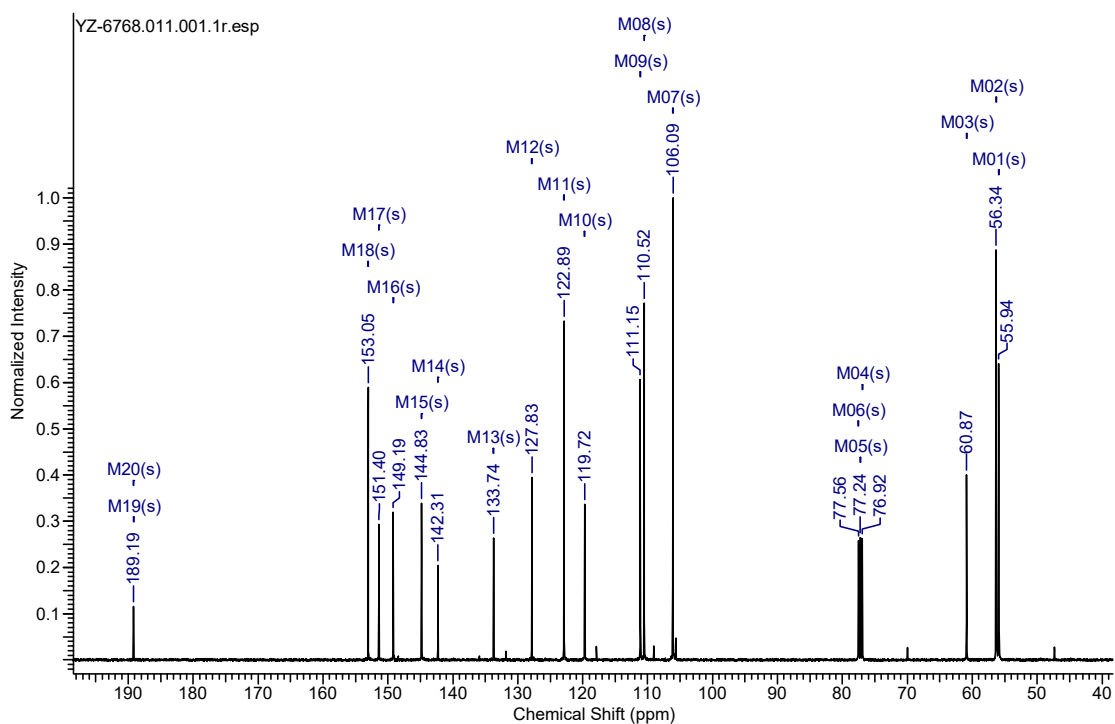


**Figure S8.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **(E)-3-(3,4-dimethoxyphenyl)-1-(3,4,5-trimethoxyphenyl)prop-2-en-1-one(3h)<sup>5</sup>**

$^1\text{H}$  NMR (400 MHz, CHLOROFORM-*d*)  $\delta$  ppm 3.90 - 3.96 (m, 15 H) 6.89 (d,  $J=8.31$  Hz, 1 H) 7.16 (d,  $J=1.71$  Hz, 1 H) 7.25 (dd,  $J=8.31, 1.96$  Hz, 1 H) 7.27 (s, 2 H) 7.36 (d,  $J=15.41$  Hz, 1 H) 7.76 (d,  $J=15.65$  Hz, 1 H)



$^{13}\text{C}$  NMR (101 MHz, CHLOROFORM-*d*)  $\delta$  189.2, 189.2, 153.1, 151.4, 149.2, 144.8, 142.3, 133.7, 127.8, 122.9, 119.7, 111.1, 110.5, 106.1, 77.6, 77.2, 76.9, 60.9, 56.3, 55.9

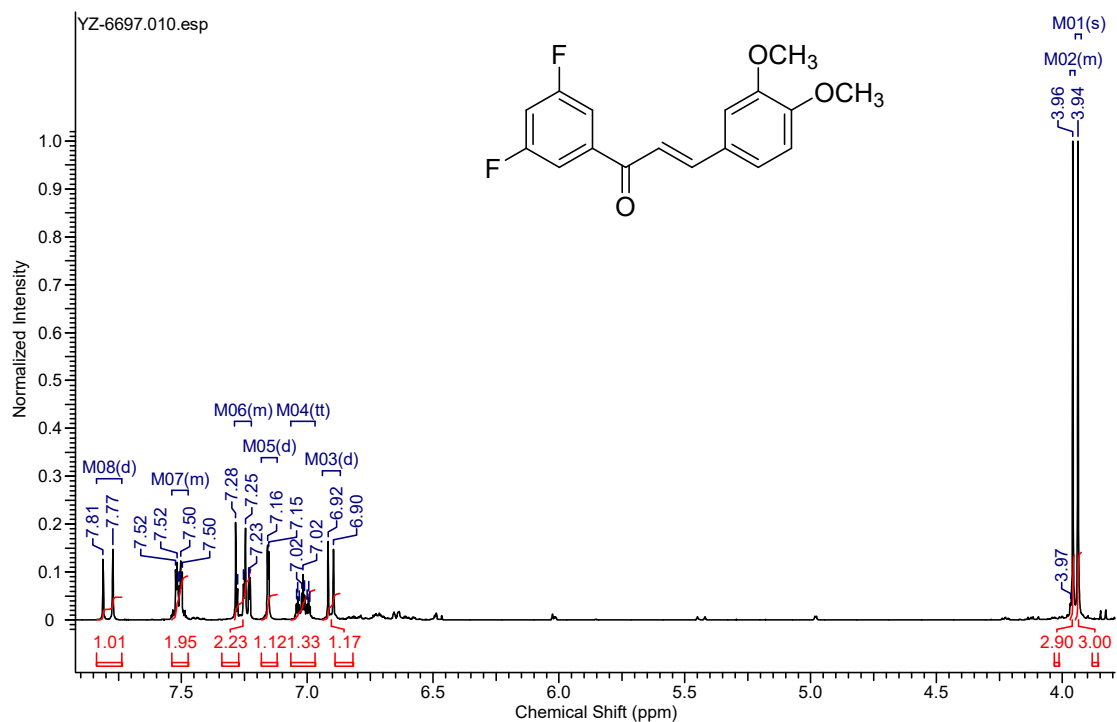


**Figure S9.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of

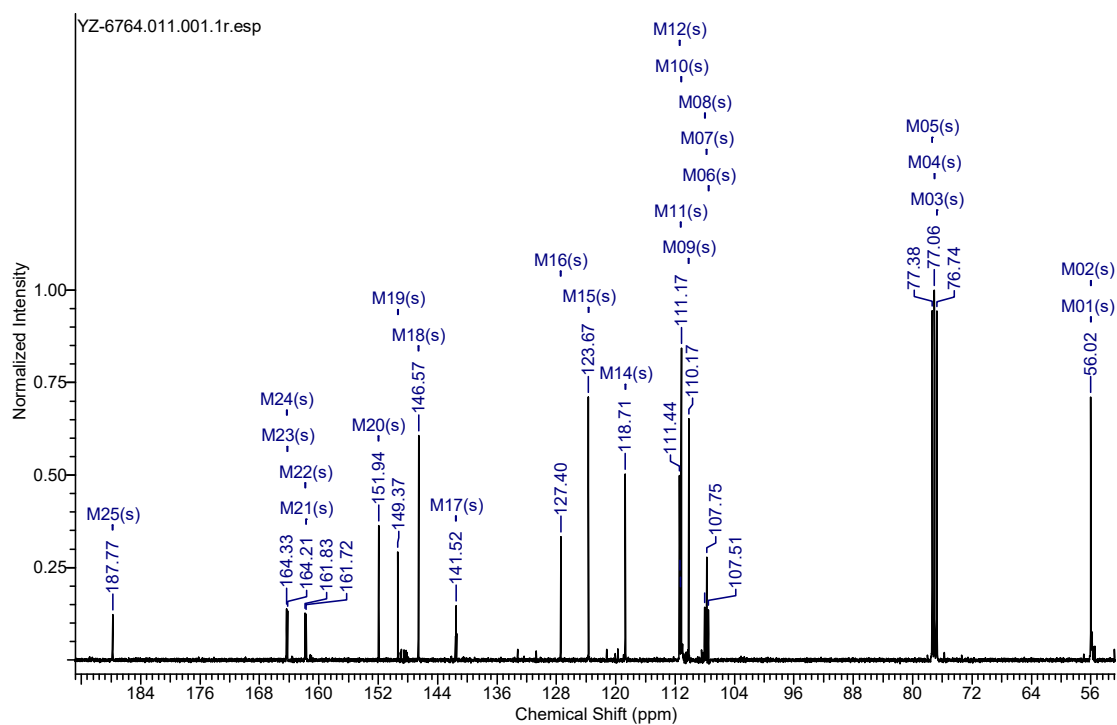
**(E)-1-(3,5-difluorophenyl)-3-(3,4-dimethoxyphenyl)prop-2-en-1-one(3i)<sup>3</sup>**

$^1\text{H}$  NMR (400 MHz, CHLOROFORM-*d*)  $\delta$  ppm 3.94 (s, 3 H) 3.95 - 3.97 (m, 3 H)

6.91 (d,  $J=8.31$  Hz, 1 H) 7.02 (tt,  $J=8.50, 2.26$  Hz, 1 H) 7.16 (d,  $J=1.96$  Hz, 1 H) 7.22 - 7.29 (m, 2 H) 7.47 - 7.54 (m, 2 H) 7.79 (d,  $J=15.65$  Hz, 1 H)

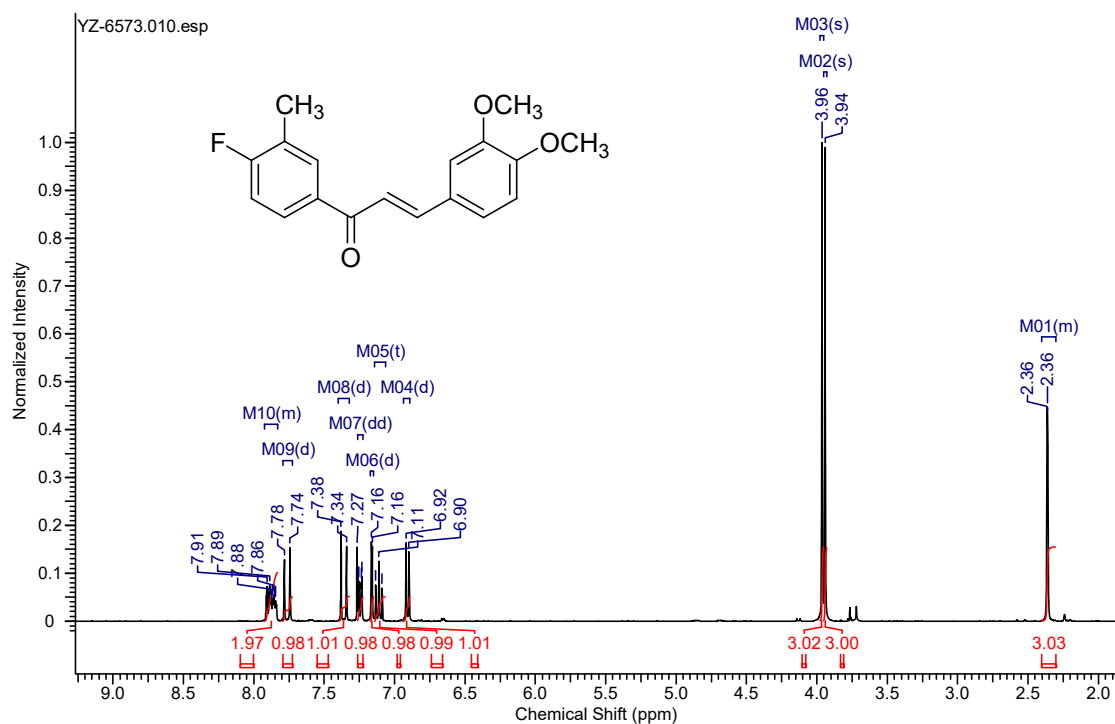


$^{13}\text{C}$  NMR (101 MHz, CHLOROFORM- $d$ )  $\delta$  187.8, 164.3, 164.2, 161.8, 161.7, 151.9, 149.4, 146.6, 141.5, 127.4, 123.7, 118.7, 111.4, 111.4, 111.3, 111.2, 110.2, 108.0, 107.8, 107.5, 77.4, 77.1, 76.7, 56.0, 56.0

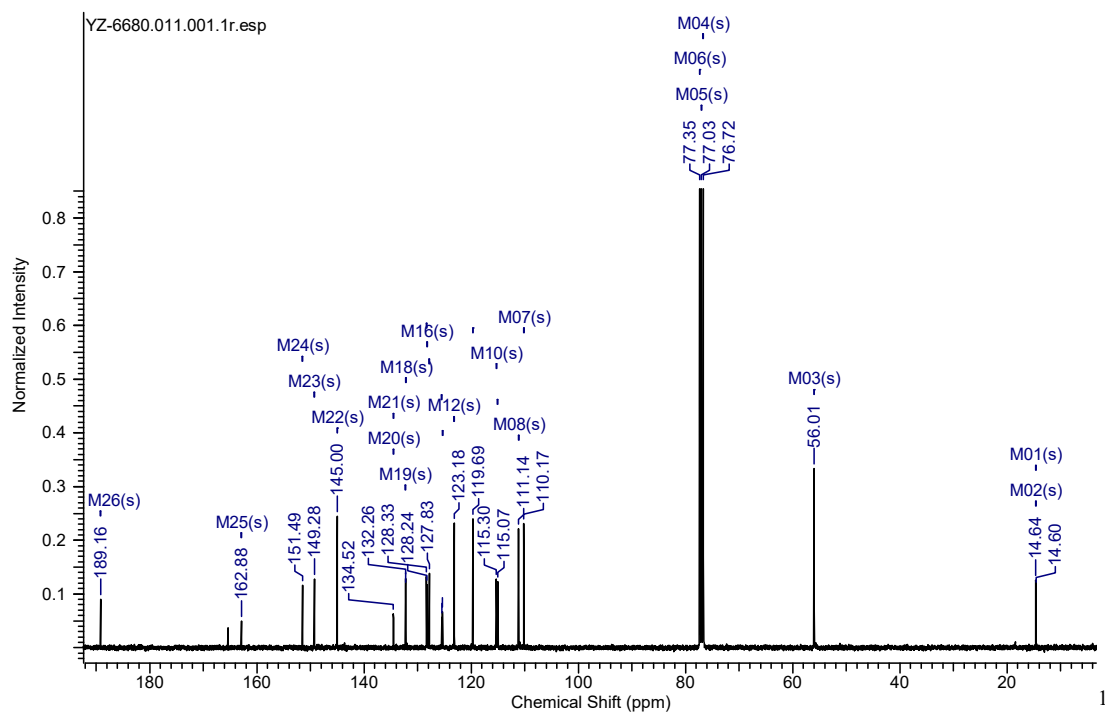


**Figure S10.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of

**(E)-3-(3,4-dimethoxyphenyl)-1-(4-fluoro-3-methylphenyl)prop-2-en-1-one(3j)**



$^1\text{H}$  NMR (400 MHz, CHLOROFORM- $d$ )  $\delta$  7.83 - 7.92 (m, 2H), 7.76 (d,  $J$  = 15.65 Hz, 1H), 7.36 (d,  $J$  = 15.65 Hz, 1H), 7.25 (dd,  $J$  = 1.83, 8.19 Hz, 1H), 7.16 (d,  $J$  = 1.96 Hz, 1H), 7.11 (t,  $J$  = 8.93 Hz, 1H), 6.91 (d,  $J$  = 8.31 Hz, 1H), 3.96 (s, 3H), 3.94 (s, 3H), 2.30 - 2.40 (m, 3H)



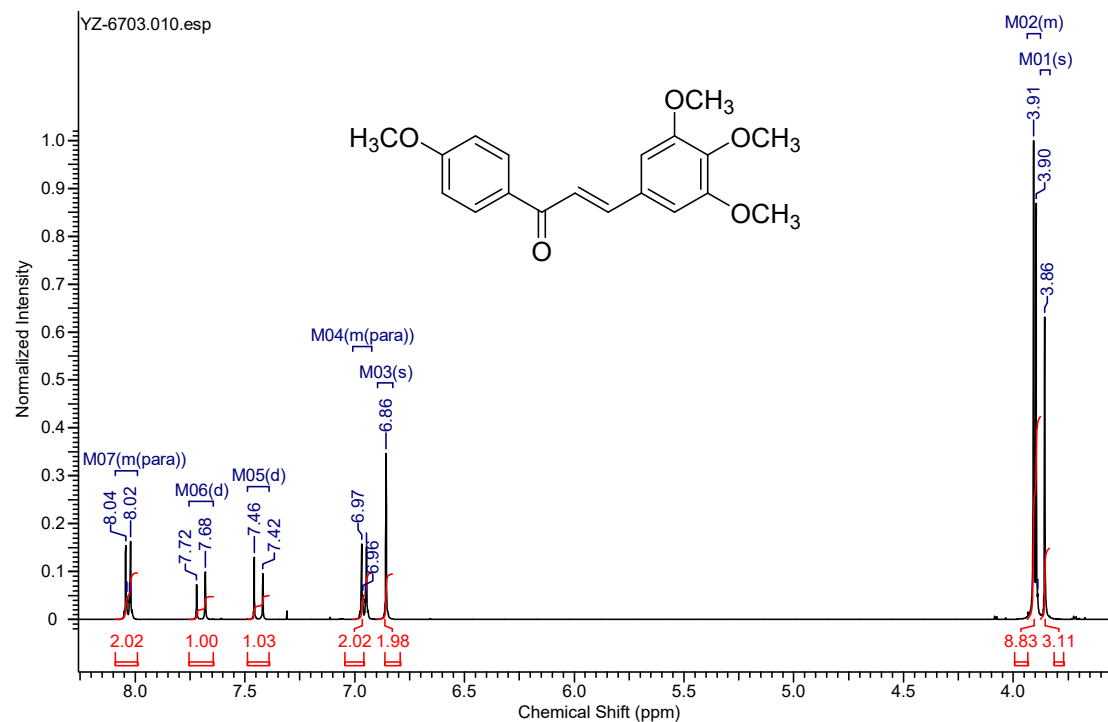
$^{13}\text{C}$  NMR (101 MHz, CHLOROFORM- $d$ )  $\delta$  189.2, 162.9, 151.5, 149.3, 145.0, 134.5, 134.5, 132.3, 132.2, 128.3, 128.2, 127.8, 125.5, 125.3, 123.2, 119.7, 115.3, 115.1,

111.1, 110.2, 77.4, 77.0, 76.7, 56.0, 14.6, 14.6

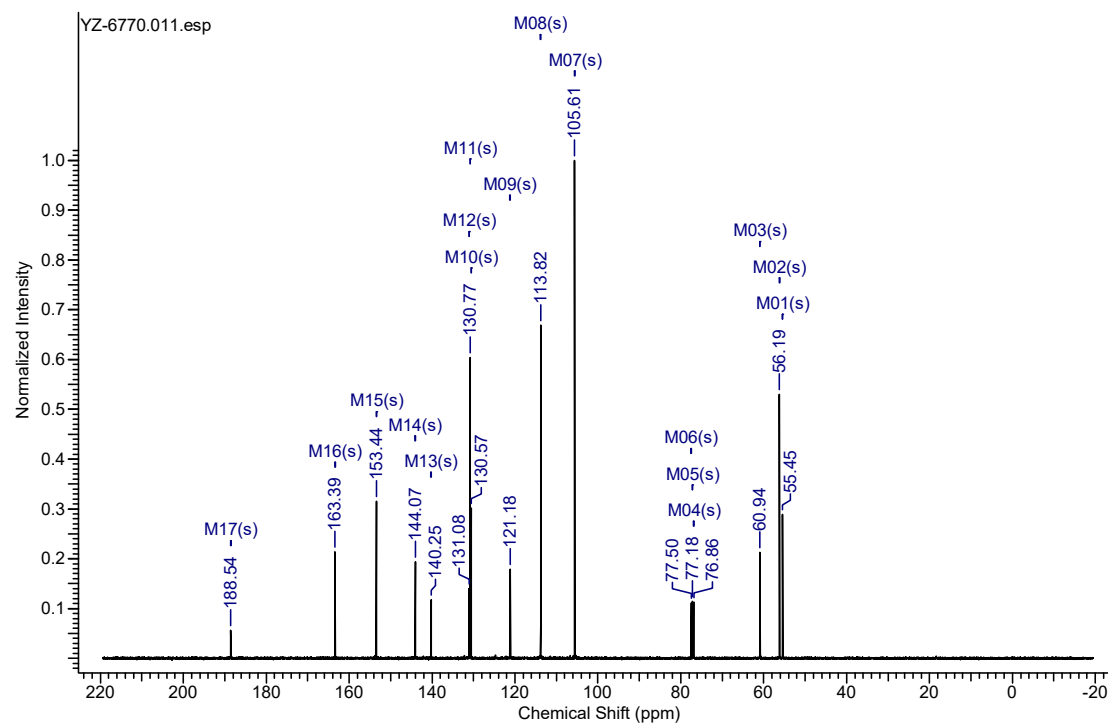
**Figure S11.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of

