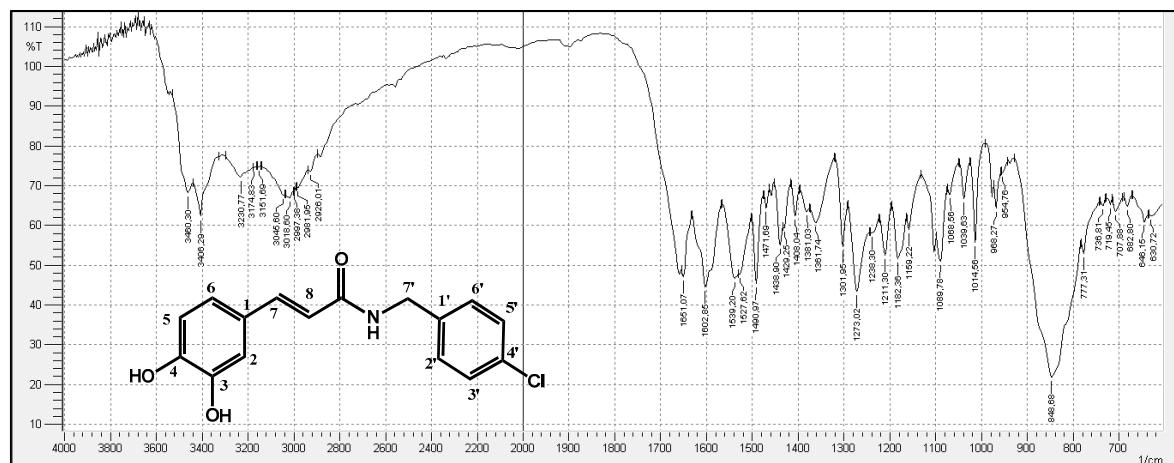
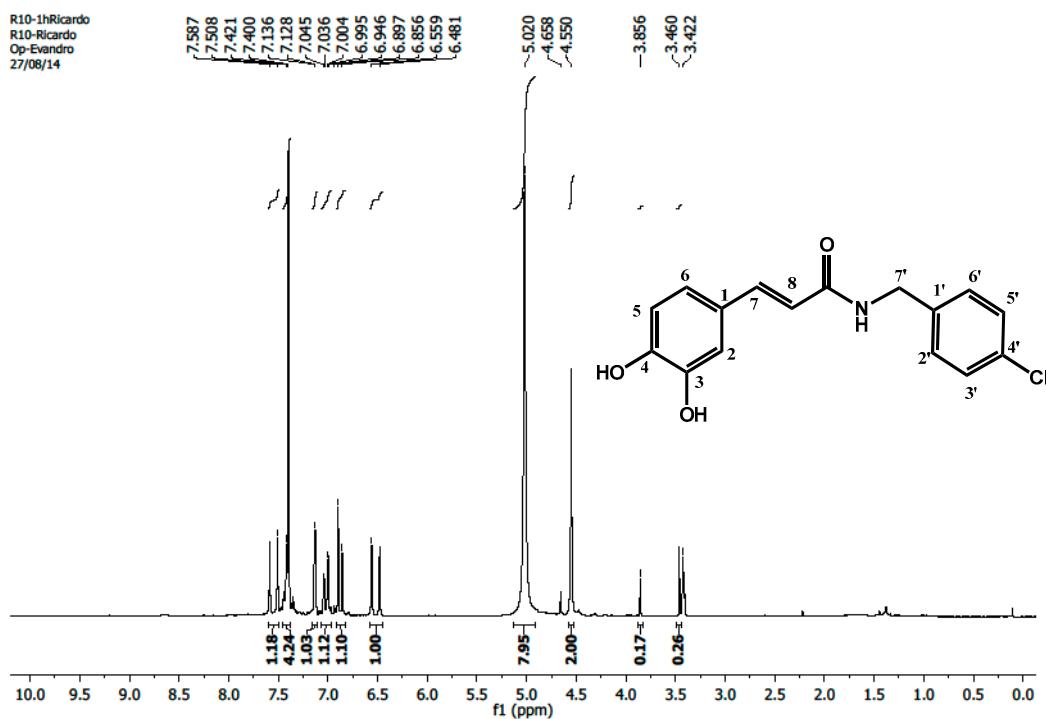


# Supplementary Material: Synthesis, Antifungal Evaluation and *In Silico* Study of N-(4-Halobenzyl)amides

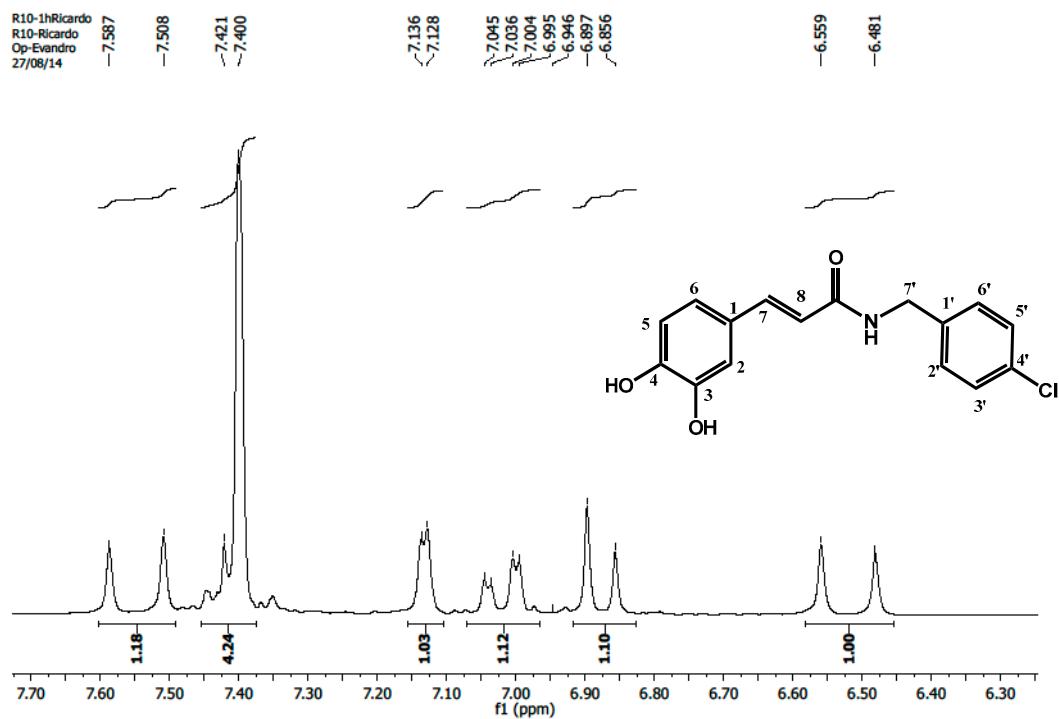
Ricardo Carneiro Montes, Ana Luiza A. L. Perez, Cássio Ilan S. Medeiros, Marianna Oliveira de Araújo, Edeltrudes de Oliveira Lima, Marcus Tullius Scotti and Damião Pergentino de Sousa



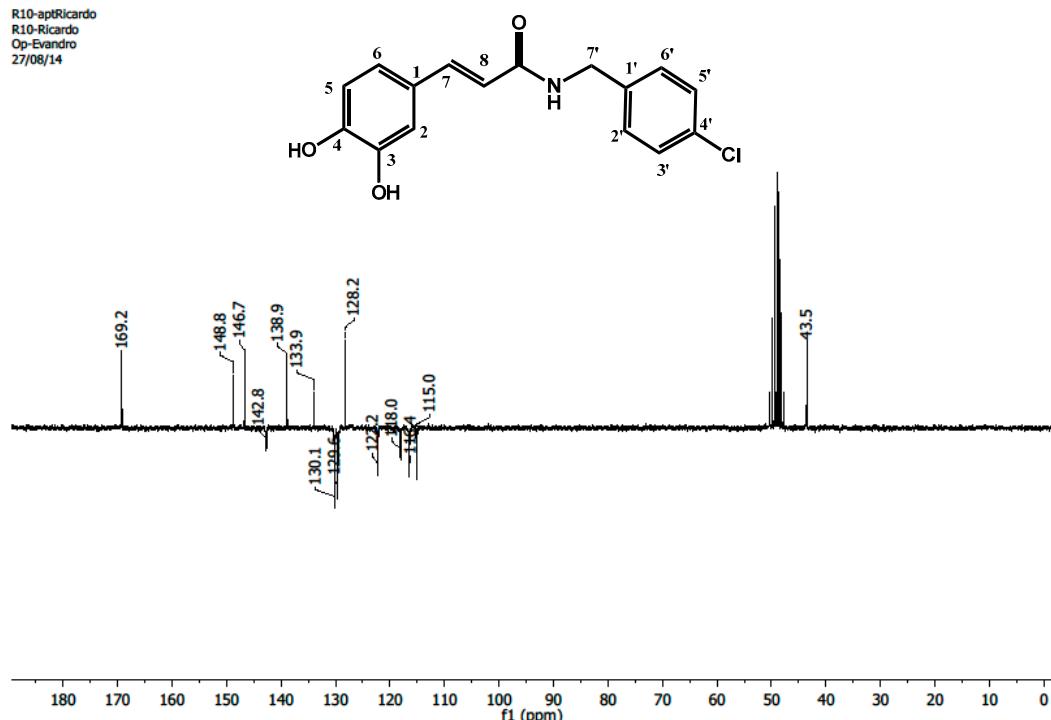
**Figure S1.** Infrared spectrum (KBr,  $\text{cm}^{-1}$ ) of (E)-N-(4-chlorobenzyl)-3-(3,4-dihydroxyphenyl)acrylamide (2).



