

Design, Synthesis and Evaluation of Novel Derivatives of Curcuminoids with Cytotoxicity

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(Total 1 pages include this cover page)

Supplementary Materials

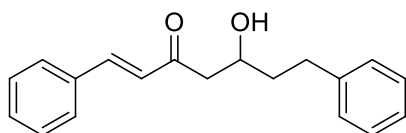
¹ H, ¹³ C NMR and mass for compound 1-24, 1a-7a, 12a, 14a, MD1-13.....	S2-19
¹ H, ¹³ C NMR spectra for compound 1-24, 1a-7a, 12a, 14a, MD1-13.....	S20-100

Supplementary Materials

Mass and ^1H and ^{13}C NMR data

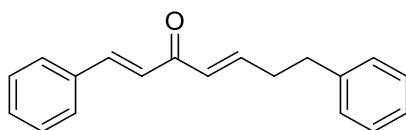
(E)-5-hydroxy-1,7-diphenylhept-1-en-3-one (1)

Reference compound [22]



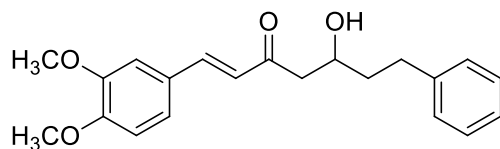
Known compound; white solid; yield 77.7%. ^1H NMR (500 MHz, CDCl_3) δ 7.49-7.46 (m, 3H), 7.34-7.32 (m, 3H), 7.21-7.11 (m, 5H), 6.63 (d, J = 15 Hz, 1H), 4.11-4.07 (m, 1H), 2.83-2.63 (m, 4H), 1.85-1.80 (m, 1H), 1.74-1.68 (m, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 201.0, 143.8, 142.1, 134.3, 131.0, 129.2, 128.6, 128.6, 126.4, 126.0, 67.3, 47.0, 38.3, 32.0; HRMS [ESI] $^+$ calculated for $\text{C}_{19}\text{H}_{21}\text{O}_2$: 281.1536 [M + H] $^+$; found: 281.1545.

(1E,4E)-1,7-diphenylhepta-1,4-dien-3-one (1a)



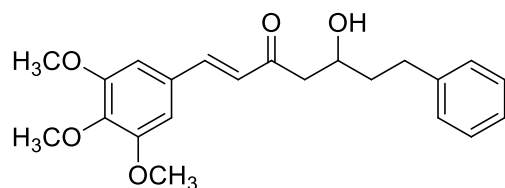
Known compound; yellow viscous oil; yield 90.2%. ^1H NMR (500 MHz, CD_3OD) δ 7.58-7.55 (m, 3H), 7.34-7.33 (m, 3H), 7.22-7.09 (m, 5H), 7.03-6.99 (m, 2H), 6.43 (d, J = 15 Hz, 1H), 2.76 (t, J = 7.5 Hz, 2H), 2.57-2.53 (m, 2H); ^{13}C NMR (125 MHz, CD_3OD) δ 191.8, 149.4, 145.2, 142.5, 136.3, 131.8, 130.8, 130.2, 129.7, 129.6, 129.6, 127.3, 125.9, 35.7, 35.6. HRMS [ESI] $^+$ calculated for $\text{C}_{19}\text{H}_{19}\text{O}$: 263.1430 [M + H] $^+$; found: 263.1429.

(E)-1-(3,4-dimethoxyphenyl)-5-hydroxy-7-phenylhept-1-en-3-one (2)



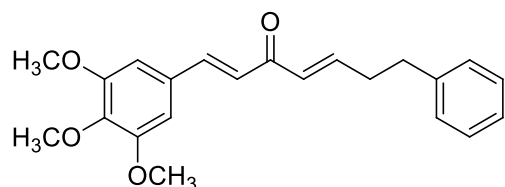
Yellowish powder; yield 80.3%; m.p.: 66.6-67.5 $^{\circ}\text{C}$. ^1H NMR (500 MHz, CD_3OD) δ 7.47 (d, J = 15 Hz, 1H), 7.17-7.04 (m, 7H), 6.84 (d, J = 5 Hz, 1H), 6.63 (d, J = 15 Hz, 1H), 4.08-4.03 (m, 1H), 3.75 (s, 6H), 2.82-2.78 (m, 1H), 2.71-2.59 (m, 2H), 2.58-2.56 (m, 1H), 1.74-1.71 (m, 2H); ^{13}C NMR (125 MHz, CD_3OD) δ 201.8, 153.2, 150.8, 145.3, 143.5, 129.3, 129.0, 126.9, 125.7, 124.7, 112.7, 111.8, 68.9, 56.6, 56.5, 49.1, 40.4, 33.0. HRMS [ESI] $^+$ calculated for $\text{C}_{21}\text{H}_{25}\text{O}_4$: 341.1747 [M + H] $^+$; found: 341.1757.

(E)-5-hydroxy-7-phenyl-1-(3,4,5-trimethoxyphenyl)hept-1-en-3-one (3)



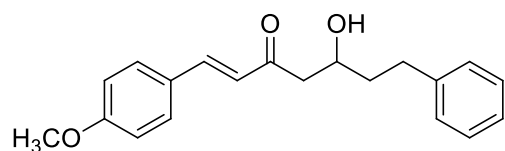
Yellow viscous oil; yield 74.3%. ^1H NMR (500 MHz, CD_3OD) δ 7.47 (d, J = 15 Hz, 1H), 7.17-7.11 (m, 4H), 7.08-7.04 (m, 1H), 6.82 (s, 1H), 6.69 (d, J = 15 Hz, 1H), 4.09-4.04 (m, 1H), 3.75 (s, 6H), 3.69 (s, 3H), 2.82-2.78 (m, 1H), 2.72-2.67 (m, 2H), 2.61-2.55 (m, 1H), 1.73-1.69 (m, 2H); ^{13}C NMR (125 MHz, CD_3OD) δ 201.7, 154.9, 145.1, 143.5, 141.6, 131.8, 129.6, 129.5, 127.2, 126.9, 107.1, 68.8, 61.3, 56.8, 49.1, 40.5, 33.0. HRMS $[\text{ESI}]^+$ calculated for $\text{C}_{22}\text{H}_{27}\text{O}_5$: 371.1853 $[\text{M} + \text{H}]^+$; found: 371.1862.

(1E,4E)-7-phenyl-1-(3,4,5-trimethoxyphenyl)hepta-1,4-dien-3-one (3a)



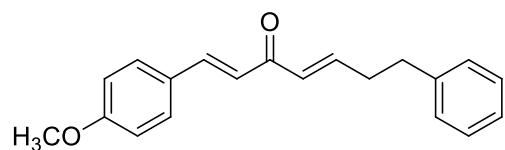
Yellow oil; yield 86.5%. ^1H NMR (500 MHz, CD_3OD) δ 7.52 (d, J = 15 Hz, 1H), 7.22-6.91 (m, 9H), 6.45 (d, J = 15 Hz, 1H), 3.82 (s, 6H), 3.73 (s, 3H), 2.79-2.76 (m, 2H), 2.61-2.54 (m, 2H); ^{13}C NMR (125 MHz, CD_3OD) δ 191.8, 155.0, 149.3, 145.4, 132.1, 130.9, 129.7, 129.6, 127.3, 125.3, 107.3, 61.4, 56.9, 35.8, 35.7. HRMS $[\text{ESI}]^+$ calculated for $\text{C}_{22}\text{H}_{25}\text{O}_4$: 353.1747 $[\text{M} + \text{H}]^+$; found: 353.1746.

(E)-5-hydroxy-1-(4-methoxyphenyl)-7-phenylhept-1-en-3-one (4)



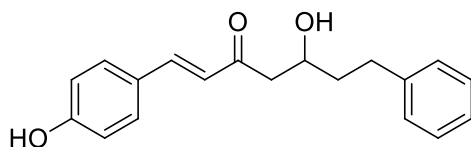
Yellow oil; yield 83.2%. ^1H NMR (500 MHz, CD_3OD) δ 7.51-7.46 (m, 3H), 7.17-7.10 (m, 4H), 7.06-7.03 (m, 1H), 6.85 (d, J = 5 Hz, 2H), 6.62 (d, J = 15 Hz, 1H), 4.78-4.01 (m, 1H), 3.72 (s, 3H), 2.81-2.77 (m, 1H), 2.74-2.67 (m, 2H), 2.61-2.55 (m, 1H), 1.76-1.73 (m, 2H); ^{13}C NMR (125 MHz, CD_3OD) δ 201.9, 163.5, 145.1, 143.5, 131.5, 129.6, 129.5, 128.6, 126.9, 125.4, 115.6, 68.9, 56.0, 48.9, 40.4, 33.0. HRMS $[\text{ESI}]^+$ calculated for $\text{C}_{20}\text{H}_{23}\text{O}_3$: 311.1642 $[\text{M} + \text{H}]^+$; found: 311.1651.

(1E,4E)-1-(4-methoxyphenyl)-7-phenylhepta-1,4-dien-3-one (4a)



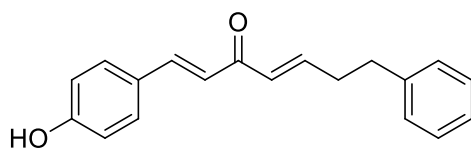
Yellow solid; yield 88.7%; m.p.: 55-54 °C. ¹H NMR (500 MHz, CD₃OD) δ 7.55-7.51 (m, 3H), 7.21-7.08 (m, 5H), 6.99-6.85 (m, 4H), 6.42 (d, *J* = 15 Hz, 1H), 3.75 (s, 3H), 2.76-2.73 (m, 2H), 2.55-2.50 (m, 2H); ¹³C NMR (125 MHz, CD₃OD) δ 191.9, 163.6, 148.8, 145.4, 142.5, 131.6, 130.8, 129.6, 129.6, 128.9, 127.3, 123.6, 115.7, 56.1, 35.7, 35.7. HRMS [ESI]⁺ calculated for C₂₀H₂₁O₂: 293.1536 [M + H]⁺; found: 293.1533.

(E)-5-hydroxy-1-(4-hydroxyphenyl)-7-phenylhept-1-en-3-one (5)



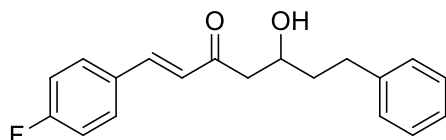
Yellow solid; yield 78.6%; m.p. 111-112 °C. NMR (500 MHz, CD₃OD) δ 7.45 (d, *J* = 15 Hz, 1H), 7.36-7.34 (m, 2H), 7.14-7.07 (m, 4H), 7.03-7.01 (m, 1H), 6.72 (d, *J* = 10 Hz, 2H), 6.54 (d, *J* = 15 Hz, 1H), 4.77 (brs, 2H), 4.04-3.99 (m, 1H), 2.78-2.72 (m, 1H), 2.70-2.62 (m, 2H), 2.59-2.53 (m, 1H), 1.71-1.66 (m, 2H); ¹³C NMR (125 MHz, CD₃OD) δ 202.0, 161.7, 145.7, 143.5, 131.8, 129.6, 129.6, 127.4, 127.0, 124.7, 117.1, 69.0, 48.8, 40.4, 33.1. HRMS [ESI]⁺ calculated for C₁₉H₁₉O₃: 295.1329 [M + H]⁺; found: 295.1339.

(1E,4E)-1-(4-hydroxyphenyl)-7-phenylhepta-1,4-dien-3-one (5a)



Yellow solid; yield 81.5%; m.p.: 130.1-131.3 °C. NMR (500 MHz, CD₃OD) δ 7.51 (d, *J* = 15 Hz, 1H), 7.43 (d, *J* = 5 Hz, 2H), 7.20-7.07 (m, 5H), 6.97-6.93 (m, 1H), 6.81 (d, *J* = 15 Hz, 1H), 6.72 (d, *J* = 5 Hz, 2H), 6.41 (d, *J* = 15 Hz, 1H), 2.76-2.73 (m, 2H), 2.54-2.50 (m, 2H); ¹³C NMR (125 MHz, CD₃OD) δ 192.0, 161.8, 148.6, 145.9, 142.5, 131.8, 129.6, 129.6, 127.7, 127.3, 122.8, 117.1, 35.7, 35.7. HRMS [ESI]⁺ calculated for C₁₉H₁₇O₂: 277.1223 [M + H]⁺; found: 277.1223.

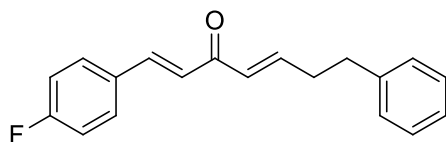
(E)-1-(4-fluorophenyl)-5-hydroxy-7-phenylhept-1-en-3-one (6)



Yellow solid; yield 73.5%; m.p.: 100.9-101.8 °C. NMR (500 MHz, CD₃OD) δ 7.59-7.57 (m, 2H), 7.52 (d, *J* = 15 Hz, 1H), 7.17-7.11 (m, 4H), 7.07-7.04 (m, 3H), 6.71 (d, *J* = 15 Hz, 1H), 4.07-4.02 (m, 1H), 2.84-2.79 (m, 1H), 2.75-2.69 (m, 2H), 2.63-2.57 (m, 1H), 1.75-1.68 (m, 2H); ¹³C NMR (125

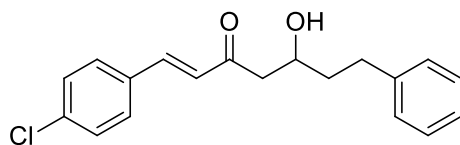
MHz, CD₃OD) δ 201.7, 166.7, 164.7, 143.6, 143.5, 132.6, 132.6, 131.9, 131.8, 129.6, 129.5, 127.7, 127.0, 117.2, 117.0, 68.8, 49.1, 40.5, 33.0. HRMS [ESI]⁺ calculated for C₁₉H₂₀O₂F: 299.1442 [M + H]⁺; found: 299.1452.

(1E,4E)-1-(4-fluorophenyl)-7-phenylhepta-1,4-dien-3-one (6a)



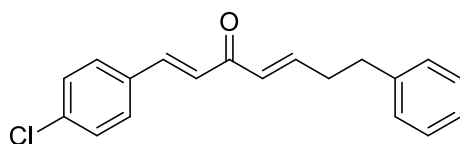
Yellow oil; yield 77.8%. NMR (500 MHz, CD₃OD) δ 7.62-7.59 (m, 2H), 7.53 (d, *J* = 10 Hz, 1H), 7.21-6.94 (m, 9H), 6.41 (d, *J* = 15 Hz, 1H), 2.76-2.73 (m, 2H), 2.55-2.51 (m, 2H); ¹³C NMR (125 MHz, CD₃OD) δ 191.6, 166.6, 164.7, 149.5, 143.8, 142.5, 132.7, 131.9, 131.9, 130.8, 129.6, 127.3, 125.7, 117.2, 117.0, 35.7, 35.6. HRMS [ESI]⁺ calculated for C₁₉H₁₈OF: 281.1336 [M + H]⁺; found: 281.1346.

(E)-1-(4-chlorophenyl)-5-hydroxy-7-phenylhept-1-en-3-one (7).



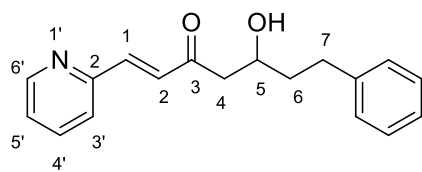
Yellow solid; yield 75.8%; m.p.: 85-85.9 °C. NMR (500 MHz, CD₃OD) δ 7.50-7.46 (m, 3H), 7.3 (d, *J* = 15 Hz, 2H), 7.20-7.10 (m, 4H), 7.06-7.03 (m, 1H), 6.73 (d, *J* = 15 Hz, 1H), 4.07-4.02 (m, 1H), 2.83-2.79 (m, 1H), 2.73-2.68 (m, 2H), 2.62-2.57 (m, 1H), 1.74-1.69 (m, 2H); ¹³C NMR (125 MHz, CD₃OD) δ 201.5, 143.5, 143.3, 137.5, 134.8, 131.1, 130.3, 129.6, 129.5, 128.4, 126.9, 68.7, 49.2, 40.4, 33.0. HRMS [ESI]⁺ calculated for C₁₉H₂₀O₂Cl: 315.1146 [M + H]⁺; found: 315.1154.

(1E,4E)-1-(4-chlorophenyl)-7-phenylhepta-1,4-dien-3-one (7a)



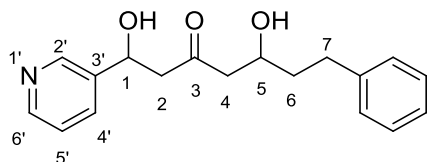
Yellow oil; yield 80.2 %. NMR (500 MHz, CD₃OD) δ 7.54-7.48 (m, 3H), 7.32-7.30 (d, *J* = 5 Hz, 2H), 7.19-7.16 (m, 2H), 7.13-7.06 (m, 3H), 7.02-6.96 (m, 2H), 6.39 (d, *J* = 15 Hz, 1H), 2.75-2.72 (m, 2H), 2.54-2.49 (m, 2H); ¹³C NMR (125 MHz, CD₃OD) δ 191.5, 149.7, 143.5, 142.4, 137.5, 135.0, 131.1, 130.8, 130.4, 129.6, 127.3, 126.5, 35.7, 35.6. HRMS [ESI]⁺ calculated for C₁₉H₁₈OCl: 297.1041 [M + H]⁺; found: 297.1048.

(E)-5-hydroxy-7-phenyl-1-(pyridin-2-yl)hept-1-en-3-one (8)



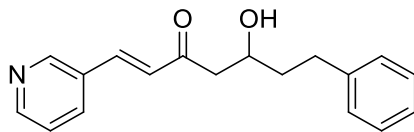
Colorless oil; yield 57%. ^1H NMR (500 MHz, CD_3OD) δ 8.49-8.48 (m, 1H), 7.76-7.73 (m, 1H), 7.57 (d, J = 5 Hz, 1H), 7.49 (d, J = 15 Hz, 1H), 7.30-7.27 (m, 1H), 7.15-7.08 (m, 1H), 7.05-7.01 (m, 7H), 4.09-4.02 (m, 1H), 2.86-2.81 (m, 1H), 2.76-2.67 (m, 2H), 2.61-2.56 (m, 1H), 1.73-1.68 (m, 2H); ^{13}C NMR (125 MHz, CD_3OD) δ 201.5, 154.5, 151.1, 143.5, 142.68, 139.0, 131.5, 129.6, 129.5, 126.9, 126.1, 126.0, 68.6, 49.5, 40.5, 33.1. HRMS $[\text{ESI}]^+$ calculated for $\text{C}_{18}\text{H}_{20}\text{NO}_2$: 282.1489 $[\text{M} + \text{H}]^+$; found: 282.1496.

1,5-dihydroxy-7-phenyl-1-(pyridin-3-yl)heptan-3-one (9)



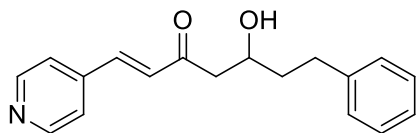
Yellow oil; yield 62.8%. ^1H NMR (500 MHz, CDCl_3) δ 8.64-8.57 (m, 2H), 7.79 (d, J = 10.0 Hz, 1H), 7.43-7.40 (m, 1H), 7.23-7.18 (m, 2H), 7.13-7.10 (m, 3H), 4.67-4.64 (m, 1H), 3.72-3.69 (m, 1H), 2.97-2.80 (brs, 2H), 2.79-2.77 (m, 1H), 2.75-2.69 (m, 1H), 2.63-2.60 (m, 1H), 2.47-2.33 (m, 3H), 2.06-2.02 (m, 1H), 1.88-1.85 (m, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 205.0, 147.1, 145.3, 141.0, 135.3, 128.5, 128.3, 126.1, 124.3, 76.7, 76.5, 48.8, 47.4, 37.6, 31.4. HRMS $[\text{ESI}]^+$ calculated for $\text{C}_{18}\text{H}_{22}\text{NO}_3$: 300.1594 $[\text{M} + \text{H}]^+$; found: 300.1600.

(E)-5-hydroxy-7-phenyl-1-(pyridin-3-yl)hept-1-en-3-one (10)



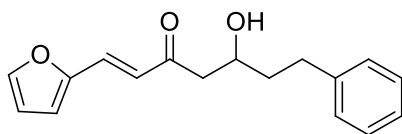
Yellow oil; yield 62.8%. ^1H NMR (500 MHz, CD_3OD) δ 8.62 (d, J = 5.0 Hz, 1H), 8.42 (d, J = 5.0 Hz, 1H), 7.96 (d, J = 5 Hz, 1H), 7.52-7.48 (m, 1H), 7.34-7.31 (m, 1H), 7.14-7.08 (m, 4H), 7.04-7.01 (m, 1H), 6.84 (d, J = 15.0 Hz, 1H), 4.78-4.03 (m, 1H), 2.85-2.81 (m, 1H), 2.74-2.67 (m, 2H), 2.60-2.54 (m, 1H), 1.75-1.68 (m, 2H); ^{13}C NMR (125 MHz, CD_3OD) δ 201.0, 151.5, 150.6, 143.4, 140.3, 136.6, 132.6, 129.6, 129.5, 126.9, 125.6, 68.6, 49.4, 40.4, 33.04. HRMS $[\text{ESI}]^+$ calculated for $\text{C}_{18}\text{H}_{20}\text{NO}_2$: 282.1489 $[\text{M} + \text{H}]^+$; found: 282.1493.

(E)-5-hydroxy-7-phenyl-1-(pyridin-4-yl)hept-1-en-3-one (11)



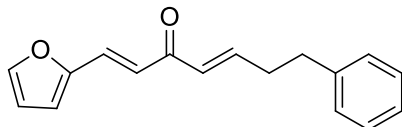
Yellow oil; yield 66.6%. ^1H NMR (500 MHz, CD_3OD) δ 8.45 (d, J = 5 Hz, 2H), 7.54-7.42 (m, 3H), 7.45-7.42 (m, 2H), 7.15-7.08 (m, 3H), 7.04-7.01 (m, 1H), 6.93 (d, J = 15 Hz, 1H), 4.78-4.02 (m, 1H), 2.85-2.81 (m, 1H), 2.75-2.67 (m, 2H), 2.60-2.54 (m, 1H), 1.73-1.68 (m, 2H); ^{13}C NMR (125 MHz, CD_3OD) δ 200.9, 151.0, 144.7, 143.5, 140.7, 133.9, 133.2, 133.1, 132.3, 130.1, 130.1, 129.6, 129.5, 127.0, 123.9, 68.5, 49.5, 40.5, 33.0. HRMS $[\text{ESI}]^+$ calculated for $\text{C}_{18}\text{H}_{20}\text{O}_2\text{N}$: 282.1483 $[\text{M} + \text{H}]^+$; found: 282.1489.

(*E*)-1-(furan-2-yl)-5-hydroxy-7-phenylhept-1-en-3-one (12)



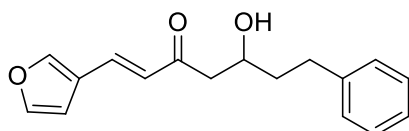
Yellowish solid; yield 63%; m.p.: 55-56 °C. ^1H NMR (500 MHz, CD_3OD) δ 7.57 (s, 1H), 7.33 (d, J = 15 Hz, 1H), 7.19-7.12 (m, 4H), 7.08-7.05 (m, 1H), 6.75 (d, J = 5 Hz, 1H), 6.56 (d, J = 15 Hz, 1H), 6.49-6.48 (m, 1H), 4.05-4.01 (m, 1H), 2.80-2.57 (m, 4H), 1.75-1.69 (m, 2H); ^{13}C NMR (125 MHz, CD_3OD) δ 201.4, 152.6, 147.0, 143.5, 131.2, 129.6, 129.5, 126.9, 124.9, 117.7, 113.9, 68.9, 49.1, 40.51, 33.0. HRMS $[\text{ESI}]^+$ calculated for $\text{C}_{17}\text{H}_{19}\text{O}_3$: 271.1329 $[\text{M} + \text{H}]^+$; found: 271.1334.

(1*E*,4*E*)-1-(furan-2-yl)-7-phenylhepta-1,4-dien-3-one (12a)



Yellow oil; yield 66%. ^1H NMR (500 MHz, CD_3OD) δ 7.56 (s, 1H), 7.34 (d, J = 15 Hz, 1H), 7.20-7.17 (m, 2H), 7.13-7.07 (m, 3H), 6.96-6.90 (m, 1H), 6.79-6.73 (m, 2H), 6.48-6.47 (m, 1H), 6.34 (d, J = 15 Hz, 1H), 2.74-2.71 (m, 2H), 2.52-2.48 (m, 2H); ^{13}C NMR (125 MHz, CD_3OD) δ 191.3, 152.8, 149.1, 147.0, 142.4, 131.3, 130.8, 129.6, 127.3, 123.0, 117.7, 114.0, 35.7, 35.6. HRMS $[\text{ESI}]^+$ calculated for $\text{C}_{17}\text{H}_{17}\text{O}_2$: 253.1223 $[\text{M} + \text{H}]^+$; found: 253.1215.

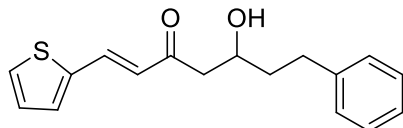
(*E*)-1-(furan-3-yl)-5-hydroxy-7-phenylhept-1-en-3-one (13)



Brown oil; yield 70.5%. ^1H NMR (500 MHz, CD_3OD) δ 7.74 (s, 1H), 7.47 (d, J = 15 Hz, 1H), 7.18-7.14 (m, 2H), 7.11-7.05 (m, 4H), 6.51 (s, 1H), 6.40 (d, J = 15 Hz, 1H), 4.78-4.01 (m, 1H), 2.64-2.55

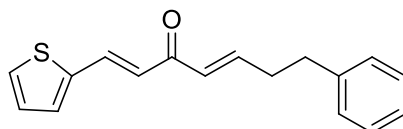
(m, 2H), 2.23 (m, 2H), 2.06-1.99 (m, 2H). HRMS [ESI]⁺ calculated for C₁₇H₁₉O₃: 271.1246 [M + H]⁺; found: 271.1245.

(E)-5-hydroxy-7-phenyl-1-(thiophen-2-yl)hept-1-en-3-one (14)



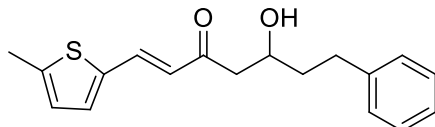
Yellow solid; yield 65%; m.p.: 94.8-95.7 °C. ¹H NMR (500 MHz, CD₃OD) δ 7.59 (s, 2H), 7.52 (d, *J* = 15 Hz, 1H), 7.31-7.27 (m, 1H), 7.16-7.09 (m, 4H), 7.06-7.03 (m, 1H), 6.55 (d, *J* = 15 Hz, 1H), 4.05 (brs, 1H), 2.81-2.76 (m, 1H), 2.72-2.65 (m, 2H), 2.64-2.56 (m, 1H), 1.73-1.68 (m, 2H); ¹³C NMR (125 MHz, CD₃OD) δ 202.0, 143.4, 139.2, 138.6, 130.8, 129.5, 129.5, 128.3, 127.4, 126.9, 126.4, 68.7, 48.9, 40.3, 33.0. HRMS [ESI]⁺ calculated for C₁₇H₁₉O₂S: 287.1100 [M + H]⁺; found: 287.1108.

(1E,4E)-7-phenyl-1-(thiophen-2-yl)hepta-1,4-dien-3-one (14a)



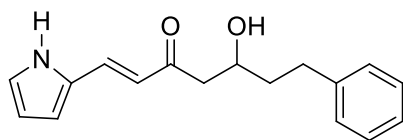
Yellowish oil; yield 72%. ¹H NMR (500 MHz, CD₃OD) δ 7.70 (s, 1H), 7.58 (d, *J* = 15 Hz, 1H), 7.40-7.38 (m, 2H), 7.22-7.14 (m, 2H), 7.12-7.09 (m, 2H), 7.01-6.96 (m, 1H), 6.85 (d, *J* = 15 Hz, 1H), 6.42 (d, *J* = 15 Hz, 1H), 2.78-2.75 (m, 2H), 2.56-2.52 (m, 2H); ¹³C NMR (125 MHz, CD₃OD) δ 192.1, 149.1, 142.5, 139.6, 138.9, 130.8, 130.7, 129.6, 128.4, 127.3, 126.5, 125.6, 35.7, 35.6. HRMS [ESI]⁺ calculated for C₁₇H₁₇OS: 269.0995 [M + H]⁺; found: 269.1000.

(E)-5-hydroxy-1-(5-methylthiophen-2-yl)-7-phenylhept-1-en-3-one (15)



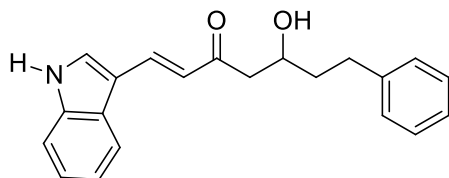
Yellowish oil; yield 60.4%. ¹H NMR (500 MHz, CDCl₃) δ 7.50 (d, *J* = 15 Hz, 1H), 7.22-7.17 (m, 2H), 7.14-7.09 (m, 3H), 7.04-7.03 (m, 1H), 6.66-6.65 (m, 1H), 6.30 (d, *J* = 15 Hz, 1H), 4.07-4.02 (m, 1H), 2.79-2.65 (m, 5H), 2.42 (s, 3H), 1.83-1.78 (m, 1H), 1.68-1.66 (m, 1H); ¹³C NMR (125 MHz, CDCl₃) δ 200.2, 145.1, 141.9, 137.5, 136.4, 133.0, 128.4, 128.3, 126.8, 125.7, 123.5, 67.2, 46.7, 38.1, 31.7, 15.8. HRMS [ESI]⁺ calculated for C₁₈H₂₁O₂S: 301.1257 [M + H]⁺; found: 301.1255.

(E)-5-hydroxy-7-phenyl-1-(1H-pyrrol-2-yl)hept-1-en-3-one (16)



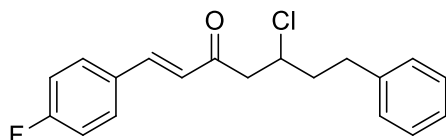
Yellow solid; yield 68.7%; m.p.: 109.5-110.3 °C. ^1H NMR (500 MHz, CD_3OD) δ 7.43 (d, J = 15 Hz, 1H), 7.18-7.11 (m, 4H), 7.07-7.05 (m, 1H), 6.91(s, 1H), 6.53-6.52 (m, 1H), 6.39 (d, J = 15 Hz, 1H), 6.15-6.14 (m, 1H), 4.05-4.01 (m, 1H), 2.77-2.57 (m, 4H), 1.76-1.69 (m, 2H); ^{13}C NMR (125 MHz, CD_3OD) δ 201.4, 143.6, 135.8, 129.6, 129.5, 126.9, 125.4, 120.5, 117.7, 111.9, 69.2, 48.7, 40.5, 33.1. HRMS $[\text{ESI}]^+$ calculated for $\text{C}_{17}\text{H}_{20}\text{O}_2\text{N}$: 279.1489 $[\text{M} + \text{H}]^+$; found: 279.1480.

(E)-5-hydroxy-1-(1H-indol-3-yl)-7-phenylhept-1-en-3-one (17)



Yellow solid; yield 62.2%; m.p.: 145.6-146.0 °C. ^1H NMR (500 MHz, CD_3OD) δ 7.84-7.79 (m, 2H), 7.61 (s, 1H), 7.35 (d, J = 5 Hz, 1H), 7.17-7.03 (m, 8H), 6.73 (d, J = 15 Hz, 1H), 4.08-4.03 (m, 1H), 2.82-2.68 (m, 3H), 2.63-2.59 (m, 1H), 1.76-1.71 (m, 2H); ^{13}C NMR (125 MHz, CD_3OD) δ 202.3, 143.6, 140.7, 139.5, 133.4, 129.6, 129.5, 126.9, 126.8, 124.2, 122.3, 121.4, 114.3, 113.4, 69.3, 48.6, 40.5, 33.1. HRMS $[\text{ESI}]^+$ calculated for $\text{C}_{21}\text{H}_{22}\text{O}_2\text{N}$: 320.1654 $[\text{M} + \text{H}]^+$; found: 320.1655.

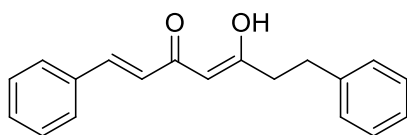
(E)-5-chloro-1-(4-fluorophenyl)-7-phenylhept-1-en-3-one (18)



Yellow oil; yield 5.3%. ^1H NMR (500 MHz, CD_3OD) δ 7.62-7.59 (m, 2H), 7.59-7.54 (m, 1H), 7.22-7.06 (m, 7H), 6.72 (d, J = 15 Hz, 1H), 4.36-4.32 (m, 1H, H5), 3.26-3.25 (m, 1H), 3.23-3.00 (m, 1H), 2.85-2.80 (m, 1H), 2.74-2.69 (m, 1H), 2.09-2.05 (m, 1H), 2.00-1.97 (m, 1H); ^{13}C NMR (125 MHz, CD_3OD) δ 198.8, 166.7, 164.7, 143.9, 142.4, 132.4, 132.0, 131.9, 129.7, 129.7, 127.3, 127.1, 117.2, 117.1, 58.5, 49.9, 41.2, 33.7. HRMS $[\text{ESI}]^+$ calculated for $\text{C}_{19}\text{H}_{19}\text{OClF}$: 317.1103 $[\text{M} + \text{H}]^+$; found: 317.1105.

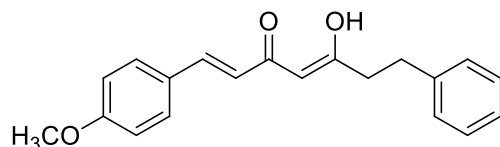
(1E,4Z)-5-hydroxy-1,7-diphenylhepta-1,4-dien-3-one (19)

Reference compound [1]



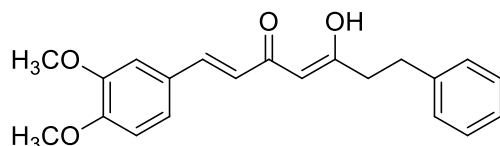
Known compound; yellow solid; yield 88%. HRMS [ESI]⁺ calculated for C₁₉H₁₇O₂: 277.1223 [M]⁺; found: 277.1232.

(1*E*,4*Z*)-5-hydroxy-1-(4-methoxyphenyl)-7-phenylhepta-1,4-dien-3-one (20)



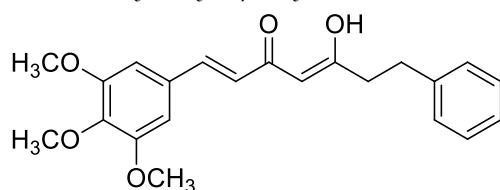
Yellow solid; yield 76%; m.p.: 80.1-81 °C. ¹H NMR (500 MHz, CD₃OD) δ 7.46-7.43 (m, 3H), 7.19-7.06 (m, 6H), 6.86 (d, *J* = 5 Hz, 2H), 6.40 (d, *J* = 15 Hz, 1H), 5.66 (s, 1H), 3.76 (s, 3H), 2.86 (t, 2H), 2.61 (t, 2H); ¹³C NMR (125 MHz, CD₃OD) δ 201.1, 179.0, 163.0, 142.4, 141.0, 130.9, 129.6, 129.5, 127.3, 121.5, 115.6, 101.4, 56.0, 43.0, 32.6. HRMS [ESI]⁺ calculated for C₂₀H₁₉O₃: 307.1329 [M]⁺; found: 307.1337.

(1*E*,4*Z*)-1-(3,4-dimethoxyphenyl)-5-hydroxy-7-phenylhepta-1,4-dien-3-one (21)



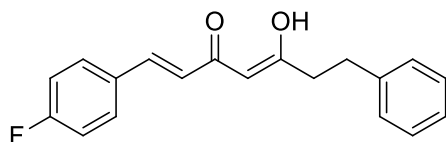
Yellow oil; yield 69.3%. ¹H NMR (500 MHz, CD₃OD) δ 7.43 (d, *J* = 15 Hz, 1H), 7.19-7.03 (m, 8H), 6.86 (d, *J* = 5 Hz, 1H), 6.41 (d, *J* = 15 Hz, 1H), 3.77-3.70 (m, 6H), 2.87-2.84 (m, 2H), 2.62-2.59 (m, 2H). HRMS [ESI]⁺ calculated for C₂₁H₂₁O₄: 337.1434 [M]⁺; found: 337.1437.

(1*E*,4*Z*)-5-hydroxy-7-phenyl-1-(3,4,5 trimethoxyphenyl)hepta-1,4-dien-3-one (22)



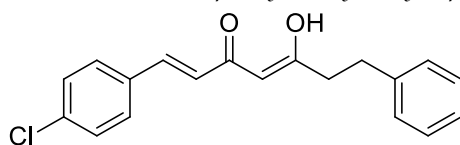
Yellow solid; yield 78%; m.p.: 82.8-83.4 °C. ¹H NMR (500 MHz, CD₃OD) δ 7.41 (d, *J* = 15 Hz, 1H), 7.19-7.06 (m, 5H), 6.78 (s, 2H), 6.47 (d, *J* = 15 Hz, 1H), 5.67 (s, 1H), 3.77 (s, 6H), 3.71 (s, 3H), 2.85 (t, *J* = 7.5 Hz, 2H), 2.63-2.60 (m, 2H); ¹³C NMR (125 MHz, CD₃OD) δ 201.8, 177.9, 154.9, 142.4, 141.1, 141.0, 132.5, 129.6, 129.5, 127.3, 123.3, 106.7, 101.9, 61.3, 56.8, 43.1, 32.4. HRMS [ESI]⁺ calculated for C₂₂H₂₃O₅: 367.1532 [M]⁺; found: 367.1540.

(1*E*,4*Z*)-1-(4-fluorophenyl)-5-hydroxy-7-phenylhepta-1,4-dien-3-one (23)



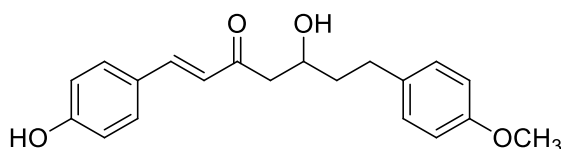
White solid; yield 62.5%; m.p.: 56-57 °C. ^1H NMR (500 MHz, CD_3OD) δ 7.53-7.51 (m, 2H), 7.45 (d, J = 15 Hz, 1H), 7.18-7.11 (m, 5H), 7.08-7.01 (m, 3H), 6.48 (d, 1H, J = 15 Hz), 5.69 (s, 1H), 2.85 (t, J = 7.5 Hz, 2H), 2.65-2.62 (m, 2H). HRMS [ESI] $^-$ calculated for $\text{C}_{19}\text{H}_{16}\text{O}_2\text{F}$: 295.1140 [M] $^-$; found: 295.1130.

(1E,4Z)-1-(4-chlorophenyl)-5-hydroxy-7-phenylhepta-1,4-dien-3-one (24)



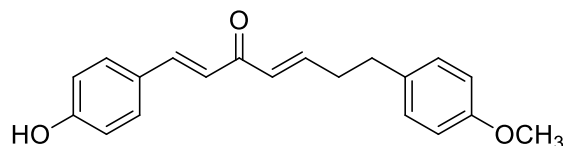
Brown solid; yield 72%; m.p.: 79.5-80.2 °C. ^1H NMR (500 MHz, CD_3OD) δ 7.56-7.50 (m, 3H), 7.38-7.37 (m, 2H), 7.27-7.20 (m, 5H), 7.17-7.14 (m, 1H), 6.62 (d, J = 15 Hz, 1H), 5.78 (s, 1H), 2.94 (t, 2H), 2.73 (t, 2H); ^{13}C NMR (125 MHz, CD_3OD) δ 202.5, 177.0, 142.4, 139.2, 136.8, 135.5, 130.5, 130.3, 129.6, 129.5, 127.3, 124.8, 102.2, 43.3, 32.4. HRMS [ESI] $^-$ calculated for $\text{C}_{19}\text{H}_{16}\text{O}_2\text{Cl}$: 311.0833 [M] $^-$; found: 311.0843.

(E)-5-hydroxy-1-(4-hydroxyphenyl)-7-(4-methoxyphenyl)hept-1-en-3-one (MD1)



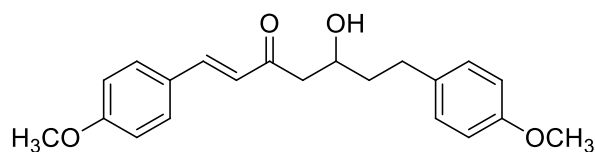
White solid; yield 70%; m.p.: 123-130 °C. ^1H NMR (500 MHz, CD_3OD) δ 7.45 (d, J = 15 Hz, 1H), 7.38 (d, J = 5 Hz, 2H), 7.01 (d, J = 5 Hz, 2H), 6.71-6.69 (m, 4H), 6.55 (d, J = 15 Hz, 1H), 4.01-3.96 (m, 1H), 3.63, (s, 3H), 2.77-2.73 (m, 1H), 2.69-2.60 (m, 2H), 2.54-2.48 (m, 1H), 1.68-1.62 (m, 2H); ^{13}C NMR (125 MHz, CD_3OD) δ 202.0, 161.8, 159.5, 145.7, 135.5, 131.8, 130.5, 127.4, 124.6, 117.1, 114.9, 68.9, 55.8, 48.9, 40.6, 32.1. HRMS [ESI] $^+$ calculated for $\text{C}_{20}\text{H}_{23}\text{O}_4$: 327.1591 [M + H] $^+$; found: 327.1585.

(1E,4E)-1-(4-hydroxyphenyl)-7-(4-methoxyphenyl)hepta-1,4-dien-3-one (MD1a)



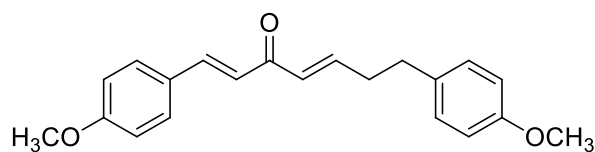
Yellow oil; yield 73%. ^1H NMR (500 MHz, CD_3OD) δ 7.50 (d, J = 15 Hz, 1H), 7.44 (d, J = 5 Hz, 2H), 7.05 (d, J = 5 Hz, 2H), 6.96-6.91 (m, 1H), 6.83-6.79 (m, 1H), 6.76-6.73 (m, 4H), 6.40 (d, J = 15 Hz, 1H), 3.67, (s, 3H), 2.70-2.67 (m, 2H), 2.51-2.47 (m, 2H); ^{13}C NMR (125 MHz, CD_3OD) δ 192.0, 161.8, 159.7, 148.8, 145.9, 134.5, 131.8, 130.8, 130.6, 127.7, 122.8, 117.1, 115.0, 55.8, 36.0, 34.8. HRMS $[\text{ESI}]^+$ calculated for $\text{C}_{20}\text{H}_{21}\text{O}_3$: 309.1485 $[\text{M} + \text{H}]^+$; found: 309.1478.

(E)-5-hydroxy-1,7-bis(4-methoxyphenyl)hept-1-en-3-one (MD2)



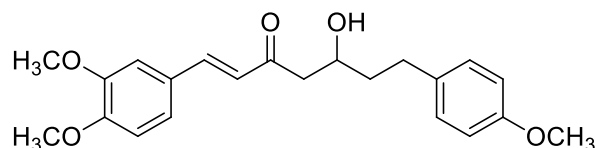
Yellow solid; yield 67.8%; m.p.: 43-44 °C. ^1H NMR (500 MHz, CD_3OD) δ 7.51-7.48 (m, 3H), 7.04 (d, J = 5 Hz, 2H), 6.88-6.86 (m, 2H), 6.73 (d, J = 5Hz, 2H), 6.62 (d, J = 15 Hz, 1H), 4.05-4.00 (m, 1H), 3.75, (s, 3H), 3.74 (s, 3H), 2.81-2.50 (m, 4H), 2.51-2.47 (m, 2H), 1.71-1.67 (m, 2H); ^{13}C NMR (125 MHz, CD_3OD) δ 202.0, 163.6, 159.4, 145.2, 135.5, 131.5, 130.5, 128.6, 125.4, 115.6, 115.0, 68.9, 56.1, 55.8, 49.01, 40.6, 32.1. HRMS $[\text{ESI}]^+$ calculated for $\text{C}_{21}\text{H}_{25}\text{O}_4$: 341.1747 $[\text{M} + \text{H}]^+$; found: 341.1744.

(1E,4E)-1,7-bis(4-methoxyphenyl)hepta-1,4-dien-3-one (MD2a)



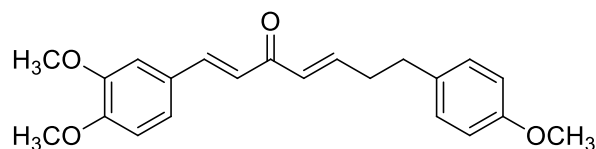
Yellow solid; yield 70.4%; m.p.: 55.5-56 °C. ^1H NMR (500 MHz, CD_3OD) δ 7.52-7.49 (m, 3H), 7.04 (d, J = 5 Hz, 2H), 6.97-6.91 (m, 1H), 6.88-6.83 (m, 3H), 6.75 (d, J = 5 Hz, 2H), 6.39 (d, J = 15 Hz, 1H), 3.74, (s, 3H), 3.66 (s, 3H), 2.69-2.66 (m, 2H), 2.50-2.46 (m, 2H); ^{13}C NMR (125 MHz, CD_3OD) δ 191.9, 163.6, 159.7, 149.0, 145.3, 134.4, 131.6, 130.8, 130.6, 128.8, 123.6, 115.7, 115.0, 56.1, 55.8, 36.0, 34.8. HRMS $[\text{ESI}]^+$ calculated for $\text{C}_{21}\text{H}_{23}\text{O}_3$: 323.1642 $[\text{M} + \text{H}]^+$; found: 323.1633.

(E)-1-(3,4-dimethoxyphenyl)-5-hydroxy-7-(4-methoxyphenyl)hept-1-en-3-one (MD3)



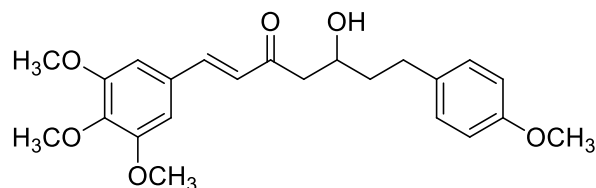
Yellow oil; yield 61%. ^1H NMR (500 MHz, CD_3OD) δ 7.49 (d, J = 15 Hz, 1H), 7.14-7.10 (m, 2H), 7.04 (d, J = 5 Hz, 2H), 6.89 (d, J = 5 Hz, 1H), 6.74 (d, J = 5 Hz, 2H), 6.65 (d, J = 15 Hz, 1H), 4.07-4.02 (m, 1H), 3.78, (s, 6H), 3.66 (s, 3H), 2.82-2.69 (m, 2H), 2.68-2.52 (m, 2H), 1.72-1.68 (m, 2H); ^{13}C NMR (125 MHz, CD_3OD) δ 201.8, 159.4, 153.2, 150.9, 145.4, 135.5, 130.5, 129.0, 125.7, 124.7, 115.0, 112.8, 111.89, 68.9, 56.6, 56.6, 55.8, 49.0, 40.6, 32.1. HRMS $[\text{ESI}]^+$ calculated for $\text{C}_{22}\text{H}_{27}\text{O}_5$: 371.1853 $[\text{M} + \text{H}]^+$; found: 371.1849.

(1E,4E)-1-(3,4-dimethoxyphenyl)-7-(4-methoxyphenyl)hepta-1,4-dien-3-one (MD3a)



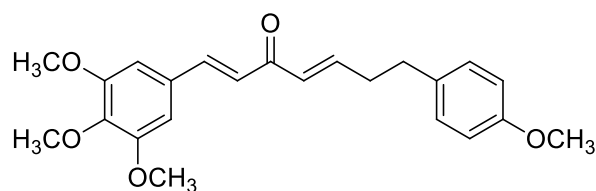
Yellow oil; yield 65.3%. ^1H NMR (500 MHz, CD_3OD) δ 7.49 (d, J = 15 Hz, 1H), 7.17-7.13 (m, 1H), 7.12-7.11 (m, 1H), 7.03 (d, J = 5 Hz, 2H), 6.98-6.95 (m, 1H), 6.94-6.86 (m, 2H), 6.75-6.73 (m, 2H), 6.39 (d, J = 15 Hz, 1H), 3.78 (s, 3H), 3.77 (s, 3H), 3.65 (s, 3H), 2.65 (t, J = 7.5 Hz, 2H), 2.50-2.45 (m, 2H); ^{13}C NMR (125 MHz, CD_3OD) δ 191.9, 159.7, 153.3, 151.0, 149.1, 145.6, 134.4, 130.8, 130.6, 129.3, 124.8, 123.8, 115.0, 112.8, 111.8, 56.7, 56.6, 55.8, 49.1, 36.0, 34.8. HRMS $[\text{ESI}]^+$ calculated for $\text{C}_{22}\text{H}_{25}\text{O}_4$: 353.1658 $[\text{M} + \text{H}]^+$; found: 353.1654.

