Electronic Supplementary Material (ESI) for RSC Advances.

Green Chemical Approach: Microwave assisted, titanium dioxide nanoparticles catalyzed, convenient and efficient C-C bond formation in the synthesis of highly functionalized quinolines and quinolinones

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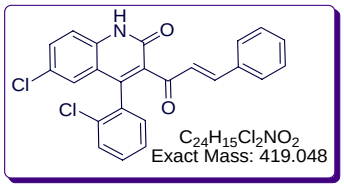
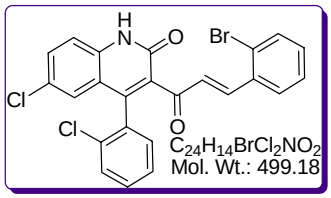
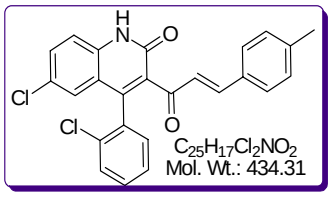


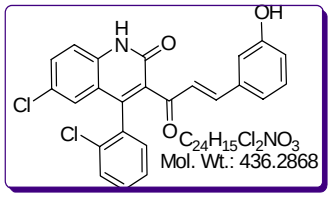
White solid, m.p 222 – 224 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.75 (s, 1H), 7.54 - 7.50 (d, *J* = 16.4 Hz, 1H), 7.48 - 7.43 (m, 3H), 7.42 - 7.42 (m, 2H), 7.39 - 7.33 (m, 5H), 7.31 - 7.29 (dd, *J* = 6.7, 2.8 Hz, 1H), 7.02 (s, 1H), 6.83 - 6.79 (d, *J* = 16.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.7, 161.5, 146.7, 146.1, 136.4, 134.1, 132.4, 132.4, 132.2, 131.7, 131.3, 130.6, 130.6, 129.7, 128.7, 128.6, 128.4, 127.0, 126.5, 126.0, 119.9, 117.9; IR (v, cm^{-1}) 3152 (-N-H), 2999, 2907, 2860, 2829, 1665, 1639, 1605, 1485, 1406, 1367, 1242, 1202, 1178, 1068, 978, 951, 885, 827, 759, 738, 712, 596, 561; UPLC - MS: m/e 420.18 [M+] , $C_{24}H_{15}Cl_2NO_2$ required Mol.Wt.: 419.05.



White solid, m.p 218 – 220 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.19 (s, 1H), 7.879 - 7.84 (d, *J* = 16.0 Hz, 1H), 7.59 - 7.58 (d, *J* = 7.6 Hz, 1H), 7.56 - 7.54 (d, *J* = 8.0 Hz, 1H), 7.47 - 7.46 (d, *J* = 7.2 Hz ,1H), 7.43 - 7.38 (m, 2H), 7.35 - 7.29 (m, 4H), 7.24 - 7.20 (t, *J* = 7.6 Hz, 1H), 7.01 (s, 1H), 6.83 - 6.79 (d, *J* = 16.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.5, 161.9, 147.6, 143.9, 136.8, 134.2, 133.6, 132.7, 132.4, 132.3, 131.9, 131.7, 131.3, 130.8, 129.9, 128.9, 128.8, 127.9, 127.7, 127.1, 126.2, 120.3, 118.3; IR (v, cm^{-1}) 3143, 3063, 3024, 2989, 2901, 2864, 2833, 2737, 1688, 1649, 1601, 1553, 1483, 1466, 1435, 1406, 1369, 1340, 1263, 1173, 1088, 1057, 1024, 978, 912, 829, 758, 744, 569; UPLC - MS: m/e 500.07 [M+], $C_{24}H_{14}BrCl_2NO_2$ required Mol.Wt.:499.18.

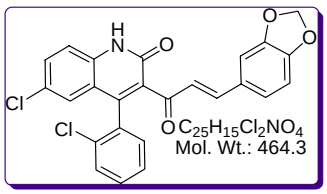


White solid, m.p 280 – 282 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.19 (s, 1H), 7.51 - 7.47 (d, *J* = 16.4, 1H), 7.44 - 7.39 (m, 3H), 7.37 - 7.33 (m, 4H), 7.31 - 7.29 (d, *J* = 6.4 Hz, 1H), 7.17 - 7.15 (m, 2H), 7.02 (s, 1H), 6.77 - 6.73 (d, *J* = 16.4 Hz, 1H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) 192.9, 161.8, 146.6, 146.5, 141.4, 136.4, 132.5, 132.5, 132.2, 131.6, 131.3, 131.3, 130.5, 129.7, 129.5, 128.5, 127.1, 125.9, 125.7, 119.9, 118.2, 21.4.; IR (v, cm^{-1}) 3144, 3076, 3021, 2986, 2903, 2862, 2829, 2787, 2733, 1682, 1643, 1595, 1560, 1433, 1408, 1367, 1180, 1030, 989, 914, 746, 559.; UPLC - MS: m/e 434.20, $C_{25}H_{17}Cl_2NO_2$ required Mol.Wt.: 434.31

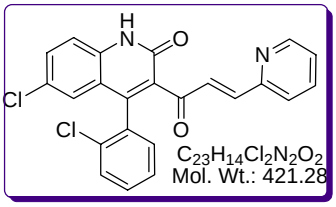


White solid, m.p 170 – 172 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.15 (s, 1H), 7.70 - 7.66 (d, *J* = 15.6 Hz, 1H), 7.47 - 7.43 (m, 4H), 7.15 - 7.12 (m, 2H), 6.95 - 6.90 (m, 3H), 6.84 - 6.79 (m, 3H); ^{13}C NMR (100 MHz, DMSO-d6) δ 193.2, 159.5, 157.5, 146.5, 144.6, 137.1, 135.1, 132.9, 131.9, 131.4, 131.2, 131.1, 130.2, 129.5, 127.5, 126.7, 126.5, 124.9, 120.0, 119.4, 118.3,

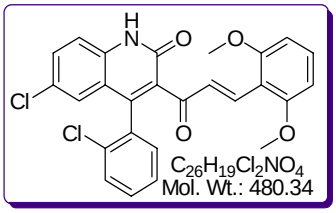
117.9, 114.6; IR (v, cm^{-1}) 3173, 3063, 2907, 2866, 2833, 2733, 1680, 1639, 1603, 1585, 1485, 1469, 1447, 1404, 1369, 1281, 1254, 1219, 1177, 1089, 1070, 1057, 1024, 982, 877, 822, 783, 766, 744, 714. UPLC - MS: m/e 436.23, $C_{24}H_{15}Cl_2NO_3$ required Mol.Wt .: 436.29.



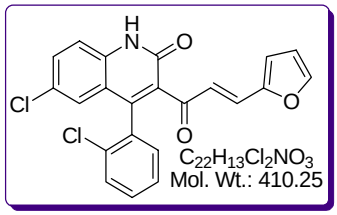
White solid, m.p 238 – 240 °C, ^{1}H NMR (400 MHz, DMSO-D6) δ 12.37 (s, 1H), 7.64 - 7.62(d, *J* = 8.8 Hz, 1H), 7.56 - 7.54 (d, *J* = 8.0 Hz, 1H), 7.49 - 7.45 (m, 2H), 7.42 - 7.36 (m, 2H), 7.31 - 7.29 (d, *J* = 7.2 Hz, 1H), 7.25 (s, 1H), 7.14 - 7.12 (d, *J* = 8.0 Hz , 1H), 6.92 - 6,89 (d, *J* = 8.0 Hz, 1H), 6.76 (s, 1H), 6.64 - 6.60 (d, *J* = 16.0 Hz, 1H), 6.03 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d6) δ 193.1, 159.5, 149.9, 148.0, 146.6, 144.4, 137.1, 133.1, 131.9, 131.3, 131.1, 131.1, 129.5, 128.2, 127.4, 126.6, 125.8, 124.9, 119.4, 117.9, 108.6, 106.8, 101.7; IR (v, cm^{-1}) 3149, 3076, 3049, 3017, 2916, 2868, 1666, 1651, 1637, 1599, 1502, 1485, 1467, 1406, 1364, 1265, 1259, 1231, 1175, 1072, 1042, 968, 933, 837, 814, 743, 552, LC - MS: m/e 464.16, $C_{25}H_{15}Cl_2NO_4$ required Mol.Wt.:464.3.



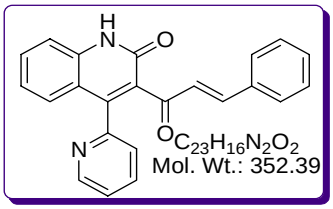
White solid, m.p 236 - 238 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.75 (s, 1H), 8.63 - 8.62 (d, *J* = 4.4 Hz, 1H), 7.71 - 7.67 (dt, *J* = 7.64, 1.6 Hz, 1H), 7.53 - 7.49 (d, *J* = 16.0 Hz, 1H), 7.46 - 7.42, (m, 2H), 7.40 - 7.34 (m, 5H), 7.31 - 7.27 (m, 2H), 7.01 (s, 2H.; ^{13}C NMR (100 MHz, DMSO-d6) δ 192.9, 161.9, 152.9, 150.2, 147.4, 144.3, 136.8, 136.7, 132.7, 132.4, 132.3, 131.9, 131.4, 130.7, 130.1, 129.9, 128.7, 127.2, 126.2, 124.8, 124.5, 120.2, 118.4; IR (v, cm^{-1}), 3149, 3071, 2997, 2909, 2870, 2841, 1666, 1634, 1616, 1603, 1578, 1564, 1487, 1469, 1429, 1408, 1371, 1283, 1244, 1089, 1061, 1049, 987, 837, 768, 743, 604, 563, UPLC -MS: m/e 421.16, $C_{23}H_{14}Cl_2N_2O_2$ required Mol.Wt.:421.28.



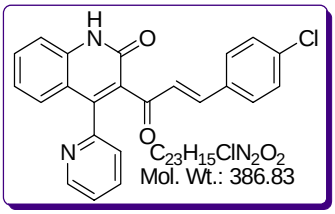
White solid, m.p 224 – 226 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.37 (s, 1H), 7.83 - 7.78 (d, *J* = 16.4 Hz, 4H), 7.45 - 7.43 (d, *J* = 7.60 Hz, 1H), 7.39 - 7.35 (m, 4H), 7.33 - 7.29 (t, *J* = 6.8 Hz, 1H), 7.01 - 6.99 (m, 2H), 6.93 - 6.85 (m, 2H), 6.79 - 6.77 (d, *J* = 9.2 Hz, 1H), 3.75 (s, 3H), 3.71 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.4, 161.9, 153.5, 153.4, 146.8, 141.7, 136.7, 133.1, 132.9, 132.6, 131.8, 131.6, 130.8, 129.9, 128.8, 127.3, 126.3, 123.8, 120.4, 118.3, 113.2, 56.0, 55.9; IR (v, cm^{-1}) 3146, 3001, 2907, 2862, 2833, 1639, 1493, 1468, 1404, 1366, 1236, 1178, 1074,1047, 986, 961, 822, 752, 716, 609, 559; UPLC-MS: m/e 480.28, $C_{26}H_{19}Cl_2NO_4$ required Mol. Wt.: 480.34.



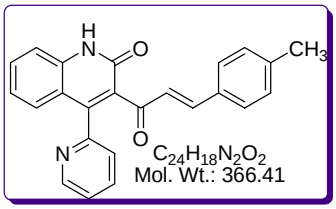
White solid, m.p 248 – 250 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.99(s, 1H), 7.74 - 7.69 (m, 2H), 7.68 (s, 2H), 7.65 - 7.59 (m, 2H), 7.54 - 7.49 (m, 3H), 6.98 - 6.94 (d, *J* = 16.0 Hz, 1H), 6.88 - 6.88 (d, *J* = 2.4 Hz, 1H), 6.72 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.4, 161.9, 151.0, 147.2, 145.6, 136.8, 132.8, 132.6, 132.6, 132.1, 131.9, 131.5, 130.8, 130.0, 128.9, 127.3, 126.3, 124.3, 120.4, 118.4, 116.9, 112.9; IR (v, cm^{-1}) 3155, 3007, 2920, 1672, 1605, 1560, 1468, 1402, 1391, 1367, 1277, 1242, 1134, 1088, 1055, 1018, 883, 835, 744, 557; UPLC - MS: m/e 410.12, $C_{26}H_{19}Cl_2NO_4$ required Mol. Wt.: 410.25



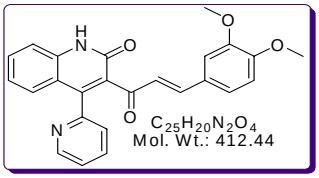
White solil, m.p 240 – 242 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.22 (s, 1H), 8.68 – 8.67 (d, *J* = 4.27 Hz, 1H), 7.80 -7.76 (td, *J* = 7.77, 2.0 Hz, 1H), 7.50 - 7.44 (m, 6H), 7.34 - 7.29 (m, 5H), 7.17 - 7.14 (t, *J* = 8.0 Hz, 1H), 6.89 - 6.85 (d, *J* = 16.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.8, 161.0, 152.9, 148.9, 147.9, 145.1, 137.9, 135.8, 133.7, 130.8, 130.2, 129.8, 127.9, 127.8, 126.5, 126.4, 124.6, 122.7, 122.4, 118.3, 115.9; IR (v, cm^{-1}) 3148, 3096, 2989, 2943, 2879, 2843, 1678, 1641, 1618, 1584, 1479, 1431, 1402, 1375, 1242, 1193, 1078, 1049, 993, 972, 768, 750, 716, 663, 569; UPLC - MS: m/e 353.26, $C_{23}H_{16}N_2O_2$ required Mol. Wt.: 352.38



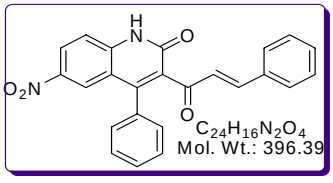
White solid, m.p 246 - 248 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.77 (s, 1H), 8.67 - 8.66 (d, *J* = 4.8 Hz, 1H), 7.81 - 7.77 (dt, *J* = 7.69, 1.2 Hz, 1H), 7.47 - 7.45 (m, 3H), 7.42 - 7.38 (m, 3H), 7.33 - 7.28 (m, 4H), 7.17 - 7.13(td , *J* = 8.3, 3.2 Hz, 1H), 6.83 - 6.87 (d, *J* = 16.00 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.2, 161.8, 153.6, 149.6, 148.8, 143.9, 138.6, 136.5, 136.4, 2845.0, 132.8, 131.5, 130.7, 129.5, 128.9, 127.4, 127.1, 125.3, 123.4, 123.1, 118.9, 116.6, 77.2, 76.5; IR (v, cm^{-1}) 3149, 3098, 3046, 2997, 2966, 2943, 2883, 1651, 1643, 1585, 1568, 1549, 1501, 1483, 1431, 1402, 1377, 1298, 1244, 1192, 1076, 993, 964, 912, 877, 822, 779. 752, 779, 669, 588; UPLC- MS: m/e 387.24, $C_{23}H_{15}ClN_2O_2$ required Mol. Wt.: 386.83



White solid, m.p 248 - 250 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.604 (s, 1H), 8.67 - 8.66 (d, *J* = 4.8 Hz, 1H), 7.79 - 7.75 (dt, *J* = 7.72, 1.6 Hz), 7.48 - 7.42 (m, 4H), 7.37 - 7.35 (d, *J* = 8.0 Hz, 2H), 7.31 - 7.28 (m, 2H), 7.18 - 7.12 (m, 3H), 6.83 - 6.79 (d, *J* =16 Hz,1H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.4, 161.5, 153.5, 149.4, 148.2, 145.9, 140.8, 138.4, 136.3, 131.4, 131.2, 130.8, 129.2, 128.3, 126.9, 125.9, 125.1, 123.1, 122.8, 118.7, 21.2, 116.4; IR (v, cm^{-1}) 3167, 3051, 3028, 2974, 2895, 2853, 1678, 1659, 1601, 1566, 1468, 1402, 1379, 1325, 1182, 1061, 993, 949, 856, 787, 752, 685, 609, 523; UPLC – MS : m/e 367.37, $C_{24}H_{18}ClN_2O_2$ required Mol. Wt.: 366.41.

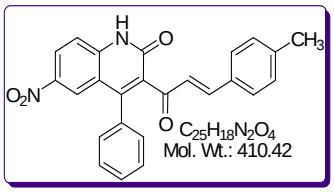


White solid, m.p 228 - 230 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.48 (s, 1H), 8.68 - 8.67 (d, *J* = 4.8 Hz, 1H), 7.81 - 7.76 (td, *J* = 7.77, 1.6 Hz, 1H), 7.49 - 7.47 (m, 3H), 7.42 - 7.38 (d, *J* = 16.4 Hz, 1H), 7.33 - 7.28 (m, 2H), 7.17 -7.13 (dt, *J* = 8.15, 2.4 Hz,1H), 7.07 - 7.05 (dd, *J* = 8.33, 1.6 Hz, 1H), 6.98 - 6.97 (d, *J* = 1.6 Hz, 1H), 6.82 - 6.79 (d, *J* = 8.4 Hz, 1H), 6.75 - 6.71 (d, *J* = 16.0 Hz, 1H), 3.89 (s, 3H), 3.84 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.6, 161.8, 153.8, 151.5, 149.7, 149.1, 148.3, 146.4, 138.7, 136.7, 131.5, 131.3, 127.3, 125.6, 125.3, 123.5, 123.4, 123.2, 119.1, 116.7, 110.9, 110.1, 55.9, 55.9; IR (v, cm^{-1}), 3157, 3042, 3001, 2957, 2938, 2843, 2760, 1663, 1643, 1616, 1595, 1584, 1510, 1468, 1425, 1402, 1379, 1273, 1240, 1074, 1024, 974, 818, 781, 675, 561; UPLC – MS : m/e 413.26., $C_{25}H_{20}N_2O_4$ required Mol. Wt.: 412.44.

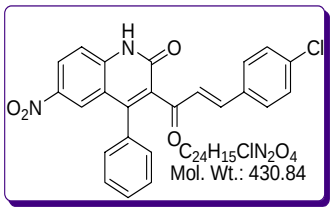


White solid, m.p 240 - 242 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 - 8.27 (dd, *J* = 8.90, 2.0 Hz, 1H), 8.25 - 8.24 (d, *J* = 2.4 Hz, 1H), 7.59 - 7.57 (d, *J* = 9.2 Hz, 1H), 7.47 - 7.46 (m, 3H), 7.42 -

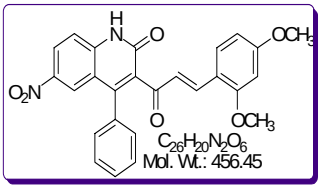
7.39 (m, 3H), 7.37 - 7.36 (m, 2H), 7.34 - 7.31 (m, 3H), 6.70 - 6.74 (d, *J* = 16.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.7, 161.1, 149.2, 145.3, 142.2, 141.2, 132.9, 131.7, 130.1, 128.9, 128.0, 127.9, 127.5, 125.8, 124.9, 123.0, 118.6, 116.7; IR (v, cm^{-1}) 3244, 3028, 2932, 2882, 1661, 1626, 1574, 1532, 1485, 1402, 1337, 1063, 979, 912, 829, 716, 559; UPLC - MS: m/e 397.32, $C_{24}H_{16}N_2O_4$ required Mol. Wt.: 396.40.



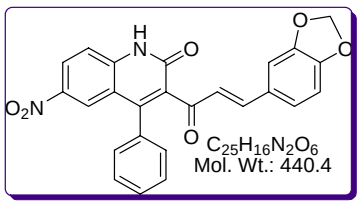
White solid, m.p 260 – 262 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 - 8.25 (dd, *J* = 8.95, 2.4 Hz, 1H), 8.26 - 8.25 (d, *J* = 2.0 Hz, 1H), 7.58 - 7.56 (d, *J* = 9.2 Hz, 1H), 7.48 - 7.46 (m, 3H), 7.38 - 7.32 (m, 5H), 7.17 - 7.15 (d, *J* = 8.0 Hz, 2H), 6.72 - 6.68 (d, *J* = 16.0 Hz, 1H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.7, 162.1, 150.2, 146.7, 143.3, 142.2, 141.9, 132.9, 132.8, 131.4, 129.9, 129.8, 129.1, 129.1, 128.6, 126.1, 125.9, 124.2, 119.7, 117.6, 21.6; IR (v, cm^{-1}) 3167, 3121, 3059, 2993, 2924, 2879, 1684, 1663, 1614, 1529, 1484, 1443, 1402, 1333, 1240, 1178, 1139, 1061, 979, 810, 764; UPLC – MS : m/e 411.25, $C_{25}H_{18}N_2O_4$ required Mol. Wt.: 410.42



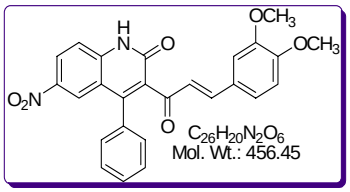
White solid, m.p 255 – 257 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.85 (s, 1H), 8.37 - 8.34 (dd, *J* = 9.05, 2.4 Hz, 1H), 8.28 - 8.28 (d, *J* = 2.4 Hz, 1H), 7.59 - 7.57 (d, *J* = 8.8 Hz, 1H), 7.49 - 7.49 (m, 3H), 7.37 - 7.32 (m, 7H), 6.71 - 6.67 (d, *J* = 16.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) 192.3, 161.9, 150.4, 144.6, 143.3, 142.1, 137.2, 132.6, 132.6, 132.5, 129.9, 129.6, 129.3, 129.1, 128.9, 126.1, 124.1, 119.6, 117.6; IR (v, cm^{-1}) 3171, 3126, 3067, 2993, 2929, 2884, 1686, 1665, 1620, 1529, 1489, 1404, 1335, 1240, 1204, 1175, 1139, 1092, 1061, 1017, 979, 914, 833, 764, 708, 563, 525; UPLC - MS: m/e 431.19, $C_{24}H_{15}ClN_2O_4$ required Mol. Wt.: 430.84.



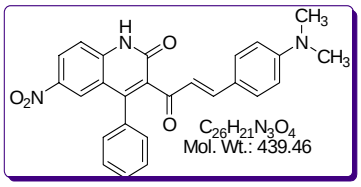
White solid, m.p 224 – 226 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 - 8.22 (m, 2H), 7.66 -7.62 (d, *J* = 16.4 Hz, 1H), 7.61 - 7.59 (d, *J* = 8.8 Hz, 1H), 7.45 - 7.44 (m, 3H), 7.35 - 7.32 (m, 3H), 6.72 - 6.68 (d, *J* = 16.0 Hz, 1H), 6.47 - 6.44 (dd, *J* = 8.64 Hz, 2.0 Hz, 1H), 6.37 - 6.37 (d, *J* = 1.6 Hz, 1H), 3.82 (s, 3H), 3.77 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.3, 163.7, 162.1, 160.1, 149.6, 143.1, 142.4, 142.2, 133.1, 132.9, 130.5, 129.6, 129.1, 128.9, 125.7, 124.9, 123.9, 119.7, 117.8, 116.1, 105.6, 98.3, 55.5, 55.5; IR (v, cm^{-1}) 3211, 3175, 3001, 2943, 2879, 2841, 1651, 1589, 1537, 1504, 1468, 1402, 1339, 1275, 1209, 1180, 1107, 1059, 1020, 966, 879, 827, 759, 712, 586; UPLC - MS: m/e 457.33, $C_{26}H_{20}N_2O_6$ required Mol. Wt.: 456.45.



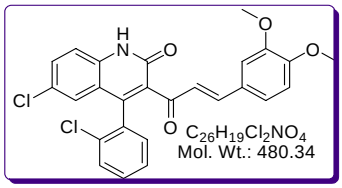
White solid, M.P-278 – 280 °C, ^{1}H-NMR (400 MHz,$CDCl_3$): δ 12.68(s, 1H), 8.30 – 8.28 (d, *J* = 7.56Hz, 1H), 8.24 – 8.23 (d, *J* = 4.96 Hz, 1H), 7.55 – 7.53 (d, 8.8 Hz, 1H), 7.46 – 7.43 (m, 3H), 7.32 – 7.30 (m, 3H), 6.91 – 6.88 (m, 2H), 6.76 – 6,74 (d, *J* = 8.47 Hz, 1H), 6.57 – 6.53 (d, *J* = 16.38 Hz, 1H), 5.99 (s, 2H); ^{13}CNMR (100 MHz, $CDCl_3$), 192.3, 161.9, 150.5, 150.1, 148.5, 146.2, 143.2, 142.1, 132.9, 132.7, 129.8, 129.0, 128.9, 128.4, 126.0, 125.5, 124.9, 124.1, 119.6, 117.5, 108.7, 106.6, 101.8; IR (v, cm^{-1}) 3163, 2932, 2783, 2735, 1659, 1639, 1620, 1599, 1533, 1489, 1448, 1402, 1359, 1337, 1257, 1230, 1138, 1099, 1065, 1038, 984, 929, 912, 833, 810, 764, 750, 702, UPLC - MS: m/e 441.20, $C_{25}H_{16}N_2O_6$ required Mol. Wt.: 440.40.



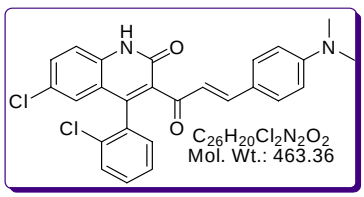
White solid, m.p 252 – 254 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 - 8.28 (d, *J* = 9.2 Hz, 1H), 8.25 - 8.25 (d, *J* = 2.0 Hz, 1H), 7.59 - 7.58 (d, *J* = 8.8 Hz, 1H), 7.47 - 7.46 (m, 3H), 7.33 - 7.29 (m, 3H), 7.02 - 7.00 (d, *J* = 8.0 Hz, 1H), 6.39 (s, 1H), 6.83 - 6.81 (d, *J* = 8.4 Hz, 1H), 6.64 - 6.59 (d, *J* = 16.0 Hz, 1H), 3.89 (s, 3H), 3.86 (s, 3H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.5, 162.1, 152.0, 150.1, 149.3, 146.8, 143.2, 142.1, 132.9, 132.8, 129.8, 129.0, 129.0, 126.9, 125.9, 124.9, 124.1, 123.6, 119.7, 117.7, 111.1, 109.9, 56.0, 55.9.; IR (v, cm^{-1}) 3177, 3082, 2934, 2837, 1653, 1620, 1597, 1512, 1487, 1487, 1464, 1443, 1334, 1265, 1238, 1139, 1063, 1022, 843, 766, 702.1, 561; UPLC - MS: m/e 457.30, $C_{26}H_{20}N_2O_6$ required Mol. Wt.: 456.45.



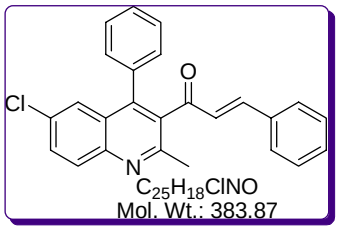
White solid, m.p 250 – 252 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.85 (s, 1H), 8.19 – 8.17 (m, 2H), 7.57 – 7.55 (d, *J* = 8.32 Hz, 1H), 7.42 – 7.39 (m, 3H), 7.31 – 7.27 (m, 5H), 6.60 – 6.52 (m, 3H), 3.01 (s, 6H);^{13}C NMR (100 MHz, $CDCl_3$) δ 191.5, 151.3, 146.9, 142.0, 141.1, 132.0, 129.6, 128.5, 127.9, 127.8, 124.6, 122.8, 121.0, 120.6, 118.7, 116.8, 110.7, 39.1; IR (v, cm^{-1}) 3153, 2993, 2924, 2858, 2822, 1659, 1589, 1528, 1487, 1435, 1400, 1373, 1337, 1267, 1242, 1169, 1061, 1029, 982, 945, 912, 831, 704, 559.; UPLC-MS: m/e 440.25 $C_{26}H_{21}N_3O_4$ required Mol. Wt.: 439.46.



White solid, m.p 214 – 216 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.91 (s, 1H), 12.91 (s, 1H), 7.48 - 7.46 (d, *J* = 7.2 Hz, 1H), 7.44 - 7.38 (m, 3H), 7.36 - 7.33 (dd, *J* = 4.34, 2.80 Hz, 1H), 7.31 - 7.30 (t, *J* = 1.6 Hz, 1H), 7.29 - 7.29 (d, *J* = 2.4 Hz, 1H), 7.06 - 7.03 (dd, *J* = 8.33, 2.0 Hz, 1H), 7.02 - 7.01 (d, *J* = 2.0 Hz, 1H), 6.98 - 6.98 (d, *J* = 1.6 Hz, 1H), 6.83 - 6.81 (d, *J* = 8.4 Hz, 1H), 6.69 - 6.65 (d, *J* = 16.0 Hz, 1H), 3.89 (s, 3H), 3.86 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.8, 161.7, 151.6, 149.1, 146.7, 146.5, 136.5, 132.7, 132.5, 132.3, 131.6, 131.4, 130.6, 129.8, 128.6, 127.2, 127.0, 125.9, 124.7, 123.5. 120.0, 118.2, 110.9, 109.9, 55.9, 55.7; IR (v, cm^{-1}) 3155, 3003, 2932, 2911, 2868, 2835, 1659, 1639, 1595, 1510, 1462, 1439, 1406, 1367, 1342, 1267, 1244, 1161, 1139, 1074, 1024, 978, 951, 881, 827, 748, 714, 671, 636; UPLC – MS : m/e 480.28, $C_{26}H_{19}Cl_2NO_4$ required Mol.Wt.: 480.34.

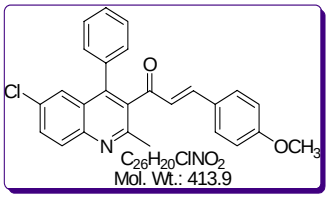


White solid, m.p 298 – 300 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.40 (s, 1H), 7.46 - 7.42 (d, *J* = 16.0 Hz,1H), 7.41 - 7.39 (m, 3H), 7.36 - 7.30 (m, 5H), 7.01 - 7.00 (t, *J* = 1.2 Hz, 1H), 6.62 - 6.62 (d, *J* = 1.6 Hz, 1H), 6.59 - 6.56 (d, *J* = 16.0 Hz, 2H), 3.02 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) 191.6, 160.7, 151.2, 146.9, 145.0, 135.4, 131.7, 131.6, 130.5, 130.5, 129.7, 129.5, 128.8, 127.5, 126.1, 125.0, 120.9, 119.2, 117.1, 110.6, 39.1; IR (v, cm^{-1}) 3148, 3084, 3005, 2993, 2907, 2862, 2826, 1651, 1593, 1553, 1526, 1485, 1435, 1406, 1366, 1341, 1263, 1240, 1132, 1186, 1171, 1072, 1053, 982, 945, 816, 750, 599, 555; UPLC – MS : m/e 463.27, $C_{26}H_{20}Cl_2N_2O_2$ required Mol. Wt.: 463.36.

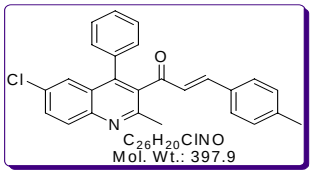


Light yellow solid, m.p 160 - 162 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 - 8.05 (d, *J* = 9.2 Hz, 1H), 7.70 - 7.68 (d, *J* = 9.2 Hz, 1H), 7.59 (s, 1H), 7.43 - 7.35 (m, 4H), 7.33 - 7.26 (m, 6H),

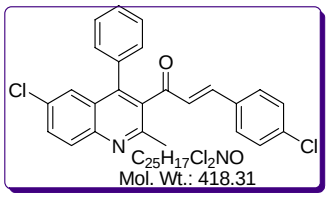
7.12 - 7.08 (d, *J* = 16.0 Hz, 1H), 6.61 - 6.57 (d, *J* = 16.4 Hz, 1H), 2.70 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.5, 155.6, 147.2, 146.4, 144.8, 134.8, 134.2, 133.6, 132.7, 131.3, 131.3, 130.8, 130.2, 129.2, 129.2, 128.8, 128.6, 127.8, 126.4, 125.3, 24.2; IR (v, cm^{-1}) 1641, 1599, 1564, 1481, 1436, 1386, 1311, 1224, 1201, 1161, 1082, 1047, 972, 881, 831, 765, 711, 702, 684, 663, 646.15, 588.; LC – MS : m/e 384.57, $C_{25}H_{18}ClNO$ required Mol. Wt.: 383.87



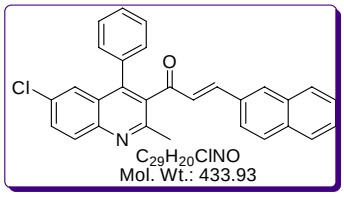
White solid, m.p 160 – 164 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 - 8.05 (d, *J* = 7.07 Hz, 1H), 7.69 - 7.67 (d, *J* = 7.84 Hz, 1H), 7.57 (s, 1H), 7.40 – 7.38 (m, 3H), 7.29 - 7.27 (m, 4H), 7.06 - 7.02 (d, *J* = 16.6 Hz, 1H), 6.85 – 6.83 (m, 2H), 6.51- 6.47 (d, *J* = 17.4 Hz, 1H), 3.81 (s, 3H), 2.69 (s, 3H); ^{13}C NMR (100MHz, $CDCl_3$) δ 197.3, 162.2, 155.6, 147.2, 146.2, 144.6, 134.7, 133.7, 132.5, 131.1, 130.7, 130.4, 129.9, 128.9, 128.7, 126.7, 126.3, 125.6, 125.2, 114.6, 55.6, 24.1, GC – MS : m/e 415.2, $C_{26}H_{20}ClNO_2$ required Mol. Wt.: 413.9.



Pale yellow solid, m.p 140 – 142 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 - 8.06 (d, *J* = 8.4 Hz, 1H), 7.70 - 7.68 (d, *J* = 8.4 Hz, 1H), 7.58 (s, 1H), 7.41 - 7.38 (m, 3H), 7.29 – 7.27 (m, 2H), 7.23 – 7.22 (m, 2H) 7.15 – 7.13 (m, 2H), 7.08 – 7.04 (d, *J* = 15.73, 1H) 6.58 - 6.54 (d, *J* = 15.84 Hz, 1H), 2.69 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.5, 155.5, 147.4, 146.2, 144.7, 141.9, 134.6, 133.5, 132.6, 131.3, 131.1, 130.6, 130.0, 129.8, 128.9, 128.7, 128.6, 126.8, 126.3, 125.2, 24.1, 21.7; IR (v, cm^{-1}) 2922, 2858, 2746, 2682, 1645, 1597, 1566, 1479, 1390, 1224, 1182, 1159, 1078, 1047, 1029, 981, 702, 497; GC – MS : m/e 397.26, $C_{26}H_{20}ClNO$ required Mol. Wt.: 397.9.

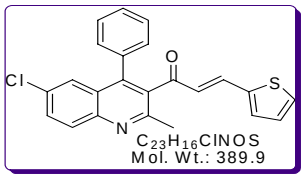


Light white solid, m.p 133 – 136 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 - 8.06 (d, *J* = 8.4 Hz, 1H), 7.71 - 7.69 (d, *J* = 8.8 Hz, 1H), 7.61 (s, 1H), 7.43 – 7.40 (m, 3H), 7.32 – 7.29 (m, 5H), 7.25 – 7.24 (d, *J* = 5.42 Hz, 1H), 7.08 - 7.04 (d, *J* = 16.4 Hz, 1H), 6.57 - 6.53 (d, *J* = 16.0 Hz, 1H), 2.71 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.0, 155.4, 146.3, 145.2, 144.7, 137.2, 134.6, 133.3, 132.7, 132.5, 131.2, 130.7, 130.0, 129.6, 129.4, 129.1, 128.8, 127.9, 126.2, 125.2, 24.1; IR (v, cm^{-1}) 3016, 2970, 2924, 1651, 1625, 1608, 1579, 1564, 1481, 1440, 1404, 1220, 1161, 1078, 983, 829, 704; LC – MS : m/e 418.57, $C_{25}H_{17}Cl_2NO$ required Mol. Wt.: 418.31.;

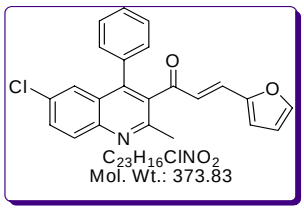


Light yellow solid, m.p 156 – 157 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 - 8.07 (d, *J* = 8.4 Hz, 1H), 7.99 - 7.95 (d, *J* = 16.0 Hz, 1H), 7.88 - 7.84 (m, 2H), 7.78 – 7.76 (d, *J* = 6.67 Hz, 1H), 7.72 - 7.70 (d, *J* = 7.6 Hz, 1H), 7.63 (s, 1H), 7.49 - 7.36 (m, 9H), 6.69 - 6.65 (d, *J* = 16.0 Hz, 1H), 2.76 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.0, 155.4, 146.2, 144.6, 143.4, 134.6, 133.6, 132.5, 131.3, 131.1, 130.6, 130.2, 130.1 129.0, 128.9, 128.7, 127.1, 126.4, 126.1, 125.5, 125.4, 125.1, 122.9, 24.1; IR (v, cm^{-1}) 2854, 1649, 1629, 1479, 1402, 1261, 1219, 1122,

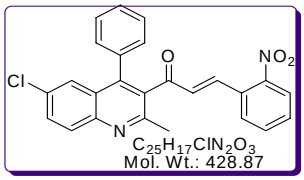
1076, 975, 945, 837, 804, 775, 700, 594; LC – MS : m/e 433.2, $C_{25}H_{17}Cl_2NO$ required Mol. Wt.: 433.93.;



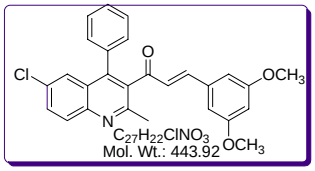
Light Brown solid, m.p 158 – 160 ^{o}C,^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 - 8.05 (d, *J* = 8.95 Hz, 1H), 7.70 - 7.67 (dd, *J* = 9.01, 2.29 Hz, 1H), 7.58-7.57 (d, *J* = 2.17 Hz, 1H), 7.55-7.53 (t, *J* = 3.5 Hz, 1H), 7.43-7.39 (m, 3H), 7.30 - 7.28 (dd, *J* = 7.72, 2.16 Hz, 2H), 7.24-7.20 (d, *J* = 15.88 Hz, 1H), 7.14-7.13 (d, *J* = 3.56 Hz, 1H), 7.03-7.01 (dd, *J* = 4.93, 3.8 Hz, 1H), 6.41-6.37 (d, *J* = 15.84 Hz, 1H), 2.70 (s, 3H); ^{13}C NMR (100MHz, $CDCl_3$) δ 195.4, 154.3, 145.1, 143.6, 138.2, 137.8, 133.4, 132.3, 131.4, 131.1, 129.9, 129.5, 128.9, 128.8, 127.9, 127.6, 127.4, 125.3, 125.1. 124.0, 22.9. GC – MS : m/e 390.4, $C_{23}H_{16}ClNOS$ required Mol. Wt.: 389.9



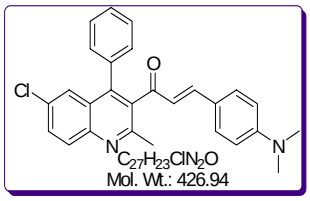
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 - 8.04 (d, *J* = 8.84 Hz, 1H), 7.69 - 7.67 (d, *J* = 8.84 Hz, 1H), 7.57 (s, 1H), 7.47 – 7.42 (m, 4H), 7.30-7.28 (m, 2H), 6.88 - 6.84 (d, *J* = 16.08 Hz, 1H), 6.56-6.55 (d, *J* = 3.13 Hz, 1H), 6.50 – 6.45 (d, *J* = 16.72 Hz, 1H), 6.45 – 6.44 (d, *J* = 3.85 Hz, 1H), 2.69 (s, 3H); ^{13}C NMR (100MHz, $CDCl_3$) δ 196.6, 155.3, 150.4, 145.7, 134.4, 133.4, 132.4, 131.0, 130.4, 129.9, 128.9, 128.6, 125.1, 124.9, 116.9, 112.8, 23.8 .; IR (v, cm^{-1}) 3028, 2920, 2850, 1666, 1643, 1624, 1595, 1546, 1479, 1444, 1390, 1340, 1311, 1280, 1263, 1222, 1192, 1155, 1124, 1080, 1045, 1008, 970, 883, 833, 761, 750; UPLC – MS : m/e 374.54, $C_{23}H_{16}ClNO_2$ required Mol. Wt.: 373.83



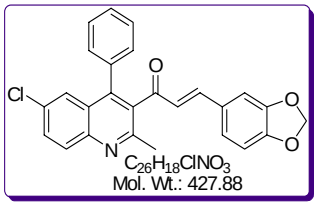
White solid, m.p 223 – 225 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 – 8.04 (d, *J* = 8.58 Hz, 1H) 8.01 - 7.99 (d, *J* = 7.05 Hz, 1H), 7.69 - 7.67 (d, *J* = 9.2 Hz, 1H), 7.58 – 7.52 (m, 4H), 7.45 – 7.42 (m, 3H), 7.34 – 7.29 (m, 3H), 2.72 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.3, 155.2, 146.4, 145.0, 142.4, 134.5, 133.8, 132.7, 132.7, 132.3, 131.4, 130.9, 130.8, 130.6, 130.4, 129.3, 129.1, 128.8, 126.1, 125.2, 24.1; IR (v, cm^{-1}) 1624, 1564, 1479, 1382, 1222, 1201, 1161, 1082, 1045, 972, 831, 765, 711, 702, 588, 484; LC – MS : m/e 429.61, $C_{25}H_{17}ClN_2O_3$ required Mol. Wt.: 428.87



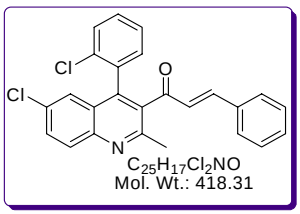
Yellow solid, Yield, m.p 166 – 169 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 - 8.05 (d, *J* = 8.92 Hz, 1H), 7.70 - 7.67 (dd, *J* = 8.96, 2.16 Hz, 1H), 7.58 - 7.57 (d, *J* = 2.04 Hz, 1H), 7.46 - 7.42 (d, *J* = 16.44 Hz, 1H), 7.41 - 7.39 (m, 3H), 7.30 - 7.29 (m, 2H), 6.92 - 6.89 (dd, *J* = 9.01, 2.92 Hz, 1H), 6.82 - 6.77 (m, 2H), 6.65 - 6.61 (d, *J* = 16.4 Hz, 1H), 3.74 (s, 3H) 3.73 (s, 3H), 2.70 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.7, 155.5, 153.4, 152.9, 146.1, 144.6, 142.5, 134.6, 133.6, 132.3, 130.9,130.6, 130.1, 128.8, 128.5, 128.2, 126.3, 125.2, 123.4, 118.3, 112.8, 112.4, 55.9, 55.8, 24.01; IR (v, cm^{-1}) 3441, 3003, 2939, 2833, 1643, 1612, 1571, 1492, 1479, 1462, 1444, 1425.40, 1390, 1309, 1288, 1276, 1240, 1222, 1205, 1186, 1163, 1124, 1080, 1047, 1024, 975, 837, 804; LC – MS : m/e 444.48, $C_{27}H_{22}ClNO_3$ required Mol. Wt.: 443.92.



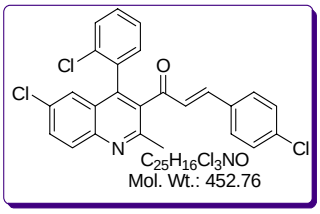
Light yellow solid, m.p 175 – 177 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 - 8.04 (d, *J* = 8.8 Hz, 1H), 7.68 - 7.65 (dd, *J* = 8.93, 2.36 Hz, 1H), 7.56 – 7.55 (d, *J* = 2.25 Hz, 1H), 7.40 – 7.37 (m, 3H), 7.30 - 7.29 (d, *J* = 2.8 Hz, 1H), 7.28 - 7.27 (d, *J* = 2.0 Hz, 1H), 7.25 – 7.24 (d, *J* = 2.18 Hz, 1H), 7.23 – 7.22 (d, *J* = 2.18 Hz, 1H), 7.02 - 6.98 (d, *J* = 16.0 Hz, 1H), 6.61 - 6.58 (d, *J* = 8.8 Hz, 2H), 6.47 - 6.43 (d, *J* = 16.0 Hz, 1H), 3.01 (s, 6H), 2.70 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.8, 150.2, 146.7, 144.0, 142.0, 140.9, 139.3, 129.4, 128.2, 127.2, 125.7, 125.3, 124.6, 123.3, 121.6, 120.5, 119.9, 118.2, 105.8 104.5, 50.7, 18.7; LC – MS : m/e 427.36, $C_{27}H_{23}ClN_2O$ required Mol. Wt.: 426.94.



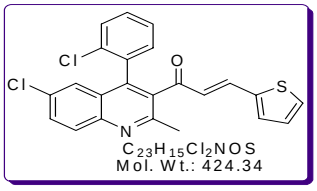
Light yellow solid, m.p 159 – 160 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 - 8.04 (d, *J* = 9.01 Hz, 1H), 7.69 - 7.66 (d, *J* = 9.09 Hz, 1H), 7.57 (s, 1H), 7.41 - 7.40 (m, 3H), 7.29 - 7.27 (m, 2H), 7.02 – 6.98 (d, *J* = 16.16 Hz, 1H), 6.82 – 6.74 (m, 3H), 6.44 – 6.40 (d, *J* = 16.13 Hz, 1H),5.99 (s, 2H), 2.69 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.9, 155.4, 150.4, 148.5, 146.8, 146.1, 144.5, 134.6, 133.5, 132.4, 130.9, 130.6, 129.9, 128.9, 128.6, 128.4, 126.2, 125.8, 125.4, 125.1, 108.6, 106.5, 101.7, 23.9; IR (v, cm^{-1}) 2964, 2920, 2854, 2791, 2700, 1643, 1620, 1598, 1566, 1500, 1489, 1448, 1390, 1261, 1215, 1107, 1080, 1035, 829, 800, 704, 609.51, 563.21, 534.2; LC – MS : m/e 428.42, $C_{26}H_{18}ClNO_3$ required Mol. Wt.: 427.88



Pale yellow solid, m.p 172 – 174 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 - 8.06 (d, *J* = 9.01 Hz , 1H), 7.71 - 7.68 (dd, *J* = 8.99, 2.16 Hz, 1H), 7.44 - 7.40 (m, 2H), 7.38 – 7.36 (m, 4H), 7.35 - 7.34 (d, *J* = 3.6 Hz, 2H), 7.32 - 7.31 (m, 2H), 7.24 – 7.2 3 (d, *J* = 2.59 Hz, 1H), 6.70 - 6.66 (d, *J* = 16.32 Hz, 1H), 2.71 (s, 3H); ^{13}C NMR (100MHz, $CDCl_3$) δ 196.8, 155.5, 147.6, 145.8, 141.8, 133.9, 133.8, 133.3, 133.2, 132.76, 132.3, 131.2, 131.1, 130.7, 130.6, 129.8, 129.0, 128.6, 127.2, 127.0, 125.5, 124.8, 23.9; LC – MS : m/e 418.07, $C_{25}H_{17}Cl_2NO$ required Mol. Wt.: 418.31.

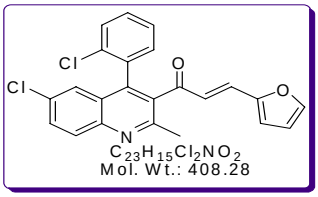


pale yellow solid, m.p 145 – 147 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 - 8.06 (d, *J* = 8.96 Hz, 1H), 7.71 - 7.68 (dd, *J* = 8.95, 2.32 Hz, 1H), 7.43 - 7.41 (dd, *J* = 5.4, 2.3 Hz, 1H), 7.39 - 7.34 (m, 2H), 7.32 - 7.31 (m, 5H), 7.24 - 7.20 (m, 2H), 6.64 - 6.60 (d, *J* = 16.28 Hz, 1H), 2.70 (s, 3H); ^{13}C NMR (100MHz, $CDCl_3$) δ 196.7, 155.6, 145.9, 142.0, 137.3, 133.8, 133.4, 133.3, 132.9, 132.5, 132.4, 131.4, 130.9, 130.9, 129.9, 129.9, 129.5, 127.5, 127.4, 125.6, 124.9, 24.0; LC – MS : m/e 452,19, $C_{26}H_{18}ClNO_3$ required Mol. Wt.: 452.76.

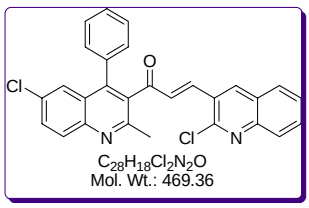


Off White solid, m.p 146 -148 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 - 8.06 (d, *J* = 8.96 Hz, 1H), 7.70 - 7.67 (dd, *J* = 8.99, 2.24 Hz, 1H), 7.46 – 7.34 (m, 5H), 7.32 - 7.31 (d, *J* = 2.19 Hz, 1H), 7.25 - 7.23 (dd, *J* = 6.94, 2.15 Hz, 2H), 7.18 – 7.17 (d, *J* = 3.42 Hz, 1H), 7.04 – 7.02 (dd, *J* = 4.83, 3.90 Hz, 2H), 6.49 - 6.45 (d, *J* = 15.99 Hz, 1H), 2.71 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.0, 155.6, 145.8, 141.9, 139.7,

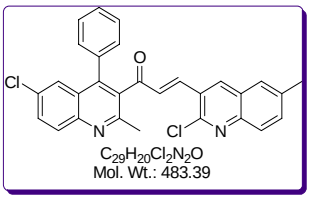
139.2, 133.7, 133.3, 133.2, 132.7, 132.6, 132.2, 131.2, 130.7, 130.6, 130.3, 129.9, 128.5, 127.2, 125.8, 125.5, 124.8, 23.9; LC – MS : m/e 424.34, $C_{26}H_{20}Cl_2N_2O_2$ required Mol. Wt.: 424.34.



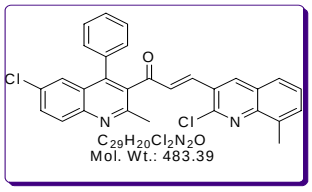
Off White solid, m.p °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 - 8.05 (d, *J* = 8.96 Hz, 1H), 7.70 - 7.67 (dd, *J* = 8.99, 2.24 Hz, 1H), 7.58 – 7.57 (d, *J* = 2.21 Hz, 1H), 7.42 - 7.40 (m, 2H), 7.29 - 7.27 (m, 2H), 7.02 - 6.98 (d, *J* = 16.12 Hz, 1H), 6.82 - 6.80 (m, 2H), 6.76 - 6.74 (d, *J* = 7.92 Hz, 1H), 6.44 - 6.40 (d, *J* = 16.12 Hz, 1H), 2.69 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.0, 155.4, 150.4, 148.5, 146.8, 146.1, 144.5, 134.6, 133.5, 132.4, 130.9, 130.6, 129.9, 128.9, 128.6, 128.4, 125.7, 125.4, 125.1, 108.6, 106.5, 101.7, 23.9; LC – MS : m/e 408.22, $C_{23}H_{15}Cl_2NO_2$ required Mol. Wt.: 408.28.



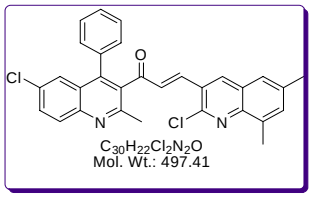
light yellow solid, m.p 203 – 205 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (s, 1H), 8.09 – 8.07 (d, *J* = 8.95 Hz, 1H), 7.99 - 7.97 (d, *J* = 8.45 Hz, 1H), 7.80 - 7.79 (d, *J* = 4.91 Hz, 1H), 7.77 – 7.75 (dd, *J* = 8.38, 1.31 Hz, 1H), 7.71 – 7.70 (dd, *J* = 8.98, 2.36 Hz, 1H), 7.64 – 7.63 (d, *J* = 2.25 Hz, 1H), 7.61 – 7.59 (dd, *J* = 7.95, 0.9 Hz, 1H), 7.57 – 7.53 (d, *J* = 16.09 Hz, 1H), 7.48 – 7.41 (m, 3H), 7.39 – 7.37 (m, 2H), 6.67 – 6.63 (d, *J* = 16.2 Hz, 1H), 2.74 (s, 3H); ^{13}C NMR (100MHz, $CDCl_3$) δ 196.7, 155.3, 149.8, 148.1, 146.3, 144.9, 140.9, 136.4, 134.5, 132.7, 132.7, 132.0, 131.3, 131.1, 130.7, 130.3, 129.1, 128.5, 128.1, 127.87, 126.9, 126.8, 125.9, 125.1, 24.1.; IR (v, cm^{-1}) 3057, 2962, 2916, 2906, 2848, 2250, 1961, 1649, 1612, 1579, 1566, 1479, 1402, 1392, 1379, 1261, 1217, 1095, 1022, 975, 866, 800, 765, 705; LC – MS : m/e 469.25, $C_{28}H_{18}Cl_2N_2O$ required Mol. Wt.: 469.36.



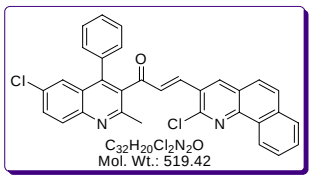
yellow solid, m.p 194 – 196 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 - 8.07 (d, *J* = 8.96 Hz, 1H), 8.02 (s, 1H), 7.87 - 7.84 (d, *J* = 8.56 Hz, 1H), 7.72 - 7.69 (dd, *J* = 8.98, 2.61 Hz, 1H), 7.63 -7.62 (d, *J* = 1.8 Hz, 1H), 7.59 - 7.57 (d, *J* = 8.84 Hz, 1H), 7.56 – 7.52 (m, 2H), 7.47 - 7.41 (m, 3H), 7.38 - 7.36 (d, *J* = 6.64 Hz, 2H), 6.65 - 6.61 (d, *J* = 16.2 Hz, 1H), 2.74 (s, 3H), 2.53 (s, 3H); ^{13}C NMR (100MHz, $CDCl_3$) δ 196.8, 155.3, 148.9, 146.7, 146.3, 144.8, 141.2, 138.0, 135.7, 134.5, 134.3, 132.8, 132.6, 131.3, 130.9, 130.7, 130.3, 129.9, 129.1, 128.7, 128.1, 126.9, 126.8, 125.9, 125.1, 24.1, 21.6; LC – MS : m/e 483.30, $C_{29}H_{20}Cl_2N_2O$ required Mol. Wt.: 483.39.



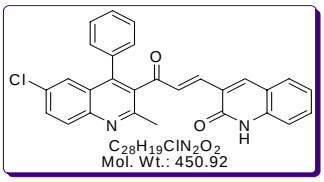
yellow solid, m.p 182 - 183 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 - 8.00 (m, 2H), 7.65 - 7.62 (dd, *J* = 9.0, 2.08 Hz, 1H), 7.56 - 7.53 (m, 2H), 7.52 - 7.46 (m, 2H), 7.38 - 7.34 (m, 3H), 7.33 - 7.30 (m, 2H), 7.19 (s, 1H), 6.59 - 6.55 (d, *J* = 16.24 Hz, 1H), 2.67 (s, 3H), 2.65 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.8, 154.3, 147.7, 146.3, 145.3, 143.8, 140.3, 135.8, 135.6, 133.4, 131.7, 131.6, 131.0, 130.2, 129.9, 129.6, 129.3, 128.0, 127.7, 126.6, 125.8, 125.5, 124.9, 124.9, 124.1, 23.0, 16.6; IR (v, cm^{-1}) 1676, 1641, 1629, 1600, 1579, 1477, 1440, 1392, 1382, 1365, 1344, 1309, 1155, 1120, 1083, 1029, 1004, 972, 833, 769, 705; LC – MS : m/e 483.37, $C_{29}H_{20}Cl_2N_2O$ required Mol. Wt.: 483.39.



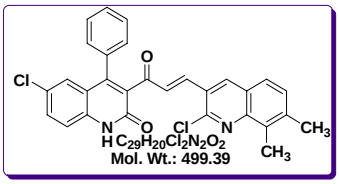
light yellow solid, m.p 172 – 175 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 - 8.07 (d, *J* = 8.96 Hz, 1H), 7.99 (s, 1H), 7.72 - 7.69 (dd, *J* = 8.96, 2.12 Hz, 1H), 7.63 - 7.62 (d, *J* = 1.8 Hz, 1H), 7.56 - 7.52 (d, *J* = 16.2 Hz, 1H), 7.46 - 7.40 (m, 4H), 7.37 - 7.36 (m, 3H), 6.65 - 6.61 (d, *J* = 16.2 Hz, 1H), 2.74 (s, 3H), 2.68 (s, 3H), 2.47 (s, 3H); ^{13}C NMR (100MHz, $CDCl_3$) δ 195.9, 154.3, 146.8, 145.3, 144.9, 143.8, 140.6, 136.6, 135.3, 134.9, 133.5, 133.4, 131.8, 131.6, 130.2, 129.6, 129.2, 128.9, 127.9, 127.7, 125.9, 125.3, 124.9, 124.1, 123.7, 23.0, 20.5, 16.5; IR (v, cm^{-1}) 1649, 1635, 1629, 1610, 1583, 1564, 1479, 1400, 1371, 1219, 1080, 975, 943, 879, 813, 759, 713, 696, 597, 557, 534.