**(E)-1-(4-methoxyphenyl)-3-(3,4,5-trimethoxyphenyl)prop-2-en-1-one(3k)<sup>6</sup>**

$^1\text{H}$  NMR (400 MHz, CHLOROFORM-*d*)  $\delta$  ppm 3.86 (s, 3 H) 3.88 - 3.94 (m, 9 H) 6.86 (s, 2 H) 6.92 - 7.01 (m, 2 H) 7.44 (d,  $J=15.65$  Hz, 1 H) 7.70 (d,  $J=15.65$  Hz, 1 H) 7.99 - 8.09 (m, 2 H)



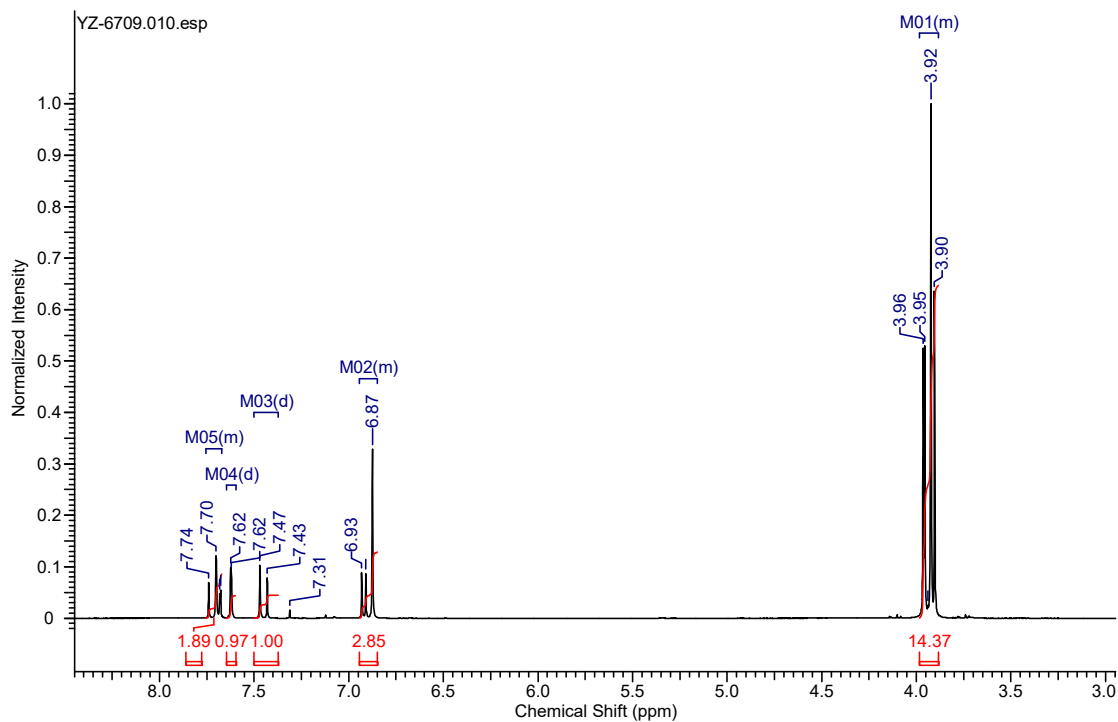
$^{13}\text{C}$  NMR (101 MHz, CHLOROFORM-*d*)  $\delta$  188.5, 163.4, 153.4, 144.1, 140.3, 131.1, 130.8, 130.6, 121.2, 113.8, 105.6, 77.5, 77.2, 76.9, 60.9, 56.2, 55.4



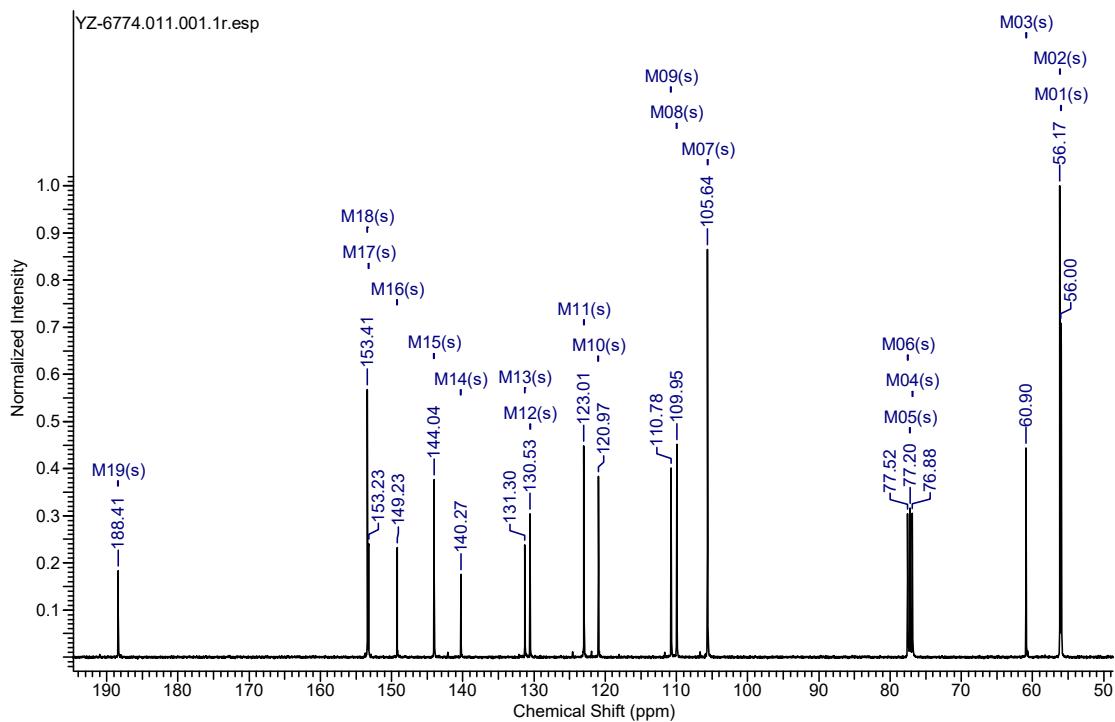
**Figure S12.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of

**(E)-1-(3,4-dimethoxyphenyl)-3-(3,4,5-trimethoxyphenyl)prop-2-en-1-one(3I)<sup>2</sup>**

$^1\text{H}$  NMR (400 MHz, CHLOROFORM-*d*)  $\delta$  7.67 - 7.76 (m, 2H), 7.62 (d,  $J = 1.96$  Hz, 1H), 7.45 (d,  $J = 15.65$  Hz, 1H), 6.85 - 6.94 (m, 3H), 3.88 - 3.98 (m, 15H)

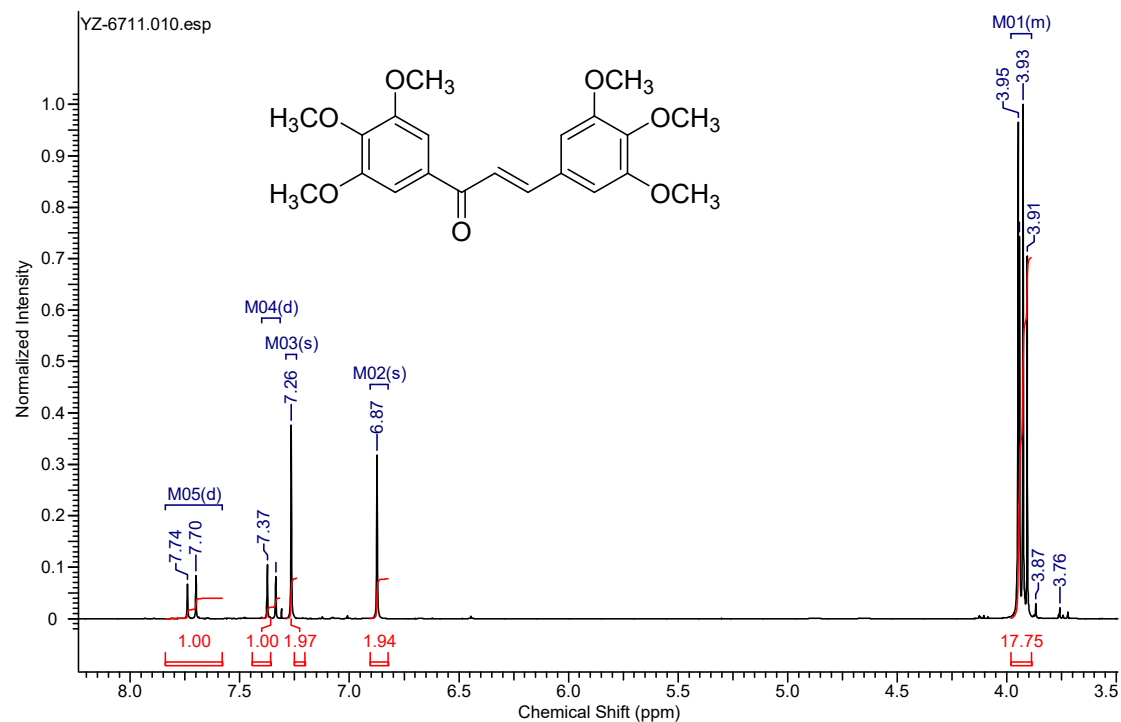


$^{13}\text{C}$  NMR (101 MHz, CHLOROFORM-*d*)  $\delta$  188.4, 153.4, 153.2, 149.2, 144.0, 140.3, 131.3, 130.5, 123.0, 121.0, 110.8, 110.0, 105.6, 77.5, 77.2, 76.9, 60.9, 56.2, 56.0

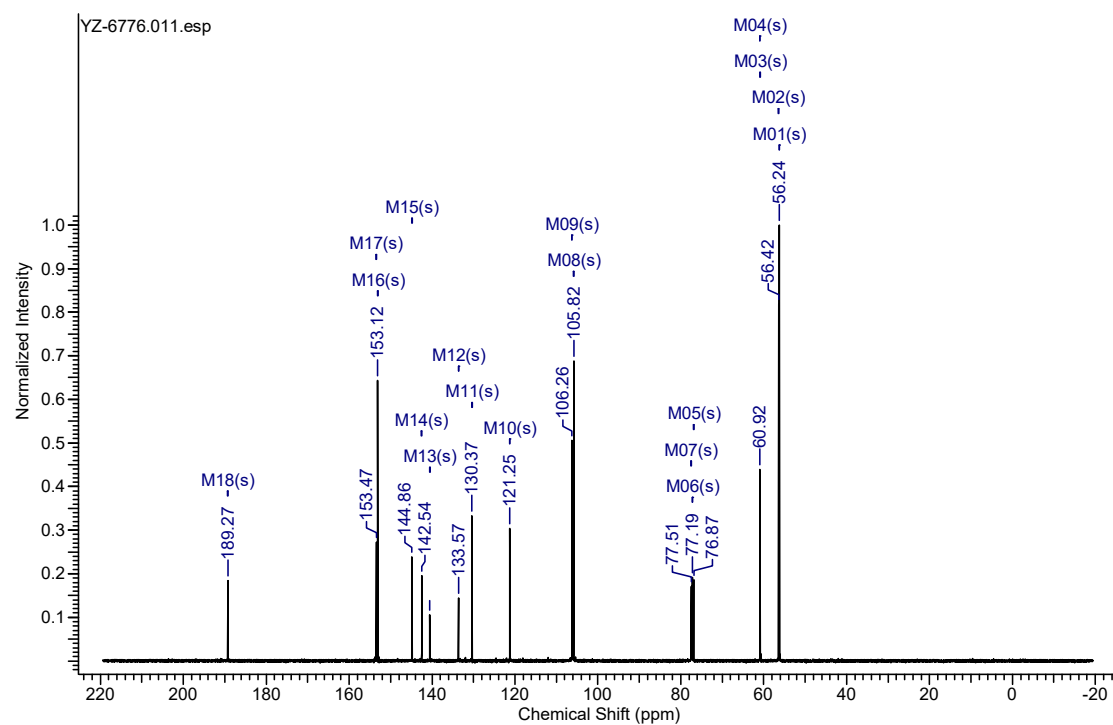


**Figure S13**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of  
**(E)-1,3-bis(3,4,5-trimethoxyphenyl)prop-2-en-1-one(3m)<sup>7</sup>**

$^1\text{H}$  NMR (400 MHz, CHLOROFORM-*d*)  $\delta$  ppm 3.89 - 3.98 (m, 18 H) 6.87 (s, 2 H)  
7.26 (s, 2 H) 7.36 (d,  $J=15.41$  Hz, 1 H) 7.72 (d,  $J=15.41$  Hz, 1 H)



$^{13}\text{C}$  NMR (101 MHz, CHLOROFORM-*d*)  $\delta$  189.3, 153.5, 153.1, 144.9, 142.5, 140.5, 133.6, 130.4, 121.3, 106.3, 105.8, 77.5, 77.2, 76.9, 60.9, 60.9, 56.4, 56.2

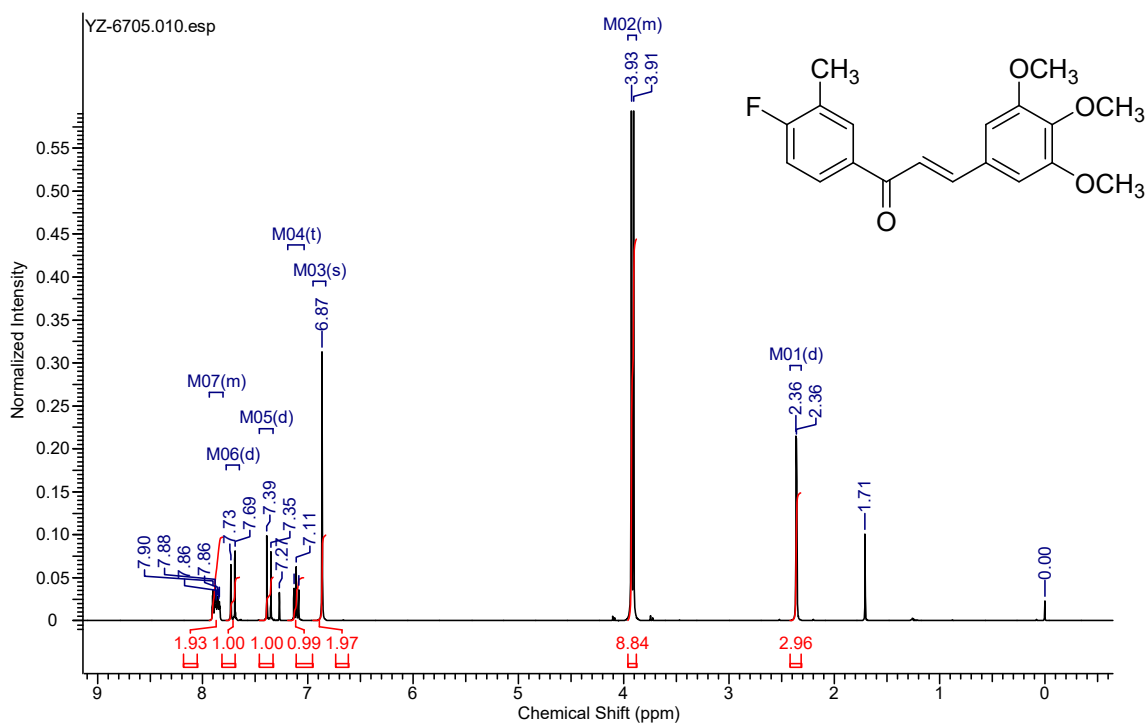




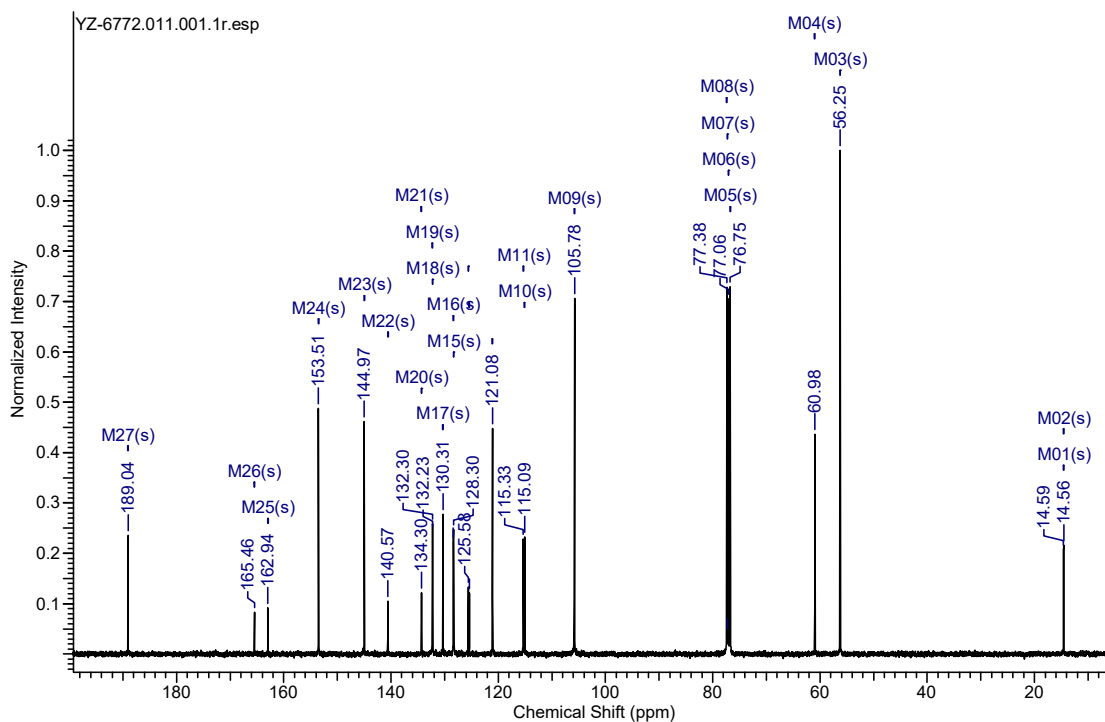
**Figure S14.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of

**(E)-1-(4-fluoro-3-methylphenyl)-3-(3,4,5-trimethoxyphenyl)prop-2-en-1-one(3n)**

$^1\text{H}$  NMR (400 MHz,  $\text{CHLOROFORM-}d$ )  $\delta$  ppm 2.36 (d,  $J=1.71$  Hz, 3 H) 3.88 - 3.96 (m, 9 H) 6.87 (s, 2 H) 7.11 (t,  $J=8.80$  Hz, 1 H) 7.37 (d,  $J=15.41$  Hz, 1 H) 7.71 (d,  $J=15.41$  Hz, 1 H) 7.81 - 7.94 (m, 2 H)

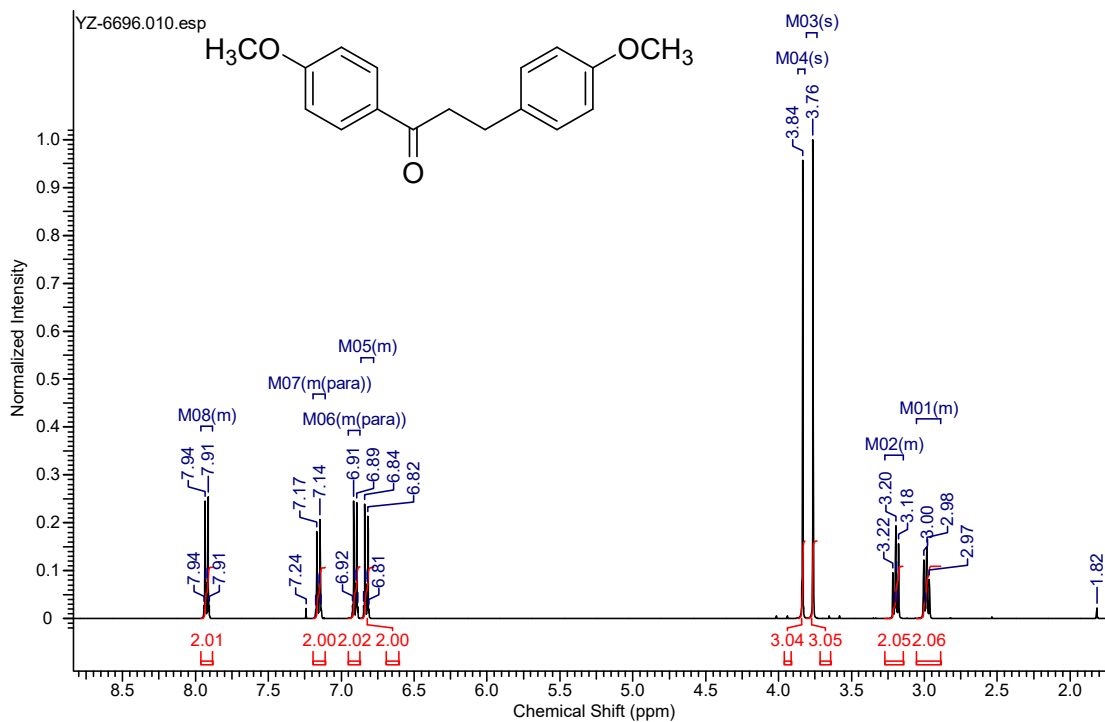


$^{13}\text{C}$  NMR (101 MHz,  $\text{CHLOROFORM-}d$ )  $\delta$  189.0, 165.5, 162.9, 153.5, 145.0, 140.6, 134.3, 134.3, 132.3, 132.2, 130.3, 128.4, 128.3, 125.6, 125.4, 121.1, 115.3, 115.1, 105.8, 77.4, 77.3, 77.1, 76.7, 61.0, 56.3, 14.6, 14.6

