# SUPPLEMENTARY MATERIAL

## Synthesis and structural studies on (E)-3-(2,6-difluorophenyl)-1-(4-fluorophenyl)prop-2-en-1-one: a promising nonlinear optical material

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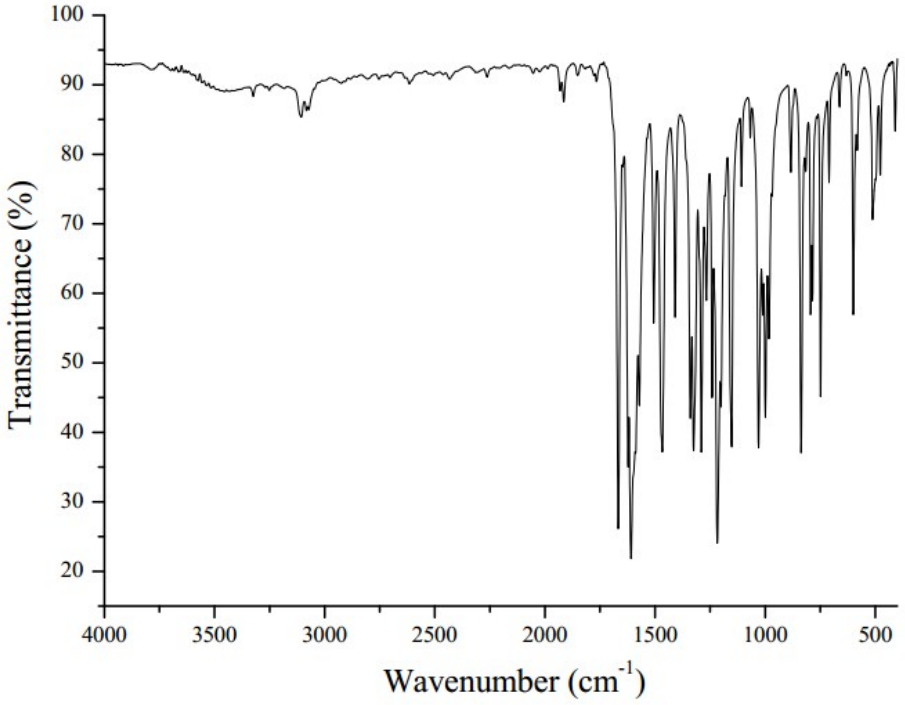


