Supplementary Material for

Synthesis of 6- and 7-alkoxy-4-methylcoumarins from corresponding hydroxy coumarins and their conversion into 6- and 7-alkoxy-4-formylcoumarin derivatives

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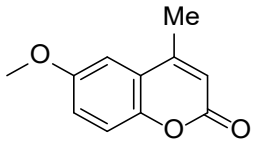
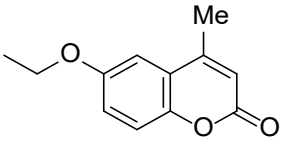
1.1. 6-Alkoxy- and 7-alkoxy-4-methylcoumarins (3 and 4)

*4-Methyl-6-methoxycoumarin (**3a**)*



From **2a** (0.02 mol, 3.52 g), methyl iodide (0.024 mol, 1.93 mL). Yield: 3.47 g (85%) of **3a** as pale-yellow crystals. M.p.: 165−167 °C (from 96% ethanol), ref.:[1] 163−167 °C (from 96% ethanol). IR (KBr), ν (cm^{-1}) 1714 ($\nu_{C=O}$ lactone), 1570, 1486 ($\nu_{C=C}$ arene), 1168 &1069 (ν_{COC} lactone); ^{1}H NMR (DMF-d_6), δ (ppm): 7.98 (s, 1H, H-5), 7.87−7.85 (m, 2H, H-7 & H-8), 6.88 (s, 1H, H-3), 2.84 (s, 3H, 6-OCH_3), 2.74 (s, 3H, 4-CH_3); ^{13}C NMR (126 MHz, DMF-d_6), δ (ppm): ^{13}C NMR (125 MHz, DMSO-d_6), δ (ppm): 160.5 (C=O lactone), 153.6 (C-6), 151.4 (C-8a), 147.4 (C-4), 126.8 (C-5), 121.2 (C-7), 118.9 (C-8), 118.4 (C-4a), 115.9 (C-3), 67.8 (6-O**C**$\mathbf{H_3}$), 18.9 (4-CH_3); ESI-MS: $C_{11}H_{10}O_3$, calc. for M+H=191.07 Da, M+Na=213.05 Da, found: *m/z* 191.13 ($[M+H]^+$), 213.15 ($[M+Na]^+$); ESI/HRMS: calcd. for M+H = 191.0708 Da, found: *m/z* 191.0713 ($[M+H]^+$, 100%); Elemental anal. for $C_{11}H_{10}O_3$, calcd.: C, 69.46; H, 5.30%; found: C, 69.57; H, 5.41%.

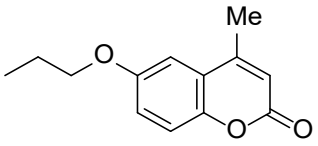
*4-Methyl-6-ethoxycoumarin (**3b**)*



From **2a** (0.02 mol, 3.52 g), ethyl iodide (0.024 mol, 1.93 mL). Yield: 3.47 g (85%) of **3b** as pale-yellow crystals. M.p.: 116−117.5 °C (from 96% ethanol), ref.:[2] 161–162 °C (from 96% ethanol). IR (KBr), ν (cm^{-1}) 1715 ($\nu_{C=O}$ lactone), 1572, 1485 ($\nu_{C=C}$ arene), 1165 &1067 (ν_{COC} lactone); ^{1}H NMR (500 MHz, DMSO-d_6, ppm), δ (ppm): 7.27 (d, J = 9.0 Hz, 1H, H-8), 7.16 (dd, J = 9.0, 2.5 Hz, 1H, H-7), 7.11 (d, J = 2.5 Hz, 1H, H-5), 6.34 (s, 1H, H-3), 4.07 (q, J = 7.0 Hz, 2H, 6-O**C**$\mathbf{H_2}$$CH_3$), 2.39 (s, 3H, 4-$CH_3$), 1.35 (t, J = 7.0 Hz, 3H, 6-OCH_2**C**$\mathbf{H_3}$); ^{13}C NMR (125 MHz, DMSO-d_6), δ (ppm): 160.3 (C=O lactone), 155.3 (C-6), 153.4 (C-8a), 147.6 (C-4), 120.5 (C-5), 119.7 (C-7), 117.8 (C-8), 115.1 (C-4a), 109.2 (C-3), 64.2 (6-O**C**$\mathbf{H_2}$$CH_3$), 18.6 (4-$CH_3$), 15.0 (6-$OCH_2$**C**$\mathbf{H_3}$); ESI-MS: $C_{12}H_{12}O_3$, calc. for M = 204.1 Da, found: *m/z* 204.2 ($[M]^+$);

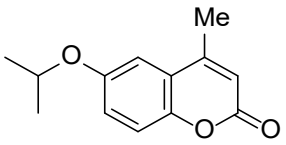
ESI/HRMS: calcd. for M+H = 205.0865 Da, found: *m/z* 205.0873 ([M+H]$^+$, 100%); Elemental anal. for $C_{12}H_{12}O_3$, calcd.: C, 70.58; H, 5.92%; found: C, 70.33; H, 5.81%.

*4-Methyl-6-propoxycoumarin (**3c**)*



From **2a** (0.02 mol, 3.52 g), propyl iodide (0.022, 2.4 mL). Yield: 3.27 g (75%) of **3c** as pale-yellow crystals. M.p.: 119−121.5 °C (from 96% ethanol). IR (KBr), ν (cm^{-1}): 1713 ($\nu_{C=O}$ lactone), 1576, 1497 ($\nu_{C=C}$ arene), 1173 &1029 (ν_{COC} lactone); ^{1}H NMR (500 MHz, $CDCl_3$, ppm), δ (ppm): 7.32 (d, *J* = 8.5 Hz, 1H, H-8), 7.22−7.18 (m, 2H, H-5 & H-7), 6.38 (s, 1H, H-3), 4.02 (t, *J* = 7.0 Hz, 2H, 6-O**CH$_2$**CH$_2$CH$_3$), 2.43 (s, 3H, 4-CH$_3$), 1.76 (sextet, *J* = 7.0 Hz, 2H, 6-OCH$_2$**CH$_2$**CH$_3$), 1.35 (t, *J* = 7.0 Hz, 3H, 6-OCH$_2$CH$_2$**CH$_3$**); ^{13}C NMR (125 MHz, DMSO-*d*$_6$), δ (ppm): 160.4 (C=O lactone), 155.5 (C-6), 153.5 (C-8a), 147.6 (C-4), 120.6 (C-5), 119.9 (C-7), 117.9 (C-8), 115.1 (C-4a), 109.4 (C-3), 70.2 (6-O**CH$_2$**CH$_2$CH$_3$), 22.5 (4-CH$_3$), 18.6 (6-OCH$_2$**CH$_2$**CH$_3$), 10.9 (6-OCH$_2$CH$_2$**CH$_3$**); ESI-MS: $C_{13}H_{14}O_3$, calcd. for M+H = 219.10 Da, M+Na = 241.08 Da, found: *m/z* 219.16 ([M+H]$^+$), 241.09 ([M+Na]$^+$); ESI-HRMS: calcd. for M+H = 219.1021 Da, found: *m/z* 219.1028 ([M+H]$^+$, 100%); Elemental anal. for $C_{13}H_{14}O_3$, calcd.: C, 71.54; H, 6.47%; found: C, 71.21; H, 6.62%.

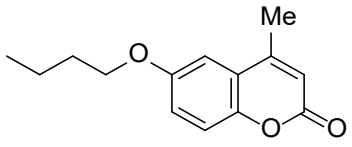
*4-Methyl-6-isopropoxycoumarin (**3d**)*



From **2a** (0.02 mol, 3.52 g), isopropyl iodide (0.022, 2.4 mL). Yield: 2.62 g (60%) of **3d** as pale-yellow crystals. M.p.: 120−122 °C (from 96% ethanol). IR (KBr), ν (cm^{-1}): 1709 ($\nu_{C=O}$ lactone), 1573, 1490 ($\nu_{C=C}$ arene), 1170 & 1020 (ν_{COC} lactone); ^{1}H NMR (500 MHz, DMSO-*d*$_6$, ppm), δ (ppm): 7.68 (d, *J* = 3.0 Hz, 1H, H-5), 6.93−6.88 (m, 2H, H-7 & H-8), 6.48 (s, 1H, H-3), 4.18 [septet, *J* = 6.5 Hz, 1H, 6-O**CH** (CH$_3$)$_2$], 1.02−0.98 [m, 6H, 6-OCH**(CH$_3$)$_2$**]; ^{13}C NMR (125 MHz, DMSO-*d*$_6$), δ (ppm): 162.2 (C=O lactone), 160.6 (C-6), 155.2 (C-4), 153.8 (C-8a), 126.8 (C-4a), 113.4 (C-8), 112.8 (C-7), 111.5 (C-3), 101.5 (C-5), 68.2 [6-O**CH**(CH$_3$)$_2$], 22.3

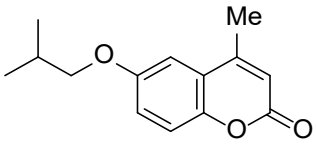
[6-OCH **(CH_3)$_2$**]; ESI-MS: $C_{13}H_{14}O_3$, calcd. for M+H = 219.10 Da, M+Na = 241.08 Da, found: *m/z* 219.15 ($[M+H]^+$), 241.15 ($[M+Na]^+$); Elemental anal. for $C_{13}H_{14}O_3$, calcd.: C, 71.54; H, 6.47%; found: C, 71.32; H, 6.24%.

*4-Methyl-6-butoxycoumarin (**3e**)*



From **2a** (0.02 mol, 3.52 g), butyl bromide (0.022 mol, 2.58 mL), and KI (0.001 mol, 0.17 g). Yield: 4.65 g (85%) of **3e** as white crystals. M.p.: 107−109 °C (from 96% ethanol). IR (KBr), ν (cm^{-1}): 1721 ($\nu_{C=O}$ lactone), 1569, 1428 ($\nu_{C=C}$ arene), 1242 &1166 (ν_{COC} lactone); ^{1}H NMR (500 MHz, DMSO-d_6), δ (ppm): 7.28 (d, J = 9.0 Hz, 1H, H-7), 7.18 (dd, J = 9.0, 3.0 Hz, 1H, H-8), 7.15 (d, J = 2.3 Hz, 1H, H-3), 6.35 (d, J = 1.0 Hz, 1H, H-5), 4.01 (t, J = 6.5 Hz, 2H, 6-O**C**$\mathbf{H}_2$$CH_2CH_2CH_3$), 2.40 (d, J = 2.0 Hz, 3H, 4-CH_3), 1.70 (quintet, J = 6.5 Hz, 2H, 6-$OCH_2C\mathbf{H}_2CH_2CH_3$), 1.44 (sextet, J = 7.0 Hz, 2H, 6-$OCH_2CH_2\mathbf{C}\mathbf{H}_2CH_3$), 0.93 (t, J = 7.0 Hz, 3H, 6-$OCH_2CH_2CH_2\mathbf{C}\mathbf{H}_3$); ^{13}C NMR (125 MHz, DMSO-d_6), δ (ppm): 159.8 (C=O lactone), 155.0 (C-6), 152.9 (C-8a), 147.0 (C-4), 120.0 (C-5), 119.3 (C-7), 117.3 (C-8), 114.6 (C-4a), 108.7 (C-3), 67.8 (6-O**C**$\mathbf{H}_2$$CH_2CH_2CH_3$), 30.7 (4-$CH_3$), 18.7 (6-$OCH_2\mathbf{C}\mathbf{H}_2CH_2CH_3$), 18.1 (6-$OCH_2CH_2\mathbf{C}\mathbf{H}_2CH_3$), 13.6 (6-$OCH_2CH_2CH_2\mathbf{C}\mathbf{H}_3$); ESI-MS: $C_{14}H_{16}O_3$, calcd. for (M+2H) = 234.2 Da, found: *m/z* 234.1 ($[M+2H]^+$); ESI-HRMS: calcd. for M+H = 233.1178 Da, found: 233.1184 ($[M+H]^+$, 100%); Elemental anal. for $C_{14}H_{16}O_3$, calcd.: C, 72.39; H, 6.94%; found: C, 72.17; H, 6.71%.

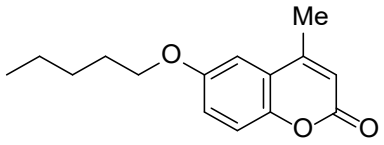
*4-Methyl-6-isobutoxycoumarin (**3f**)*



From **2a** (0.02 mol, 3.52 g), isobutyl bromide (0.022 mol, 2.59 mL), and KI (0.1 mmol, 0.17 g). Yield: 3.49 g (75%) of **3f** as white crystals. M.p.: 103−105 °C (from 96% ethanol). IR (KBr), ν (cm^{-1}): 1718 ($\nu_{C=O}$ lactone), 1520, 1500, 1480 ($\nu_{C=C}$ arene), 1248 & 1167 (ν_{COC} lactone); ^{1}H NMR (500 MHz, DMSO-d_6), δ (ppm): 7.60 (d, J = 8.75 Hz, 1H, H-7), 6.92−6.87 (m, 2H, H-5 & H-8), 6.16 (s, 1H, H-3), 4.04 [d, J = 5.0 Hz, 2H, 6-O**C**$\mathbf{H}_2$CH (CH_3)$_2$], 2.36 (s,

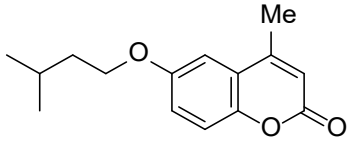
3H, 4-CH_3), 1.73−1.67 [m, 1H, 6-OCH_2**C**H (CH_3)$_2$], 0.98 [d, *J* = 7.0 Hz, 6H, 6-OCH_2CH (**CH_3)$_2$**]; ^{13}C NMR (125 MHz, DMSO-*d*$_6$), δ (ppm): 162.2 (C=O lactone), 160.6 (C-6), 155.2 (C-4), 153.8 (C-8a), 126.8 (C-4a), 113.4 (C-8), 112.8 (C-7), 111.5 (C-3), 101.5 (C-5), 68.4 [6-O**CH_2**CH (CH_3)$_2$], 31.0 [6-OCH_2**C**H (CH_3)$_2$], 19.1 [6-OCH_2CH **(CH_3)$_2$**], 18.5 (4-CH_3), 14.1 [6-OCH_2**C**H (CH_3)$_2$]; ESI-MS: $C_{14}H_{16}O_3$, calcd. for M+H = 233.12 Da, M+Na = 255.10 Da, found: *m/z* 233.19 ([M+H]$^+$), 255.08 ([M+Na]$^+$); ESI-HRMS: calcd. for M+H = 233.1178 Da, found: 233.1185 ([M+H]$^+$, 100%); Elemental anal. for $C_{14}H_{16}O_3$, calcd.: C, 72.39; H, 6.94%; found: C, 72.57; H, 6.61%.

*4-Methyl-6-pentoxycoumarin (**3g**)*



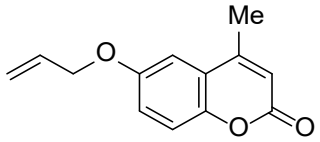
From **2a** (0.02 mol, 3.52 g), pentyl bromide (0.022 mol, 3.12 mL), and KI (0.001 mol, 0.17 g). Yield: 4.88 g (84%) of **3g** as white crystals. M.p.: 90−92 °C (from 96% ethanol). IR (KBr), ν (cm^{-1}): 1719 ($\nu_{C=O}$ lactone), 1568, 1492 ($\nu_{C=C}$ arene), 1248 &1170 (ν_{COC} lactone); ^{1}H NMR (500 MHz, DMSO-*d*$_6$), δ (ppm): 7.28 (d, *J* = 9.0 Hz, 1H, H-7), 7.18 (dd, *J* = 8.75, 2.3 Hz, 1H, H-8), 7.15 (d, *J* = 3.0 Hz, 1H, H-3), 6.45 (d, *J* = 0.5 Hz, 1H, H-3), 4.00 (t, *J* = 6.5 Hz, 2H, 6-O**CH_2**$CH_2CH_2CH_2CH_3$), 2.40 (d, 3H, *J* = 1.0 Hz, 4-CH_3), 1.72 (quintet, *J* = 6.5 Hz, 2H, 6-OCH_2**CH_2**$CH_2CH_2CH_3$), 1.37−1.35 (m, 4H, 6-OCH_2CH_2**CH_2CH_2**CH_3), 0.88 (t, *J* = 7.0 Hz, 3H, 6-$OCH_2CH_2CH_2CH_2$**C**H$_3$); ^{13}C NMR (125 MHz, DMSO-*d*$_6$), δ (ppm): 159.9 (C=O lactone), 155.0 (C-6), 153.0 (C-8a), 147.1 (C-4), 120.1 (C-5), 119.3 (C-7), 117.4 (C-8), 114.6 (C-4a), 108.8 (C-3), 68.1 (6-O**CH_2**$(CH_2)_3CH_3$], 28.3 (4-CH_3), 27.7 (6-OCH_2**CH_2**$CH_2CH_2CH_3$), 21.8 (6-OCH_2CH_2**CH_2**CH_2CH_3), 18.1 [6-$OCH_2CH_2CH_2$**CH_2**CH_3), 13.9 (6-$OCH_2CH_2CH_2CH_2$**C**H$_3$]; ESI-MS: $C_{15}H_{18}O_3$, calcd. for (M+H) = 247.1 Da, found: *m/z* 247.2 ([M+H]$^+$); ESI-HRMS: calcd. for M+H = 247.1334 Da, found: *m/z* 247.1339 ([M+H]$^+$, 100%); Elemental anal. for $C_{15}H_{18}O_3$, calcd.: C, 73.15; H, 7.37%; found: 73.35; H, 7.12%.

*4-Methyl-6-isopentoxycoumarin (**3h**)*



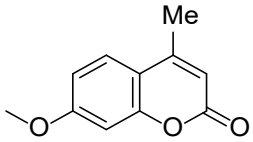
From **2a** (0.02 mol, 3.52 g), isopentyl bromide (0.024 mol, 2.88 mL), and KI (0.1 mmol, 0.17 g). Yield: 3.85 g (79%) of **3h** as white crystals. M.p.: 99−101 °C (from 96% ethanol). IR (KBr), ν (cm^{-1}): 1708 ($\nu_{C=O}$ lactone), 1571 ($\nu_{C=C}$ arene), 1243 & 1169 (ν_{COC} lactone); ^{1}H NMR (500 MHz, DMSO-d_6), δ (ppm): 7.24 (t, J = 6.0 Hz, 1H, H-7), 7.14 (dd, J = 8.75, 3.0 Hz, 1H, H-8), 7.10 (s, 1H, H-3), 6.31 (d, J = 1.0 Hz, 1H, H-5), 4.00 [t, J = 6.5 Hz, 2H, 6-O**C**$\mathbf{H}_2$$CH_2CH(CH_3)_2$], 2.37 (s, 3H, 4-$CH_3$), 1.76−1.74 [m, 1H, 6-$OCH_2CH_2$**C**$\mathbf{H}$ $(CH_3)_2$], 1.59 [q, J = 13.5, 6.5 Hz, 2H, 6-OCH_2**C**$\mathbf{H}_2$$CH(CH_3)_2$], 0.91 [t, J = 7.0 Hz, 6H, 6-OCH_2CH_2CH (**C**$\mathbf{H_3)_2}$]; ^{13}C NMR (125 MHz, DMSO-d_6), δ (ppm): 159.8 (C=O lactone), 154.9 (C-6), 152.9 (C-4), 147.0 (C-8a), 120.0 (C-4a), 119.3 (C-8), 117.3 (C-7), 114.6 (C-3), 108.8 (C-5), 66.5 [6-O**C**$\mathbf{H_2}$$CH_2CH(CH_3)_2$], 37.6 [6-$OCH_2$**C**$\mathbf{H_2}$$CH(CH_3)_2$], 24.5 [6-$OCH_2CH_2$**C**$\mathbf{H}$ $(CH_3)_2$], 22.3 [6-OCH_2CH_2CH **(C**$\mathbf{H_3)_2}$], 18.1 (4-CH_3); ESI-MS: $C_{15}H_{18}O_3$, calcd. for M+H = 247.1 Da, found: *m/z* 247.3 ($[M+H]^+$); ESI-HRMS: calcd. for M+H = 247.1334 Da, found: *m/z* 247.1341 ($[M+H]^+$, 100%); Elemental anal. for $C_{15}H_{18}O_3$, calcd.: C, 73.15; H, 7.37%; found: 73.42; H, 7.57%.

*4-Methyl-6-allyloxycoumarin (**3i**)*



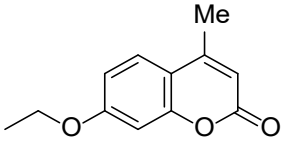
From **2a** (0.02 mol, 3.52 g), allyl bromide (0.024 mol, 2.1 mL), and KI (0.1 mmol, 0.17 g). Yield: 3.67 g (85%) of **3i** as white crystals. M.p.: 70−73 °C (from 96% ethanol). IR (KBr), ν (cm^{-1}): 1712 ($\nu_{C=O}$ lactone), 1570, 1490 ($\nu_{C=C}$ arene), 1245 & 1164 (ν_{COC} lactone); ^{1}H NMR (500 MHz, DMSO-d_6), δ (ppm): 7.32−7.24 (m, 1H, H-7), 7.24−7.18 (m, 2H, H-5 & H-8), 6.37 (s, 1H, H-3), 6.09−6.05 (m, 1H, 6-OCH_2**C**$\mathbf{H}$=CH_2), 5.44 (d, J = 14.0 Hz, 1H, 6-OCH_2CH=**C**$\mathbf{H_2}$), 5.29 (d, J = 14.0 Hz, 1H, 6-OCH_2CH=**C**$\mathbf{H_2}$), 4.66 (s, 2H, O**C**$\mathbf{H_2}$$CH$=$CH_2$), 2.417 (s, 3H, 4-$CH_3$); ^{13}C NMR (125 MHz, DMSO-d_6), δ (ppm): 160.3 (C=O lactone), 154.9 (C-6), 153.4 (C-4), 147.8 (C-8a), 134.0 (6-OCH_2**C**$\mathbf{H}$=CH_2), 120.6 (C-4a), 120.0 (C-8), 118.2 (6-OCH_2CH=**C**$\mathbf{H_2}$), 117.9 (C-7), 115.2 (C-3), 109.7 (C-5), 69.4 (6-O**C**$\mathbf{H_2}$$CH$=$CH_2$), 18.6 (4-$CH_3$); ESI-MS: $C_{13}H_{12}O_3$, calcd. for M+H = 217.09 Da, M+Na = 239.07, found: *m/z* 217.11 ($[M+H]^+$), 239.12 ($[M+H]^+$); ESI-HRMS: calcd. for M+H = 217.0865 Da, found: *m/z* 217.0871 ($[M+H]^+$, 100%); Elemental anal. for $C_{13}H_{12}O_3$, calcd.: C, 72.21; H, 5.59%; found: C, 72.59; H, 5.27%.

*4-Methyl-7-methoxycoumarin (**4a**)*



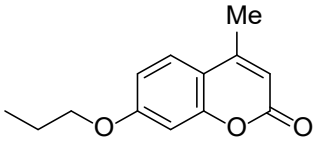
From **4** (0.02 mol, 3.52 g), methyl iodide (0.024 mol, 1.93 mL). Yield: 3.47 g (85%) of **4a** as pale-yellow crystals. M.p.: 159−162 °C (from 96% ethanol); ref.:[3] 158−160 °C. IR (KBr), ν (cm^{-1}) 1720 ($\nu_{C=O}$ lactone), 1575, 1490 ($\nu_{C=C}$ arene), 1198 & 1069 (ν_{COC} lactone); ^{1}H NMR (DMF-d_6), δ (ppm): 7.98 (s, 1H, H-5), 7.87−7.85 (m, 2H, H-6 & H-8), 6.88 (s, 1H, H-3), 2.84 (s, 3H, 7-OCH_3), 2.74 (s, 3H, 4-CH_3); ^{13}C NMR (126 MHz, DMF-d_6), δ (ppm): ^{13}C NMR (125 MHz, DMSO-d_6), δ (ppm): 162.7 (C=O lactone), 160.6 (C-7), 155.4 (C-8a), 153.4 (C-4), 126.8 (C-5), 113.2 (C-3), 112.9 (C-4a), 111.4 (C-6), 105.9 (C-8), 67.8 (7-O**C**$\mathbf{H_3}$), 18.9 (4-CH_3); ESI-MS: $C_{11}H_{10}O_3$, calcd. for $[M+H]^+$=191.07 Da, found: *m/z* 191.14; Elemental anal. for $C_{11}H_{10}O_3$, calcd.: C, 69.46; H, 5.30%; found: C, 69.21; H, 5.46%.

*4-Methyl-7-ethoxycoumarin (**4b**)*



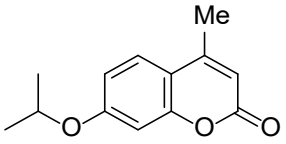
From **2b** (0.02 mol, 3.52 g), ethyl iodide (0.024 mol, 1.93 mL). Yield: 4.09 g (85%) of **4b** as white crystals. M.p.: 115−117°C (from 96% ethanol); ref.:[4] 113−115 °C,[5] ref.[6] described the synthesis method for this compound, but there was not melting point data. IR (KBr), ν cm^{-1}: 1737 ($\nu_{C=O}$ lactone), 1540, 1500, 1480 ($\nu_{C=C}$ arene), 1145 &1069 (ν_{COC} lactone); ^{1}H NMR (500 MHz, DMSO-d_6), δ (ppm): 7.66 (d, J = 9.5 Hz, 1H, H-5), 6.95−6.93 (m, 2H, H-6 & H-8), 6.19 (s, 1H, H-3), 4.13 (q, J = 7.0 Hz, 2H, 7-O**C**$\mathbf{H_2}$$CH_3$), 2.39 (s, 3H, 4-$CH_3$), 1.36 (t, J = 7.0 Hz, 3H, 7-OCH_2**C**$\mathbf{H_3}$); ^{13}C NMR (125 MHz, DMSO-d_6), δ (ppm): 162.1 (C=O lactone), 160.6 (C-6), 155.3 (C-8a), 153.9 (C-4), 126.9 (C-5), 113.5 (C-7), 112.8 (C-8), 111.5 (C-4a), 101.6 (C-3), 64.4 (7-O**C**$\mathbf{H_2}$$CH_3$), 18.6 (4-$CH_3$), 14.9 (7-$OCH_2$**C**$\mathbf{H_3}$); ESI-MS: $C_{12}H_{12}O_3$, calc. for M+H = 205.09 Da, M+Na = 227.07 Da, found: *m/z* 205.08 ($[M+H]^+$), 227.15 ($[M+Na]^+$); ESI/HRMS: calcd. for M+H = 205.0865 Da, found: *m/z* 205.0871 ($[M+H]^+$, 100%); Elemental anal. for $C_{12}H_{12}O_3$, calcd.: C, 70.58; H, 5.92%; found: C, 70.27; H, 5.79%.

*4-Methyl-7-propoxycoumarin (**4c**)*



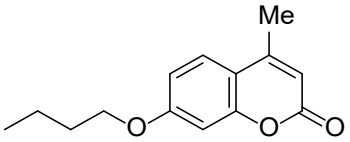
From **2b** (0.02 mol, 3.52 g), propyl iodide (0.024 mol, 2.34 mL), and K_2CO_3 (0.04 mol, 5.5 g). Yield: 3.05 g (70%) of **4c** as white crystals. M.p.: 78−80 °C (from 96% ethanol). IR (KBr), ν (cm^{-1}): 1718 ($\nu_{C=O}$ lactone), 1550, 1520, 1480 ($\nu_{C=C}$ arene), 1147 &1064 (ν_{COC} lactone); ^{1}H NMR (500 MHz, DMSO-d_6), δ (ppm): 7.62 (d, J = 8.5 Hz, 1H, H-5), 6.93−6.90 (m, 2H, H-6 & H-8), 6.17 (s, 1H, H-3), 4.01 (q, J = 7.0 Hz, 2H, 7-O**C**$\mathbf{H_2}$$CH_2CH_3$), 3.34 (s, 3H, 4-$CH_3$), 1.76 (sextet, J = 7.0 Hz, 2H, 7-OCH_2**C**$\mathbf{H_2}$$CH_3$), 0.99 (t, J = 7.0 Hz, 3H, 7-OCH_2CH_2**C**$\mathbf{H_3}$); ^{13}C NMR (125 MHz, DMSO-d_6), δ (ppm): 162.2 (C=O lactone), 160.6 (C-7), 155.2 (C-8a), 153.8 (C-4), 126.8 (C-5), 113.4 (C-6), 112.8 (C-4a), 111.5 (C-3), 101.5 (C-8), 70.2 (7-O**C**$\mathbf{H_2}$$CH_2CH_3$), 22.3 (4-$CH_3$), 18.5 (7-$OCH_2$**C**$\mathbf{H_2}$$CH_3$), 10.7 (7-$OCH_2CH_2$**C**$\mathbf{H_3}$); ESI-MS: $C_{13}H_{14}O_3$, calcd. for M+H = 219.10 Da, M+Na = 241.08 Da, found: *m/z* 219.15 ($[M+H]^+$), 241.15 ($[M+Na]^+$); Elemental anal. for $C_{13}H_{14}O_3$, calcd.: C, 71.54; H, 6.47%; found: C, 71.72; H, 6.61%

*4-Methyl-7-isopropoxycoumarin (**4d**)*



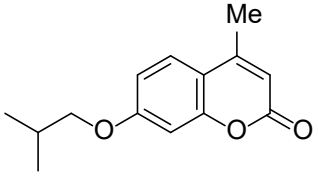
From **2b** (0.02 mol, 3.52 g), propyl iodide (0.024 mol, 2.34 mL), and K_2CO_3 (0.04 mol, 5.5 g). Yield: 3.27 g (75%) of **4d** as white crystals. M.p.: 80−82 °C (from 96% ethanol). IR (KBr), ν (cm^{-1}): 1721 ($\nu_{C=O}$ lactone), 1602 ($\nu_{C=C}$ alkene), 1520, 1500, 1483 ($\nu_{C=C}$ arene), 1145 & 1011 (ν_{COC} lactone); ^{1}H NMR (500 MHz, DMSO-d_6, ppm), δ (ppm): 7.68 (d, J = 3.0 Hz, 1H, H-5), 6.93−6.88 (m, 2H, H-7 & H-8), 6.48 (s, 1H, H-3), 4.18 [septet, J = 6.5 Hz, 1H, 7-O**C**$\mathbf{H}$$(CH_3)_2$], 1.02−0.98 [m, 6H, 7-OCH$\mathbf{(CH_3)_2}$]; ^{13}C NMR (125 MHz, DMSO-d_6), δ (ppm): 162.2 (C=O lactone), 160.6 (C-6), 155.2 (C-4), 153.8 (C-8a), 126.8 (C-4a), 113.4 (C-8), 112.8 (C-7), 111.5 (C-3), 101.7 (C-5), 68.5 [7-O**C**$\mathbf{H}$ $(CH_3)_2$], 21.3 [7-OCH$\mathbf{(CH_3)_2}$]; ESI-MS: $C_{13}H_{14}O_3$, calcd. for M+H = 219.10 Da, M+Na = 241.08 Da, found: *m/z* 219.18 ($[M+H]^+$), 241.17 ($[M+Na]^+$); Elemental anal. for $C_{13}H_{14}O_3$, calcd.: C, 71.54; H, 6.47%; found: C, 71.32; H, 6.21%

*4-Methyl-7-butoxycoumarin (**4e**)*



From **2a** (0.02 mol, 3.52 g), butyl bromide (0.022 mol, 2.58 mL), and KI (0.1 mmol, 0.17 g). Yield: 4.65 g (85%) of **4e** as white crystals. M.p.: 107−109 °C (from 96% ethanol). IR (KBr), ν (cm^{-1}): 1721 ($\nu_{C=O}$ lactone), 1569, 1428 ($\nu_{C=C}$ arene), 1242 & 1166 (ν_{COC} lactone); ^{1}H NMR (500 MHz, DMSO-d_6), δ (ppm): 7.28 (d, J = 9.0 Hz, 1H, H-7), 7.18 (dd, J = 9.0, 3.0 Hz, 1H, H-8), 7.15 (s, 1H, H-3), 6.35 (d, J = 1.0 Hz, 1H, H-5), 4.01 (t, J = 6.5 Hz, 2H, 7-O**C**$\mathbf{H}_2$$CH_2CH_2CH_3$), 2.40 (s, 3H, 4-$CH_3$), 1.70 (quintet, J = 6.5 Hz, 2H, 7-$OCH_2C\mathbf{H}_2CH_2CH_3$), 1.44 (sextet, J = 7.0 Hz, 2H, 7-$OCH_2CH_2\mathbf{CH}_2CH_3$), 0.93 (t, J = 7.0 Hz, 3H, 7-$OCH_2CH_2CH_2\mathbf{CH}_3$); ^{13}C NMR (125 MHz, DMSO-d_6), δ (ppm): 159.8 (C=O lactone), 155.0 (C-6), 152.9 (C-4), 147.0 (C-8a), 120.0 (C-4a), 119.3 (C-8), 117.3 (C-7), 114.6 (C-3), 108.7 (C-5), 67.8 (7-O**C**$\mathbf{H}_2$$CH_2CH_2CH_3$), 30.7 (7-$OCH_2\mathbf{CH}_2CH_2CH_3$), 18.7 (4-$CH_3$), 18.1 (7-$O(CH_2CH_2\mathbf{CH}_2CH_3$), 13.6 (7-$OCH_2CH_2CH_2\mathbf{CH}_3$); ESI-MS: $C_{14}H_{16}O_3$, calcd. for [M+H = 233.12 Da, M+Na = 255.10 Da, found: *m/z* 233.15 ($[M+H]^+$), 255.17 ($[M+Na]^+$); Elemental anal. for $C_{14}H_{16}O_3$, calcd.: C, 72.39; H, 6.94%; found: C, 72.67; H, 6.72%.

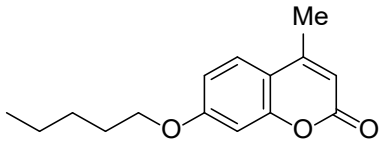
*4-Methyl-7-isobutoxycoumarin (**4f**)*



From **2b** (0.02 mol, 3.52 g), isobutyl bromide (0.022 mol, 2.59 mL), and KI (0.1 mmol, 0.17 g). Yield: 3.12 g (57%) of **4f** as white crystals. M.p.: 57−60 °C (from 96% ethanol). IR (KBr), ν (cm^{-1}): 1714 ($\nu_{C=O}$ lactone), 1570, 1486 ($\nu_{C=C}$ arene), 1281 & 1142 (ν_{COC} lactone); ^{1}H NMR (500 MHz, DMSO-d_6), δ (ppm): 7.63 (d, J = 8.5 Hz, 1H, H-5), 6.94 (d, J = 2.3 Hz, 1H, H-8), 6.91 (d, J = 1.5 Hz, 1H, H-6), 6.17 (s, 1H, H-3), 3.83 [d, J = 6.5 Hz, 2H, 7-O**C**$\mathbf{H}_2$$CH(CH_3)_2$], 2.37 (s, 3H, 4-$CH_3$), 2.03 [septet, J = 6.5 Hz, 1H, 7-$OCH_2\mathbf{CH}(CH_3)_2$], 0.98 [d, J = 7.0 Hz, 6H, 7-$OCH_2CH(\mathbf{CH_3)_2}$]; ^{13}C NMR (125 MHz, DMSO-d_6), δ (ppm): 161.8 (C=O lactone), 160.1 (C-7), 154.7 (C-8a), 153.3 (C-4), 126.3 (C-5), 112.9 (C-3), 112.3 (C-4a), 111.0 (C-6), 101.1 (C-8), 74.3 [7-O**C**$\mathbf{H_2}$$CH(CH_3)_2$], 27.5 [7-$OCH_2\mathbf{CH}(CH_3)_2$], 18.9 [7-$OCH_2CH$ **(**$\mathbf{CH_3)_2}$], 18.1

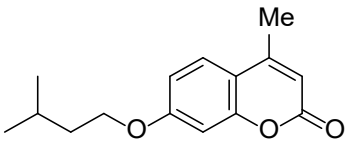
(4-CH_3); ESI-MS: $C_{14}H_{16}O_3$, calcd. for $[M+2H]^+$=234.2 Da, found: *m/z* 234.1; Elemental anal. for $C_{14}H_{16}O_3$, calcd.: C, 72.39; H, 6.94%; found: C, 72.69; H, 6.71%.

*4-Methyl-7-pentoxycoumarin (**4g**)*



From **2b** (0.02 mol, 3.52 g), pentyl bromide (0.024 mol, 2.88 mL), and KI (0.001 mol, 0.17 g). Yield: 4.88 g (84%) of **4d** as white crystals. M.p.: 48−50 °C (from 96% ethanol). IR (KBr), ν (cm^{-1}): 1722 ($\nu_{C=O}$ lactone), 1616 ($\nu_{C=C}$ arene), 1279 & 1157 (ν_{COC} lactone); ^{1}H NMR (500 MHz, DMSO-d_6), δ (ppm): 7.60 (d, *J* = 8.0 Hz, 1H, H-5), 6.93−6.89 (m, 2H, H-6 & H-8), 6.45 (s, 1H, H-3), 4.00 (t, *J* = 6.5 Hz, 2H, 7-O**CH₂**$CH_2CH_2CH_2CH_3$], 2.40 (s, 3H, 4-CH_3), 1.72 (quintet, *J* = 6.5 Hz, 2H, 7-OCH_2**CH₂**$CH_2CH_2CH_3$), 1.37−1.35 (m, 4H, 7-OCH_2CH_2**CH₂CH₂**CH_3), 0.89 (t, *J* = 7.0 Hz, 3H, 7-$OCH_2CH_2CH_2CH_2$**CH₃**); ^{13}C NMR (125 MHz, DMSO-d_6), δ (ppm): 162.2 (C=O lactone), 160.6 (C-7), 155.2 (C-8a), 153.7 (C-4), 126.7 (C-5), 113.4 (C-3), 112.8 (C-4a), 111.5 (C-6), 101.5 (C-8), 68.7 (7-O**CH₂**$CH_2CH_2CH_2CH_3$), 28.6 (7-OCH_2**CH₂**$CH_2CH_2CH_3$), 28.1 (7-OCH_2CH_2**CH₂**CH_2CH_3), 22.3 (7-$OCH_2CH_2CH_2$**CH₂**CH_3), 18.5 (4-CH_3), 14.3 (7-$OCH_2CH_2CH_2CH_2$**CH₃**); ESI-MS: $C_{15}H_{18}O_3$, calcd. for M+H = 247.13 Da, M+Na = 269.12 Da, found: *m/z* 247.17 ($[M+H]^+$), 269.21 ($[M+Na]^+$); ESI-HRMS: calcd. for M+H = 247.1334 Da, found: *m/z* 247.1339 ($[M+H]^+$, 100%); Elemental anal. for $C_{15}H_{18}O_3$, calcd.: C, 73.15; H, 7.37%; found: 73.41; H, 7.12%.

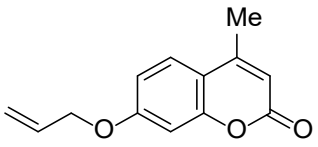
*4-Methyl-7-isopentoxycoumarin (**4h**)*



From **2b** (0.02 mol, 3.52 g), isopentyl bromide (0.024 mol, 2.88 mL), and KI (0.1 mmol, 0.17 g). Yield: 4.76 g (82%) of **4h** as white crystals. M.p.: 57−60 °C (from 96% ethanol). IR (KBr), ν cm^{-1}: 1722 ($\nu_{C=O}$ lactone), 1616 ($\nu_{C=C}$ arene), 1279 & 1157 (ν_{COC} lactone); ^{1}H NMR (500 MHz, DMSO-d_6), δ (ppm): 7.61 (d, *J* = 8.5 Hz, 1H, H-5), 6.91 (d, *J* = 1.5 Hz, 1H, H-8), 6.90 (s, 1H, H-3), 6.15 (d, *J* = 1.5 Hz, 1H, H-6), 4.06 [t, *J* = 7.0 Hz, 2H, 7-O**CH₂**$CH_2CH(CH_3)_2$],

2.36 (s, 3H, 4-CH_3), 1.76 (septet, J = 6.5 Hz, 1H, 7-OCH_2CH_2**CH** $(CH_3)_2$), 1.61 [q, J = 13.5, 6.5 Hz, 2H, 7-OCH_2**CH_2**$CH(CH_3)_2$], 0.91 [d, J = 7.0 Hz, 6H, 7-OCH_2CH_2CH **$(CH_3)_2$**]; ^{13}C NMR (125 MHz, DMSO-d_6), δ (ppm): 161.6 (C=O lactone), 160.0 (C-7), 154.6 (C-8a), 153.0 (C-4), 126.0 (C-5), 112.8 (C-3), 110.9 (C-4a), 110.9 (C-6), 100.8 (C-8), 66.6 [7-O**CH_2**$CH_2CH(CH_3)_2$], 37.1 [7-OCH_2**CH_2**$CH(CH_3)_2$], 24.5 [7-OCH_2CH_2**CH**$(CH_3)_2$], 22.3 [7-OCH_2CH_2CH**$(CH_3)_2$**], 17.9 (4-CH_3); ESI-MS: $C_{15}H_{18}O_3$, calcd. for M+H = 247.1 Da, found: *m/z* 247.2 ($[M+H]^+$); ESI-HRMS: calcd. for M+H = 247.1334 Da, found: *m/z* 247.1329 ($[M+H]^+$, 100%); Elemental anal. for $C_{15}H_{18}O_3$, calcd.: C, 73.15; H, 7.37%; found: 73.39; H, 7.17%.

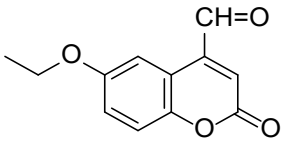
*4-Methyl-7-allyloxycoumarin (**4i**)*



From **2b** (0.02 mol, 3.52 g), allyl bromide (0.024 mol, 2.1 mL), and KI (0.1 mmol, 0.17 g). Yield: 4.43 g (87%) of **4i** as white crystals. M.p.: 97−100 °C (from 96% ethanol). IR (KBr), ν (cm^{-1}): 1724 ($\nu_{C=O}$ lactone), 1614 ($\nu_{C=C}$ arene), 1293 & 1152 (ν_{COC} lactone); ^{1}H NMR (500 MHz, DMSO-d_6), δ (ppm): 7.33−7.24 (m, 1H, H-5), 7.23−7.18 (m, 2H, H-6 & H-8), 6.38 (s, 1H, H-3), 6.09−6.05 (m, 1H, 7-OCH_2**CH**=CH_2), 5.45 (d, J = 17.5 Hz, 1H, 7-OCH_2CH=**CH_2**), 5.29 (d , J = 10.5 Hz, 7-OCH_2CH=**CH_2**), 4.66 (s, 2H, 7-O**CH_2**CH=CH_2), 2.41 (s, 3H, 4- CH_3); ^{13}C NMR (125 MHz, DMSO-d_6), δ (ppm): 160.3 (C=O lactone), 154.9 (C-7), 153.4 (C-8a), 147.8 (C-4), 134.0 (7-OCH_2**CH**=CH_2), 120.6 (C-5), 120.0 (C-3), 118.2 (7-OCH_2CH=**CH_2**), 117.9 (C-4a), 115.2 (C-6), 109.7 (C-8), 69.4 (7-O**CH_2**CH=CH_2), 18.6 (4-CH_3); ESI-MS: $C_{13}H_{12}O_3$, calcd. for M+H = 217.09 Da, M+Na = 239.07, found: *m/z* 217.17 ($[M+H]^+$), 239.19 ($[M+H]^+$); ESI-HRMS: calcd. for M+H = 217.0865 Da, found: *m/z* 217.0872 ($[M+H]^+$, 100%); Elemental anal. for $C_{13}H_{12}O_3$, calcd.: C, 72.21; H, 5.59%; found: C, 72.43; H, 5.31%.

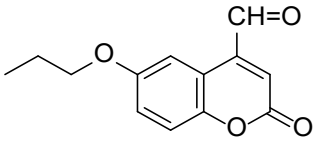
1.2. 6-Alkoxy- and 7-alkoxy-4-formylcoumarins (5 and 6)

*4-Formyl-6-ethoxycoumarin (**5b**)*



From **3b** (2 mmol, 408 mg). Yield: 283 mg (65%, method A), 392 mg (90%, method B) of **5b** as yellow crystals. M.p.: 167−168 °C (from toluene). IR (KBr), ν cm^{-1}: 1736 ($\nu_{C=O}$ lactone), 1708 ($\nu_{C=O}$ aldehyde), 1565, 1430 ($\nu_{C=C}$ arene), 1243 &1054 (ν_{COC} lactone); ^{1}H NMR (500 MHz, DMSO-d_6), δ (ppm): 10.15 (s, 4-CHO), 7.96 (d, J = 3.0 Hz, 1H, H-5), 7.40 (d, J = 9.0 Hz, 1H, H-8), 7.27 (dd, J = 9.5, 3.0 Hz, 1H, H-7), 7.16 (s, H, 1H, H-3), 4.09 (q, J = 7.0 Hz, 2H, 6-O**CH_2**CH_3), 1.37 (t, J = 7.0 Hz, 3H, 6-OCH_2**CH_3**); ^{13}C NMR (125 MHz, DMSO-d_6), δ (ppm): 193.6 (4-CHO), 160.1 (C=O lactone), 155.0 (C-6), 148.2 (C-4), 143.0 (C-8a), 125.3 (C-4a), 119.9 (C-7), 117.3 (C-8), 109.1 (C-3), 63.7 (6-O**CH_2**CH_3), 14.5 (6-OCH_2**CH_3**); ESI-MS: $C_{12}H_{10}O_4$, calcd. for M+H = 219.07 Da, M+Na = 241.05 Da, found: *m/z* 219.15 ($[M+H]^+$), 241.11 ($[M+Na]^+$); ESI-MS: calcd. for M+H = 219.0657 Da, found: *m/z* 219.0685 ($[M+H]^+$, 100%); ESI-HRMS: calcd. for M+H = 219.0657 Da, found: *m/z* 219.0661 ($[M+H]^+$, 100%); Elemental anal. for $C_{12}H_{10}O_4$, calcd.: C, 69.46; H, 5.30%; found: C, 69.57; H, 5.41%.

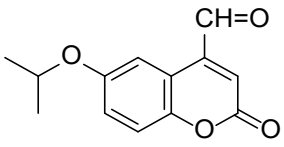
*4-Formyl-6-propoxycoumarin (**5c**)*



From **3c** (2 mmol, 440 mg). Yield: 310 mg (67%, method A), 392 mg (93%, method B) of **5c** as yellow crystals. M.p.: 143−145 °C (from toluene). IR (KBr), ν (cm^{-1}): 1723 ($\nu_{C=O}$ lactone), 1703 ($\nu_{C=O}$ aldehyde), 1542, 1434 ($\nu_{C=C}$ arene), 1244 &1045 (ν_{COC} lactone); ^{1}H NMR (500 MHz, DMSO-d_6), δ (ppm): 10.16 (s, 4-CHO), 7.99 (d, J = 3.0 Hz, 1H, H-5), 7.43 (d, J = 9.0 Hz, 1H, H-8), 7.30 (dd, J = 9.5, 2.5 Hz, 1H, H-7), 7.19 (s, H, 1H, H-3), 3.98 (t, J = 7.0 Hz, 2H, 6-O**CH_2**CH_2CH_3), 1.77 (sextet, J = 7.0 Hz, 2H, 6-OCH_2**CH_2**CH_3), 1.01 (t, J = 7.0 Hz, 2H, 6-OCH_2CH_2**CH_3**); ^{13}C NMR (125 MHz, DMSO-d_6), δ (ppm): 194.1 (4-CHO), 160.6 (C=O lactone), 155.8 (C-6), 148.7 (C-4), 143.6 (C-8a), 125.9 (C-4a), 120.5 (C-7), 118.2 (C-8), 115.9 (C-3), 109.7 (C-5), 70.2 (6-O**CH_2**CH_2CH_3), 22.4 (6-OCH_2**CH_2**CH_3), 10.8 (6-OCH_2CH_2**CH_3**);

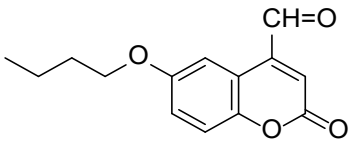
ESI-MS: $C_{13}H_{12}O_4$, calcd. for M+H = 233.08 Da, M+Na = 255.06 Da, found: *m/z* 233.12 ($[M+H]^+$), 255.17 ($[M+Na]^+$); ESI-HRMS: calcd. for M+H = 233.0814 Da, found: *m/z* 233.0817 ($[M+H]^+$, 100%); Elemental anal. for $C_{13}H_{12}O_4$, calcd.: C, 67.23; H, 5.21%; found: C, 67.39; H, 5.12%.

*4-Formyl-6-isopropoxycoumarin (**5d**)*



From **3d** (2 mmol, 440 mg). Yield: 232 mg (50%, method A), 427 mg (92%, method B) of **5d** as yellow crystals. M.p.: 134−135 °C (from toluene). IR (KBr), ν (cm^{-1}): 1734 ($\nu_{C=O}$ lactone), 1704 ($\nu_{C=O}$ aldehyde), 1525, 1432 ($\nu_{C=C}$ arene), 1246 & 1054 (ν_{COC} lactone); ^{1}H NMR (500 MHz, DMSO-d_6), δ (ppm): 10.12 (s, 4-CHO), 8.54 (d, *J* = 9.0 Hz, 1H, H-5), 6.92 (m, 1H, H-3), 6.96−6.94 (m, 1H, H-8), 6.35−6.34 (d, *J* = 8.0 Hz, 1H, H-6), 4.05−4.03 [m, 1H, 6-O**CH**$(CH_3)_2$], 0.99−0.96 [m, 6H, 6-OCH**$(CH_3)_2$**]; ^{13}C NMR (125 MHz, DMSO-d_6), δ (ppm): 194.2 (4-CHO), 161.5 (C-4), 161.3 (C-7), 156.4 (C=O lactone), 143.4 (C-8a), 121.5 (C-5), 112.6 (C-3), 110.9 (C-4a), 108.1 (C-6), 101.4 (C-8), 70.1 [6-O**CH**$(CH_3)_2$], 10.6 [6-OCH**$(CH_3)_2$**]; ESI-MS: $C_{13}H_{12}O_4$, calcd. for M+H = 233.08 Da, M+Na = 255.06 Da, found: *m/z* 233.15 ($[M+H]^+$), 255.19 ($[M+Na]^+$); ESI-HRMS: calcd. for M+H = 233.0814 Da, found: *m/z* 233.0819 ($[M+H]^+$, 100%); Elemental anal. for $C_{13}H_{12}O_4$, calcd.: C, 67.23; H, 5.21%; found: C, 67.41; H, 5.09%.

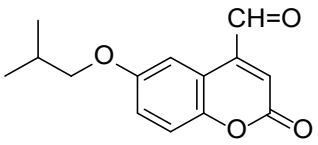
*4-Formyl-6-butoxycoumarin (**5e**)*



From **3e** (2 mmol, 464 mg). Yield: 331 mg (67%, method A), 449 mg (91%, method B) of **5e** as yellow crystals. M.p.: 110−112 °C (from toluene). IR (KBr), ν (cm^{-1}): 1735 ($\nu_{C=O}$ lactone), 1700 ($\nu_{C=O}$ aldehyde), 1565, 1435 ($\nu_{C=C}$ arene), 1244 & 1150 (ν_{COC} lactone); ^{1}H NMR (500 MHz, DMSO-d_6), δ (ppm): 10.16 (s, 4-CHO), 7.99 (d, *J* = 3.0 Hz, 1H, H-5), 7.46 (d, *J* = 9.0 Hz, 1H, H-8), 7.32 (dd, *J* = 9.5, 2.5 Hz, 1H, H-7), 7.17 (s, H, 1H, H-3), 4.04−4.01 (m, 2H, 6-

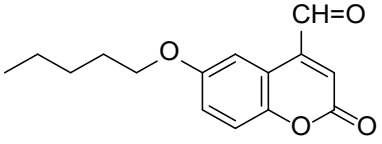
O**CH₂**$CH_2CH_2CH_3$), 1.76−1.70 (m, 2H, 6-OCH_2**CH_2**CH_2CH_3), 1.50−1.42 (m, 2H, 6-OCH_2CH_2**CH_2**CH_3), 0.95 (t, *J* = 7.0 Hz, 3H, 6-$OCH_2CH_2CH_2$**CH_3**); ^{13}C NMR (125 MHz, DMSO-d_6), δ (ppm): 194.1 (4-CHO), 160.6 (C=O lactone), 155.8 (C-6), 148.7 (C-4), 143.5 (C-8a), 125.8 (C-4a), 120.5 (C-7), 119.5 (C-8), 118.2 (C-3), 112.0 (C-5), 68.4 (6-O**CH₂**$CH_2CH_2CH_3$), 31.1 (6-OCH_2**CH_2**CH_2CH_3), 19.2 (6-OCH_2CH_2**CH_2**CH_3), 14.1 (6-$OCH_2CH_2CH_2$**CH_3**); ESI-MS: $C_{14}H_{14}O_4$, calcd. for M+H = 247.10 Da, M+Na = 269.08 Da, found: *m/z* 247.12 ($[M+H]^+$), 269.15 ($[M+Na]^+$); ESI-HRMS: calcd. for M+H = 247.0970 Da, found: *m/z* 247.0977 ($[M+H]^+$, 100%); Elemental anal. for $C_{14}H_{14}O_4$, calcd.: C, 68.28; H, 5.73%; found: C, 68.41; H, 5.53%.

*4-Formyl-6-isobutoxycoumarin (**5f**)*



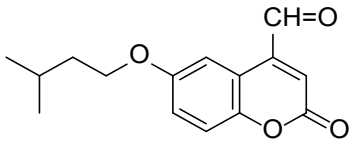
From **3f** (2 mmol, 464 mg). Yield: 338 mg (65%, method A), 478 mg (92%, method B) of **5f** as yellow crystals. M.p.: 123−125 °C (from toluene). IR (KBr), ν (cm^{-1}): 1733 ($\nu_{C=O}$ lactone), 1694 ($\nu_{C=O}$ aldehyde), 1515, 1425 ($\nu_{C=C}$ arene), 1250 & 1154 (ν_{COC} lactone); ^{1}H NMR (500 MHz, DMSO-d_6), δ (ppm): 10.16 (s, 4-CHO), 7.99 (d, *J* = 3.0 Hz, 1H, H-5), 7.43 (d, *J* = 9.0 Hz, 1H, H-8), 7.29 (dd, *J* = 9.0, 3.0 Hz, 1H, H-7), 7.19 (s, H, 1H, H-3), 3.83 [d, *J* = 6.5 Hz, 2H, 6-O**CH₂**$CH(CH_3)_2$], 2.37 (s, 3H, 4-CH_3), 2.03 [septet, *J* = 6.5 Hz, 1H, 6-OCH_2**CH**$(CH_3)_2$], 0.98 [d, *J* = 7.0 Hz, 6H, 6-OCH_2CH(**CH_3)₂**]; ^{13}C NMR (125 MHz, DMSO-d_6), δ (ppm): 194.1 (4-CHO), 160.6 (C-4), 155.8 (C-6), 148.7 (C=O lactone), 143.6 (C-8a), 125.9 (C-4a), 120.5 (C-3), 118.2 (C-8), 115.9 (C-7), 109.7 (C-5), 74.3 [6-O**CH₂**$CH(CH_3)_2$], 27.5 [6-OCH_2**CH**$(CH_3)_2$], 18.9 [6-OCH_2CH**$(CH_3)_2$**], 18.1 (4-CH_3); ESI-MS: $C_{14}H_{14}O_4$, calcd. for M+H = 247.10 Da, M+Na = 269.08 Da, found: *m/z* 247.15 ($[M+H]^+$), 269.17 ($[M+Na]^+$); ESI-HRMS: calcd. for M+H = 247.0970 Da, found: *m/z* 247.0978 ($[M+H]^+$, 100%); Elemental anal. for $C_{14}H_{14}O_4$, calcd.: C, 68.28; H, 5.73%; found: C, 68.47; H, 5.51%.

*4-Formyl-6-pentoxycoumarin (**5g**)*



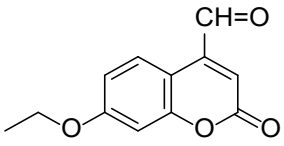
From **3g** (2 mmol, 492 mg). Yield: 322 mg (61%, method A), 475 mg (90%, method B) of **5g** as yellow crystals. M.p.: 112−114 °C. IR (KBr), ν (cm^{-1}): 1738 ($\nu_{C=O}$ lactone), 1703 ($\nu_{C=O}$ aldehyde), 1567, 1437 ($\nu_{C=C}$ arene), 1243 &1156 (ν_{COC} lactone); ^{1}H NMR (500 MHz, DMSO-d_6), δ (ppm): 10.14 (s, 4-CHO), 7.94 (d, J = 3.5 Hz, 1H, H-5), 7.39 (d, J = 9.0 Hz, 1H, H-8), 7.32 (dd, J = 9.0, 3.5 Hz, 1H, H-7), 7.16 (s, H, 1H, H-3), 3.98 (t, 2H, J = 7.0 Hz, 6-O**CH$_2$**CH$_2$CH$_2$CH$_2$CH$_3$), 1.74 (quintet, 2H, J = 7.0 Hz, 6-OCH$_2$**CH$_2$**CH$_2$CH$_2$CH$_3$), 1.43−1.33 (m, 4H, 6-OCH$_2$CH$_2$**CH$_2$CH$_2$**CH$_3$), 0.91 (t, J = 7.0 Hz, 3H, 6-OCH$_2$CH$_2$CH$_2$CH$_2$**CH$_3$**); ^{13}C NMR (125 MHz, DMSO-d_6), δ (ppm): 194.1 (4-CHO), 160.6 (C=O lactone), 155.7 (C-6), 148.7 (C-4), 143.5 (C-8a), 125.8 (C-4a), 120.4 (C-7), 118.2 (C-8), 115.8 (C-3), 109.6 (C-5), 68.6 (6-O**CH$_2$**CH$_2$CH$_2$CH$_2$CH$_3$), 28.7 (6-OCH$_2$**CH$_2$**CH$_2$CH$_2$CH$_3$), 28.1 (6-OCH$_2$CH$_2$**CH$_2$**CH$_2$CH$_3$), 22.4 (6-OCH$_2$CH$_2$CH$_2$**CH$_2$**CH$_3$), 14.4 (6-OCH$_2$CH$_2$CH$_2$CH$_2$**CH$_3$**); ESI-MS: $C_{15}H_{16}O_4$, calcd. for M = 260.1 Da, found: *m/z* 260.8 ($[M]^+$); Elemental anal. for $C_{15}H_{16}O_4$, calcd.: C, 69.22; H, 6.20%; found: C, 69.05; H, 6.49%.