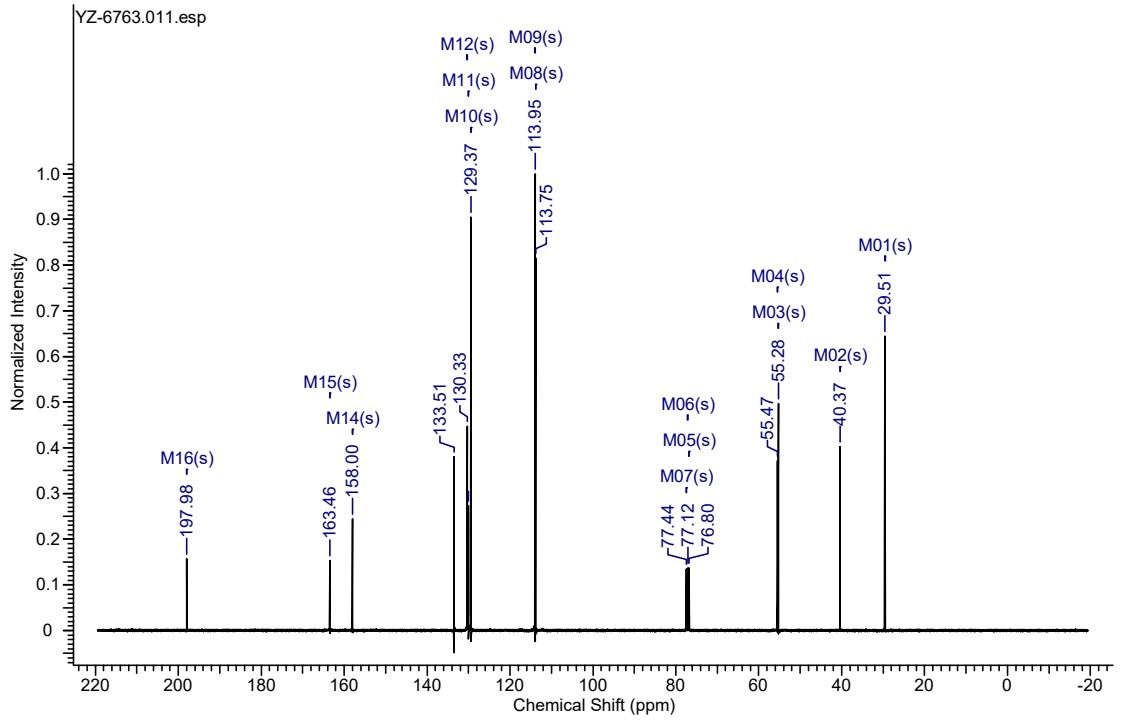


**Figure S15.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **1,3-bis(4-methoxyphenyl)propan-1-one(4a)<sup>2</sup>**

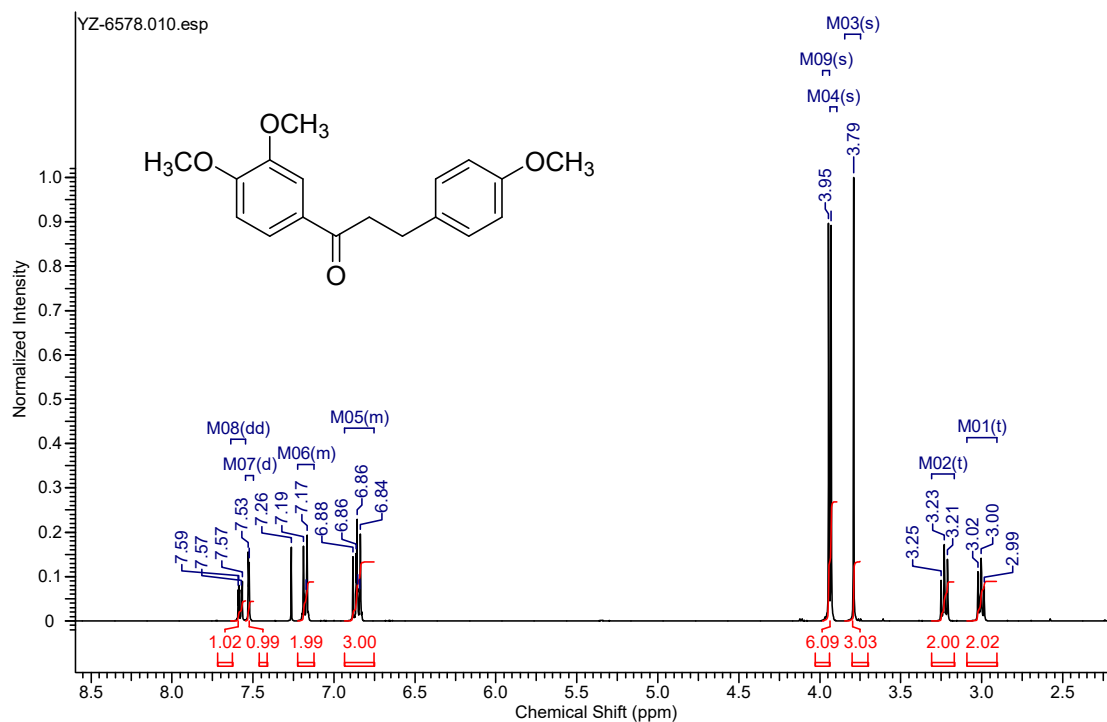
$^1\text{H}$  NMR (400 MHz, CHLOROFORM-*d*)  $\delta$  ppm 2.89 - 3.05 (m, 2 H) 3.15 - 3.27 (m, 2 H) 3.76 (s, 3 H) 3.84 (s, 3 H) 6.78 - 6.87 (m, 2 H) 6.87 - 6.95 (m, 2 H) 7.11 - 7.19 (m, 2 H) 7.88 - 7.96 (m, 2 H)



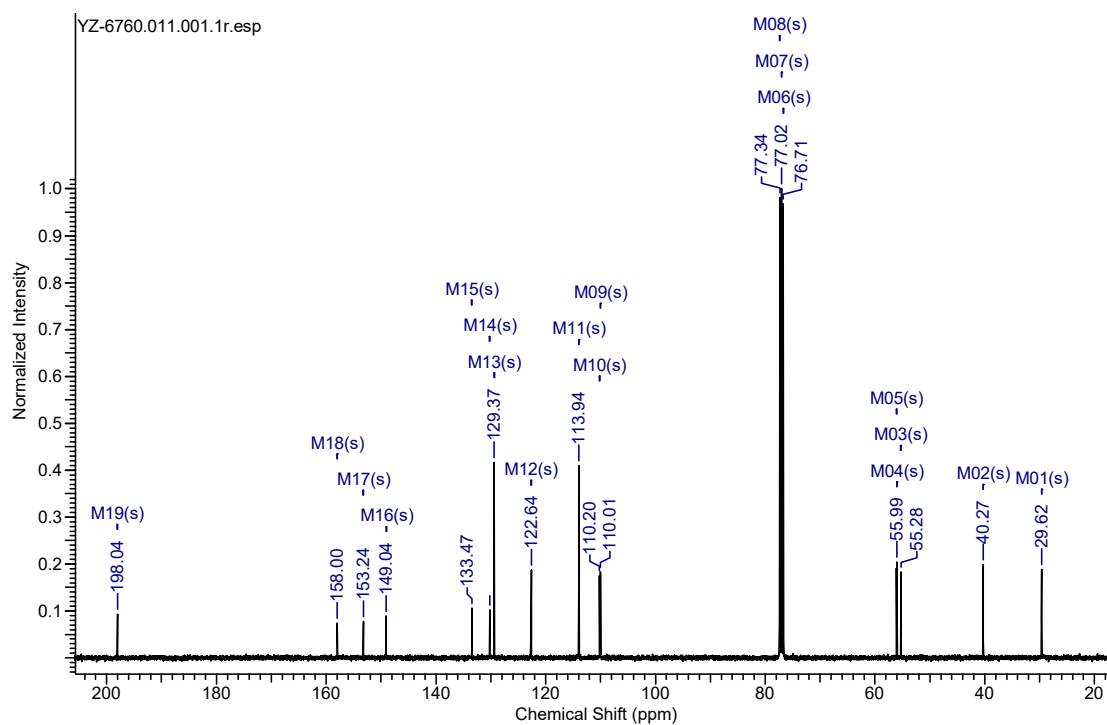
$^{13}\text{C}$  NMR (101 MHz, CHLOROFORM-*d*)  $\delta$  198.0, 163.5, 158.0, 133.5, 130.3, 130.1, 129.4, 114.0, 113.7, 77.4, 77.1, 76.8, 55.5, 55.3, 40.4, 29.5



**Figure S16.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **1-(3,4-dimethoxyphenyl)-3-(4-methoxyphenyl)propan-1-one(4b)<sup>1</sup>**

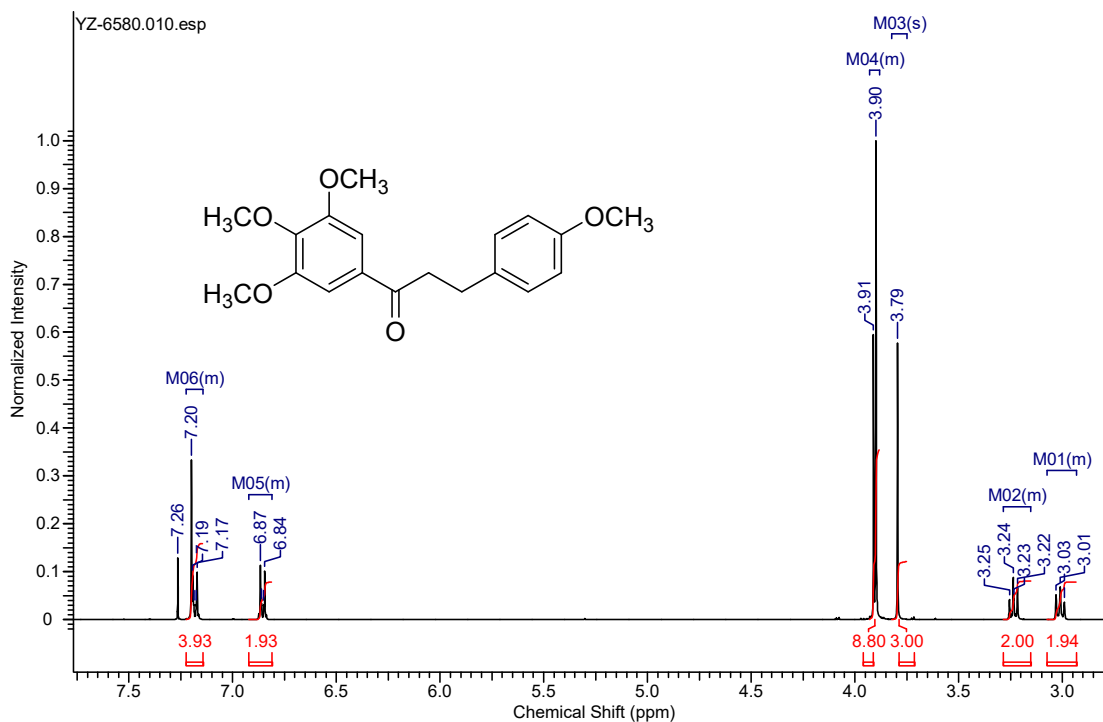


$^1\text{H}$  NMR (400 MHz, CHLOROFORM-*d*)  $\delta$  7.58 (dd,  $J = 1.96$ , 8.56 Hz, 1H), 7.53 (d,  $J = 1.96$  Hz, 1H), 7.12 - 7.23 (m, 2H), 6.75 - 6.94 (m, 3H), 3.93 (s, 3H), 3.95 (s, 3H), 3.79 (s, 3H), 3.23 (t,  $J = 7.70$  Hz, 2H), 3.00 (t,  $J = 7.70$  Hz, 2H)

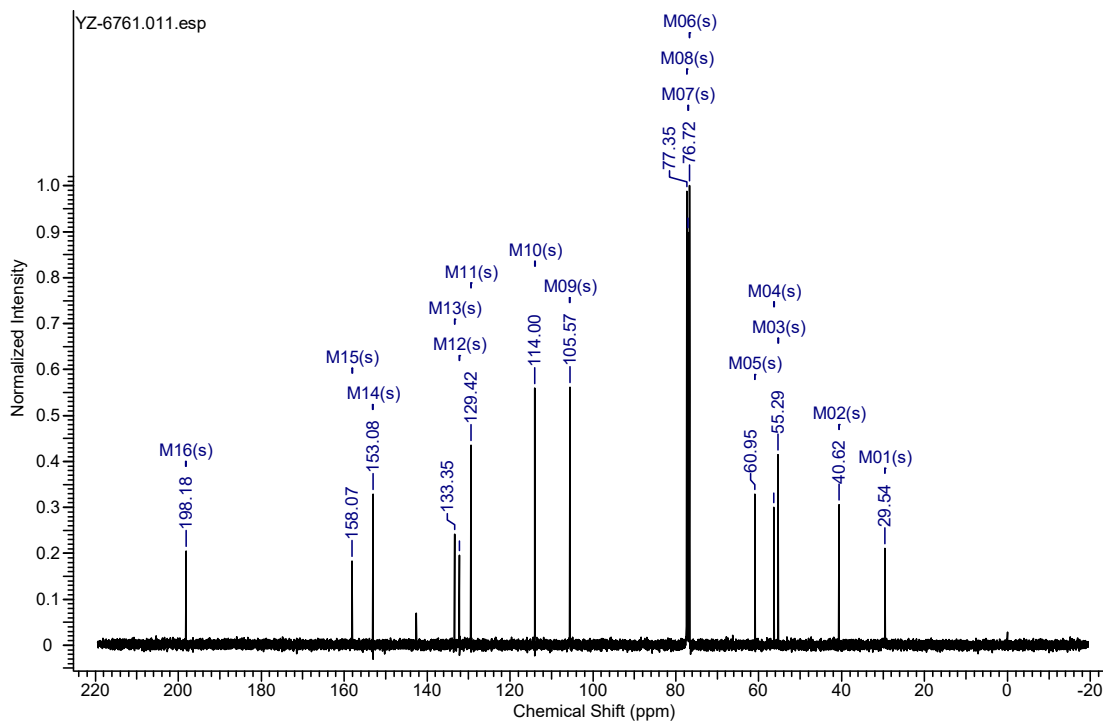


$^{13}\text{C}$  NMR (101 MHz, CHLOROFORM-*d*)  $\delta$  198.0, 158.0, 153.2, 149.0, 133.5, 130.2, 129.4, 122.6, 113.9, 110.2, 110.0, 77.3, 77.0, 76.7, 56.1, 56.0, 55.3, 40.3, 29.6

**Figure S17.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **3-(4-methoxyphenyl)-1-(3,4,5-trimethoxyphenyl)propan-1-one(4c)<sup>2</sup>**



$^1\text{H}$  NMR (400 MHz, CHLOROFORM-*d*)  $\delta$  7.14 - 7.22 (m, 4H), 6.81 - 6.92 (m, 2H), 3.88 - 3.93 (m, 9H), 3.79 (s, 3H), 3.15 - 3.28 (m, 2H), 2.93 - 3.07 (m, 2H)

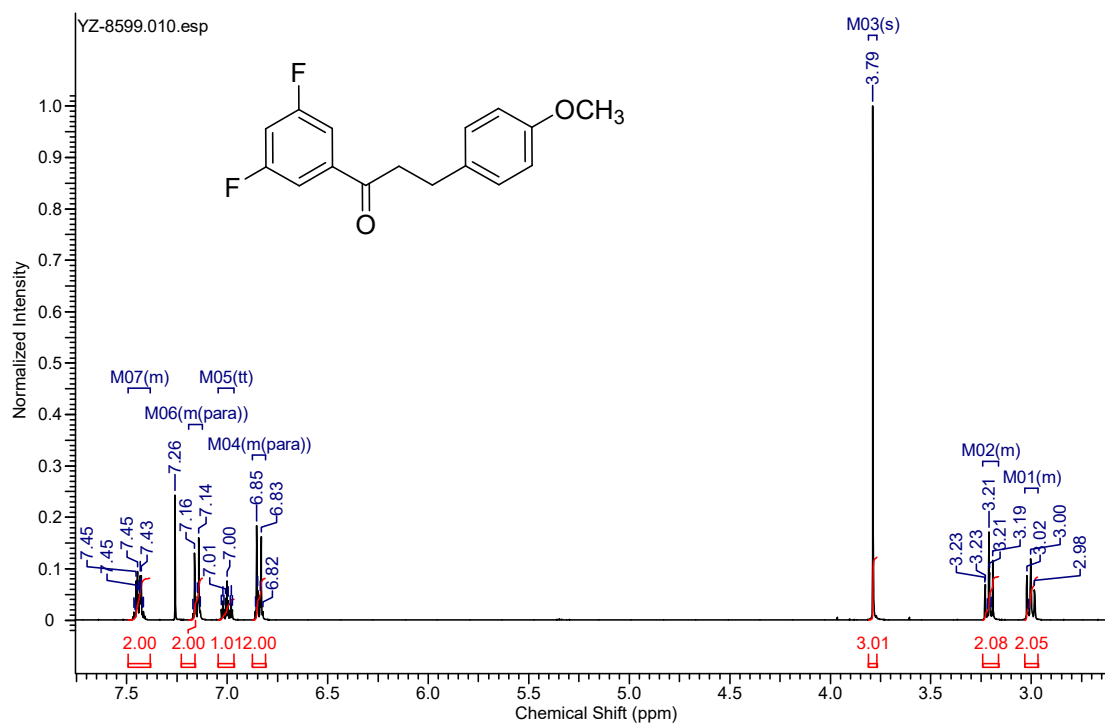


$^{13}\text{C}$  NMR (101 MHz, CHLOROFORM-*d*)  $\delta$  198.2, 158.1, 153.1, 133.3, 132.2, 129.4, 114.0, 105.6, 77.3, 77.0, 76.7, 61.0, 56.3, 55.3, 40.6, 29.5

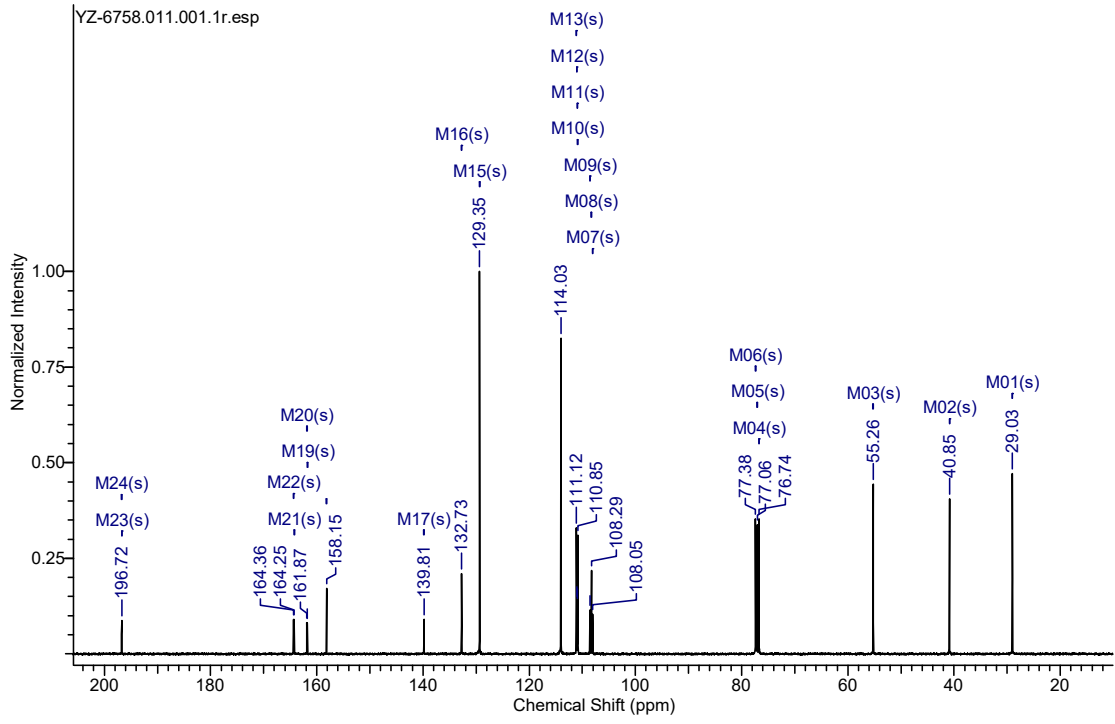
**Figure S18.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of