(E)-5-hydroxy-7-(4-methoxyphenyl)-1-(3,4,5-trimethoxyphenyl)hept-1-en-3-one (MD4)



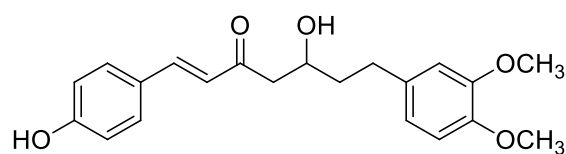
Yellow oil; yield 63.7%. ^1H NMR (500 MHz, CD_3OD) δ 7.46 (d, J = 15 Hz, 1H), 7.03 (d, J = 5 Hz, 2H), 6.84 (s, 2H), 6.73-6.67 (m, 3H), 4.07-4.01 (m, 1H), 3.78 (s, 6H), 3.71 (s, 3H), 3.64 (s, 3H), 2.83-2.78 (m, 1H), 2.72-2.62 (m, 2H), 2.59-2.50 (m, 1H), 1.71-1.67 (m, 2H); ^{13}C NMR (125 MHz, $\text{MeOD}-d_4$) δ 201.8, 159.4, 154.9, 145.2, 141.6, 135.4, 131.9, 130.5, 130.4, 127.2, 115.0, 107.2, 68.8, 61.4, 56.9, 56.6, 56.9, 55.8, 40.6, 32.1. HRMS $[\text{ESI}]^+$ calculated for $\text{C}_{23}\text{H}_{29}\text{O}_6$: 401.1884 $[\text{M} + \text{H}]^+$; found: 401.1890.

(1E,4E)-7-(4-methoxyphenyl)-1-(3,4,5-trimethoxyphenyl)hepta-1,4-dien-3-one (MD4a)



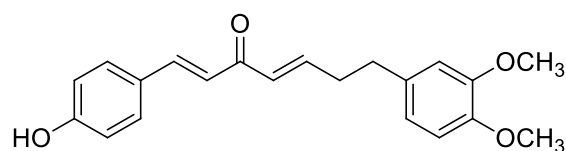
Yellow solid; yield 68.6%; m.p.: 59-60 °C. ^1H NMR (500 MHz, CDCl_3) δ 7.50 (d, J = 15 Hz, 1H), 7.09 (d, J = 5 Hz, 1H), 7.02-6.96 (m, 1H), 6.83-6.76 (m, 5H), 6.43 (d, J = 15 Hz, 1H), 3.88 (s, 9H), 3.76 (s, 3H), 2.77-2.74 (m, 2H), 2.57-2.53 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 189.0, 158.0, 153.4, 146.9, 143.2, 140.3, 132.8, 130.2, 129.3, 129.3, 124.4, 113.9, 105.4, 61.0, 56.1, 55.2, 34.6, 33.6. HRMS [ESI] $^+$ calculated for $\text{C}_{23}\text{H}_{27}\text{O}_5$: 383.1756 [M + H] $^+$; found: 383.1753.

(*E*)-7-(3,4-dimethoxyphenyl)-5-hydroxy-1-(4-hydroxyphenyl)hept-1-en-3-one (MD5)



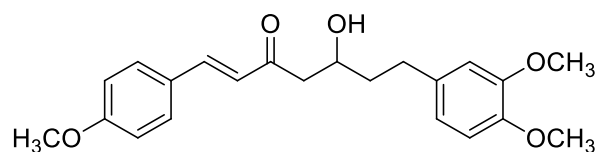
A yellowish oil; yield 60.2%. ^1H NMR (500 MHz, CD_3OD) δ 7.46 (d, J = 15 Hz, 1H), 7.38 (d, J = 5 Hz, 2H), 6.74-6.72 (m, 4H), 6.66-6.65 (m, 1H), 6.56 (d, J = 15 Hz, 1H), 4.04-3.99 (m, 1H), 3.70 (s, 3H), 3.68 (s, 3H), 2.79-2.75 (m, 1H), 2.70-2.62 (m, 2H), 2.57-2.51 (m, 1H), 1.72-1.67 (m, 2H); ^{13}C NMR (125 MHz, CD_3OD) δ 202.0, 161.7, 150.4, 148.7, 145.7, 136.5, 131.7, 127.3, 124.6, 121.8, 117.1, 113.7, 113.3, 68.9, 56.7, 56.5, 48.8, 40.4, 32.5. ESI-MS (positive, m/z): 357.3 [M+H]

(1*E*,4*E*)-7-(3,4-dimethoxyphenyl)-1-(4-hydroxyphenyl)hepta-1,4-dien-3-one (MD5a)



Yellow oil; yield 68%. ^1H NMR (500 MHz, CDCl_3) δ 7.53 (d, J = 15 Hz, 1H), 7.38 (d, J = 5 Hz, 2H), 6.99-6.93 (m, 1H), 6.81 (d, J = 5 Hz, 2H), 6.75-6.72 (m, 2H), 6.67-6.65 (m, 2H), 6.39 (d, J = 15 Hz, 1H), 3.78 (s, 3H), 3.74 (s, 3H), 2.71-2.68 (m, 2H), 2.53-2.49 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 189.8, 158.7, 148.8, 147.3, 147.0, 143.9, 133.4, 130.3, 129.5, 126.9, 122.2, 120.2, 116.0, 111.7, 111.3, 55.9, 55.8, 34.6, 34.1. HRMS [ESI] $^+$ calculated for $\text{C}_{21}\text{H}_{23}\text{O}_4$: 339.1591 [M + H] $^+$; found: 339.1584.

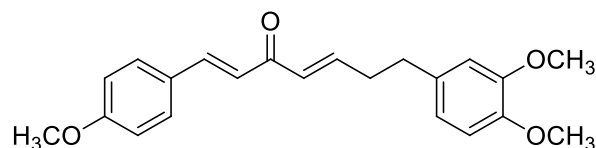
(*E*)-7-(3,4-dimethoxyphenyl)-5-hydroxy-1-(4-methoxyphenyl)hept-1-en-3-one (MD6)



White solid; yield 61.3%; m.p.: 50-51 °C. ^1H NMR (500 MHz, CD_3OD) δ 7.50-7.47 (m, 3H), 6.86

(m, 2H), 6.75-6.73 (m, 2H), 6.67-6.59 (m, 2H), 4.02 (brs, 1H), 3.73 (s, 3H), 3.71 (s, 3H), 3.68 (s, 3H), 2.81-2.76 (m, 1H), 2.71-2.63 (m, 2H), 2.57-2.51 (m, 1H), 1.70 (brs, 2H); ^{13}C NMR (125 MHz, CD_3OD) δ 201.9, 163.6, 150.5, 148.8, 145.2, 136.5, 131.5, 128.6, 125.5, 121.9, 115.7, 113.7, 113.4, 68.9, 56.7, 56.6, 56.1, 49.02, 40.4, 32.5. HRMS $[\text{ESI}]^+$ calculated for $\text{C}_{22}\text{H}_{27}\text{O}_5$: 371.1853 $[\text{M} + \text{H}]^+$; found: 371.1846..

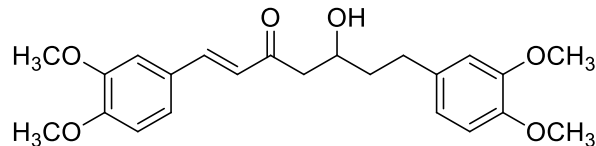
(1E,4E)-7-(3,4-dimethoxyphenyl)-1-(4-methoxyphenyl)hepta-1,4-dien-3-one (MD6a)



Yellow oil; yield 72.5%. ^1H NMR (500 MHz, CD_3OD) δ 7.52-7.49 (m, 3H), 6.97-6.91 (m, 1H), 6.87-6.83 (m, 3H), 6.77-6.73 (m, 2H), 6.66 (d, $J = 5$ Hz, 1H), 6.39 (d, $J = 15$ Hz, 1H), 3.73 (s, 3H), 3.70 (s, 3H), 3.68 (s, 3H), 2.69-2.66 (m, 2H), 2.51-2.47 (m, 2H); ^{13}C NMR (125 MHz, CD_3OD) δ 191.9, 163.6, 150.5, 149.0, 145.4, 135.5, 131.6, 130.8, 128.8, 123.6, 121.9, 115.7, 113.8, 113.3, 56.7, 56.6, 56.1, 35.9, 35.3. HRMS $[\text{ESI}]^+$ calculated for $\text{C}_{22}\text{H}_{25}\text{O}_4$: 353.1747 $[\text{M} + \text{H}]^+$; found: 353.1738.

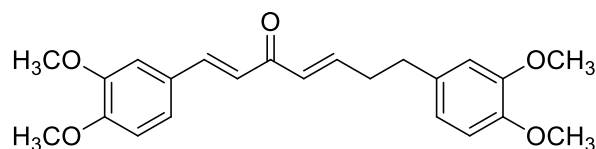
(E)-1,7-bis(3,4-dimethoxyphenyl)-5-hydroxyhept-1-en-3-one (MD7)

Reference compound [12]



Known compound; yellow solid; yield 66.1%; m.p.: 87-88 °C. ^1H NMR (500 MHz, CD_3OD) δ 7.47 (d, $J = 15$ Hz, 1H), 7.12-7.08 (m, 2H), 6.87 (d, $J = 5$ Hz, 1H), 6.74-6.72 (m, 2H), 6.66-6.61 (m, 2H), 4.04-4.00 (m, 1H), 3.76 (s, 6H), 3.70 (s, 3H), 3.67 (s, 3H), 2.80-2.76 (m, 1H), 2.71-2.62 (m, 2H), 2.59-2.50 (m, 1H), 1.72-1.66 (m, 2H); ^{13}C NMR (125 MHz, CD_3OD) δ 201.9, 153.3, 151.0, 150.5, 148.8, 145.4, 136.5, 129.1, 125.7, 124.7, 121.9, 113.7, 113.4, 112.8, 111.8, 68.9, 56.7, 56.6, 56.5, 49.07, 40.5, 32.5. HRMS $[\text{ESI}]^+$ calculated for $\text{C}_{23}\text{H}_{29}\text{O}_6$: 401.1959 $[\text{M} + \text{H}]^+$; found: 401.1948.

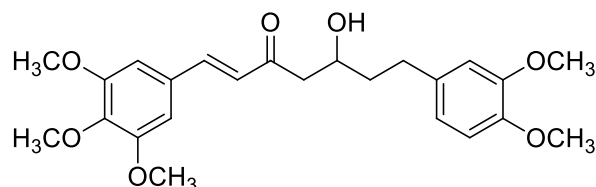
(1E,4E)-1,7-bis(3,4-dimethoxyphenyl)hepta-1,4-dien-3-one (MD7a)



Yellow oil; yield 70.5%. ^1H NMR (500 MHz, CD_3OD) δ 7.51 (d, $J = 15$ Hz, 1H), 7.18 (s, 1H), 7.13 (d, $J = 5$ Hz, 1H), 6.99-6.94 (m, 1H), 6.90-6.87 (m, 2H), 6.78-6.74 (m, 2H), 6.68 (d, $J = 5$ Hz, 1H), 6.41 (d, $J = 15$ Hz, 1H), 3.79(s, 3H), 3.78 (s, 3H), 3.72 (s, 3H), 3.70 (s, 3H), 2.69 (t, $J = 7.5$ Hz, 2H),

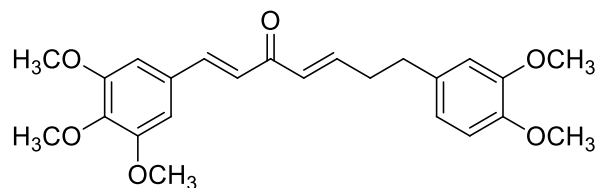
2.55-2.49 (m, 2H); ^{13}C NMR (125 MHz, CD_3OD) δ 191.8, 153.3, 151.0, 150.6, 149.1, 149.0, 145.6, 135.5, 130.9, 129.3, 124.8, 123.9, 121.9, 113.8, 113.3, 112.8, 111.9, 56.7, 56.6, 35.9, 35.2. HRMS $[\text{ESI}]^+$ calculated for $\text{C}_{23}\text{H}_{26}\text{O}_5$: 382.1780 $[\text{M} + \text{H}]^+$; found: 382.1779.

(E)-7-(3,4-dimethoxyphenyl)-5-hydroxy-1-(3,4,5-trimethoxyphenyl)hept-1-en-3-one (MD8)



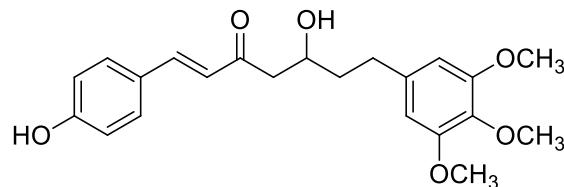
Colorless oil; yield 62%. ^1H NMR (500 MHz, CD_3OD) δ 7.47 (d, $J = 15$ Hz, 1H), 6.86 (s, 2H), 6.76-6.67 (m, 4H), 4.08-4.00 (m, 1H), 3.79 (s, 3H), 3.73 (s, 3H), 3.69 (s, 9H), 2.84-2.80 (m, 1H), 2.75-2.65 (m, 2H), 2.61-2.53 (m, 1H), 1.75-1.70 (m, 2H); ^{13}C NMR (125 MHz, CD_3OD) δ 201.7, 154.9, 150.5, 148.8, 145.1, 141.7, 136.5, 131.8, 127.2, 121.8, 113.8, 113.4, 107.2, 68.8, 61.3, 56.9, 56.7, 56.5, 49.1, 40.4, 32.5. HRMS $[\text{ESI}]^+$ calculated for $\text{C}_{24}\text{H}_{31}\text{O}_7$: 431.2064 $[\text{M} + \text{H}]^+$; found: 431.2055.

(1E,4E)-7-(3,4-dimethoxyphenyl)-1-(3,4,5-trimethoxyphenyl)hepta-1,4-dien-3-one (MD8a)



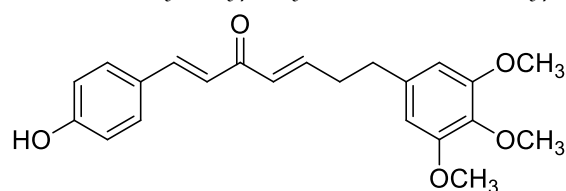
Yellow solid; yield 65.6%; m.p.: 86-87 °C. ^1H NMR (500 MHz, CD_3OD) δ 7.46 (d, $J = 15$ Hz, 1H), 7.01-6.92 (m, 2H), 6.85 (s, 2H), 6.75-6.72 (m, 2H), 6.64 (m, 1H), 6.39 (d, $J = 15$ Hz, 1H), 3.77 (s, 6H), 3.71 (s, 3H), 3.70 (s, 3H), 3.69 (s, 3H), 2.67-2.64 (m, 2H), 2.49-2.45 (m, 2H); ^{13}C NMR (125 MHz, CD_3OD) δ 191.6, 154.9, 150.5, 149.3, 149.0, 145.3, 141.7, 135.4, 132.0, 130.8, 125.3, 121.9, 113.7, 113.3, 107.2, 61.3, 56.8, 56.6, 56.5, 35.8, 35.2. HRMS $[\text{ESI}]^+$ calculated for $\text{C}_{24}\text{H}_{29}\text{O}_6$: 413.1959 $[\text{M} + \text{H}]^+$; found: 413.1954.

(E)-5-hydroxy-1-(4-hydroxyphenyl)-7-(3,4,5-trimethoxyphenyl)hept-1-en-3-one (MD9)



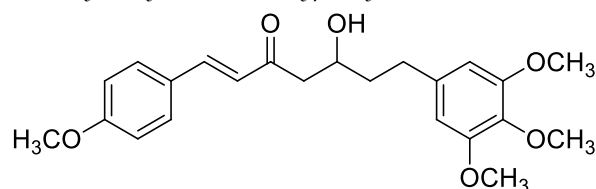
Yellow oil; yield 73 %. ^1H NMR (500 MHz, CD_3OD) δ 7.50-7.39 (m, 3H), 6.73 (d, $J = 5$ Hz, 2H), 6.58 (d, $J = 15$ Hz, 1H), 6.43 (s, 2H), 4.05-4.00 (m, 1H), 3.71 (s, 6H), 3.63 (s, 3H), 2.81-2.77 (m, 1H), 2.72-2.64 (m, 2H), 2.58-2.52 (m, 1H), 1.75-1.67 (m, 2H); ^{13}C NMR (125 MHz, CD_3OD) δ 202.0, 161.8, 154.5, 145.7, 139.8, 137.3, 131.7, 127.3, 124.6, 117.1, 106.9, 68.9, 61.3, 56.7, 48.9, 40.2, 33.3. HRMS $[\text{ESI}]^+$ calculated for $\text{C}_{22}\text{H}_{27}\text{O}_6$: 387.1802 $[\text{M} + \text{H}]^+$; found: 387.1792.

(1E,4E)-1-(4-hydroxyphenyl)-7-(3,4,5-trimethoxyphenyl)hepta-1,4-dien-3-one (MD9a)



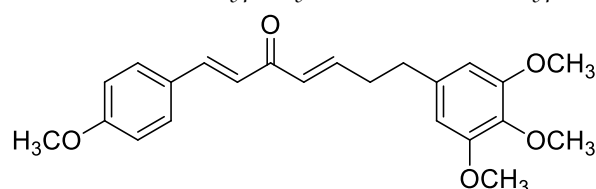
Yellow oil; yield 77 %. ^1H NMR (500 MHz, CDCl_3) δ 7.58 (d, J = 15 Hz, 1H), 7.44 (d, J = 5 Hz, 2H), 7.03-6.97 (m, 1H), 6.85 (d, J = 5 Hz, 2H), 6.79 (d, J = 15 Hz, 1H), 6.45 (d, J = 15 Hz, 1H), 6.39-6.37 (m, 2H), 3.82 (s, 6H), 3.81 (s, 3H), 2.76-2.73 (m, 2H), 2.59-2.55 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 189.5, 158.3, 153.1, 146.5, 143.5, 136.6, 136.3, 130.3, 129.6, 127.2, 122.4, 116.0, 105.3, 60.8, 56.0, 34.9, 34.6. HRMS [ESI] $^+$ calculated for $\text{C}_{22}\text{H}_{25}\text{O}_5$: 369.1697 [M + H] $^+$; found: 369.1687.

(E)-5-hydroxy-1-(4-methoxyphenyl)-7-(3,4,5-trimethoxyphenyl)hept-1-en-3-one (MD10)



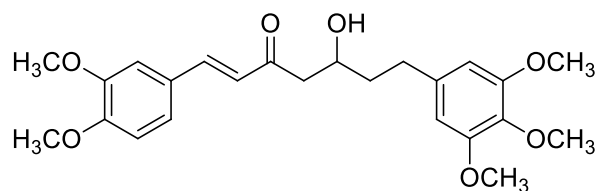
Yellow oil; yield 64 %. ^1H NMR (500 MHz, CD_3OD) δ 7.53-7.49 (m, 3H), 6.88 (d, J = 5 Hz, 2H), 6.64 (d, J = 15 Hz, 1H), 6.44 (s, 2H), 4.08-4.00 (m, 1H), 3.75 (s, 3H), 3.72 (m, 6H), 3.63 (s, 3H), 2.84-2.80 (m, 1H), 2.79-2.65 (m, 2H), 2.60-2.54 (m, 1H), 1.79-1.73 (m, 2H); ^{13}C NMR (125 MHz, CD_3OD) δ 201.9, 163.6, 154.5, 145.2, 139.8, 137.3, 133.4, 131.5, 128.6, 125.5, 115.7, 106.9, 68.8, 61.3, 56.7, 56.1, 49.0, 40.3, 33.3. HRMS [ESI] $^+$ calculated for $\text{C}_{23}\text{H}_{29}\text{O}_6$: 401.1959 [M + H] $^+$; found: 401.1956.

(1E,4E)-1-(4-methoxyphenyl)-7-(3,4,5-trimethoxyphenyl)hepta-1,4-dien-3-one (MD10a)



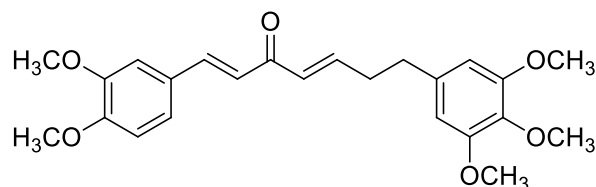
Yellow oil; yield 65.7%. ^1H NMR (500 MHz, CDCl_3) δ 7.58 (d, J = 15 Hz, 1H), 7.50 (d, J = 5 Hz, 2H), 7.02-6.96 (m, 1H), 6.91-6.88 (m, 2H), 6.80 (d, J = 15 Hz, 1H), 6.44 (d, J = 15 Hz, 1H), 6.39 (s, 2H), 3.82 (s, 9H), 3.80 (s, 3H), 2.76-2.73 (m, 2H), 2.59-2.55 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 189.1, 161.6, 153.1, 146.1, 143.1, 136.6, 130.0, 129.7, 127.4, 122.7, 114.4, 105.3, 60.8, 56.0, 55.3, 34.9, 34.4. HRMS [ESI] $^+$ calculated for $\text{C}_{23}\text{H}_{27}\text{O}_5$: 383.1853 [M + H] $^+$; found: 383.1844.

(E)-1-(3,4-dimethoxyphenyl)-5-hydroxy-7-(3,4,5-trimethoxyphenyl) hept-1-en-3-one (MD11)



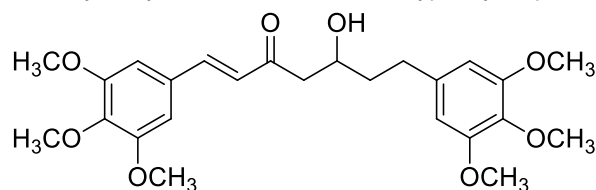
Yellow oil; yield 62.4%. ^1H NMR (500 MHz, CD_3OD) δ 7.49 (d, J = 15 Hz, 1H), 7.14-7.10 (m, 2H), 6.88 (d, J = 5 Hz, 1H), 6.66-6.63 (m, 1H), 6.44-6.40 (m, 2H), 4.05-4.03 (m, 1H), 3.77-3.70 (m, 12H), 3.63 (s, 3H), 2.83-2.79 (m, 1H), 2.74-2.66 (m, 2H), 2.58-2.56 (m, 1H), 1.74-1.71 (m, 2H); ^{13}C NMR (125 MHz, CD_3OD) δ 201.9, 154.5, 153.3, 150.9, 145.4, 139.8, 137.3, 129.0, 125.7, 124.7, 112.8, 111.9, 106.9, 68.8, 61.3, 56.7, 56.6, 49.05, 40.3, 33.3. HRMS [ESI] $^+$ calculated for $\text{C}_{24}\text{H}_{31}\text{O}_7$: 431.2064 [M + H] $^+$; found: 431.2054.

(1E,4E)-1-(3,4-dimethoxyphenyl)-7-(3,4,5-trimethoxyphenyl)hepta-1,4-dien-3-one (MD11a)



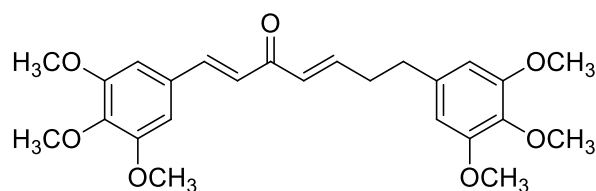
Yellow oil; yield 67.5%. ^1H NMR (500 MHz, CDCl_3) δ 7.55 (d, J = 15 Hz, 1H), 7.14-7.12 (m, 1H), 7.06 (s, 1H), 7.02-6.98 (m, 1H), 6.85 (d, J = 5 Hz, 1H), 6.78 (d, J = 15 Hz, 1H), 6.46 (d, J = 15 Hz, 1H), 6.39 (s, 2H), 3.90 (s, 6H), 3.82 (s, 6H), 3.80 (s, 3H), 2.76-2.73 (m, 2H), 2.59-2.55 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 189.0, 153.1, 151.3, 149.2, 146.1, 143.3, 136.6, 129.4, 127.6, 123.1, 123.0, 111.0, 109.8, 105.3, 60.8, 56.0, 55.9, 55.9, 34.9, 34.4. HRMS [ESI] $^+$ calculated for $\text{C}_{24}\text{H}_{29}\text{O}_6$: 413.1959 [M + H] $^+$; found: 413.1951.

(E)-5-hydroxy-1,7-bis(3,4,5-trimethoxyphenyl)hept-1-en-3-one (MD12)



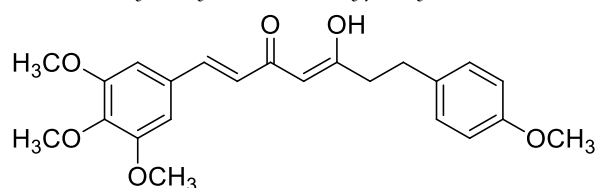
Yellow oil; yield 69.1%. ^1H NMR (500 MHz, CD_3OD) δ 7.48 (d, J = 15 Hz, 1H), 6.86 (s, 2H), 6.71 (d, J = 15 Hz, 1H), 6.45 (s, 2H), 4.07-4.05 (m, 1H), 3.79 (s, 6H), 3.73 (s, 9H), 3.64 (s, 3H), 2.85-2.81 (m, 1H), 2.76-2.66 (m, 2H), 2.62-2.54 (m, 1H), 1.77-1.70 (m, 2H); ^{13}C NMR (125 MHz, CD_3OD) δ 201.7, 155.0, 154.5, 145.1, 141.7, 139.8, 137.3, 131.9, 127.2, 107.2, 106.9, 68.7, 61.3, 61.2, 56.9, 56.7, 49.1, 40.3, 33.6. HRMS [ESI] $^+$ calculated for $\text{C}_{25}\text{H}_{33}\text{O}_8$: 461.2170 [M + H] $^+$; found: 461.2161.

(1E,4E)-1,7-bis(3,4,5-trimethoxyphenyl)hepta-1,4-dien-3-one (MD12a)



Yellow solid; yield 66.5%; m.p.: 98-99 °C. ^1H NMR (500 MHz, CDCl_3) δ 7.51 (d, J = 15 Hz, 1H), 7.04-6.98 (m, 1H), 6.81-6.77 (m, 2H), 6.46 (d, J = 15 Hz, 1H), 6.39 (s, 2H), 3.88 (s, 6H), 3.86 (s, 3H), 3.82 (s, 6H), 3.80 (m, 3H), 2.77-2.74 (m, 2H), 2.60-2.56 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 188.9, 153.4, 153.2, 146.5, 143.3, 140.3, 136.5, 136.4, 130.1, 129.3, 124.5, 105.5, 105.3, 60.9, 60.8, 56.1, 56.0, 55.9, 34.9, 34.4. HRMS $[\text{ESI}]^+$ calculated for $\text{C}_{25}\text{H}_{31}\text{O}_7$: 443.2064 $[\text{M} + \text{H}]^+$; found: 443.2058.

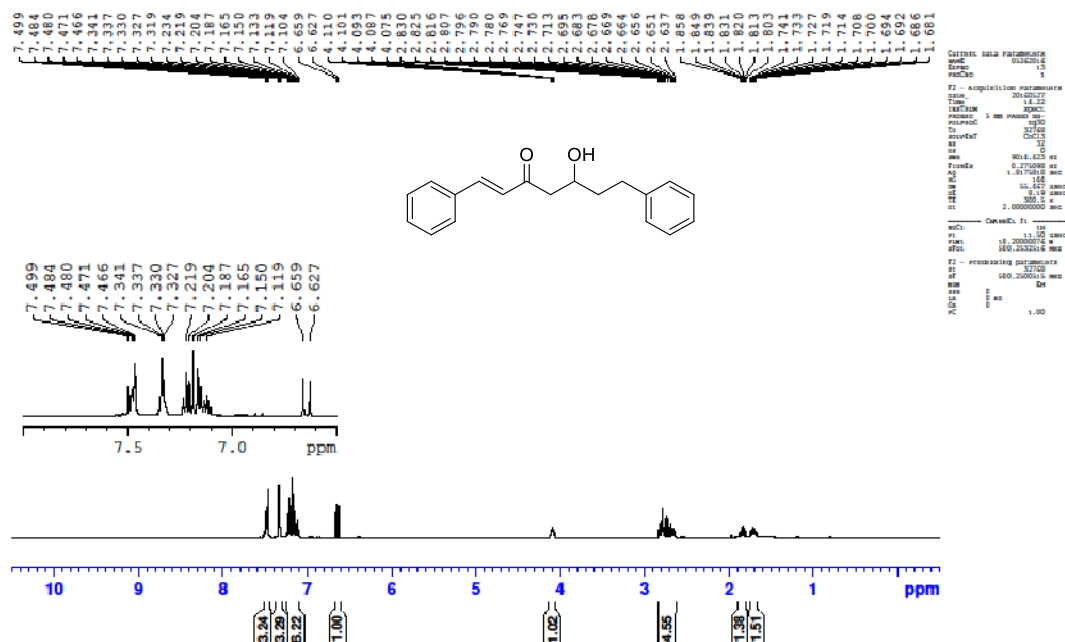
(1E,4Z)-5-hydroxy-7-(4-methoxyphenyl)-1-(3,4,5-trimethoxyphenyl)hepta-1,4-dien-3-one (MD13)

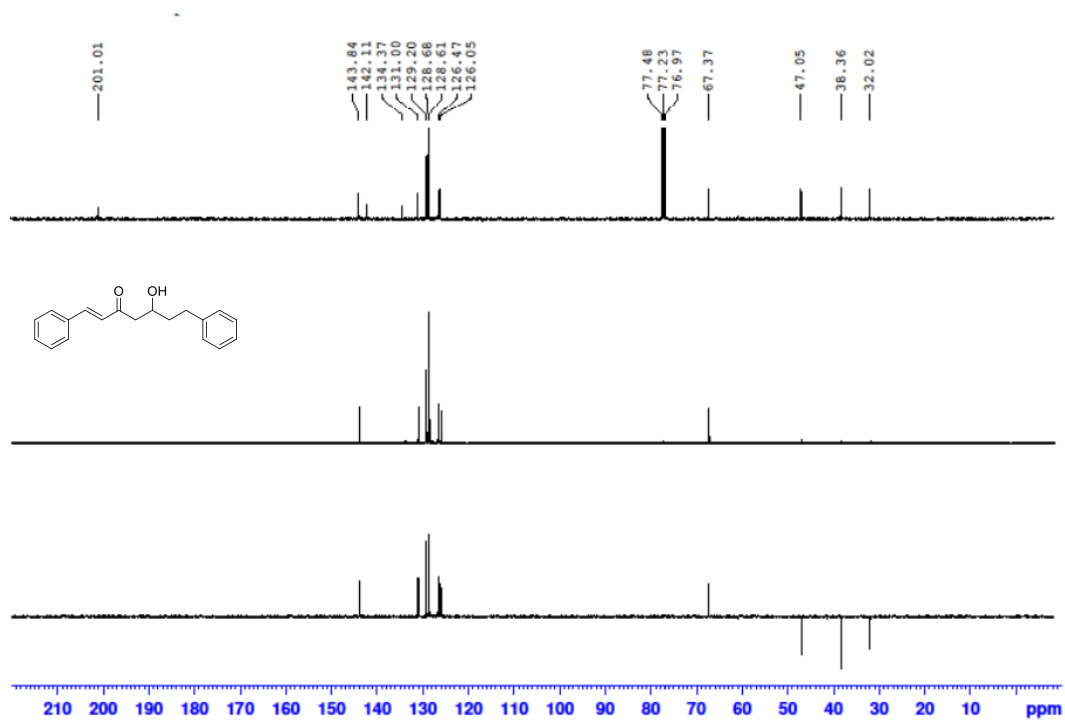


Yellow oil; yield 69.3%; m.p.: 98-99 °C. ^1H NMR (500 MHz, $\text{DMSO}-d_6$) δ 7.48 (d, J = 15 Hz, 1H), 7.15-7.14 (m, 2H), 7.02 (s, 2H), 6.84-6.78 (m, 3H), 5.90 (s, 1H), 5.73 (s, 1H), 3.81 (s, 6H), 3.70 (s, 6H), 2.83 (brs, 2H), 2.71-2.70 (m, 2H); ^{13}C NMR (125 MHz, $\text{DMSO}-d_6$) δ 200.2, 176.4, 157.6, 153.1, 139.5, 132.6, 130.4, 129.2, 122.3, 113.8, 105.7, 100.7, 60.1, 56.0, 55.0, 41.4, 29.63. HRMS $[\text{ESI}]^+$ calculated for $\text{C}_{23}\text{H}_{27}\text{O}_6$: 399.1802 $[\text{M} + \text{H}]^+$; found: 399.1791.

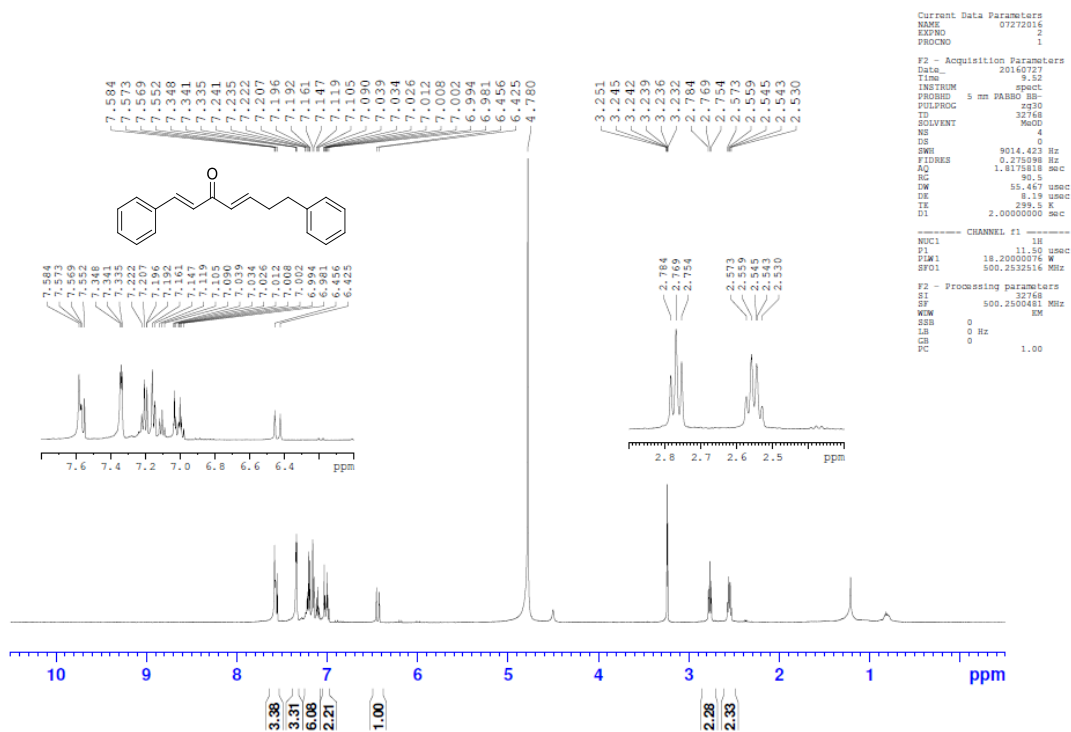
NMR Spectra ¹H and ¹³C

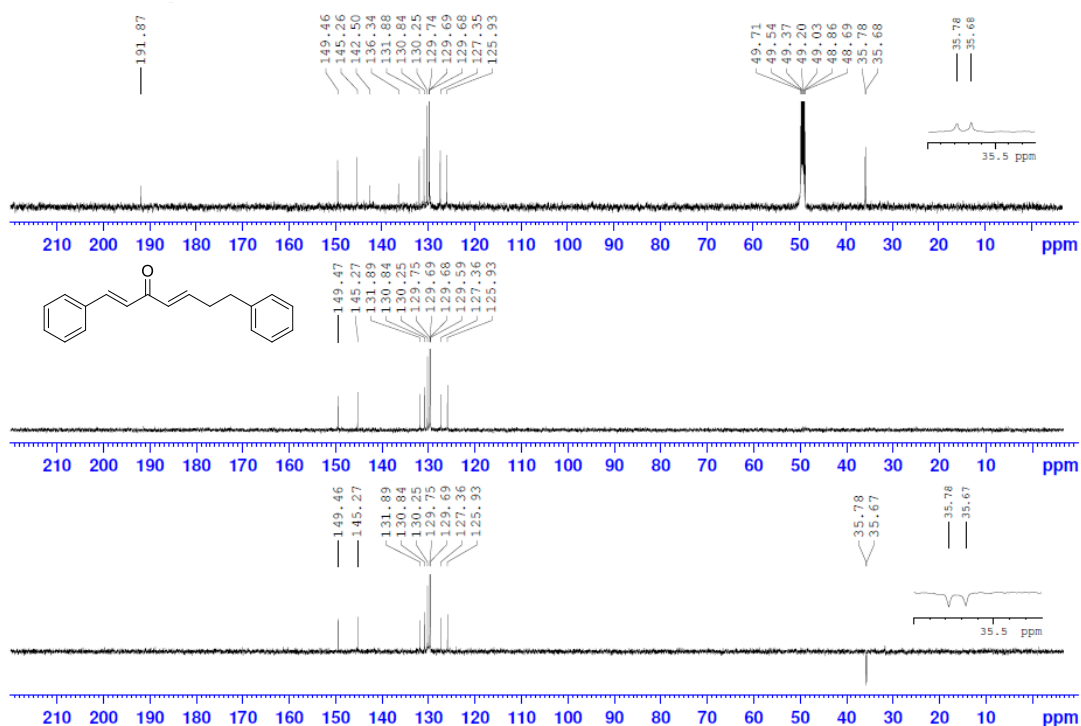
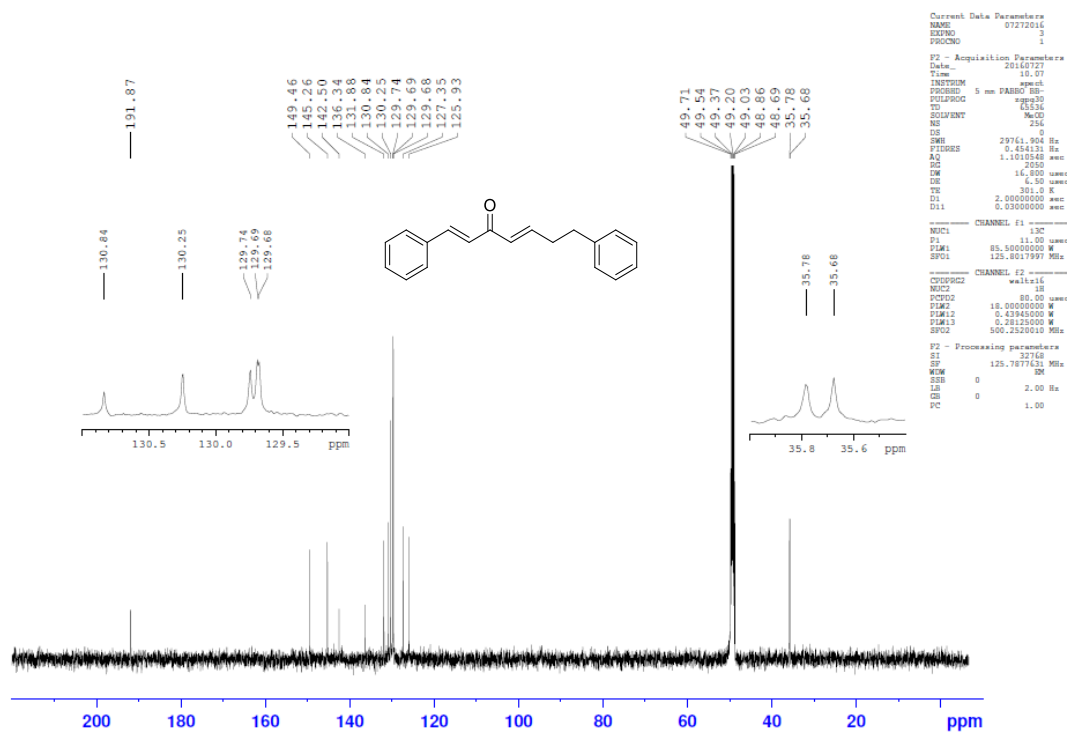
Compound 1



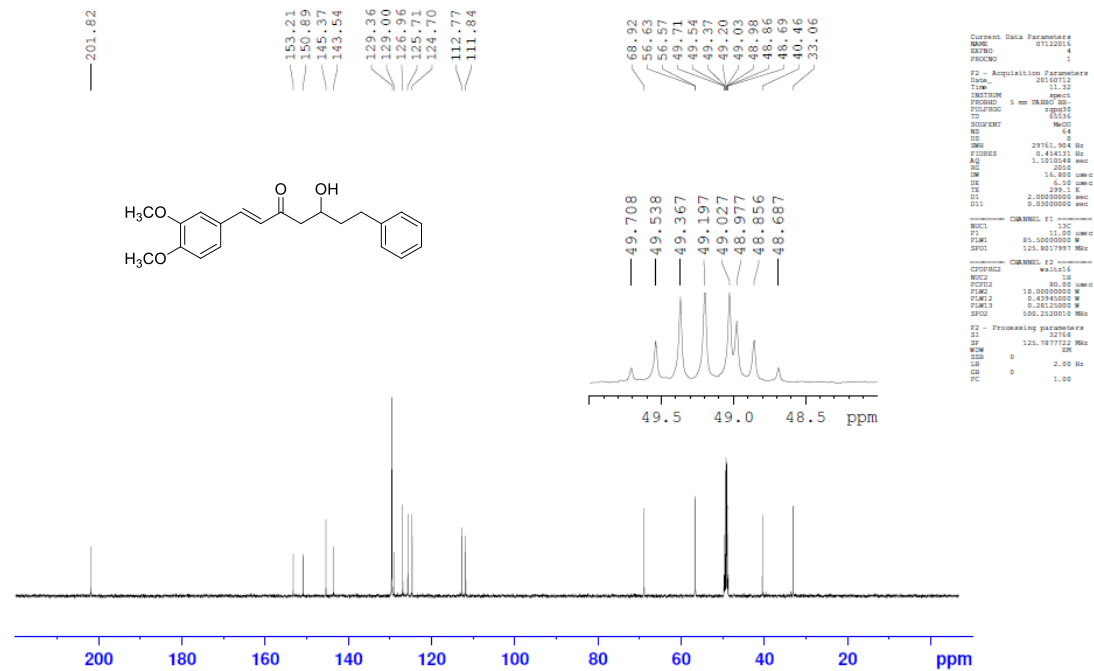
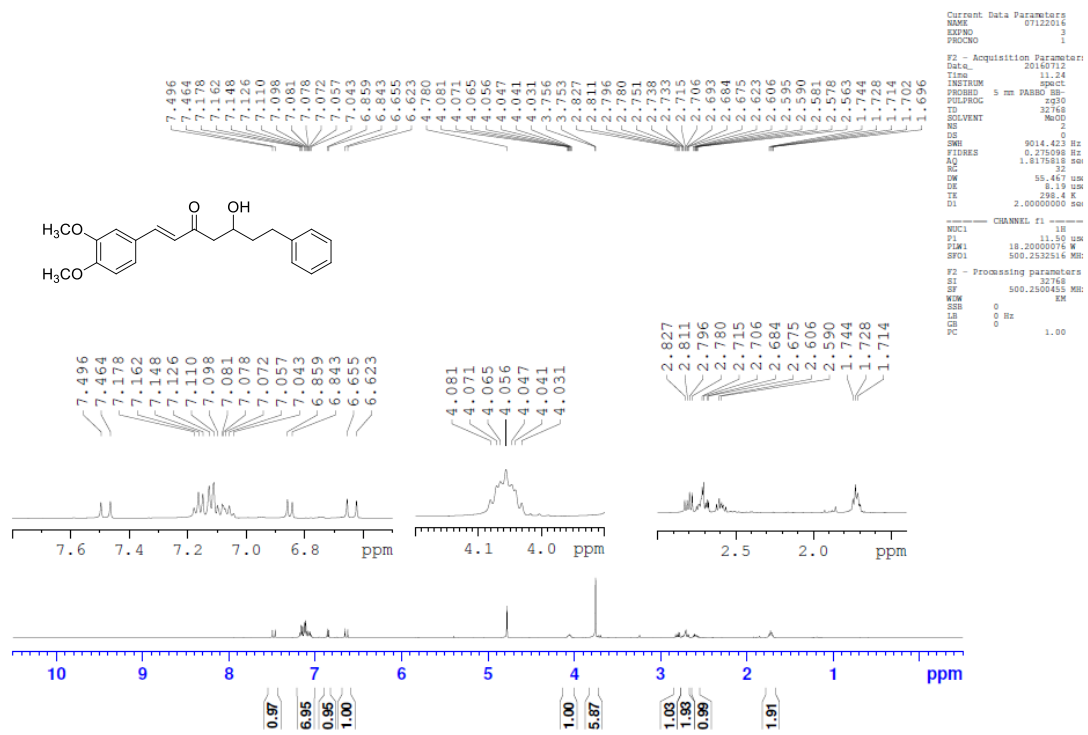


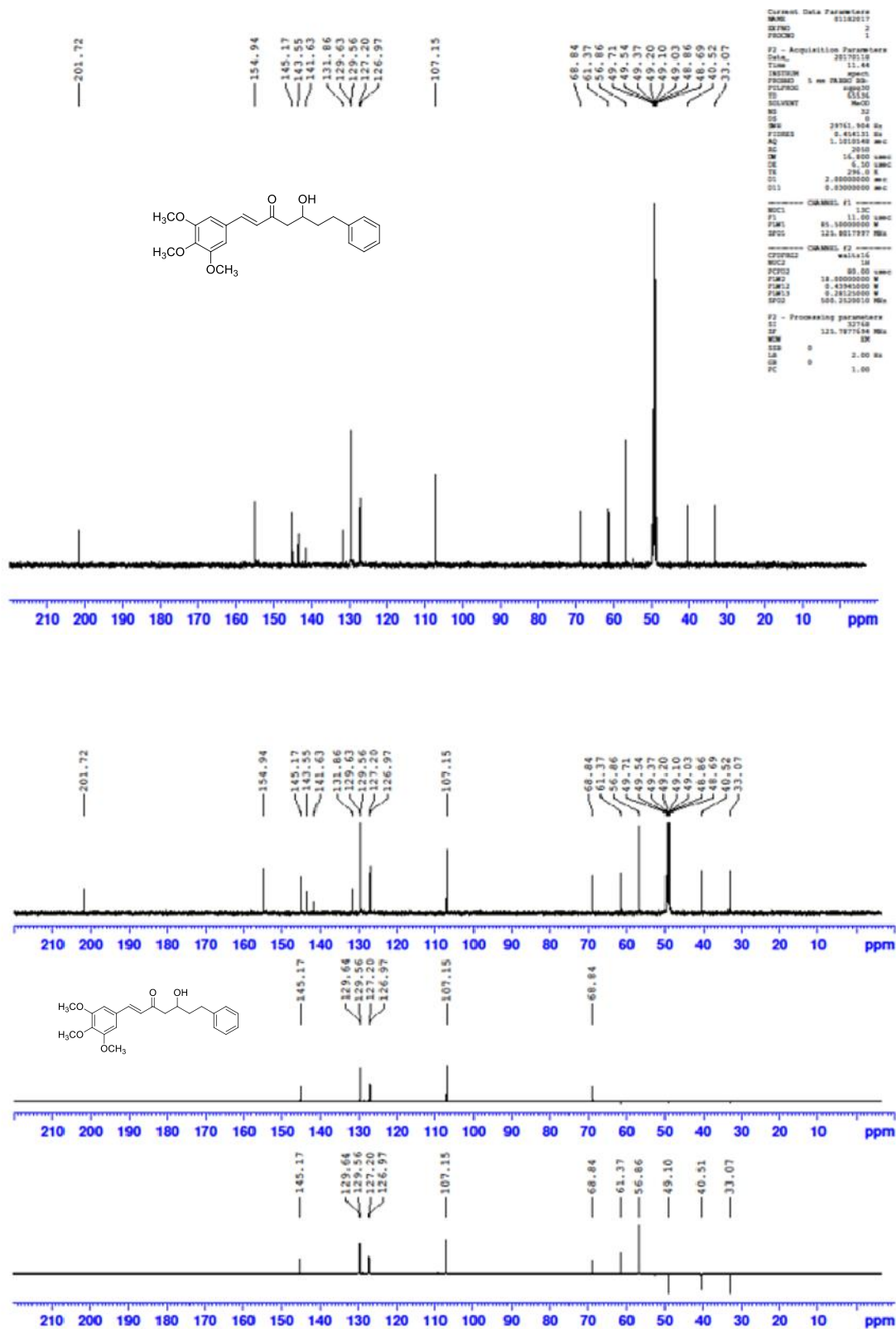
Compound 1a



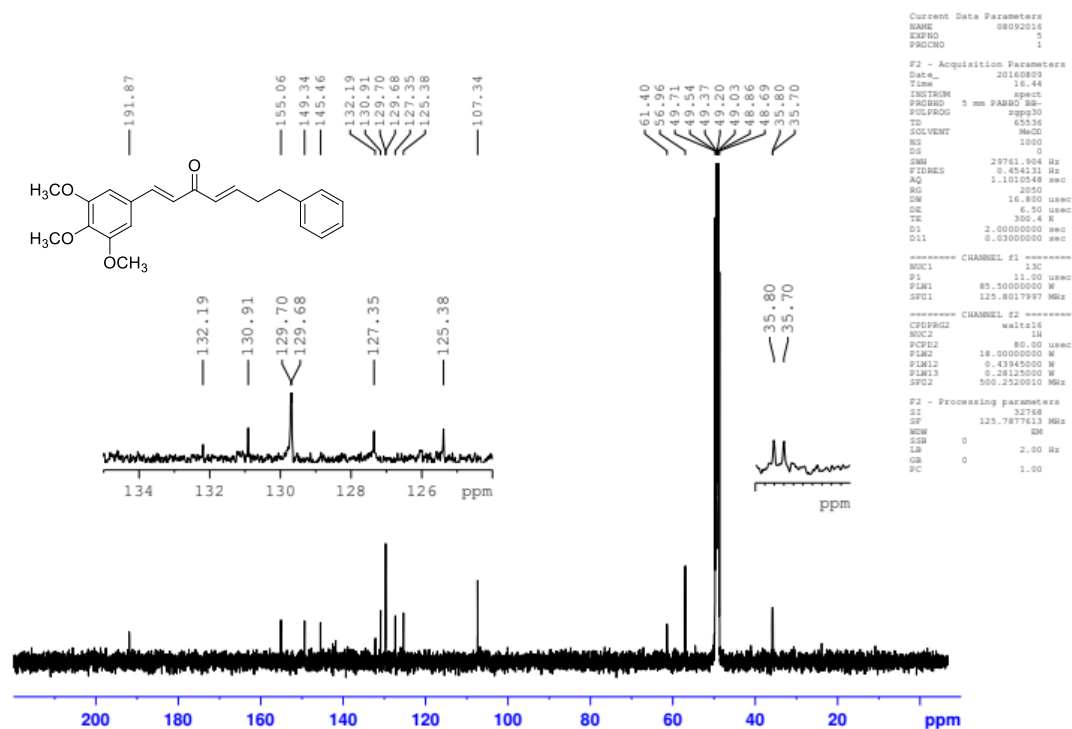
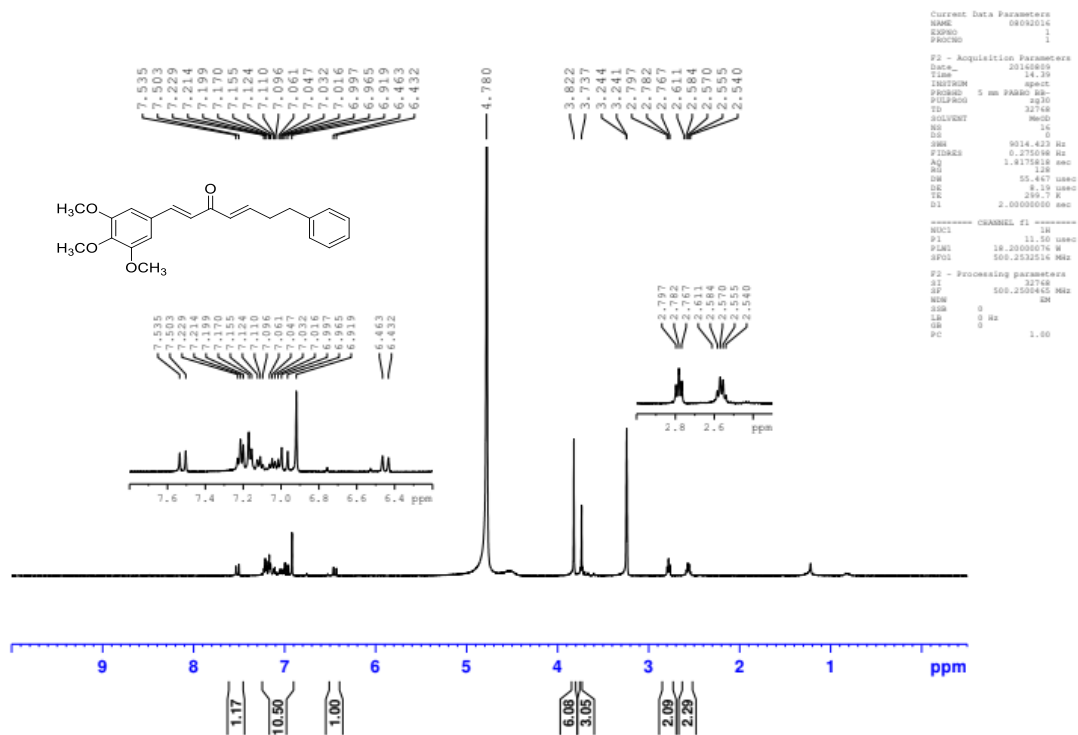