*4-Formyl-6-isopentoxycoumarin (**5h**)*



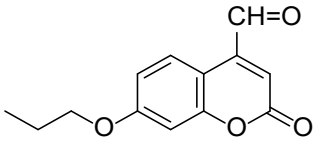
From **3h** (2 mmol, 492 mg). Yield: 260 mg (50%, method A), 468 mg (90%, method B) of **5h** as yellow crystals. M.p.: 114−116 °C (from toluene). IR (KBr), ν (cm^{-1}): 1738 ($\nu_{C=O}$ lactone), 1700 ($\nu_{C=O}$ aldehyde), 1562, 1438 ($\nu_{C=C}$ arene), 1273 & 1156 (ν_{COC} lactone); ^{1}H NMR (500 MHz, DMSO-d_6), δ (ppm): 10.16 (s, 4-CHO), 7.97 (d, J = 3.0 Hz, 1H, H-5), 7.45−7.39 (m, 1H, H-8), 7.33−7.27 (m, 1H, H-7), 7.18 (s, 1H, H-3), 4.03 [t, J = 6.75 Hz, 2H, 6-O**CH$_2$**CH$_2$CH(CH$_3$)$_2$], 1.84−1.76 [m, 1H, 6-OCH$_2$CH$_2$**CH**(CH$_3$)$_2$], 1.66−1.61 [m, 2H, 6-OCH$_2$**CH$_2$**CH(CH$_3$)$_2$], 0.94 [d, 6H, J = 6.5 Hz, 6-OCH$_2$CH$_2$CH**(CH$_3$)$_2$**]; ^{13}C NMR (125 MHz, DMSO-d_6), δ (ppm): 193.6 (4-CHO), 160.1 (C-4), 154.5 (C-6), 148.2 (C=O lactone), 143.1 (C-8a), 125.2 (C-4a), 119.9 (C-3), 117.7 (C-8), 117.3 (C-7), 109.3 (C-5), 66.6 [6-O**CH$_2$**CH$_2$CH(CH$_3$)$_2$], 37.3 [6-OCH$_2$**CH$_2$**CH(CH$_3$)$_2$], 24.6 [6-OCH$_2$CH$_2$**CH**(CH$_3$)$_2$], 22.4 [6-OCH$_2$CH$_2$CH**(CH$_3$)$_2$**]; ESI-MS: $C_{15}H_{16}O_4$, calcd. for M+H = 261.11 Da, M+Na = 283.09 Da, found: *m/z* 261.18 ($[M+H]^+$), 283.21 ($[M+Na]^+$); ESI-HRMS: calcd. for M+H = 261.1127 Da, found: 261.1121 ($[M+H]^+$, 100%); Elemental anal. for $C_{15}H_{16}O_4$, calcd.: C, 69.22; H, 6.20%; found: C, 69.39; H, 6.04%.

*4-Formyl-7-ethoxycoumarin (**6b**)*



From **4b** (2 mmol, 408 mg). Yield: 283 mg (65%, method A), 401 mg (92%, method B) of **6b** as yellow crystals. M.p.: 163−165 °C; ref. [6], m.p. 113 °C, this reference described the synthesis method for this compound, but there was not any physical and spectral data. IR (KBr), ν (cm^{-1}): 1739 ($\nu_{C=O}$ lactone), 1704 ($\nu_{C=O}$ aldehyde), 1570, 1514, 1490 ($\nu_{C=C}$ arene), 1265 & 1054 (ν_{COC} lactone); ^{1}H NMR (500 MHz, DMSO-d_6), δ (ppm): 10.08 (s, 4-CHO), 8.34 (d, J = 8.75 Hz, 1H, H-5), 7.79 (d, J = 8.75 Hz, 1H, H-6), 7.23 (d, J = 5.5 Hz, 1H, H-8), 6.33 (s, 1H, H-3), 4.15−4.09 (m, 2H, 7-O**CH$_2$**CH$_3$), 1.36−1.33 (m, 3H, 7-OCH$_2$**CH$_3$**); ^{13}C NMR (125 MHz, DMSO-d_6), δ (ppm): 193.7 (4-CHO), 161.2 (C-4), 160.7 (C-7), 155.5 (C=O lactone), 143.5 (C-8a), 121.2 (C-5), 113.1 (C-3), 112.3 (C-4a), 110.6 (C-6), 101.0 (C-8), 63.9 (7-O**CH$_2$**CH$_3$), 14.4 (7-OCH$_2$**CH$_3$**); ESI-MS: $C_{12}H_{10}O_4$, calc. for M+H = 219.07 Da, M+Na = 241.05 Da, found: *m/z* 219.12 ([M+H]$^+$), 241.13 ([M+Na]$^+$); ESI-HRMS: calcd. for M+H = 219.0657 Da, found: *m/z* 219.0662 ([M+H]$^+$, 100%); Elemental anal. for $C_{12}H_{10}O_4$, calcd.: C, 66.05; H, 4.62%; found: C, 66.25; H, 4.51%.

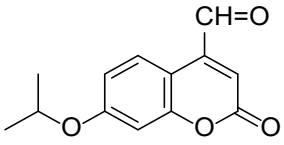
*4-Formyl-7-propoxycoumarin (**6c**)*



From **4b** (2 mmol, 440 mg). Yield: 278 mg (60%, method A), 421 mg (91%, method B) of **6b** as yellow crystals. M.p.: 131−133 °C (from toluene). IR (KBr), ν (cm^{-1}): 1731 ($\nu_{C=O}$ lactone), 1700 ($\nu_{C=O}$ aldehyde), 1570, 1515, 1490 ($\nu_{C=C}$ arene), 1209 & 1064 (ν_{COC} lactone); ^{1}H NMR (500 MHz, DMSO-d_6), δ (ppm): 10.08 (s, 4-CHO), 8.32 (d, J = 9.0 Hz, 1H, H-5), 6.99−6.97 (m, 1H, H-3), 6.93 (s, 1H, H-8), 6.91−6.89 (m, 1H, H-6), 4.01 (q, 2H, J = 6.75 Hz, 7-O**CH$_2$**CH$_2$CH$_3$), 1.78−1.71 (m, 2H, 7-OCH$_2$**CH$_2$**CH$_3$), 0.99-0.96 (m, 3H, 7-OCH$_2$CH$_2$**CH$_3$**); ^{13}C NMR (125 MHz, DMSO-d_6), δ (ppm): 193.6 (4-CHO), 161.9 (C=O lactone), 160.3 (C-7), 155.8 (C-8a), 143.3(C-4), 121.2 (C-5), 110.6 (C-4a), 107.1 (C-3), 101.4 (C-6), 100.9 (C-8),

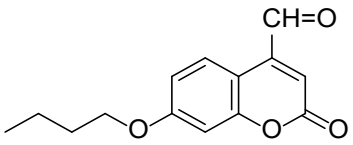
69.6 (7-O**C**H$_2$CH$_2$CH$_3$), 21.8 (7-OCH$_2$**C**H$_2$CH$_3$), 10.2 (7-OCH$_2$CH$_2$**C**H$_3$); ESI-MS: $C_{13}H_{12}O_4$, calcd. for M+H = 233.08 Da, M+Na = 255.06 Da, found: *m/z* 233.12 ([M+H]$^+$), 255.17 ([M+Na]$^+$); Elemental anal. for $C_{15}H_{16}O_4$, calcd.: C, 67.23; H, 5.21%; found: C, 67.47; H, 5.39%.

*4-Formyl-7-isopropoxycoumarin (**6d**)*



From **4d** (2 mmol, 440 mg). Yield: 232 mg (50%, method A), 418 mg (90%, method B) of **4d** as yellow crystals. M.p.: 130−132 °C (from toluene). IR (KBr), ν (cm^{-1}): 1725 ($\nu_{C=O}$ lactone), 1703 ($\nu_{C=O}$ aldehyde), 1510, 1490 ($\nu_{C=C}$ arene), 1250 & 1059 (ν_{COC} lactone); ^{1}H NMR (500 MHz, DMSO-d_6), δ (ppm): 10.08 (s, 4-CHO), 8.34 (d, *J* = 9.0 Hz, 1H, H-5), 6.96 (m, 1H, H-3), 6.94−6.91 (m, 1H, H-8), 6.35−6.33 (d, *J* = 8.0 Hz, 1H, H-6), 4.04−4.00 [m, 1H, 7-O**C**H(CH$_3$)$_2$], 0.99−0.96 [m, 6H, 7-OCH**(CH$_3$)$_2$**]; ^{13}C NMR (125 MHz, DMSO-d_6), δ (ppm): 193.9 (4-CHO), 161.8 (C-4), 161.6 (C-7), 156.1 (C=O lactone), 143.7 (C-8a), 121.5 (C-5), 112.6 (C-3), 110.9 (C-4a), 108.1 (C-6), 101.4 (C-8), 70.1 [7-O**C**H(CH$_3$)$_2$], 10.6 [7-OCH**(CH$_3$)$_2$**]; ESI-MS: $C_{13}H_{24}O_4$, calcd. for M+H = 233.08 Da, 255.06 Da, found: *m/z* 233.13 ([M+H]$^+$), 255.19 ([M+Na]$^+$); ESI-HRMS: calcd. for M+H = 233.0814 Da, found: *m/z* 233.0819 ([M+H]$^+$, 100%); Elemental anal. for $C_{15}H_{16}O_4$, calcd.: C, 67.23; H, 5.21%; found: C, 67.41; H, 5.09%.

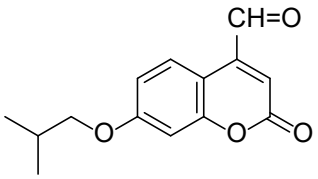
*4-Formyl-7-butoxycoumarin (**6e**)*



From **4e** (2 mmol, 464 mg). Yield: 295 mg (60%, method A), 452 mg (92%, method B) of **6e** as yellow crystals. M.p.: 140−142 °C; ref. [6] described the synthesis method for this compound, but there was not any physical and spectral data. IR (KBr), ν (cm^{-1}): 1729 ($\nu_{C=O}$ lactone), 1704 ($\nu_{C=O}$ aldehyde), 1509, 1425 ($\nu_{C=C}$ arene), 1266 & 1056 (ν_{COC} lactone); ^{1}H NMR (500 MHz, DMSO-d_6), δ (ppm): 10.18 (s, 4-CHO), 8.34 (d, *J* = 9.0 Hz, 1H, H-5), 6.96−6.91 (m, 1H, H-

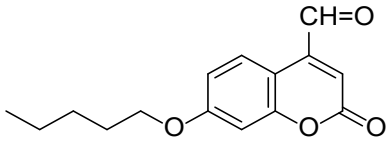
8), 6.93 (s, 1H, H-3), 6.91−6.89 (m, 1H, H-6), 4.01 (t, 2H, J = 6.75 Hz, 7-O**C**$\mathbf{H_2}$$CH_2CH_2CH_3$), 1.78−1.71 (m, 4H, 7-$OCH_2$$\mathbf{CH_2CH_2}$$CH_3$), 0.99−0.96 (t, J = 7.0 Hz, 3H, 7-$OCH_2CH_2CH_2$$\mathbf{CH_3}$); ^{13}C NMR (125 MHz, DMSO-d_6), δ (ppm): 159.8 (C=O lactone), 155.0 (C-6), 152.9 (C-4), 147.0 (C-8a), 120.0 (C-4a), 119.3 (C-8), 117.3 (C-7), 114.6 (C-3), 108.7 (C-5), 67.8 (7-O**C**$\mathbf{H_2}$$CH_2CH_2CH_3$), 30.7 (7-$OCH_2$$\mathbf{CH_2}$$CH_2CH_3$), 18.7 (4-$CH_3$), 18.1 (7-$OCH_2CH_2$$\mathbf{CH_2}$$CH_3$), 13.6 (7-$OCH_2CH_2CH_2$$\mathbf{CH_3}$); ESI-MS: $C_{14}H_{14}O_4$, calcd. for M+H = 247.09 Da, 269.08 Da, found: *m/z* 247.15 ($[M+H]^+$), 269.17 ($[M+Na]^+$); ESI-HRMS: calcd. for M+H = 247.0970 Da, found: *m/z* 247.0981 ($[M+H]^+$, 100%); Elemental anal. for $C_{14}H_{14}O_4$, calcd.: C, 68.28; H, 5.73%; found: C, 68.46; H, 5.61%.

4-Formyl-7-isobutoxycoumarin ***(6f)***



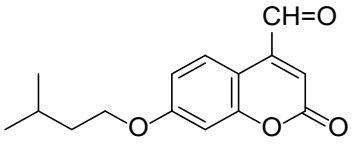
From **4f** (2 mmol, 464 mg). Yield: 226 mg (46%, method A), 452 mg (92%, method B) of **6f** as yellow crystals. M.p.: 127−129 °C (from toluene). M.p.: 127−129 °C (from toluene). IR (KBr), ν (cm^{-1}): 1734 ($\nu_{C=O}$ lactone), 1698 ($\nu_{C=O}$ aldehyde), 1616, 1514 ($\nu_{C=C}$ arene), 1270 & 1149 (ν_{COC} lactone); ^{1}H NMR (500 MHz, DMSO-d_6), δ (ppm): 10.16 (s, 4-CHO), 8.25 (d, J = 9.0 Hz, 1H, H-5), 7.42 (d, J = 2.5 Hz, 1H, H-8), 7.18 (s, 1H, H-3), 6.95−6.89 (m, 1H, H-6), 4.12 [q, 2H, J = 6.75 Hz, 7-O**C**$\mathbf{H_2}$$CH(CH_3)_2$], 1.78−1.71 (m, 1H, 7-$OCH_2$**C**$\mathbf{H}$$(CH_3)_2$), 0.99−0.96 [m, 6H, 7-$OCH_2CH$$\mathbf{(CH_3)_2}$]; ^{13}C NMR (125 MHz, DMSO-d_6), δ (ppm): 194.1 (4-CHO), 160.2 (C-4), 155.8 (C-7), 148.7 (C=O lactone), 143.5 (C-8a), 125.9 (C-5), 120.5 (C-3), 118.2 (C-4a), 109.7 (C-6), 87.0 (C-8), 66.7 [7-O**C**$\mathbf{H_2}$$CH(CH_3)_2$], 32.4 [7-$OCH_2$**C**$\mathbf{H}$$(CH_3)_2$], 20.8 [7-$OCH_2CH$$\mathbf{(CH_3)_2}$]; ESI-MS: $C_{14}H_{14}O_4$, calcd. for M+H = 247.09 Da, 269.08 Da, found: *m/z* 247.16 ($[M+H]^+$), 269.15 ($[M+Na]^+$); ESI-HRMS: calcd. for M+H = 247.0970 Da, found: *m/z* 247.0965 ($[M+H]^+$, 100%); Elemental anal. for $C_{14}H_{14}O_4$, calcd.: C, 68.28; H, 5.73%; found: C, 68.11; H, 5.91%.

*4-Formyl-7-pentoxycoumarin (**6g**)*



From **4g** (2 mmol, 492 mg). Yield: 338 mg (65%, method A), 473 mg (91%, method B) of **6g** as yellow crystals. M.p.: 135−137 °C (from toluene). IR (KBr), ν (cm^{-1}): 1729 ($\nu_{C=O}$ lactone), 1701 ($\nu_{C=O}$ aldehyde), 1614, 1510 ($\nu_{C=C}$ arene), 1266 & 1149 (ν_{COC} lactone); ^{1}H NMR (500 MHz, DMSO-d_6), δ (ppm): 10.16 (s, 4-CHO), 7.84 (d, J = 3.0 Hz, 1H, H-5), 7.45−7.39 (m, 1H, H-8), 7.32−7.27 (m, 1H, H-7), 7.15 (s, 1H, H-3), 4.03 (d, 2H, J = 6.75 Hz, 7-O**CH$_2$**$CH_2CH_2CH_2CH_3$), 1.84−1.76 (m, 2H, 7-OCH_2**CH$_2$**$CH_2CH_2CH_3$), 1.66−1.61 (m, 4H, 7-OCH_2CH_2**CH$_2$CH$_2$**CH_3), 0.96 (d, 3H, J = 6.5 Hz, 7-$OCH_2CH_2CH_2CH_2$**CH$_3$**); ^{13}C NMR (125 MHz, DMSO-d_6), δ (ppm): 193.6 (4-CHO), 160.1 (C-4), 154.5 (C-7), 148.2 (C=O lactone), 143.1 (C-8a), 125.2 (C-5), 119.9 (C-3), 117.7 (C-4a), 117.3 (C-6), 109.3 (C-8), 66.8 (7-O**CH$_2$**$CH_2CH_2CH_2CH_3$), 37.4 (7-OCH_2**CH$_2$**$CH_2CH_2CH_3$), 24.5 (7-OCH_2CH_2**CH$_2$**CH_2CH_3), 22.6 (7-$OCH_2CH_2CH_2$**CH$_2$**CH_3), 14.6 (7-$OCH_2CH_2CH_2CH_2$**CH$_3$**); ESI-MS: $C_{15}H_{16}O_4$, calcd. for M+H = 261.11 Da, M+Na = Da, 283.09 Da, found: *m/z* 261.21 ($[M+H]^+$), 283.17 ($[M+Na]^+$); ESI-HRMS: calcd. for M+H = 261.1127 Da, found: 261.1138 ($[M+H]^+$, 100%); Elemental anal. for $C_{15}H_{16}O_4$, calcd.: C, 69.22; H, 6.20%; found: C, 69.51; H, 6.43%.

*4-Formyl-7-isopentoxycoumarin (**6h**)*



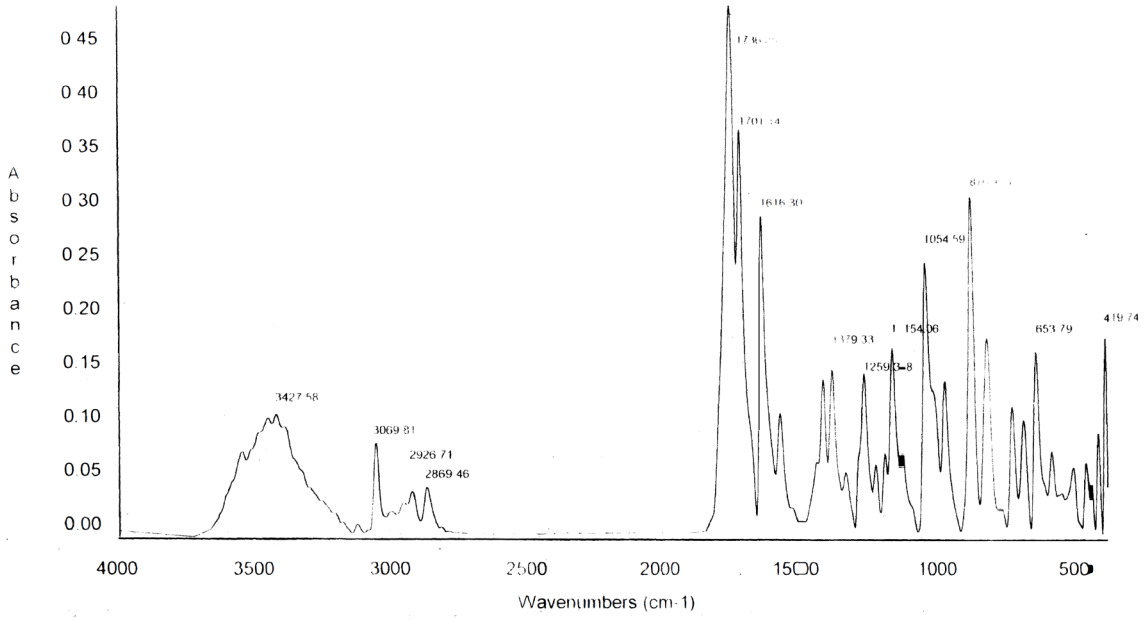
From **4h** (2 mmol, 492 mg). Yield: 322 mg (62%, method A), 473 mg (91%, method B) of **6h** as yellow crystals. M.p.: 116−118 °C (from toluene). IR (KBr), ν (cm^{-1}): 1729 ($\nu_{C=O}$ lactone), 1701 ($\nu_{C=O}$ aldehyde), 1614, 1510 ($\nu_{C=C}$ arene), 1266 & 1149 (ν_{COC} lactone); ^{1}H NMR (500 MHz, DMSO-d_6), δ (ppm): 10.16 (s, 4-CHO), 7.84 (d, J = 3.0 Hz, 1H, H-5), 7.45−7.39 (m, 1H, H-8), 7.32−7.27 (m, 1H, H-7), 7.15 (s, 1H, H-3), 4.03 (dd, 2H, J = 13.75, 6.75 Hz, 7-O**CH$_2$**$CH_2CH(CH_3)_2$], 1.84−1.76 [m, 1H, 7-OCH_2CH_2**CH**$(CH_3)_2$], 1.66−1.61 [m, 2H, 7-OCH_2**CH$_2$**$CH(CH_3)_2$], 0.96 [d, 6H, J = 6.5 Hz, 7-OCH_2CH_2CH**(CH$_3$)$_2$**]; ^{13}C NMR (125 MHz, DMSO-d_6), δ (ppm): 193.6 (4-CHO), 160.1 (C-4), 154.5 (C-7), 148.2 (C=O lactone), 143.1 (C-8a), 125.2 (C-5), 119.9 (C-3), 117.7 (C-4a), 117.3 (C-6), 109.3 (C-8), 66.8 [7-

O**CH$_2$**CH$_2$CH(CH$_3$)$_2$], 37.4 [7-OCH$_2$**CH$_2$**CH(CH$_3$)$_2$], 24.5 [7-OCH$_2$CH$_2$**CH**(CH$_3$)$_2$], 22.6 [7-OCH$_2$CH$_2$CH**(CH$_3$)$_2$**]; ESI-MS: $C_{15}H_{16}O_4$, calcd. for M+H = 261.11 Da, M+Na = Da, 283.09 Da, found: *m/z* 261.19 ([M+H]$^+$), 283.15 ([M+Na]$^+$); ESI-HRMS: calcd. for M+H = 261.1127 Da, found: 261.1121 ([M+H]$^+$, 100%); Elemental anal. for $C_{15}H_{16}O_4$, calcd.: C, 69.22; H, 6.20%; found: C, 69.55; H, 6.42%.

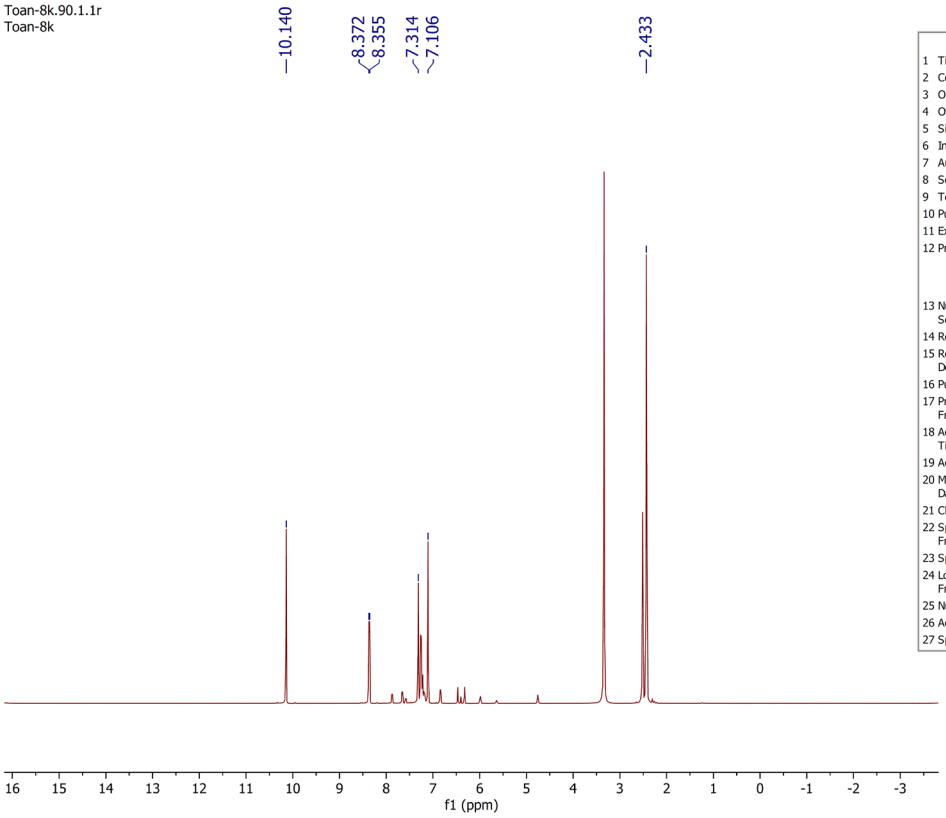
2. Selected spectra

2.1. Selected spectra of 6- and 7-alkoxy-4-methylcoumarins (5 and 6)

*4-Methyl-6-methoxycoumarin **(3a)***



Toan-8k.90.1.1r
Toan-8k



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5	Site	
6	Instrument	spect
7	Author	
8	Solvent	DMSO
9	Temperature	299.8
10	Pulse Sequence	zg30
11	Experiment	1D
12	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0186
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15	Relaxation Delay	1.0000
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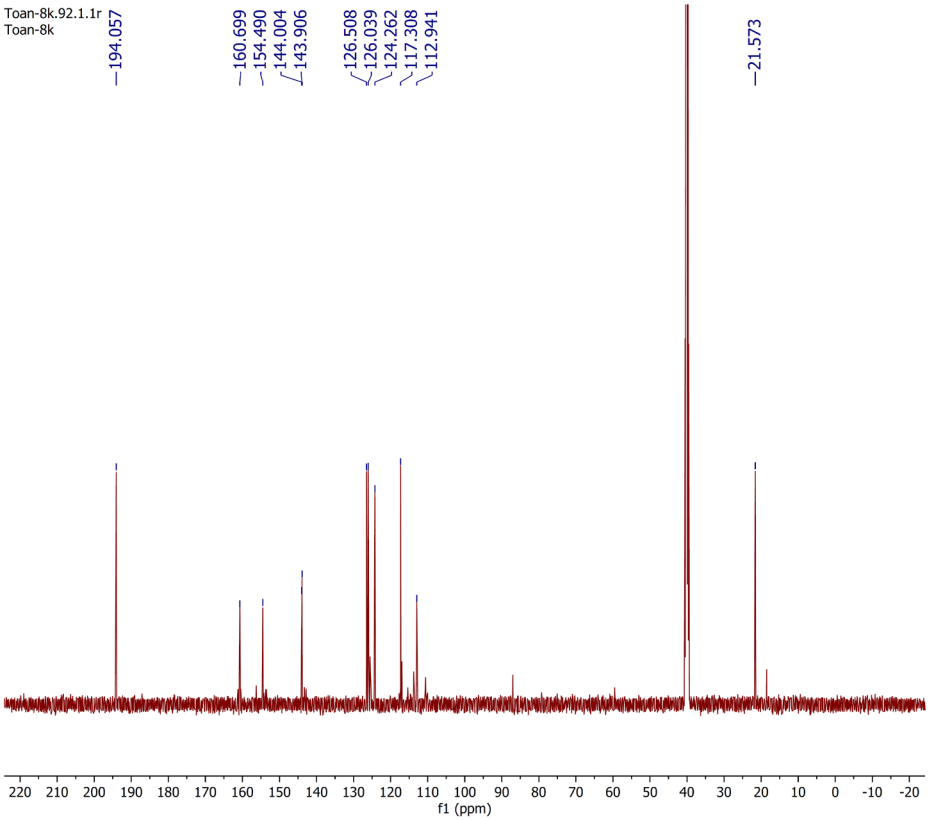
27	Spectral Size	65536

Toan-8k.92.1.1r
Toan-8k



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7	Author	
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10	Pulse Sequence	zgpg30
11	Experiment	1D
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25	Nucleus	13C
26	Acquired Size	32768

Lab: Materials chemistry, Faculty of Chemistry, HUS-VNU
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Tel: 844.38.253.053; **Fax**: 844.38.241.140 **Mail**: Chem.vnu@.edu.vn

Operator: Ms. Dao Thi Nhung
Mobile: 0948 119 043; Email: daothinhungtn@yahoo.com

Mass Spectrometter
LTQ Orbitrap XL™

Sample name : 5b- 6OMe4MeCou
Mode: ESI, M+H

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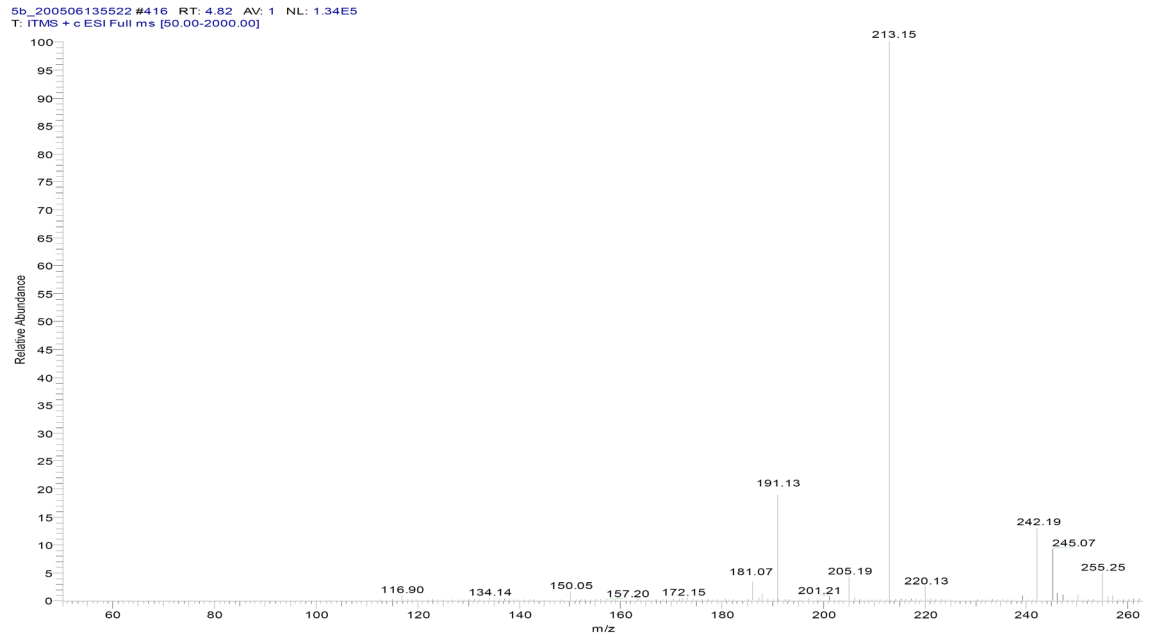
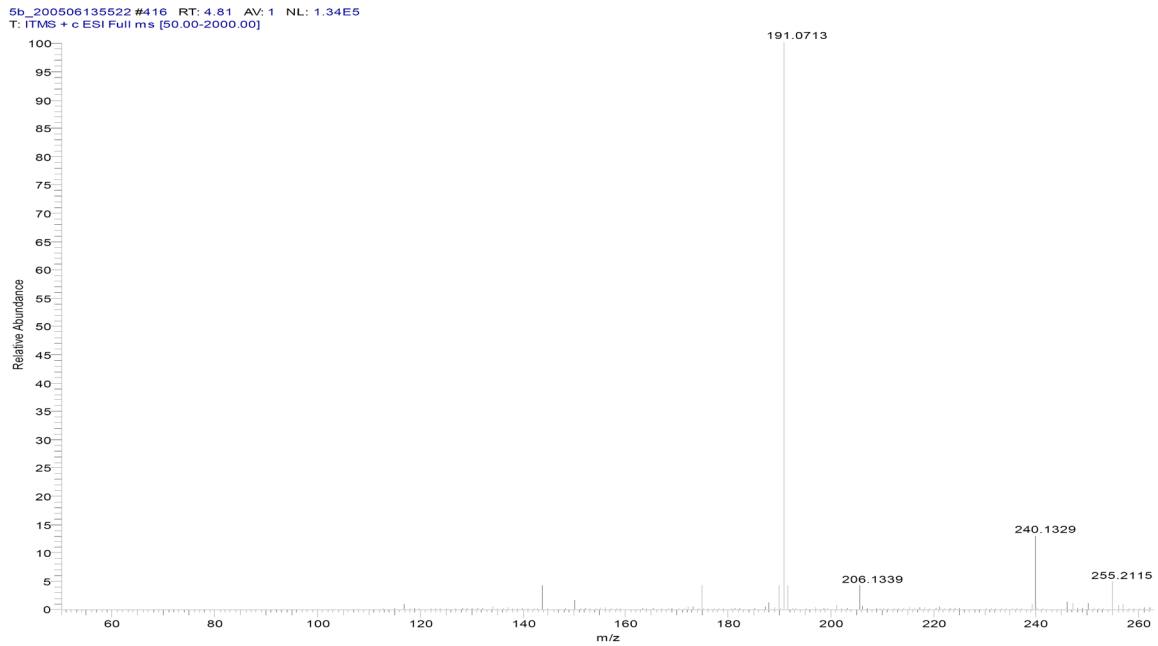
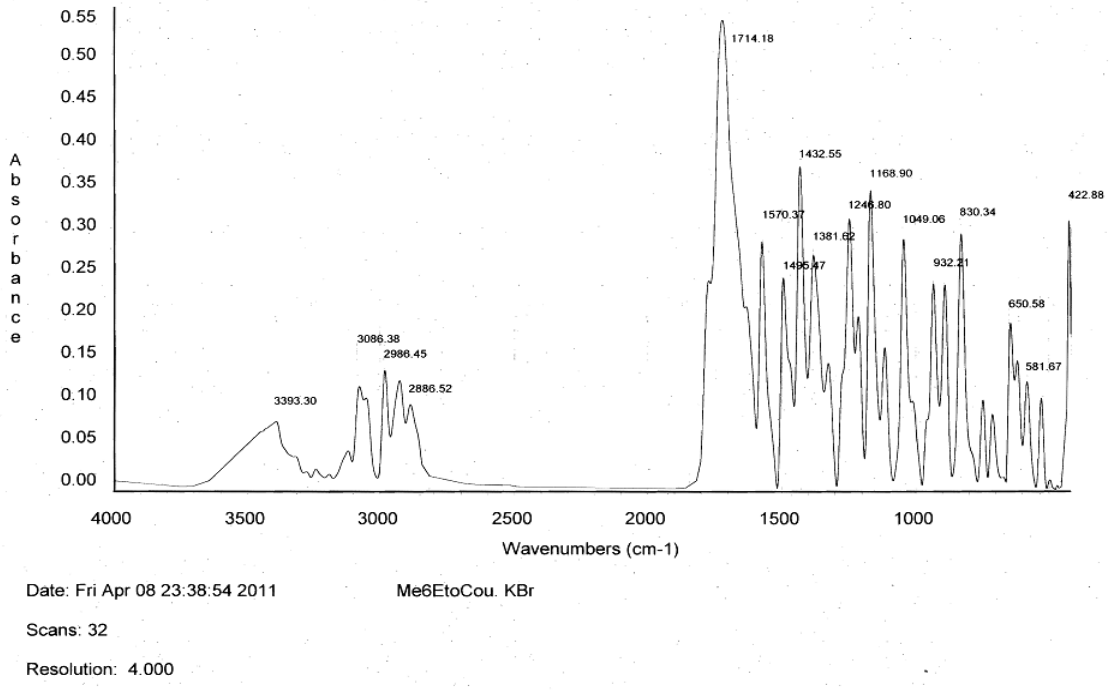
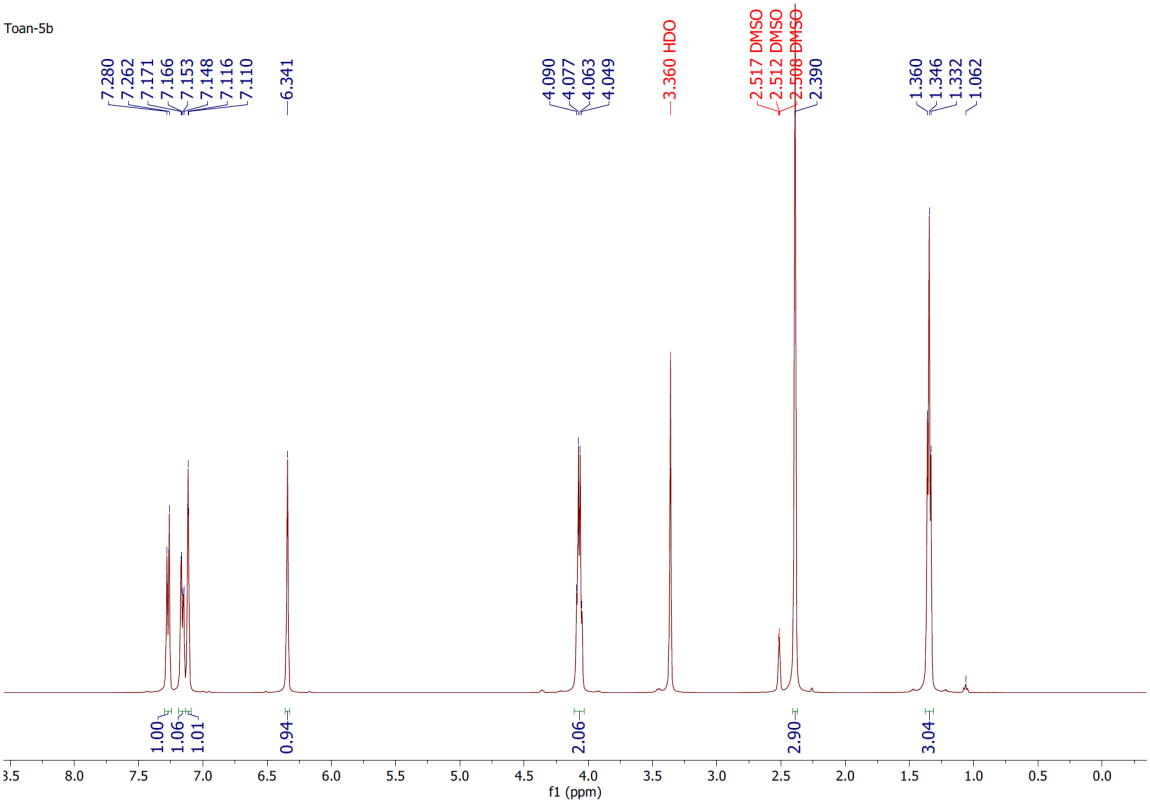
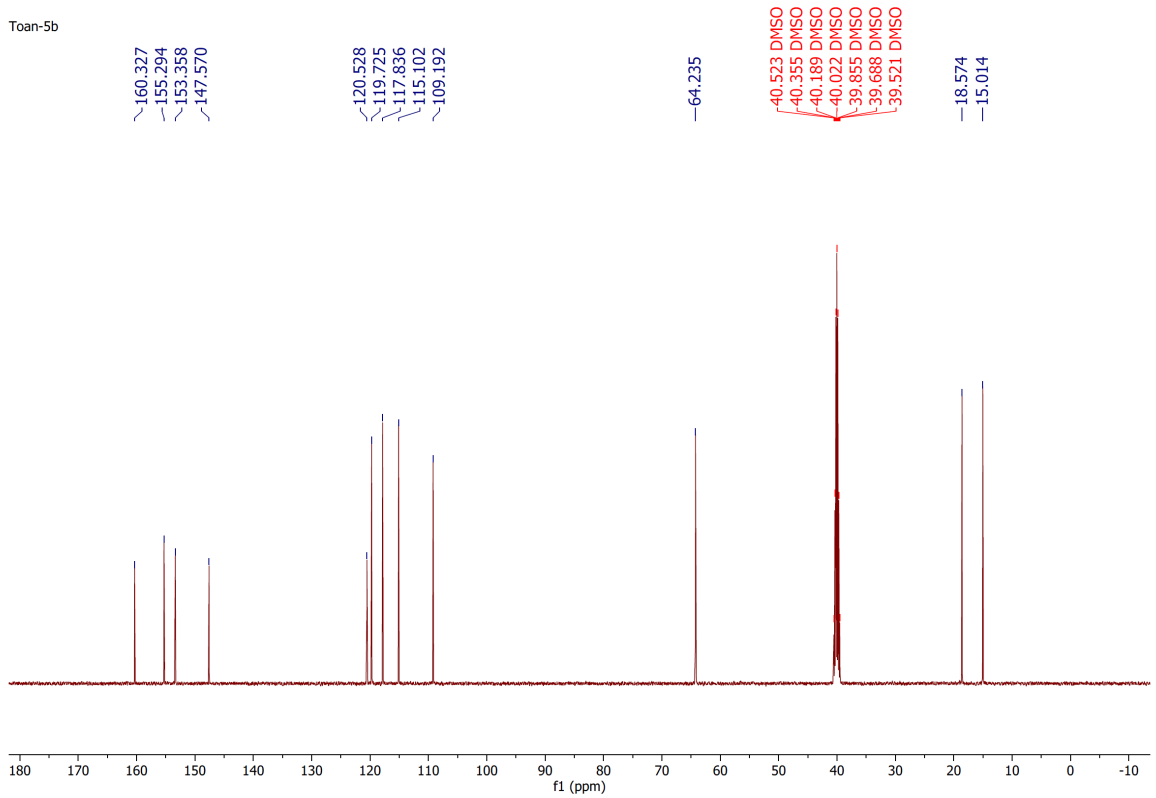




*4-Methyl-6-ethoxycoumarin (**3b**)*







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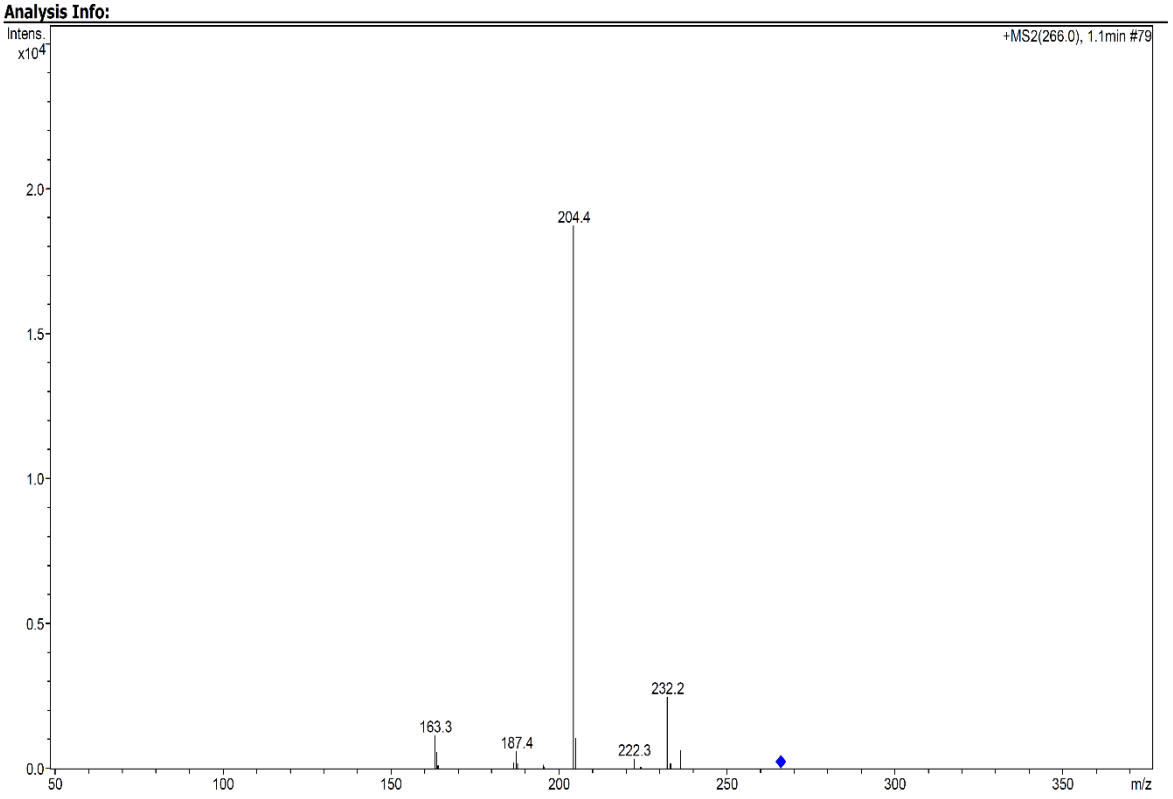
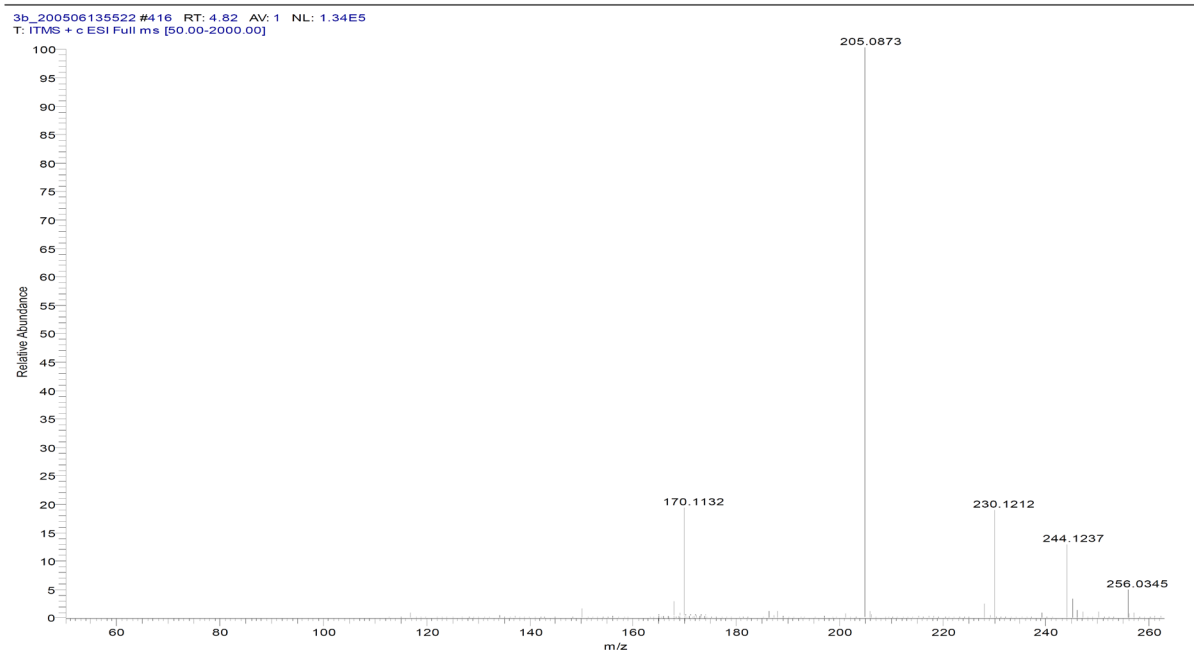
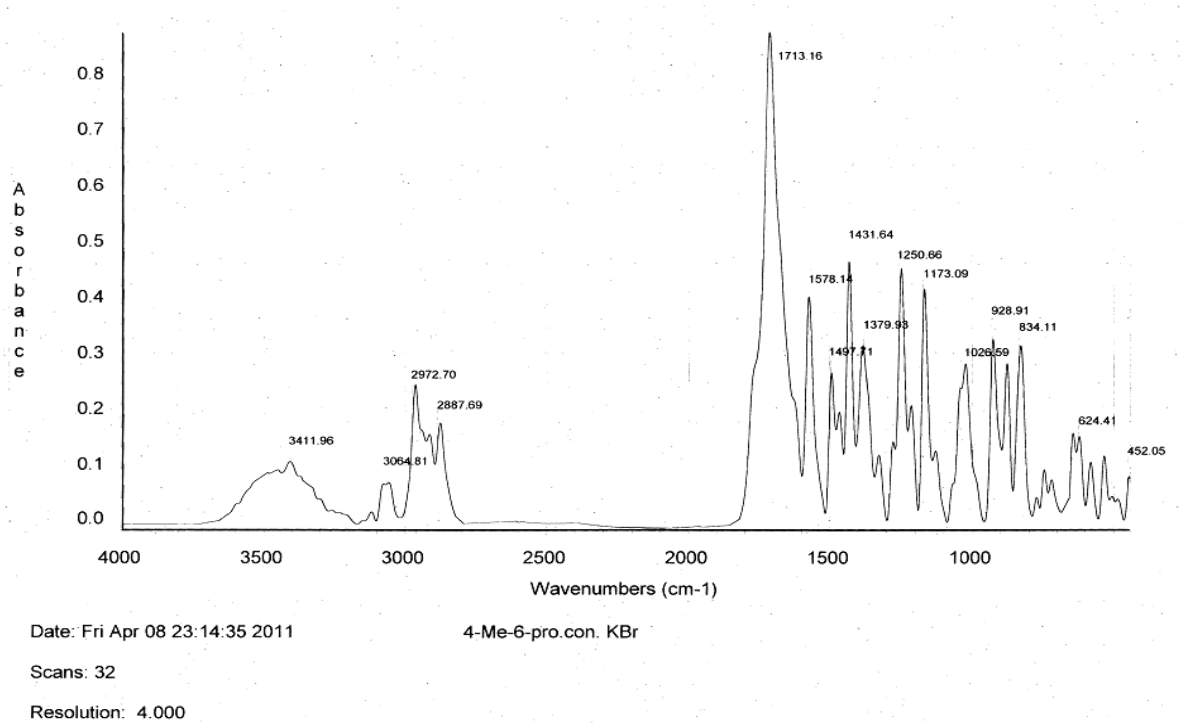
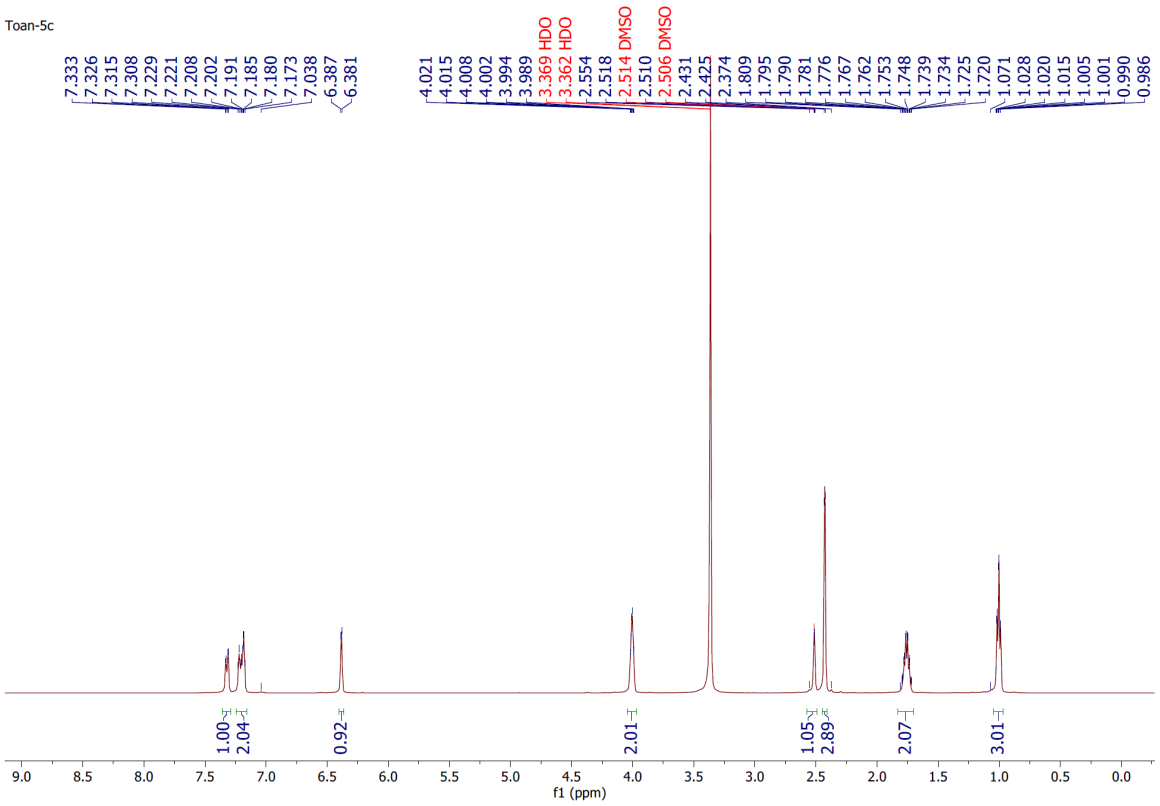




*4-Methyl-6-propoxycoumarin (**3c**)*

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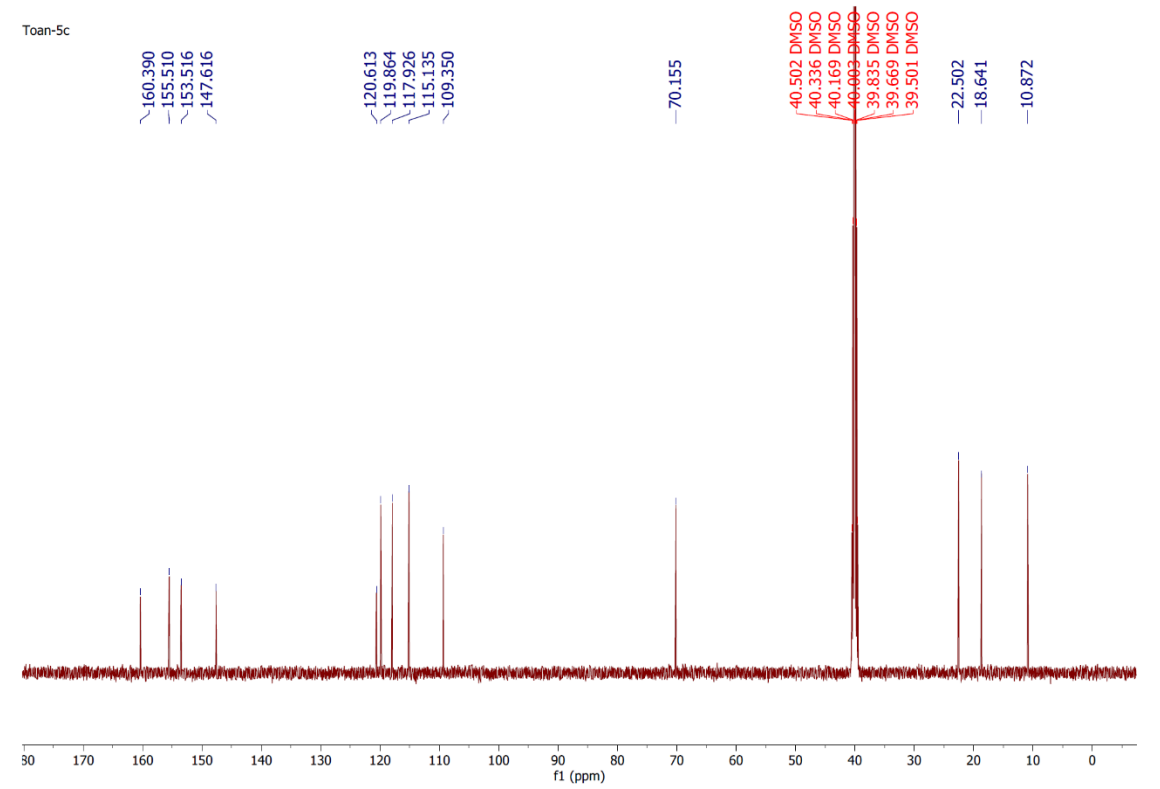
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39.669 DMSO
39.501 DMSO
22.502
18.641
10.872
f1 (ppm)

Lab: Materials chemistry, Faculty of Chemistry, HUS-VNU
19 Le Thanh Tong, Hoan Kiem, Ha Noi

