

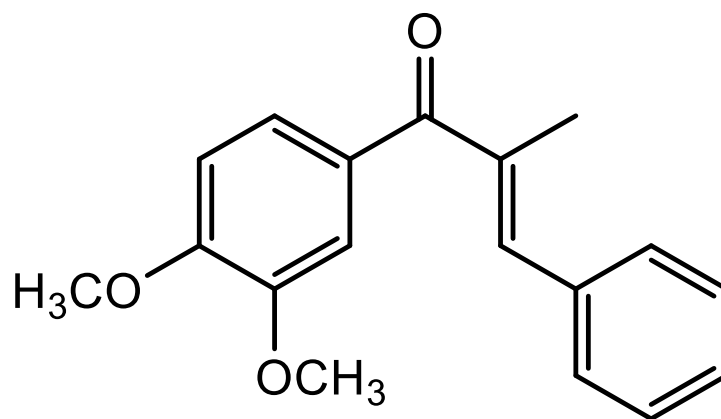
# Supporting Information

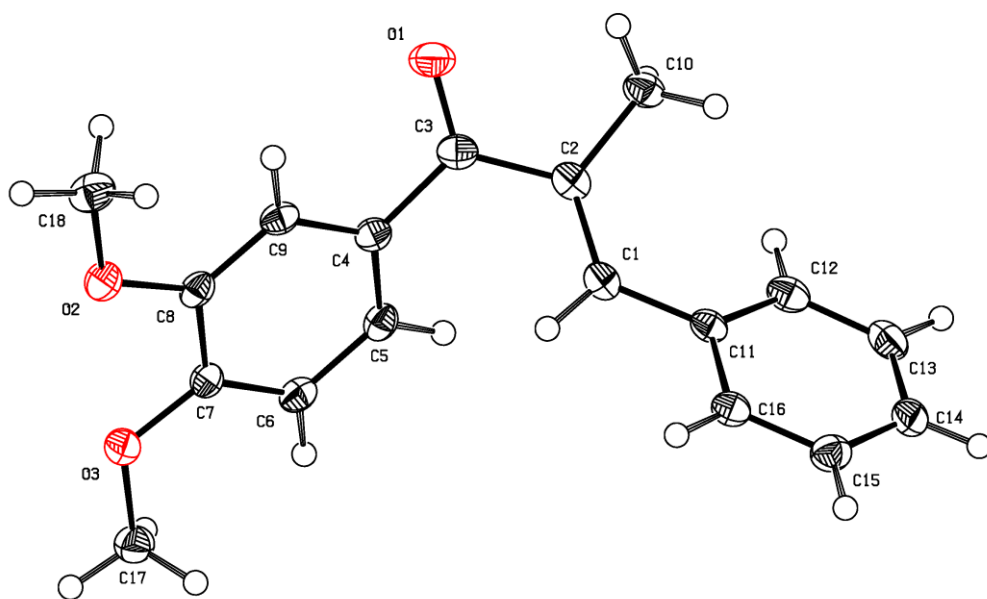
for

## **(E)-1-(3,4-Dimethoxy-phenyl)-2-methyl-3-phenylprop-2-en-1-one: a P-type acid-stable photochromic $\alpha$ -methylchalcone**

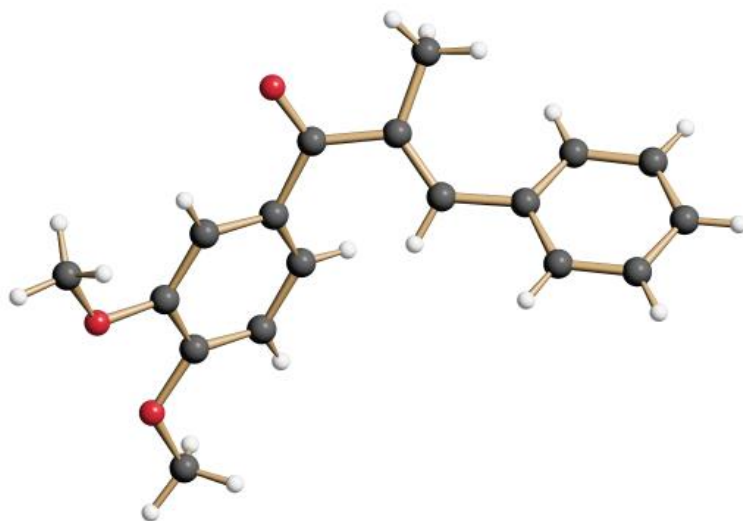
Banu Öngel, Jörg M. Neudörfl, Axel G. Griesbeck, Department of Chemistry,  
University of Cologne