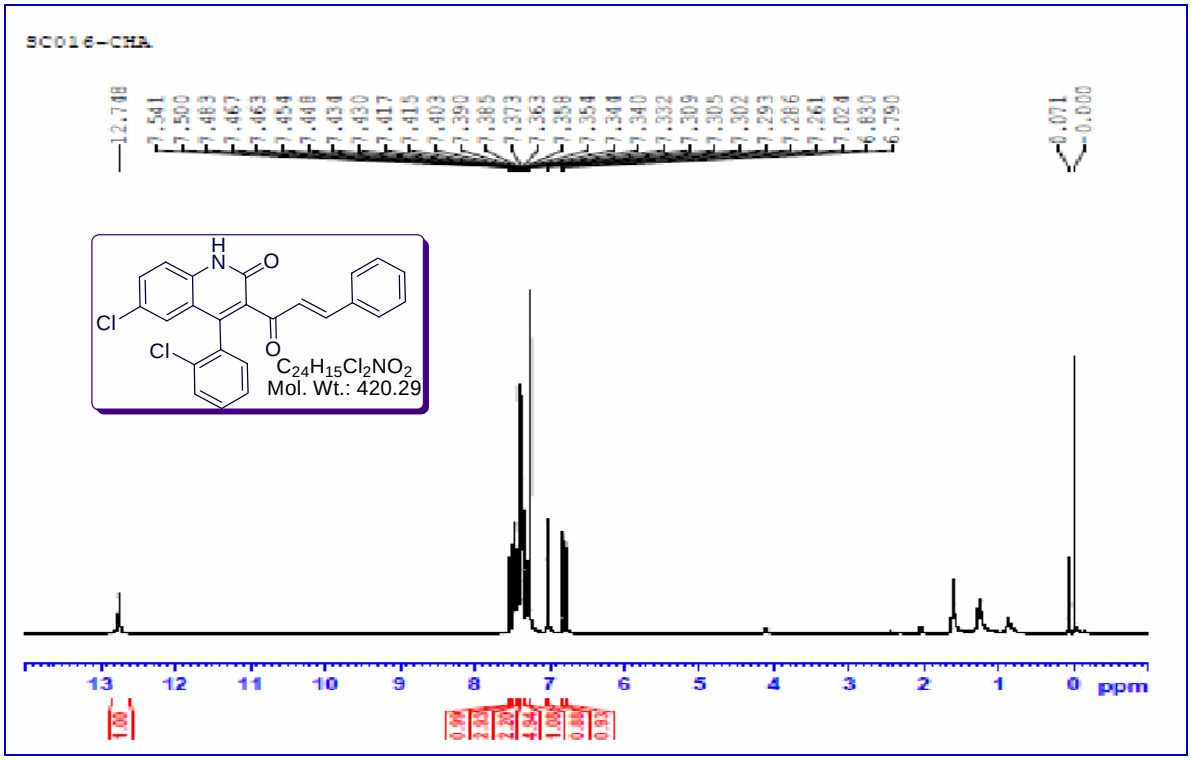
light yellow solid, Yield, m.p 235 - 237 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.12 - 9.10 (t**,** *J* = 5.08, 3.6 Hz, 1H), 8.10 - 8.07 (m, 2H), 7.88 - 7.86 (d, *J* = 4.92 Hz, 1H), 7.82 - 7.80 (d, *J* = 8.84 Hz, 1H), 7.72 - 7.71 (m, 3H), 7.64 - 7.58 (m, 3H), 7.48 - 7.38 (m, 5H), 6.70 - 6.66 (d, *J* = 16.24 Hz, 1H), 2.75 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.8, 155.3, 149.2, 147.2, 146.3, 144.9, 141.2, 135.7, 134.5, 134.3, 132.8, 132.6, 131.3, 130.8, 130.7, 130.3, 130.0, 129.6, 129.1, 129.1, 128.7, 127.9, 127.7, 126.9, 125.9, 125.1, 124.9, 124.3, 24.1; LC – MS : m/e 519.37, $C_{32}H_{20}Cl_2N_2O$ required Mol. Wt.: 519.42.



yellow solid, m.p 165 – 166 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.03 (s, 1H), 8.09 - 8.07 (d, *J* = 8.96 Hz, 1H), 7.83 (s, 1H), 7.72 - 7.69 (dd, *J* = 8.97, 2.16 Hz, 1H), 7.61 - 7.60 (d, *J* = 2.04 Hz, 1H), 7.54 - 7.52 (d, *J* = 7.96 Hz, 2H), 7.49 - 7.48 (d, *J* = 7.32 Hz, 1H), 7.39 – 7.34 (m, 5H), 7.28 – 7.25 (m, 2H), 7.09 - 7.07 (d, *J* = 6.76 Hz, 1H), 2.73 (s, 3H); ^{13}C NMR (100MHz, $CDCl_3$) δ 197.9, 162.1, 155.4, 146.2, 144.7, 141.6, 138.5, 134.6, 133.4, 132.4, 131.0, 130.6, 130.3, 130.1, 129.9, 129.3, 128.9, 128.9, 128.6, 126.2, 125.1, 124.9, 123.3, 119.5, 115.6, 24.1; IR (v, cm^{-1}) 2997, 2960, 2922, 2850, 1737, 1701, 1676, 1575, 1556, 1467, 1438, 1390, 1377, 1354, 1201, 1166, 1080, 1028, 960, 837, 765, 734, 711, 636, 621; LC – MS : m/e 451.19, $C_{29}H_{20}Cl_2N_2O$ required Mol. Wt.: 450.92.



yellow solid, m.p 165 – 166 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.76 (s, 1H), 8.19 (s, 1H), 7.82 – 7.78(d, *J* = 16.01 Hz, 1H), 7.54 – 7.36 (m, 10H), 6.82 – 6.78 (d, *J* = 15.90 Hz, 1H), 2.65 (s, 3H), 2.49 (s, 3H).;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0
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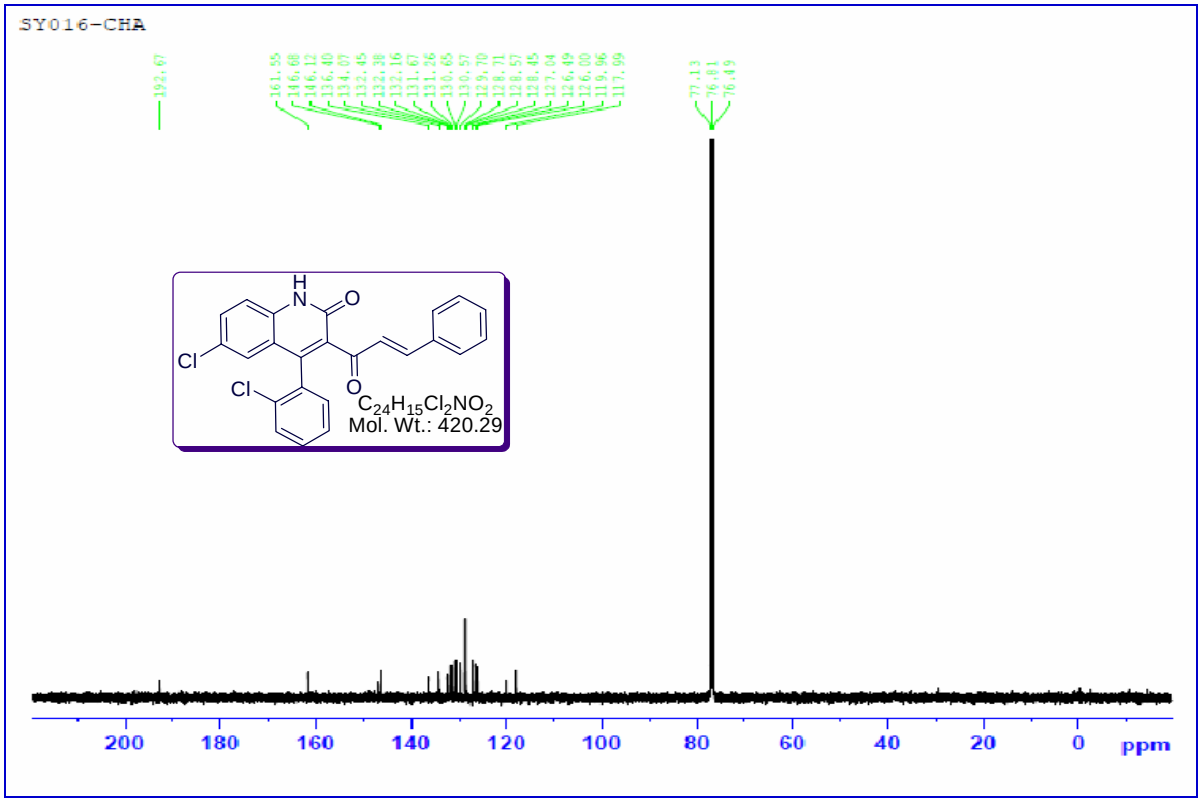
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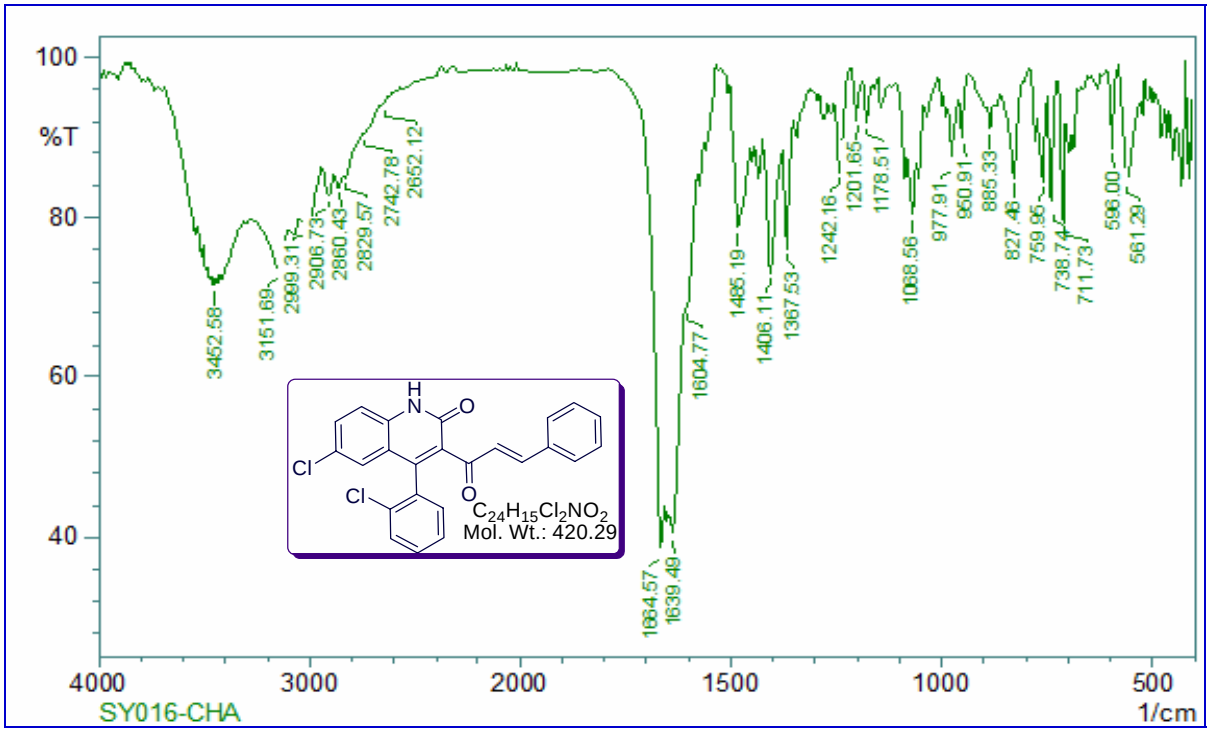
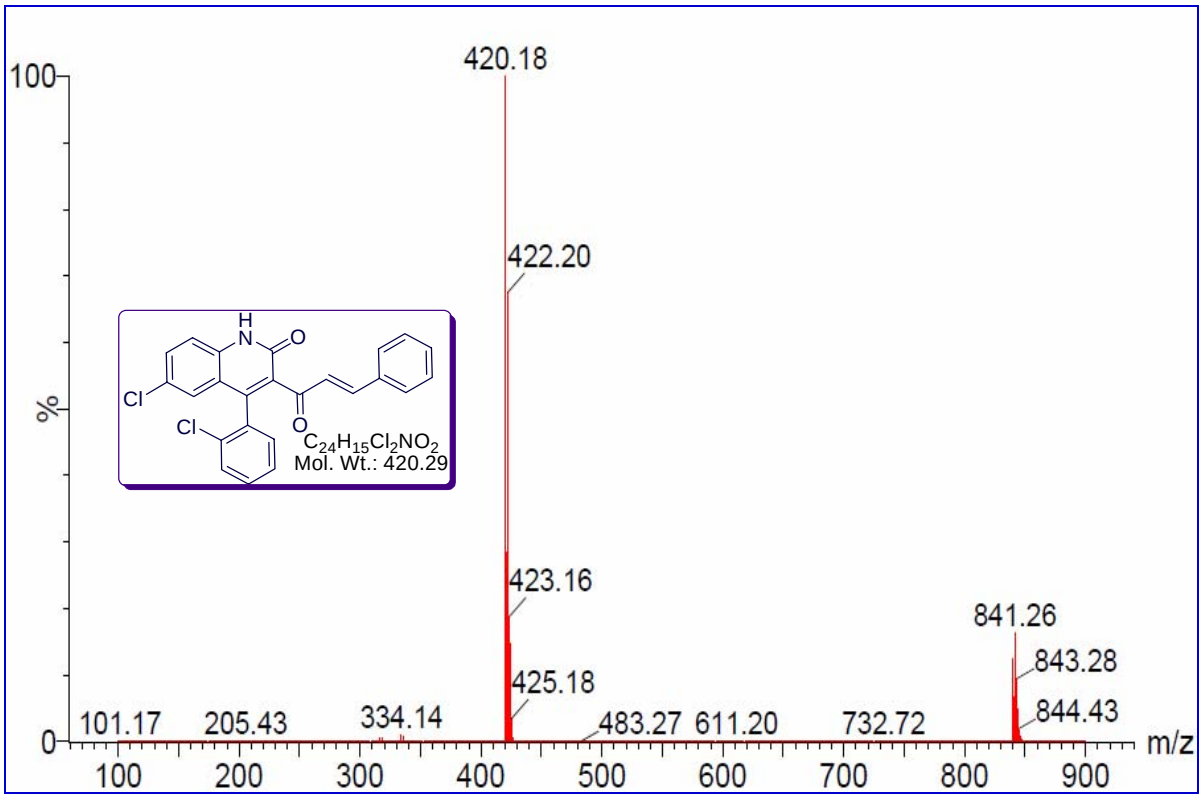
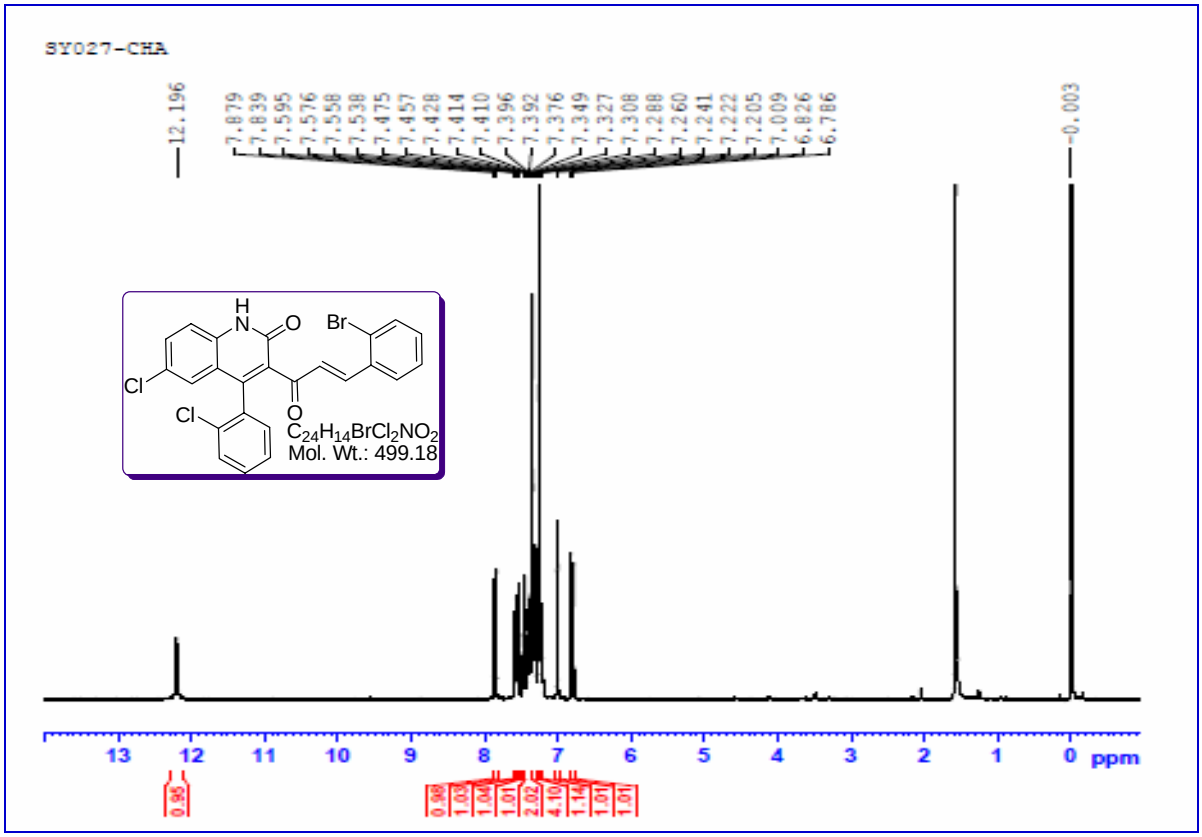
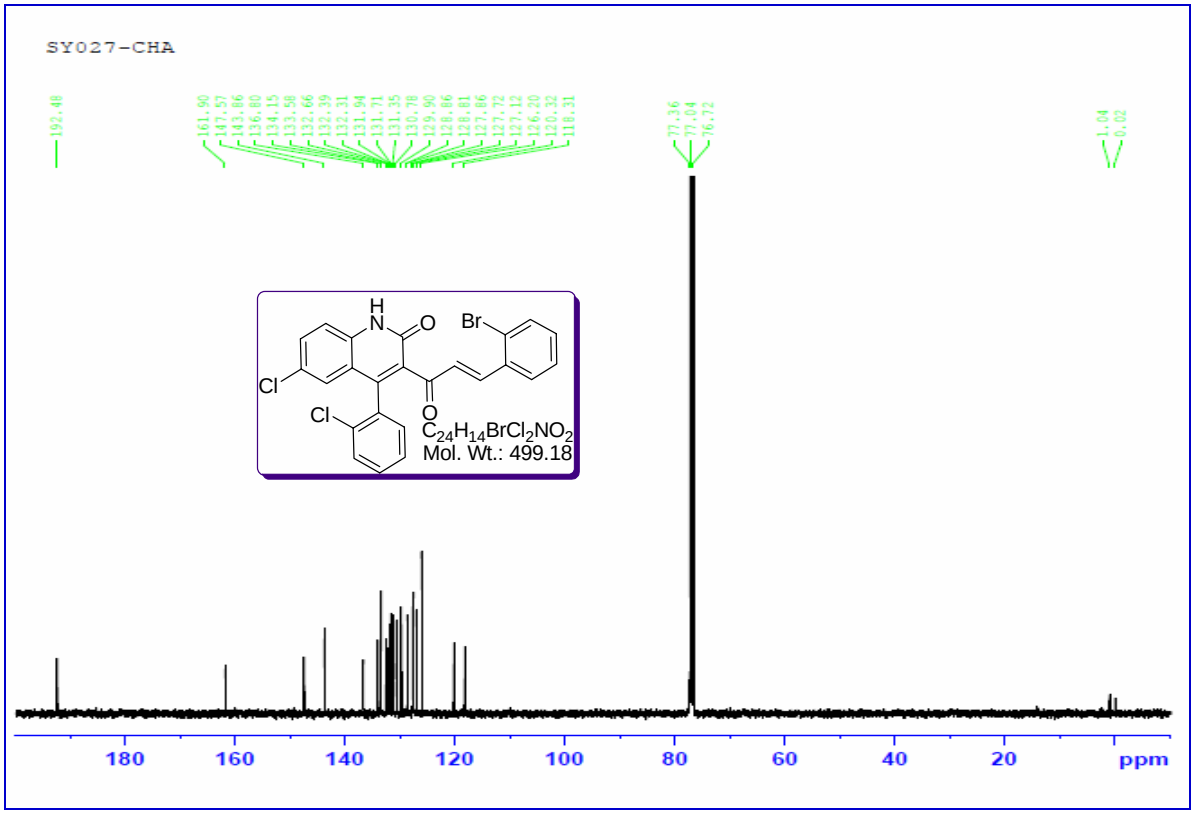
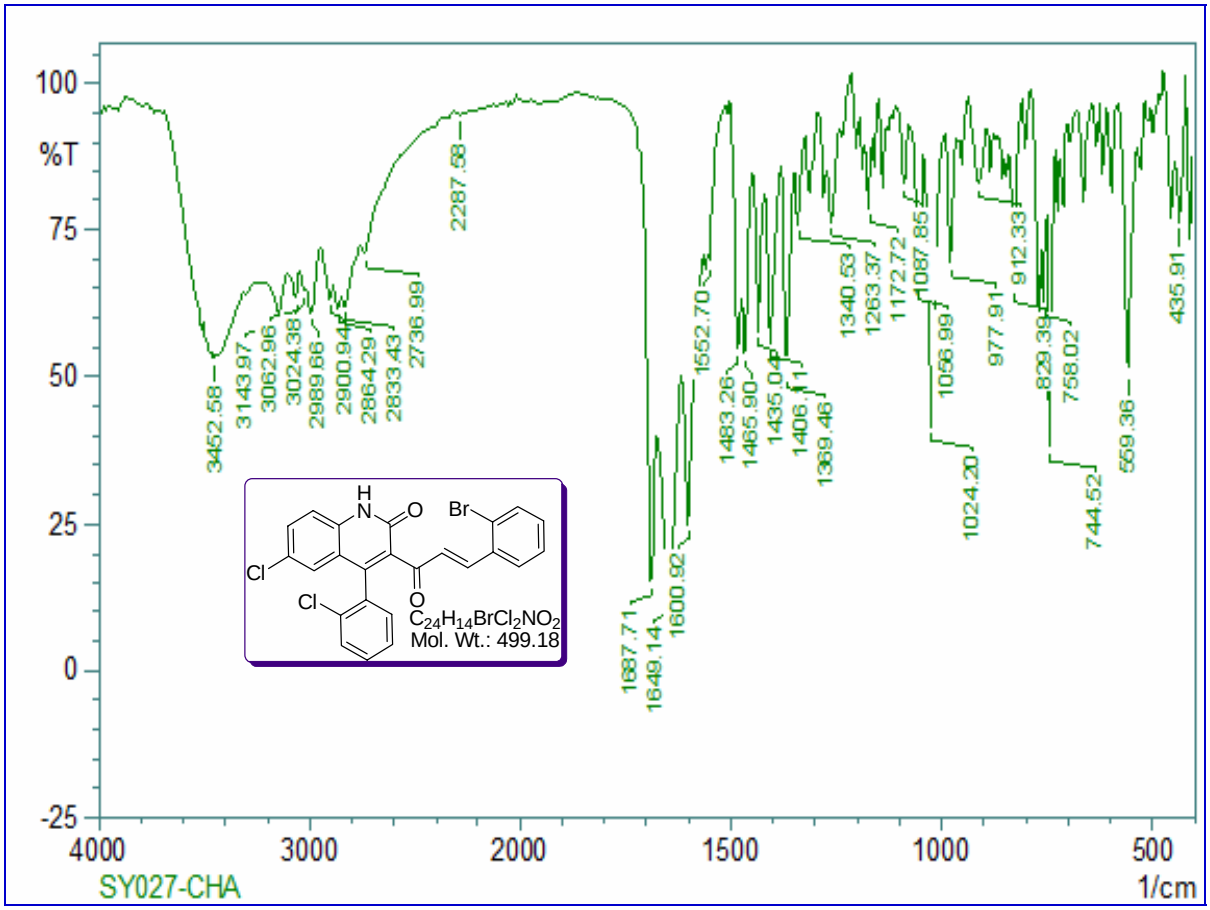
127.04
126.49
126.00
119.96
117.99
77.13
76.81
76.49
H
N
O
Cl
Cl
O
C24H15Cl2NO2
Mol. Wt.: 420.29
200
180
160
140
120
100
80
60
40
20
0
ppm

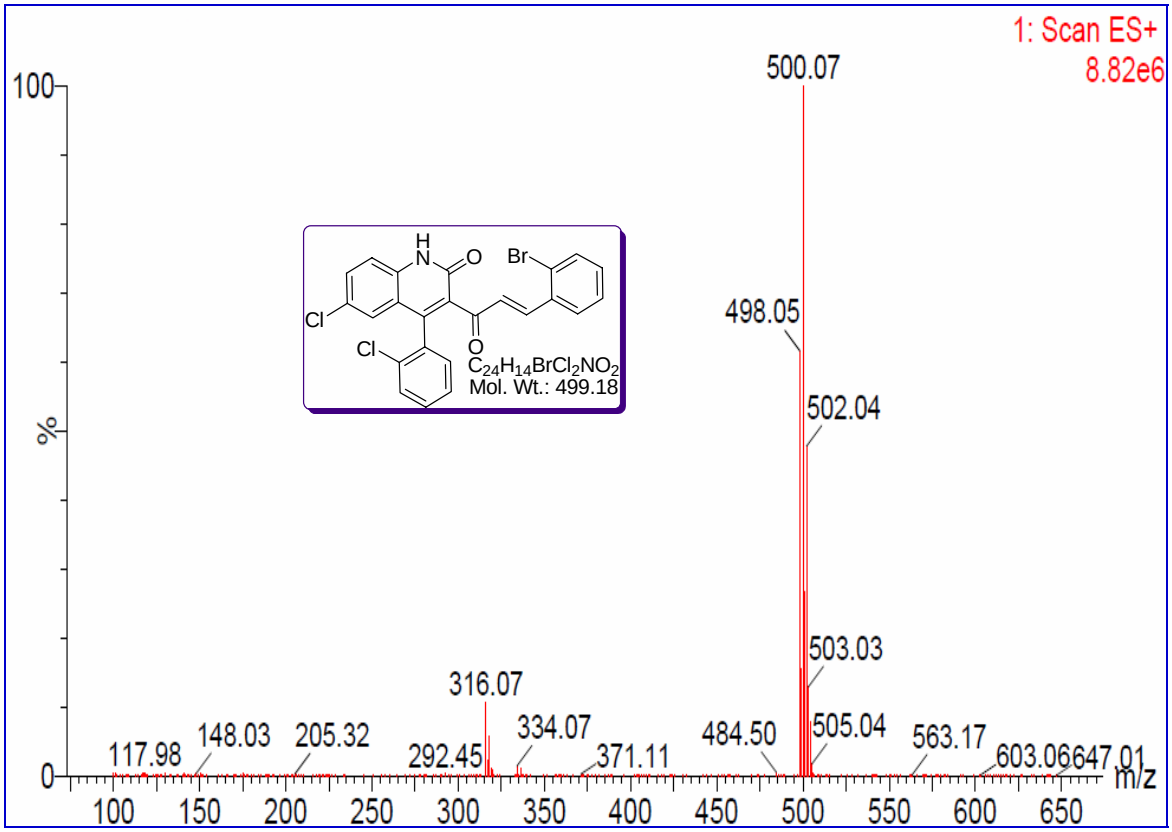

100
%T
80
60
40
4000
3000
2000
1500
1000
500
1/cm
SY016-CHA
3452.58
3151.69
2999.31
2906.73
2860.43
2829.57
2742.78
2652.12
1664.57
1639.49
1604.77
1485.19
1406.11
1367.53
1242.16
1201.65
1178.51
1068.56
977.91
960.91
885.33
827.46
759.95
738.74
711.73
596.00
561.29
Cl
Cl
H
N
O
O
$C_{24}H_{15}Cl_2NO_2$
Mol. Wt.: 420.29

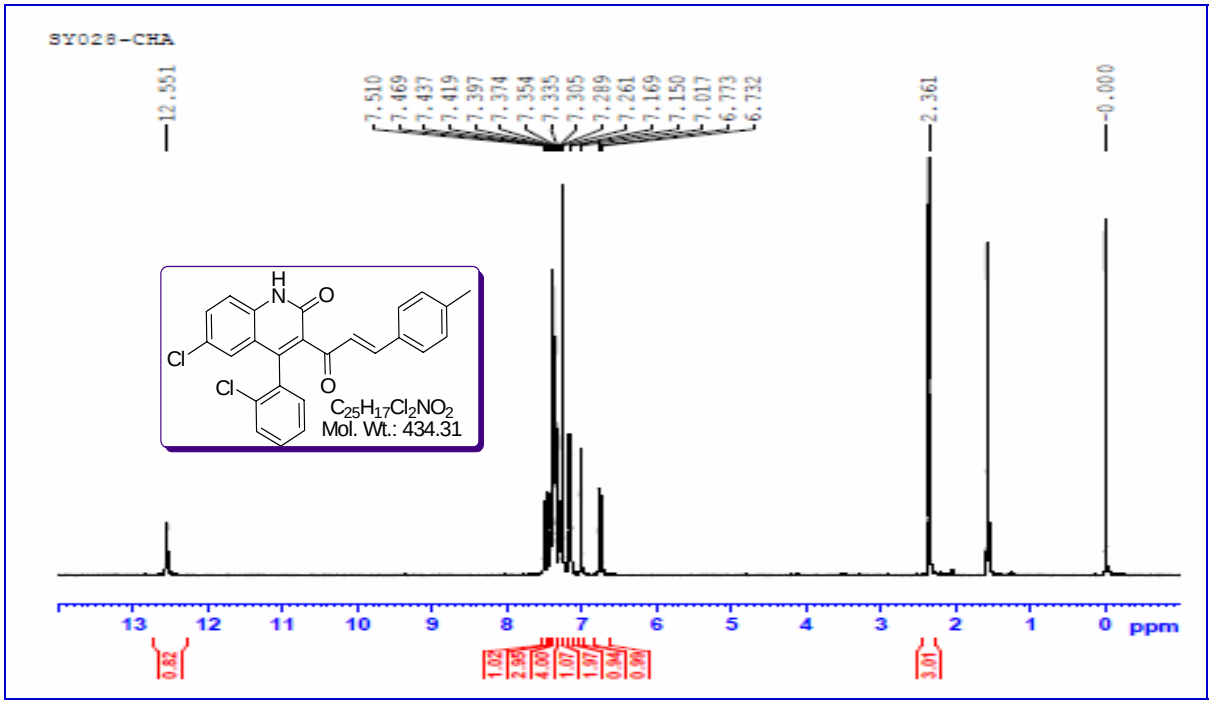

100
%
0
420.18
422.20
423.16
425.18
841.26
843.28
844.43
101.17
205.43
334.14
483.27
611.20
732.72
100
200
300
400
500
600
700
800
900
m/z
Cl
Cl
H
N
O
O
$C_{24}H_{15}Cl_2NO_2$
Mol. Wt.: 420.29

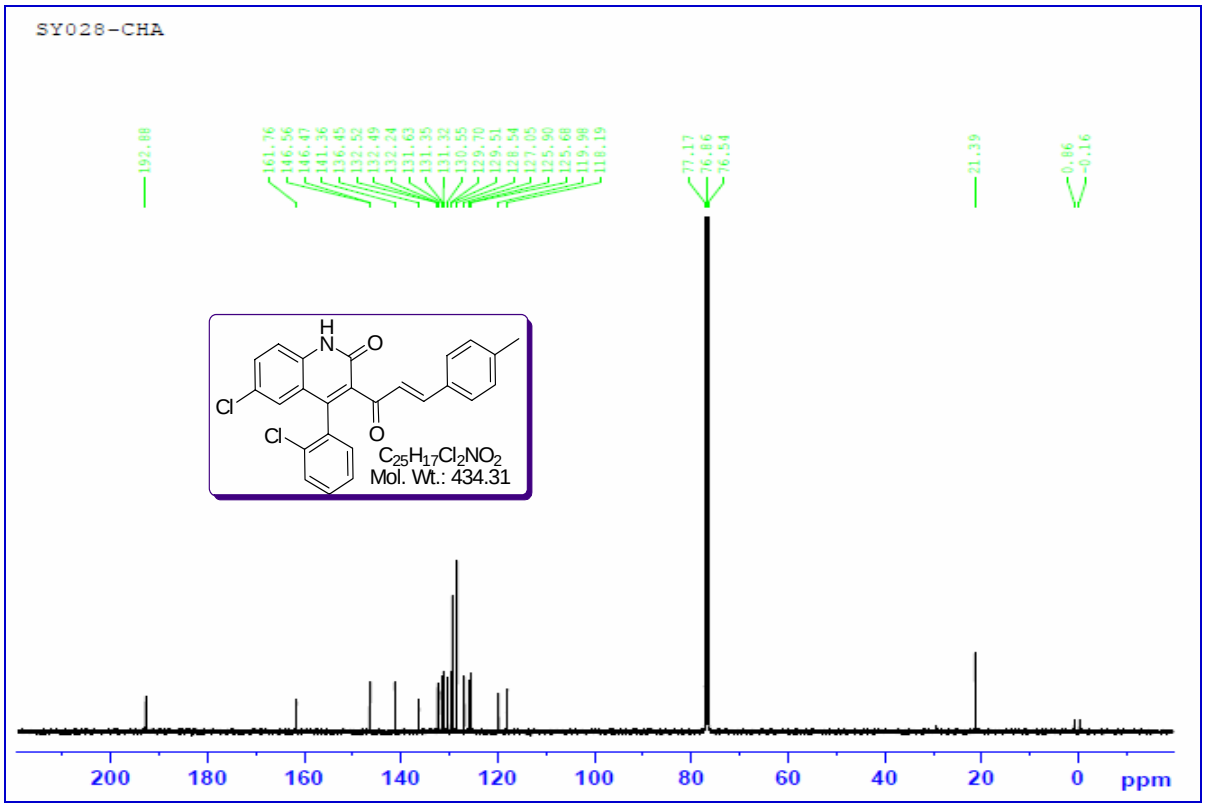

SY027-CHA
12.196
7.879
7.839
7.595
7.576
7.558
7.538
7.475
7.457
7.428
7.414
7.410
7.396
7.392
7.376
7.349
7.327
7.308
7.288
7.260
7.241
7.222
7.205
7.009
6.826
6.786
-0.003
H
N
O
Br
Cl
Cl
O
C24H14BrCl2NO2
Mol. Wt.: 499.18
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.98
1.03
1.04
1.01
1.01
2.02
4.10
1.14
1.01
1.01

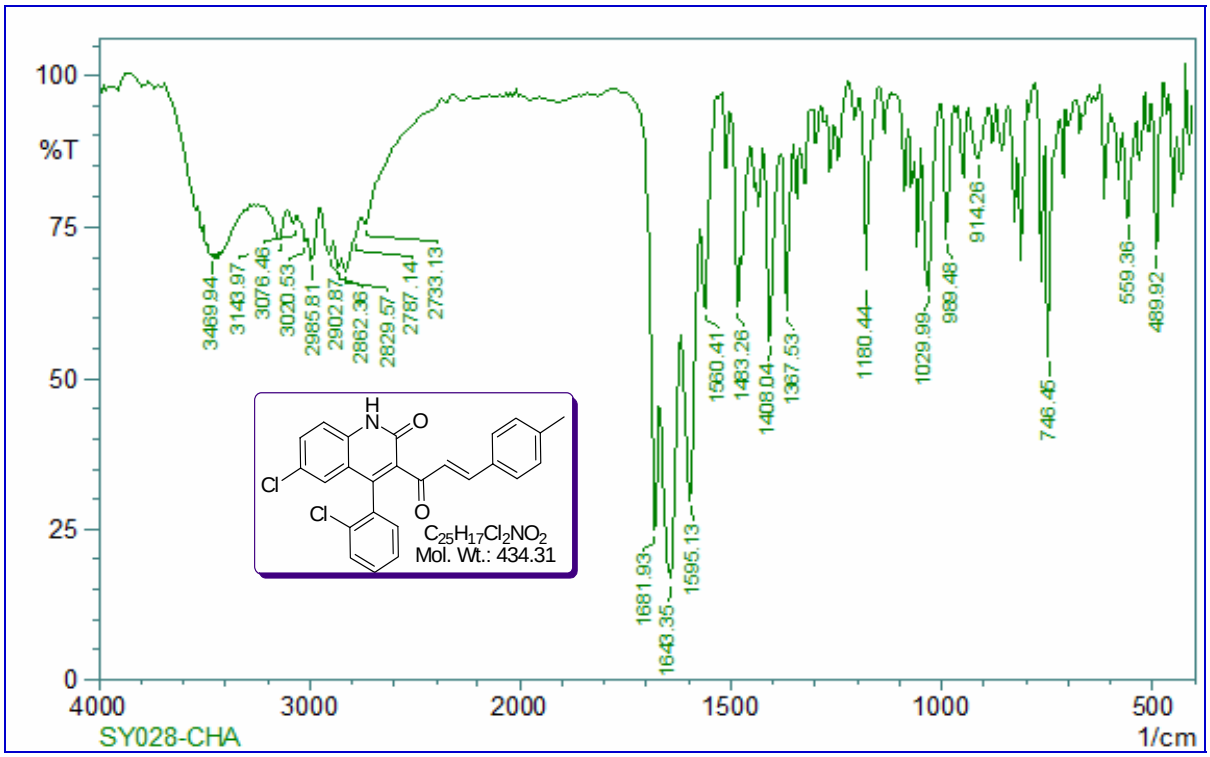

SY027-CHA
192.48
161.90
147.57
143.86
136.80
134.15
133.58
132.66
132.39
132.31
131.94
131.71
131.35
130.78
129.90
128.86
128.81
127.86
127.72
127.12
126.20
120.32
118.31
77.36
77.04
76.72
1.04
0.02
H
N
O
Br
Cl
Cl
O
C24H14BrCl2NO2
Mol. Wt.: 499.18
180
160
140
120
100
80
60
40
20
ppm

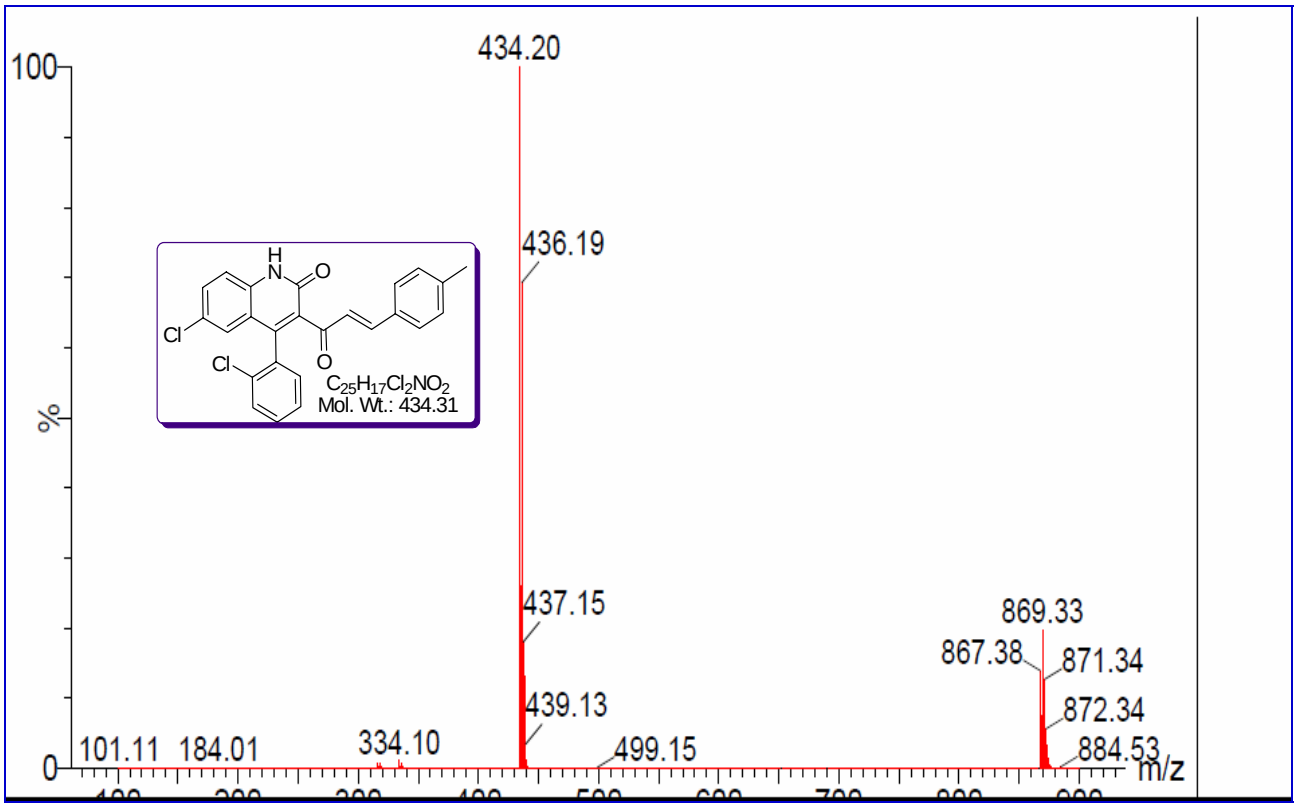

100
%T
75
50
25
0
-25
4000
3000
2000
1500
1000
500
1/cm
SY027-CHA
3452.58
3143.97
3062.96
3024.38
2989.66
2900.94
2864.29
2833.43
2736.99
2287.68
1687.71
1649.14
1600.92
1552.70
1483.26
1465.90
1435.04
1406.11
1389.46
1340.53
1263.37
1172.72
1087.85
1056.99
1024.20
977.91
912.33
829.39
758.02
744.52
659.36
435.91
H
N
O
Br
Cl
Cl
O
C24H14BrCl2NO2
Mol. Wt.: 499.18

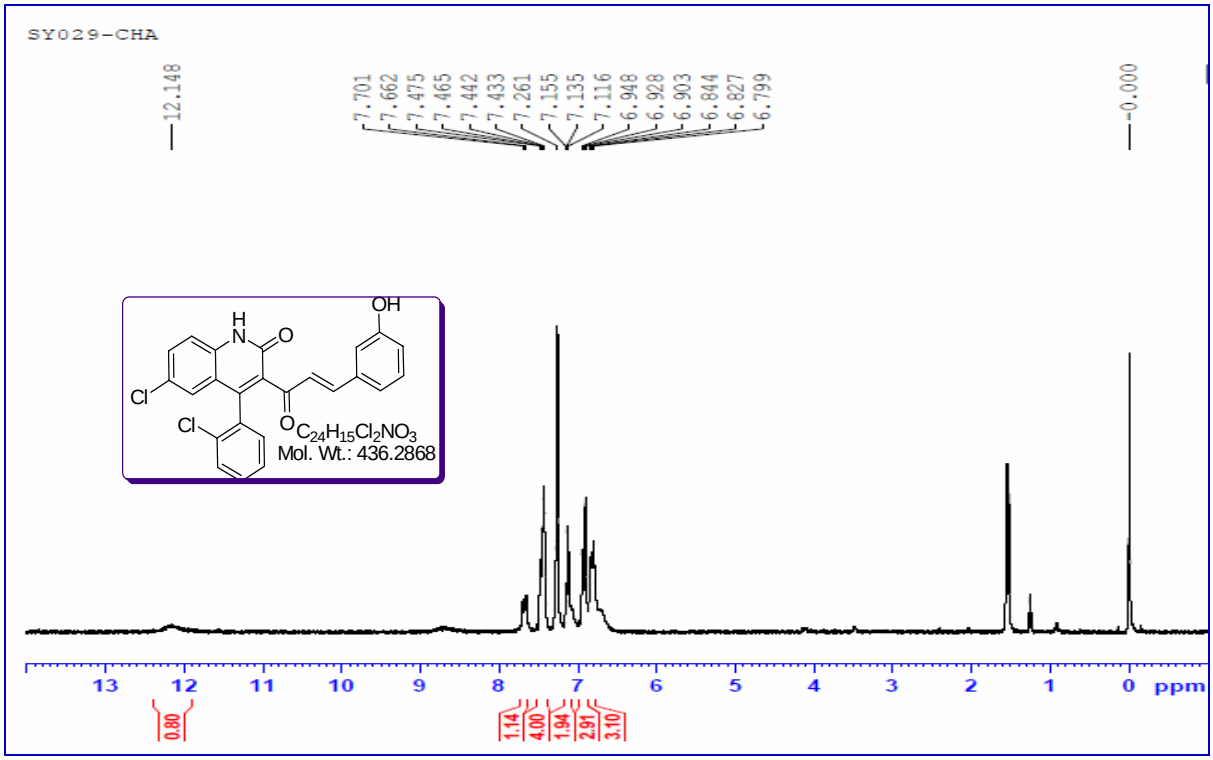

1: Scan ES+
8.82e6
100
%
0
500.07
498.05
502.04
503.03
316.07
334.07
505.04
563.17
603.06
647.01
117.98
148.03
205.32
292.45
371.11
484.50
100
150
200
250
300
350
400
450
500
550
600
650
m/z
H
N
O
Br
Cl
Cl
O
C24H14BrCl2NO2
Mol. Wt.: 499.18

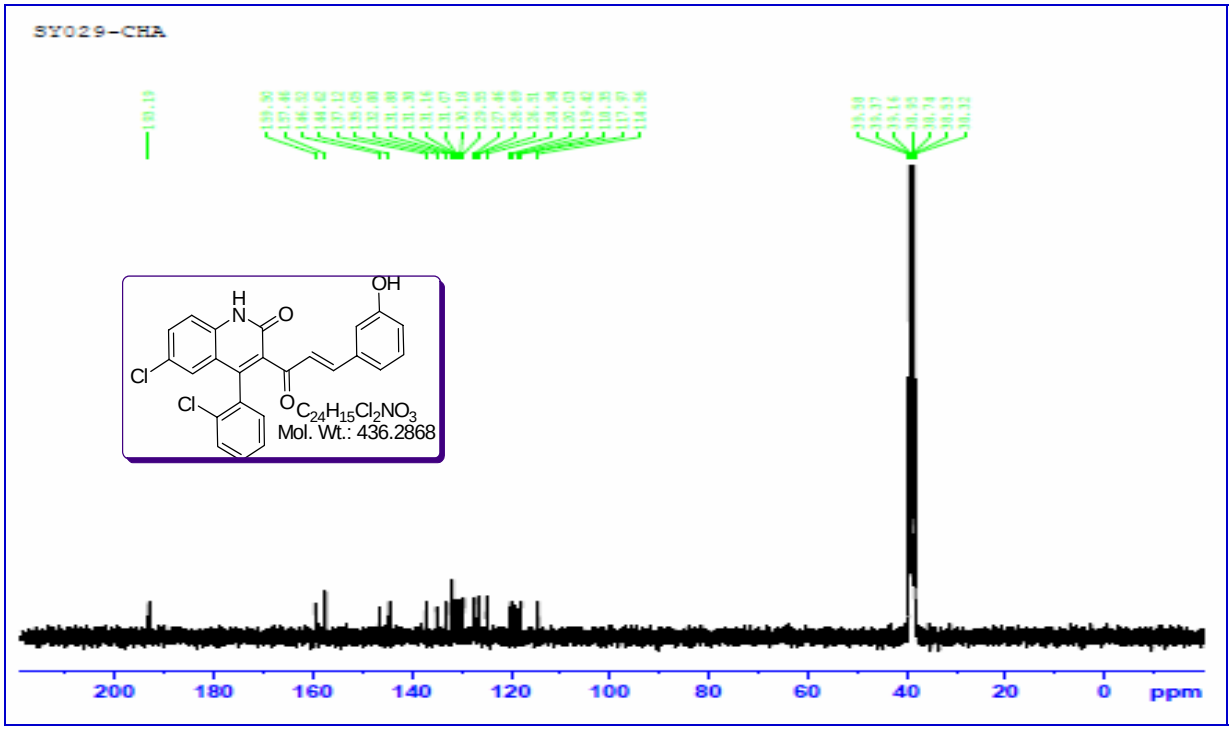

SY028-CHA
12.551
7.510
7.469
7.437
7.419
7.397
7.374
7.354
7.335
7.305
7.289
7.261
7.169
7.150
7.017
6.773
6.732
2.361
-0.000
Cl
Cl
O
H
N
O
C25H17Cl2NO2
Mol. Wt.: 434.31
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.82
1.02
2.90
4.00
1.07
1.97
1.97
0.94
0.99
3.01

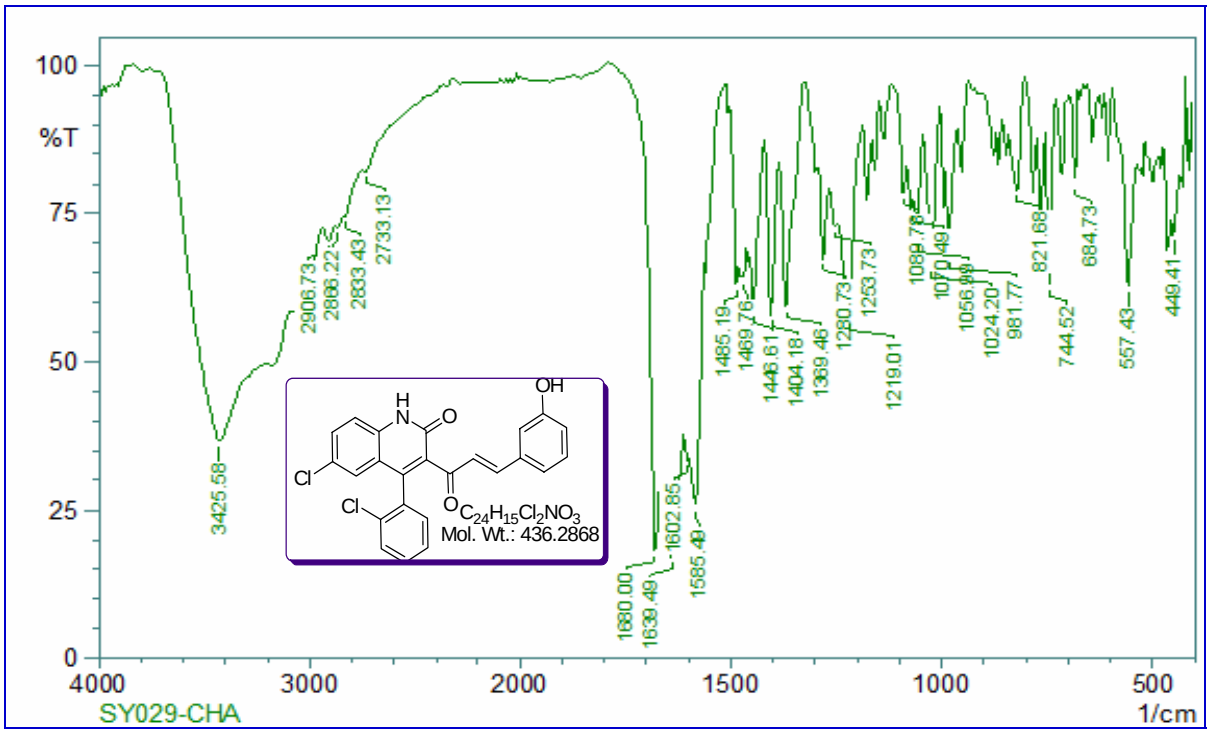

SY028-CHA
192.88
161.76
146.56
146.47
141.36
136.45
132.52
132.49
132.24
131.63
131.35
131.32
130.55
129.70
129.51
128.54
127.05
125.90
125.68
119.98
118.19
77.17
76.86
76.54
21.39
0.86
-0.16
Cl
Cl
O
H
N
O
C25H17Cl2NO2
Mol. Wt.: 434.31
200
180
160
140
120
100
80
60
40
20
0
ppm

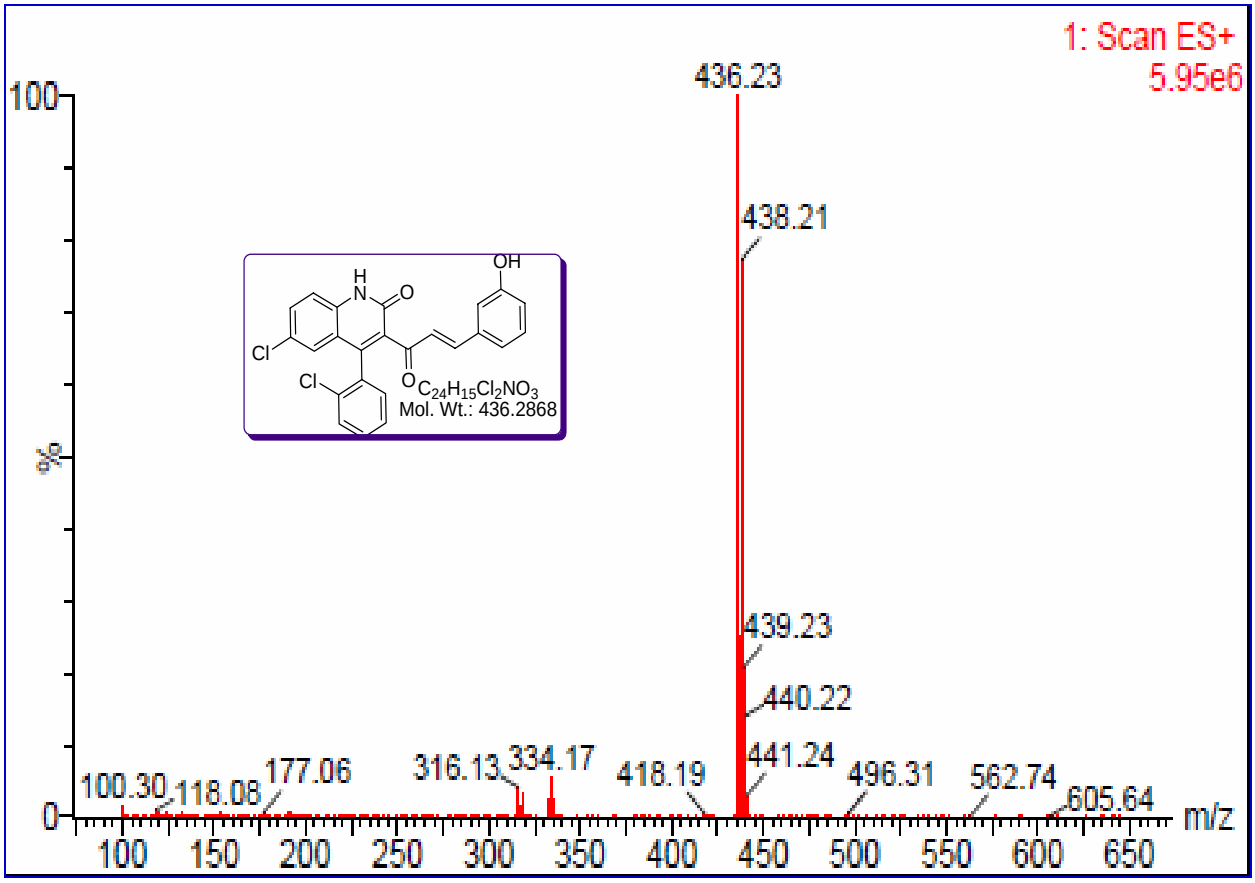

100
%T
75
50
25
0
4000
3000
2000
1500
1000
500
1/cm
SY028-CHA
3469.94
3143.97
3076.46
3020.53
2985.81
2902.87
2862.36
2829.57
2787.14
2733.13
1681.93
1643.35
1595.13
1560.41
1483.26
1408.04
1367.53
1180.44
1029.99
989.48
914.26
746.45
559.36
489.92
H
N
O
Cl
Cl
O
C25H17Cl2NO2
Mol. Wt.: 434.31

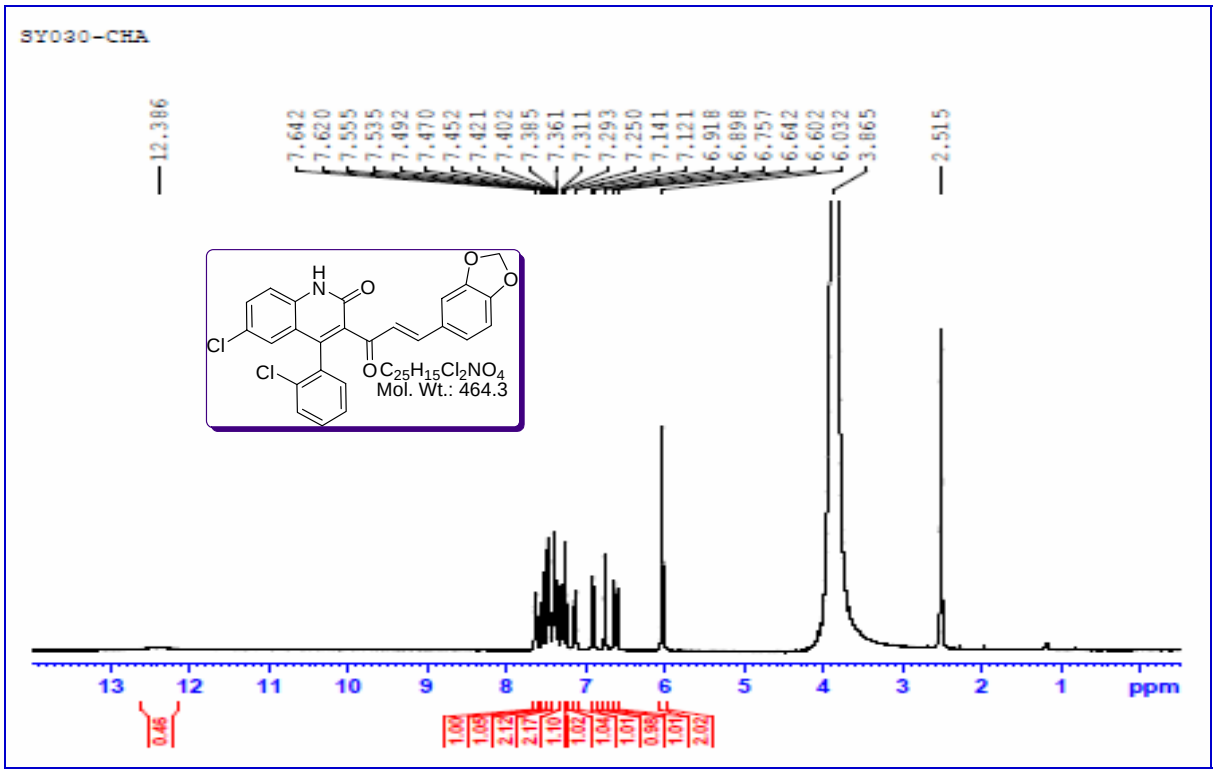

100
%
0
434.20
436.19
437.15
439.13
101.11
184.01
334.10
499.15
867.38
869.33
871.34
872.34
884.53
m/z
H
N
O
Cl
Cl
O
C25H17Cl2NO2
Mol. Wt.: 434.31

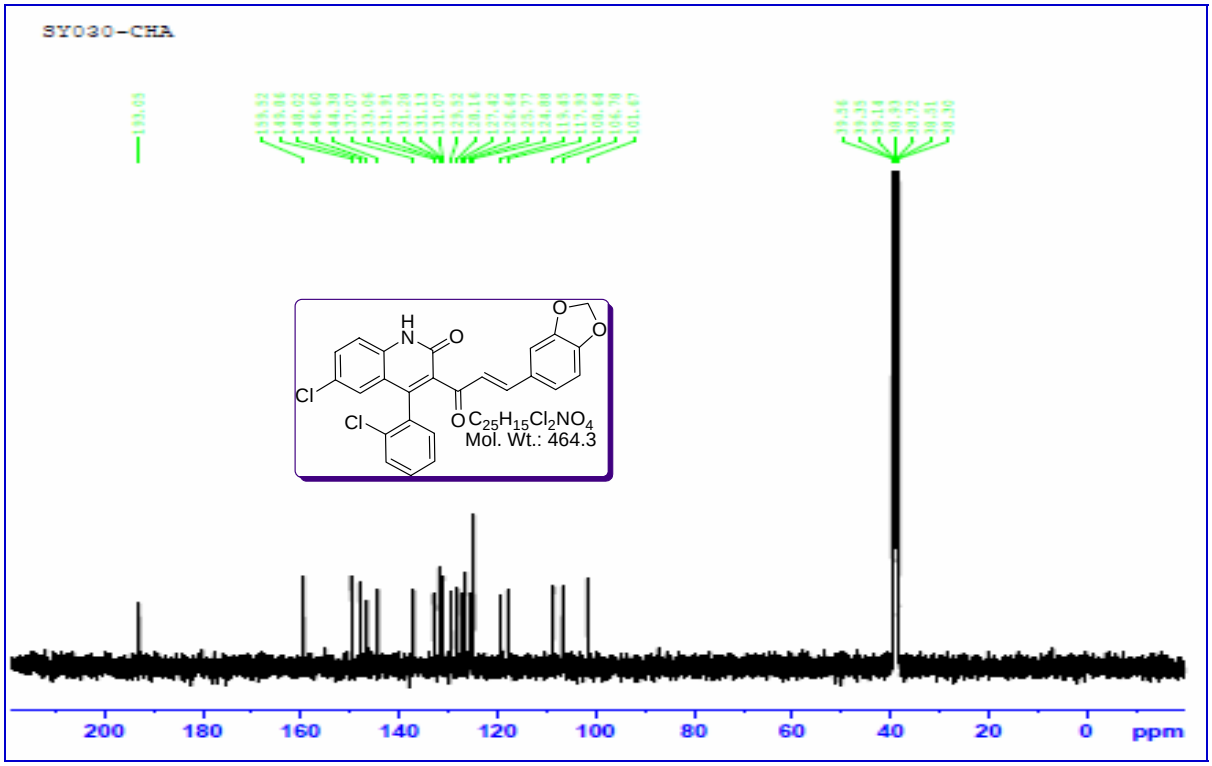

SY029-CHA
12.148
7.701
7.662
7.475
7.465
7.442
7.433
7.261
7.155
7.135
7.116
6.948
6.928
6.903
6.844
6.827
6.799
0.000
OH
H
N
O
Cl
Cl
O
C24H15Cl2NO3
Mol. Wt.: 436.2868
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.80
1.14
4.00
1.94
2.91
3.10

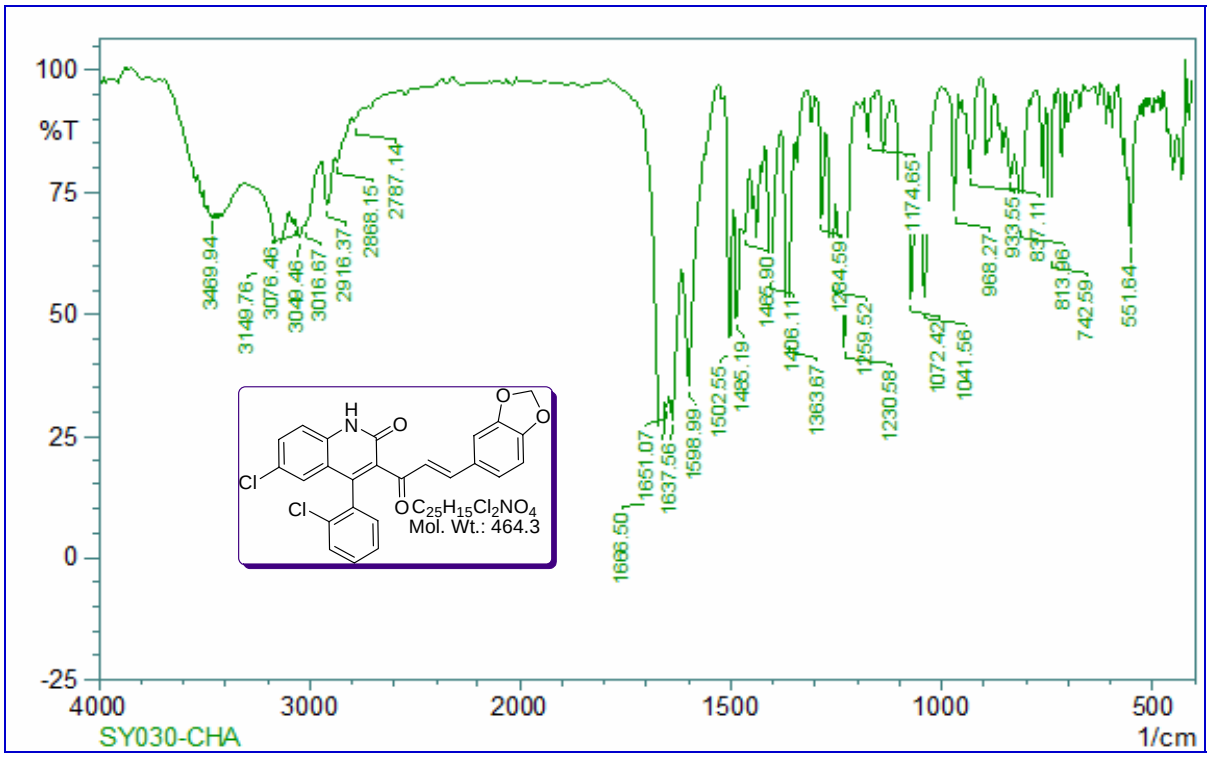

SY029-CHA
OH
H
N
O
Cl
Cl
O
C24H15Cl2NO3
Mol. Wt.: 436.2868
200
180
160
140
120
100
80
60
40
20
0
ppm