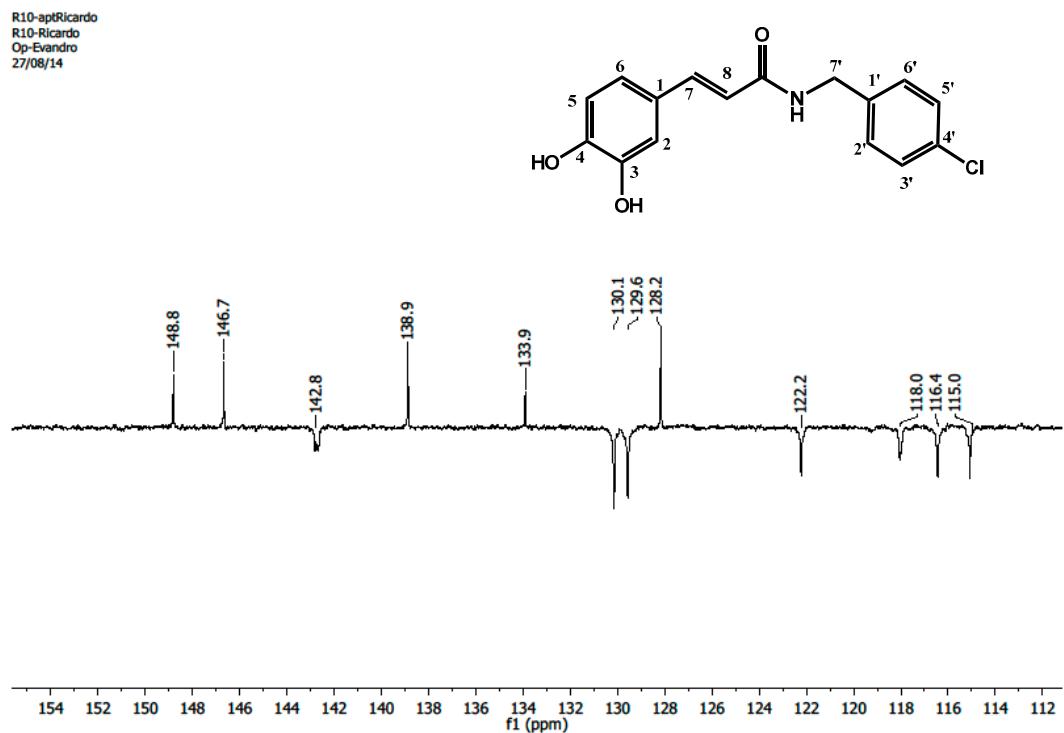
**Figure S2.** <sup>1</sup>H-NMR spectrum of (E)-N-(4-chlorobenzyl)-3-(3,4-dihydroxyphenyl)acrylamide (MeOD, 200 MHz).



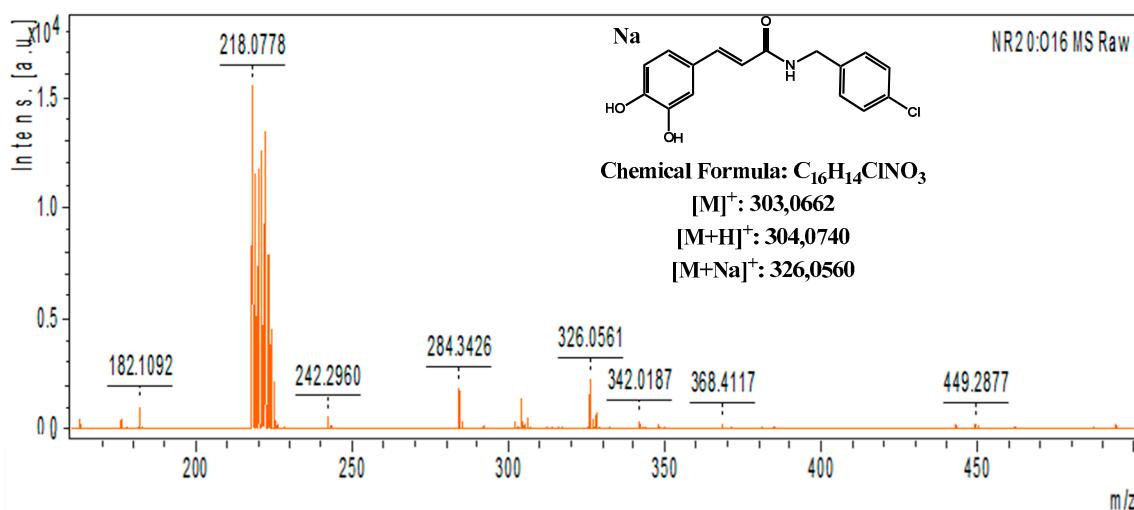
**Figure S3.** Expansion of the  $^1\text{H}$ -NMR spectrum of (*E*)-*N*-(4-chlorobenzyl)-3-(3,4-dihydroxyphenyl)acrylamide (2) (MeOD, 200 MHz).



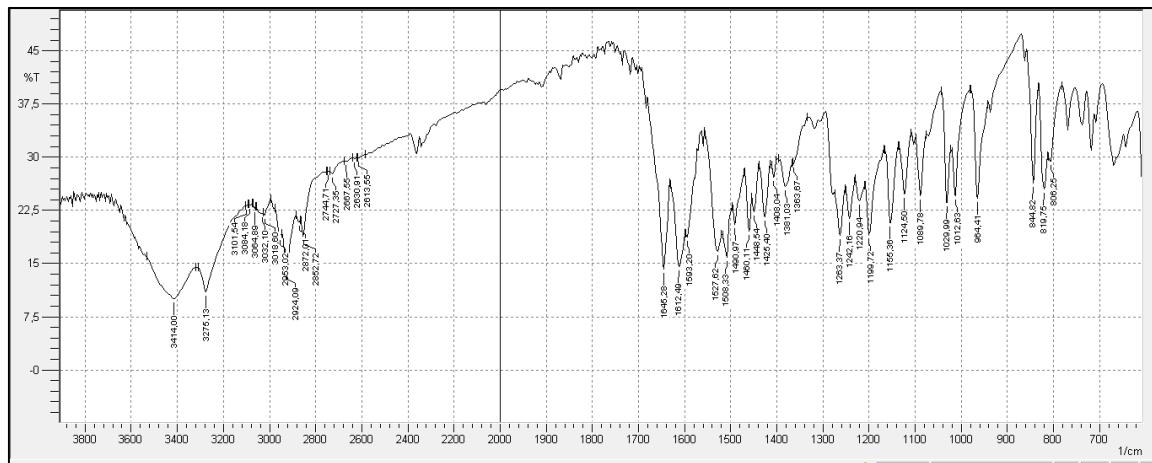
**Figure S4.**  $^{13}\text{C}$ -APT NMR spectrum of (*E*)-*N*-(4-chlorobenzyl)-3-(3,4-dihydroxyphenyl)acrylamide (2) (MeOD, 50 MHz).



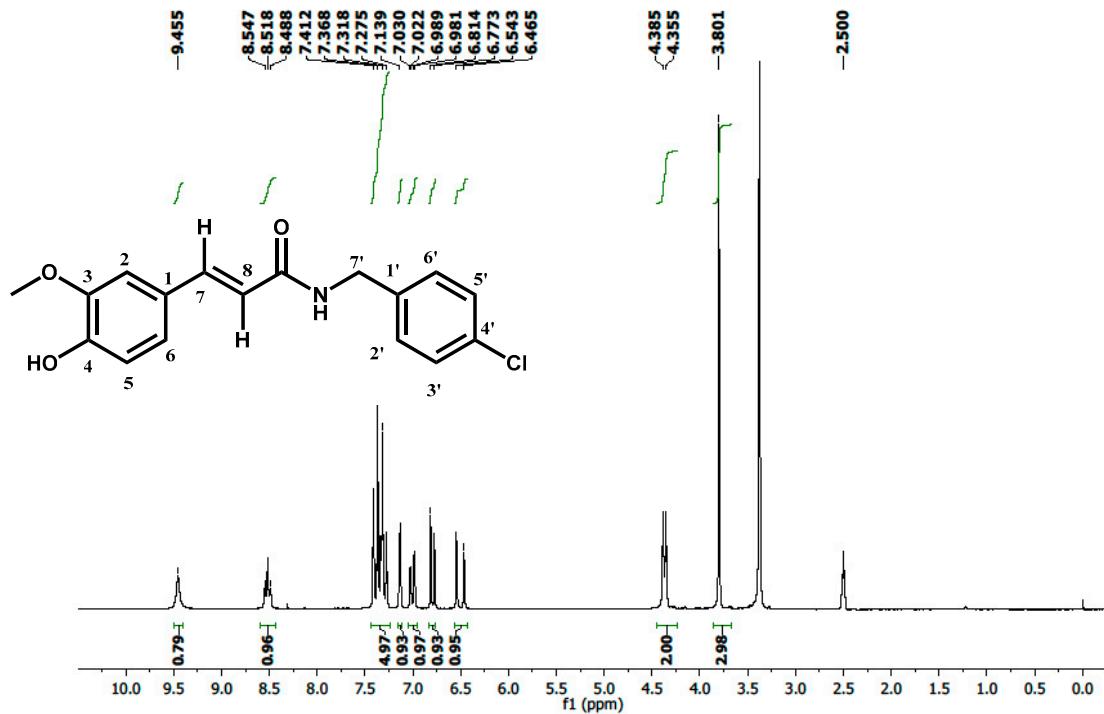
**Figure S5.** Expansion of the <sup>13</sup>C-APT NMR spectrum of (E)-N-(4-chlorobenzyl)-3-(3,4-dihydroxyphenyl)acrylamide (2) (MeOD, 50 MHz).