Compound <b>3</b> ChemDraw, MDL molfile enclosed	I
X-ray ellipsoid and ball/stick pictures data for X-ray structure analysis	II III
$^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ -spectra	IV
MS data and IR-spectrum	V





**Figure S1.** Chalcone 3: X-ray ellipsoid picture.



**Figure S2.** Chalcone 3: ball/stick picture.

Compound name and <b>CCDC-number</b>	( <i>E</i> )-1-(3,4-Dimethoxy-phenyl)-2-methyl-3-phenylprop-2-en-1-one; CCDC 2081479
Moiety formula	C <sub>18</sub> H <sub>18</sub> O <sub>3</sub>
Formula weight	282.32 g/mol
Temperature	100(2) K
Wavelength	1.54178 Å
Crystal system	monoclinic
Space group	P2 <sub>1</sub> /n
Unit cell dimensions	a= 12.9441(5) Å      α= 90° b= 8.6844(3) Å      β= 114.7361(17)° c= 14.4820(5) Å      γ= 90°
Volume	1478.57(9) Å <sup>3</sup>
Z	4
Density (calculated)	1.268 Mg/m <sup>3</sup>
Absorption coefficient	0.688 mm <sup>-1</sup>
F(000)	600
Crystal size	0.150 x 0.070 x 0.070 mm <sup>3</sup>
θ-range for data collection	3.854 bis 72.134°
Index ranges	-15<=h<=15, -10<=k<=10, -16<=l<=17
Collected / Independent reflections	16151
Data / restraints / parameters	2898 [R(int) = 0.0520]
max. and min. transmission	0.7536 and 0.6581
Data / restraints / parameters	2898 / 0 / 193
Goodness-of-fit on F <sup>2</sup>	1.055
Final R indices [I>2σ(I)]	R1 = 0.0424, wR2 = 0.0937
R indices (all data)	R1 = 0.0543, wR2 = 0.1003
Largest diff. peak and hole	0.216 and 0.236 e.Å <sup>-3</sup>