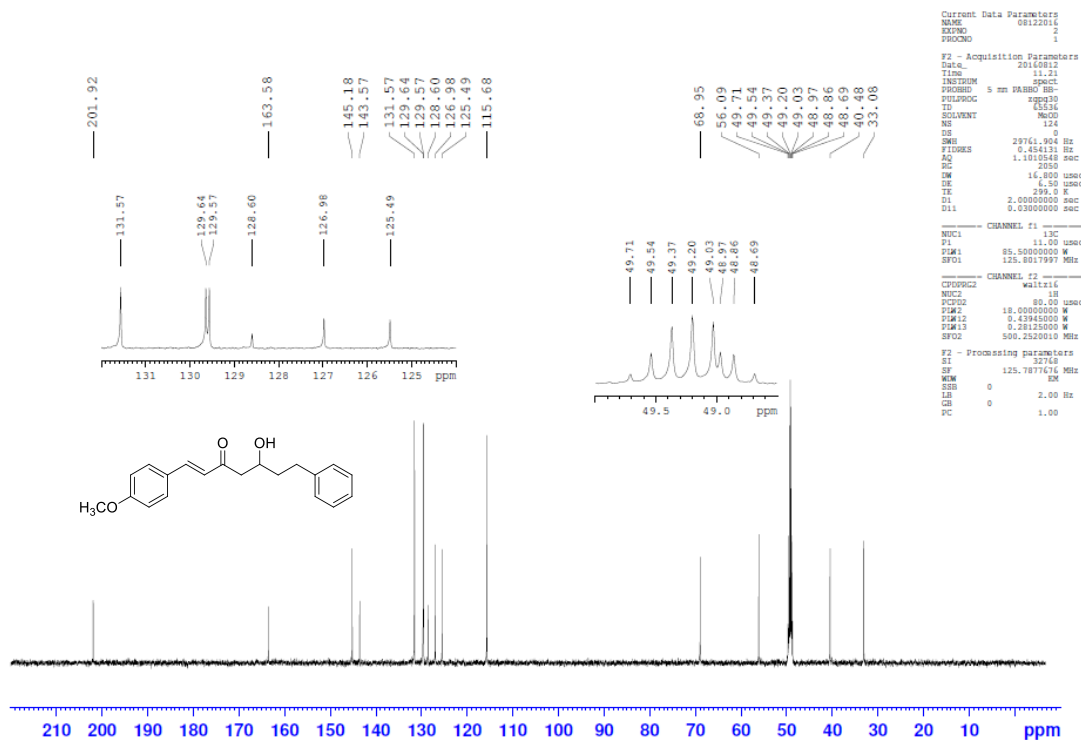
Compound 2





Compound 3a



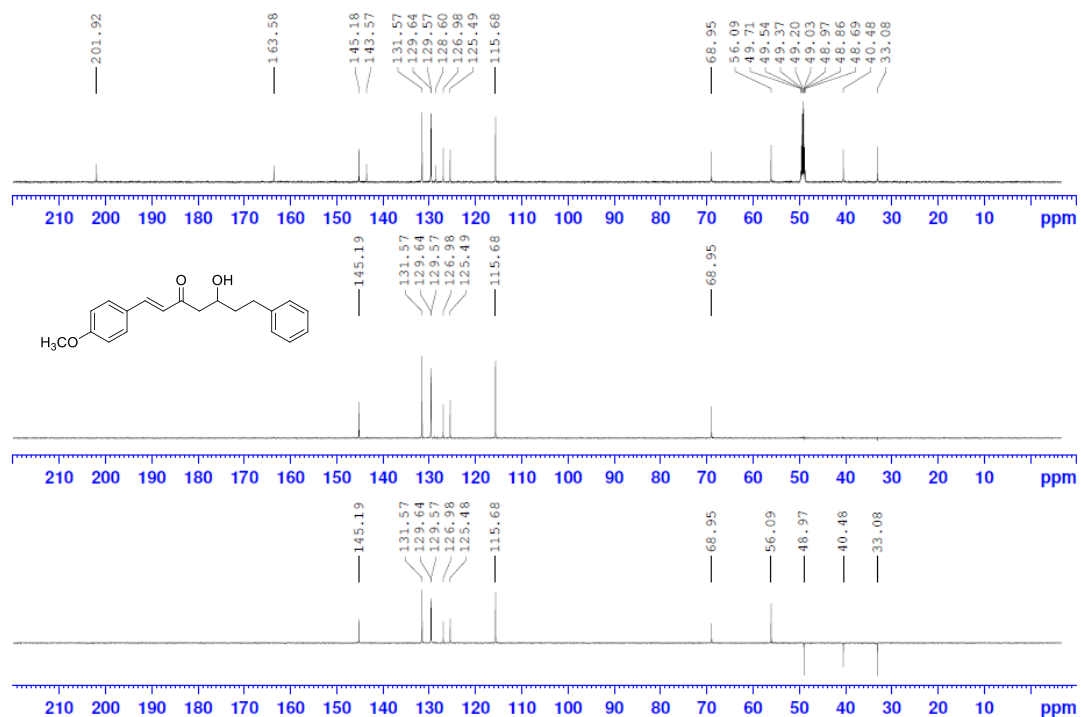


Current Data Parameters
NAME 08122016
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160612
Time 11.21
INSTRUM spect
PROBHD 5 mm QNP1H
PULPROG zgpg30
TD 65536
SOLVENT Me2O
NS 124
DS 0
SFO1 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1810540 sec
RG 2050
SW 16.000 USMC
LB 6.50 USMC
JT 299.0 K
D1 2.00000000 sec
D11 0.03000000 sec

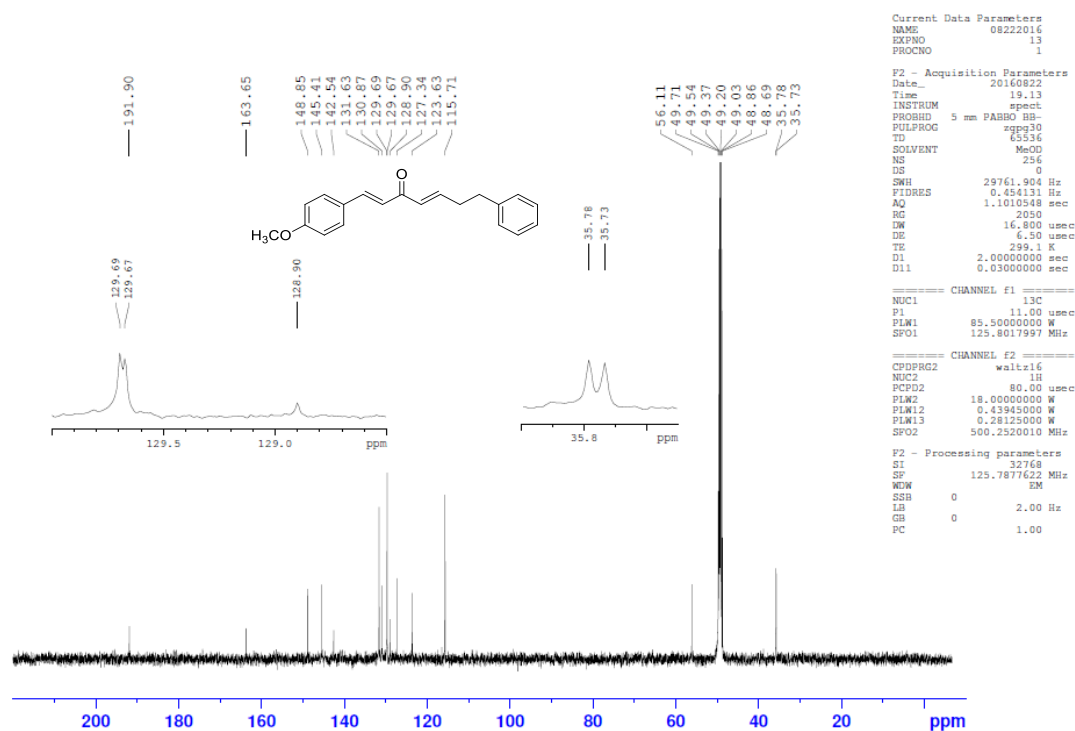
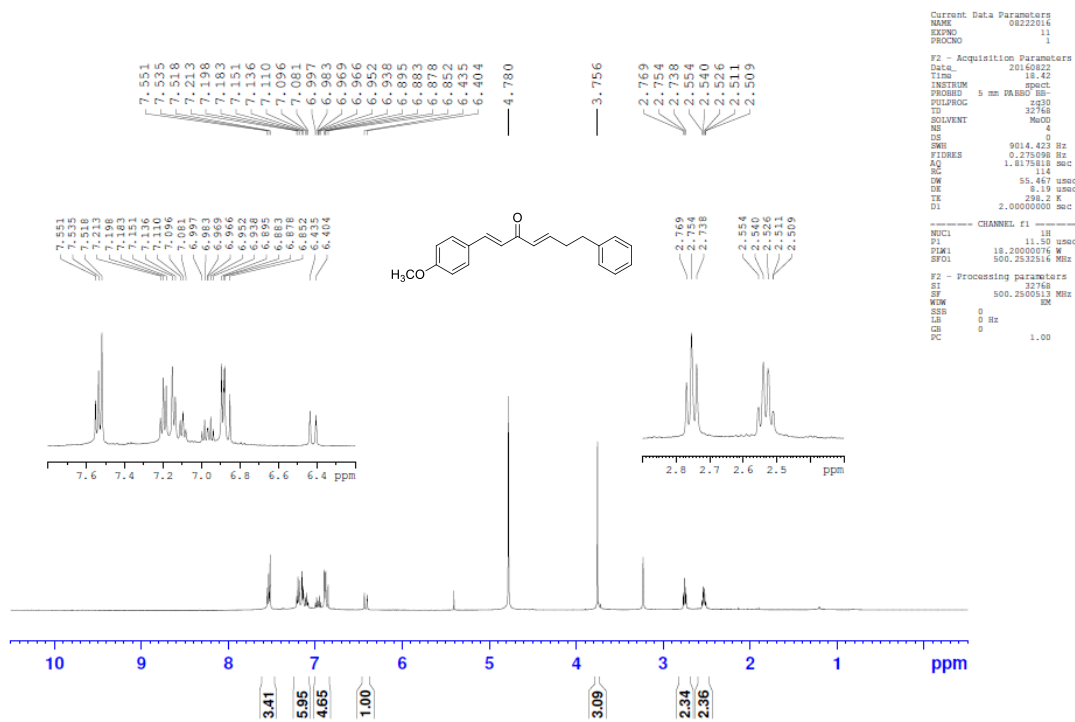
CHANNEL F1
NUC1 13C
P1 11.00 USMC
PL1 85.50000000 W
SFO1 125.6017997 MHz

CHANNEL F2
CPDPRG2 waltz16
NUC2 1H
P2 90.00 USMC
PL2 18.00000000 W
PL12 0.43840000 W
PL13 0.28125000 W
SFO2 500.2520010 MHz

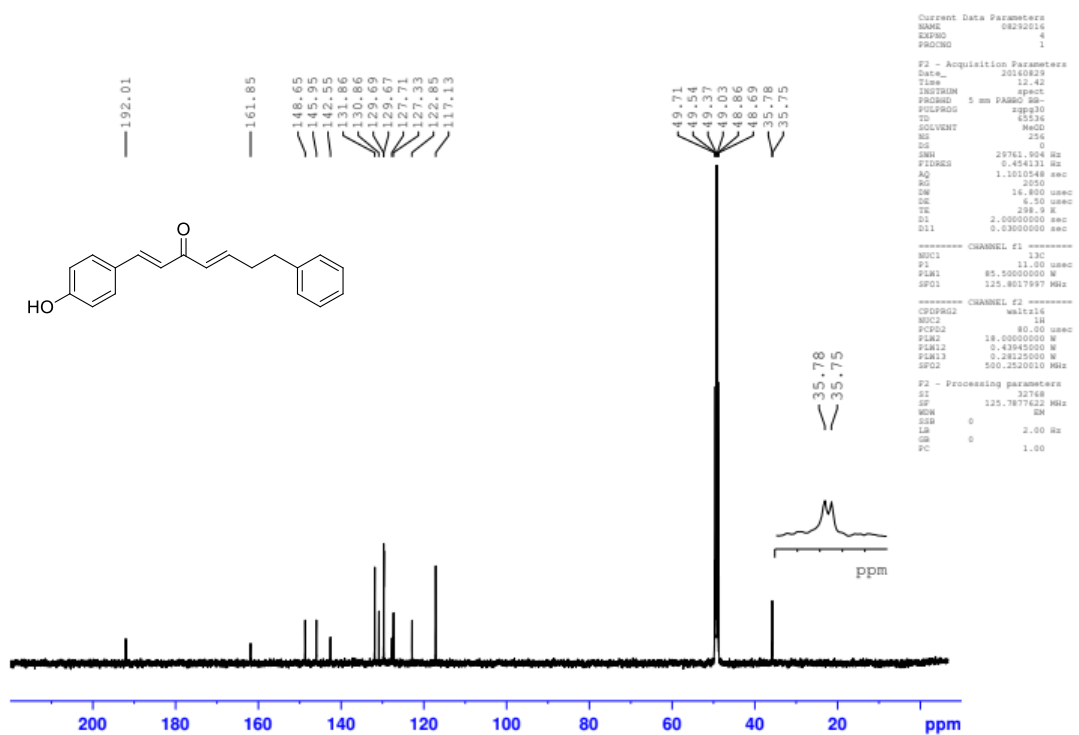
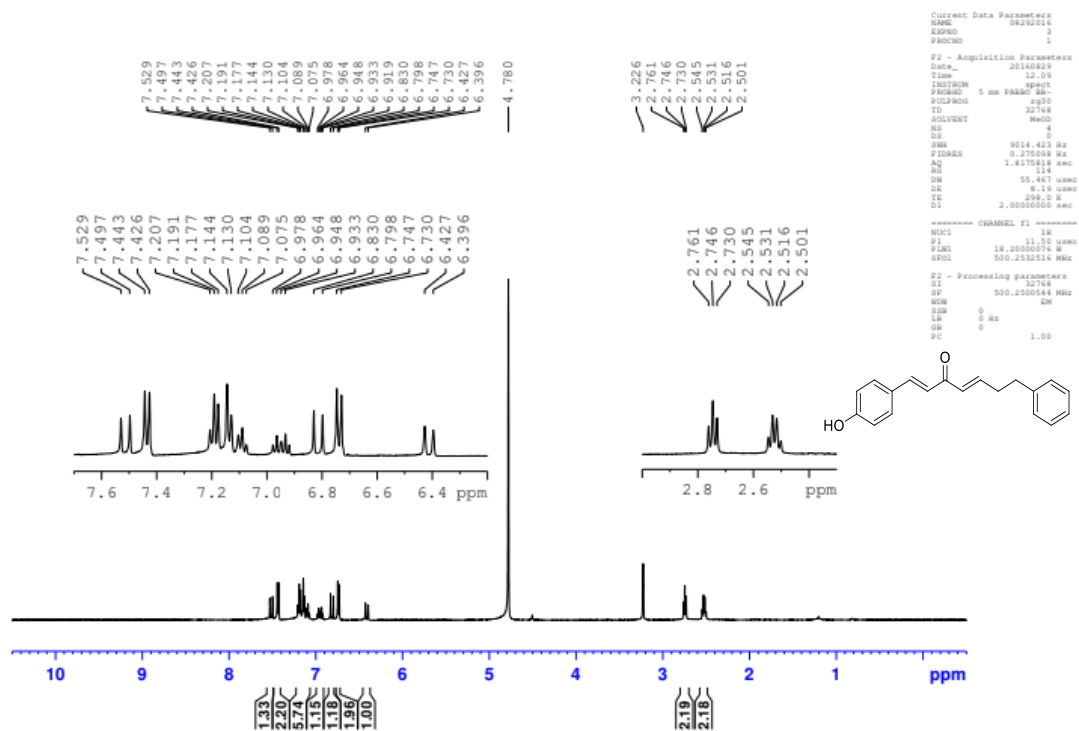
F2 - Processing parameters
SI 32768
SF 125.7677616 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

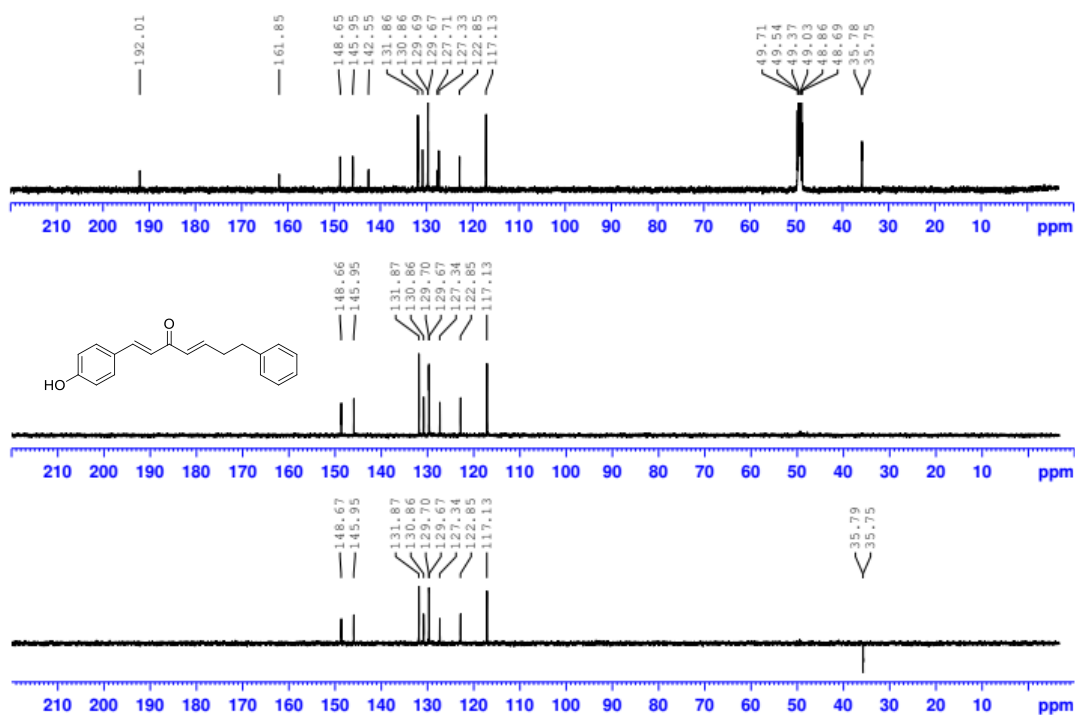


Compound 4a

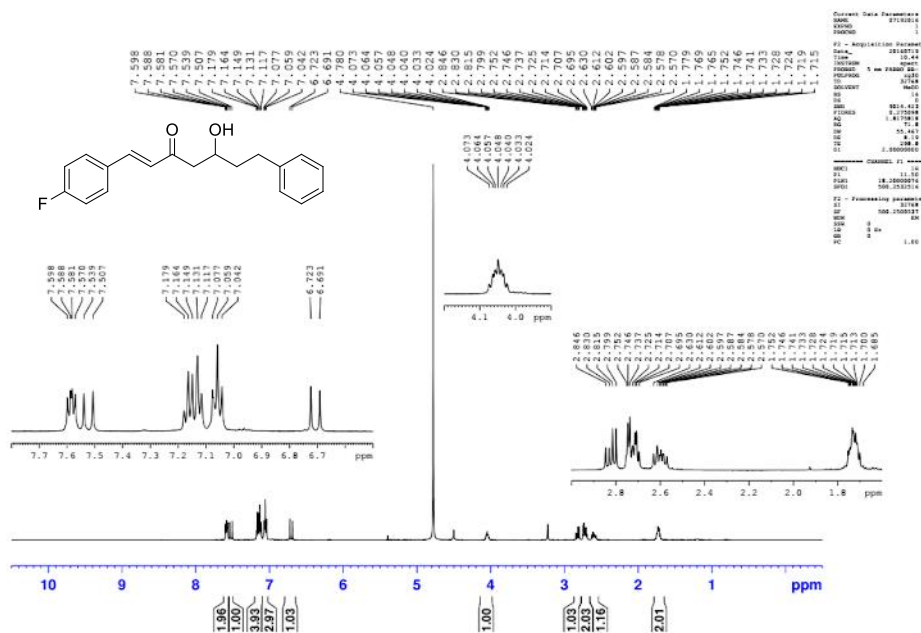


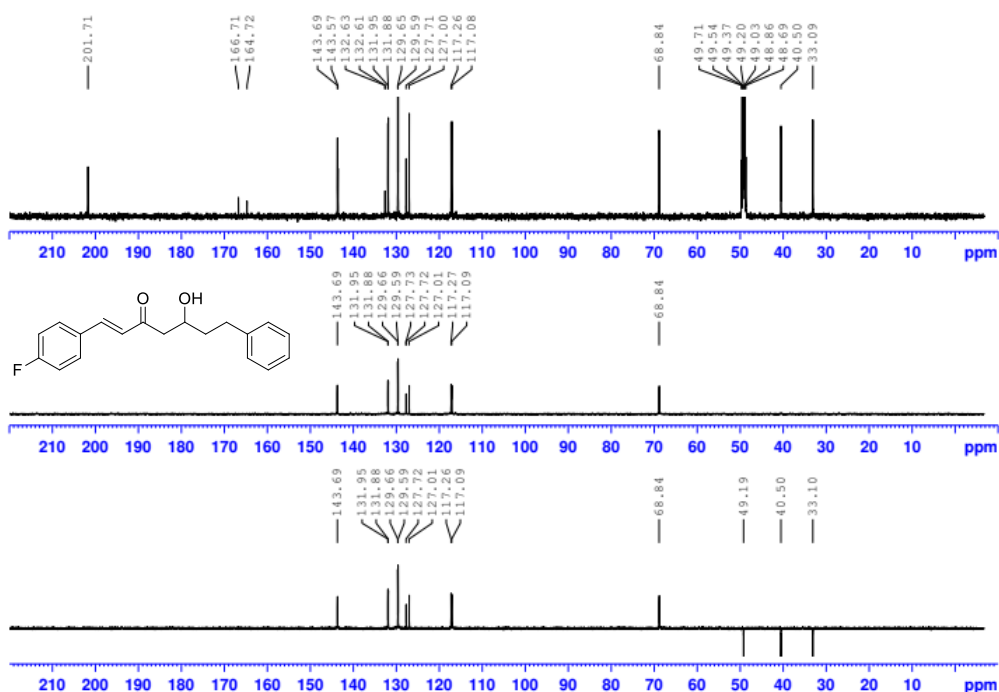
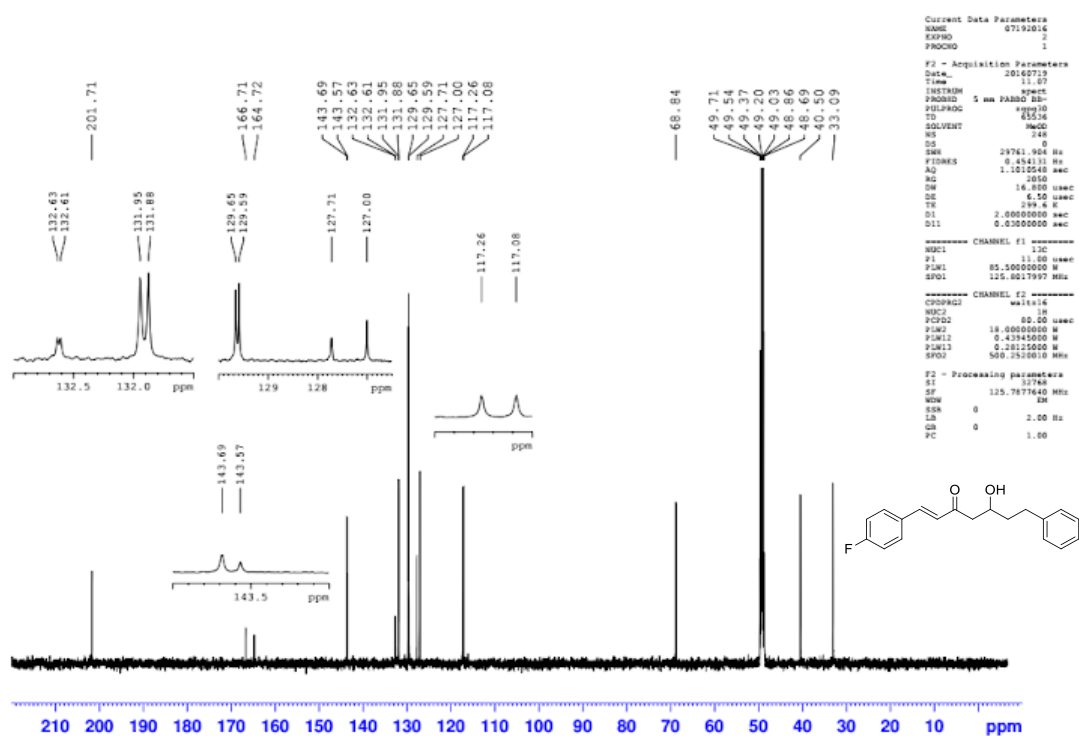




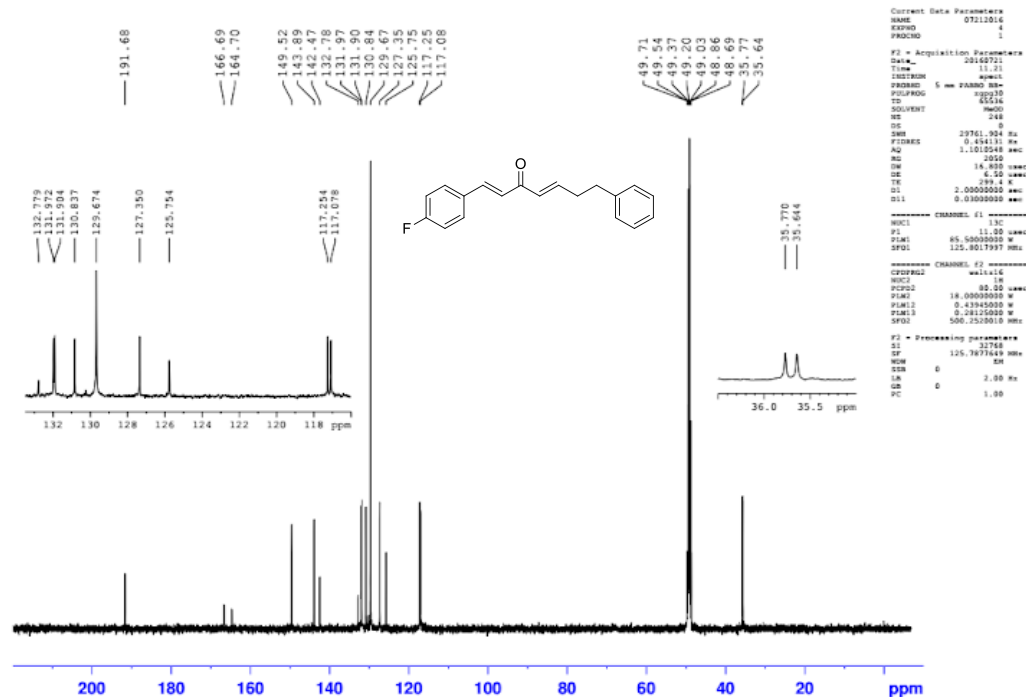
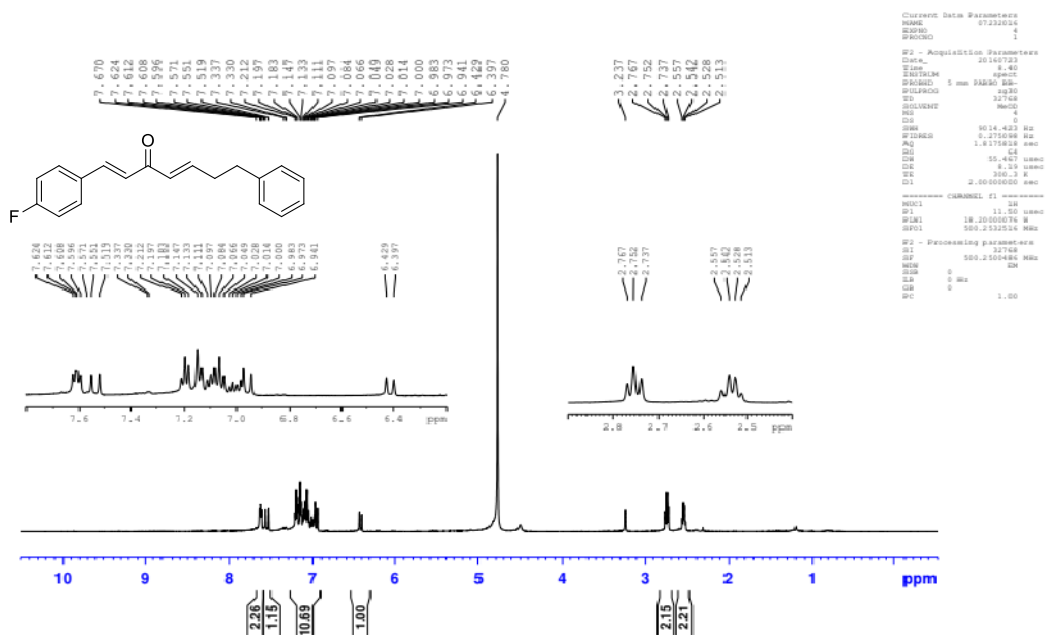


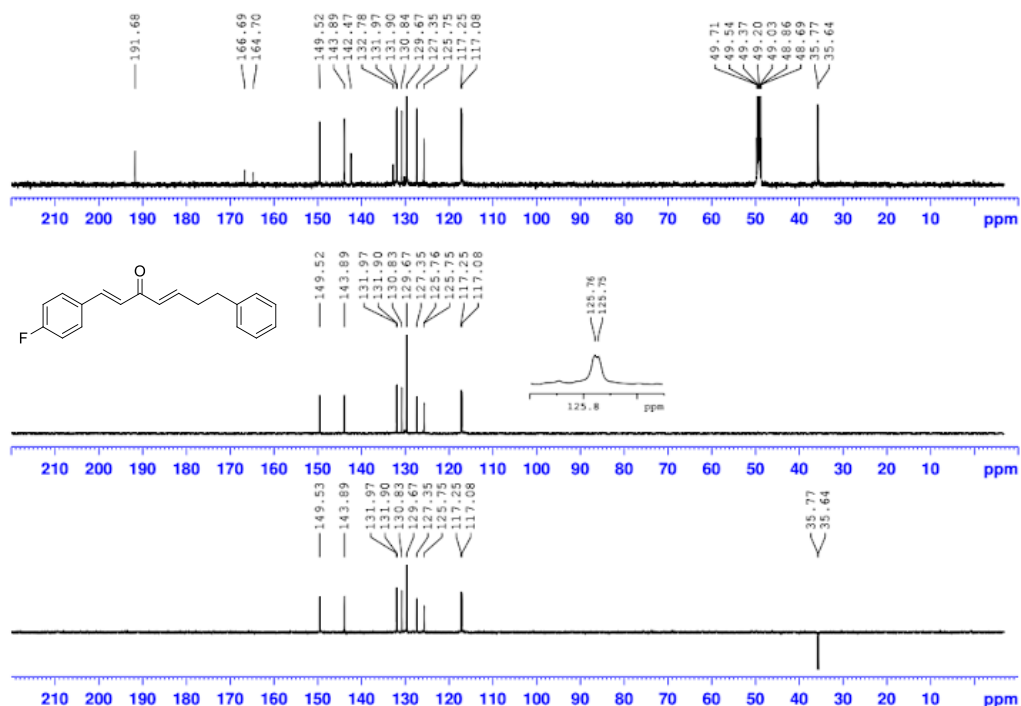
Compound 6



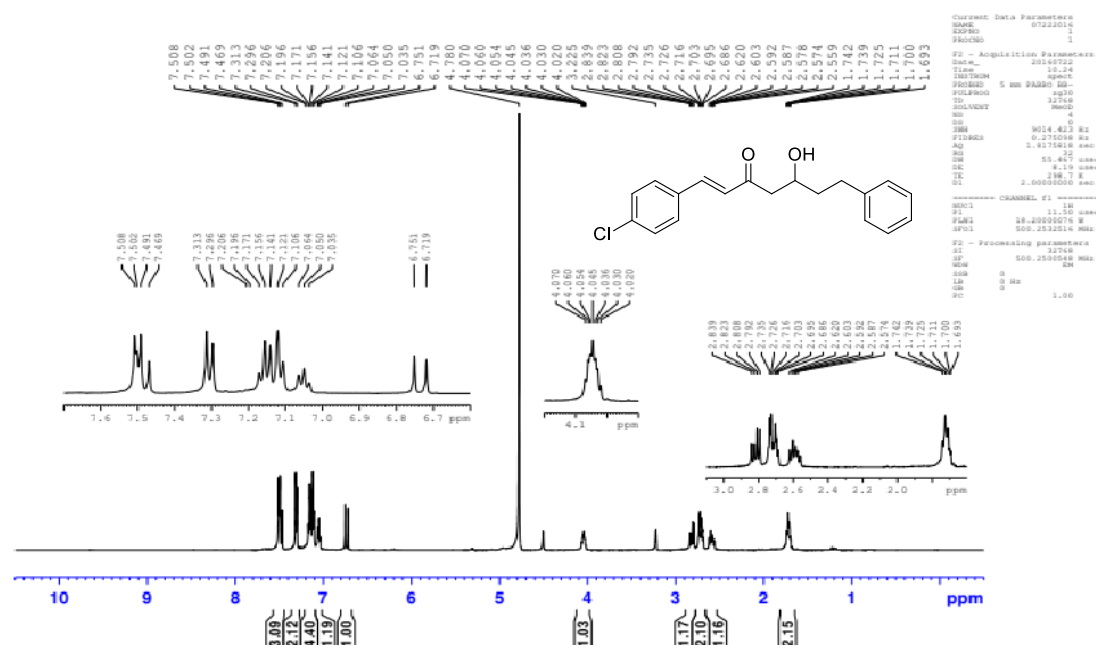


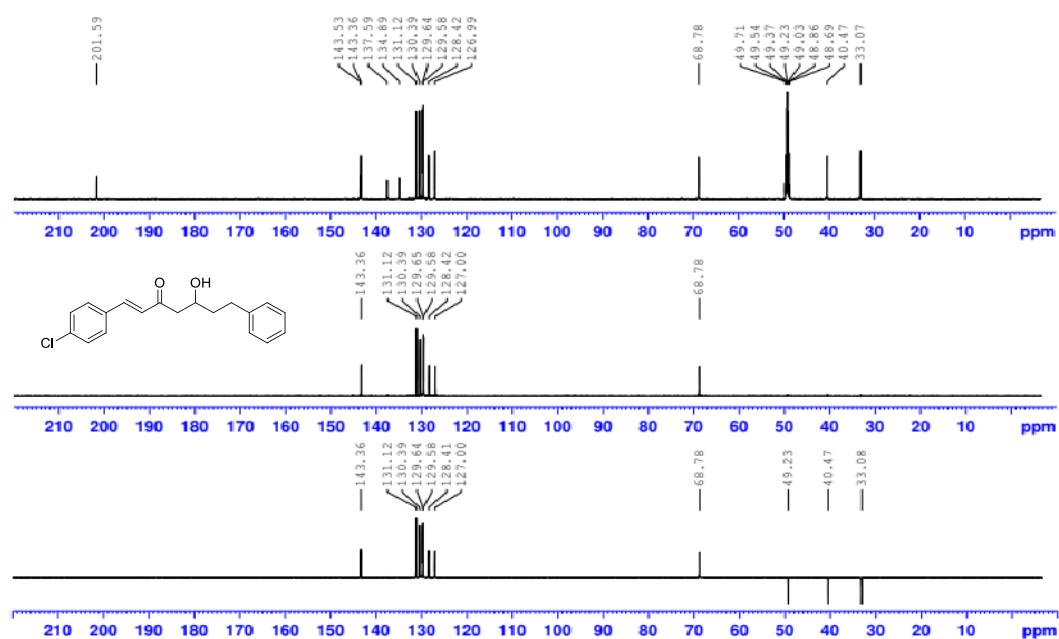
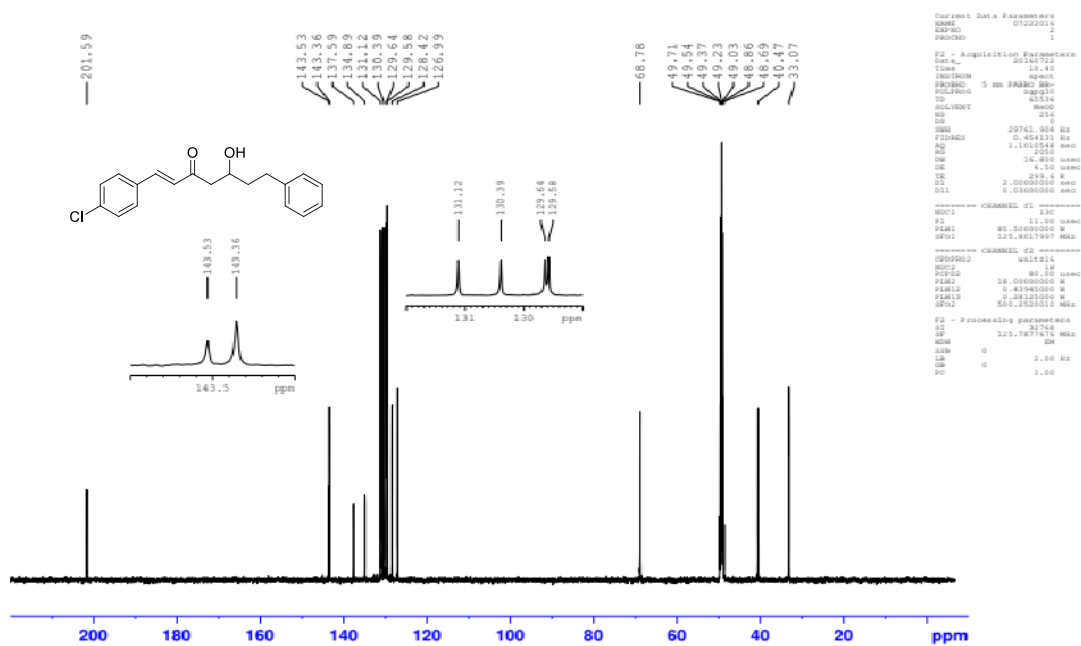
Compound 6a



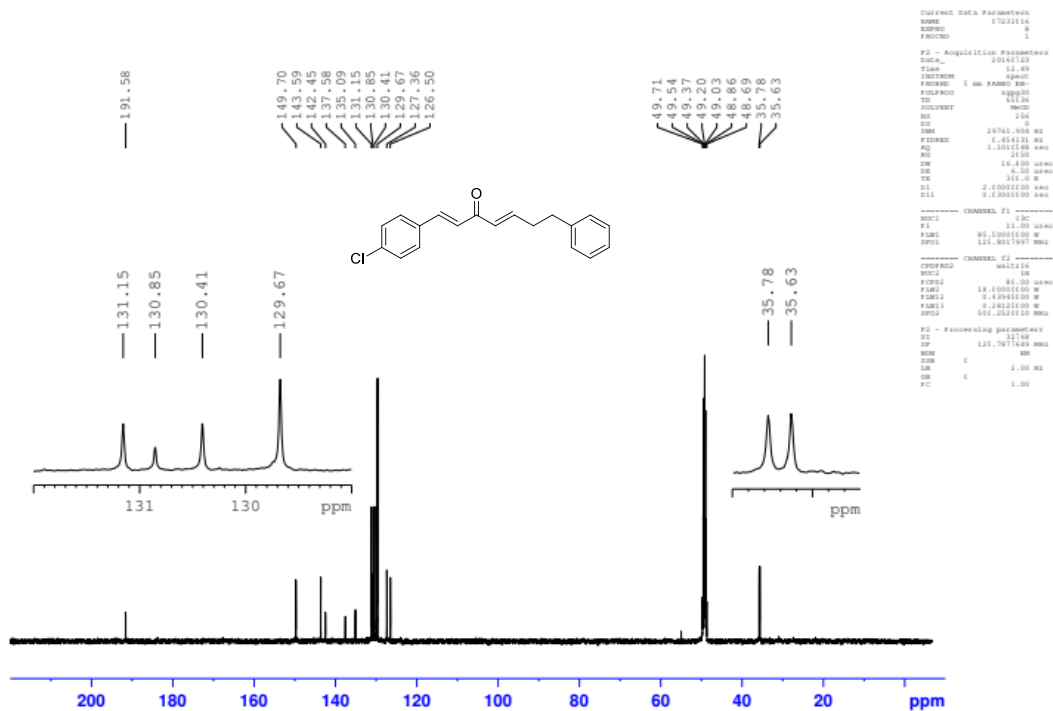
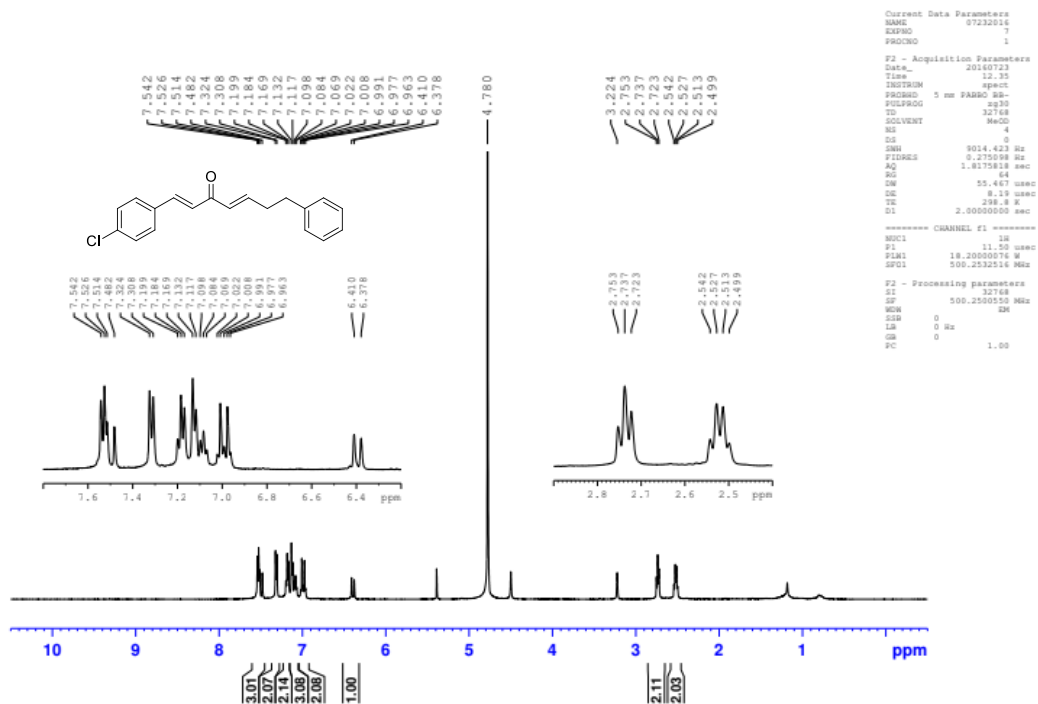