Tel: 844.38.253.053; **Fax**: 844.38.241.140 **Mail**: Chem.vnu@.edu.vn

Operator: Ms. Dao Thi Nhung
Mobile: 0948 119 043; Email: daothinhungtn@yahoo.com

Sample name: 6c-OPr4MeCou
Mode: ESI, M+H

Mass Spectrometter
LTQ Orbitrap XL™
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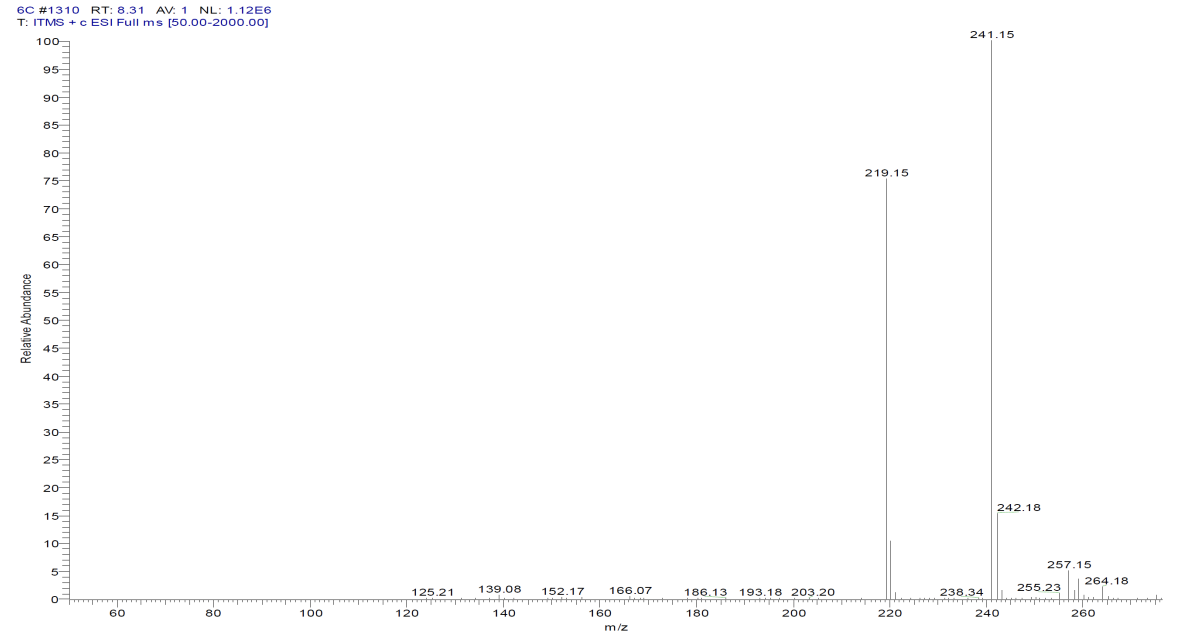
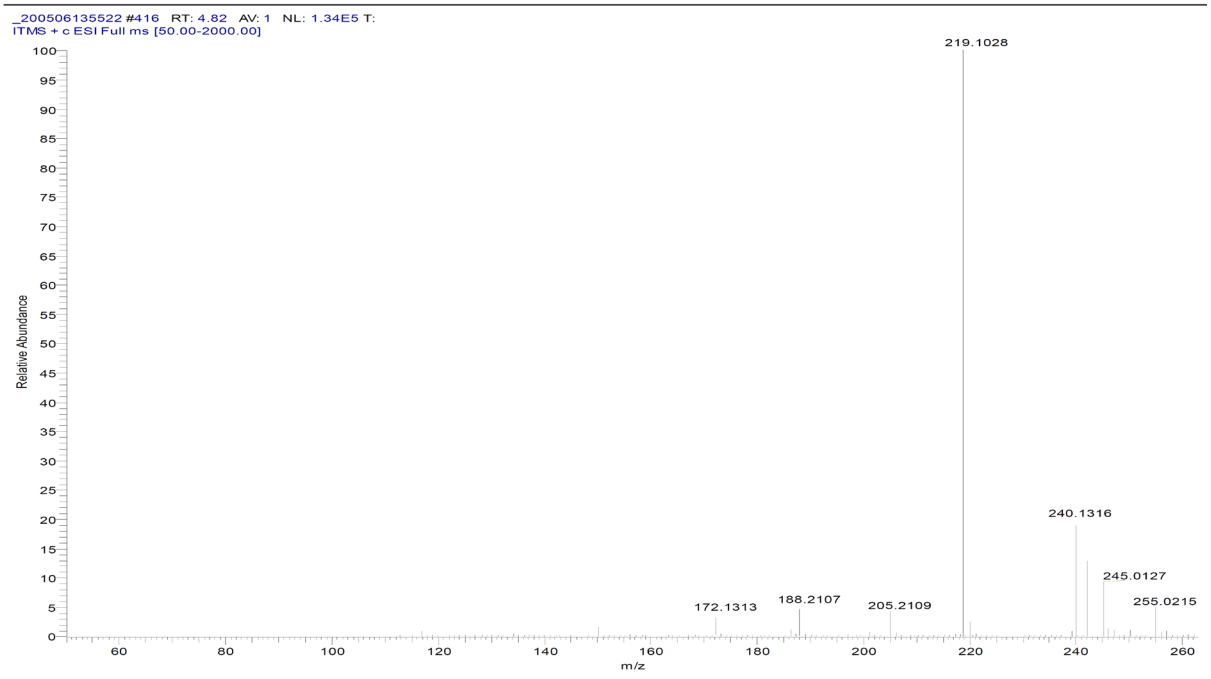
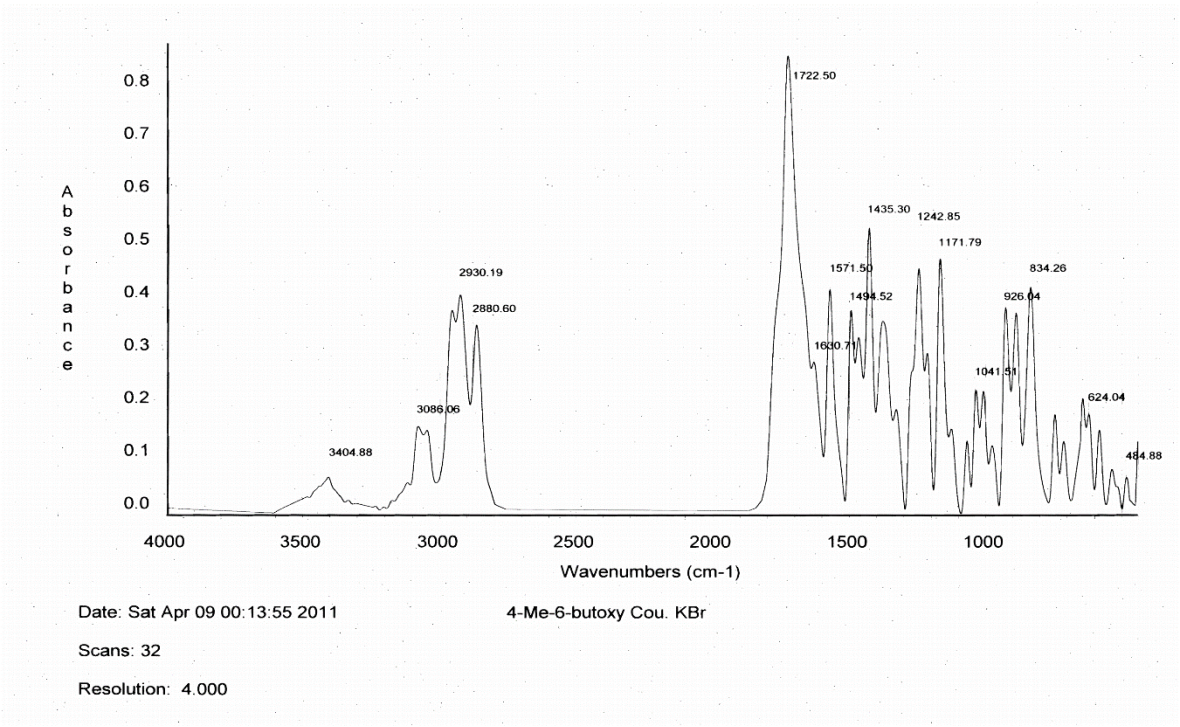
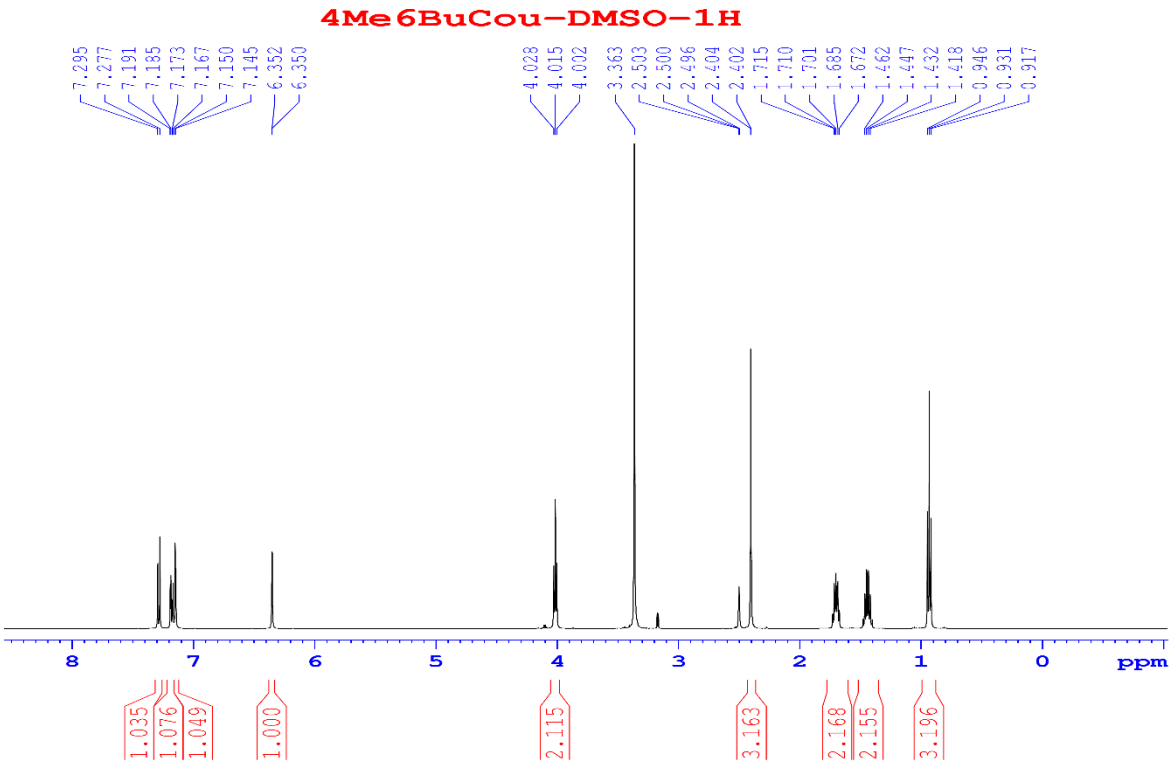
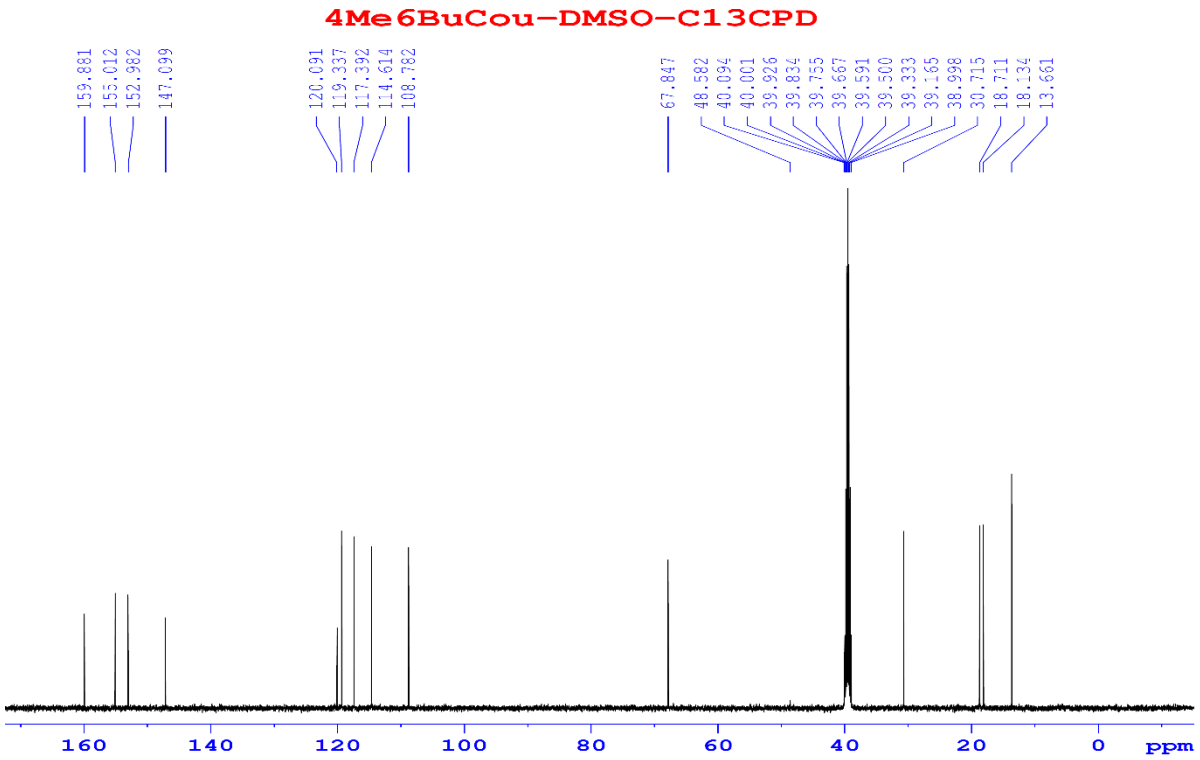




*4-Methyl-6-butoxycoumarin (**3e**)*







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Method: DO MS.m
Sample Name: 4-Me-6-butoxy cou
Analysis Info:

Instrument: Agilent 6310 Ion Trap
Operator: Phong PTHC, Vien Hoa HCTN

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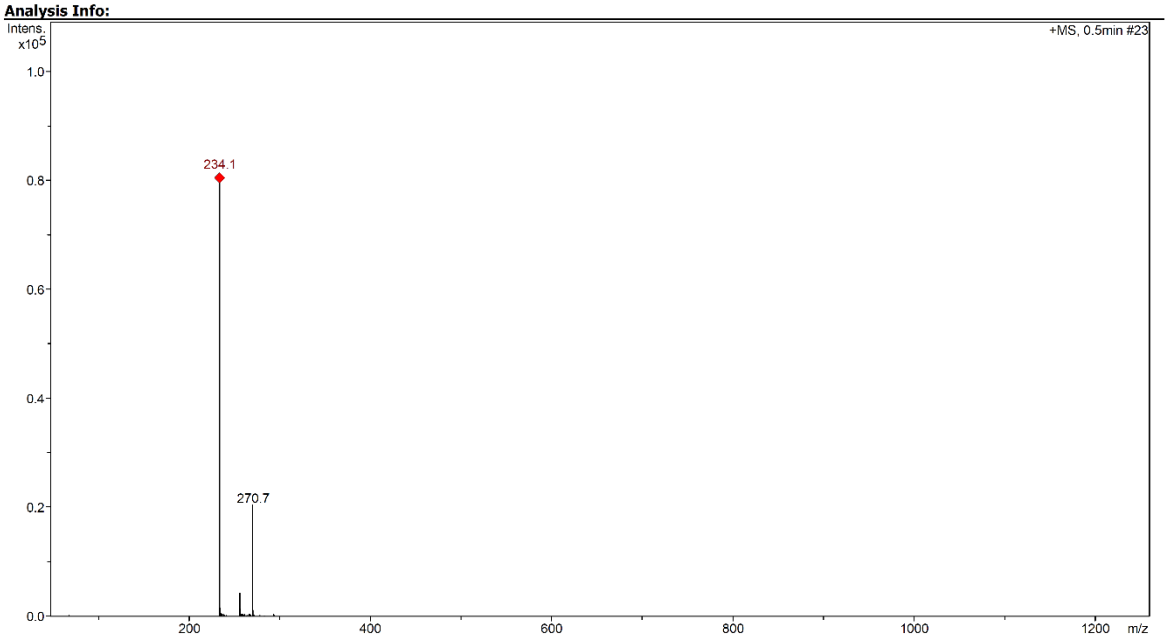
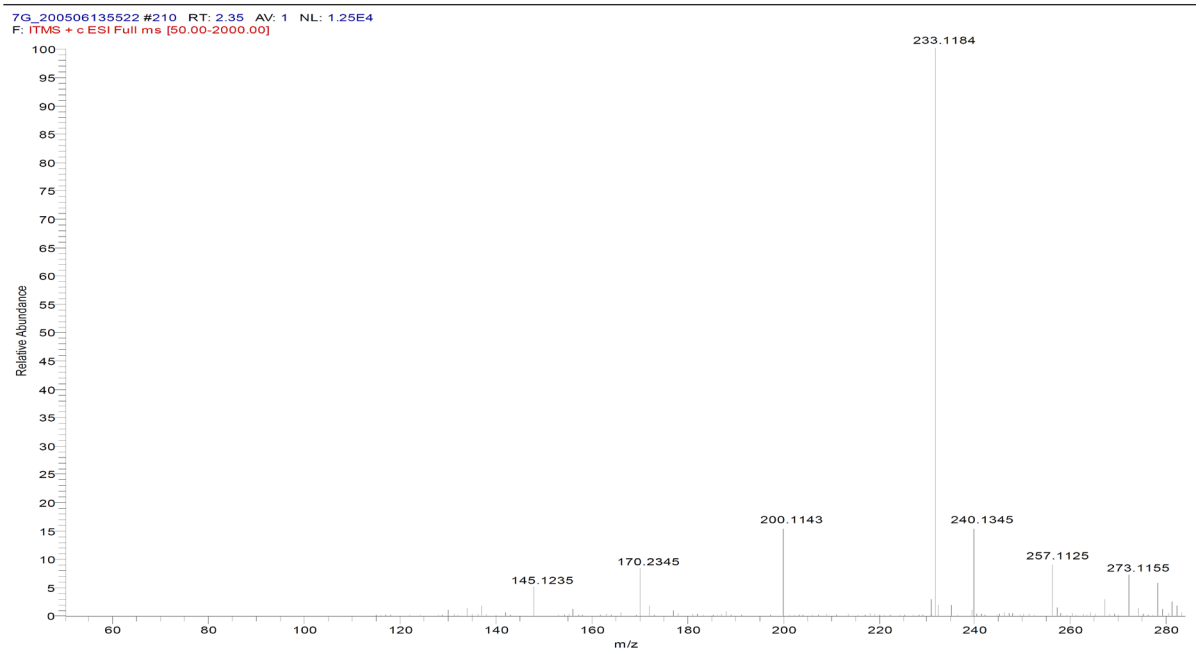


MSD Trap Report v 4 (A4-Opt2)

Page 1 of 1

Agilent Technologies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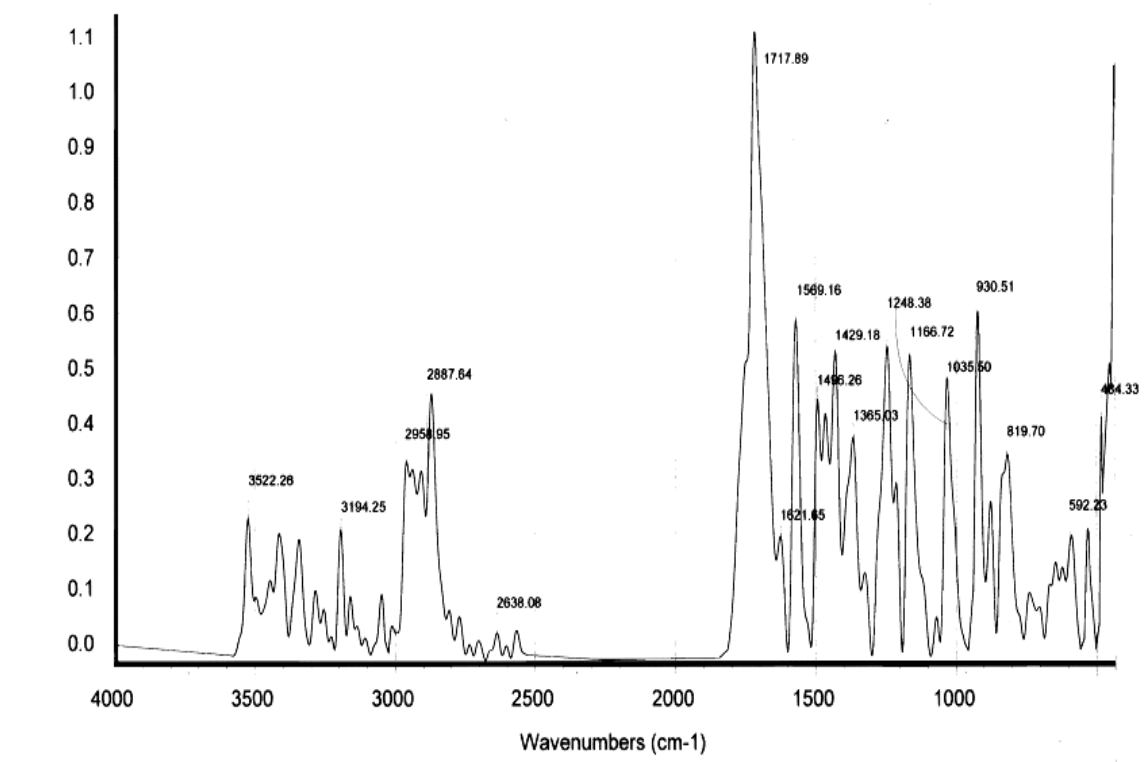
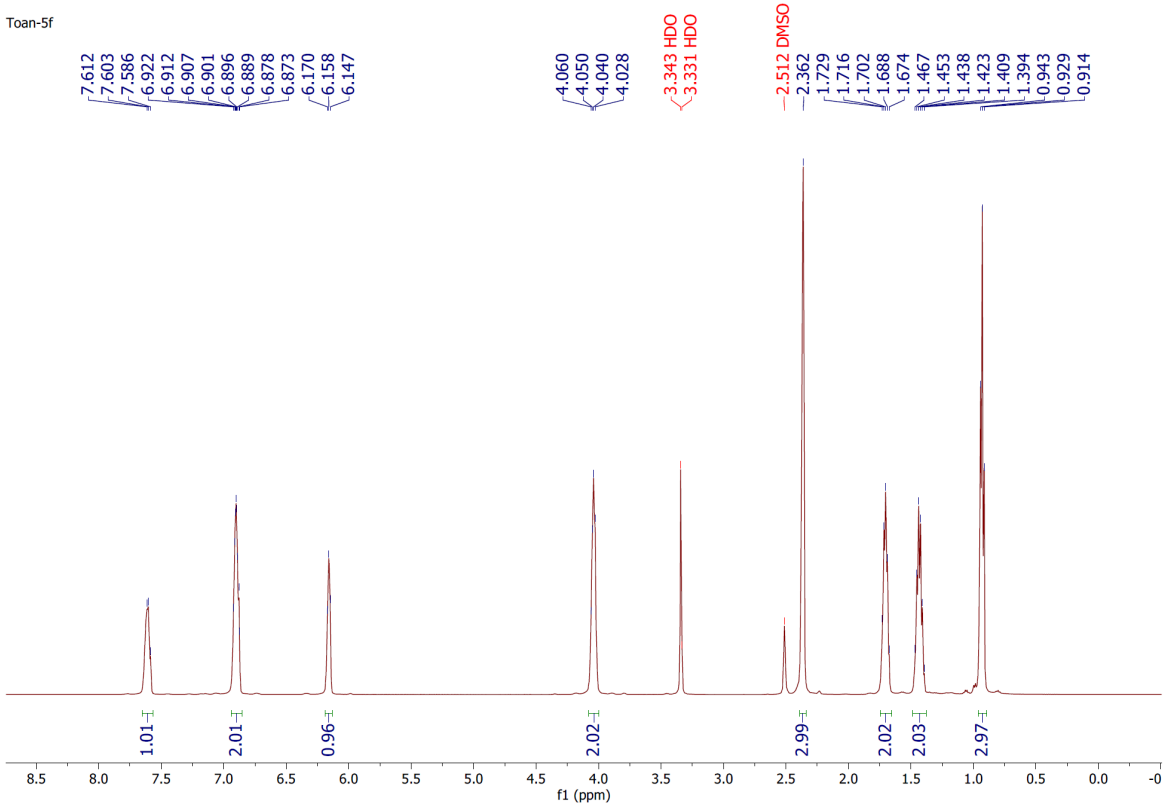
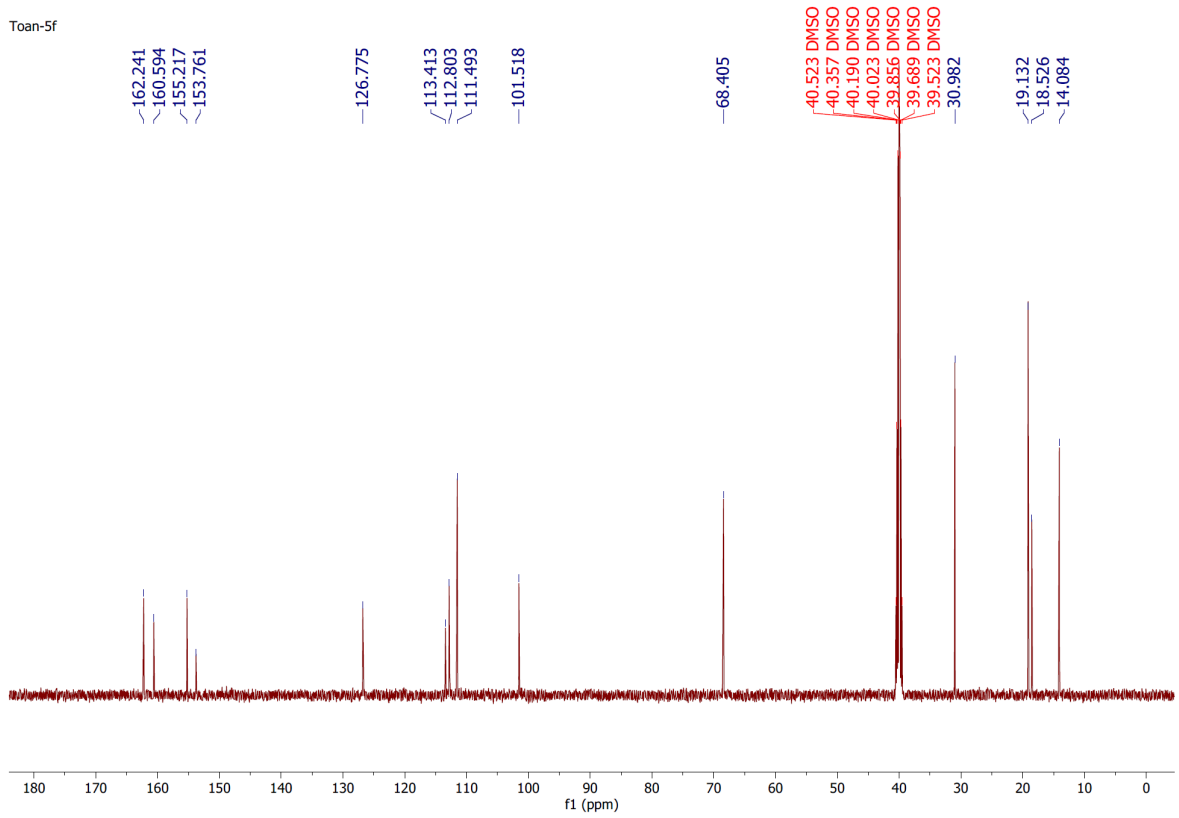
Relative Abundance
m/z

*4-Methyl-6-isobutoxycoumarin (**3f**)*



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40
30
20
10
0
f1 (ppm)

Lab: Materials chemistry, Faculty of Chemistry, HUS-VNU
19 Le Thanh Tong, Hoan Kiem, Ha Noi

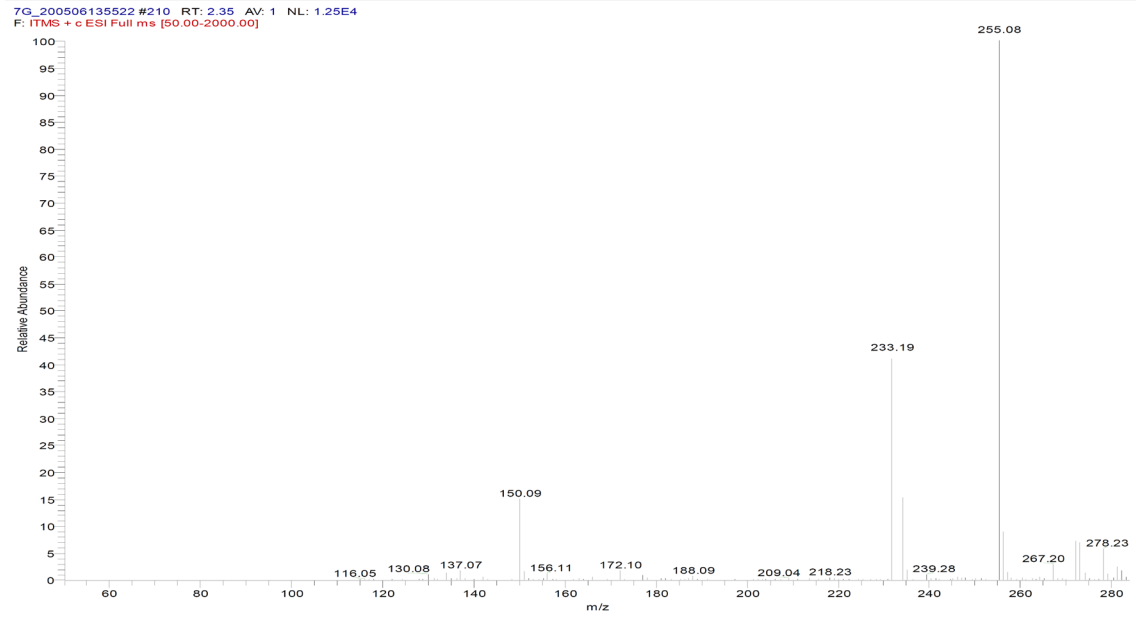
Tel: 844.38.253.053; **Fax**: 844.38.241.140 **Mail**: Chem.vnu@.edu.vn

Operator: Ms. Dao Thi Nhung
Mobile: 0948 119 043; Email: daothinhungtn@yahoo.com

Sample name : 5f-6OiBu4MeCou
Mode: ESI, M+H

Mass Spectrometter
LTQ Orbitrap XL™

C:\LTQ Orbitrap\...\7G_200506135522 5/6/2020 1:55:22 PM



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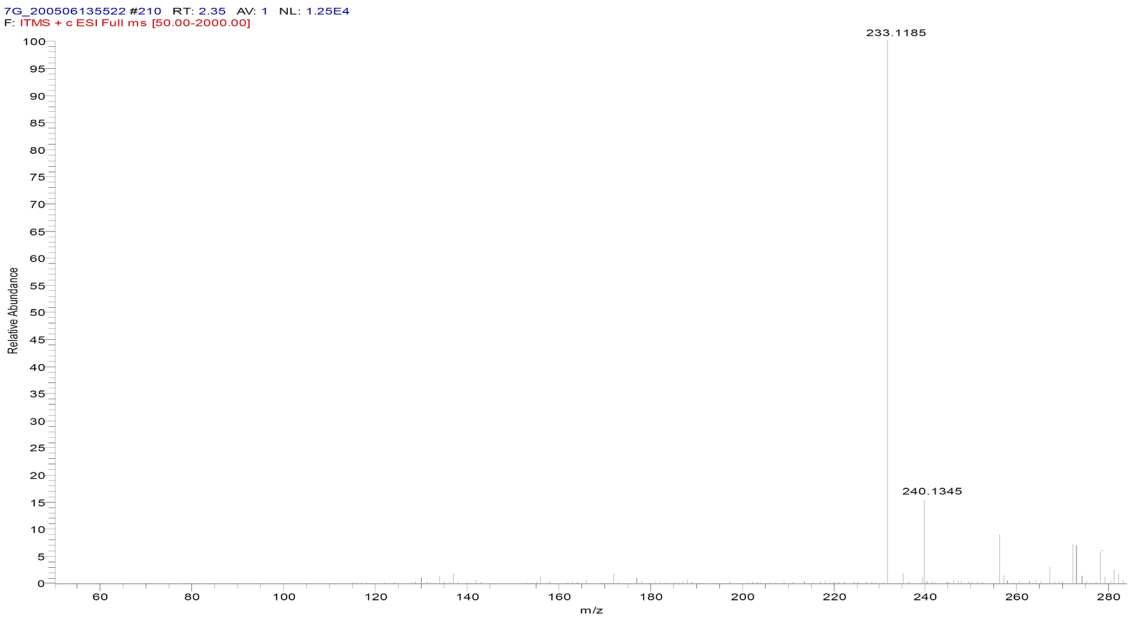
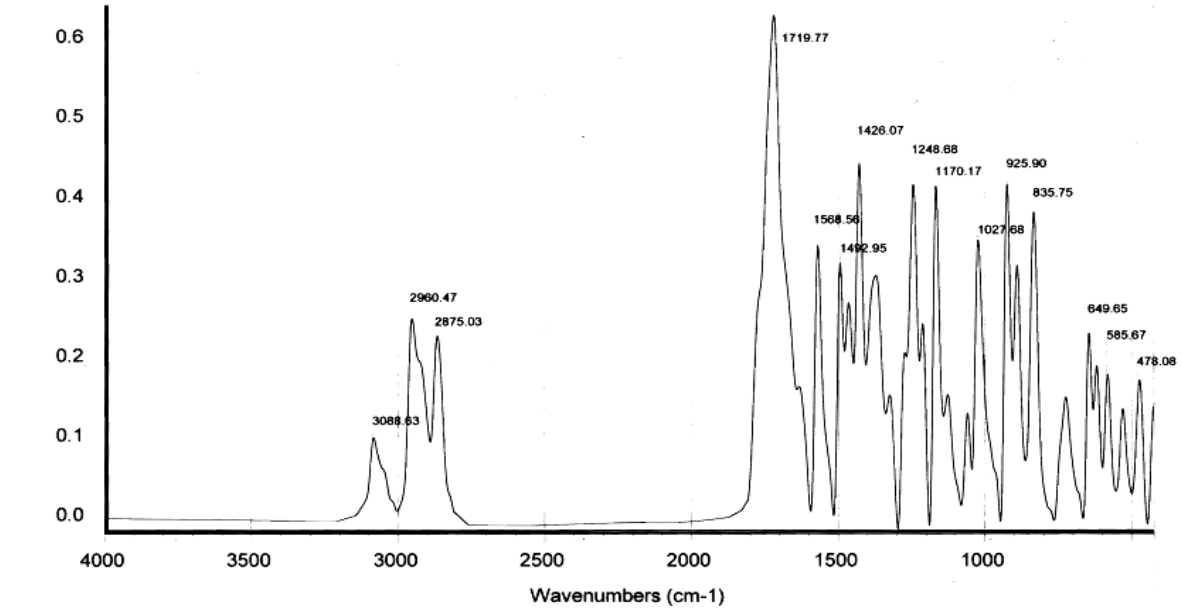


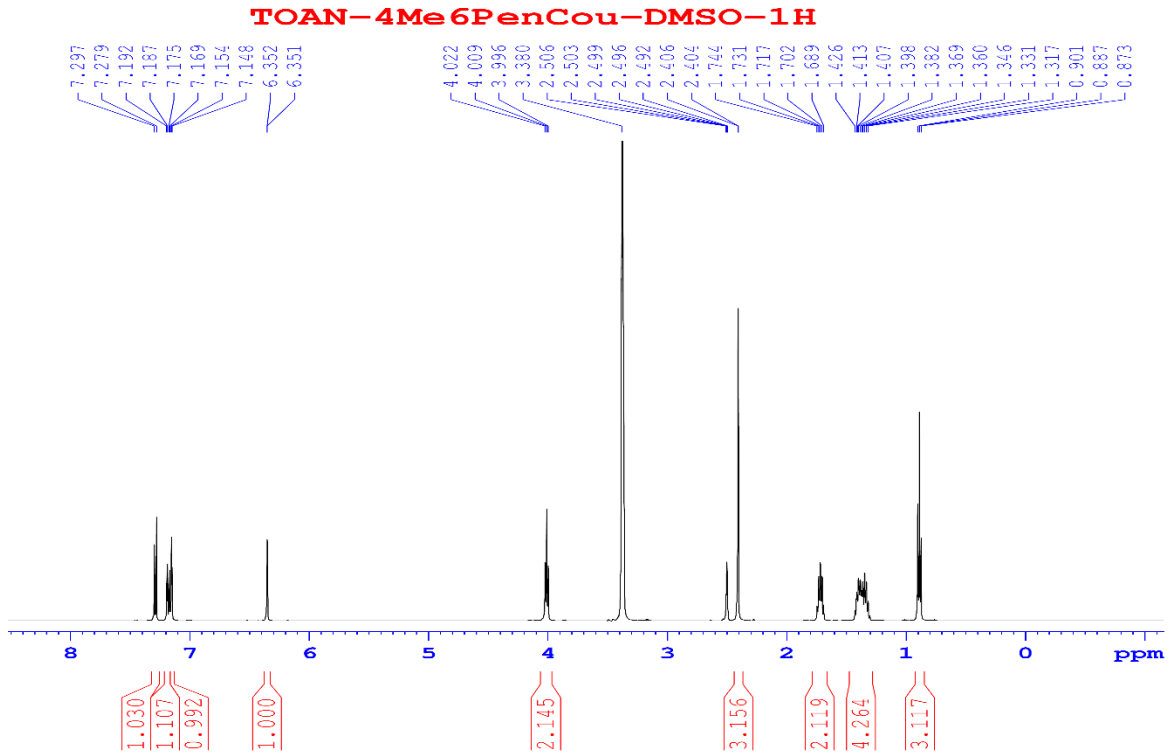
*4-Methyl-6-pentoxycoumarin (**3g**)*

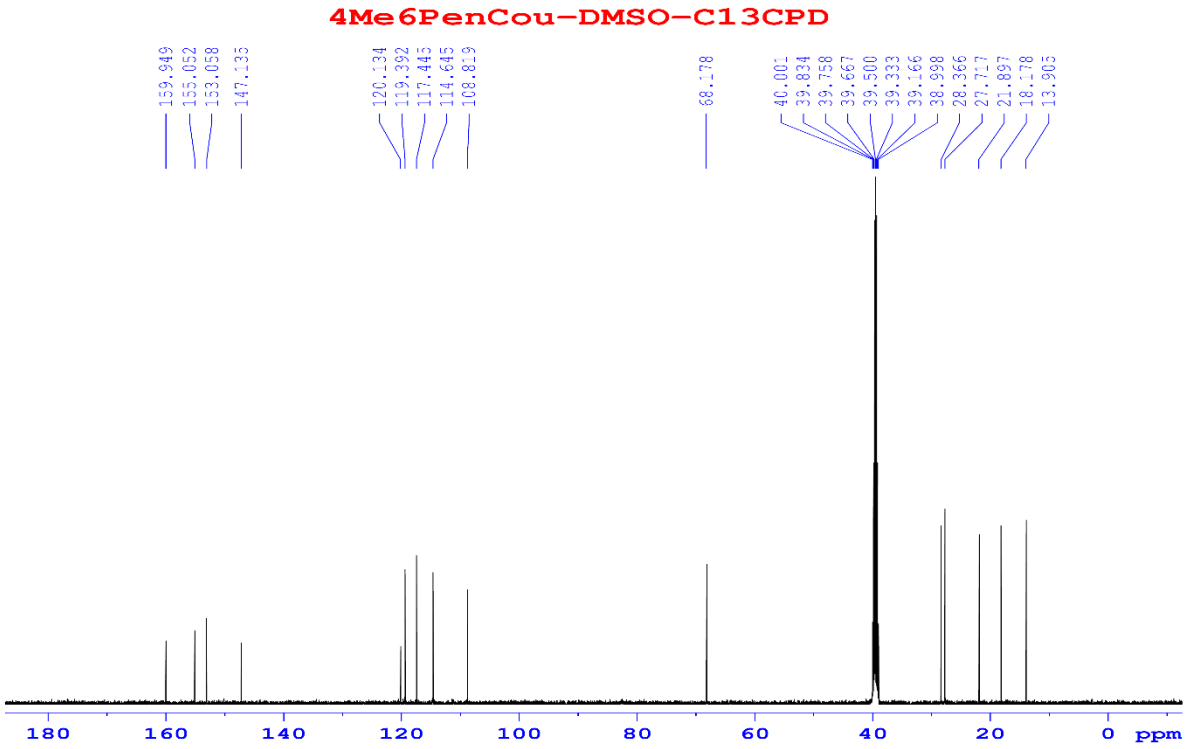


Date: Thu Nov 15 21:00:12 2012 4-Me-6-pentoxy cou- Ngay do 17/4/203. KBr

Scans: 32

Resolution: 4.000



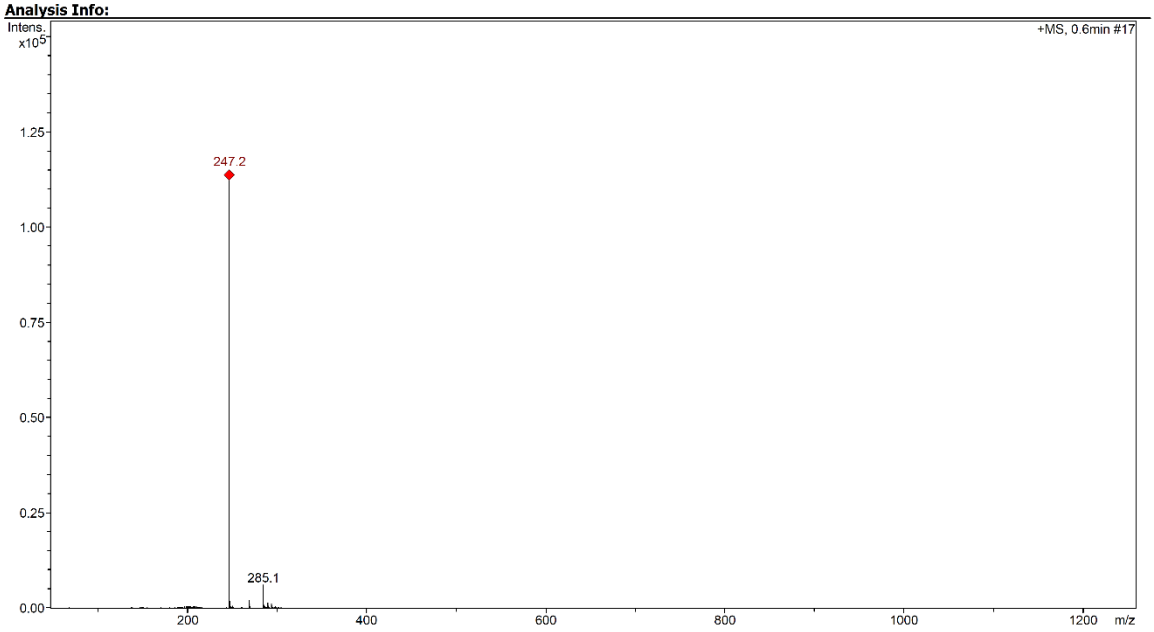


Display Report - Selected Window Selected Analysis

Analysis Name: 14011608.d
Method: def_lcms.m
Sample Name: 4-Me-6- pentoxy-cou 1H
Analysis Info:

Instrument: Agilent 6310 Ion Trap
Operator: Phong PTHC, Vien Hoa HCTN

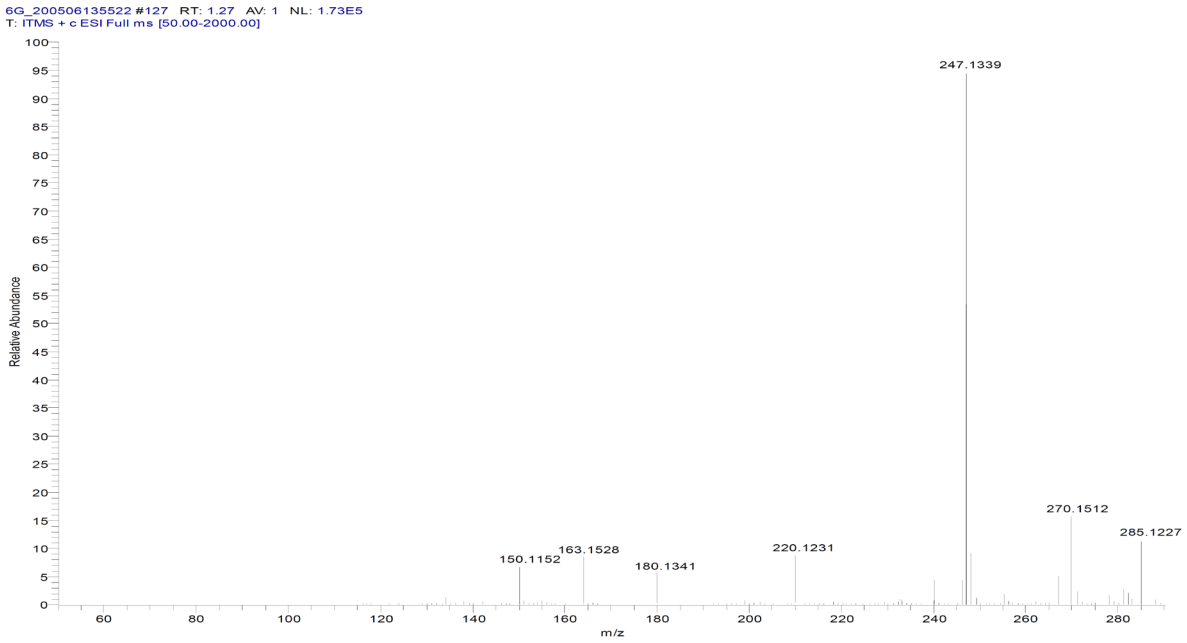
Print Date: 1/16/2014 11:32:27
Acq. Date: 1/16/2014 11:16:16 AM



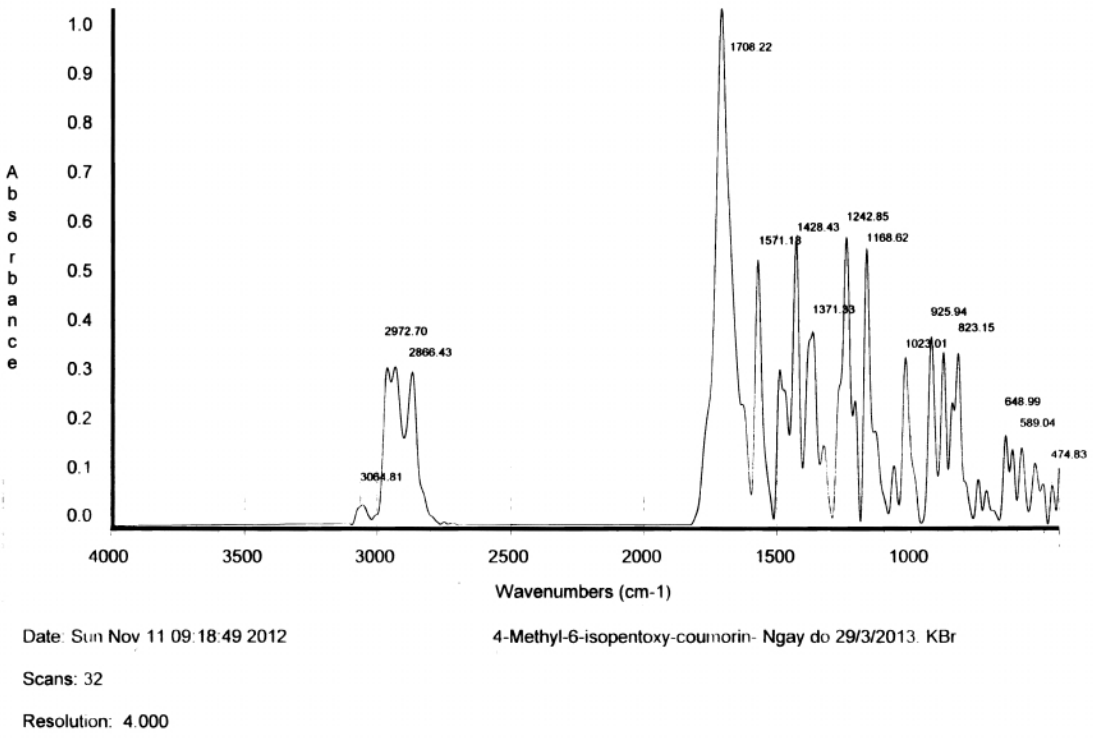
MSD Trap Report v 4 (A4-Opt2)

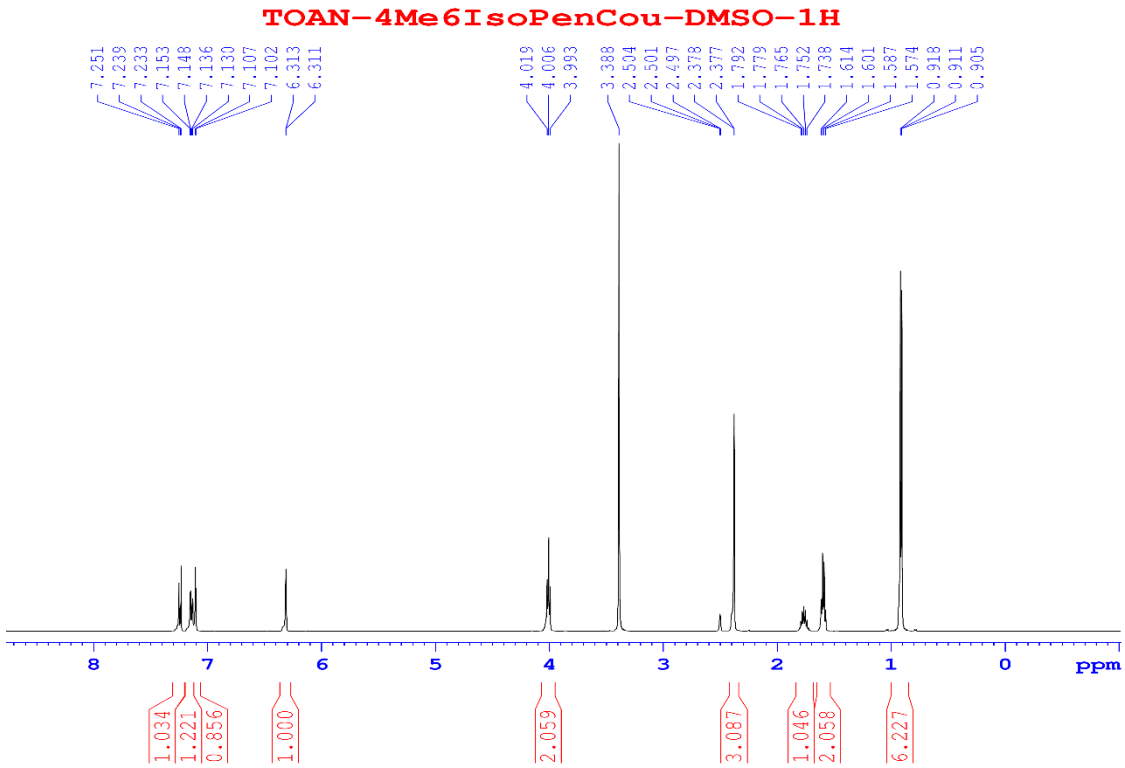
Page 1 of 1

Agilent Technologies



*4-Methyl-6-isopentoxycoumarin (**3h**)*

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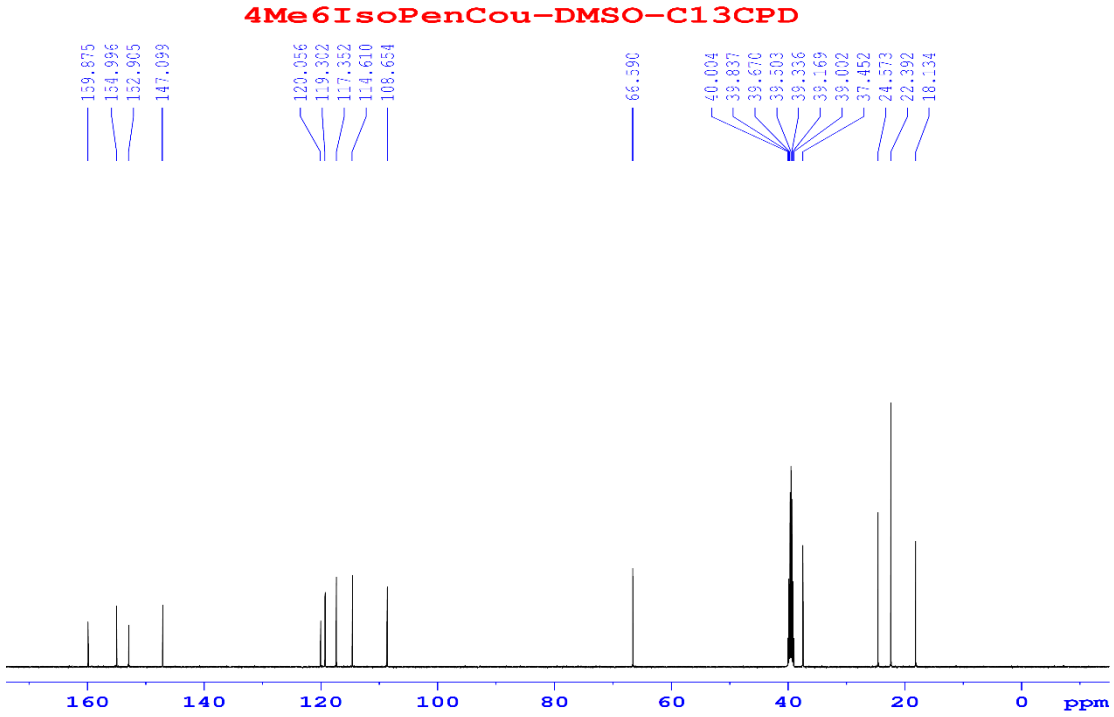
7.239
7.233
7.153
7.148
7.136
7.130
7.107
7.102
6.313
6.311
4.019
4.006
3.993
3.388
2.504
2.501
2.497
2.378
2.377
1.792
1.779
1.765
1.752
1.738
1.614
1.601
1.587
1.574
0.918
0.911
0.905
8
7
6
5
4
3
2
1
0
ppm
1.034
1.221
0.856
1.000
2.059
3.087
1.046
2.058
6.227

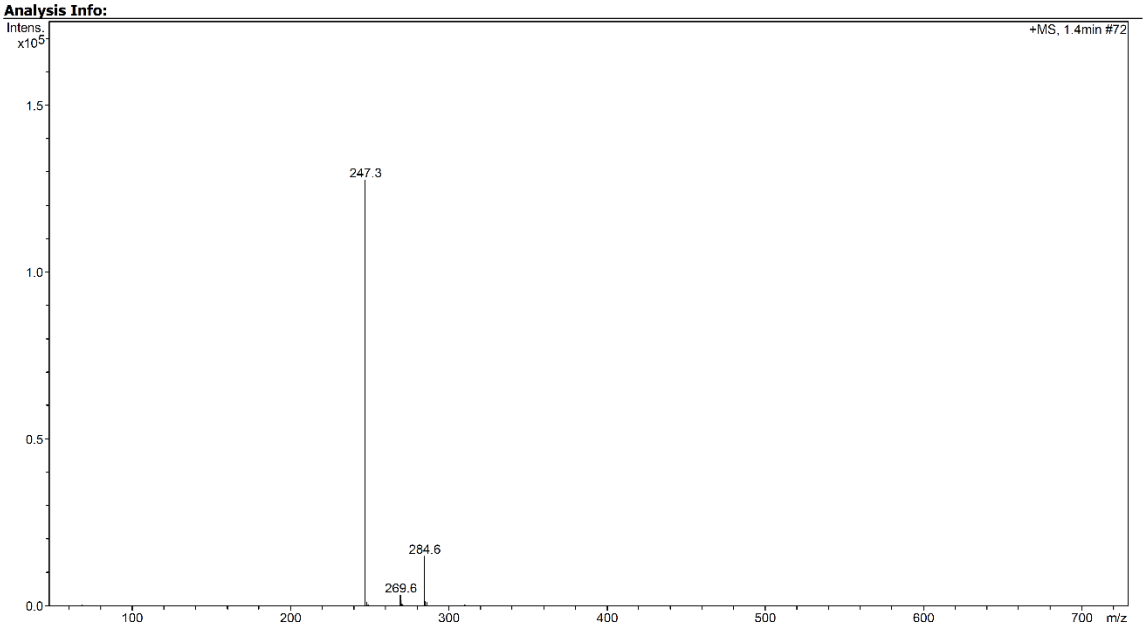

4Me6IsoPenCou-DMSO-C13CPD
159.875
154.996
152.965
147.099
120.056
119.302
117.352
114.610
108.654
66.590
40.004
39.837
39.670
39.503
39.336
39.169
39.002
37.452
24.573
22.392
18.234
160
140
120
100
80
60
40
20
0
ppm

Display Report - Selected Window Selected Analysis

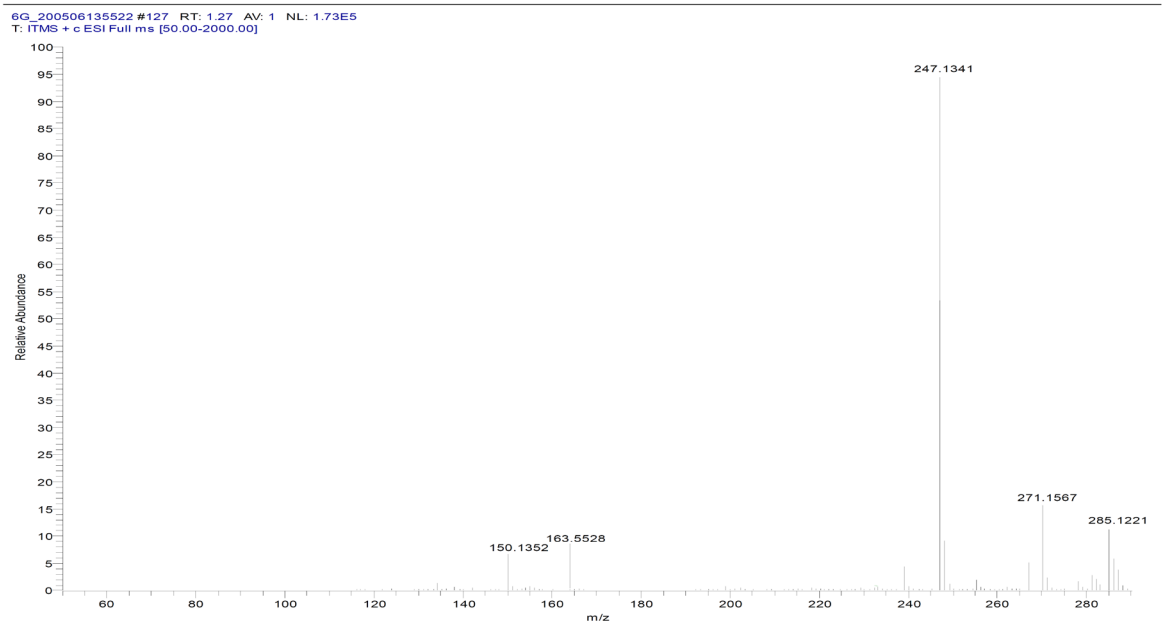
Analysis Name: 14011614.d
Method: DO MS.m
Sample Name: 4Me-6 isopentoxy cou 1H
Analysis Info:

Instrument: Agilent 6310 Ion Trap
Operator: Phong PTHC, Vien Hoa HCTN

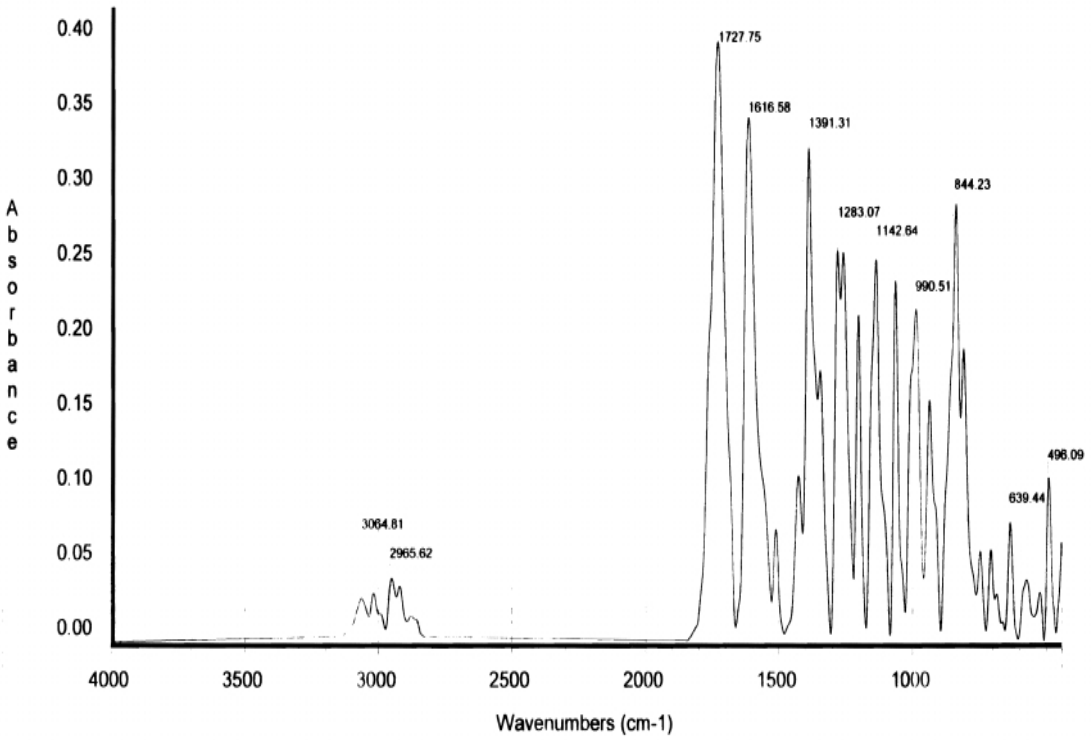
Print Date: 1/16/2014 1:25:09 PM
Acq. Date: 1/16/2014 1:19:23 PM