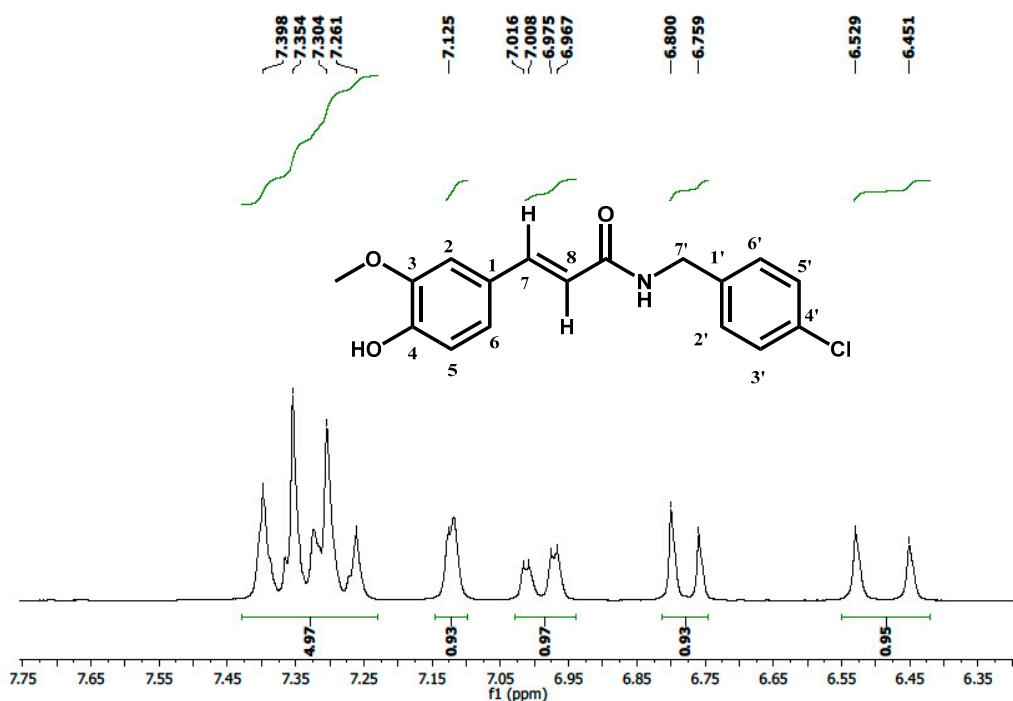
**Figure S6.** High resolution mass spectrum—MALDI of (E)-N-(4-chlorobenzyl)-3-(3,4-dihydroxyphenyl)acrylamide (2).



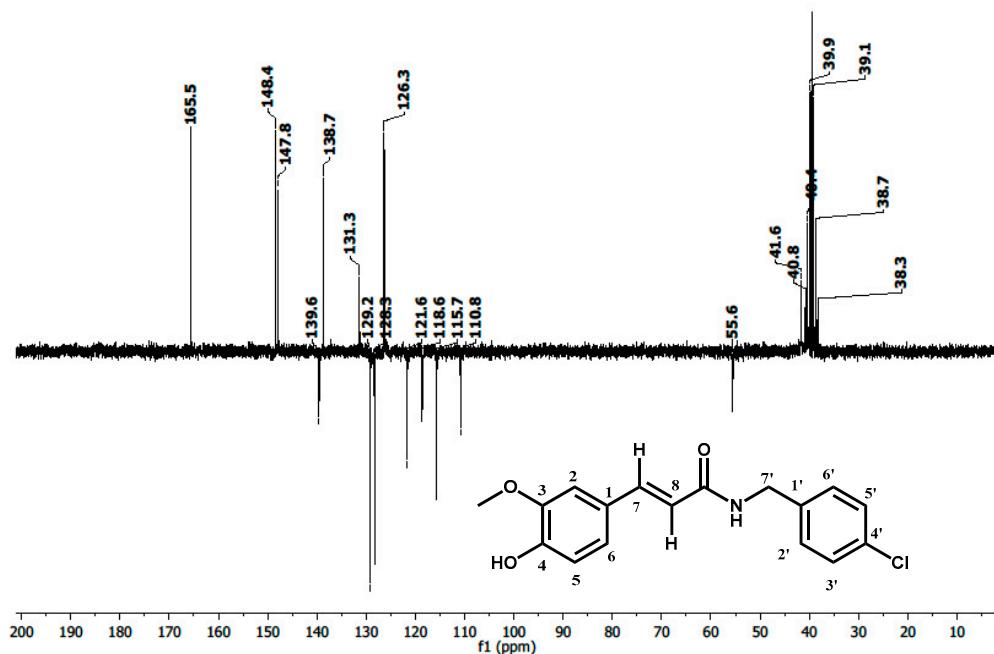
**Figure S7.** Infrared spectrum (KBr,  $\text{cm}^{-1}$ ) of (*E*)-*N*-(4-chlorobenzyl)-3-(4-hydroxy-3-methoxyphenyl)acrylamide (3).



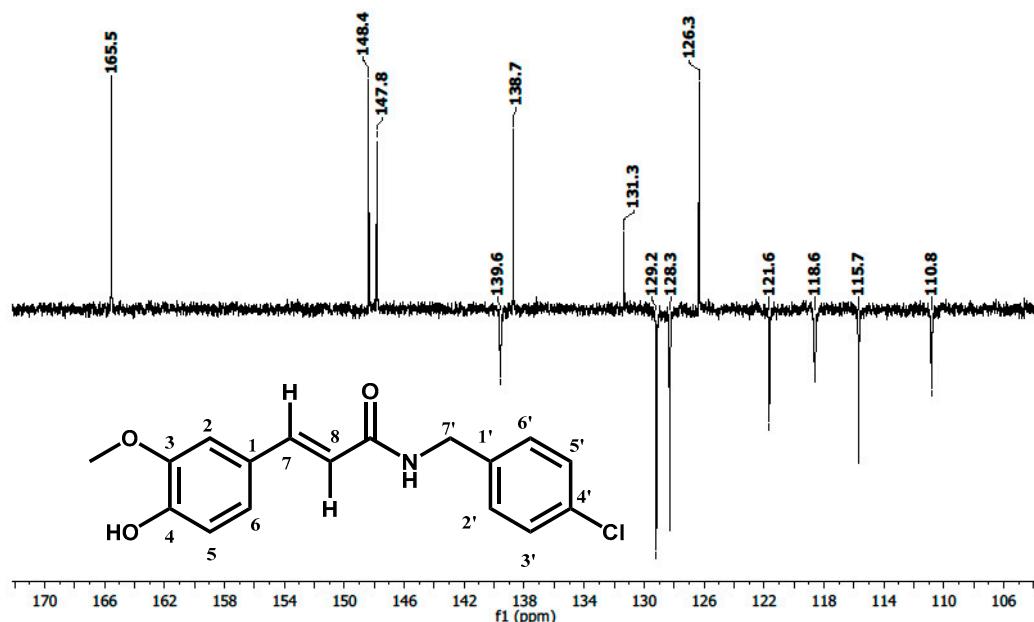
**Figure S8.**  $^1\text{H}$ -NMR spectrum of (*E*)-*N*-(4-chlorobenzyl)-3-(4-hydroxy-3-methoxyphenyl)acrylamide (3) ( $\text{DMSO}-d_6$ , 200 MHz).



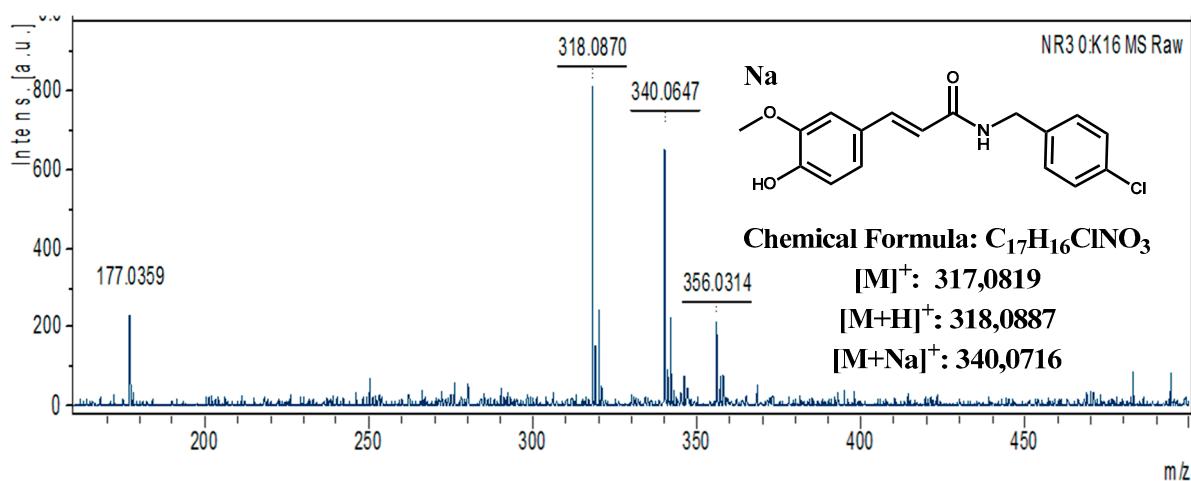
**Figure S9.** Expansion of the  $^1\text{H}$ -NMR spectrum of (*E*)-*N*-(4-chlorobenzyl)-3-(4-hydroxy-3-methoxyphenyl)acrylamide (**3**) ( $\text{DMSO}-d_6$ , 200 MHz).



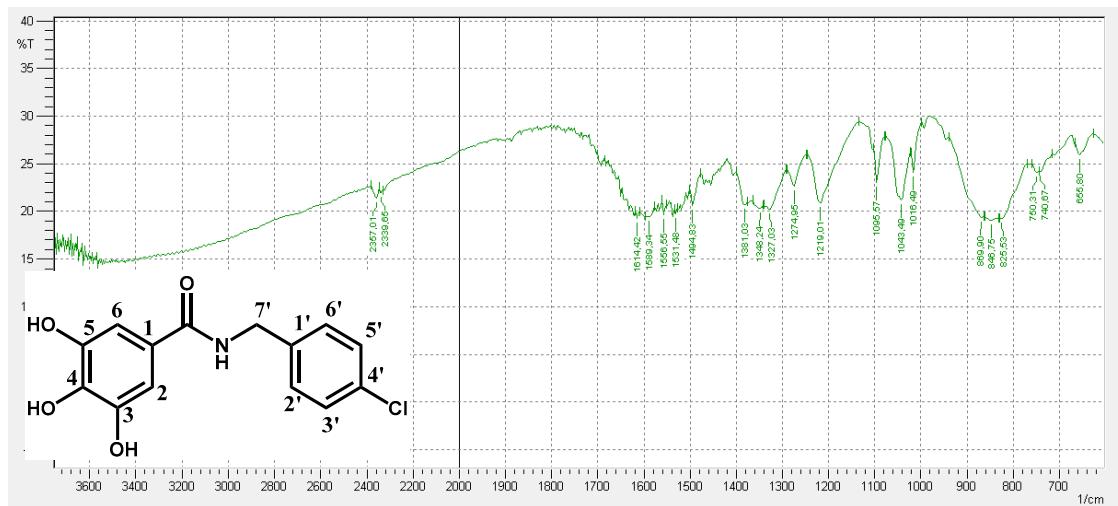
**Figure S10.**  $^{13}\text{C}$ -APT NMR spectrum of (*E*)-*N*-(4-chlorobenzyl)-3-(4-hydroxy-3-methoxyphenyl)acrylamide (**3**) ( $\text{DMSO}-d_6$ , 50 MHz).