**1-(3,5-difluorophenyl)-3-(4-methoxyphenyl)propan-1-one(4d)**

$^1\text{H}$  NMR (400 MHz, CHLOROFORM- $d$ )  $\delta$  7.38 - 7.49 (m, 2H), 7.12 - 7.19 (m, 2H), 7.00 (tt,  $J = 2.32, 8.44$  Hz, 1H), 6.81 - 6.87 (m, 2H), 3.79 (s, 3H), 3.16 - 3.24 (m, 2H), 2.97 - 3.03 (m, 2H)



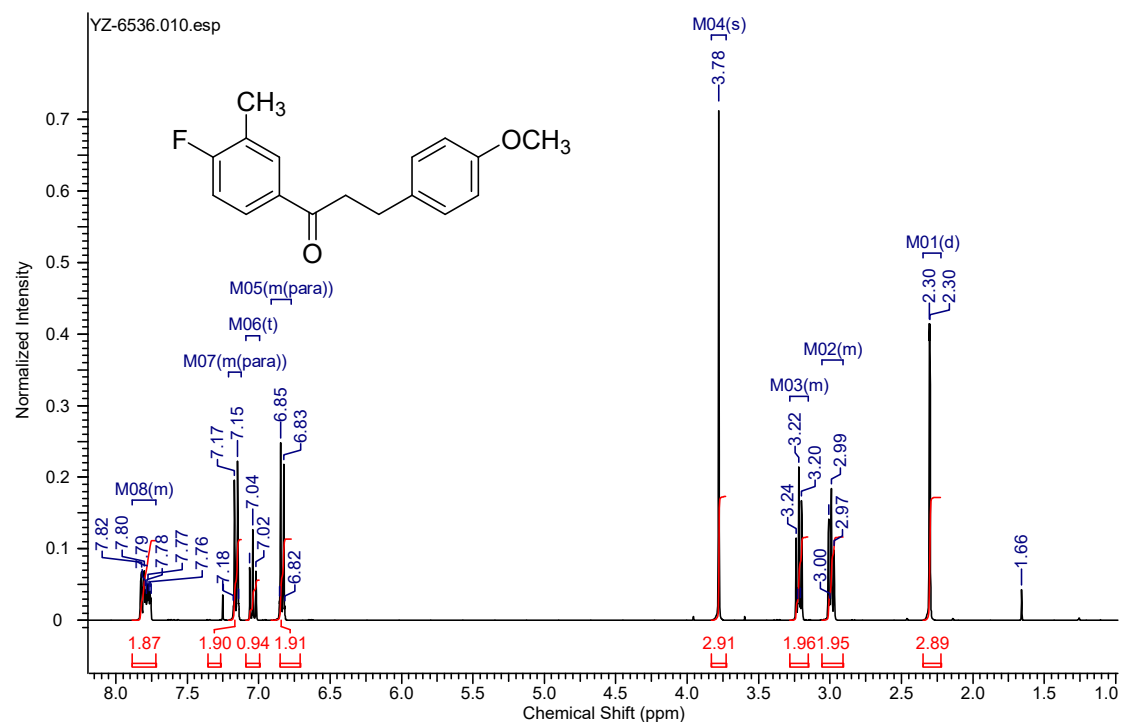
$^{13}\text{C}$  NMR (101 MHz, CHLOROFORM- $d$ )  $\delta$  196.7, 196.7, 164.4, 164.2, 161.9, 161.8, 158.2, 139.8, 132.7, 129.4, 114.0, 111.1, 111.0, 110.9, 110.9, 108.5, 108.3, 108.0, 77.4, 77.1, 76.7, 55.3, 40.8, 29.0



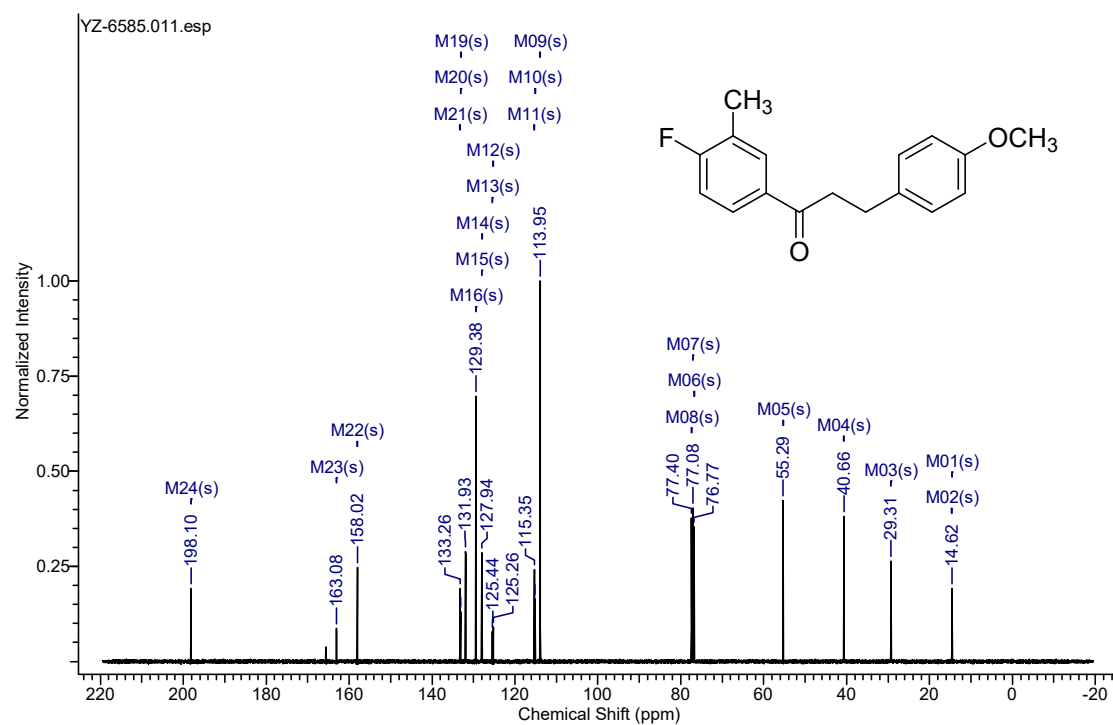
**Figure S19.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of

**1-(4-fluoro-3-methylphenyl)-3-(4-methoxyphenyl)propan-1-one(4e)**

$^1\text{H}$  NMR (400 MHz, CHLOROFORM- $d$ )  $\delta$  7.72 - 7.89 (m, 2H), 7.12 - 7.21 (m, 2H), 7.04 (t,  $J = 8.80$  Hz, 1H), 6.77 - 6.91 (m, 2H), 3.78 (s, 3H), 3.15 - 3.28 (m, 2H), 2.91 - 3.06 (m, 2H), 2.30 (d,  $J = 1.71$  Hz, 3H)

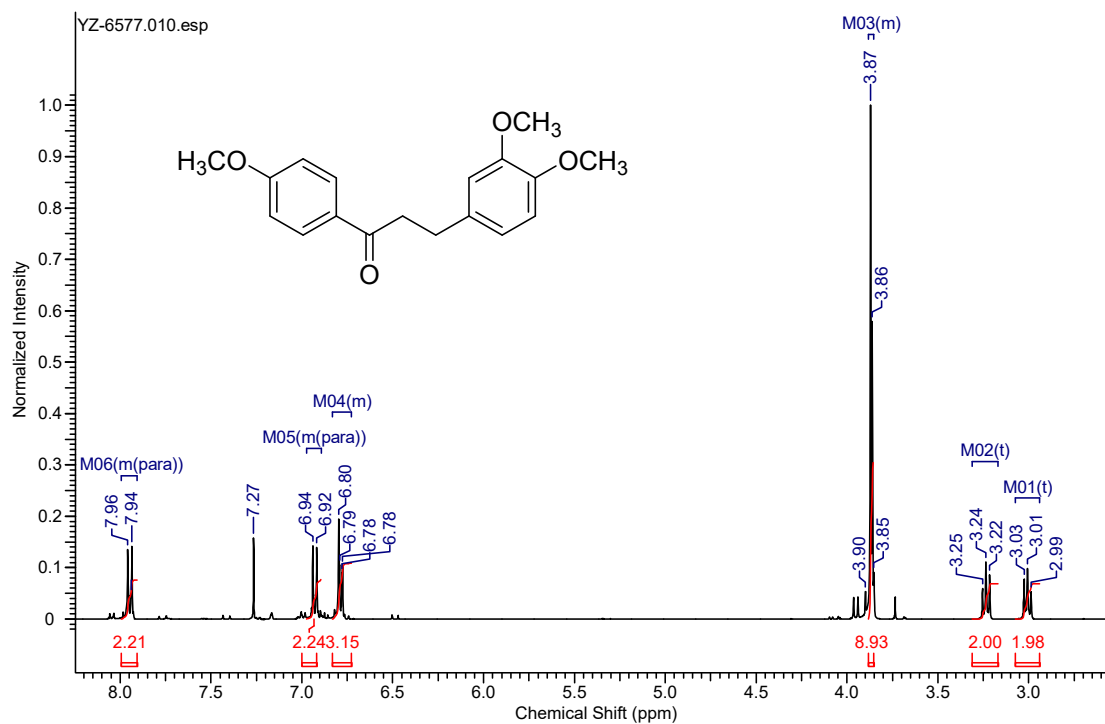


$^{13}\text{C}$  NMR (101 MHz, CHLOROFORM- $d$ )  $\delta$  198.1, 163.1, 158.0, 133.3, 133.1, 133.0, 131.9, 131.9, 129.4, 128.0, 127.9, 125.4, 125.3, 115.4, 115.1, 113.9, 77.4, 77.1, 76.8, 55.3, 40.7, 29.3, 14.6, 14.6

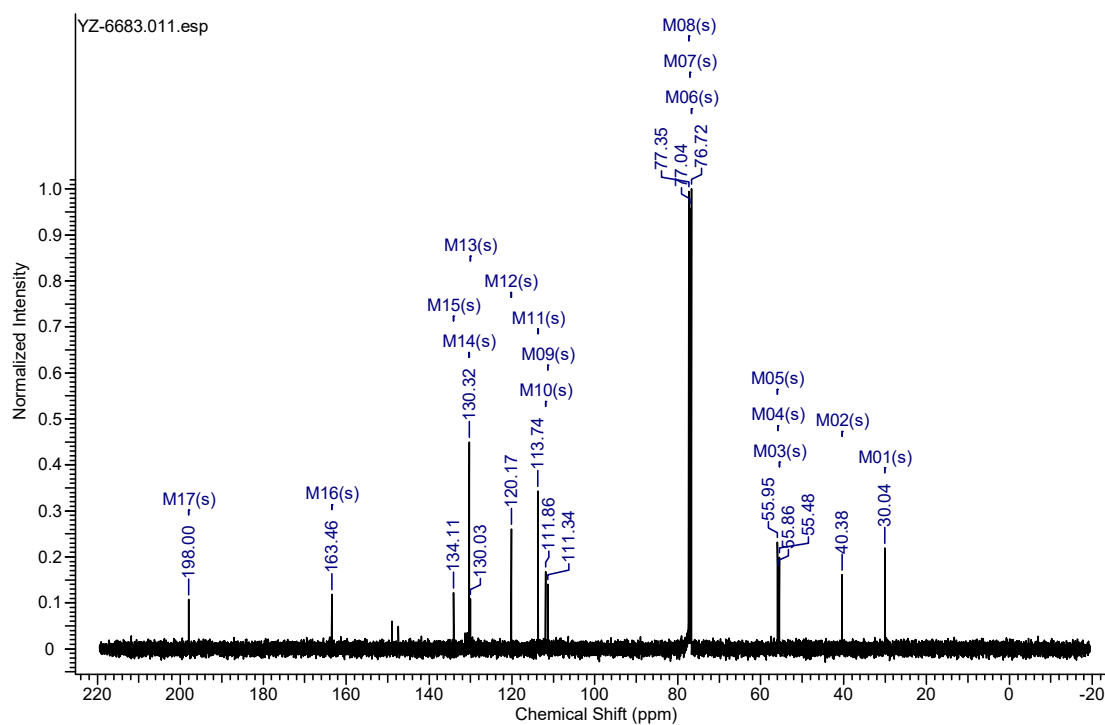




**Figure S20.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **3-(3,4-dimethoxyphenyl)-1-(4-methoxyphenyl)propan-1-one(4f)<sup>8</sup>**



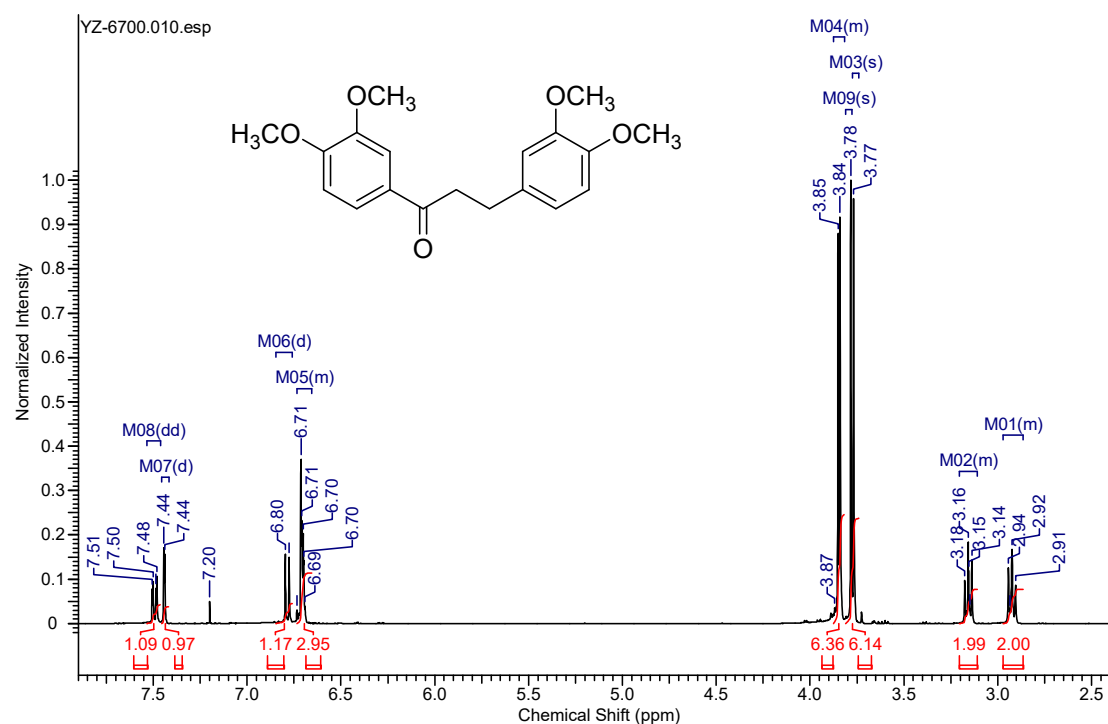
$^1\text{H}$  NMR (400 MHz,  $\text{CHCl}_3$ -d)  $\delta$  7.91 - 7.99 (m, 2H), 6.89 - 6.98 (m,  $J = 8.80$  Hz, 2H), 6.73 - 6.83 (m, 3H), 3.85 - 3.88 (m, 9H), 3.23 (t,  $J = 7.70$  Hz, 2H), 3.01 (t,  $J = 7.70$  Hz, 2H)



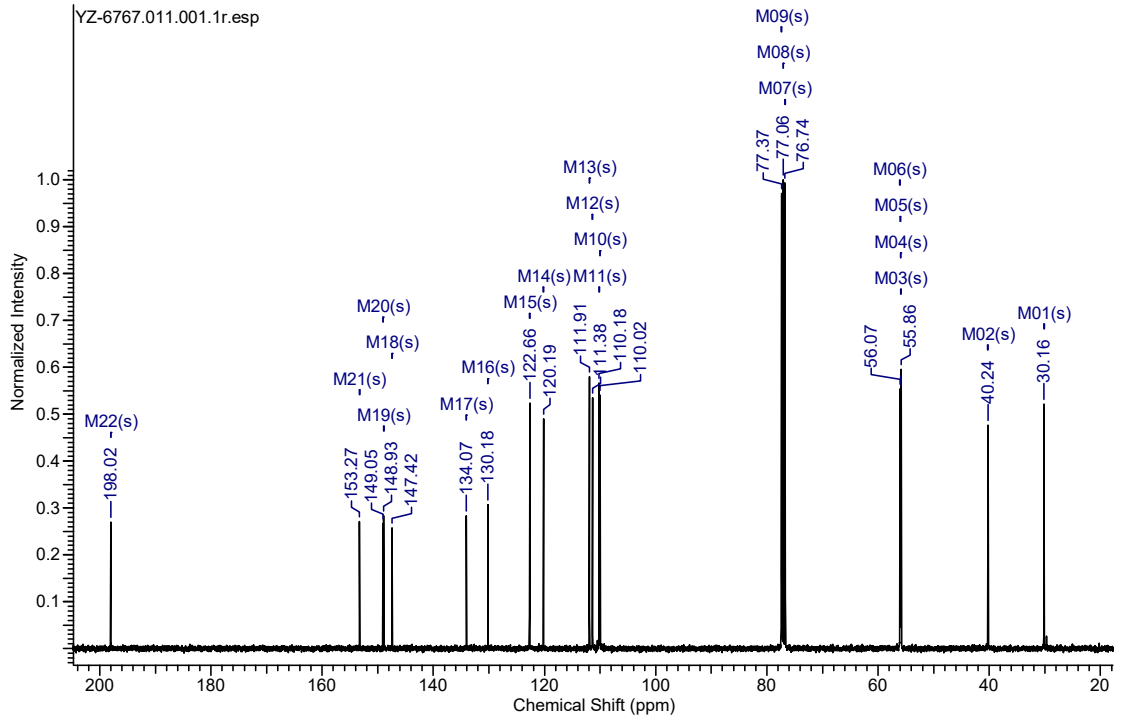
$^{13}\text{C}$  NMR (101 MHz, CHLOROFORM- $d$ )  $\delta$  198.0, 163.5, 134.1, 130.3, 130.0, 120.2, 113.7, 111.9, 111.3, 77.4, 77.0, 76.7, 56.0, 55.9, 55.5, 40.4, 30.0

**Figure S21.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **1,3-bis(3,4-dimethoxyphenyl)propan-1-one(4g)<sup>1</sup>**

$^1\text{H}$  NMR (400 MHz, CHLOROFORM- $d$ )  $\delta$  ppm 2.87 - 2.97 (m, 2 H) 3.11 - 3.20 (m, 2 H) 3.78 (s, 3 H) 3.77 (s, 3 H) 3.82 - 3.88 (m, 6 H) 6.66 - 6.73 (m, 3 H) 6.79 (d,  $J=8.31$  Hz, 1 H) 7.44 (d,  $J=1.96$  Hz, 1 H) 7.49 (dd,  $J=8.44, 2.08$  Hz, 1 H)



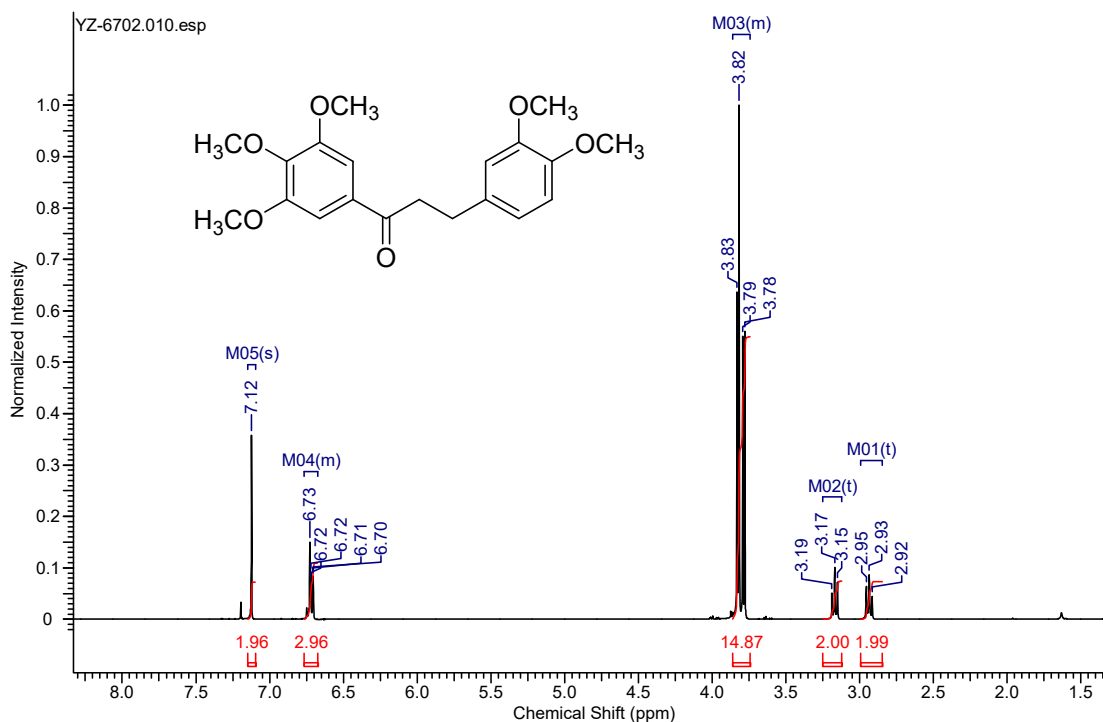
$^{13}\text{C}$  NMR (101 MHz, CHLOROFORM- $d$ )  $\delta$  198.0, 153.3, 149.1, 148.9, 147.4, 134.1, 130.2, 122.7, 120.2, 111.9, 111.4, 110.2, 110.0, 77.4, 77.1, 76.7, 56.1, 56.0, 56.0, 55.9, 40.2, 30.2