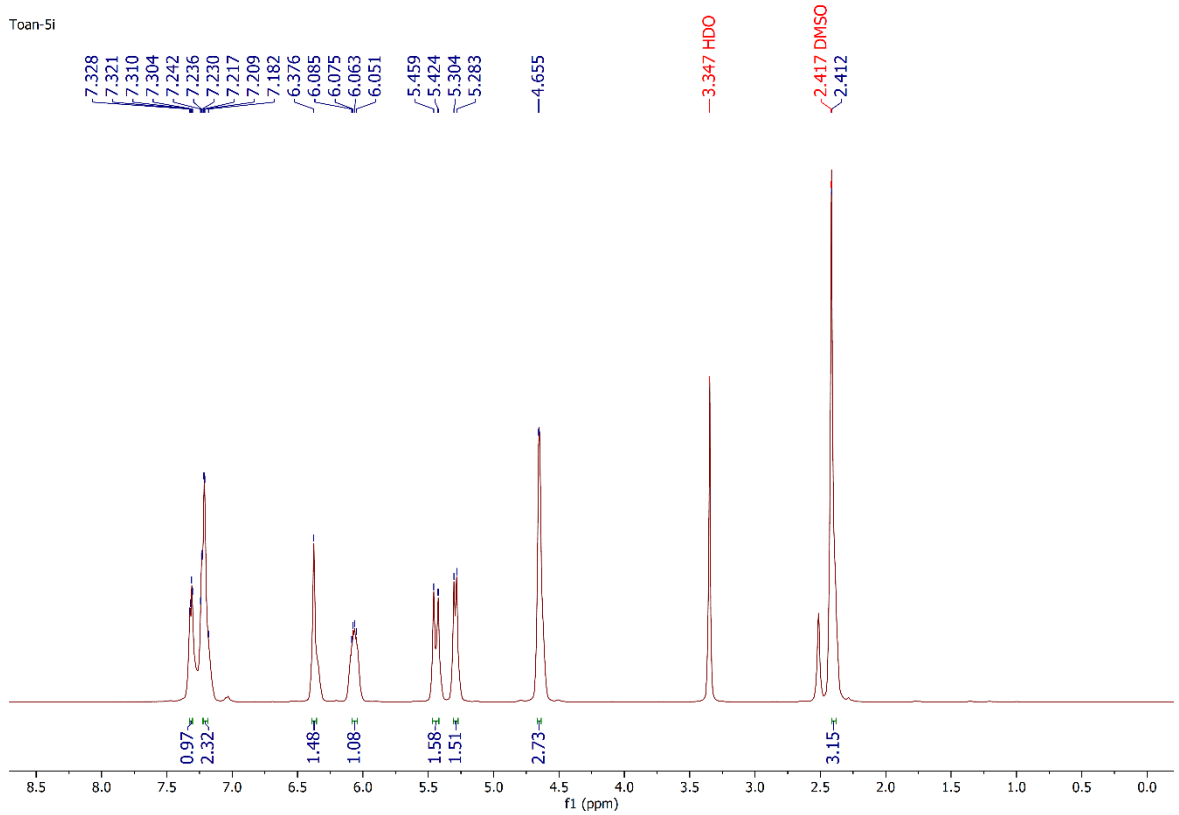


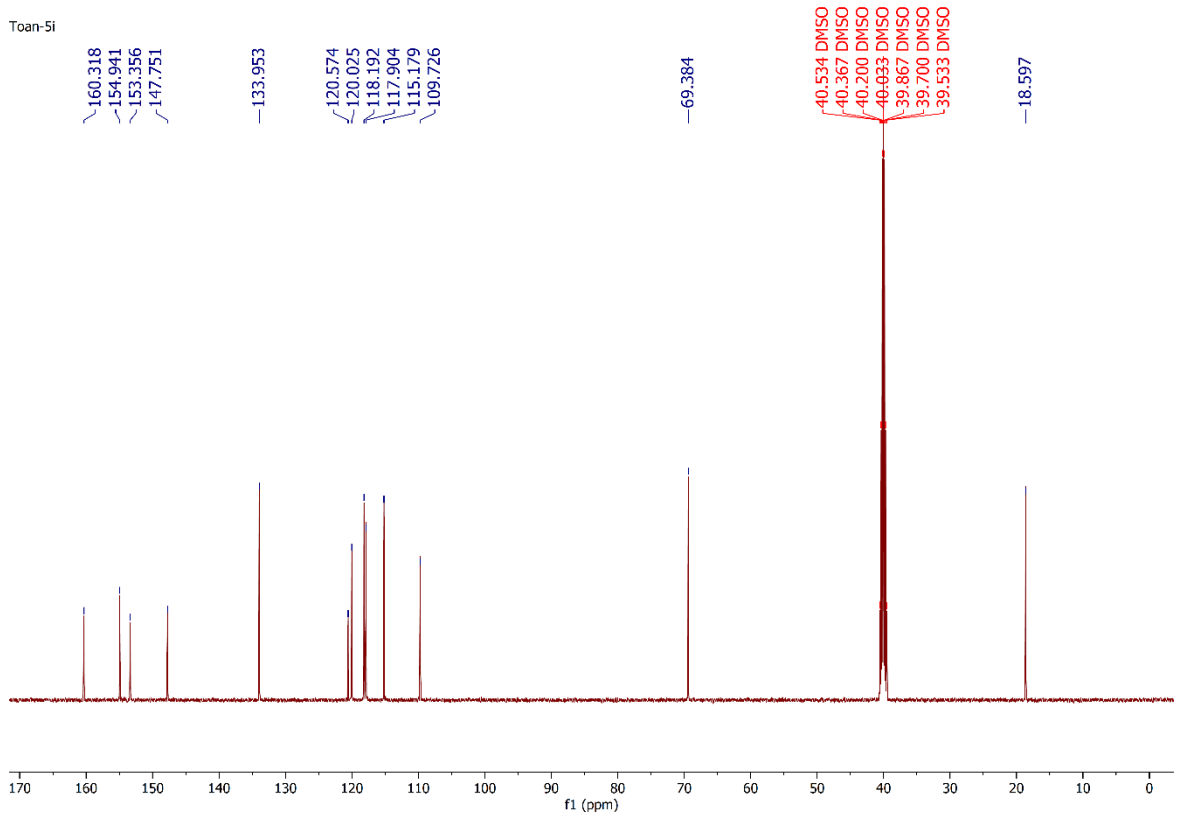
MSD Trap Report v 4 (A4-Opt2) Page 1 of 1 Agilent Technologies



*4-Methyl-6-allyloxycoumarin (**3i**)*







Lab: Materials chemistry, Faculty of Chemistry, HUS-VNU
19 Le Thanh Tong, Hoan Kiem, Ha Noi

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Operator: Ms. Dao Thi Nhung
Mobile: 0948 119 043; Email: daothinhungtn@yahoo.com

SAMPLE:5i-6OAllyl4MeCou
Mode: ESI, M+H

Mass Spectrometter
LTQ Orbitrap XL™
Solvent: MeOH/DCM

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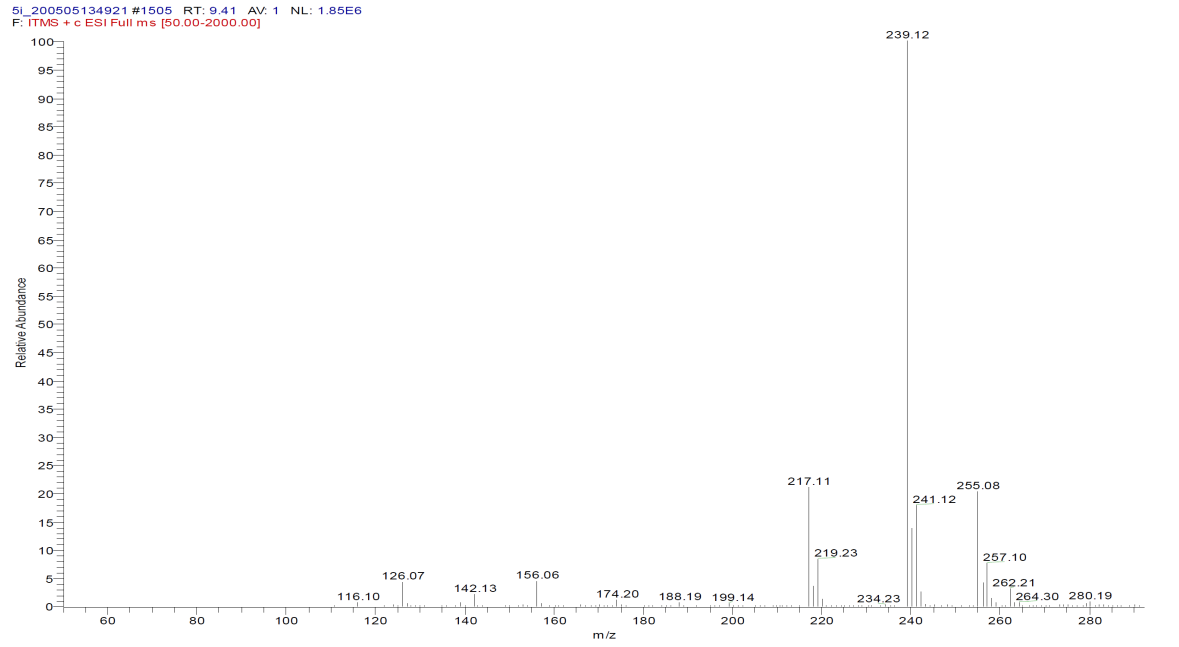
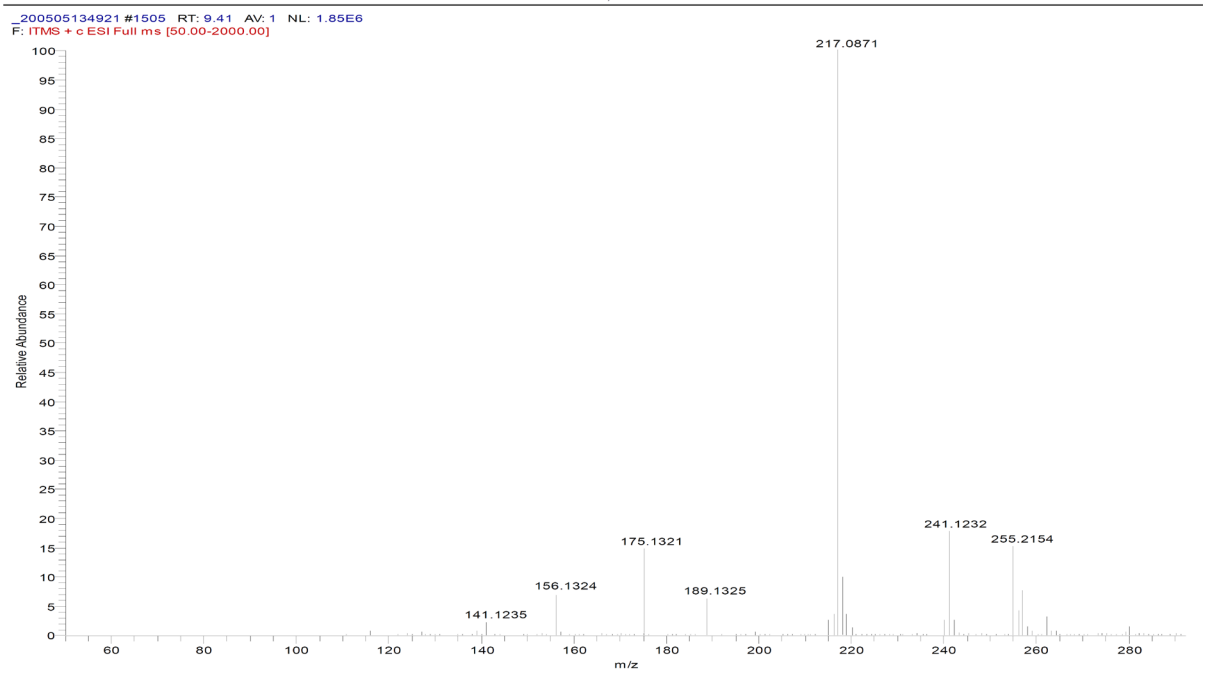
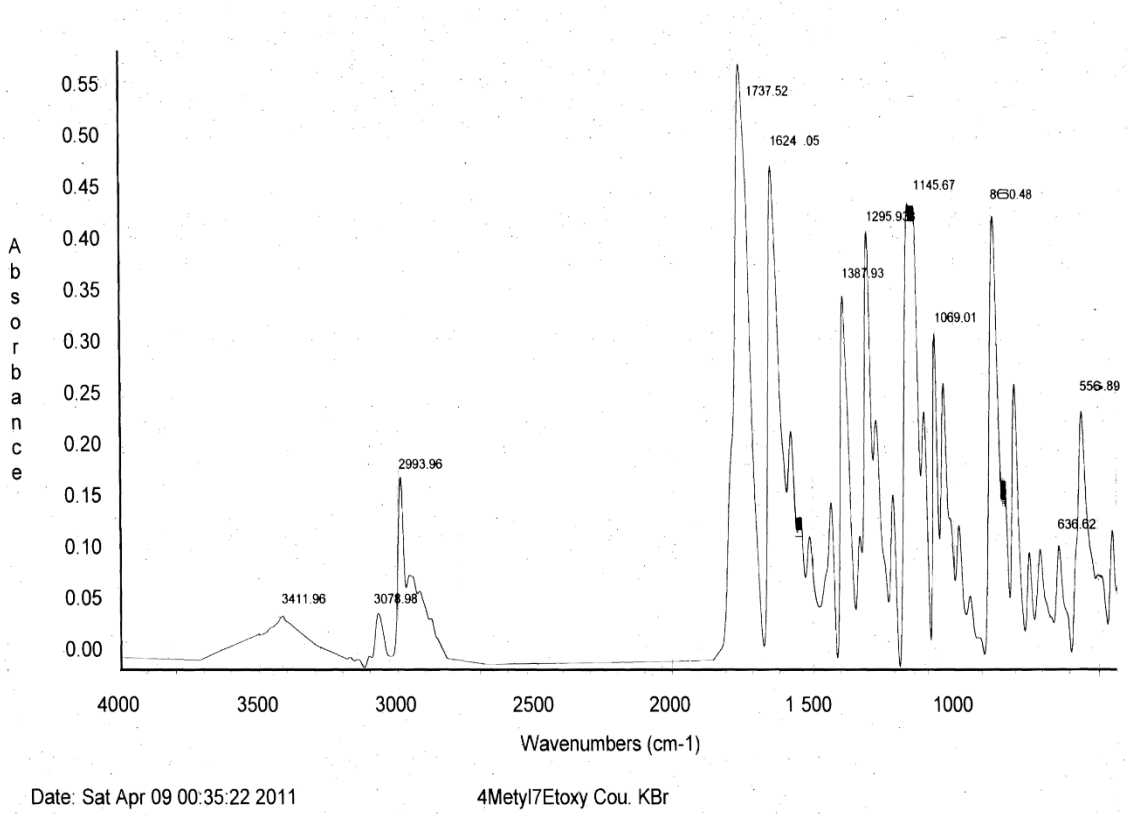
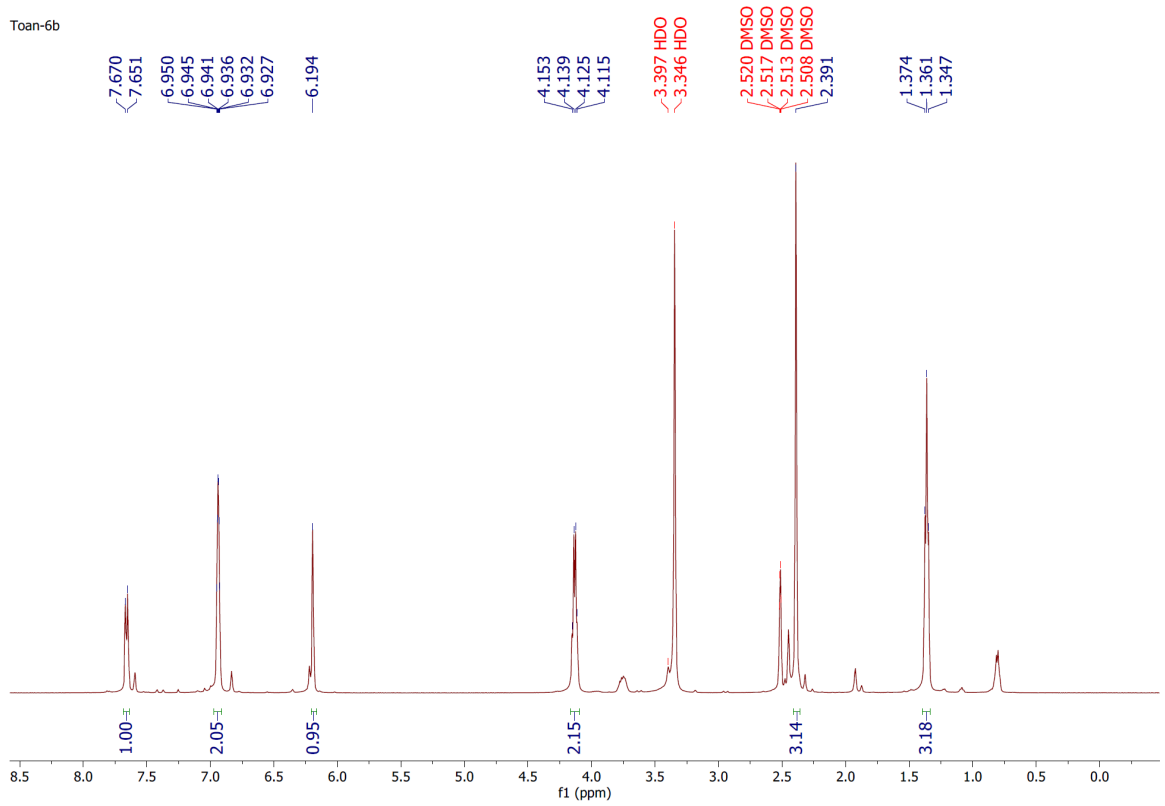
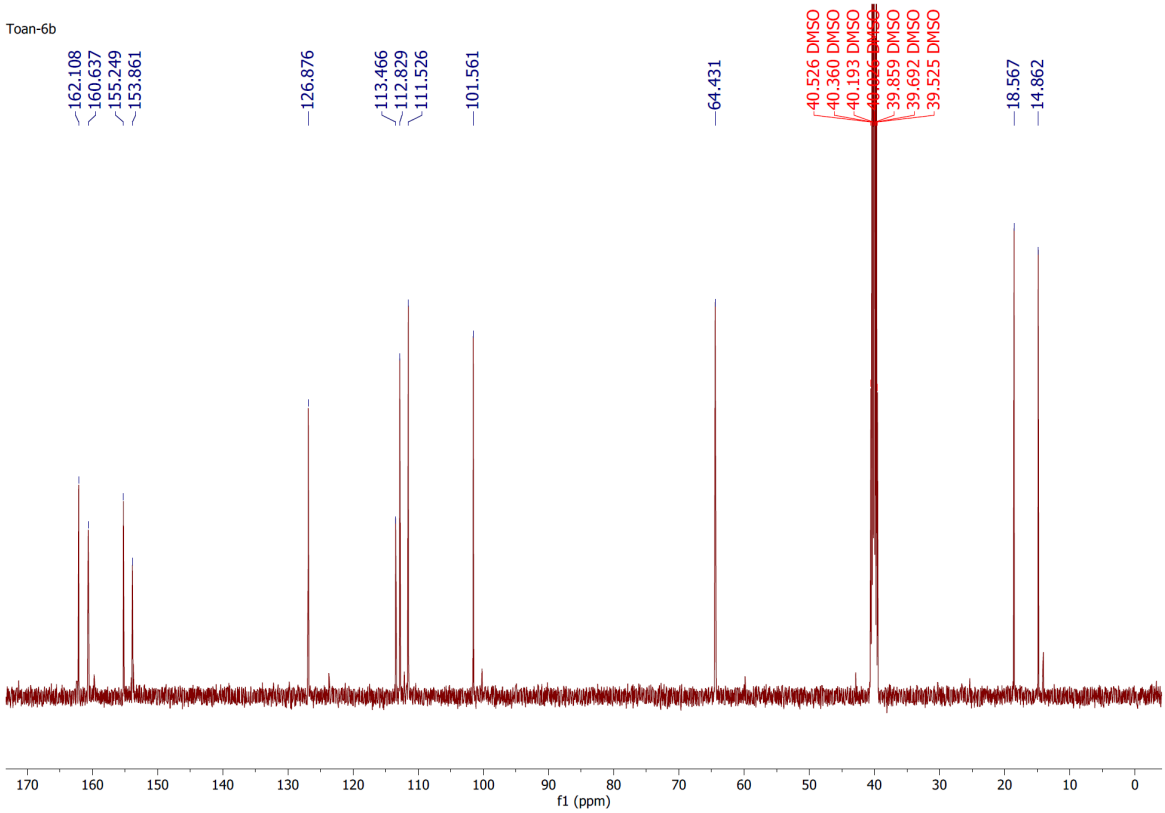




*4-Methyl-7-ethoxycoumarin (**4b**)*




Toan-6b
7.670
7.651
6.950
6.945
6.941
6.936
6.932
6.927
6.194
4.153
4.139
4.125
4.115
3.397 HDO
3.346 HDO
2.520 DMSO
2.517 DMSO
2.513 DMSO
2.508 DMSO
2.391
1.374
1.361
1.347
1.00
2.05
0.95
2.15
3.14
3.18
f1 (ppm)


Toan-6b
162.108
160.637
155.249
153.861
126.876
113.466
112.829
111.526
101.561
64.431
40.526 DMSO
40.360 DMSO
40.193 DMSO
39.859 DMSO
39.692 DMSO
39.525 DMSO
18.567
14.862
f1 (ppm)

Lab: Materials chemistry, Faculty of Chemistry, HUS-VNU
19 Le Thanh Tong, Hoan Kiem, Ha Noi

Tel: 844.38.253.053; **Fax**: 844.38.241.140 **Mail**: Chem.vnu@.edu.vn

Operator: Ms. Dao Thi Nhung
Mobile: 0948 119 043; Email: daothinhungtn@yahoo.com

Mass Spectrometter
LTQ Orbitrap XL™

Sample name : 5b-4MeCou
Mode: ESI, M+H

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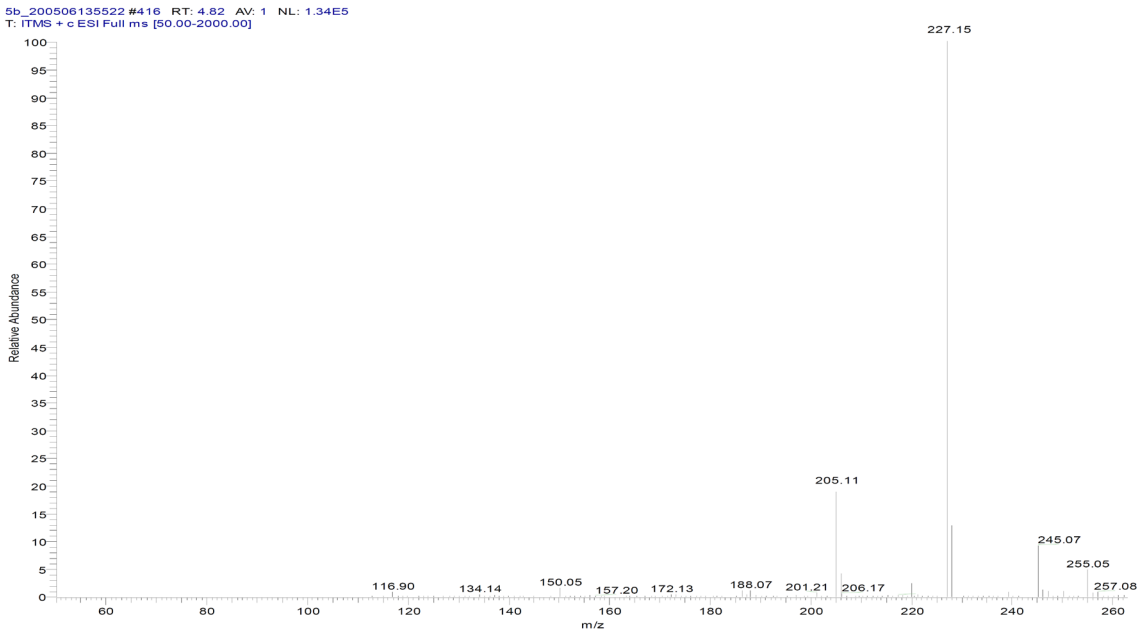
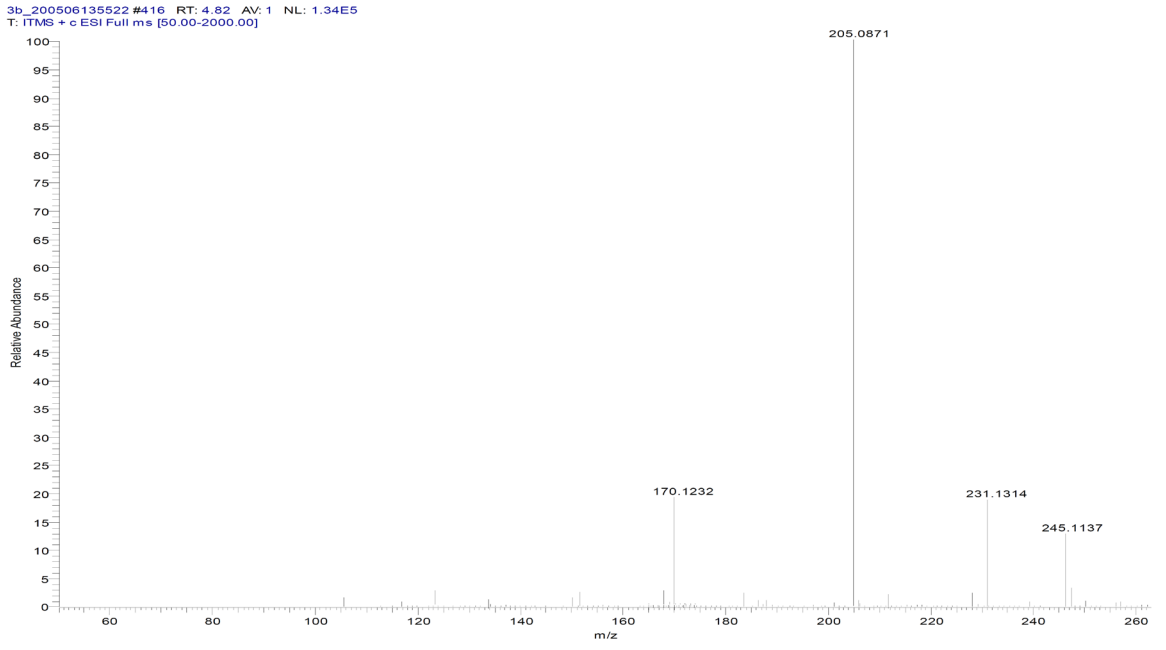
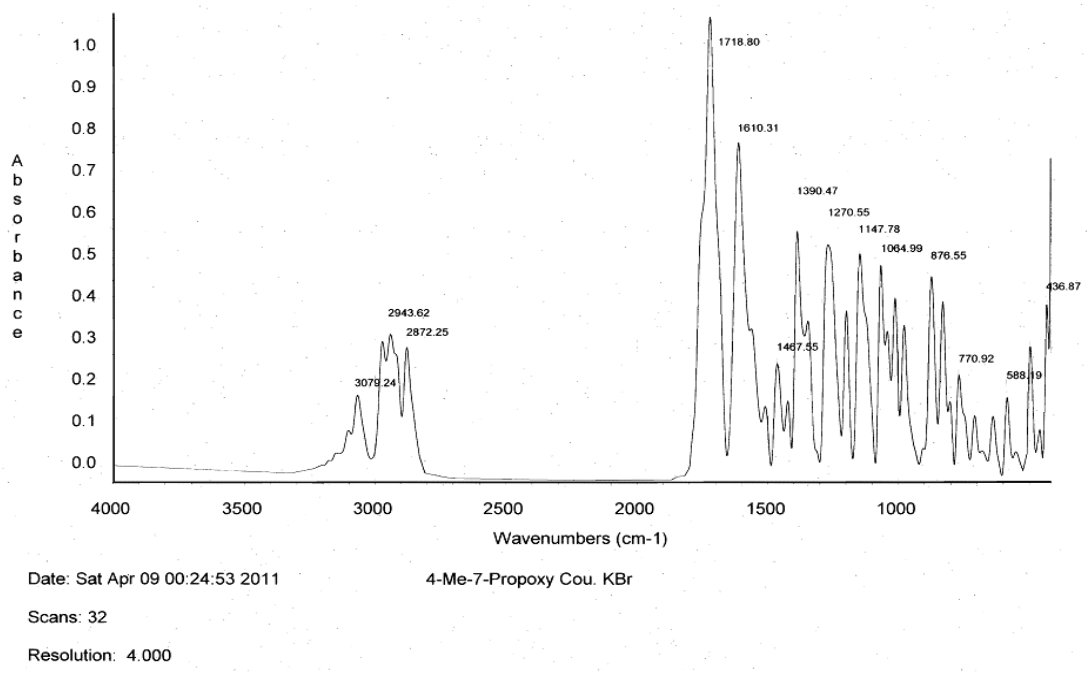
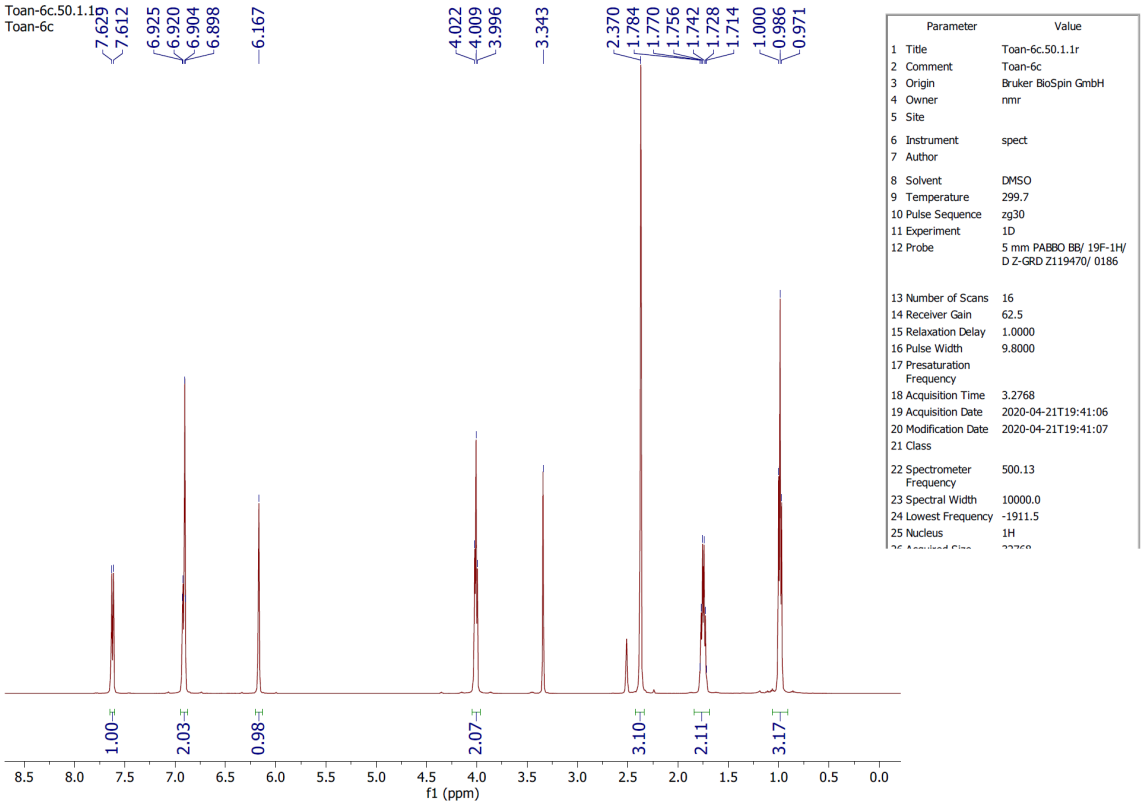
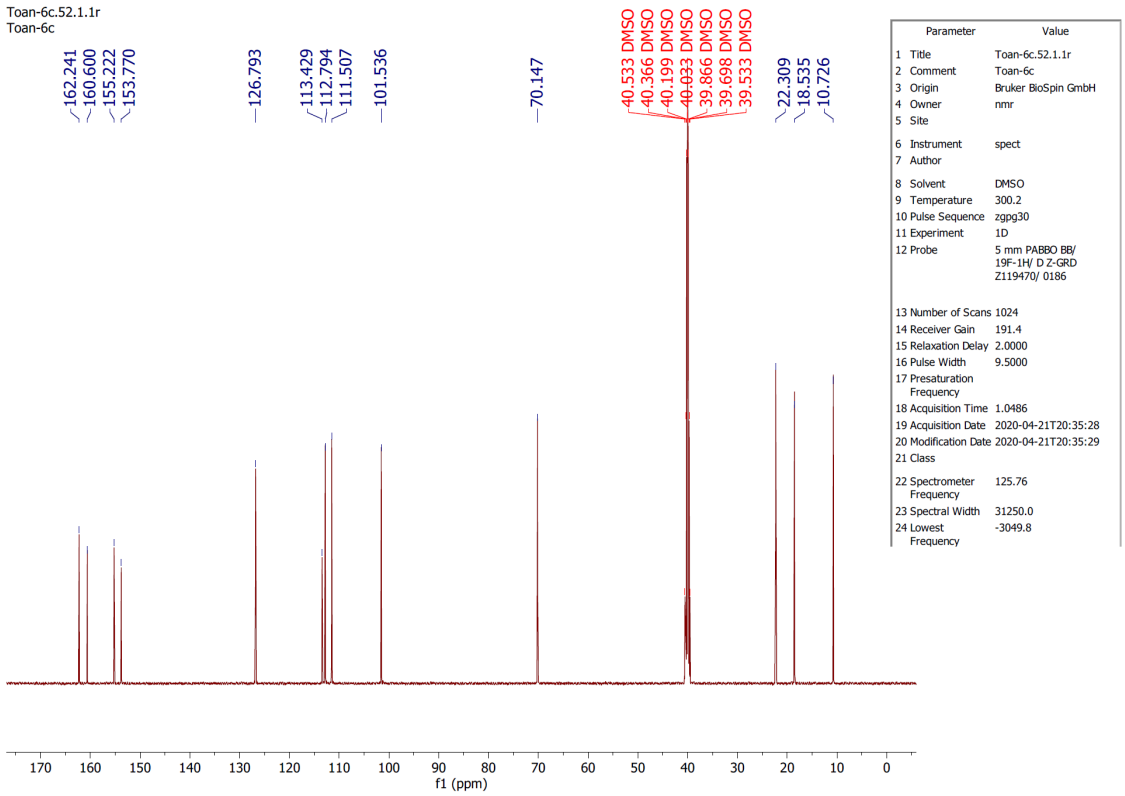




*4-Methyl-7-propoxycoumarin (**4c**)*







Parameter	Value
1 Title	Toan-6c.52.1.1r
2 Comment	Toan-6c
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Instrument	spect
7 Author	
8 Solvent	DMSO
9 Temperature	300.2
10 Pulse Sequence	zgpg30
11 Experiment	1D
12 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0186
13 Number of Scans	1024
14 Receiver Gain	191.4
15 Relaxation Delay	2.0000
16 Pulse Width	9.5000
17 Presaturation Frequency	
18 Acquisition Time	1.0486
19 Acquisition Date	2020-04-21T20:35:28
20 Modification Date	2020-04-21T20:35:29
21 Class	
22 Spectrometer Frequency	125.76
23 Spectral Width	31250.0
24 Lowest Frequency	-3049.8

Lab: Materials chemistry, Faculty of Chemistry, HUS-VNU
19 Le Thanh Tong, Hoan Kiem, Ha Noi

Tel: 844.38.253.053; **Fax**: 844.38.241.140 **Mail**: Chem.vnu@.edu.vn

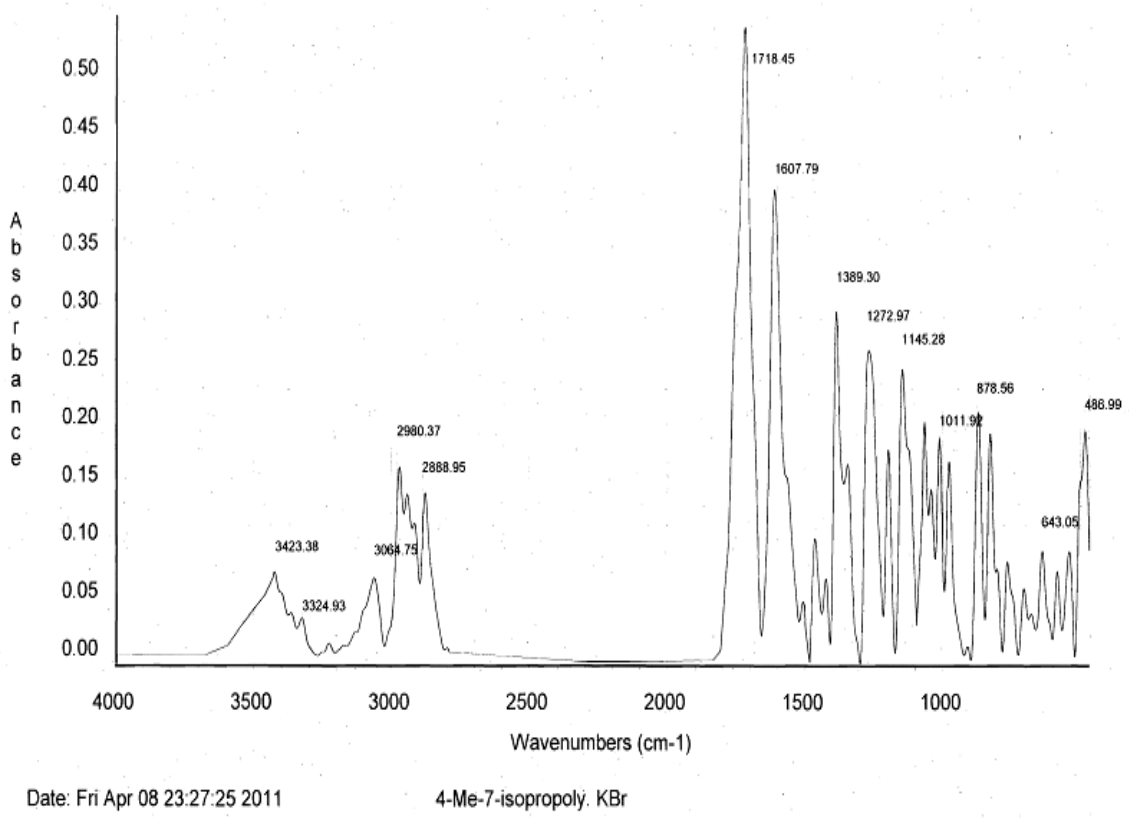
Operator: Ms. Dao Thi Nhung
Mobile: 0948 119 043; Email: daothinhungtn@yahoo.com

Sample name : 7OEt4MeCou
Mode: ESI, M+H

Mass Spectrometer
LTQ Orbitrap XL™

C:\LTQ Orbitrap\...\5b_200506135522 5/7/2020 4:10:35 PM

*4-Methyl-7-isopropoxycoumarin (**4d**)*



Lab: Materials chemistry, Faculty of Chemistry, HUS-VNU
19 Le Thanh Tong, Hoan Kiem, Ha Noi

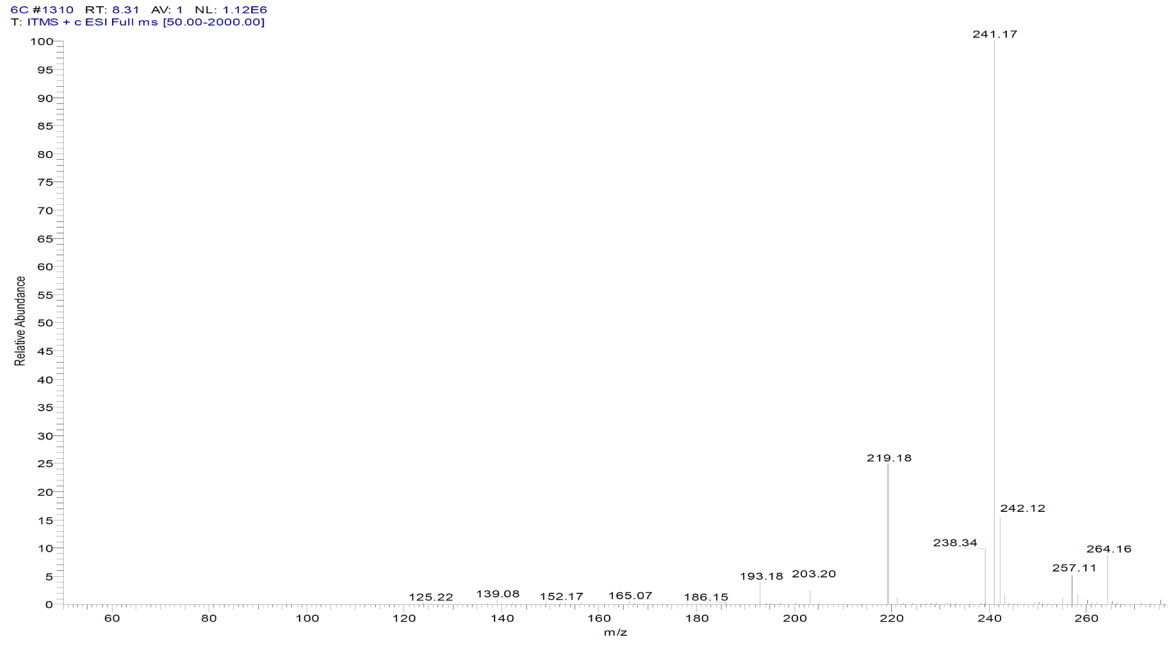
Tel: 844.38.253.053; **Fax**: 844.38.241.140 **Mail**: Chem.vnu@.edu.vn

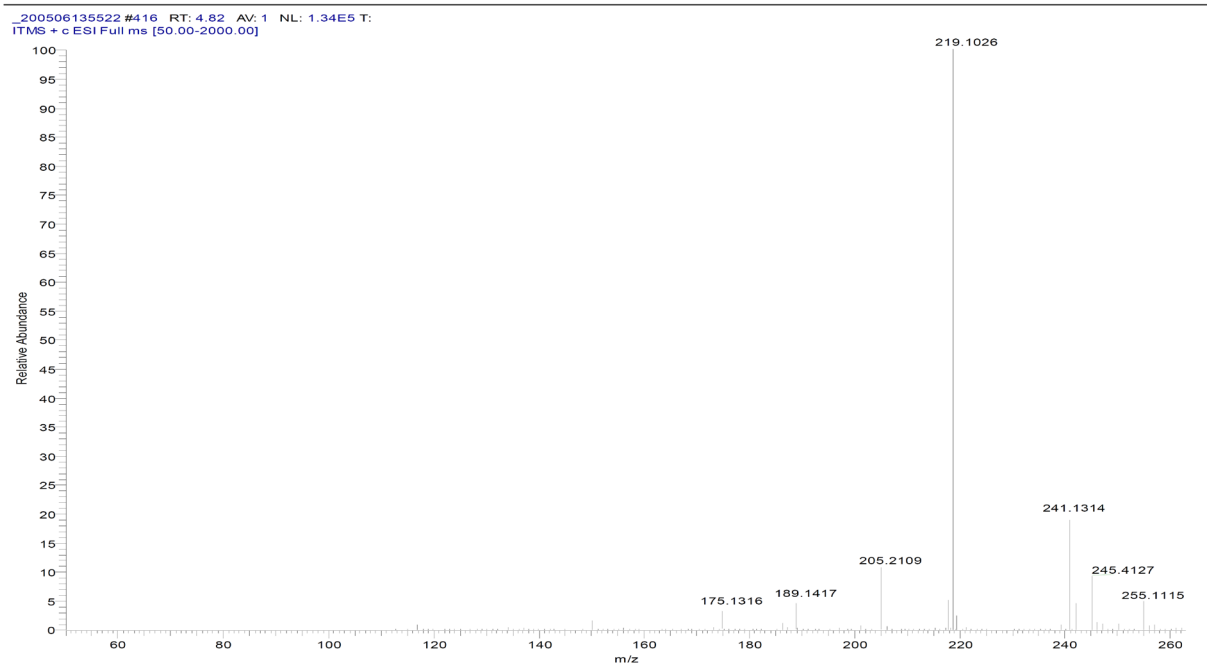
Operator: Ms. Dao Thi Nhung
Mobile: 0948 119 043; Email: daothinhungtn@yahoo.com

Sample name: 6c-7OEt4MeCou
Mode: ESI, M+H

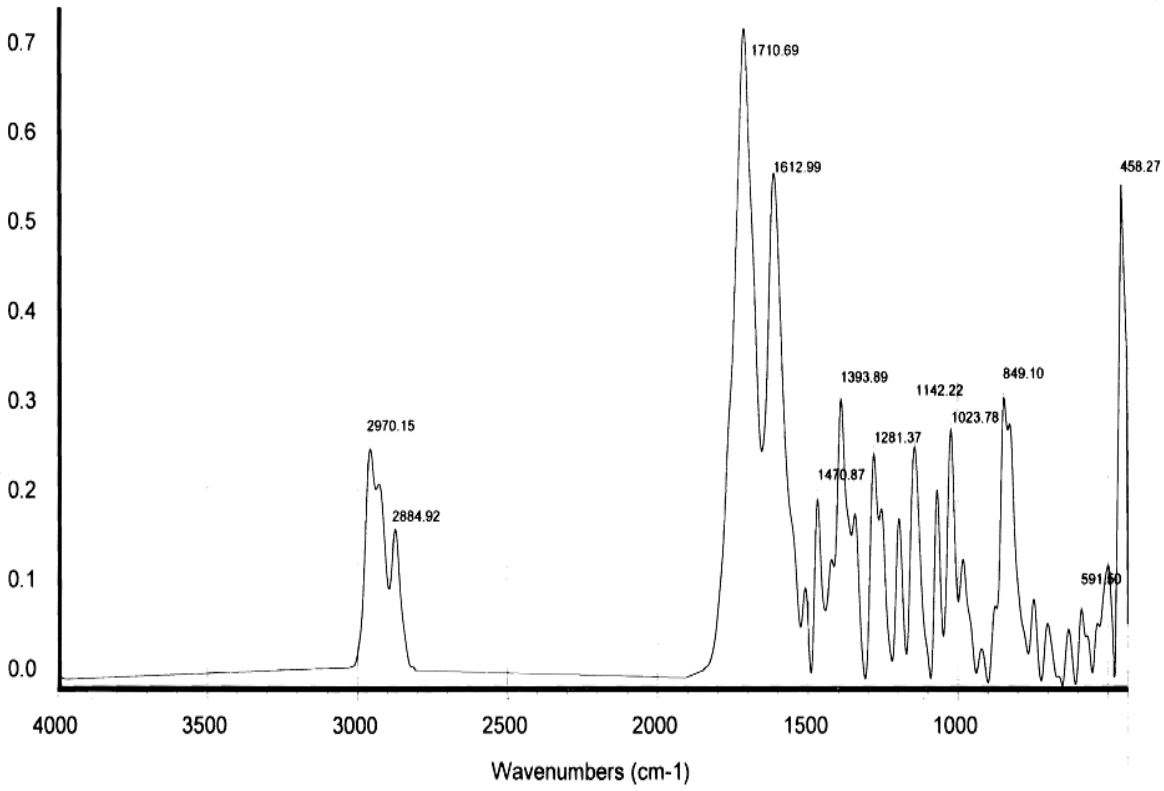
Mass Spectrometter
LTQ Orbitrap XL™
Solvent: MeOH/DCM

C:\LTQ Orbitrap\Nhung\1Nam 2020\6C 5/5/2020 1:10:06 PM

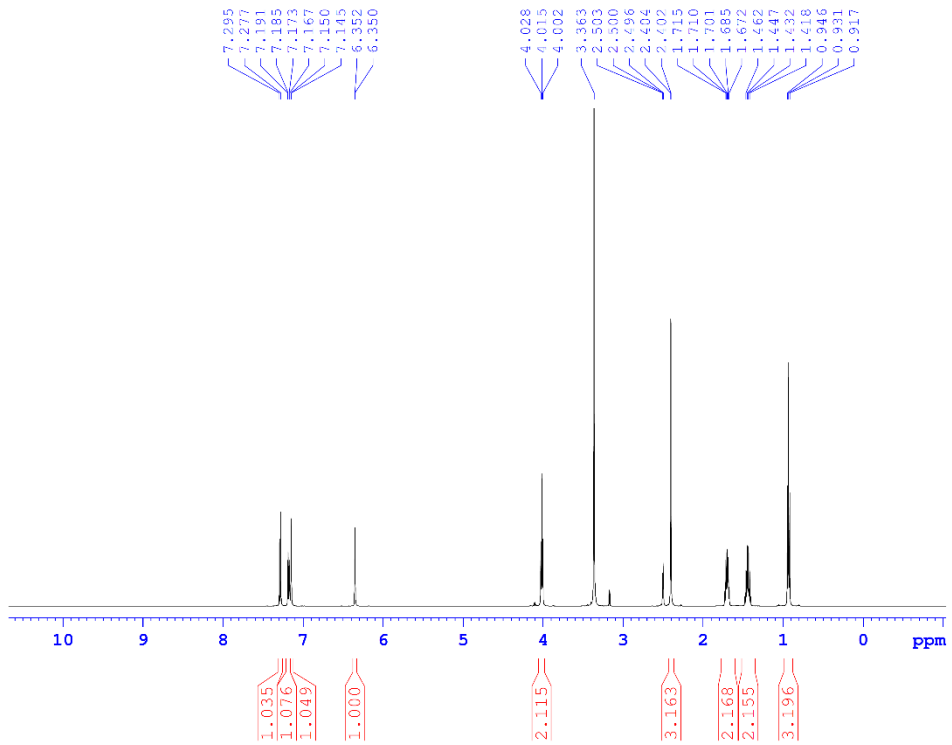




*4-Methyl-7-butoxycoumarin (**4e**)*



4Me7BuCou-DMSO-1H

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NAME       TOAN.4Me6BuCou
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameter
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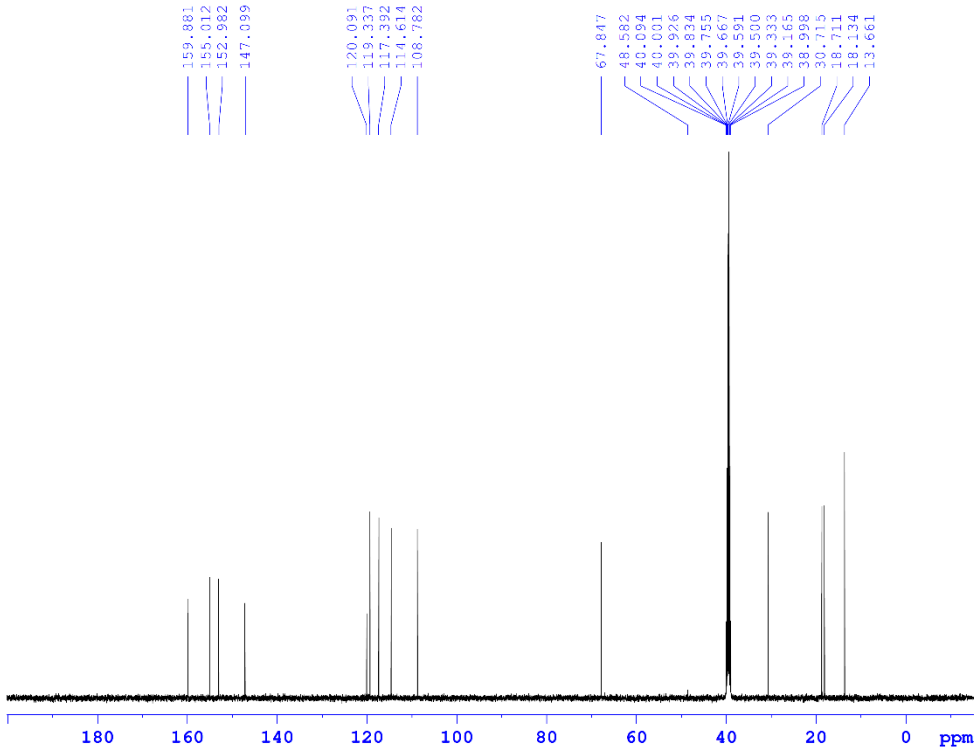
Time                11.15
INSTRUM             spect
PROBHD   5 mm Multinucl
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     0
SWH           10000.000 Hz
FIDRES        0.152588 Hz
AQ            3.2769001 se
RG                  71.8
DW                50.000 us
DE                 6.00 us
TE                300.0 K
D1            1.00000000 se
MCREST        0.00000000 se
MCWRK         0.01500000 se

======== CHANNEL f1 ======
NUC1                   1H
P1                  10.30 us
PL1                 1.00 dB
SFO1         500.1335009 MH