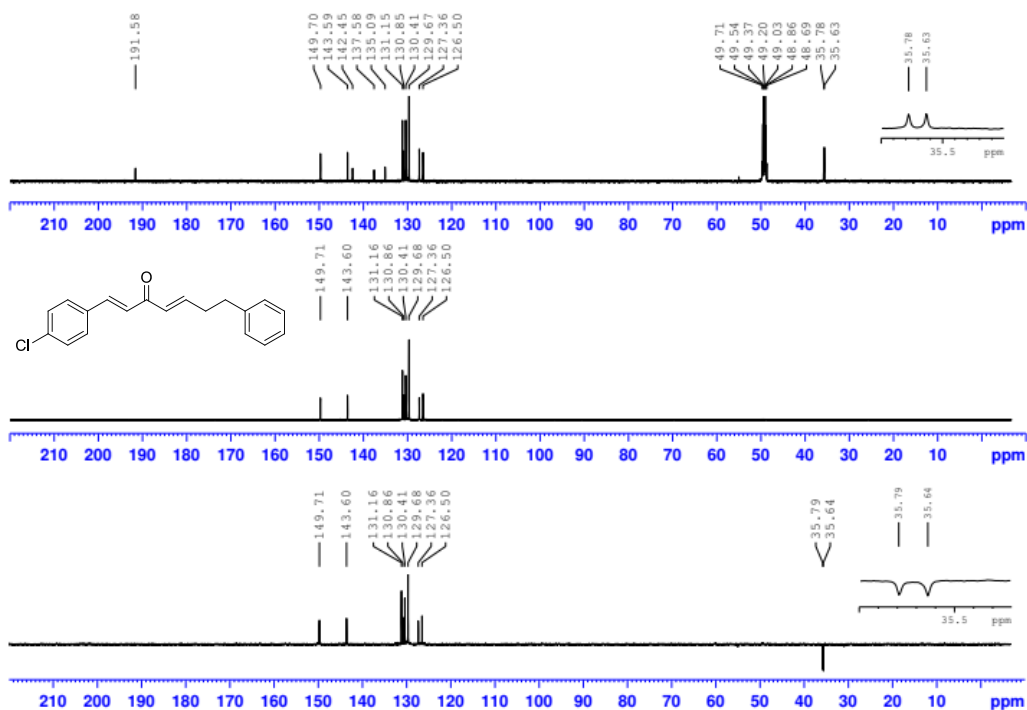
Compound 7



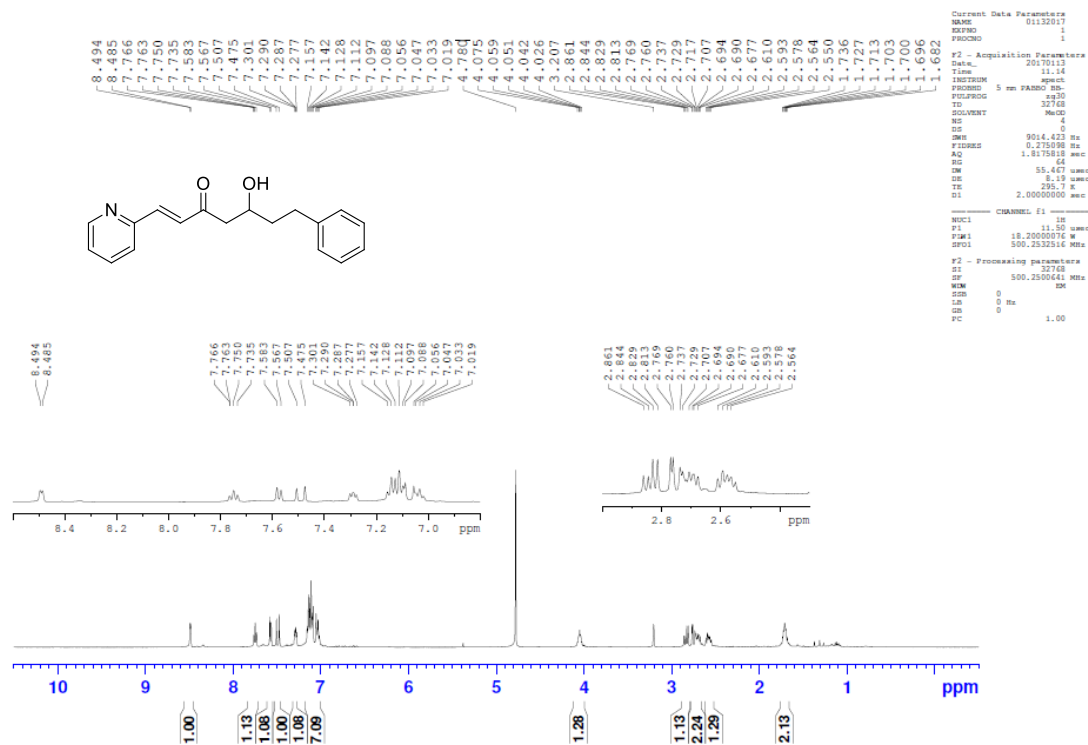


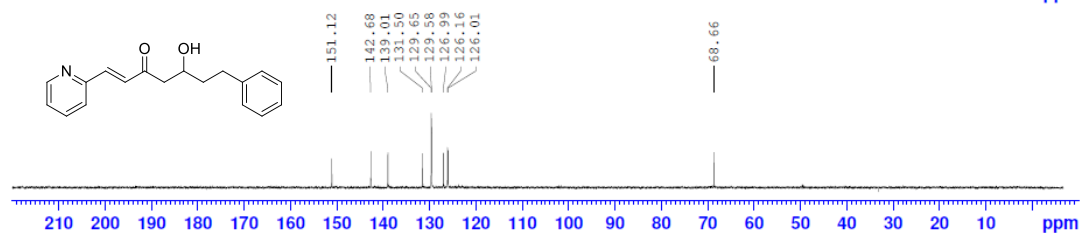
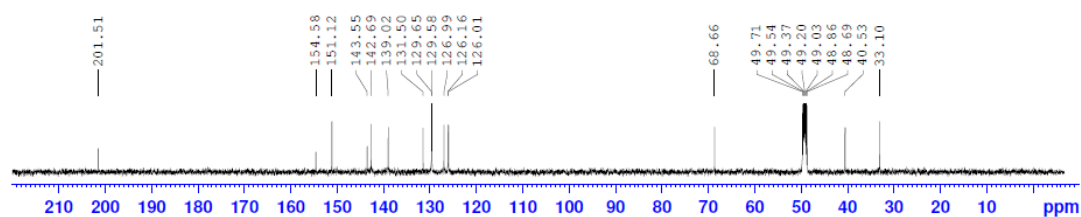
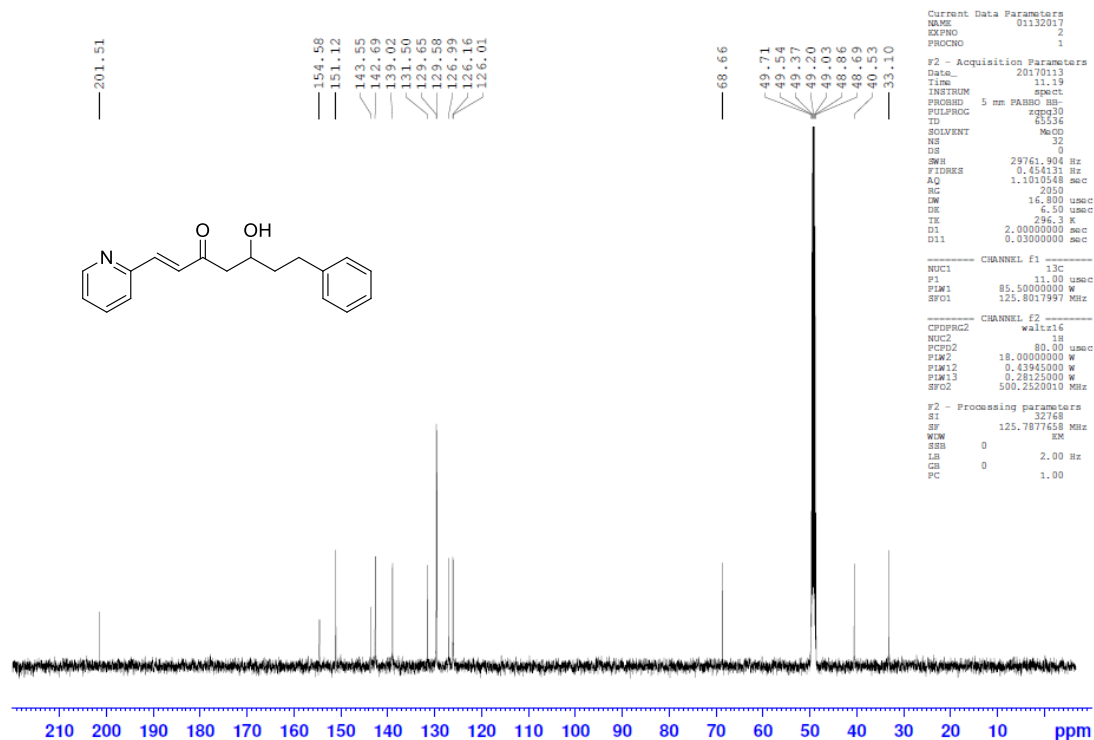
Compound 7a



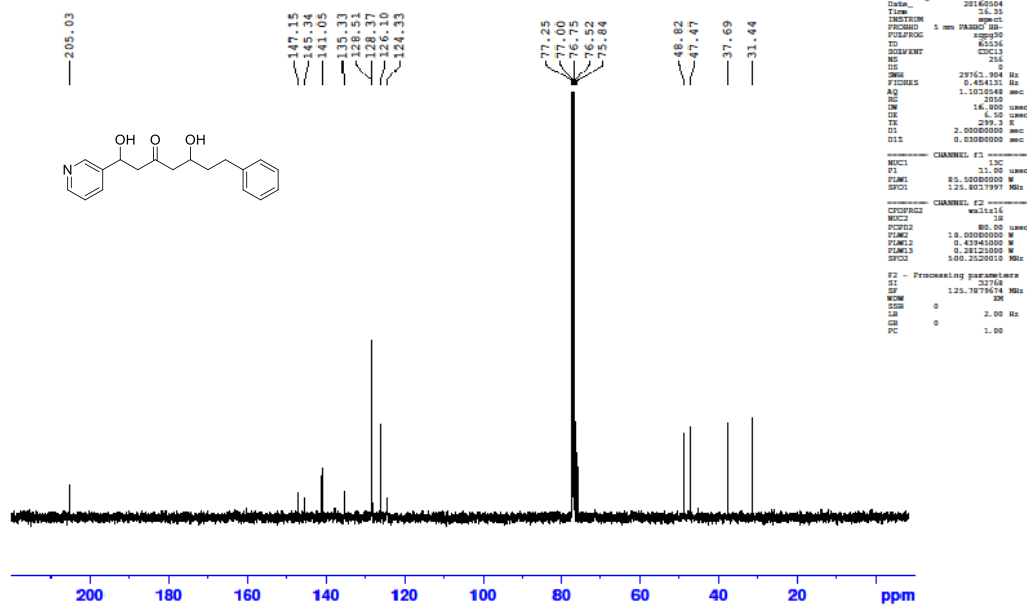
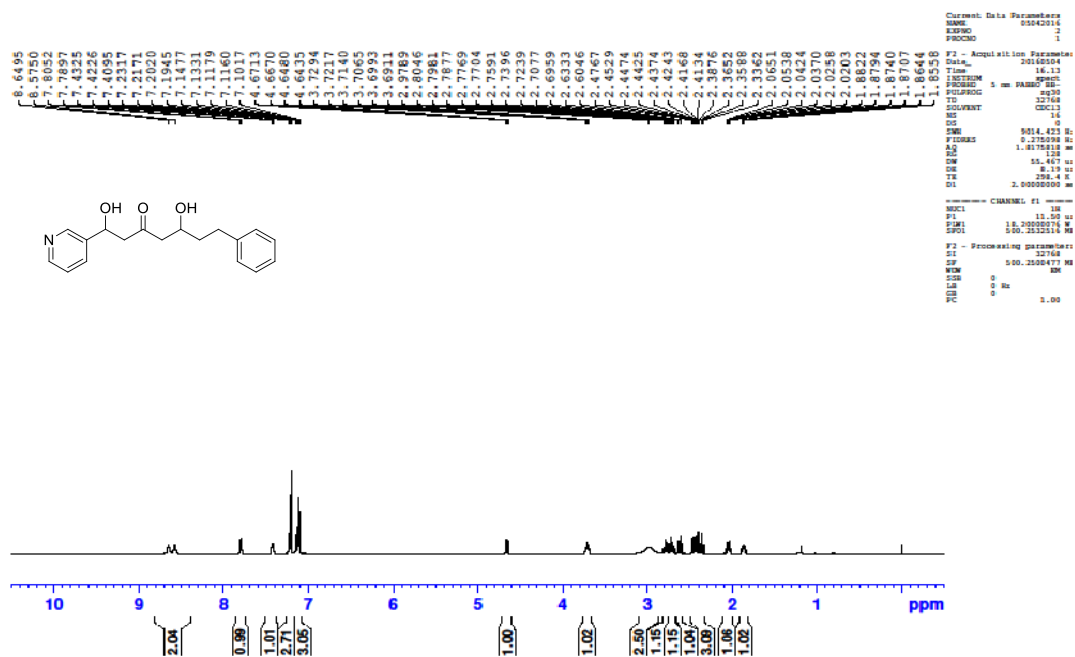


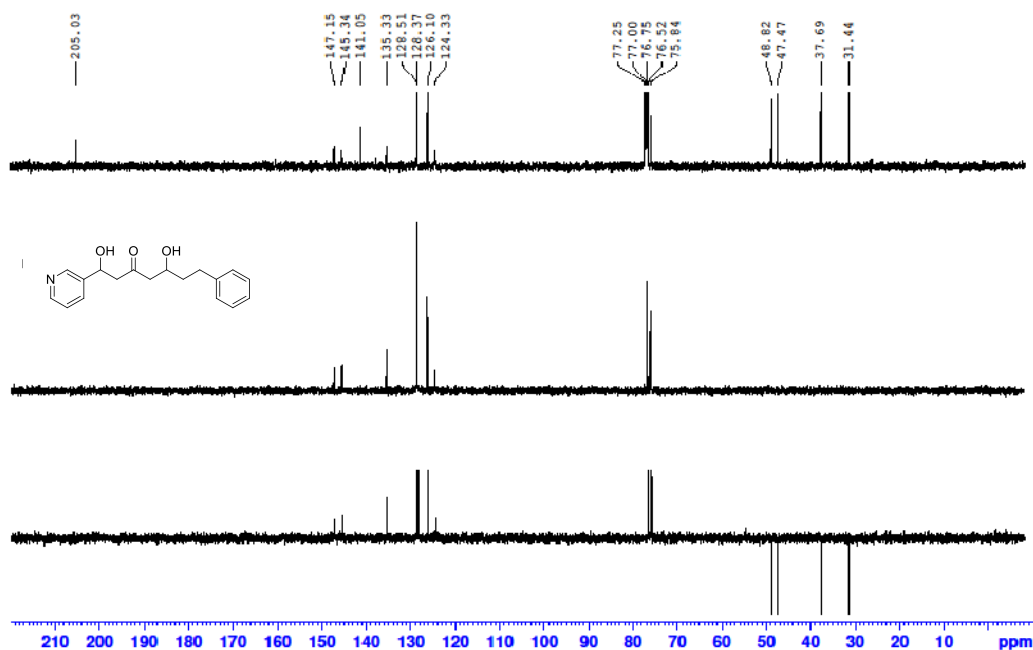
Compound 8



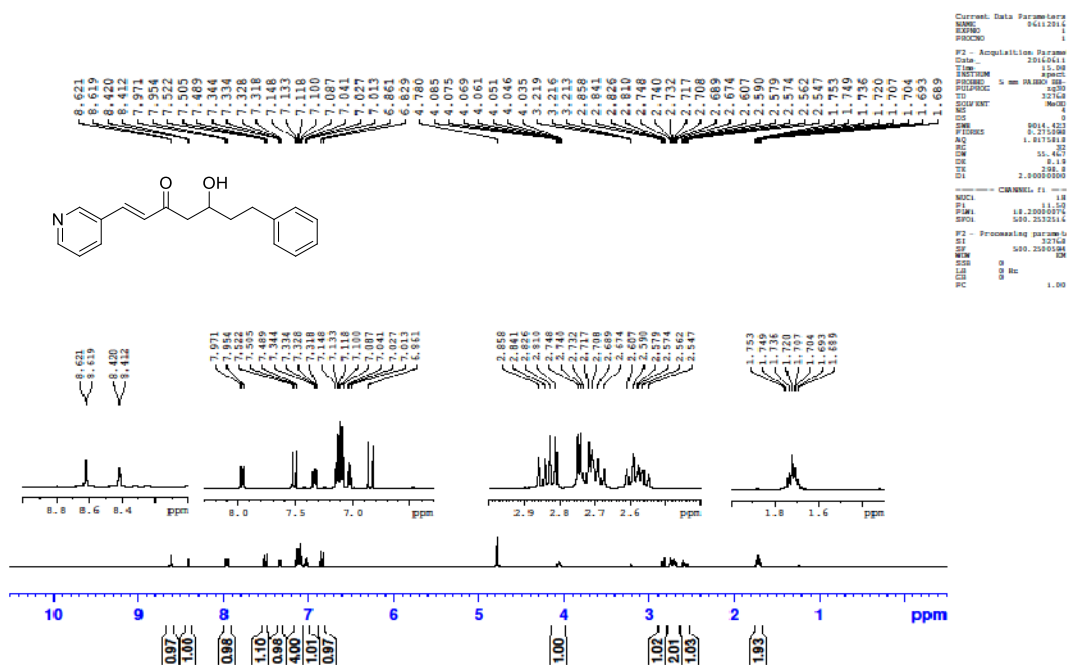


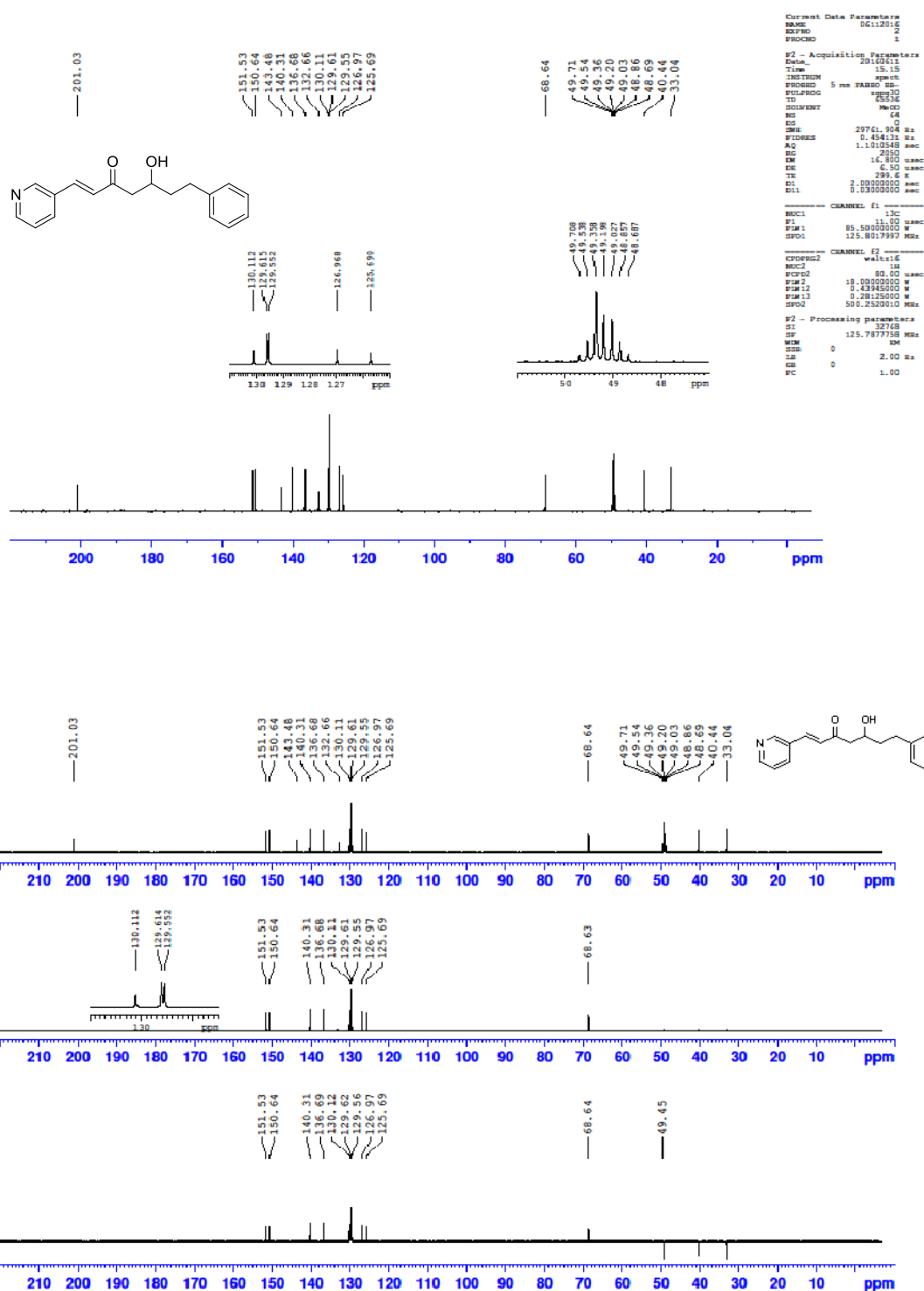
Compound 9



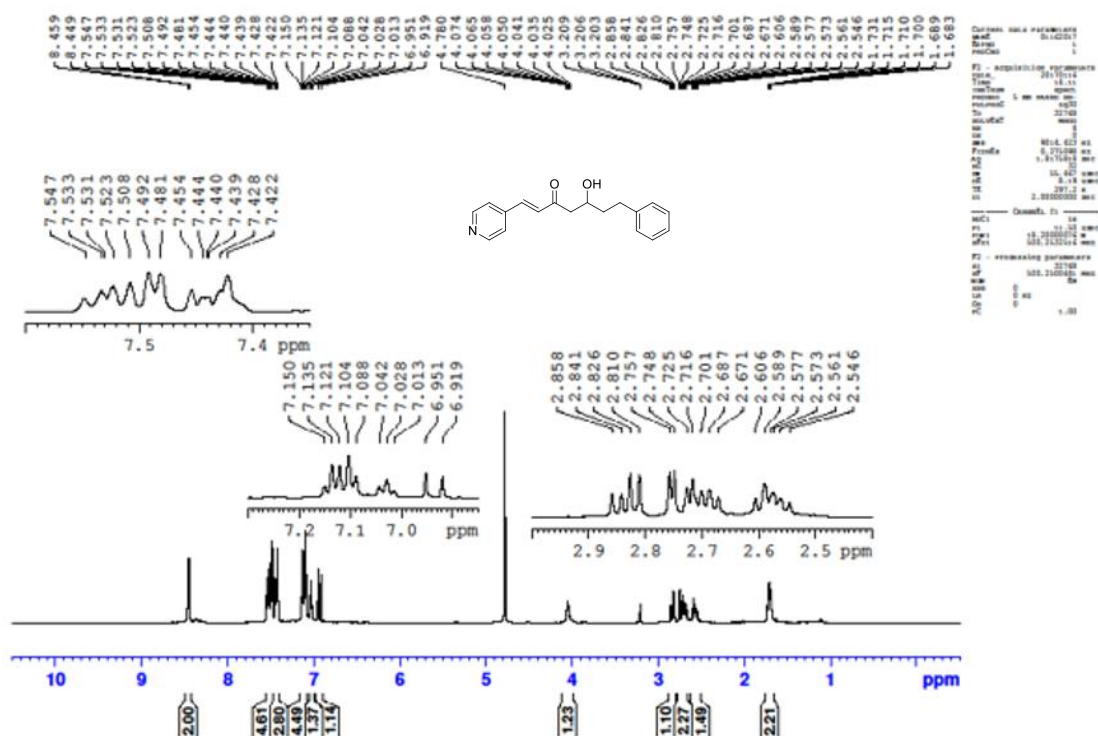


Compound 10

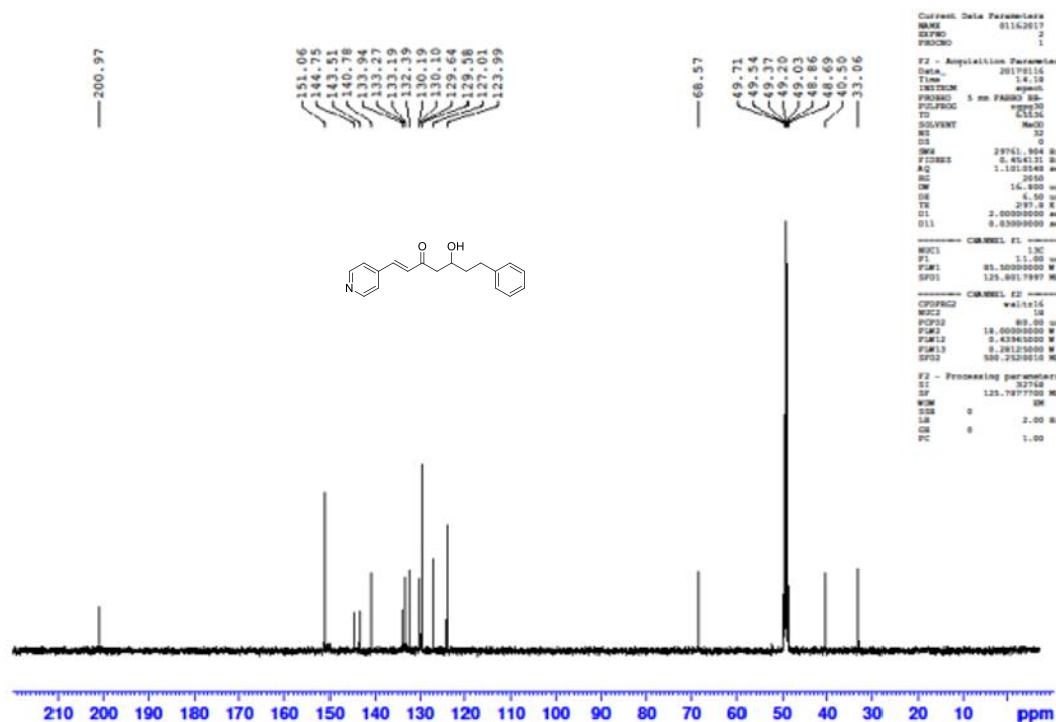




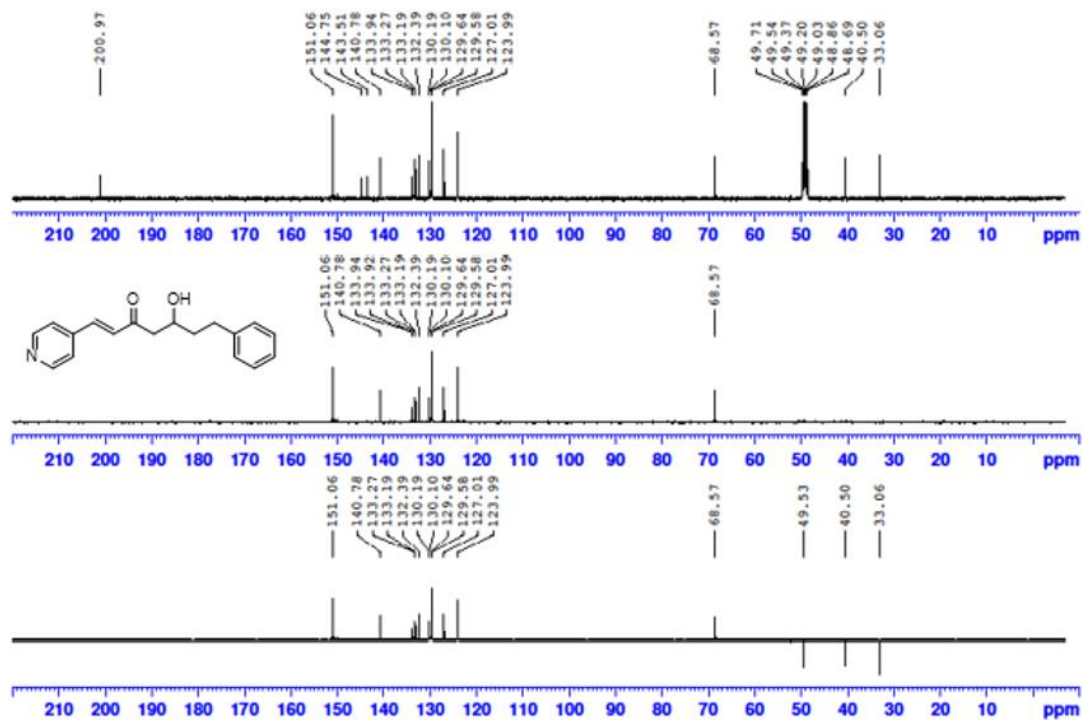
Compound 11



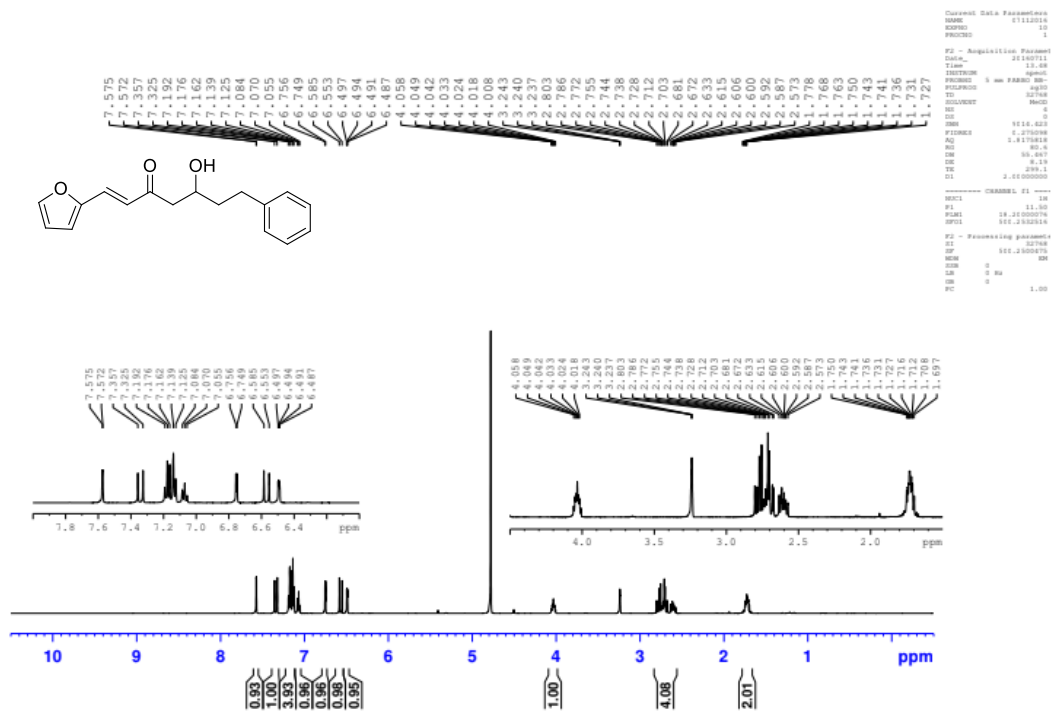
Current Data Parameters
 Name: 01162017
 Date: 10/10/16
 Time: 14:11
 Location: 400MHz
 Sample: 1
 Volume: 0.500
 Concent: 0.500
 Solvent: MeOH
 NS: 2
 DS: 4
 SWH: 6014.875 Hz
 FIDRES: 0.271266 Hz
 AQ: 1.8716151 sec
 RG: 327.40
 GB: 0
 PC: 0
 LB: 0.0000000 Hz
 GB: 0
 PC: 0
 LB: 0.0000000 Hz
 GB: 0
 PC: 0

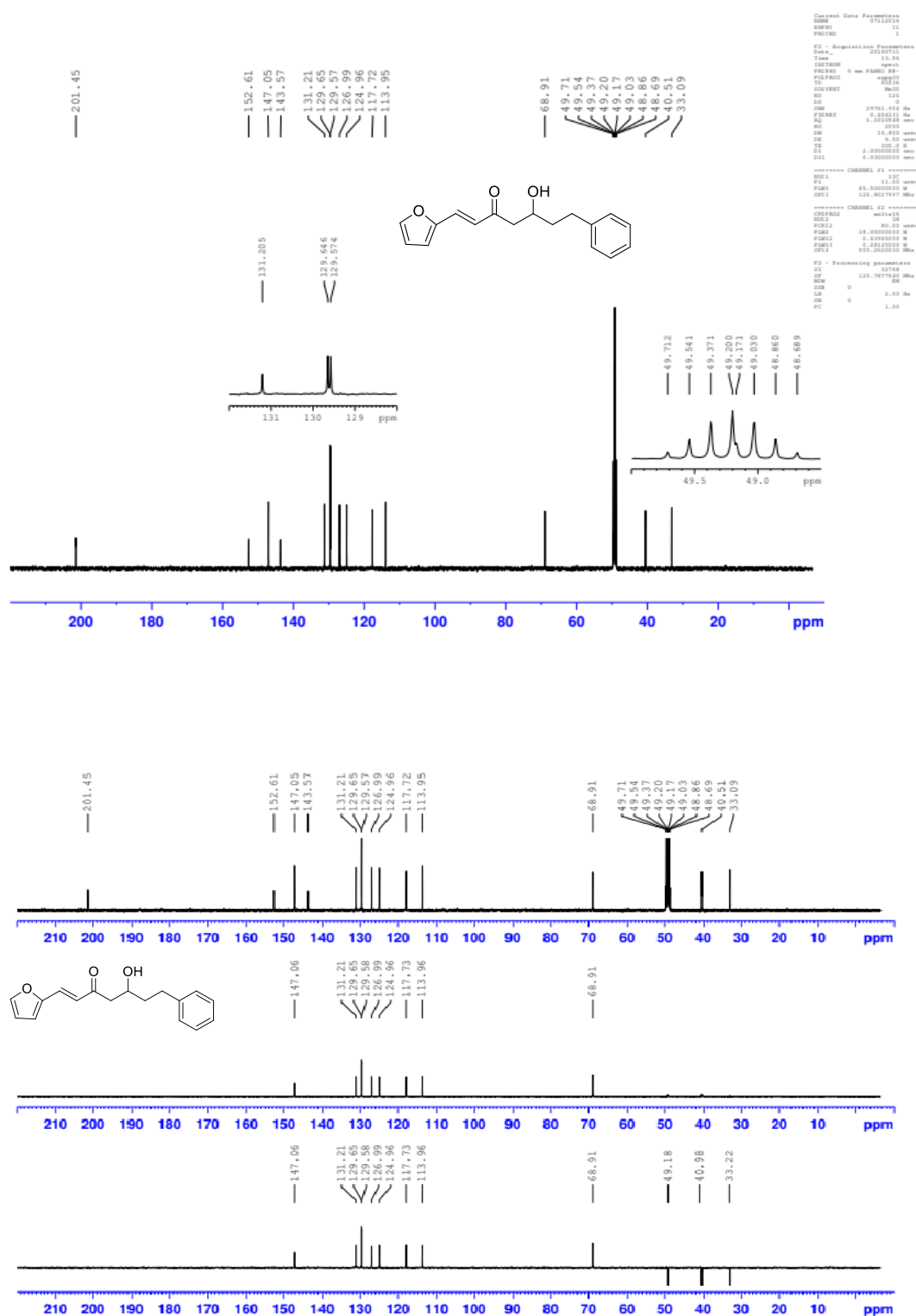


Current Data Parameters
 Name: 01162017
 Date: 10/10/16
 Time: 14:18
 Location: 400MHz
 Sample: 1
 Volume: 0.500
 Concent: 0.500
 Solvent: MeOH
 NS: 2
 DS: 4
 SWH: 6014.875 Hz
 FIDRES: 0.271266 Hz
 AQ: 1.8716151 sec
 RG: 327.40
 GB: 0
 PC: 0
 LB: 0.0000000 Hz
 GB: 0
 PC: 0
 LB: 0.0000000 Hz
 GB: 0
 PC: 0

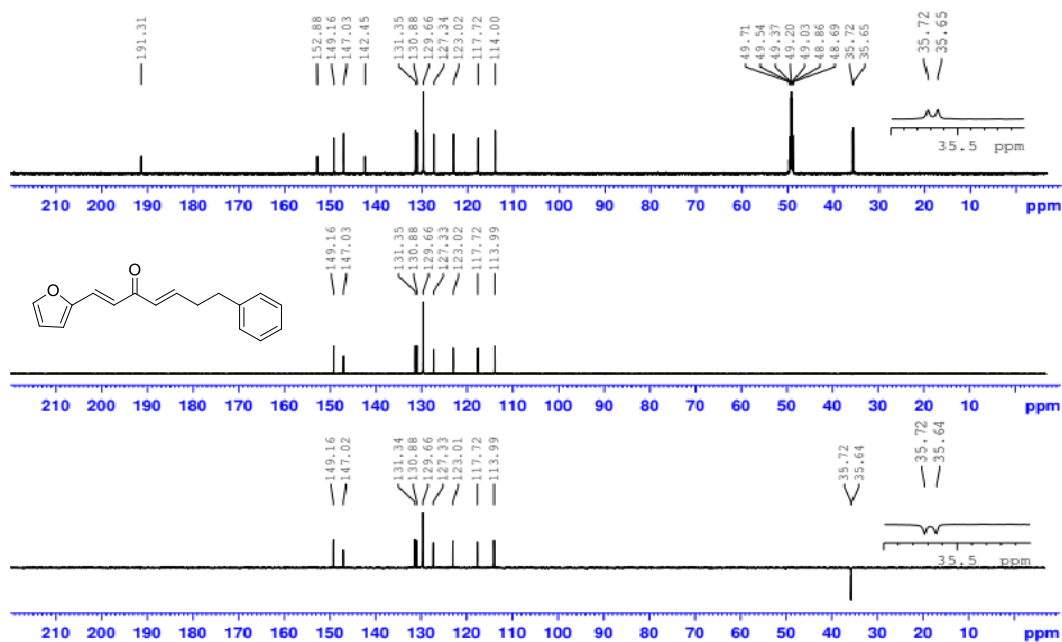


Compound 12

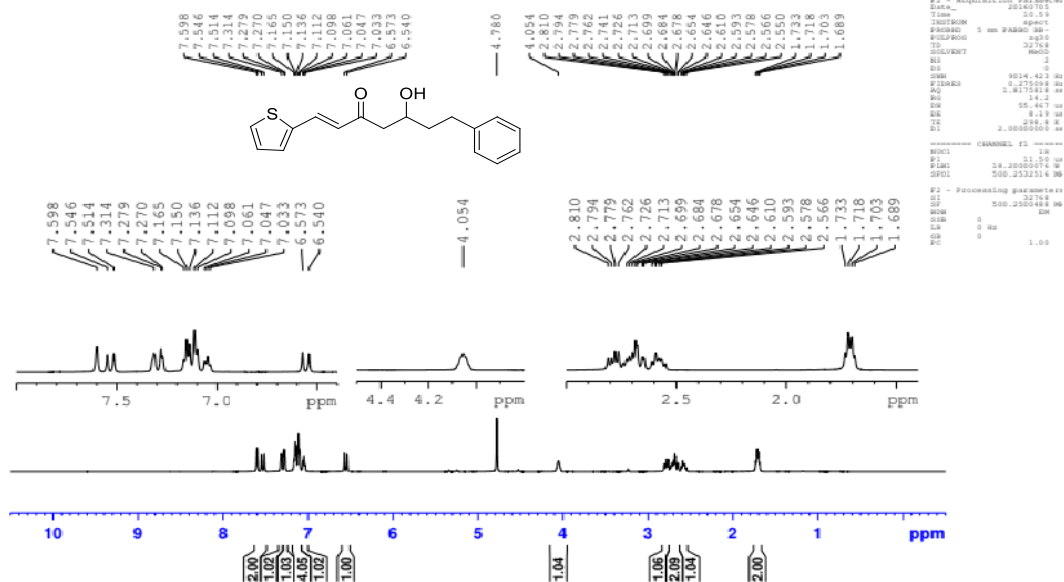


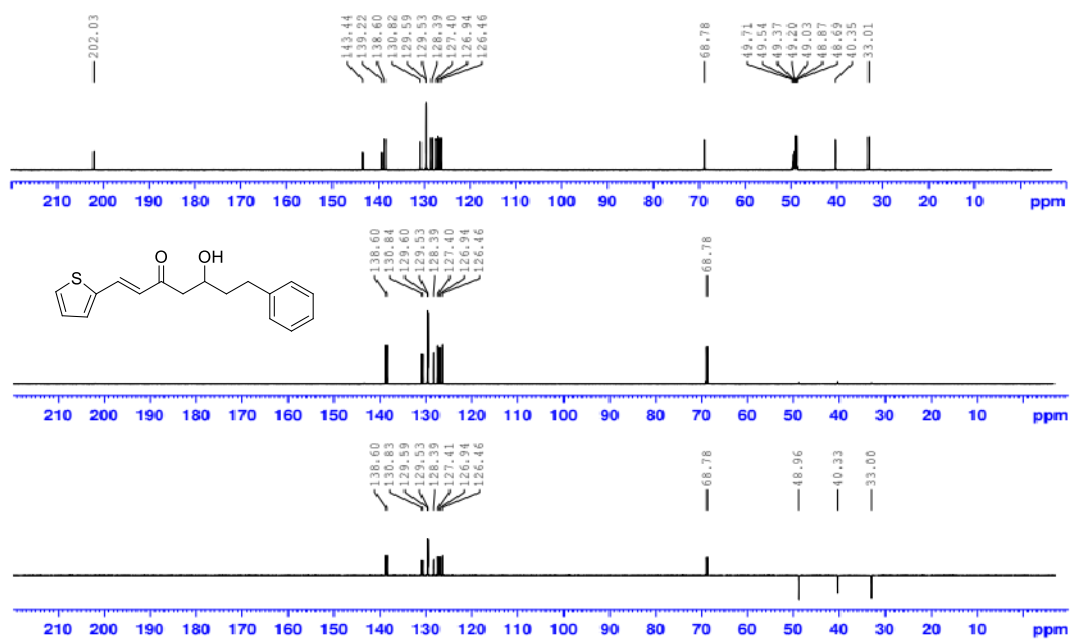
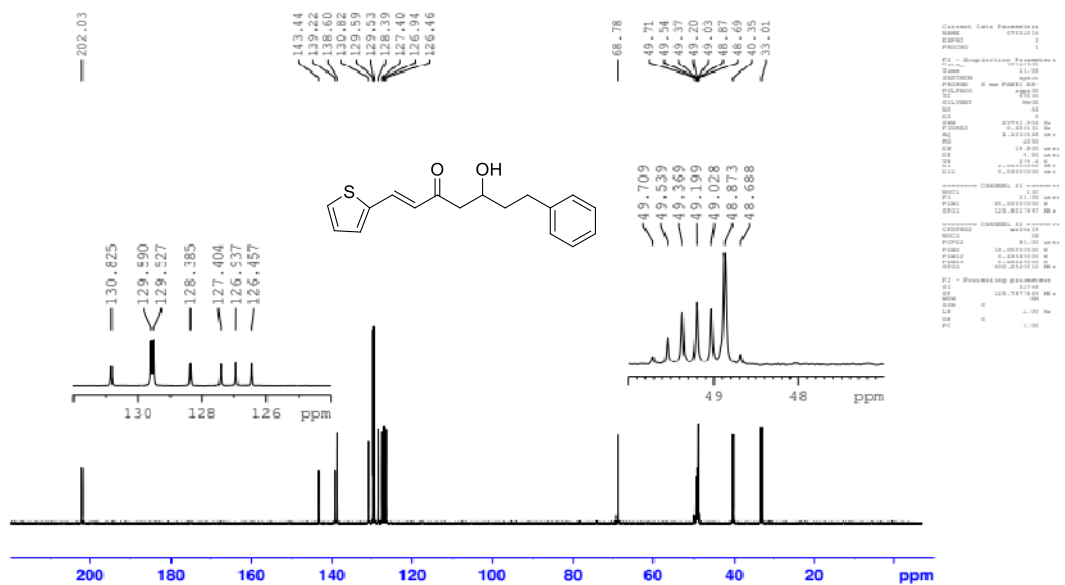


Compound 12a

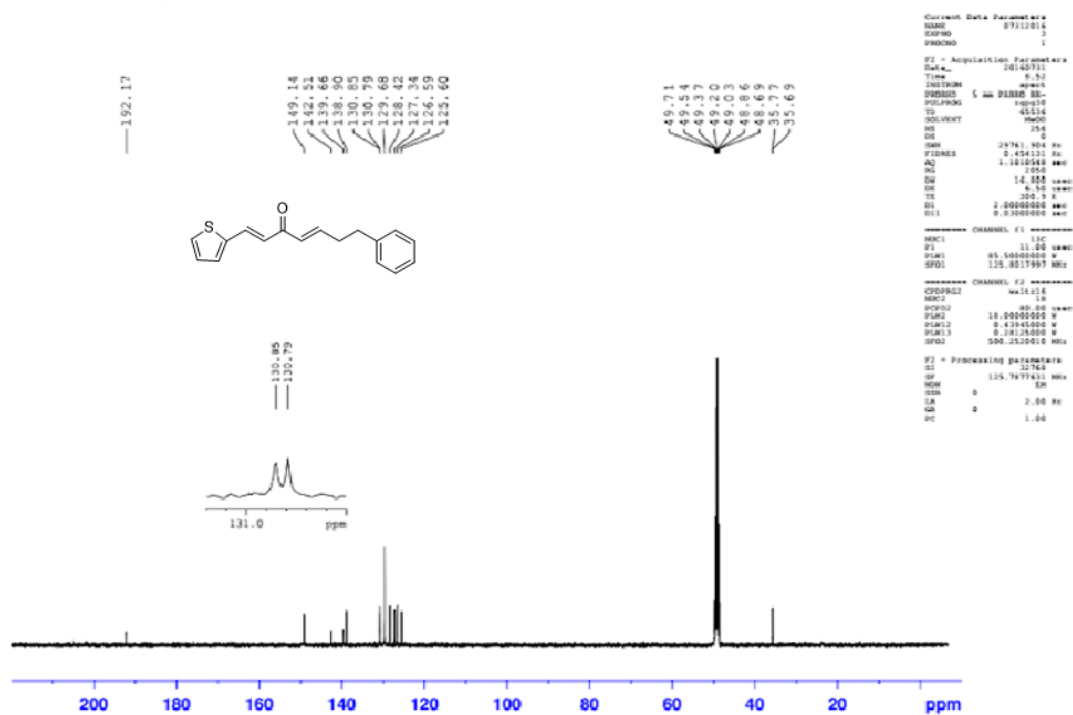
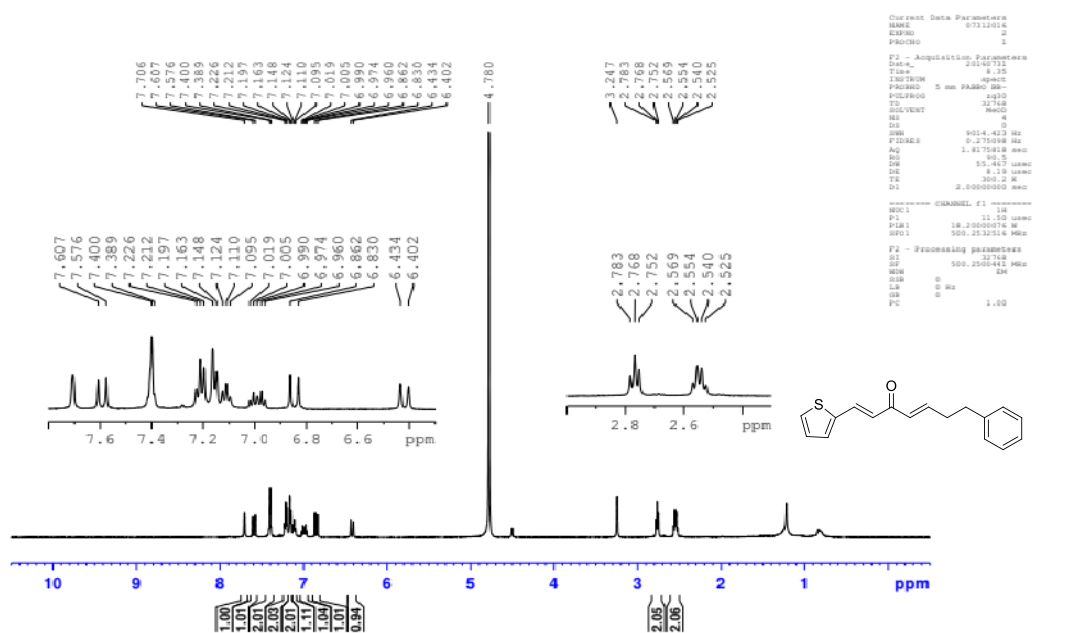