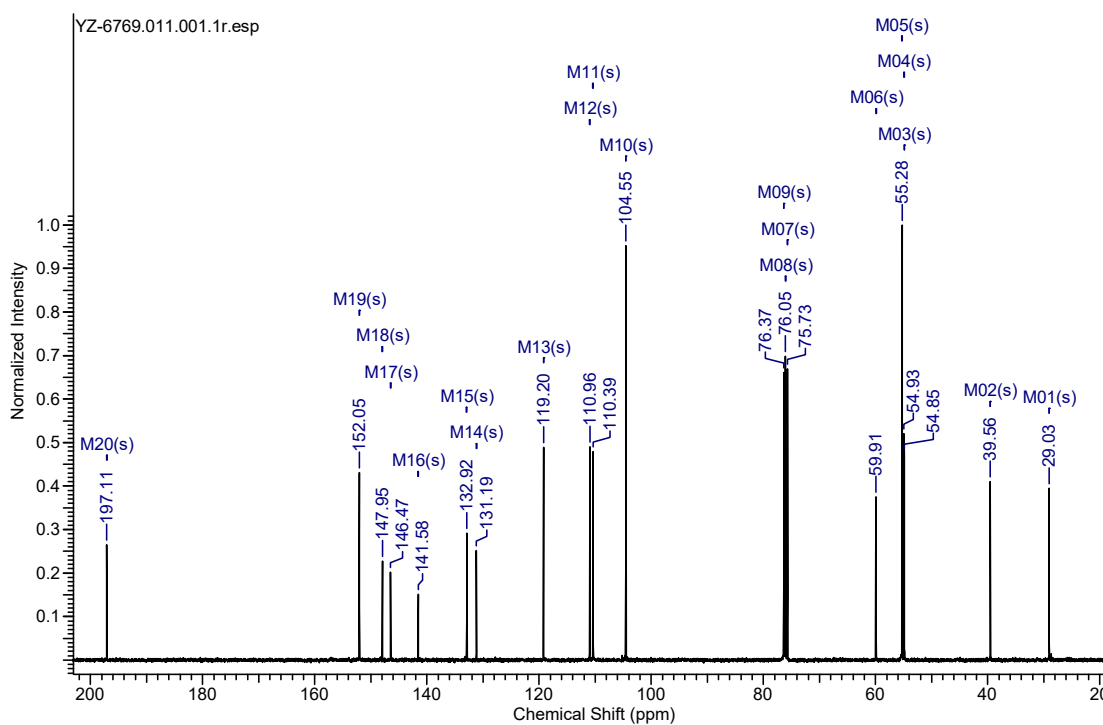
**Figure S22.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of

**3-(3,4-dimethoxyphenyl)-1-(3,4,5-trimethoxyphenyl)propan-1-one(4h)<sup>5</sup>**

$^1\text{H}$  NMR (400 MHz, CHLOROFORM-*d*)  $\delta$  ppm 2.93 (t,  $J=7.58$  Hz, 2 H) 3.17 (t,  $J=7.70$  Hz, 2 H) 3.74 - 3.86 (m, 15 H) 6.67 - 6.77 (m, 3 H) 7.12 (s, 2 H)



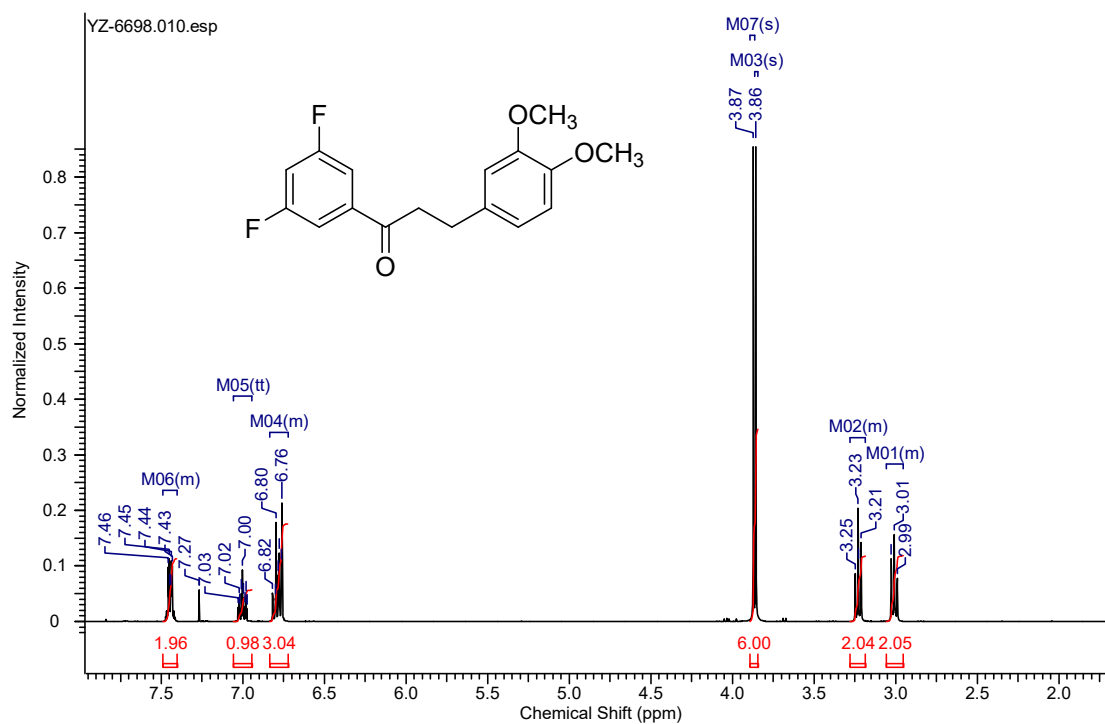
$^{13}\text{C}$  NMR (101 MHz, CHLOROFORM-*d*)  $\delta$  197.1, 152.1, 147.9, 146.5, 141.6, 132.9, 131.2, 119.2, 111.0, 110.4, 104.6, 76.4, 76.0, 75.7, 59.9, 55.3, 54.9, 54.9, 39.6, 29.0



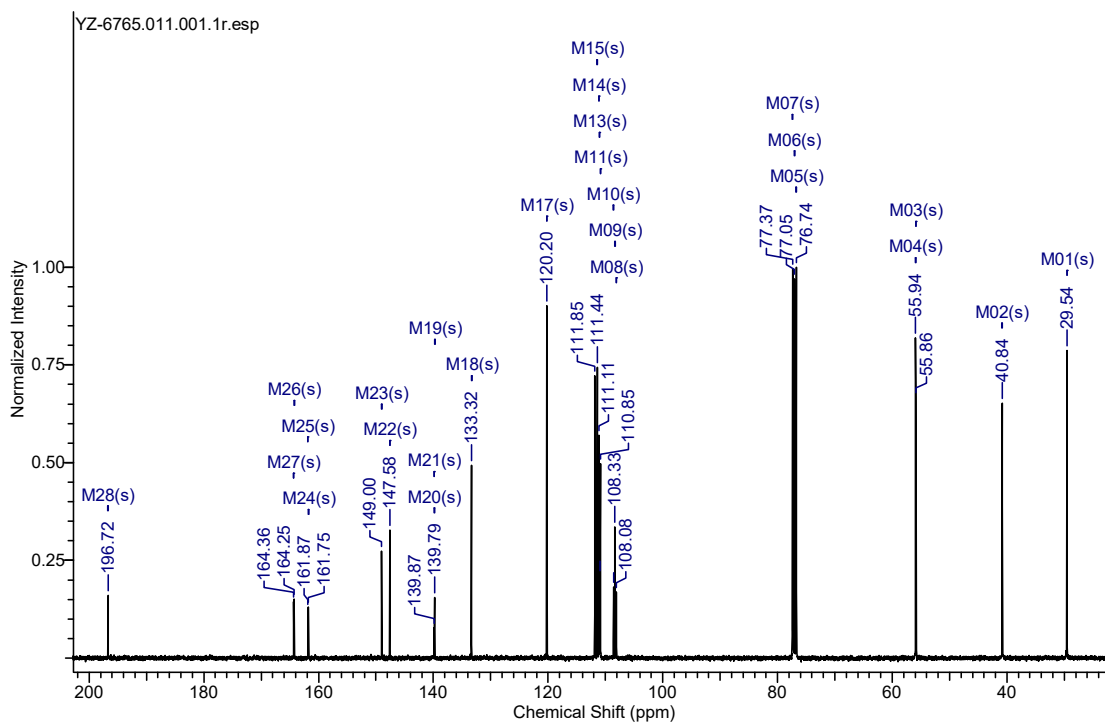
**Figure S23.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of

**1-(3,5-difluorophenyl)-3-(3,4-dimethoxyphenyl)propan-1-one(4i)**

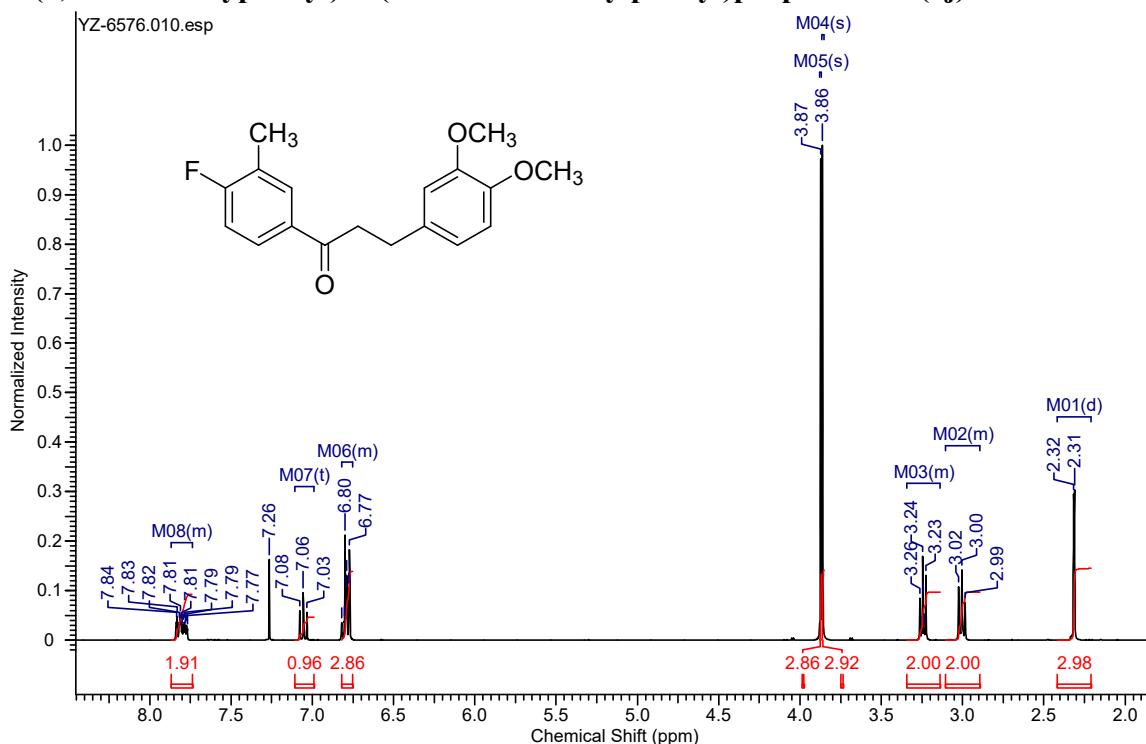
$^1\text{H}$  NMR (400 MHz,  $\text{CHLOROFORM-}d$ )  $\delta$  ppm 2.95 - 3.06 (m, 2 H) 3.18 - 3.28 (m, 2 H) 3.87 (s, 3 H) 3.86 (s, 3 H) 6.72 - 6.84 (m, 3 H) 7.00 (tt,  $J=8.38, 2.38$  Hz, 1 H) 7.40 - 7.49 (m, 2 H)



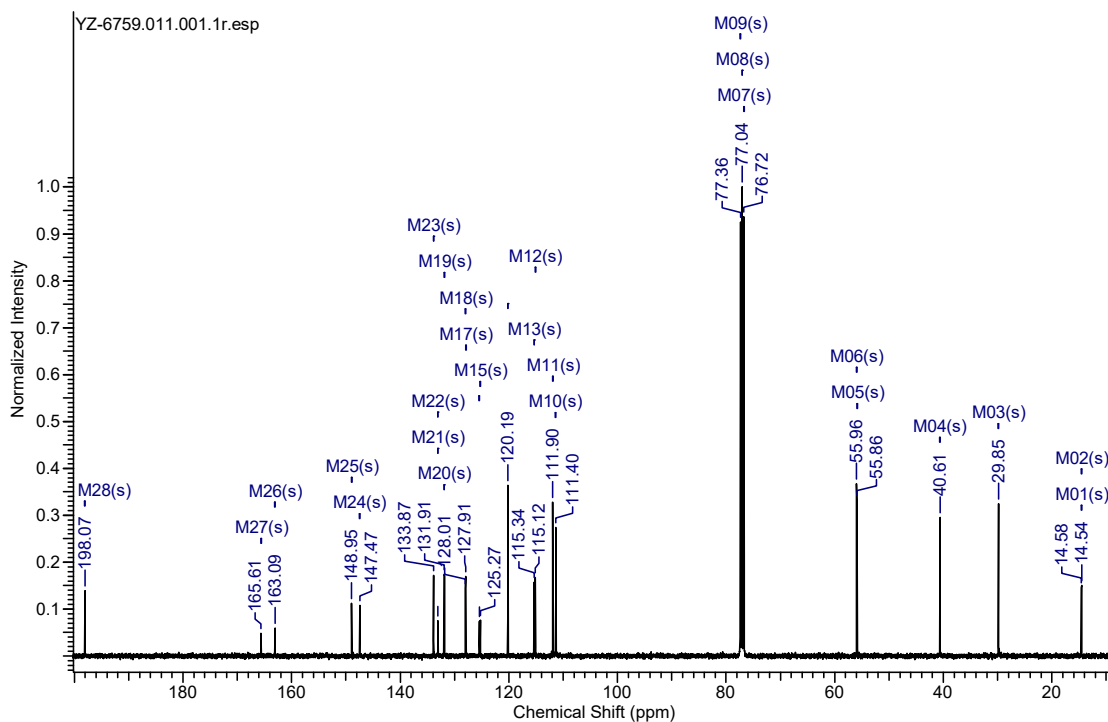
$^{13}\text{C}$  NMR (101 MHz,  $\text{CHLOROFORM-}d$ )  $\delta$  196.7, 164.4, 164.2, 161.9, 161.8, 149.0, 147.6, 139.9, 139.8, 139.7, 133.3, 120.2, 111.9, 111.4, 111.1, 111.0, 110.9, 110.8, 108.6, 108.3, 108.1, 77.4, 77.1, 76.7, 55.9, 55.9, 40.8, 29.5



**Figure S24.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **3-(3,4-dimethoxyphenyl)-1-(4-fluoro-3-methylphenyl)propan-1-one(4j)**



$^1\text{H}$  NMR (400 MHz, CHLOROFORM- $d$ )  $\delta$  7.74 - 7.87 (m, 2H), 7.06 (t,  $J$  = 8.80 Hz, 1H), 6.75 - 6.82 (m, 3H), 3.87 (s, 3H), 3.86 (s, 3H), 3.14 - 3.34 (m, 2H), 2.89 - 3.11 (m, 2H), 2.31 (d,  $J$  = 1.96 Hz, 3H)

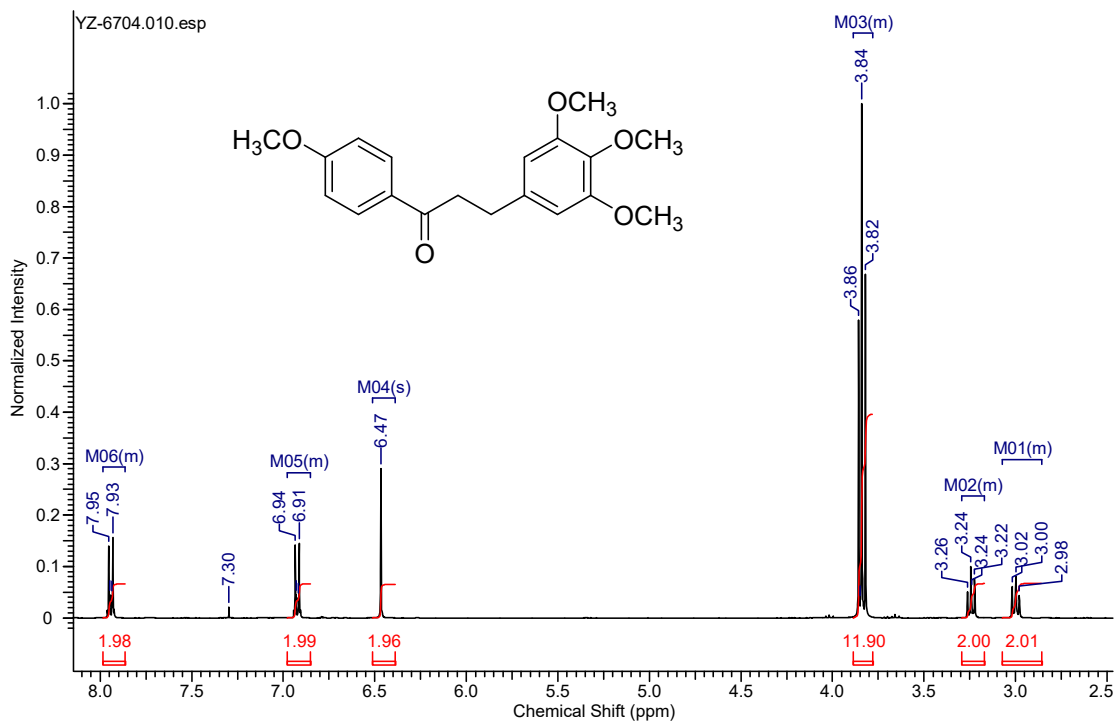


$^{13}\text{C}$  NMR (101 MHz, CHLOROFORM- $d$ )  $\delta$  198.1, 165.6, 163.1, 149.0, 147.5, 133.9, 133.1, 133.1, 131.9, 131.8, 128.0, 127.9, 125.4, 125.3, 120.2, 115.3, 115.1, 111.9, 111.4, 77.4, 77.0, 76.7, 56.0, 55.9, 40.6, 29.8, 14.6, 14.5

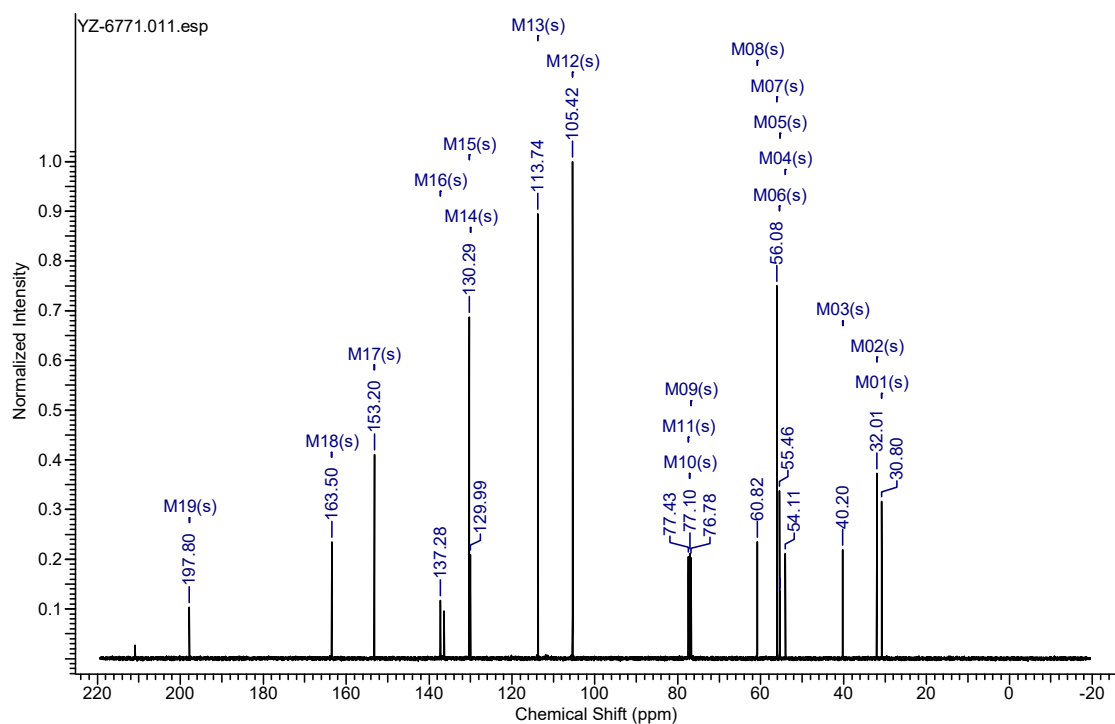
**Figure S25.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of