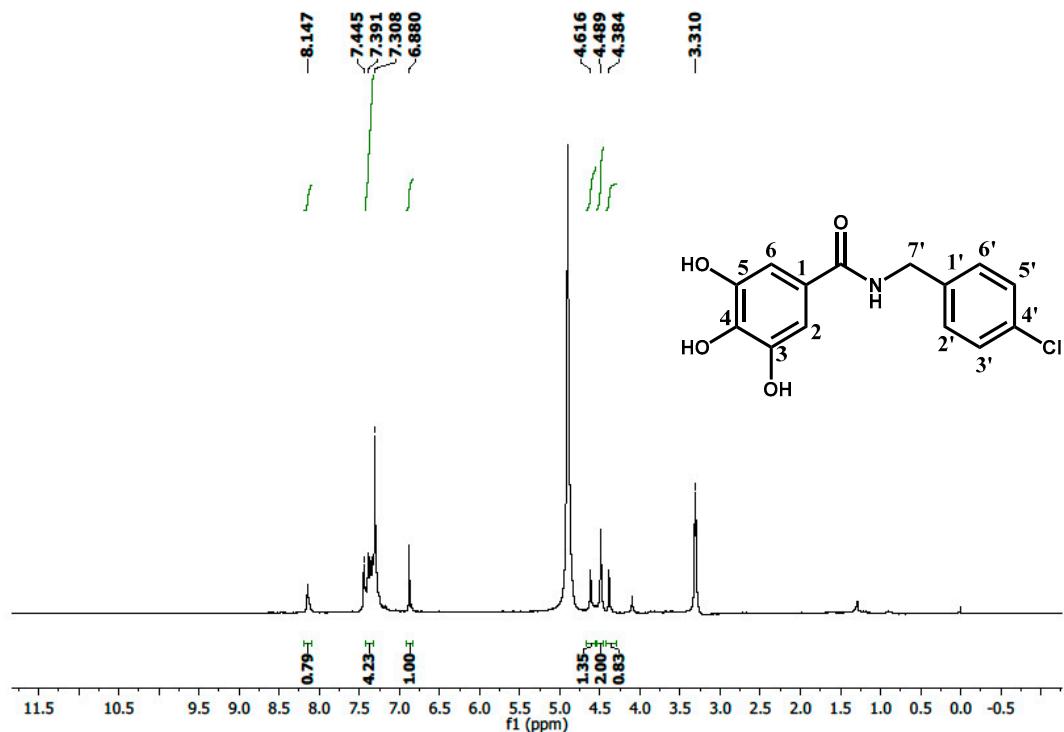
**Figure S11.** Expansion of the  $^{13}\text{C}$ -APT NMR spectrum of (*E*)-*N*-(4-chlorobenzyl)-3-(4-hydroxy-3-methoxyphenyl)acrylamide (**3**) ( $\text{DMSO}-d_6$ , 50 MHz).



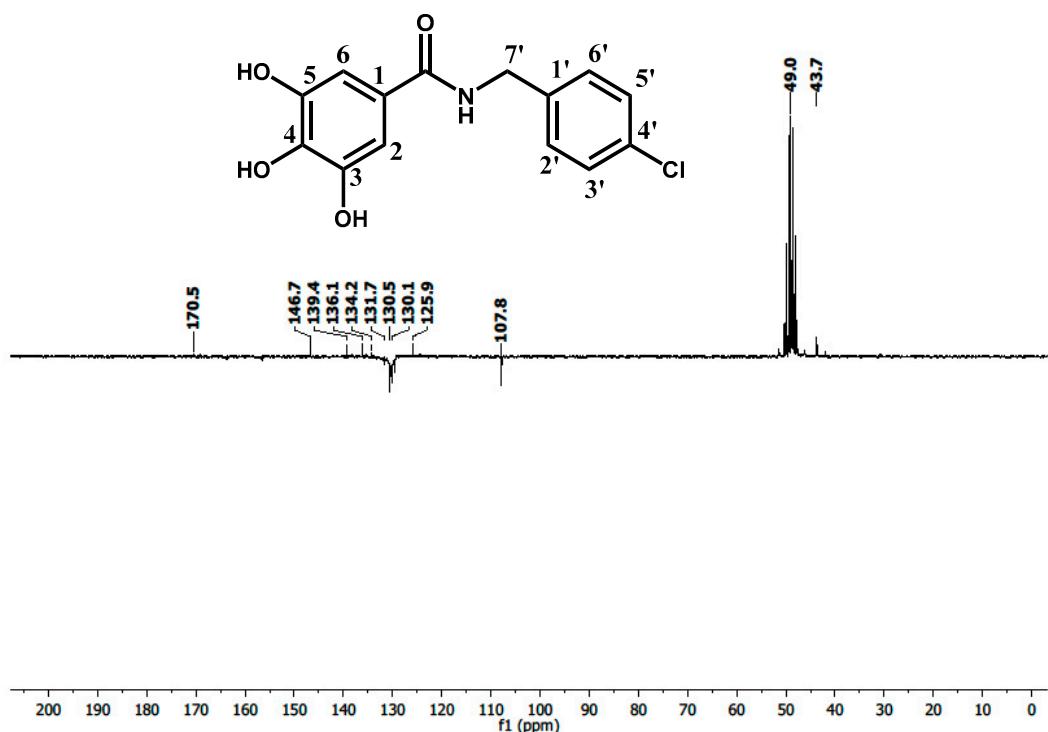
**Figure S12.** High resolution mass spectrum—MALDI of (*E*)-*N*-(4-chlorobenzyl)-3-(4-hydroxy-3-methoxyphenyl) (**3**).



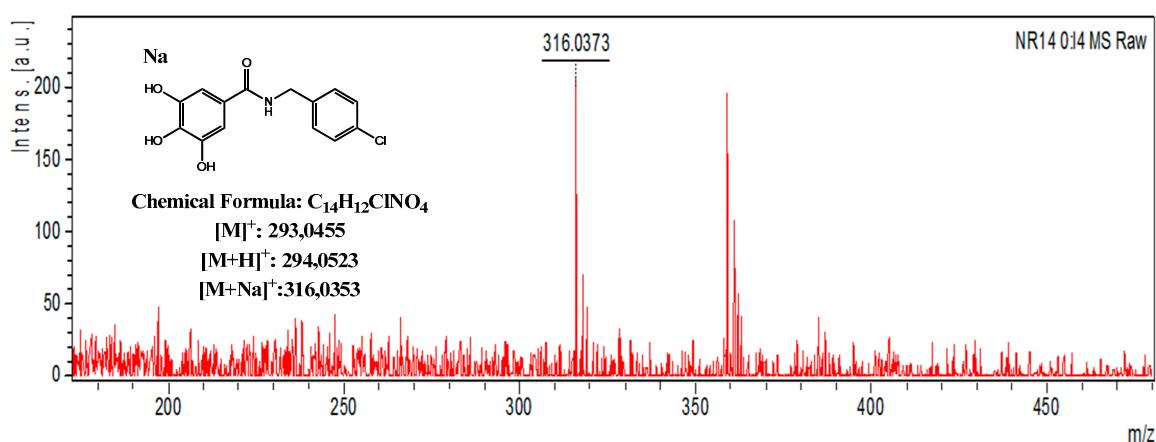
**Figure S13.** Infrared spectrum (KBr,  $\text{cm}^{-1}$ ) de *N*-(4-chlorobenzyl)-3,4,5-trihydroxybenzamide (**14**).



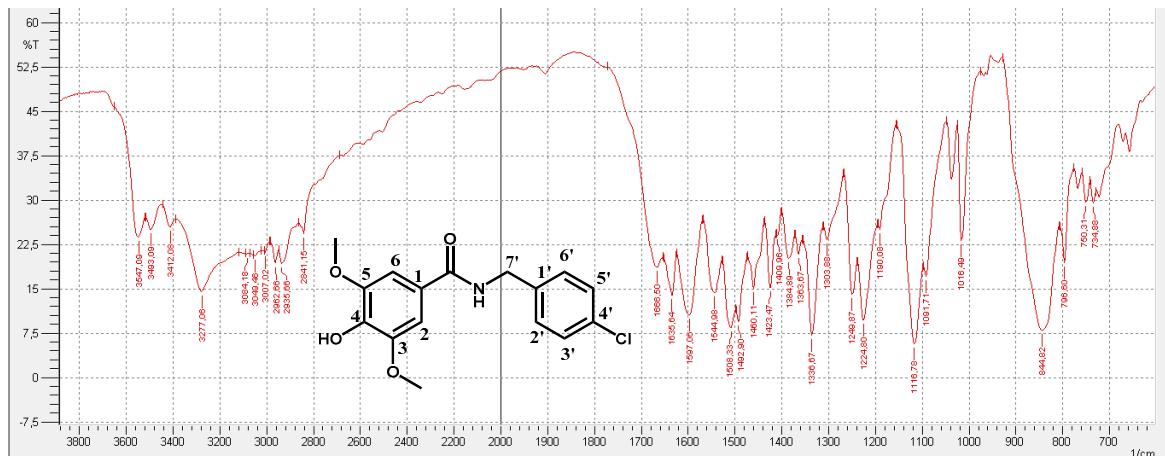
**Figure S14.** <sup>1</sup>H-NMR spectrum of *N*-(4-chlorobenzyl)-3,4,5-trihydroxybenzamide (**14**) (MeOD, 200 MHz).