F2 - Processing parameters
SI                  32768
SF          500.1300066 MH
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                   1.00
```

4Me7BuCou-DMSO-C13CPD

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Current Data Parameters
NAME       TOAN.4Me6BuCou
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parame
Date_           20131030
Time                10.20
INSTRUM             spect
PROBHD   5 mm Multinucl
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   128
DS                     2
SWH           31446.541
FIDRES        0.479836
AQ            1.0420883
RG                  32768
DW                15.900
DE                 6.00
TE                303.0
D1            2.00000000
d11           0.03000000
DELTA         1.89999998
MCREST        0.00000000
MCWRK         0.01500000

======== CHANNEL f1 ======
NUC1                  13C
P1                   5.20
PL1                  0.00
SFO1         125.7716224

======== CHANNEL f2 ======
CPDPRG2          waltz16
NUC2                   1H
PCPD2               80.00
PL2                 -1.00
PL12                16.81
PL13                22.00
SFO2         500.1320005

F2 - Processing parameto
SI                  32768
SF          125.7578490
WDW                    EM
SSB                     0
LB                  1.00
GB                      0
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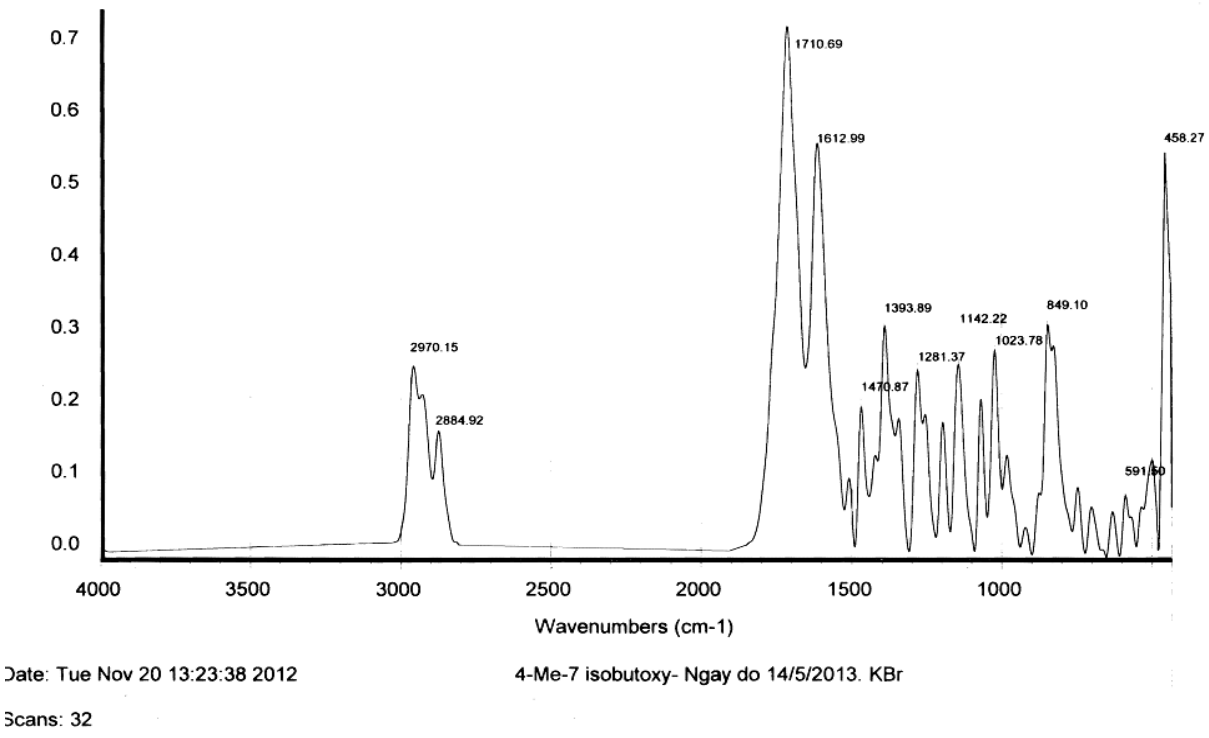
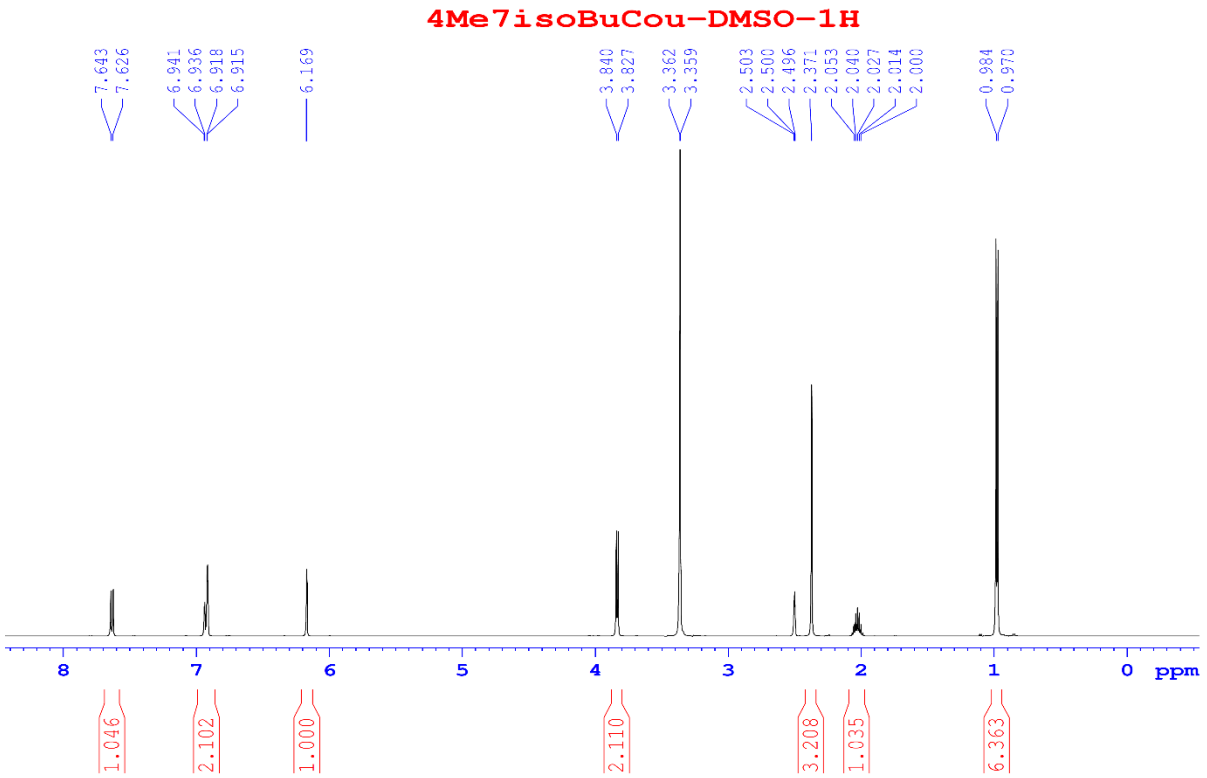
*4-Methyl-7-isobutoxycoumarin (**4f**)*




4Me7isoBuCou-DMSO-1H
7.643
7.626
6.941
6.936
6.918
6.915
6.169
3.840
3.827
3.362
3.359
2.503
2.500
2.496
2.371
2.053
2.040
2.027
2.014
2.000
0.984
0.970
8
7
6
5
4
3
2
1
0
ppm
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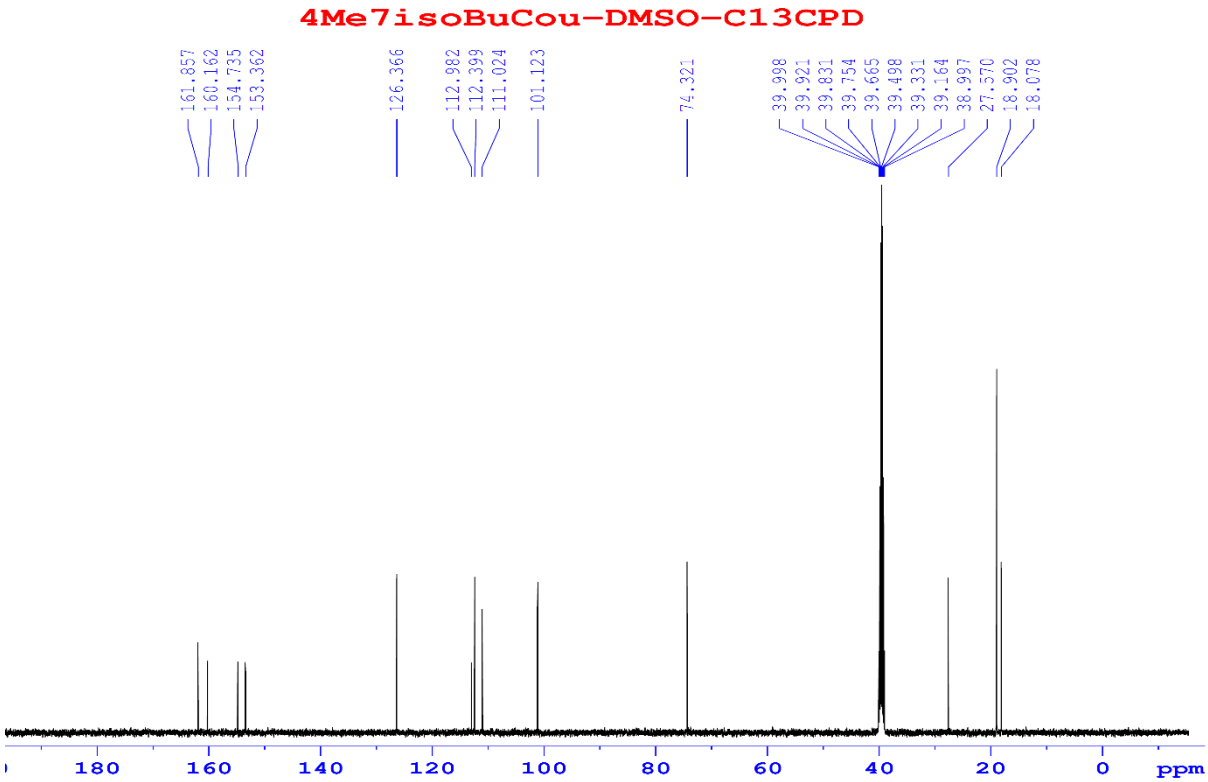
2.102
1.000
2.110
3.208
1.035
6.363


4Me7isoBuCou-DMSO-C13CPD
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154.735
153.362
126.366
112.982
112.399
111.024
101.123
74.321
39.998
39.921
39.831
39.754
39.665
39.498
39.331
39.164
38.997
27.570
18.902
18.078
180
160
140
120
100
80
60
40
20
0
ppm

Display Report - Selected Window Selected Analysis

Analysis Name: 14011621.d
Method: DO MS.m
Sample Name: 4-Me-7 iso butoxy cou 1H
Analysis Info:

Instrument: Agilent 6310 Ion Trap
Operator: Phong PTHC, Vien Hoa HCTN

Print Date: 1/16/2014 3:54:39 PM
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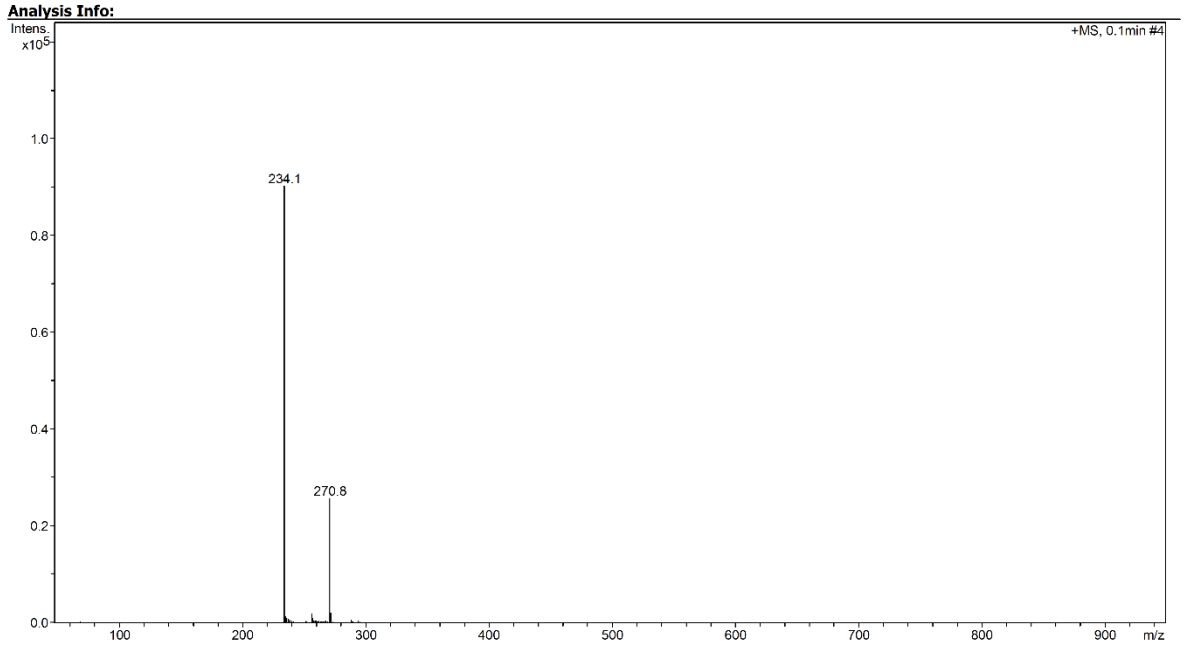
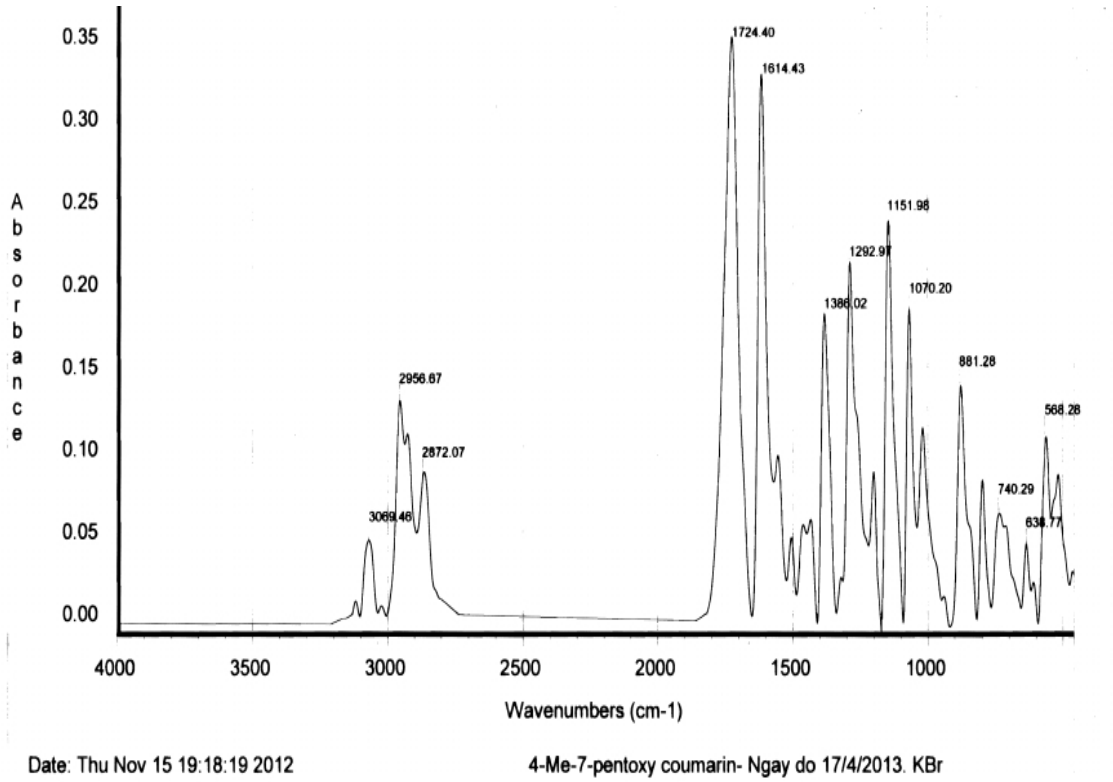
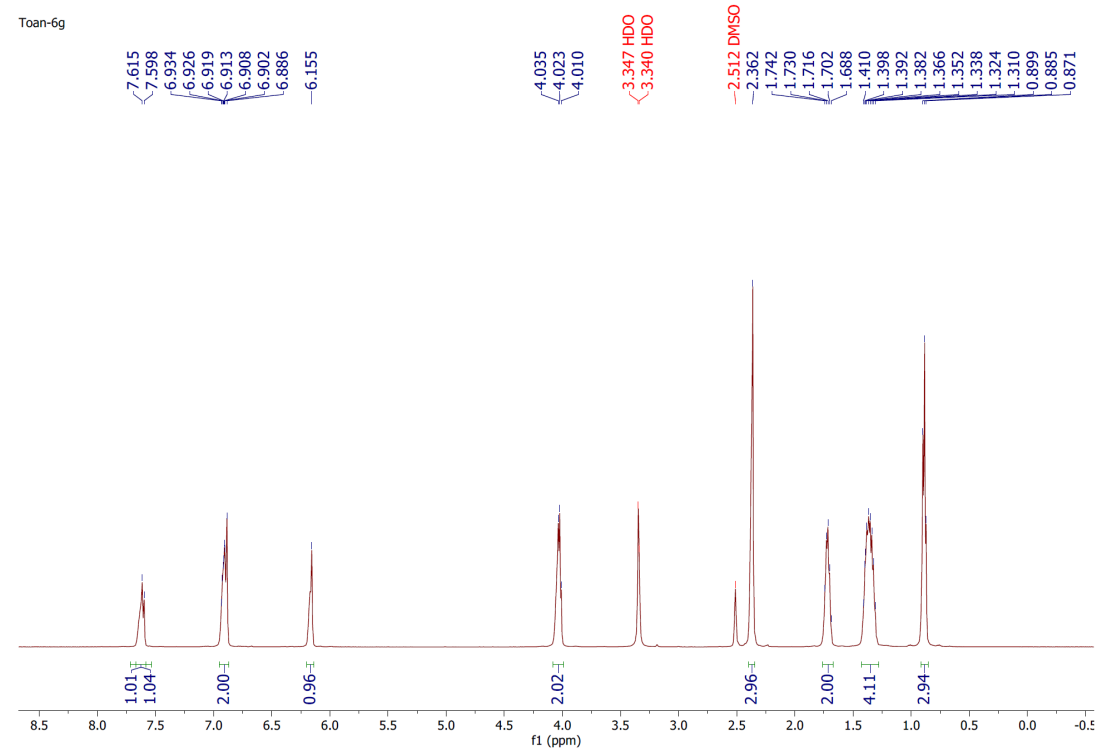


MSD Trap Report v 4 (A4-Opt2) Page 1 of 1 Agilent Technologies

*4-Methyl-7-pentoxycoumarin (**4g**)*

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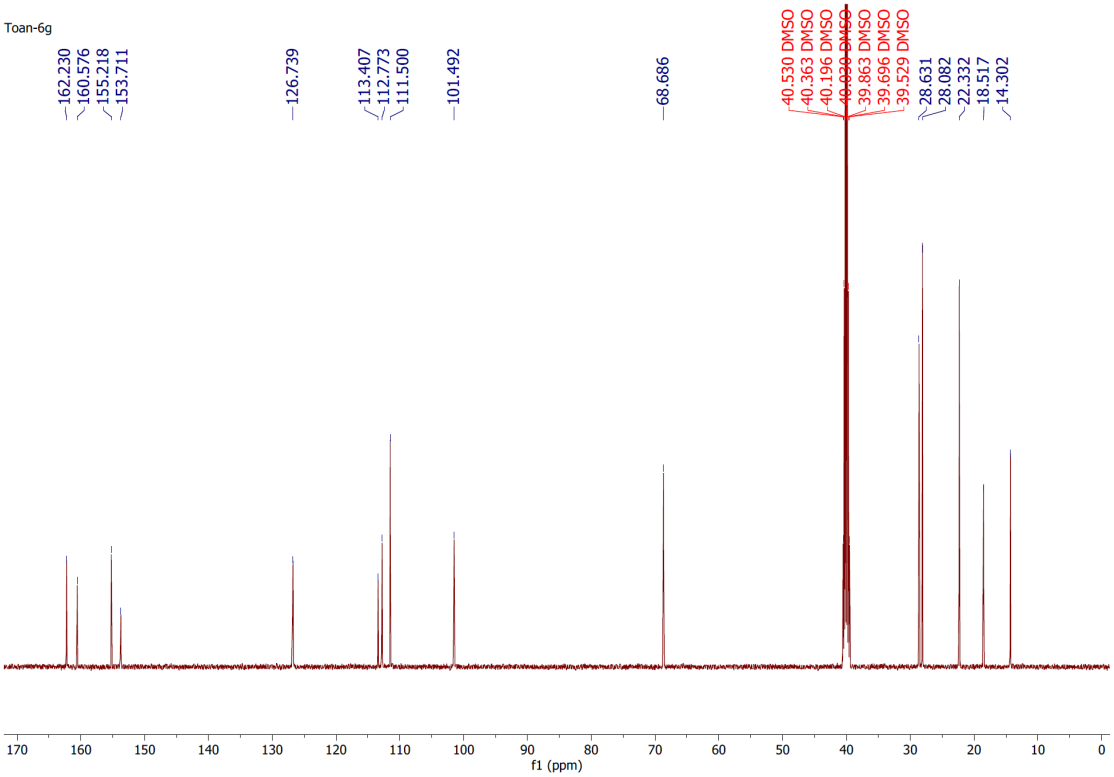
7.615
7.598
6.934
6.926
6.919
6.913
6.908
6.902
6.886
6.155
4.035
4.023
4.010
3.347 HDO
3.340 HDO
2.512 DMSO
2.362
1.742
1.730
1.716
1.702
1.688
1.410
1.398
1.392
1.382
1.366
1.352
1.338
1.324
1.310
0.899
0.885
0.871
1.01
1.04
2.00
0.96
2.02
2.96
2.00
4.11
2.94
f1 (ppm)


Toan-6g
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160.576
155.218
153.711
126.739
113.407
112.773
111.500
101.492
68.686
40.530 DMSO
40.363 DMSO
40.196 DMSO
40.030 DMSO
39.863 DMSO
39.696 DMSO
39.529 DMSO
28.631
28.082
22.332
18.517
14.302
f1 (ppm)

Lab: Materials chemistry, Faculty of Chemistry, HUS-VNU
19 Le Thanh Tong, Hoan Kiem, Ha Noi

Tel: 844.38.253.053; **Fax**: 844.38.241.140 **Mail**: Chem.vnu@.edu.vn

Operator: Ms. Dao Thi Nhung
Mobile: 0948 119 043; Email: daothinhungtn@yahoo.com

Sample name :6g-7OPn4MeCou
Mode: ESI, M+H

Mass Spectrometter
LTQ Orbitrap XL™

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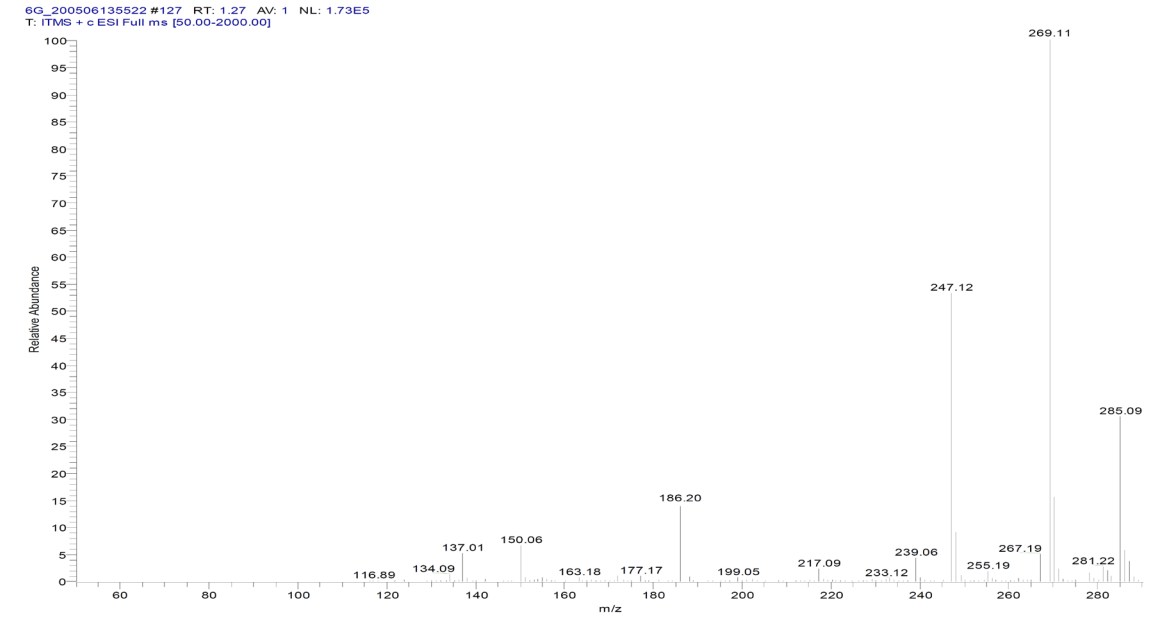
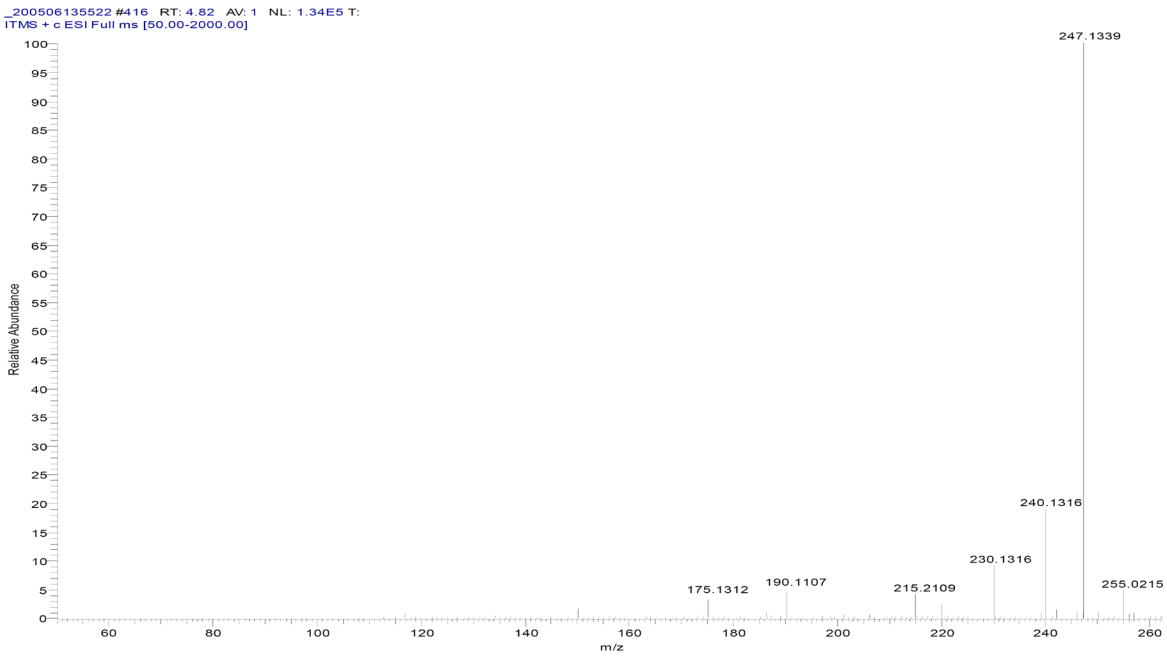
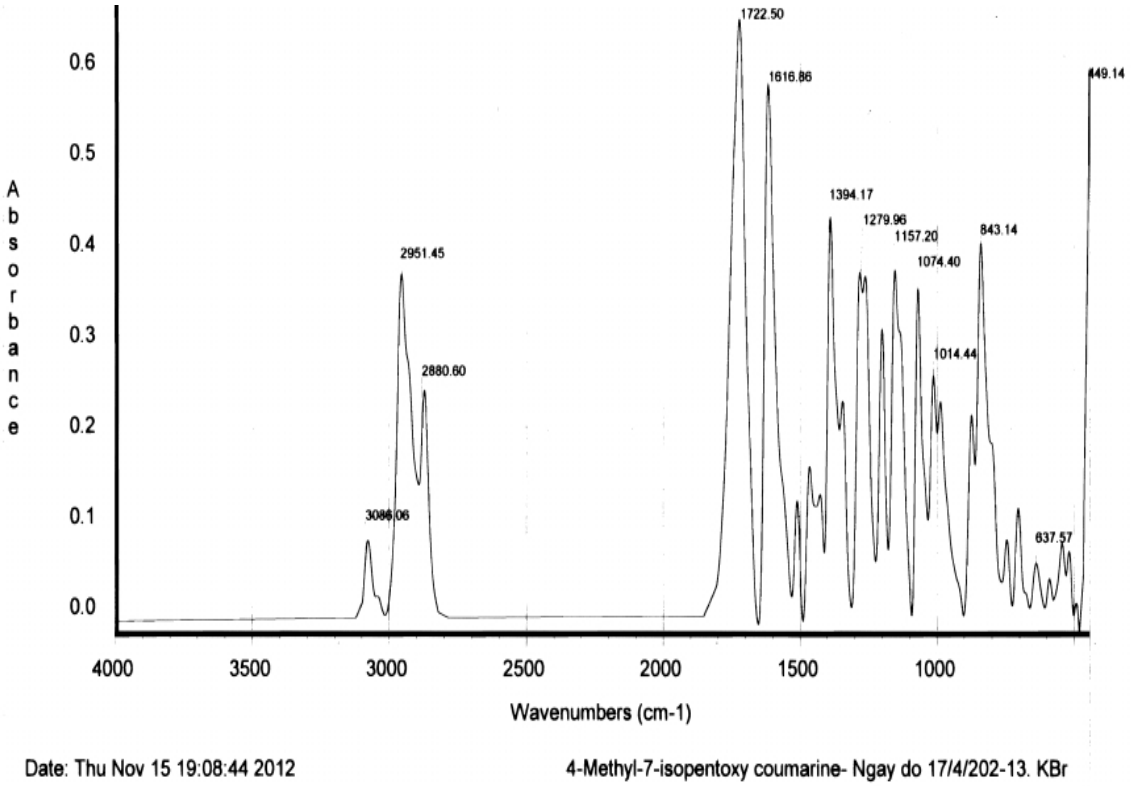
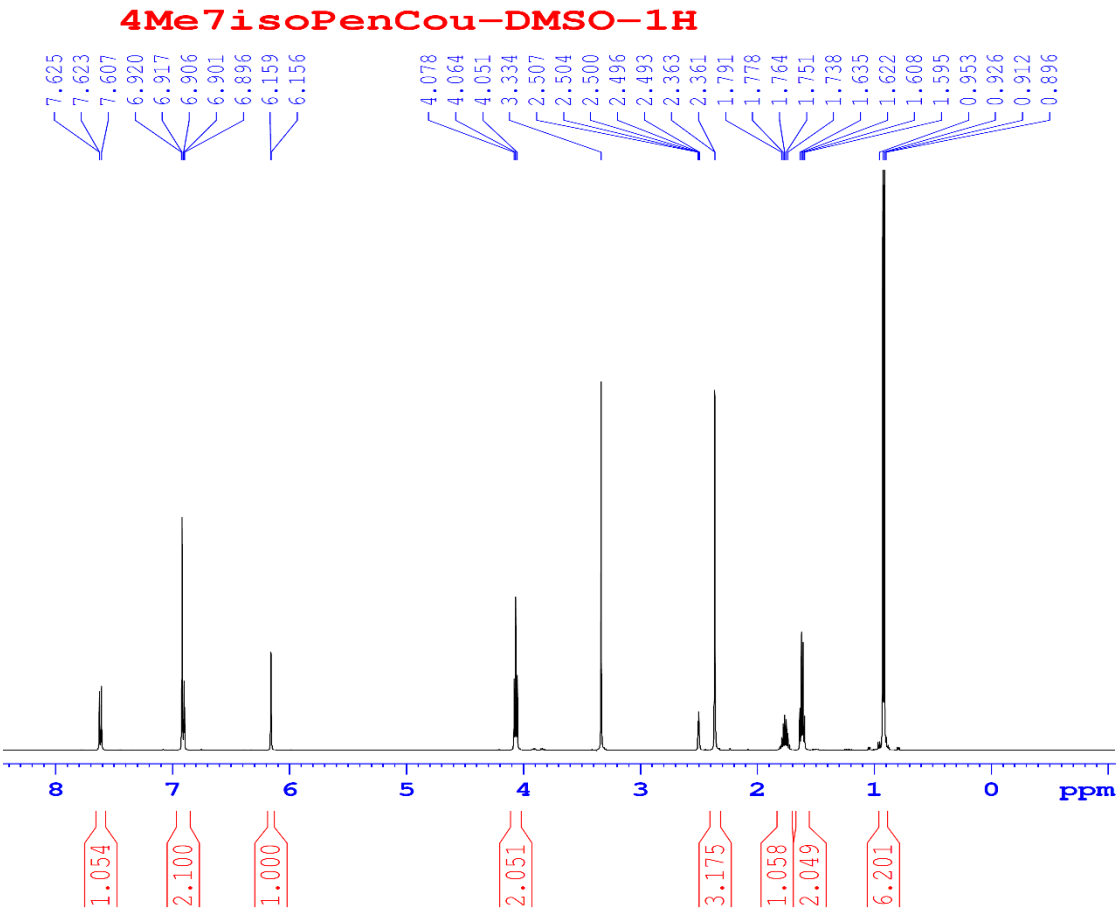
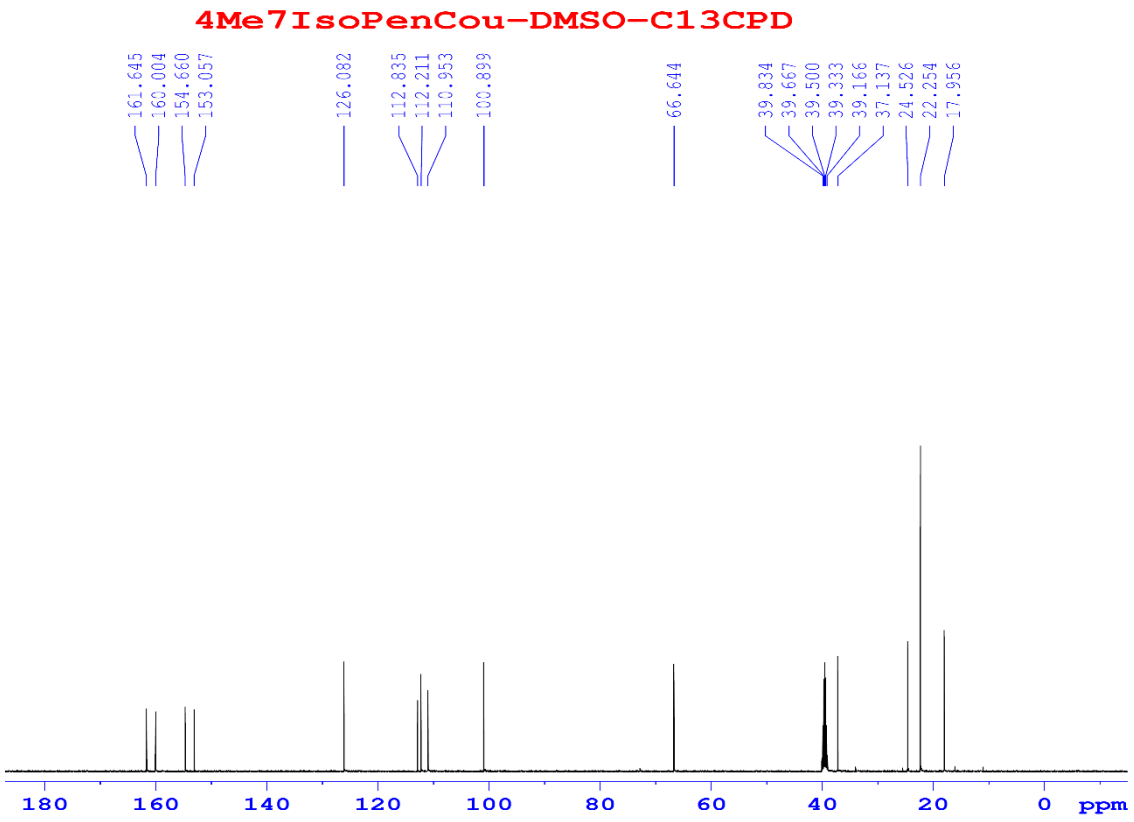




*4-Methyl-7-isopentoxycoumarin (**4h**)*







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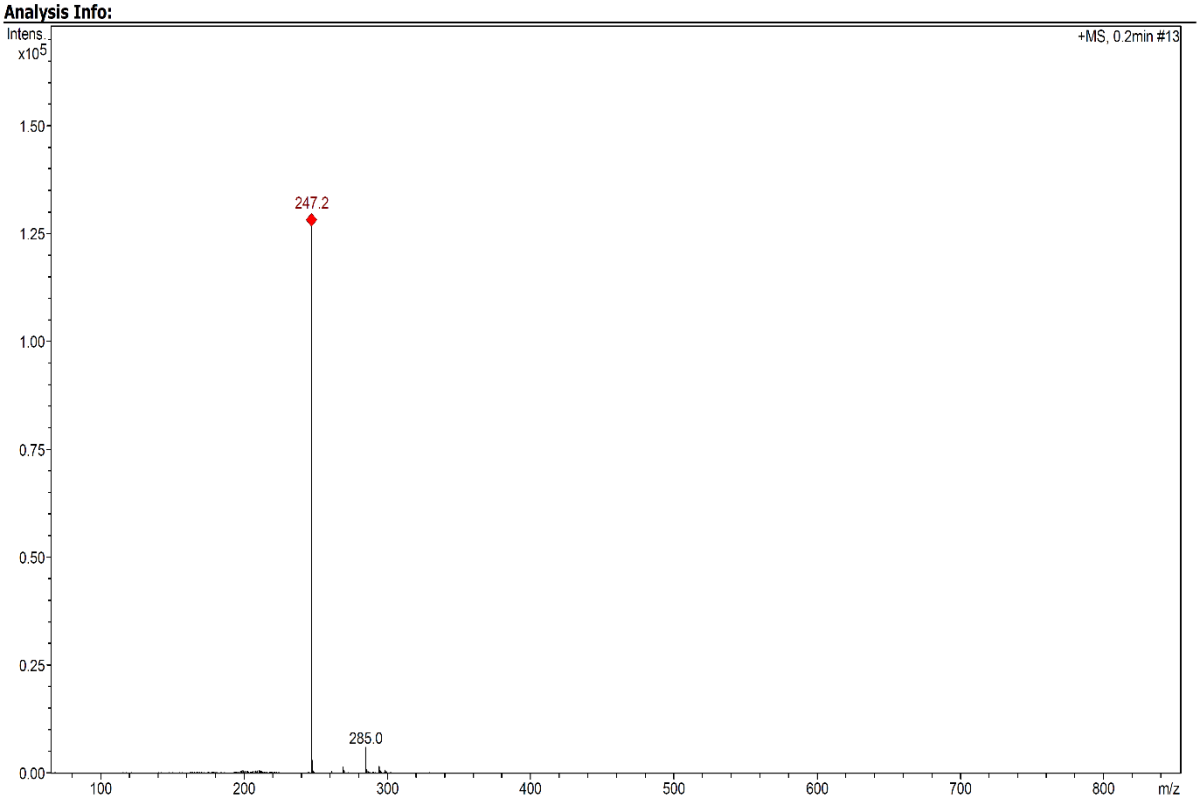
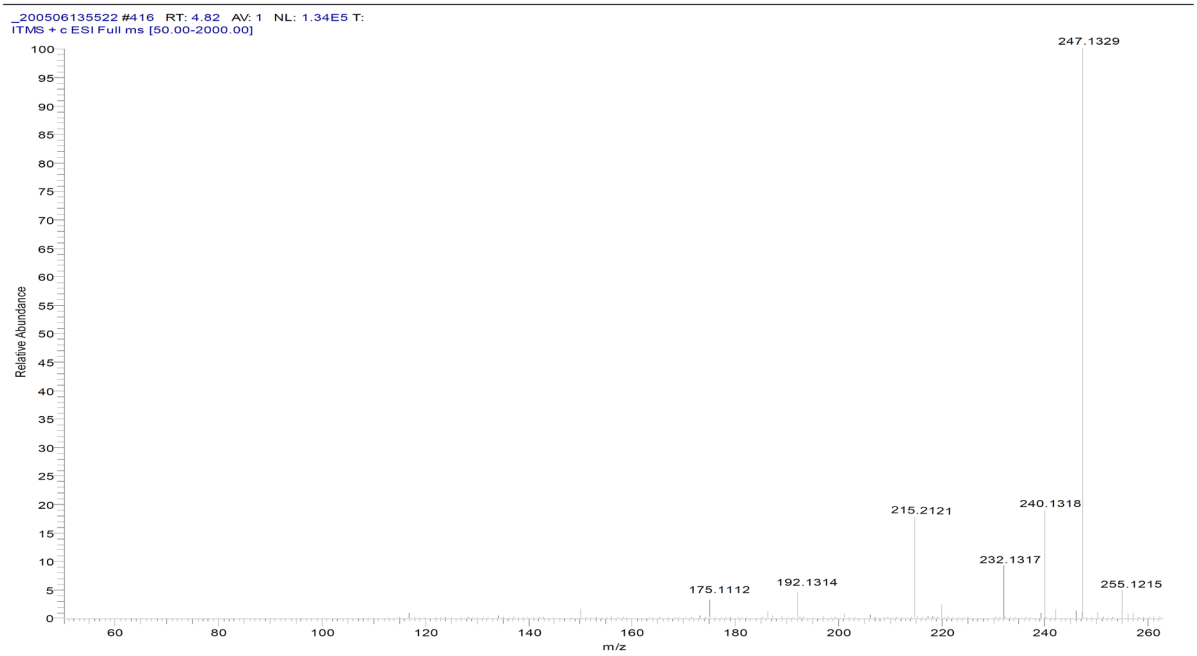
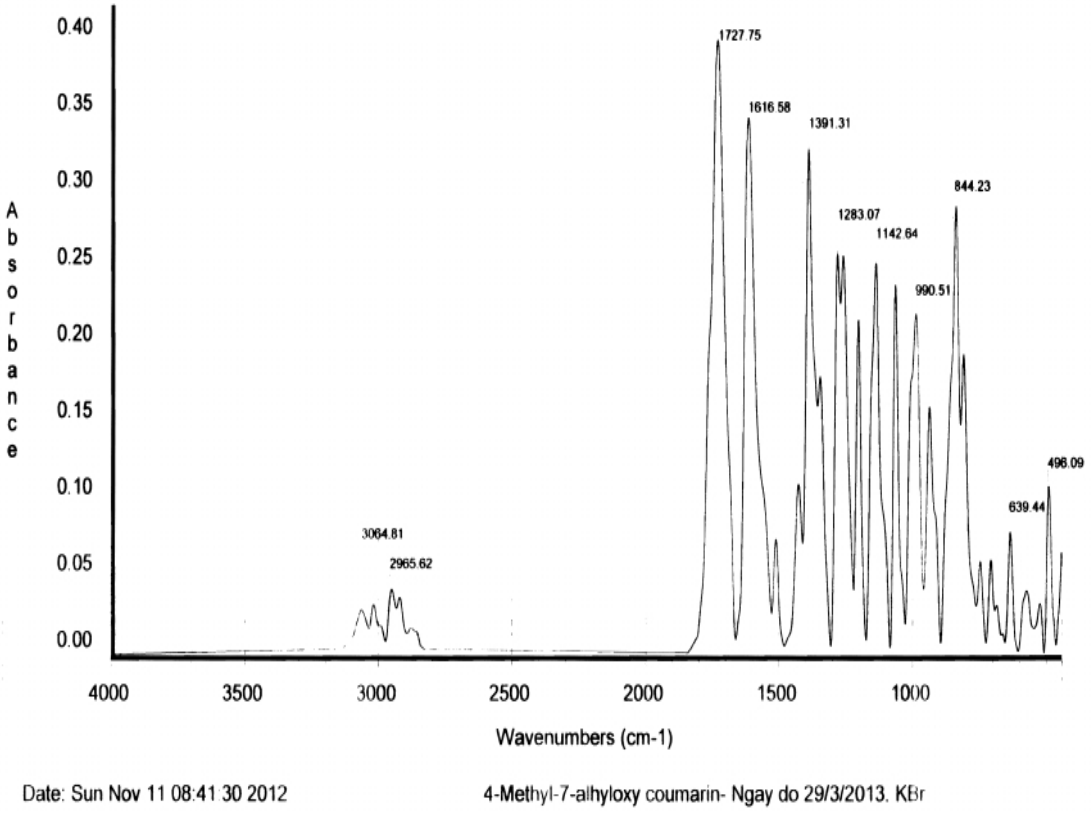
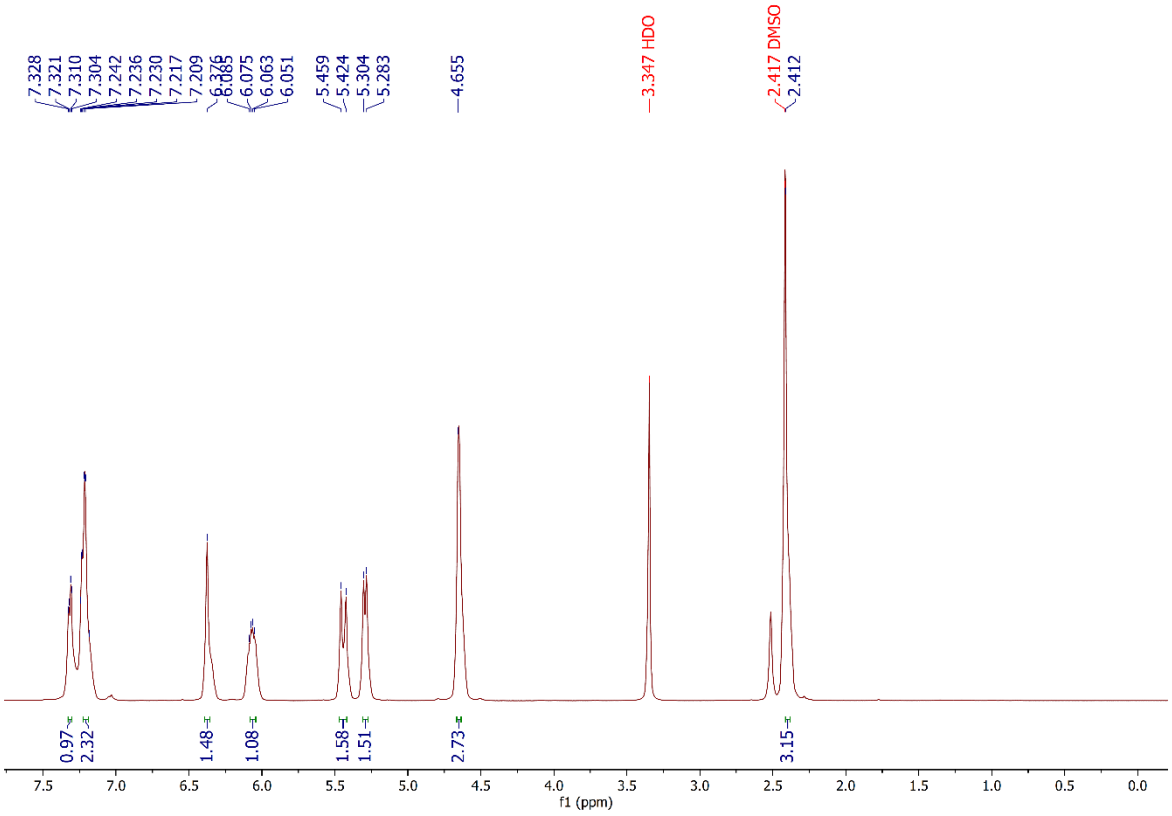




*4-Methyl-7-allyloxycoumarin (**4i**)*

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7.321
7.310
7.304
7.242
7.236
7.230
7.217
7.209
6.085
6.075
6.063
6.051
5.459
5.424
5.304
5.283
4.655
3.347 HDO
2.417 DMSO
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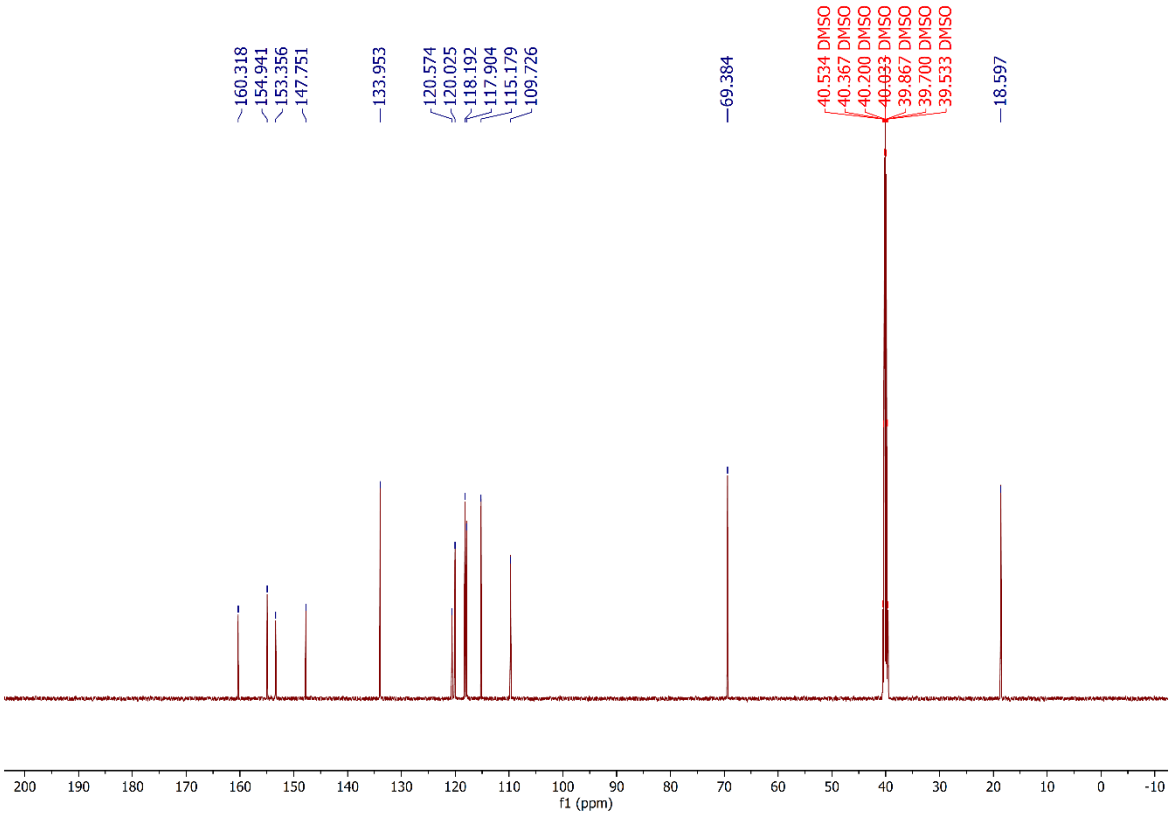
0.97
2.32
1.48
1.08
1.58
1.51
2.73
3.15
f1 (ppm)


160.318
154.941
153.356
147.751
133.953
120.574
120.025
118.192
117.904
115.179
109.726
69.384
40.534 DMSO
40.367 DMSO
40.200 DMSO
40.033 DMSO
39.867 DMSO
39.700 DMSO
39.533 DMSO
18.597
f1 (ppm)

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Operator: Ms. Dao Thi Nhung
Mobile: 0948 119 043; Email:
daothinhungtn@yahoo.com

Mass Spectrometter
LTQ Orbitrap XL™
Solvent: MeOH/DCM

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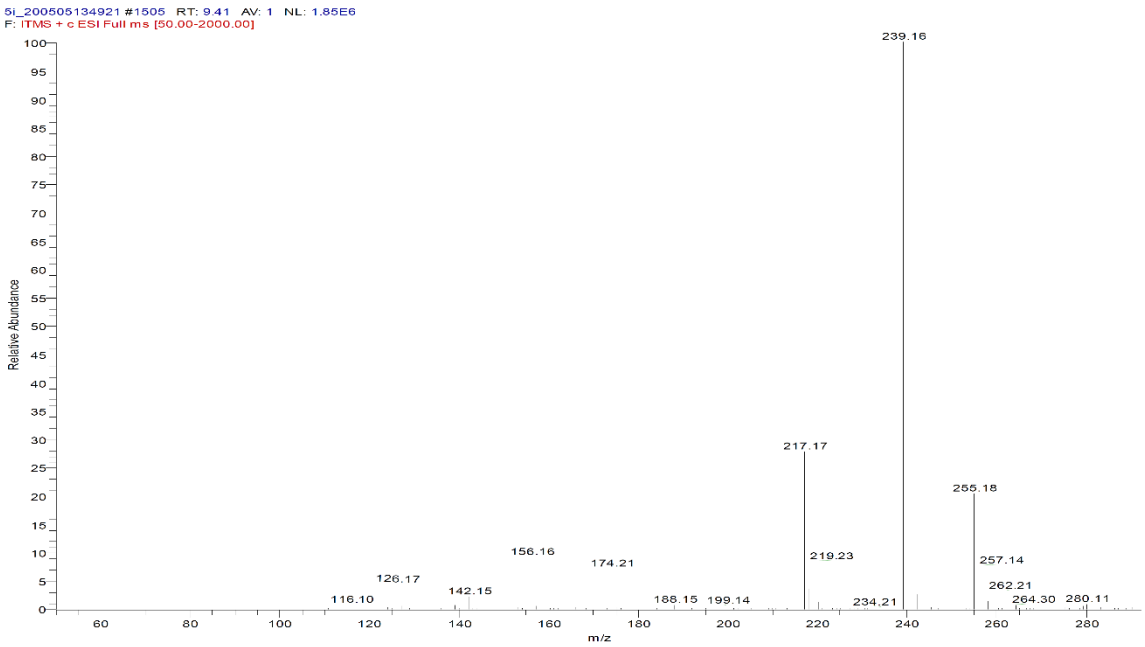