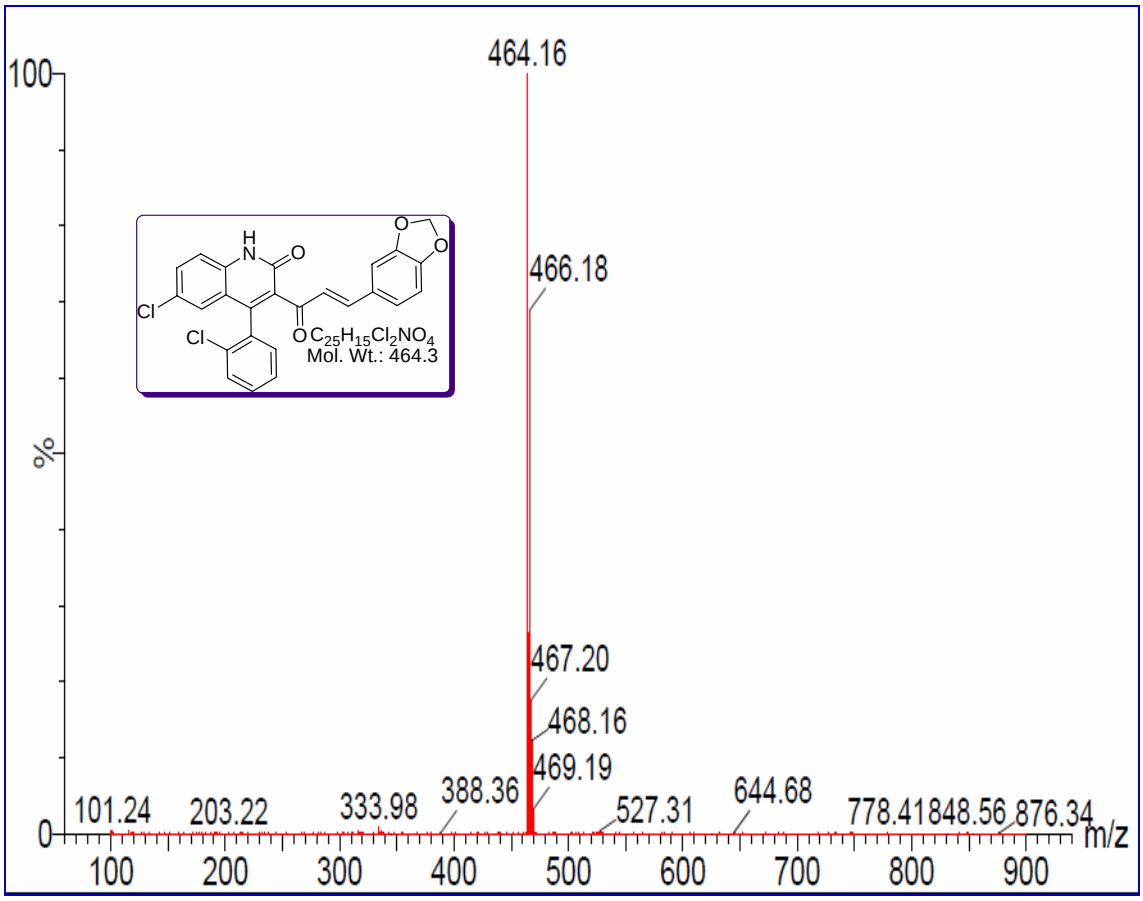

100
%T
75
50
25
0
4000
3000
2000
1500
1000
500
1/cm
SY029-CHA
3425.58
2906.73
2886.22
2833.43
2733.13
1680.00
1639.49
1602.85
1585.49
1485.19
1469.76
1446.61
1404.18
1369.46
1280.73
1253.73
1219.01
1089.78
1070.49
1056.99
1024.20
981.77
821.68
744.52
684.73
557.43
449.41
OH
H
N
O
Cl
Cl
O
C24H15Cl2NO3
Mol. Wt.: 436.2868

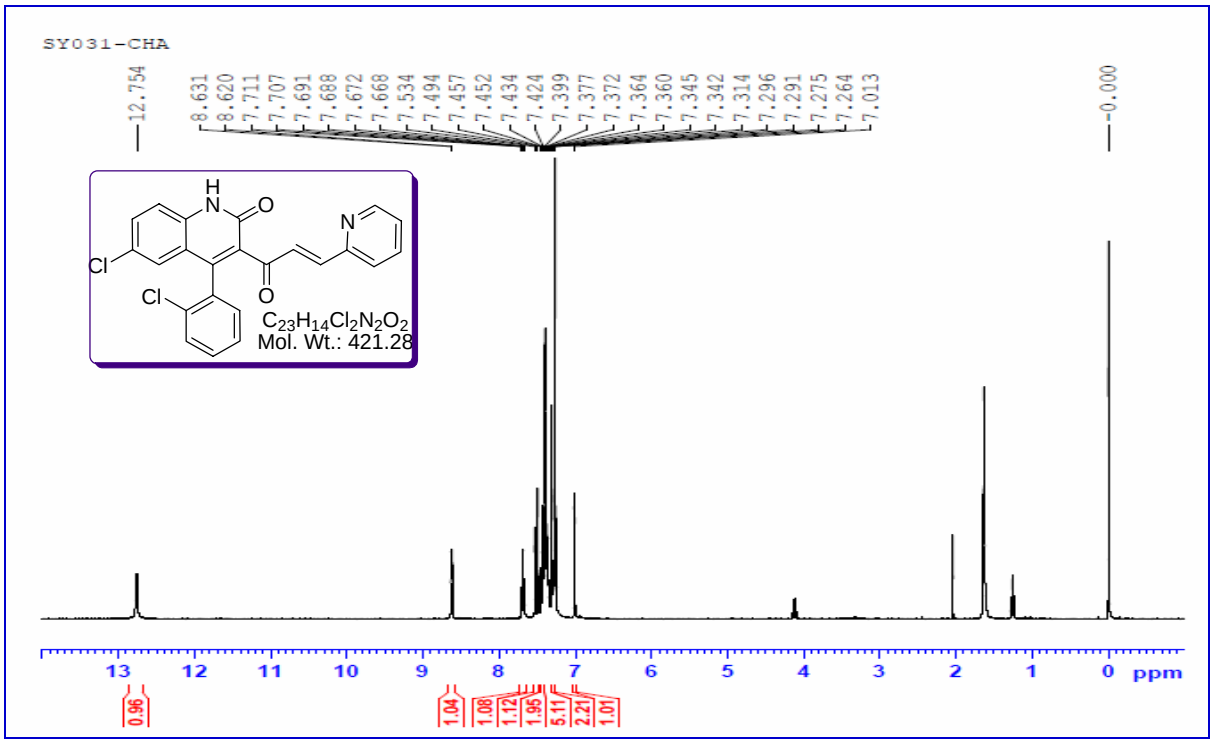

1: Scan ES+
5.95e6
100
%
0
436.23
438.21
439.23
440.22
441.24
100.30
118.08
177.06
316.13
334.17
418.19
496.31
562.74
605.64
m/z
100
150
200
250
300
350
400
450
500
550
600
650
OH
H
N
O
Cl
Cl
O
C24H15Cl2NO3
Mol. Wt.: 436.2868

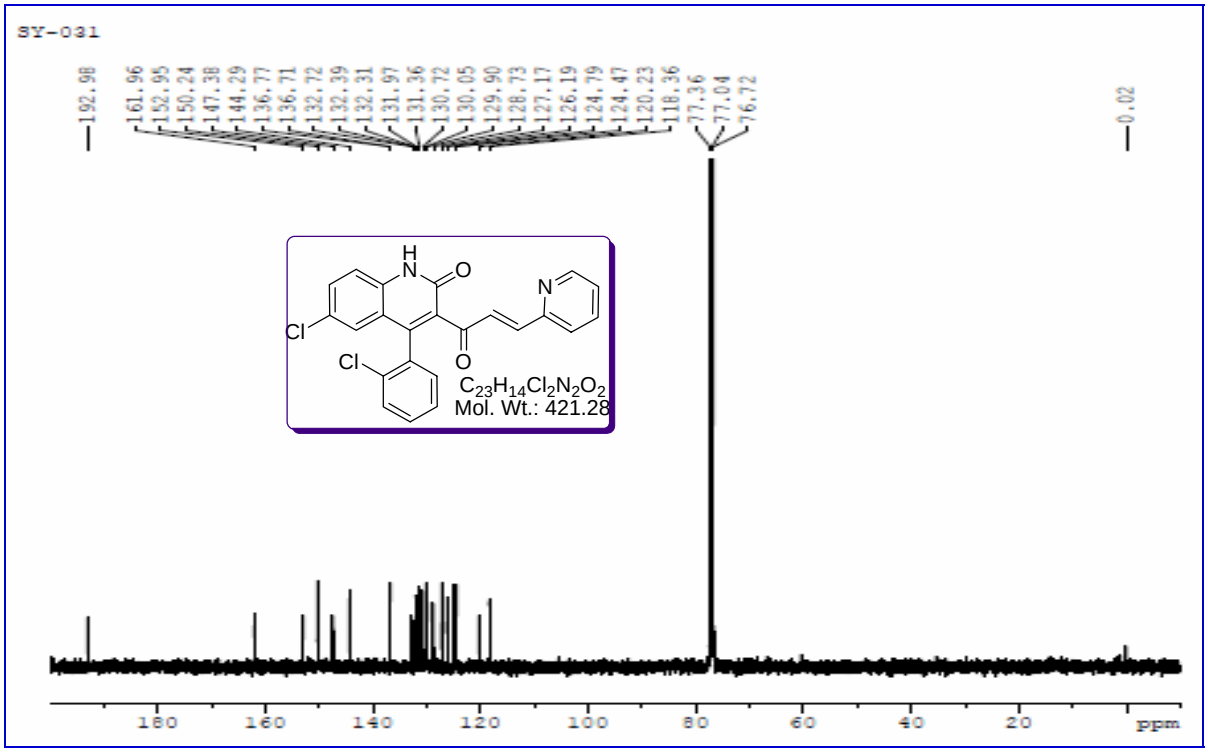

SY030-CHA
12.386
7.642
7.620
7.555
7.535
7.492
7.470
7.452
7.421
7.402
7.385
7.361
7.311
7.293
7.250
7.141
7.121
6.918
6.898
6.757
6.642
6.602
6.032
3.865
2.515
O
H
N
O
Cl
Cl
O
O
O C25H15Cl2NO4
Mol. Wt.: 464.3
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
0.46
1.00
1.05
2.12
2.17
1.10
1.02
1.04
1.01
0.98
1.01
2.02

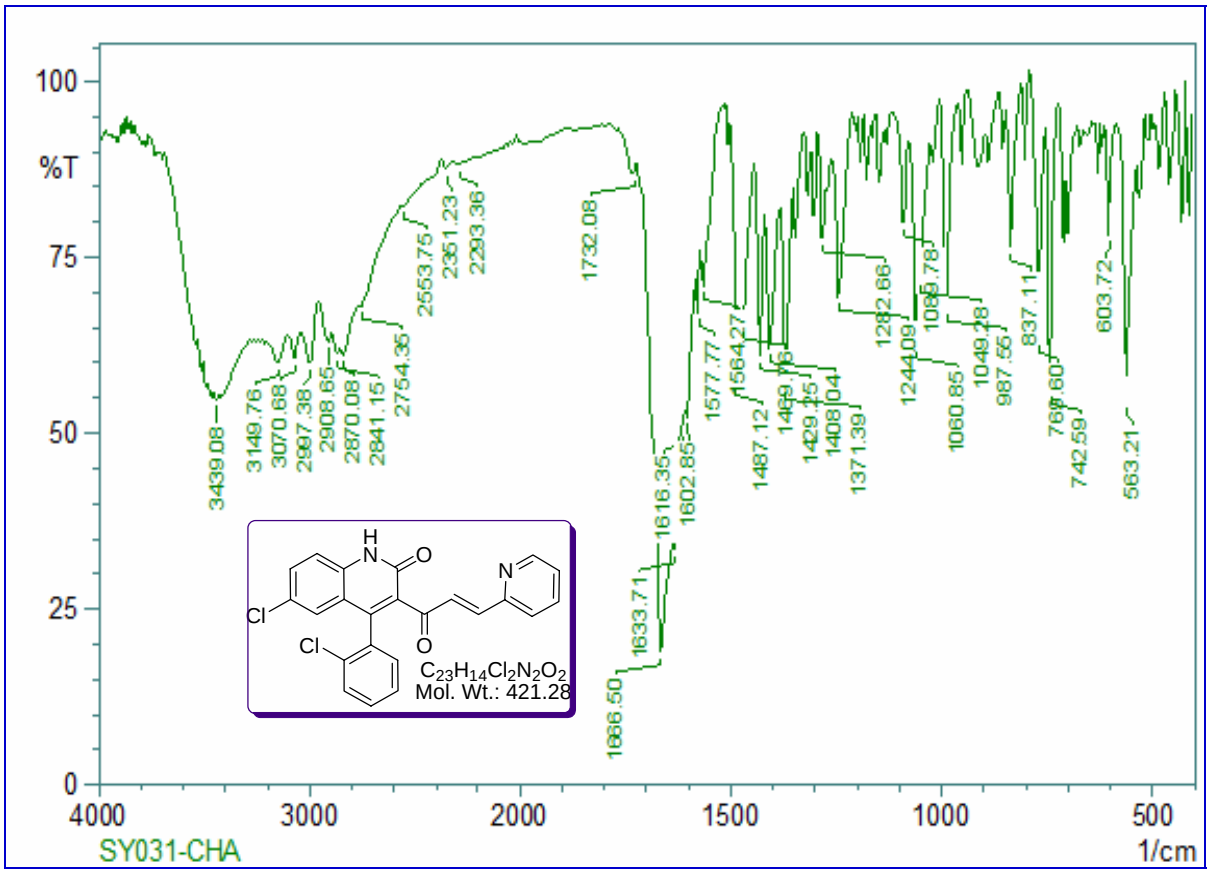

SY030-CHA
193.03
159.52
148.86
148.02
146.60
144.39
137.07
133.06
131.91
131.28
131.13
131.07
129.92
129.16
127.42
126.64
125.77
124.88
115.45
113.93
108.64
106.78
101.67
39.36
39.33
39.14
38.93
38.72
38.51
38.30
O
H
N
O
Cl
Cl
O
O
O C25H15Cl2NO4
Mol. Wt.: 464.3
200
180
160
140
120
100
80
60
40
20
0
ppm

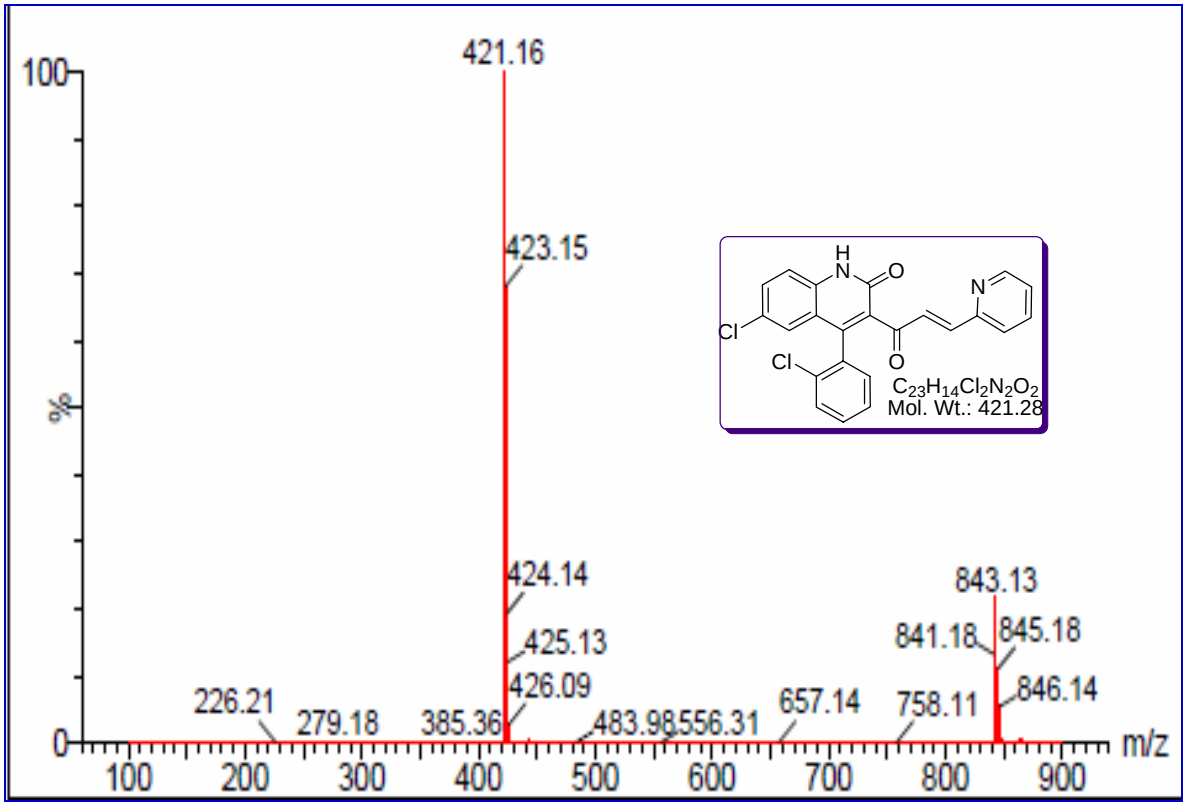

100
%T
75
50
25
0
-25
4000
3000
2000
1500
1000
500
1/cm
SY030-CHA
3469.94
3149.76
3076.46
3043.46
3016.67
2916.37
2868.15
2787.14
1686.50
1651.07
1637.56
1598.99
1502.55
1485.19
1465.90
1406.11
1363.67
1284.59
1259.52
1230.58
1174.65
1072.42
1041.56
968.27
933.55
837.11
813.86
742.59
551.64
Cl
Cl
O
$C_{25}H_{15}Cl_2NO_4$
Mol. Wt.: 464.3

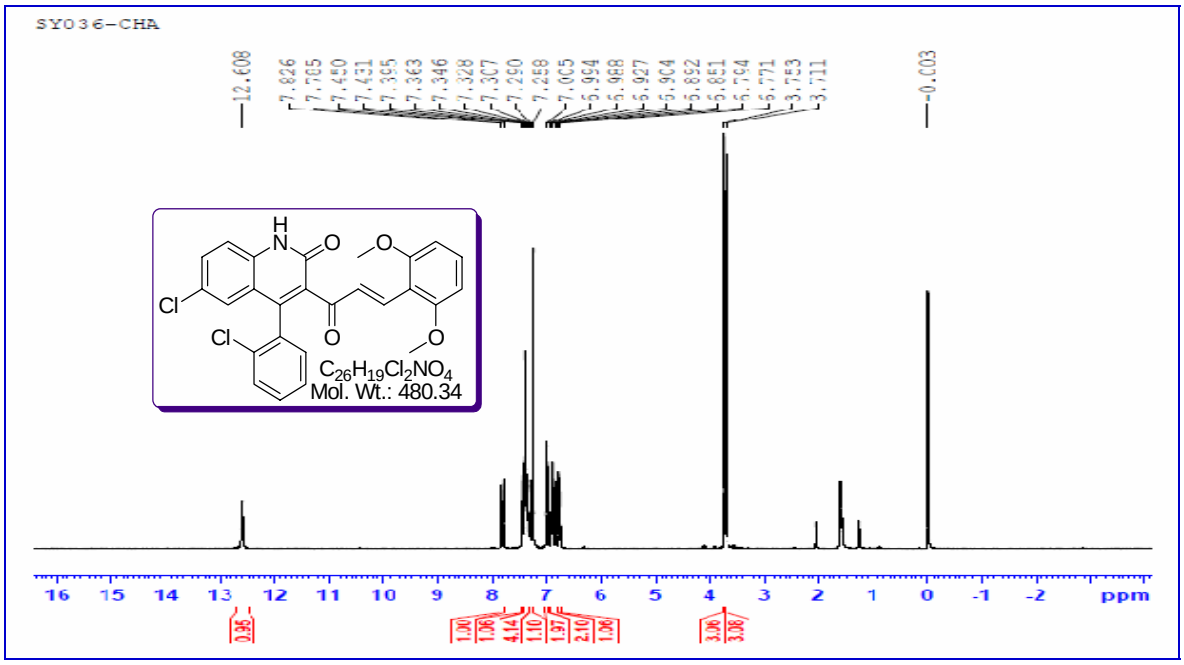

100
%
0
464.16
466.18
467.20
468.16
469.19
101.24
203.22
333.98
388.36
527.31
644.68
778.41
848.56
876.34
100
200
300
400
500
600
700
800
900
m/z
Cl
Cl
O
$C_{25}H_{15}Cl_2NO_4$
Mol. Wt.: 464.3

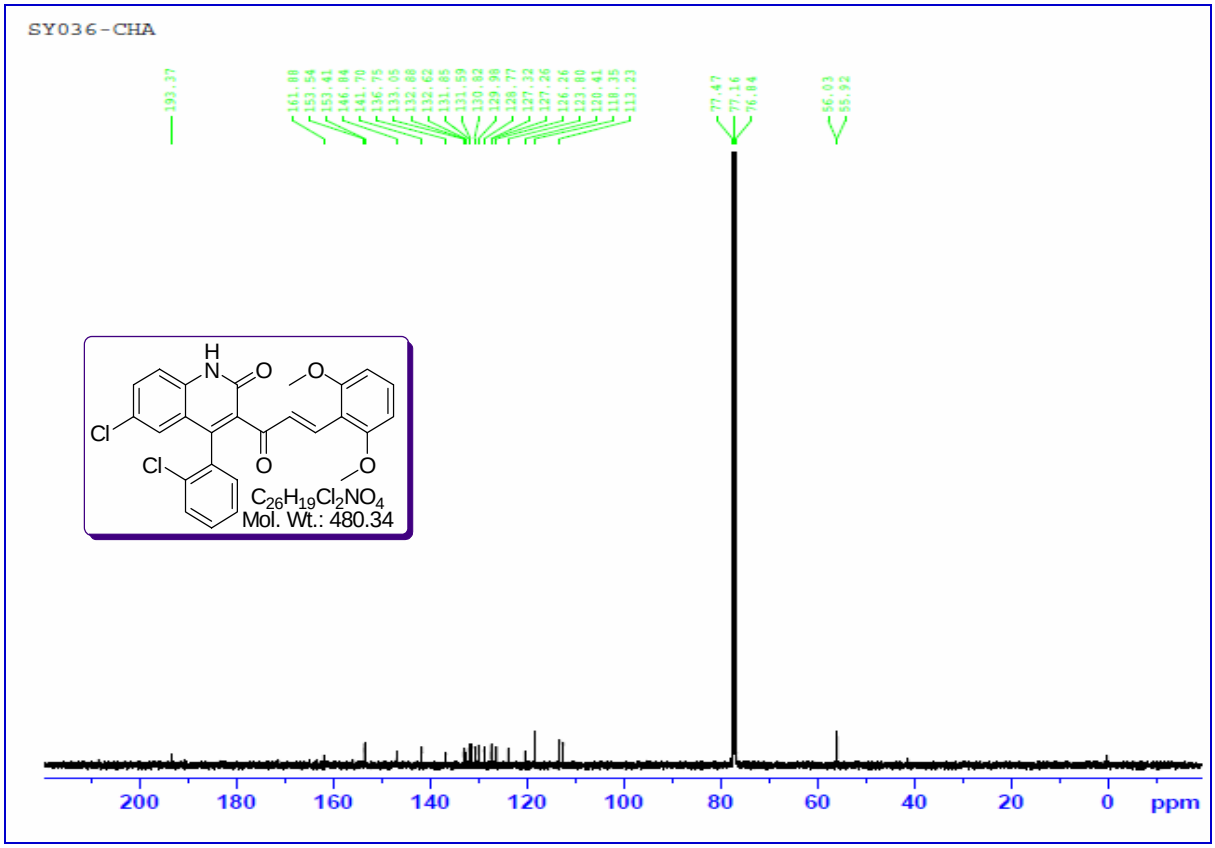

SY031-CHA
12.754
8.631
8.620
7.711
7.707
7.691
7.688
7.672
7.668
7.534
7.494
7.457
7.452
7.434
7.424
7.399
7.377
7.372
7.364
7.360
7.345
7.342
7.314
7.296
7.291
7.275
7.264
7.013
0.000
H
N
O
N
Cl
Cl
O
C23H14Cl2N2O2
Mol. Wt.: 421.28
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.96
1.04
1.08
1.12
1.95
5.11
2.21
1.01

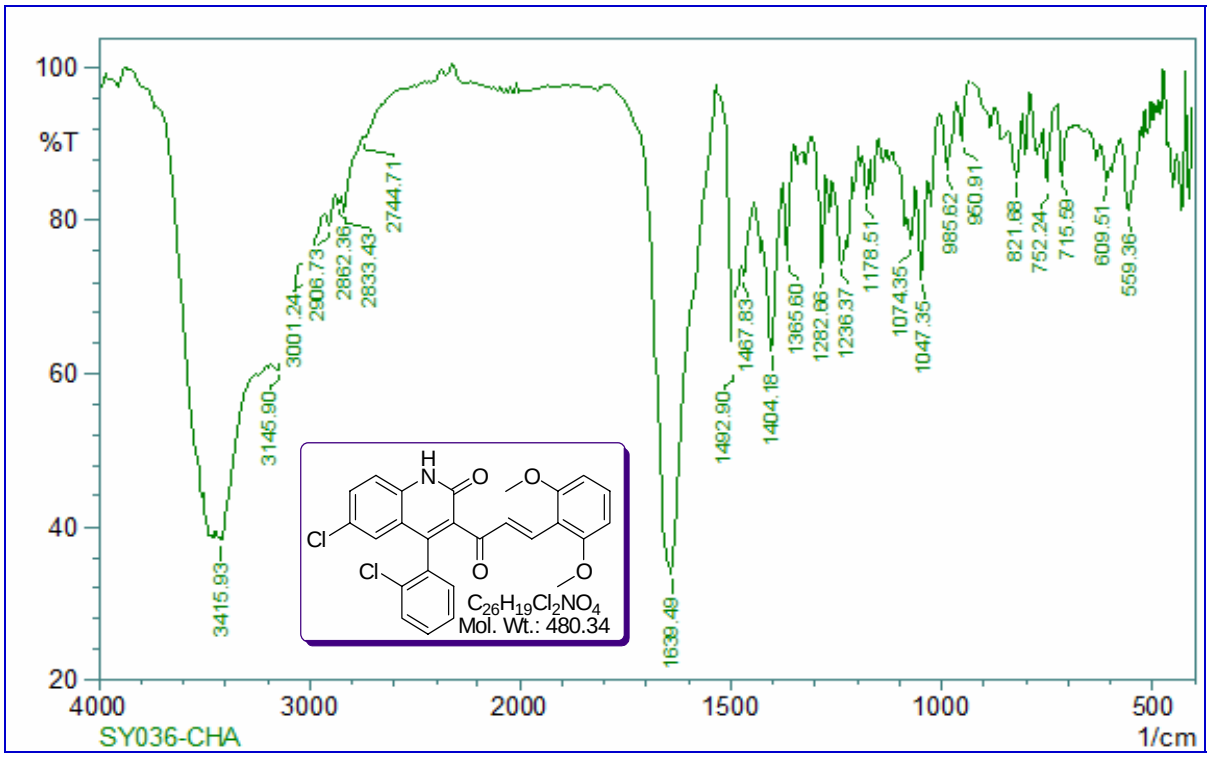

SY-031
192.98
161.96
152.95
150.24
147.38
144.29
136.77
136.71
132.72
132.39
132.31
131.97
131.36
130.72
130.05
129.90
128.73
127.17
126.19
124.79
124.47
120.23
118.36
77.36
77.04
76.72
0.02
H
N
O
N
Cl
Cl
O
C23H14Cl2N2O2
Mol. Wt.: 421.28
180
160
140
120
100
80
60
40
20
ppm

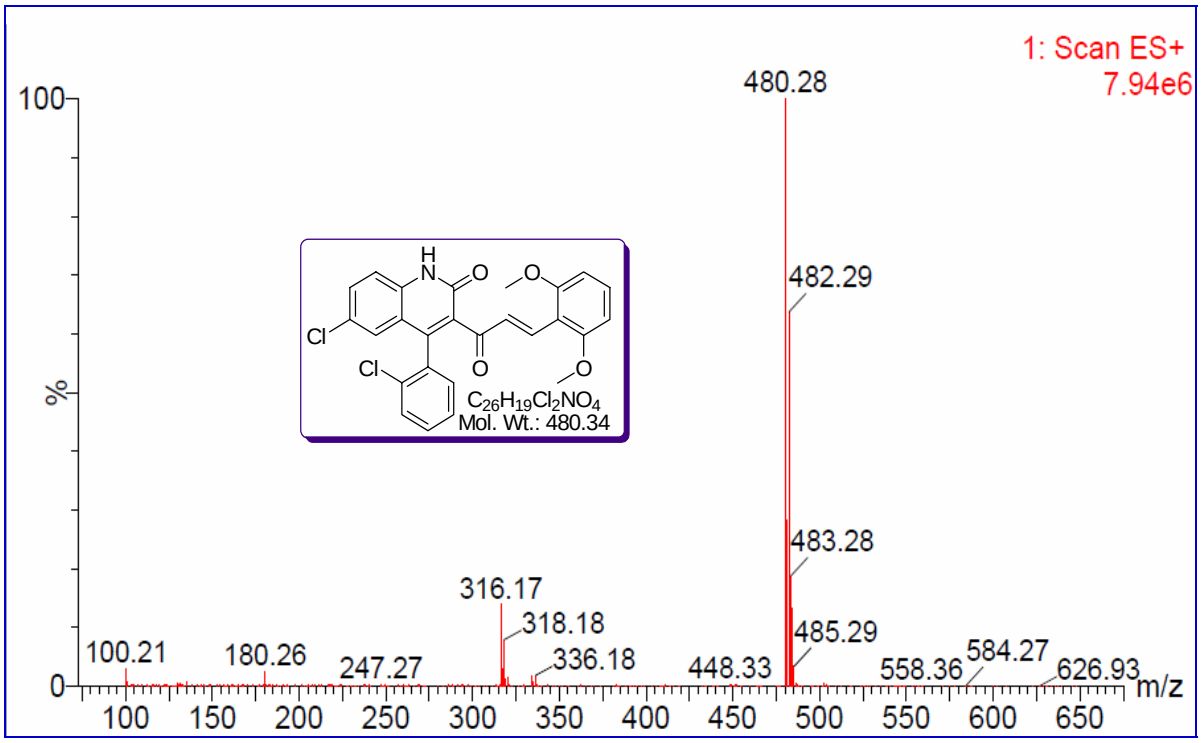

100
%T
75
50
25
0
4000
3000
2000
1500
1000
500
1/cm
SY031-CHA
3439.08
3149.76
3070.68
2997.38
2908.65
2870.08
2841.15
2754.35
2553.75
2361.23
2293.36
1732.08
1666.50
1633.71
1616.35
1602.85
1577.77
1564.27
1487.12
1469.76
1429.25
1408.04
1371.39
1282.66
1244.09
1085.78
1060.85
1049.28
987.55
837.11
768.60
742.59
603.72
563.21
H
N
O
Cl
N
Cl
O
C23H14Cl2N2O2
Mol. Wt.: 421.28

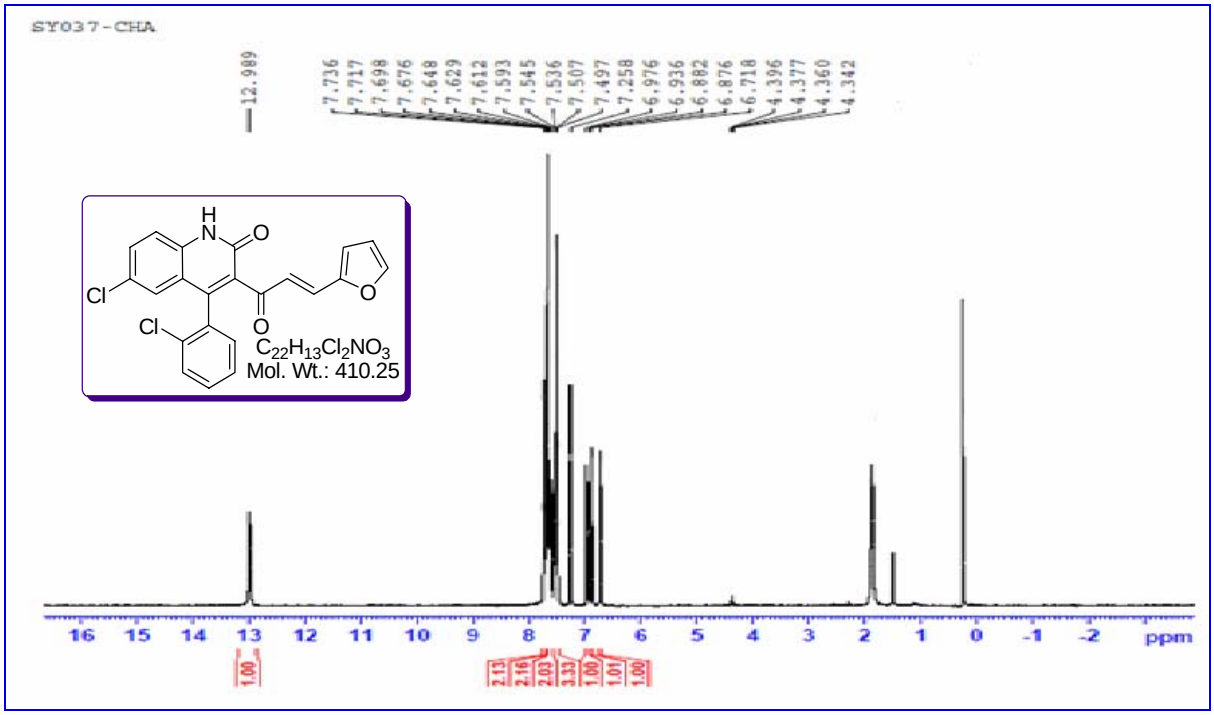

100
%
0
421.16
423.15
424.14
425.13
426.09
843.13
841.18
845.18
846.14
226.21
279.18
385.36
483.98
556.31
657.14
758.11
100
200
300
400
500
600
700
800
900
m/z
H
N
O
Cl
N
Cl
O
C23H14Cl2N2O2
Mol. Wt.: 421.28

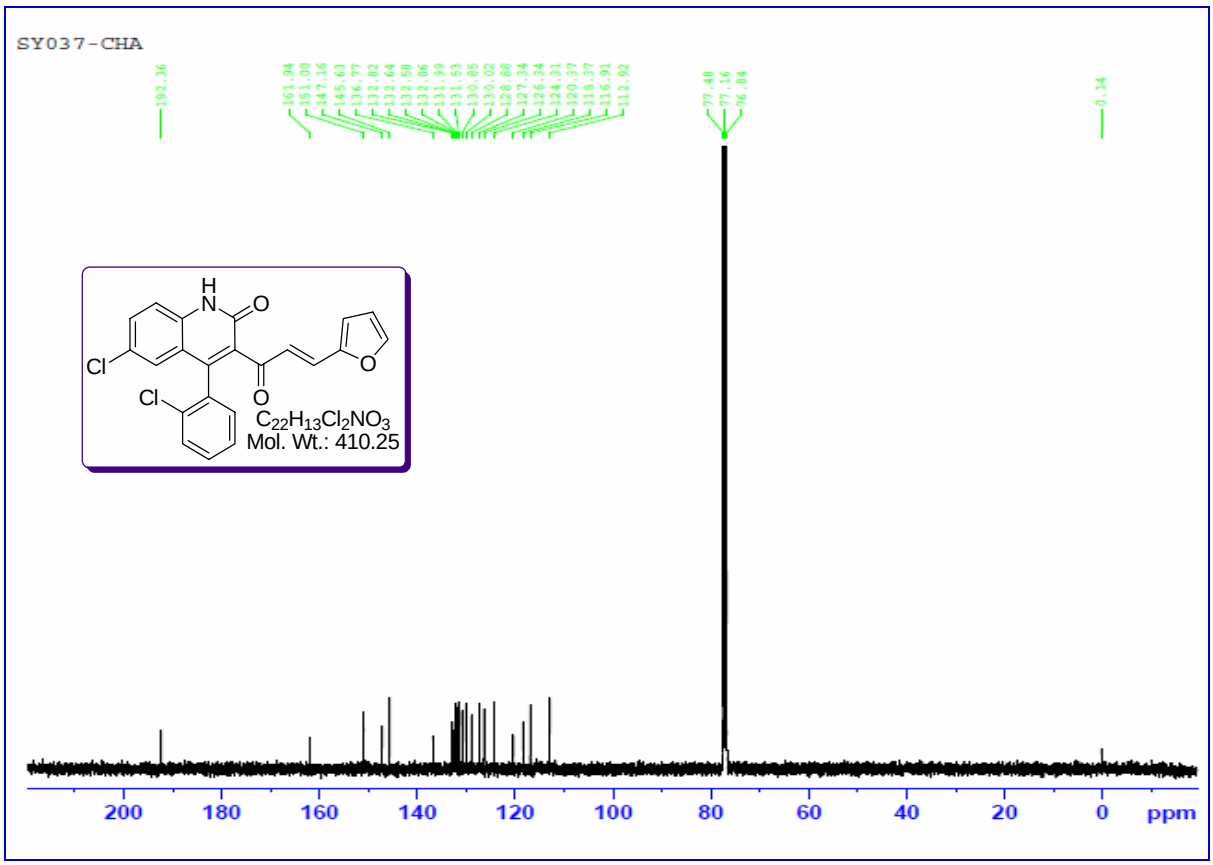

SY036-CHA
12.608
7.826
7.765
7.450
7.431
7.395
7.363
7.346
7.328
7.307
7.290
7.258
7.065
5.994
5.988
5.927
5.904
5.892
5.851
5.794
5.771
3.753
3.711
0.003
H
N
O
O
O
Cl
Cl
O
O
C26H19Cl2NO4
Mol. Wt.: 480.34
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
0.85
1.00
1.08
4.14
1.10
1.97
2.10
1.06
3.06
3.00

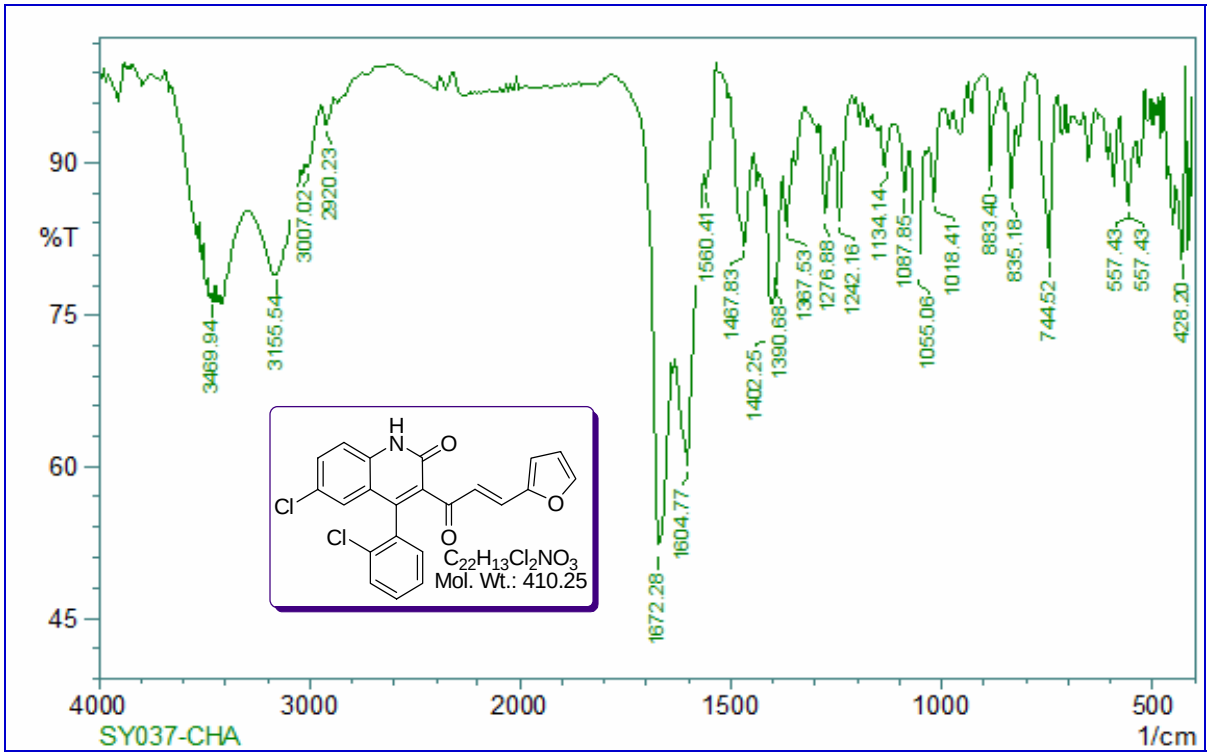

SY036-CHA
193.37
161.88
153.54
153.41
146.84
141.70
136.75
133.05
132.88
132.62
131.85
131.59
130.82
129.98
128.77
127.32
127.26
126.26
123.80
120.41
110.35
113.23
77.47
77.16
76.84
56.03
55.92
H
N
O
O
O
Cl
Cl
O
O
C26H19Cl2NO4
Mol. Wt.: 480.34
200 180 160 140 120 100 80 60 40 20 0 ppm

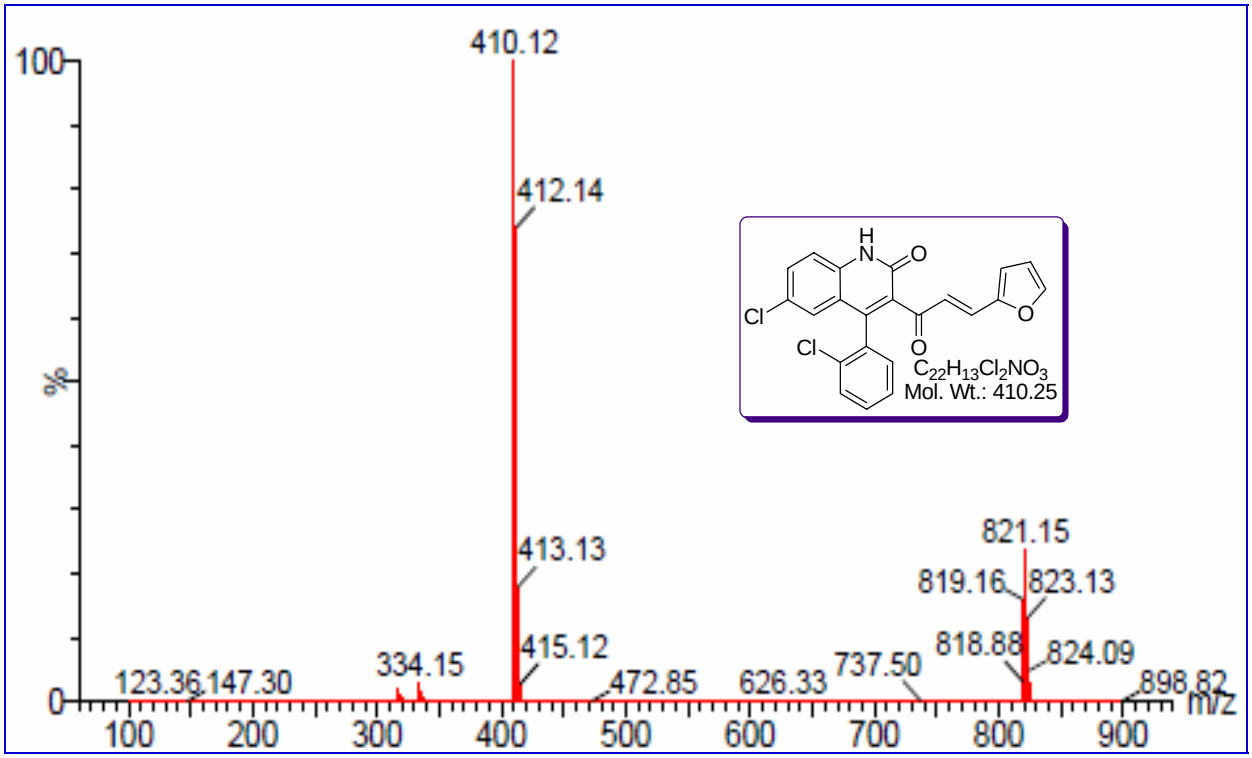

100
%T
80
60
40
20
4000
3000
2000
1500
1000
500
1/cm
SY036-CHA
3415.93
3145.90
3001.24
2906.73
2862.36
2833.43
2744.71
1639.49
1492.90
1467.83
1404.18
1365.60
1282.86
1236.37
1178.51
1074.35
1047.35
985.62
950.91
821.88
752.24
715.59
609.51
559.36
Cl
Cl
O
O
O
O
H
N
O
C26H19Cl2NO4
Mol. Wt.: 480.34

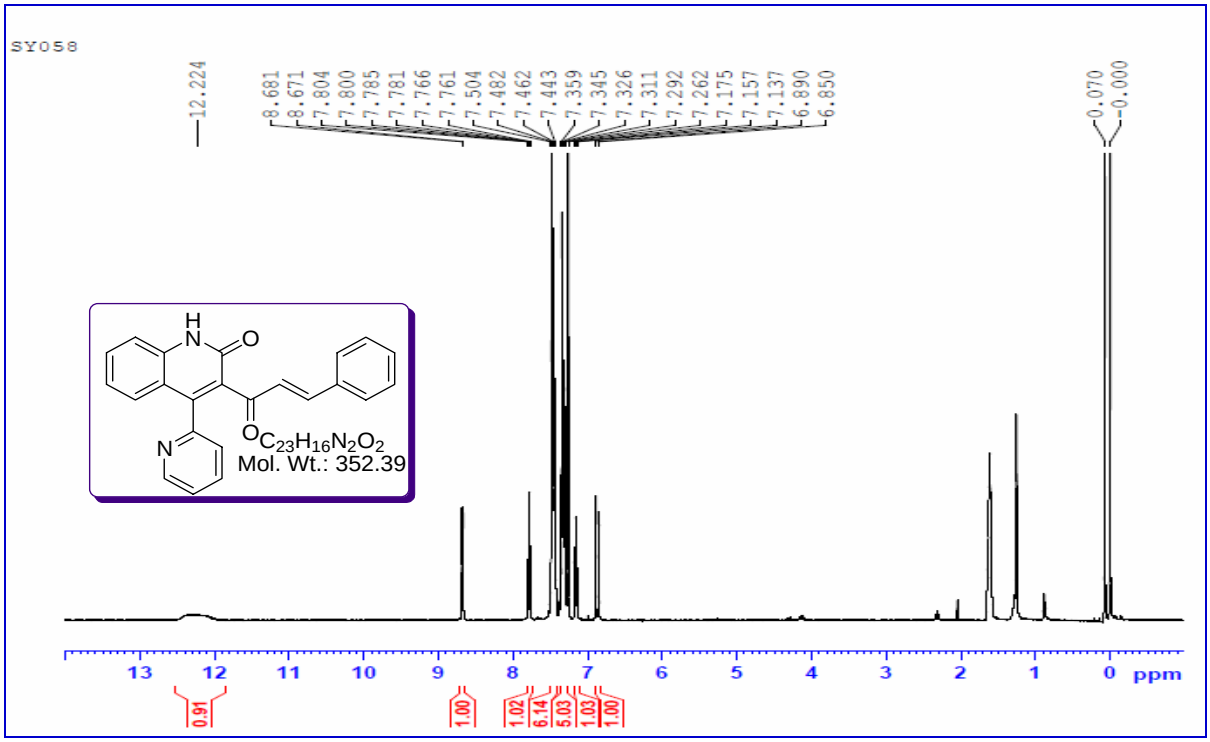

1: Scan ES+
7.94e6
100
%
0
480.28
482.29
483.28
485.29
316.17
318.18
336.18
100.21
180.26
247.27
448.33
558.36
584.27
626.93
m/z
100
150
200
250
300
350
400
450
500
550
600
650
Cl
Cl
O
O
O
O
H
N
O
C26H19Cl2NO4
Mol. Wt.: 480.34

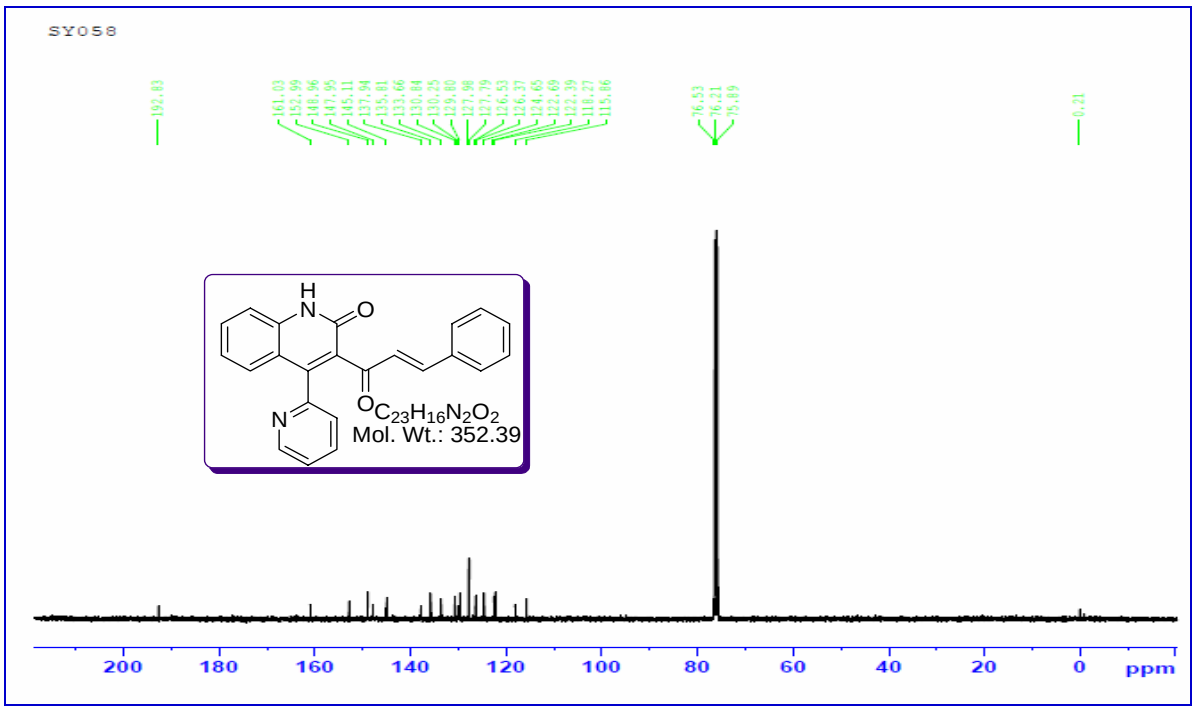

SY037-CHA
12.989
7.736
7.717
7.698
7.676
7.648
7.629
7.612
7.593
7.545
7.536
7.507
7.497
7.258
6.976
6.936
6.882
6.876
6.718
4.396
4.377
4.360
4.342
H
N
O
Cl
O
Cl
O
$C_{22}H_{13}Cl_2NO_3$
Mol. Wt.: 410.25
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
1.00
2.13 2.16 2.03 3.33 1.00 1.01 1.00

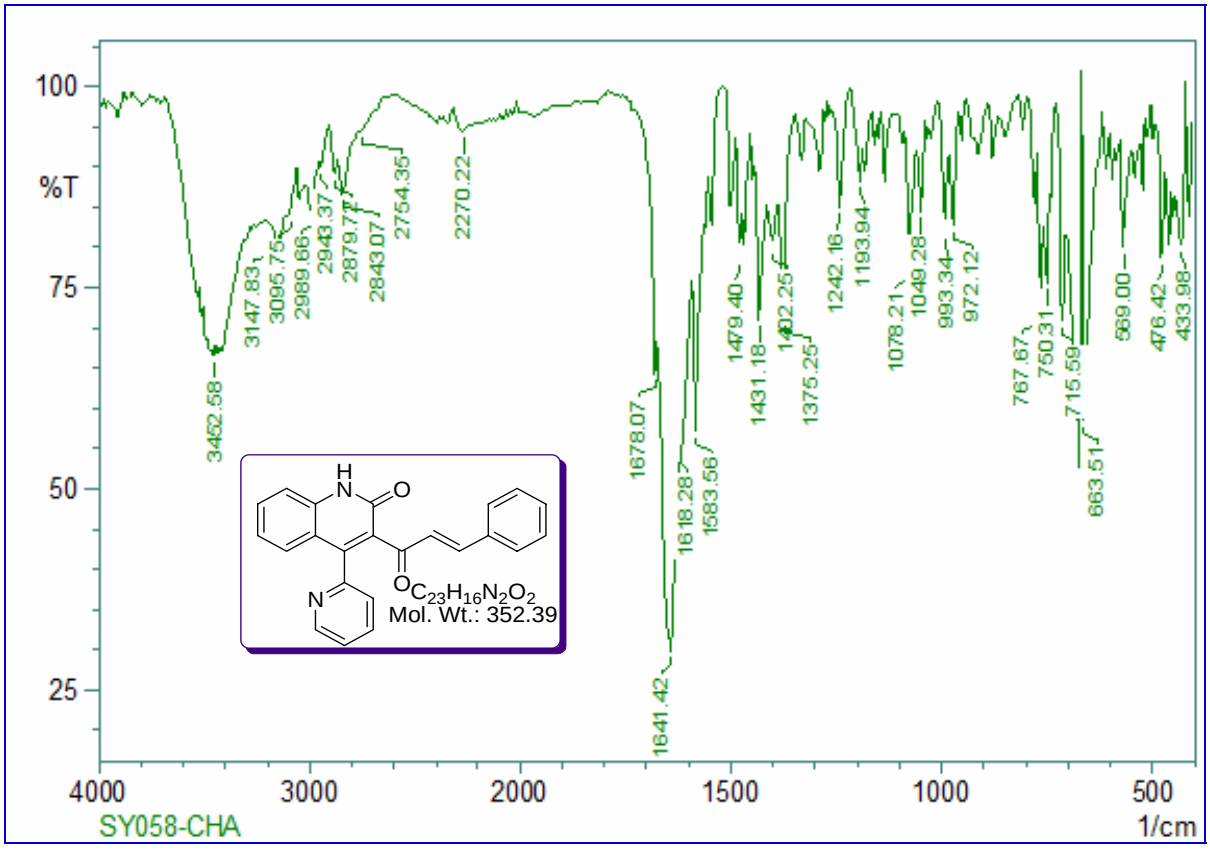

SY037-CHA
192.36
161.94
151.00
147.16
145.63
136.77
132.82
132.64
132.58
132.06
131.99
131.53
130.85
130.02
128.88
127.34
126.34
124.31
120.37
118.37
116.91
112.92
77.48
77.16
76.84
0.14
H
N
O
Cl
O
Cl
O
$C_{22}H_{13}Cl_2NO_3$
Mol. Wt.: 410.25
200 180 160 140 120 100 80 60 40 20 0 ppm

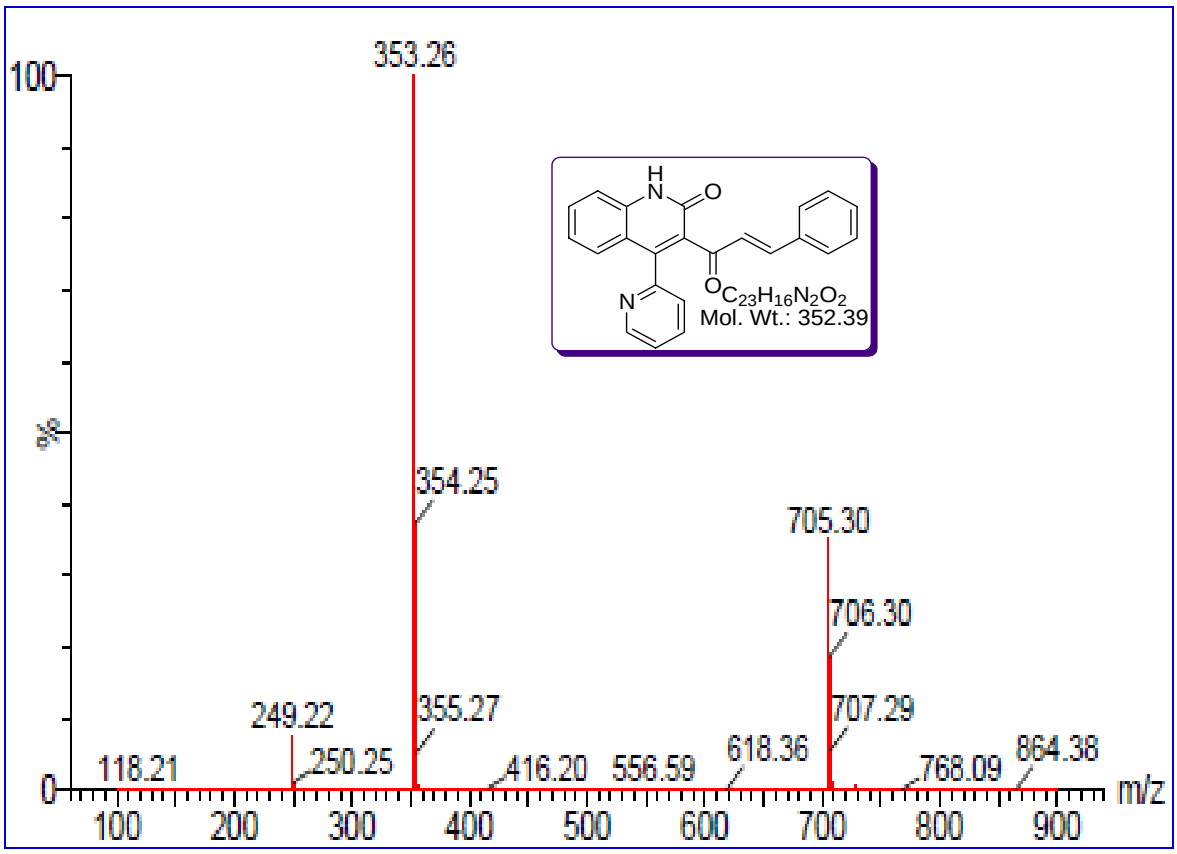

90
%T
75
60
45
3469.94
3155.54
3007.02
2920.23
1672.28
1604.77
1560.41
1467.83
1402.25
1390.68
1367.53
1276.88
1242.16
1134.14
1087.85
1055.06
1018.41
883.40
835.18
744.52
557.43
557.43
428.20
H
N
O
Cl
Cl
O
O
$C_{22}H_{13}Cl_2NO_3$
Mol. Wt.: 410.25
4000
3000
2000
1500
1000
500
1/cm
SY037-CHA

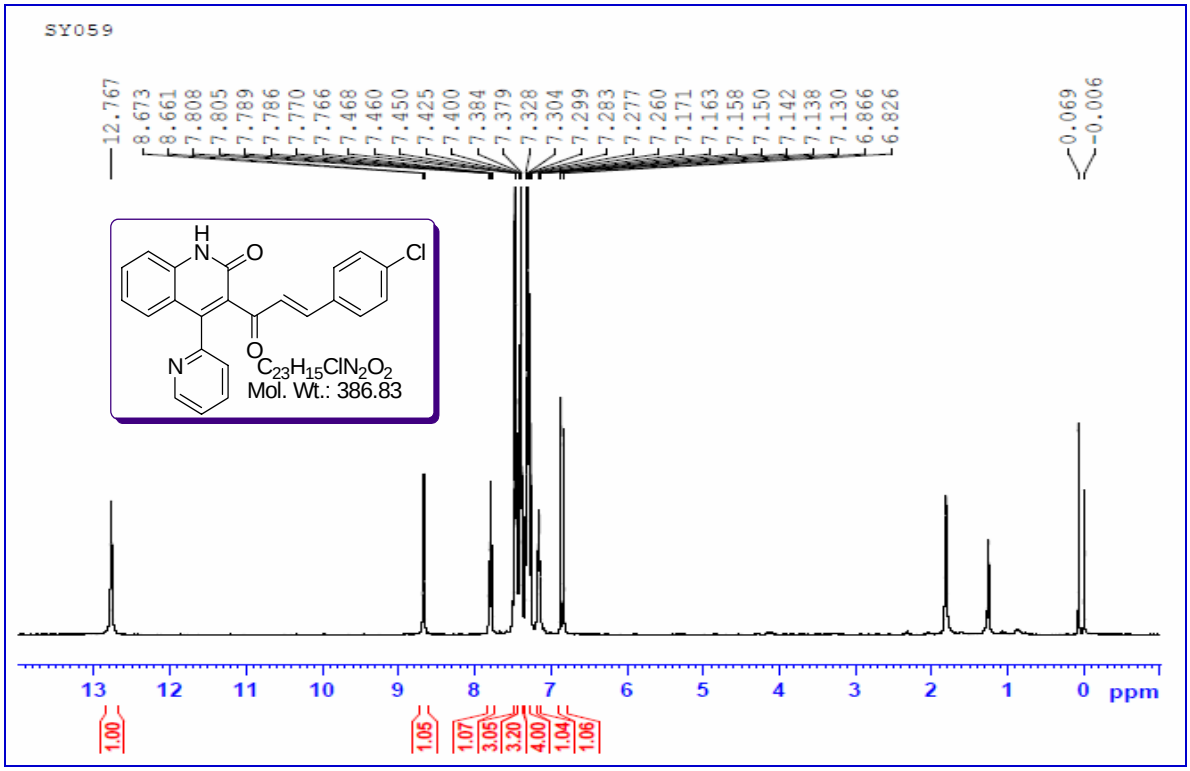

100
%
0
410.12
412.14
413.13
415.12
821.15
819.16
823.13
818.88
824.09
123.36
147.30
334.15
472.85
626.33
737.50
898.82
H
N
O
Cl
Cl
O
O
$C_{22}H_{13}Cl_2NO_3$
Mol. Wt.: 410.25
100
200
300
400
500
600
700
800
900
m/z

