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Supplementary Information

Biological and Structure-Activity Evaluation of Chalcone Derivatives against Bacteria and Fungi

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Table S1. Crystal and refinement data for compounds **3a**, **3f**, **3i**, **3n**, **3o**, **3q** and **3t**

Compound	**3a**	**3f**	**3i**	**3n**	**3o**	**3q**	**3t**
Formula	$C_{16}H_{12}O_3$	$C_{16}H_{11}O_4Br$	$C_{15}H_{11}N_1O_3$	$C_{15}H_{12}O_2$	$C_{15}H_{12}O_2$	$C_{15}H_{11}NO_3$	$C_{13}H_{10}O_3$
F(000)	1056	508	352	336	608	528	572
Crystal size / mm	0.15 × 0.15 × 0.20	0.33 × 0.23 × 0.20	0.35 × 0.25 × 0.05	0.35 × 0.30 × 0.20	0.35 × 0.25 × 0.20	0.35 × 0.13 × 0.10	0.28 × 0.25 × 0.13
Crystal habit/color	prism/yellow	prism/yellow	prism/yellow	prism/yellow	block/colorless	block/colorless	block/colorless
Crystal system	orthorhombic	monoclinic	triclinic	triclinic	monoclinic	monoclinic	monoclinic
Space group	Pcab	$P2_1/c$	P1	P-1	$P2_1/c$	$P2_1/c$	$P2_1/n$
a / Å	7.809(2)	4.160(3)	4.7580(9)	6.822(2)	12.641(1)	6.299(3)	3.9530(9)
b / Å	11.176(1)	11.757(2)	6.096(1)	10.474(4)	12.066(2)	13.226(3)	14.583(2)
c / Å	28.679(1)	27.598(7)	10.658(2)	17.097(2)	7.813(1)	14.809(3)	17.893(5)
α / degree	90	90	95.807(2)	73.88(2)	90	90	90
β / degree	90	92.87(1)	90.482(2)	84.29(2)	101.278(1)	93.73(2)	92.16(1)
γ / degree	90	90	96.397(2)	87.66(2)	90	90	90
V / Å^3	2496.1(8)	1348(1)	305.6(1)	1167.7(6)	1455.6(3)	1231.1	1168.6(4)
Z	8	4	1	2	4	4	4
ρ_{calc} / (g cm^{-3})	1.343	1.710	1.208	1.291	1.274	1.366	1.387
μ / mm^{-1}	0.756	4.291	0.799	0.673	0.814	0.793	0.672
Rad. Cu K_α / Å	1.54180	1.54180	1.54180	1.54180	1.54180	1.54180	1.54180
Difractometer	Nonius CAD-4	Nonius CAD-4	Nonius CAD-4	Nonius CAD-4	Nonius CAD-4	Nonius CAD-4	Nonius CAD-4
θ min/max / degree	3.25/70.09	3.63/66.99	3.89/67.13	4.61/67.06	4.06/67.15	4.36/67.90	2.96/67.16
Refl. collected	2201	2795	1771	4330	2832	4082	2170
Data/restr/param	2126/0/173	1995/0/156	1764/1/209	4185/0/314	2465/0/185	3528/0/274	4885/0/344
Abs. cor. T_{mx}/T_{mn}	none	0.6568/0.5180	none	none	none	none	none
R_{int}	0.0111	0.0219	0.0330	0.0248	0.0157	0.0596	0.0245
R	0.0557	0.0809	0.0492	0.0701	0.0820	0.0660	0.0680
R_w	0.1557	0.2286	0.1547	0.1953	0.3328	0.1611	0.1987
S on F^2	1.084	1.103	1.080	1.168	1.099	1.150	1.078
Max/min peaks / (e Å^{-3})	0.360/-0.357	0.328/-0.232	0.223/-0.267	0.357/-0.374	0.528/-0.420	0.417/-0.409	0.234/-0.287

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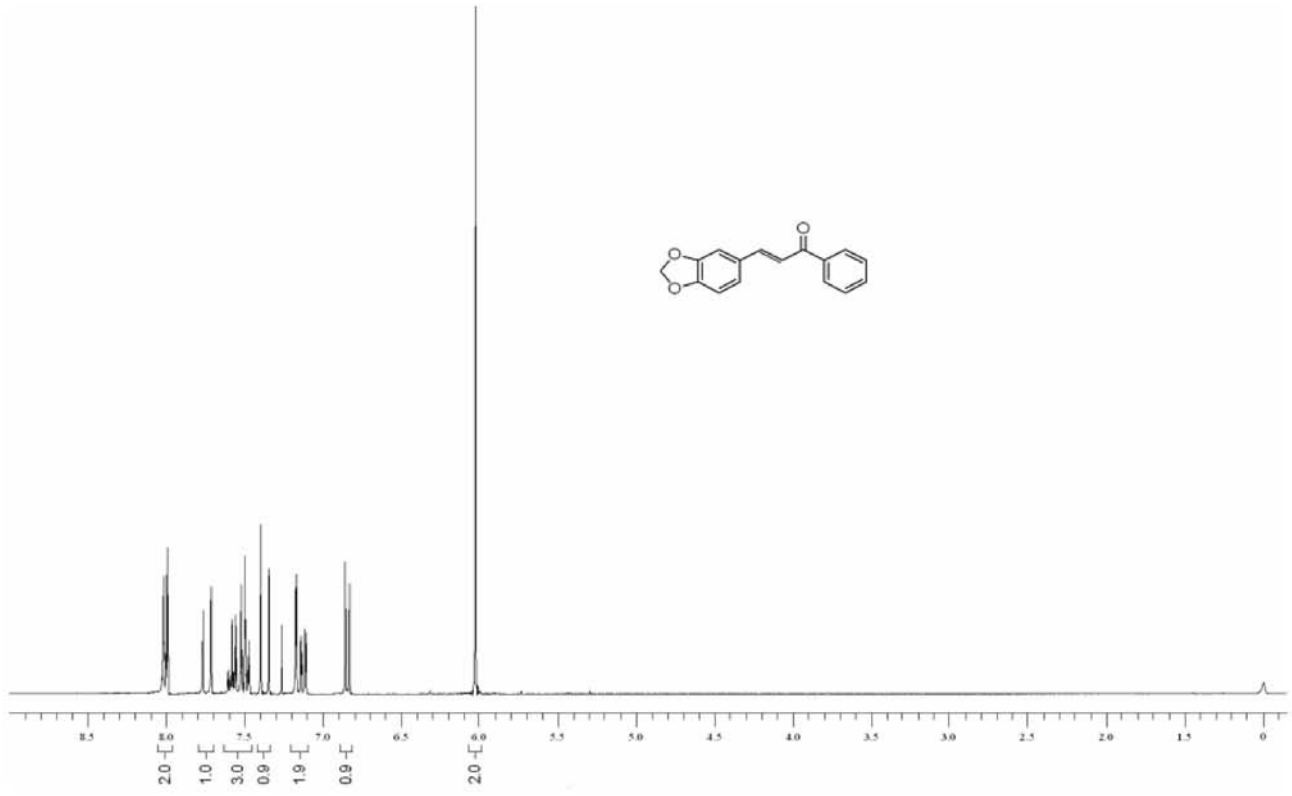

Figure S1. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **3a**.

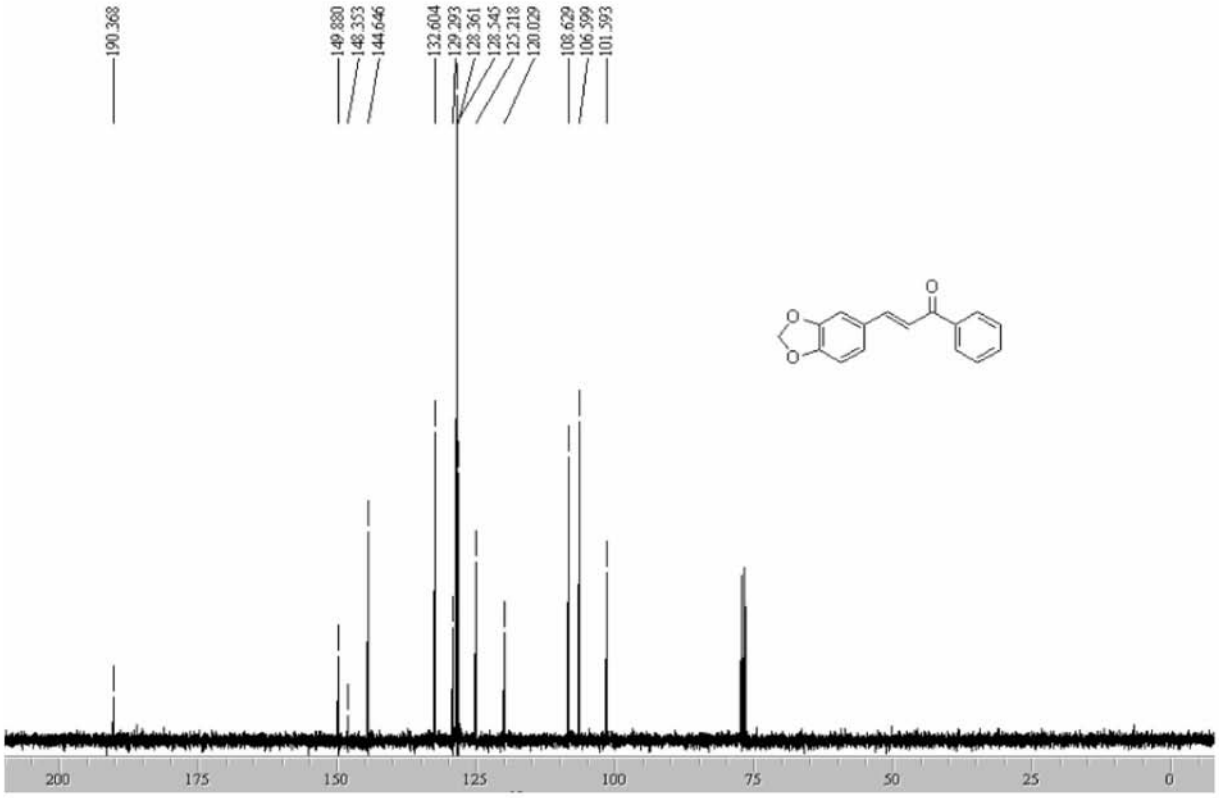

Figure S2. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **3a**.

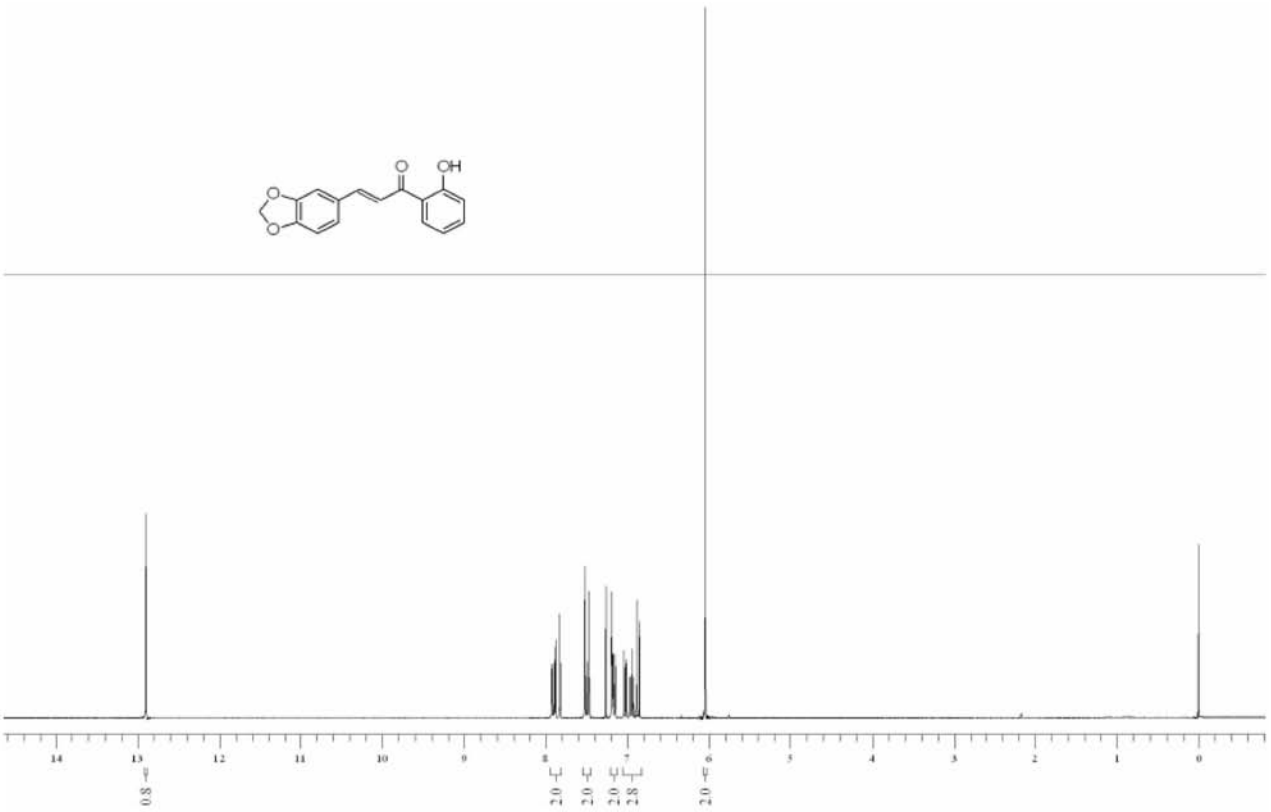

Figure S3. [1]H NMR (300 MHz, $CDCl_3$) spectrum of compound **3b**.

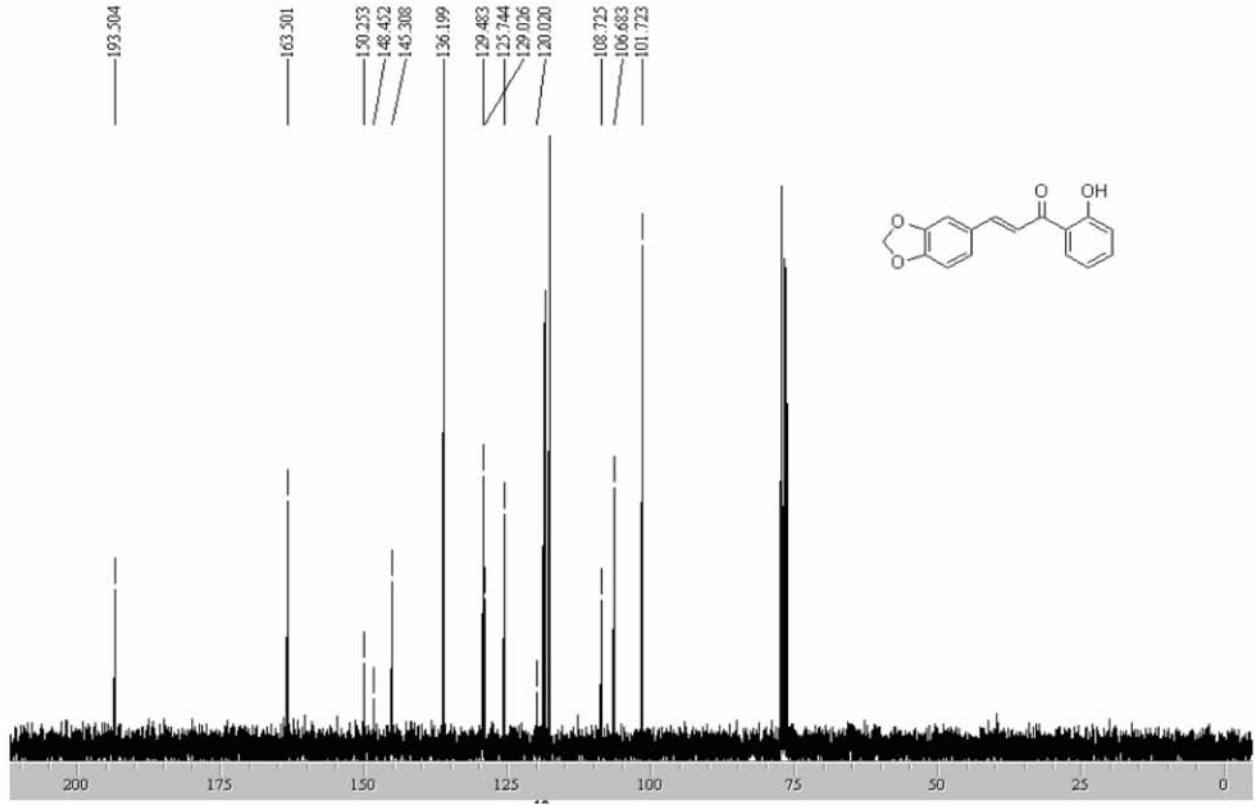

Figure S4. [13]C NMR (75 MHz, $CDCl_3$) spectrum of compound **3b**.