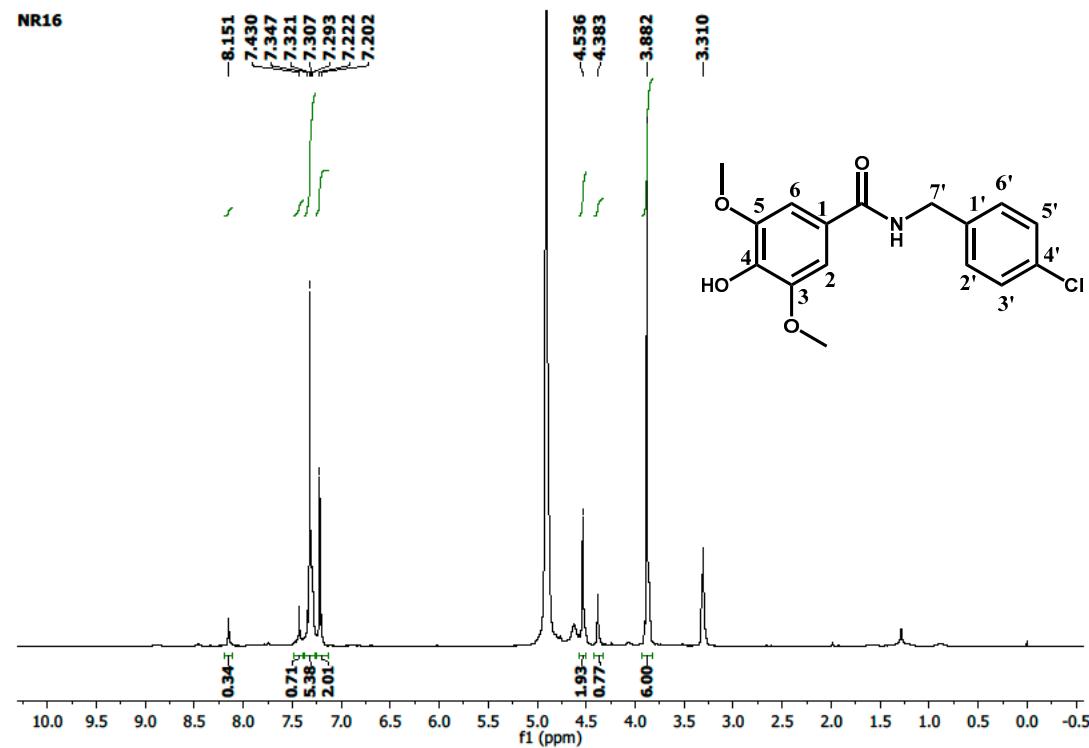
**Figure S15.**  $^{13}\text{C}$ -APT NMR spectrum of *N*-(4-chlorobenzyl)-3,4,5-trihydroxybenzamide (**14**) (MeOD, 50 MHz).



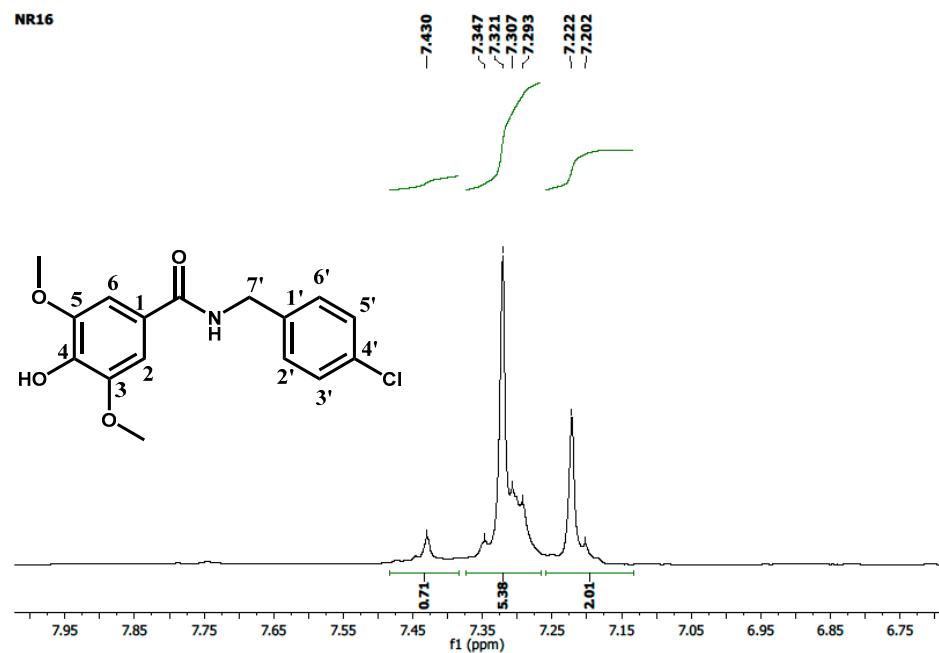
**Figure S16.** High resolution mass spectrum—MALDI of *N*-(4-chlorobenzyl)-3,4,5-trihydroxybenzamide (**14**).



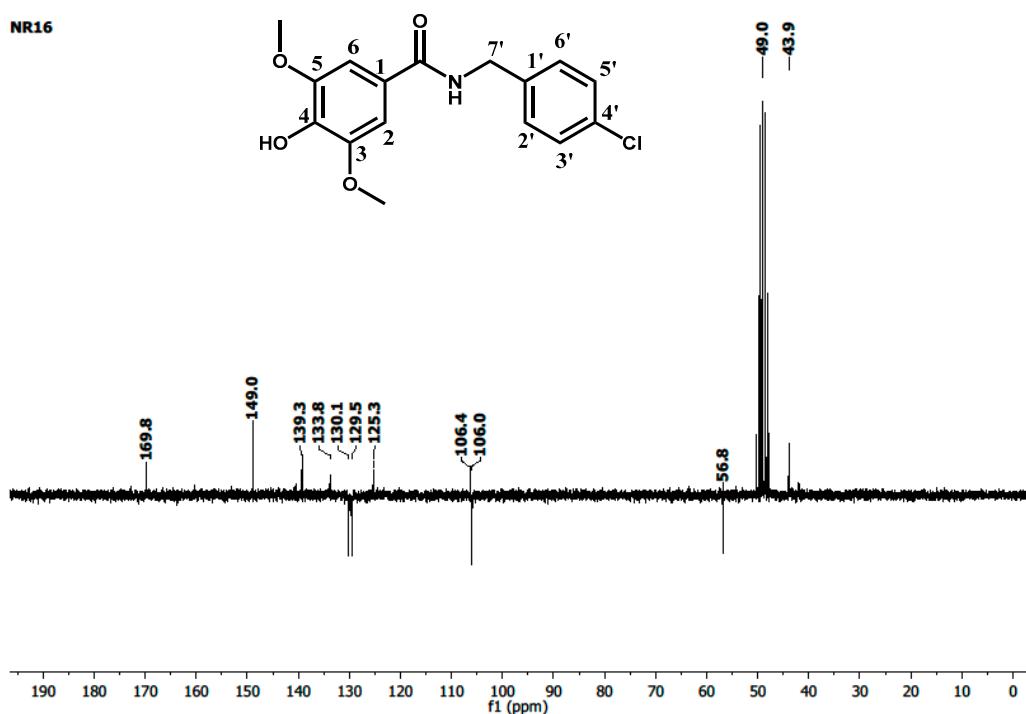
**Figure S17.** Infrared spectrum (KBr,  $\text{cm}^{-1}$ ) of *N*-(4-chlorobenzyl)-4-hydroxy-3,5-dimethoxybenzamide (**16**).



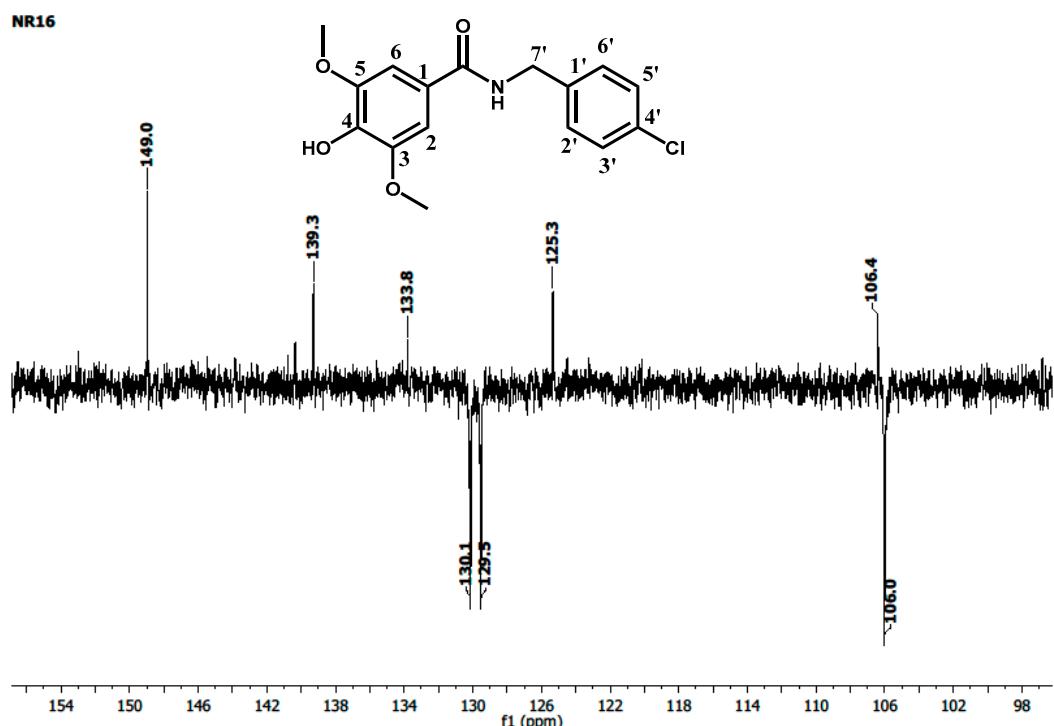
**Figure S18.** <sup>1</sup>H-NMR spectrum of *N*-(4-chlorobenzyl)-4-hydroxy-3,5-dimethoxybenzamide (**16**) ( $\text{DMSO}-d_6$ , 200 MHz).