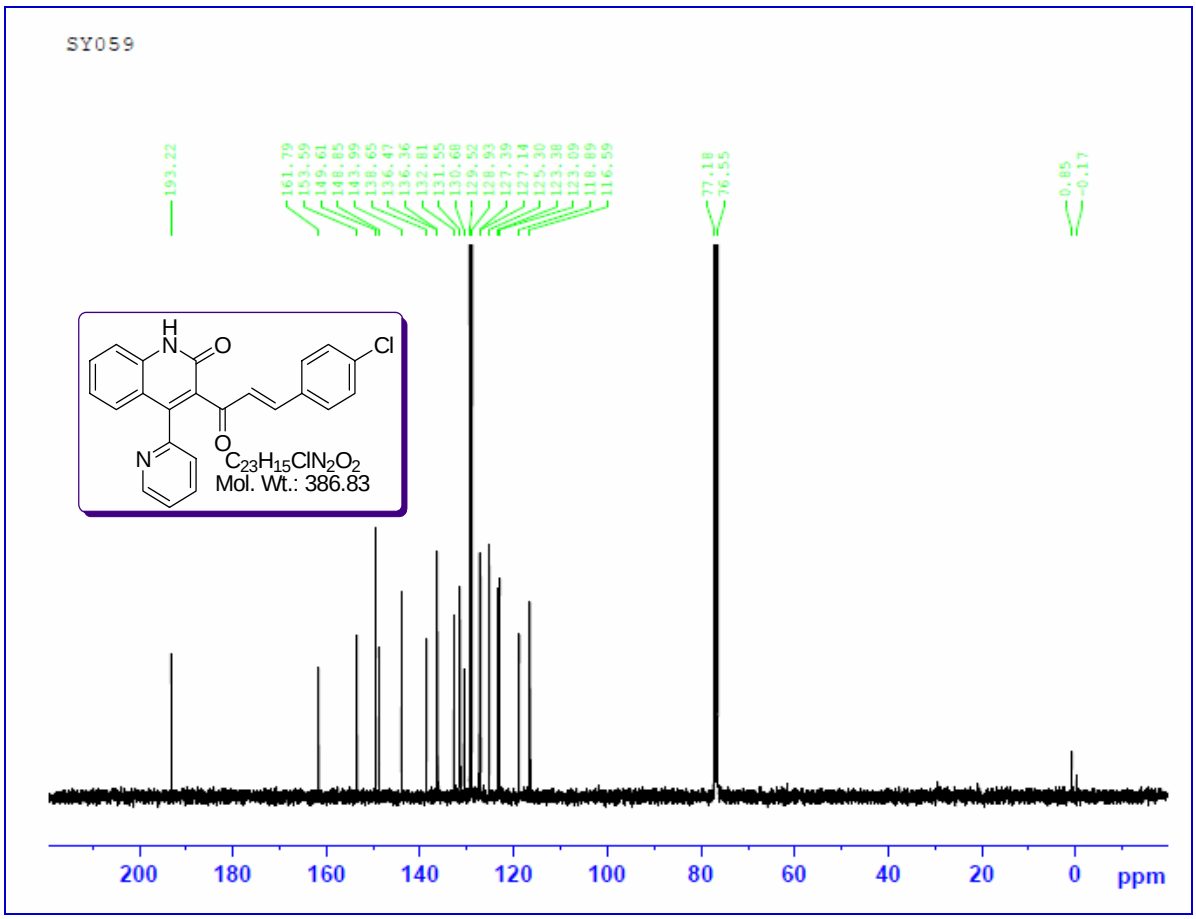

SY058
12.224
8.681
8.671
7.804
7.800
7.785
7.781
7.766
7.761
7.504
7.482
7.462
7.443
7.359
7.345
7.326
7.311
7.292
7.262
7.175
7.157
7.137
6.890
6.850
0.070
0.000
H
N
O
O
N
C23H16N2O2
Mol. Wt.: 352.39
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.91
1.00
1.02
6.14
5.03
1.03
1.00

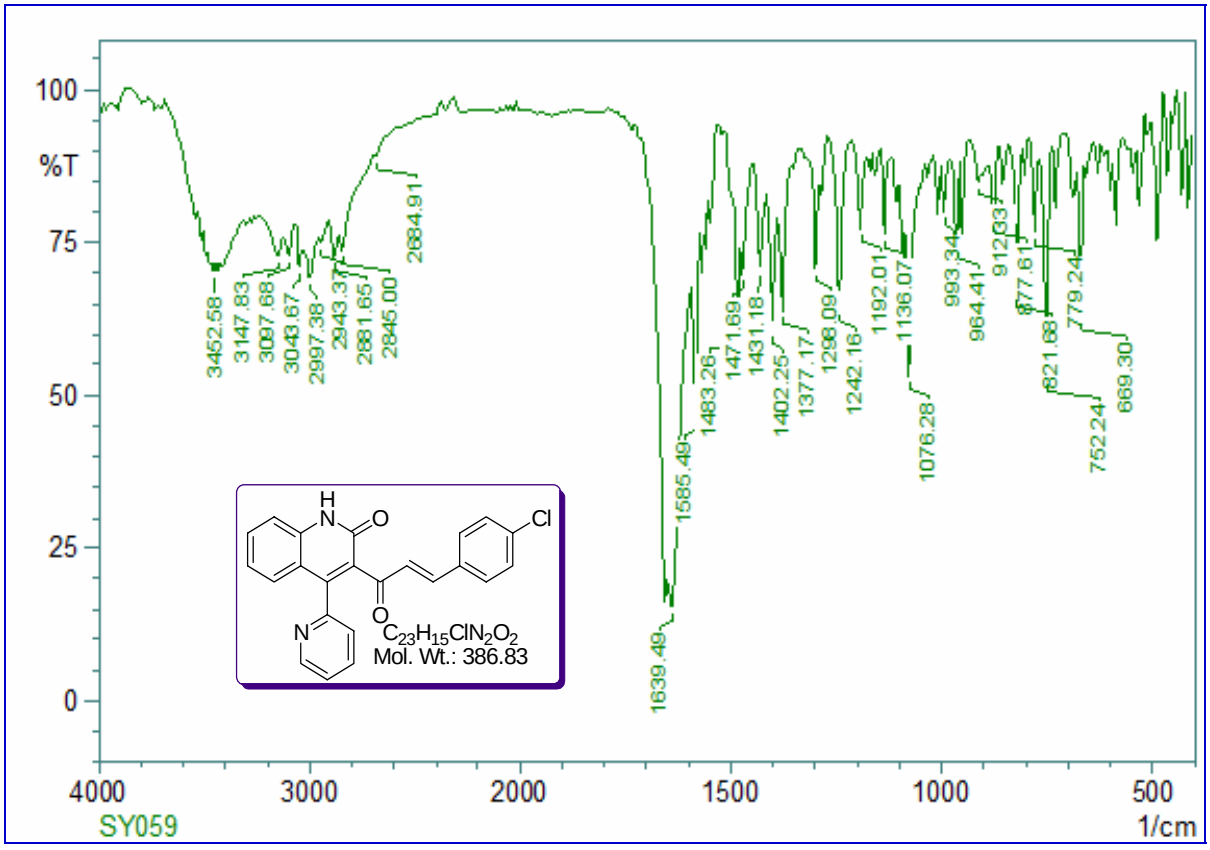

SY058
192.83
161.03
152.99
148.96
147.95
145.11
137.94
135.81
133.66
130.84
130.25
129.80
127.98
127.79
126.53
126.37
124.65
122.69
122.39
118.27
115.86
76.53
76.21
75.89
1.21
H
N
O
O
N
C23H16N2O2
Mol. Wt.: 352.39
200
180
160
140
120
100
80
60
40
20
0
ppm

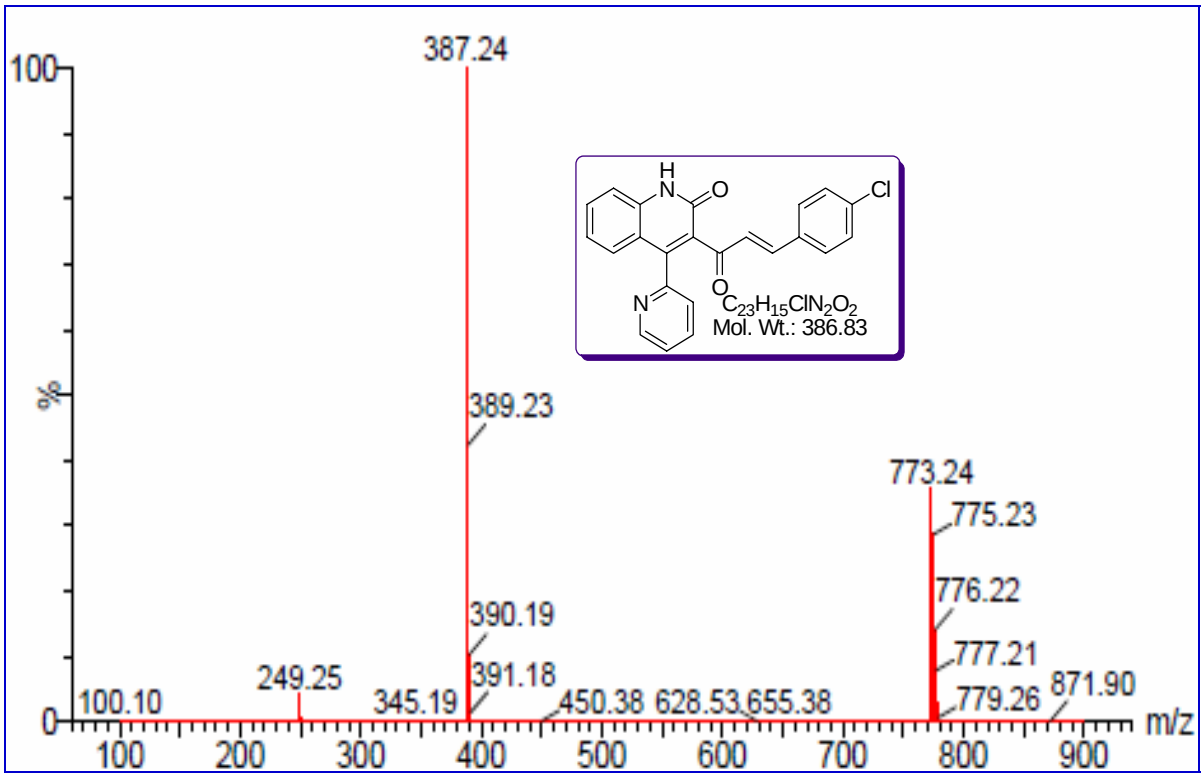

100
%T
75
50
25
3452.58
3147.83
3095.75
2989.66
2943.37
2879.77
2843.07
2754.35
2270.22
1678.07
1641.42
1618.28
1583.56
1479.40
1431.18
1402.25
1375.25
1242.16
1193.94
1078.21
1049.28
993.34
972.12
767.67
750.31
715.59
663.51
569.00
476.42
433.98
H
N
O
O
N
$C_{23}H_{16}N_2O_2$
Mol. Wt.: 352.39
4000
3000
2000
1500
1000
500
SY058-CHA
1/cm

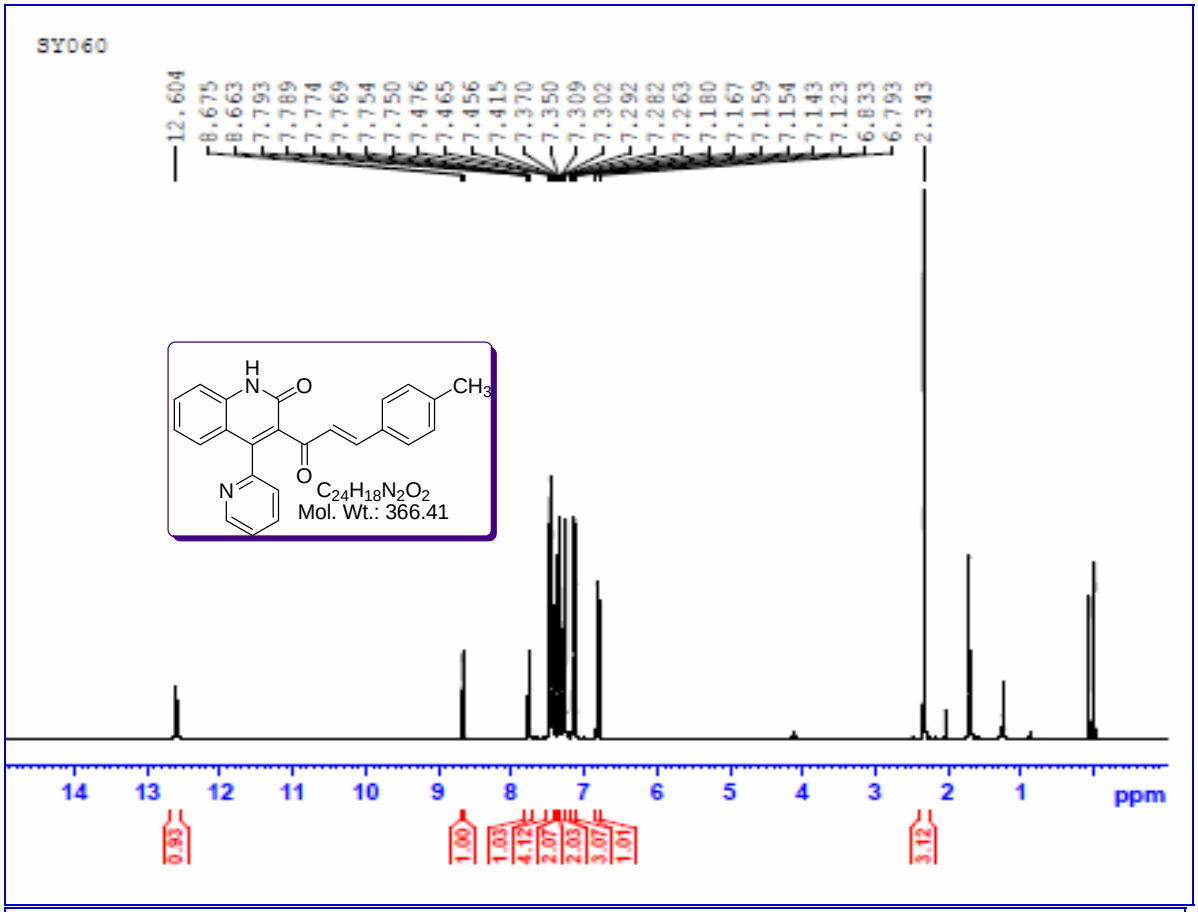

100
%
0
353.26
354.25
705.30
706.30
707.29
249.22
355.27
118.21
250.25
416.20
556.59
618.36
768.09
864.38
H
N
O
O
N
$C_{23}H_{16}N_2O_2$
Mol. Wt.: 352.39
100
200
300
400
500
600
700
800
900
m/z

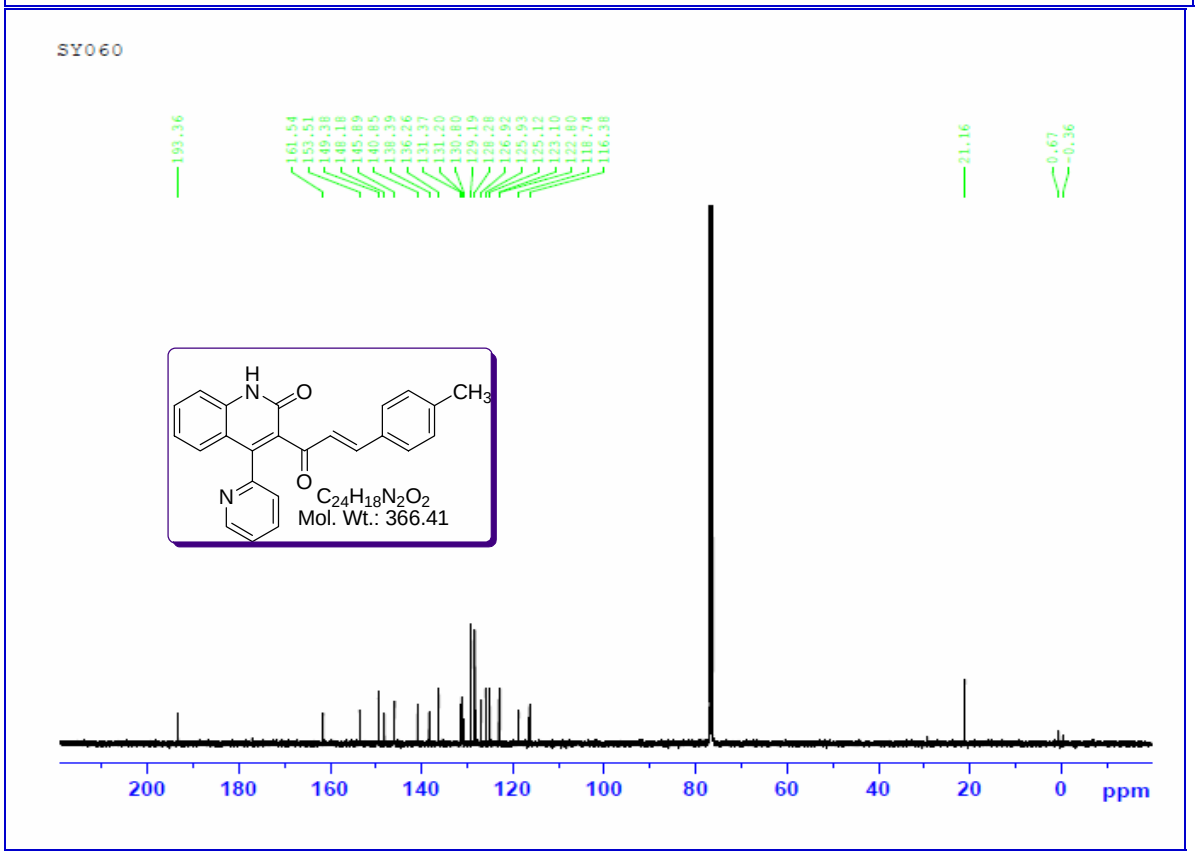

SY059
12.767
8.673
8.661
7.808
7.805
7.789
7.786
7.770
7.766
7.468
7.460
7.450
7.425
7.400
7.384
7.379
7.328
7.304
7.299
7.283
7.277
7.260
7.171
7.163
7.158
7.150
7.142
7.138
7.130
6.866
6.826
0.069
-0.006
H
N
O
Cl
O
N
C23H15ClN2O2
Mol. Wt.: 386.83
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.05
1.07
3.05
3.20
4.00
1.04
1.06

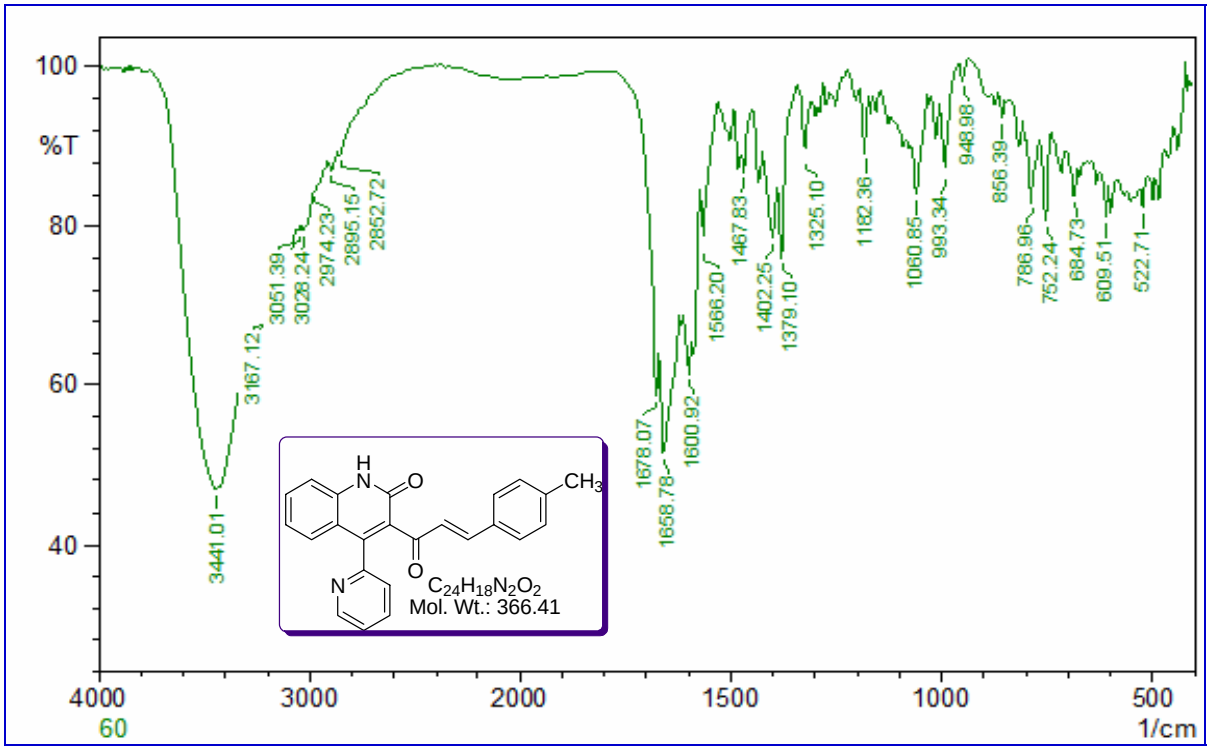

SY059
193.22
161.79
153.59
149.61
148.85
143.99
138.65
136.47
136.36
132.81
131.55
130.68
129.52
128.93
127.39
127.14
125.30
123.38
123.09
118.89
116.59
77.18
76.55
0.85
-0.17
H
N
O
Cl
O
N
C23H15ClN2O2
Mol. Wt.: 386.83
200
180
160
140
120
100
80
60
40
20
0
ppm

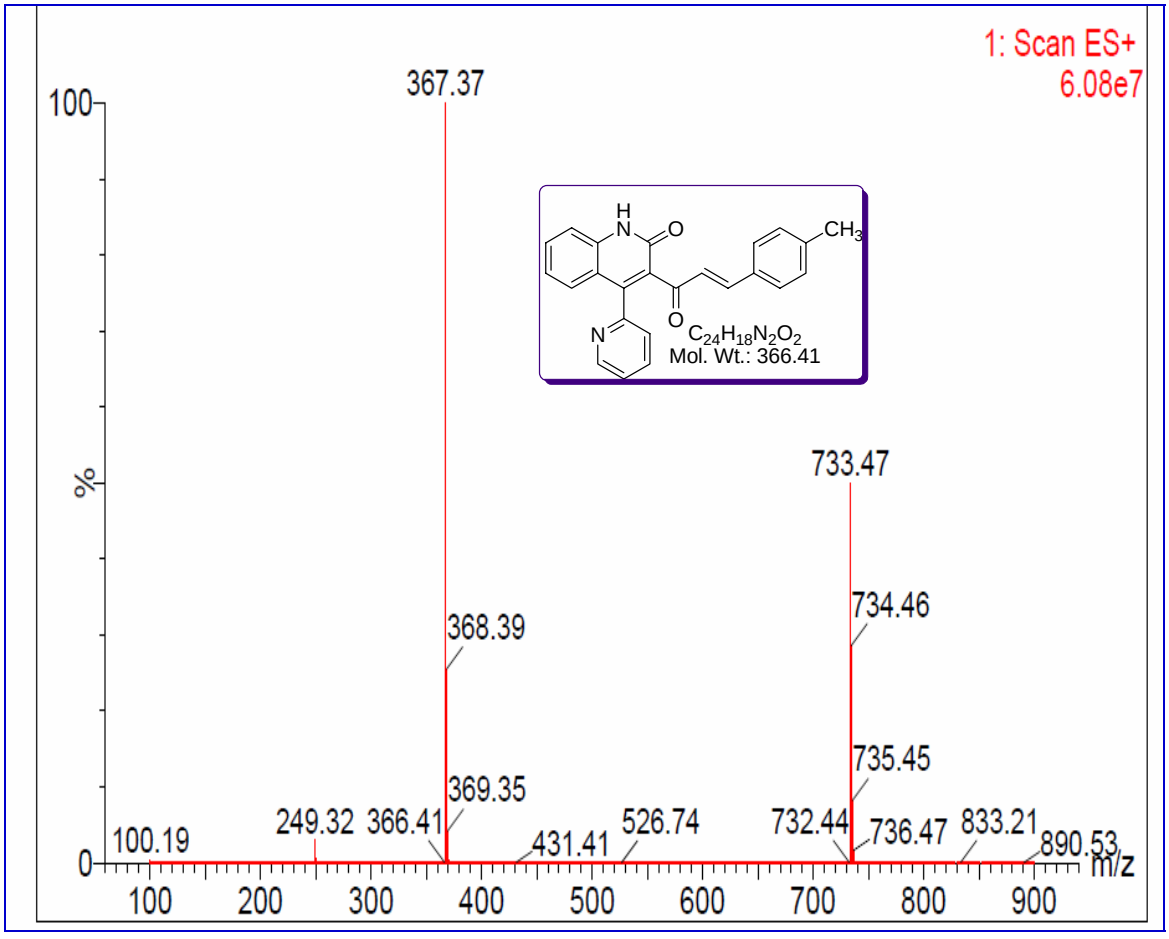

100
%T
75
50
25
0
3452.58
3147.83
3097.68
3043.67
2997.38
2943.37
2881.65
2845.00
2634.91
1639.49
1585.49
1483.26
1471.69
1431.18
1402.25
1377.17
1298.09
1242.16
1192.01
1136.07
1076.28
993.34
964.41
912.63
877.61
821.68
779.24
752.24
669.30
H
N
O
Cl
O
N
C23H15ClN2O2
Mol. Wt.: 386.83
4000
3000
2000
1500
1000
500
SY059
1/cm

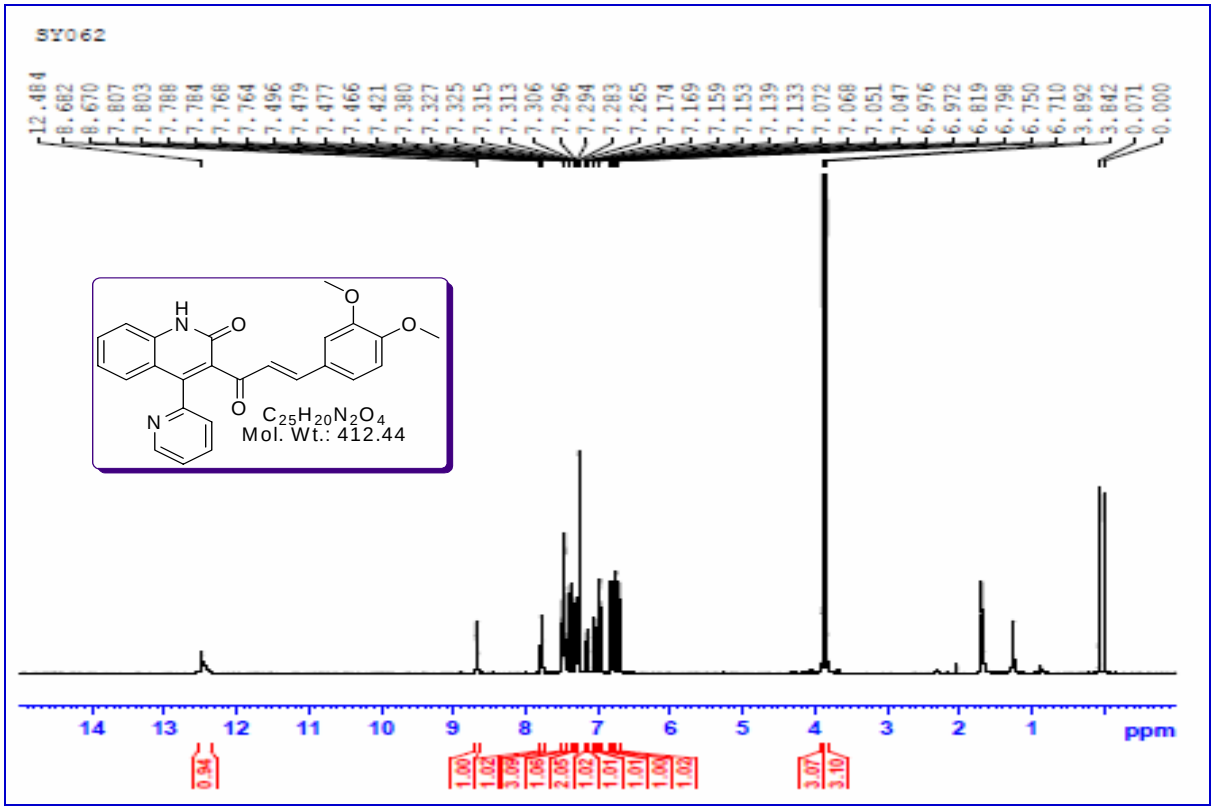

100
%
0
387.24
389.23
390.19
391.18
773.24
775.23
776.22
777.21
779.26
871.90
249.25
345.19
450.38
628.53
655.38
100.10
H
N
O
Cl
O
N
C23H15ClN2O2
Mol. Wt.: 386.83
100
200
300
400
500
600
700
800
900
m/z

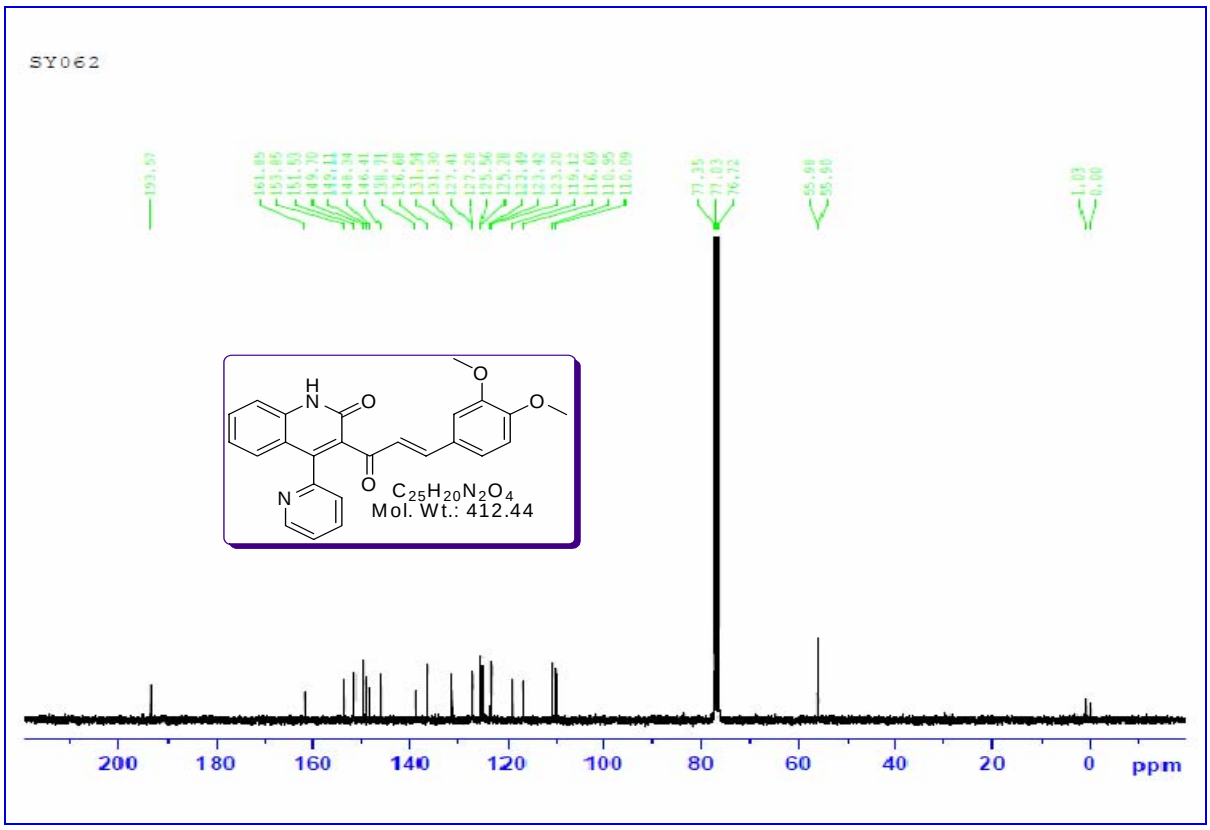

SY060
12.604
8.675
8.663
7.793
7.789
7.774
7.769
7.754
7.750
7.476
7.465
7.456
7.415
7.370
7.350
7.309
7.302
7.292
7.282
7.263
7.180
7.167
7.159
7.154
7.143
7.123
6.833
6.793
2.343
H
N
O
CH3
O
N
C24H18N2O2
Mol. Wt.: 366.41
14
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
0.83
1.00
1.03
4.12
2.07
2.03
3.07
1.01
3.12

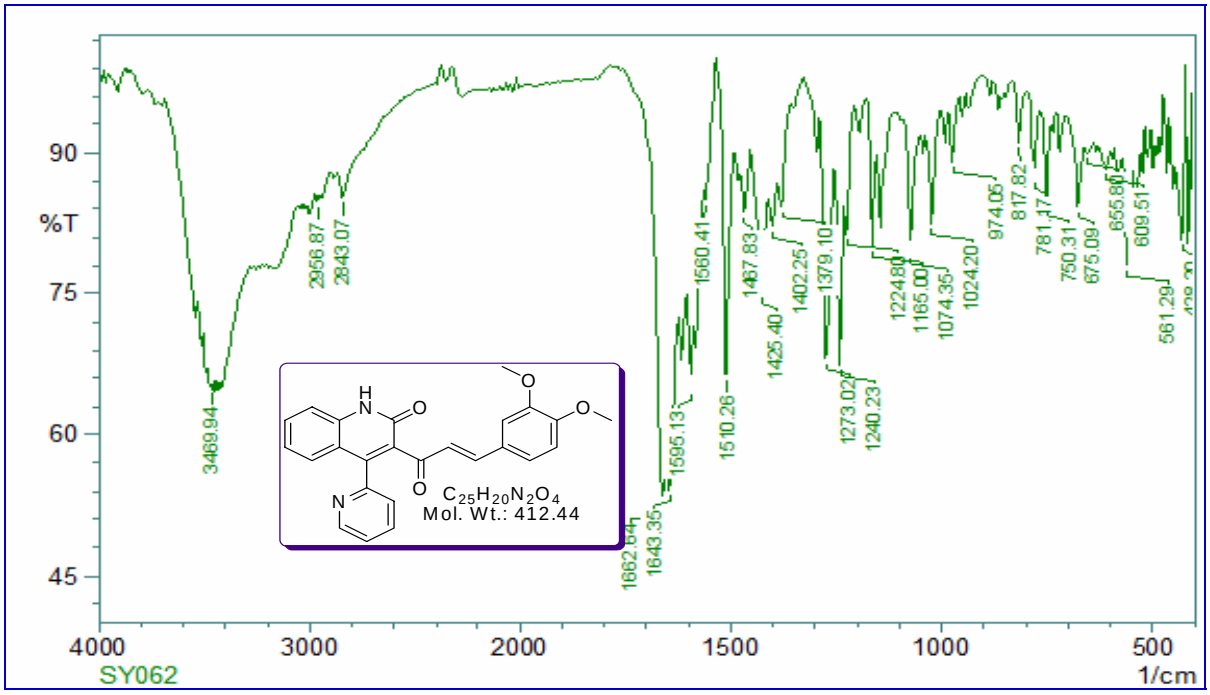

SY060
193.36
161.54
153.51
149.38
148.18
145.89
140.85
138.39
136.26
131.37
131.20
130.80
129.19
128.28
126.92
125.93
125.12
123.10
122.80
118.74
116.38
21.16
0.67
0.36
H
N
O
CH3
O
N
C24H18N2O2
Mol. Wt.: 366.41
200
180
160
140
120
100
80
60
40
20
0
ppm

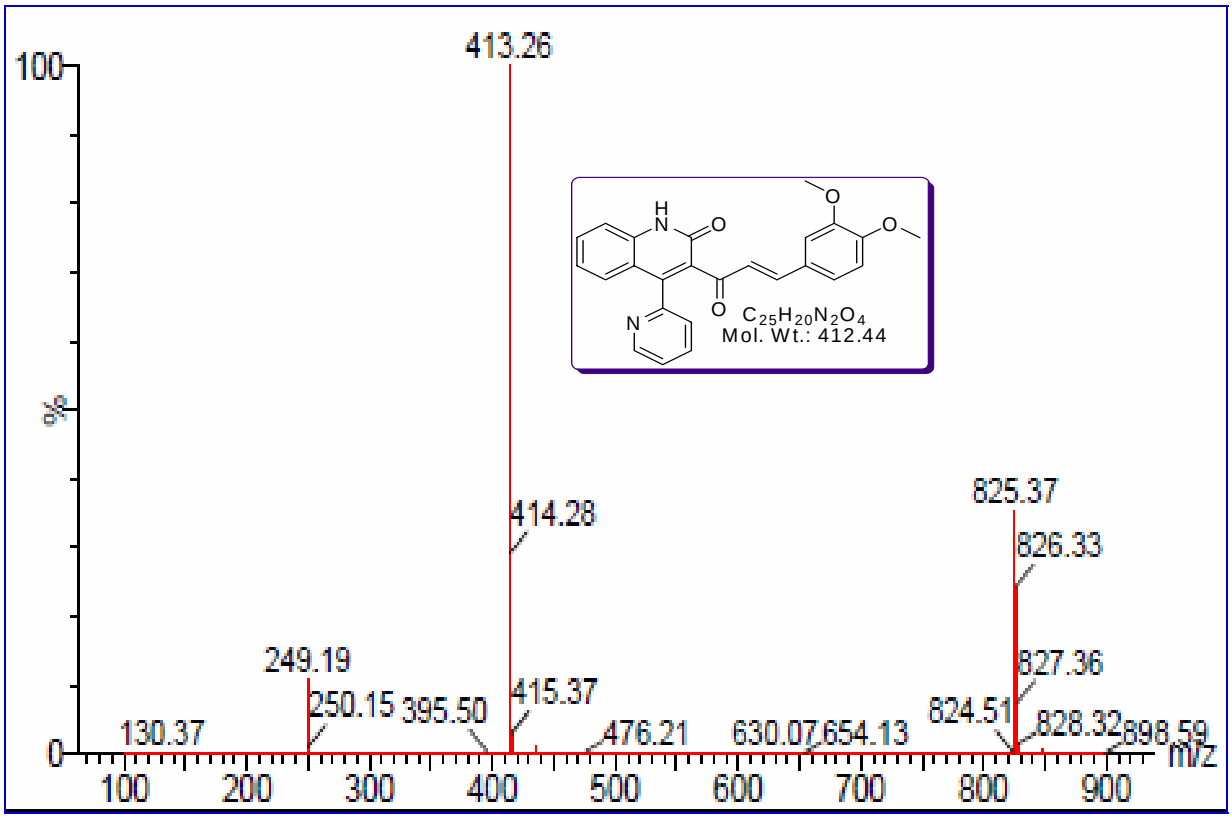

100
%T
80
60
40
3441.01
3167.12
3051.39
3028.24
2974.23
2895.15
2852.72
1678.07
1658.78
1600.92
1566.20
1467.83
1402.25
1379.10
1325.10
1182.36
1060.85
993.34
948.98
856.39
786.96
752.24
684.73
609.51
522.71
4000
3000
2000
1500
1000
500
60
1/cm
H
N
O
CH3
O
N
C24H18N2O2
Mol. Wt.: 366.41

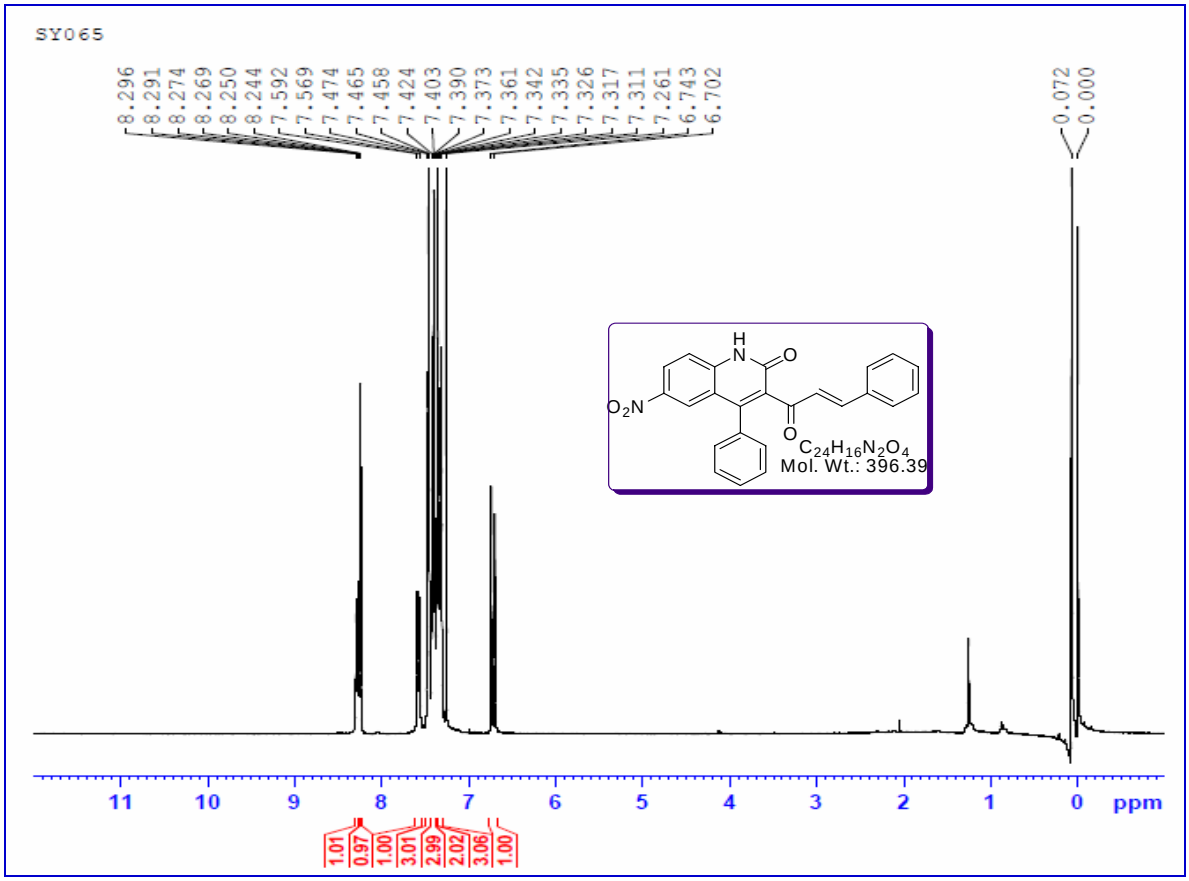

1: Scan ES+
6.08e7
100
%
0
367.37
368.39
369.35
733.47
734.46
735.45
100.19
249.32
366.41
431.41
526.74
732.44
736.47
833.21
890.53
m/z
100
200
300
400
500
600
700
800
900
H
N
O
CH3
O
N
C24H18N2O2
Mol. Wt.: 366.41

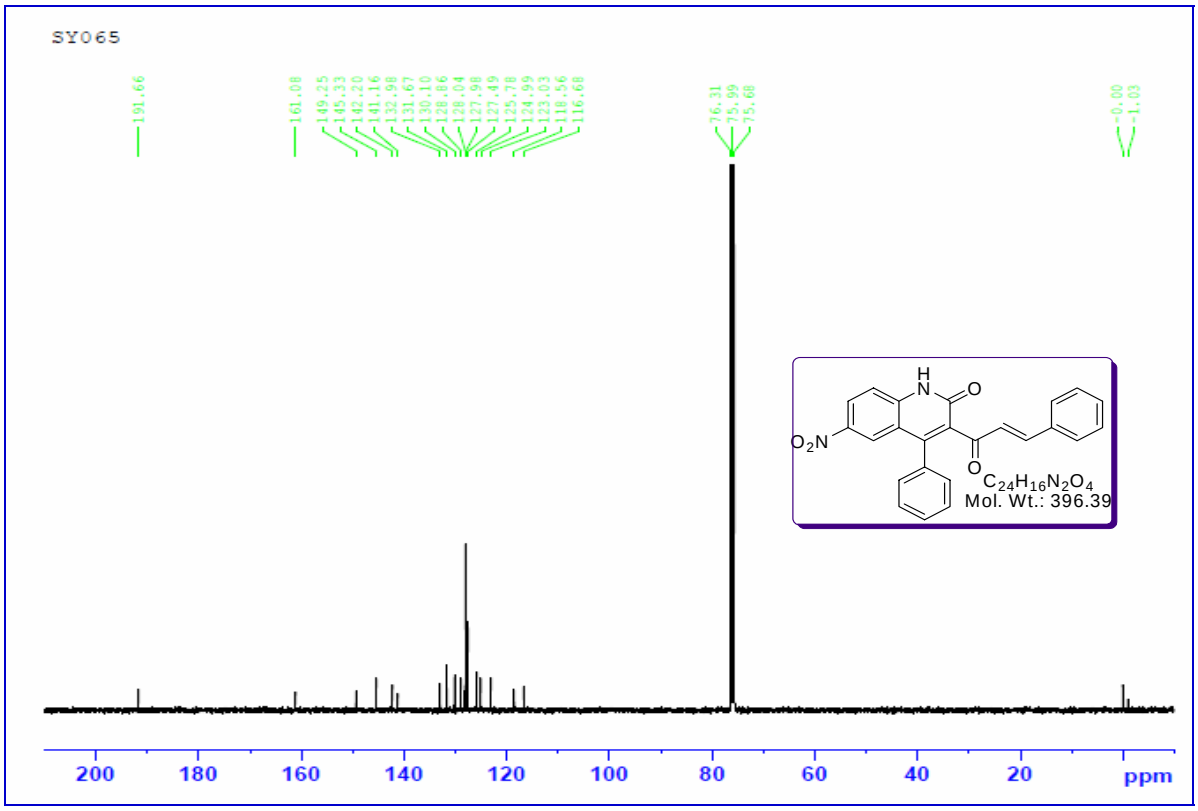

SY062
12.484
8.682
8.670
7.807
7.803
7.788
7.784
7.768
7.764
7.496
7.479
7.477
7.466
7.421
7.380
7.327
7.325
7.315
7.313
7.306
7.296
7.294
7.283
7.265
7.174
7.169
7.159
7.153
7.139
7.133
7.072
7.068
7.051
7.047
6.976
6.972
6.819
6.798
6.750
6.710
3.892
3.842
0.071
0.000
H
N
O
O
O
O
N
C25H20N2O4
Mol. Wt.: 412.44
14
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
0.94
1.00
1.02
3.08
1.06
2.05
1.02
1.01
1.01
1.00
1.02
3.07
3.10

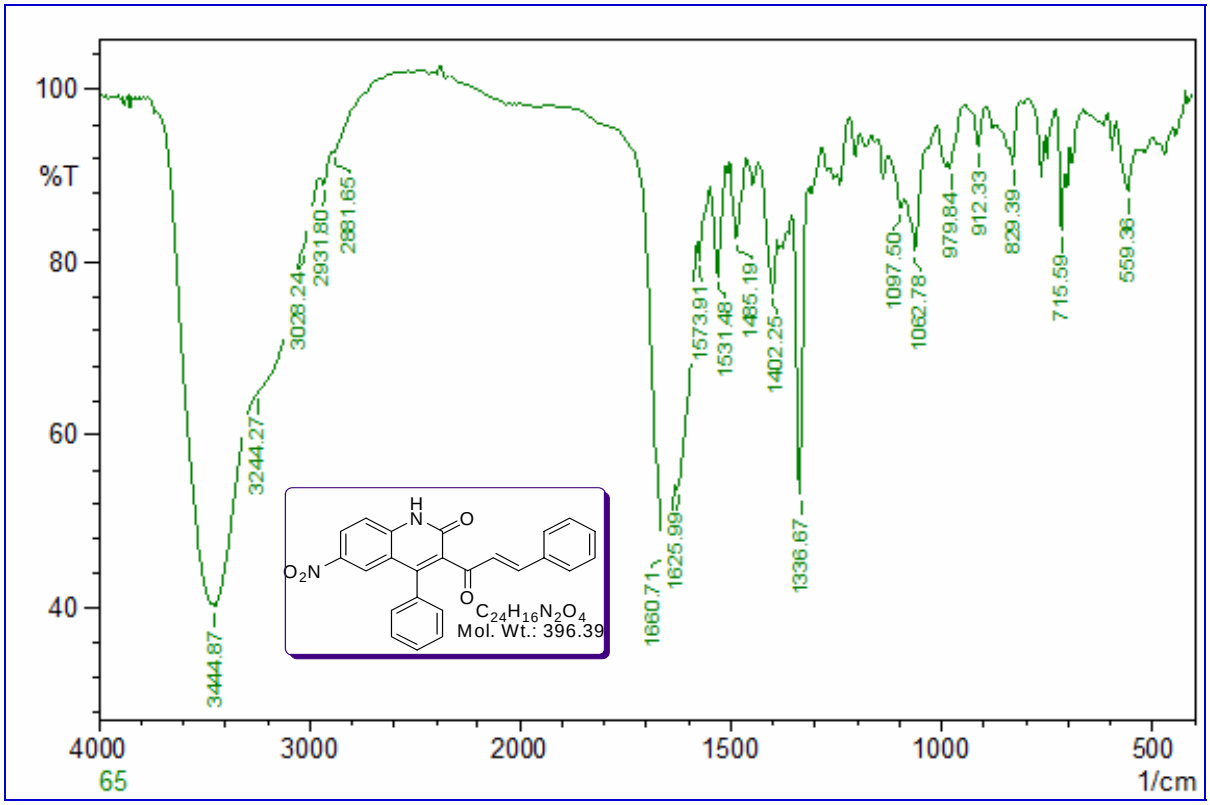

SY062
193.57
161.85
153.85
151.53
149.70
149.11
148.34
146.41
138.71
136.68
131.54
131.30
127.41
127.28
125.56
125.28
123.49
123.42
123.20
119.12
116.69
110.95
110.09
77.35
77.03
76.72
55.96
55.90
1.03
0.00
H
N
O
O
O
O
N
C25H20N2O4
Mol. Wt.: 412.44
200
180
160
140
120
100
80
60
40
20
0
ppm

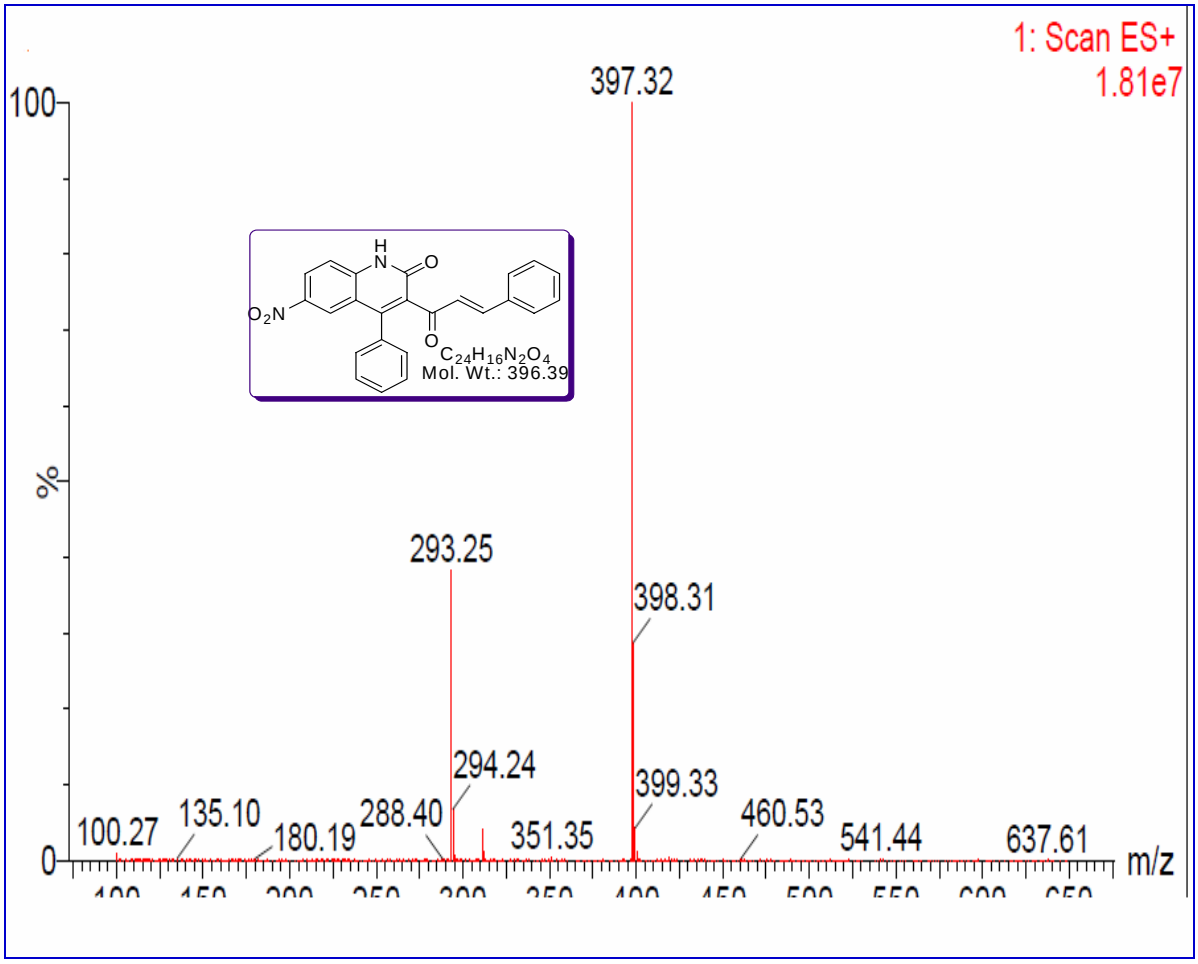

90
%T
75
60
45
4000
3000
2000
1500
1000
500
1/cm
SY062
3469.94
2956.87
2843.07
1662.84
1643.35
1595.13
1560.41
1510.26
1457.83
1425.40
1402.25
1379.10
1273.02
1240.23
1224.80
1165.00
1074.35
1024.20
974.05
817.82
781.17
750.31
675.09
655.80
609.51
561.29
O
H
N
O
O
O
N
C25H20N2O4
Mol. Wt.: 412.44

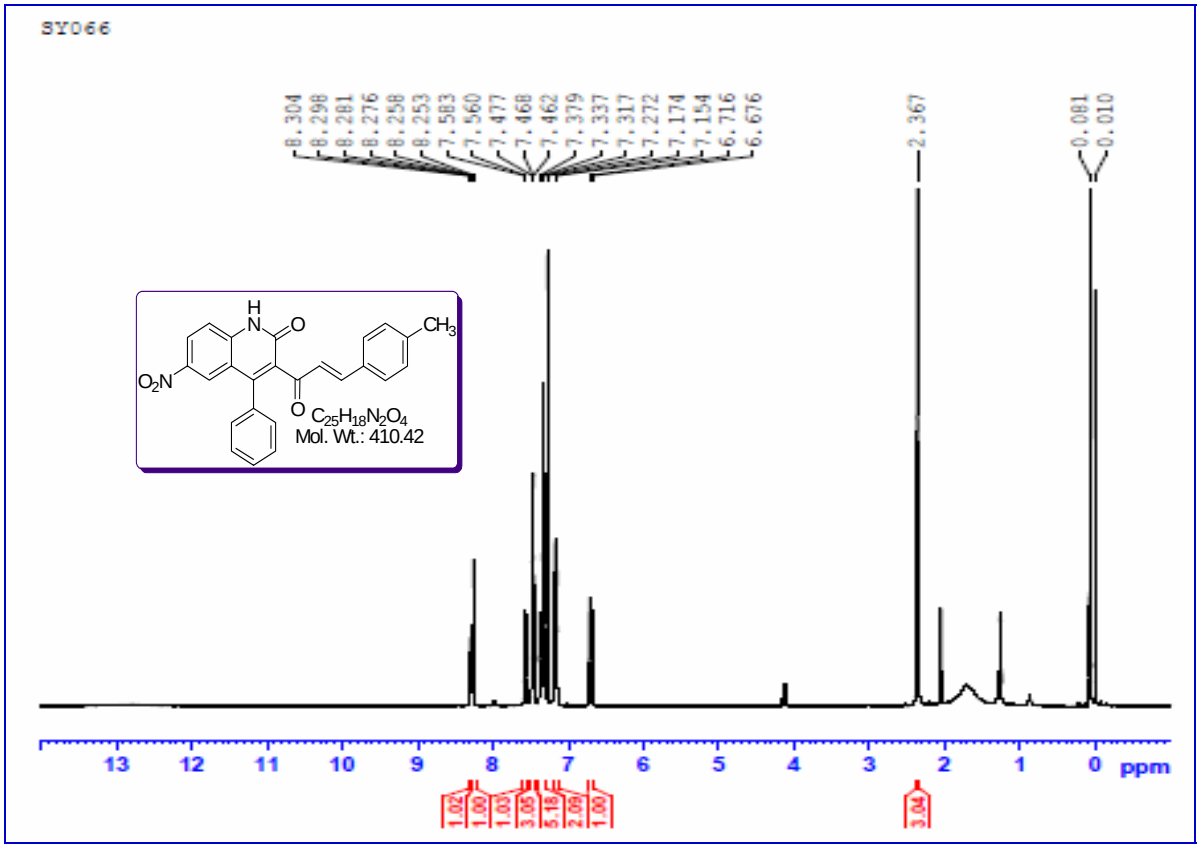

100
%
0
413.26
414.28
825.37
826.33
827.36
249.19
250.15
395.50
415.37
824.51
828.32
898.59
130.37
476.21
630.07
654.13
100
200
300
400
500
600
700
800
900
m/z
O
H
N
O
O
O
N
C25H20N2O4
Mol. Wt.: 412.44

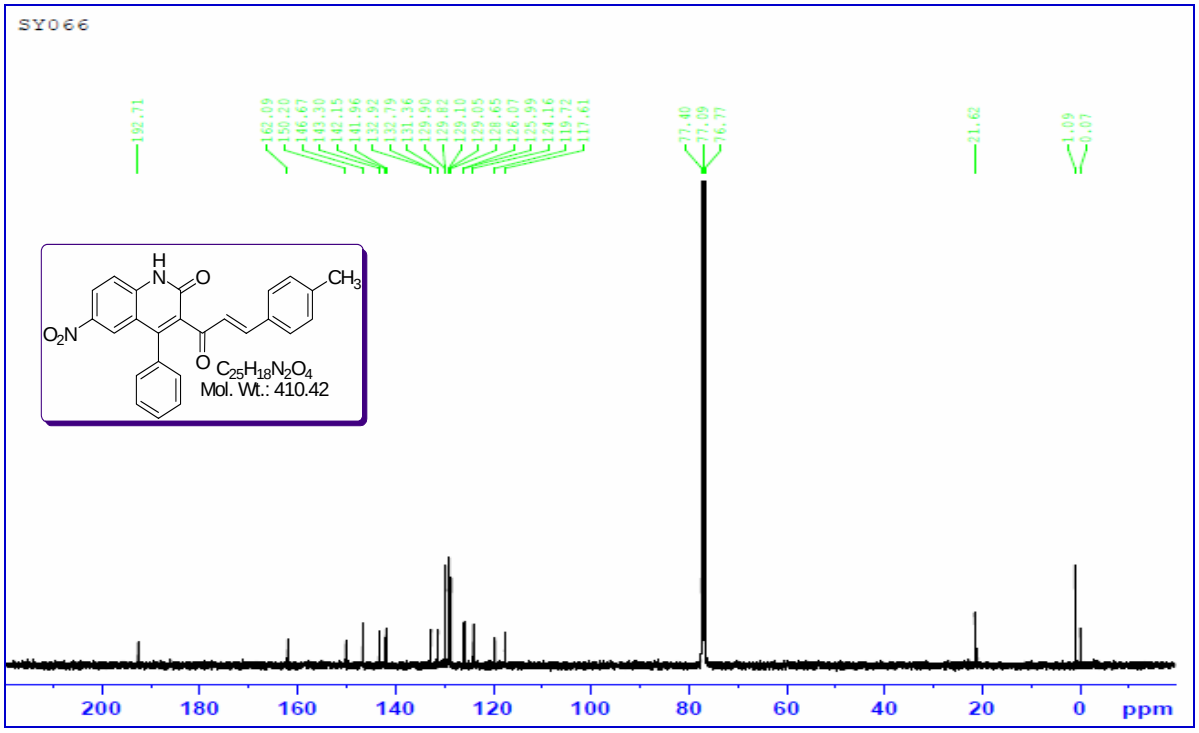

SY065
8.296
8.291
8.274
8.269
8.250
8.244
7.592
7.569
7.474
7.465
7.458
7.424
7.403
7.390
7.373
7.361
7.342
7.335
7.326
7.317
7.311
7.261
6.743
6.702
0.072
0.000
H
N
O
O2N
O
C24H16N2O4
Mol. Wt.: 396.39
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.01
0.97
1.00
3.01
2.99
2.02
3.06
1.00