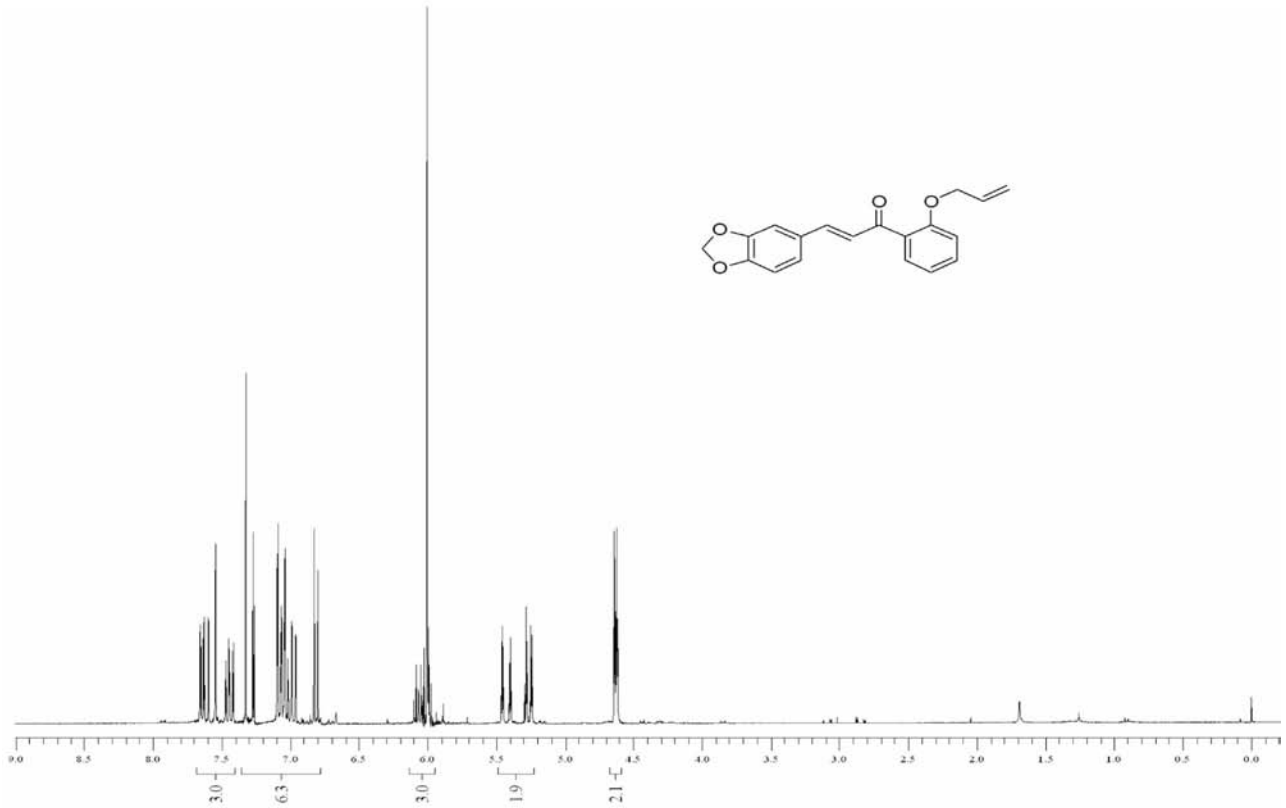

Figure S5. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **3c**.

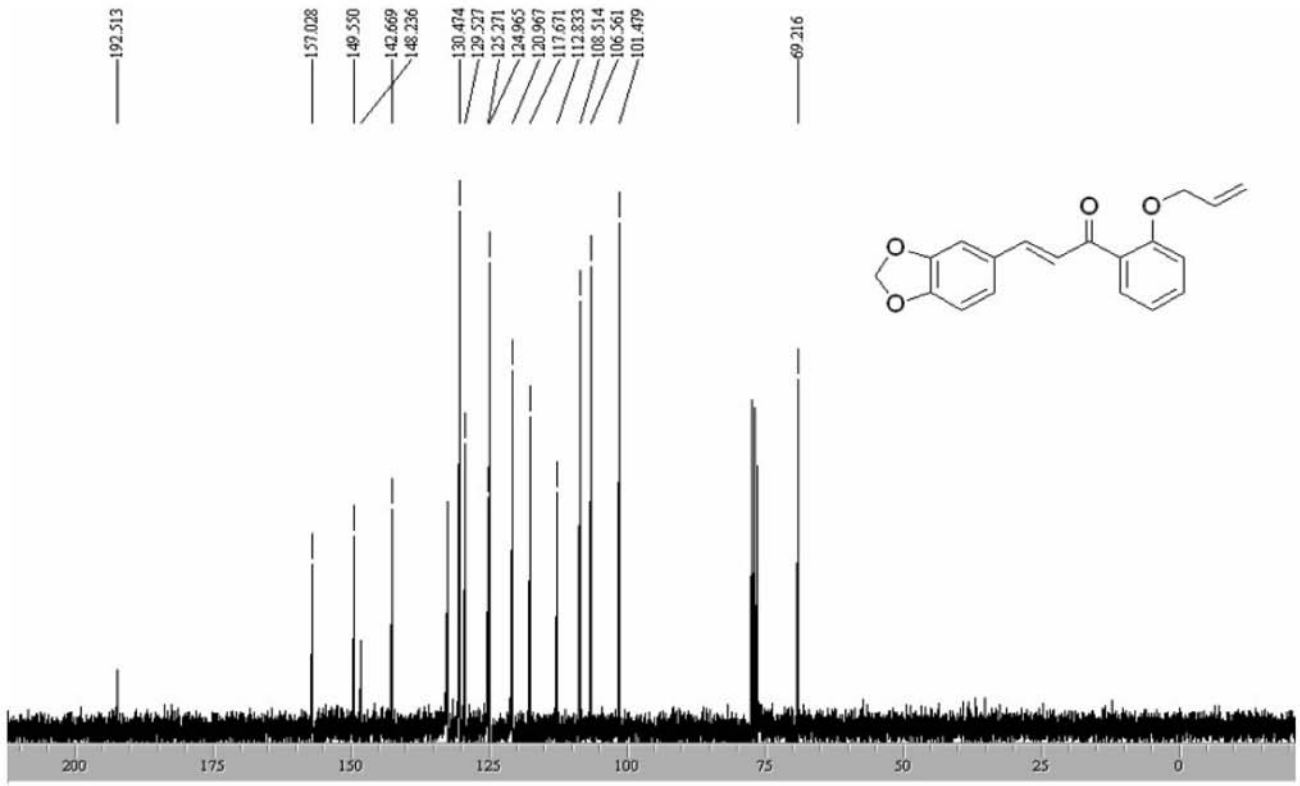

Figure S6. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **3c**.

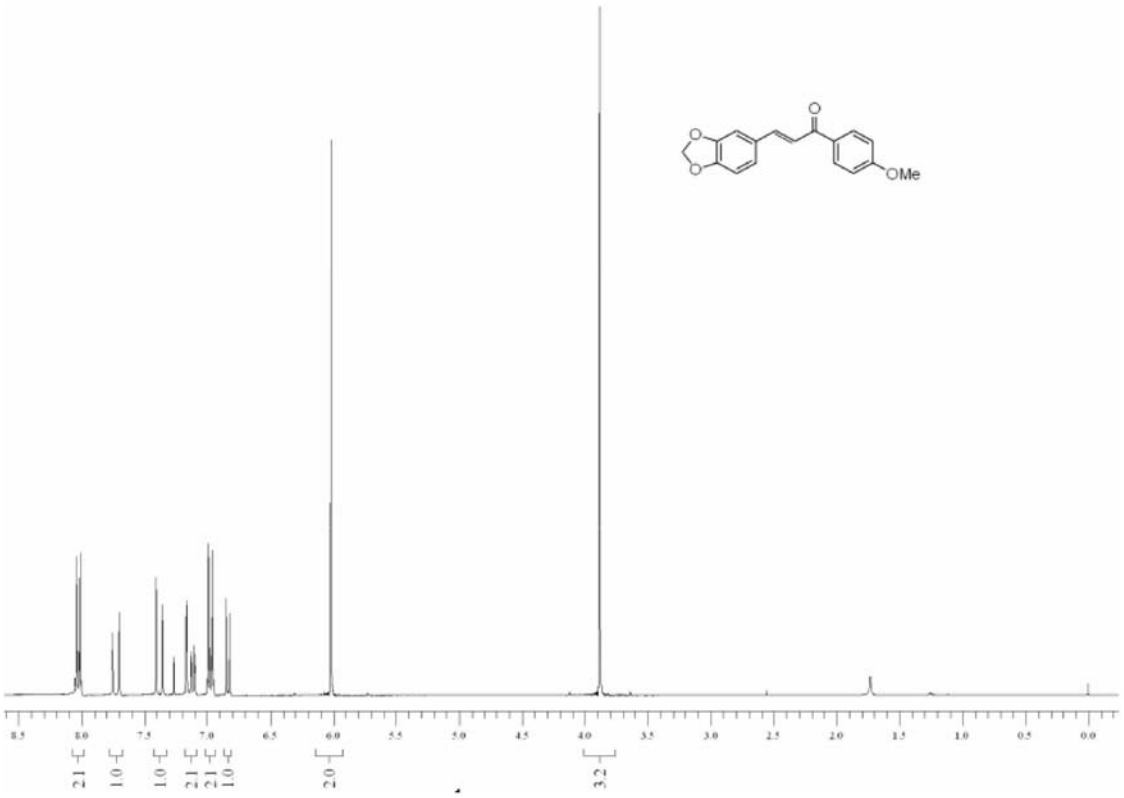

Figure S7. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **3d**.

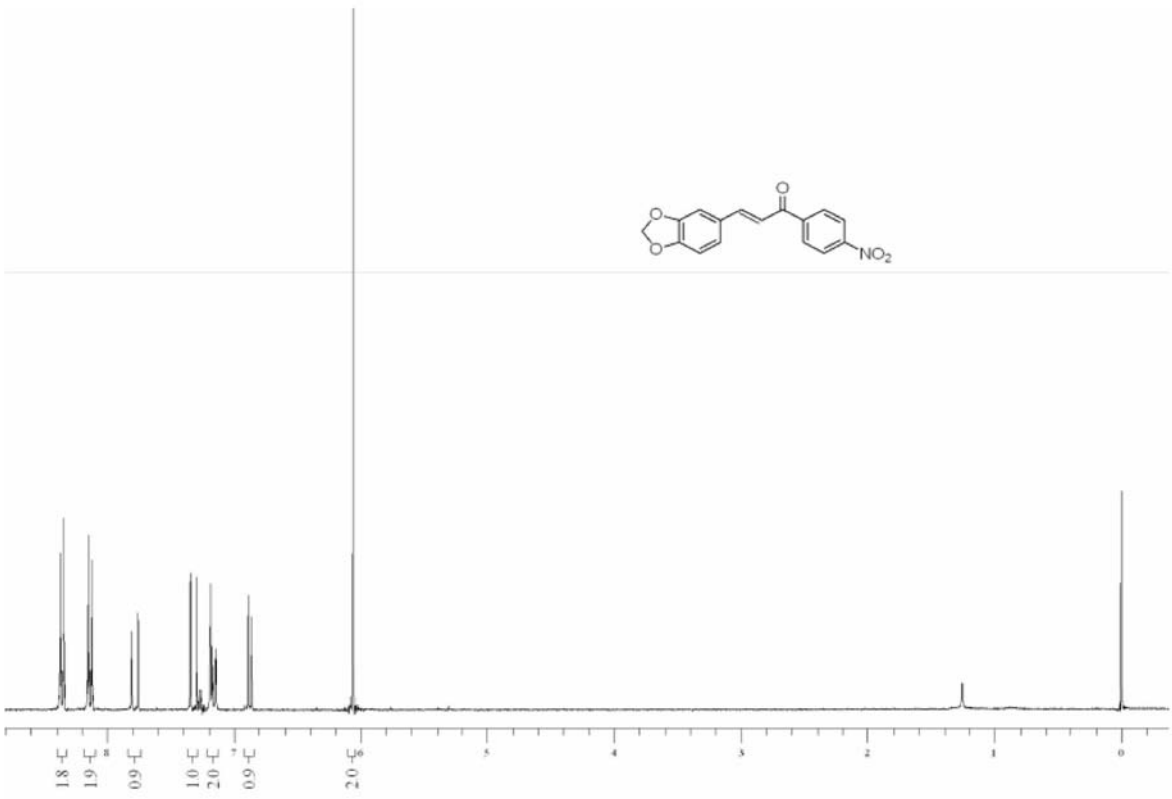

Figure S8. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **3e**.

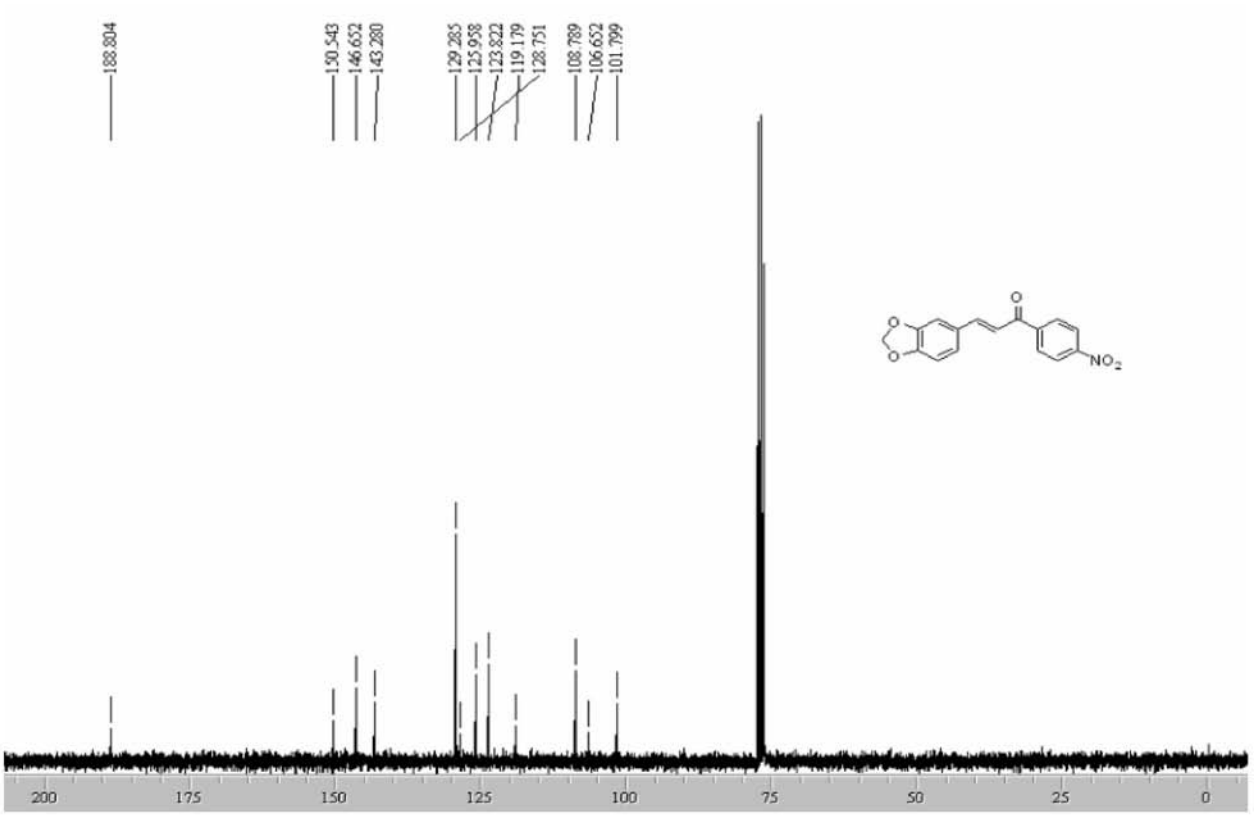

Figure S9. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **3e**.