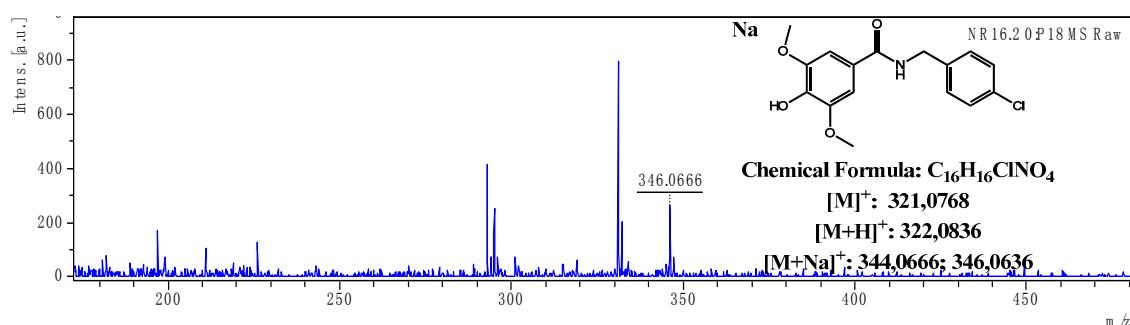
**Figure S19.** Expansion of the <sup>1</sup>H-NMR spectrum of *N*-(4-chlorobenzyl)-4-hydroxy-3,5-dimethoxybenzamide (**16**) (DMSO-*d*<sub>6</sub>, 200 MHz).



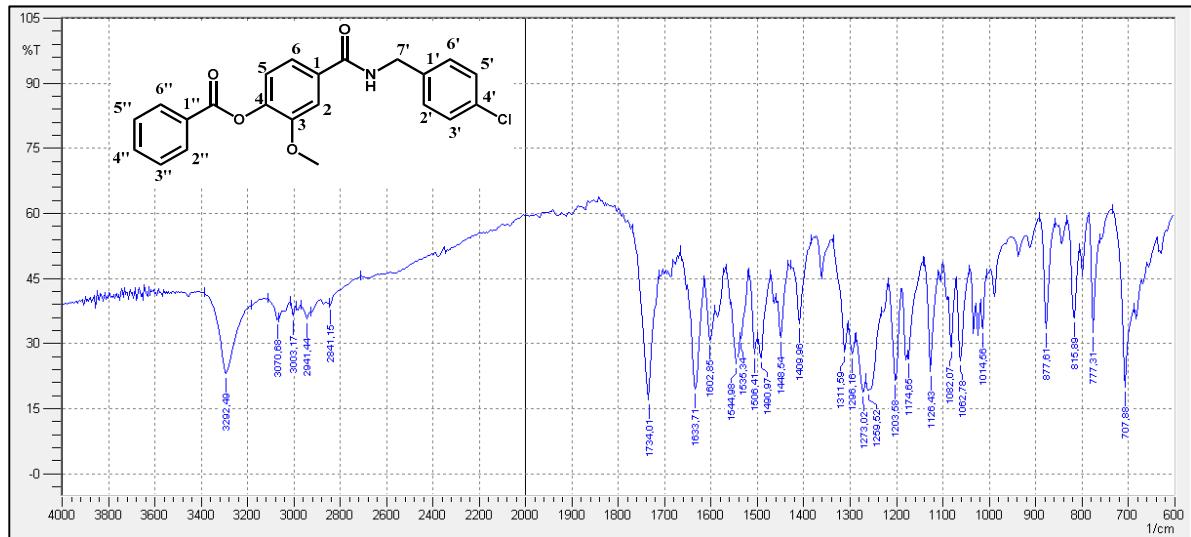
**Figure S20.** <sup>13</sup>C-APT NMR spectrum of *N*-(4-chlorobenzyl)-4-hydroxy-3,5-dimethoxybenzamide (**16**) (DMSO-*d*<sub>6</sub>, 50 MHz).



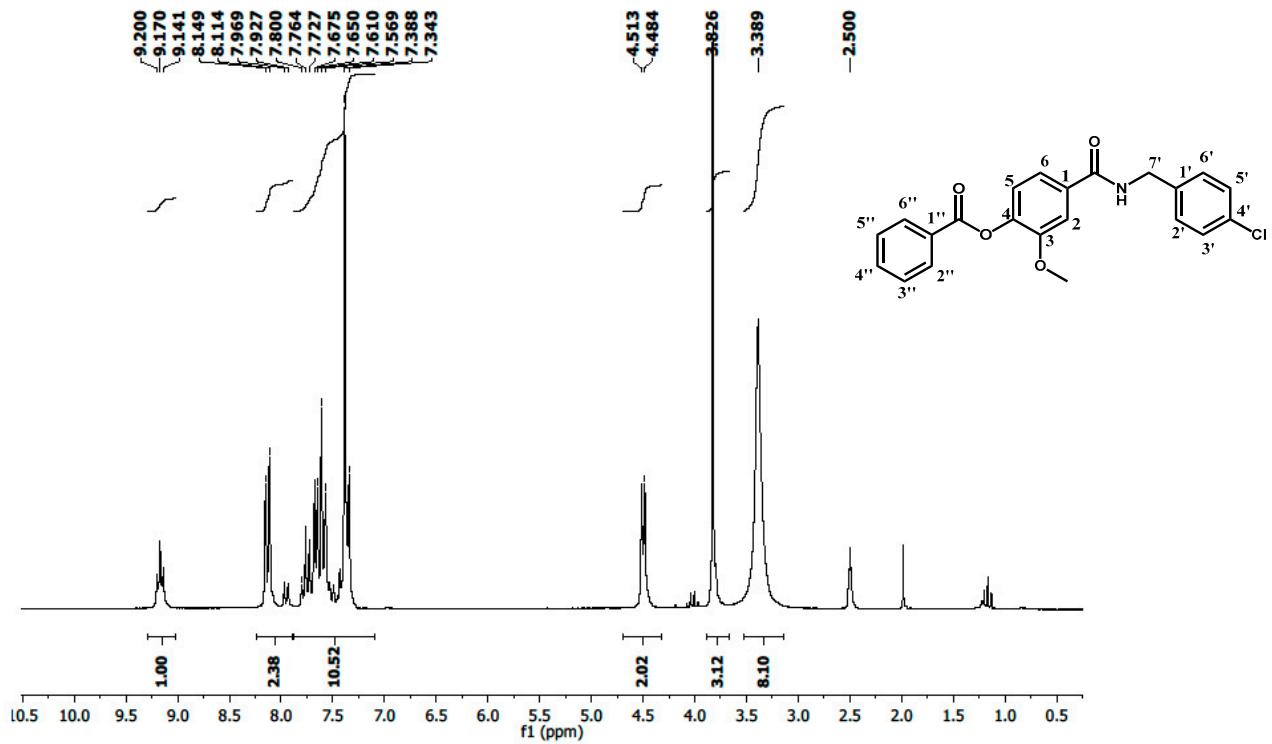
**Figure S21.** Expansion of the spectrum of  $^{13}\text{C}$ -APT NMR of *N*-(4-chlorobenzyl)-4-hydroxy-3,5-dimethoxybenzamide (**16**) (DMSO- $d_6$ , 50 MHz).



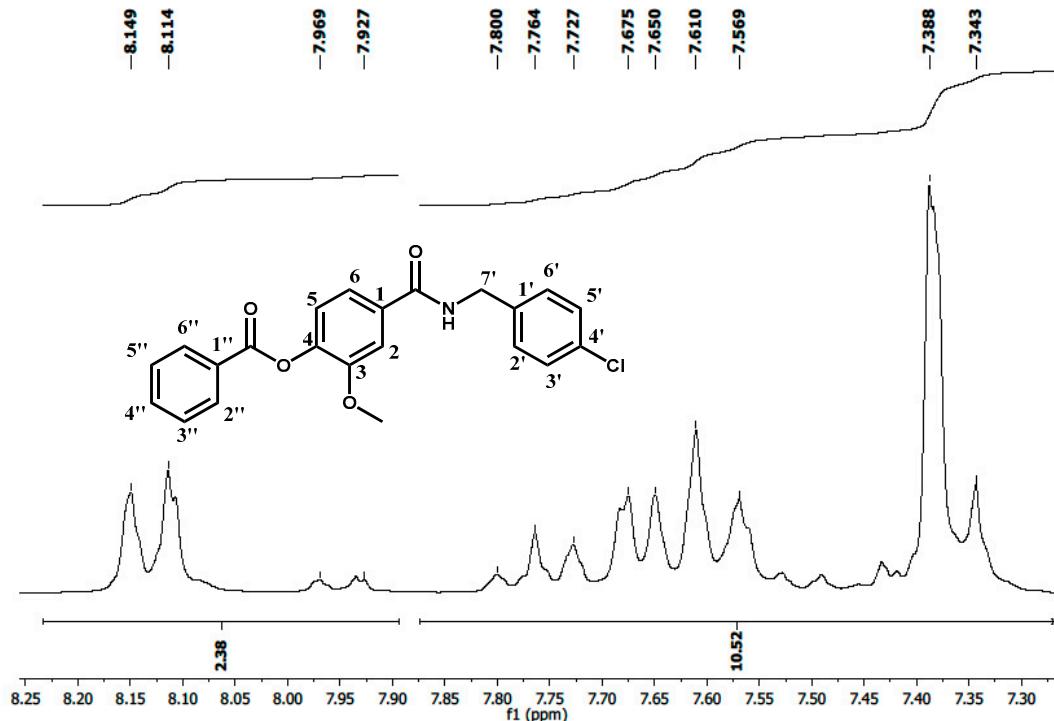
**Figure S22.** High resolution mass spectrum—MALDI of *N*-(4-chlorobenzyl)-4-hydroxy-3,5-dimethoxybenzamide (**16**).