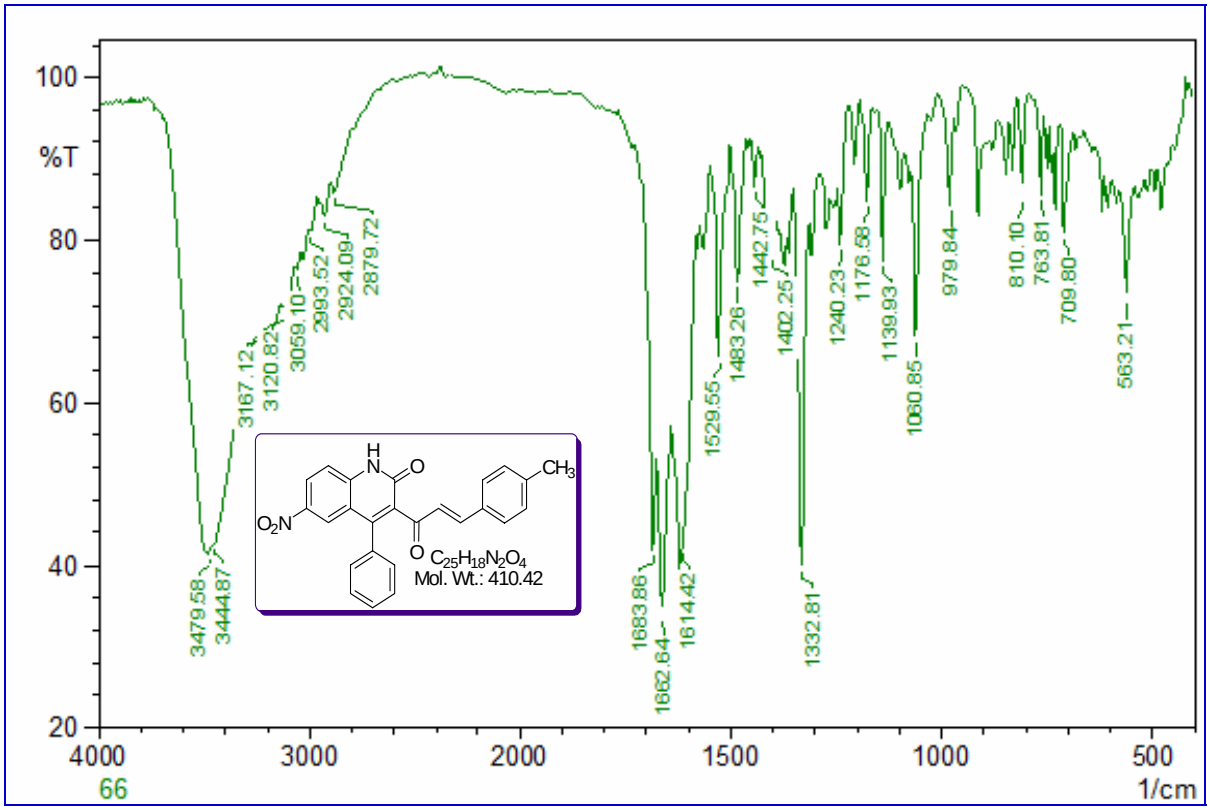

SY065
191.66
161.08
149.25
145.33
142.20
141.16
132.98
131.67
130.10
128.86
128.04
127.98
127.49
125.78
124.99
123.03
118.56
116.68
76.31
75.99
75.68
0.00
-1.03
H
N
O
O2N
O
C24H16N2O4
Mol. Wt.: 396.39
200
180
160
140
120
100
80
60
40
20
ppm

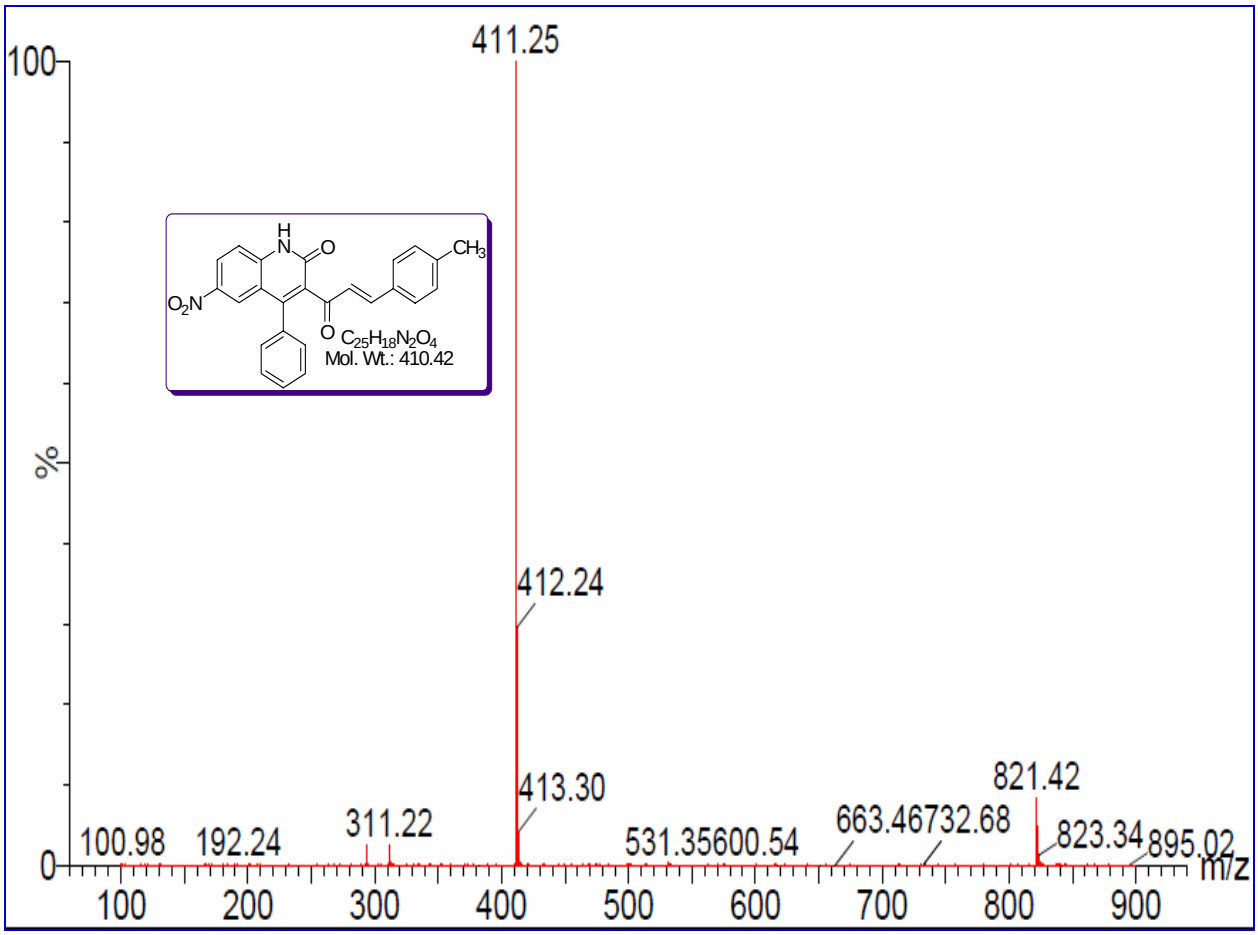

100
%T
80
60
40
3444.87
3244.27
3028.24
2931.80
2881.65
1660.71
1625.99
1573.91
1531.48
1485.19
1402.25
1336.67
1097.50
1062.78
979.84
912.33
829.39
715.59
559.36
$C_{24}H_{16}N_2O_4$
Mol. Wt.: 396.39
4000
3000
2000
1500
1000
500
65
1/cm

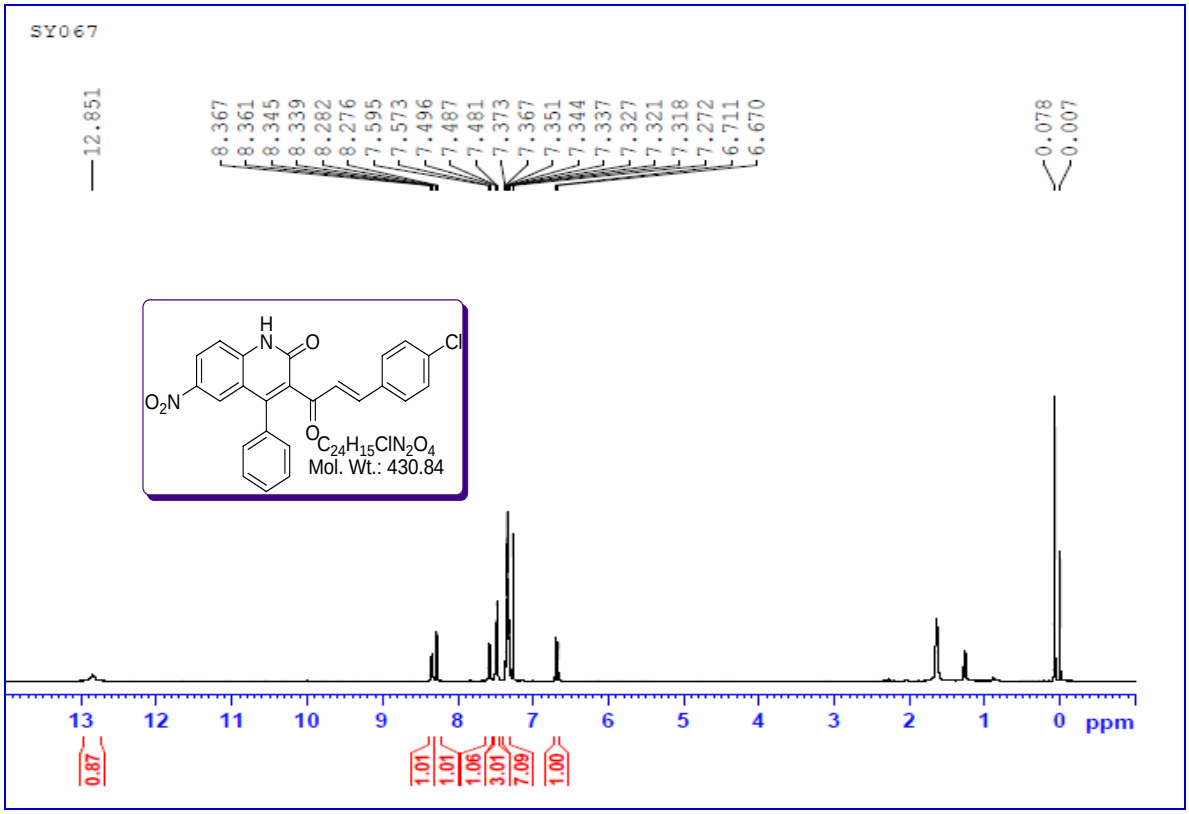

1: Scan ES+
1.81e7
100
%
0
397.32
398.31
293.25
294.24
399.33
100.27
135.10
180.19
288.40
351.35
460.53
541.44
637.61
m/z
$C_{24}H_{16}N_2O_4$
Mol. Wt.: 396.39

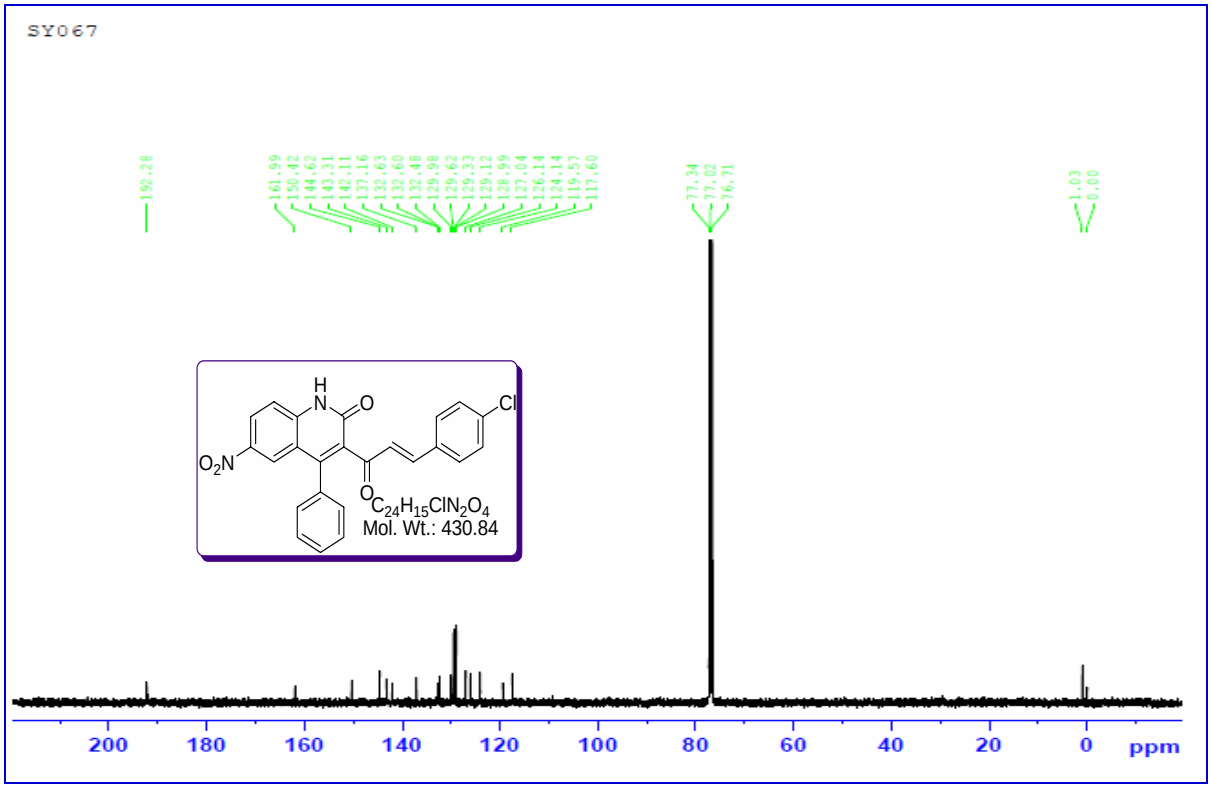

SY066
8.304
8.298
8.281
8.276
8.258
8.253
7.583
7.560
7.477
7.468
7.462
7.379
7.337
7.317
7.272
7.174
7.154
6.716
6.676
2.367
0.081
0.010
H
N
O
CH3
O2N
O
C25H18N2O4
Mol. Wt.: 410.42
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.02
1.00
1.03
3.05
5.18
2.09
1.00
3.04

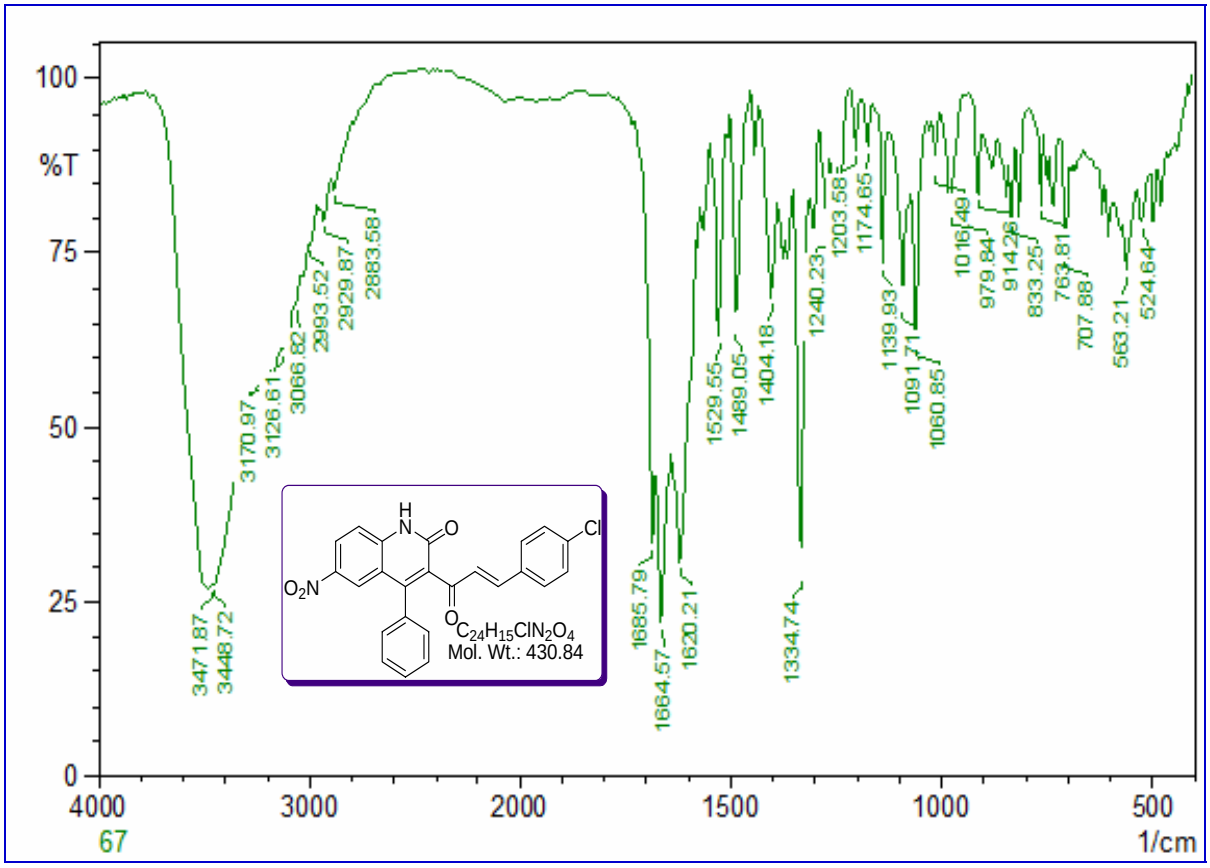

SY066
192.71
162.09
150.20
146.67
143.30
142.15
141.96
132.92
132.79
131.36
129.90
129.82
129.10
129.05
128.65
126.07
125.99
124.16
119.72
117.61
77.40
77.09
76.77
21.62
1.09
0.07
H
N
O
CH3
O2N
O
C25H18N2O4
Mol. Wt.: 410.42
200
180
160
140
120
100
80
60
40
20
0
ppm

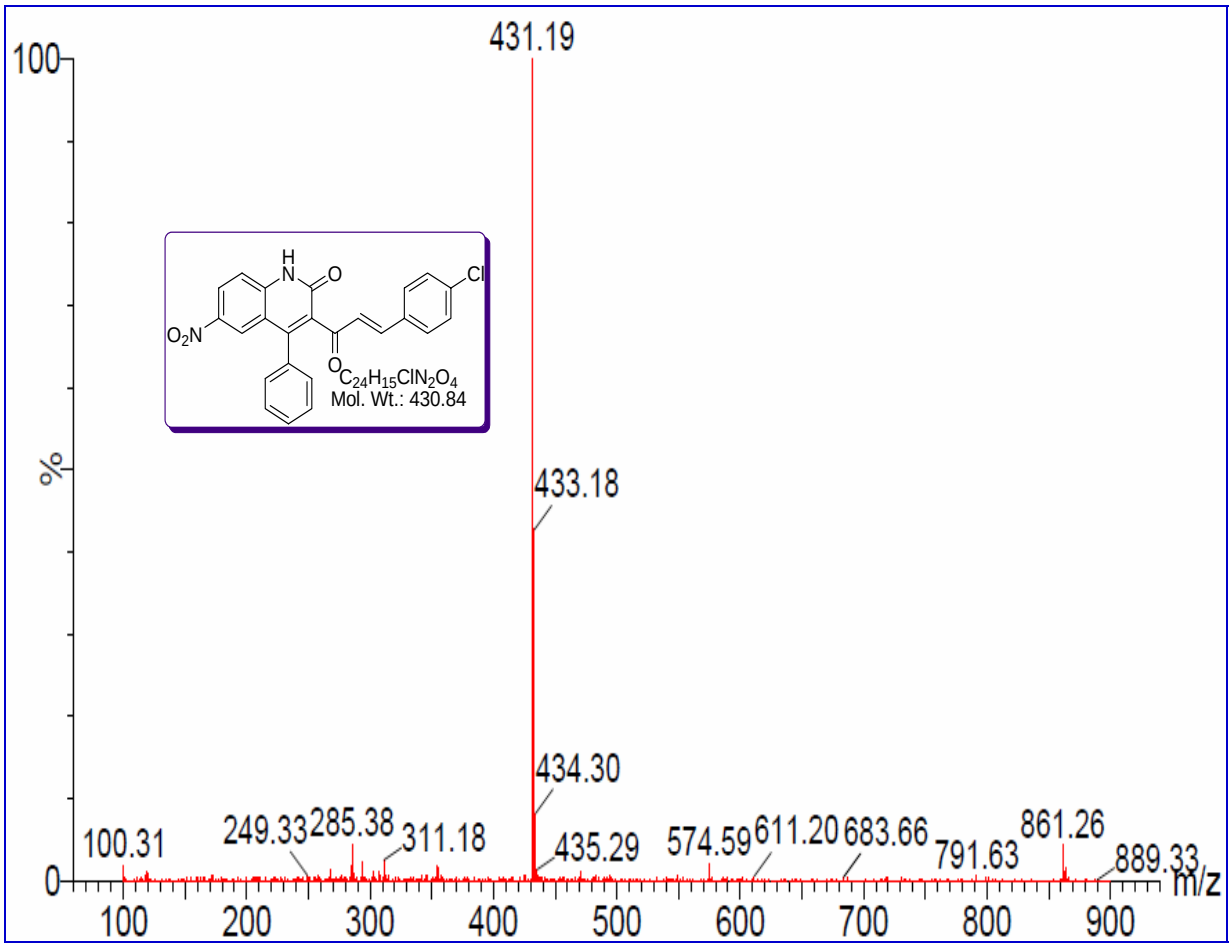

100
%T
80
60
40
20
4000
3000
2000
1500
1000
500
66
1/cm
3479.58
3444.87
3167.12
3120.82
3059.10
2993.52
2924.09
2879.72
1683.86
1662.64
1614.42
1529.55
1483.26
1442.75
1402.25
1332.81
1240.23
1176.68
1139.93
1060.85
979.84
810.10
763.81
709.80
563.21
O2N
CH3
C25H18N2O4
Mol. Wt.: 410.42

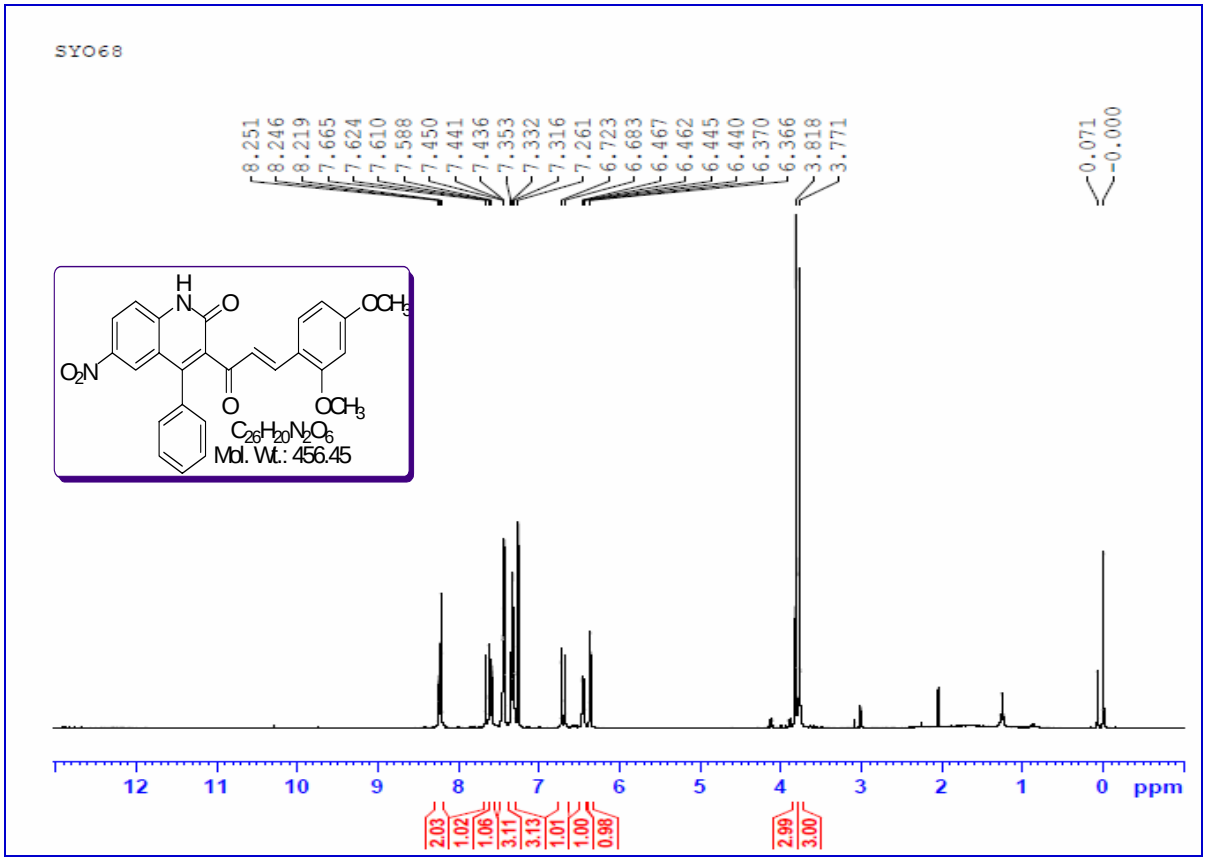

100
%
0
411.25
412.24
413.30
821.42
100.98
192.24
311.22
531.35600.54
663.46732.68
823.34
895.02
m/z
100
200
300
400
500
600
700
800
900
O2N
CH3
C25H18N2O4
Mol. Wt.: 410.42

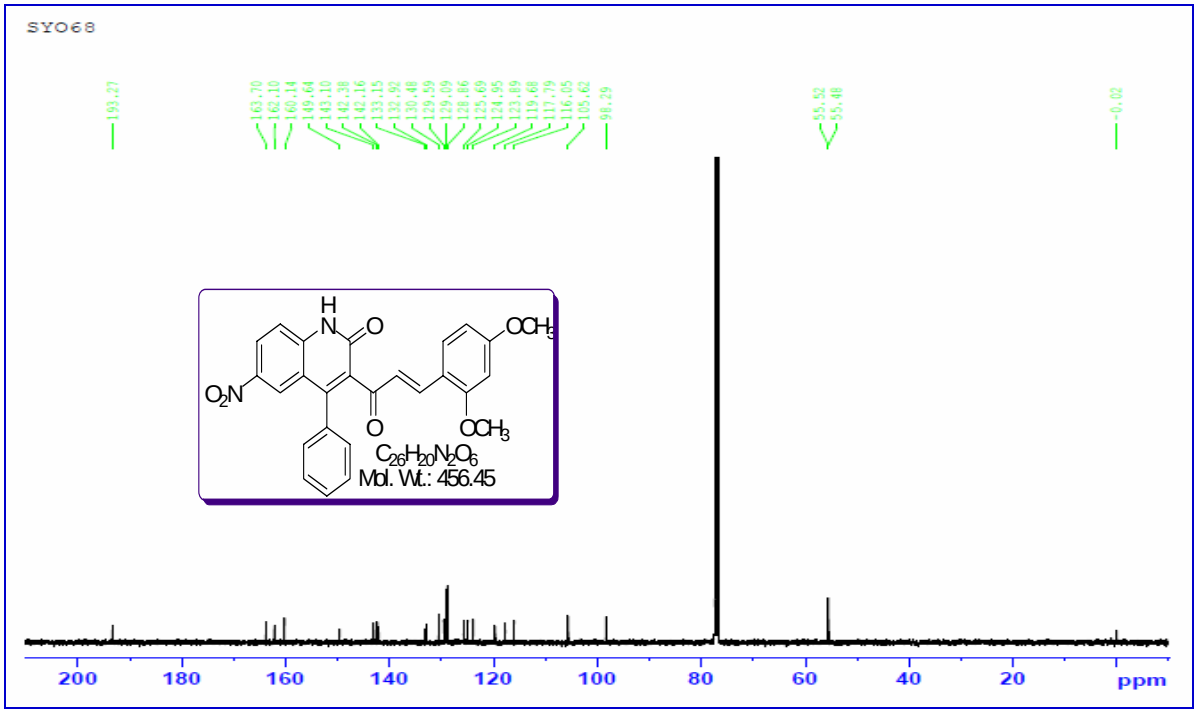

SY067
12.851
8.367
8.361
8.345
8.339
8.282
8.276
7.595
7.573
7.496
7.487
7.481
7.373
7.367
7.351
7.344
7.337
7.327
7.321
7.318
7.272
6.711
6.670
0.078
0.007
H
N
O
Cl
O2N
O
C24H15ClN2O4
Mol. Wt.: 430.84
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.87
1.01
1.01
1.06
3.01
7.09
1.00

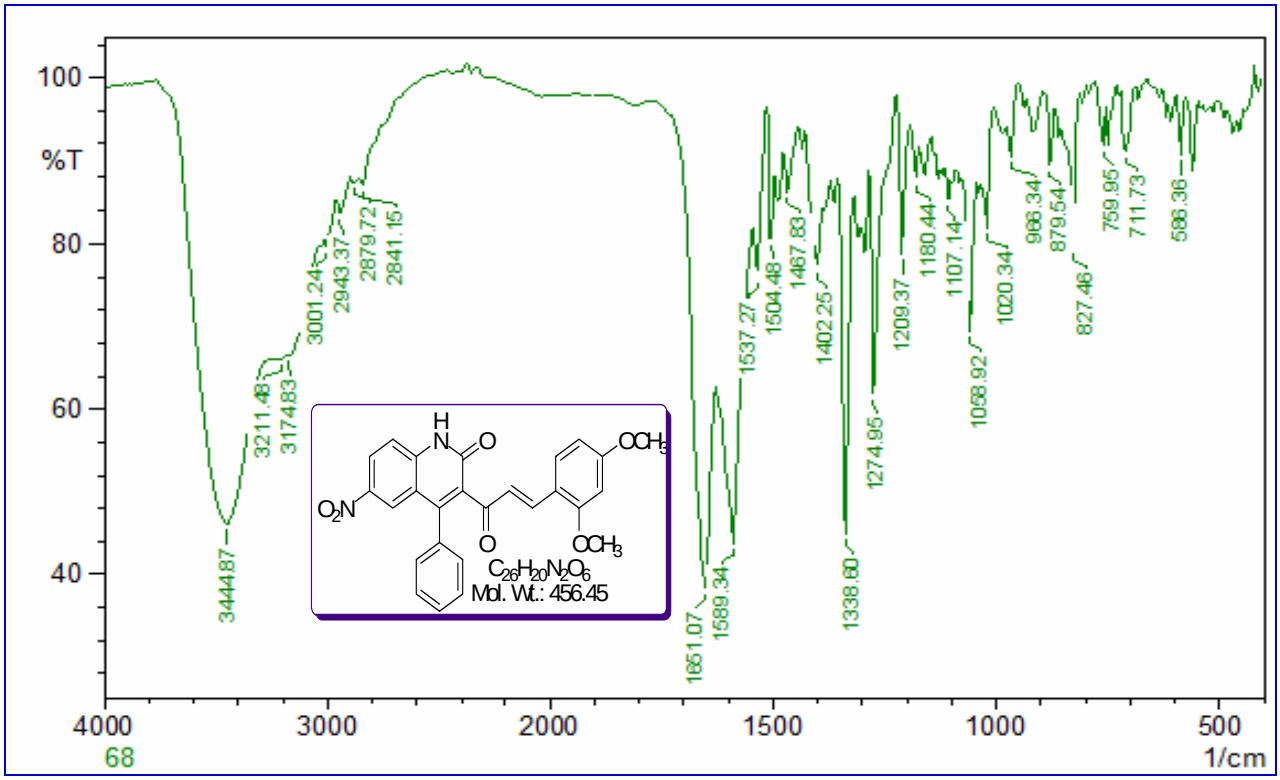

SY067
192.28
161.99
150.42
144.62
143.31
142.11
137.16
132.63
132.60
132.48
129.98
129.62
129.33
129.12
128.99
127.04
126.14
124.14
119.57
117.60
77.34
77.02
76.71
1.03
0.00
H
N
O
Cl
O2N
O
C24H15ClN2O4
Mol. Wt.: 430.84
200
180
160
140
120
100
80
60
40
20
0
ppm

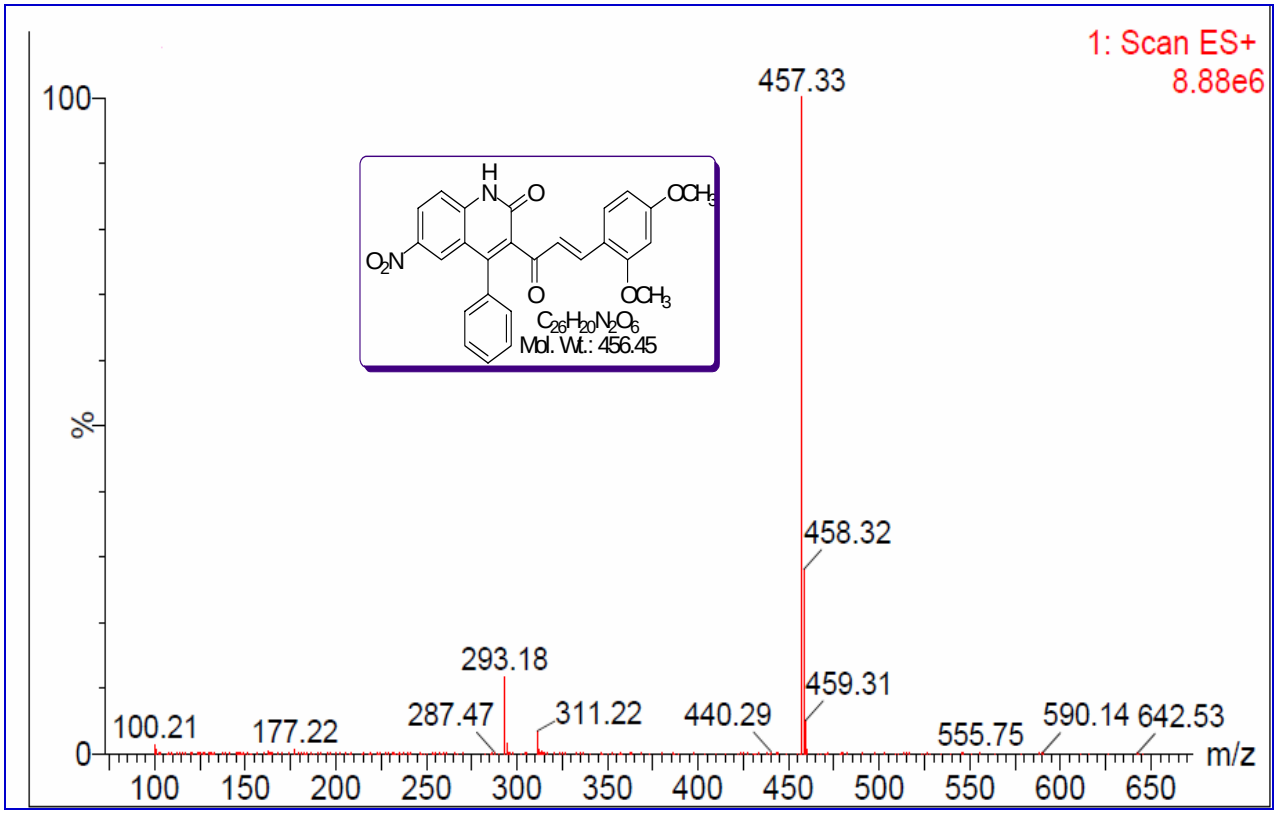

100
%T
75
50
25
0
4000
3000
2000
1500
1000
500
1/cm
67
3471.87
3448.72
3170.97
3126.61
3066.82
2993.52
2929.87
2883.58
1685.79
1664.57
1620.21
1529.55
1489.05
1404.18
1334.74
1240.23
1203.58
1174.65
1139.93
1091.71
1060.85
1016.49
979.84
914.26
833.25
763.81
707.88
563.21
524.64
H
N
O
Cl
O_2N
O
$C_{24}H_{15}ClN_2O_4$
Mol. Wt.: 430.84

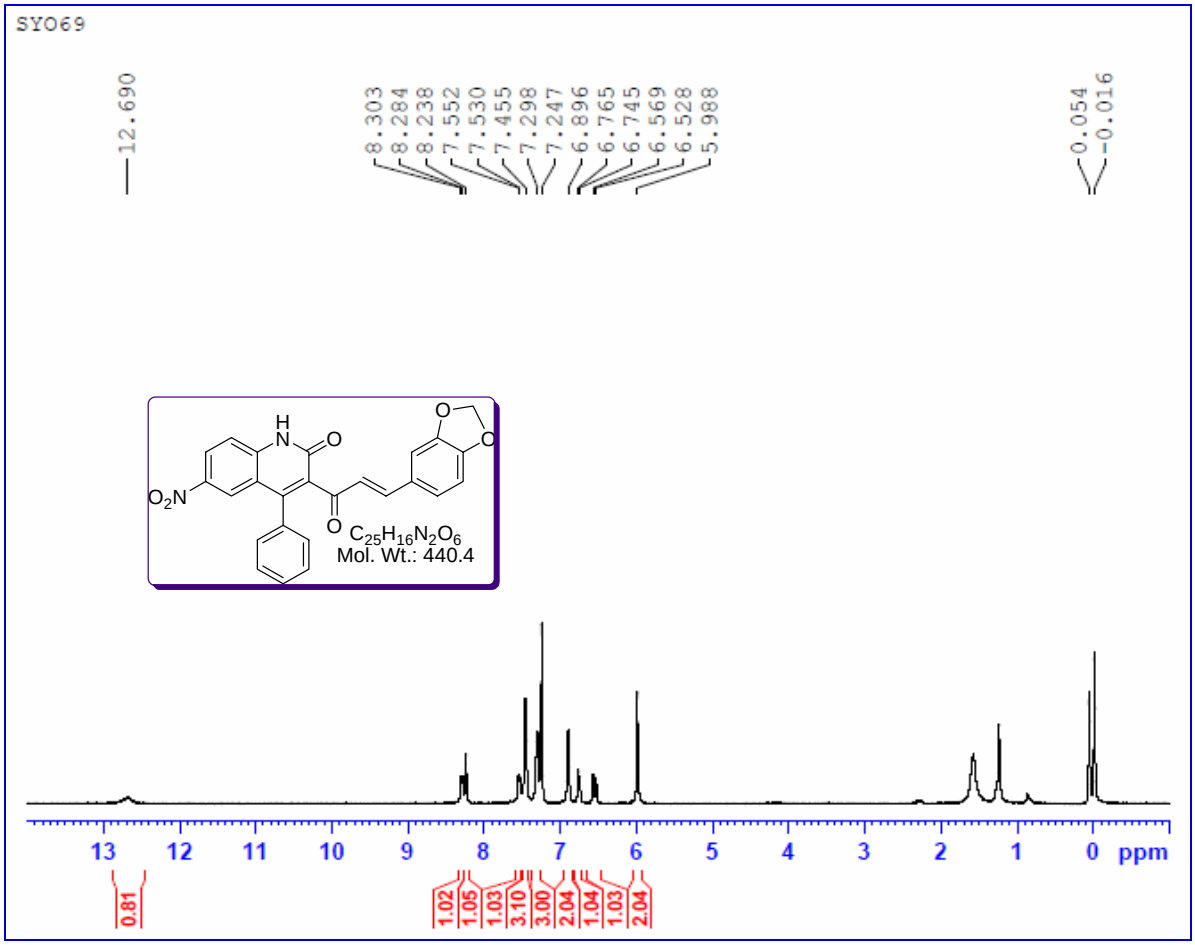

100
%
0
431.19
433.18
434.30
100.31
249.33
285.38
311.18
435.29
574.59
611.20
683.66
791.63
861.26
889.33
m/z
100
200
300
400
500
600
700
800
900
H
N
O
Cl
O_2N
O
$C_{24}H_{15}ClN_2O_4$
Mol. Wt.: 430.84

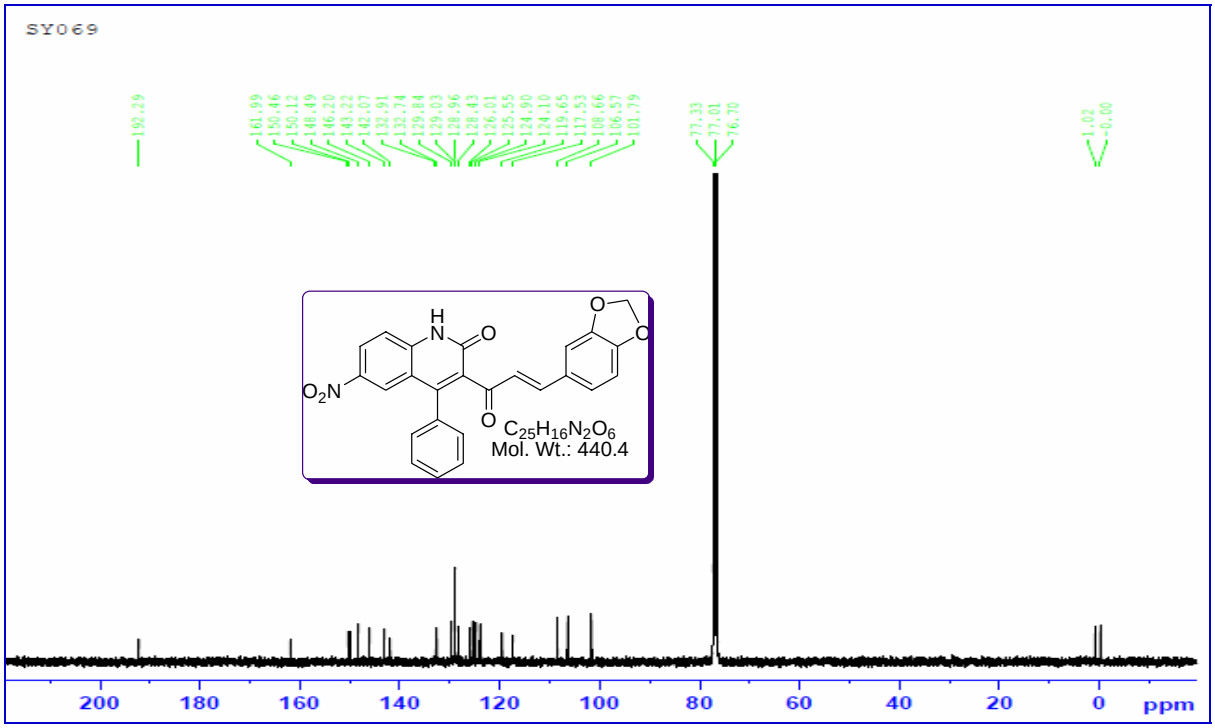

SYO68
8.251
8.246
8.219
7.665
7.624
7.610
7.588
7.450
7.441
7.436
7.353
7.332
7.316
7.261
6.723
6.683
6.467
6.462
6.445
6.440
6.370
6.366
3.818
3.771
0.071
-0.000
H
N
O
OCH3
O2N
O
OCH3
C26H20N2O6
Mol. Wt.: 456.45
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.03
1.02
1.06
3.11
3.13
1.01
1.00
0.98
2.99
3.00

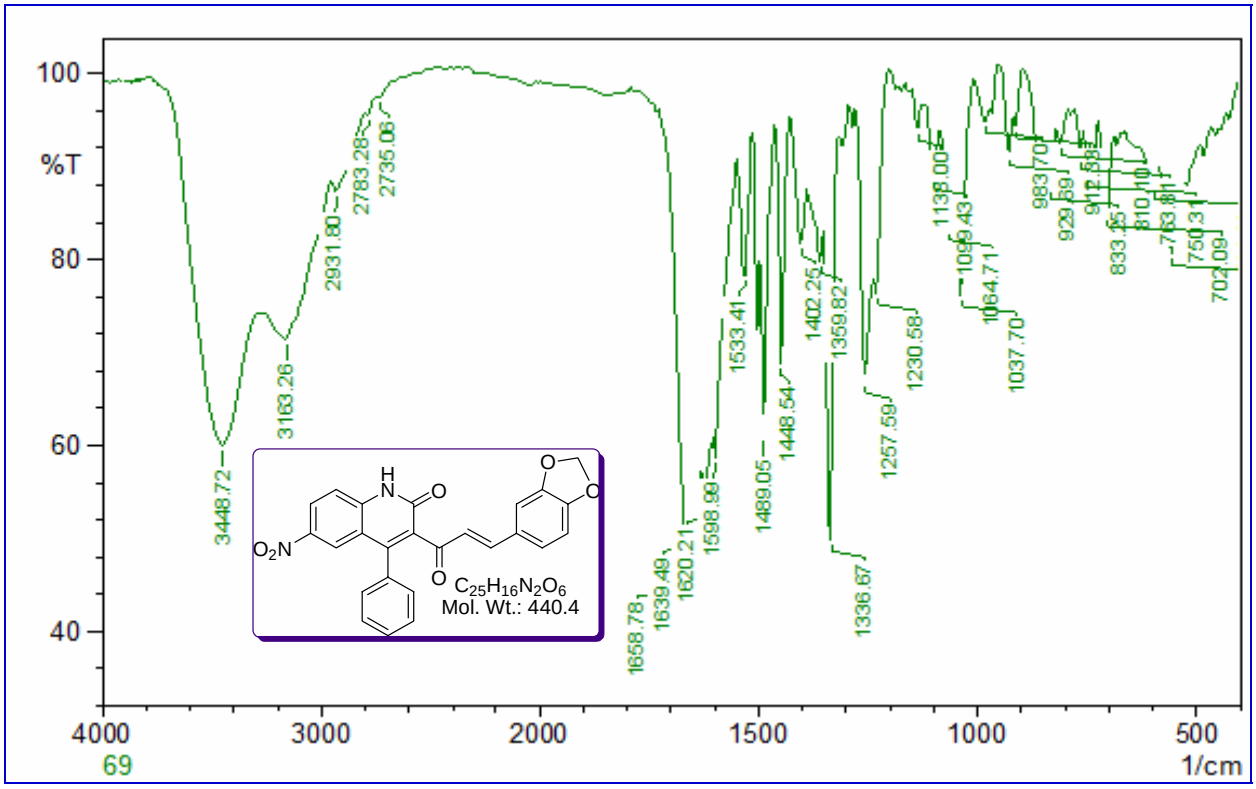

SYO68
193.27
163.70
162.10
160.14
149.64
143.10
142.38
142.16
133.15
132.92
130.48
129.59
129.09
128.86
125.69
124.95
123.89
119.68
117.79
116.05
105.62
98.29
55.52
55.48
-0.02
H
N
O
OCH3
O2N
O
OCH3
C26H20N2O6
Mol. Wt.: 456.45
200
180
160
140
120
100
80
60
40
20
ppm

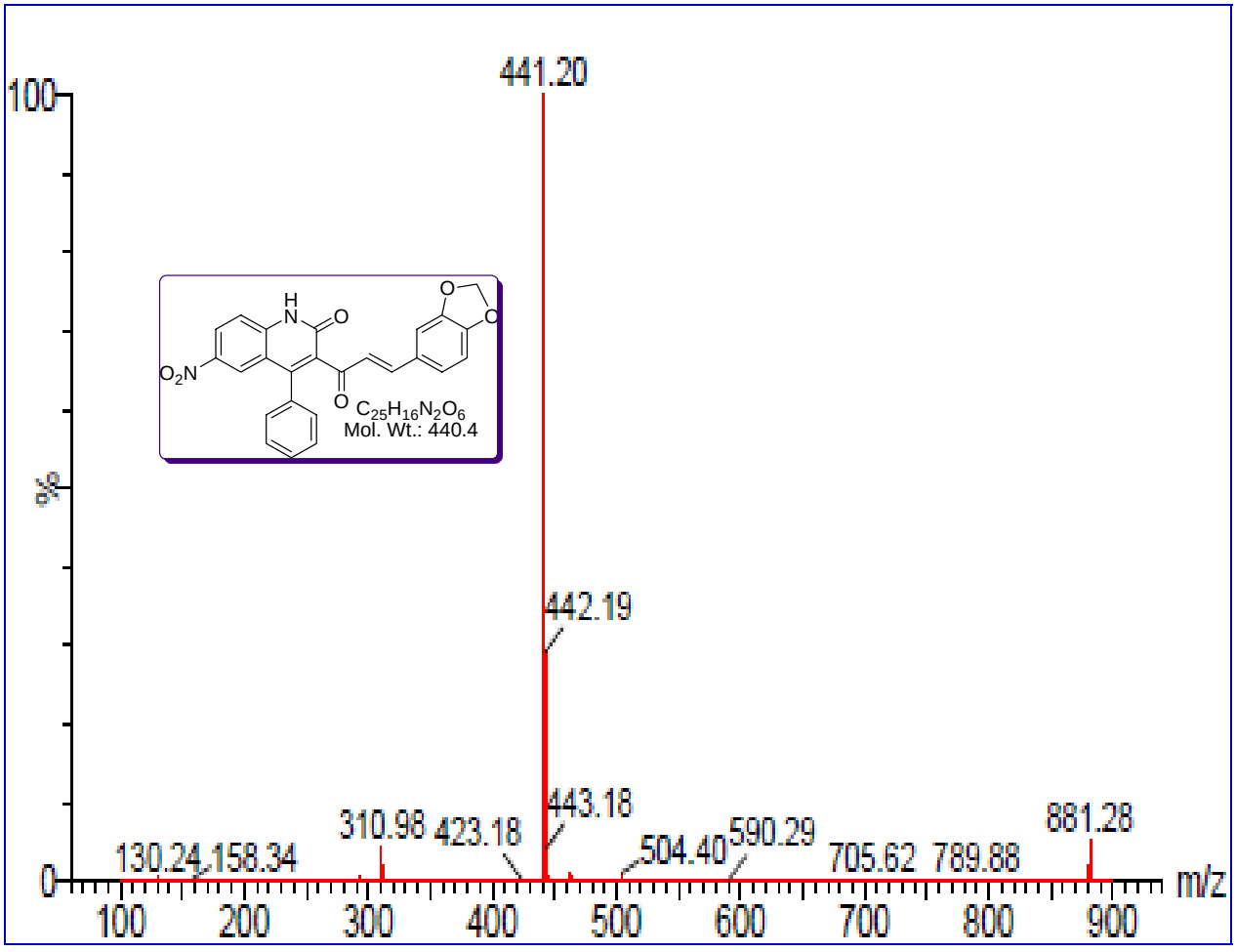

100
%T
80
60
40
3444.87
3211.48
3174.83
3001.24
2943.37
2879.72
2841.15
1651.07
1589.34
1537.27
1504.48
1467.83
1402.25
1338.60
1274.95
1209.37
1180.44
1107.14
1058.92
1020.34
966.34
879.54
827.46
759.95
711.73
586.36
H
N
O
O2N
OCH3
O
OCH3
C26H20N2O6
Mol. Wt.: 456.45
4000
3000
2000
1500
1000
500
1/cm
68

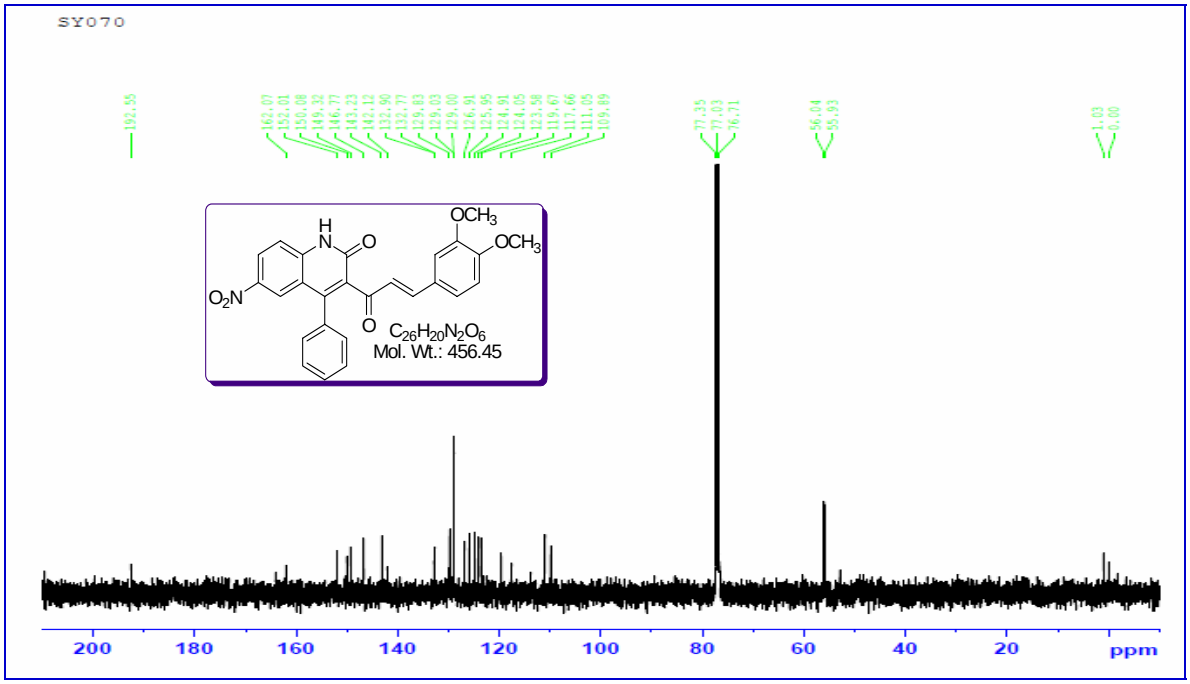

1: Scan ES+
8.88e6
100
%
0
457.33
458.32
459.31
293.18
100.21
177.22
287.47
311.22
440.29
555.75
590.14
642.53
H
N
O
O2N
OCH3
O
OCH3
C26H20N2O6
Mol. Wt.: 456.45
100
150
200
250
300
350
400
450
500
550
600
650
m/z

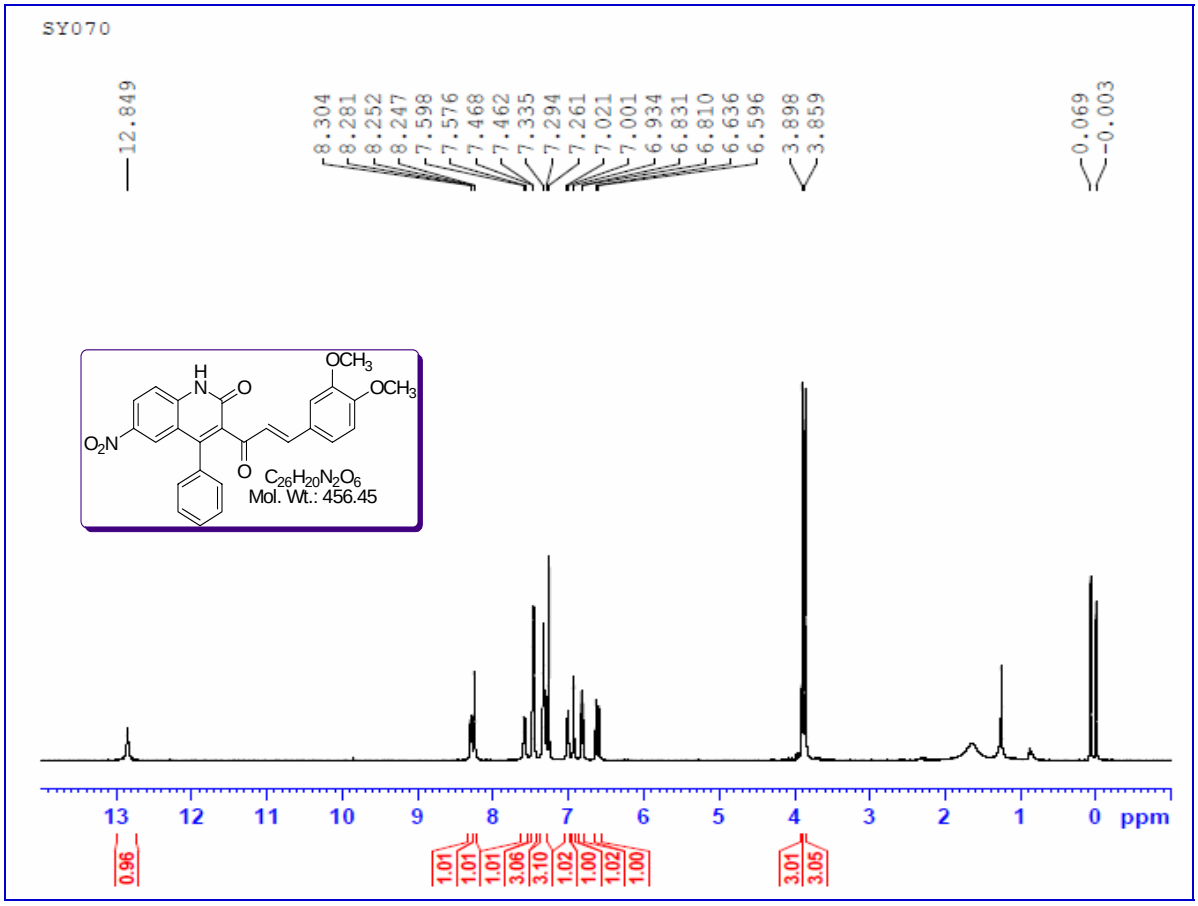

SY069
12.690
8.303
8.284
8.238
7.552
7.530
7.455
7.298
7.247
6.896
6.765
6.745
6.569
6.528
5.988
0.054
-0.016
$C_{25}H_{16}N_2O_6$
Mol. Wt.: 440.4
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.81
1.02
1.05
1.03
3.10
3.00
2.04
1.04
1.03
2.04

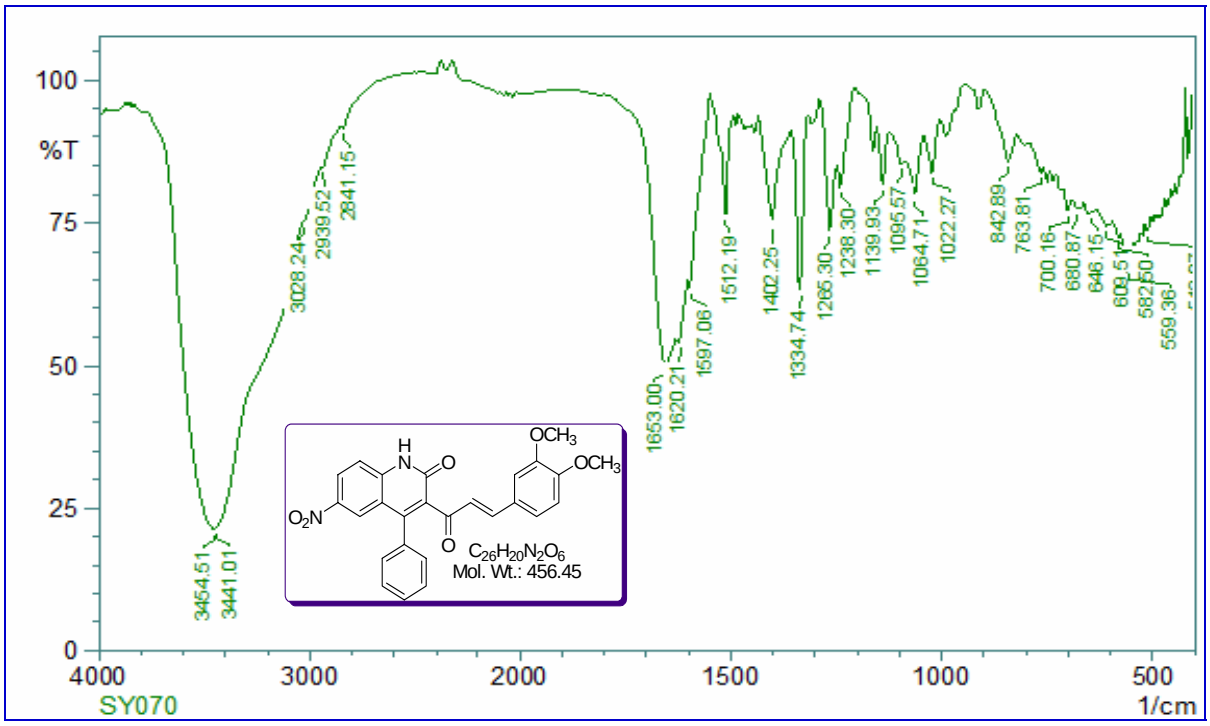

SY069
192.29
161.99
150.46
150.12
148.49
146.20
143.22
142.07
132.91
132.74
129.84
129.03
128.96
128.43
126.01
125.55
124.90
124.10
119.65
117.53
108.66
106.57
101.79
77.33
77.01
76.70
1.02
-0.00
$C_{25}H_{16}N_2O_6$
Mol. Wt.: 440.4
200
180
160
140
120
100
80
60
40
20
0
ppm