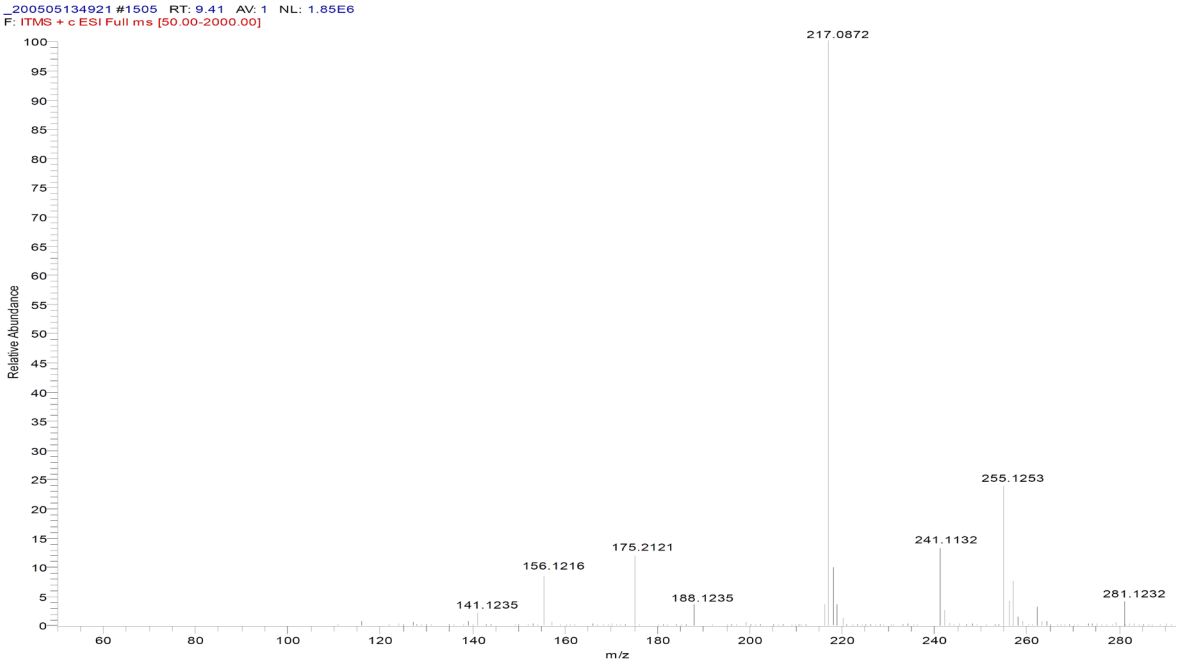
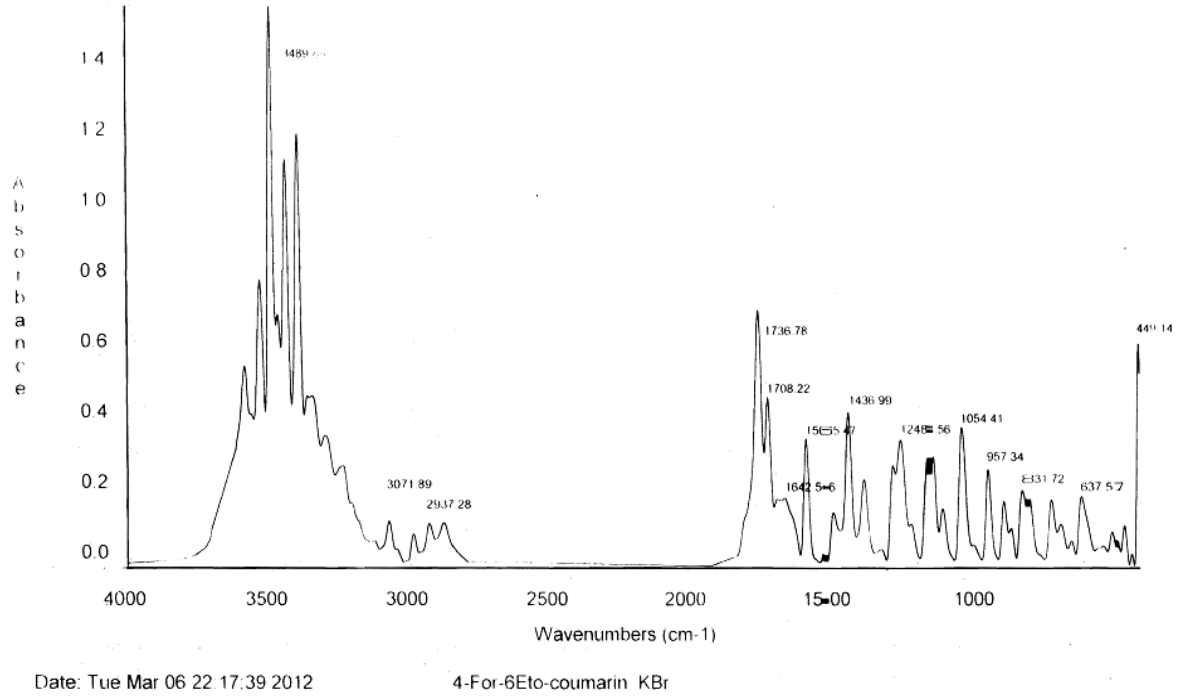
SAMPLE:7OAllyl4MeCou
Mode: ESI, M+H

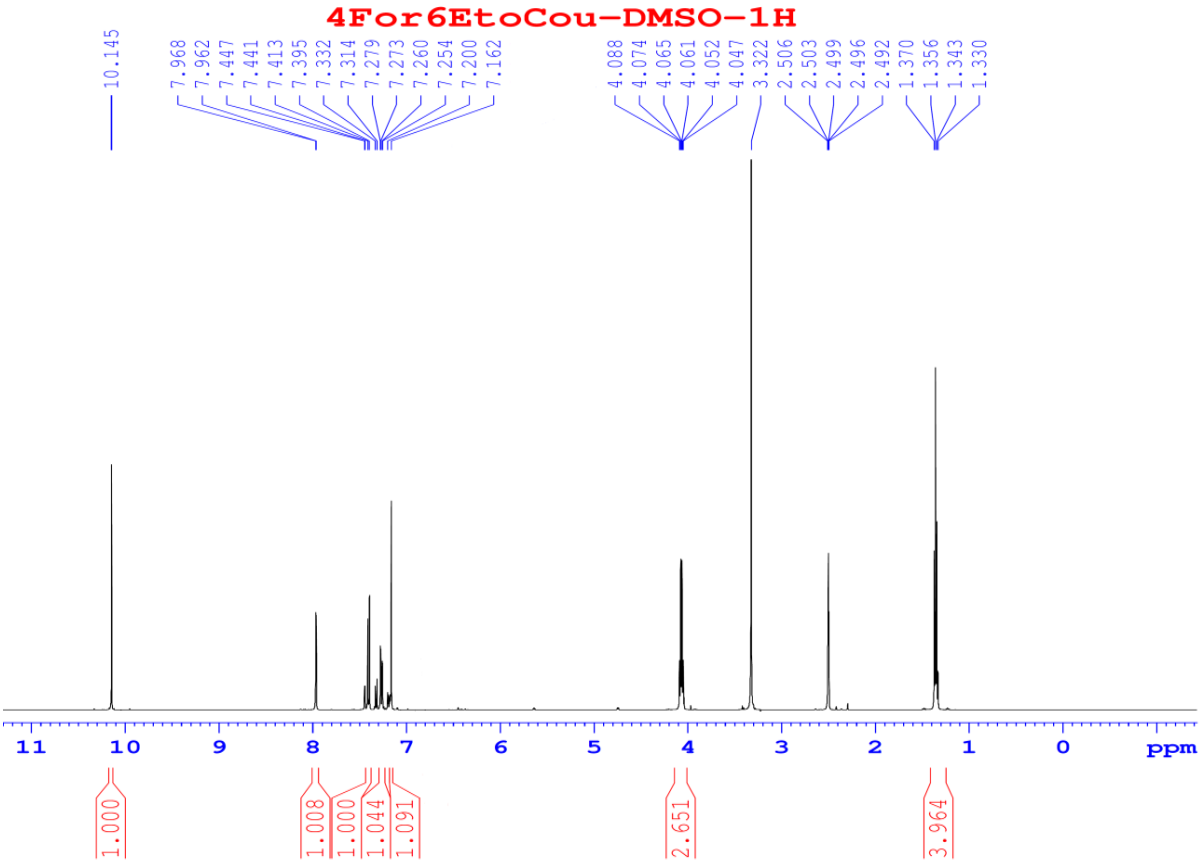


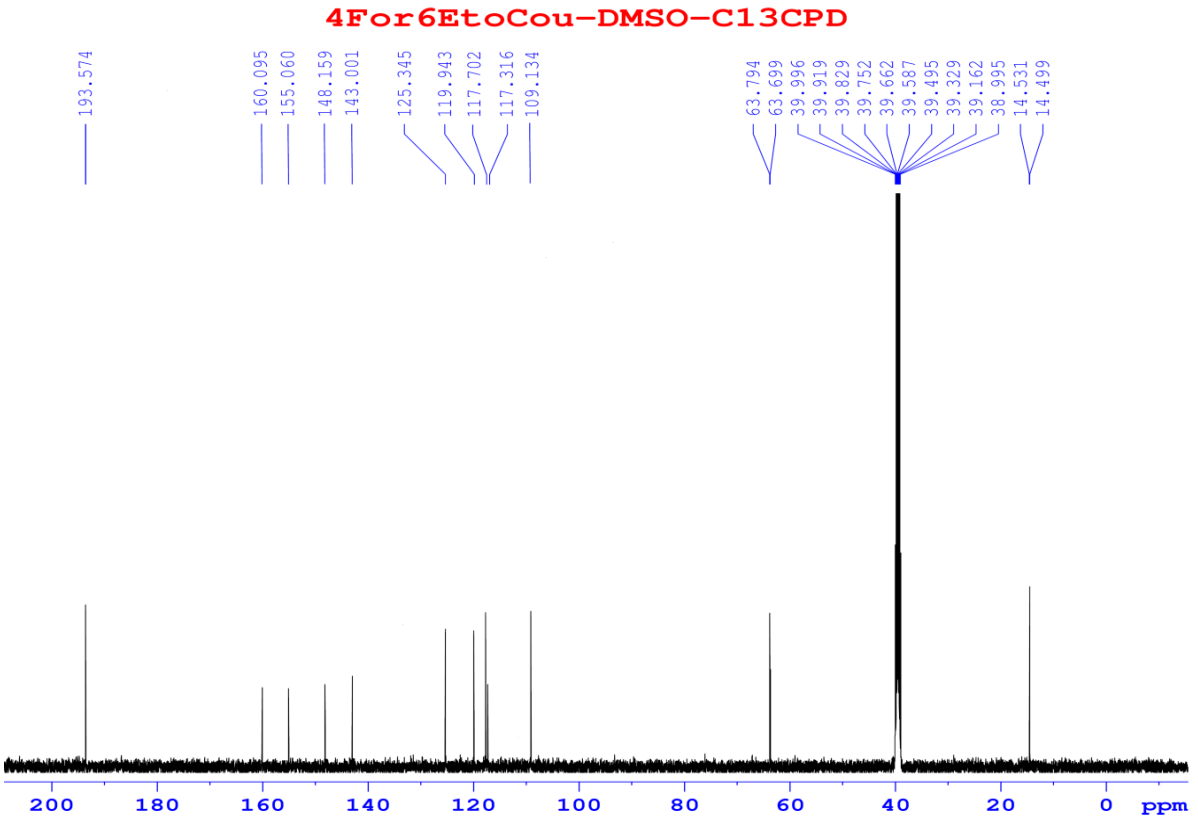


2.2. Selected spectra of 6- and 7-alkoxy-4-formylcoumarins 5a-h and 6a-j

*4-Formyl-6-ethoxycoumarin (**5b**)*







Lab: Materials chemistry, Faculty of Chemistry, HUS-VNU
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Mobile: 0948 119 043; Email: daothinhungtn@yahoo.com

Sample name : 5b ForCou
Mode: ESI, M+H

Mass Spectrometter
LTQ Orbitrap XL™

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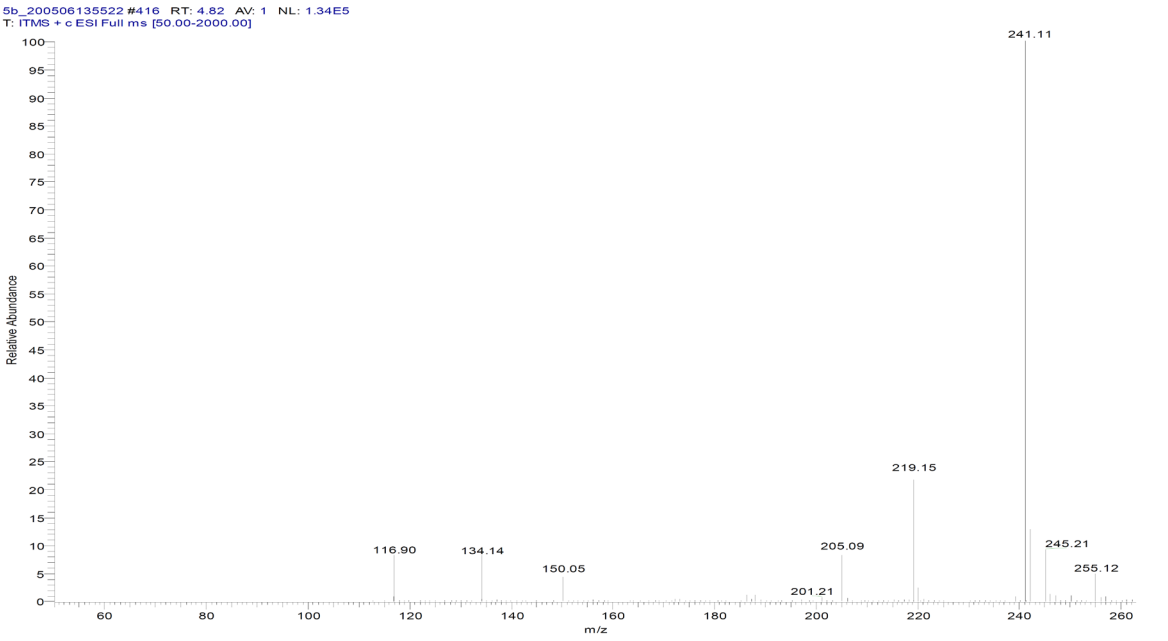
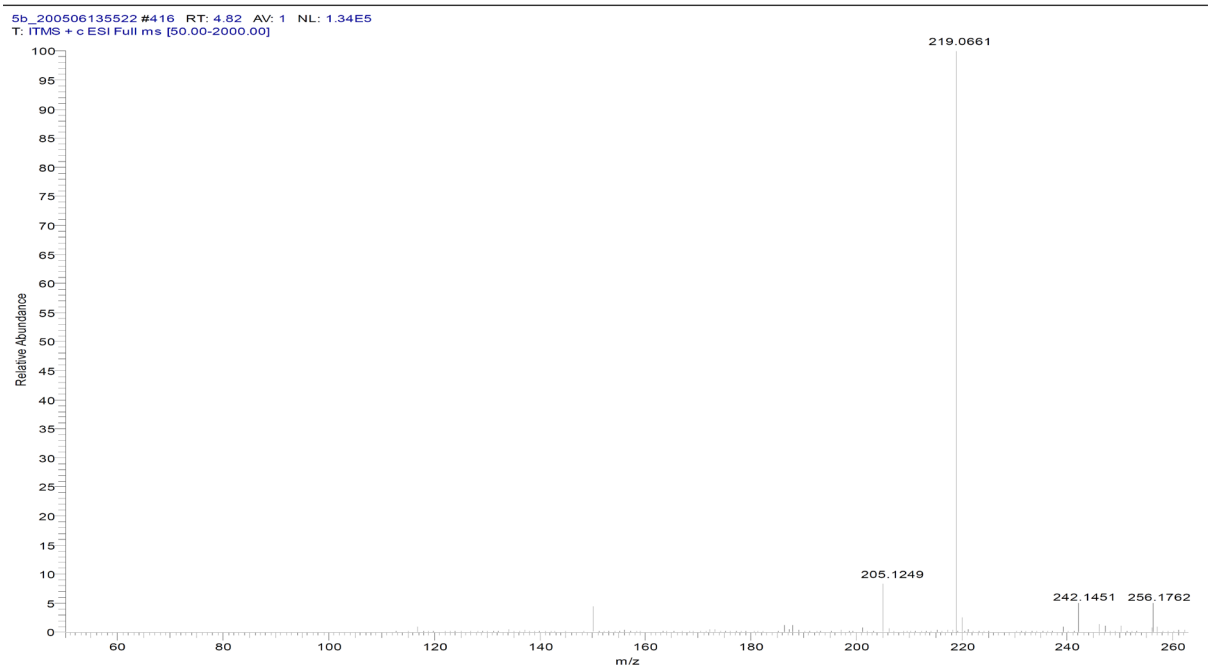
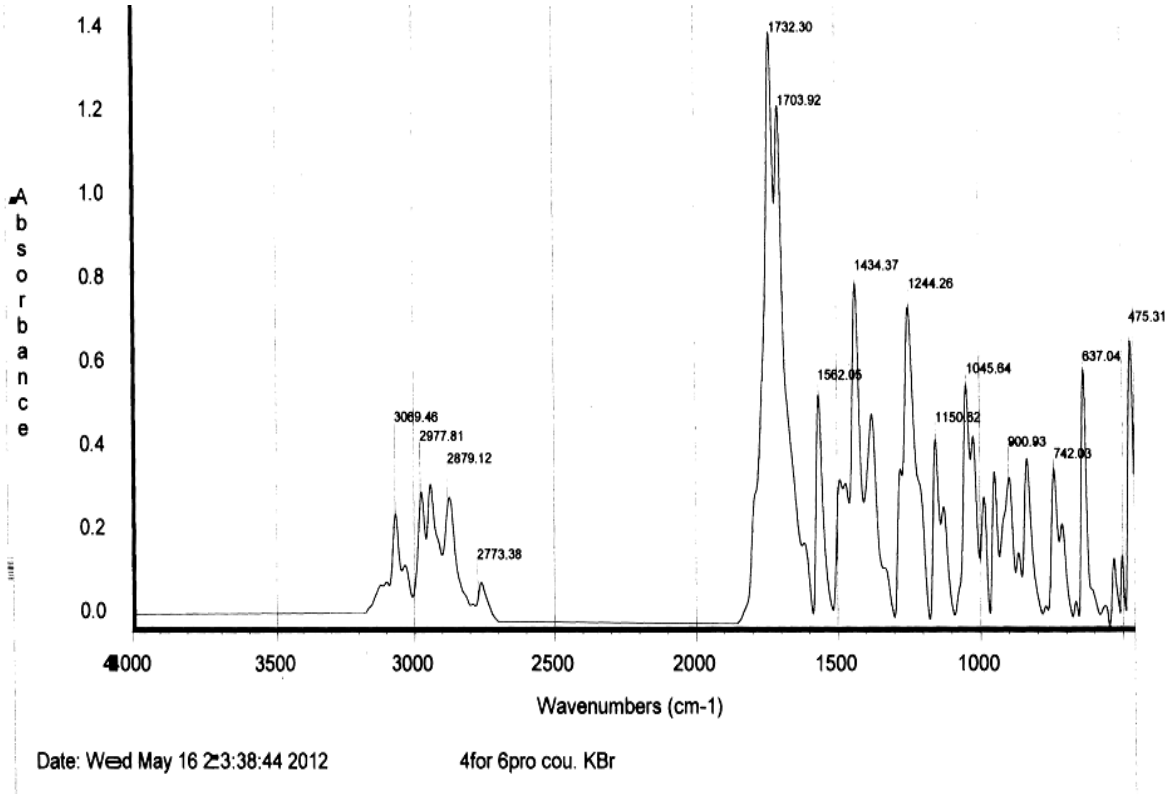
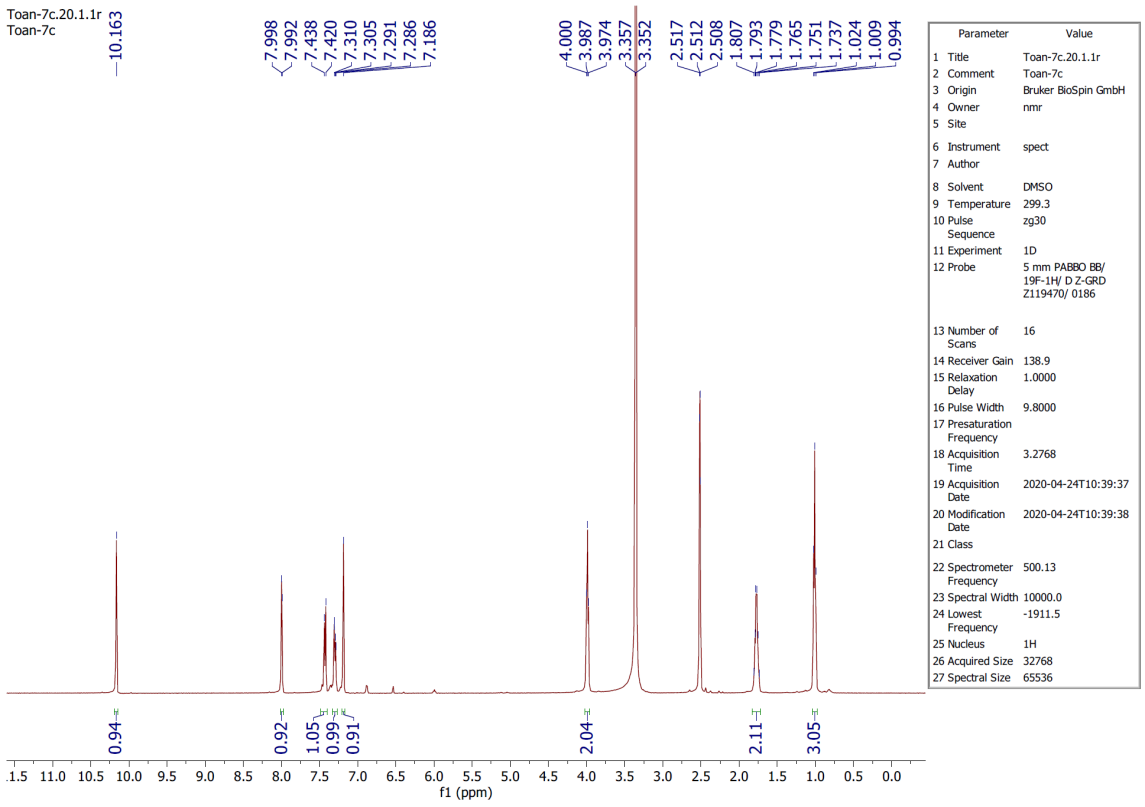




*4-Formyl-6-propoxycoumarin (**5c**)*





Parameter	Value
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4 Owner	nmr
5 Site	
6 Instrument	spect
7 Author	
8 Solvent	DMSO
9 Temperature	299.3
10 Pulse Sequence	zg30
11 Experiment	1D
12 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0186
13 Number of Scans	16
14 Receiver Gain	138.9
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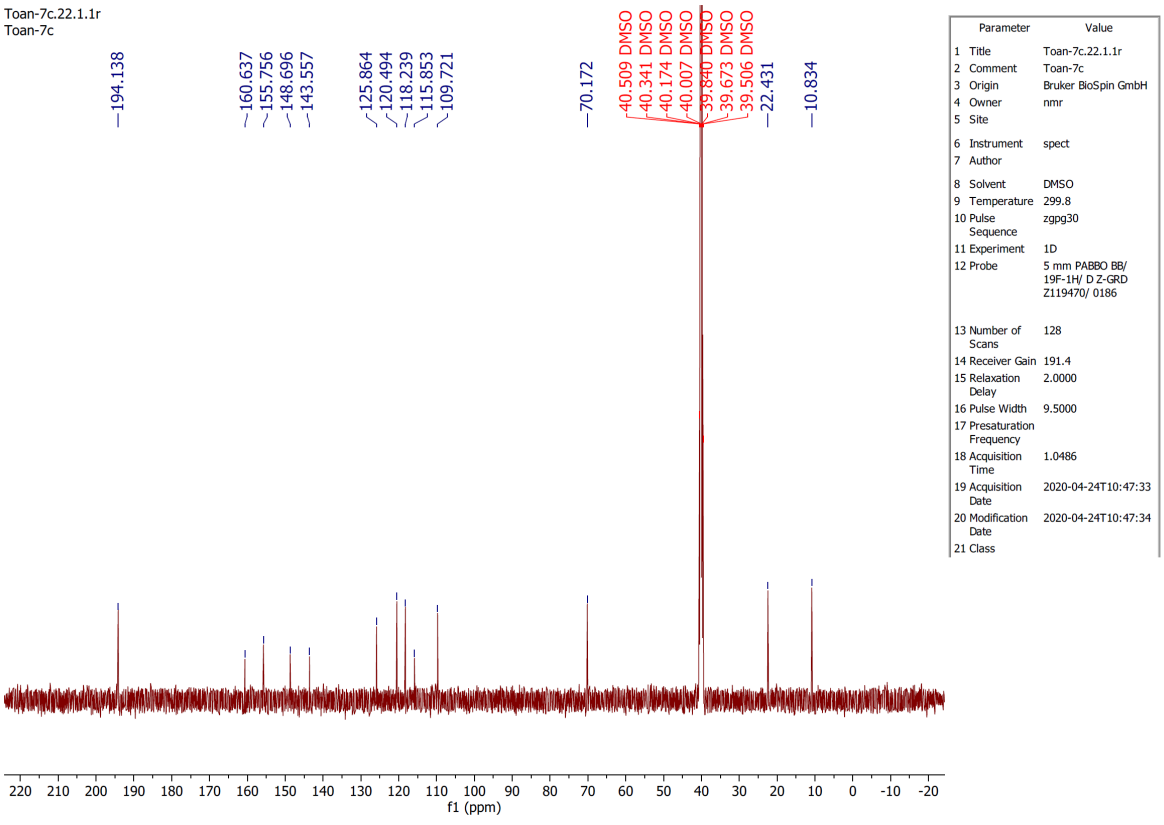
16 Pulse Width	9.8000
17 Presaturation Frequency	
18 Acquisition Time	3.2768
19 Acquisition Date	2020-04-24T10:39:37
20 Modification Date	2020-04-24T10:39:38
21 Class	
22 Spectrometer Frequency	500.13
23 Spectral Width	10000.0
24 Lowest Frequency	-1911.5
25 Nucleus	1H
26 Acquired Size	32768
27 Spectral Size	65536



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5 Site	
6 Instrument	spect
7 Author	
8 Solvent	DMSO
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10 Pulse Sequence	zgpg30
11 Experiment	1D
12 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0186
13 Number of Scans	128
14 Receiver Gain	191.4
15 Relaxation Delay	2.0000
16 Pulse Width	9.5000
17 Presaturation Frequency	
18 Acquisition Time	1.0486
19 Acquisition Date	2020-04-24T10:47:33
20 Modification Date	2020-04-24T10:47:34
21 Class	

Lab: Materials chemistry, Faculty of Chemistry, HUS-VNU
19 Le Thanh Tong, Hoan Kiem, Ha Noi

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Operator: Ms. Dao Thi Nhung
Mobile: 0948 119 043; Email: daothinhungtn@yahoo.com

Sample name : 6OPr4ForCou
Mode: ESI, M+H

Mass Spectrometter
LTQ Orbitrap XL™

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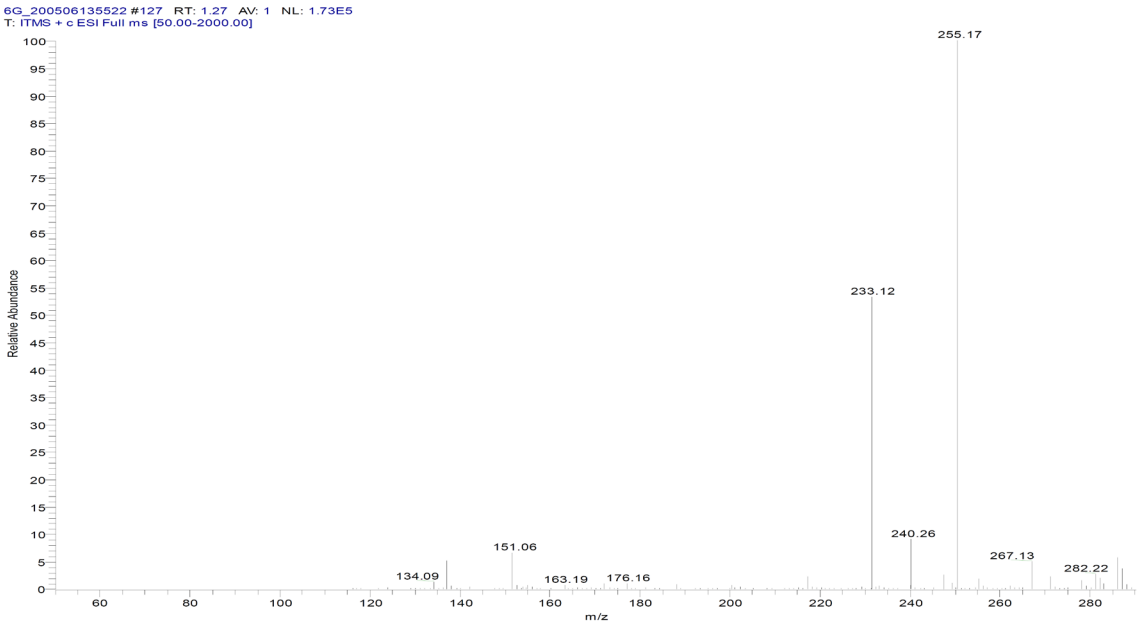
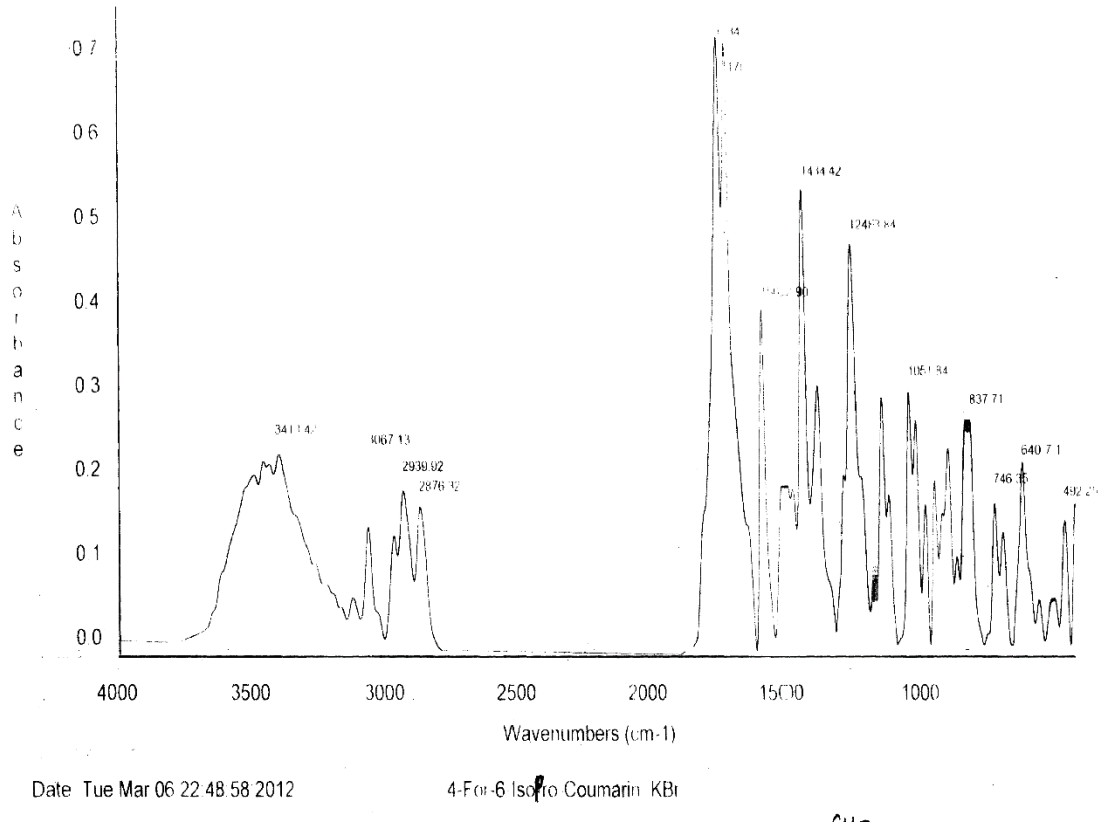
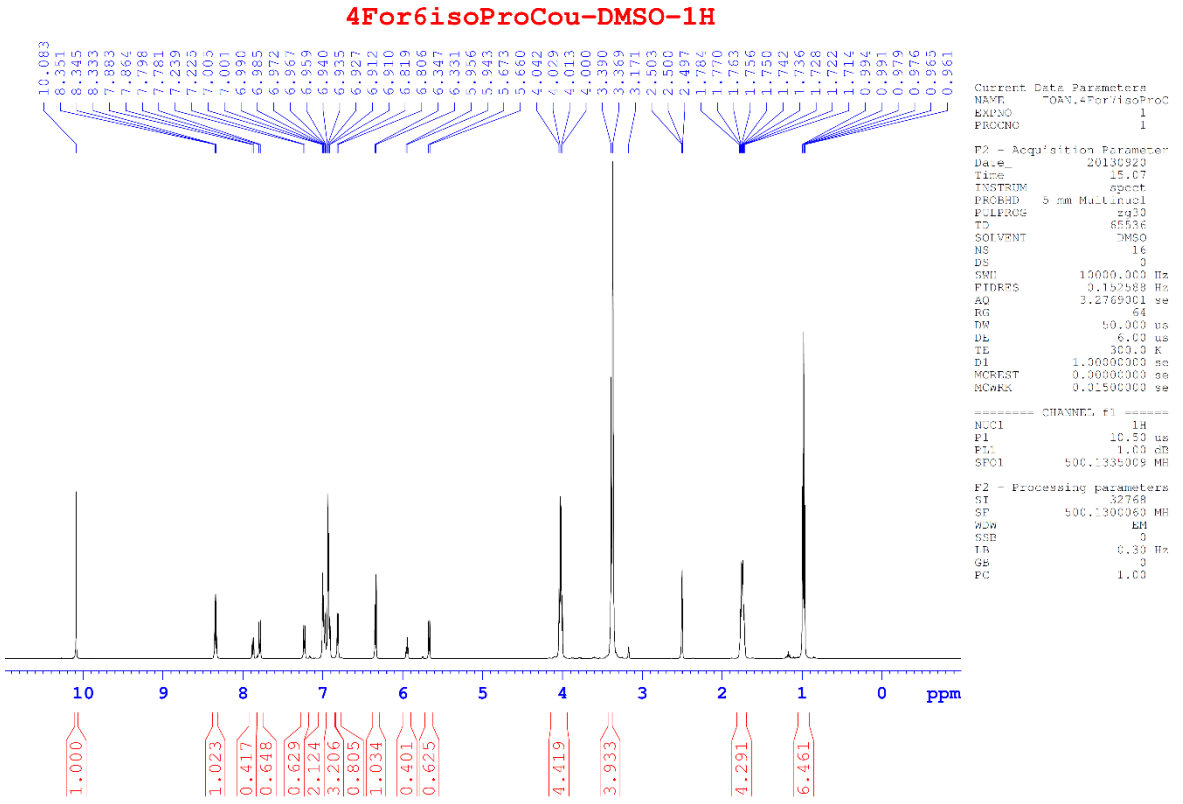


*4-Formyl-6-isopropoxycoumarin (**5d**)*





Lab: Materials chemistry, Faculty of Chemistry, HUS-VNU
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Operator: Ms. Dao Thi Nhung
Mobile: 0948 119 043; Email: daothinhungtn@yahoo.com

Sample name :6OPr4ForCou
Mode: ESI, M+H

Mass Spectrometter
LTQ Orbitrap XL™

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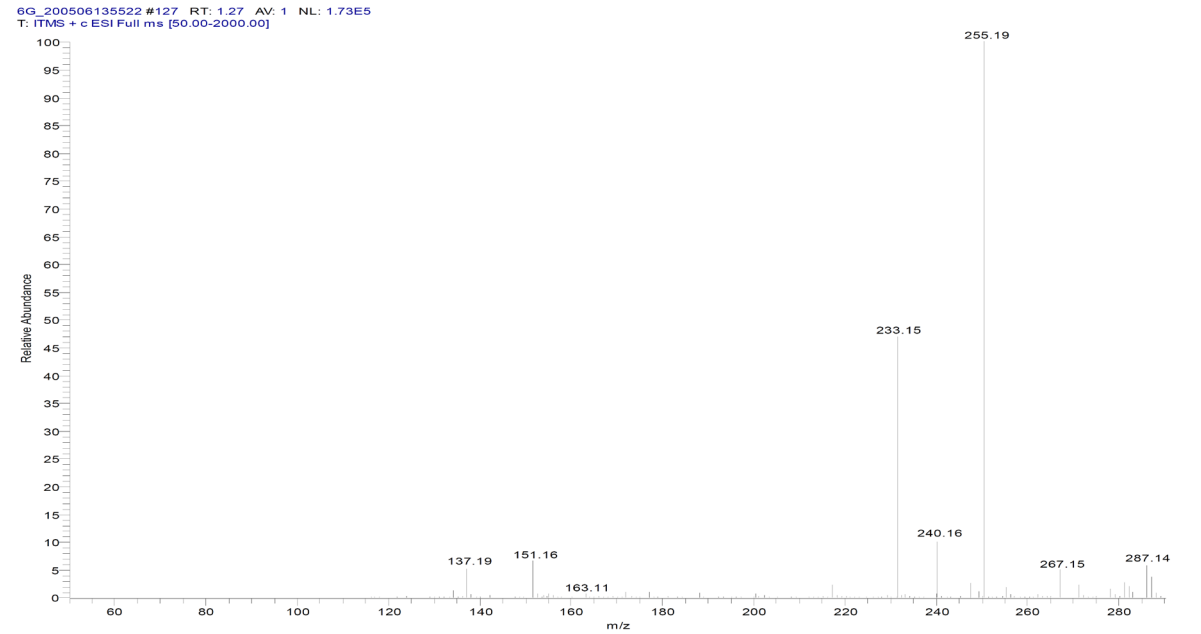
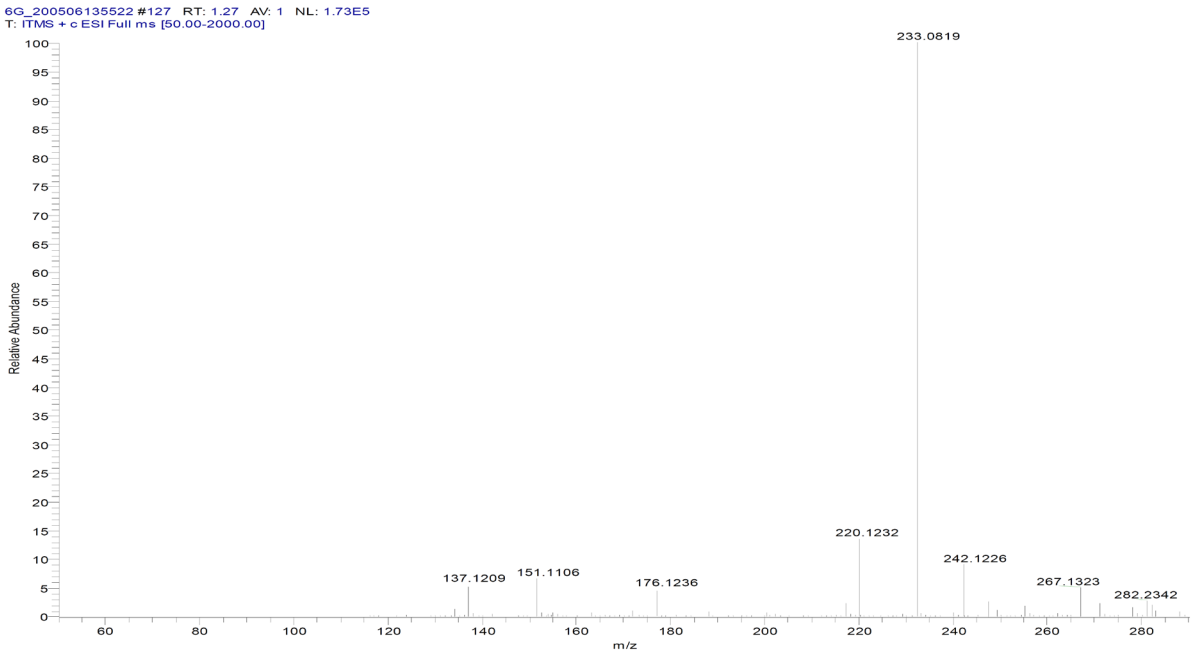
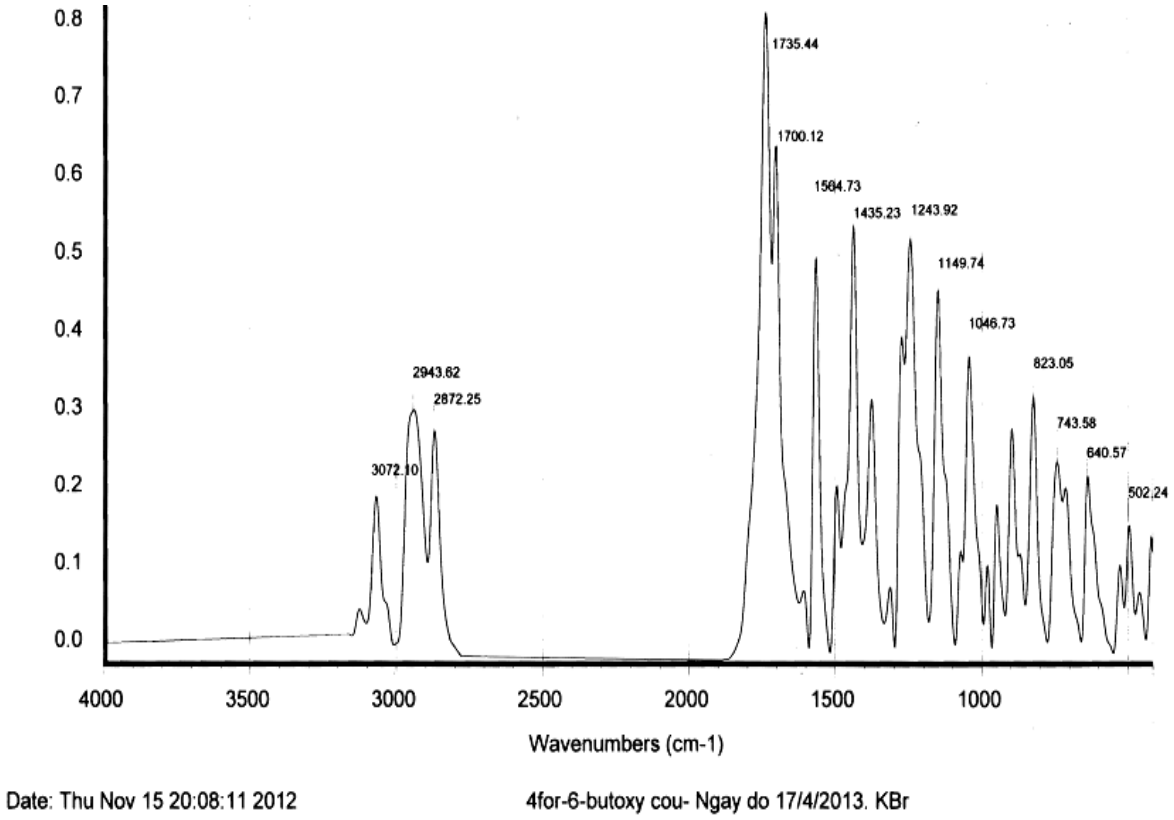
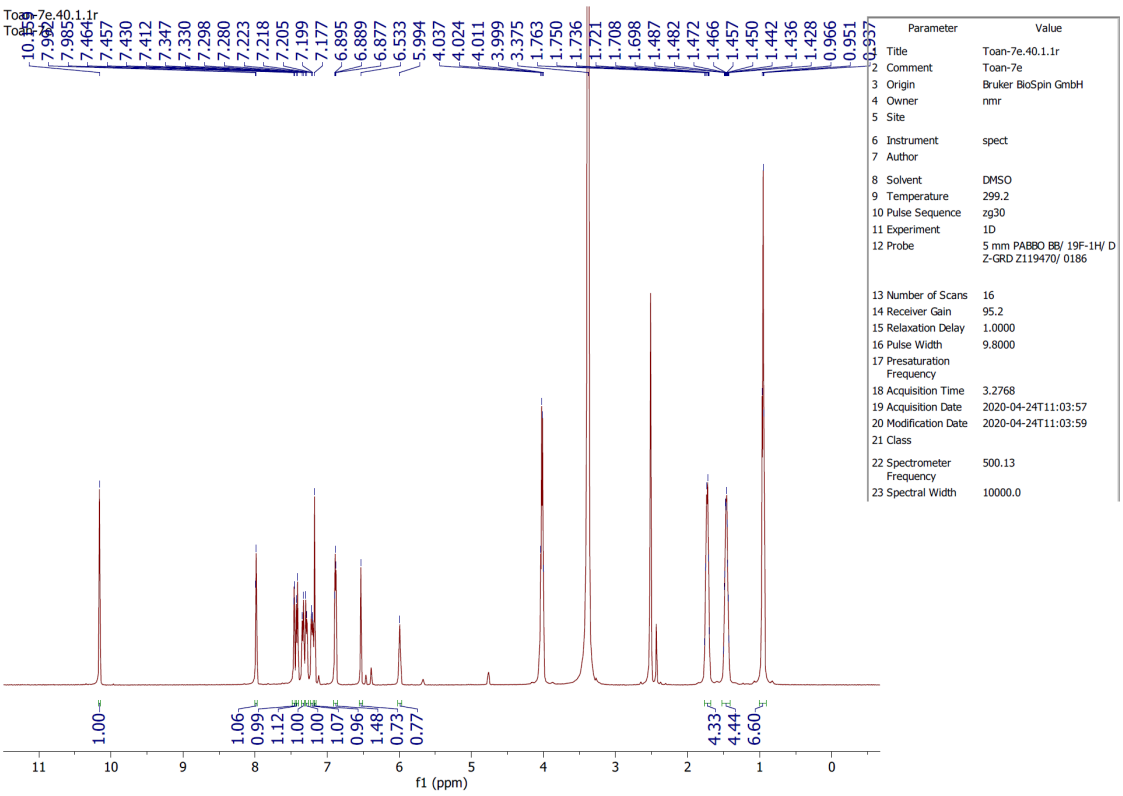
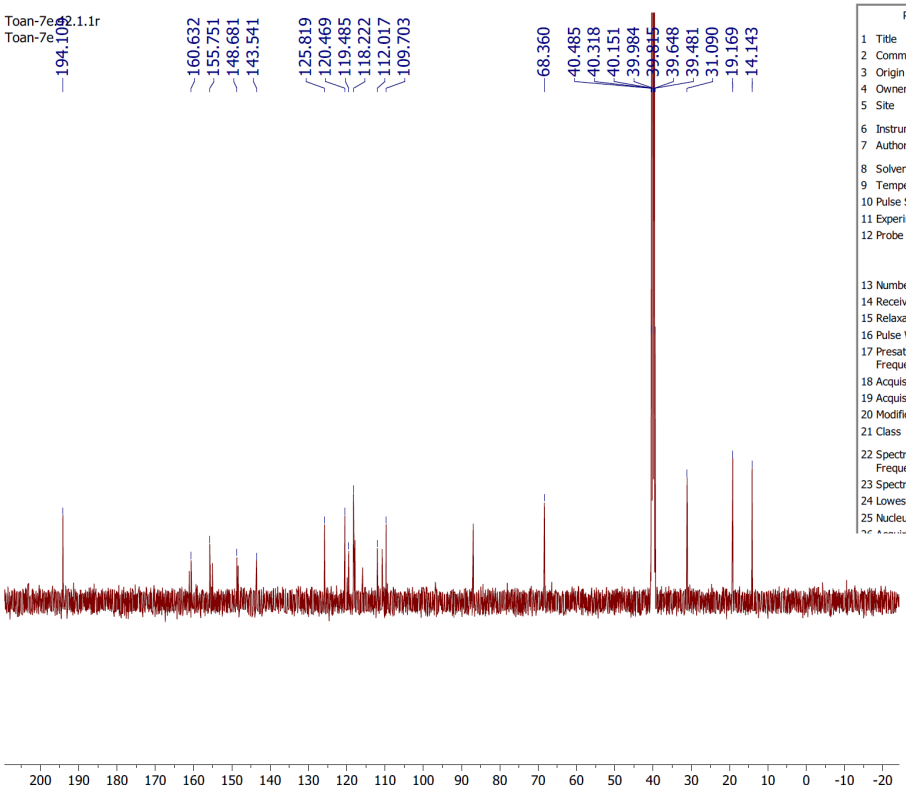




*4-Formyl-6-butoxycoumarin (**5e**)*







Parameter	Value
1 Title	Toan-7e.42.1.1r
2 Comment	Toan-7e
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Instrument	spect
7 Author	
8 Solvent	DMSO
9 Temperature	299.7
10 Pulse Sequence	zgpg30
11 Experiment	1D
12 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0186
13 Number of Scans	128
14 Receiver Gain	191.4
15 Relaxation Delay	2.0000
16 Pulse Width	9.5000
17 Presaturation Frequency	
18 Acquisition Time	1.0486
19 Acquisition Date	2020-04-24T11:11:51
20 Modification Date	2020-04-24T11:11:52
21 Class	
22 Spectrometer Frequency	125.76
23 Spectral Width	31250.0
24 Lowest Frequency	-3049.8
25 Nucleus	13C

Lab: Materials chemistry, Faculty of Chemistry, HUS-VNU
19 Le Thanh Tong, Hoan Kiem, Ha Noi

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Operator: Ms. Dao Thi Nhung
Mobile: 0948 119 043; Email: daothinhungtn@yahoo.com

Sample name :6-6OBu4ForCou
Mode: ESI, M+H

Mass Spectrometer
LTQ Orbitrap XL™

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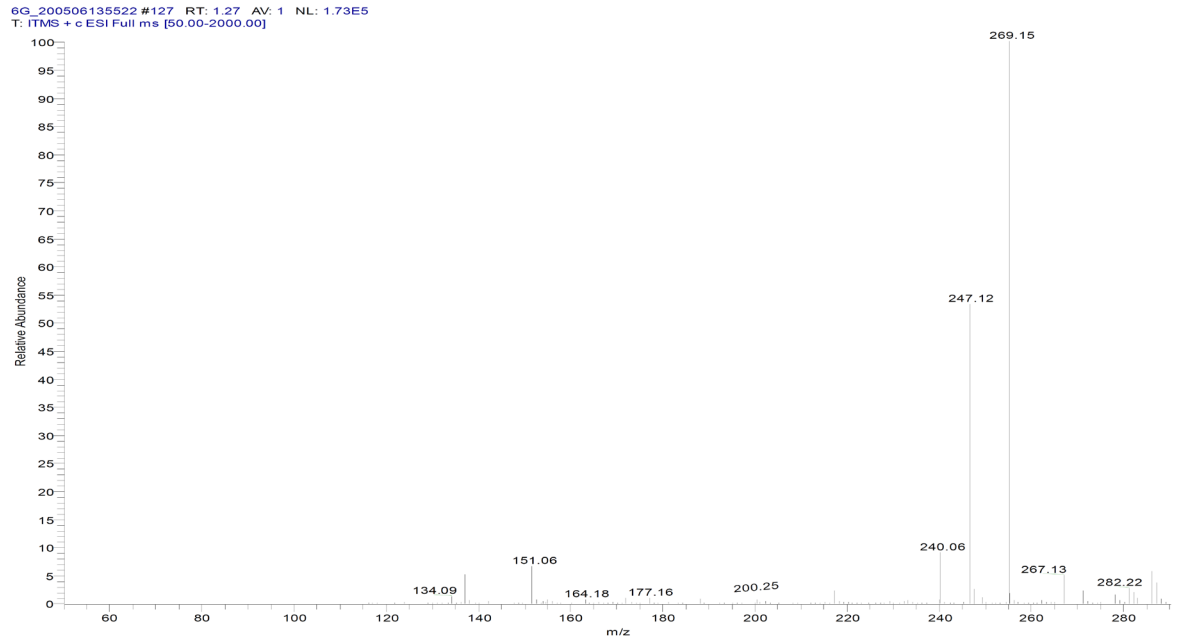
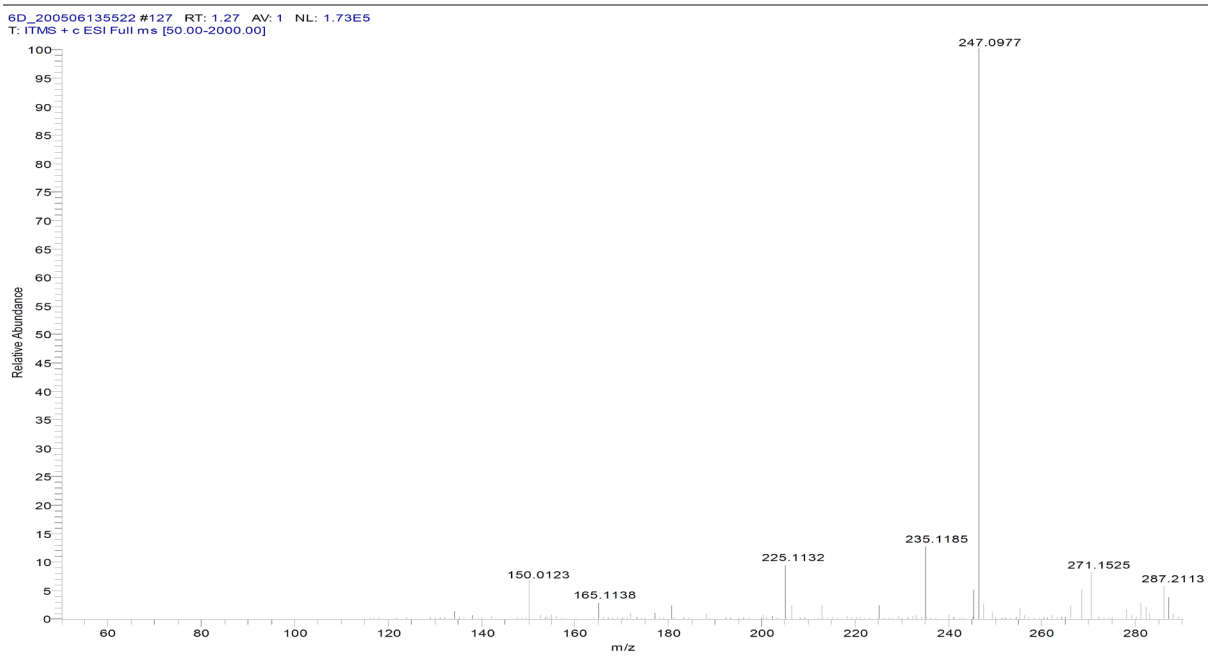
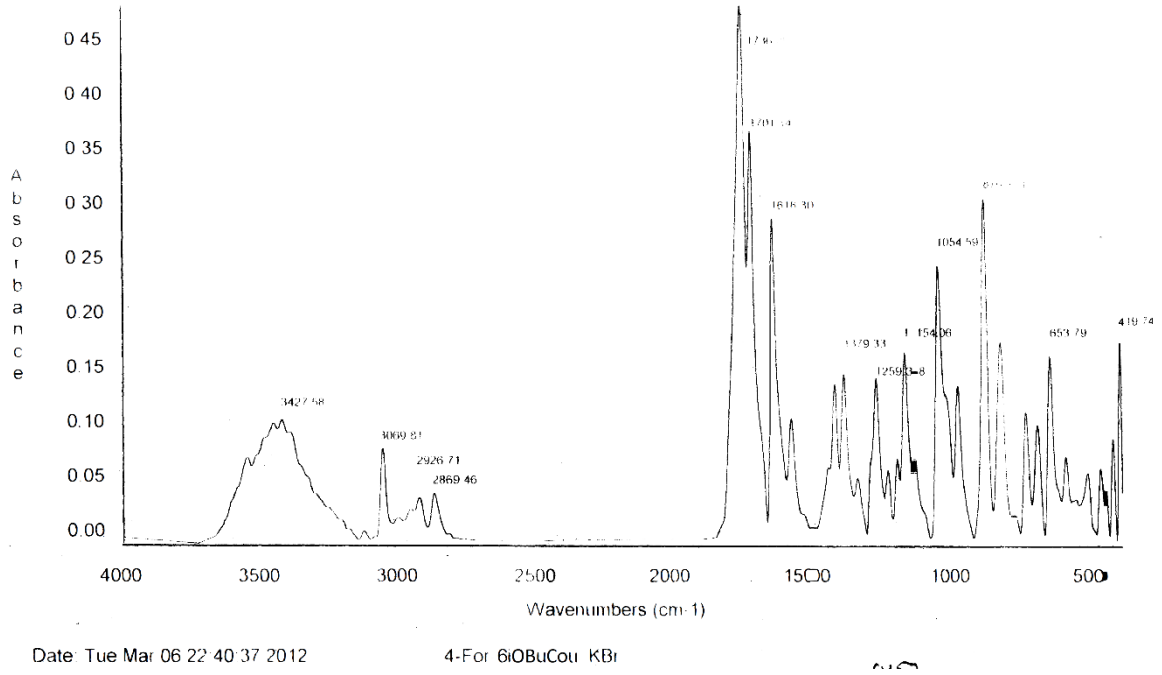




*4-Formyl-6-isobutoxycoumarin (**5f**)*



Lab: Materials chemistry, Faculty of Chemistry, HUS-VNU
19 Le Thanh Tong, Hoan Kiem, Ha Noi

Tel: 844.38.253.053; **Fax**: 844.38.241.140 **Mail**: Chem.vnu@.edu.vn

Operator: Ms. Dao Thi Nhung
Mobile: 0948 119 043; Email: daothinhungtn@yahoo.com

Sample name :6iOBu4ForCou
Mode: ESI, M+H

Mass Spectrometter
LTQ Orbitrap XL™

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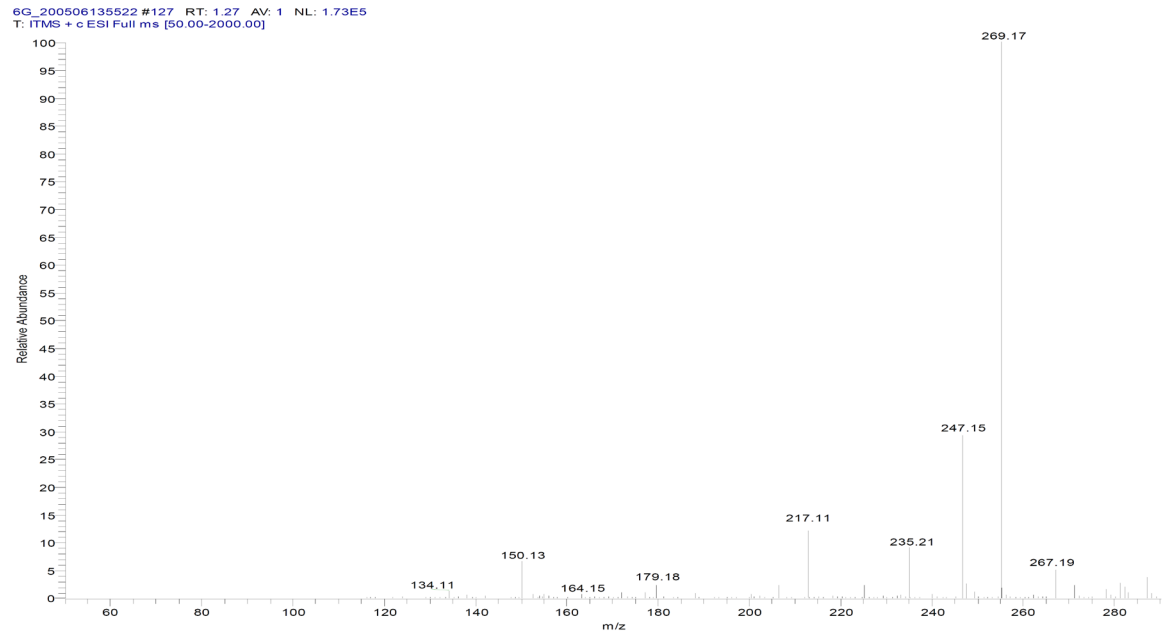
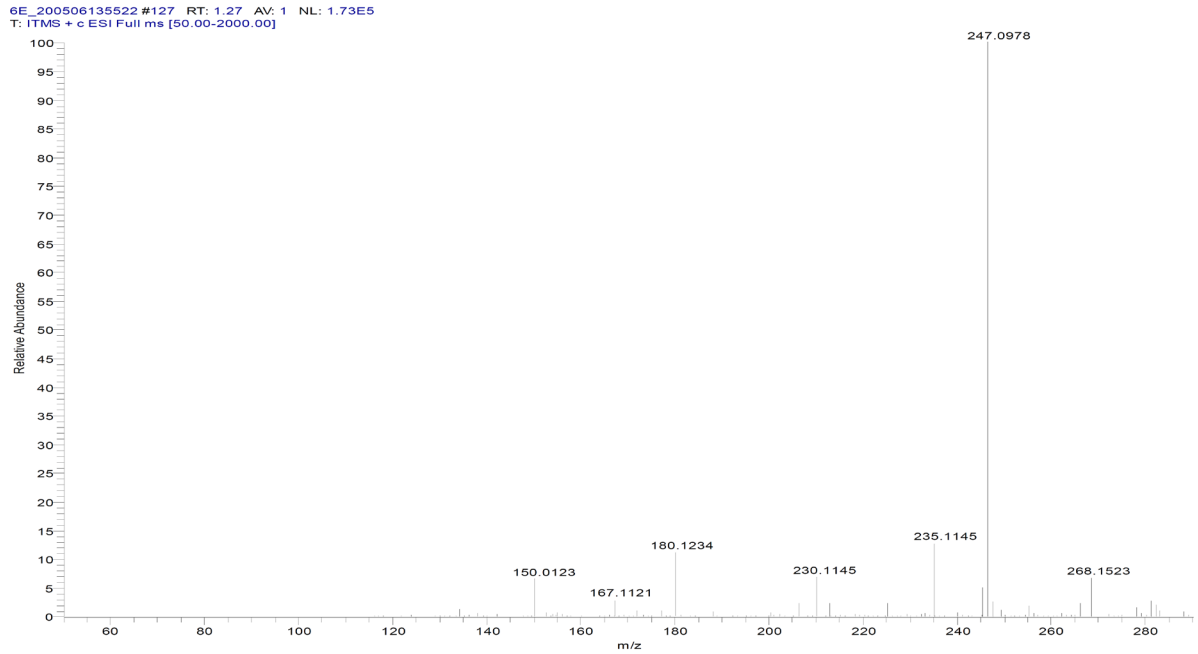
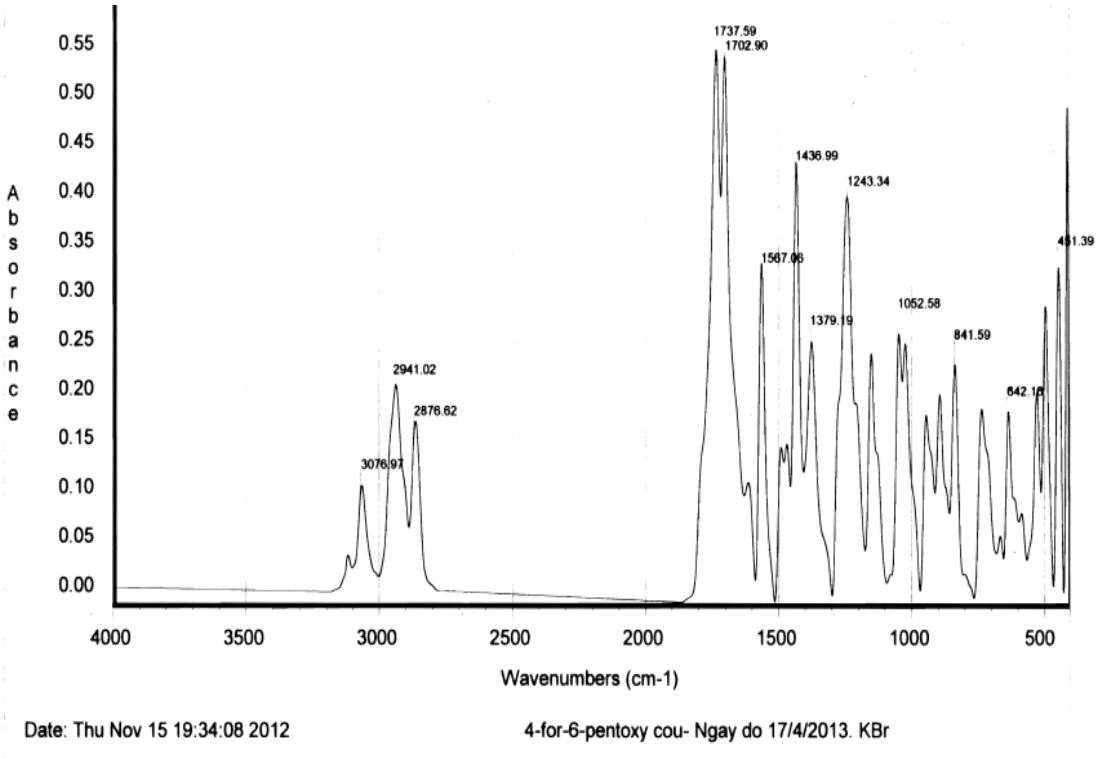
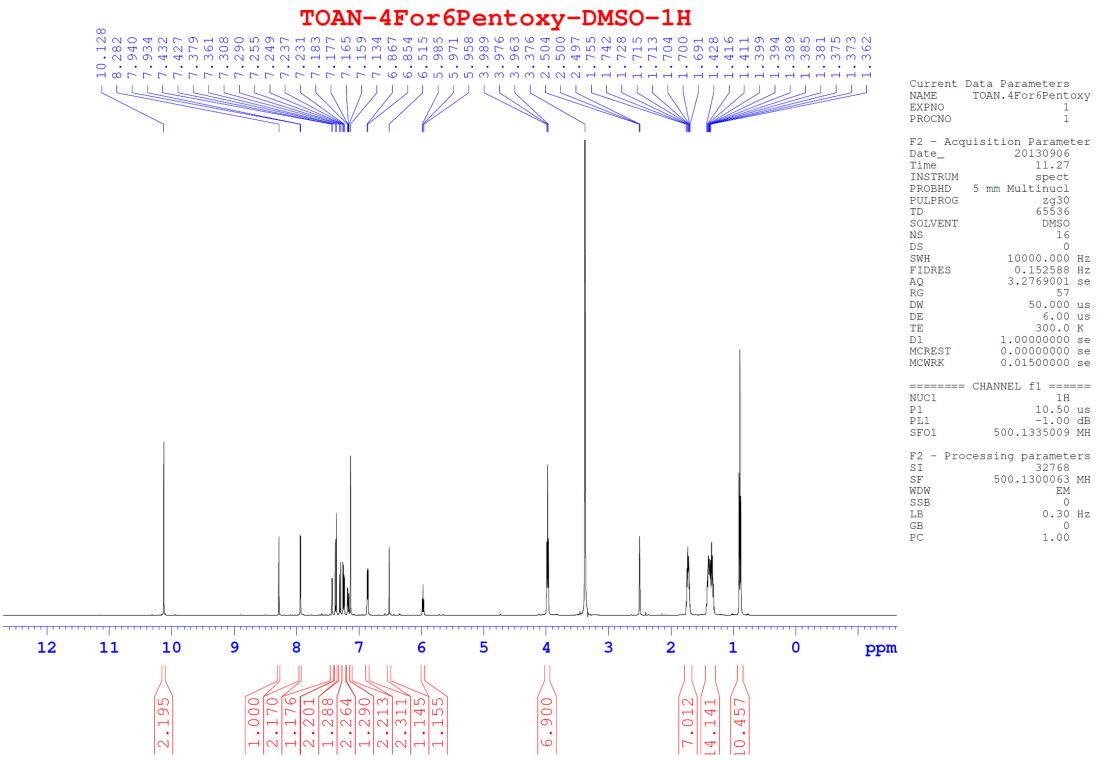


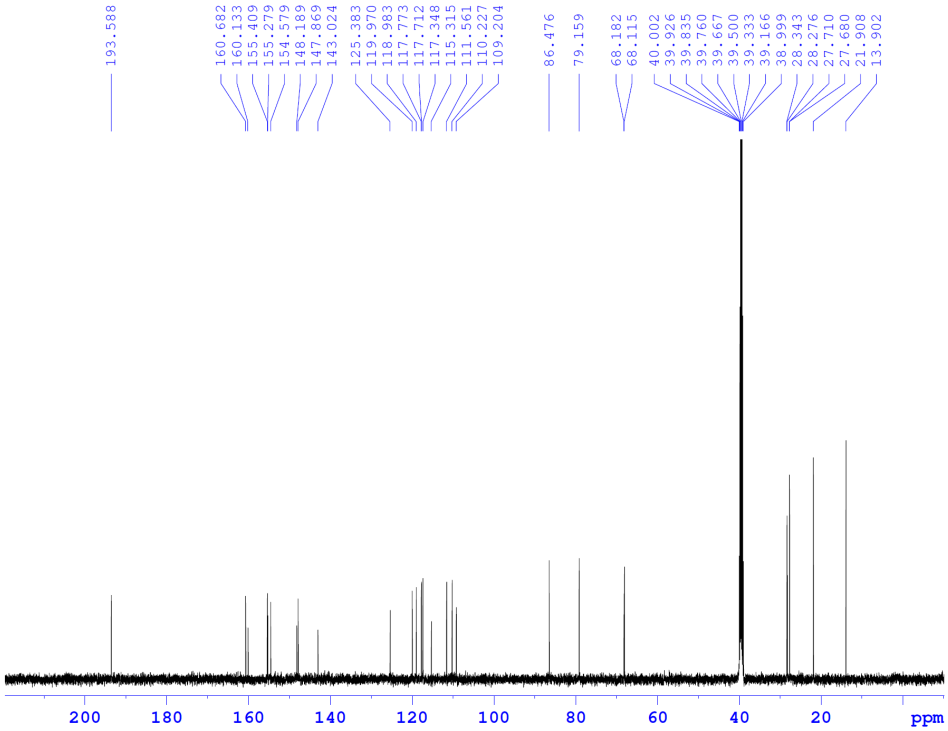


*4-Formyl-6-pentoxycoumarin (**5g**)*





4For6Pentoxy-DMSO-C13CPD