**Table S1.** Chalcone **3**: data for X-ray structure analysis

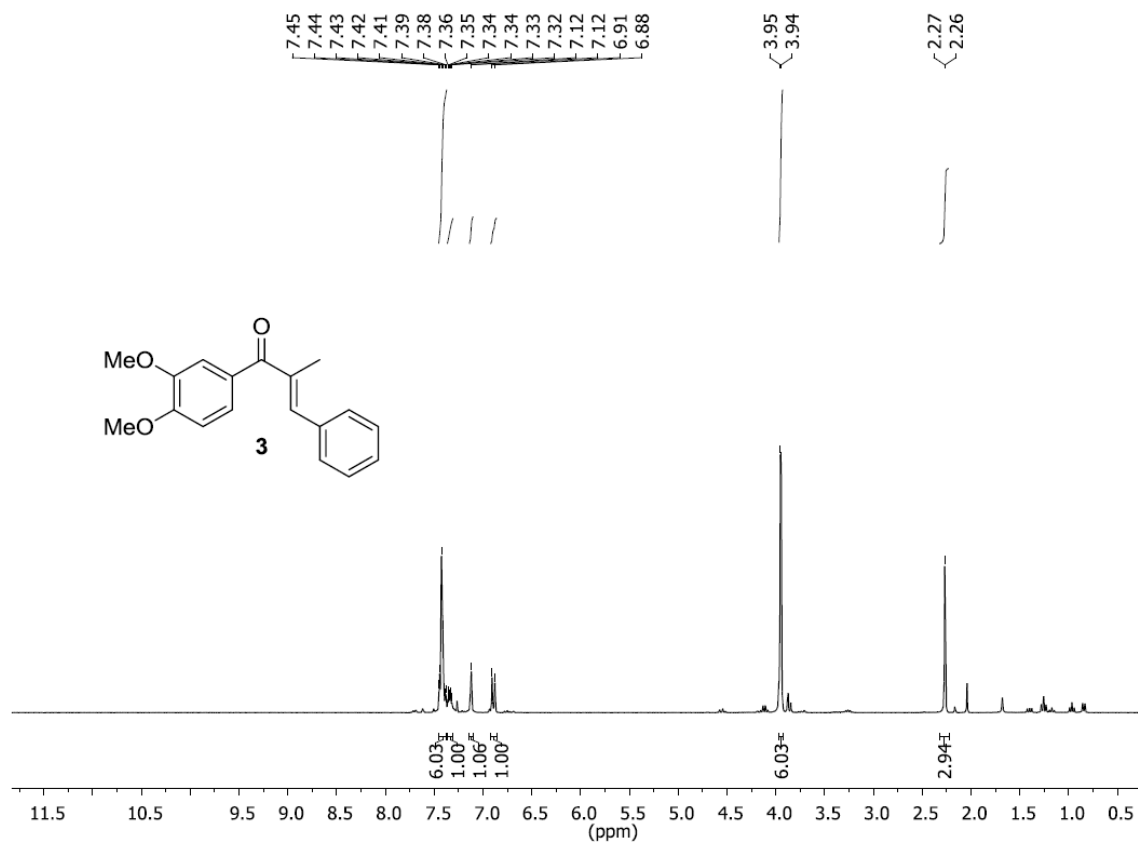


Figure S3. Chalcone 3: <sup>1</sup>H-NMR spectrum.

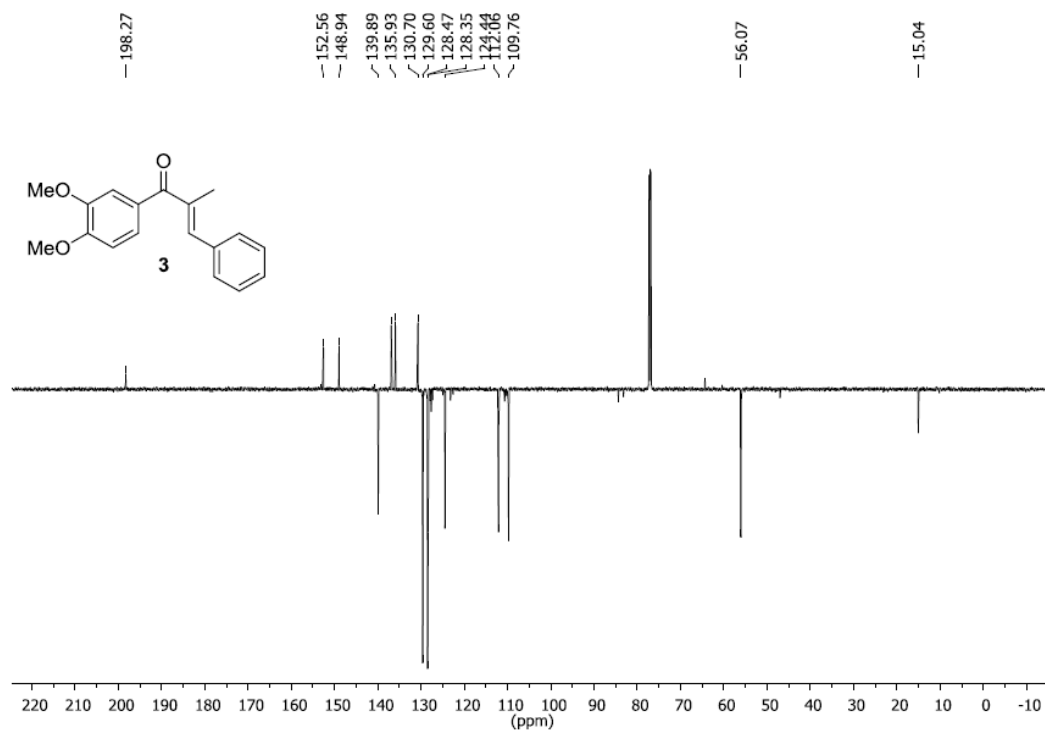


Figure S4. Chalcone 3: <sup>13</sup>C-NMR spectrum.