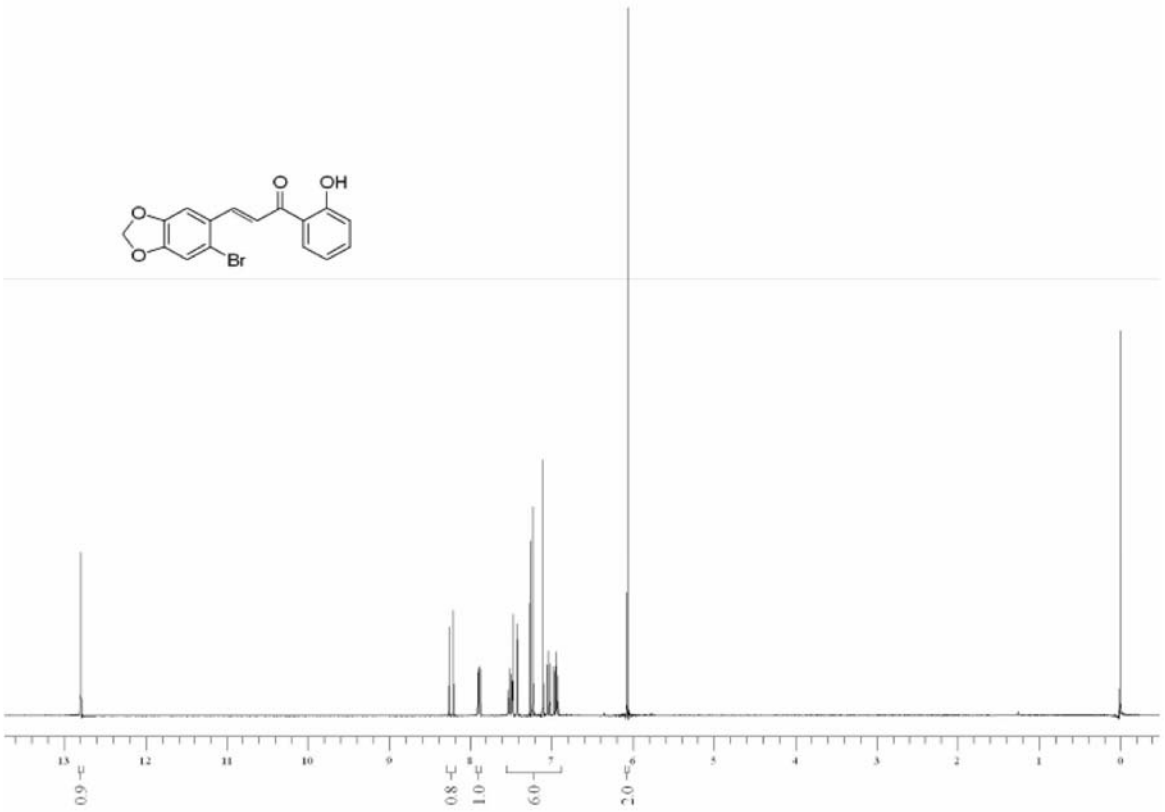

Figure S10. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **3f**.

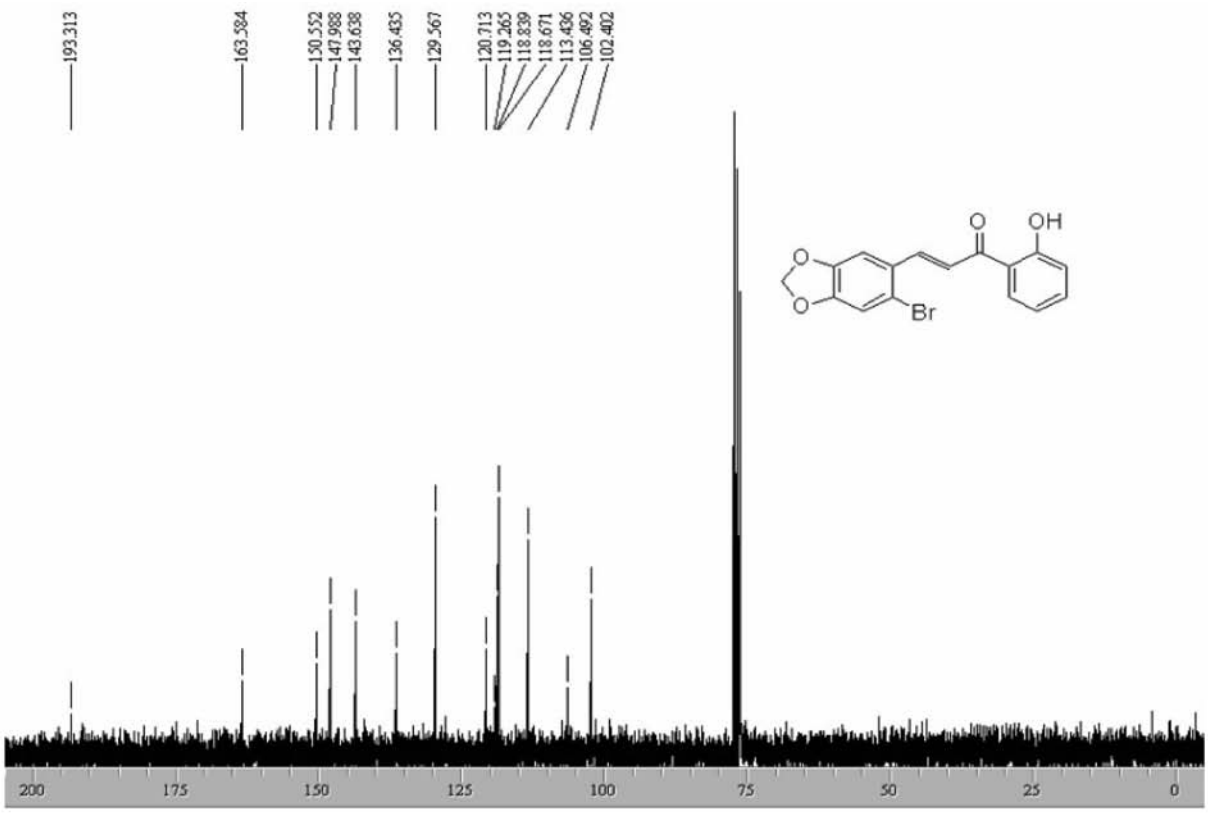

Figure S11. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **3f**.

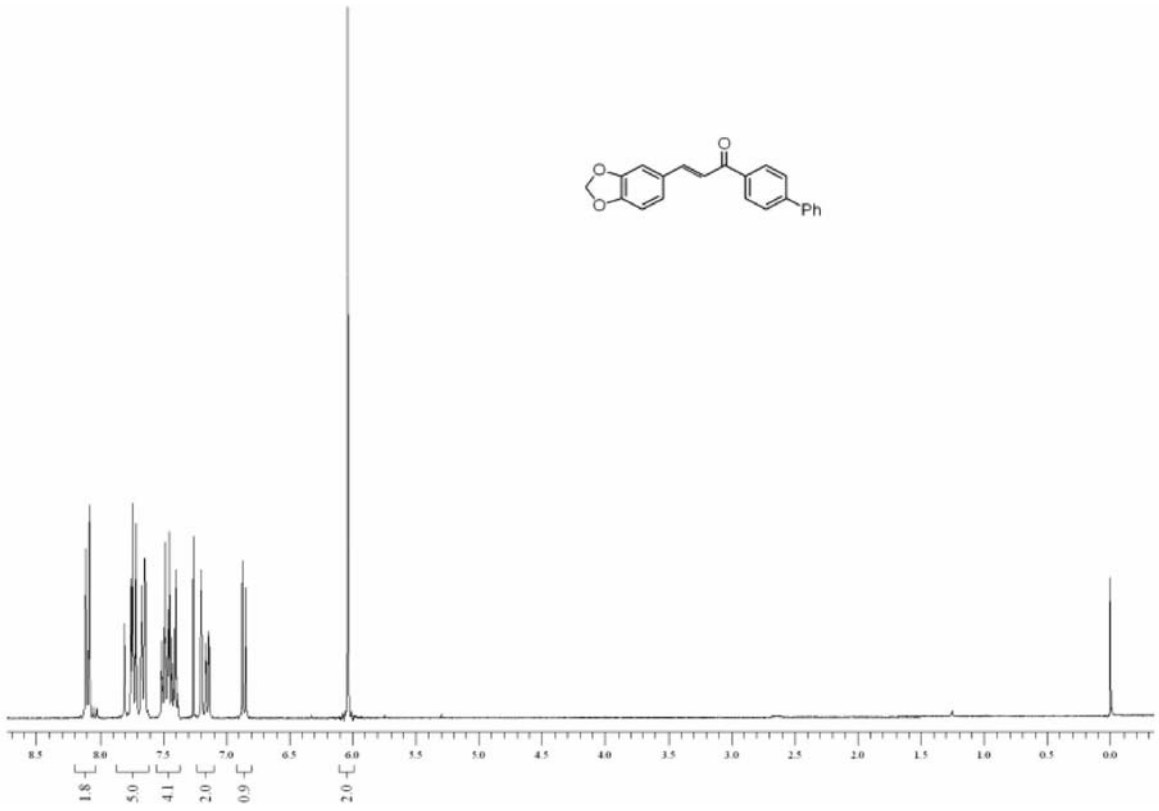

Figure S12. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **3g**.

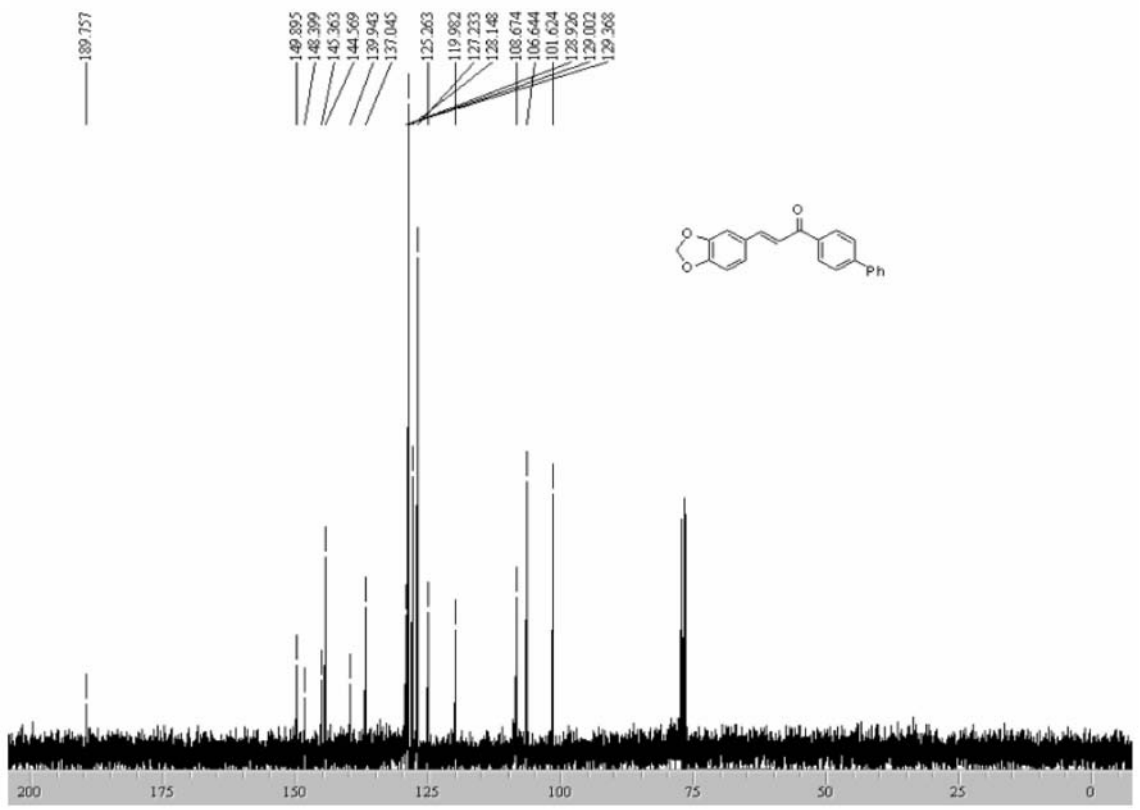

Figure S13. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **3g**.

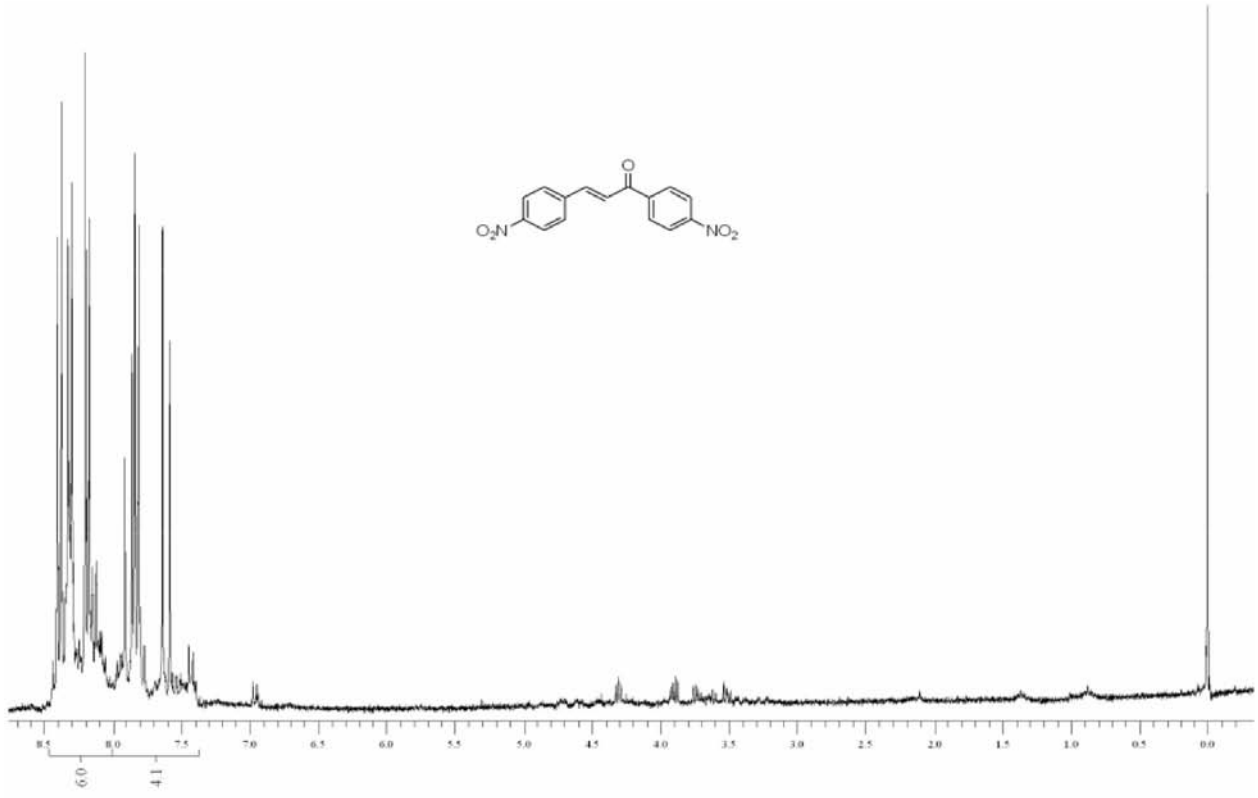

Figure S14. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **3h**.