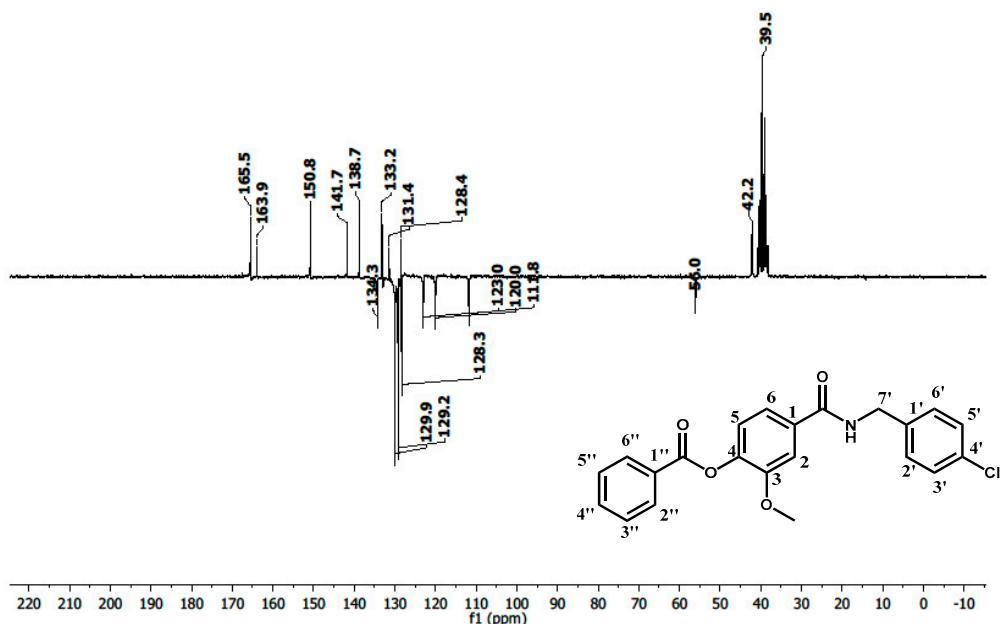
**Figure S23.** Infrared spectrum (KBr,  $\text{cm}^{-1}$ ) of 4-((4-chlorobenzyl) carbamoyl)-2-methoxyphenyl benzoate (23).



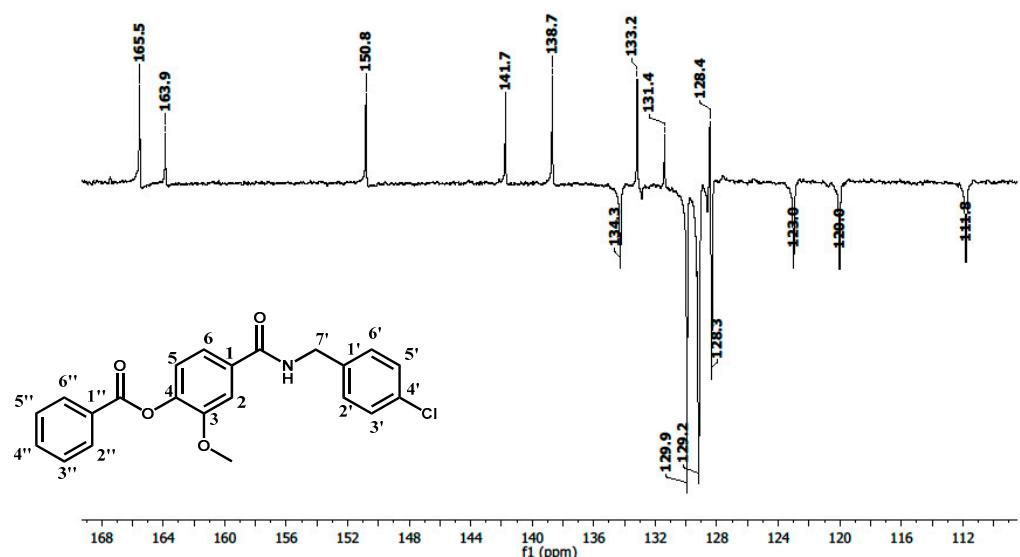
**Figure S24.**  $^1\text{H}$ -NMR spectrum of 4-((4-chlorobenzyl) carbamoyl)-2-methoxyphenyl benzoate (23) ( $\text{DMSO}-d_6$ , 200 MHz).



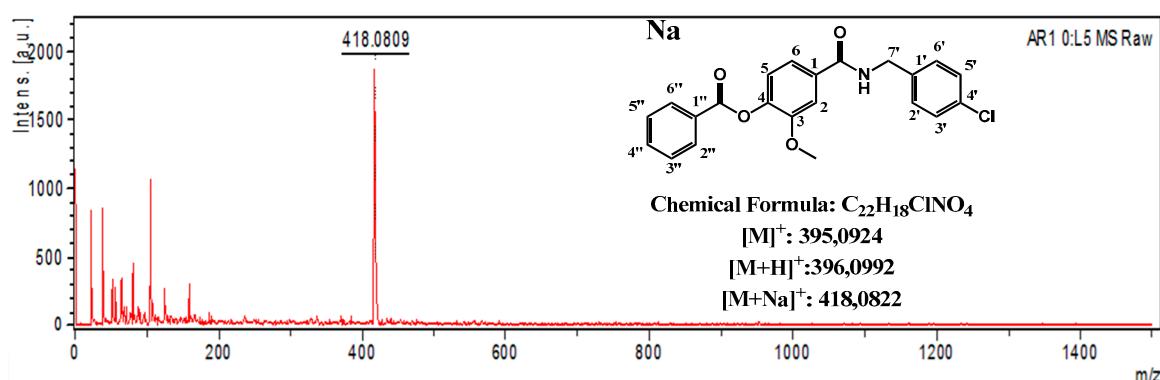
**Figure S25.** Expansion of the <sup>1</sup>H-NMR spectrum of 4-((4-chlorobenzyl) carbamoyl)-2-methoxyphenyl benzoate (**23**) (DMSO-*d*<sub>6</sub>, 200 MHz).



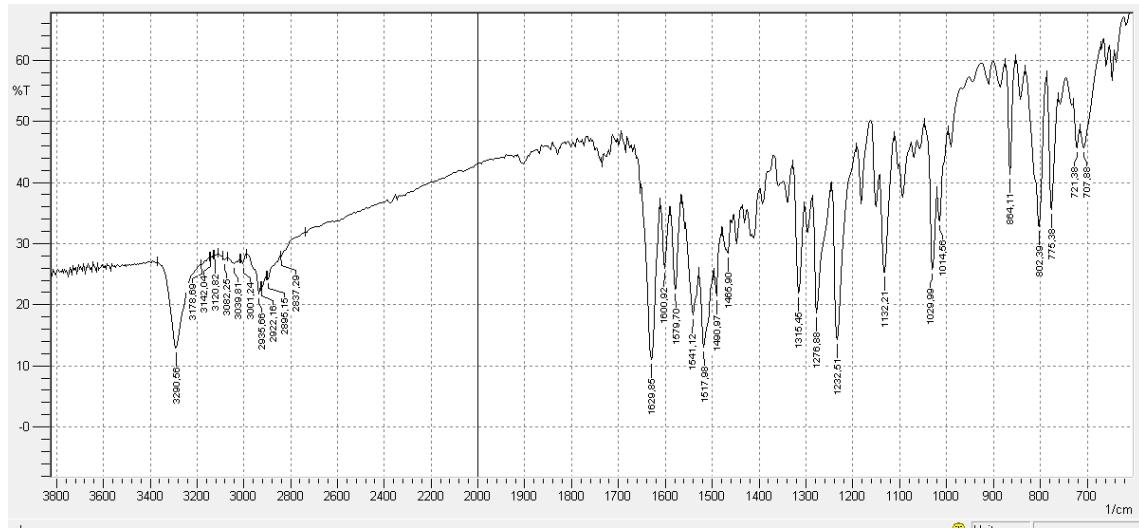
**Figure S26.** <sup>13</sup>C-APT NMR spectrum of 4-((4-chlorobenzyl) carbamoyl)-2-methoxyphenyl benzoate (**23**) (DMSO-*d*<sub>6</sub>, 50 MHz).



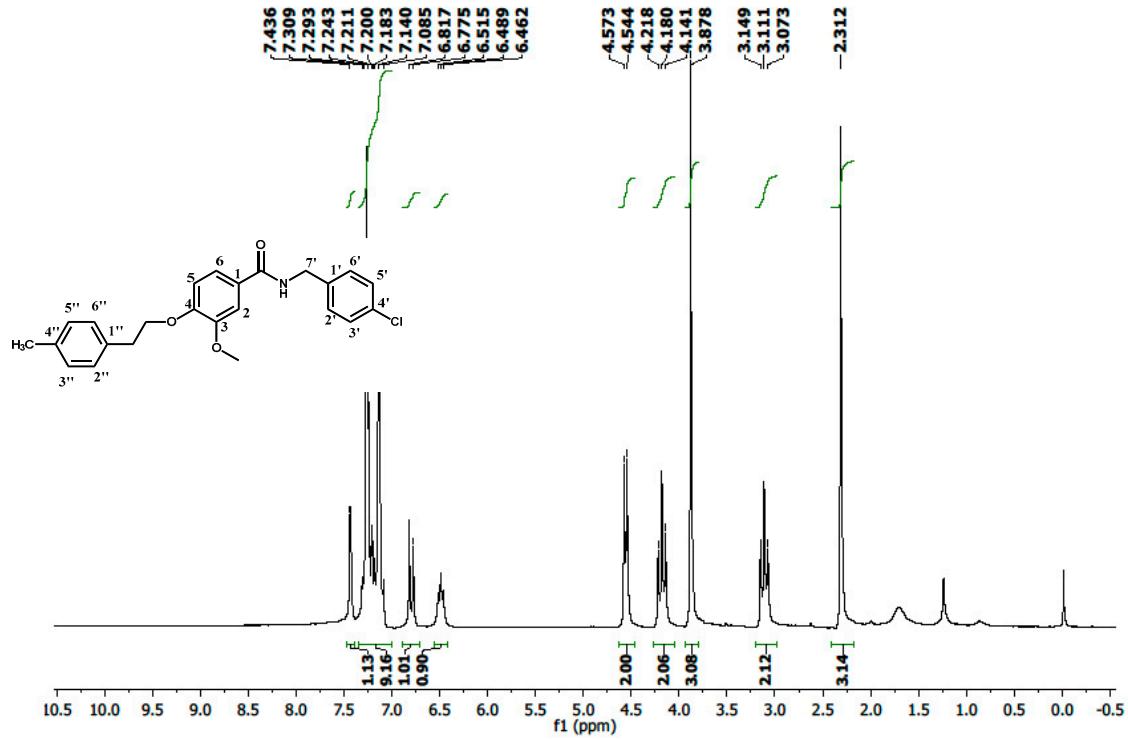
**Figure S27.** Expansion of the <sup>13</sup>C-APT NMR spectrum of 4-((4-chlorobenzyl) carbamoyl)-2-methoxyphenyl benzoate (**23**) (DMSO-*d*<sub>6</sub>, 50 MHz).