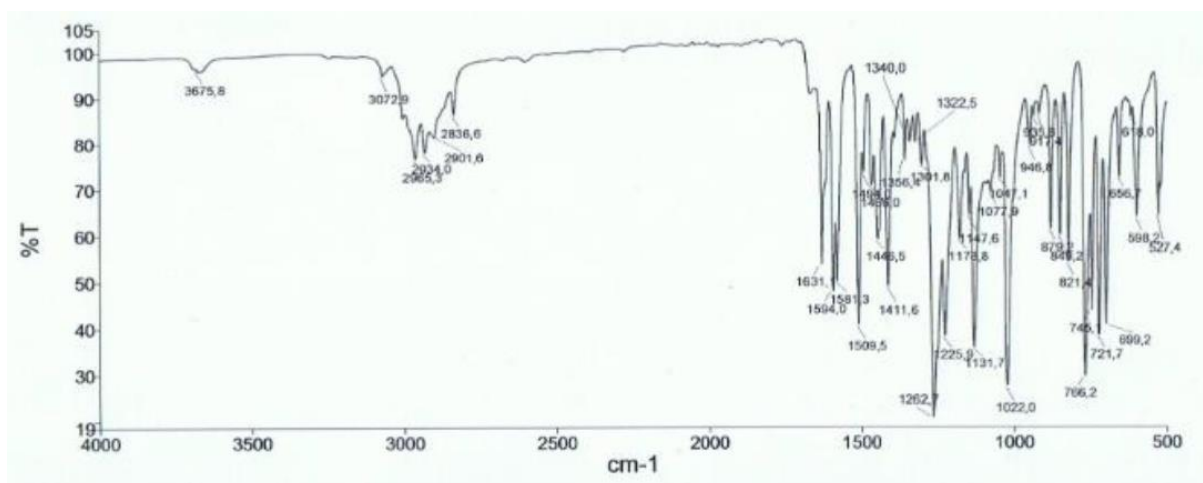


Figure S5. Chalcone 3: IR spectrum.

bby349 #225-288 RT: 2.10-2.60 AV: 64 NL: 1.41E7  
T: FTMS + c ESI Full ms [100.00-800.00]

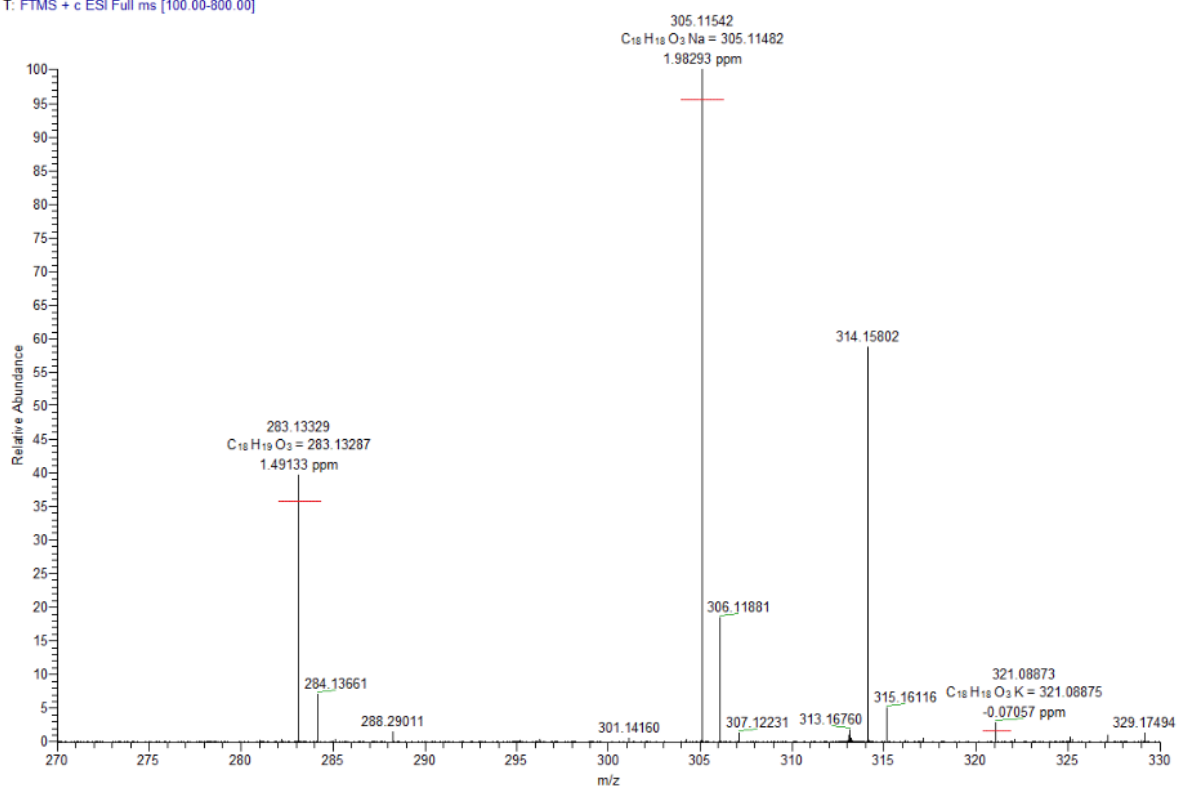


Figure S6. Chalcone 3: mass spectrometric analysis.