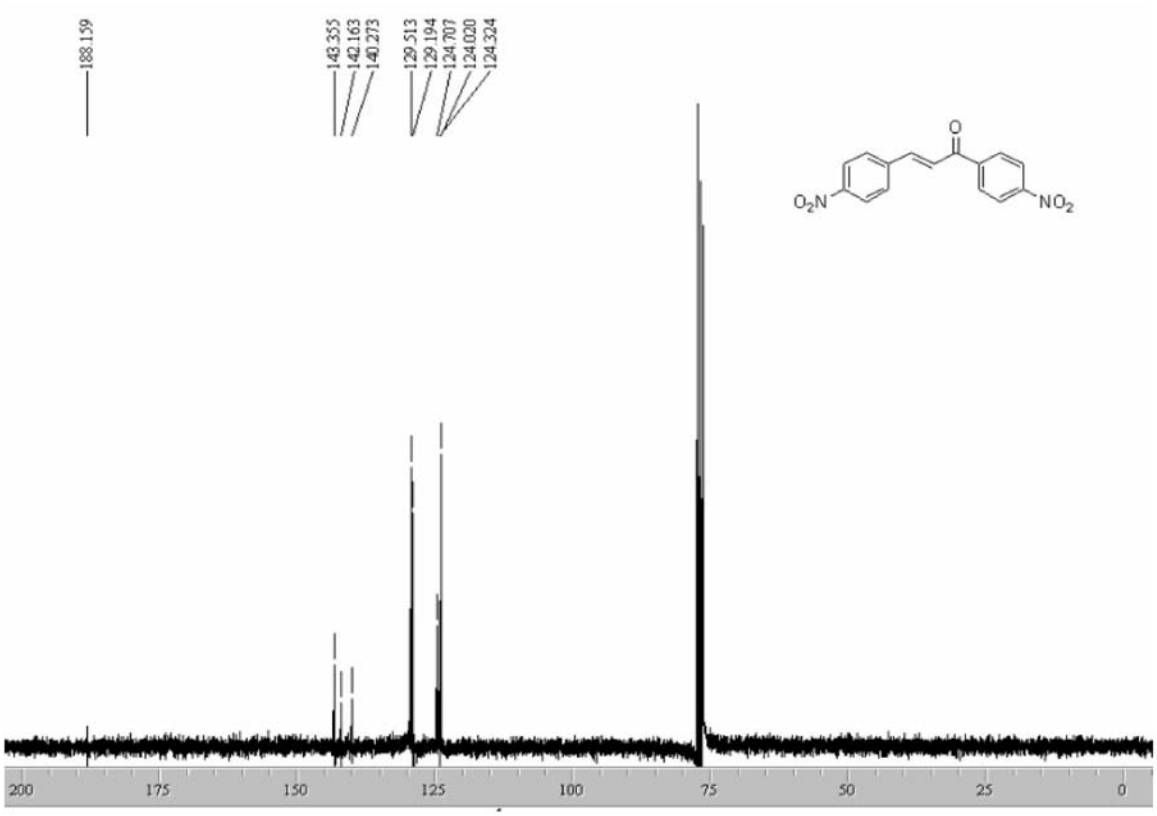

Figure S15. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **3h**.

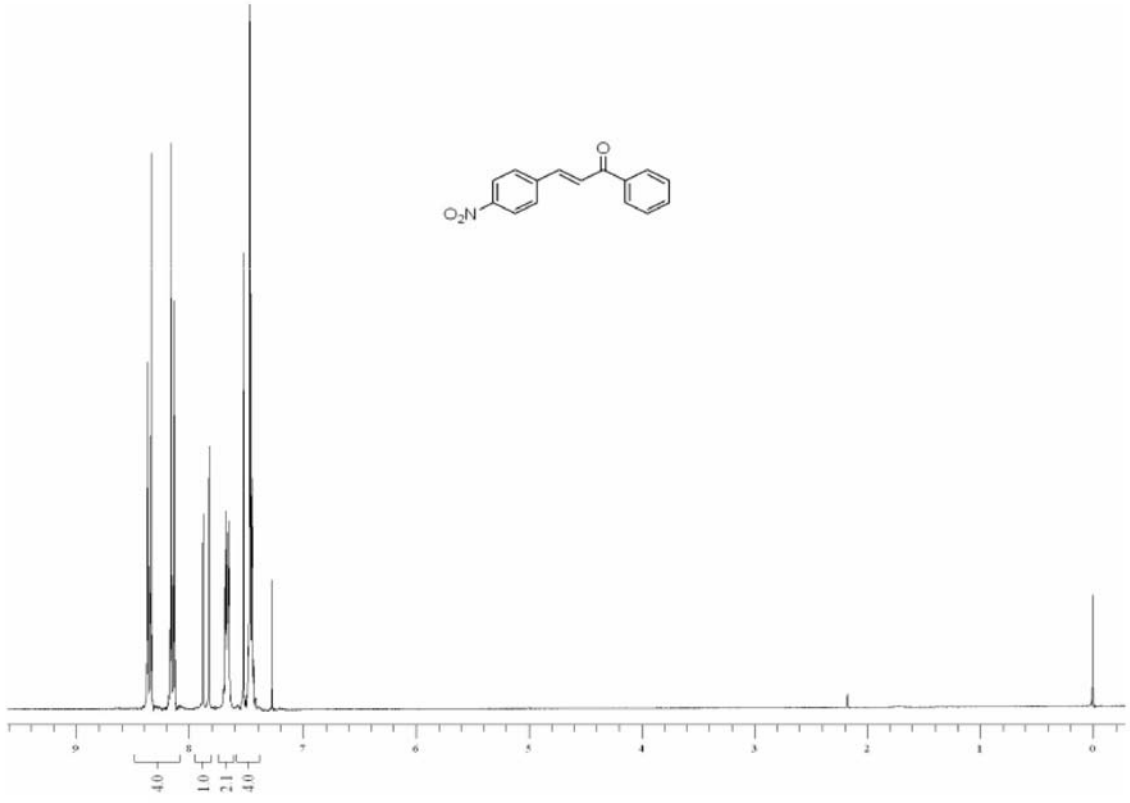

Figure S16. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **3i**.

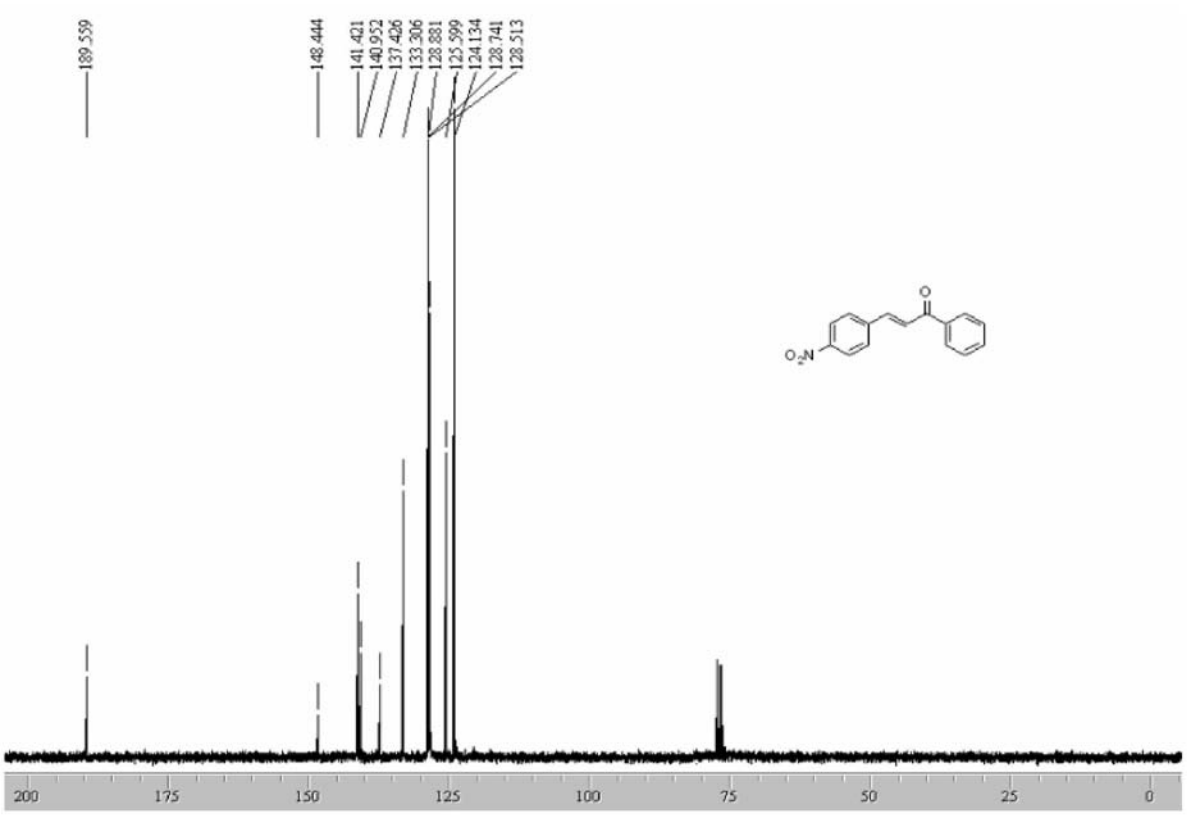

Figure S17. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **3i**.

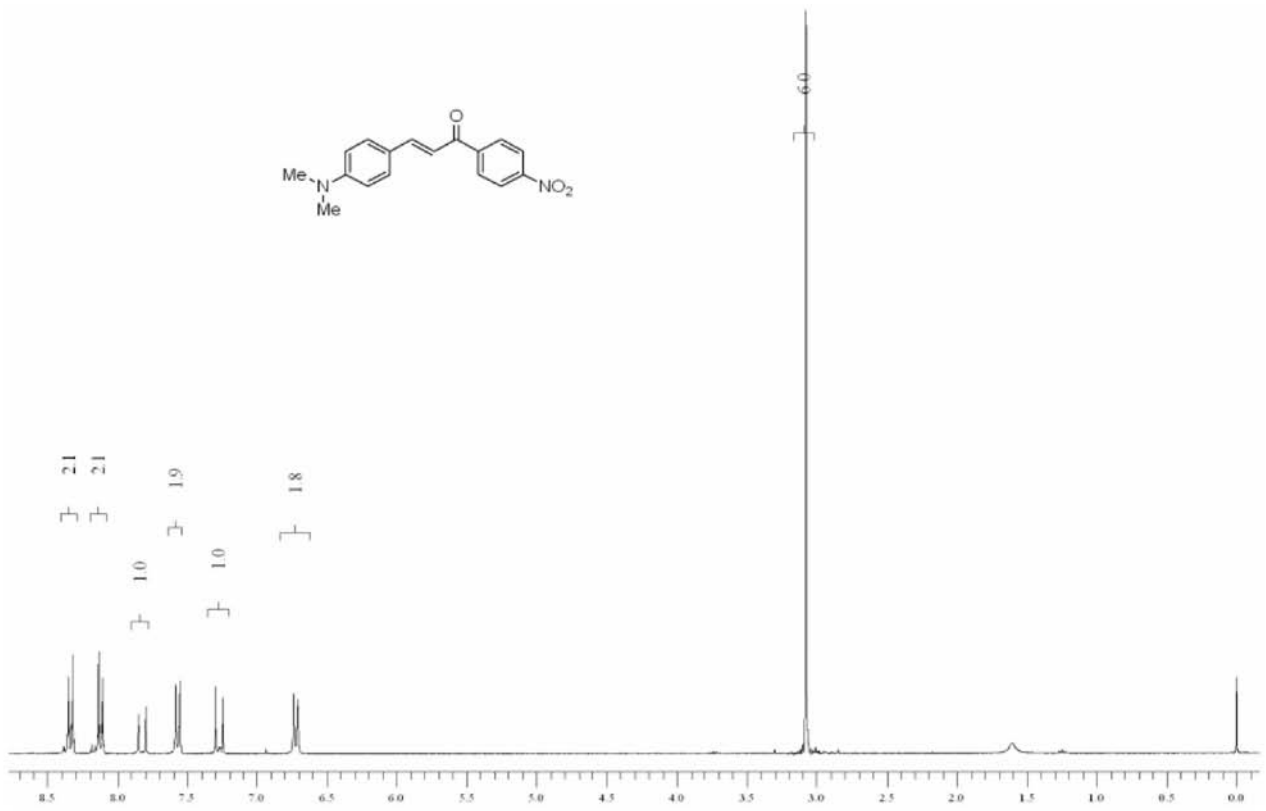

Figure S18. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **3j**.

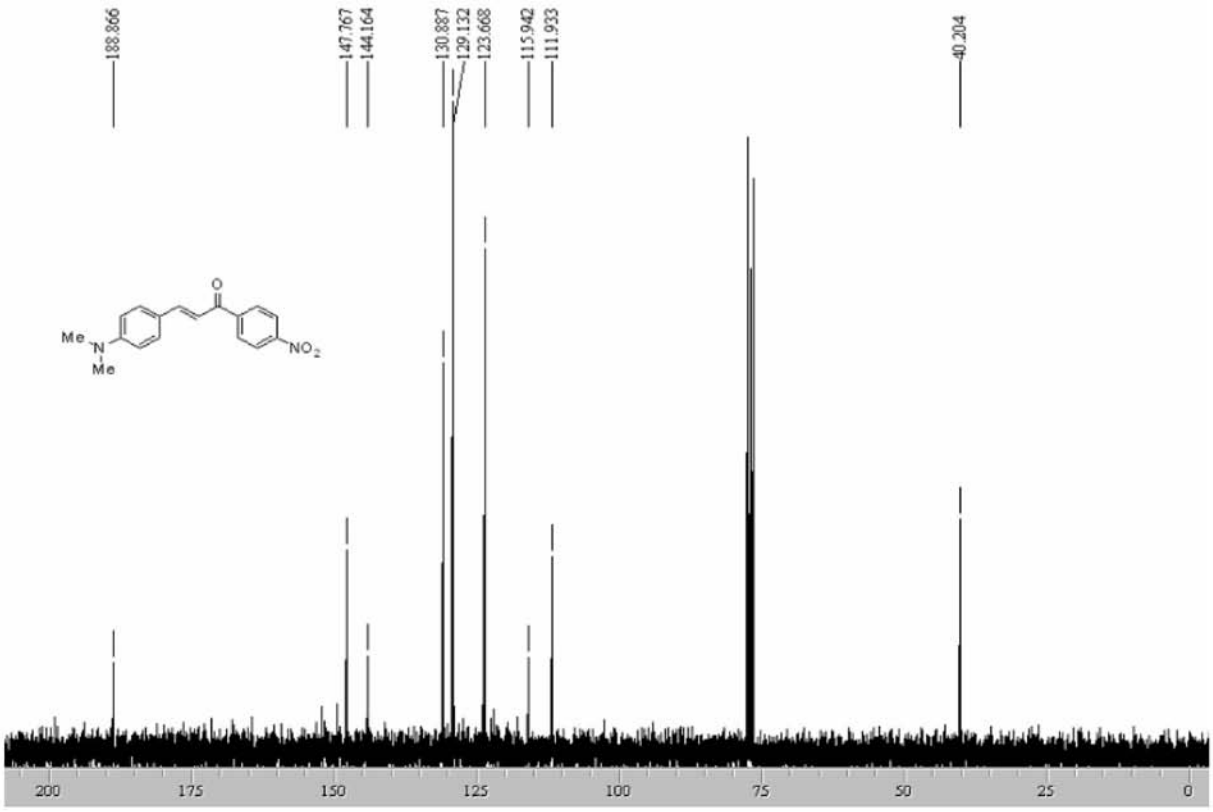

Figure S19. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **3j**.