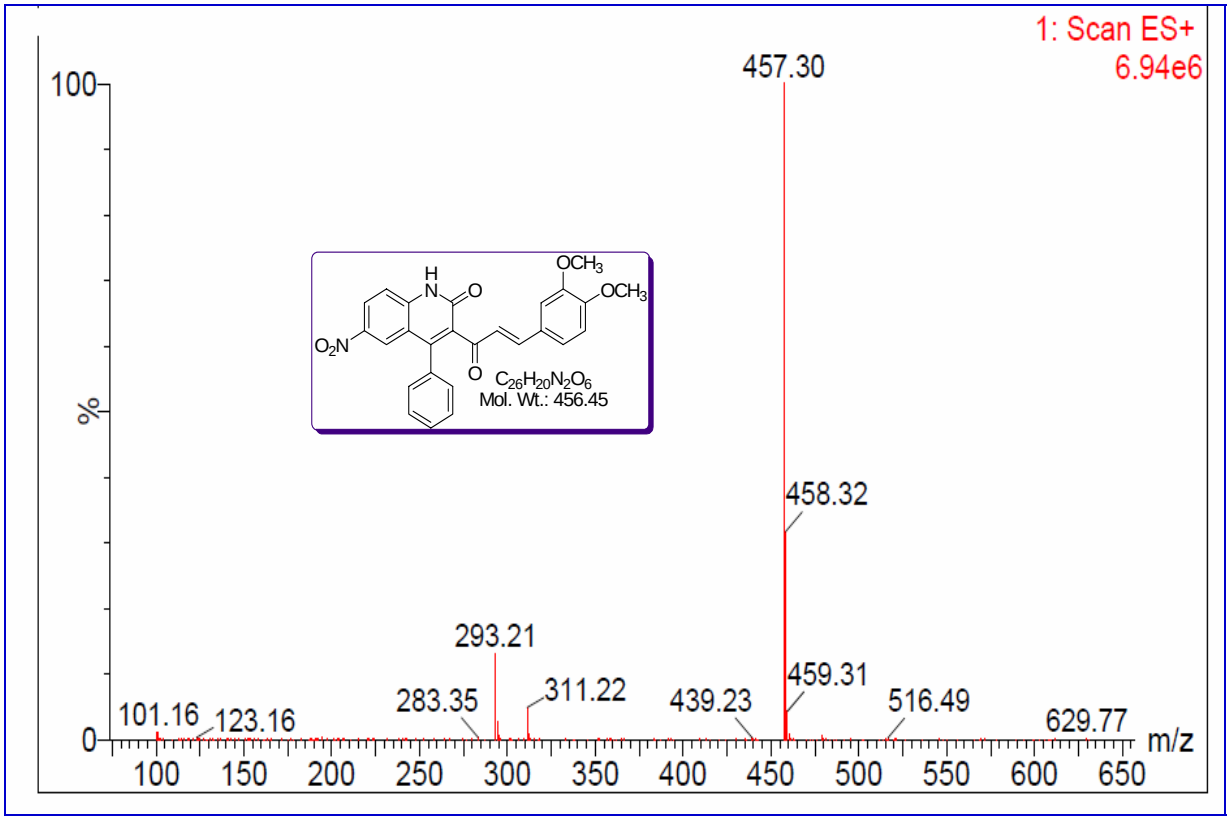

100
%T
80
60
40
4000
3000
2000
1500
1000
500
1/cm
3448.72
3163.26
2931.80
2783.28
2735.06
1658.78
1639.49
1620.21
1598.99
1533.41
1489.05
1448.54
1402.25
1359.82
1336.67
1257.59
1230.58
1138.00
1096.43
1064.71
1037.70
983.70
929.59
833.25
810.10
763.81
750.31
702.09
$C_{25}H_{16}N_2O_6$
Mol. Wt.: 440.4

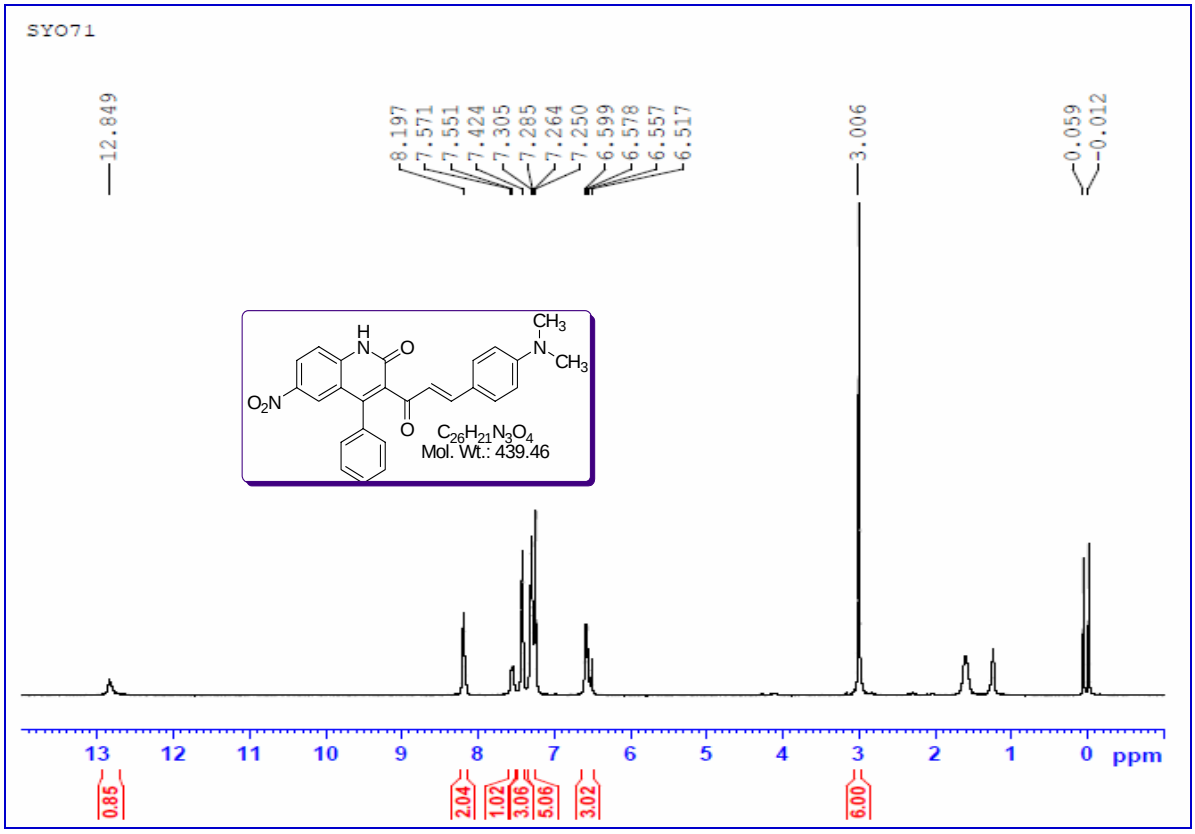

100
%
0
441.20
442.19
443.18
310.98
423.18
130.24
158.34
504.40
590.29
705.62
789.88
881.28
100
200
300
400
500
600
700
800
900
m/z
$C_{25}H_{16}N_2O_6$
Mol. Wt.: 440.4

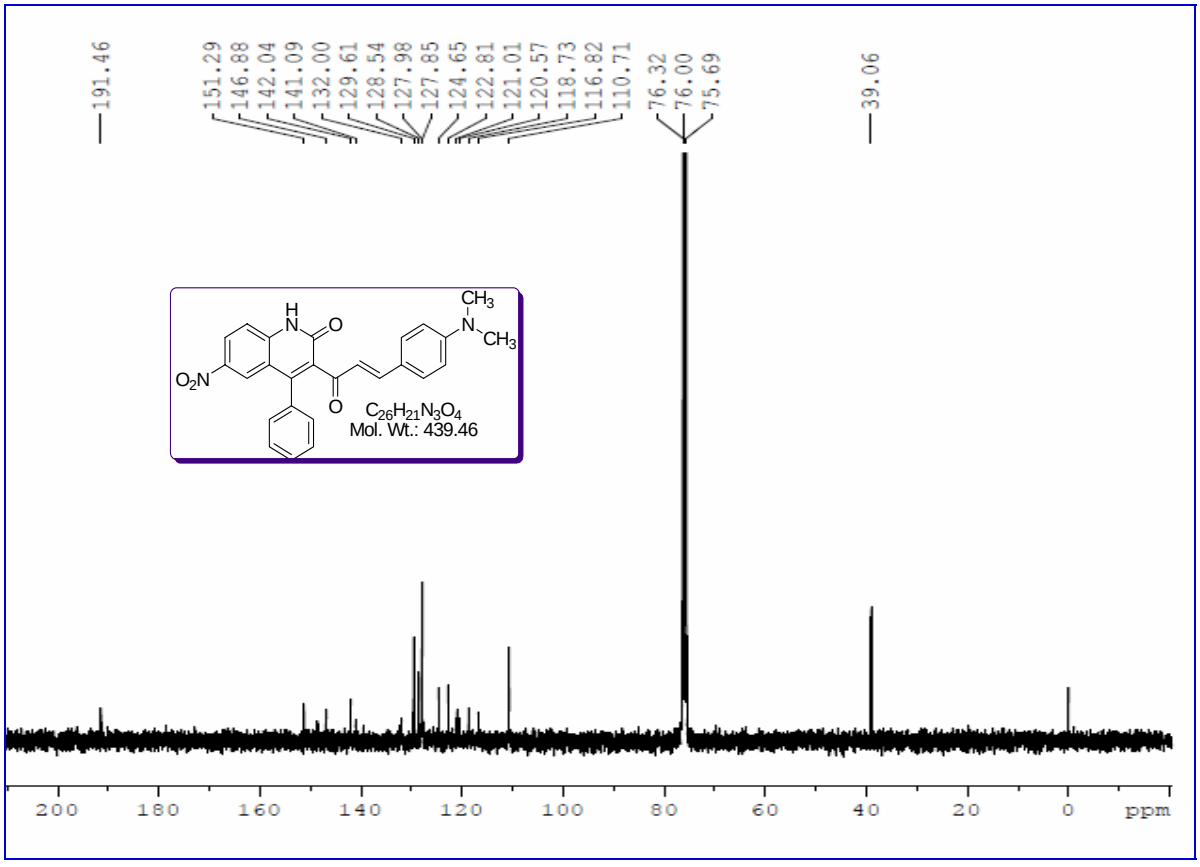

SY070
192.55
162.07
152.01
150.08
149.32
146.77
143.23
142.12
132.90
132.77
129.83
129.03
129.00
126.91
125.95
124.91
124.05
123.58
119.67
117.66
111.05
109.89
77.35
77.03
76.71
56.04
55.93
1.03
0.00
OCH3
OCH3
H
N
O
O2N
O
C26H20N2O6
Mol. Wt.: 456.45
200
180
160
140
120
100
80
60
40
20
ppm

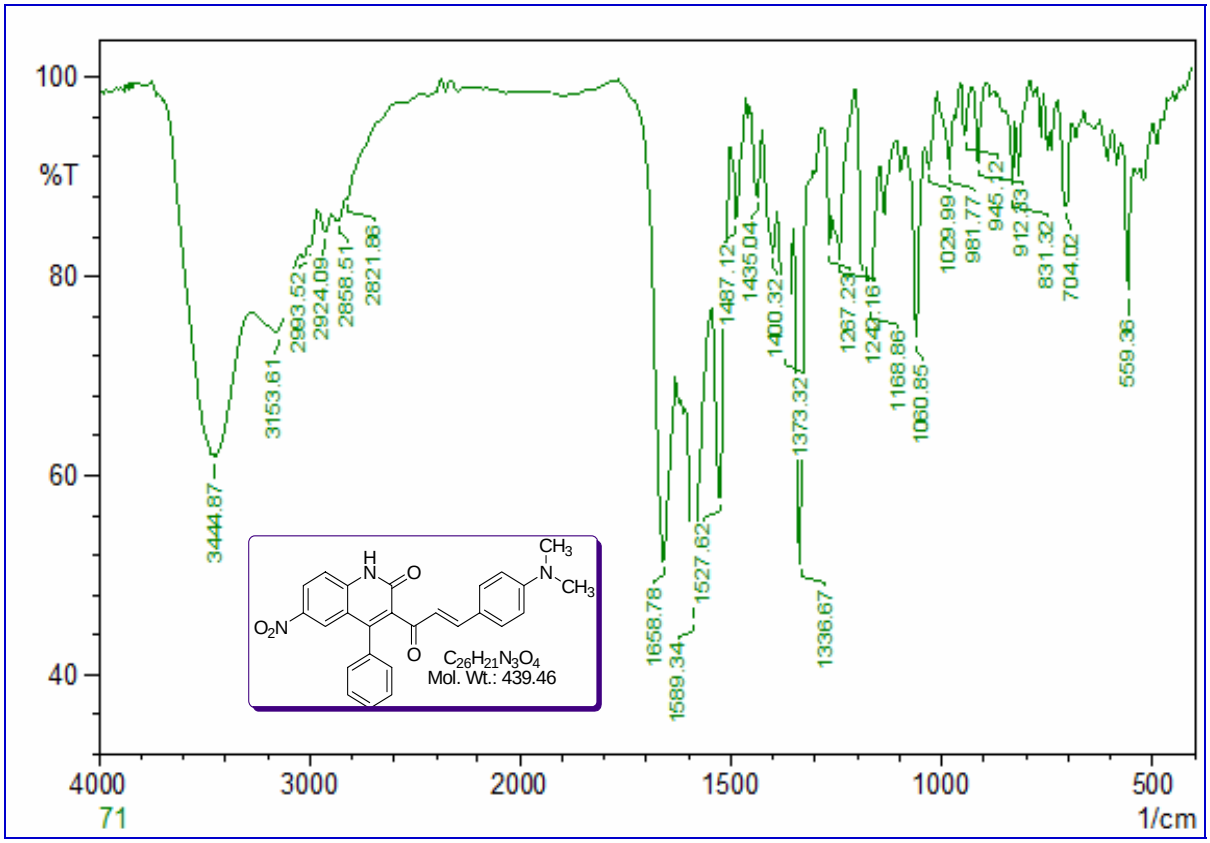

SY070
12.849
8.304
8.281
8.252
8.247
7.598
7.576
7.468
7.462
7.335
7.294
7.261
7.021
7.001
6.934
6.831
6.810
6.636
6.596
3.898
3.859
0.069
-0.003
OCH3
OCH3
H
N
O
O2N
O
C26H20N2O6
Mol. Wt.: 456.45
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.96
1.01
1.01
1.01
3.06
3.10
1.02
1.00
1.02
1.00
3.01
3.05

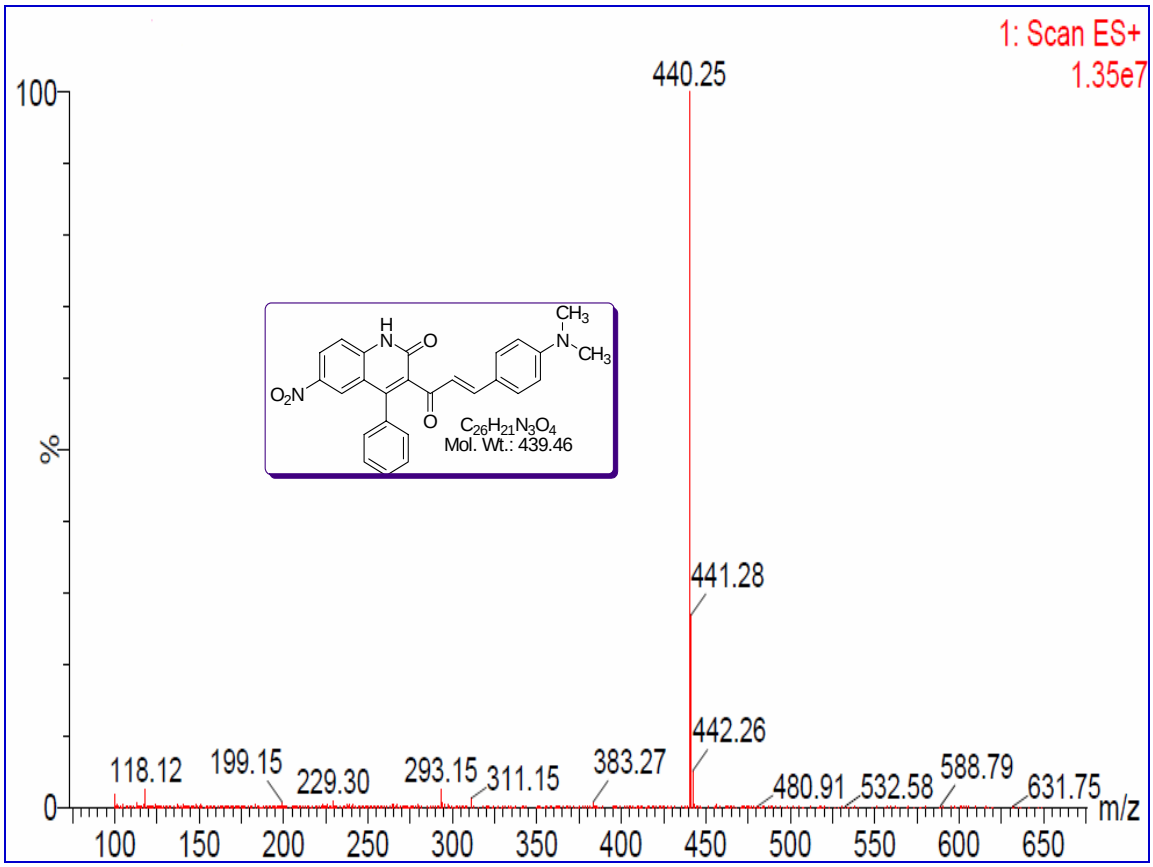

100
%T
75
50
25
0
4000
3000
2000
1500
1000
500
1/cm
SY070
3454.51
3441.01
3028.24
2939.52
2841.15
1653.00
1620.21
1597.06
1512.19
1402.25
1334.74
1285.30
1238.30
1139.93
1095.57
1064.71
1022.27
842.89
763.81
700.16
680.87
646.15
609.51
582.50
559.36
OCH3
OCH3
H
N
O
O2N
O
C26H20N2O6
Mol. Wt.: 456.45

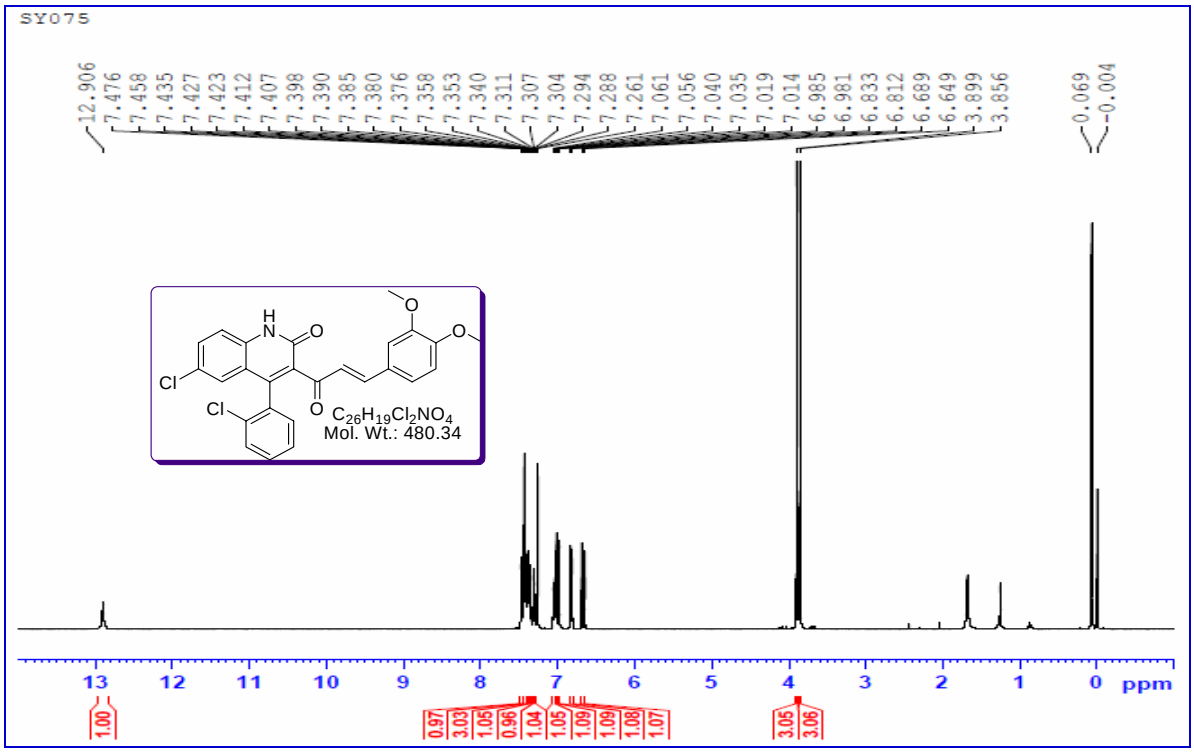

1: Scan ES+
6.94e6
100
%
0
457.30
458.32
459.31
293.21
311.22
283.35
439.23
516.49
629.77
101.16
123.16
100
150
200
250
300
350
400
450
500
550
600
650
m/z
OCH3
OCH3
H
N
O
O2N
O
C26H20N2O6
Mol. Wt.: 456.45

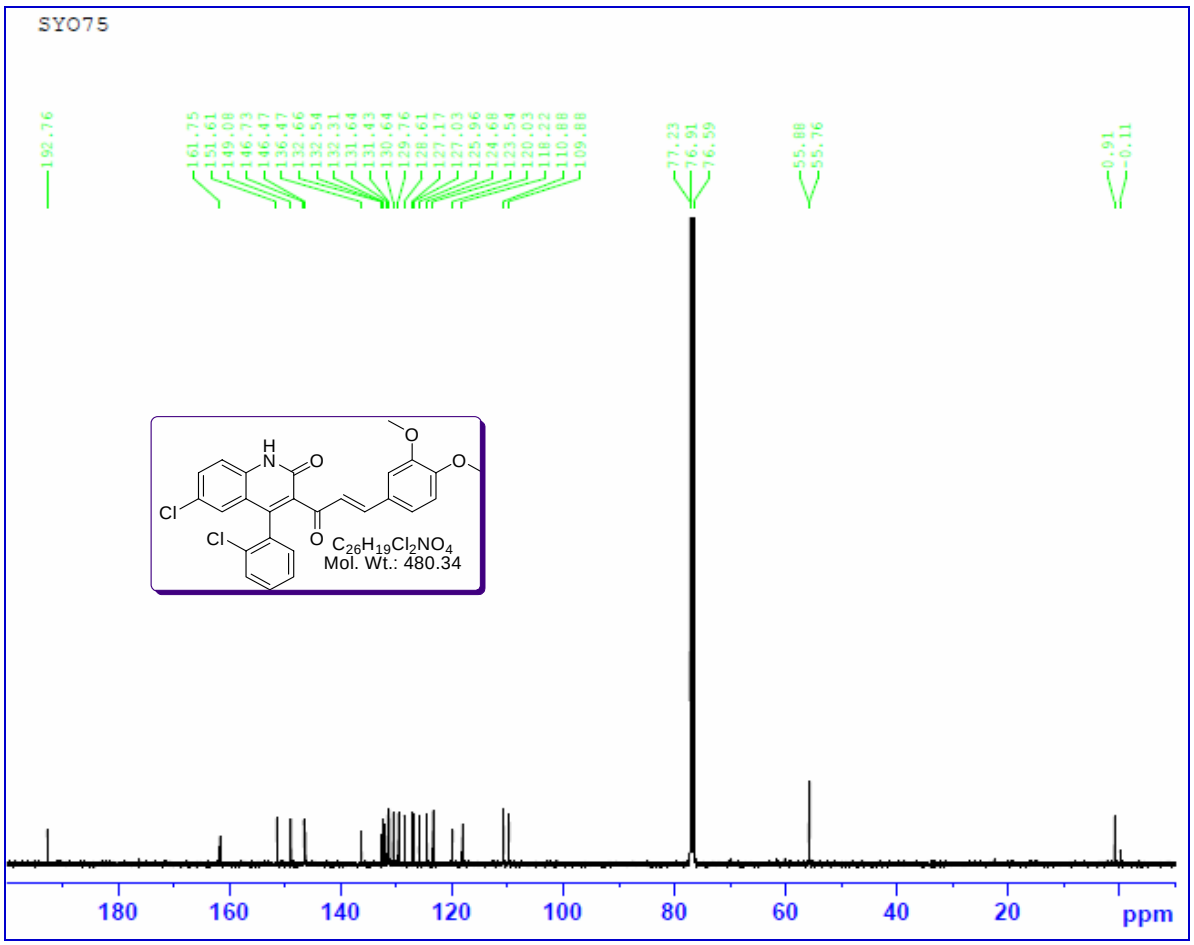

SYO71
12.849
8.197
7.571
7.551
7.424
7.305
7.285
7.264
7.250
6.599
6.578
6.557
6.517
3.006
0.059
0.012
$C_{26}H_{21}N_3O_4$
Mol. Wt.: 439.46
13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.85
2.04
1.02
3.06
5.06
3.02
6.00

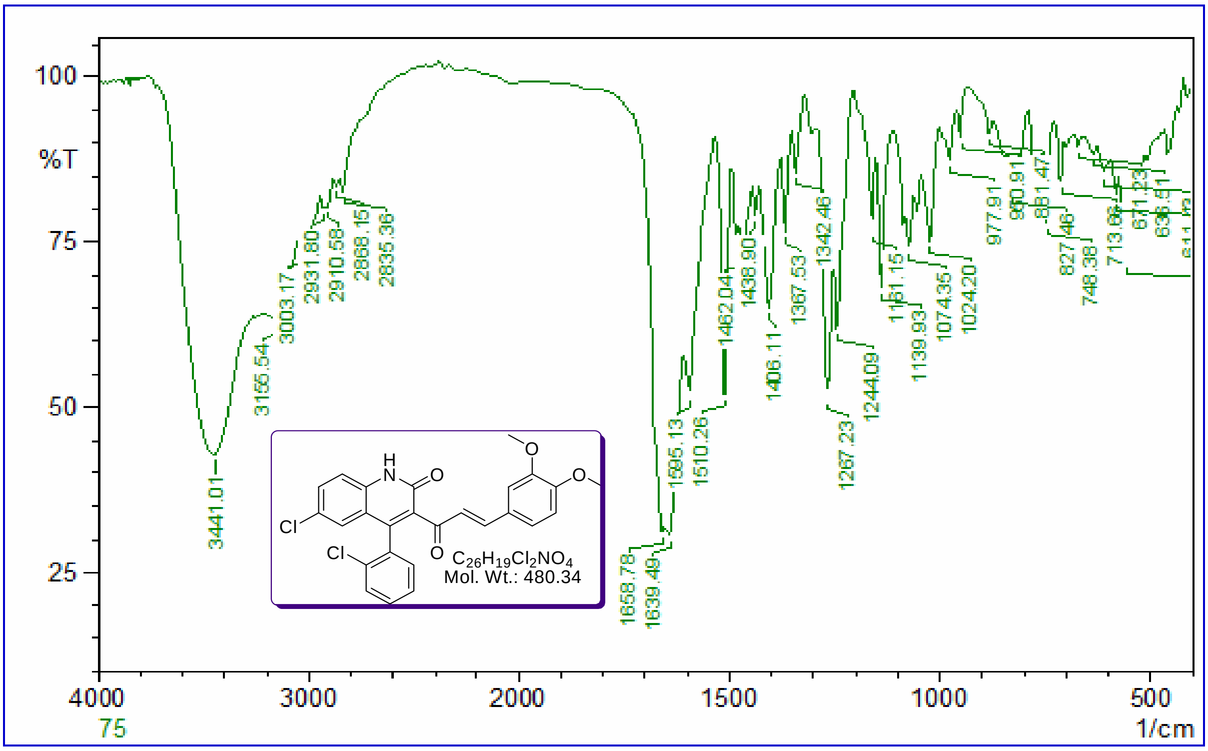

191.46
151.29
146.88
142.04
141.09
132.00
129.61
128.54
127.98
127.85
124.65
122.81
121.01
120.57
118.73
116.82
110.71
76.32
76.00
75.69
39.06
$C_{26}H_{21}N_3O_4$
Mol. Wt.: 439.46
200 180 160 140 120 100 80 60 40 20 0 ppm

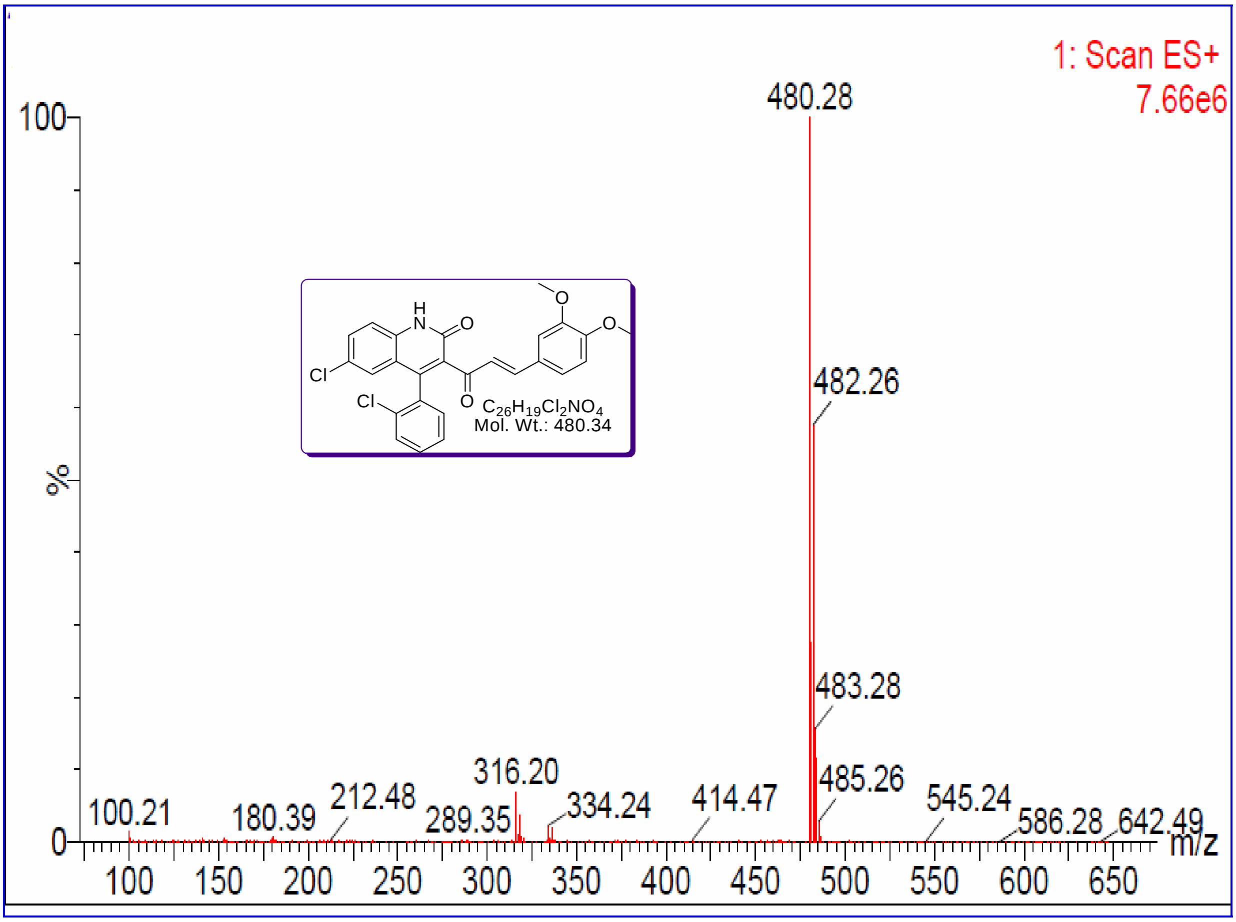

100
%T
80
60
40
4000
3000
2000
1500
1000
500
1/cm
71
3444.87
3153.61
2924.09
2858.51
2821.86
1658.78
1589.34
1527.62
1487.12
1435.04
1400.32
1373.32
1336.67
1267.23
1168.86
1060.85
1029.99
981.77
945.21
912.63
831.32
704.02
559.36
$C_{26}H_{21}N_3O_4$
Mol. Wt.: 439.46

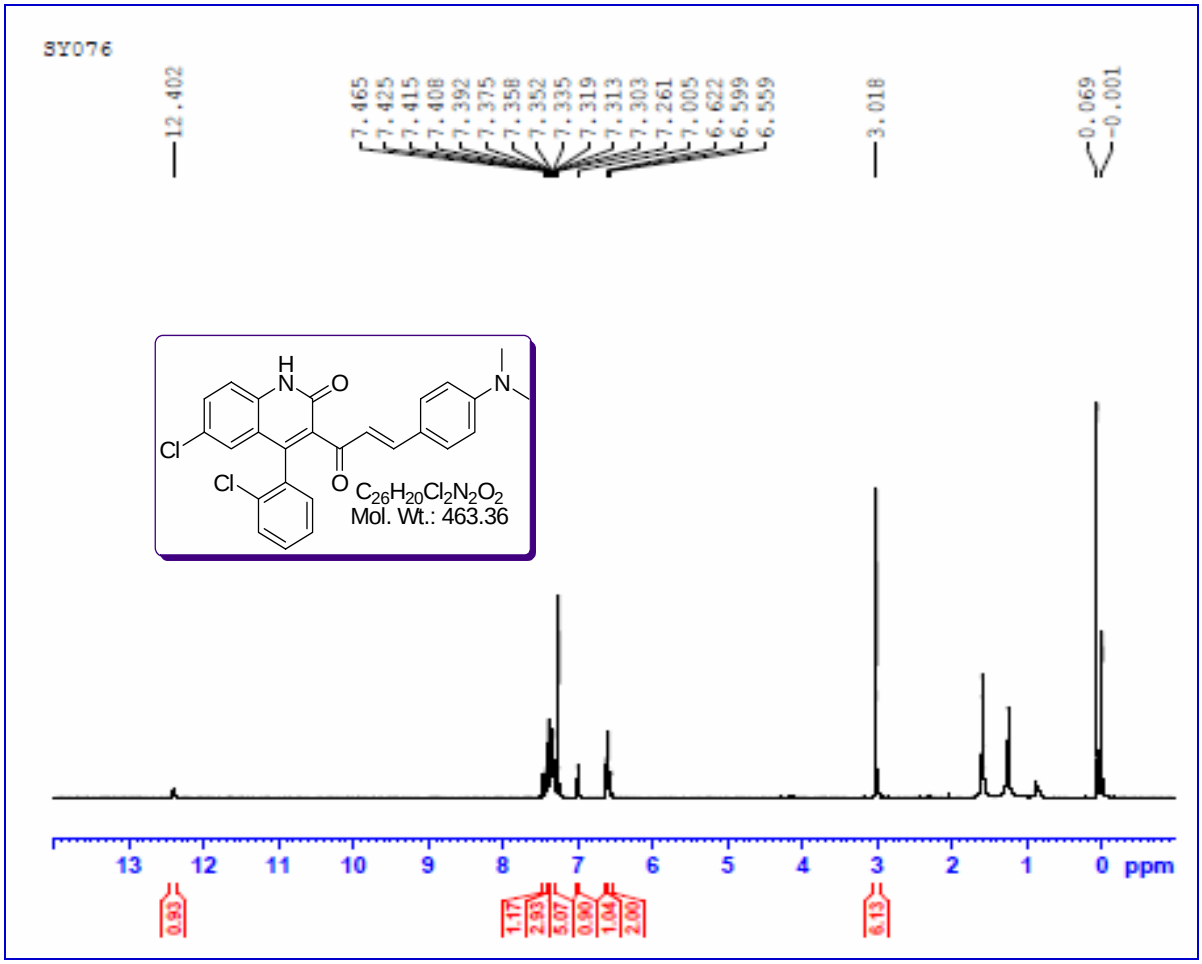

1: Scan ES+
1.35e7
100
%
0
440.25
441.28
442.26
118.12
199.15
229.30
293.15
311.15
383.27
480.91
532.58
588.79
631.75
m/z
100
150
200
250
300
350
400
450
500
550
600
650
$C_{26}H_{21}N_3O_4$
Mol. Wt.: 439.46

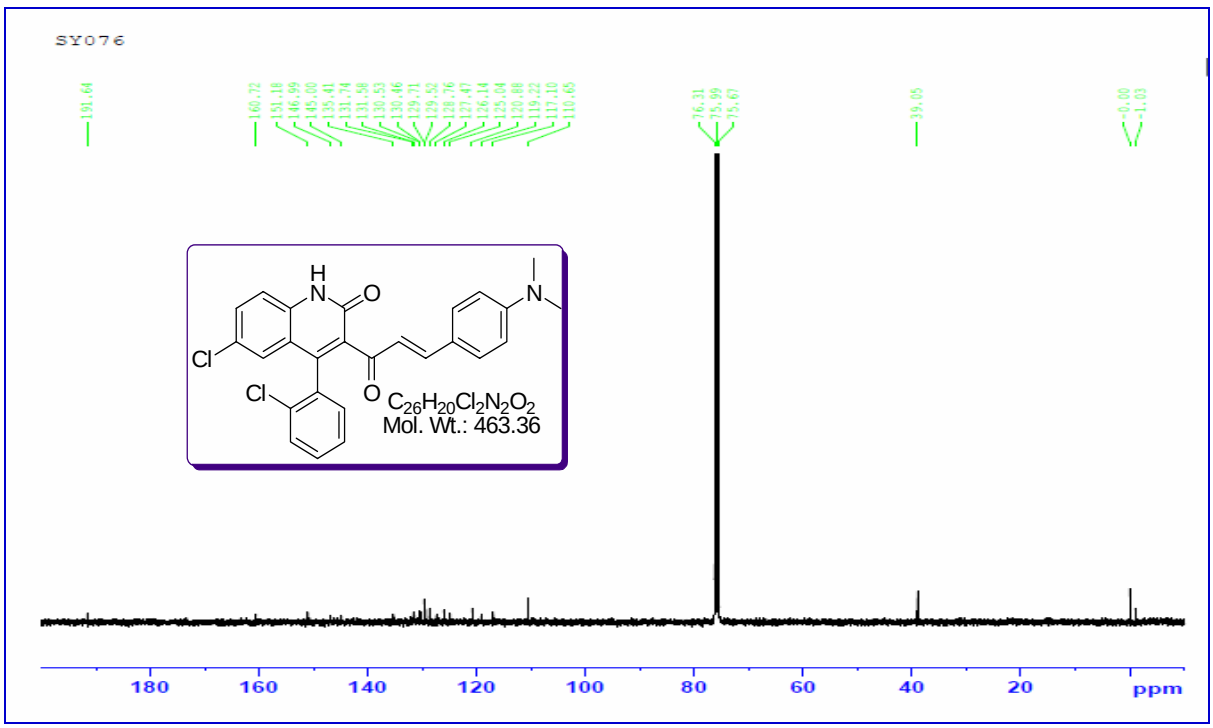

SY075
12.906
7.476
7.458
7.435
7.427
7.423
7.412
7.407
7.398
7.390
7.385
7.380
7.376
7.358
7.353
7.340
7.311
7.307
7.304
7.294
7.288
7.261
7.061
7.056
7.040
7.035
7.019
7.014
6.985
6.981
6.833
6.812
6.689
6.649
3.899
3.856
0.069
-0.004
H
N
O
O
O
Cl
Cl
O
C26H19Cl2NO4
Mol. Wt.: 480.34
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
0.97
3.03
1.05
0.96
1.04
1.05
1.09
1.09
1.08
1.07
3.05
3.06

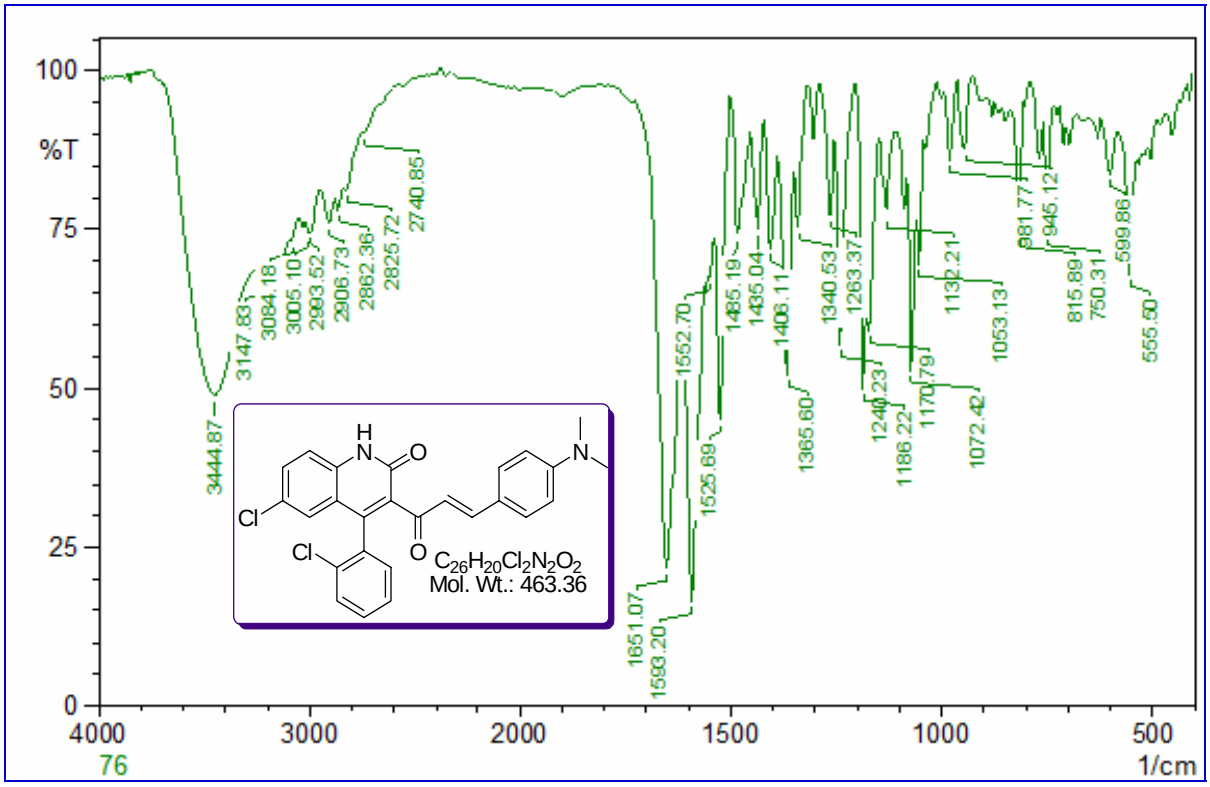

SYO75
192.76
161.75
151.61
149.08
146.73
146.47
136.47
132.66
132.54
132.31
131.64
131.43
130.64
129.76
128.61
127.17
127.03
125.96
124.68
123.54
120.03
118.22
110.88
109.88
77.23
76.91
76.59
55.88
55.76
0.91
-0.11
H
N
O
O
O
Cl
Cl
O
C26H19Cl2NO4
Mol. Wt.: 480.34
180
160
140
120
100
80
60
40
20
ppm

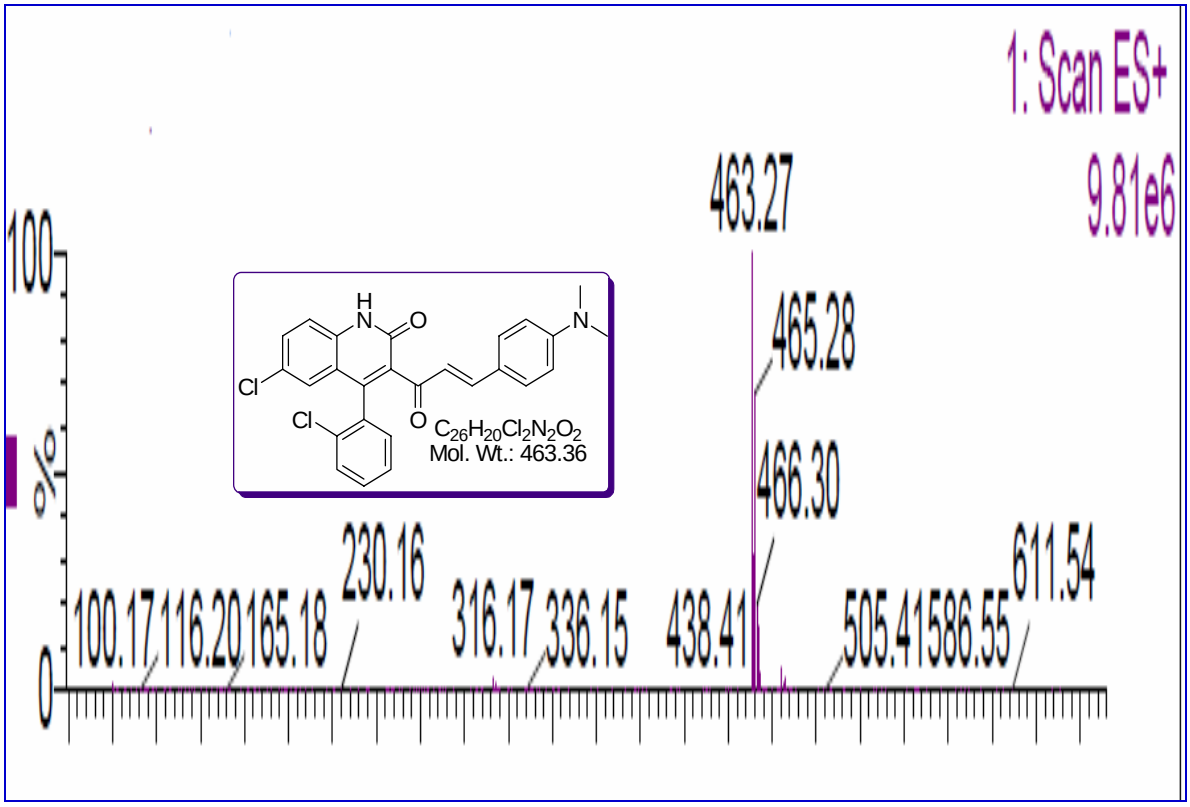

100
%T
75
50
25
3441.01
3155.54
3003.17
2931.80
2910.58
2868.15
2835.36
1658.78
1639.49
1595.13
1510.26
1462.04
1438.90
1406.11
1367.53
1342.46
1267.23
1244.09
1161.15
1139.93
1074.35
1024.20
977.91
950.91
881.47
827.46
748.38
713.66
671.23
636.51
Cl
Cl
H
N
O
O
O
O
$C_{26}H_{19}Cl_2NO_4$
Mol. Wt.: 480.34
4000
3000
2000
1500
1000
500
75
1/cm

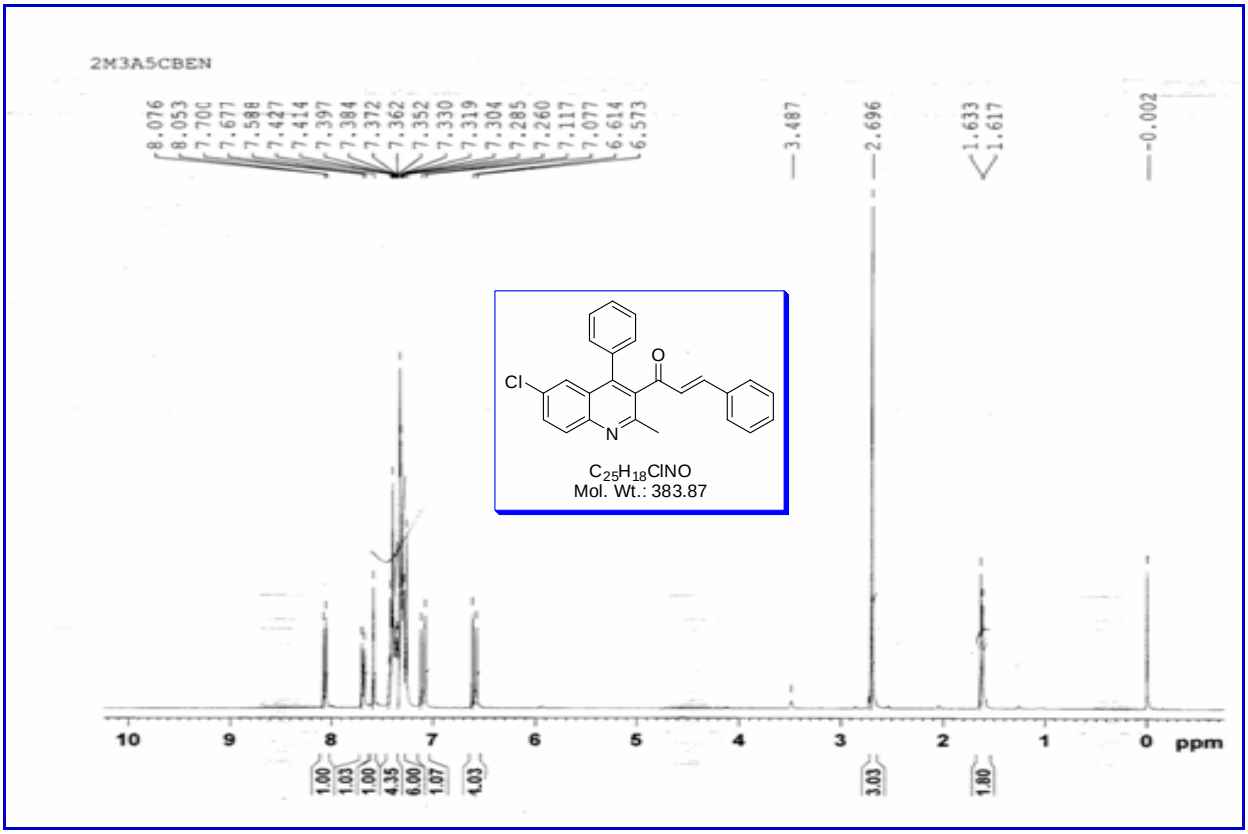

1: Scan ES+
7.66e6
100
%
0
480.28
482.26
483.28
485.26
100.21
180.39
212.48
289.35
316.20
334.24
414.47
545.24
586.28
642.49
Cl
Cl
H
N
O
O
O
O
$C_{26}H_{19}Cl_2NO_4$
Mol. Wt.: 480.34
100
150
200
250
300
350
400
450
500
550
600
650
m/z

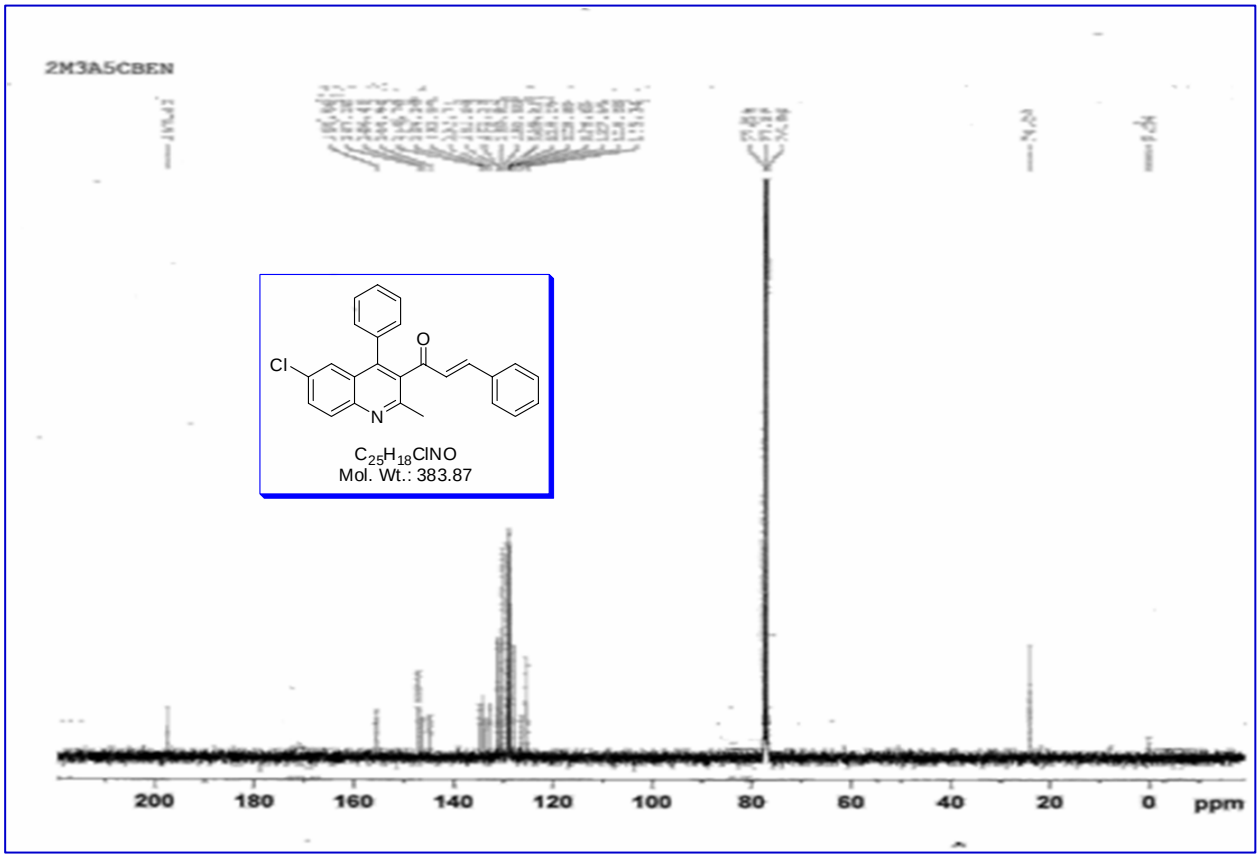

SY076
12.402
7.465
7.425
7.415
7.408
7.392
7.375
7.358
7.352
7.335
7.319
7.313
7.303
7.261
7.005
6.622
6.599
6.559
3.018
0.069
-0.001
H
N
O
Cl
Cl
O
N
C26H20Cl2N2O2
Mol. Wt.: 463.36
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.93
1.17
2.93
5.07
0.90
1.04
2.00
6.13

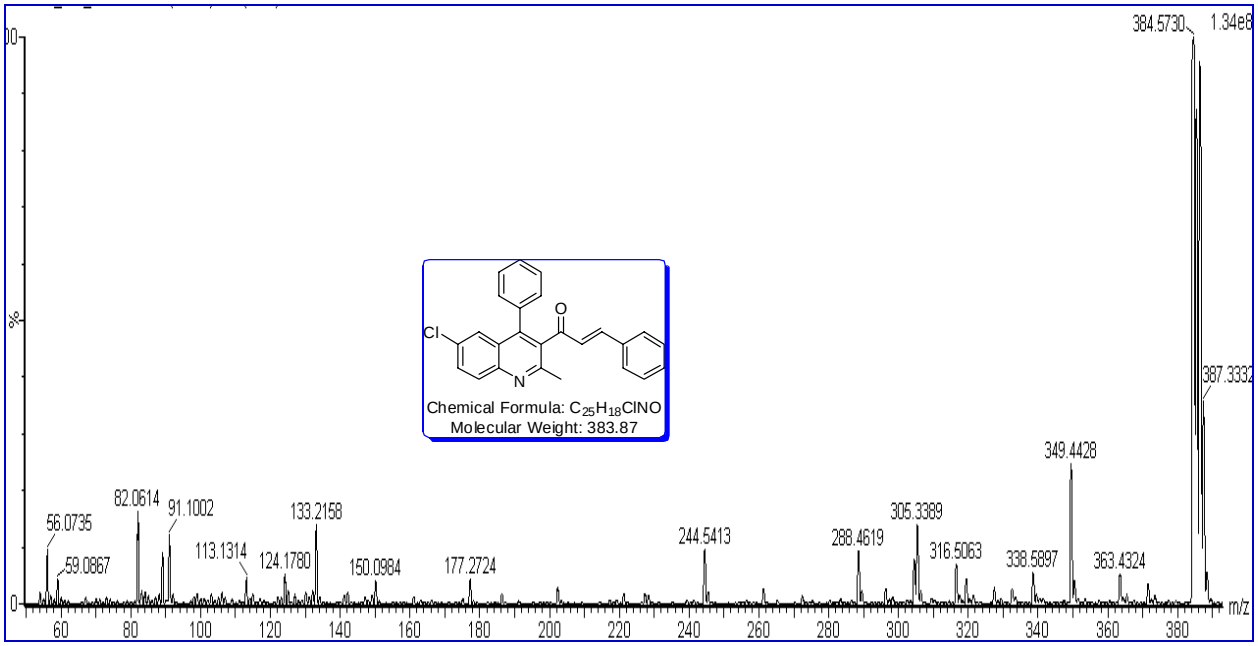

SY076
191.64
160.72
151.18
146.99
145.00
135.41
131.74
131.58
130.53
130.46
129.71
129.52
128.76
127.47
126.14
125.04
120.88
119.22
117.10
110.65
76.31
75.99
75.67
39.05
0.00
-1.03
H
N
O
Cl
Cl
O
N
C26H20Cl2N2O2
Mol. Wt.: 463.36
180
160
140
120
100
80
60
40
20
ppm

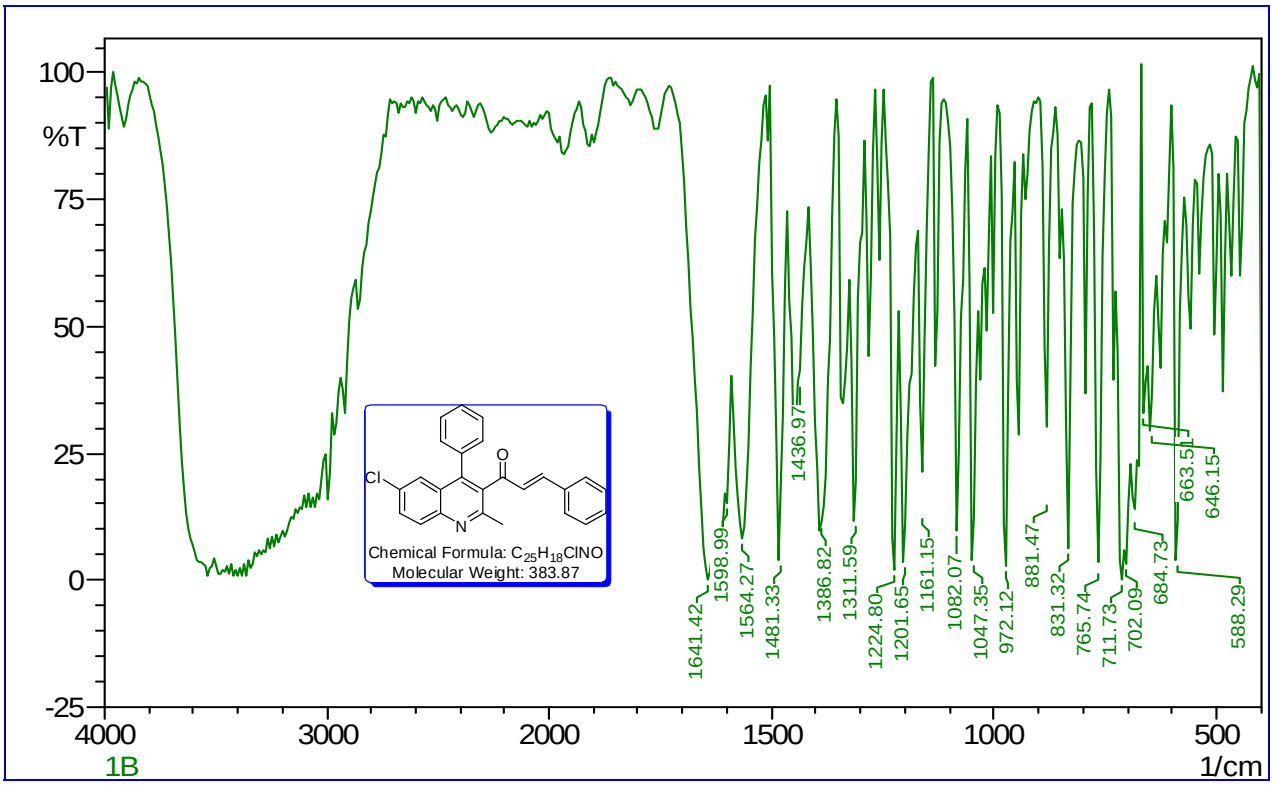

100
%T
75
50
25
0
4000
3000
2000
1500
1000
500
1/cm
3444.87
3147.83
3084.18
3005.10
2993.52
2906.73
2862.36
2825.72
2740.85
1651.07
1593.20
1552.70
1525.69
1485.19
1435.04
1406.11
1365.60
1340.53
1263.37
1240.23
1186.22
1170.79
1132.21
1072.42
1053.13
981.77
945.12
815.89
750.31
599.86
555.50
H
N
O
N
Cl
Cl
O
C26H20Cl2N2O2
Mol. Wt.: 463.36