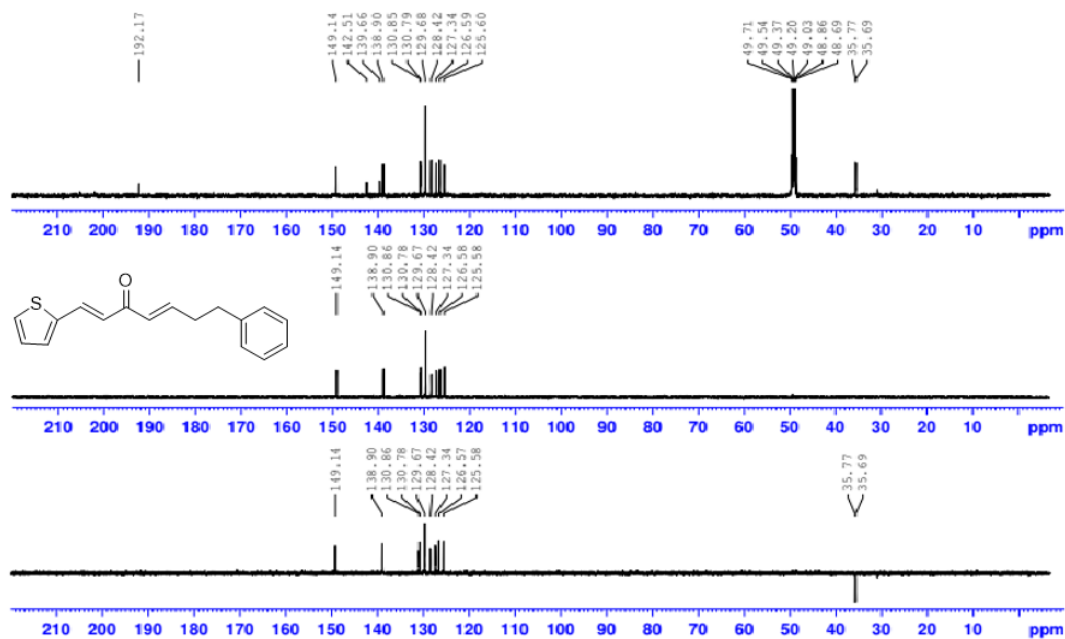
Compound 14



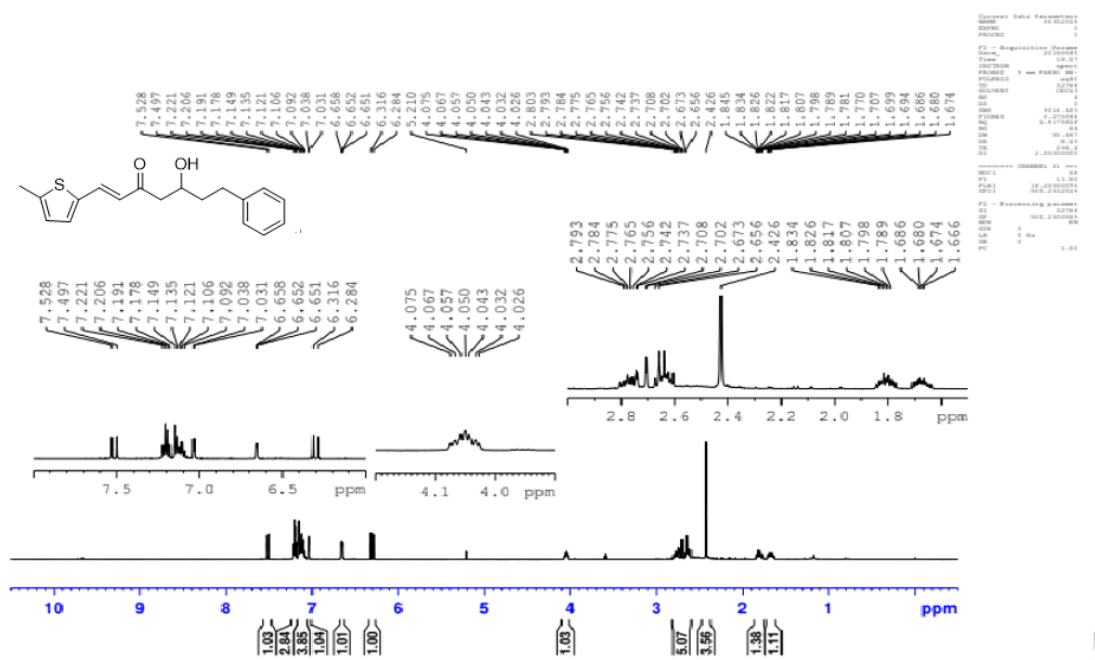


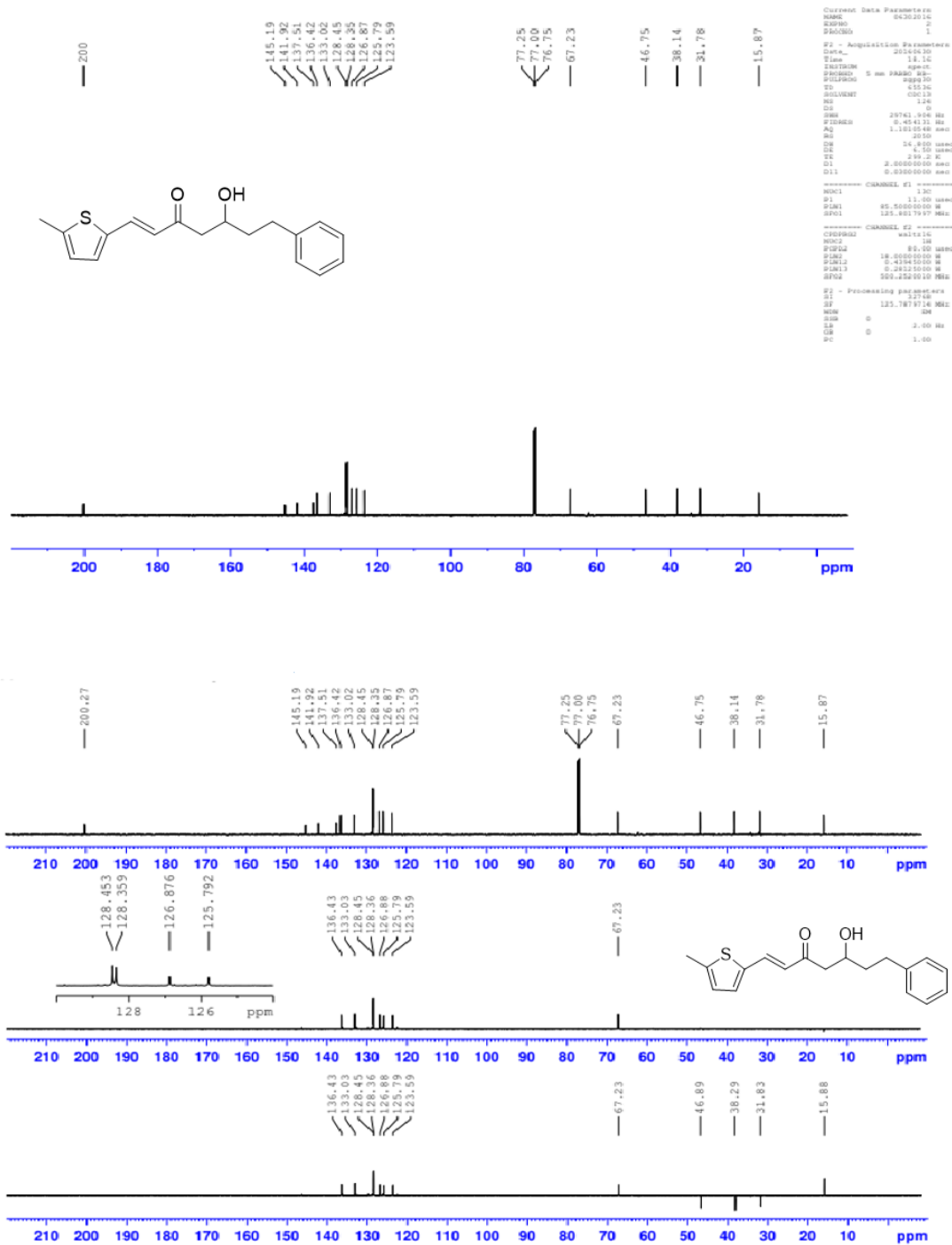
Compound 14a



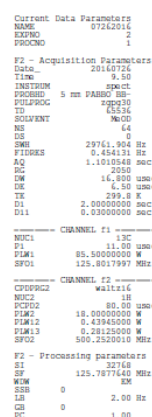
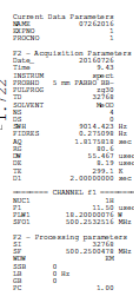


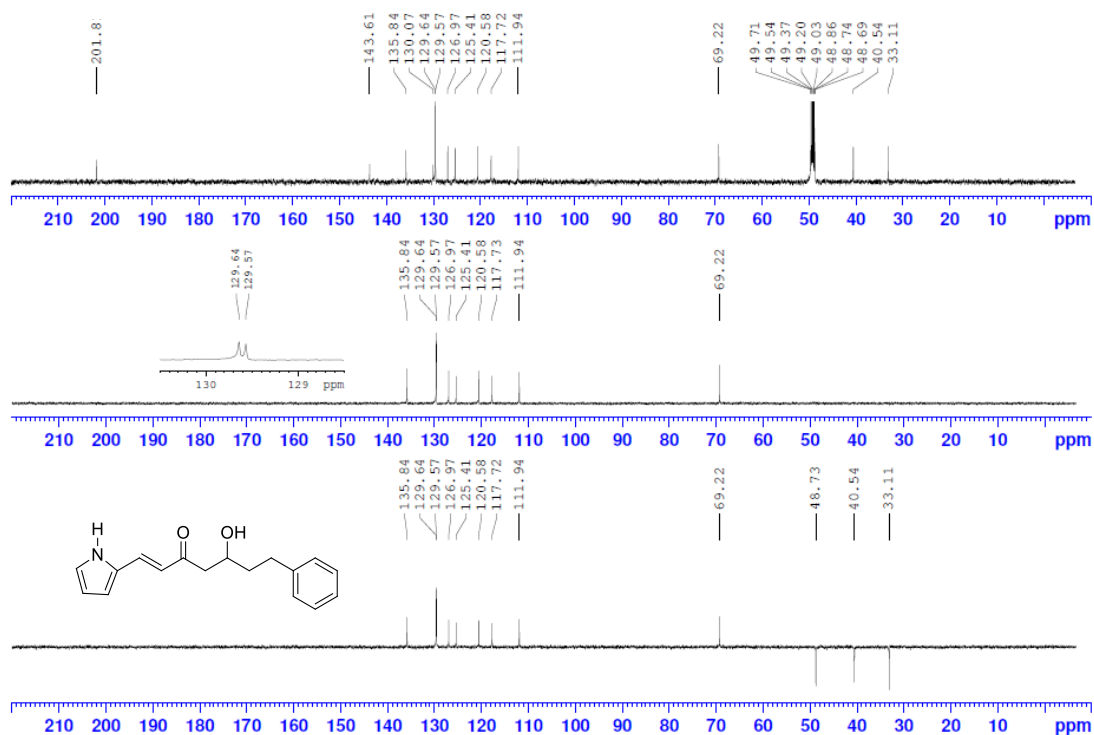
Compound 15



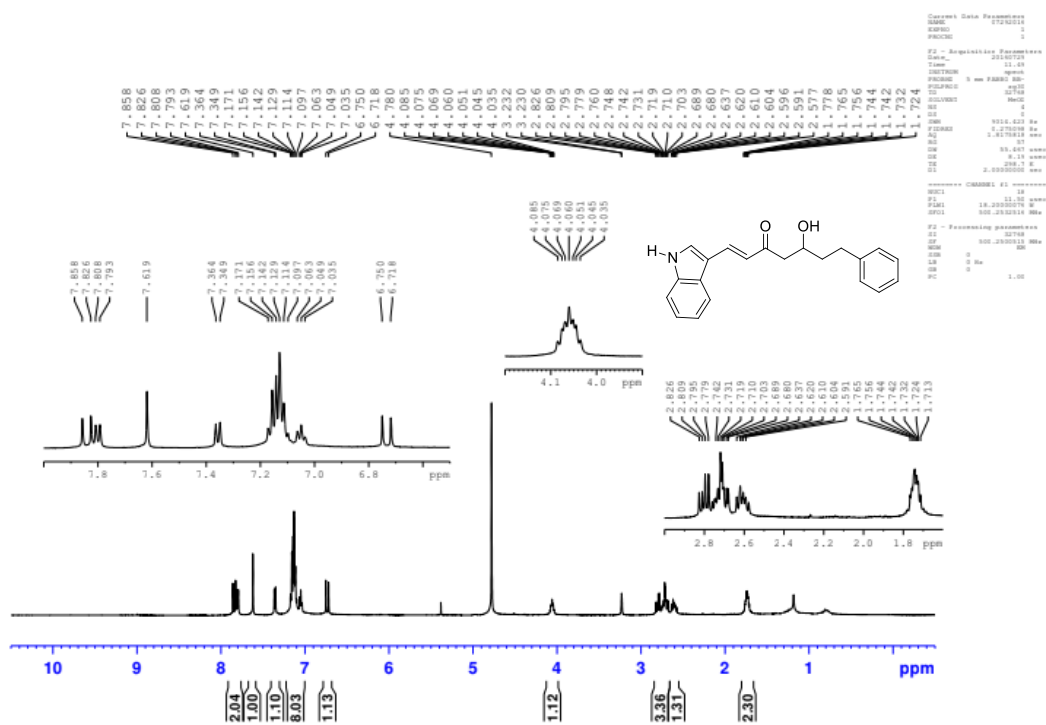


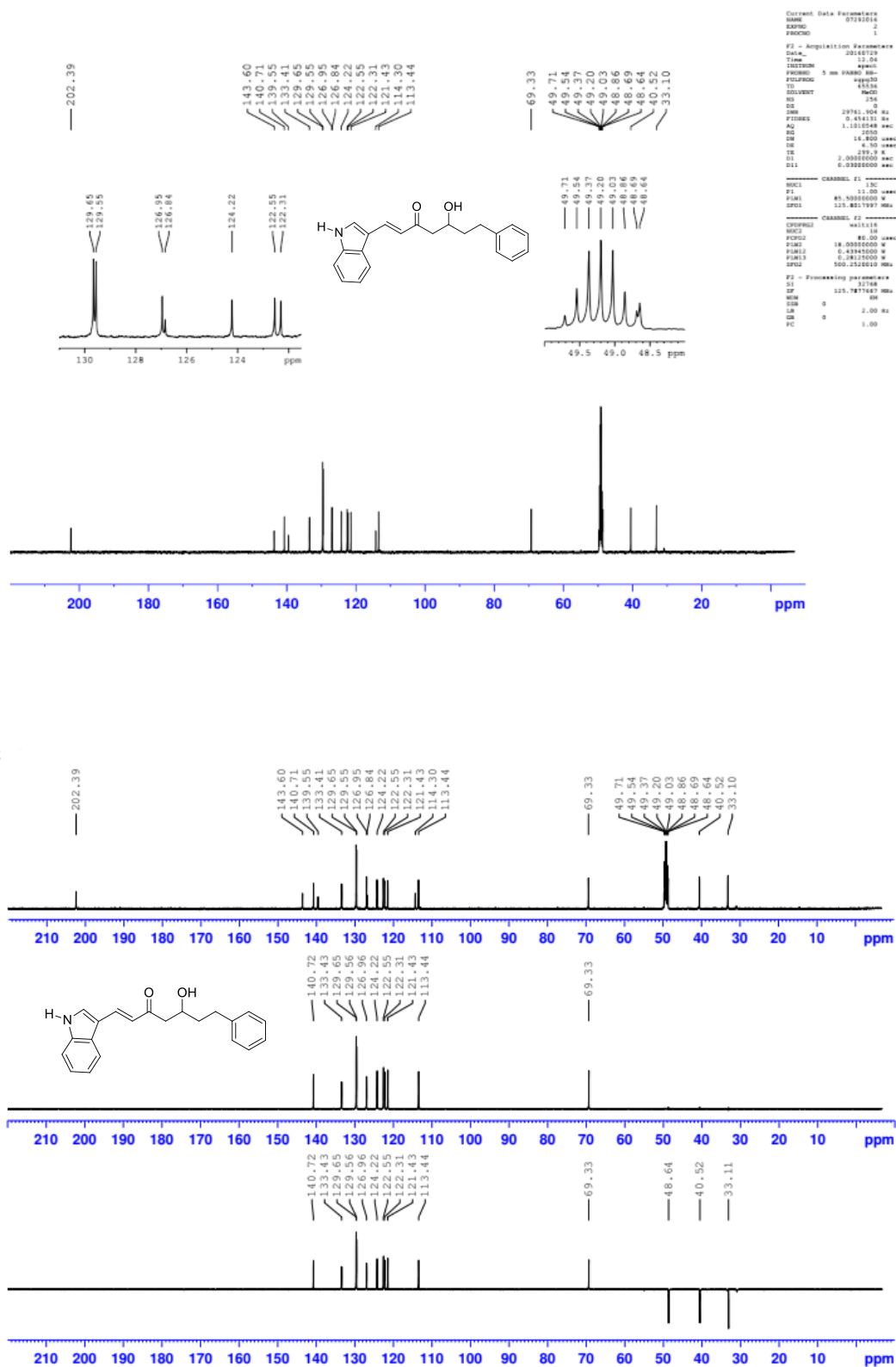
Compound 16





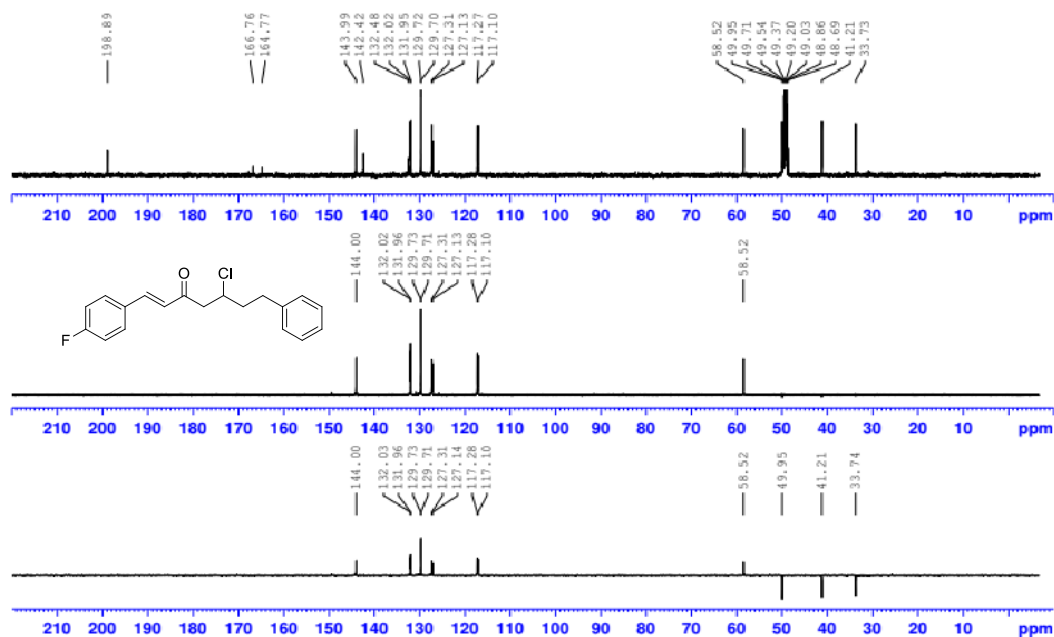
Compound 17



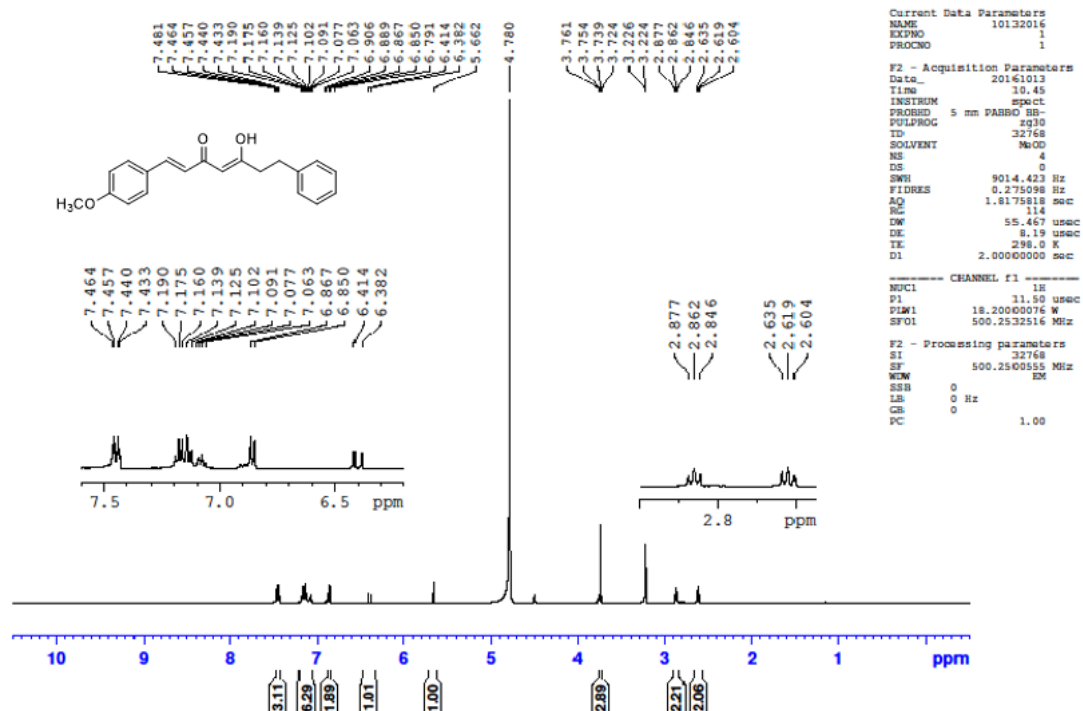


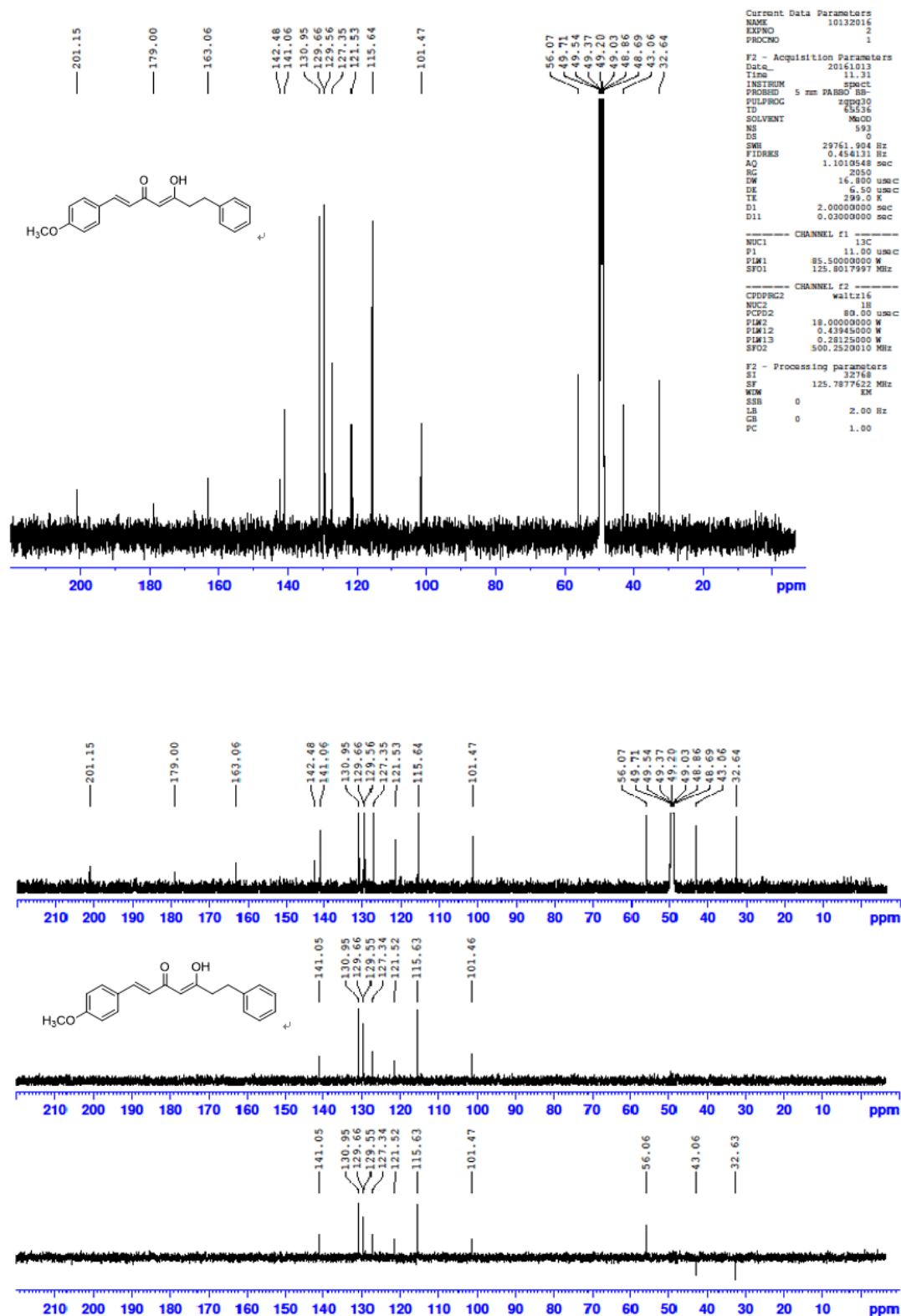
Compound 18



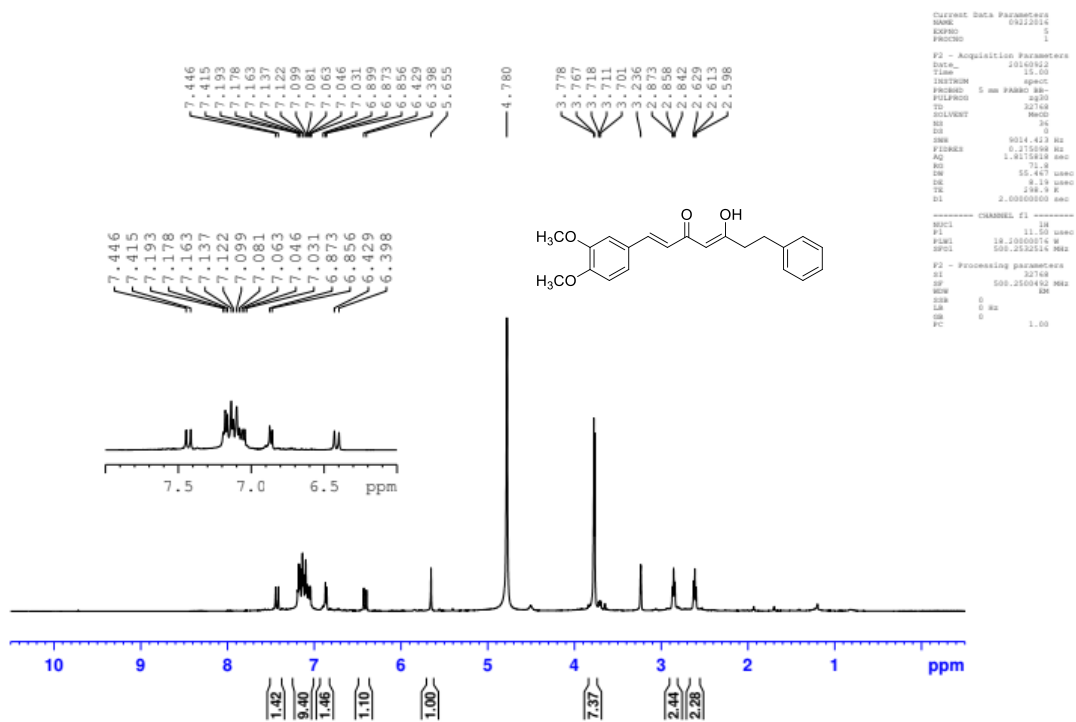


Compound 20

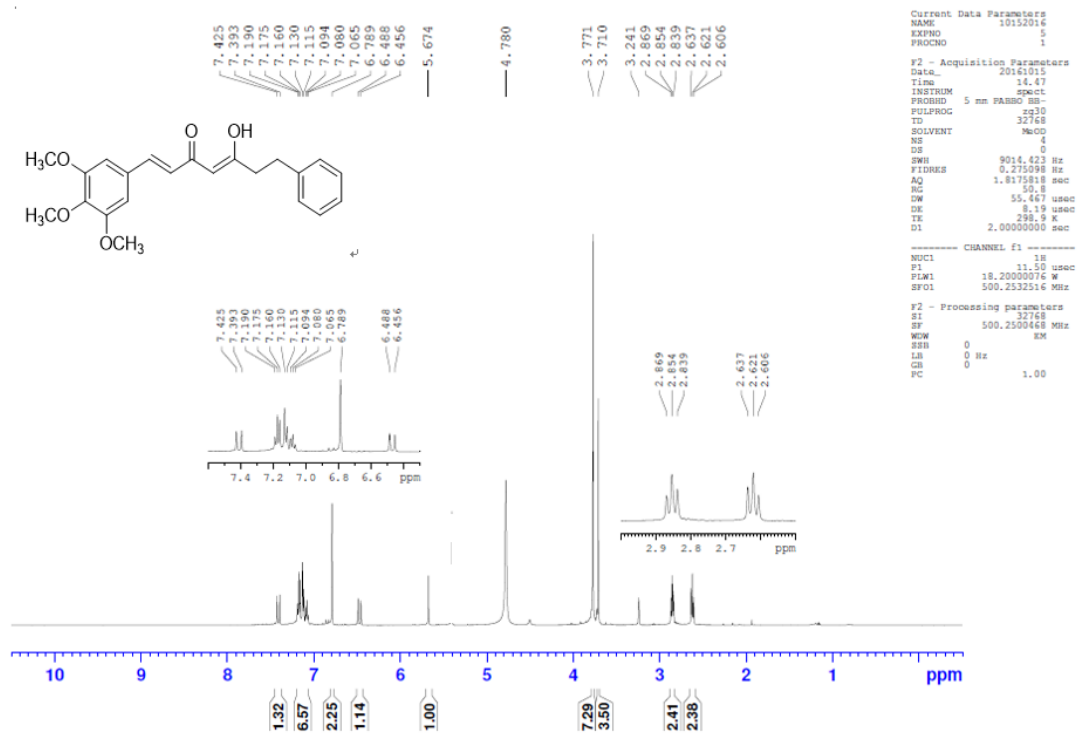


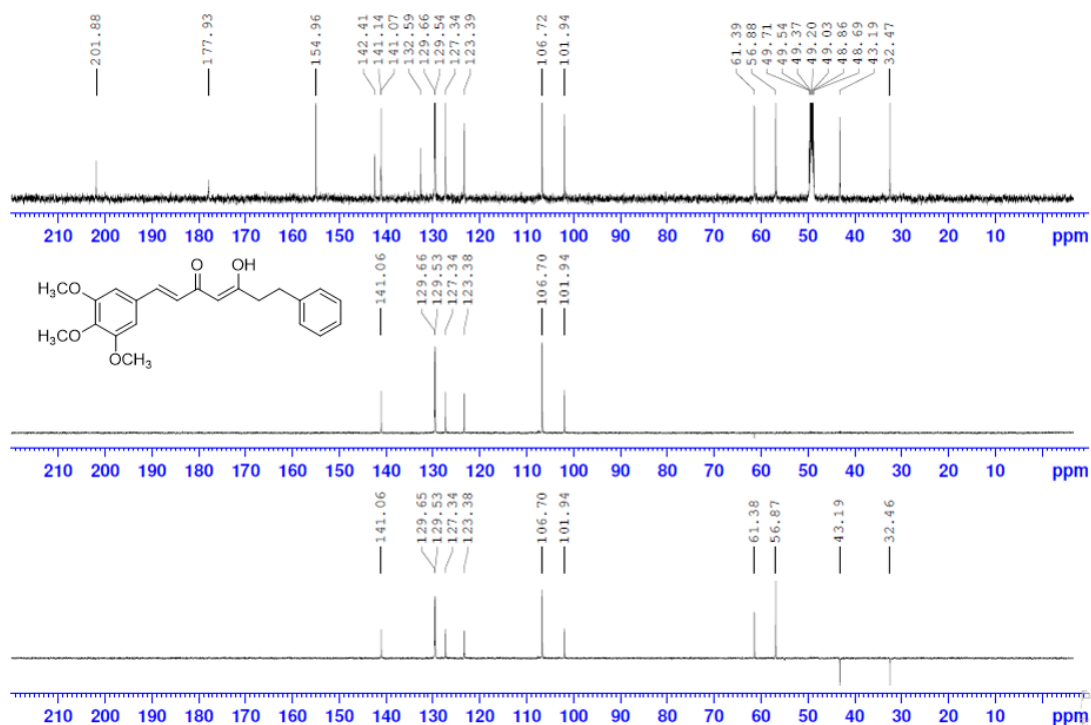
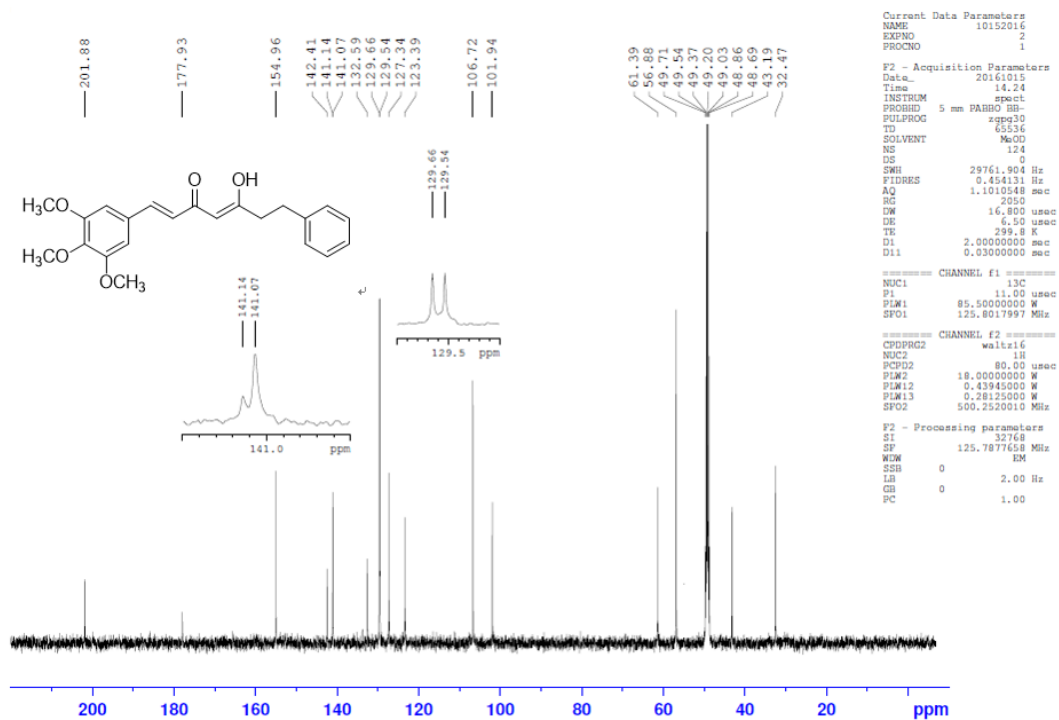


Compound 21

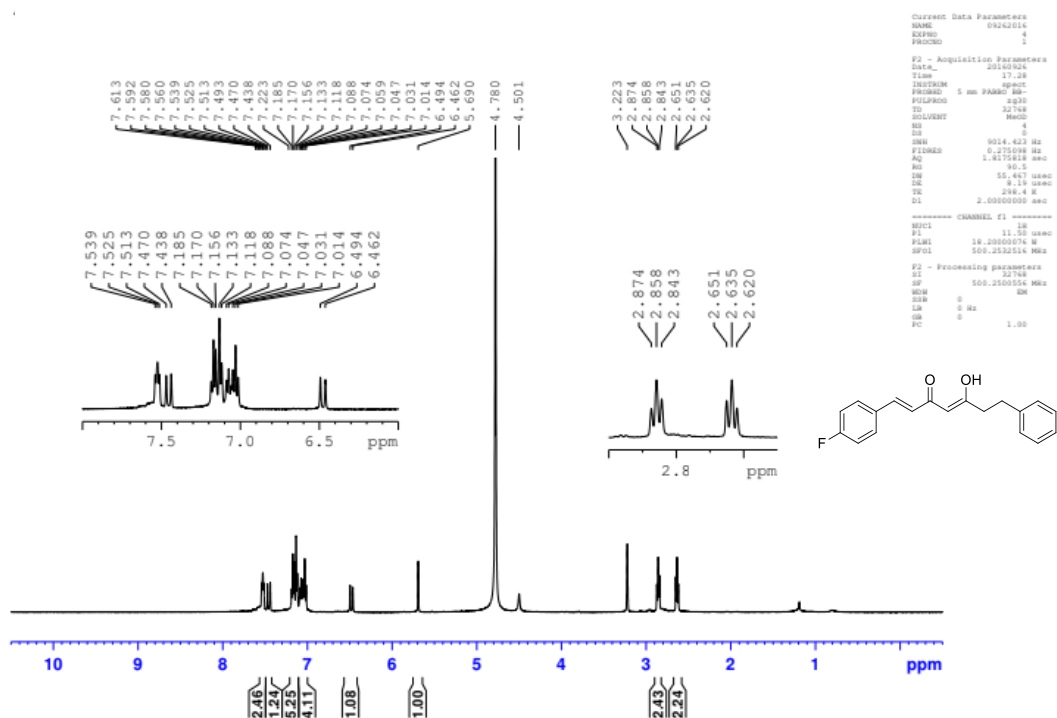


Compound 22

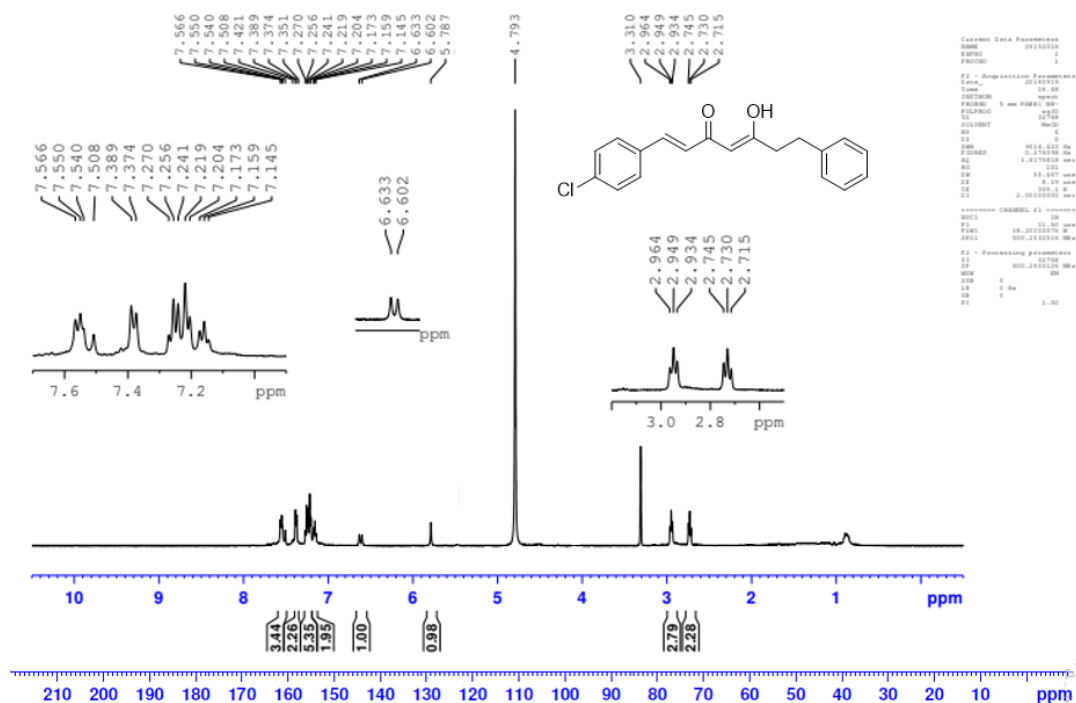


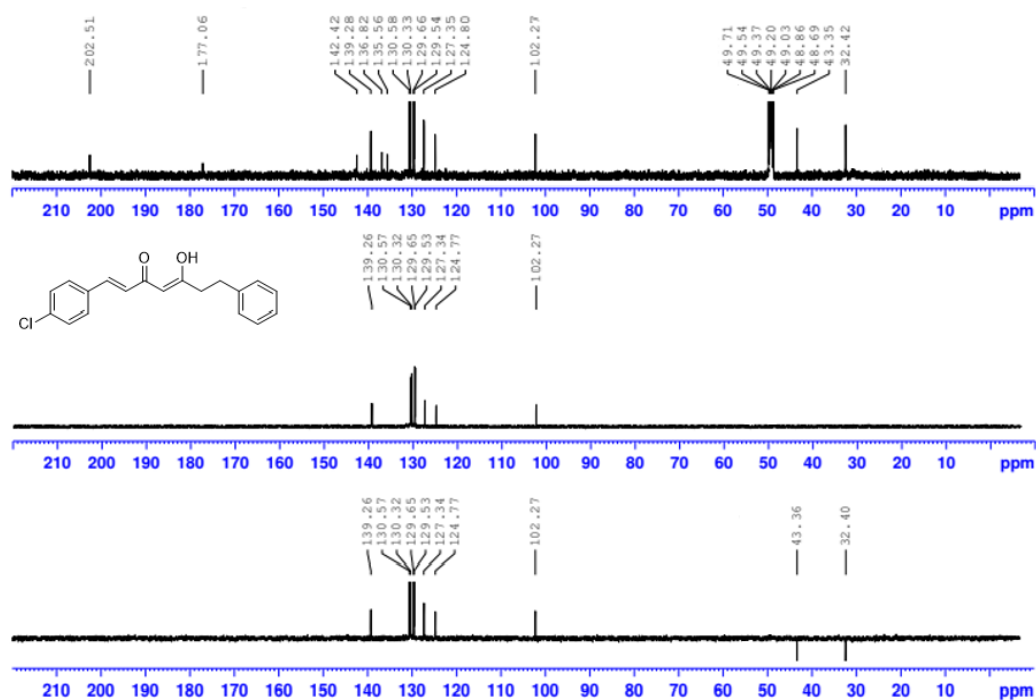
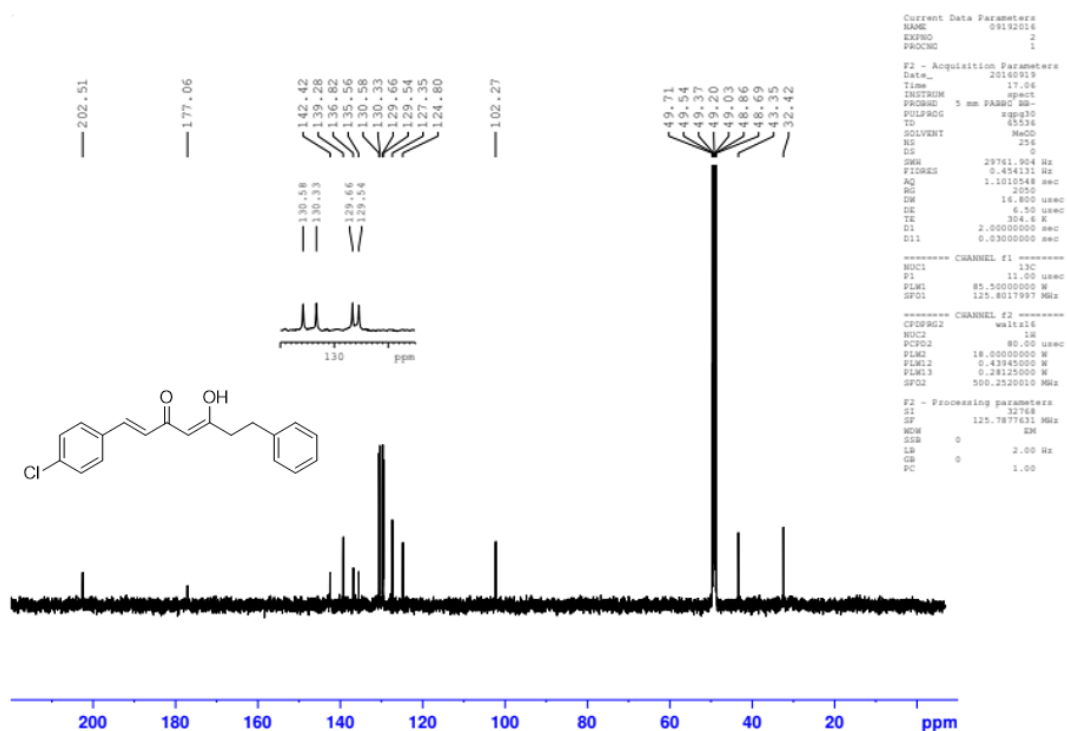


Compound 23

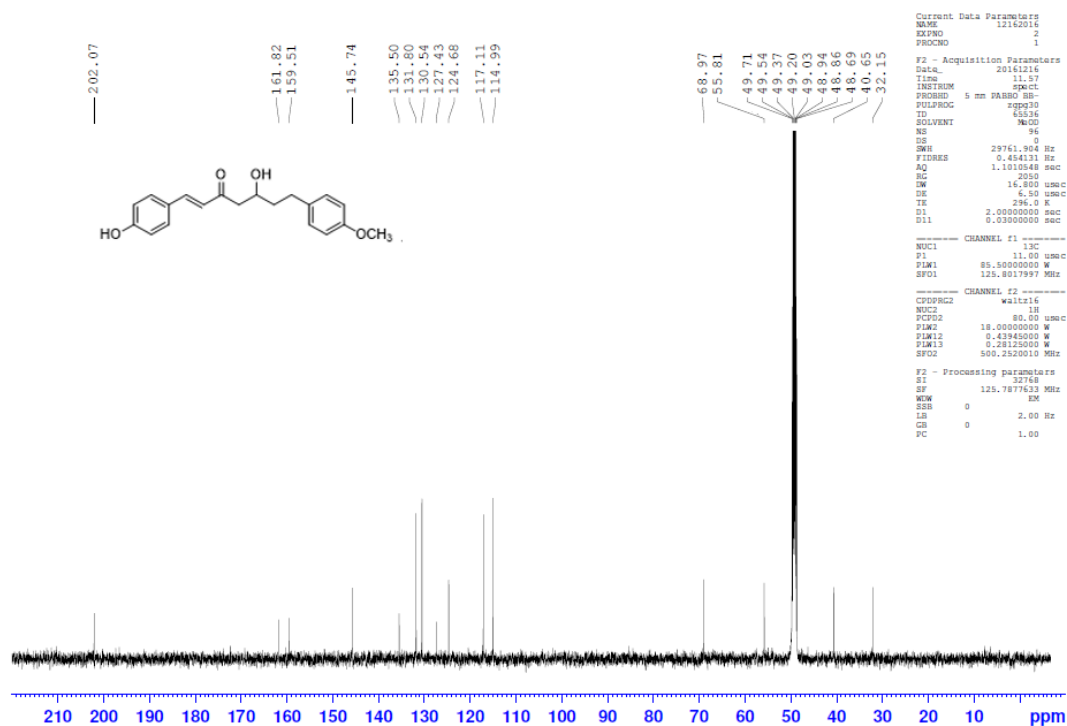
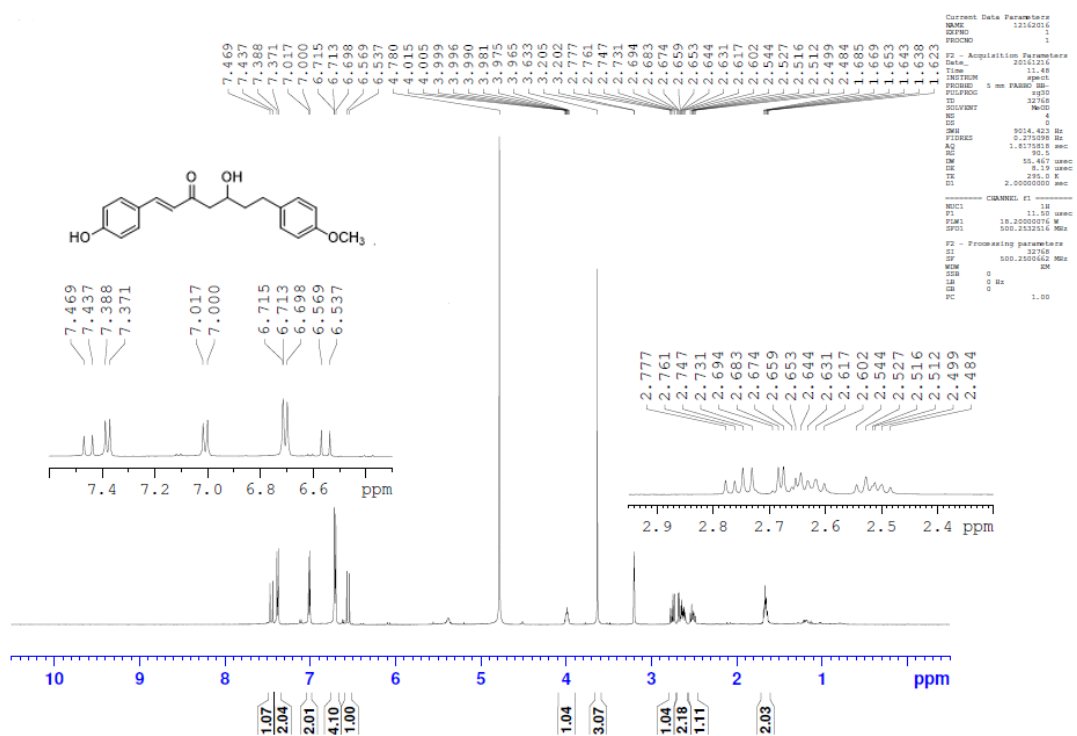