```
Current Data Parameters
NAME      TOAN.4For6Pentox
EXPNO                    2
PROCNO                   1

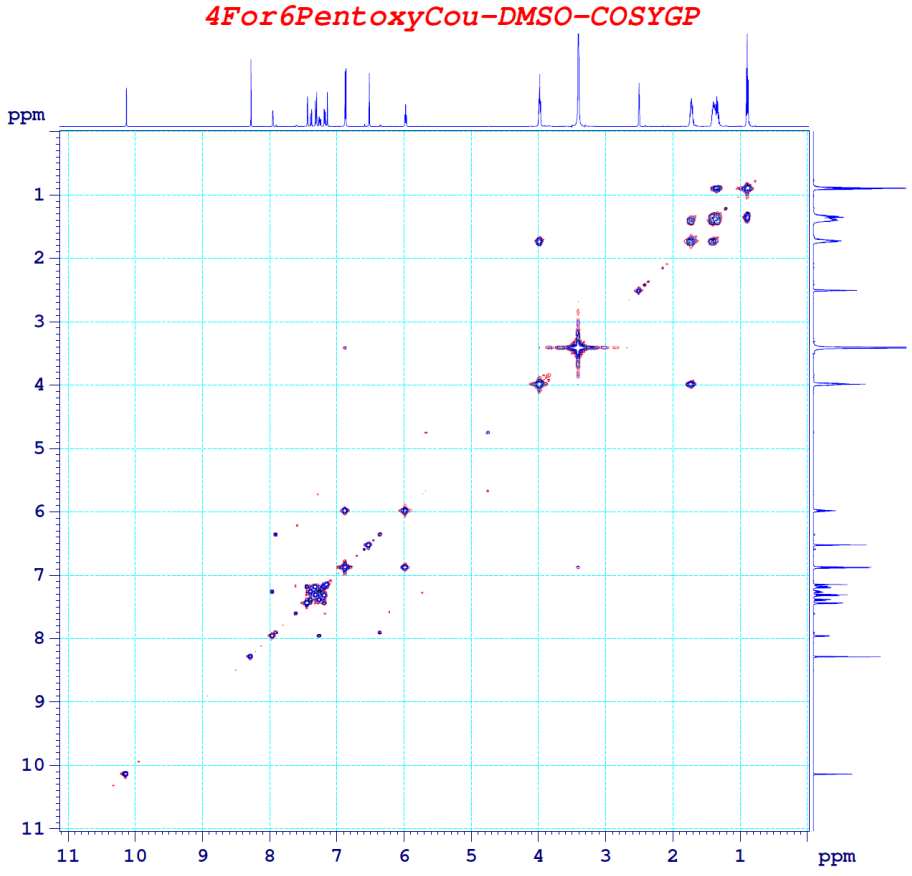
F2 - Acquisition Paramet
Date_             20130917
Time                 13.43
INSTRUM              spect
PROBHD   5 mm Multinucl
PULPROG             zgpg30
TD                   65536
SOLVENT               DMSO
NS                     128
DS                       2
SWH              31446.541
FIDRES           0.479836
AQ               1.0420883
RG                   32768
DW                  15.900
DE                    6.00
TE                  300.0
D1               2.00000000
d11              0.03000000
DELTA            1.89999998
MCREST           0.00000000
MCWRK            0.01500000

======== CHANNEL f1 =====
NUC1                   13C
P1                    5.00
PL1                  -1.00
SFO1           125.7716224

======== CHANNEL f2 =====
CPDPRG2            waltz16
NUC2                   1H
PCPD2                80.00
PL2                  -1.00
PL12                 16.64
PL13                 22.00
SFO2           500.1320005

F2 - Processing paramete
SI                   32768
SF             125.7578442
WDW                     EM
SSB                      0
LB                    1.00
GB                       0
```

4For6PentoxyCou-DMSO-COSYGP




```
Current Data Parameters
NAME      TOAN.4For6PenCou
EXPNO                    5
PROCNO                   1

F2 - Acquisition Parameters
Date_             20130925
Time                 9.46
INSTRUM              spect
PROBHD   5 mm Multinucl
PULPROG          cosygpqf
TD                   2048
SOLVENT              CDCl3
NS                       8
DS                       8
SWH              6009.615 Hz
FIDRES           2.934382 Hz
AQ               0.1705268 sec
RG                    90.5
DW                  83.200 usec
DE                    6.00 usec
TE                  300.0 K
d0               0.00000300 sec
D1               1.48689198 sec
d13              0.00000400 sec
D16              0.00020000 sec
IN0              0.00016663 sec
MCREST           0.00000000 sec
MCWRK            1.48689198 sec

======== CHANNEL f1 ========
NUC1                     1H
P0                    10.30 usec
P1                    10.30 usec
PL1                   -1.00 dB
SFO1          500.1332508 MHz

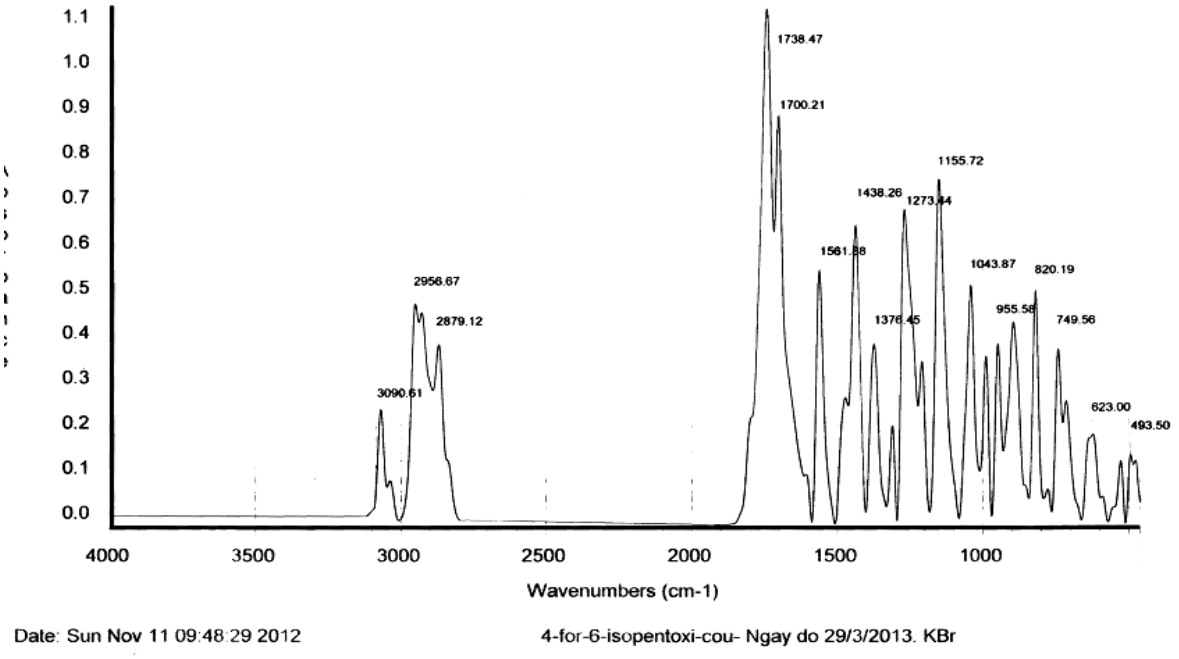
====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPX1                  0.00 %
GPX2                  0.00 %
GPY1                  0.00 %
GPY2                  0.00 %
GPZ1                 10.00 %
GPZ2                 10.00 %
P16                1000.00 usec

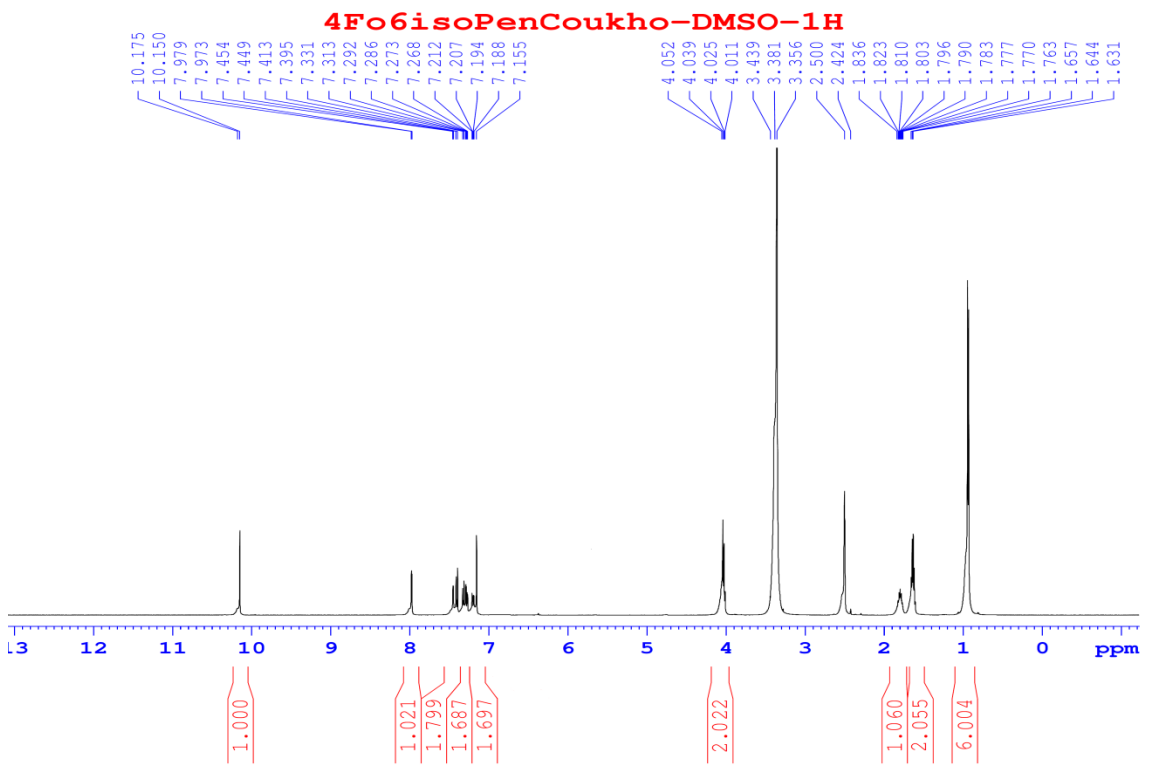
F1 - Acquisition parameters
ND0                      1
TD                     256
SFO1           500.1323 MHz
FIDRES         23.443361 Hz
SW                12.000 ppm
FnMODE                  QF

F2 - Processing parameters
SI                    1024
SF           500.1300049 MHz
WDW                   SINE
SSB                      0
LB                    0.00 Hz
GB                       0
PC                    1.00

F1 - Processing parameters
SI                    1024
MC2                     QF
SF           500.1290066 MHz
WDW                   SINE
SSB                      0
LB                    0.00 Hz
GB                       0
```

*4-Formyl-6-isopentoxycoumarin (**5h**)*

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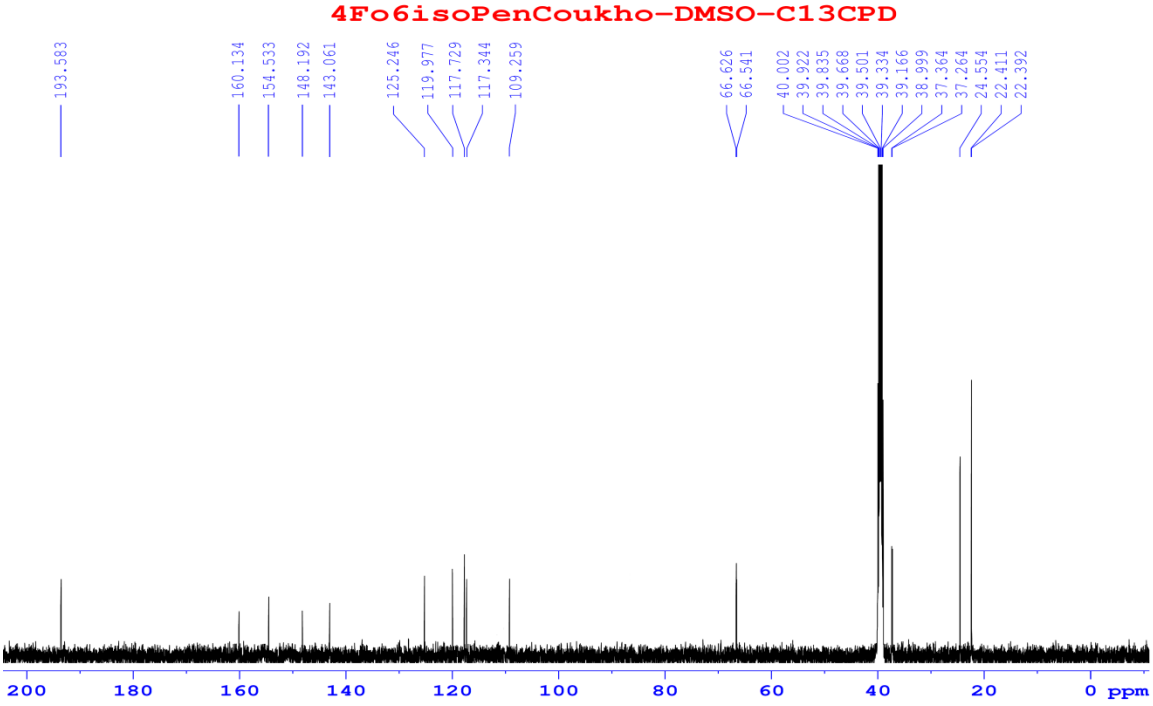
10.175
10.150
7.979
7.973
7.454
7.449
7.413
7.395
7.331
7.313
7.292
7.286
7.273
7.268
7.212
7.207
7.194
7.188
7.155
4.052
4.039
4.025
4.011
3.439
3.381
3.356
2.500
2.424
1.836
1.823
1.810
1.803
1.796
1.790
1.783
1.777
1.770
1.763
1.657
1.644
1.631
13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.000
1.021
1.799
1.687
1.697
2.022
1.060
2.055
6.004


4Fo6isoPenCoukho-DMSO-C13CPD
193.583
160.134
154.533
148.192
143.061
125.246
119.977
117.729
117.344
109.259
66.626
66.541
40.002
39.922
39.835
39.668
39.501
39.334
39.166
38.999
37.364
37.264
24.554
22.411
22.392
200 180 160 140 120 100 80 60 40 20 0 ppm

Lab: Materials chemistry, Faculty of Chemistry, HUS-VNU
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Tel: 844.38.253.053; **Fax**: 844.38.241.140 **Mail**: Chem.vnu@.edu.vn

Operator: Ms. Dao Thi Nhung
Mobile: 0948 119 043; Email: daothinhungtn@yahoo.com

SAMPLE: 6OiPn4ForCou
Mode: ESI, M+H

Mass Spectrometter
LTQ Orbitrap XL™
Solvent: MeOH/DCM

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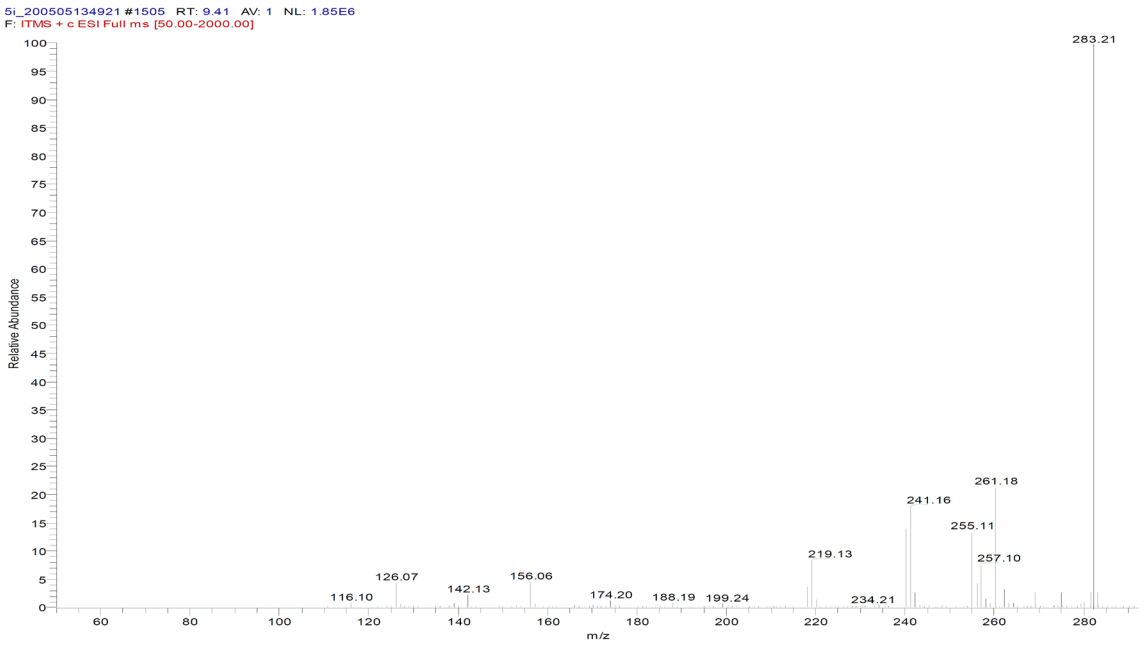
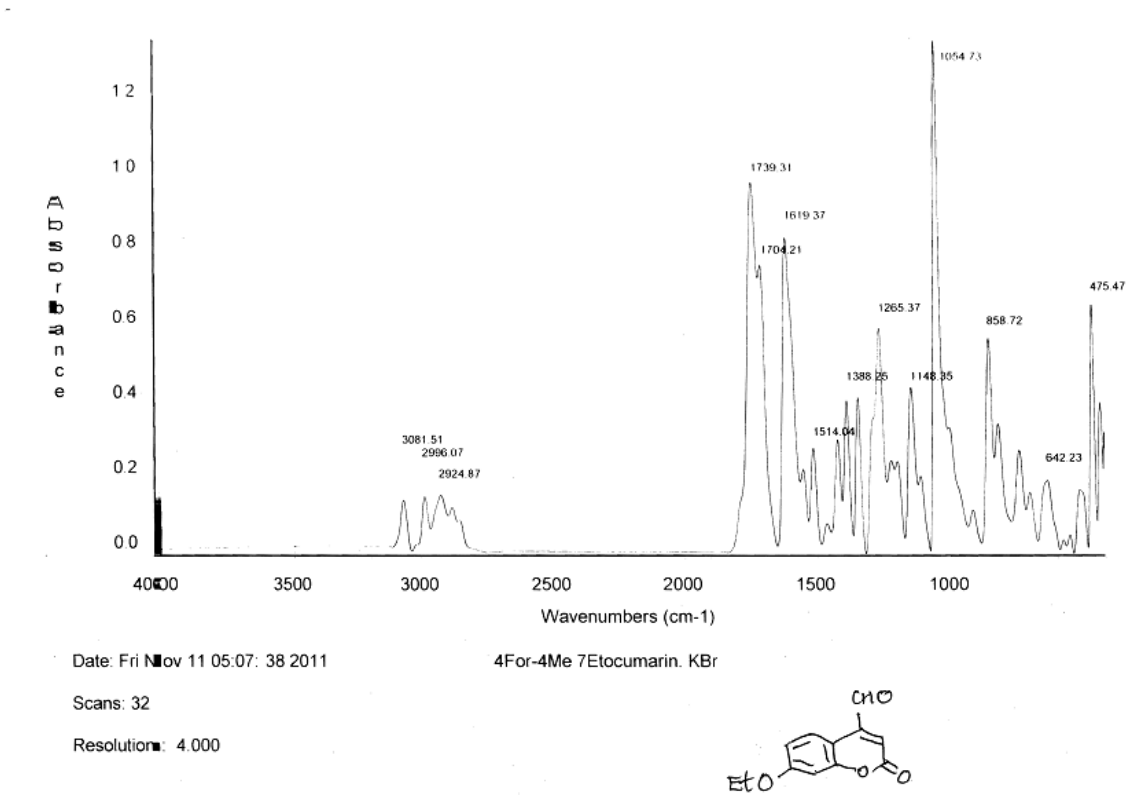
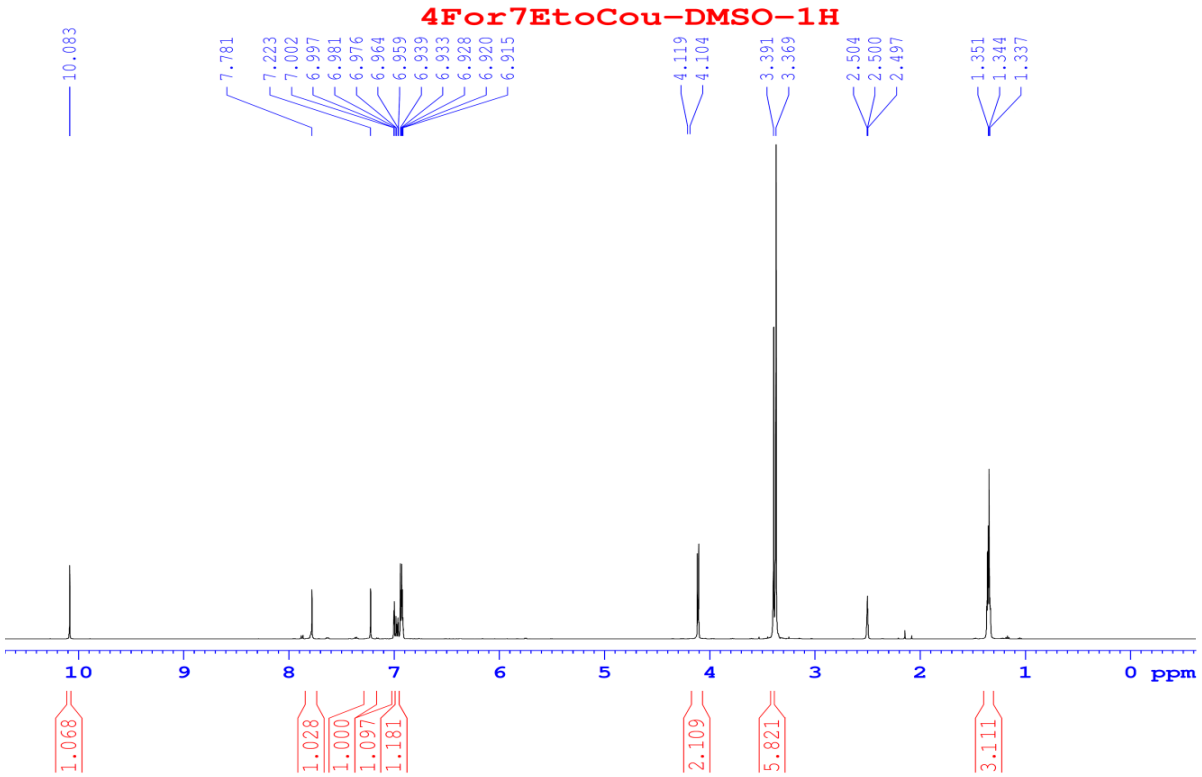
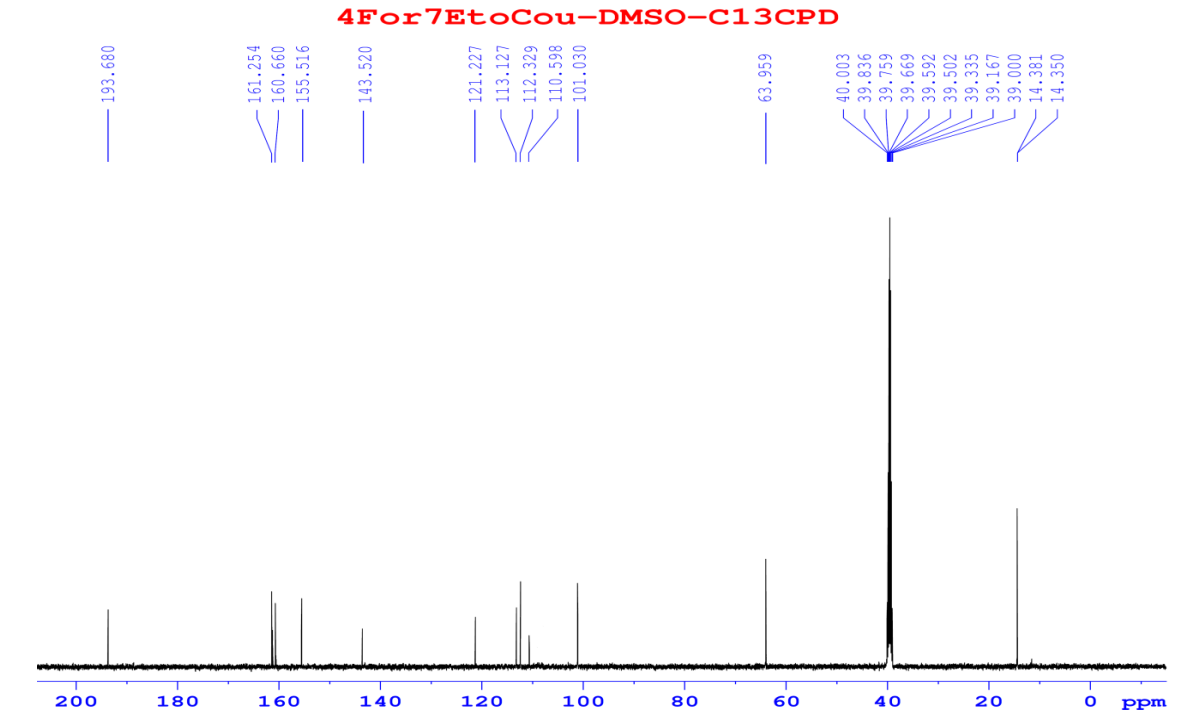


4-Formyl-7-ethoxycoumarin (***6b***)




4For7EtoCou-DMSO-1H
10.083
7.781
7.223
7.002
6.997
6.981
6.976
6.964
6.959
6.939
6.933
6.928
6.920
6.915
4.119
4.104
3.391
3.369
2.504
2.500
2.497
1.351
1.344
1.337
10
9
8
7
6
5
4
3
2
1
0 ppm
1.068
1.028
1.000
1.097
1.181
2.109
5.821
3.111


4For7EtoCou-DMSO-C13CPD
193.680
161.254
160.660
155.516
143.520
121.227
113.127
112.329
110.598
101.030
63.959
40.003
39.836
39.759
39.669
39.592
39.502
39.335
39.167
39.000
14.381
14.350
200
180
160
140
120
100
80
60
40
20
0 ppm

Lab: Materials chemistry, Faculty of Chemistry, HUS-VNU
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Operator: Ms. Dao Thi Nhung
Mobile: 0948 119 043; Email: daothinhungtn@yahoo.com

Sample name : -7OEt4ForCou
Mode: ESI, M+H

Mass Spectrometter
LTQ Orbitrap XL™

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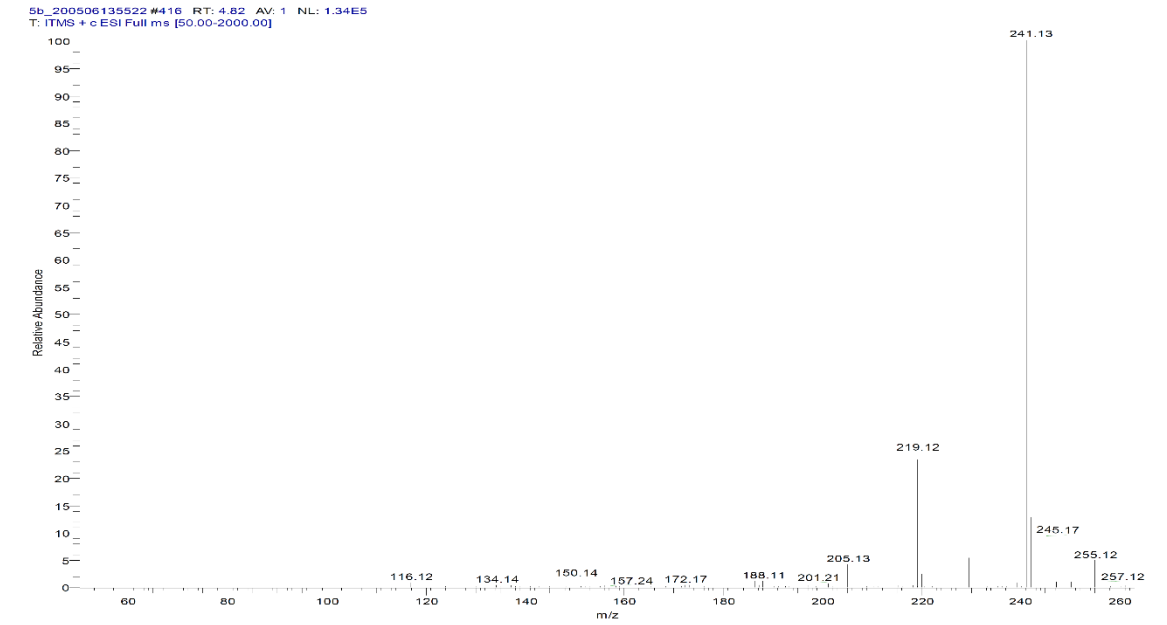
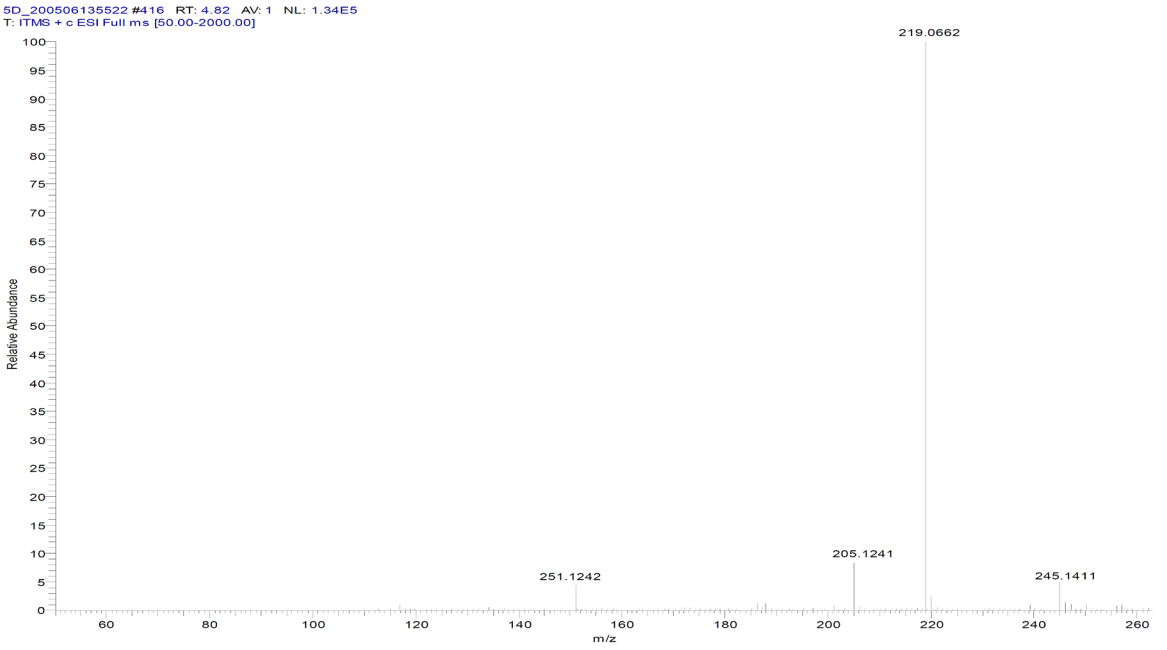
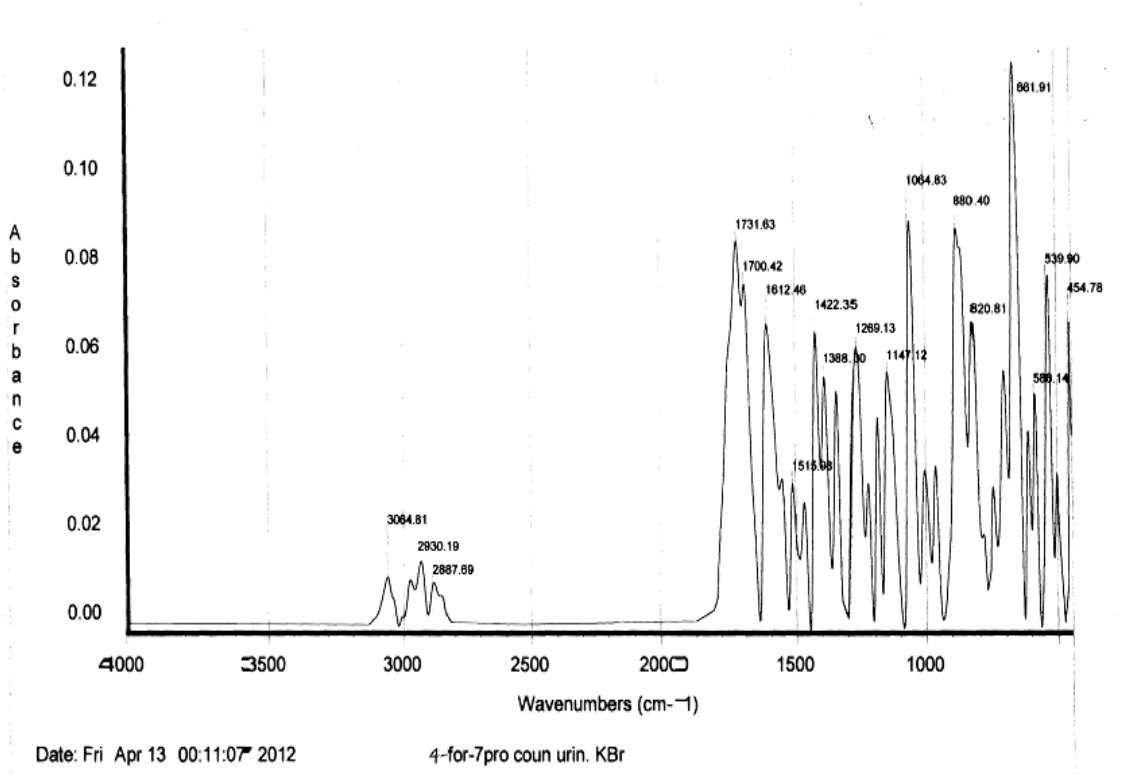
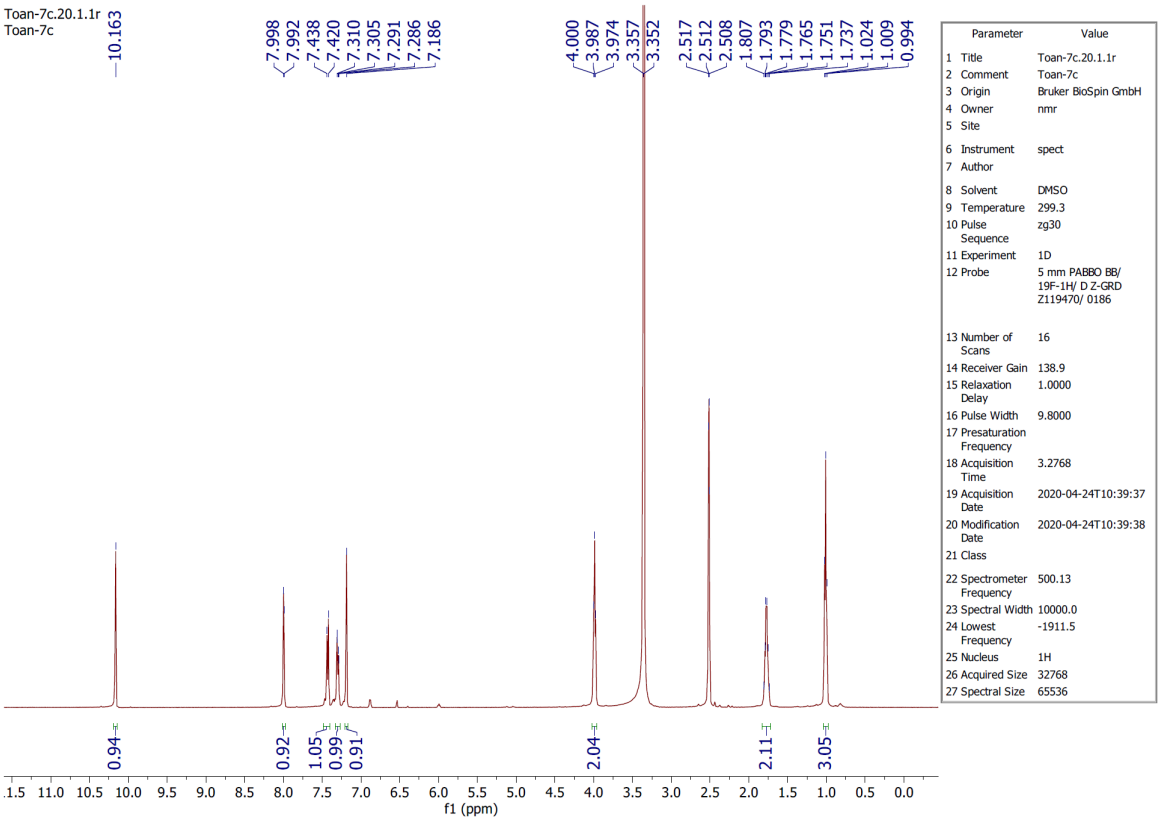
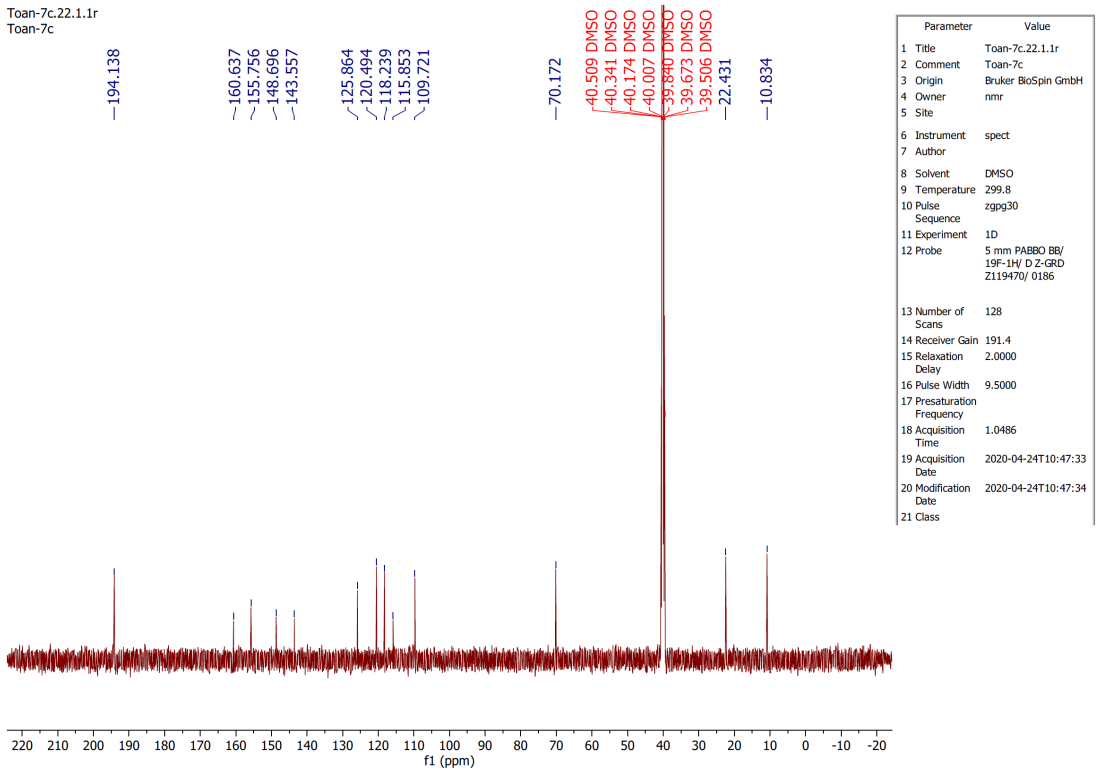




4-Formyl-7-propoxycoumarin ***(6c)***







	Parameter	Value
1	Title	Toan-7c.22.1.1r
2	Comment	Toan-7c
3	Origin	Bruker BioSpin GmbH
4	Owner	nmr
5	Site	
6	Instrument	spect
7	Author	
8	Solvent	DMSO
9	Temperature	299.8
10	Pulse Sequence	zgpg30
11	Experiment	1D
12	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0186
13	Number of Scans	128
14	Receiver Gain	191.4
15	Relaxation Delay	2.0000
16	Pulse Width	9.5000
17	Presaturation Frequency	
18	Acquisition Time	1.0486
19	Acquisition Date	2020-04-24T10:47:33
20	Modification Date	2020-04-24T10:47:34
21	Class	

Lab: Materials chemistry, Faculty of Chemistry, HUS-VNU
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Operator: Ms. Dao Thi Nhung
Mobile: 0948 119 043; Email: daothinhungtn@yahoo.com

Mass Spectrometer
LTQ Orbitrap XL™

Sample name :7OPr4ForCou
Mode: ESI, M+H

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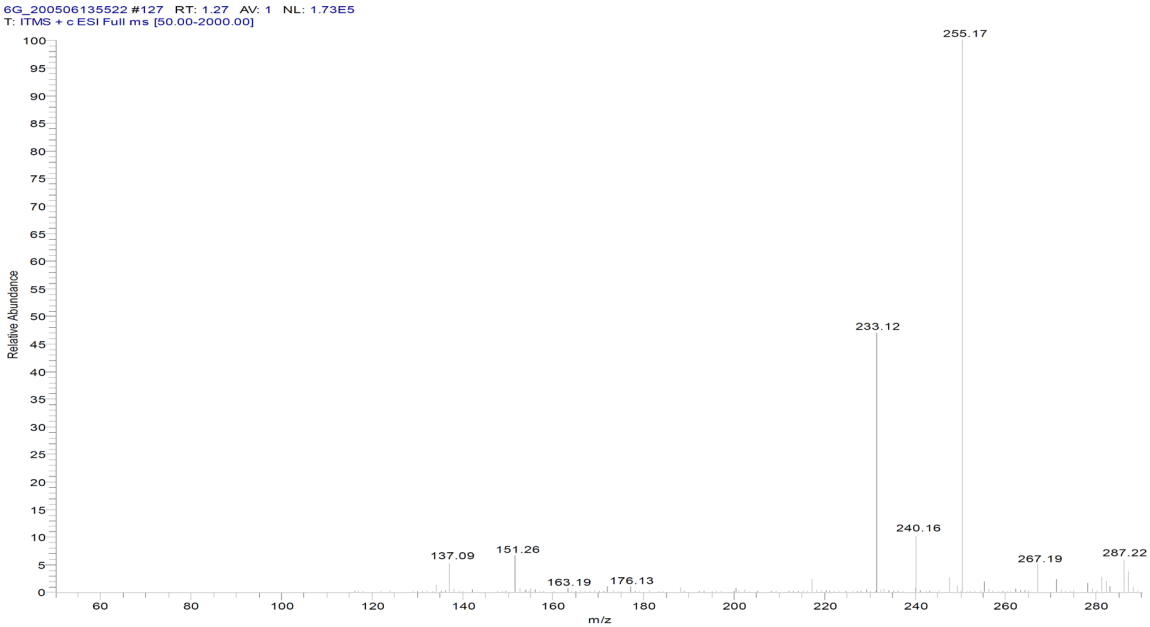
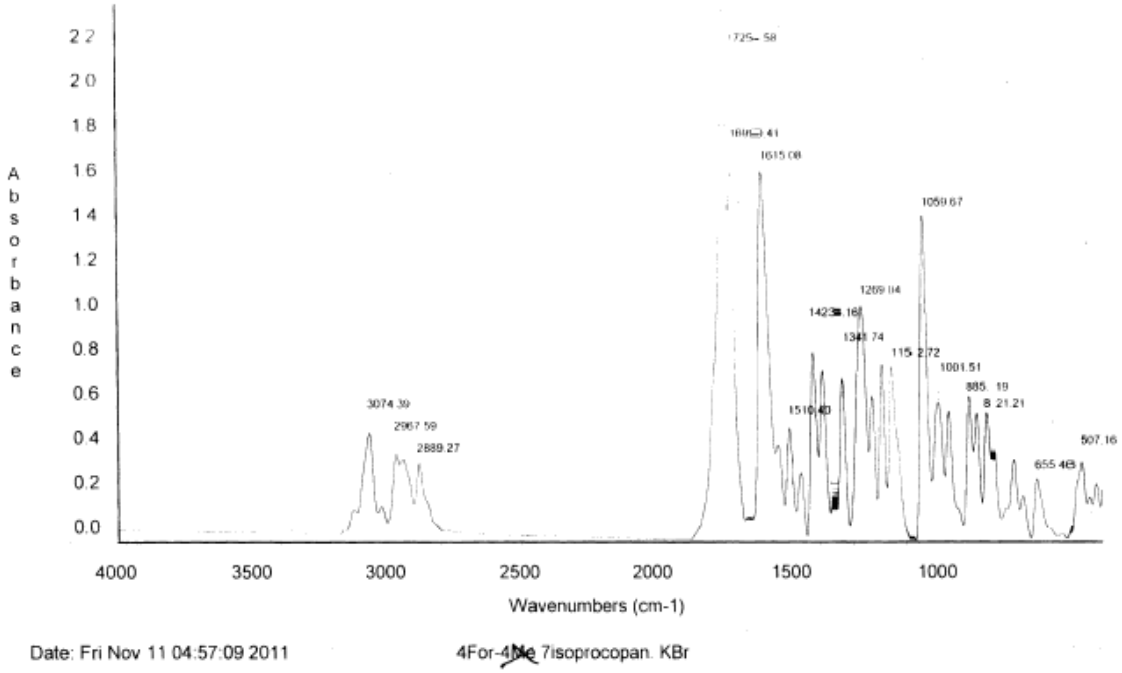
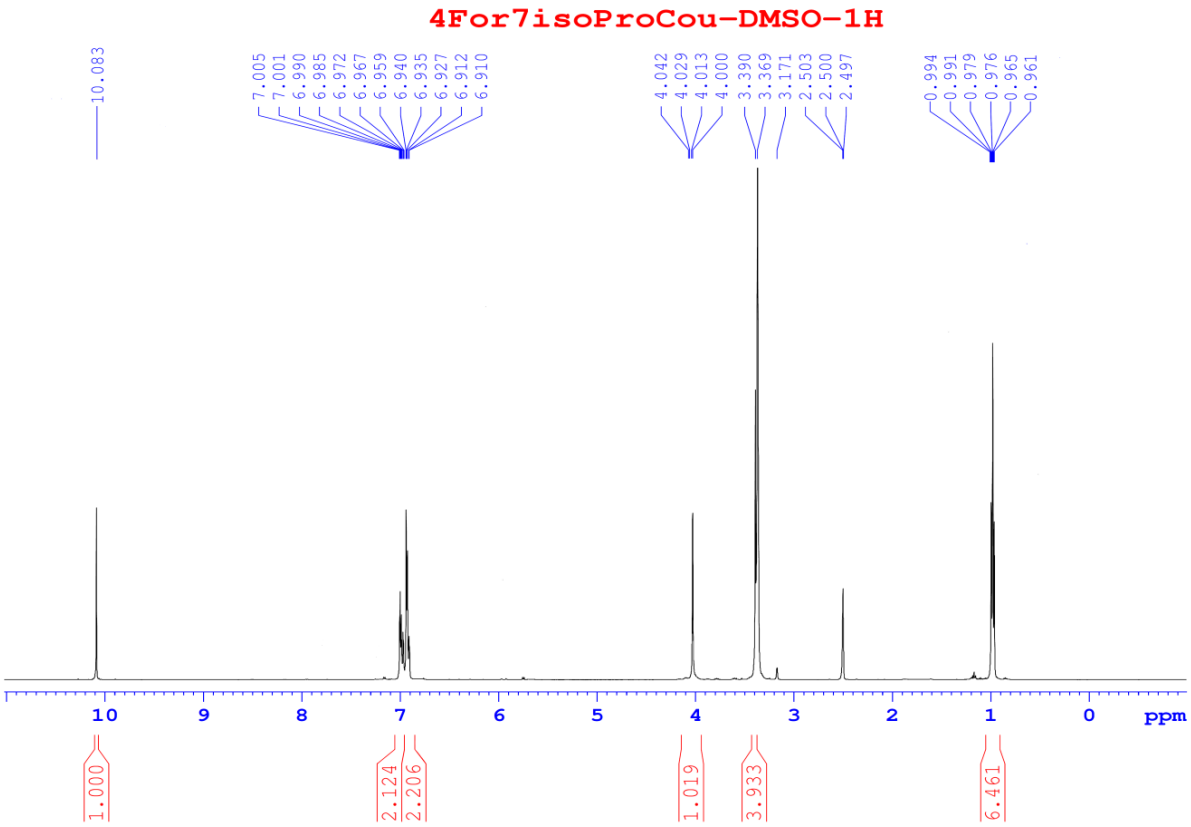
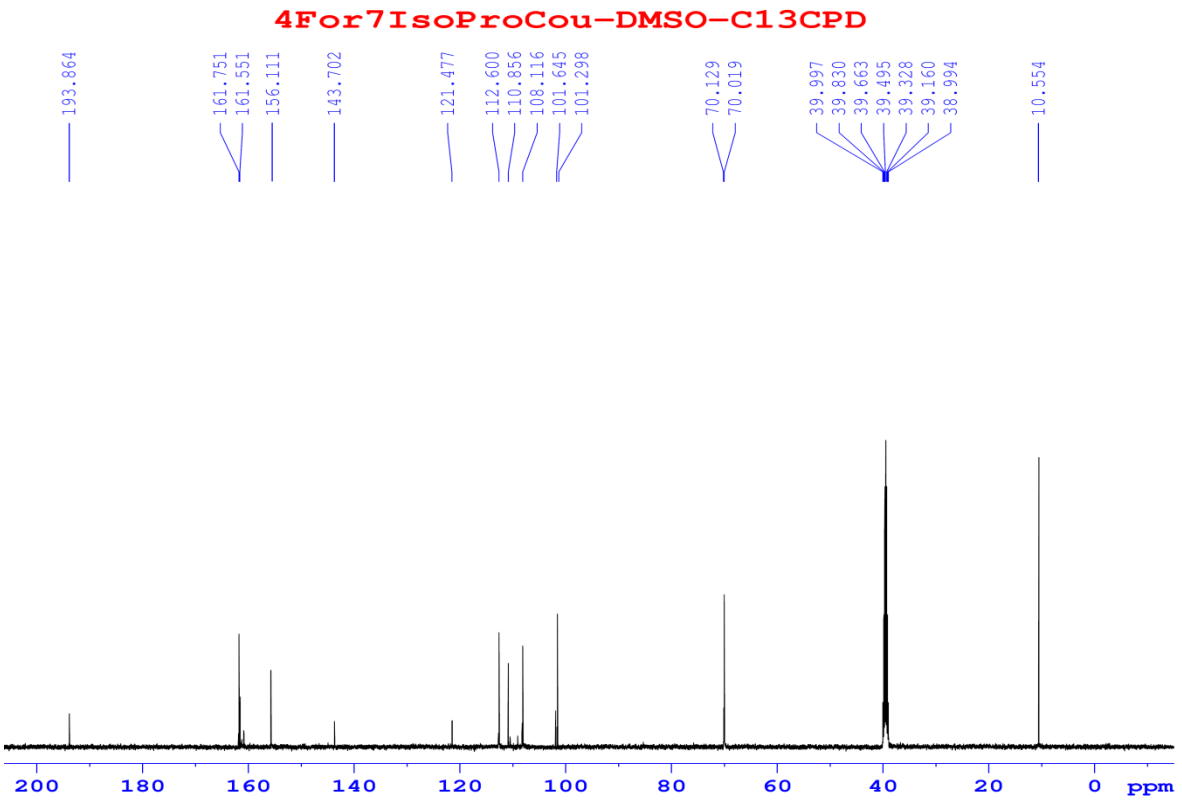


4-Formyl-7-isopropoxycoumarin ***(6d)***







Lab: Materials chemistry, Faculty of Chemistry, HUS-VNU
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Operator: Ms. Dao Thi Nhung
Mobile: 0948 119 043; Email: daothinhungtn@yahoo.com

Sample name : 7iOPr4ForCou
Mode: ESI, M+H

Mass Spectrometter
LTQ Orbitrap XL™

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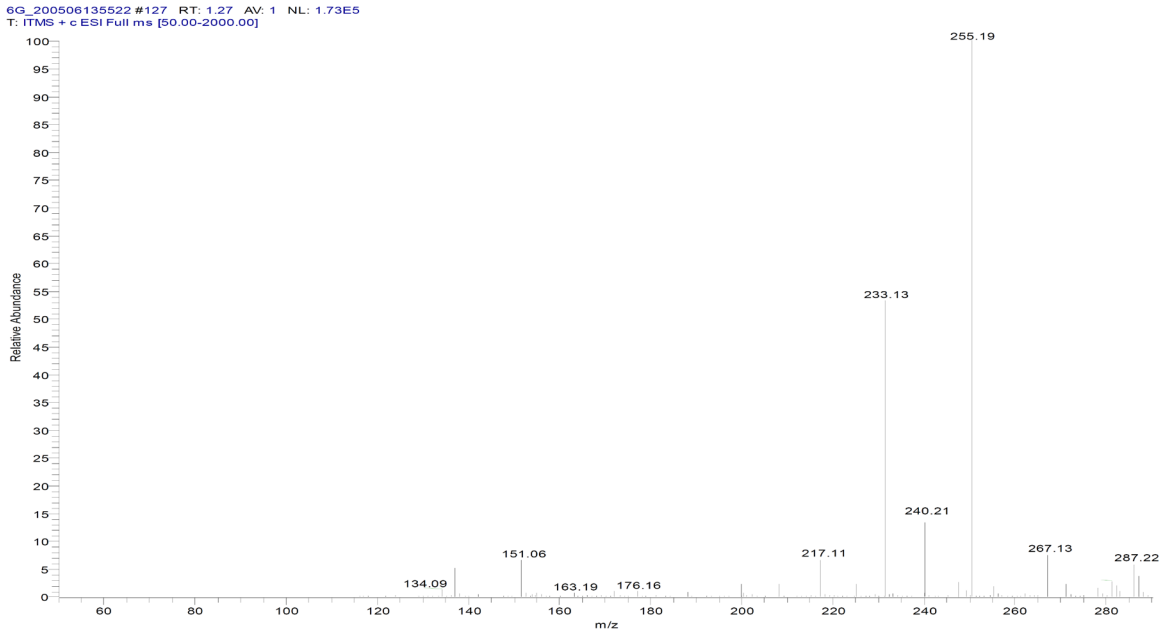
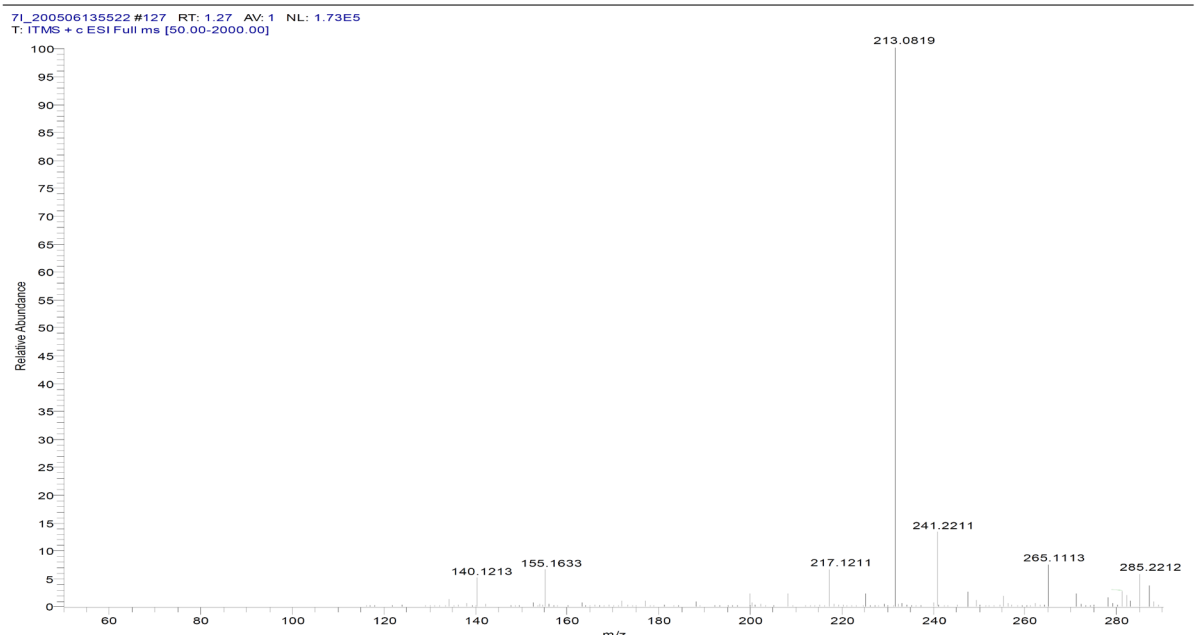
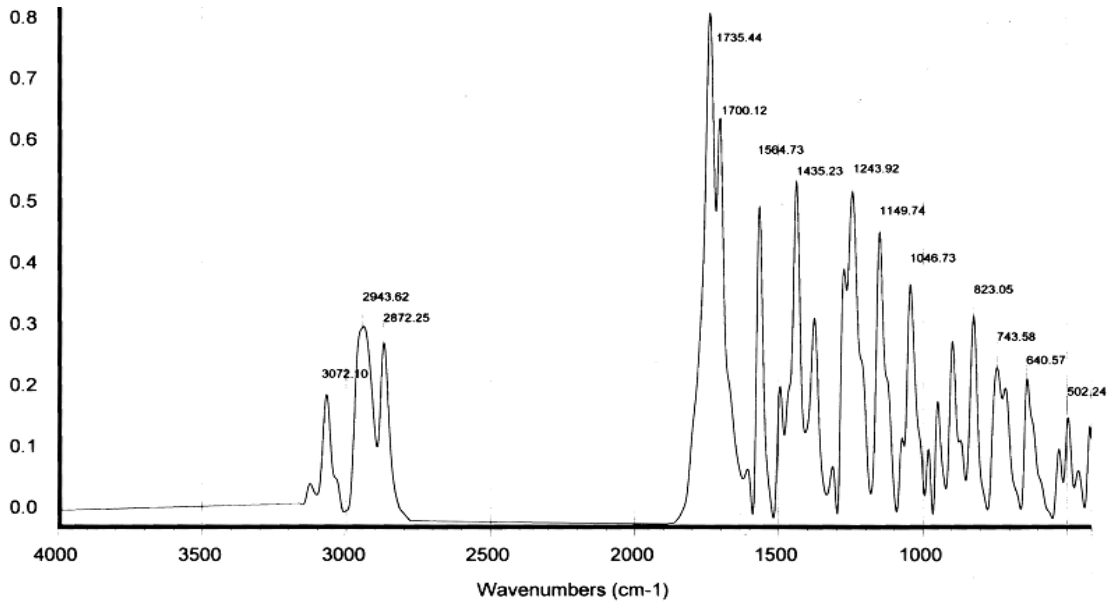
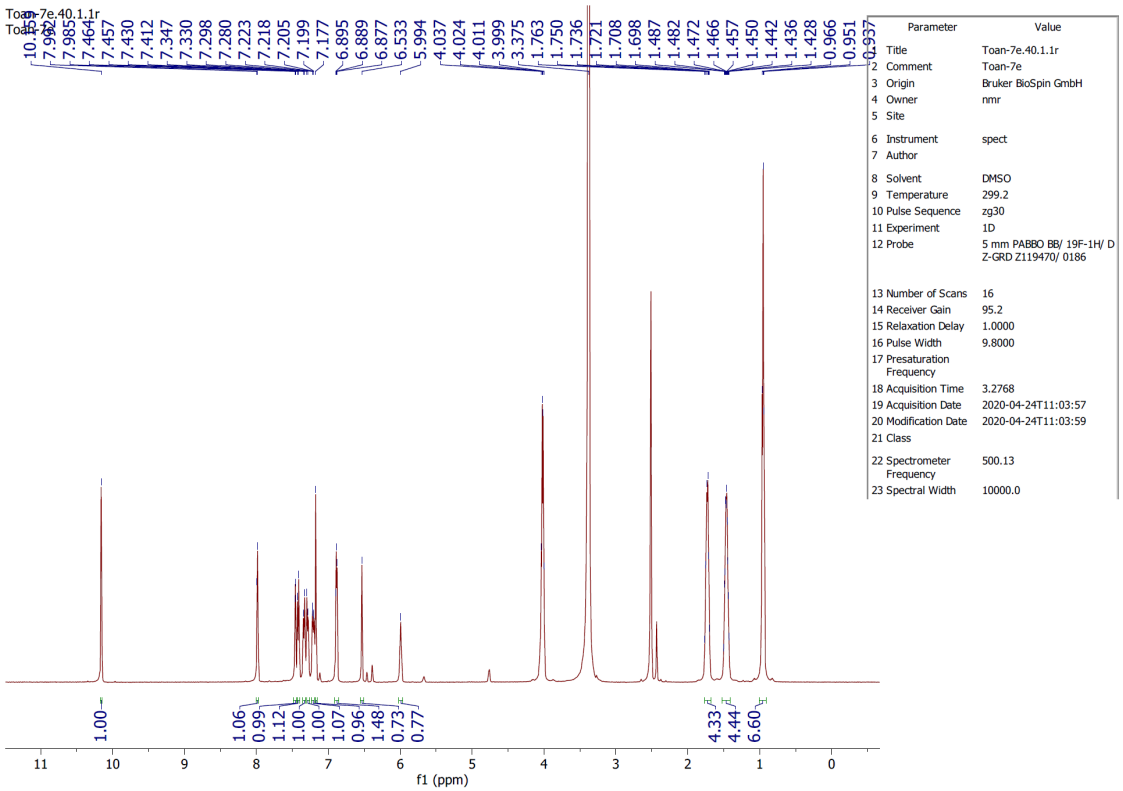
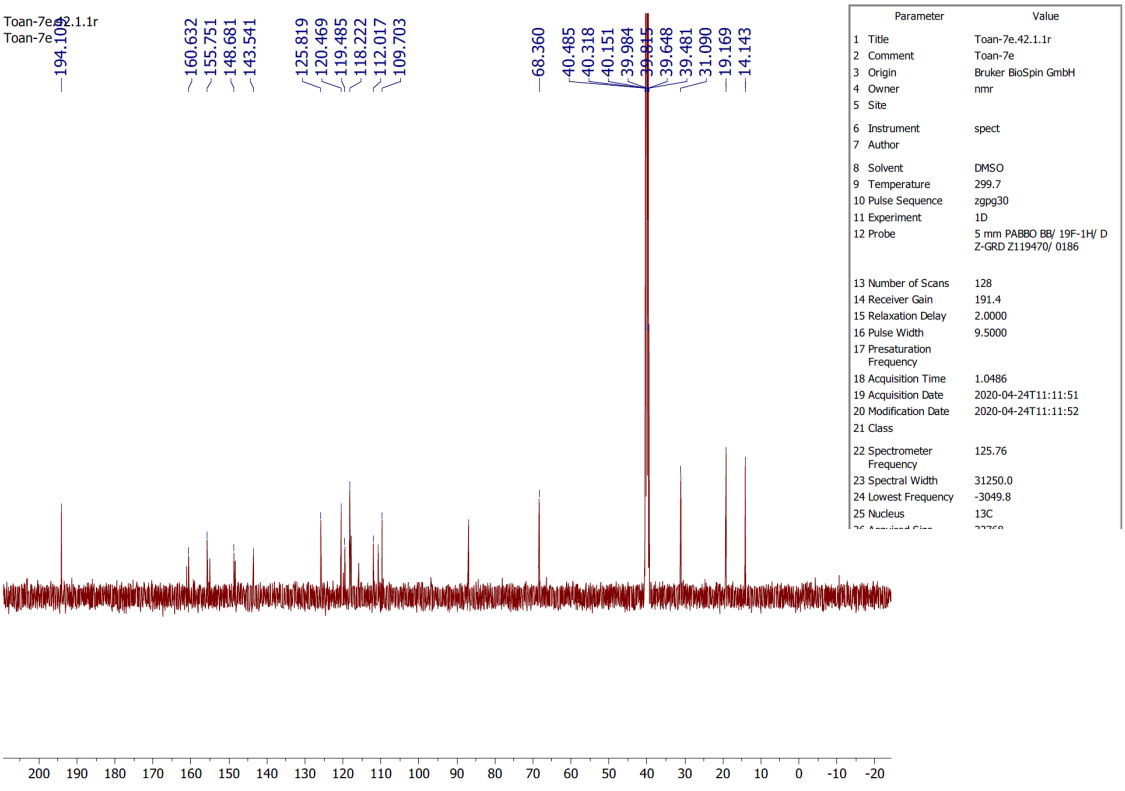




*4-Formyl-7-butoxycoumarin (**6e**)*




Toan-7e.40.1.1r
Toan-7e
10.132
7.992
7.985
7.464
7.457
7.430
7.412
7.347
7.330
7.298
7.280
7.223
7.218
7.205
7.199
7.177
6.895
6.889
6.877
6.533
5.994
4.037
4.024
4.011
3.999
3.375
1.763
1.750
1.736
1.721
1.708
1.698
1.487
1.482
1.472
1.466
1.457
1.450
1.442
1.436
1.428
0.966
0.951
0.937
1.00
1.06
0.99
1.12
1.00
1.00
1.07
0.96
1.48
0.73
0.77
4.33
4.44
6.60
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)
Parameter
Value
1 Title
Toan-7e.40.1.1r
2 Comment
Toan-7e
3 Origin
Bruker BioSpin GmbH
4 Owner
nmr
5 Site
6 Instrument
spect
7 Author
8 Solvent
DMSO
9 Temperature
299.2
10 Pulse Sequence
zg30
11 Experiment
1D
12 Probe
5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0186
13 Number of Scans
16
14 Receiver Gain
95.2
15 Relaxation Delay
1.0000
16 Pulse Width
9.8000
17 Presaturation Frequency
18 Acquisition Time
3.2768
19 Acquisition Date
2020-04-24T11:03:57
20 Modification Date
2020-04-24T11:03:59
21 Class
22 Spectrometer Frequency
500.13
23 Spectral Width
10000.0


Toan-7e.42.1.1r
Toan-7e
194.102
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143.541
125.819
120.469
119.485
118.222
112.017
109.703
68.360
40.485
40.318
40.151
39.984
39.815
39.648
39.481
31.090
19.169
14.143
200
190
180
170
160
150
140
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120
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80
70
60
50
40
30
20
10
0
-10
-20
Parameter
Value
1 Title
Toan-7e.42.1.1r
2 Comment
Toan-7e
3 Origin
Bruker BioSpin GmbH
4 Owner
nmr
5 Site
6 Instrument
spect
7 Author
8 Solvent
DMSO
9 Temperature
299.7
10 Pulse Sequence
zgpg30
11 Experiment
1D
12 Probe
5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0186
13 Number of Scans
128
14 Receiver Gain
191.4
15 Relaxation Delay
2.0000
16 Pulse Width
9.5000
17 Presaturation Frequency
18 Acquisition Time
1.0486
19 Acquisition Date
2020-04-24T11:11:51
20 Modification Date
2020-04-24T11:11:52
21 Class
22 Spectrometer Frequency
125.76
23 Spectral Width
31250.0
24 Lowest Frequency
-3049.8
25 Nucleus
13C

Lab: Materials chemistry, Faculty of Chemistry, HUS-VNU
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Operator: Ms. Dao Thi Nhung
Mobile: 0948 119 043; Email: daothinhungtn@yahoo.com

Sample name :7OBu4ForCou
Mode: ESI, M+H

Mass Spectrometter
LTQ Orbitrap XL™

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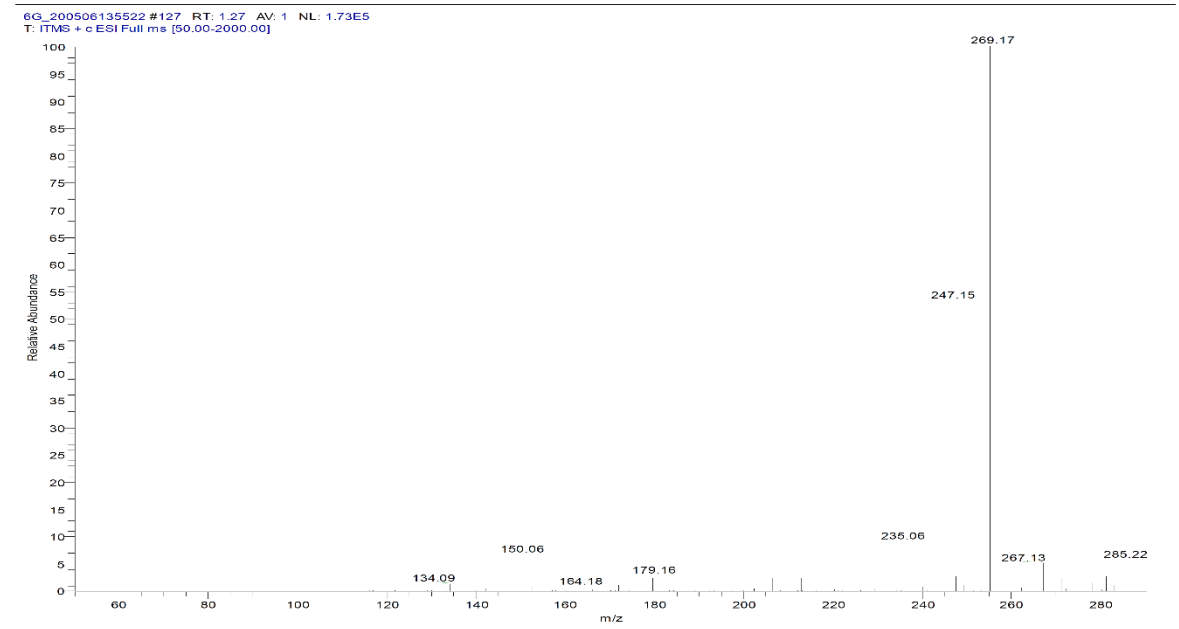
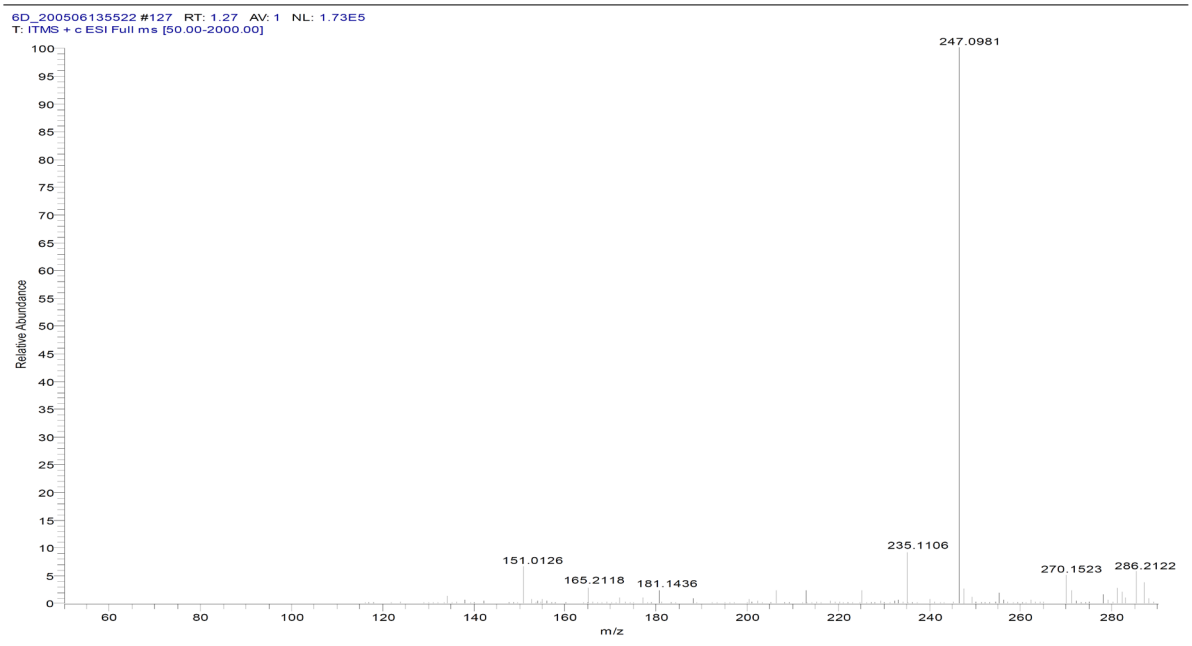
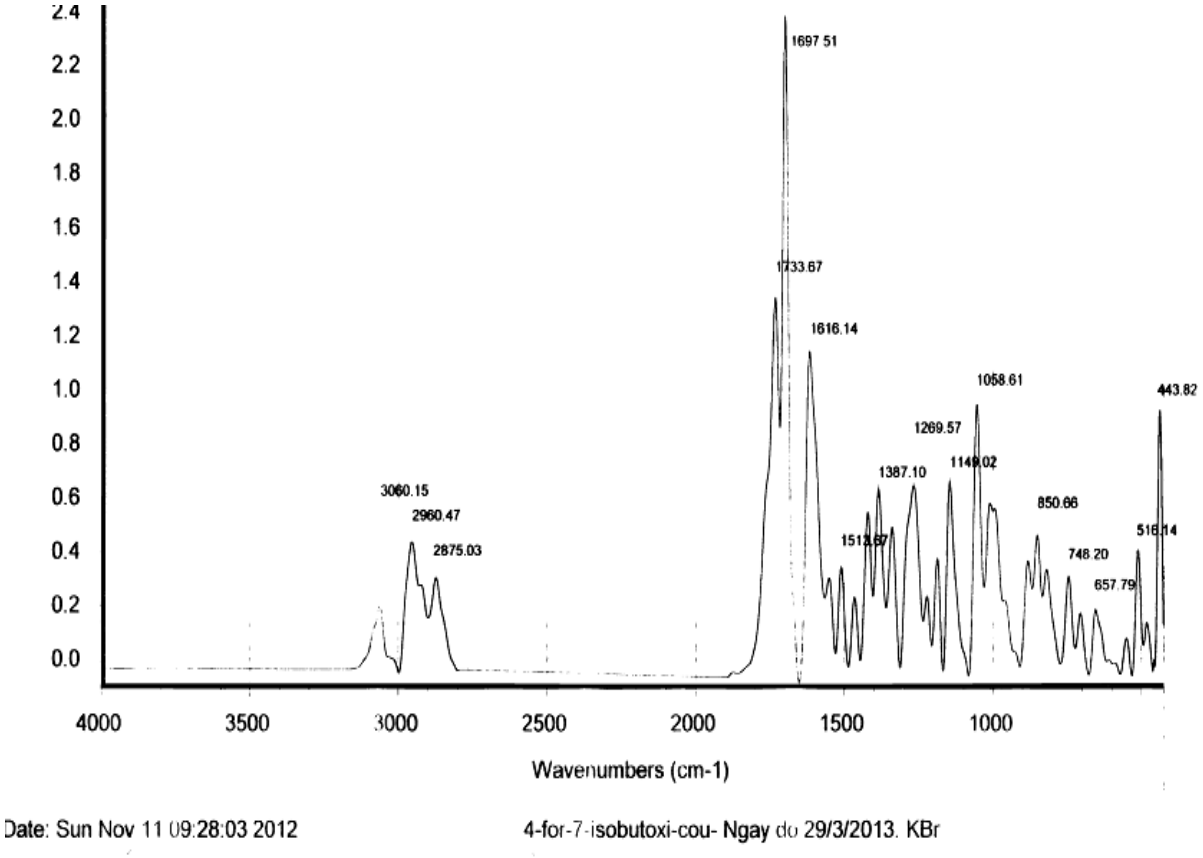
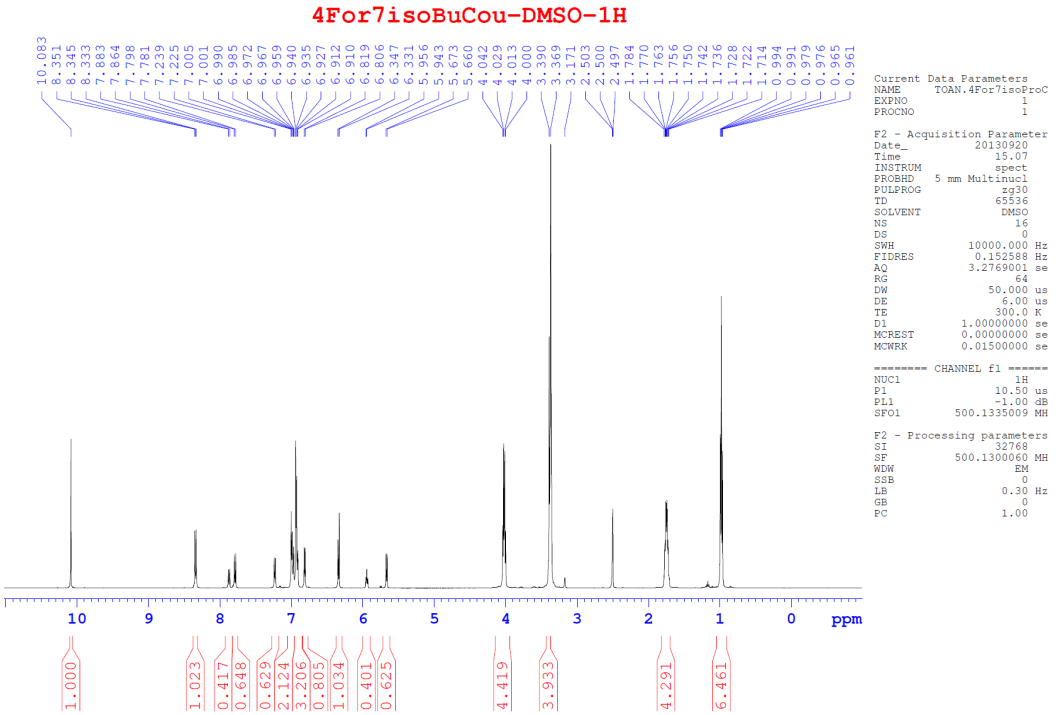
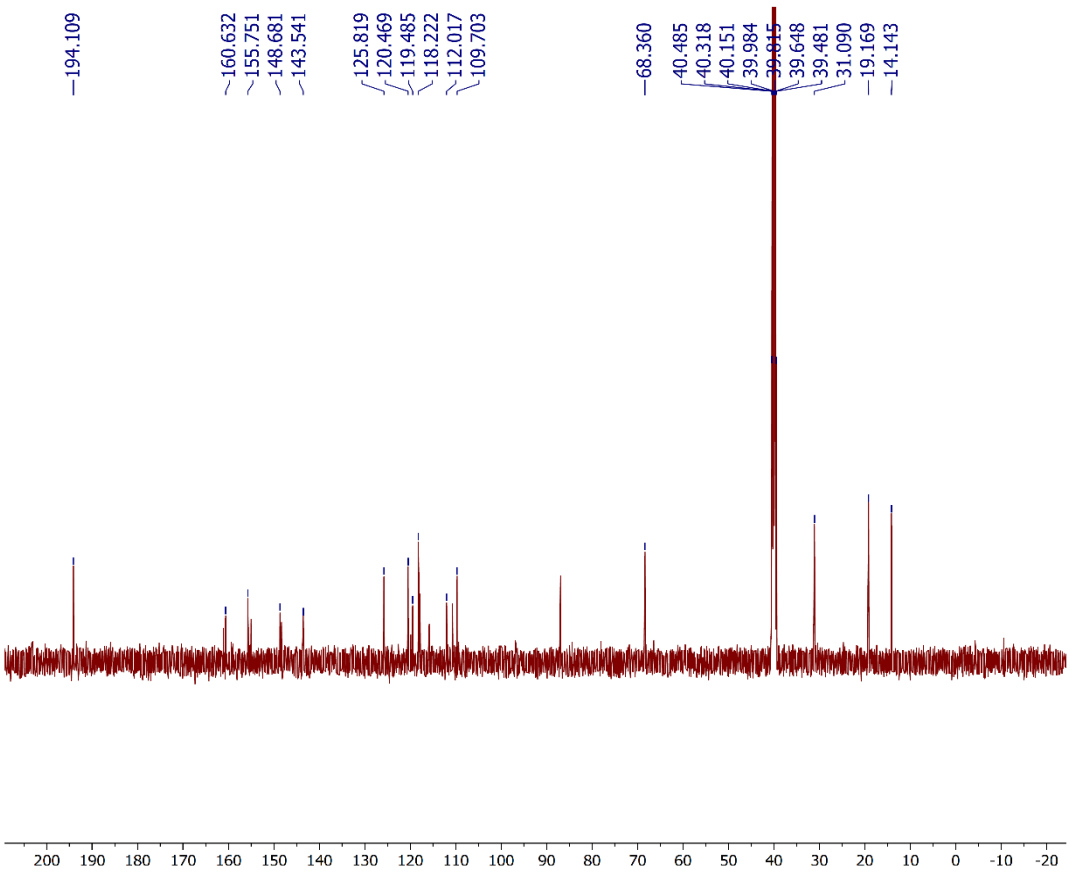




*4-Formyl-7-isobutoxycoumarin (**6f**)*







Lab: Materials chemistry, Faculty of Chemistry, HUS-VNU
19 Le Thanh Tong, Hoan Kiem, Ha Noi

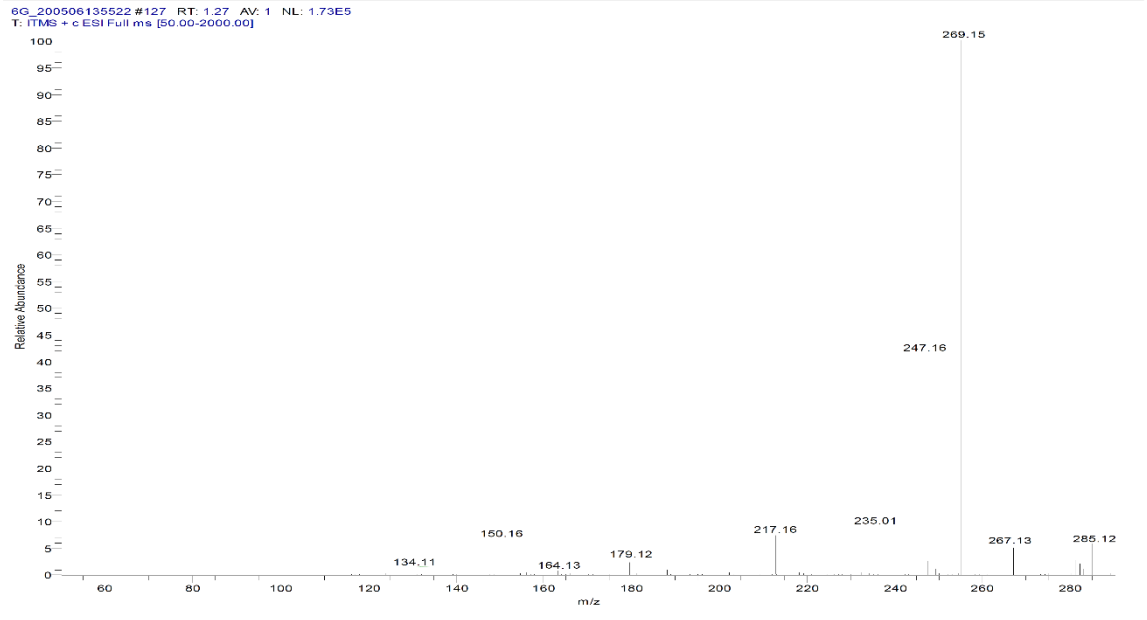
Tel: 844.38.253.053; **Fax**: 844.38.241.140 **Mail**: Chem.vnu@.edu.vn

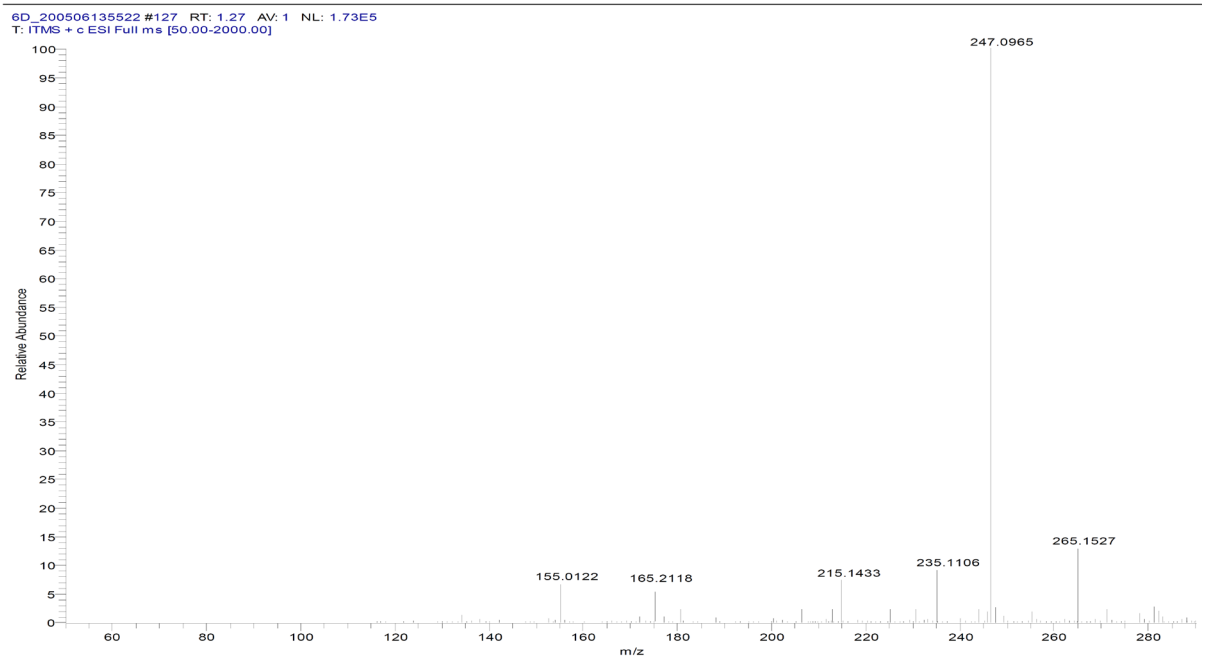
Operator: Ms. Dao Thi Nhung
Mobile: 0948 119 043; Email: daothinhungtn@yahoo.com

Sample name :7OBu4ForCou
Mode: ESI, M+H

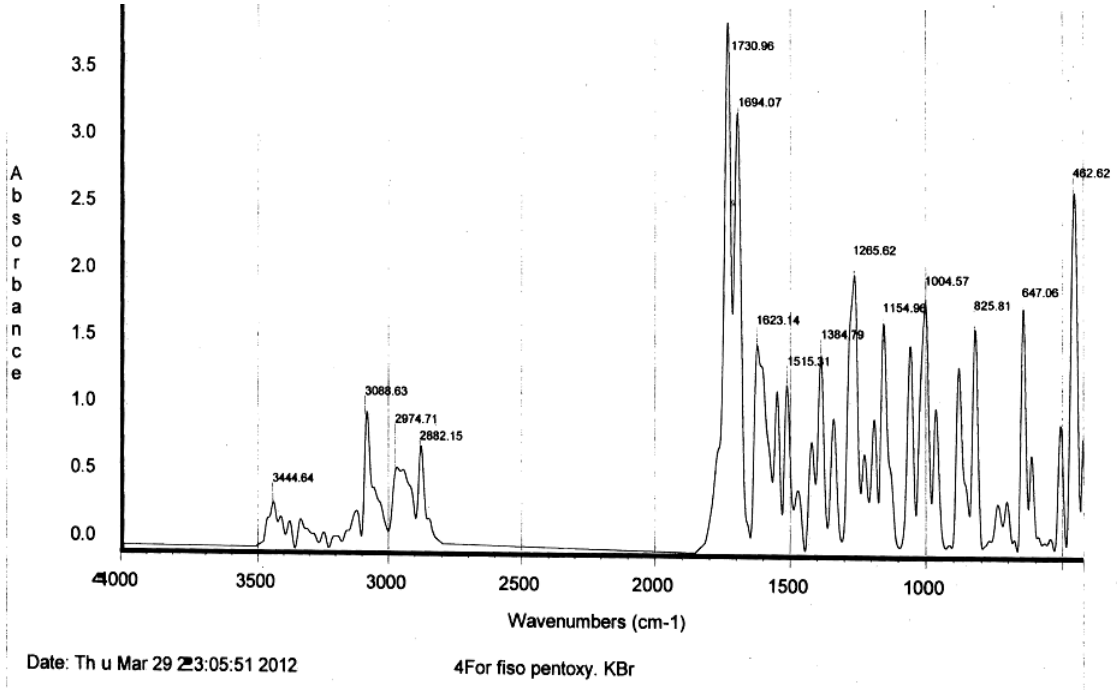
Mass Spectrometter
LTQ Orbitrap XL™

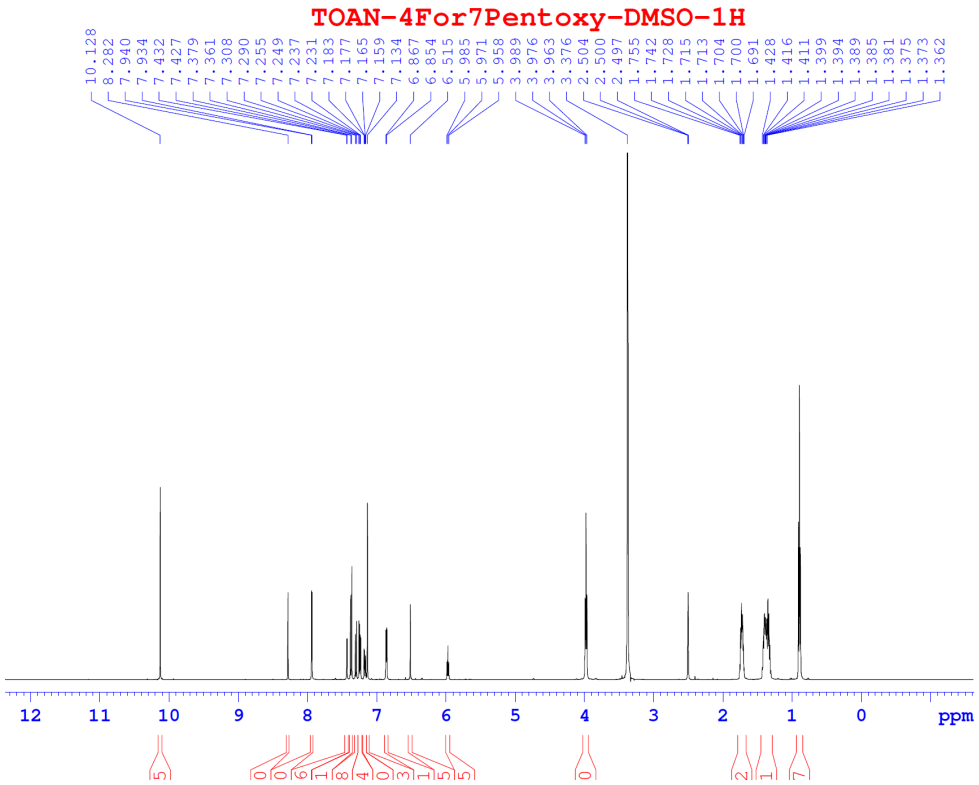
C:\LTQ Orbitrap\...\6G_200506135533 5/8/2020 5:06:43 PM





*4-Formyl-7-pentoxycoumarin (**6g**)*



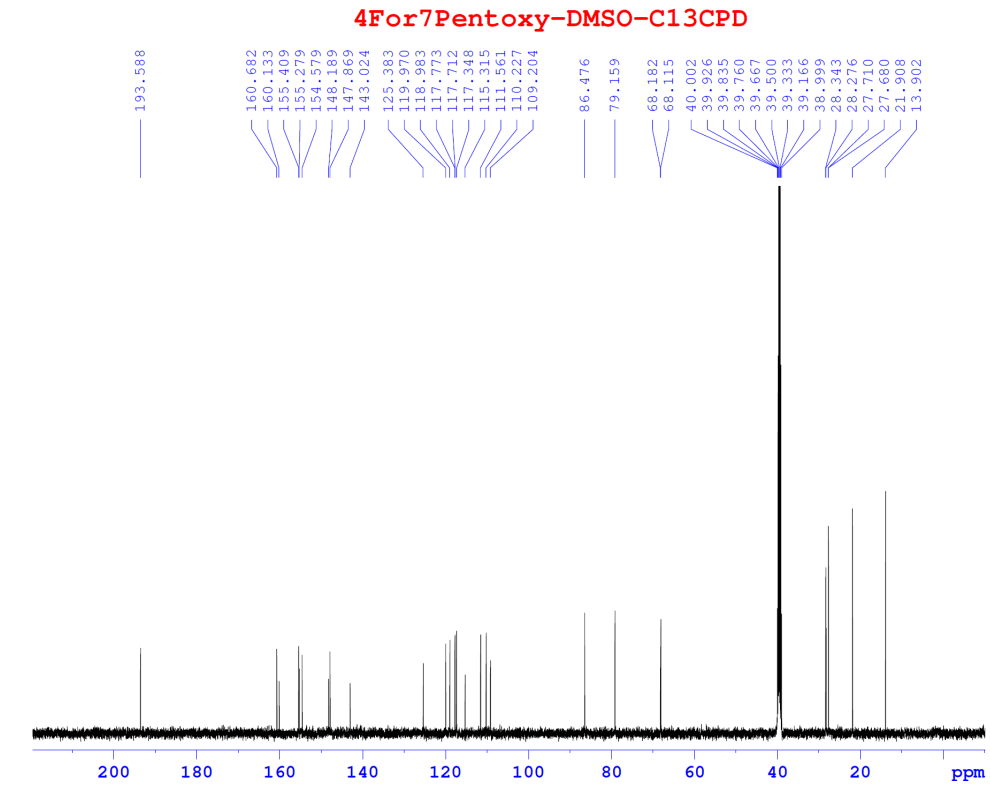