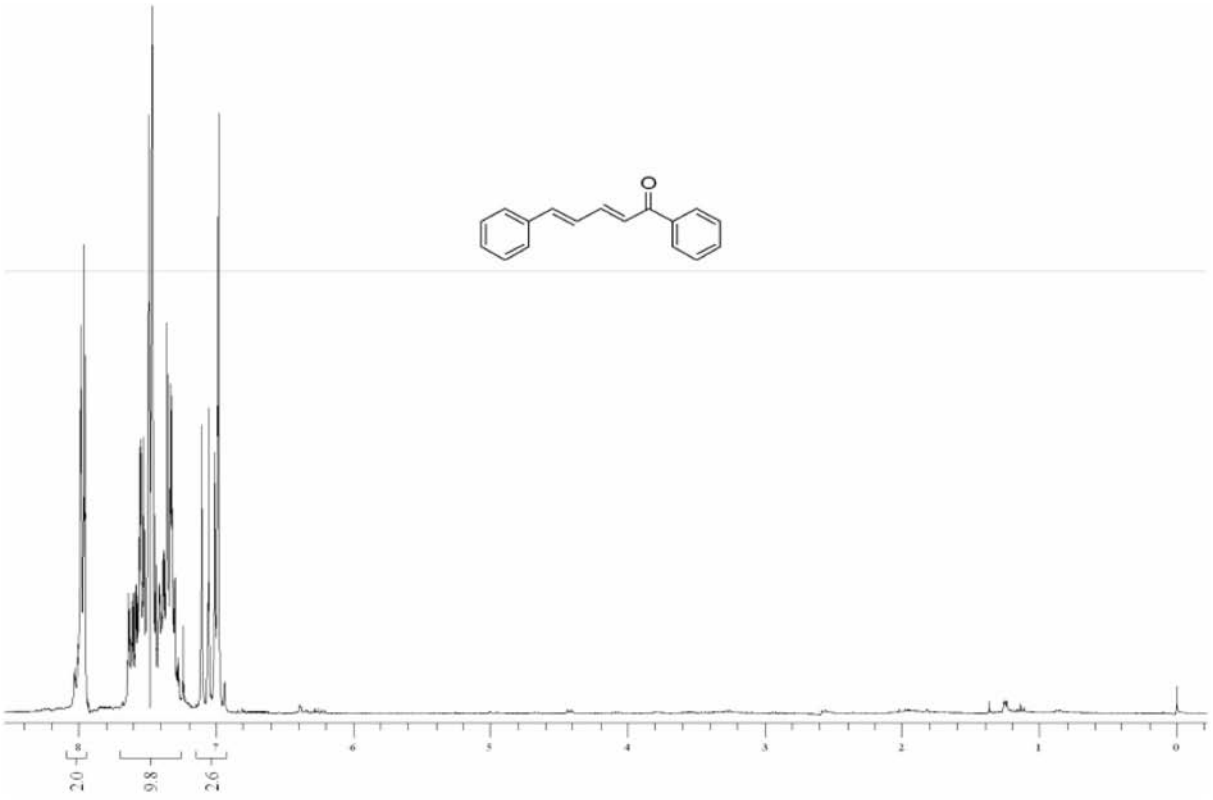

Figure S20. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **3k**.

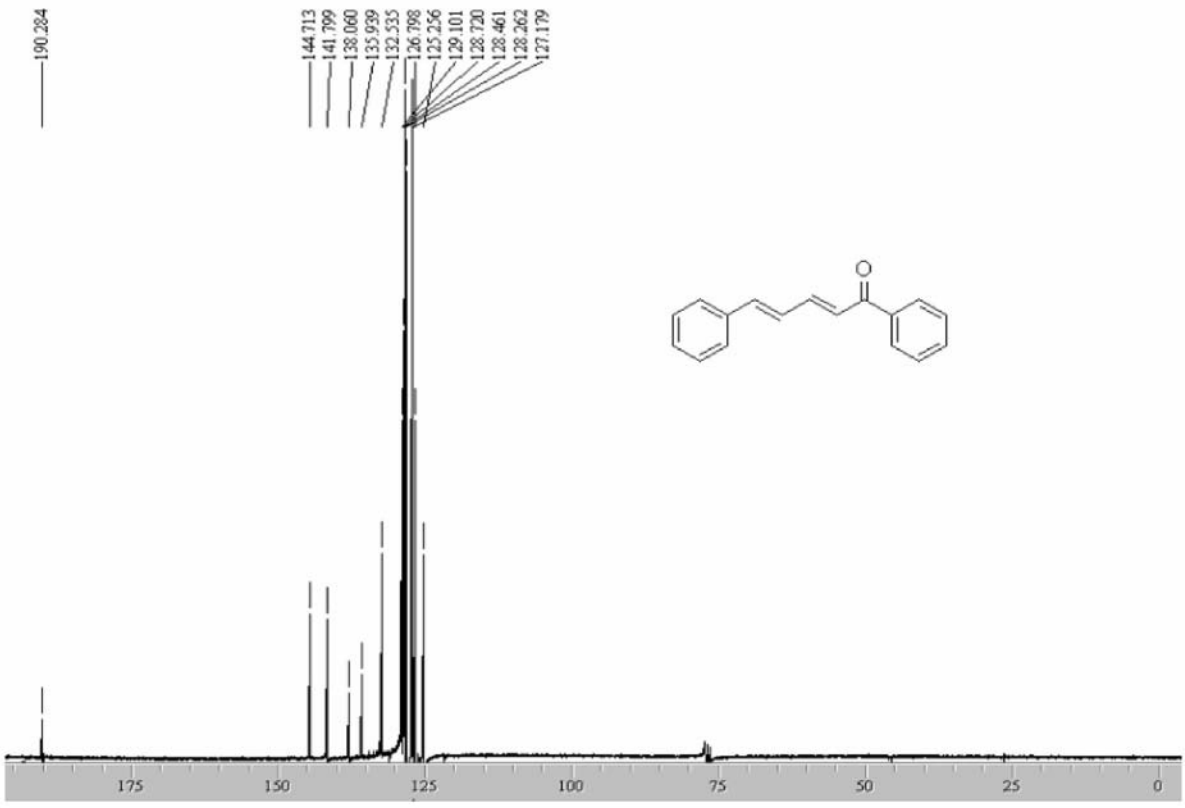

Figure S21. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **3k**.

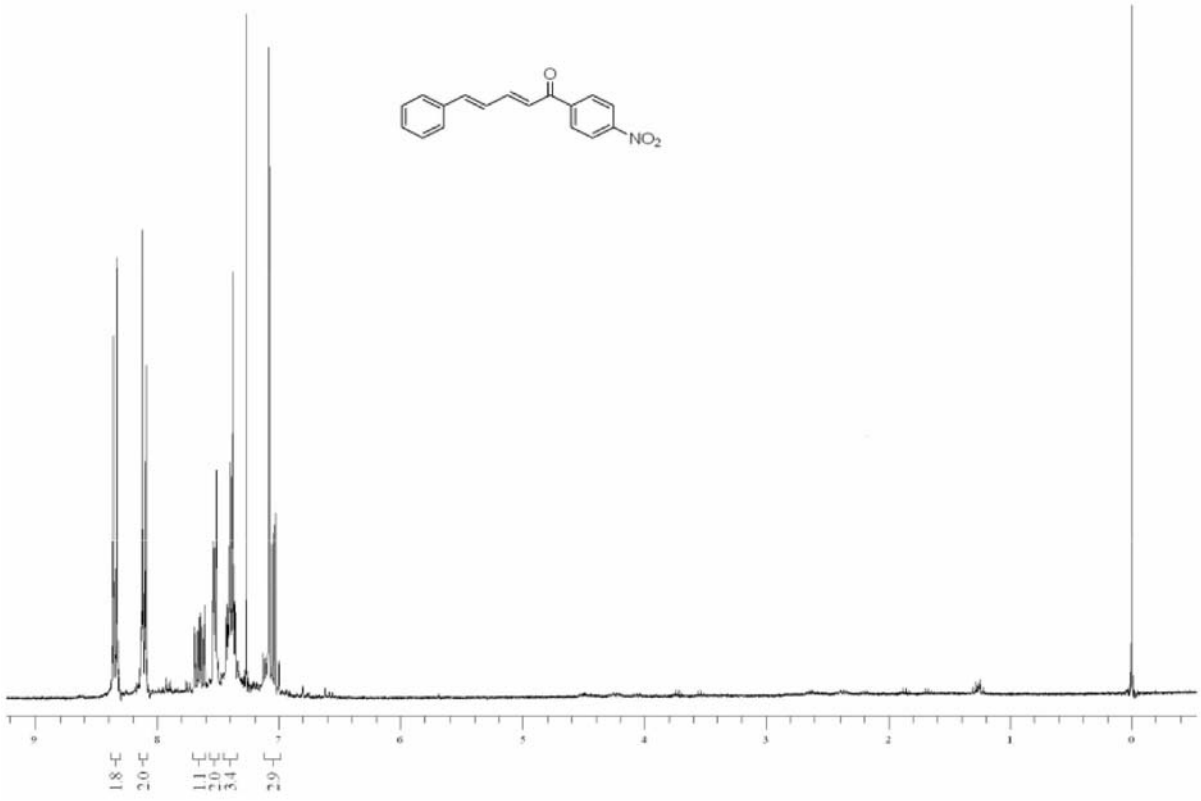

Figure S22. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **3l**.

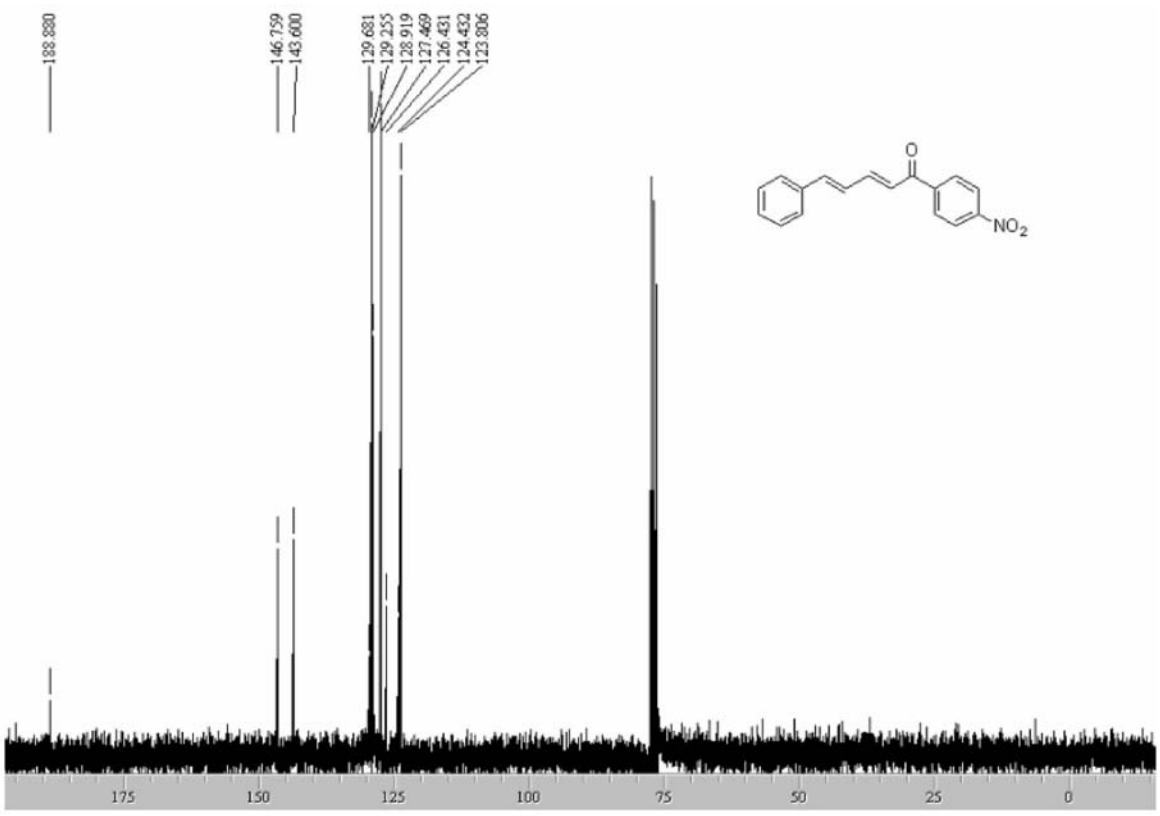

Figure S23. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **3l**.

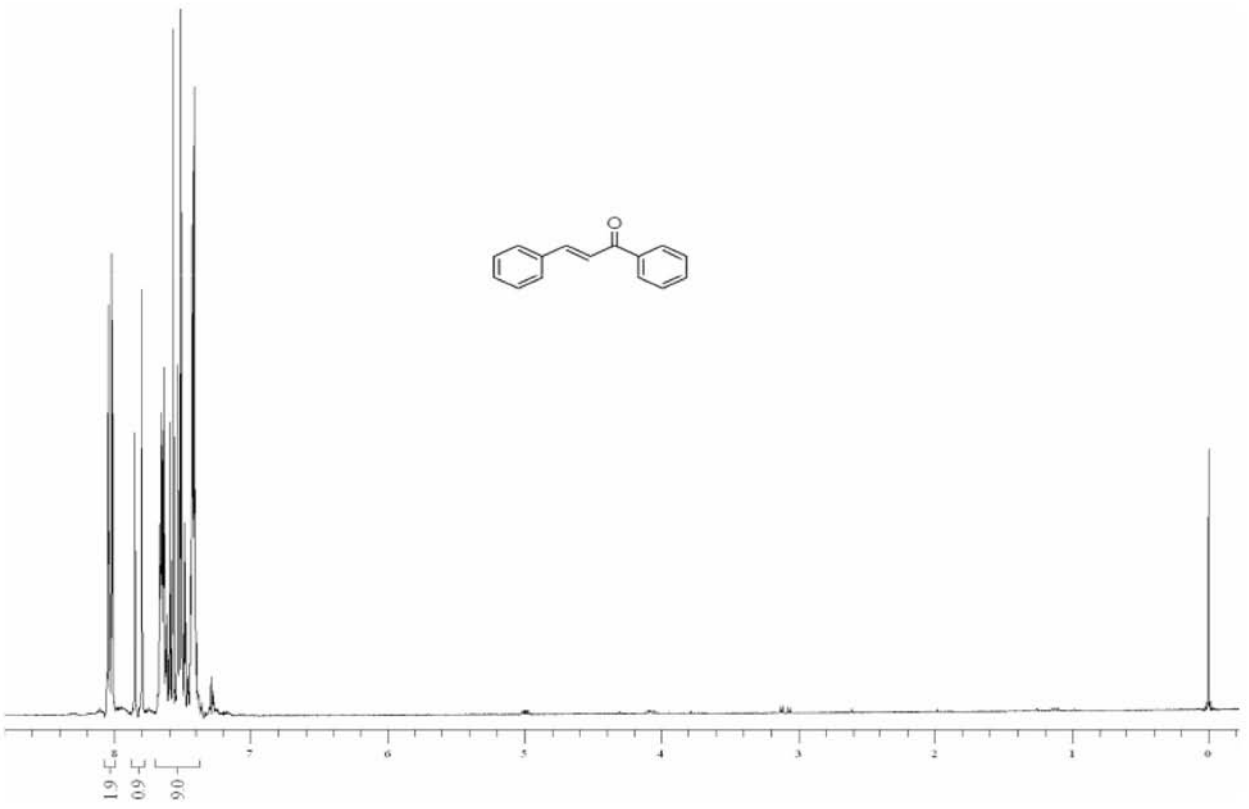

Figure S24. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **3m**.