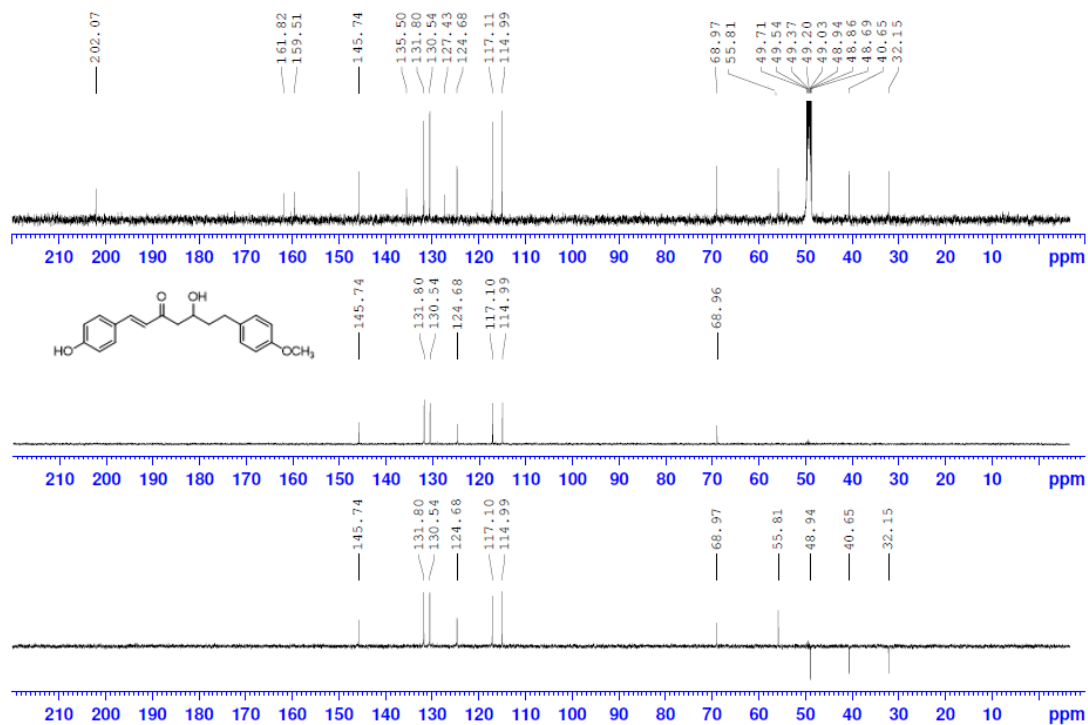
Compound 24



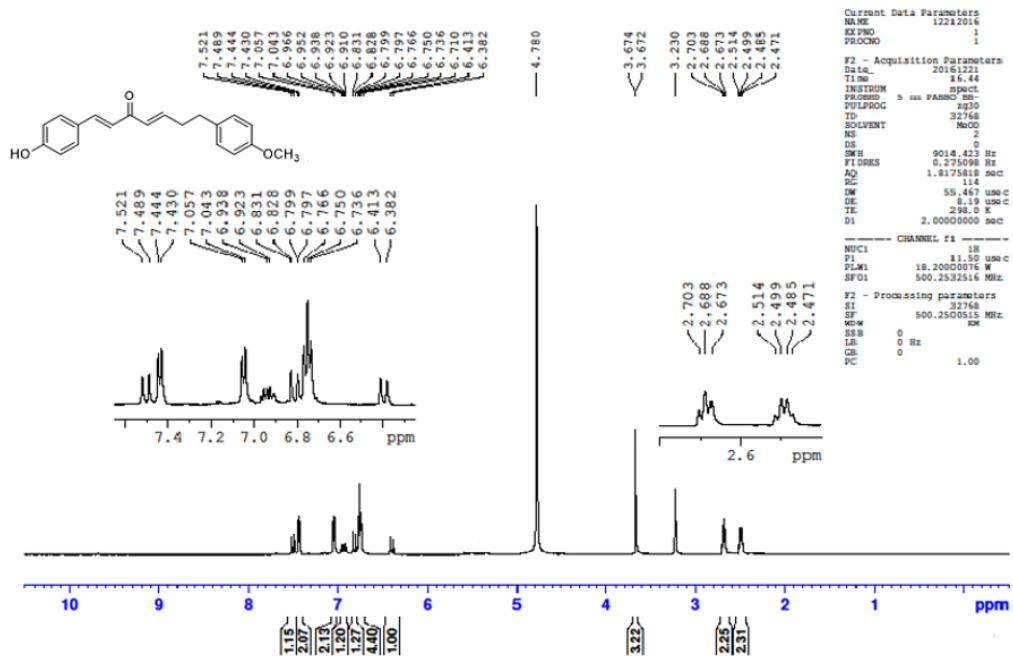


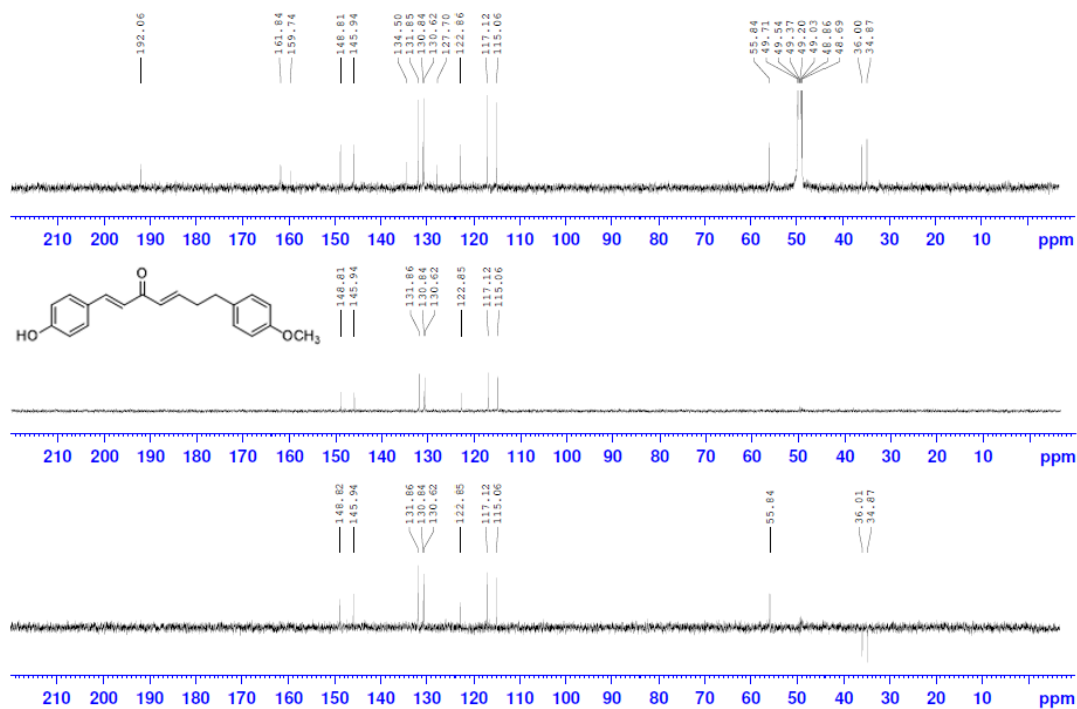
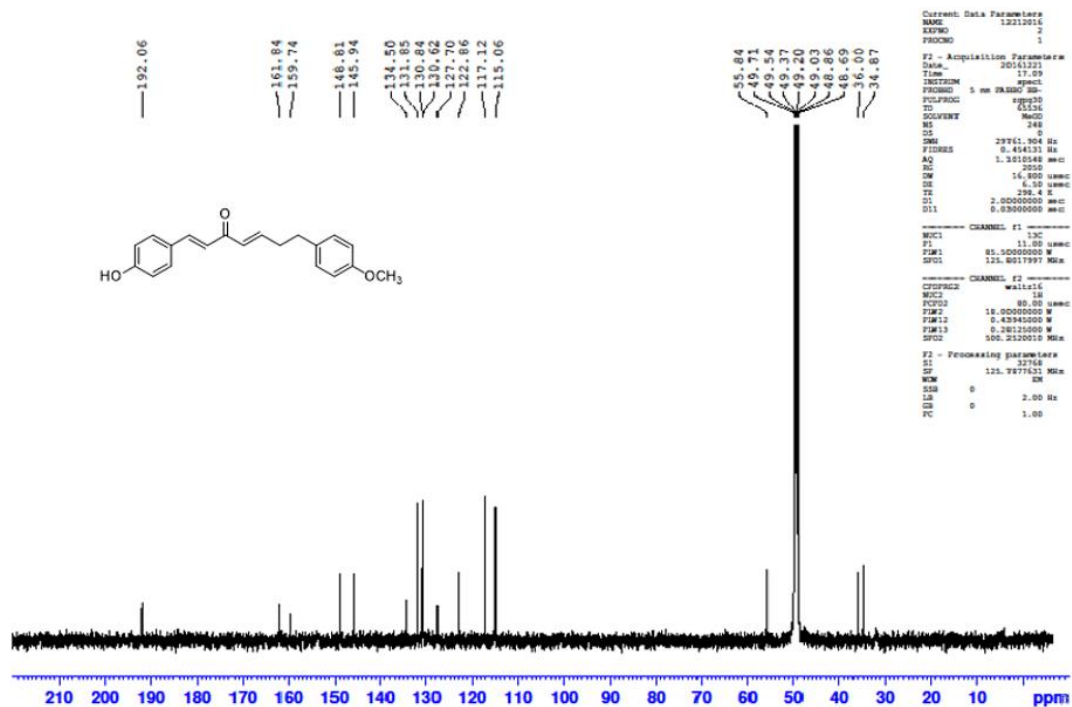
MD1



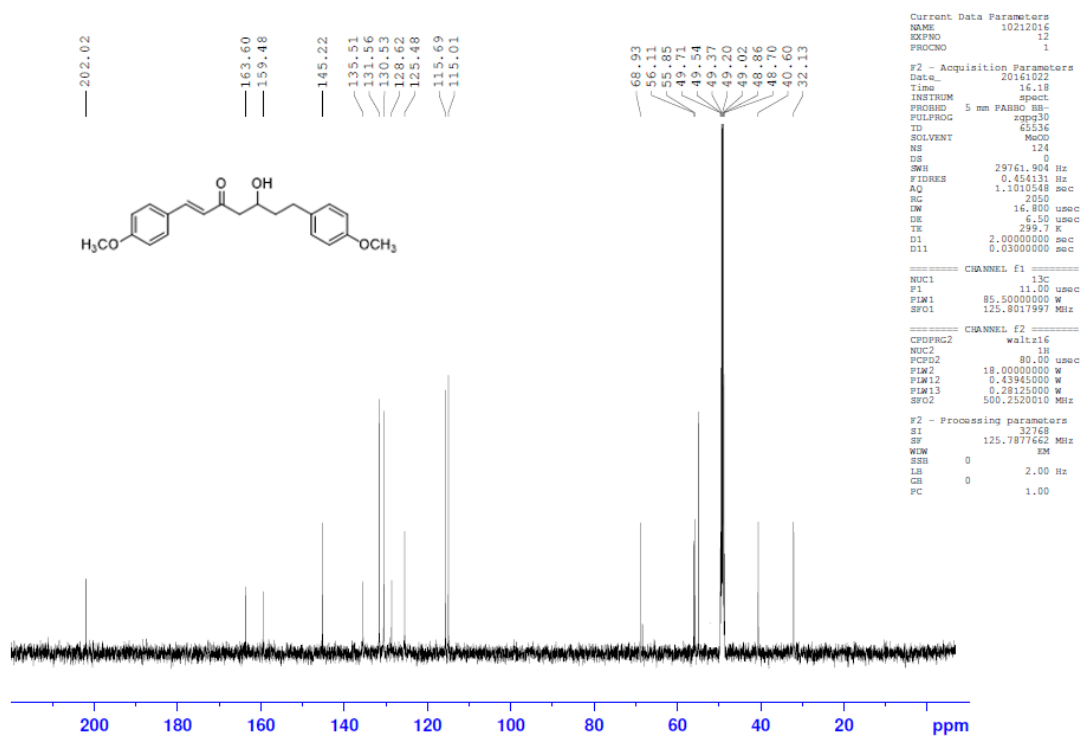
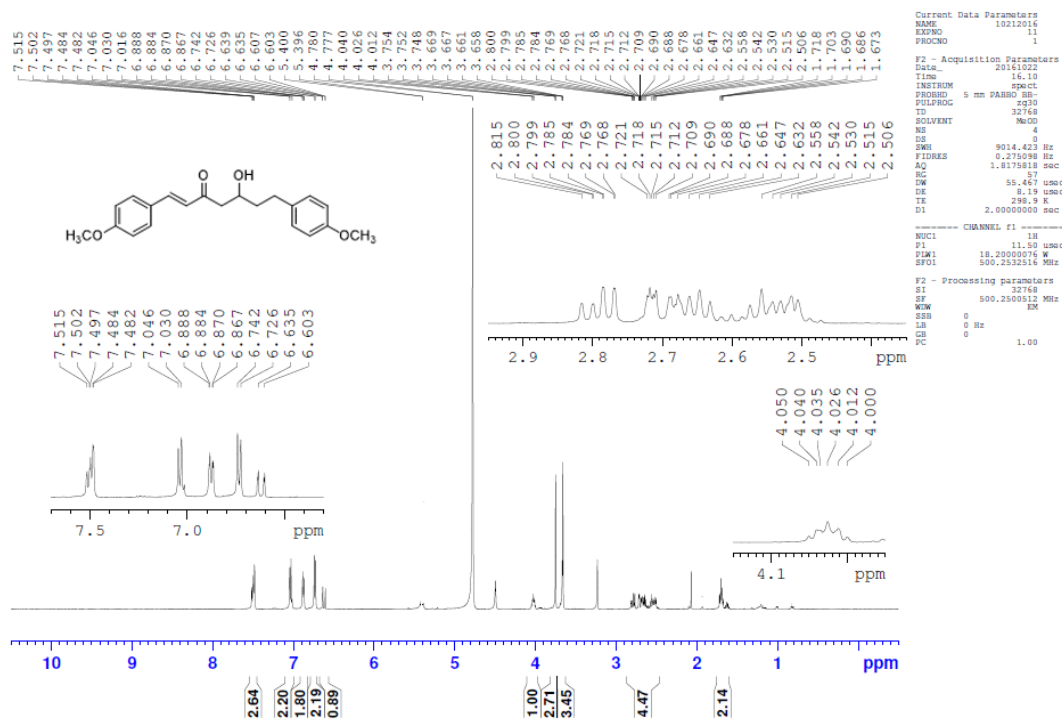


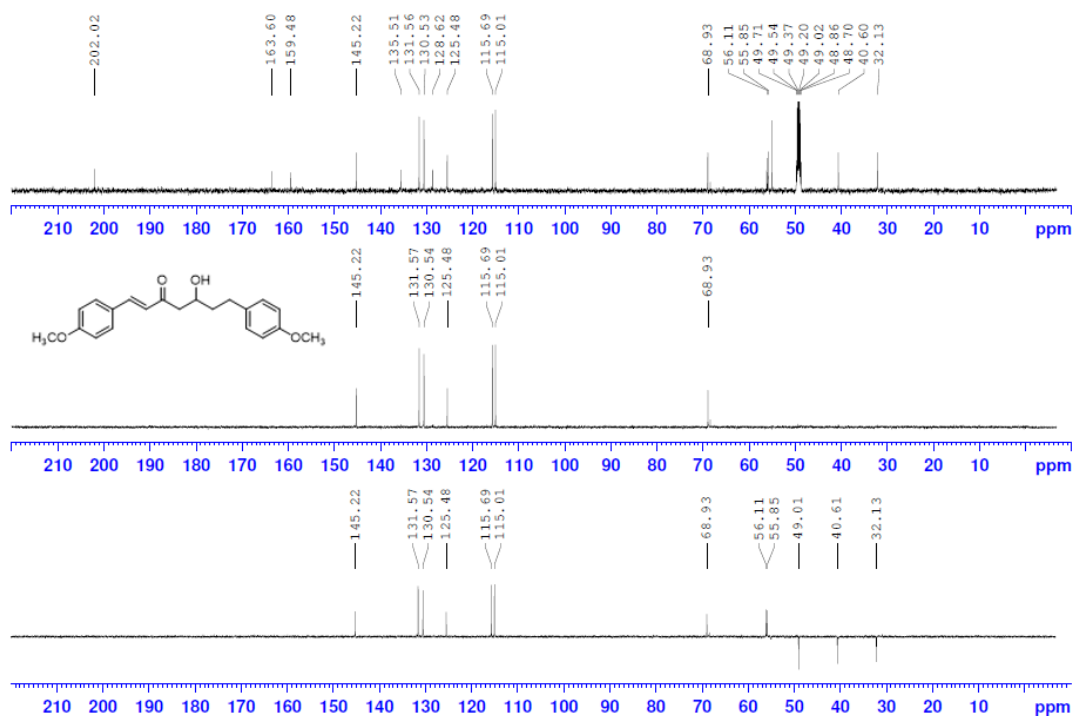
MD1a



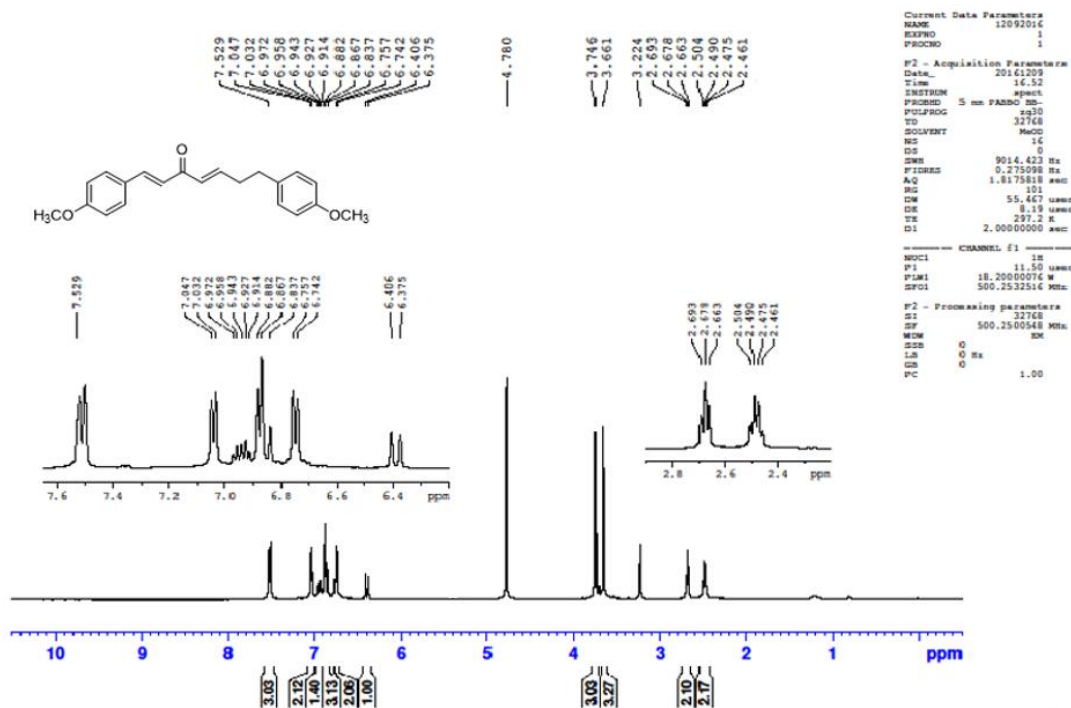


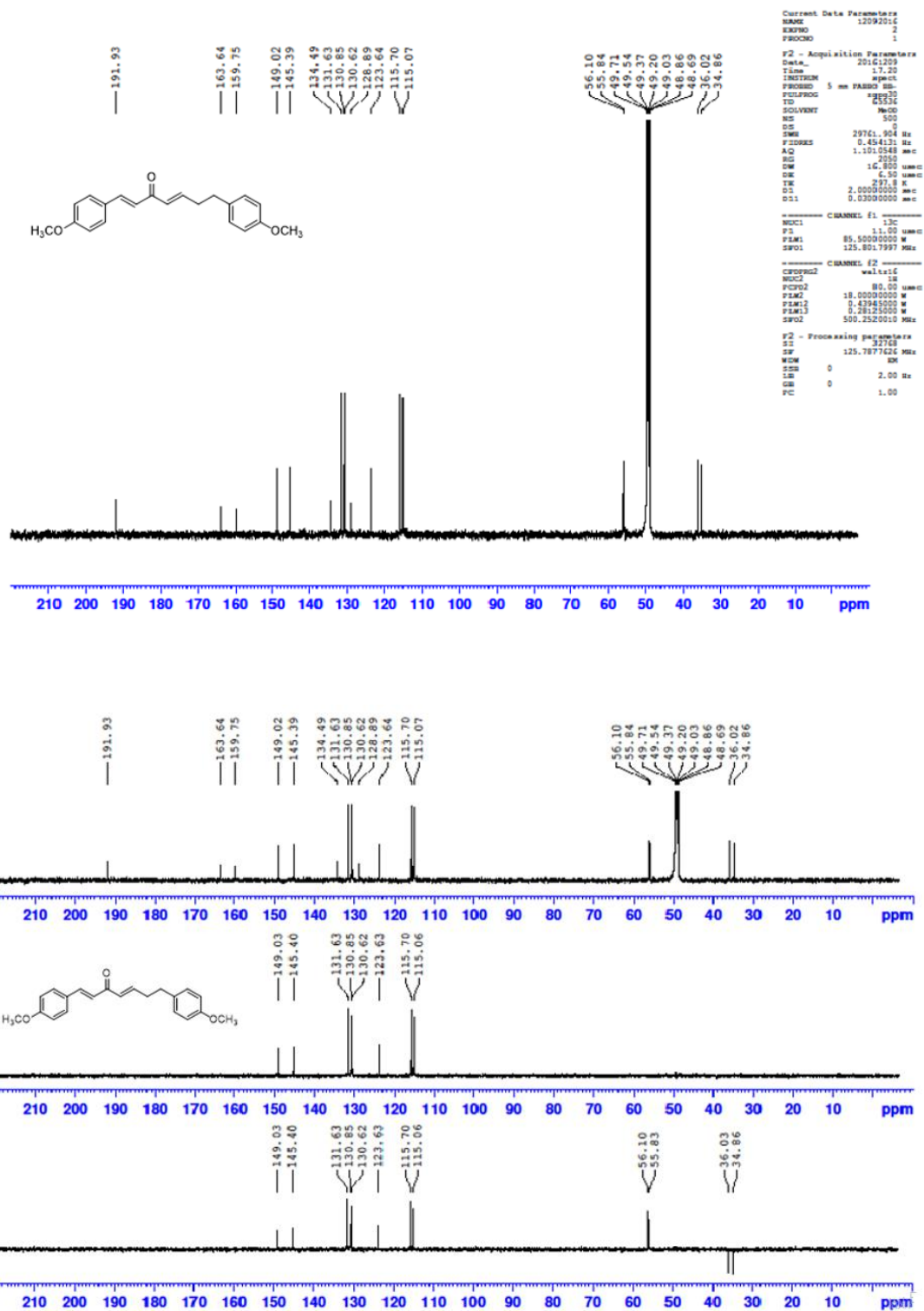
MD2



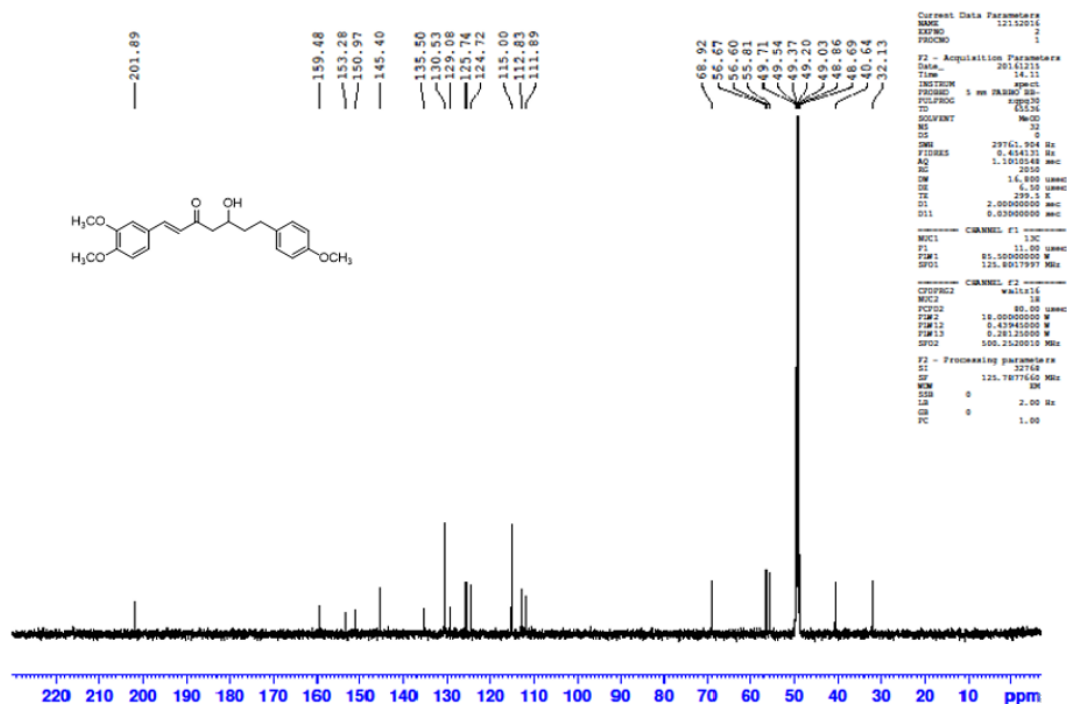
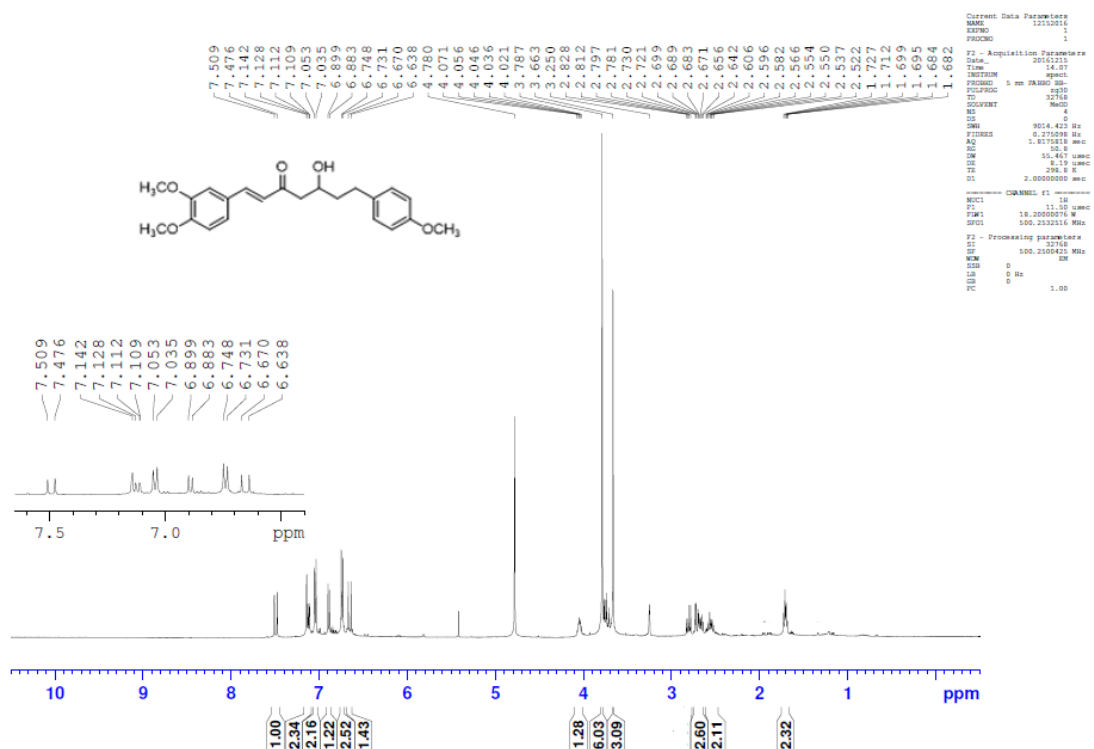


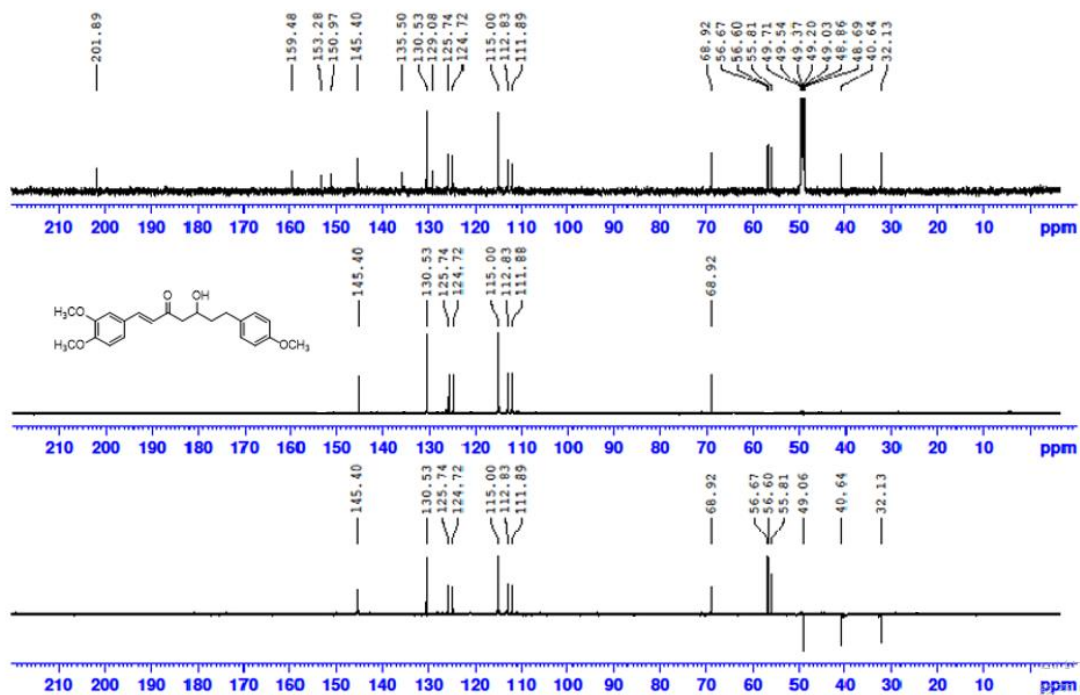
MD2a



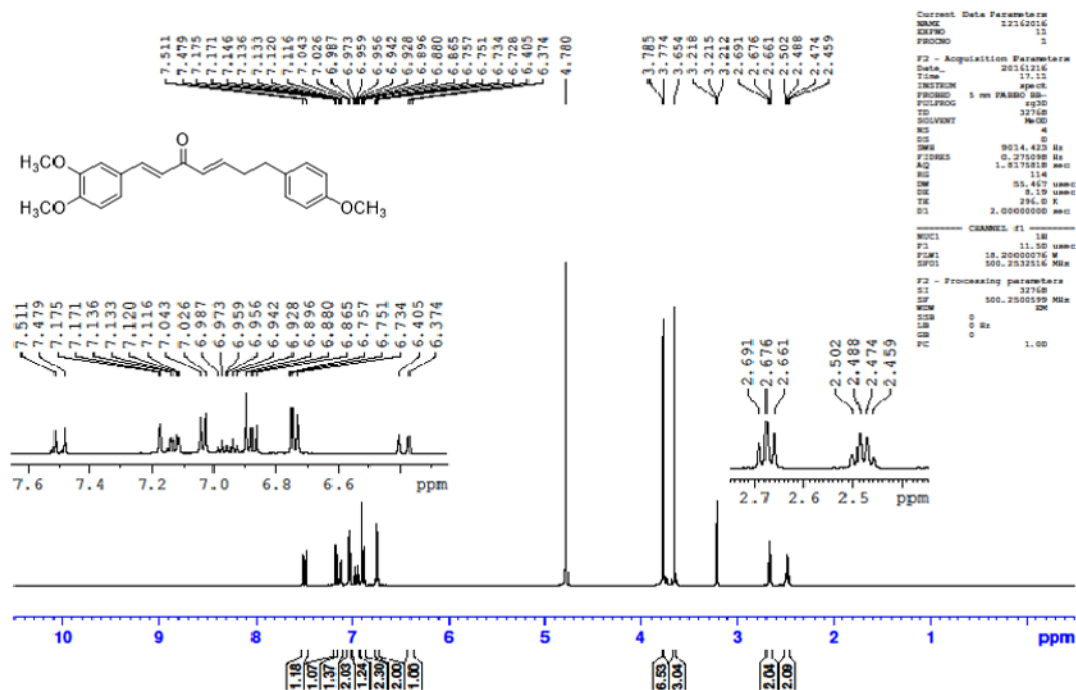


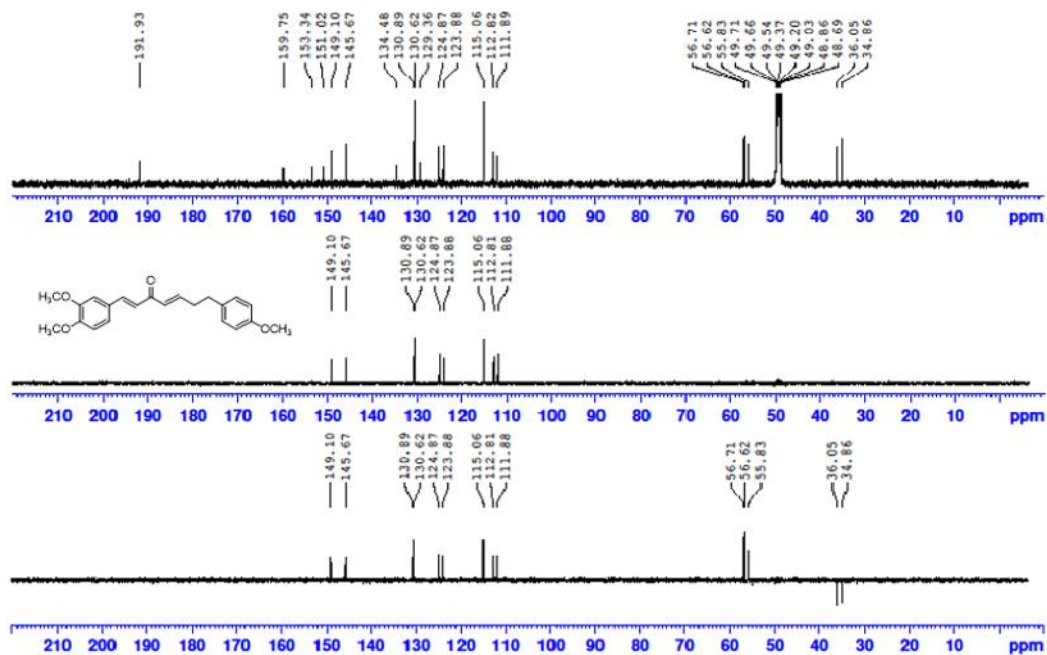
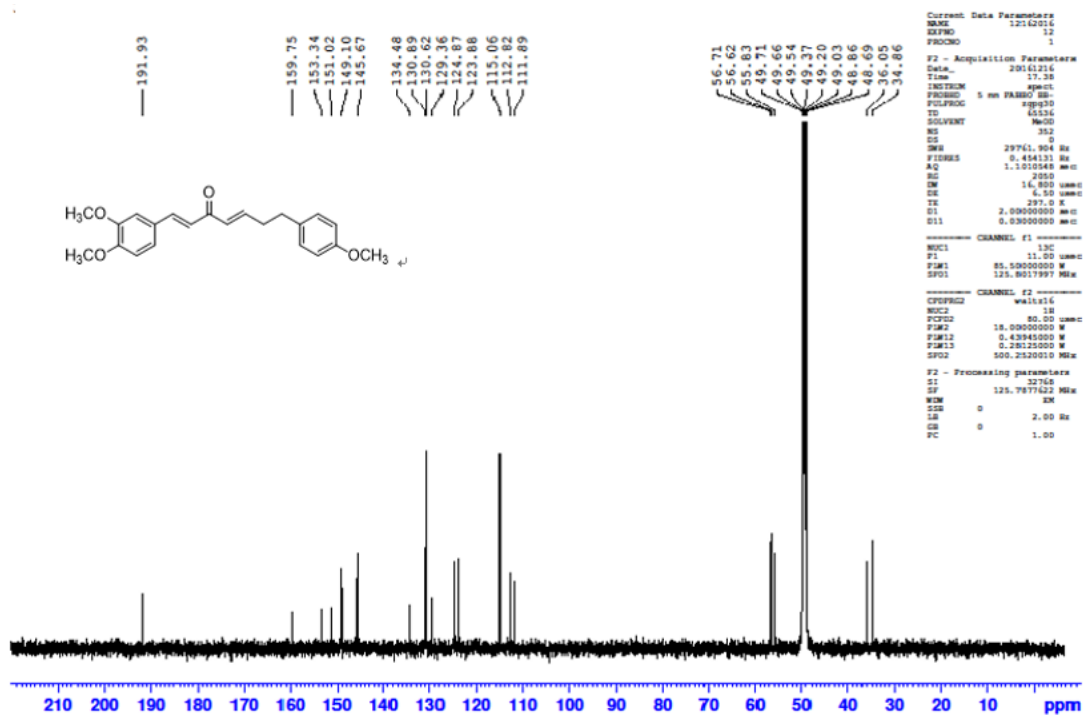
MD3



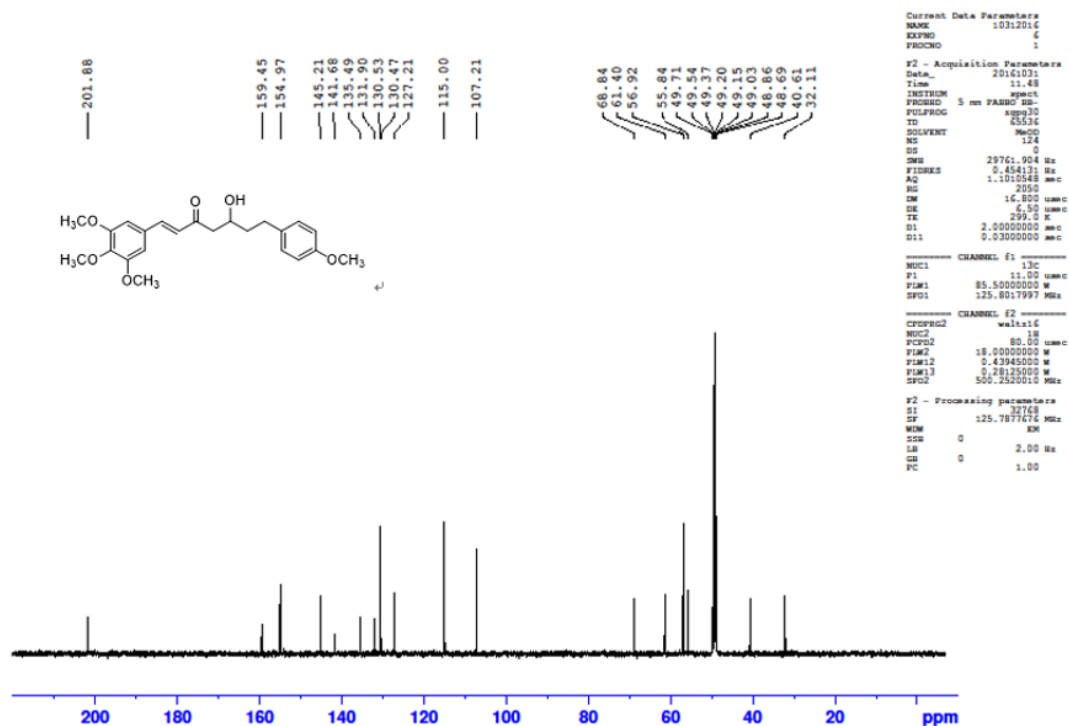
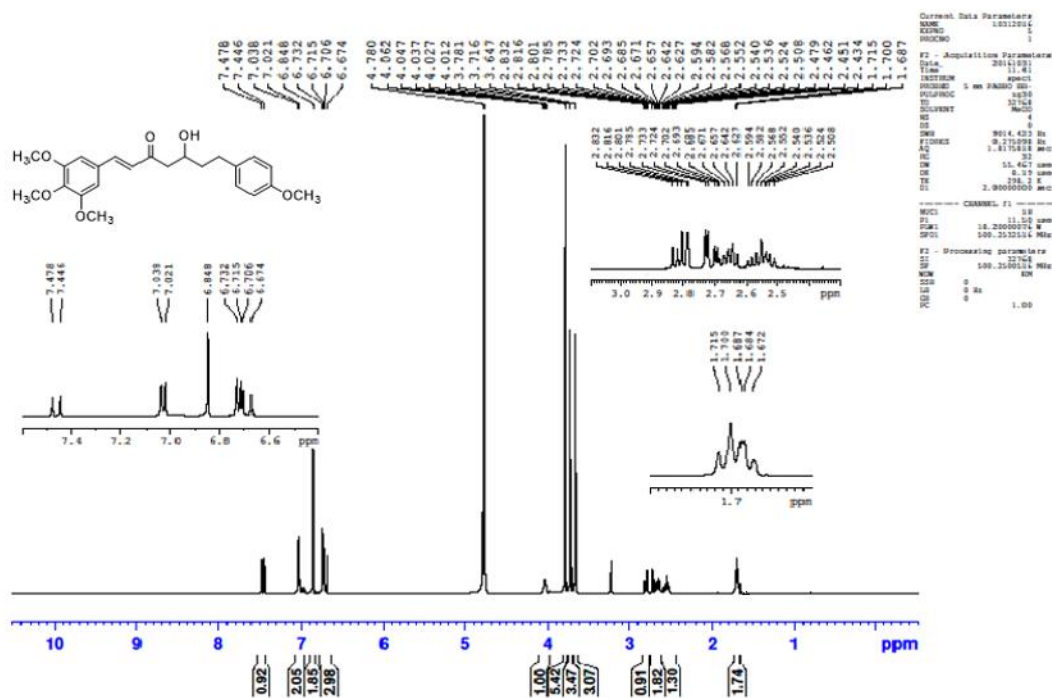


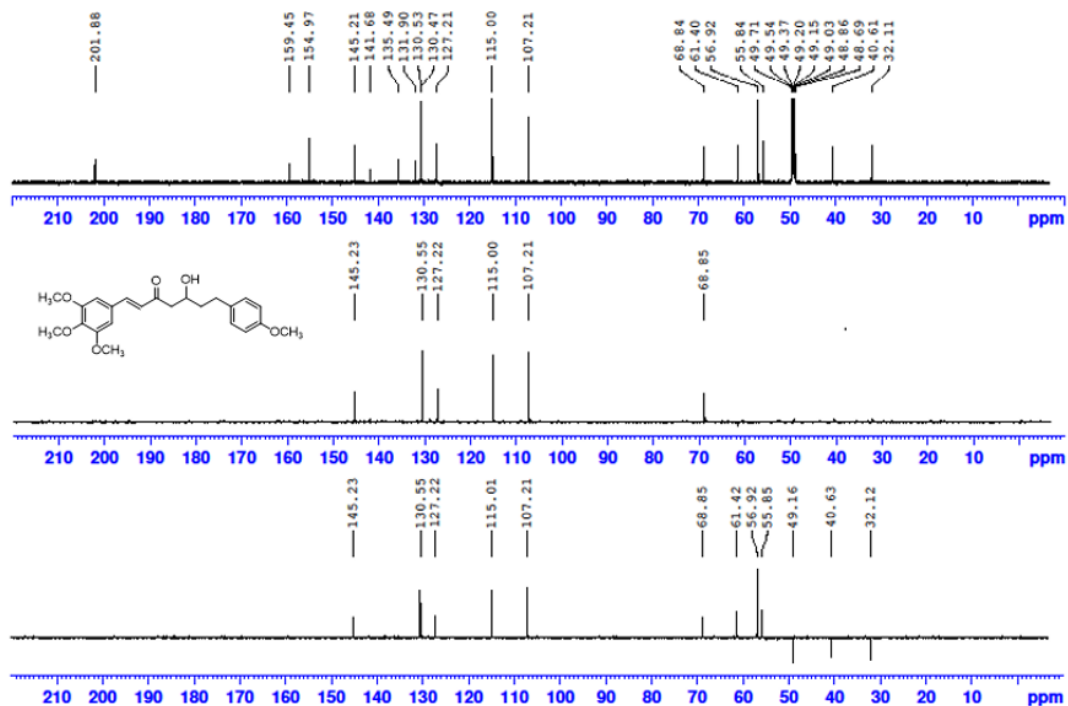
MD3a



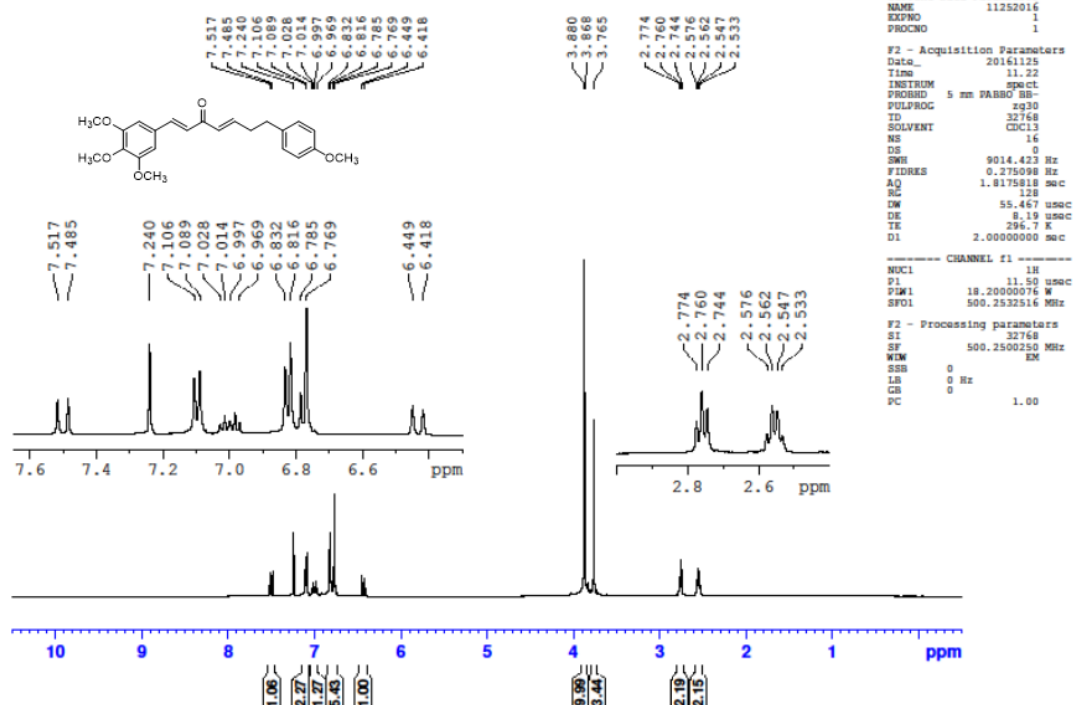


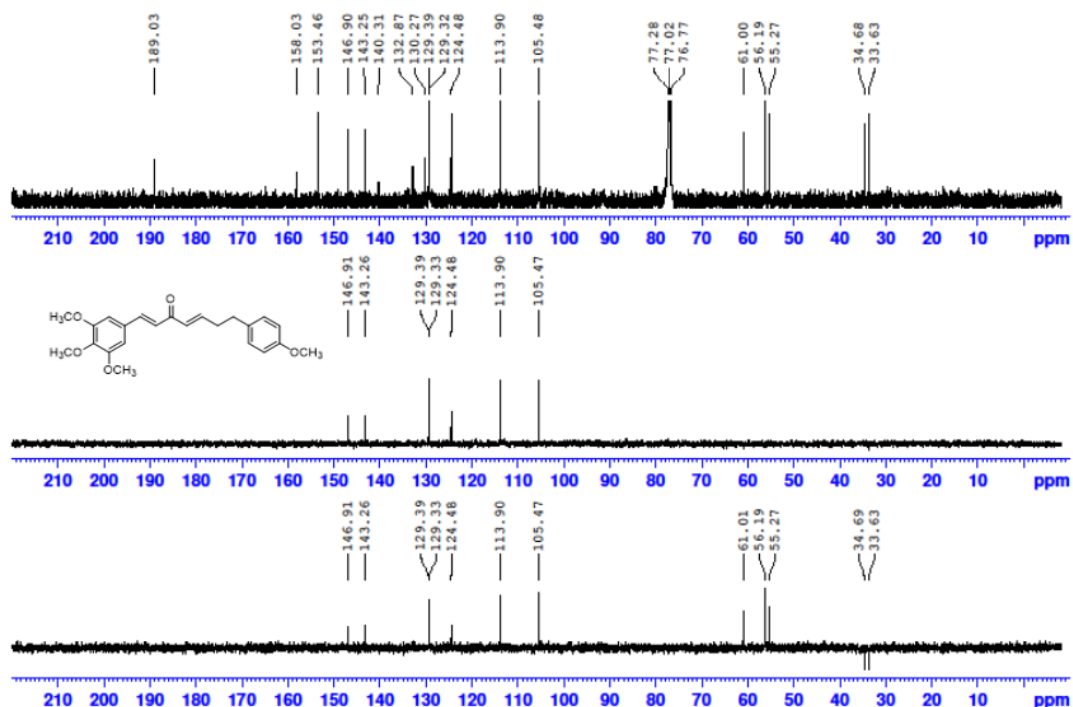
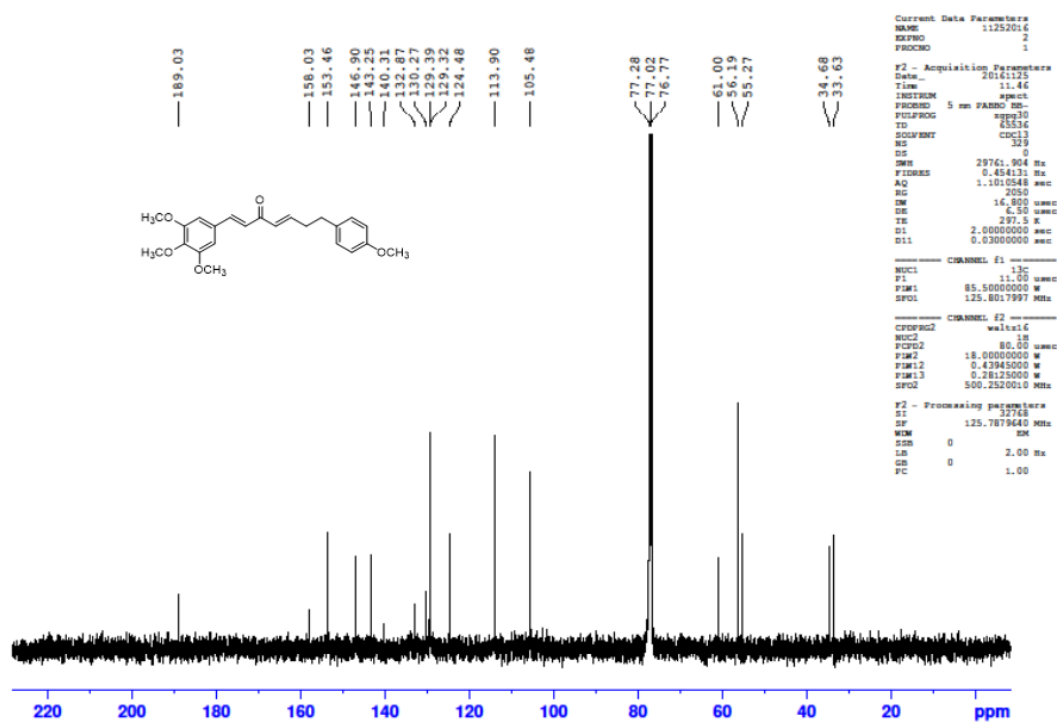
MD4