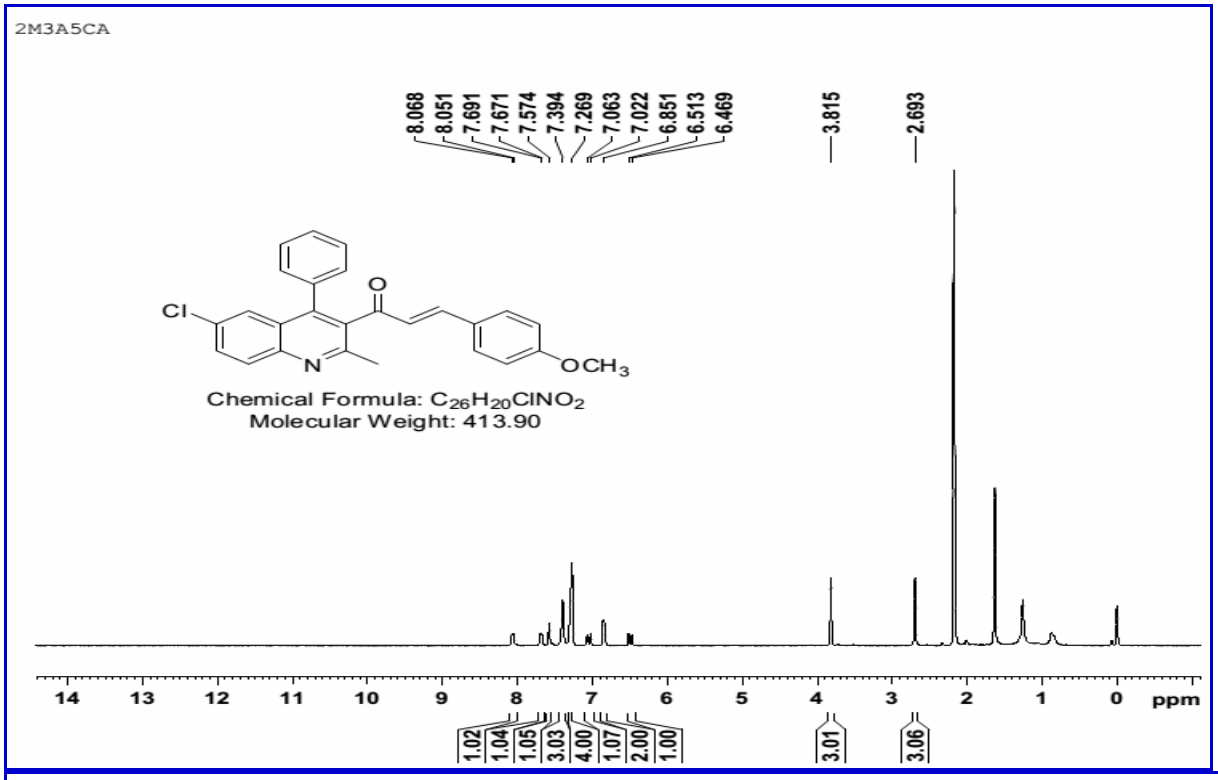

1: Scan ES+
9.81e6
100
%
0
463.27
465.28
466.30
100.17
116.20
165.18
230.16
316.17
336.15
438.41
505.41
586.55
611.54
H
N
O
N
Cl
Cl
O
C26H20Cl2N2O2
Mol. Wt.: 463.36

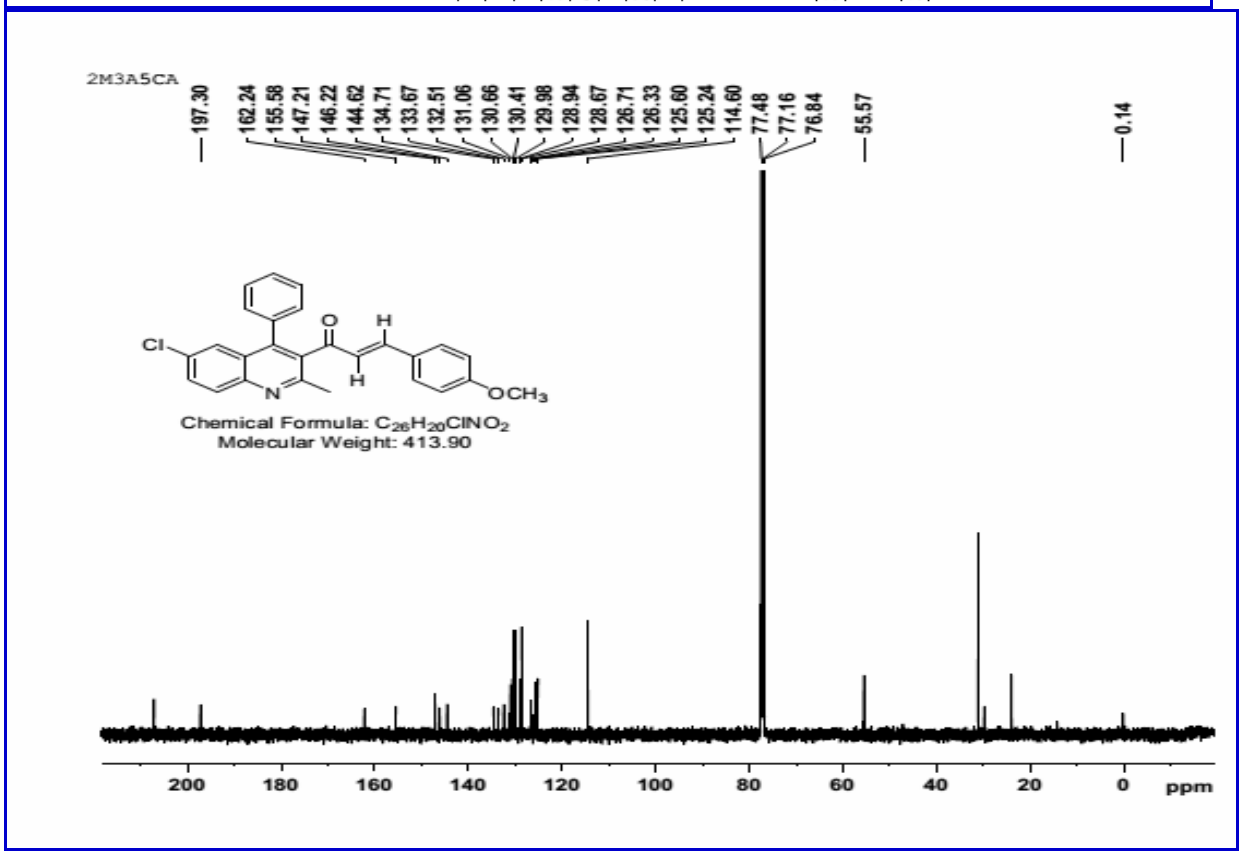

2M3A5CBEN
8.076
8.053
7.700
7.677
7.588
7.427
7.414
7.397
7.384
7.372
7.362
7.352
7.330
7.319
7.304
7.285
7.260
7.117
7.077
6.614
6.573
3.487
2.696
1.633
1.617
0.002
Cl
O
N
C25H18ClNO
Mol. Wt.: 383.87
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.03
1.00
4.35
6.00
1.07
4.03
3.03
1.80

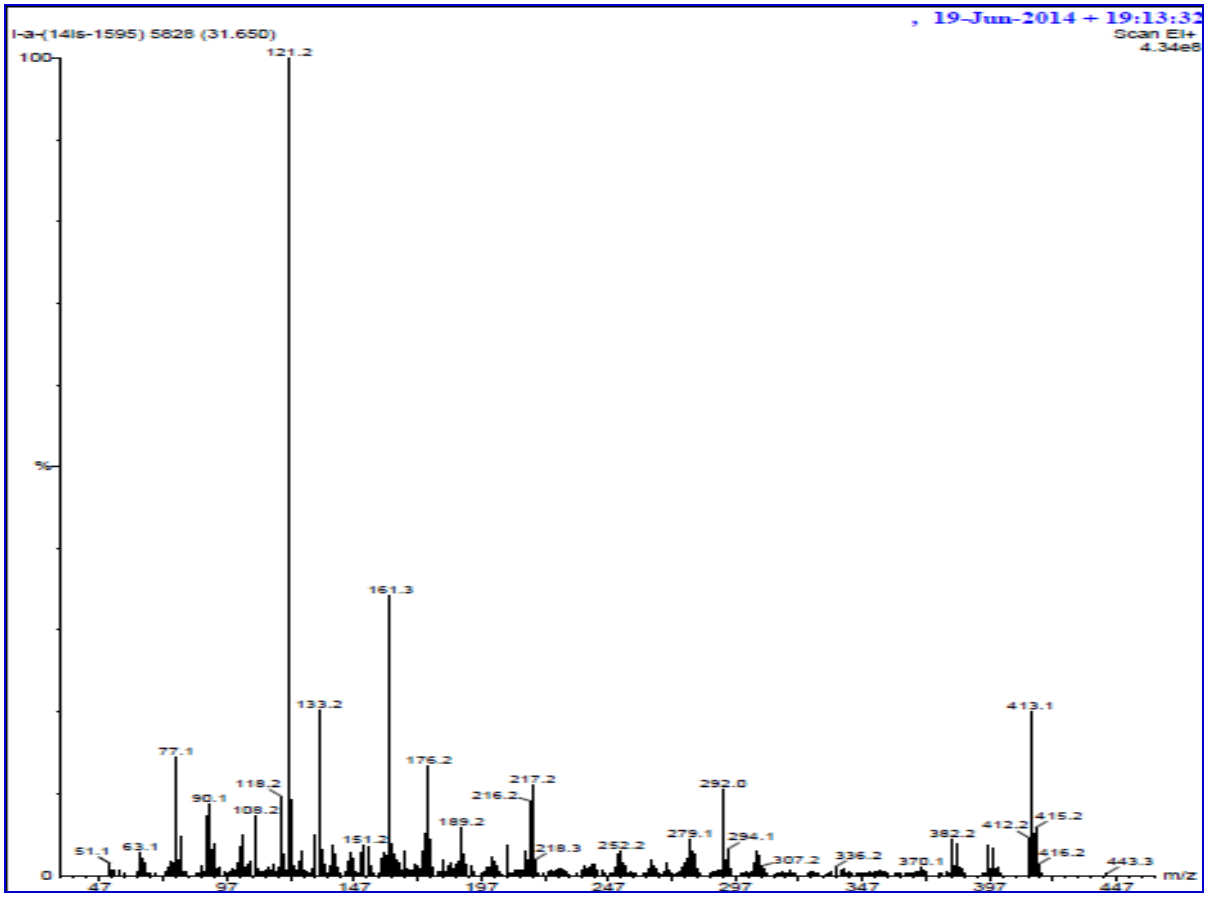

2M3A5CBEN
Cl
O
N
C25H18ClNO
Mol. Wt.: 383.87
200
180
160
140
120
100
80
60
40
20
0
ppm

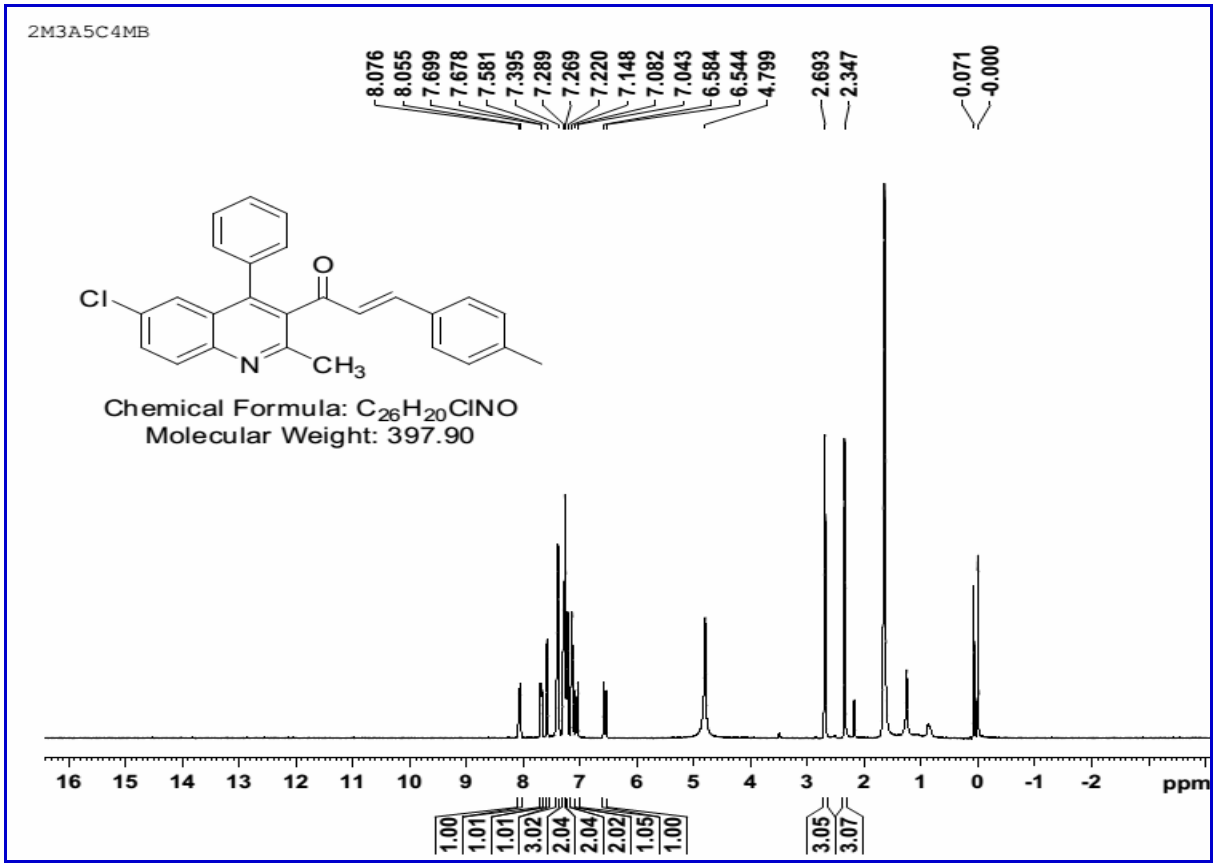

384.5730
1.34e8
387.3332
349.4428
82.0614
91.1002
56.0735
133.2158
59.0867
113.1314
124.1780
150.0984
177.2724
244.5413
288.4619
305.3389
316.5063
338.5897
363.4324
%
m/z
Cl
O
N
Chemical Formula: C25H18ClNO
Molecular Weight: 383.87

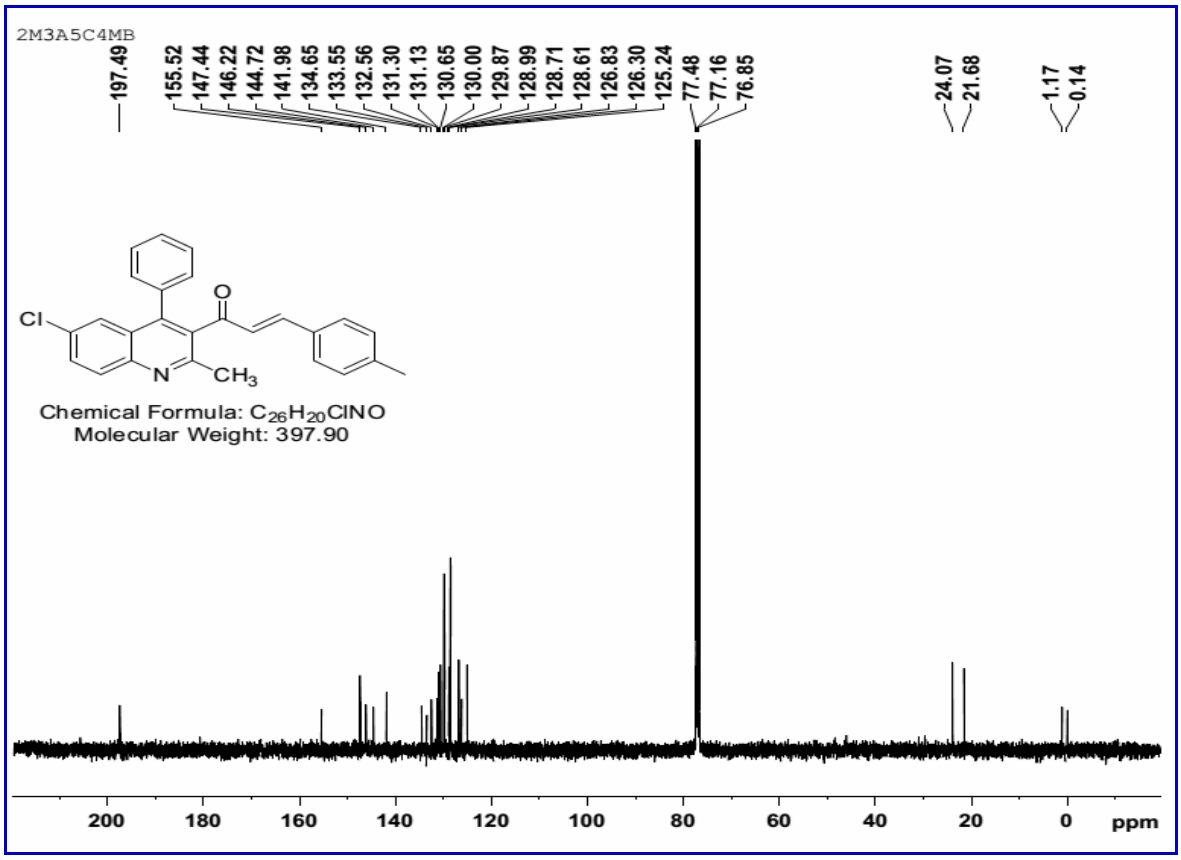

100
%T
75
50
25
0
-25
4000
3000
2000
1500
1000
500
1/cm
1B
1641.42
1598.99
1564.27
1481.33
1436.97
1386.82
1311.59
1224.80
1201.65
1161.15
1082.07
1047.35
972.12
881.47
831.32
765.74
711.73
702.09
684.73
663.51
646.15
588.29
Cl
O
N
Chemical Formula: C25H18ClNO
Molecular Weight: 383.87

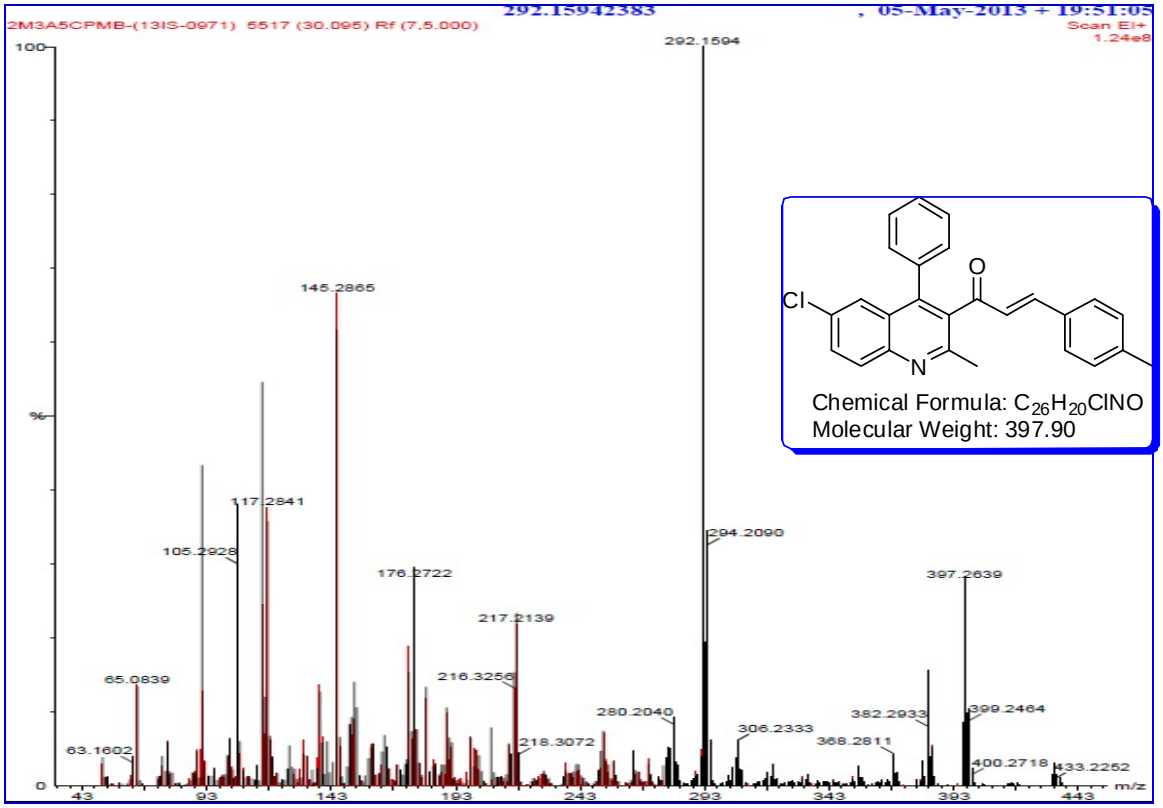

2M3A5CA
8.068
8.051
7.691
7.671
7.574
7.394
7.269
7.063
7.022
6.851
6.513
6.469
3.815
2.693
Cl
O
N
OCH3
Chemical Formula: C26H20ClNO2
Molecular Weight: 413.90
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.02 1.04 1.05 3.03 4.00 1.07 2.00 1.00 3.01 3.06

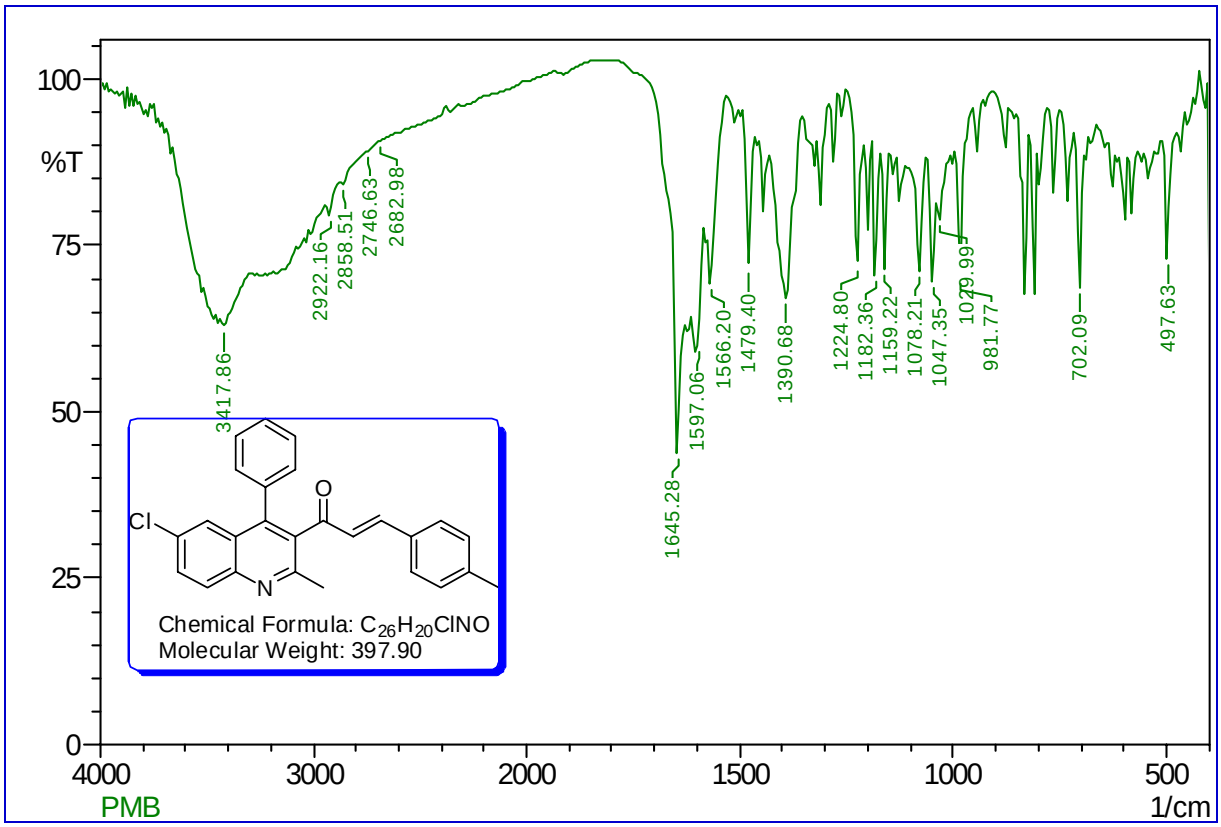

2M3A5CA
197.30
162.24
155.58
147.21
146.22
144.62
134.71
133.67
132.51
131.06
130.66
130.41
129.98
128.94
128.67
126.71
126.33
125.60
125.24
114.60
77.48
77.16
76.84
55.57
0.14
Cl
O
H
H
N
OCH3
Chemical Formula: C26H20ClNO2
Molecular Weight: 413.90
200 180 160 140 120 100 80 60 40 20 0 ppm

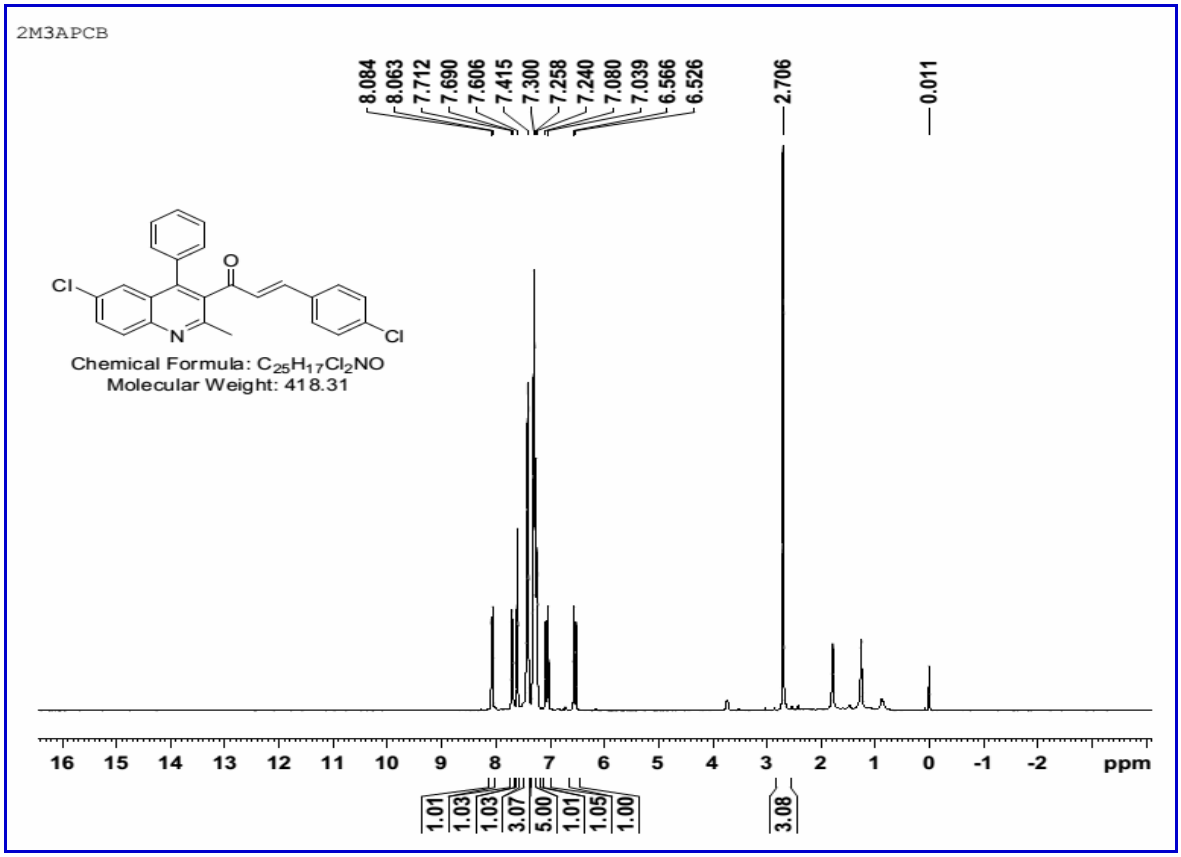

I-a-(14Is-1595) 5828 (31.650)
, 19-Jun-2014 + 19:13:32
Scan EI+
4.34e8
100
%
0
121.2
161.3
133.2
413.1
77.1
176.2
118.2
217.2
292.0
216.2
90.1
109.2
189.2
279.1
294.1
415.2
412.2
382.2
51.1
63.1
151.2
218.3
252.2
307.2
336.2
370.1
416.2
443.3
47
97
147
197
247
297
347
397
447
m/z

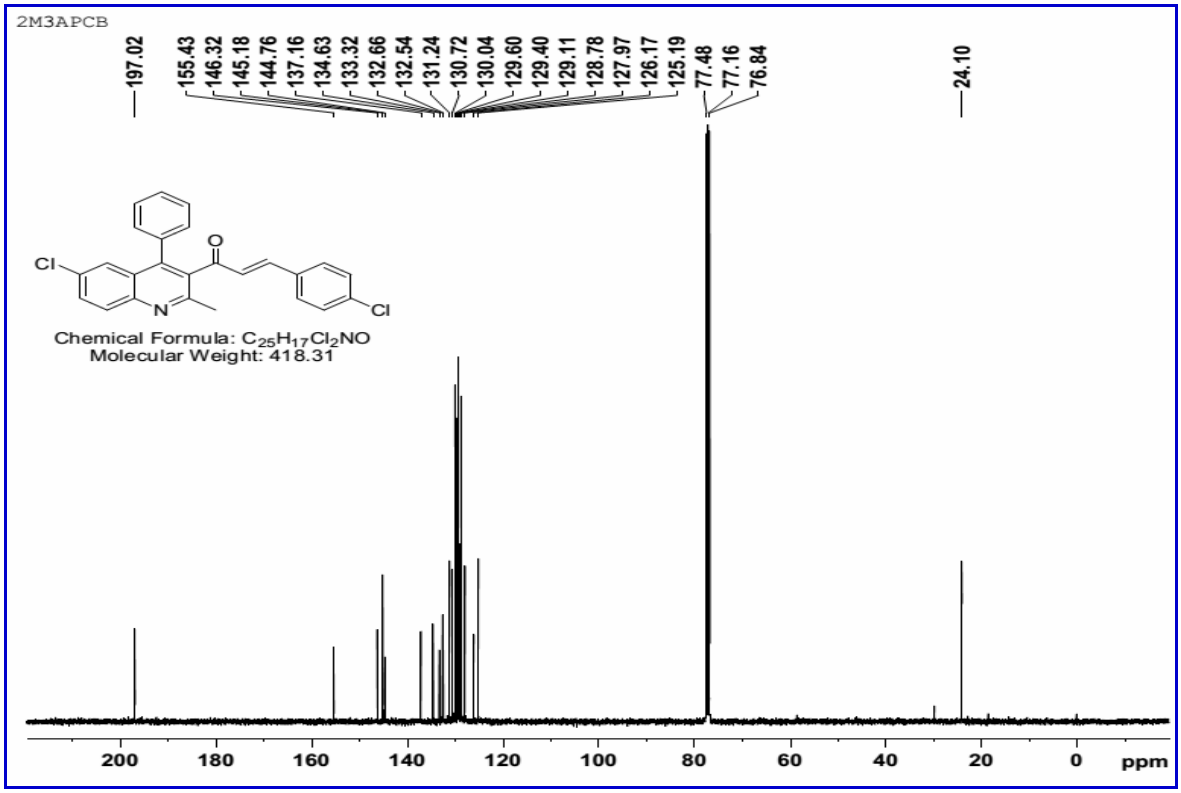

2M3A5C4MB
8.076
8.055
7.699
7.678
7.581
7.395
7.289
7.269
7.220
7.148
7.082
7.043
6.584
6.544
4.799
2.693
2.347
0.071
-0.000
Cl
O
N
CH3
Chemical Formula: C26H20ClNO
Molecular Weight: 397.90
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
1.00 1.01 1.01 3.02 2.04 2.04 2.02 1.05 1.00
3.05 3.07

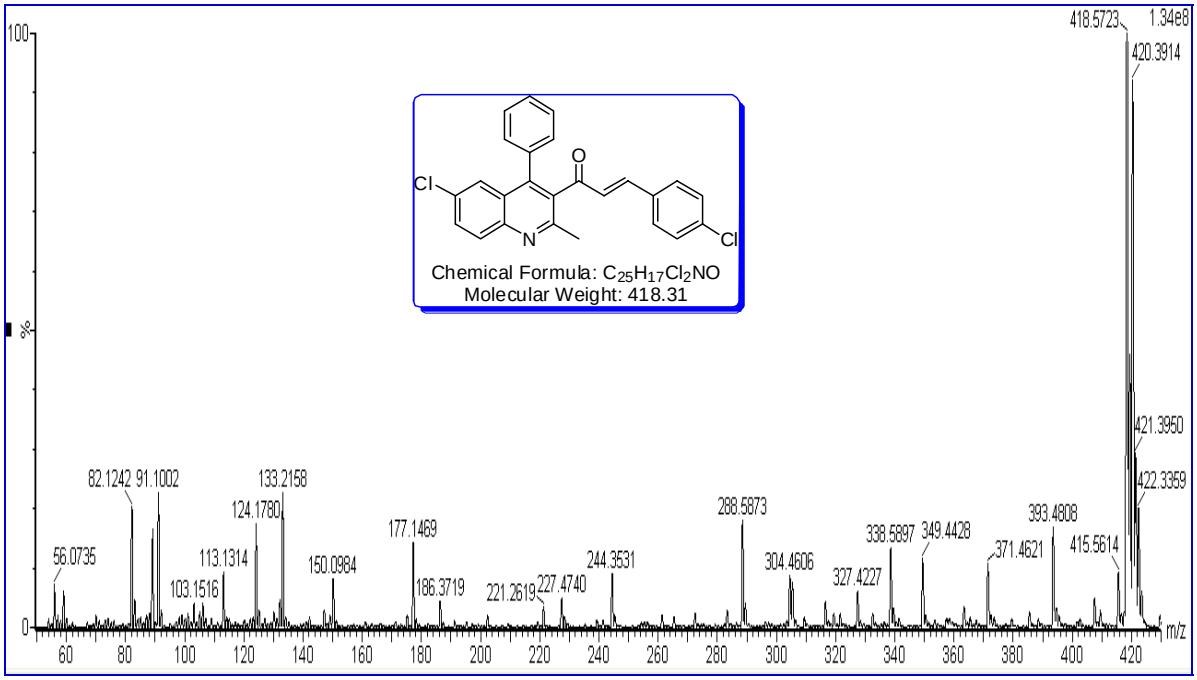

2M3A5C4MB
197.49
155.52
147.44
146.22
144.72
141.98
134.65
133.55
132.56
131.30
131.13
130.65
130.00
129.87
128.99
128.71
128.61
126.83
126.30
125.24
77.48
77.16
76.85
24.07
21.68
1.17
0.14
Cl
O
N
CH3
Chemical Formula: C26H20ClNO
Molecular Weight: 397.90
200 180 160 140 120 100 80 60 40 20 0 ppm

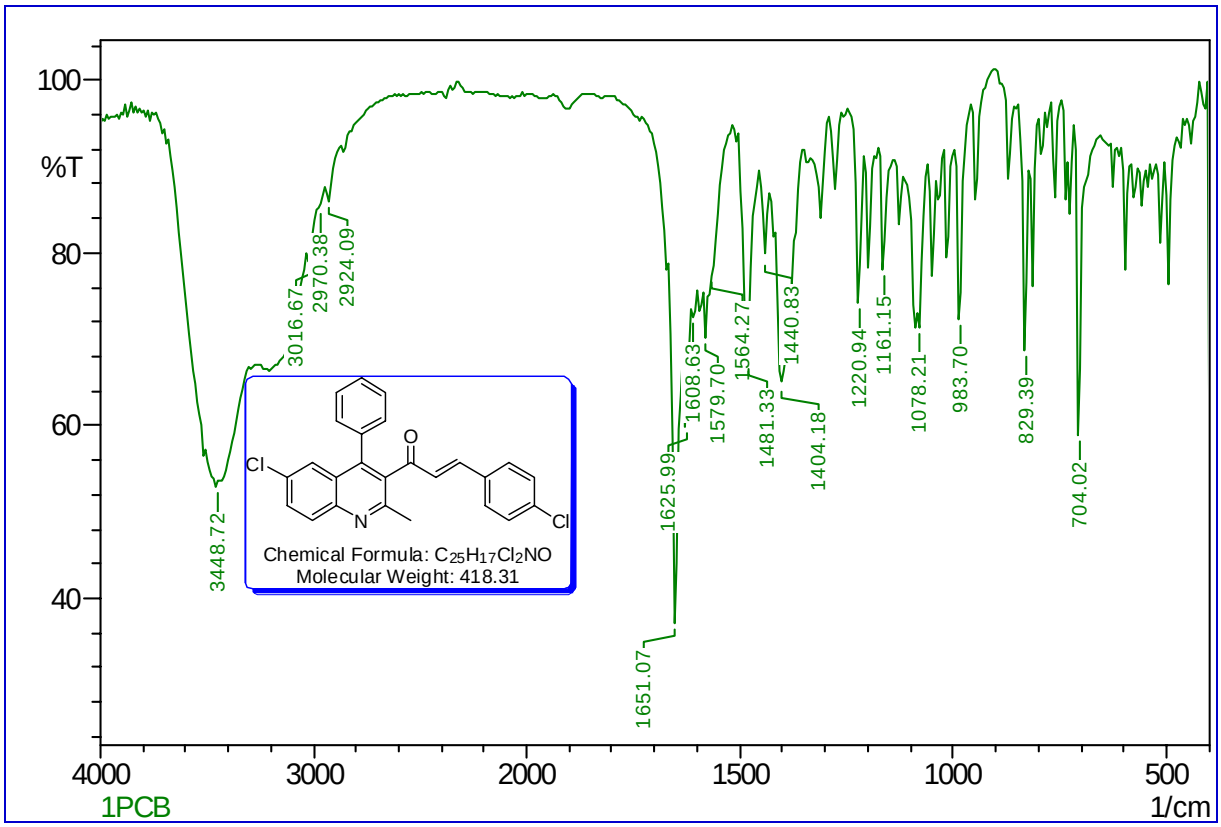

292.15942383
, 05-May-2013 + 19:51:05
2M3A5CPMB-(13IS-0971) 5517 (30.095) Rf (7.5.000)
Scan EI+
1.24e8
292.1594
145.2865
117.2841
105.2928
294.2090
176.2722
397.2639
217.2139
65.0839
216.3256
280.2040
382.2933
399.2464
306.2333
368.2811
63.1602
218.3072
400.2718
433.2252
Cl
O
N
Chemical Formula: C26H20ClNO
Molecular Weight: 397.90
m/z

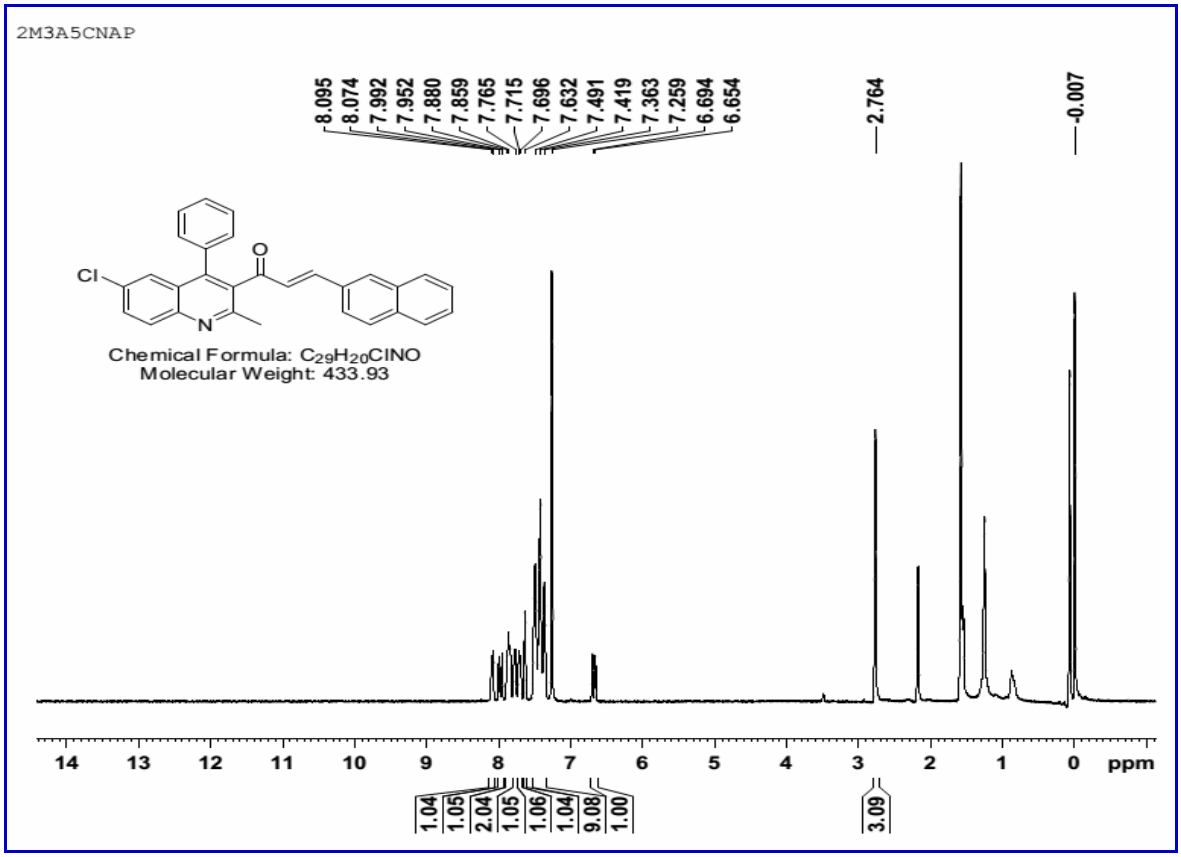

%T
3417.86
2922.16
2858.51
2746.63
2682.98
1645.28
1597.06
1566.20
1479.40
1390.68
1224.80
1182.36
1159.22
1078.21
1047.35
981.77
702.09
497.63
Cl
O
N
Chemical Formula: C26H20ClNO
Molecular Weight: 397.90
PMB
1/cm

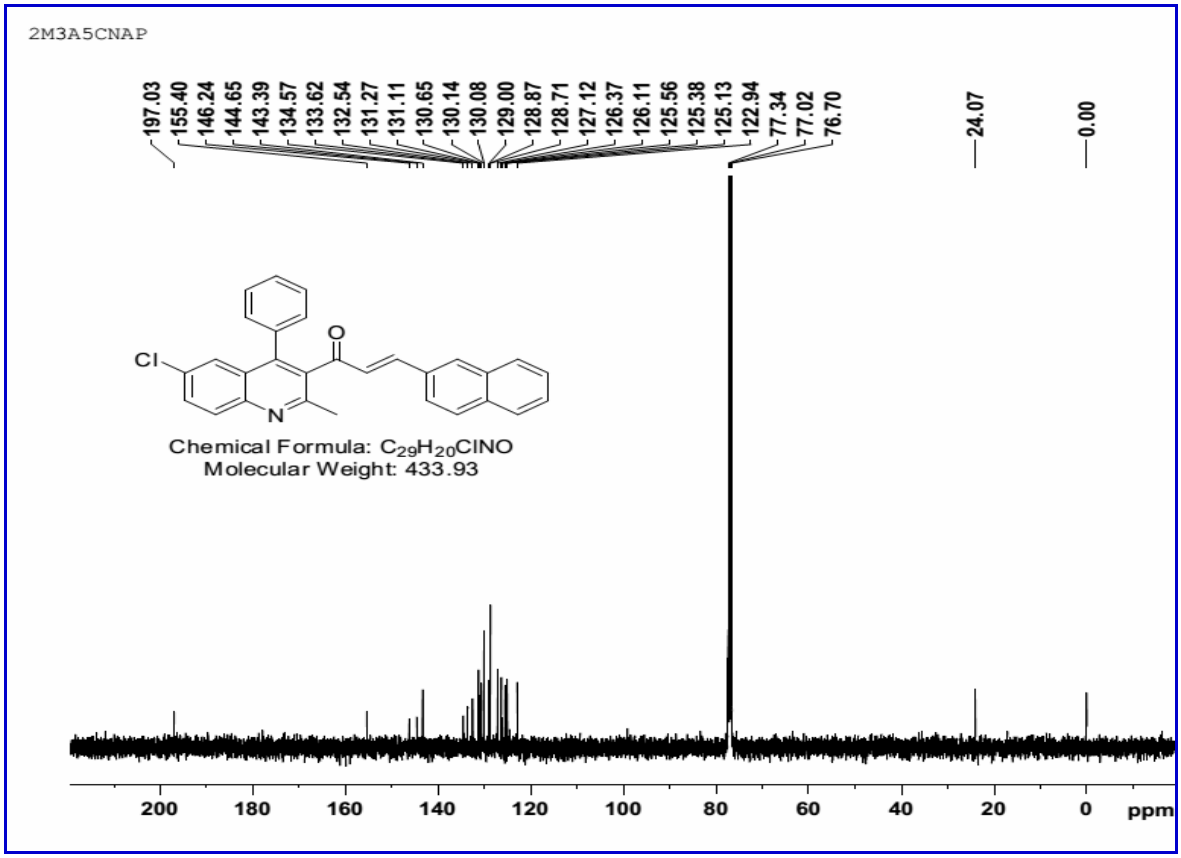

2M3APCB
8.084
8.063
7.712
7.690
7.606
7.415
7.300
7.258
7.240
7.080
7.039
6.566
6.526
2.706
0.011
Cl
O
N
Cl
Chemical Formula: C25H17Cl2NO
Molecular Weight: 418.31
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
1.01
1.03
1.03
3.07
5.00
1.01
1.05
1.00
3.08

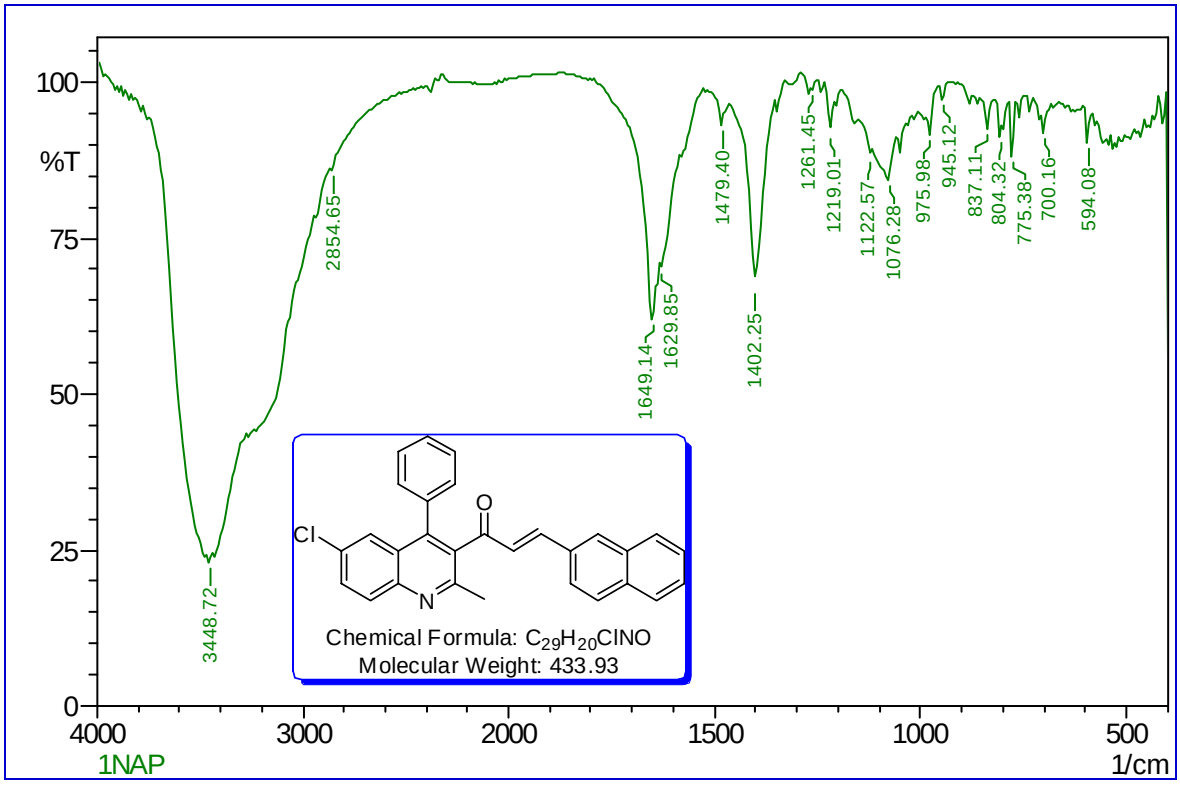

2M3APCB
197.02
155.43
146.32
145.18
144.76
137.16
134.63
133.32
132.66
132.54
131.24
130.72
130.04
129.60
129.40
129.11
128.78
127.97
126.17
125.19
77.48
77.16
76.84
24.10
Cl
O
N
Cl
Chemical Formula: C25H17Cl2NO
Molecular Weight: 418.31
200 180 160 140 120 100 80 60 40 20 0 ppm

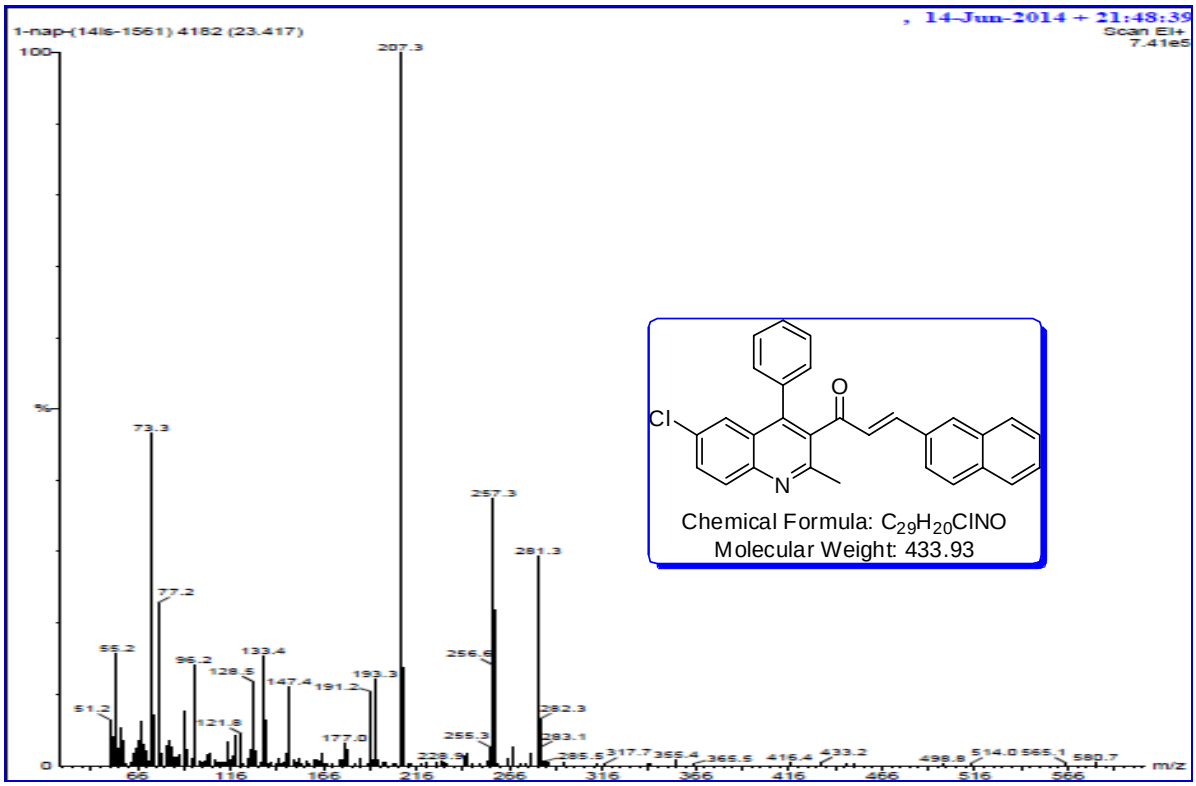

100
%
0
418.5723
1.34e8
420.3914
421.3950
422.3369
82.1242
91.1002
133.2158
124.1780
177.1469
288.5873
56.0735
113.1314
103.1516
150.0984
186.3719
221.2619
227.4740
244.3531
304.4606
327.4227
338.5897
349.4428
371.4621
393.4808
415.5614
Cl
O
N
Cl
Chemical Formula: C25H17Cl2NO
Molecular Weight: 418.31
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
400
420
m/z


100
%T
80
60
40
3448.72
3016.67
2970.38
2924.09
1651.07
1625.99
1608.63
1579.70
1564.27
1481.33
1440.83
1404.18
1220.94
1161.15
1078.21
983.70
829.39
704.02
Cl
O
N
Cl
Chemical Formula: C25H17Cl2NO
Molecular Weight: 418.31
4000
3000
2000
1500
1000
500
1/cm
1PCB

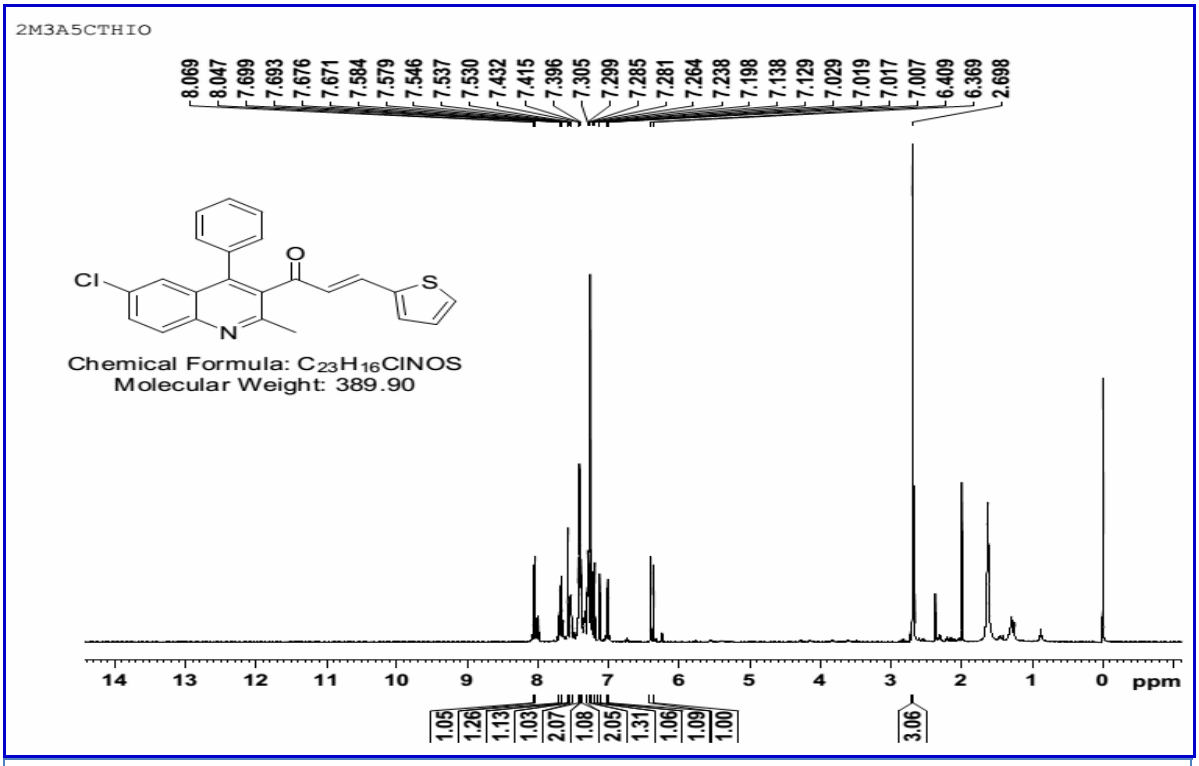

2M3A5CNAP
8.095
8.074
7.992
7.952
7.880
7.859
7.765
7.715
7.696
7.632
7.491
7.419
7.363
7.259
6.694
6.654
2.764
-0.007
Cl
O
N
Chemical Formula: C29H20ClNO
Molecular Weight: 433.93
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.04 1.05 2.04 1.05 1.06 1.04 9.08 1.00
3.09


2M3A5CNAP
197.03
155.40
146.24
144.65
143.39
134.57
133.62
132.54
131.27
131.11
130.65
130.14
130.08
129.00
128.87
128.71
127.12
126.37
126.11
125.56
125.38
125.13
122.94
77.34
77.02
76.70
24.07
0.00
Cl
O
N
Chemical Formula: C29H20ClNO
Molecular Weight: 433.93
200 180 160 140 120 100 80 60 40 20 0 ppm

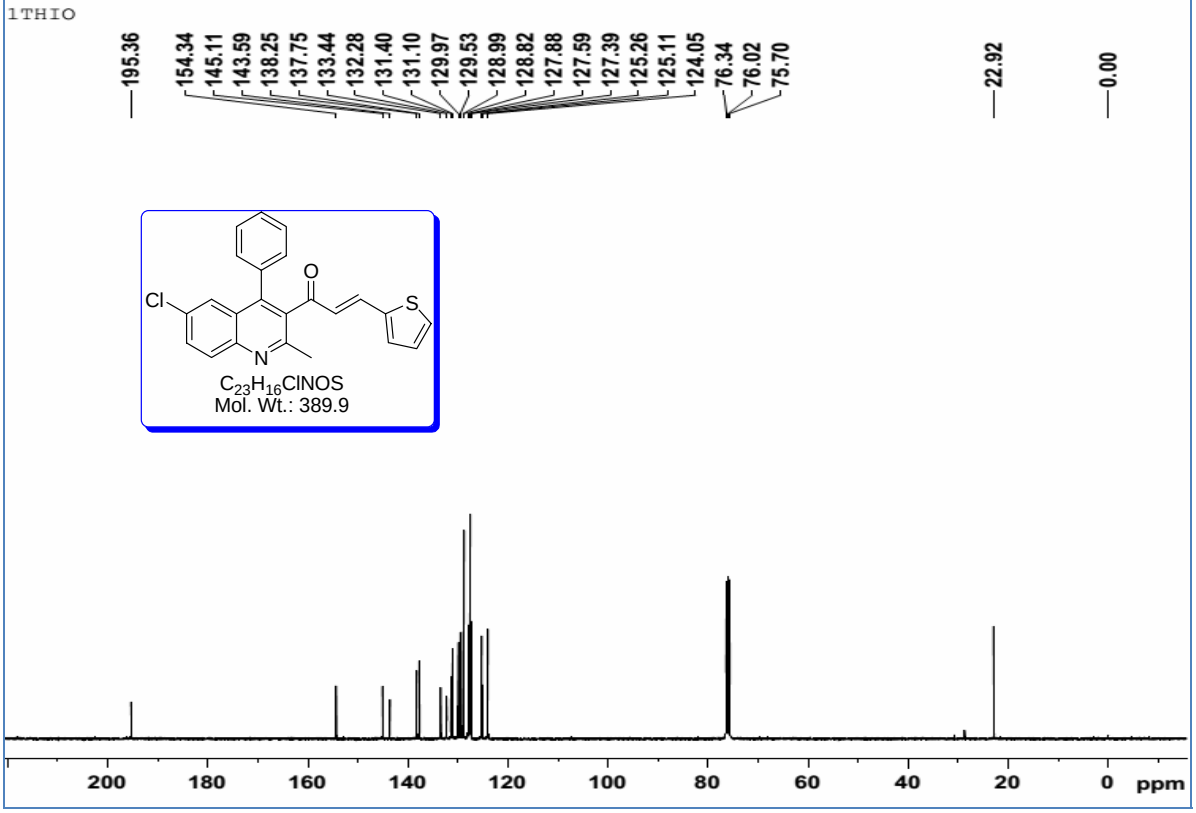

100
%T
75
50
25
0
4000
3000
2000
1500
1000
500
1/cm
1NAP
3448.72
2854.65
1649.14
1629.85
1479.40
1402.25
1261.45
1219.01
1122.57
1076.28
975.98
945.12
837.11
804.32
775.38
700.16
594.08
Cl
O
N
Chemical Formula: C29H20ClNO
Molecular Weight: 433.93