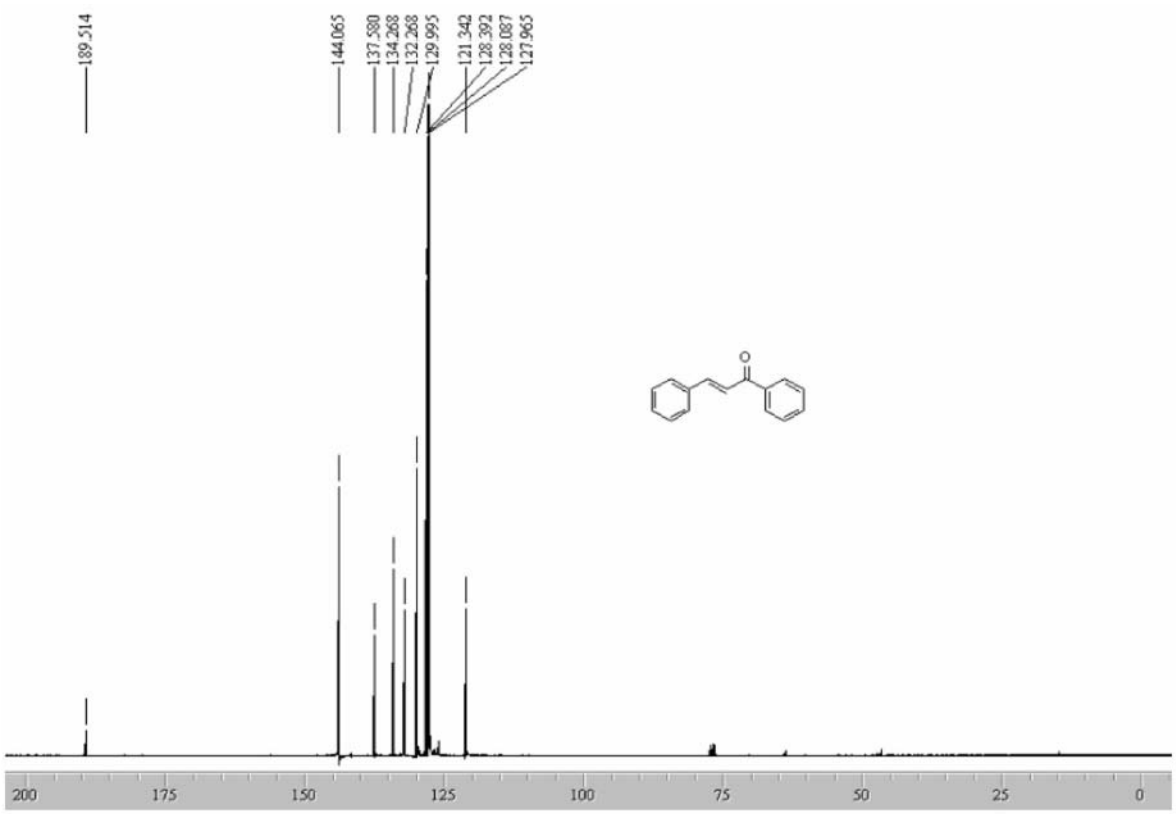

Figure S25. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **3m**.

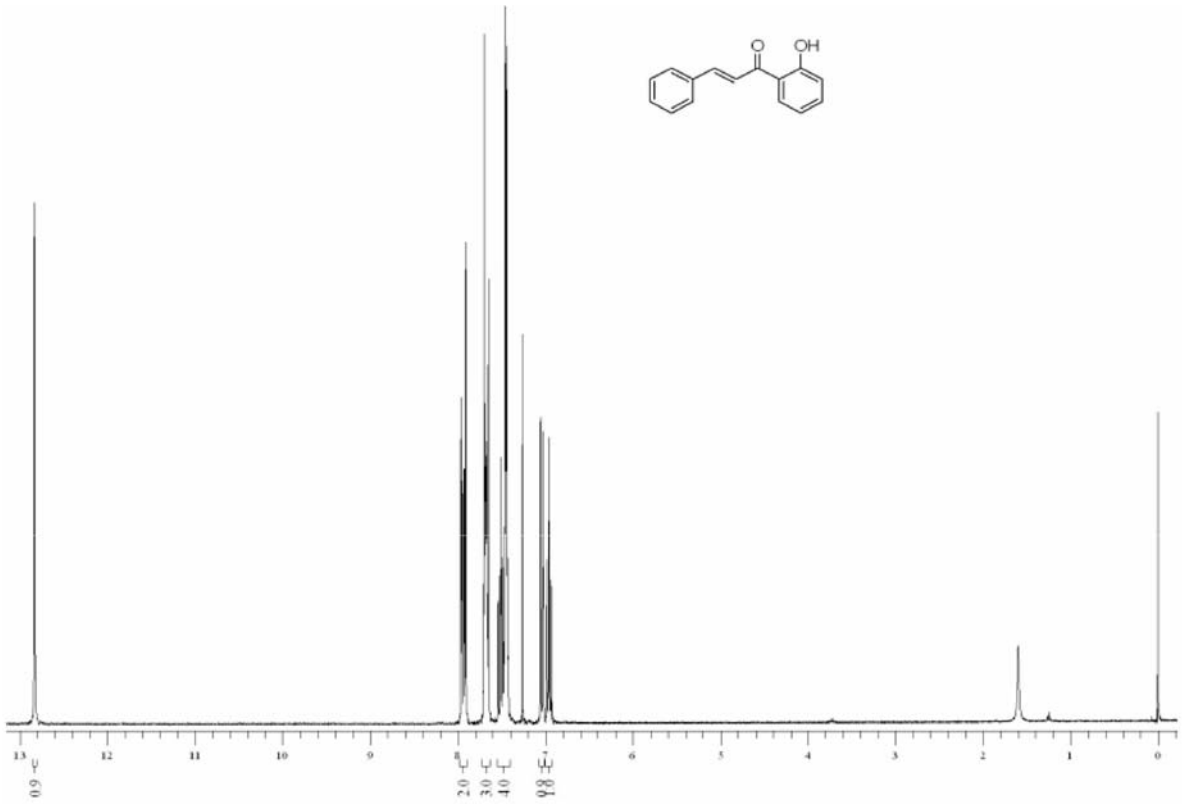

Figure S26. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **3n**.

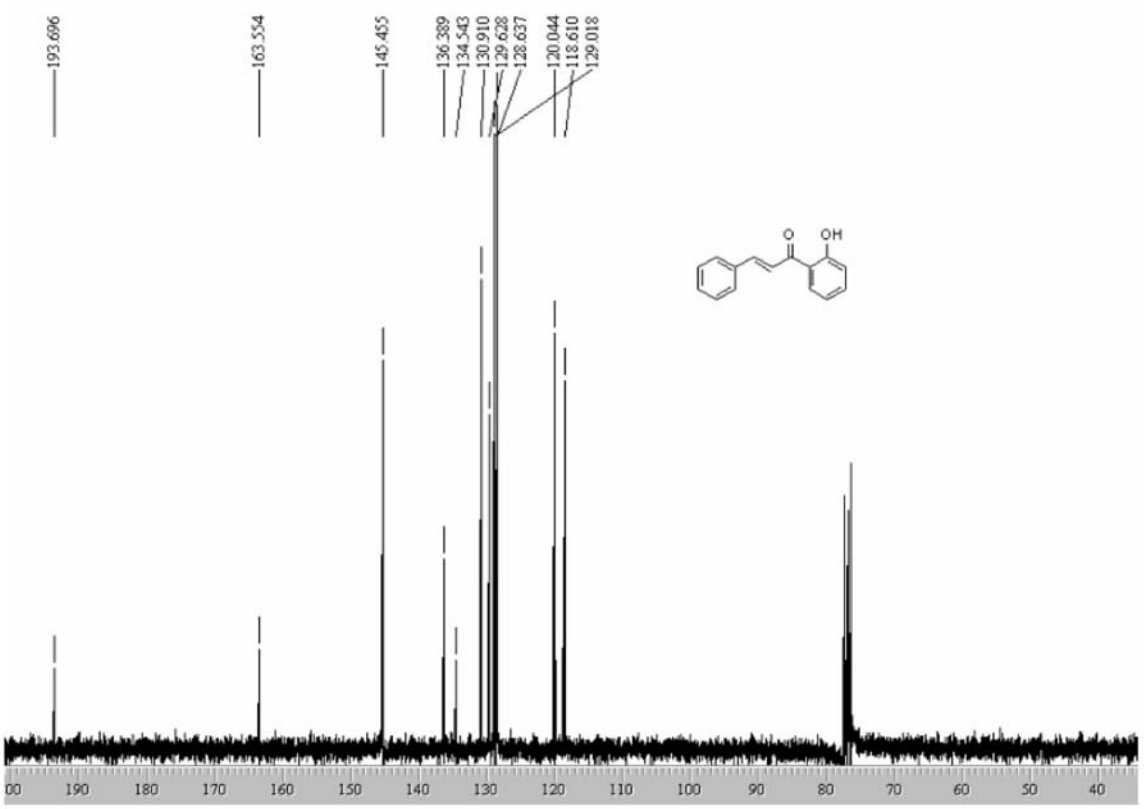

Figure S27. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **3n**.

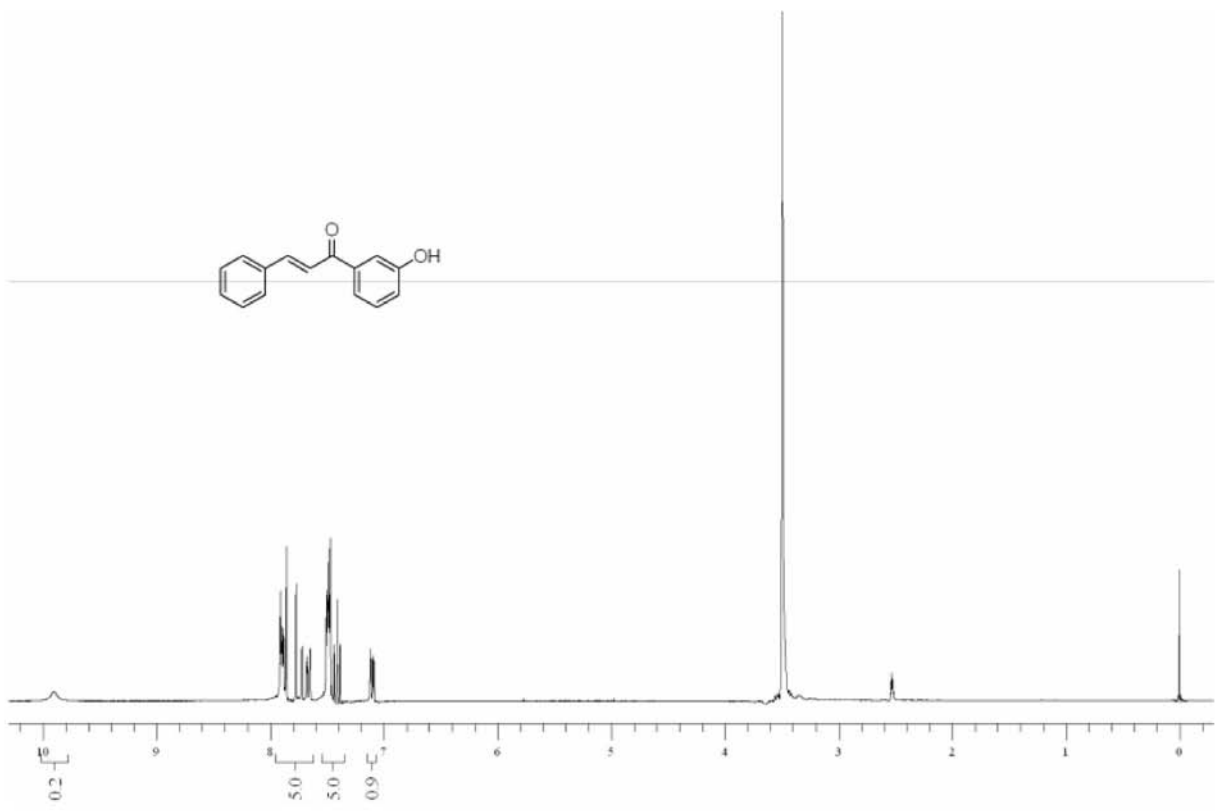

Figure S28. ^{1}H NMR (300 MHz, d_6-DMSO) spectrum of compound **3o**.

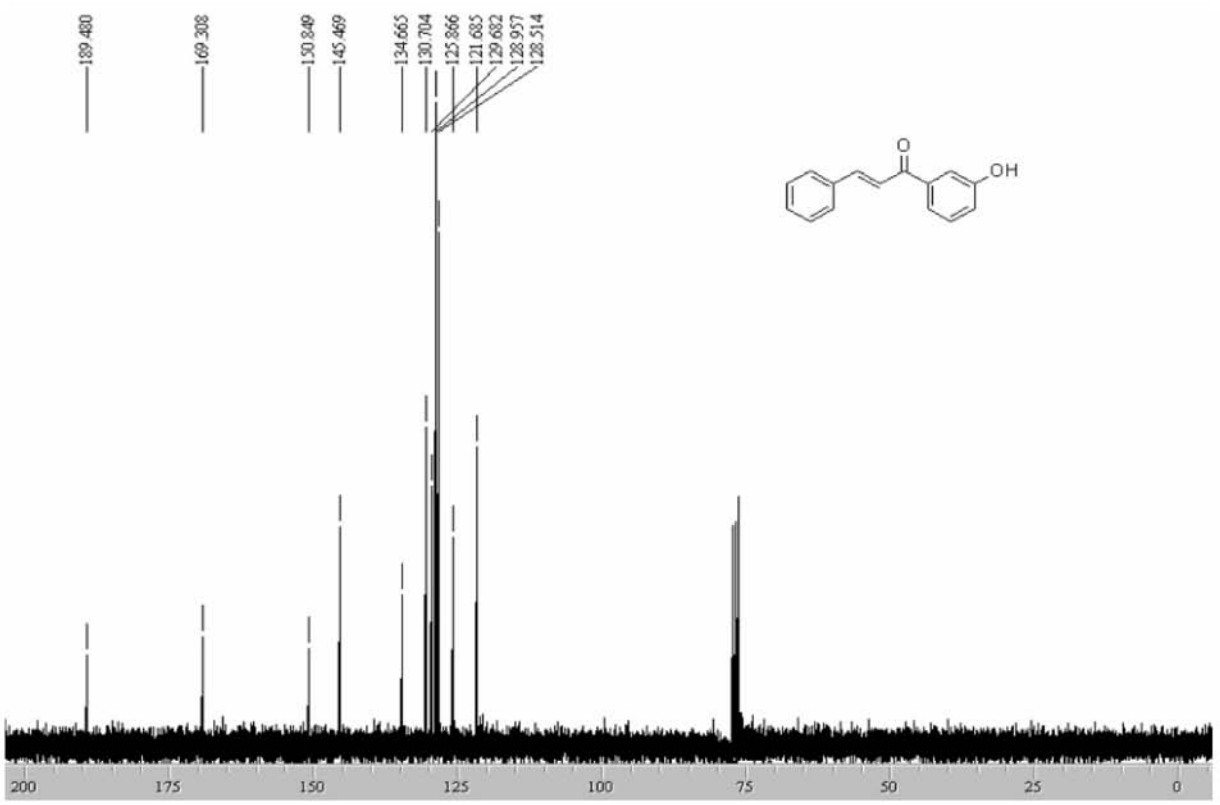

Figure S29. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **3o**.