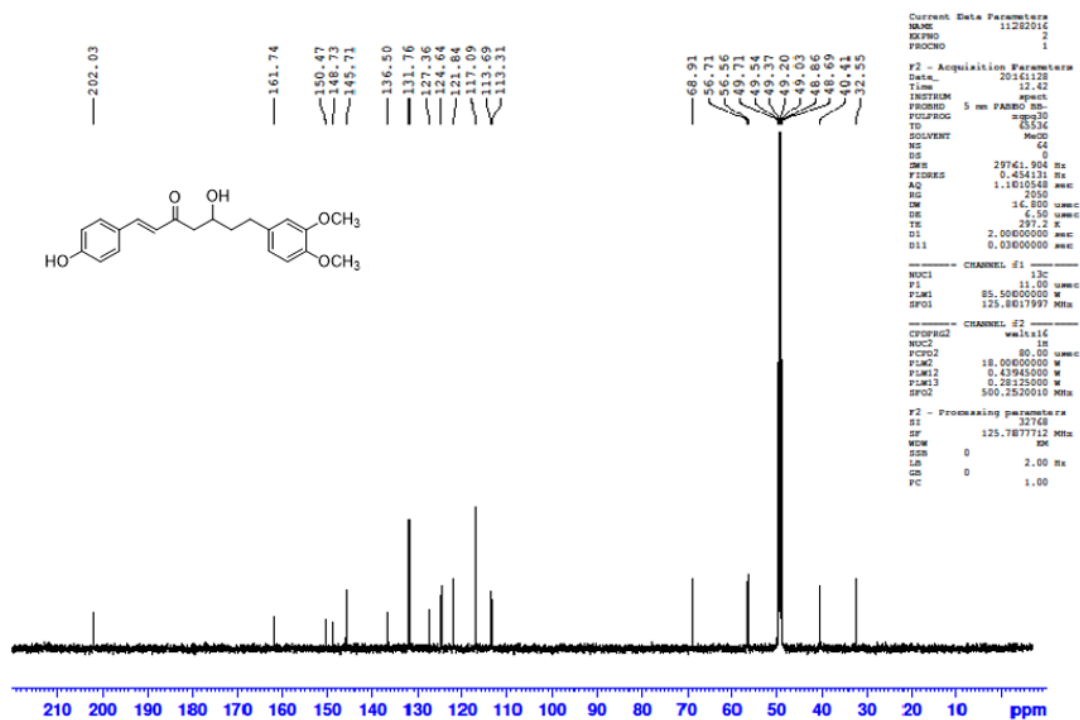
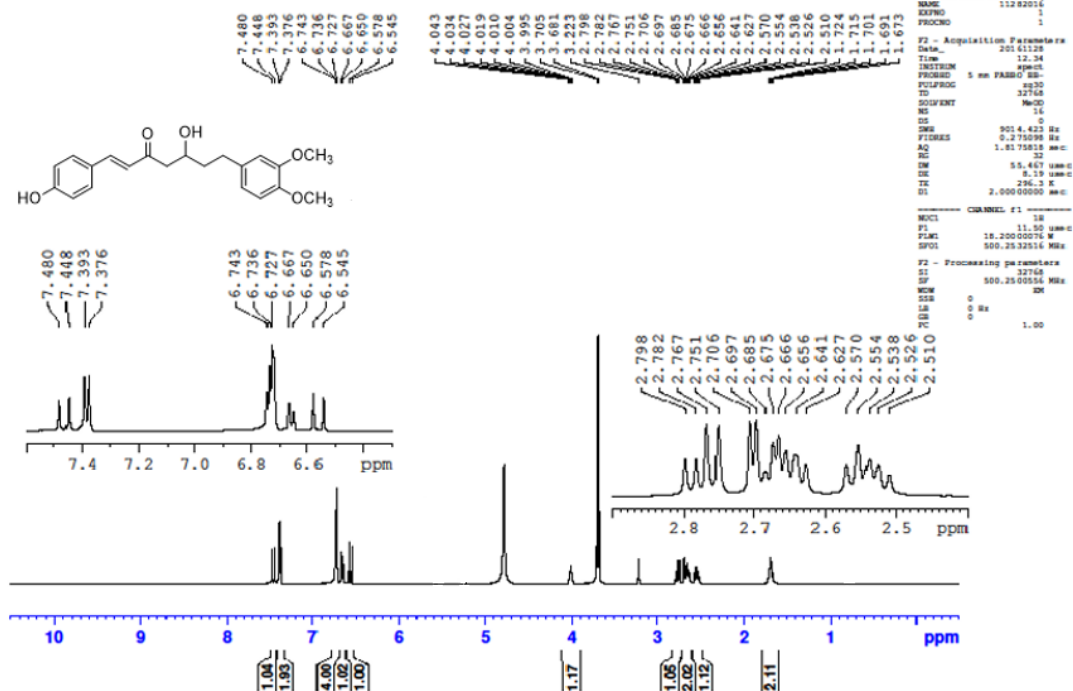


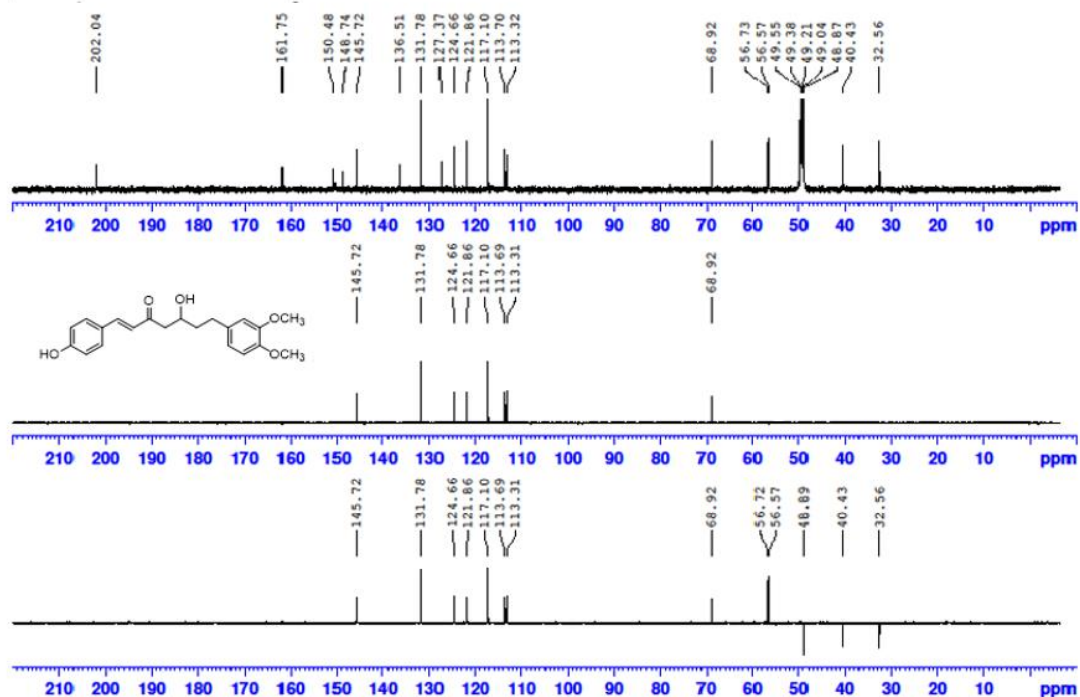
MD4a



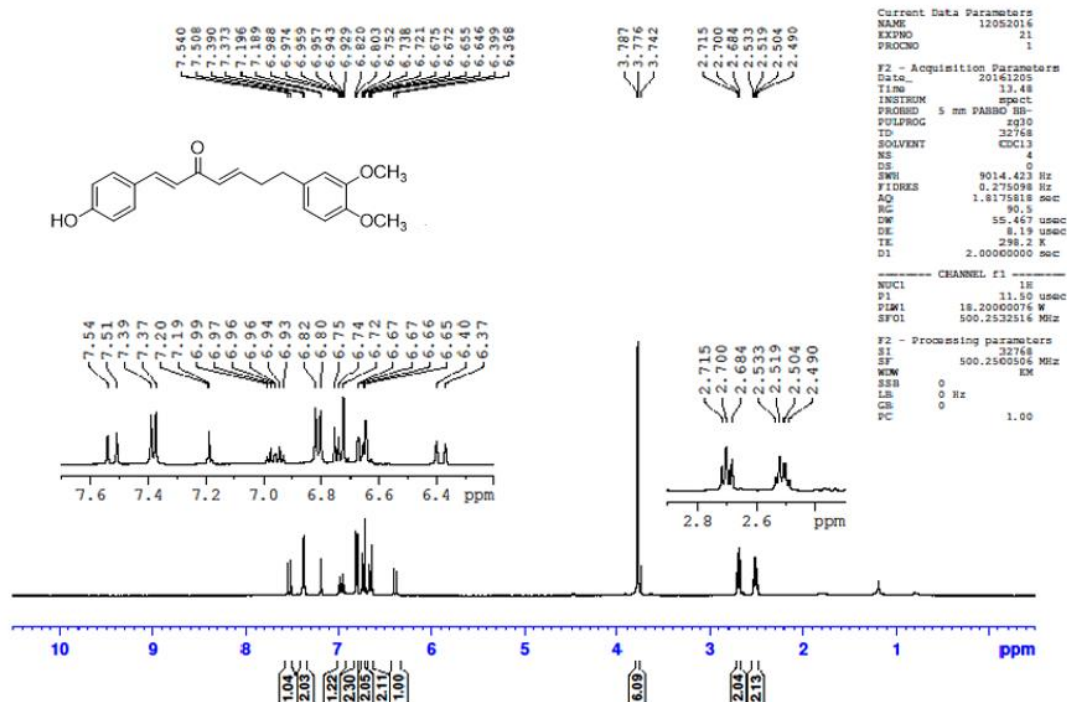


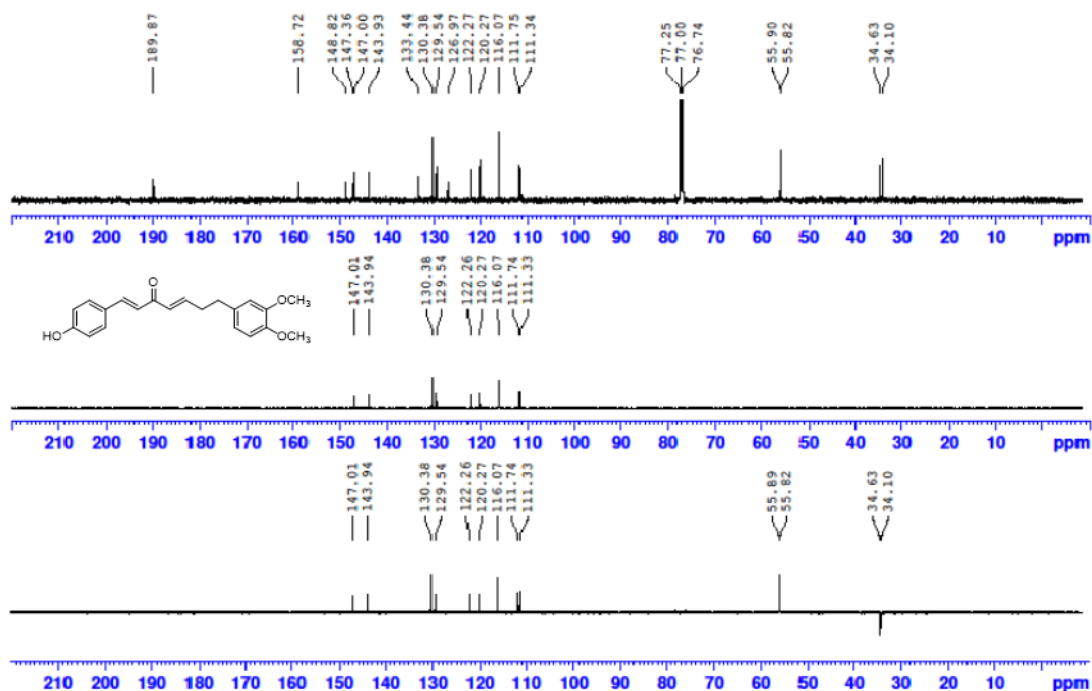
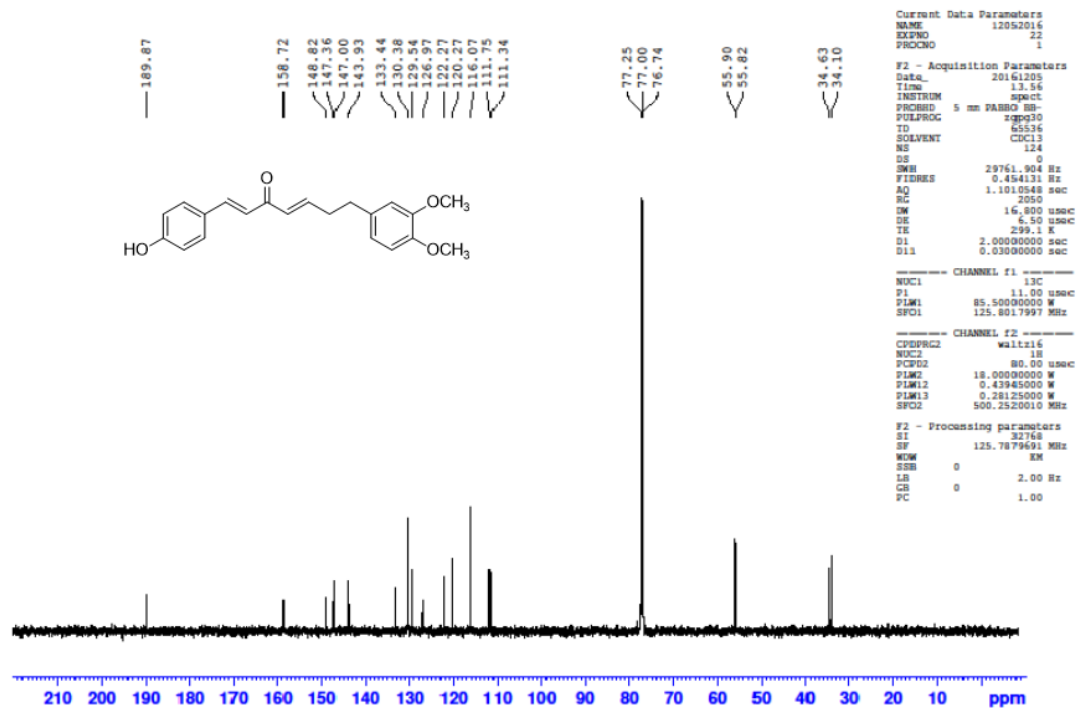
MD5



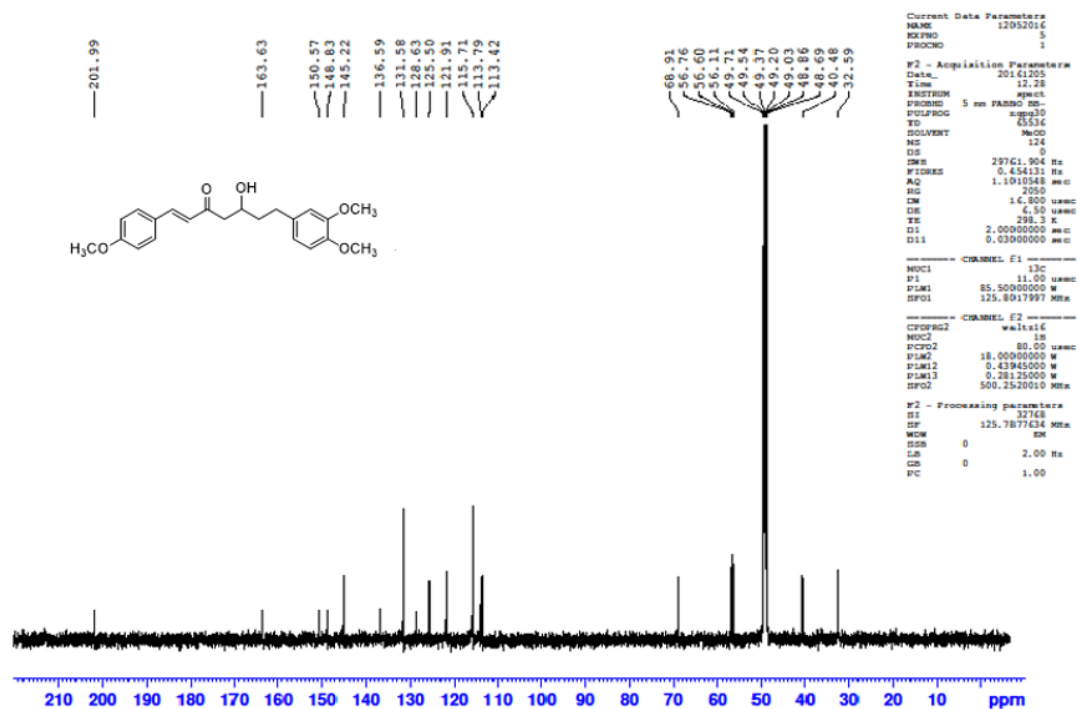
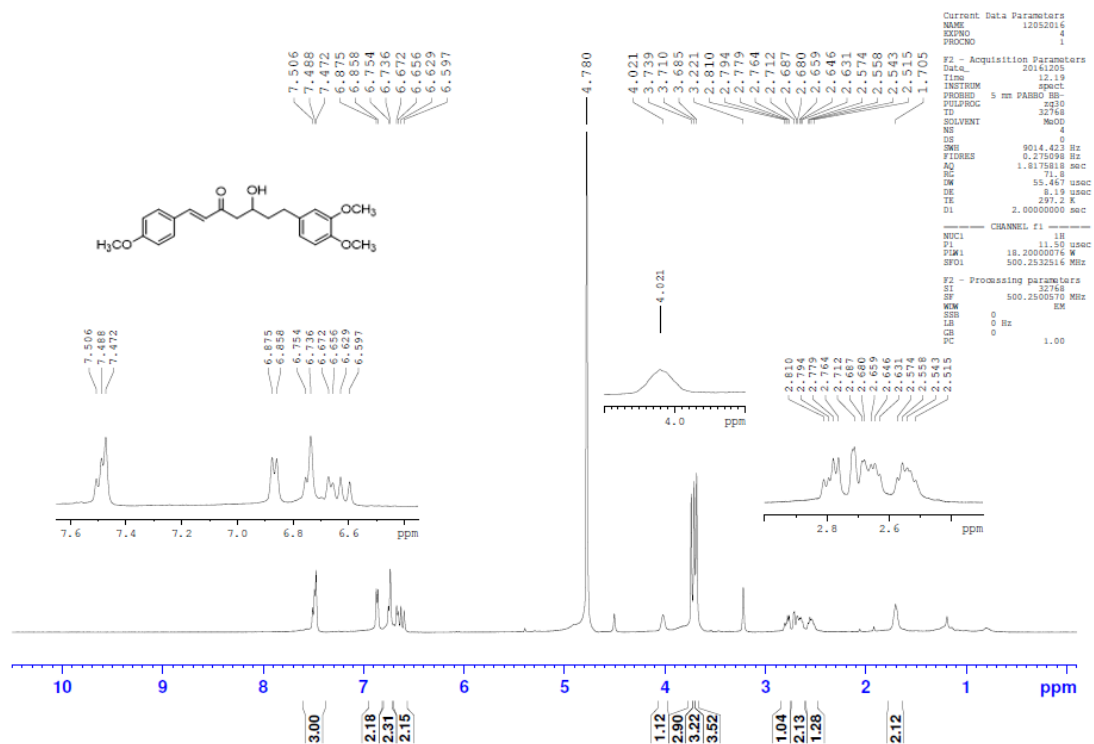


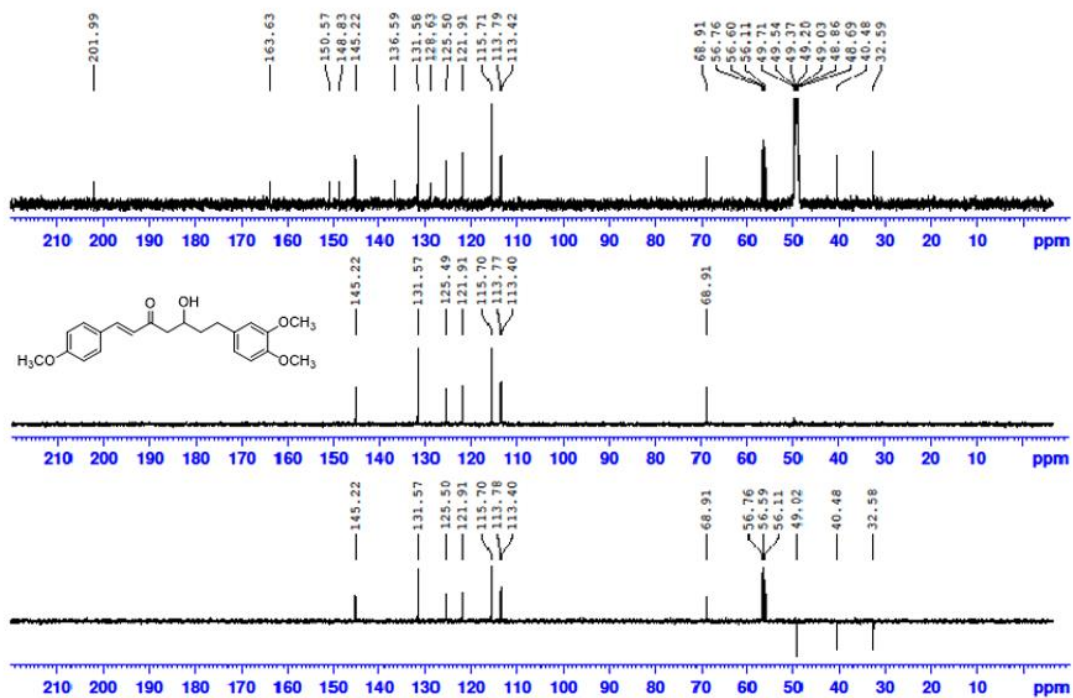
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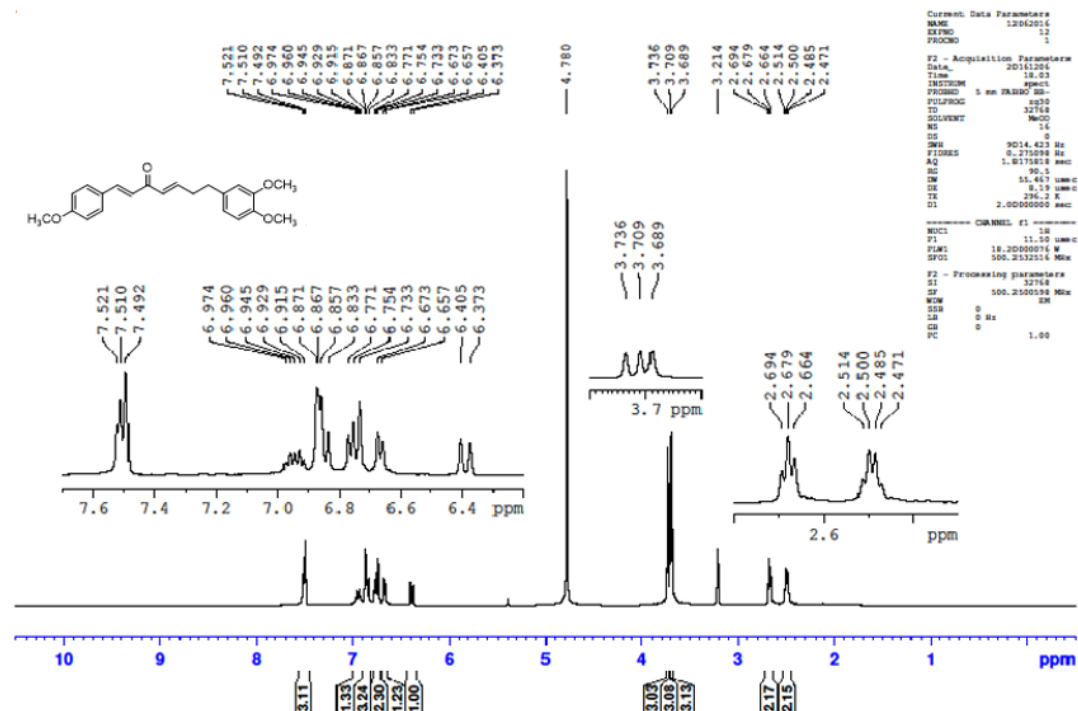


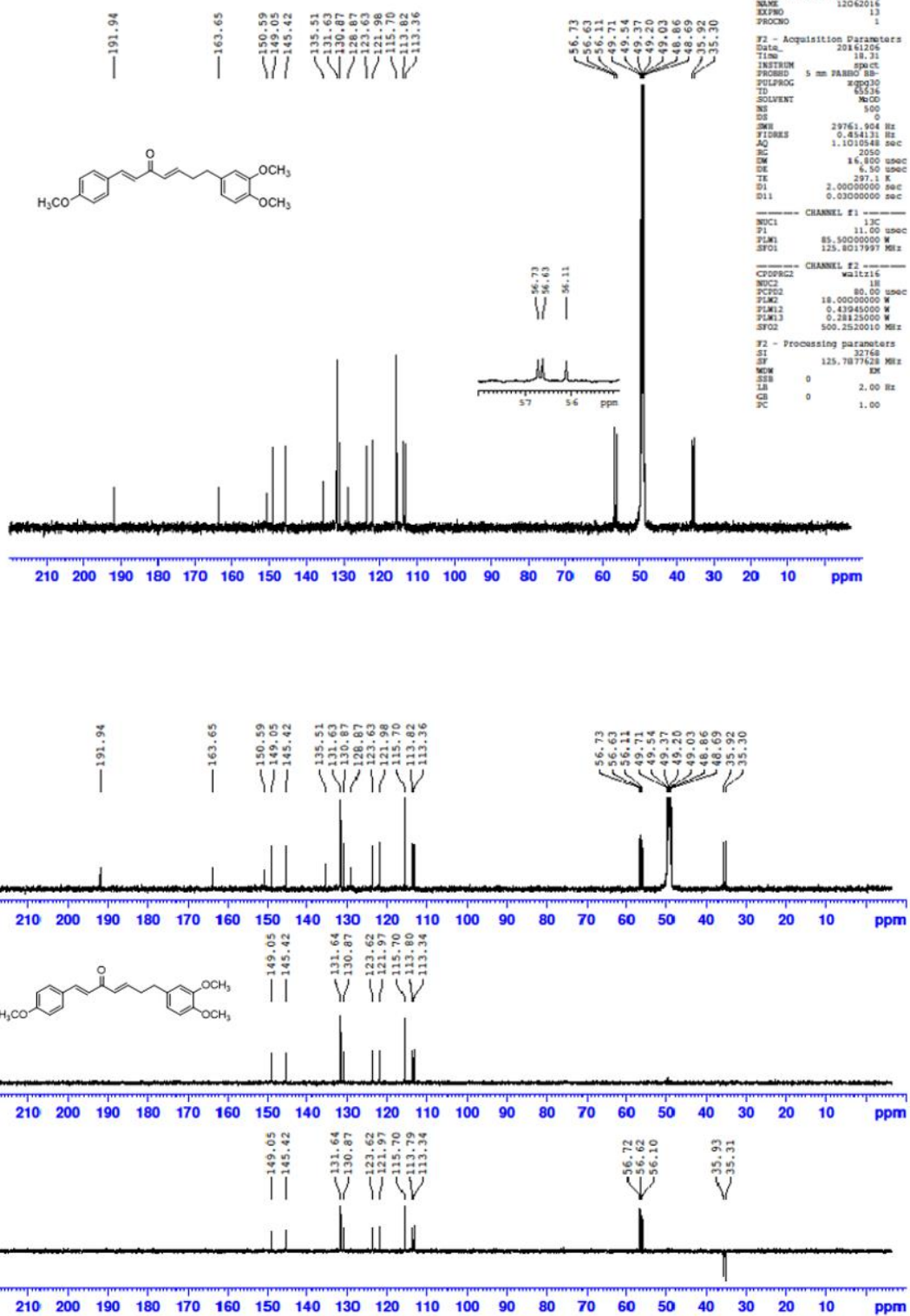
MD6



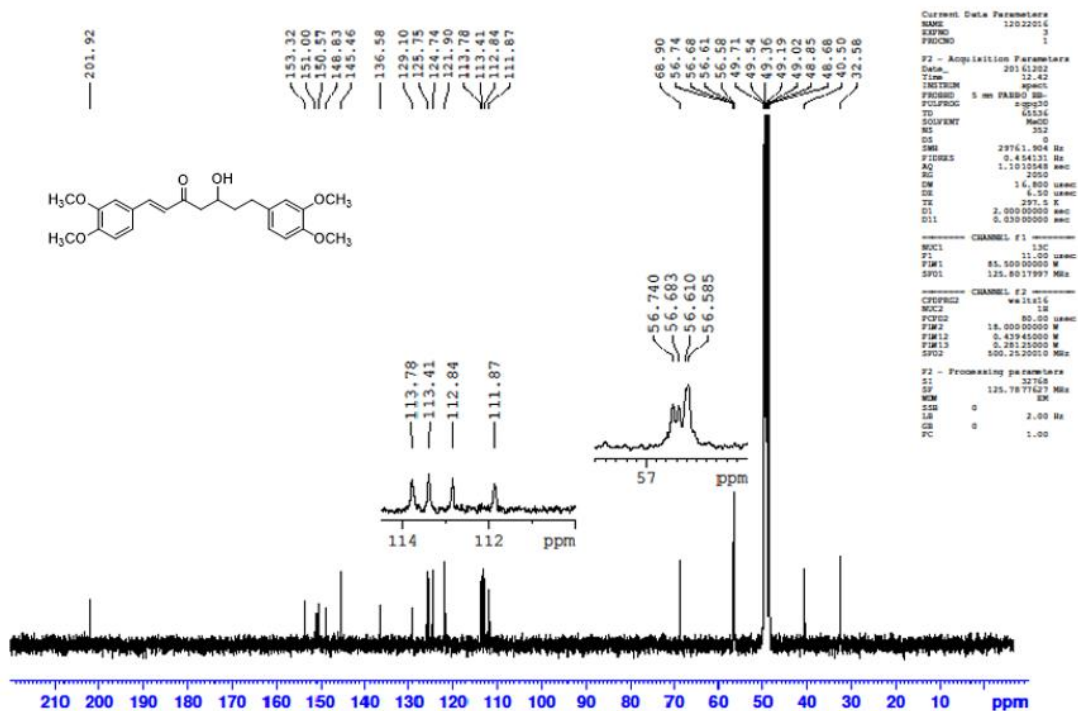
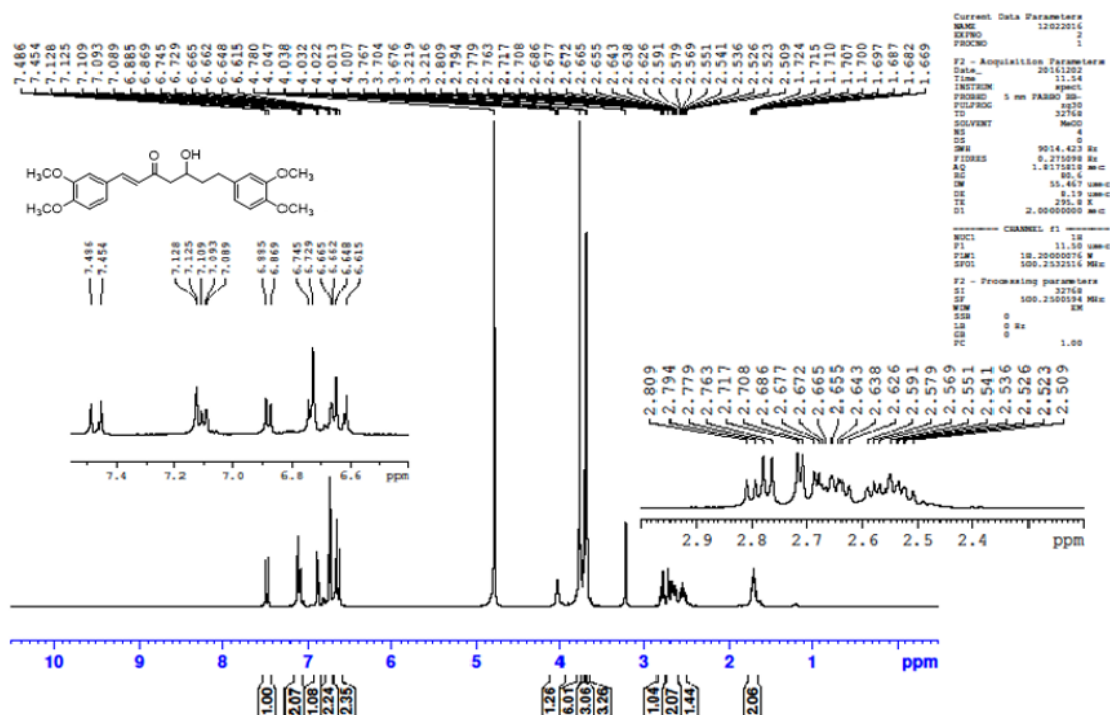


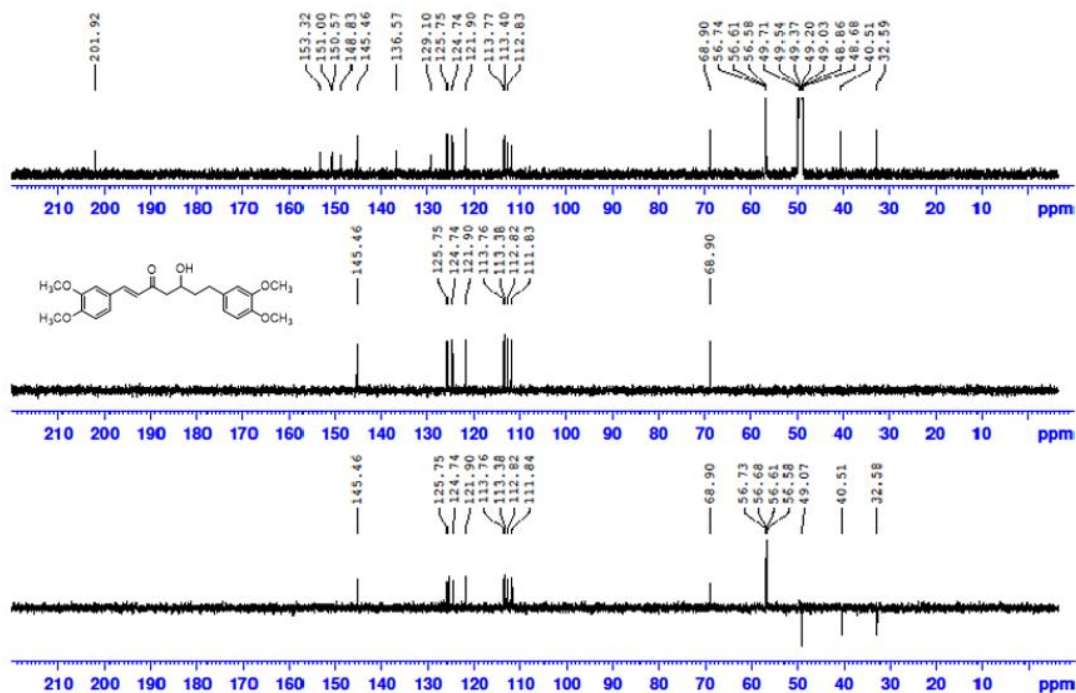
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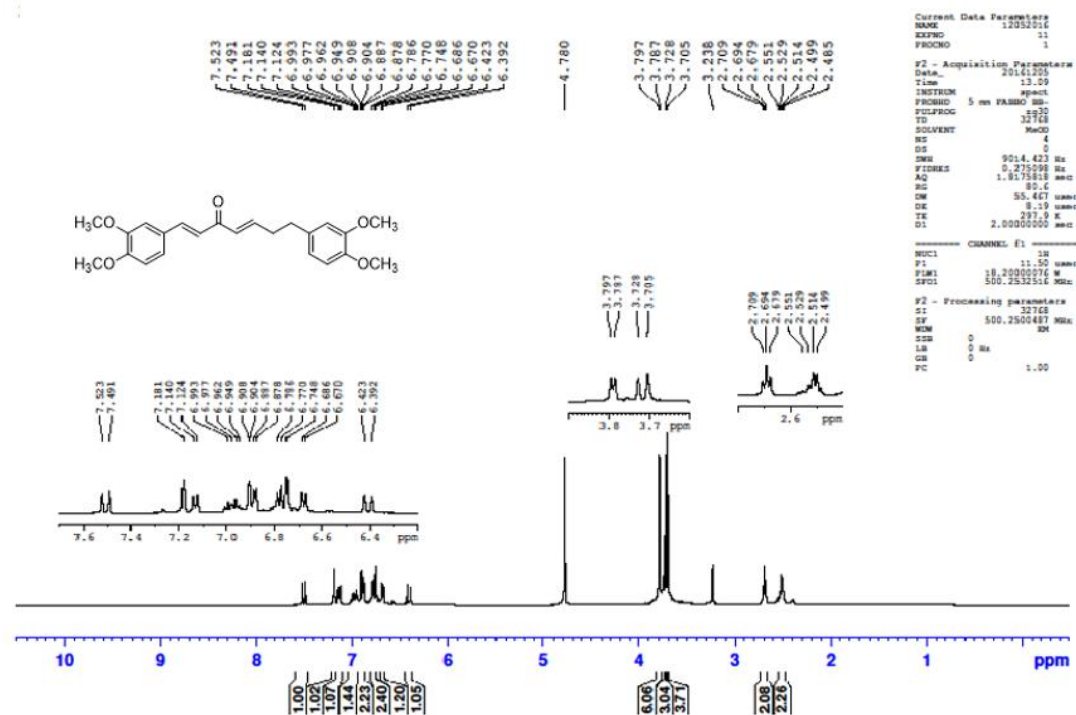


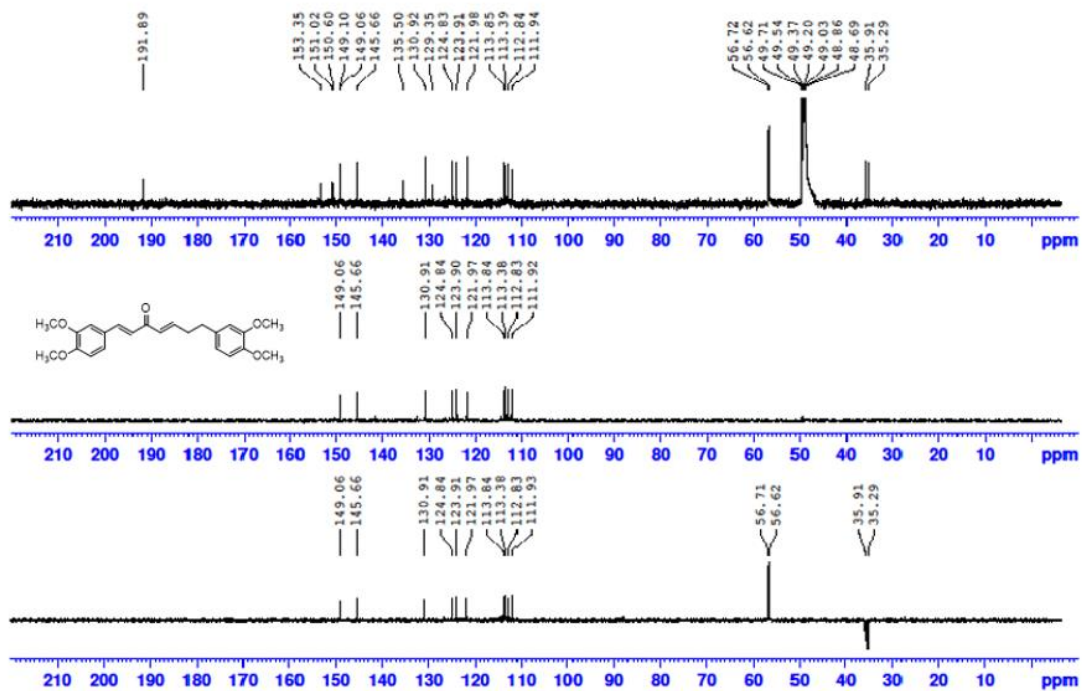
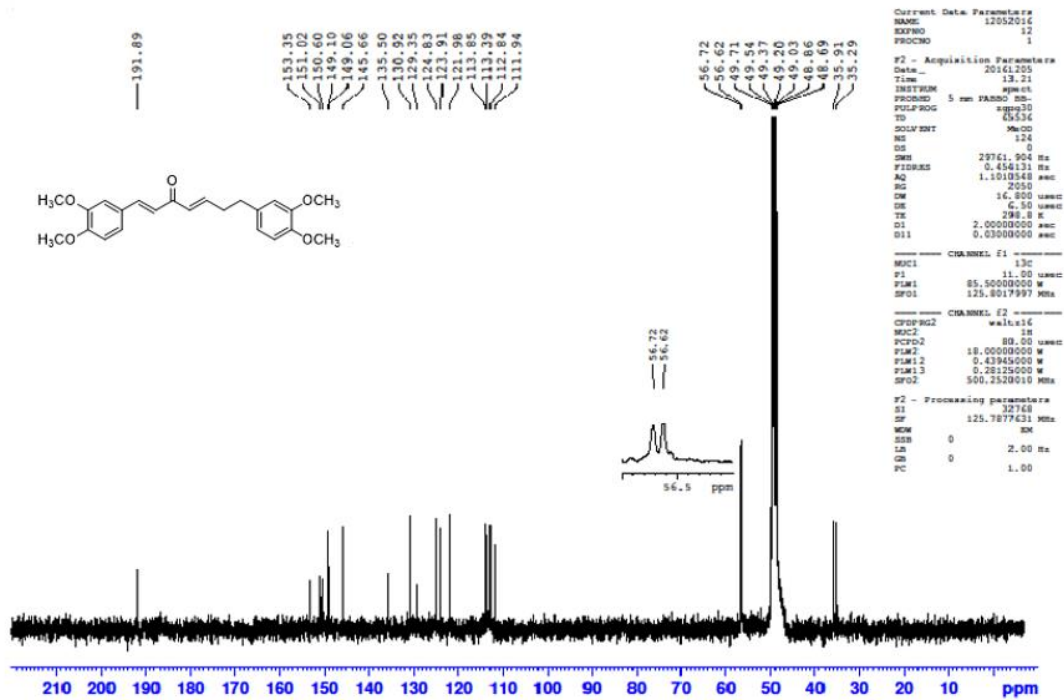
MD7



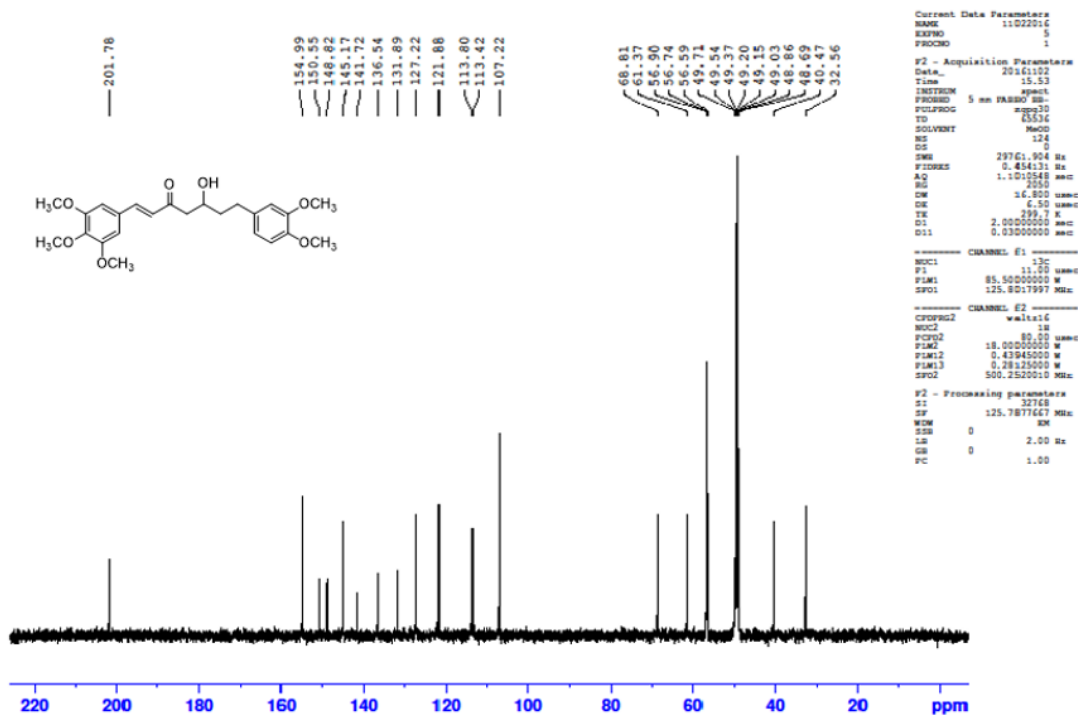
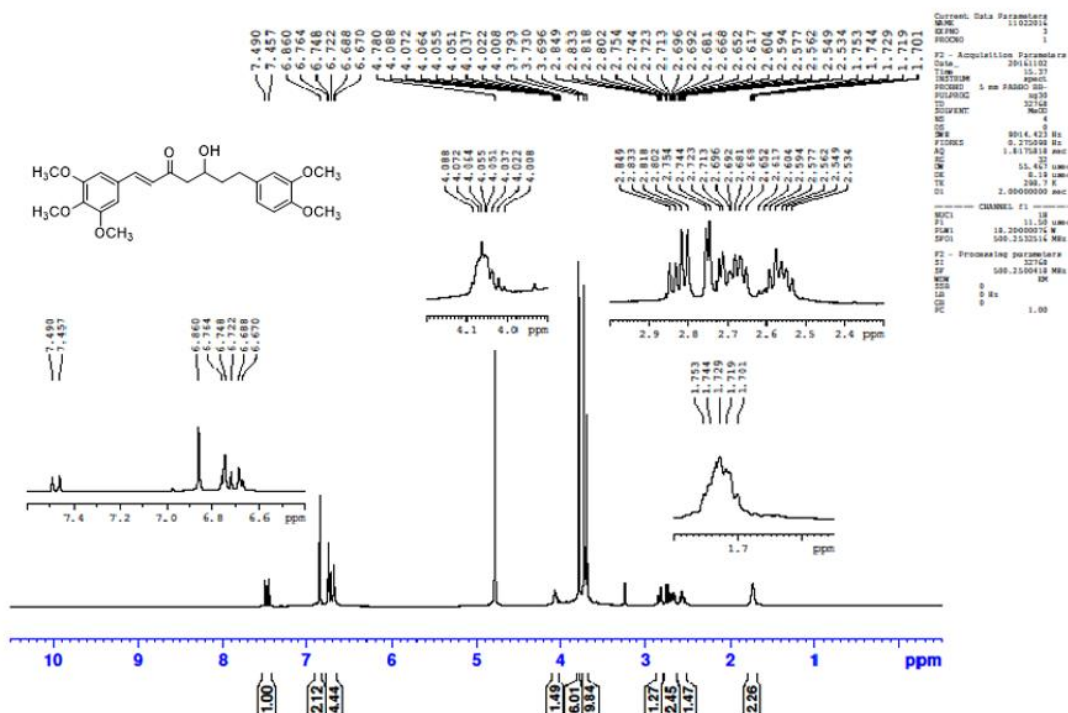


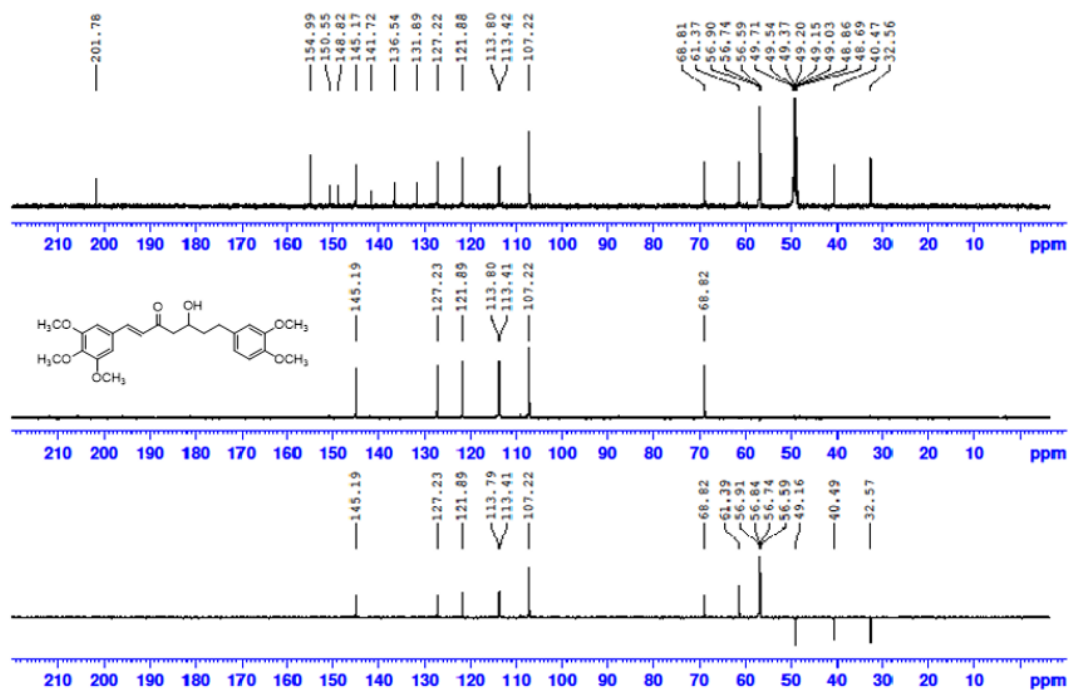
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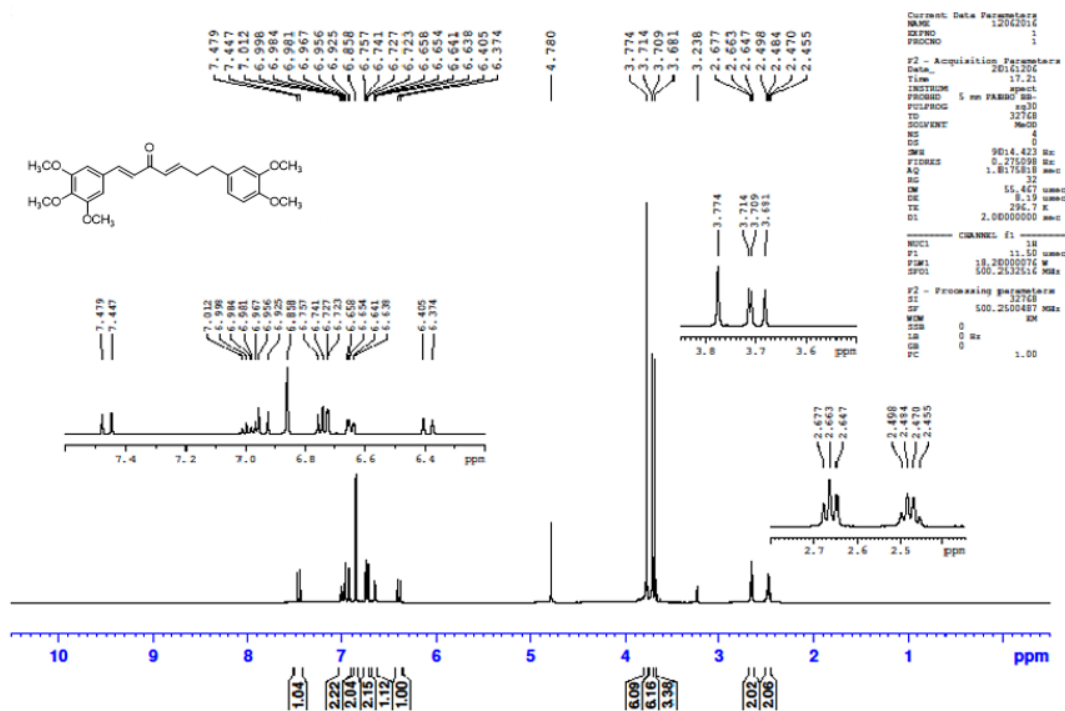