**Figure S1.** Infrared spectrum of *(E)-3-(2,6-difluorophenyl)-1-(4-fluorophenyl)prop-2-en-1-one.*

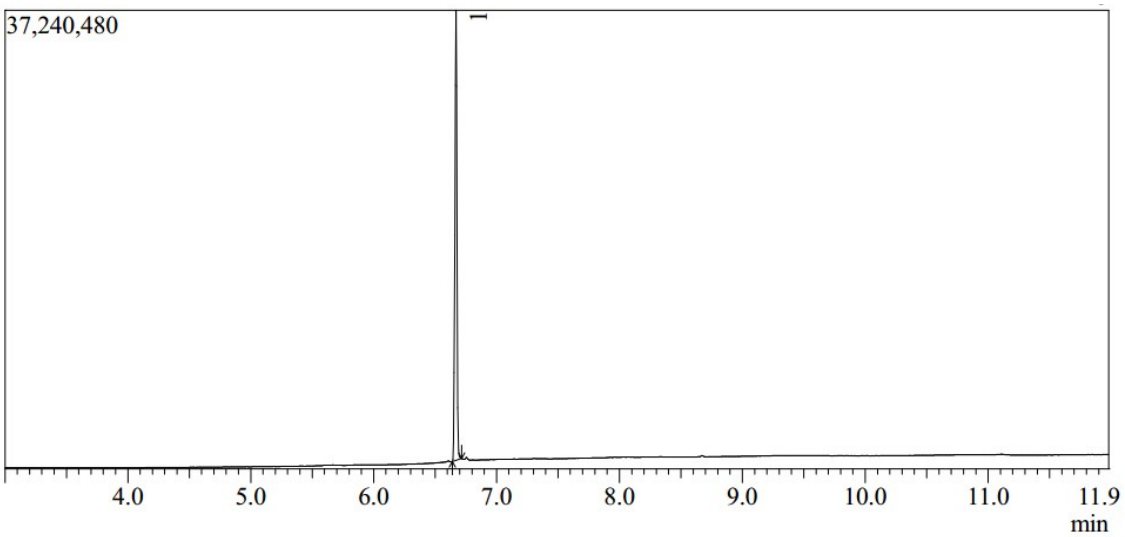


**Figure S2.** GC chromatogram of *(E)-3-(2,6-difluorophenyl)-1-(4-fluorophenyl)prop-2-en-1-one.*

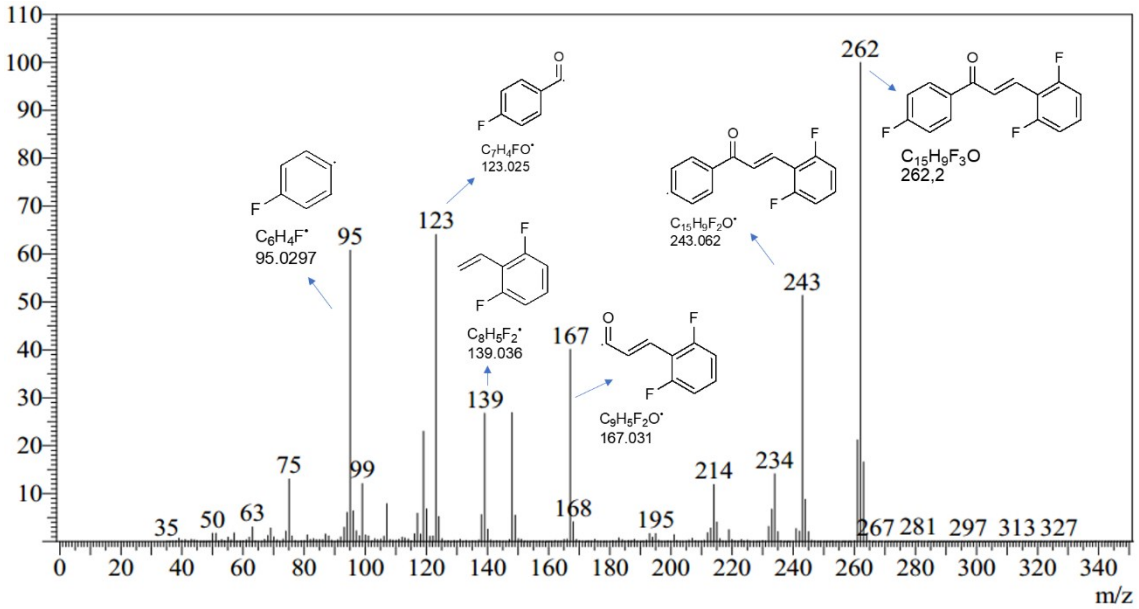


**Figure S3.** Mass scan spectrum of *(E)-3-(2,6-difluorophenyl)-1-(4-fluorophenyl)prop-2-en-1-one.*

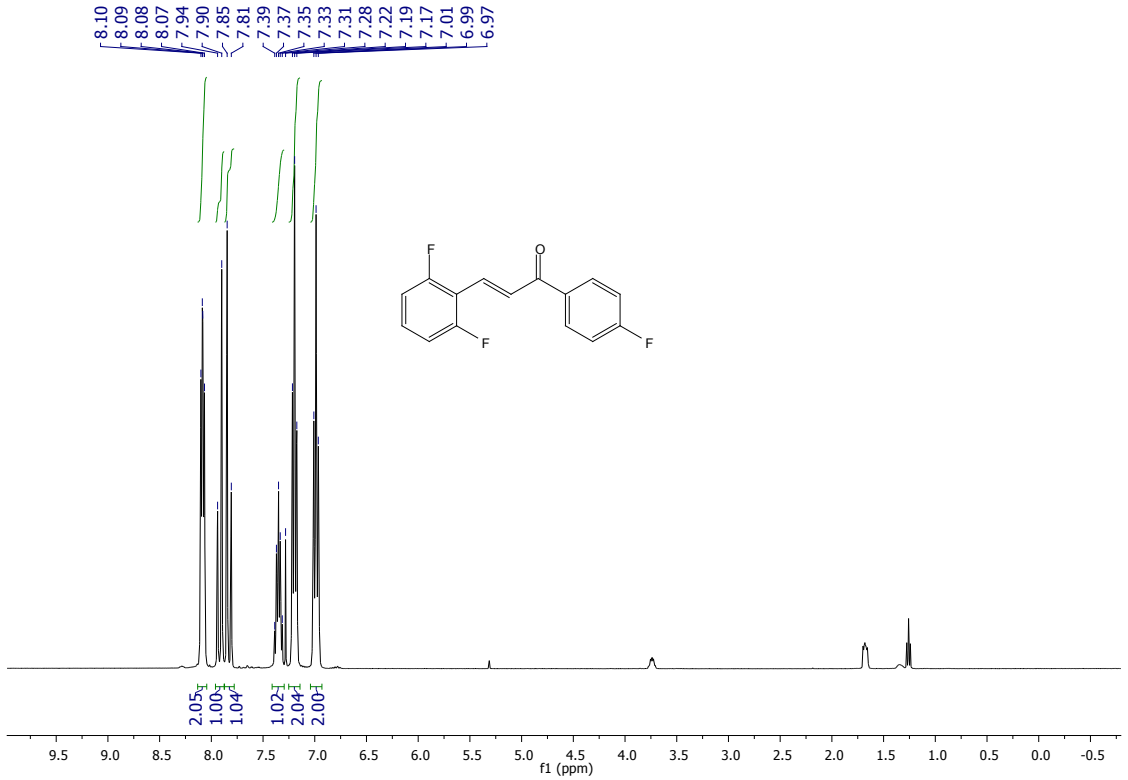


**Figure S4.** $^{1}$H-NMR of *(E)-3-(2,6-difluorophenyl)-1-(4-fluorophenyl)prop-2-en-1-one* (500 MHz, $CDCl_3$).

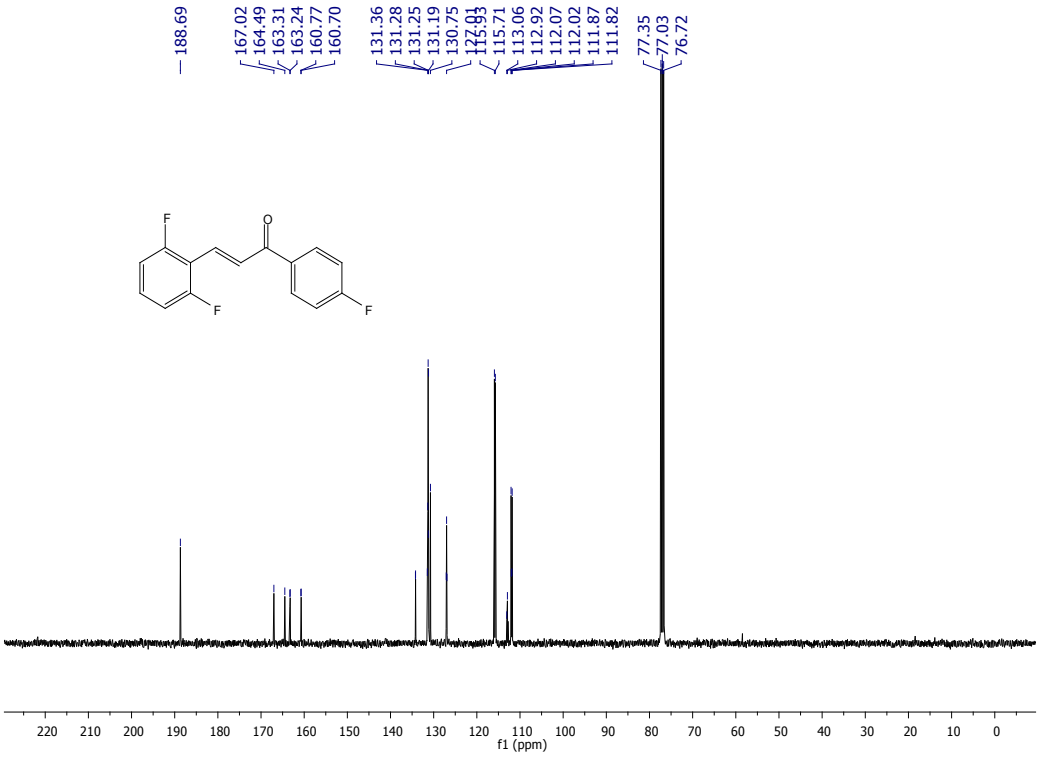