```
Current Data Parameters
NAME      TOAN.4For6Pentoxy
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameter
Date_           20130906
Time               11.27
INSTRUM            spect
PROBHD   5 mm Multinucl
PULPROG            zg30
TD                65536
SOLVENT            DMSO
NS                    16
DS                     0
SWH            10000.000 Hz
FIDRES             0.152588 Hz
AQ             3.2769001 se
RG                    57
DW                50.000 us
DE                 6.00 us
TE                300.0 K
D1             1.00000000 se
MCREST         0.00000000 se
MCWRK          0.01500000 se

======== CHANNEL f1 ======
NUC1                  1H
P1                10.50 us
PL1               -1.00 dB
SFO1         500.1335009 MH

F2 - Processing parameters
SI                32768
SF           500.1300063 MH
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

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Current Data Parameters
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EXPNO                     2
PROCNO                    1

F2 - Acquisition Paramet
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Time               13.43
INSTRUM            spect
PROBHD   5 mm Multinucl
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                   128
DS                     2
SWH            31446.541
FIDRES             0.479836
AQ             1.0420883
RG                 32768
DW                15.900
DE                 6.00
TE                300.0
D1             2.00000000
d11            0.03000000
DELTA          1.89999998
MCREST         0.00000000
MCWRK          0.01500000

======== CHANNEL f1 =====
NUC1                 13C
P1                 5.00
PL1               -1.00
SFO1         125.7716224

======== CHANNEL f2 =====
CPDPRG2          waltz16
NUC2                  1H
PCPD2             80.00
PL2               -1.00
PL12              16.64
PL13              22.00
SFO2         500.1320005

F2 - Processing paramete
SI                32768
SF           125.7578442
WDW                  EM
SSB                   0
LB                 1.00
GB                    0
```

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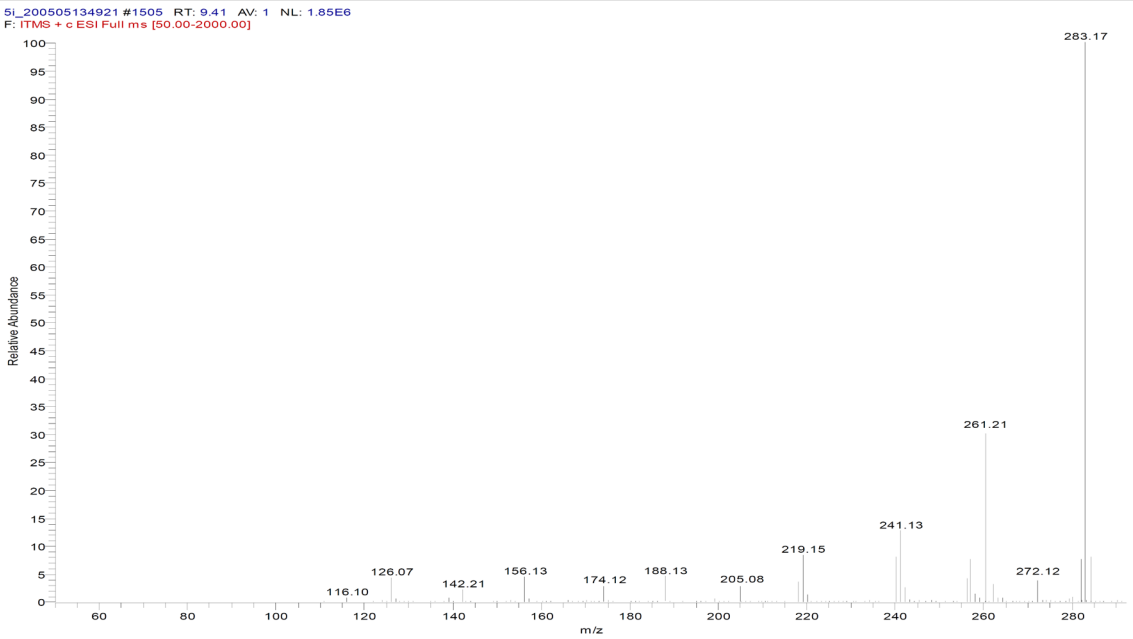
Tel: 844.38.253.053; **Fax**: 844.38.241.140 **Mail**: Chem.vnu@.edu.vn

Operator: Ms. Dao Thi Nhung
Mobile: 0948 119 043; Email: daothinhungtn@yahoo.com

SAMPLE:7OPn4ForCou
Mode: ESI, M+H

Mass Spectrometter
LTQ Orbitrap XL™
Solvent: MeOH/DCM

C:\LTQ Orbitrap\...\5i_200505134921 5/5/2020 1:49:21 PM



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Operator: Ms. Dao Thi Nhung
Mobile: 0948 119 043; Email: daothinhungtn@yahoo.com

SAMPLE:7OPn4ForCou
Mode: ESI, M+H

Mass Spectrometter
LTG Orbitrap XL™
ThermoSCIENTIFIC company

Resolution: >60 000 Dt
Sensitivity: 10^{-14}
Tandem: n>= 15
Mass Accuracy: <= 2ppm

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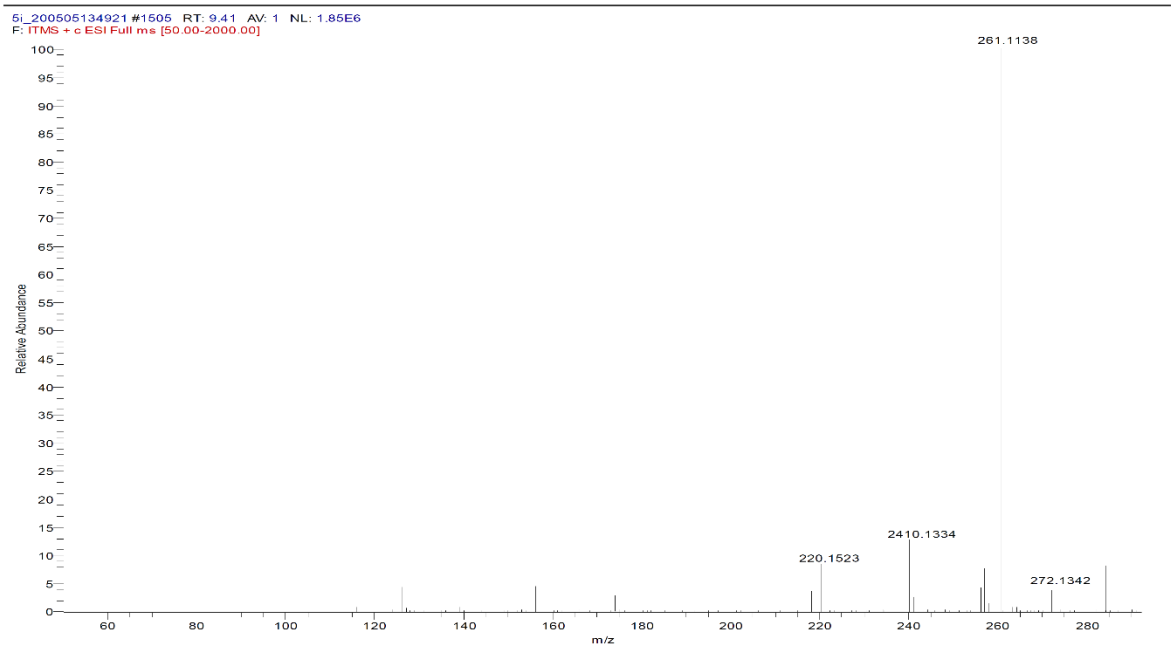

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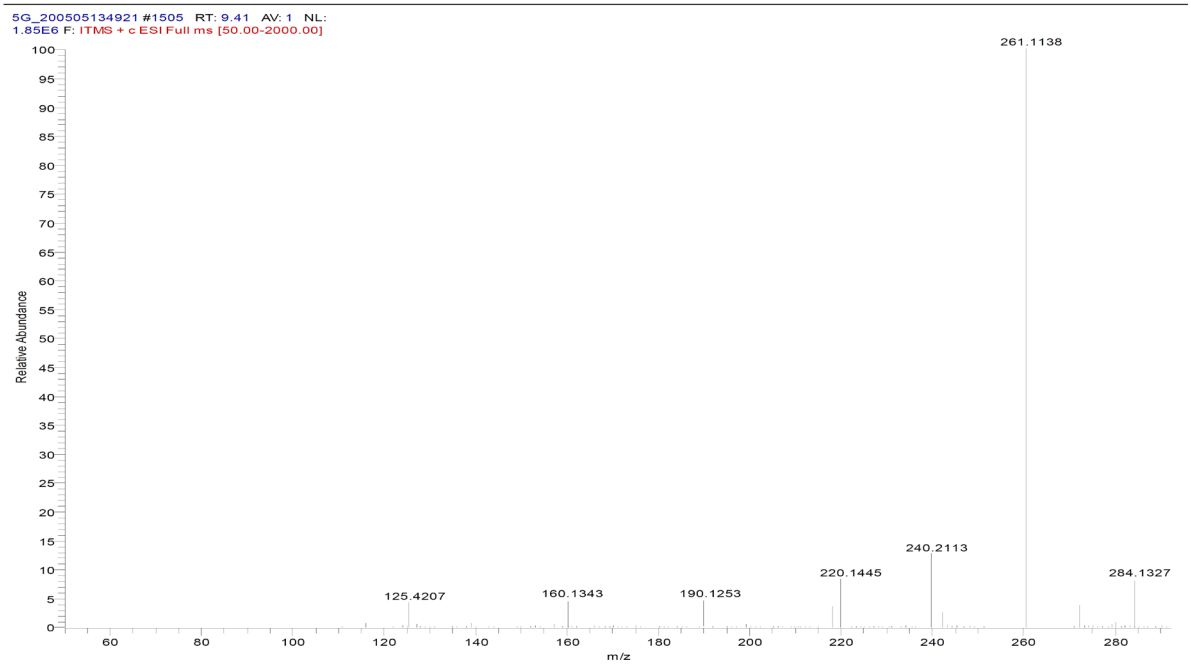
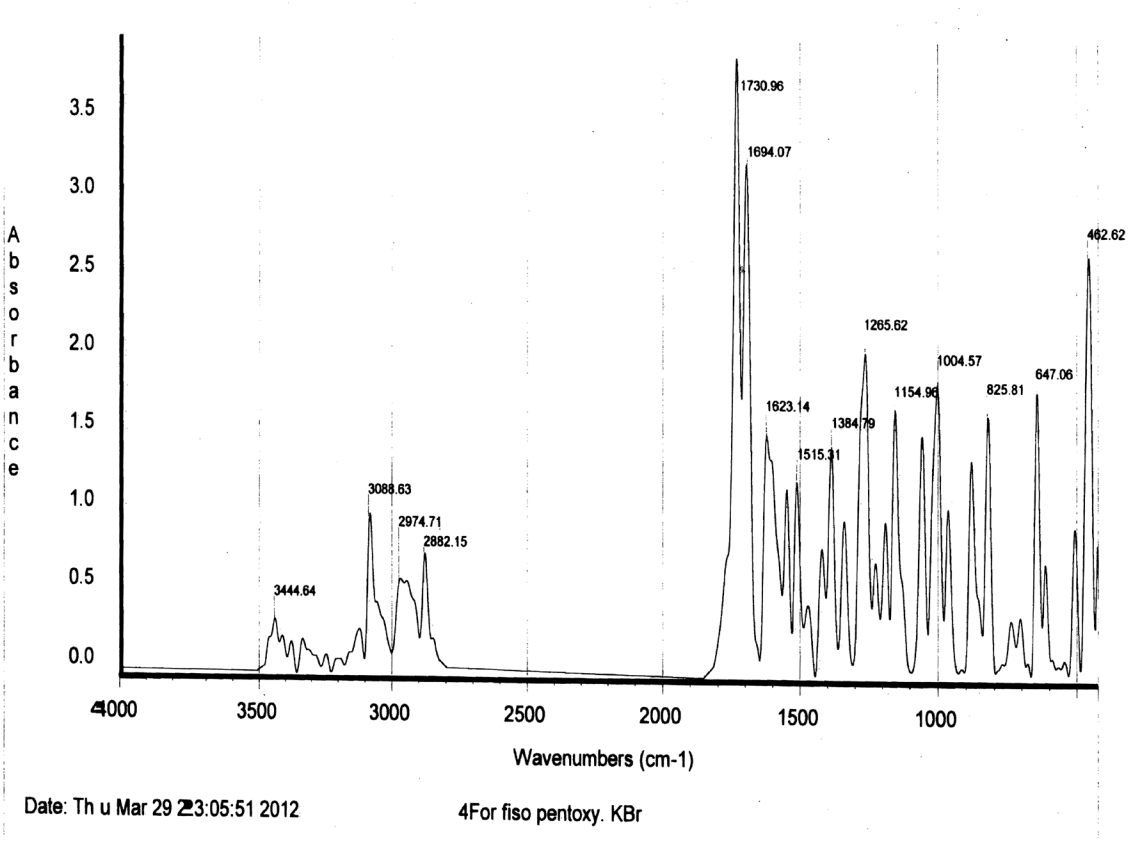
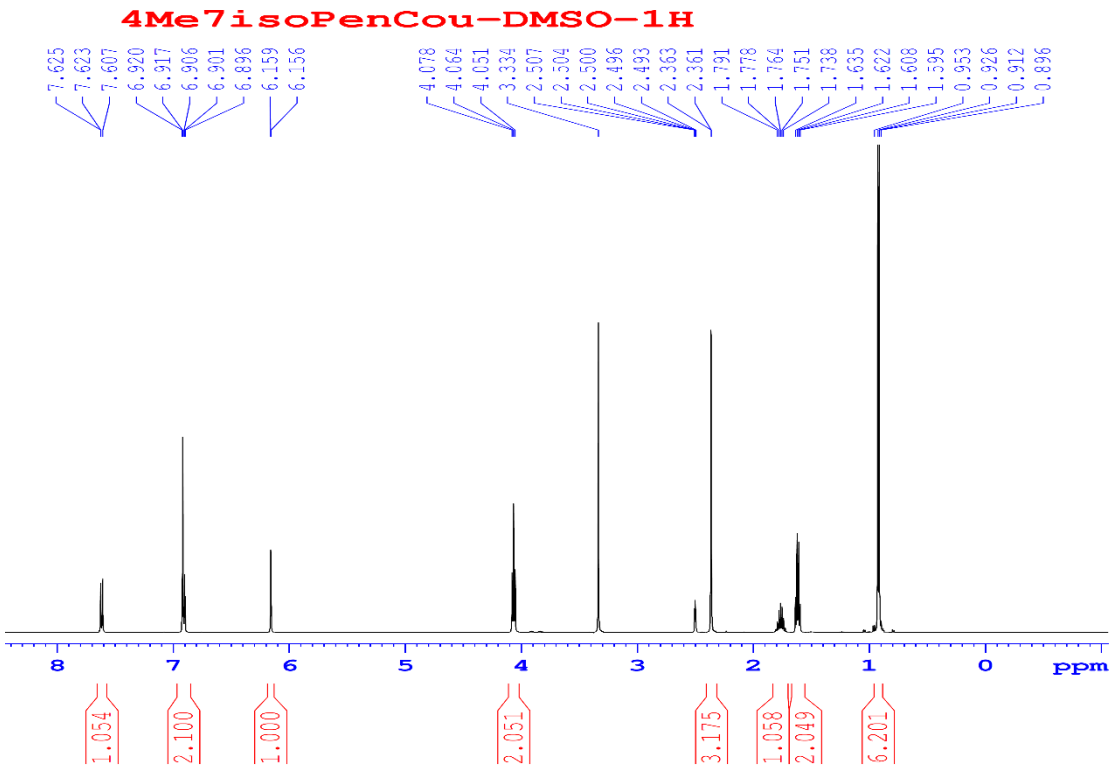
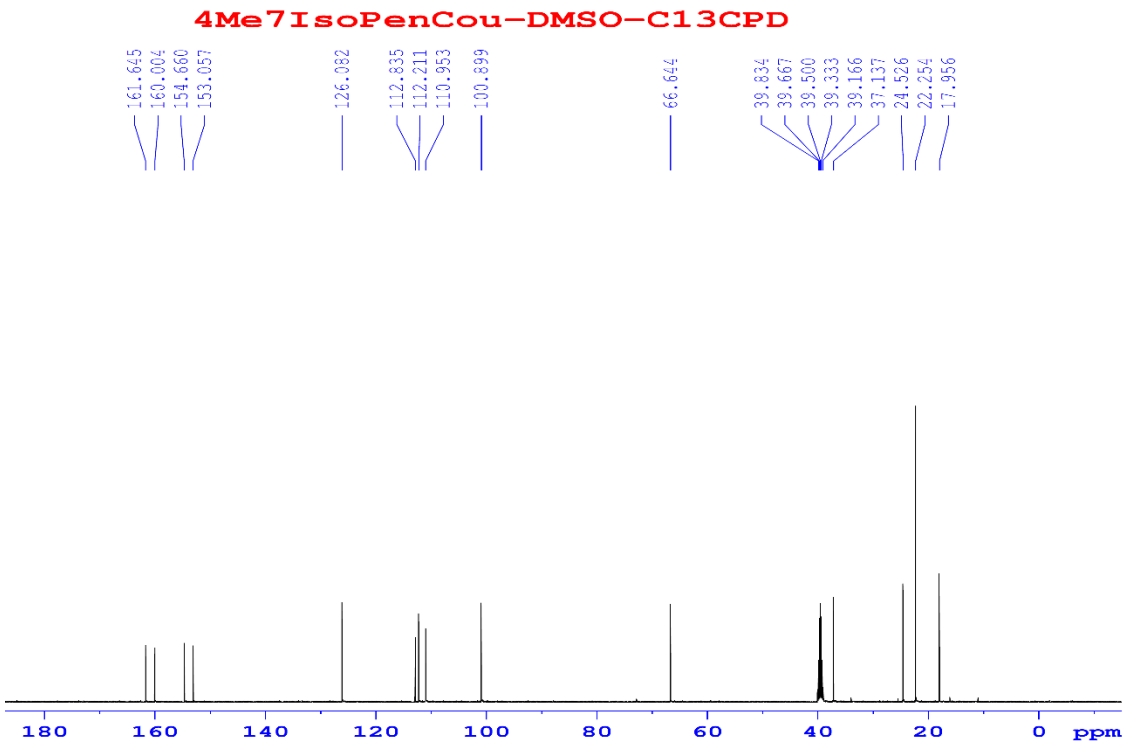


*4-Formyl-7-isopentoxycoumarin (**6h**)*







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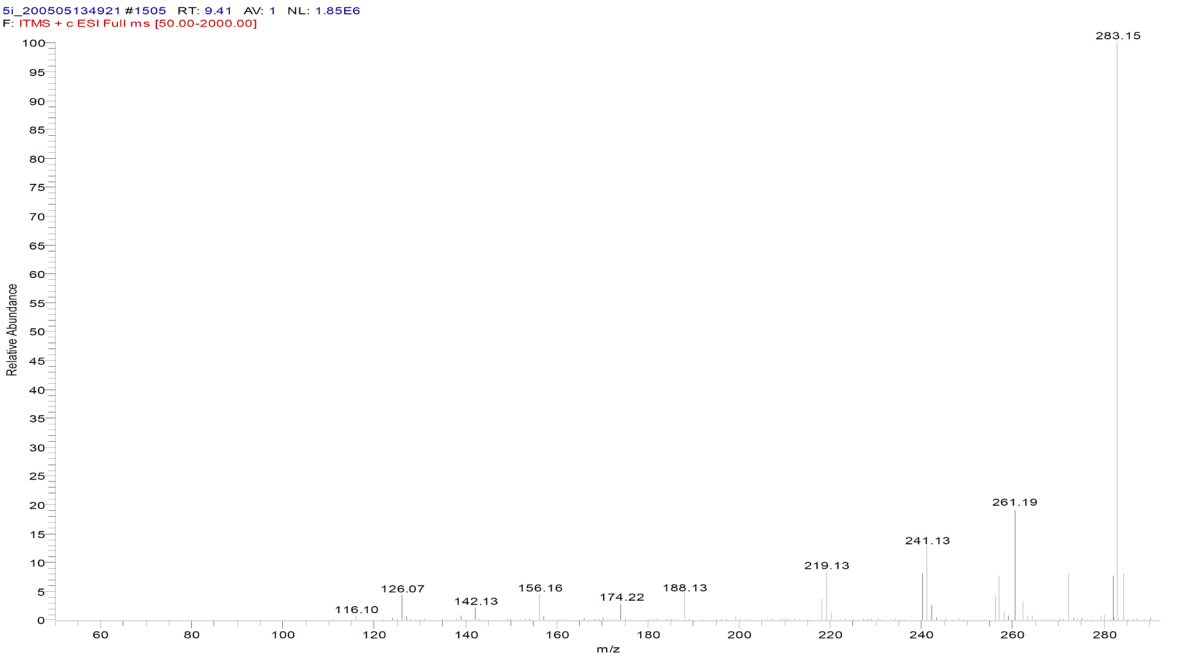
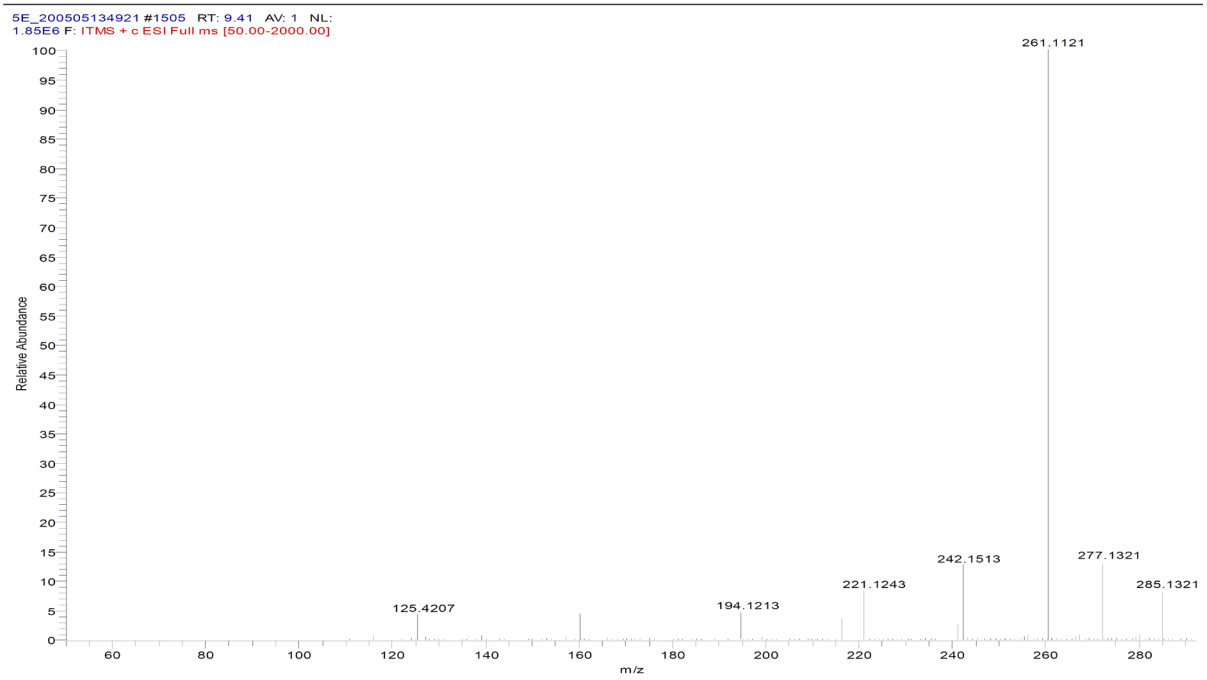
Operator: Ms. Dao Thi Nhung
Mobile: 0948 119 043; Email: daothinhungtn@yahoo.com

SAMPLE:7OiPn4ForCou
Mode: ESI, M+H

Mass Spectrometter
LTQ Orbitrap XL™
Solvent: MeOH/DCM

C:\LTQ Orbitrap\...\5i_200505134921 5/5/2020 1:49:21 PM





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