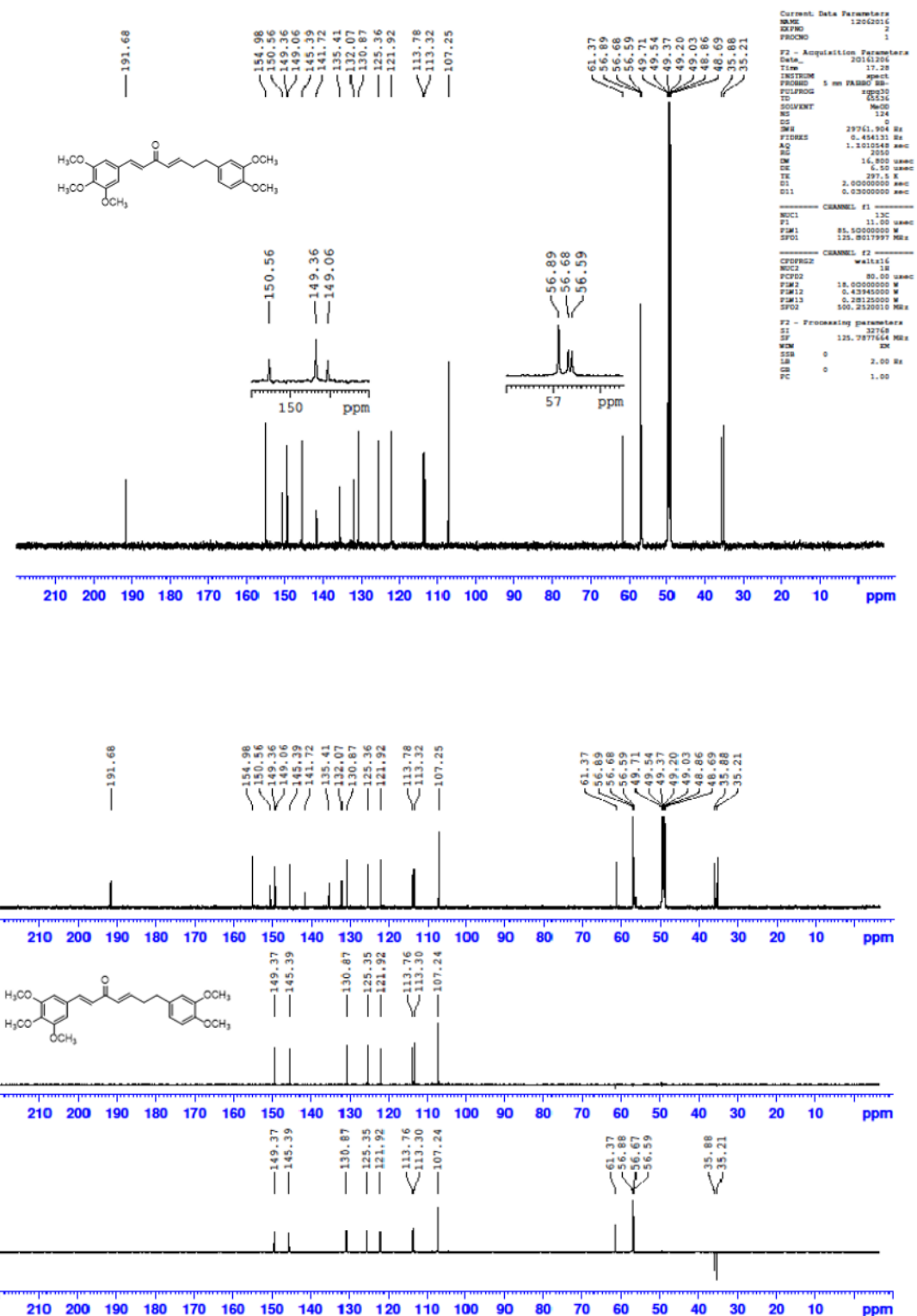
MD8



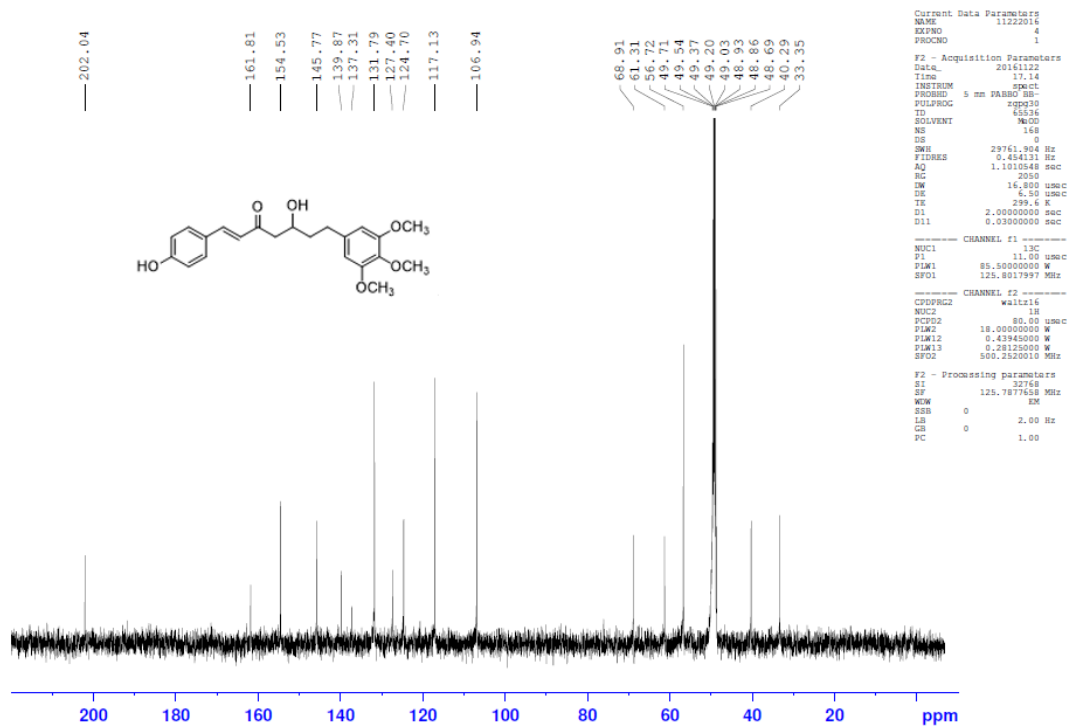
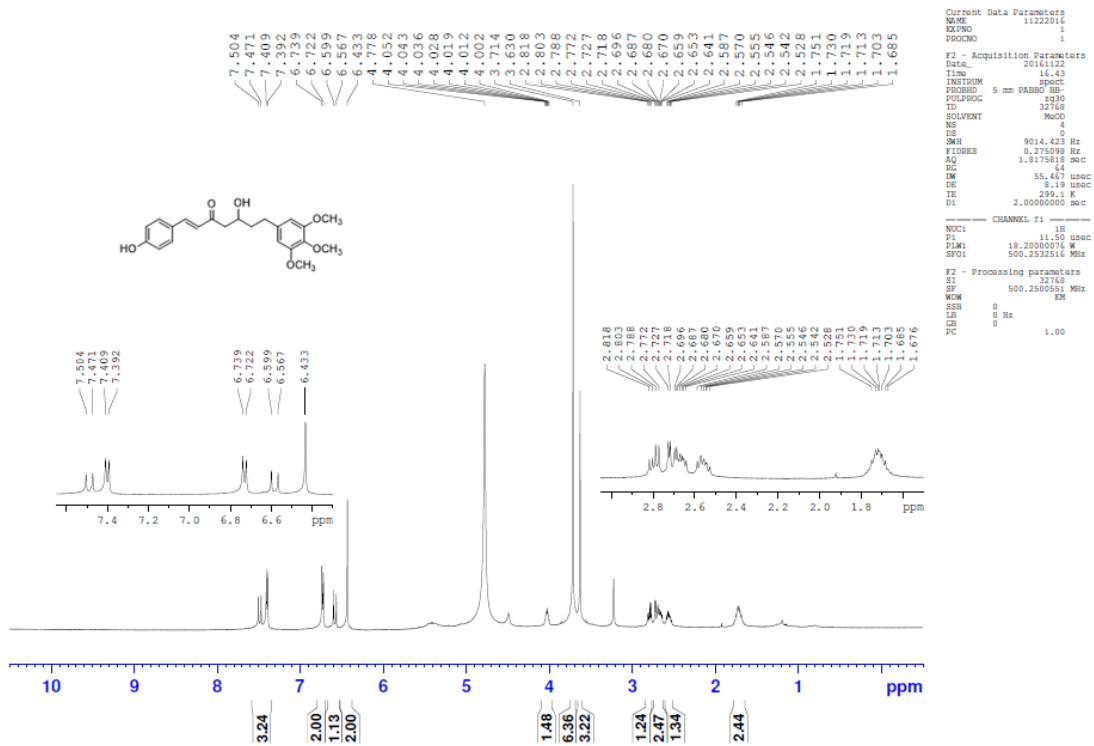


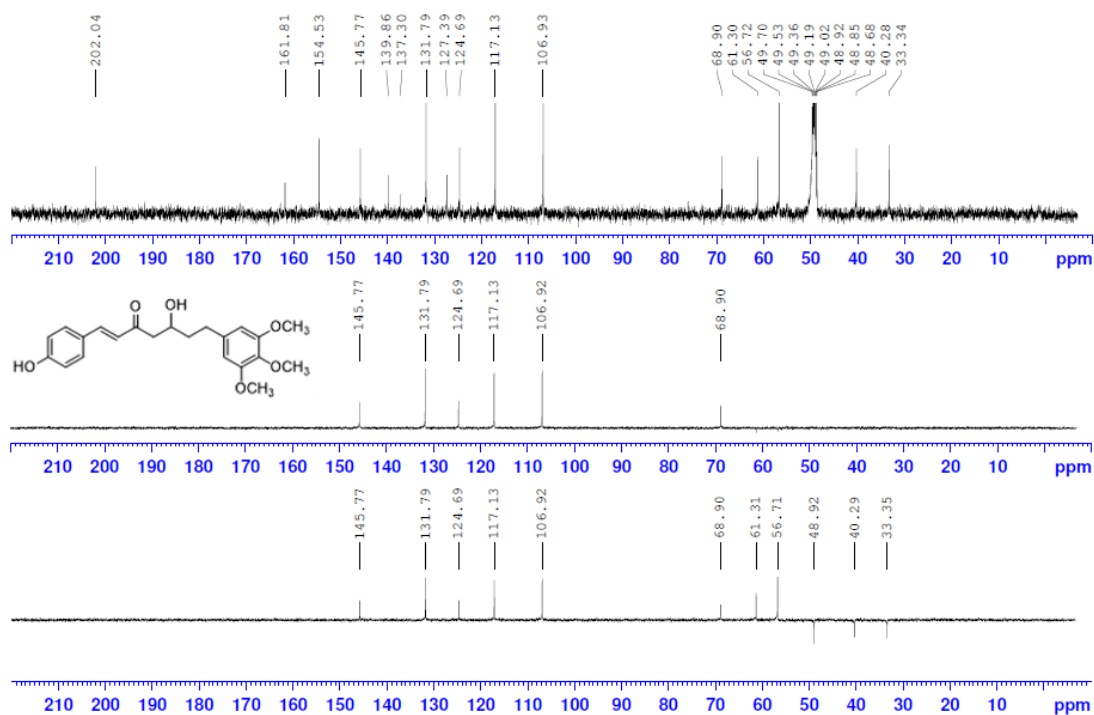
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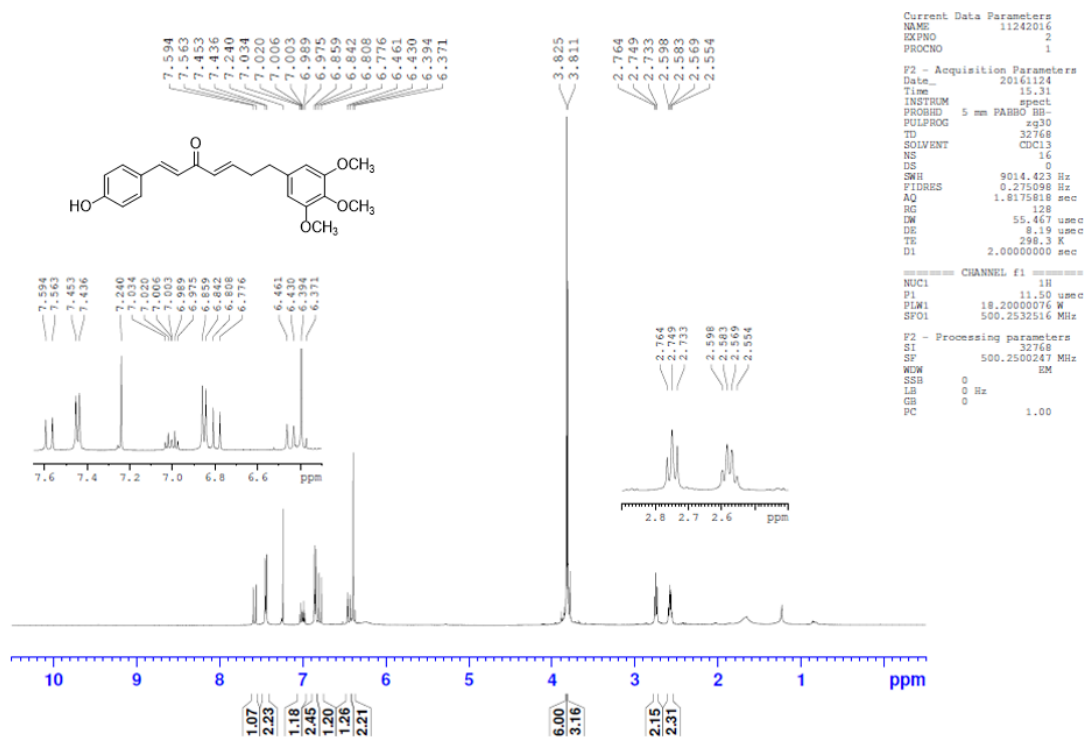


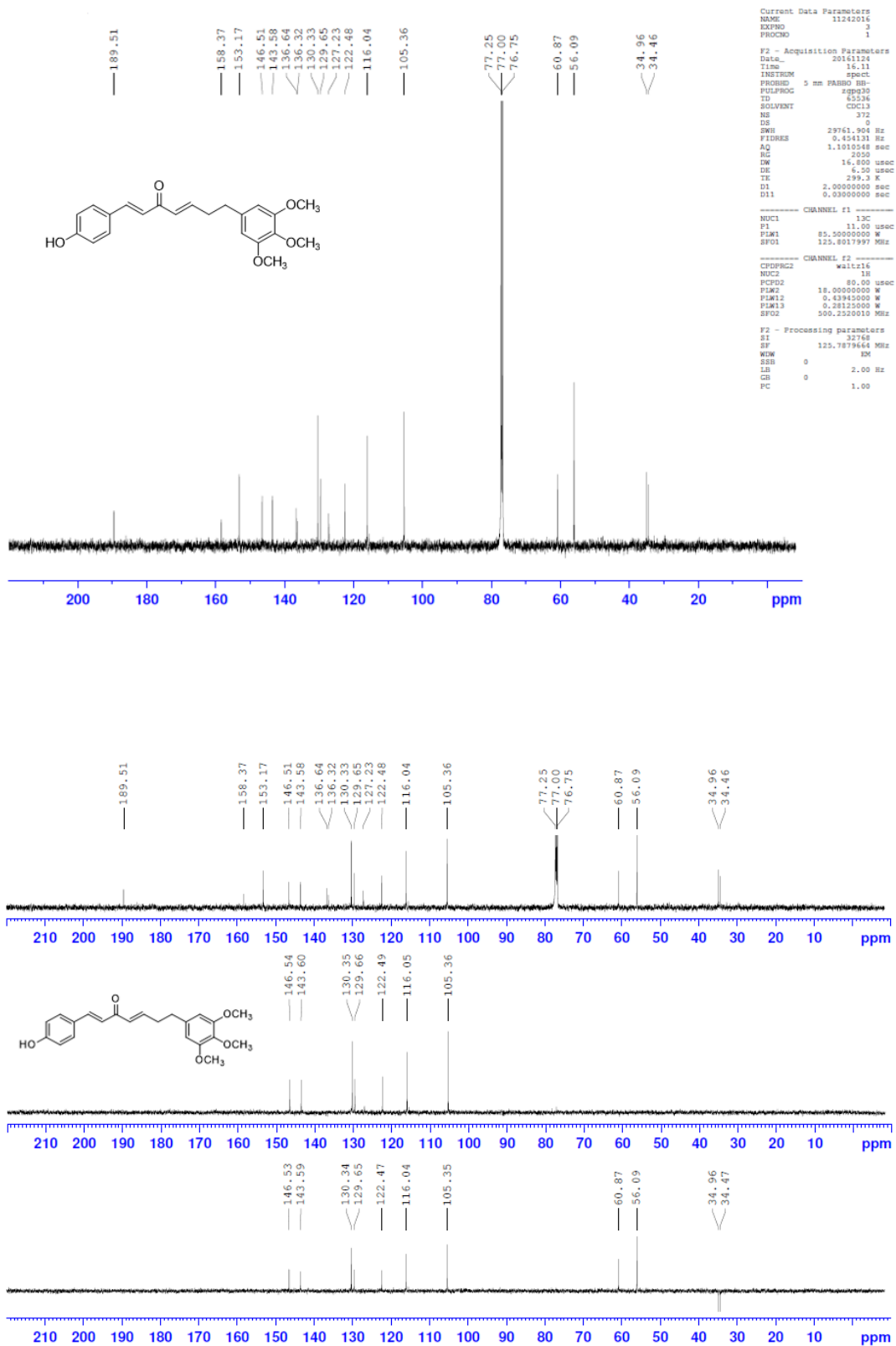
MD9



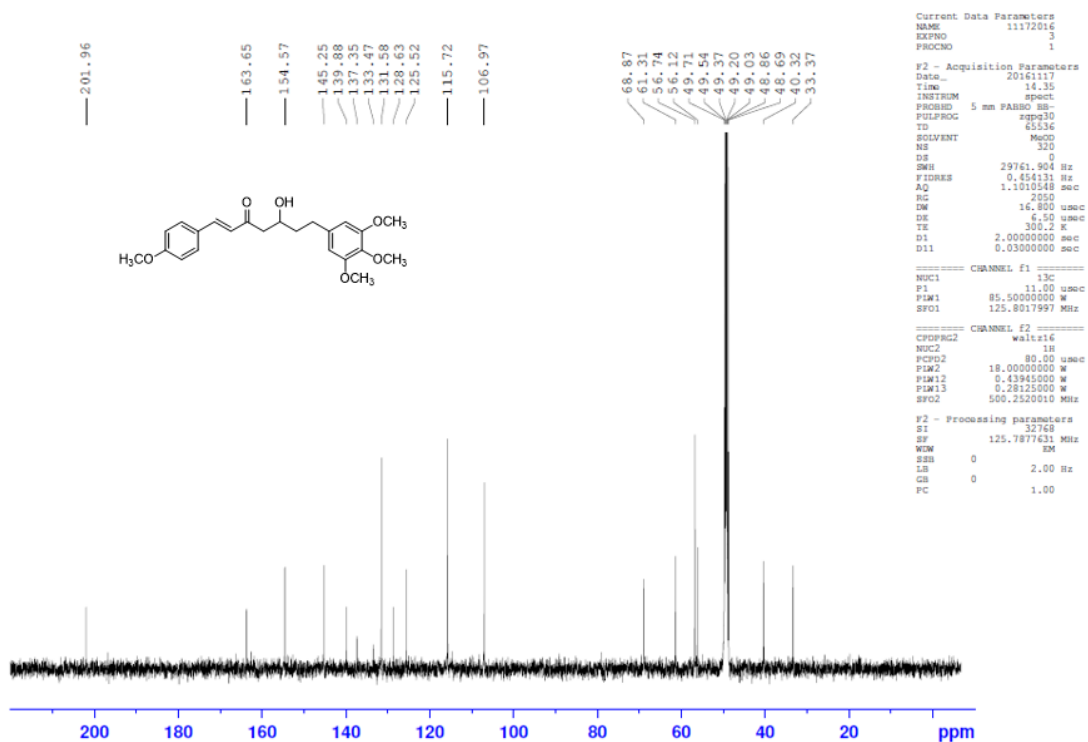
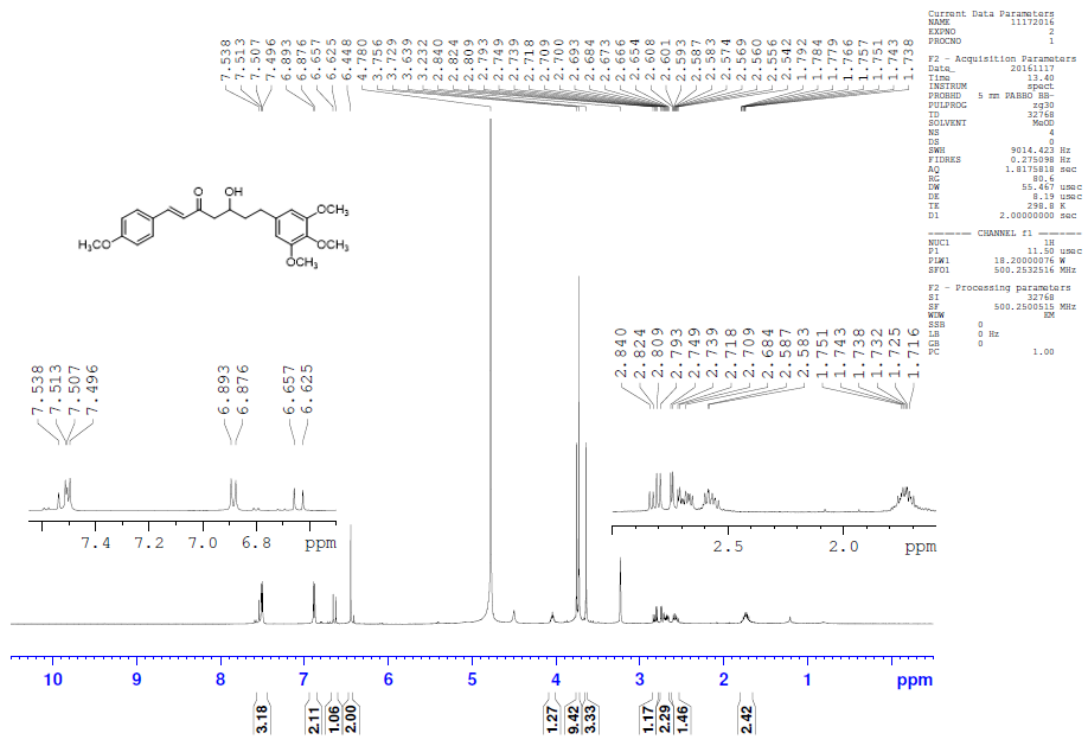


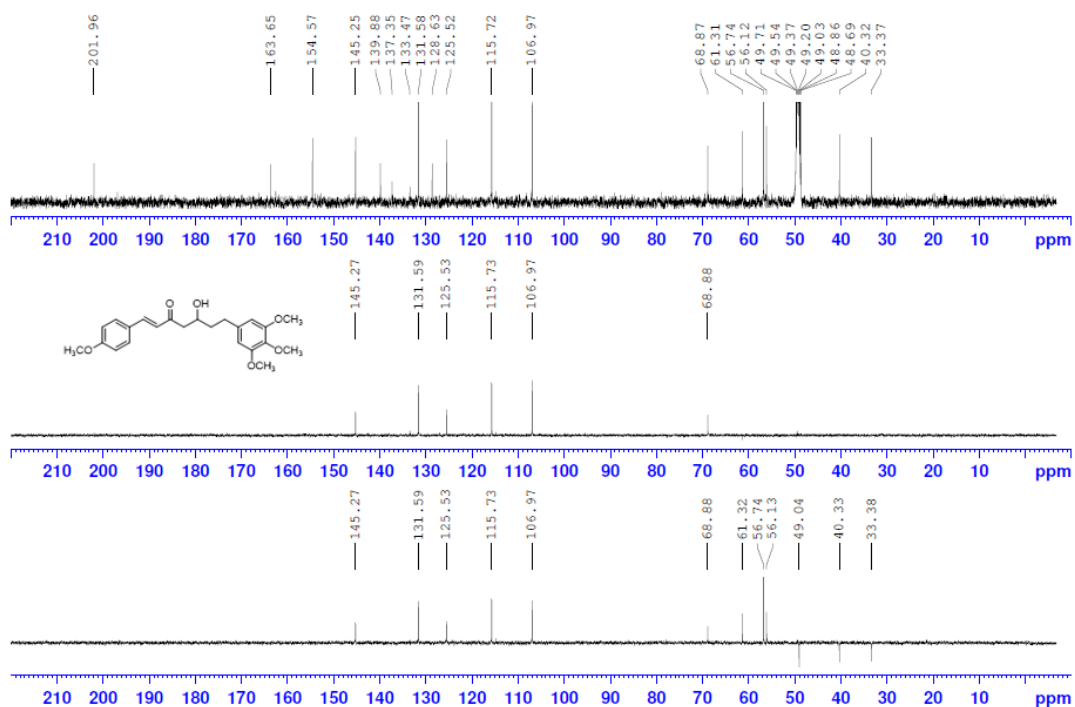
MD9a



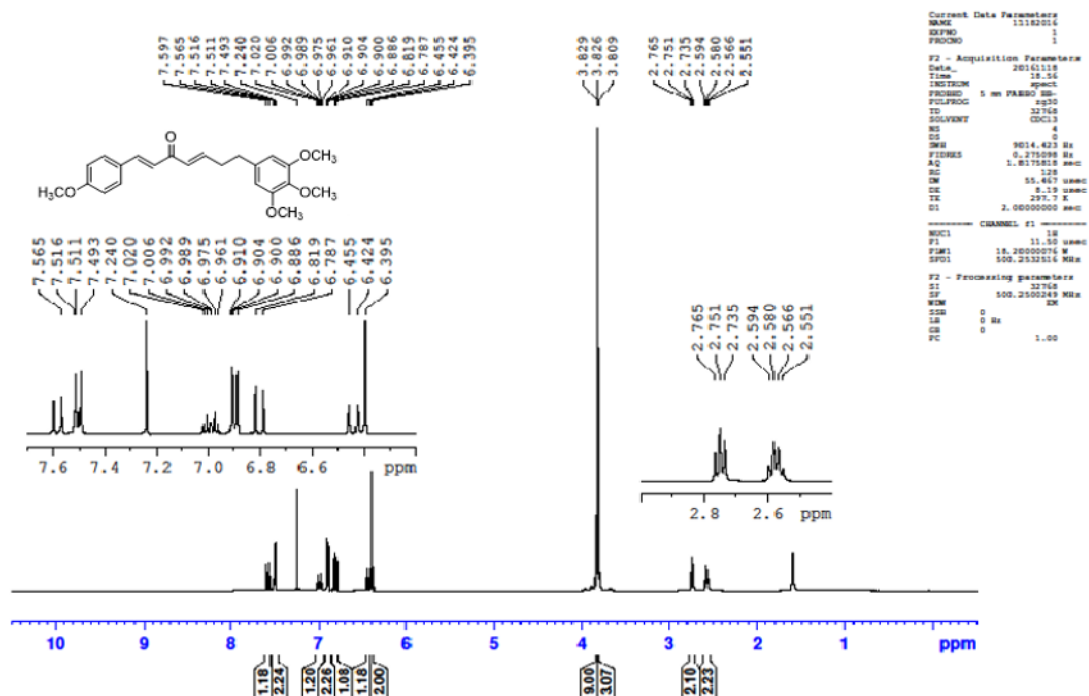


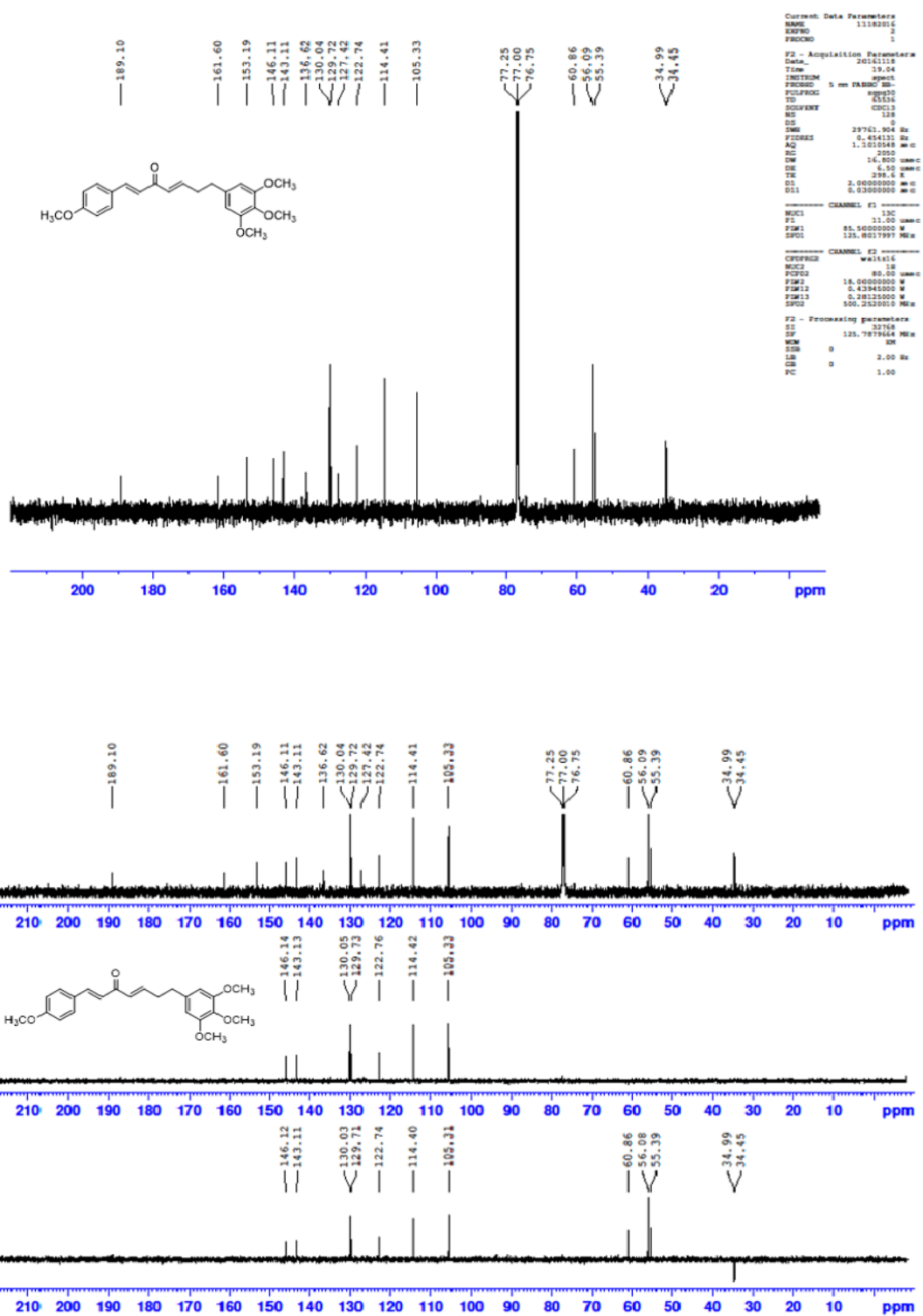
MD10



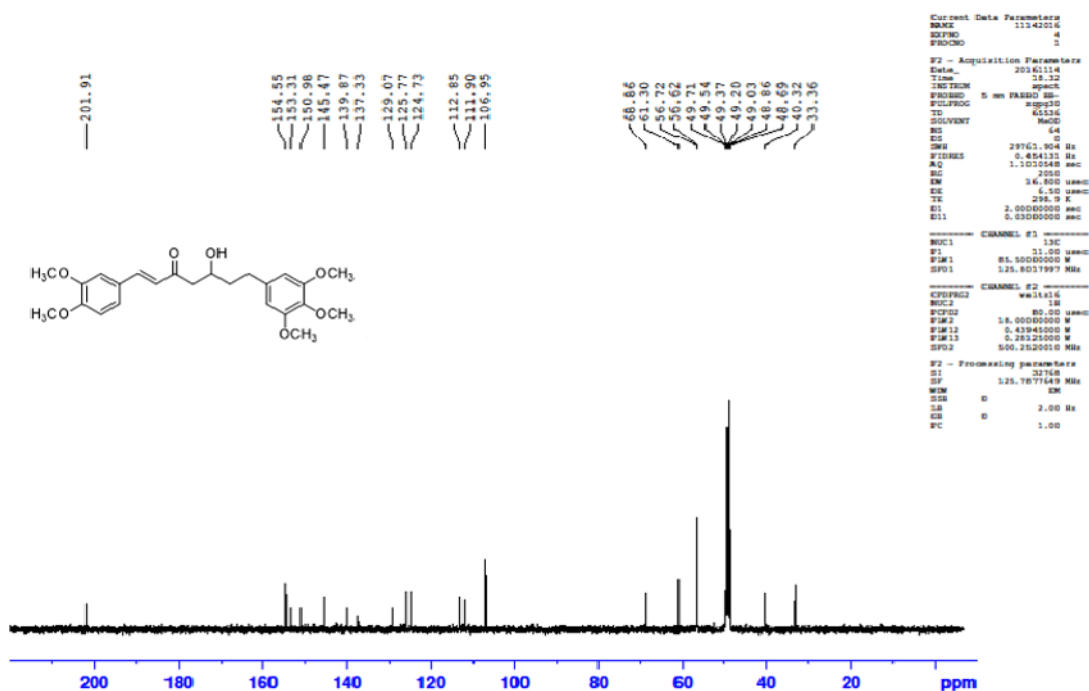
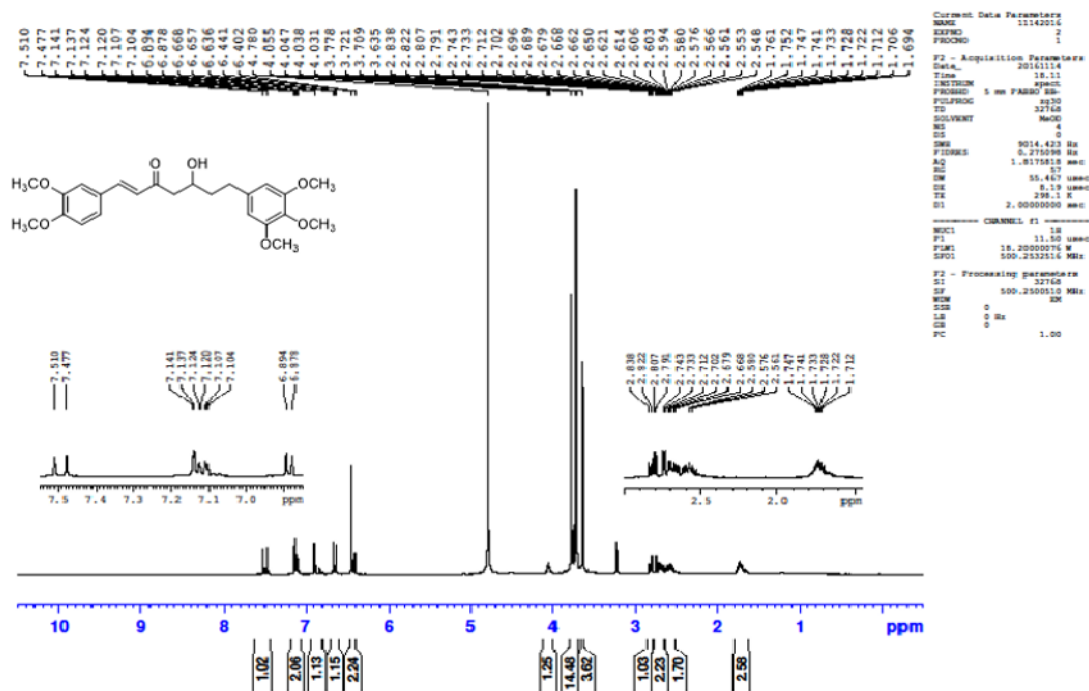


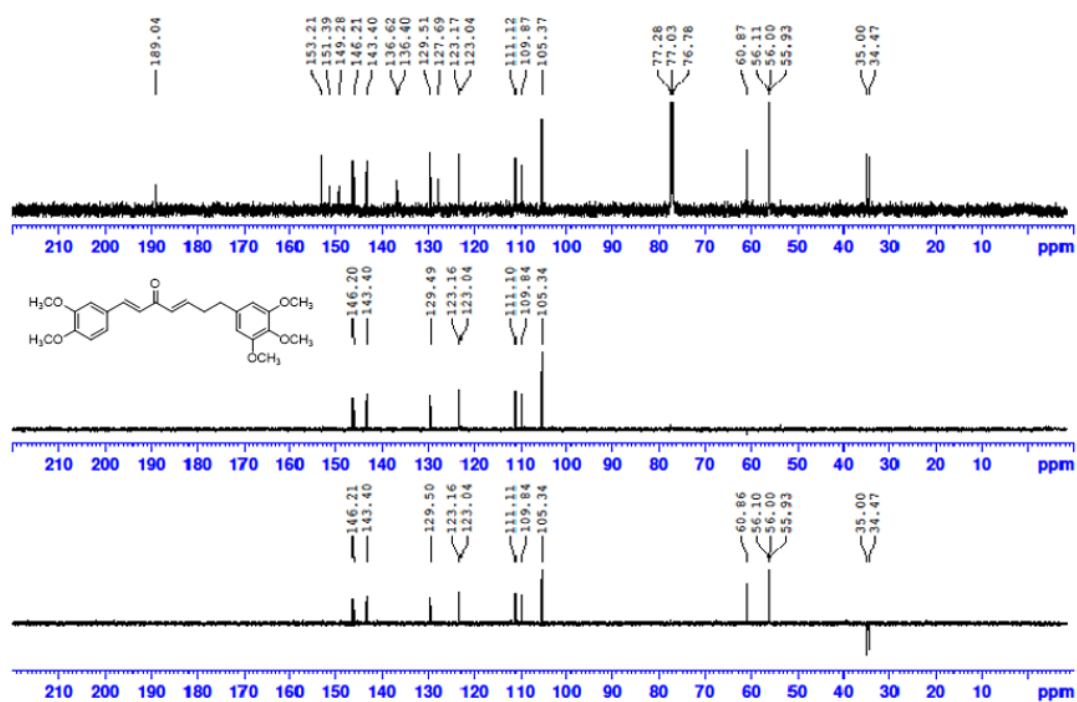
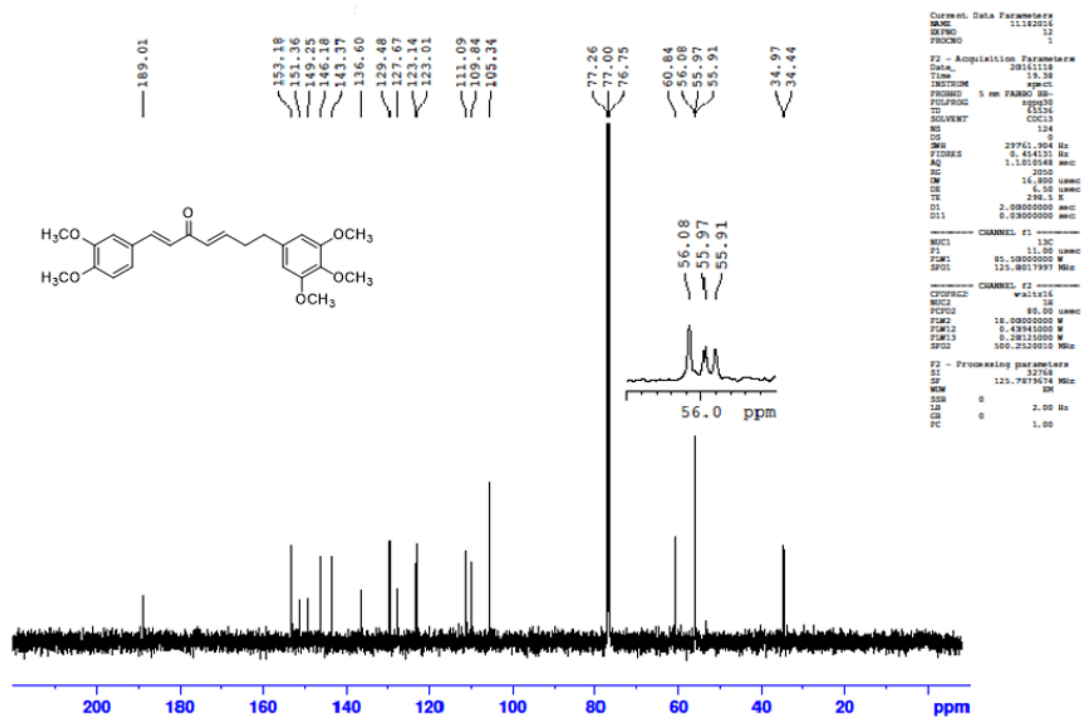
MD10a



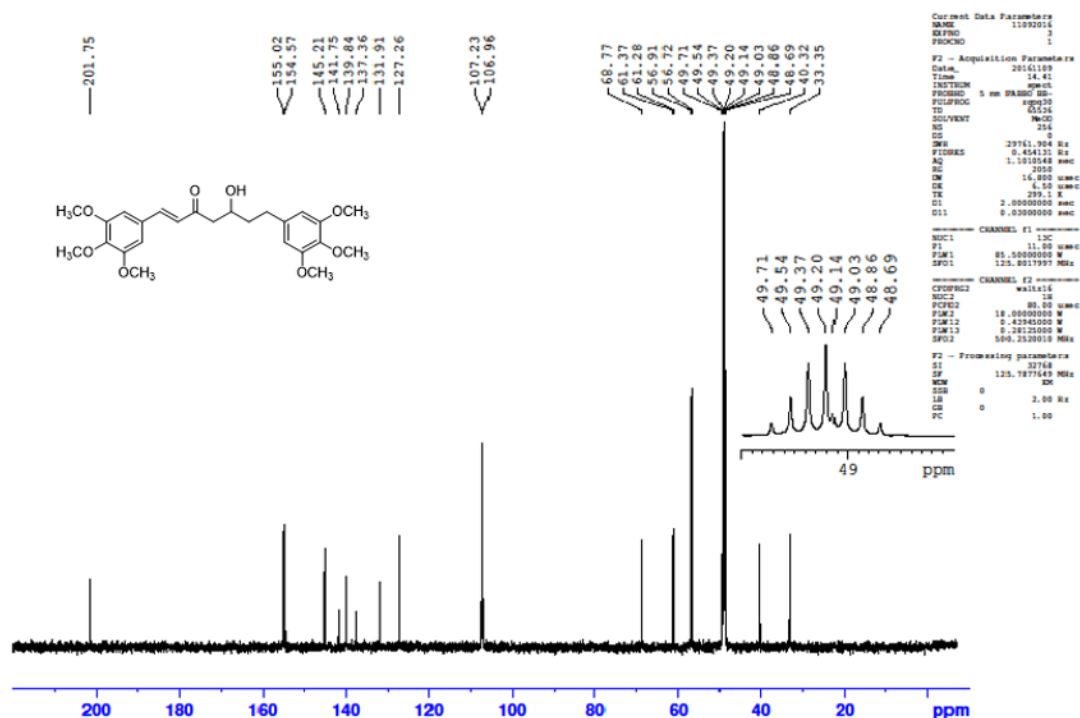
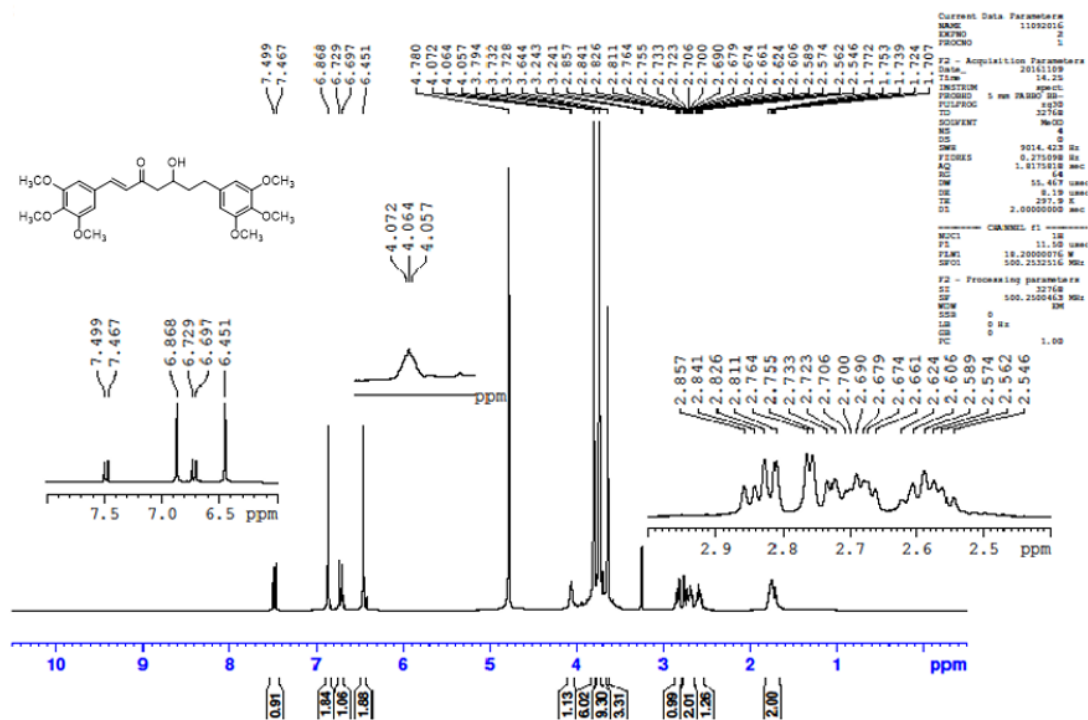


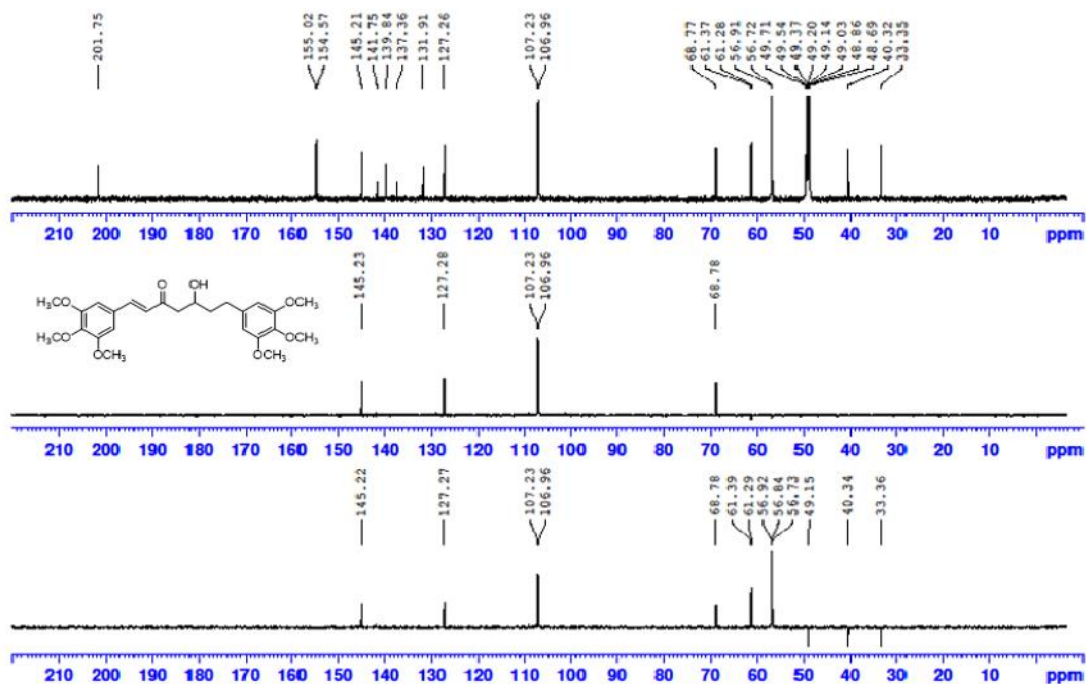
MD11





MD12





MD12a