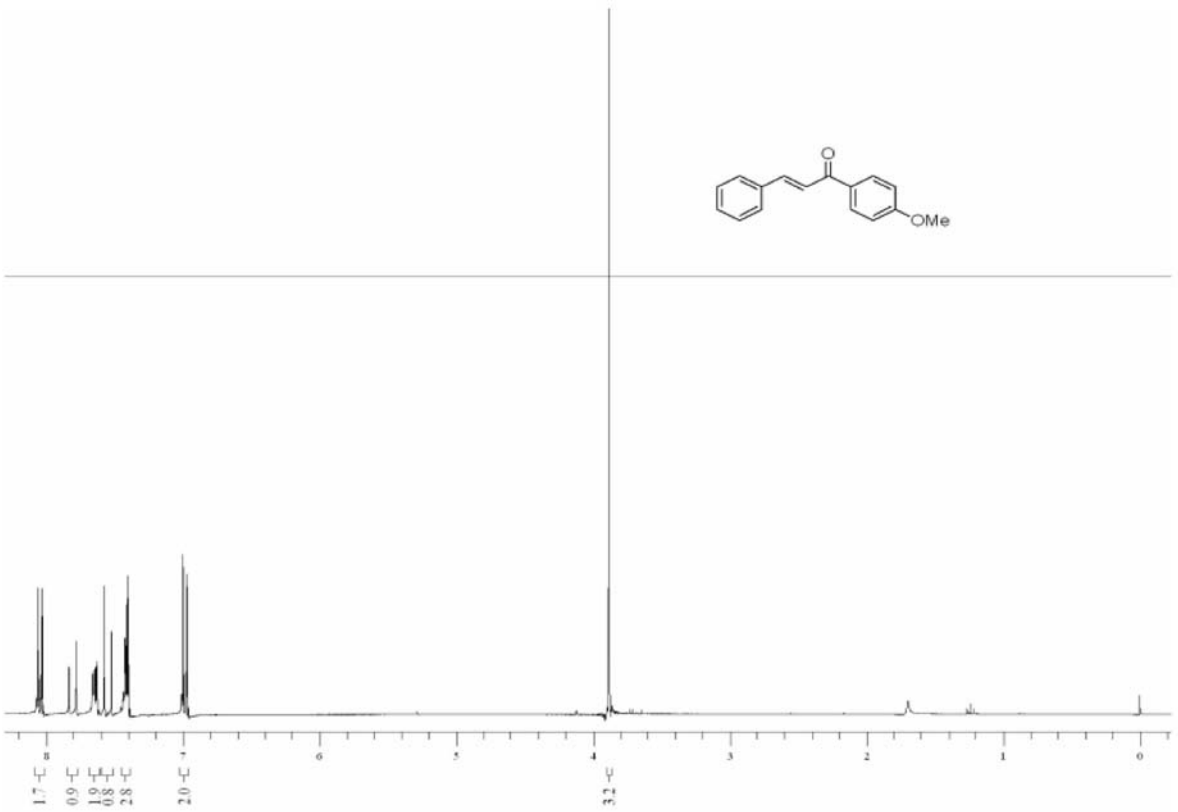

Figure S30. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **3p**.

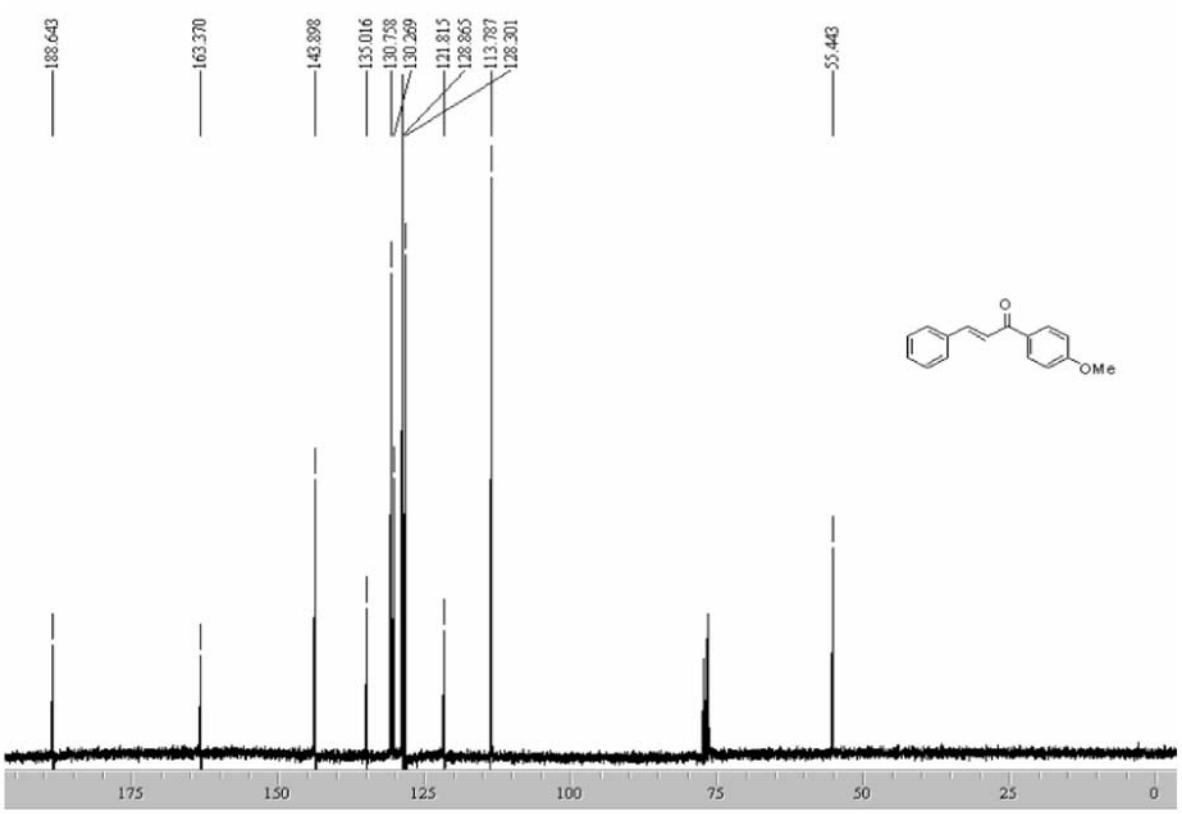

Figure S31. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **3p**.

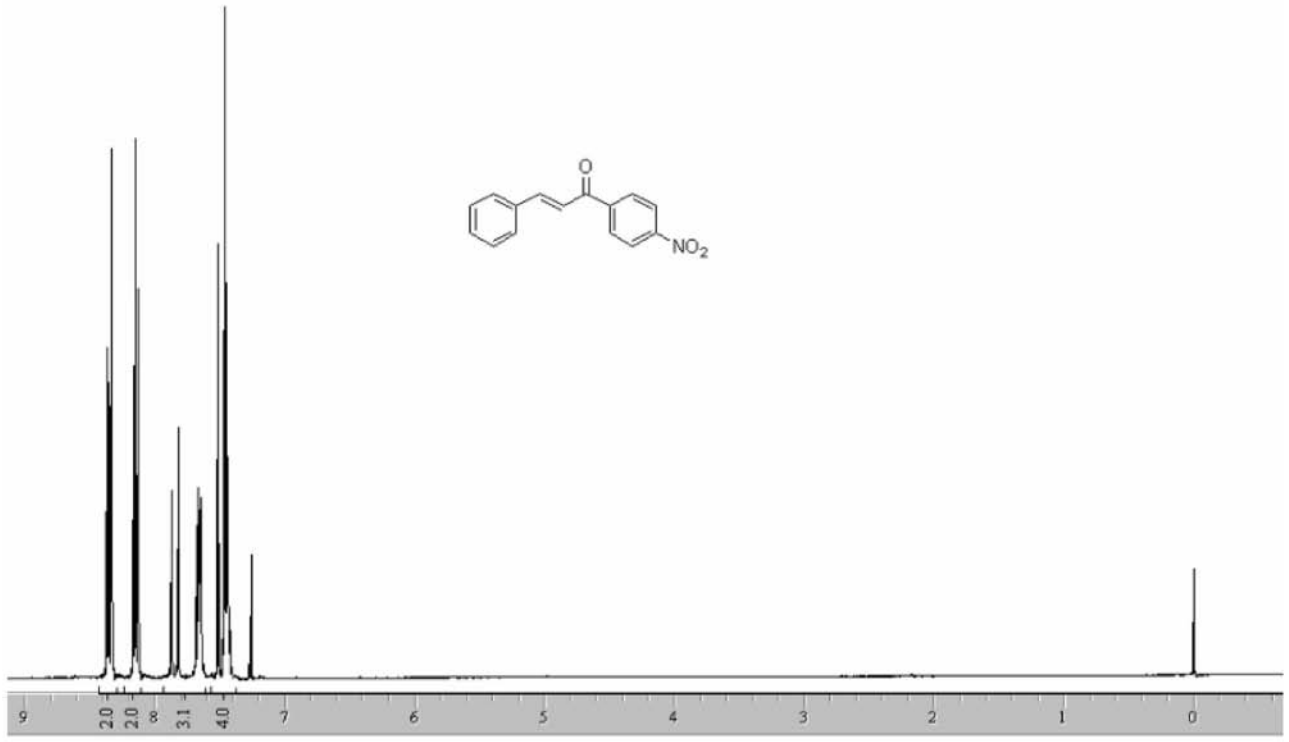

Figure S32. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **3q**.

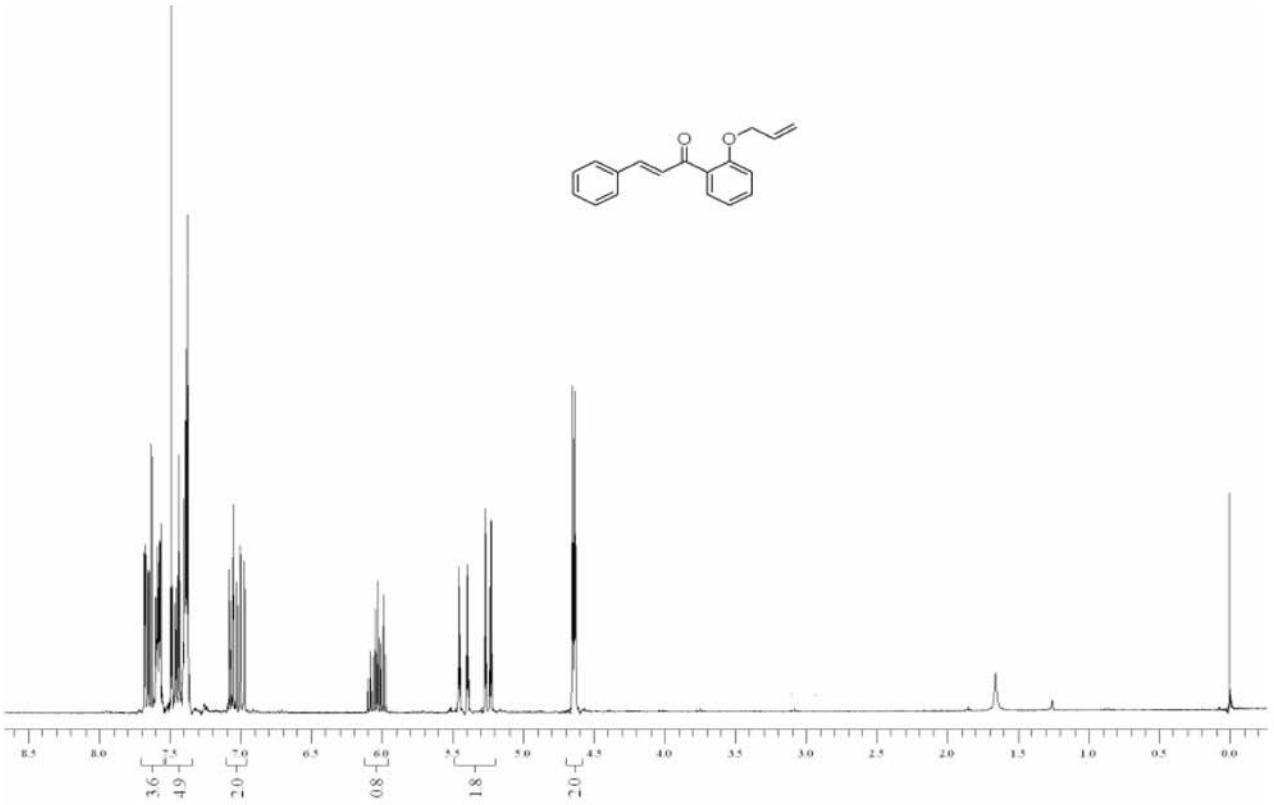

Figure S33. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **3r**.

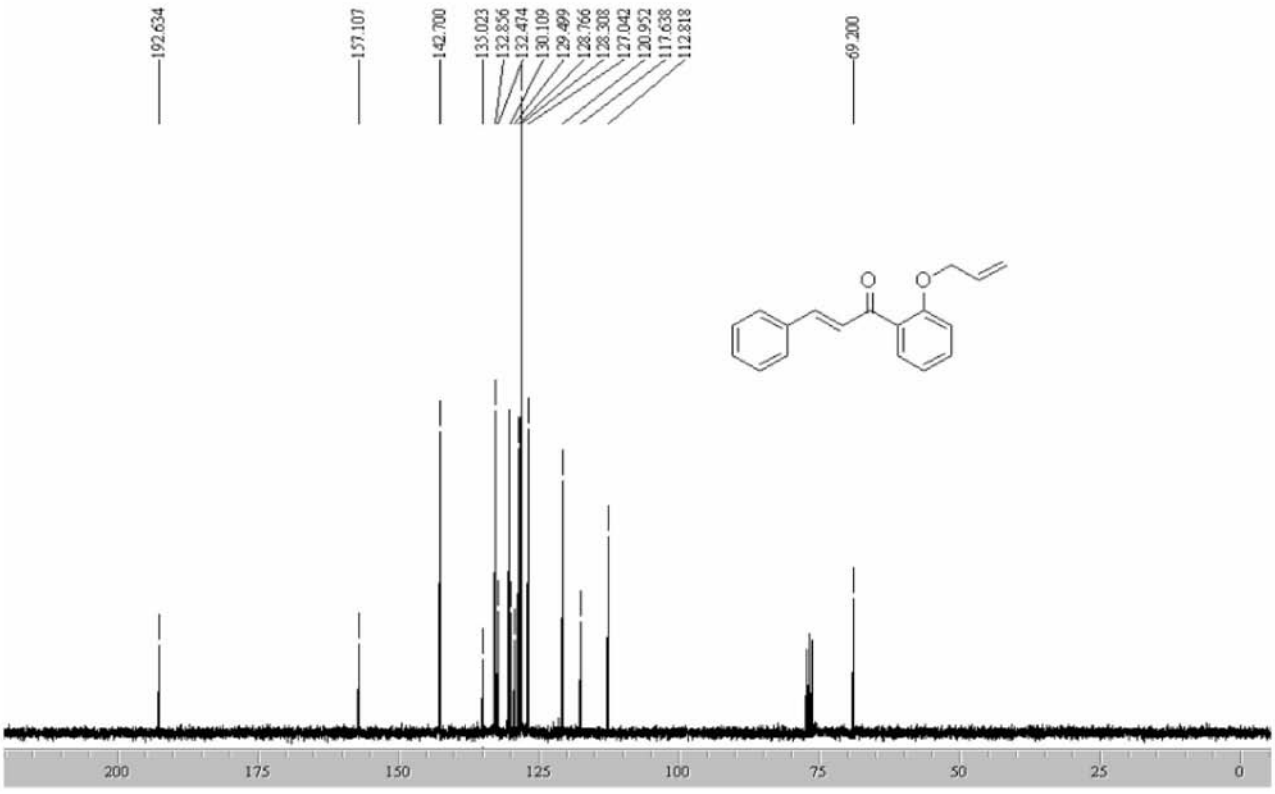

Figure S34. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **3r**.