**1-(4-methoxyphenyl)-3-(3,4,5-trimethoxyphenyl)propan-1-one(4k)<sup>6</sup>**

$^1\text{H}$  NMR (400 MHz, CHLOROFORM- $d$ )  $\delta$  ppm 2.86 - 3.07 (m, 2 H) 3.17 - 3.29 (m, 2 H) 3.78 - 3.89 (m, 12 H) 6.47 (s, 2 H) 6.85 - 6.98 (m, 2 H) 7.87 - 7.98 (m, 2 H)



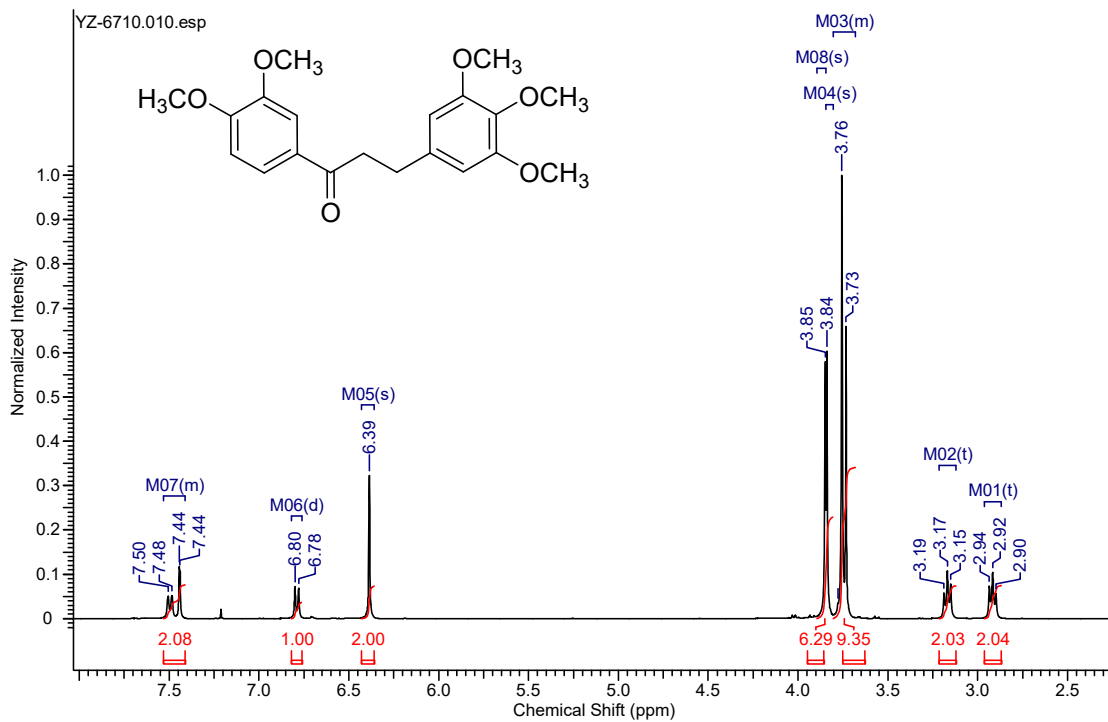
$^{13}\text{C}$  NMR (101 MHz, CHLOROFORM- $d$ )  $\delta$  197.8, 163.5, 153.2, 137.3, 130.3, 130.0, 113.7, 105.4, 77.4, 77.1, 76.8, 60.8, 56.1, 55.5, 55.3, 54.1, 40.2, 32.0, 30.8



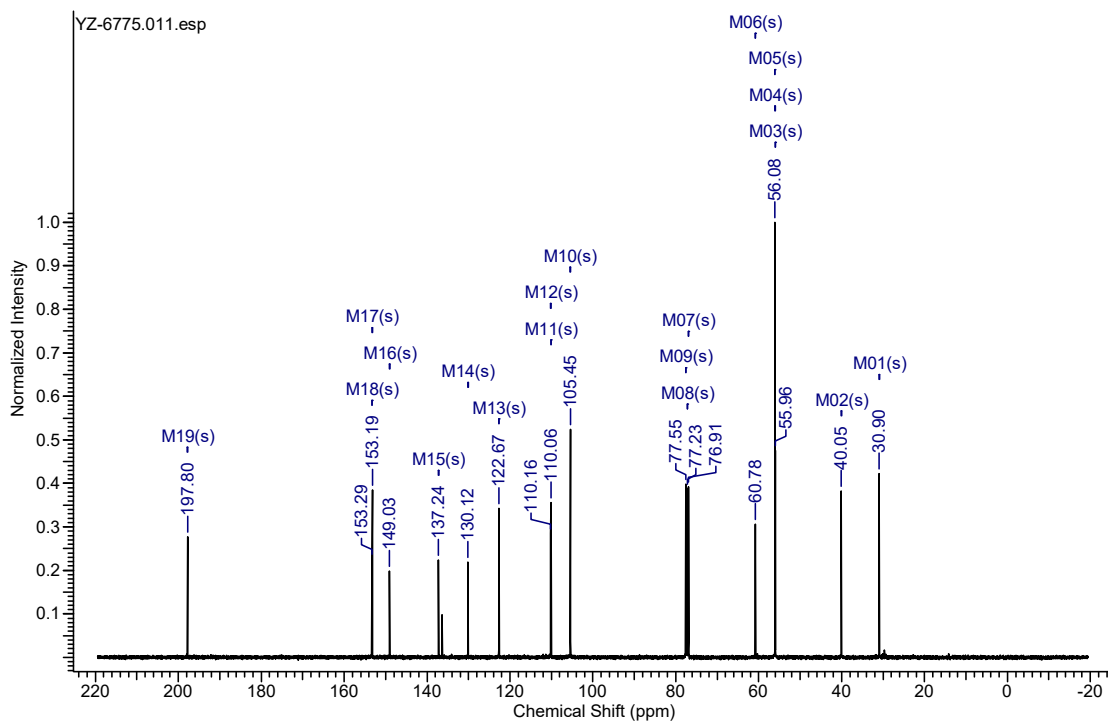
**Figure S26.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **1-(3,4-dimethoxyphenyl)-3-(3,4,5-trimethoxyphenyl)propan-1-one(4I) $^2$**

$^1\text{H}$  NMR (400 MHz, CHLOROFORM- $d$ )  $\delta$  7.41 - 7.53 (m, 2H), 6.79 (d,  $J = 8.31$  Hz, 1H), 6.39 (s, 2H), 3.84 (s, 3H), 3.85 (s, 3H), 3.68 - 3.81 (m, 9H), 3.17 (t,  $J = 7.58$  Hz, 2H), 2.92 (t,  $J = 7.46$  Hz, 2H)



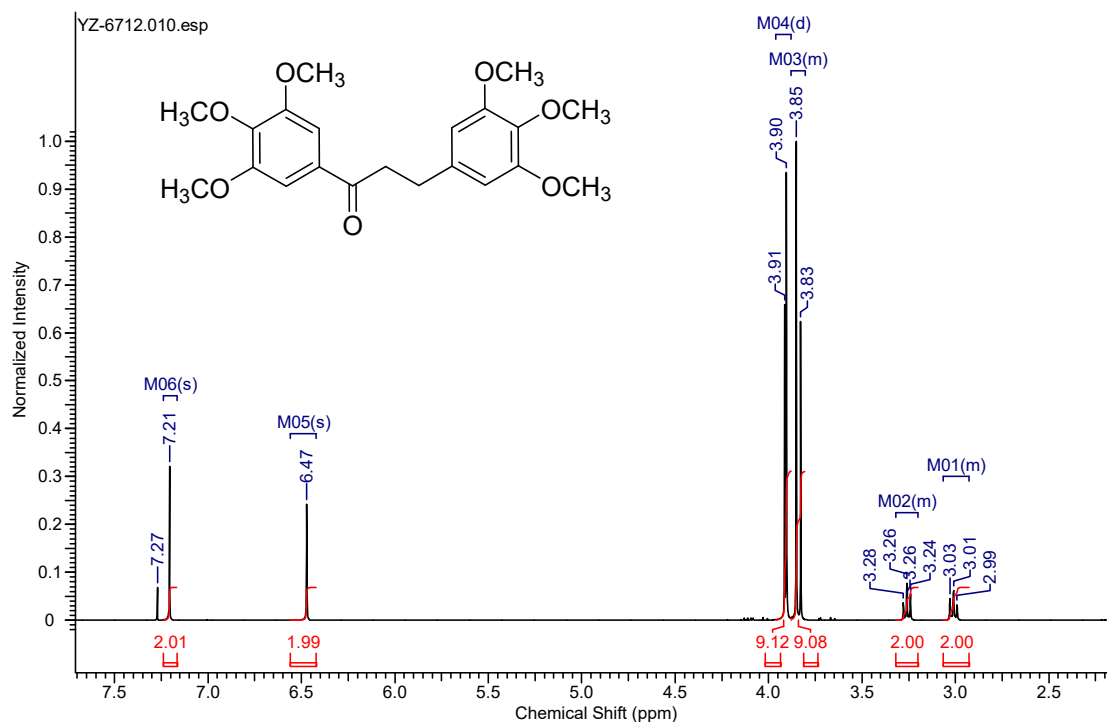


$^{13}\text{C}$  NMR (101 MHz, CHLOROFORM- $d$ )  $\delta$  197.8, 153.3, 153.2, 149.0, 137.2, 130.1, 122.7, 110.2, 110.1, 105.5, 77.5, 77.2, 76.9, 60.8, 56.1, 56.0, 56.0, 40.1, 30.9

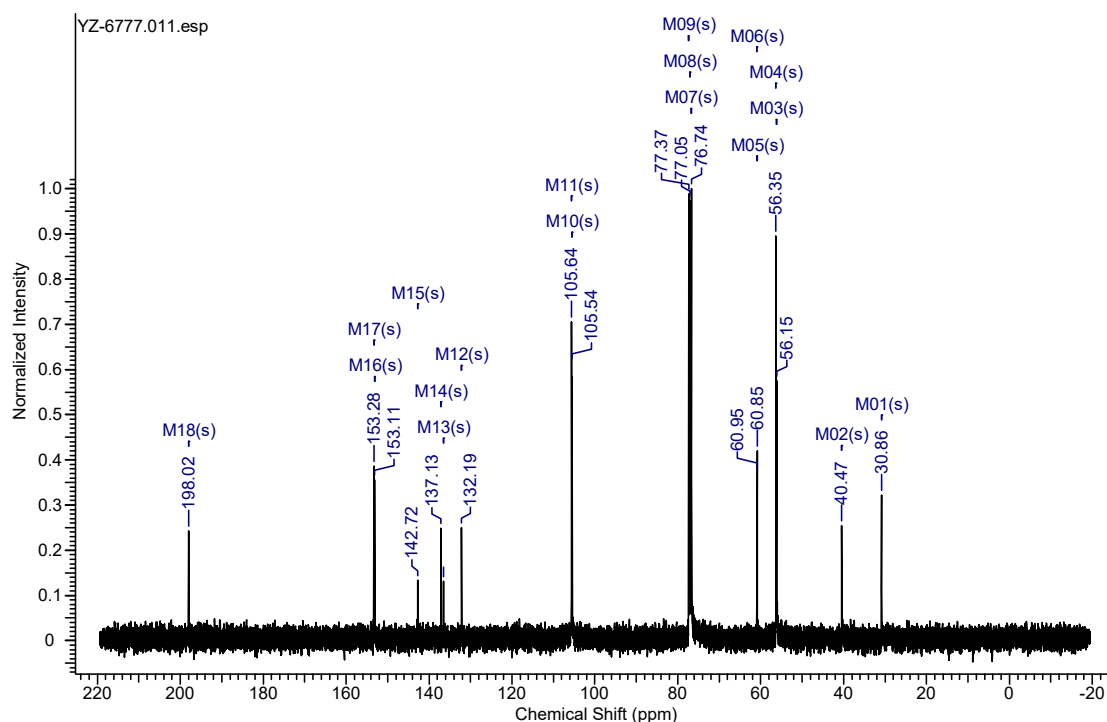


**Figure S27.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **1,3-bis(3,4,5-trimethoxyphenyl)propan-1-one(4m)**

$^1\text{H}$  NMR (400 MHz, CHLOROFORM-*d*)  $\delta$  ppm 2.93 - 3.07 (m, 2 H) 3.20 - 3.32 (m, 2 H) 3.80 - 3.88 (m, 9 H) 3.91 (d,  $J=3.91$  Hz, 9 H) 6.47 (s, 2 H) 7.21 (s, 2 H)



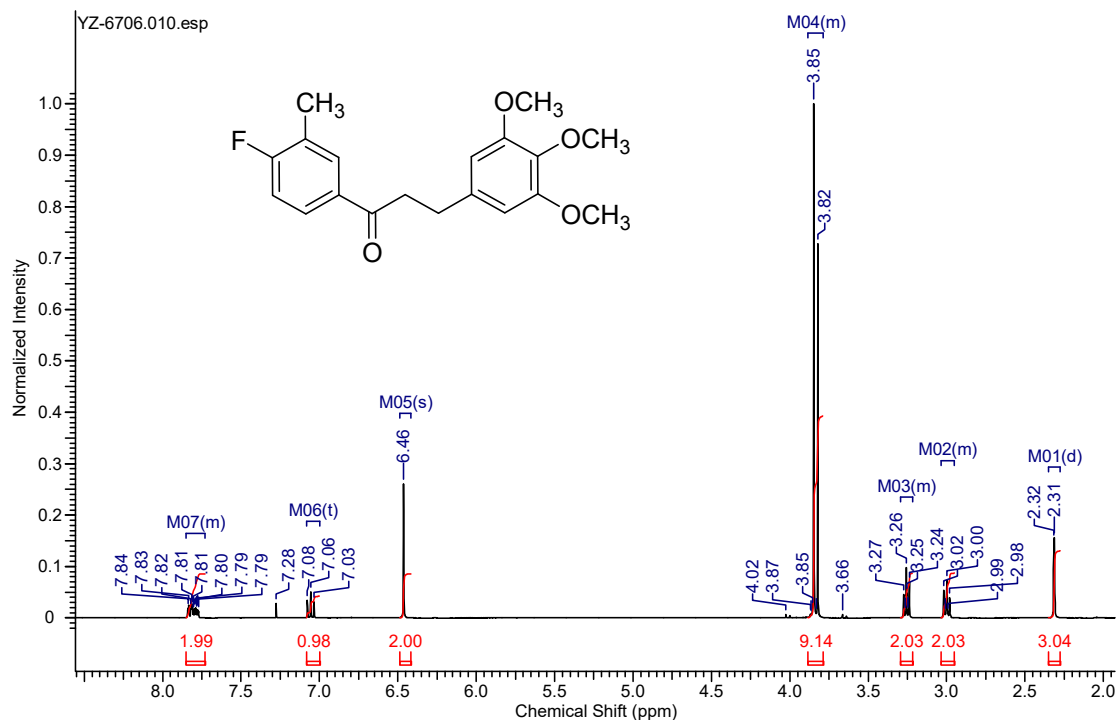
$^{13}\text{C}$  NMR (101 MHz, CHLOROFORM-*d*)  $\delta$  198.0, 153.3, 153.1, 142.7, 137.1, 136.5, 132.2, 105.6, 105.5, 77.4, 77.1, 76.7, 60.9, 60.9, 56.4, 56.1, 40.5, 30.9



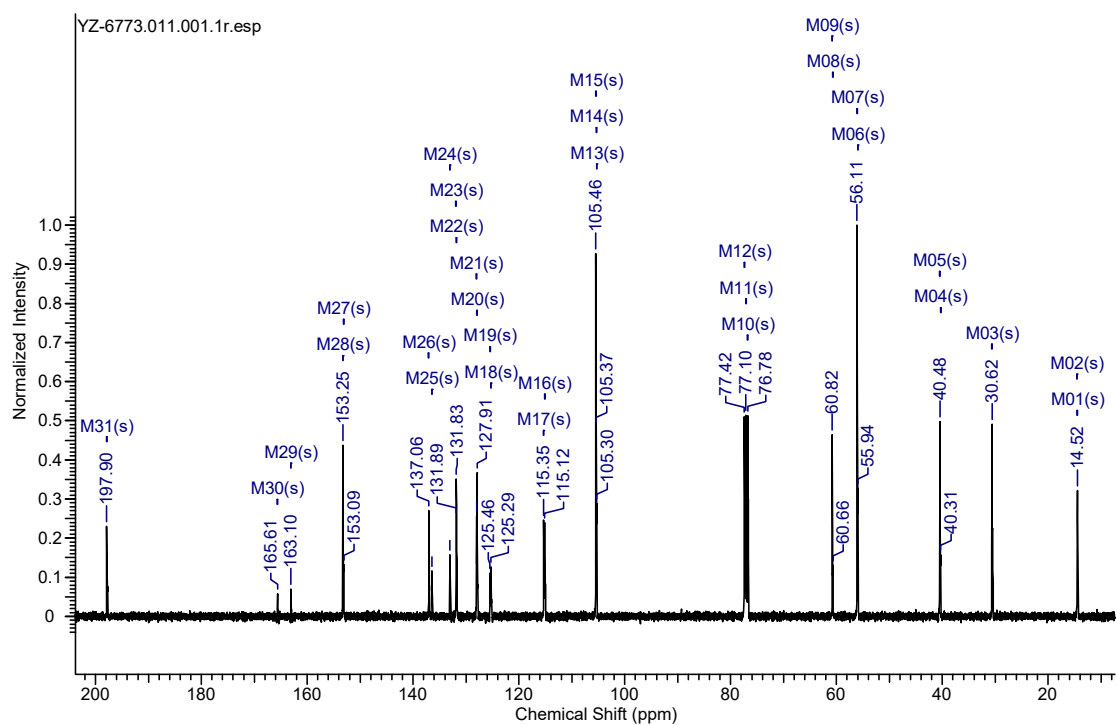
**Figure S28.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of

**1-(4-fluoro-3-methylphenyl)-3-(3,4,5-trimethoxyphenyl)propan-1-one(4n)**

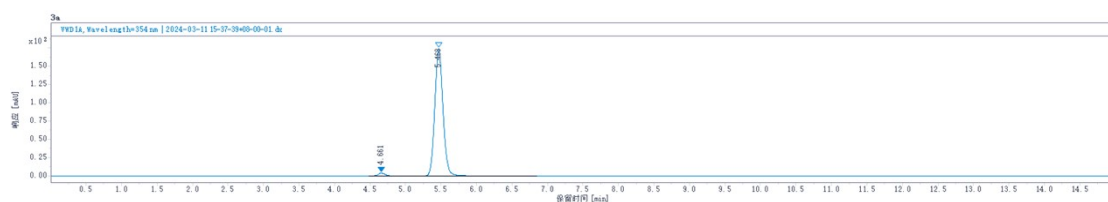
$^1\text{H}$  NMR (400 MHz, CHLOROFORM- $d$ )  $\delta$  7.73 - 7.85 (m, 2H), 7.06 (t,  $J$  = 8.80 Hz, 1H), 6.46 (s, 2H), 3.79 - 3.88 (m, 9H), 3.22 - 3.29 (m, 2H), 2.95 - 3.04 (m, 2H), 2.31 (d,  $J$  = 1.96 Hz, 3H)



$^{13}\text{C}$  NMR (101 MHz, CHLOROFORM- $d$ )  $\delta$  197.9, 165.6, 163.1, 153.3, 153.1, 137.1, 136.4, 133.0, 131.9, 131.8, 128.0, 127.9, 125.5, 125.3, 115.4, 115.1, 105.5, 105.4, 105.3, 77.4, 77.1, 76.8, 60.8, 60.7, 56.1, 55.9, 40.5, 40.3, 30.6, 14.6, 14.5