**Figure S5.** $^{13}$C-NMR of *(E)-3-(2,6-difluorophenyl)-1-(4-fluorophenyl)prop-2-en-1-one* (126 MHz, $CDCl_3$).

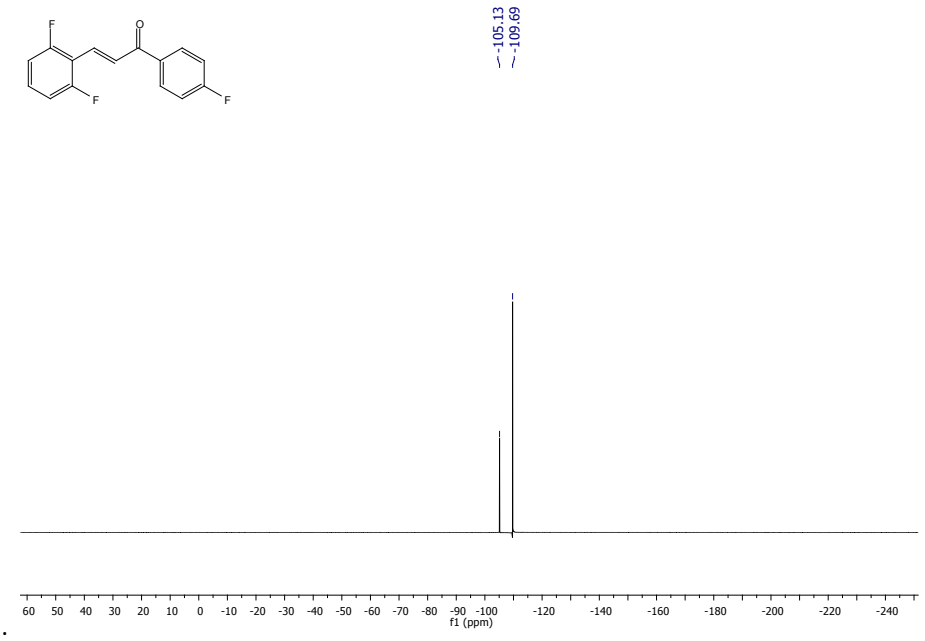


**Figure S6.** $^{19}$F NMR of *(E)-3-(2,6-difluorophenyl)-1-(4-fluorophenyl)prop-2-en-1-one* (376 MHz, $CDCl_3$).

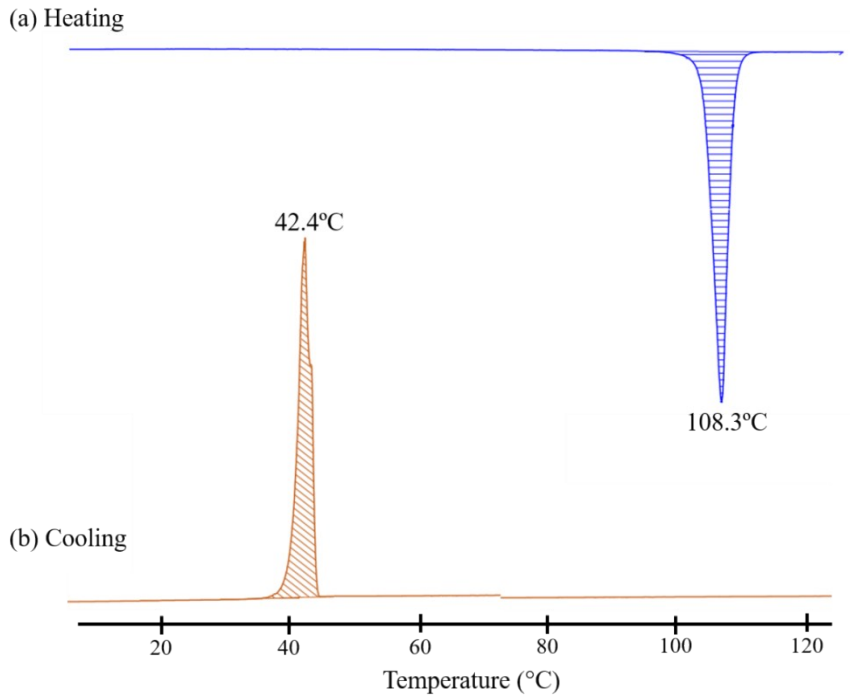


**Figure S7.** DSC thermogram of *(E)-3-(2,6-difluorophenyl)-1-(4-fluorophenyl)prop-2-en-1-one.*

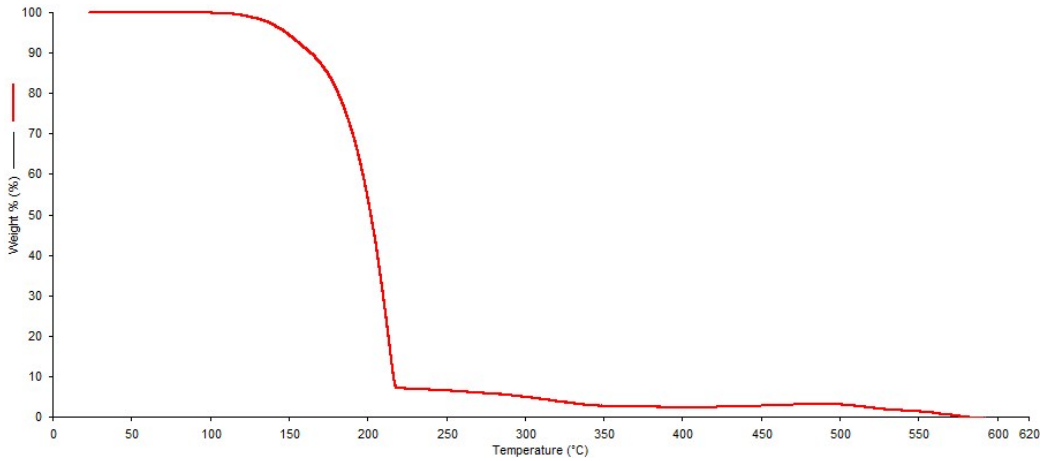


**Figure S8.** TGA thermogram of *(E)-3-(2,6-difluorophenyl)-1-(4-fluorophenyl)prop-2-en-1-one.*

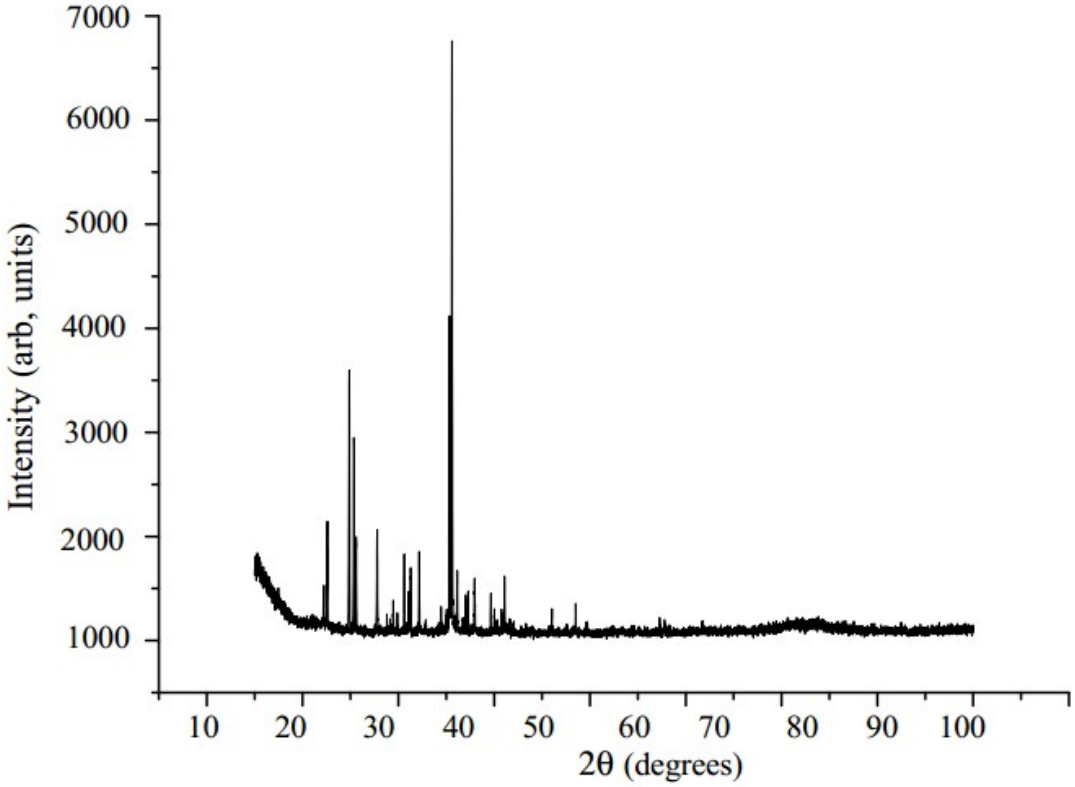