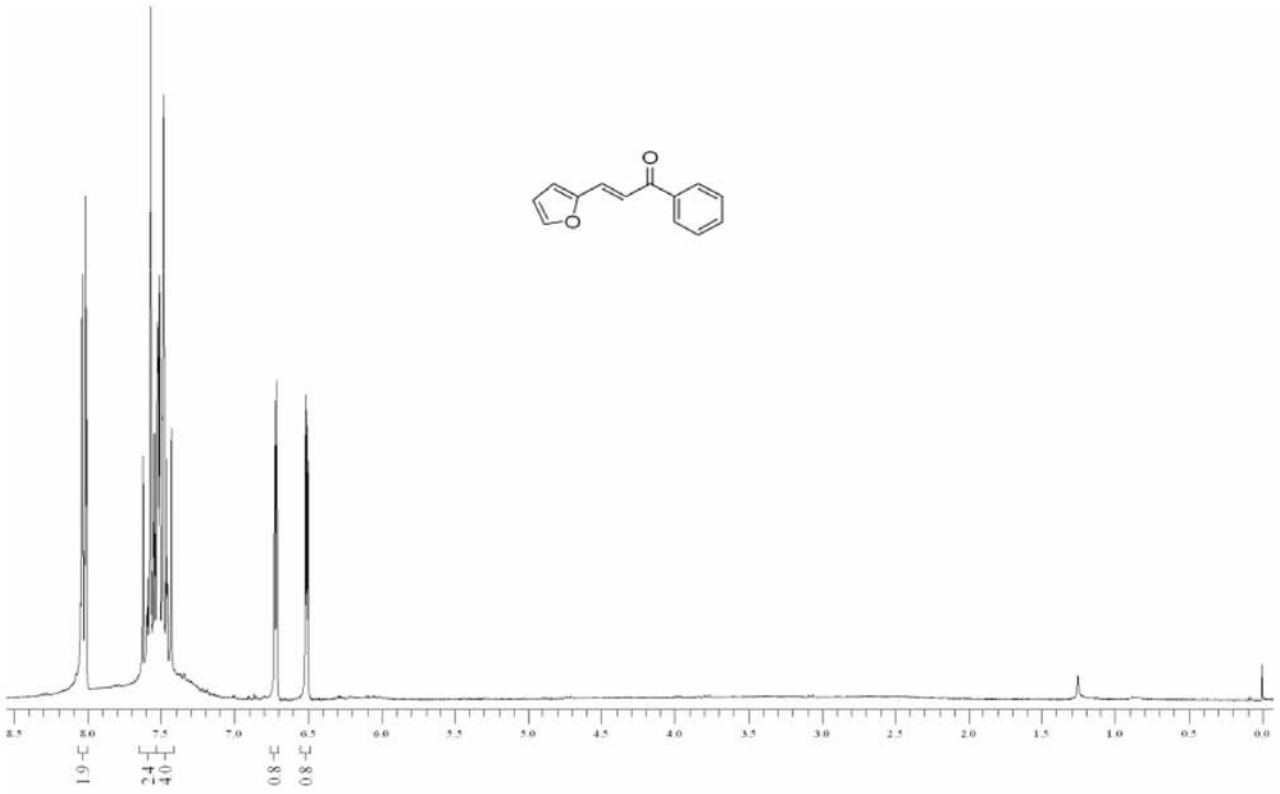

Figure S35. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **3s**.

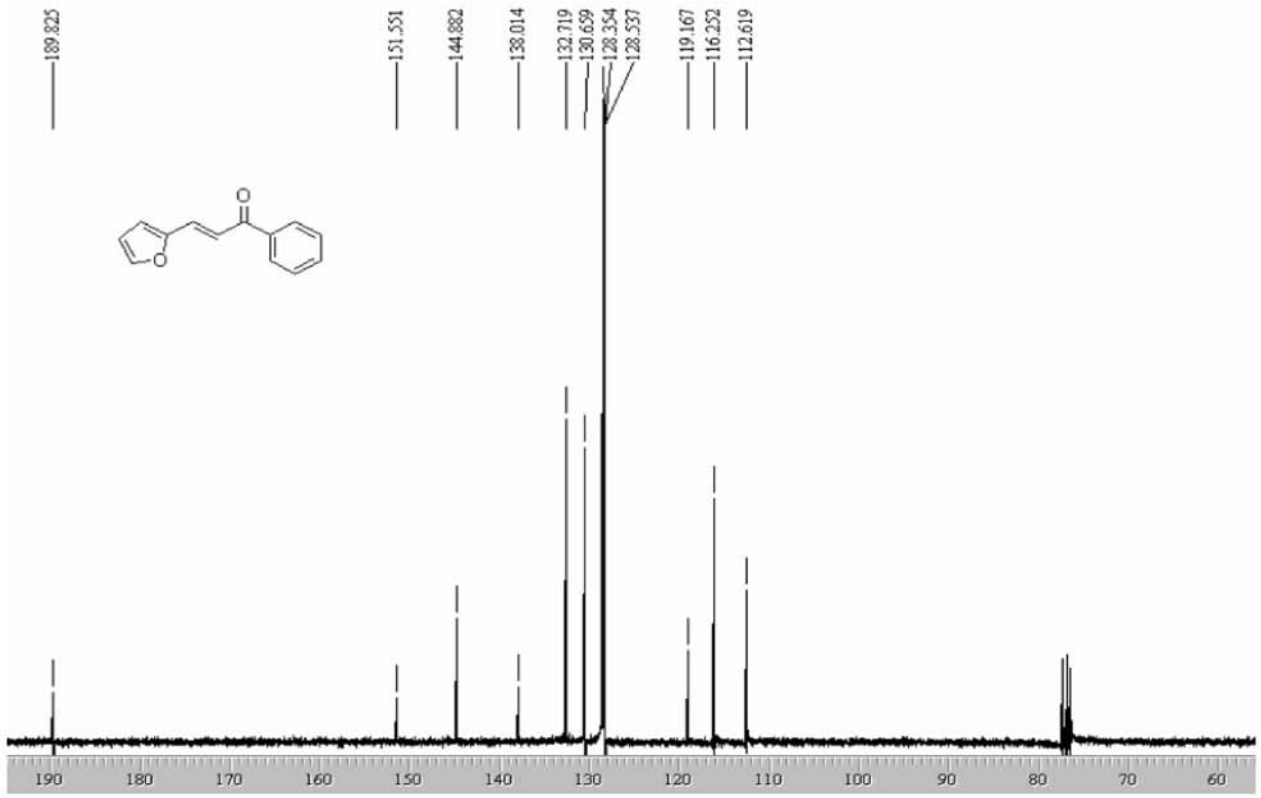

Figure S36. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **3s**.

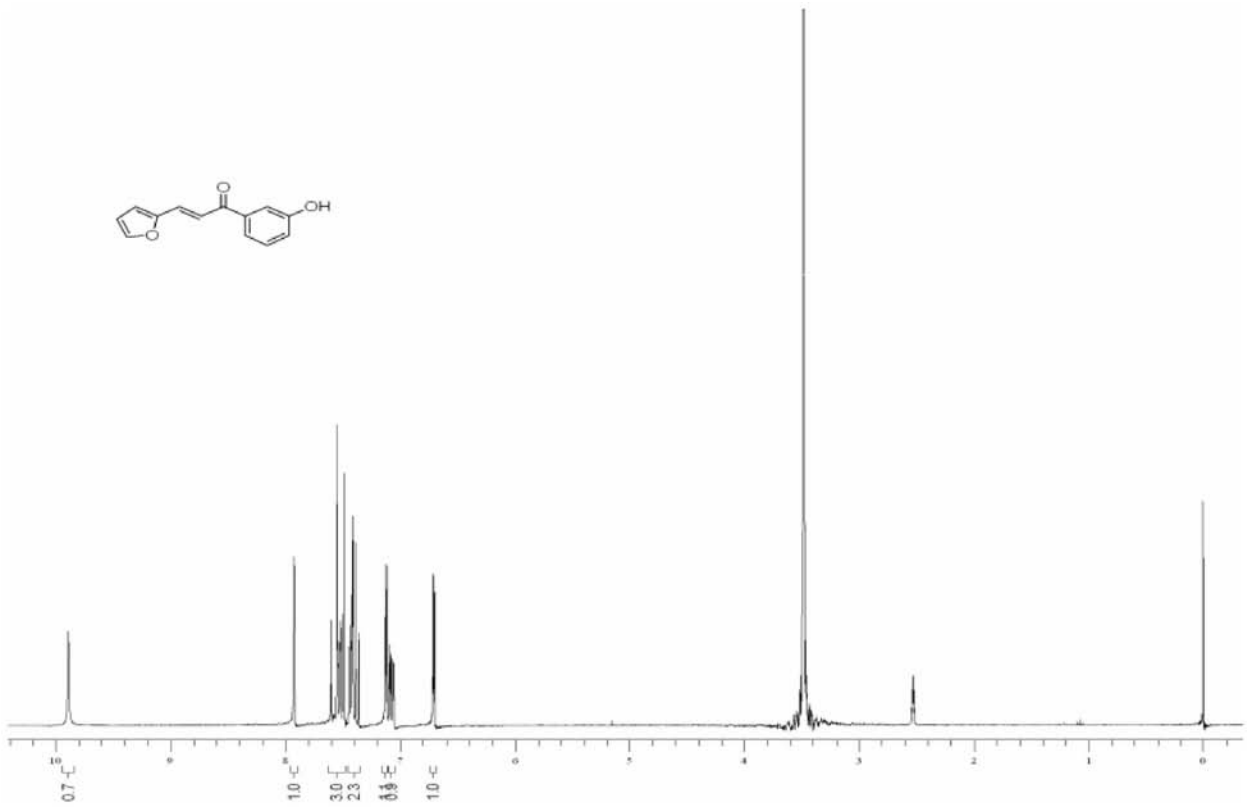

Figure S37. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **3t**.

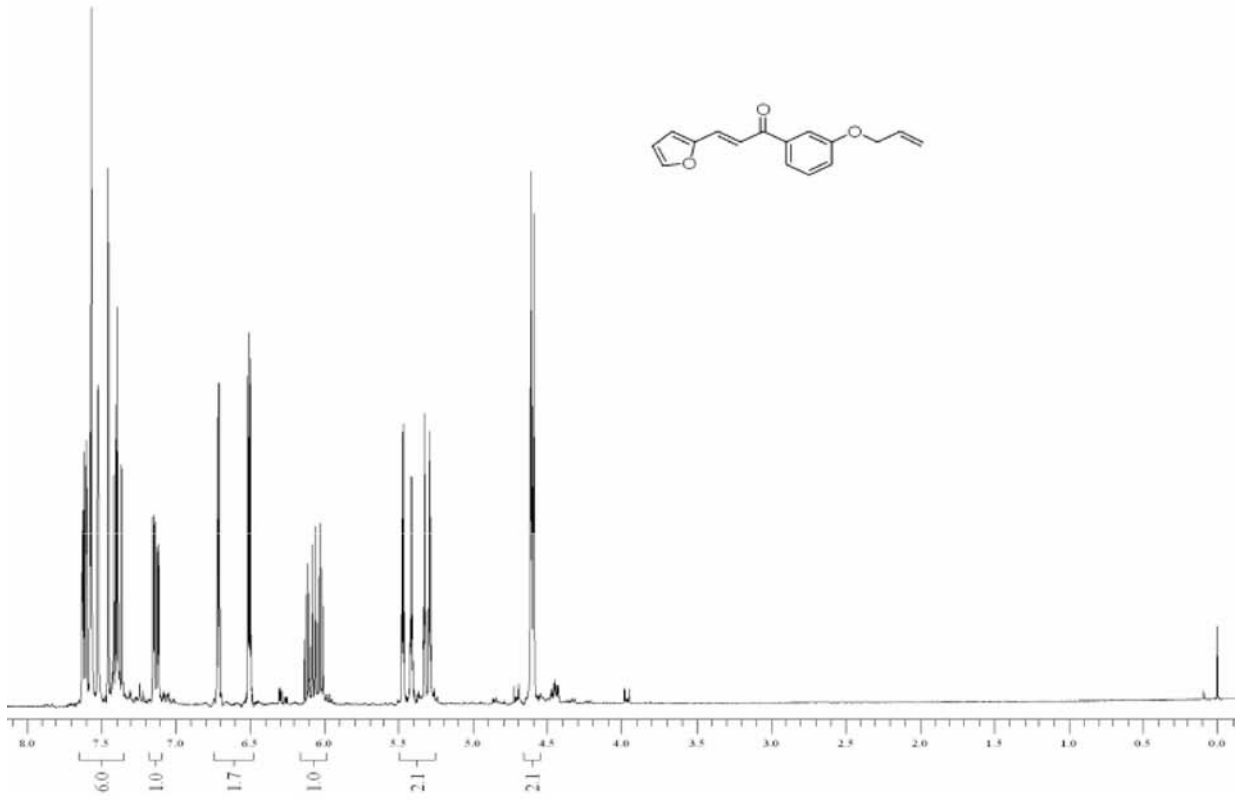

Figure S38. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **3u**.

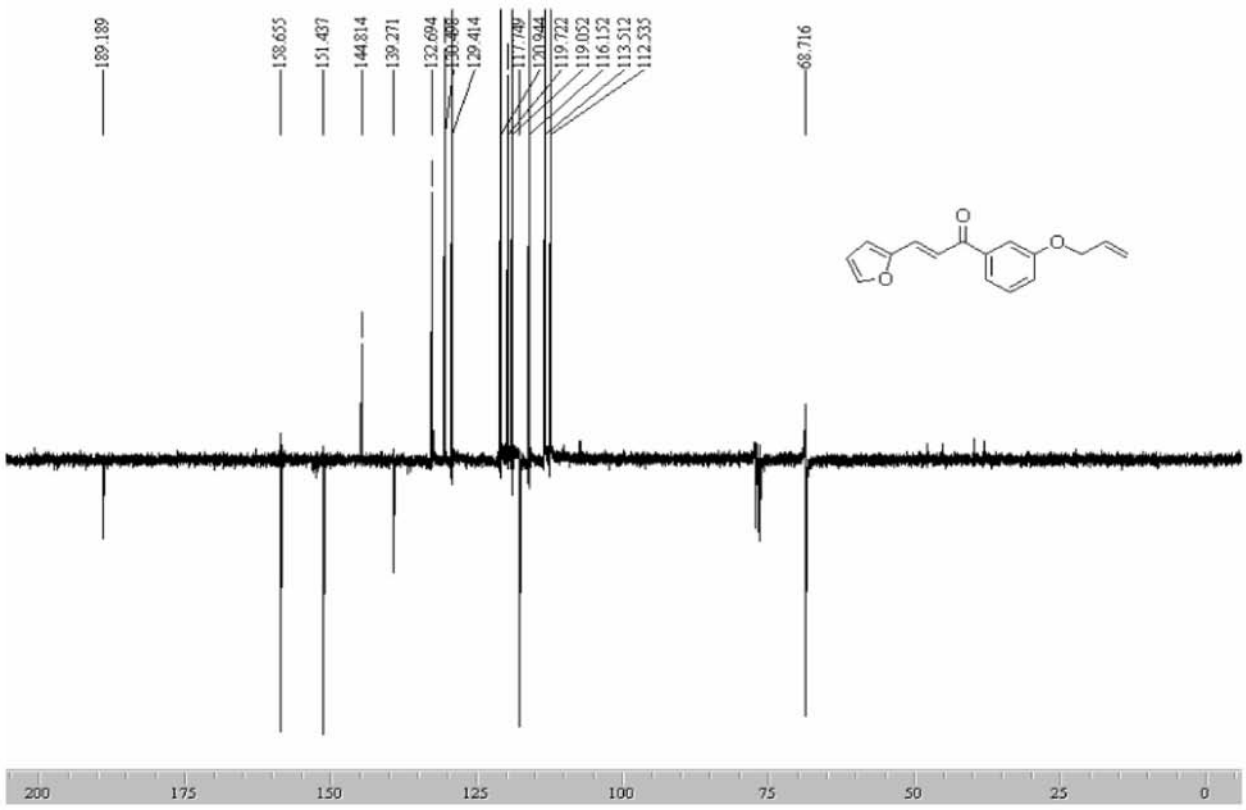

Figure S39. ^{13}C APT (75 MHz, $CDCl_3$) spectrum of compound **3u**.