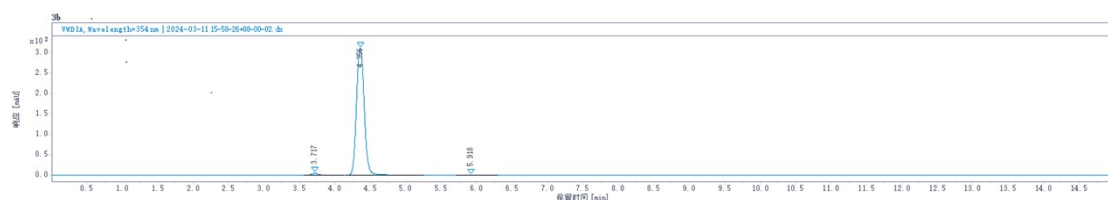


**Figure S29. HPLC-purity spectra of (E)-1,3-bis(4-methoxyphenyl)prop-2-en-1-one(3a)**



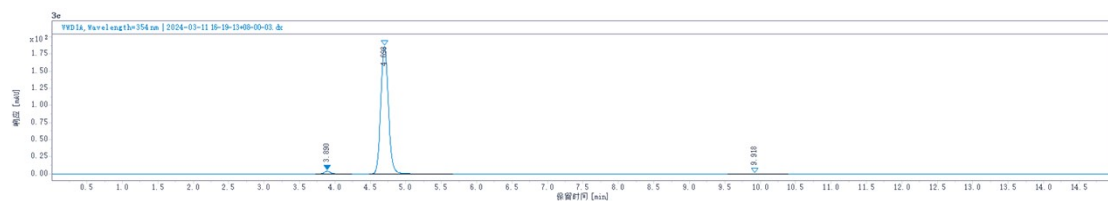
RT (min)	A (mAU·s)	A %	H(mAU)	H%
5.468	14049.819	98.235	1744.983	97.94

**Figure S30. HPLC-purity spectra of (E)-1-(3,4-dimethoxyphenyl)-3-(4-methoxyphenyl)prop-2-en-1-one(3b)**



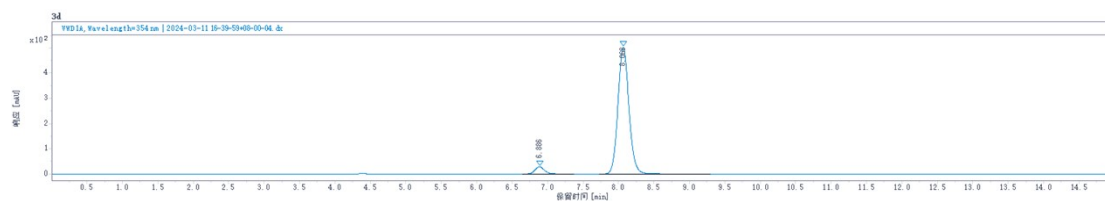
RT (min)	A (mAU·s)	A %	H(mAU)	H%
4.356	23751.979	98.840	3101.850	98.53

**Figure S31. HPLC-purity spectra of (E)-3-(4-methoxyphenyl)-1-(3,4,5-trimethoxyphenyl)prop-2-en-1-one(3c)**



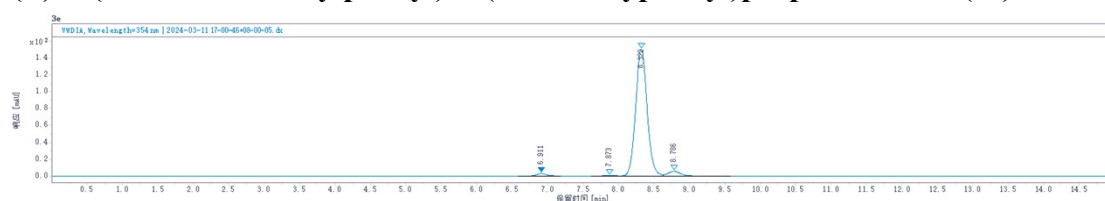
RT (min)	A (mAU·s)	A %	H(mAU)	H%
4.698	13895.724	98.201	1861.197	97.95

**Figure S32. HPLC-purity spectra of (E)-1-(3,5-difluorophenyl)-3-(4-methoxyphenyl)prop-2-en-1-one(3d)**



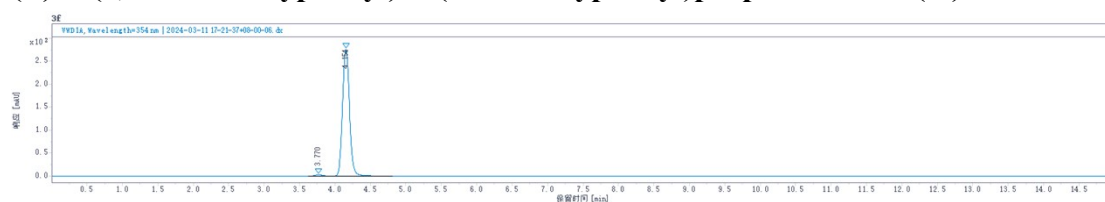
RT (min)	A (mAU·s)	A %	H(mAU)	H%
8.068	5413.124	95.385	502.750	94.63

**Figure S33.** HPLC-purity spectra of **(E)-1-(4-fluoro-3-methylphenyl)-3-(4-methoxyphenyl)prop-2-en-1-one(3e)**



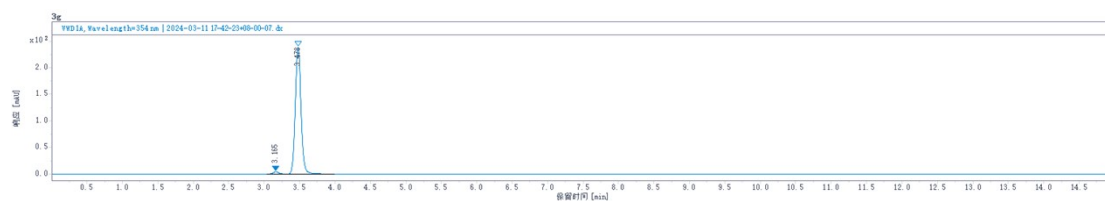
RT (min)	A (mAU·s)	A %	H(mAU)	H%
8.322	16918.283	95.223	1505.866	94.27

**Figure S34.** HPLC-purity spectra of **(E)-3-(3,4-dimethoxyphenyl)-1-(4-methoxyphenyl)prop-2-en-1-one(3f)**



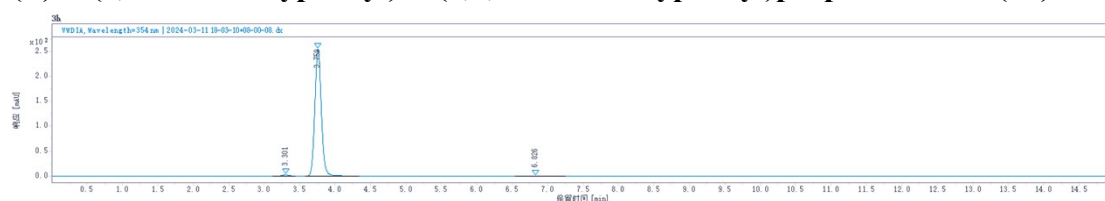
RT (min)	A (mAU·s)	A %	H(mAU)	H%
4.154	18831.46	98.910	2762.747	98.72

**Figure S35.** HPLC-purity spectra of **(E)-1,3-bis(3,4-dimethoxyphenyl)prop-2-en-1-one(3g)**



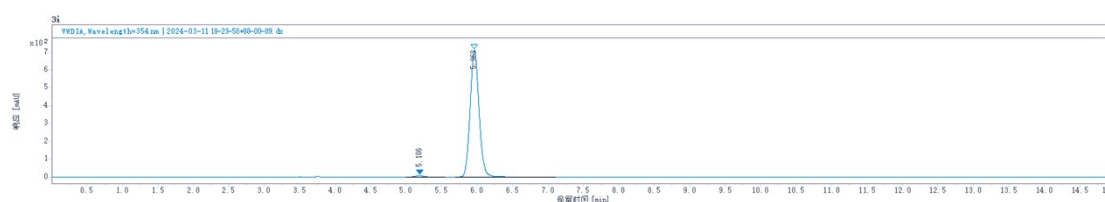
RT (min)	A (mAU·s)	A %	H(mAU)	H%
3.478	13510.705	98.482	2387.008	98.4

**Figure S36.** HPLC-purity spectra of  
**(E)-3-(3,4-dimethoxyphenyl)-1-(3,4,5-trimethoxyphenyl)prop-2-en-1-one(3h)**



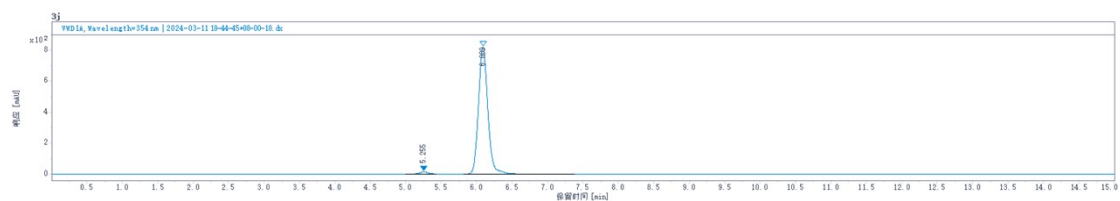
RT (min)	A (mAU·s)	A %	H(mAU)	H%
3.759	16322.255	98.954	2542.324	98.96

**Figure S37.** HPLC-purity spectra of  
**(E)-1-(3,5-difluorophenyl)-3-(3,4-dimethoxyphenyl)prop-2-en-1-one(3i)**



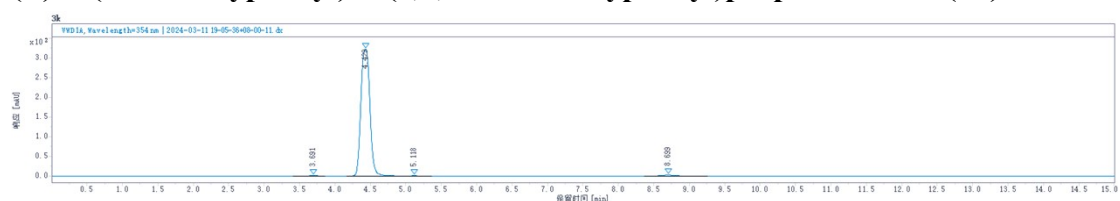
RT (min)	A (mAU·s)	A %	H(mAU)	H%
5.963	6239.909	99.062	711.151	98.93

**Figure S38.** HPLC-purity spectra of  
**(E)-3-(3,4-dimethoxyphenyl)-1-(4-fluoro-3-methylphenyl)prop-2-en-1-one(3j)**



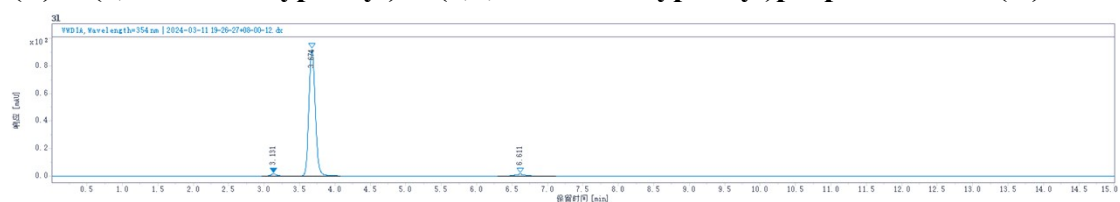
RT (min)	A (mAU·s)	A %	H(mAU)	H%
6.089	7511.836	98.572	818.616	98.35

**Figure S39.** HPLC-purity spectra of **(E)-1-(4-methoxyphenyl)-3-(3,4,5-trimethoxyphenyl)prop-2-en-1-one(3k)**



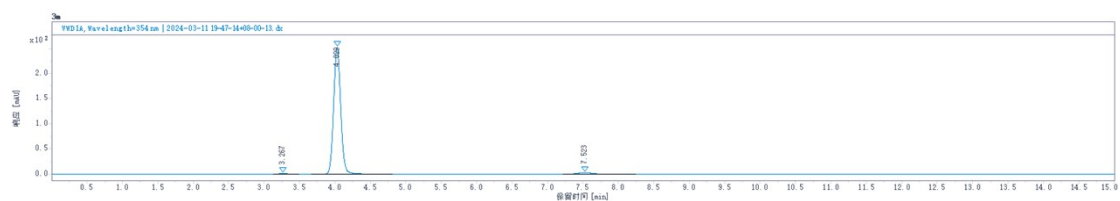
RT (min)	A (mAU·s)	A %	H(mAU)	H%
4.429	28579.264	98.276	3222.672	98.51

**Figure S40.** HPLC-purity spectra of **(E)-1-(3,4-dimethoxyphenyl)-3-(3,4,5-trimethoxyphenyl)prop-2-en-1-one(3l)**



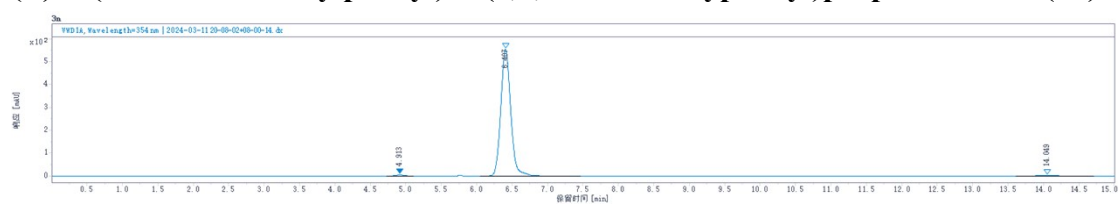
RT (min)	A (mAU·s)	A %	H(mAU)	H%
3.674	5726.501	96.403	921.734	97.11

**Figure S41.** HPLC-purity spectra of **(E)-1,3-bis(3,4,5-trimethoxyphenyl)prop-2-en-1-one(3m)**



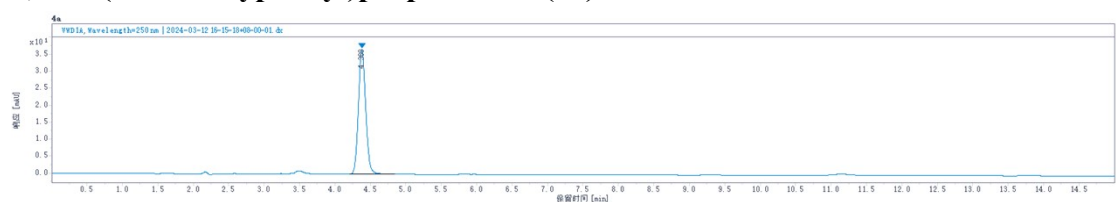
RT (min)	A (mAU·s)	A %	H(mAU)	H%
4.029	17553.933	97.446	2523.966	98.27

**Figure S42.** HPLC-purity spectra of **(E)-1-(4-fluoro-3-methylphenyl)-3-(3,4,5-trimethoxyphenyl)prop-2-en-1-one(3n)**



RT (min)	A (mAU·s)	A %	H(mAU)	H%
6.407	5391.019	98.733	554.526	98.81

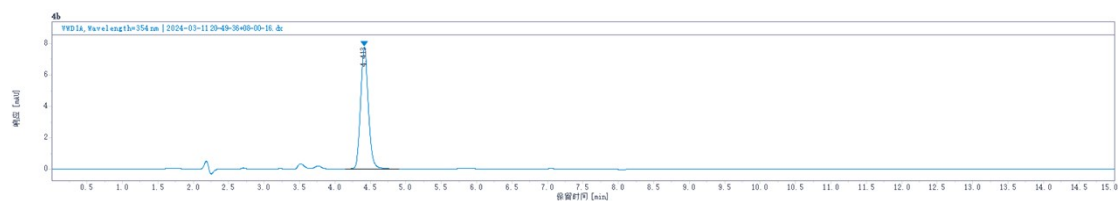
**Figure S43.** HPLC-purity spectra of **1,3-bis(4-methoxyphenyl)propan-1-one(4a)**



RT (min)	A (mAU·s)	A %	H(mAU)	H%
4.380	264.727	100.000	36.785	100.00

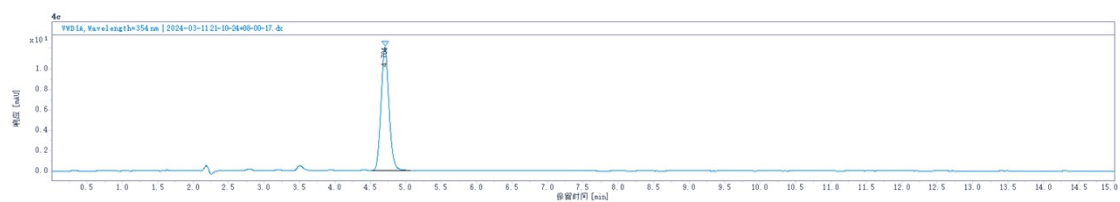
**Figure S44.** HPLC-purity spectra of **1-(3,4-dimethoxyphenyl)-3-(4-methoxyphenyl)propan-1-one(4b)**





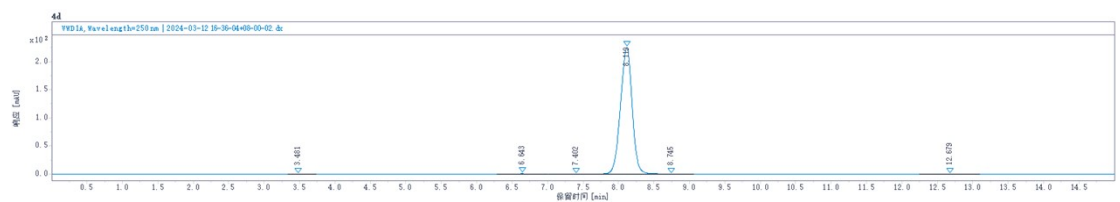
RT (min)	A (mAU·s)	A %	H(mAU)	H%
4.413	59.679	100.000	7.767	100.00

**Figure S45.** HPLC-purity spectra of **3-(4-methoxyphenyl)-1-(3,4,5-trimethoxyphenyl)propan-1-one(4c)**



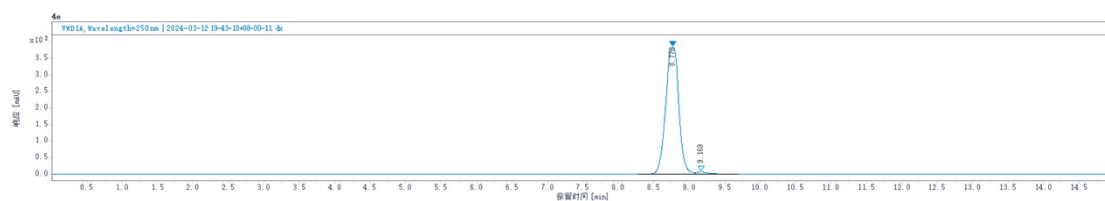
RT (min)	A (mAU·s)	A %	H(mAU)	H%
4.704	93.805	100.000	12.027	100.00

**Figure S46.** HPLC-purity spectra of **1-(3,5-difluorophenyl)-3-(4-methoxyphenyl)propan-1-one(4d)**



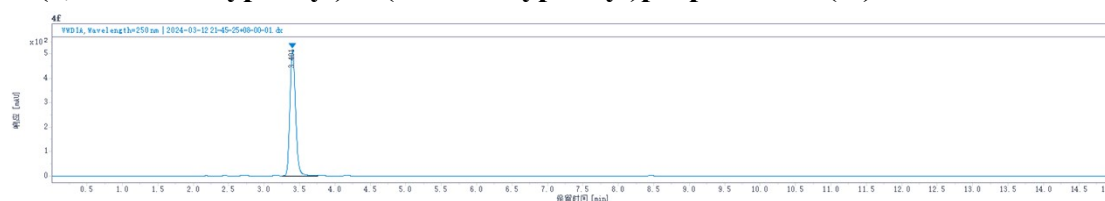
RT (min)	A (mAU·s)	A %	H(mAU)	H%
8.119	25828.361	99.432	2256.125	99.40

**Figure S47.** HPLC-purity spectra of **1-(4-fluoro-3-methylphenyl)-3-(4-methoxyphenyl)propan-1-one(4e)**



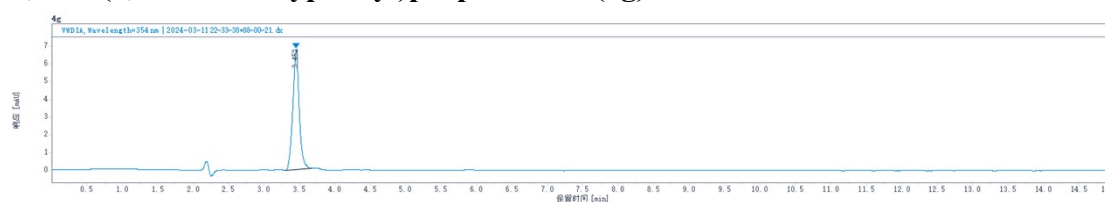
RT (min)	A (mAU·s)	A %	H(mAU)	H%
8.770	49187.772	98.639	3832.089	98.58