**Figure S9.** Powder diffraction patterns of *(E)-3-(2,6-difluorophenyl)-1-(4-fluorophenyl)prop-2-en-1-one.*

**Table S1:** Cartesian coordinates of the optimized structures using M062X exchange-correlation functional and basis set 6-311++G(d,p) for (*E*)-3-(2,6-difluorophenyl)-1-(4-fluorophenyl)prop-2-en-1-one.

| Atom | x | y | z |
|---|---|---|---|
| F | -1.77988000 | -2.07750900 | -0.30132300 |
| F | -3.69902100 | 2.16856400 | 0.30642100 |
| F | 6.20411700 | -1.08401600 | 0.11565900 |
| C | -2.64381700 | 0.09418600 | 0.00062100 |
| C | 2.41897800 | 0.48205700 | -0.02102800 |
| C | -2.84955000 | -1.28029500 | -0.15847500 |
| O | 0.95502700 | 2.32555100 | -0.09490200 |
| C | -1.34757000 | 0.76950600 | 0.02436800 |
| H | -1.38664200 | 1.84551100 | 0.16731900 |
| C | 2.618’03600 | -0.84781400 | 0.35471200 |
| H | 1.78044700 | -1.47613100 | 0.63032900 |
| C | -0.13122000 | 0.22581800 | -0.11141200 |
| H | 0.01212800 | -0.83107800 | -0.27186700 |
| C | 3.52464200 | 1.27712900 | -0.33778400 |
| H | 3.35367800 | 2.31067100 | -0.61362700 |
| C | -3.81711000 | 0.84415300 | 0.14715400 |
| C | 3.89901000 | -1.38296800 | 0.41142700 |
| H | 4.07999500 | -2.40764700 | 0.70907700 |
| C | 4.96634500 | -0.56999600 | 0.07540000 |
| C | 1.06350900 | 1.11795100 | -0.07135400 |
| C | -4.09570100 | -1.87386000 | -0.17510700 |
| H | -4.16475500 | -2.94594600 | -0.30309600 |
| C | 4.80717900 | 0.75485700 | -0.30017700 |
| H | 5.67770400 | 1.34698400 | -0.55231000 |
| C | -5.22060700 | -1.07080000 | -0.02673600 |
| H | -6.20616400 | -1.51854600 | -0.03845700 |
| C | -5.08754800 | 0.30211900 | 0.13680100 |
| H | -5.94101700 | 0.95616300 | 0.25456800 |