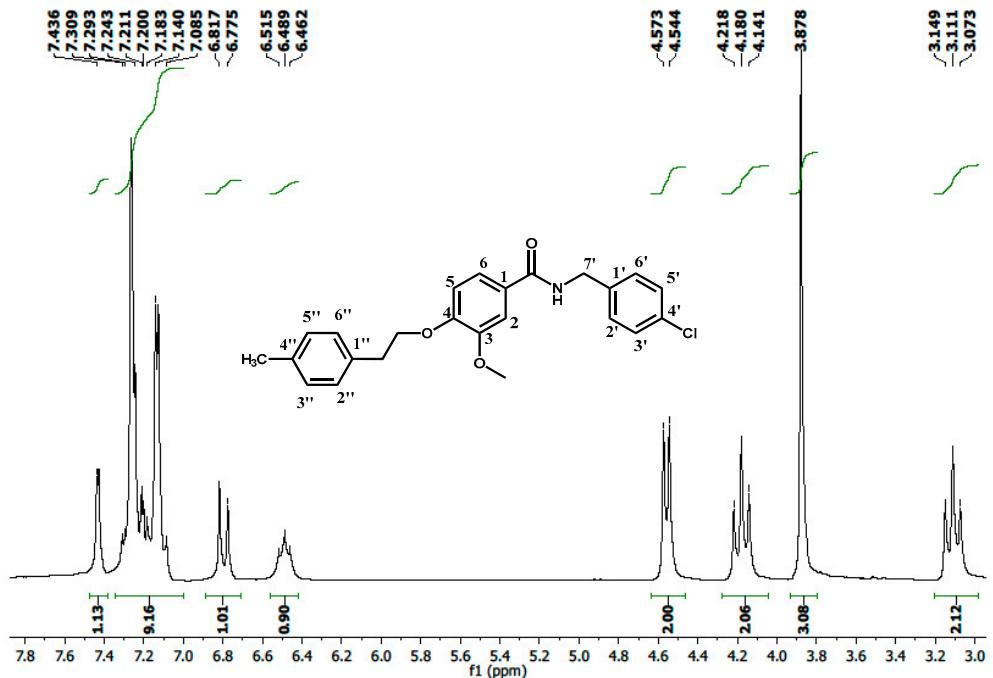
**Figure S28.** High resolution mass spectrum—MALDI of 4-((4-chlorobenzyl)carbamoyl)-2-methoxyphenyl benzoate (**23**).



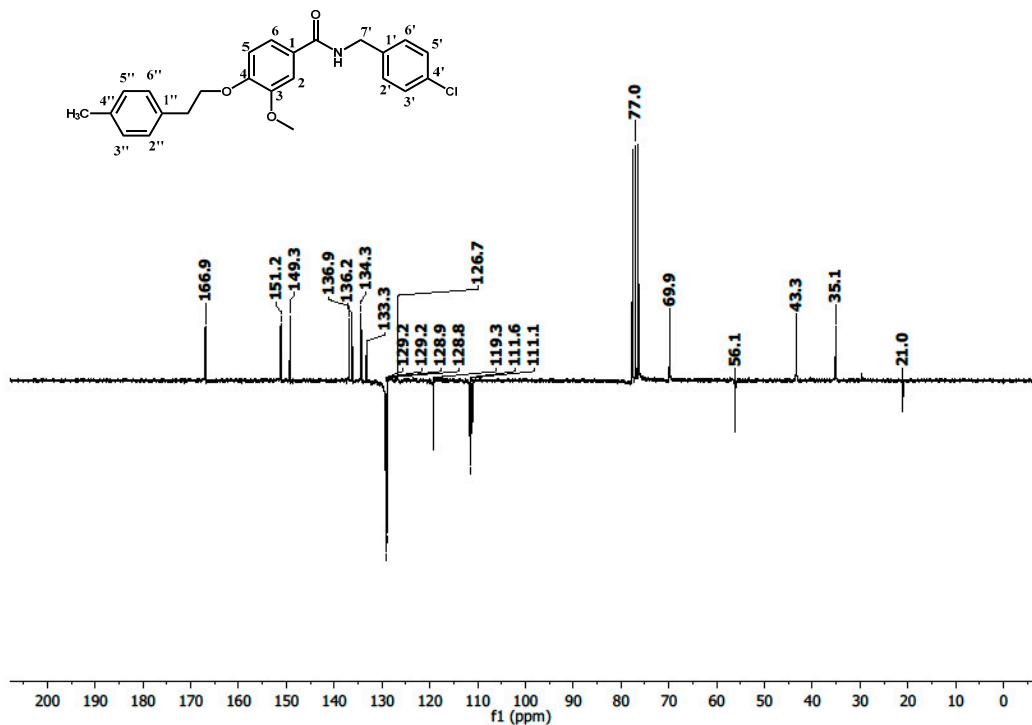
**Figure S29.** Infrared spectrum (KBr,  $\text{cm}^{-1}$ ) of *N*-(4-chlorobenzyl)-3-methoxy-4-(4-methylphenetoxy) (28).



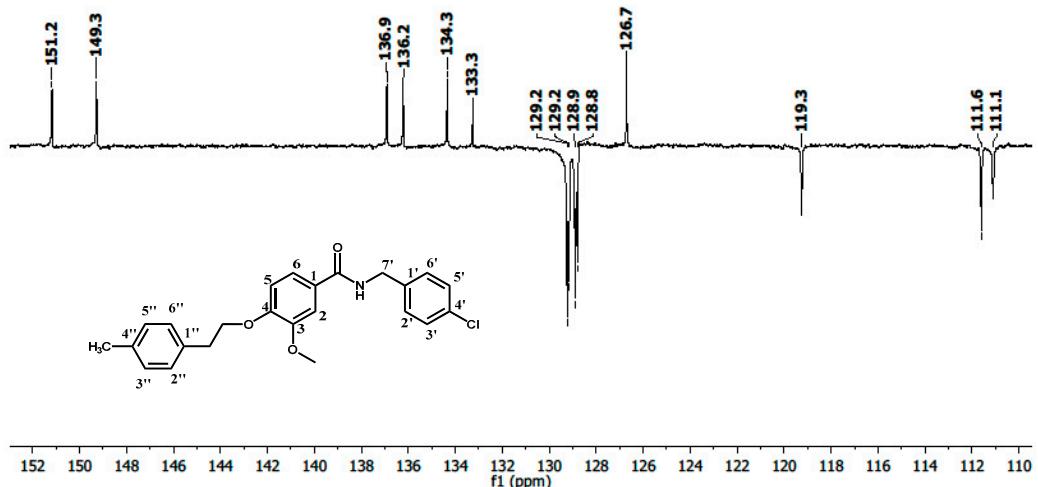
**Figure S30.**  $^1\text{H}$ -NMR spectrum of *N*-(4-chlorobenzyl)-3-methoxy-4-(4-methylphenetoxy) (28) ( $\text{CDCl}_3$ , 200 MHz).



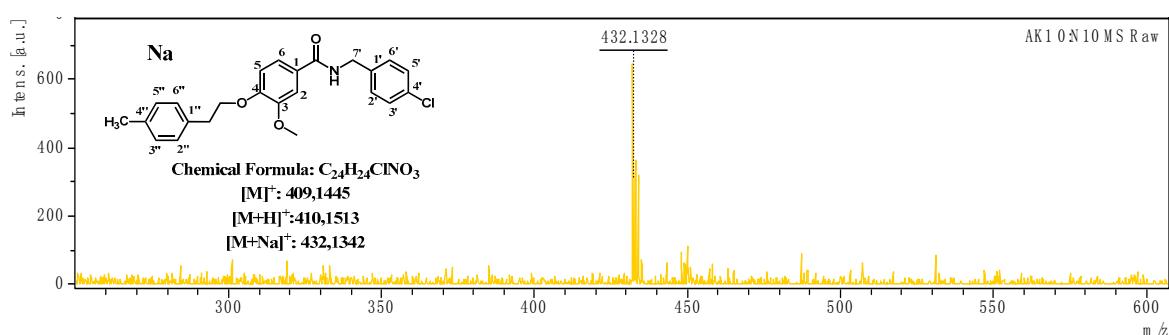
**Figure S31.** Expansion of the spectrum of <sup>1</sup>H NMR of *N*-(4-chlorobenzyl)-3-methoxy-4-(4-methylphenetoxy) (**28**) (CDCl<sub>3</sub>, 200 MHz).



**Figure S32.** <sup>13</sup>C-APT NMR spectrum of *N*-(4-chlorobenzyl)-3-methoxy-4-(4-methylphenetoxy) (**28**) (CDCl<sub>3</sub>, 50 MHz).



**Figure S33.** Expansion of the <sup>13</sup>C-APT NMR spectrum of *N*-(4-chlorobenzyl)-3-methoxy-4-(4-methylphenetoxy) (28) ( $\text{CDCl}_3$ , 50 MHz).



**Figure S34.** High resolution mass spectrum—MALDI of *N*-(4-chlorobenzyl)-3-methoxy-4-(4-methylphenetoxy) (28).