**Figure S48.** HPLC-purity spectra of **3-(3,4-dimethoxyphenyl)-1-(4-methoxyphenyl)propan-1-one(4f)**



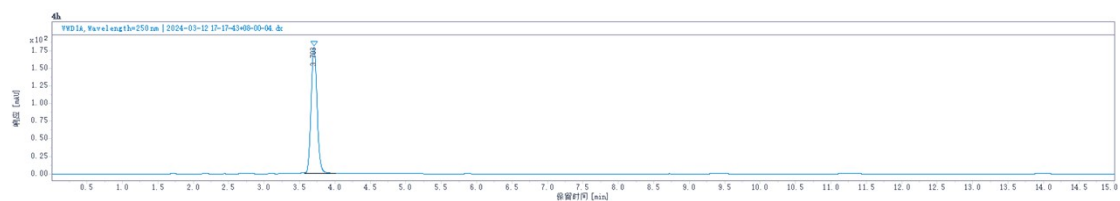
RT (min)	A (mAU·s)	A %	H(mAU)	H%
3.401	2854.960	100.000	519.424	100.00

**Figure S49.** HPLC-purity spectra of **1,3-bis(3,4-dimethoxyphenyl)propan-1-one(4g)**



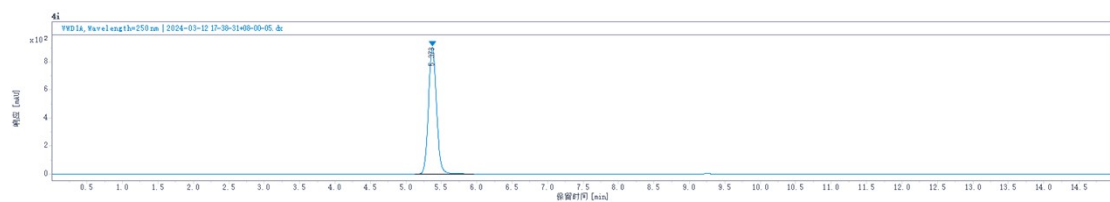
RT (min)	A (mAU·s)	A %	H(mAU)	H%
3.452	42.727	100.000	6.781	100.00

**Figure S50.** HPLC-purity spectra of **3-(3,4-dimethoxyphenyl)-1-(3,4,5-trimethoxyphenyl)propan-1-one(4h)**



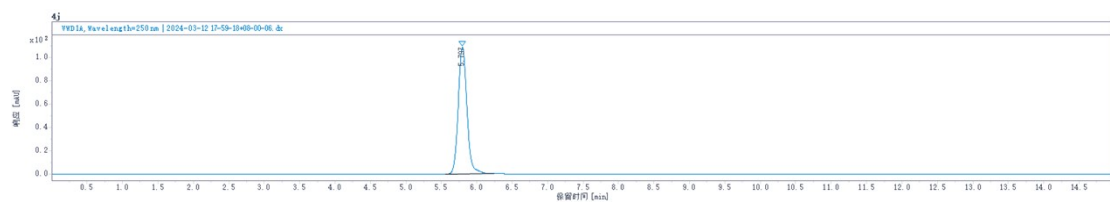
RT (min)	A (mAU·s)	A %	H(mAU)	H%
3.703	1067.594	100.000	180.457	100.00

**Figure S51.** HPLC-purity spectra of **1-(3,5-difluorophenyl)-3-(3,4-dimethoxyphenyl)propan-1-one(4i)**



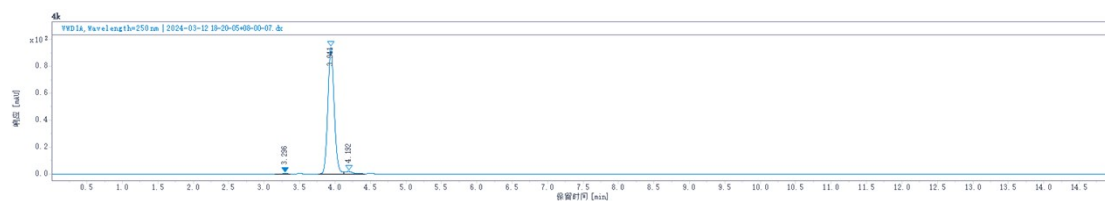
RT (min)	A (mAU·s)	A %	H(mAU)	H%
5.373	7143.652	100.000	904.950	100.00

**Figure S52.** HPLC-purity spectra of **3-(3,4-dimethoxyphenyl)-1-(4-fluoro-3-methylphenyl)propan-1-one(4j)**



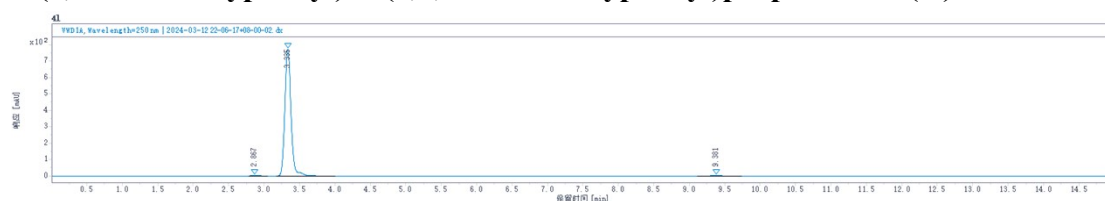
RT (min)	A (mAU·s)	A %	H(mAU)	H%
5.797	9298.015	100.000	1088.935	100.00

**Figure S53.** HPLC-purity spectra of **1-(4-methoxyphenyl)-3-(3,4,5-trimethoxyphenyl)propan-1-one(4k)**



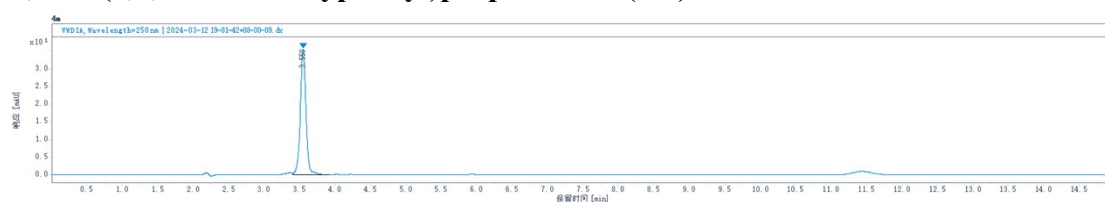
RT (min)	A (mAU·s)	A %	H(mAU)	H%
3.941	5934.708	97.561	941.638	97.91

**Figure S54.** HPLC-purity spectra of **1-(3,4-dimethoxyphenyl)-3-(3,4,5-trimethoxyphenyl)propan-1-one(4l)**



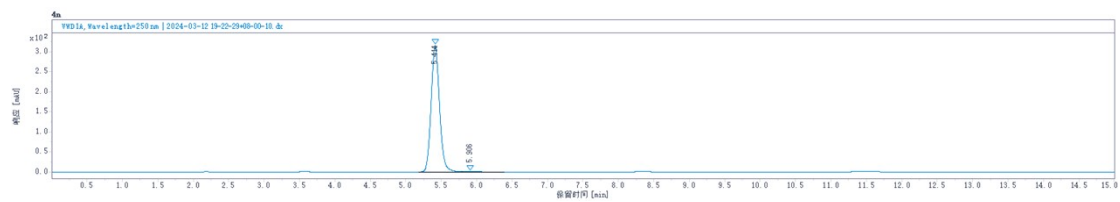
RT (min)	A (mAU·s)	A %	H(mAU)	H%
3.335	4676.390	98.942	772.720	99.19

**Figure S55.** HPLC-purity spectra of **1,3-bis(3,4,5-trimethoxyphenyl)propan-1-one(4m)**



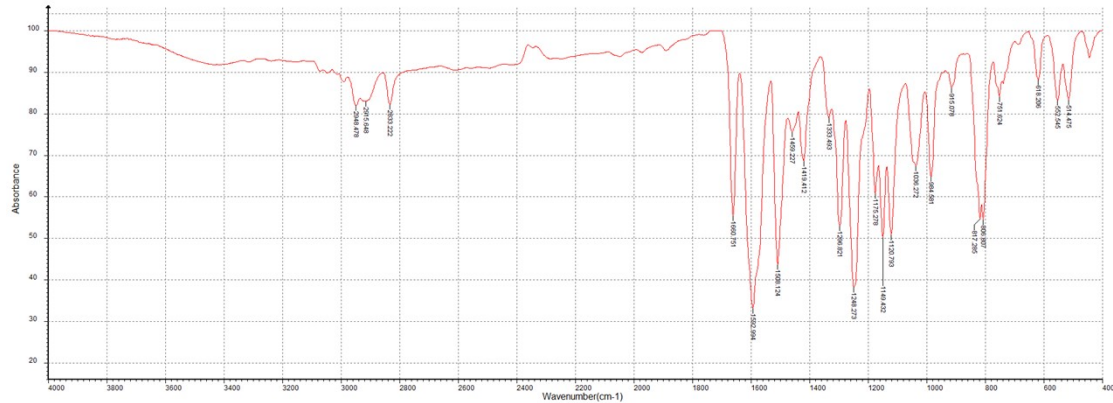
RT (min)	A (mAU·s)	A %	H(mAU)	H%
3.550	196.473	100.000	35.503	100.00

**Figure S56.** HPLC-purity spectra of **1-(4-fluoro-3-methylphenyl)-3-(3,4,5-trimethoxyphenyl)propan-1-one(4n)**

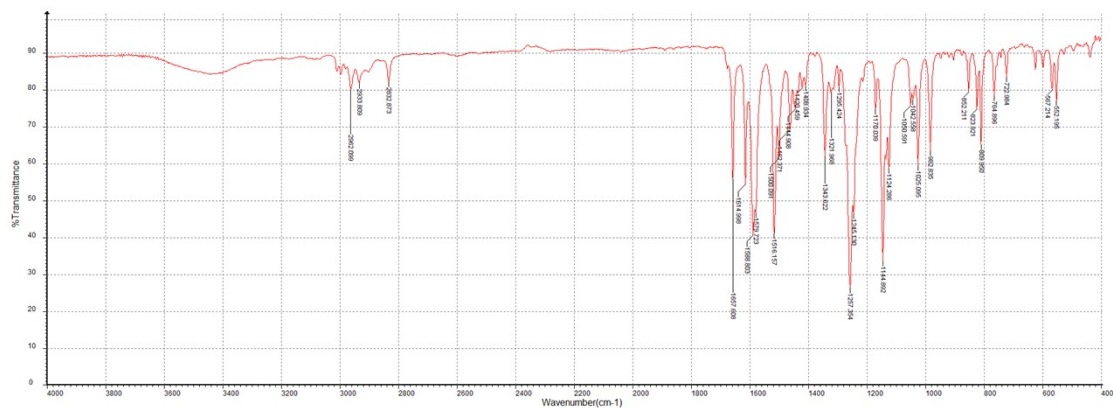


RT (min)	A (mAU·s)	A %	H(mAU)	H%
5.414	2615.111	99.235	315.734	99.38

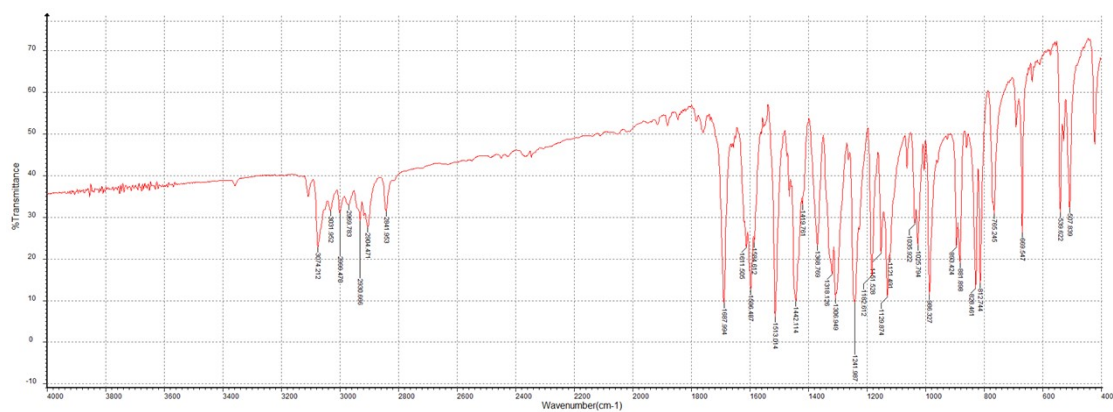
**Figure S57.** IR spectra of  
**(E)-1-(4-fluoro-3-methylphenyl)-3-(4-methoxyphenyl)prop-2-en-1-one(3e)**



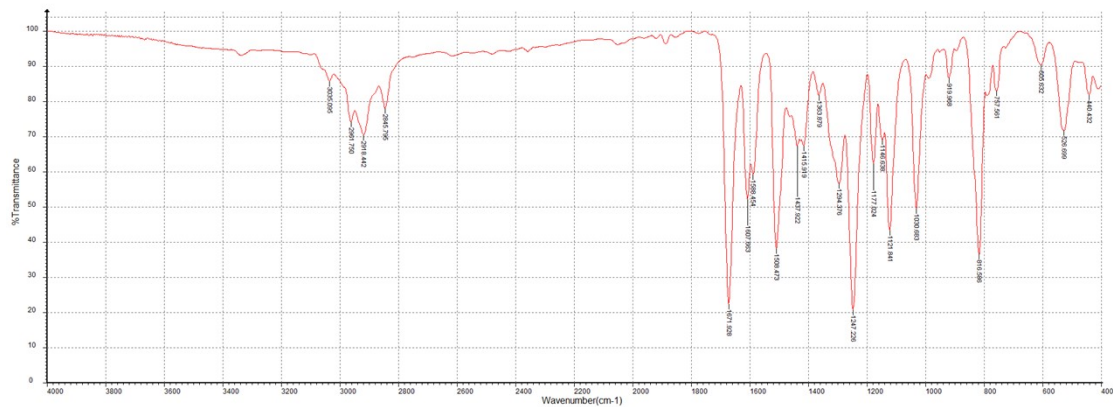
**Figure S58.** IR spectra of  
**(E)-3-(3,4-dimethoxyphenyl)-1-(4-fluoro-3-methylphenyl)prop-2-en-1-one(3j)**



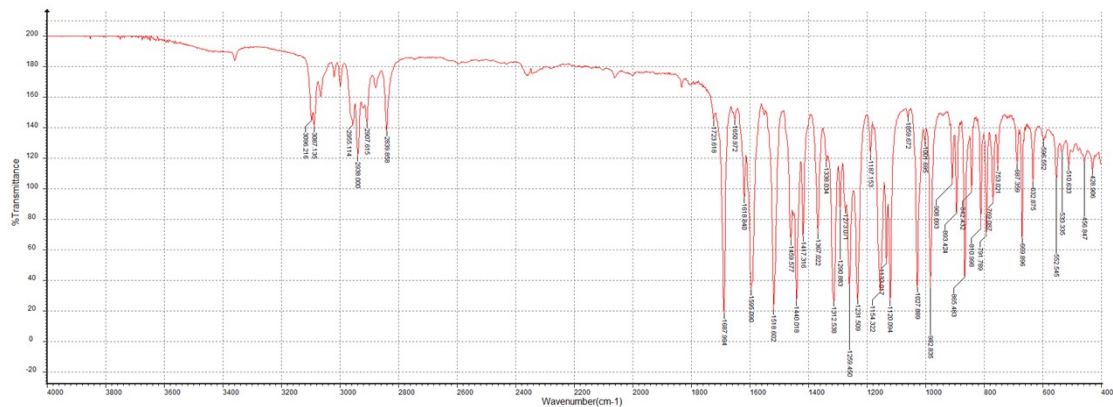
**Figure S59.** IR spectra of  
**1-(3,5-difluorophenyl)-3-(4-methoxyphenyl)propan-1-one(4d)**



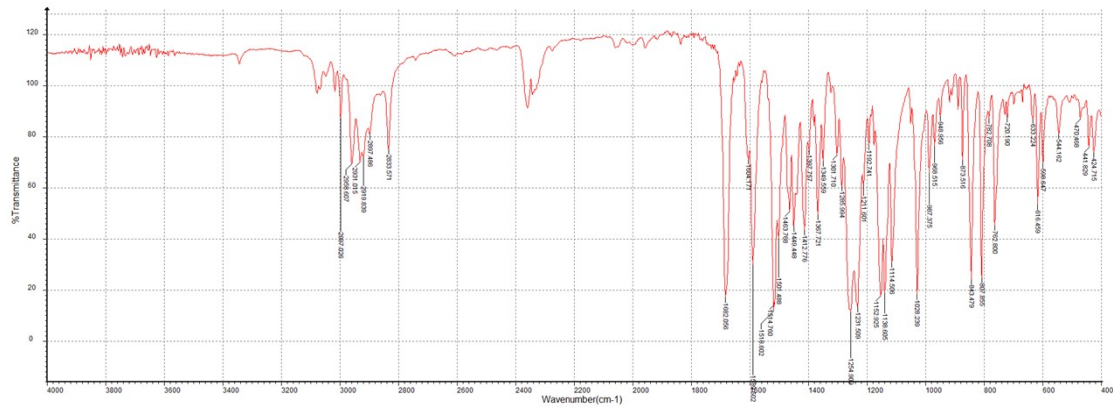
**Figure S60.** IR spectra of  
**1-(4-fluoro-3-methylphenyl)-3-(4-methoxyphenyl)propan-1-one(4e)**



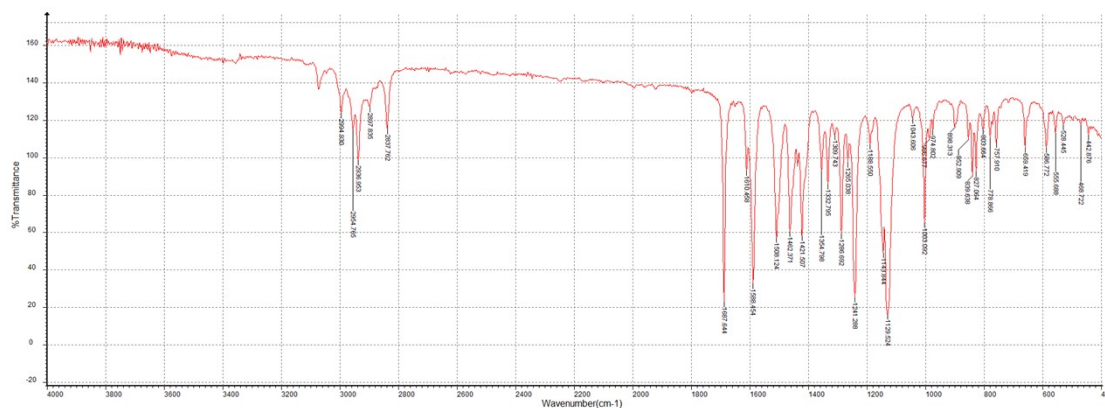
**Figure S61.** IR spectra of  
**1-(3,5-difluorophenyl)-3-(3,4-dimethoxyphenyl)propan-1-one(4i)**



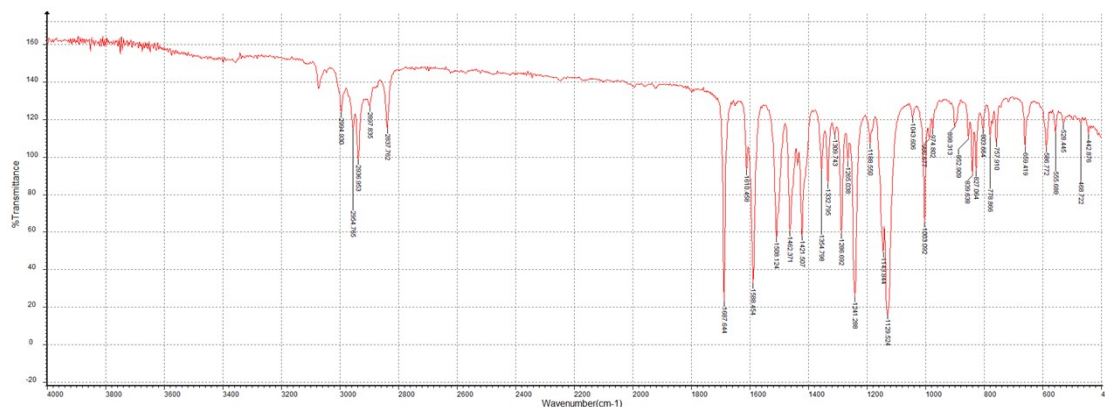
**Figure S62.** IR spectra of  
**3-(3,4-dimethoxyphenyl)-1-(4-fluoro-3-methylphenyl)propan-1-one(4j)**



**Figure S63.** IR spectra of  
**1,3-bis(3,4,5-trimethoxyphenyl)propan-1-one(4m)**



**Figure S64.** IR spectra of  
**1-(4-fluoro-3-methylphenyl)-3-(3,4,5-trimethoxyphenyl)propan-1-one(4n)**



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