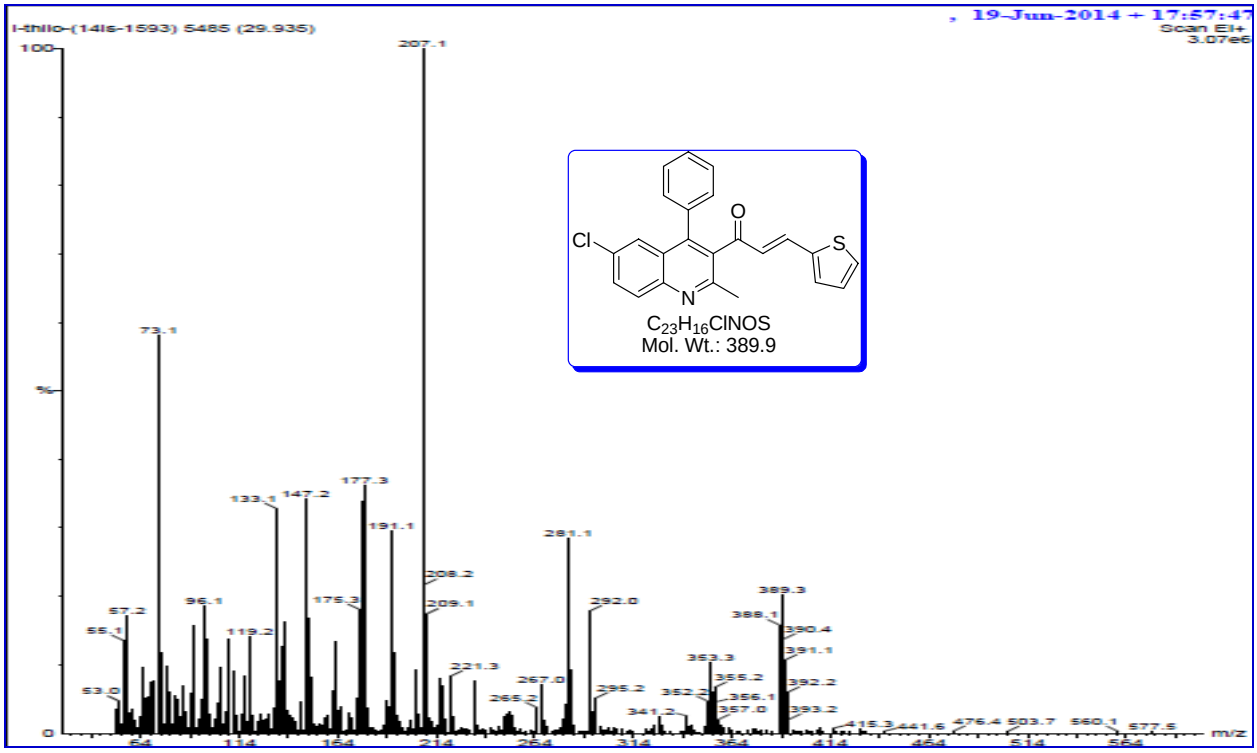

1-nap-(14lis-1561) 4182 (23.417)
14-Jun-2014 + 21:48:39
Scan EI+
7.41e5
100
%
0
207.3
73.3
257.3
281.3
77.2
55.2
96.2
133.4
128.5
147.4
191.2
193.3
51.2
121.8
177.0
256.6
282.3
255.3
283.1
m/z
Cl
O
N
Chemical Formula: C29H20ClNO
Molecular Weight: 433.93

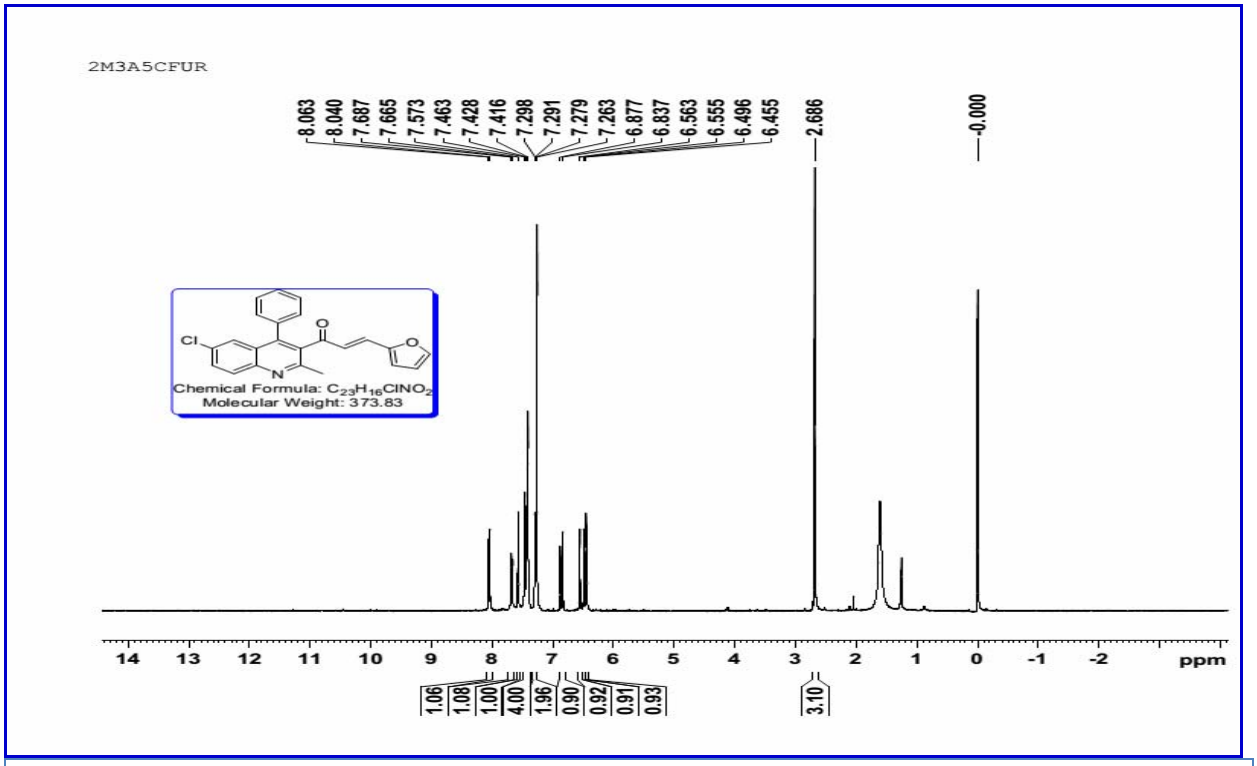
2M3A5CTHIO

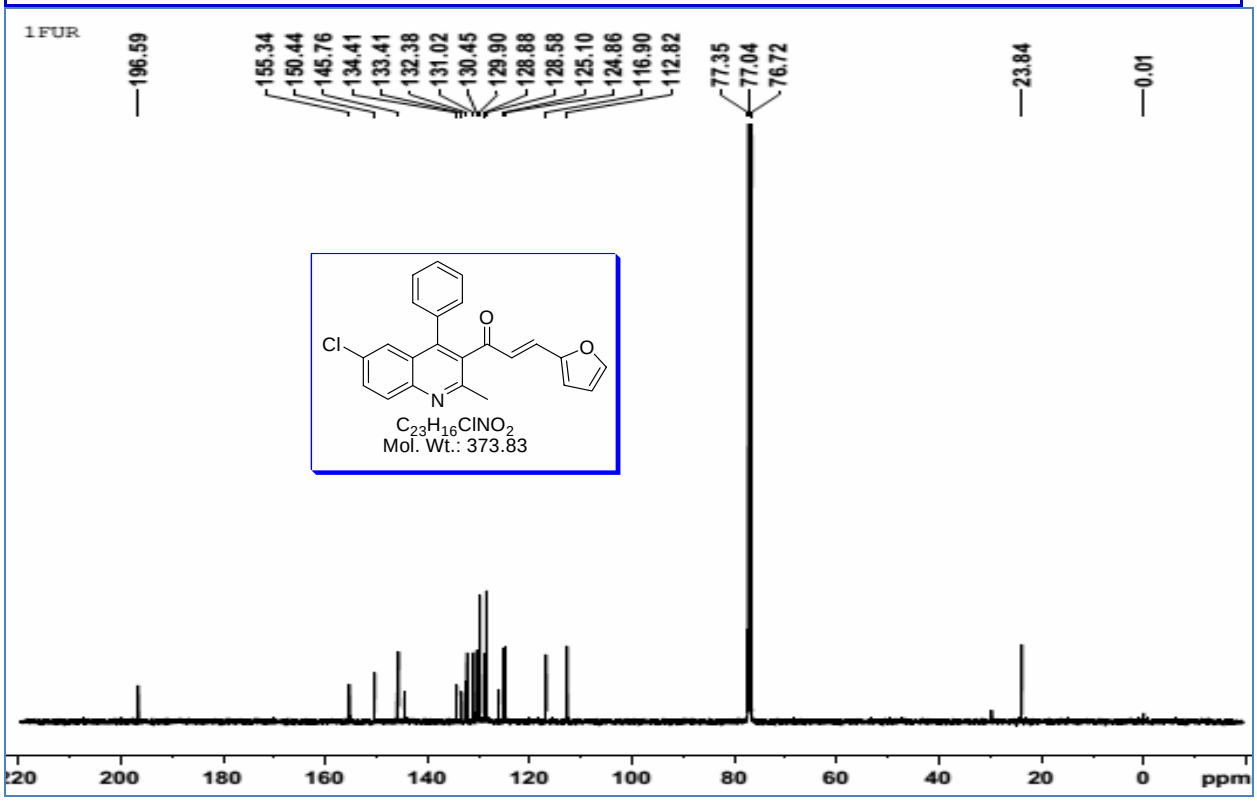


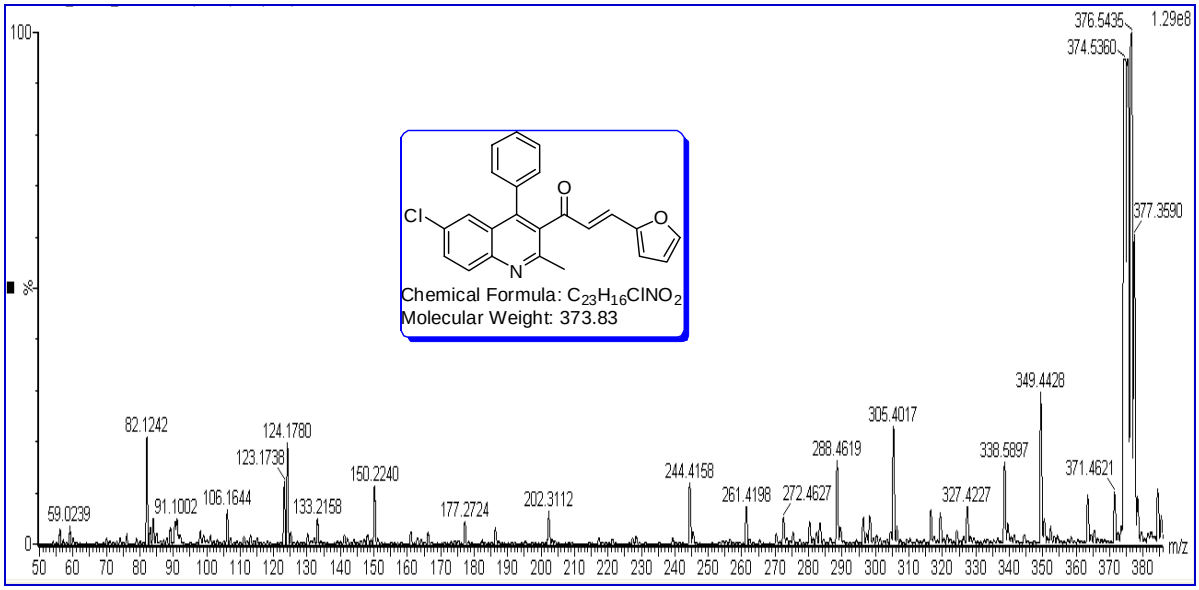
1THIO

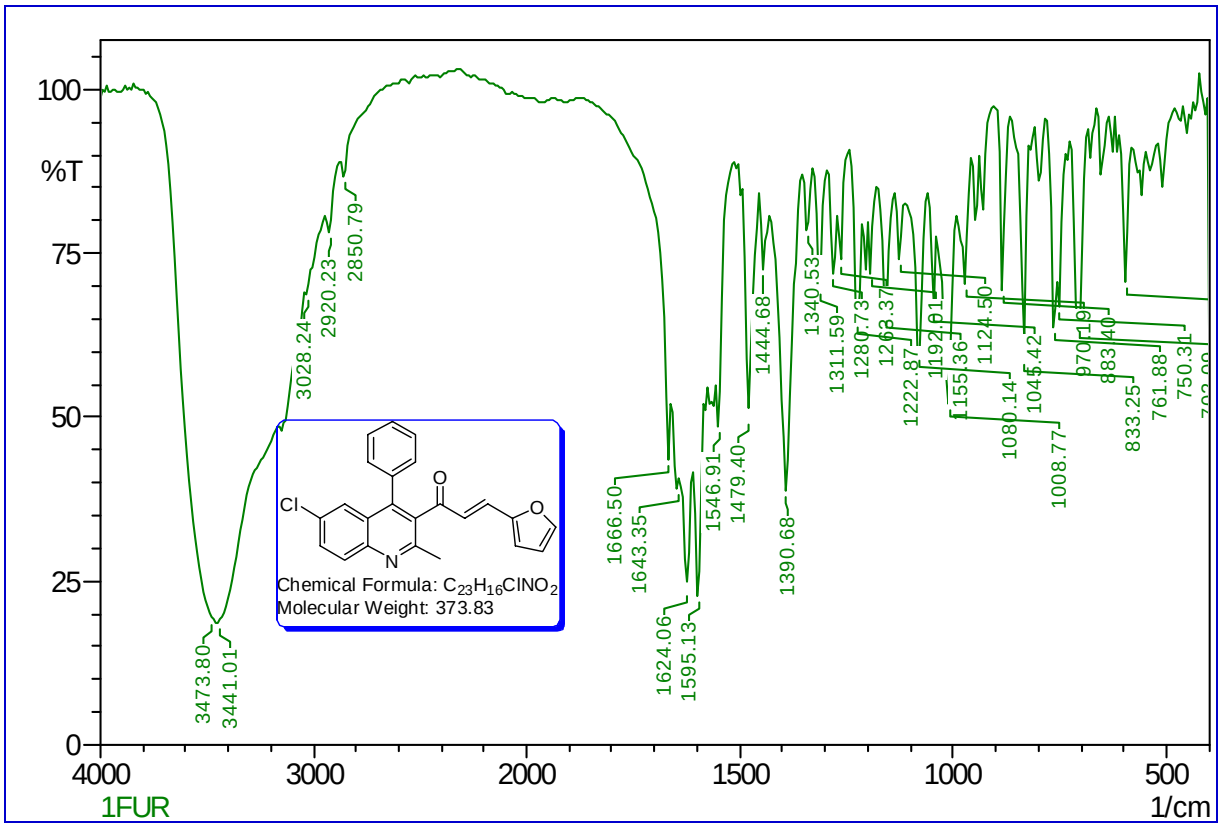


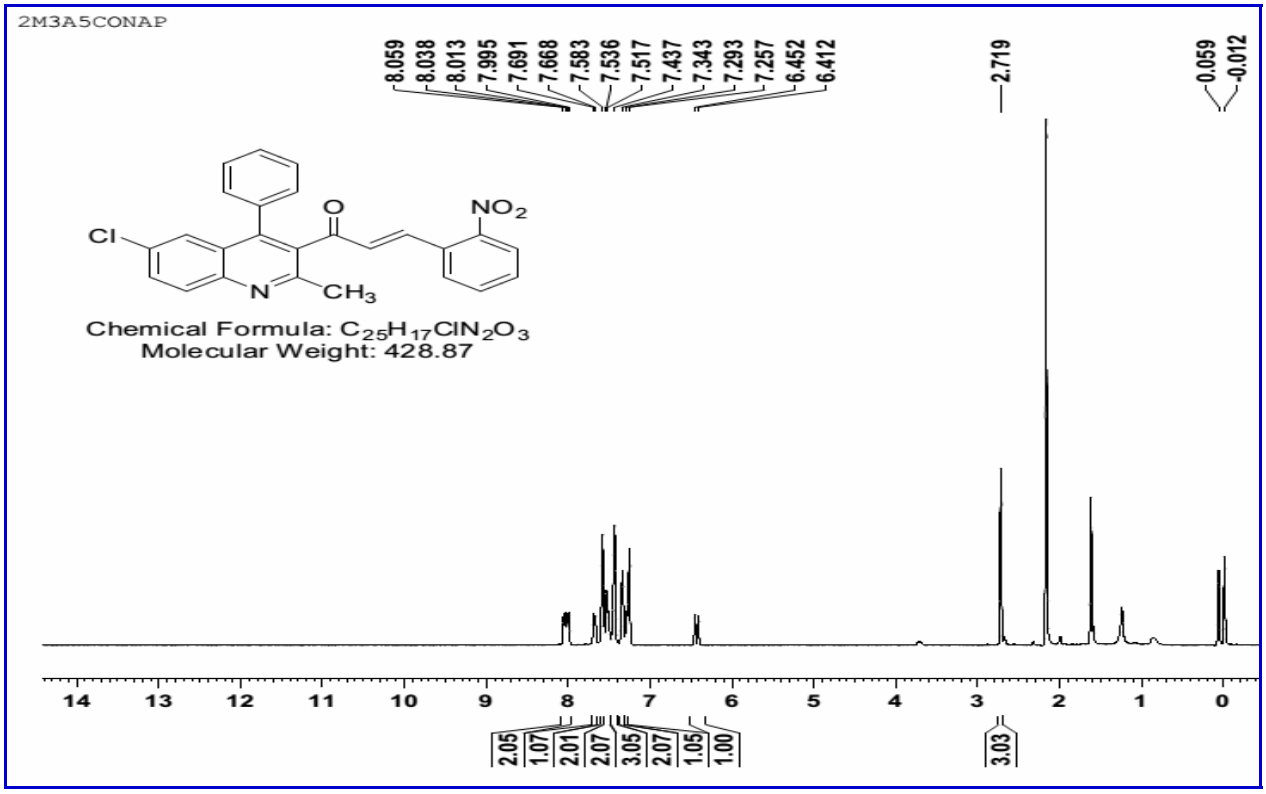

I-thllo-(14ls-1593) 5485 (29.935)
, 19-Jun-2014 + 17:57:47
Scan EI+
3.07e6
100
%
0
m/z
Cl
O
S
N
C23H16ClNOS
Mol. Wt.: 389.9

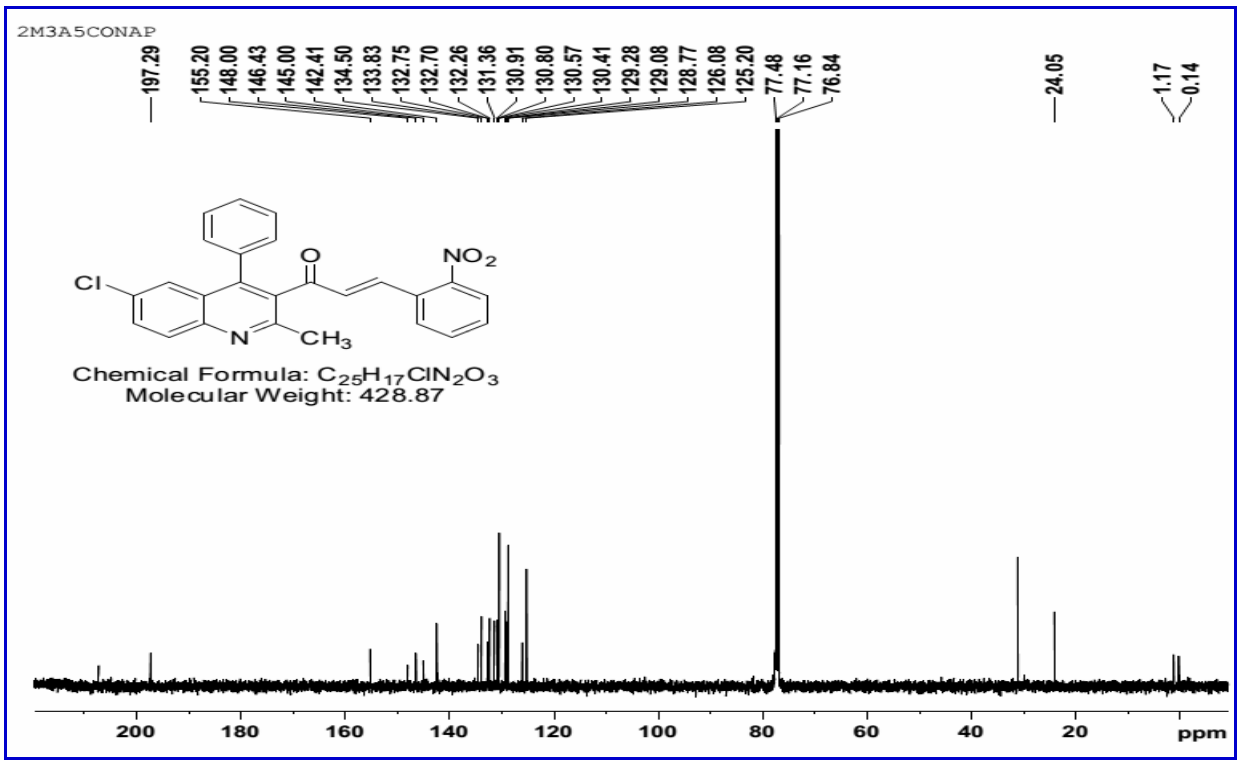

2M3A5CFUR
8.063
8.040
7.687
7.665
7.573
7.463
7.428
7.416
7.298
7.291
7.279
7.263
6.877
6.837
6.563
6.555
6.496
6.455
2.686
-0.000
Cl
O
N
O
Chemical Formula: C23H16ClNO2
Molecular Weight: 373.83
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
1.06
1.08
1.00
4.00
1.96
0.90
0.92
0.91
0.93
3.10

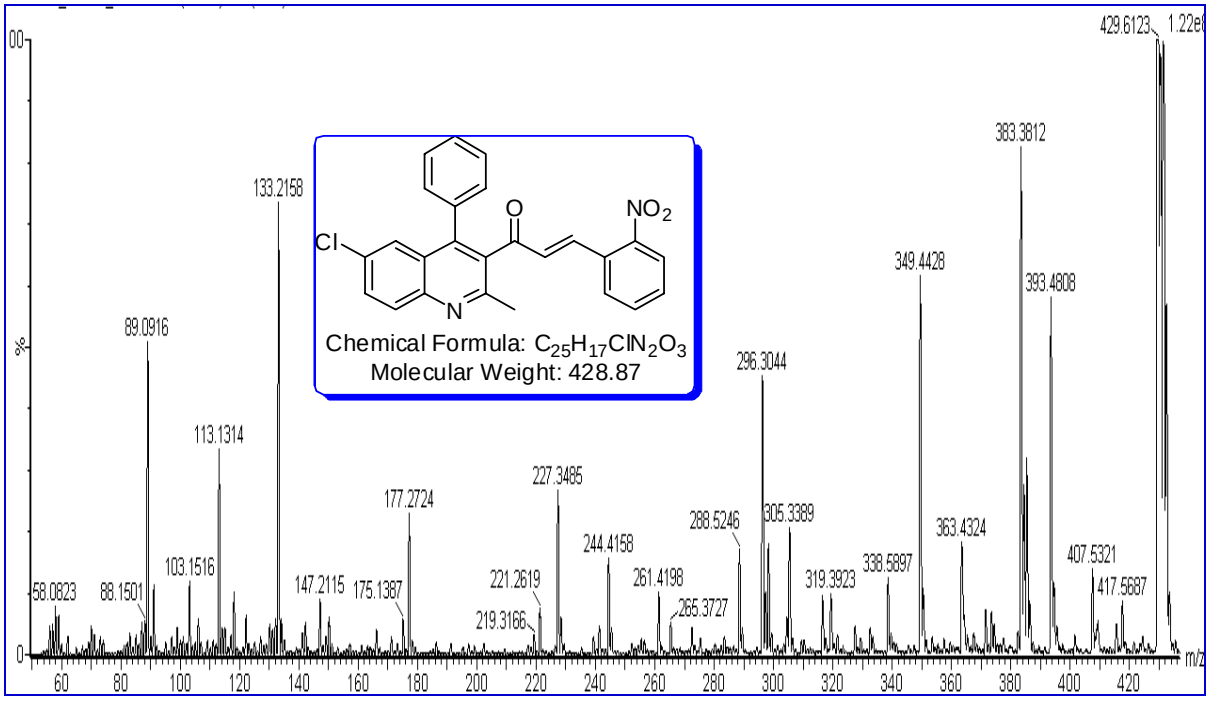

1FUR
196.59
155.34
150.44
145.76
134.41
133.41
132.38
131.02
130.45
129.90
128.88
128.58
125.10
124.86
116.90
112.82
77.35
77.04
76.72
23.84
0.01
Cl
O
N
O
C23H16ClNO2
Mol. Wt.: 373.83
220 200 180 160 140 120 100 80 60 40 20 0 ppm

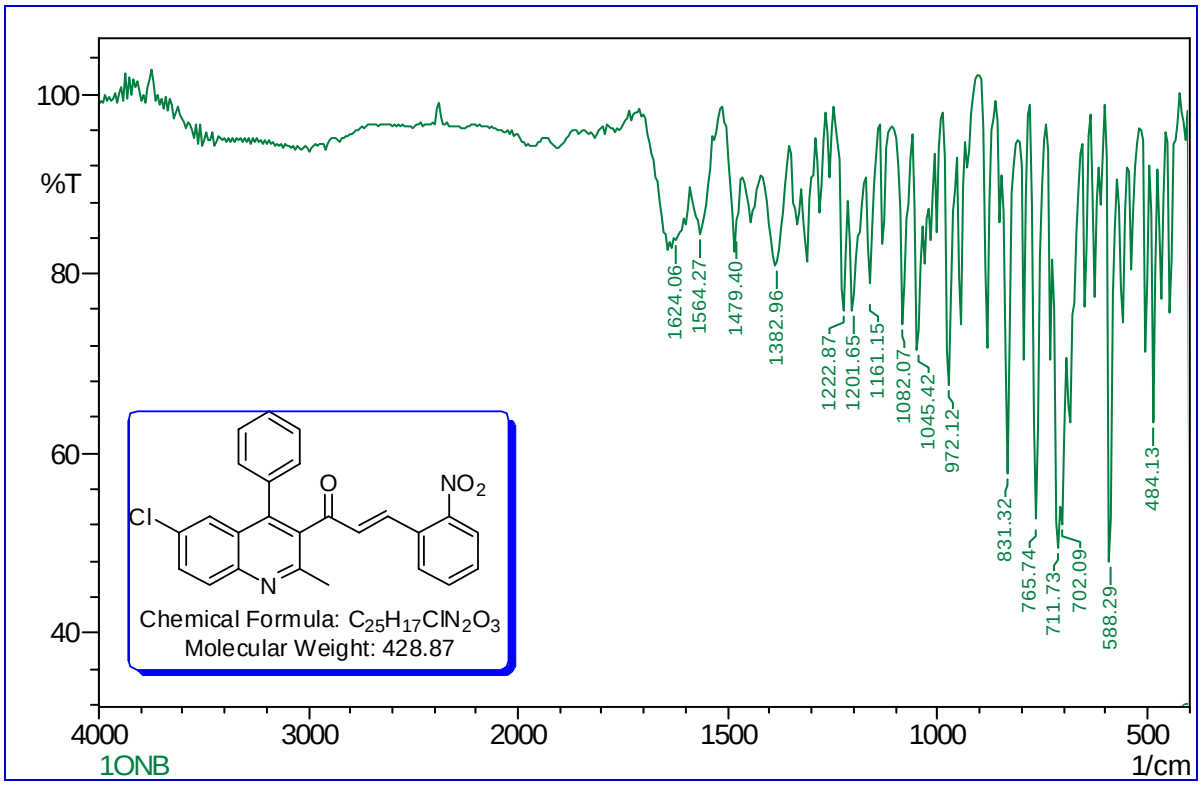

100
%
0
376.5435
1.29e8
374.5360
377.3590
349.4428
305.4017
288.4619
338.5897
371.4621
327.4227
244.4158
261.4198
272.4627
82.1242
124.1780
123.1738
150.2240
91.1002
106.1644
133.2158
177.2724
202.3112
59.0239
Cl
O
N
Chemical Formula: C23H16ClNO2
Molecular Weight: 373.83
50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 260 270 280 290 300 310 320 330 340 350 360 370 380
m/z

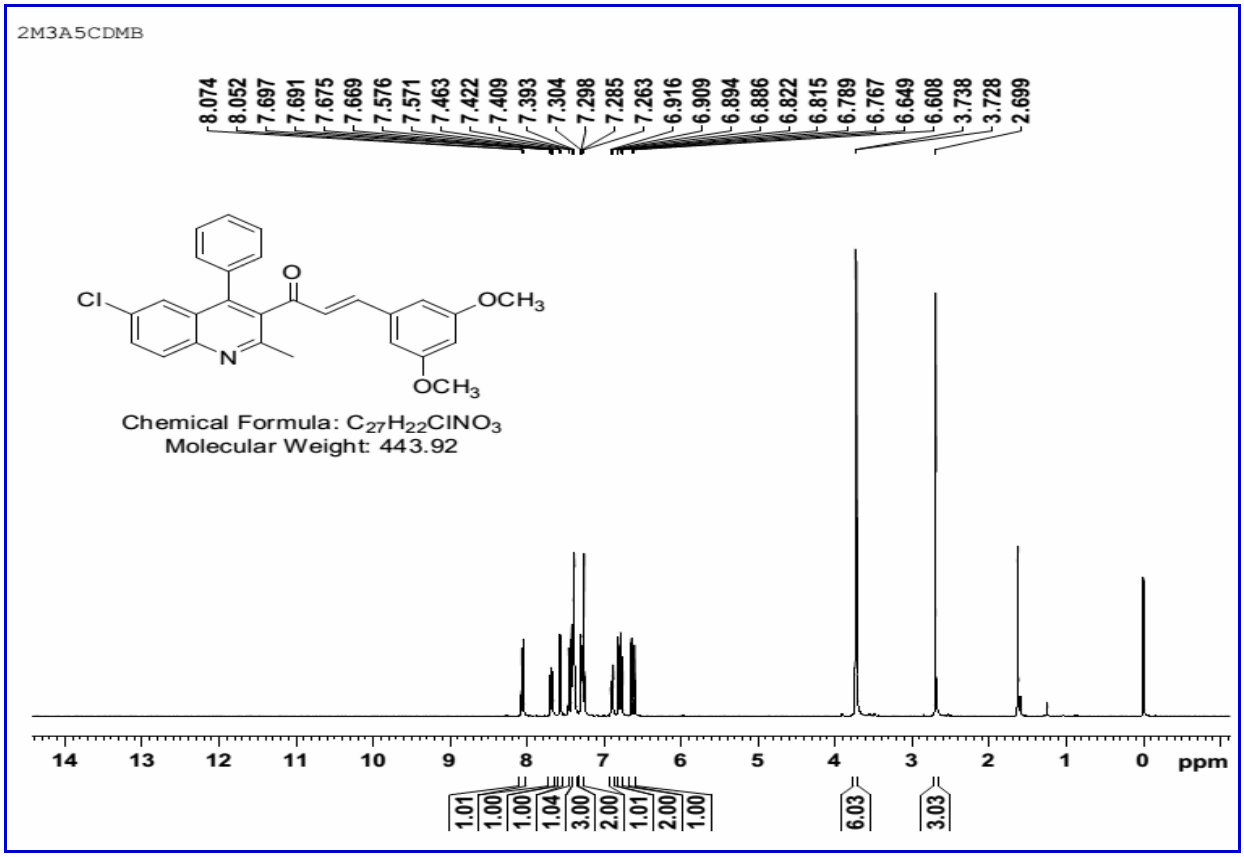

100
%T
75
50
25
0
3473.80
3441.01
3028.24
2920.23
2850.79
1666.50
1643.35
1624.06
1595.13
1546.91
1479.40
1444.68
1390.68
1340.53
1311.59
1280.73
1268.37
1222.87
1192.91
1155.36
1124.50
1080.14
1045.42
1008.77
970.19
883.40
833.25
761.88
750.31
Cl
O
N
Chemical Formula: C23H16ClNO2
Molecular Weight: 373.83
4000
3000
2000
1500
1000
500
1/cm
1FUR

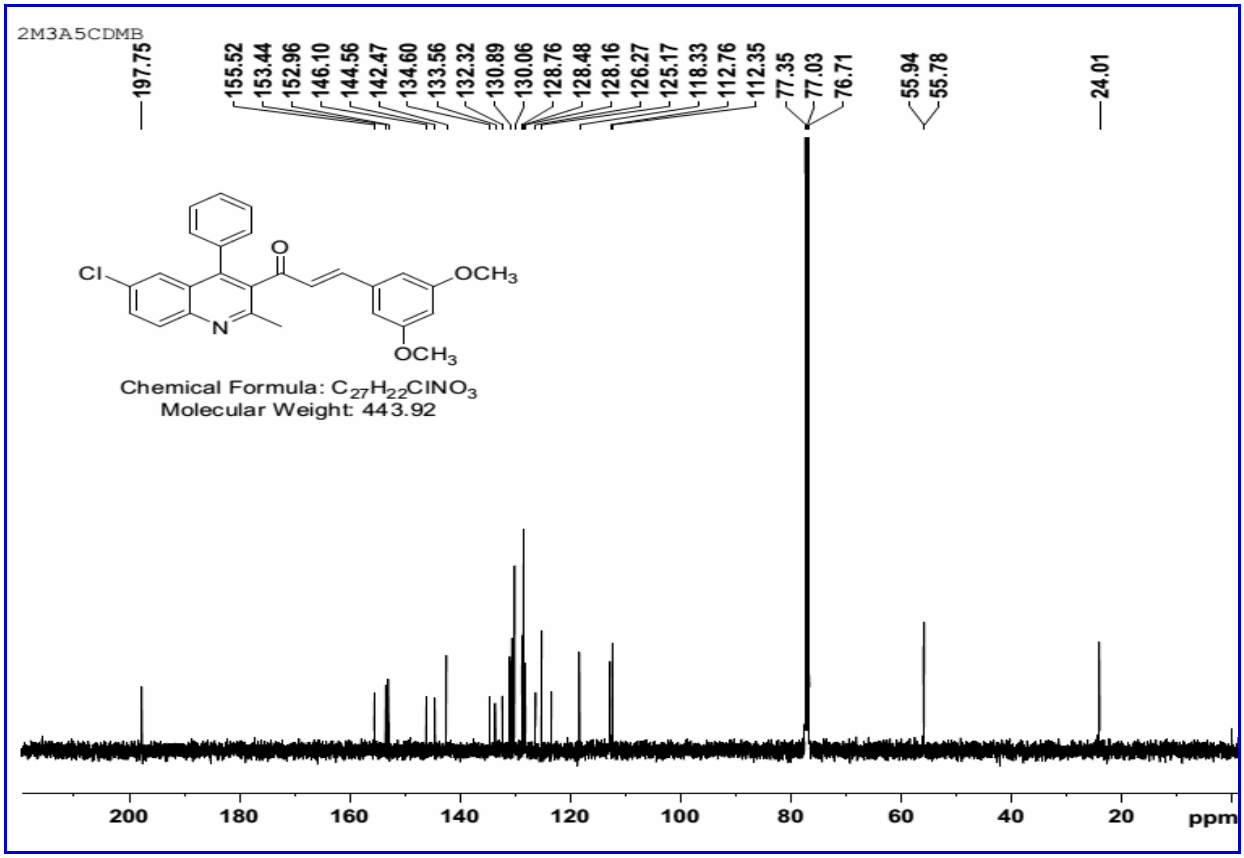

2M3A5CONAP
8.059
8.038
8.013
7.995
7.691
7.668
7.583
7.536
7.517
7.437
7.343
7.293
7.257
6.452
6.412
2.719
0.059
-0.012
Cl
O
NO2
N
CH3
Chemical Formula: C25H17ClN2O3
Molecular Weight: 428.87
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
2.05
1.07
2.01
2.07
3.05
2.07
1.05
1.00
3.03

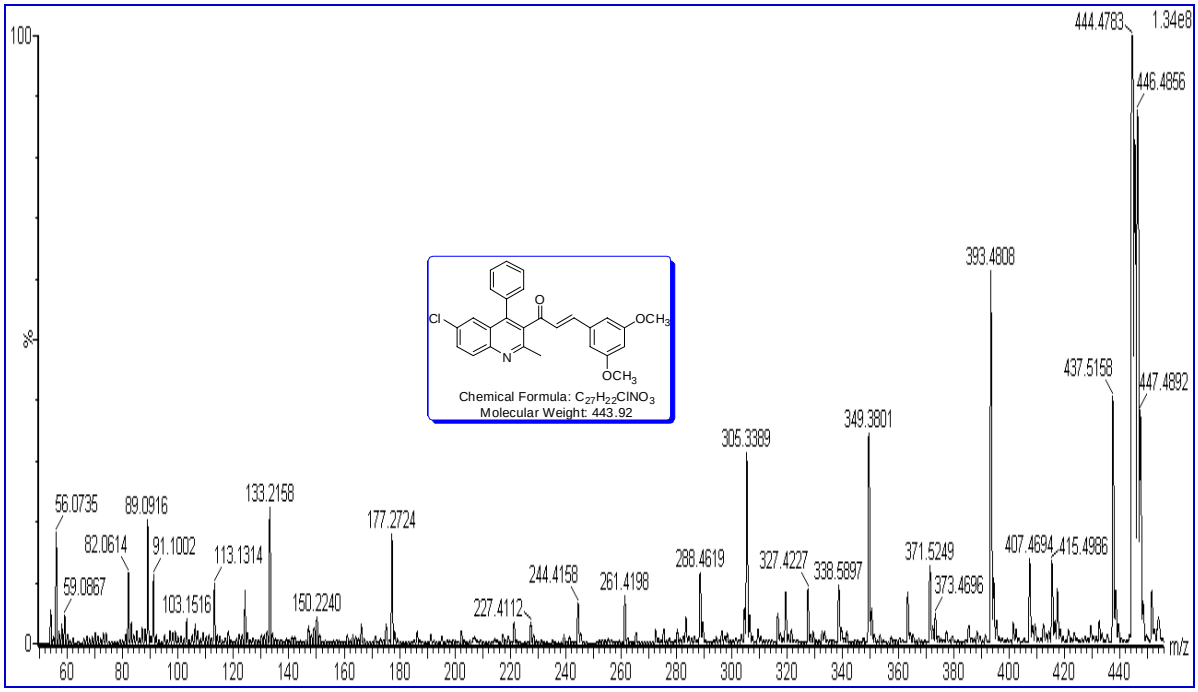

2M3A5CONAP
197.29
155.20
148.00
146.43
145.00
142.41
134.50
133.83
132.75
132.70
132.26
131.36
130.91
130.80
130.57
130.41
129.28
129.08
128.77
126.08
125.20
77.48
77.16
76.84
24.05
1.17
0.14
Cl
O
NO2
N
CH3
Chemical Formula: C25H17ClN2O3
Molecular Weight: 428.87
200
180
160
140
120
100
80
60
40
20
ppm

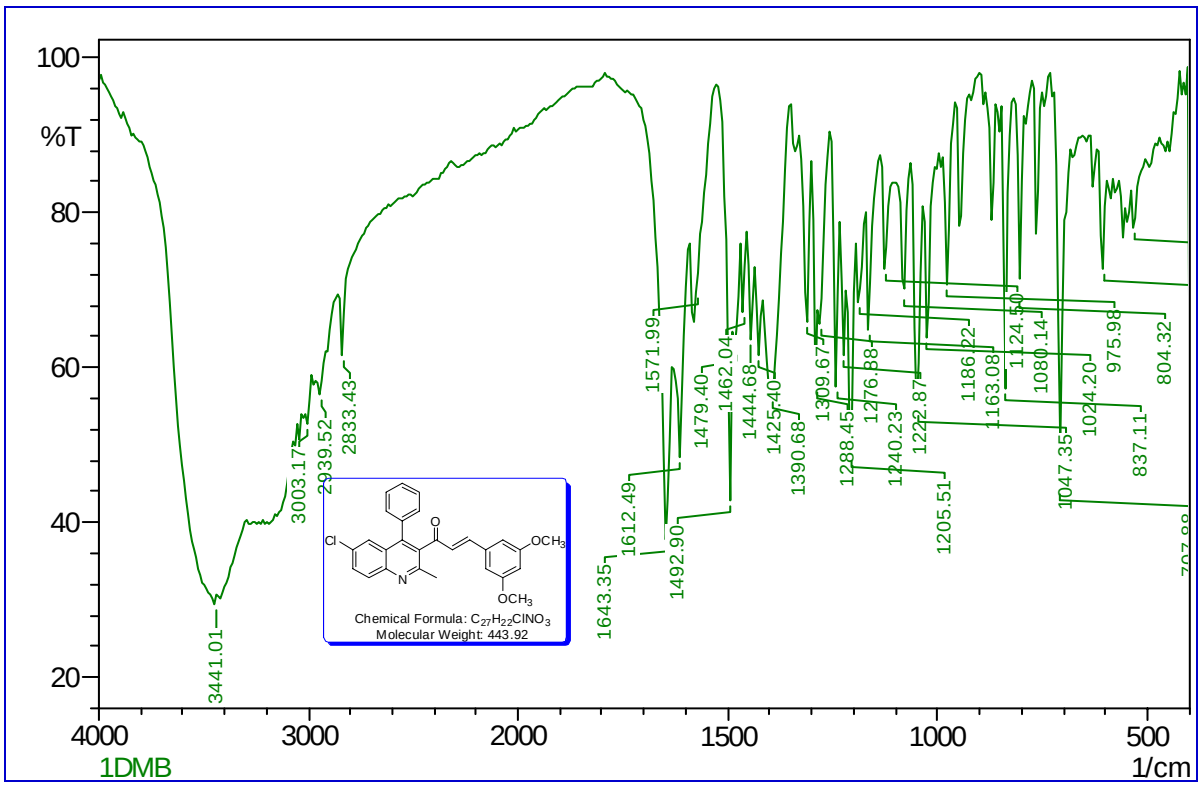

Chemical Formula: $C_{25}H_{17}ClN_2O_3$
Molecular Weight: 428.87
429.6123
383.3812
349.4428
393.4808
296.3044
133.2158
89.0916
113.1314
227.3485
177.2724
288.5246
305.3389
244.4158
363.4324
407.5321
103.1516
338.5897
221.2619
261.4198
319.3923
417.5687
147.2115
175.1387
265.3727
219.3166
58.0823
88.1501

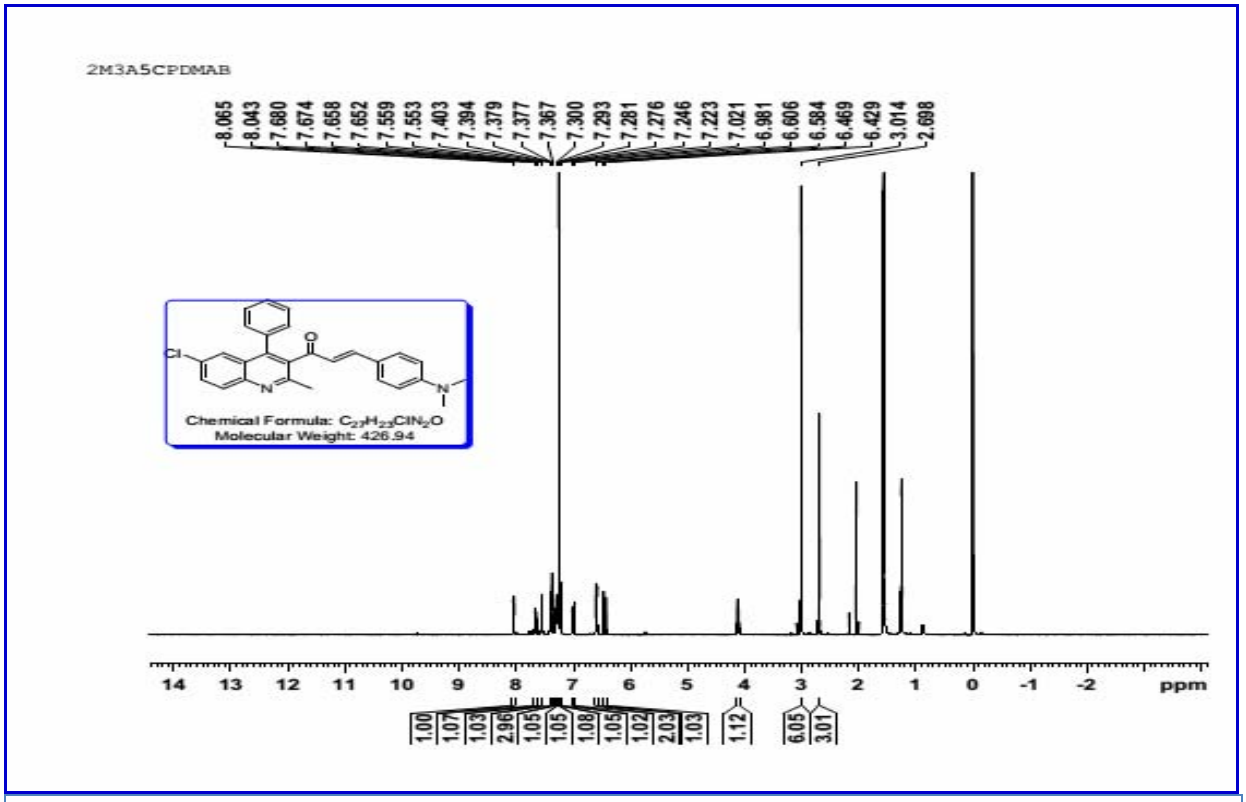

Chemical Formula: $C_{25}H_{17}ClN_2O_3$
Molecular Weight: 428.87
%T
1624.06
1564.27
1479.40
1382.96
1222.87
1201.65
1161.15
1082.07
1045.42
972.12
831.32
765.74
711.73
702.09
588.29
484.13
1ONB
1/cm

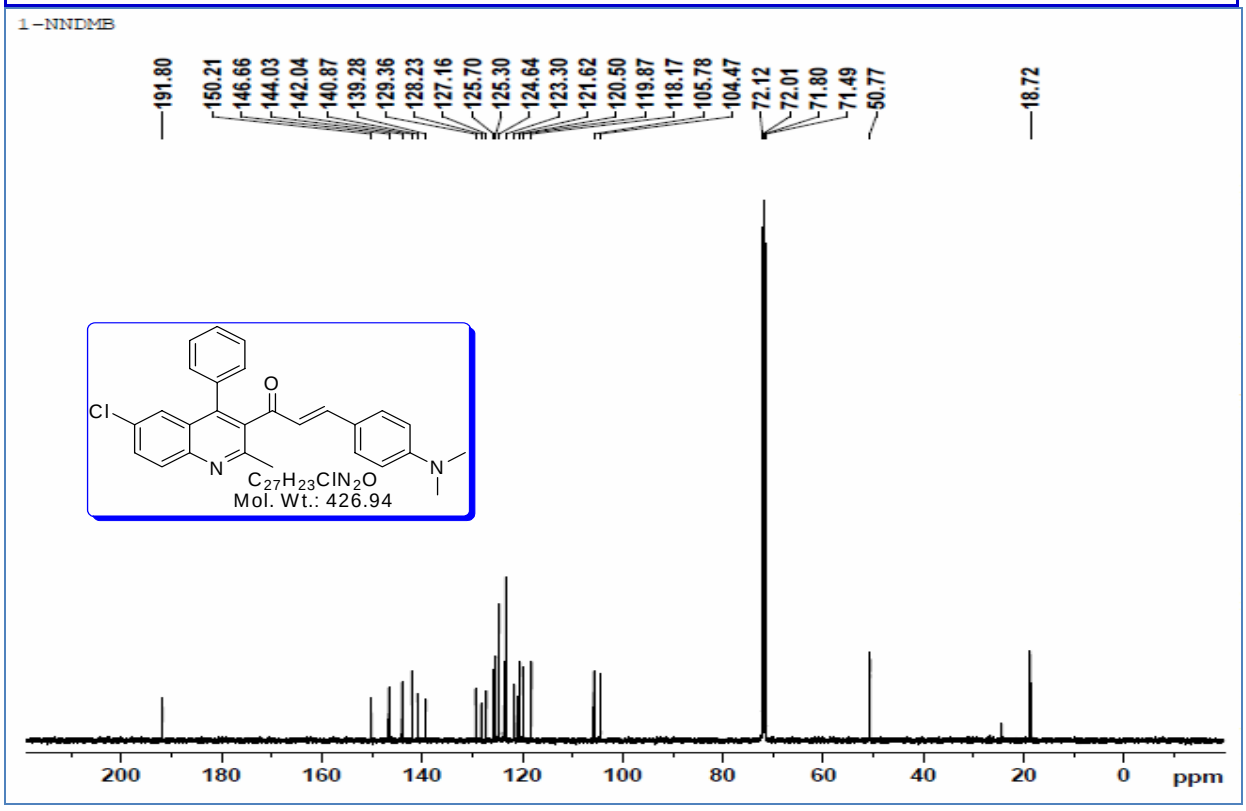

2M3A5CDMB
8.074
8.052
7.697
7.691
7.675
7.669
7.576
7.571
7.463
7.422
7.409
7.393
7.304
7.298
7.285
7.263
6.916
6.909
6.894
6.886
6.822
6.815
6.789
6.767
6.649
6.608
3.738
3.728
2.699
Cl
O
OCH3
N
OCH3
Chemical Formula: C27H22ClNO3
Molecular Weight: 443.92
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.01
1.00
1.00
1.04
3.00
2.00
1.01
2.00
1.00
6.03
3.03

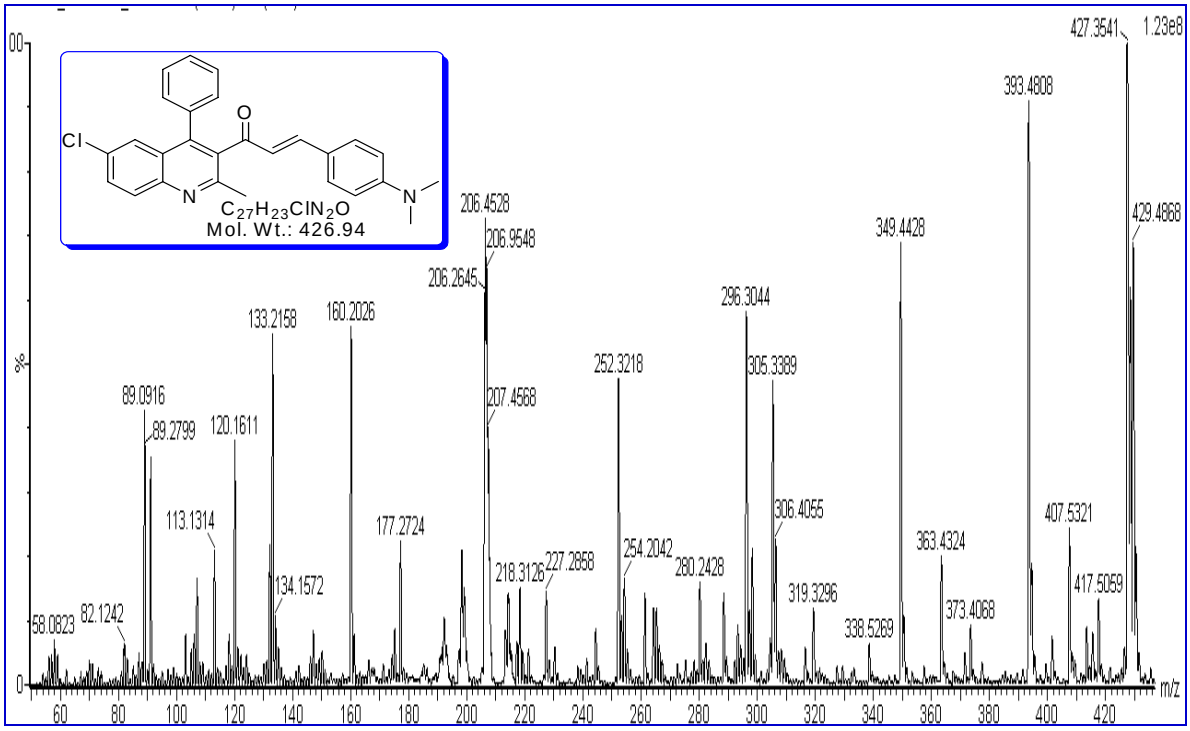

2M3A5CDMB
197.75
155.52
153.44
152.96
146.10
144.56
142.47
134.60
133.56
132.32
130.89
130.06
128.76
128.48
128.16
126.27
125.17
118.33
112.76
112.35
77.35
77.03
76.71
55.94
55.78
24.01
Cl
O
OCH3
N
OCH3
Chemical Formula: C27H22ClNO3
Molecular Weight: 443.92
200
180
160
140
120
100
80
60
40
20
ppm

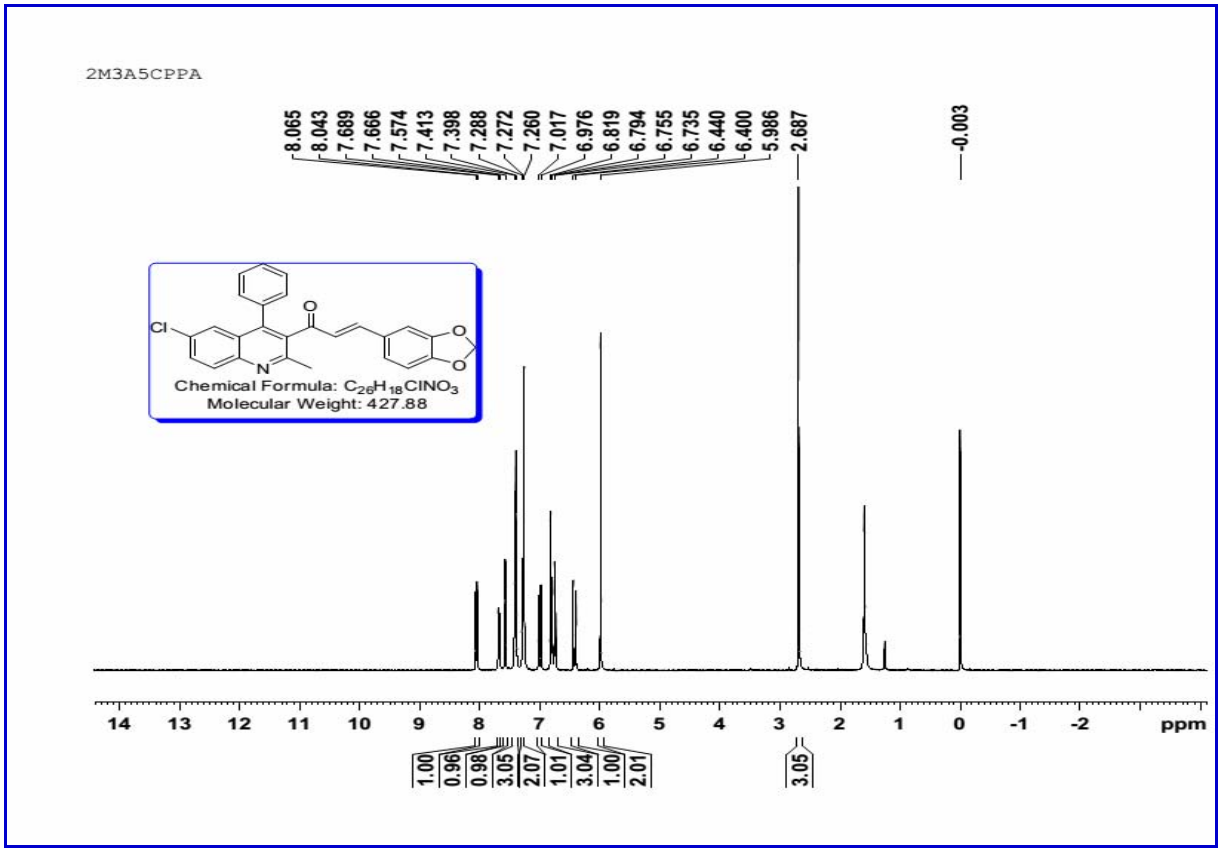

100
%
0
444.4783
1.34e8
446.4856
393.4808
437.5158
447.4892
349.3801
305.3389
56.0735
89.0916
82.0614
91.1002
113.1314
133.2158
59.0867
103.1516
150.2240
177.2724
227.4112
244.4158
261.4198
286.4619
327.4227
338.5897
371.5249
373.4696
407.4694
415.4986
Cl
O
OCH3
N
OCH3
Chemical Formula: C27H22ClNO3
Molecular Weight: 443.92
60 80 100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 420 440
m/z

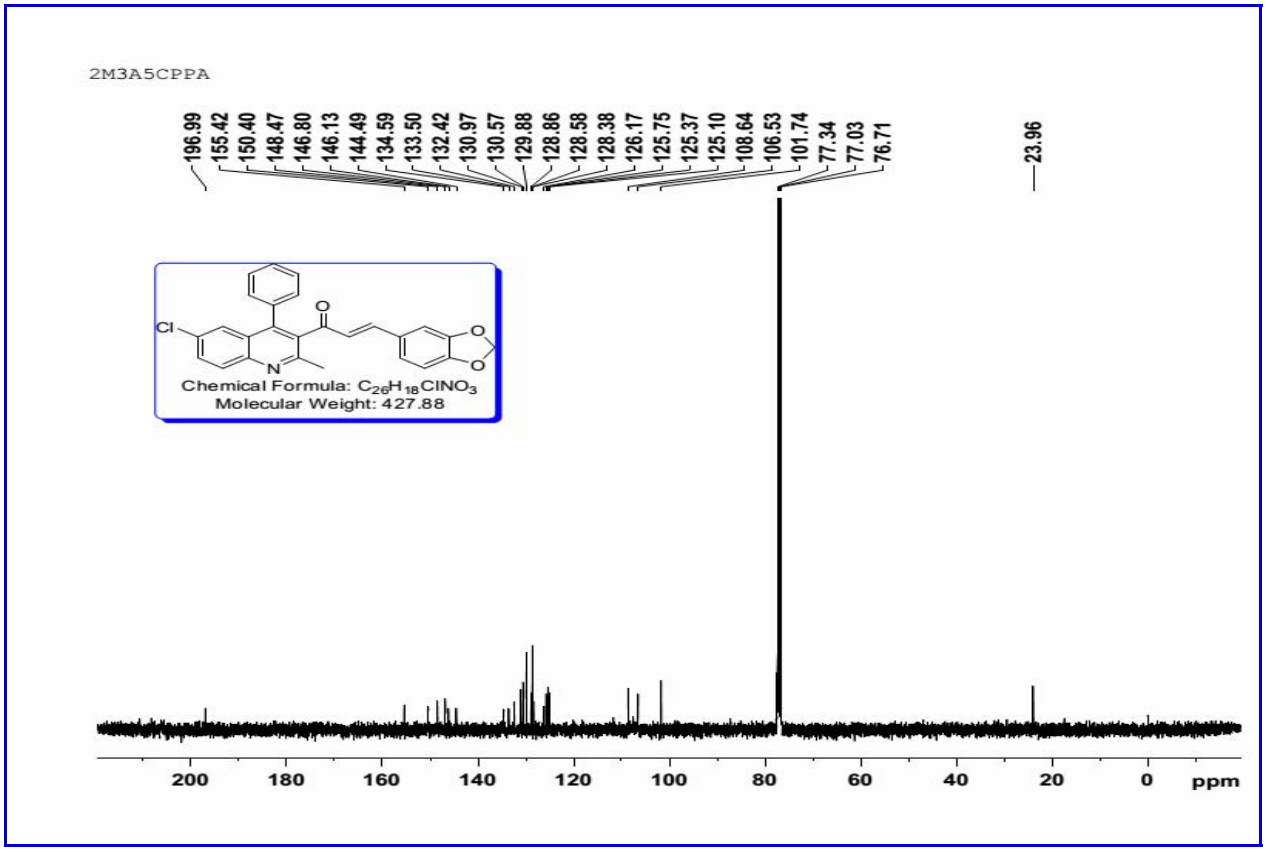

100
%T
80
60
40
20
3441.01
3003.17
2939.52
2833.43
1643.35
1612.49
1571.99
1492.90
1479.40
1462.04
1444.68
1425.40
1390.68
1309.67
1288.45
1276.88
1240.23
1222.87
1205.51
1186.22
1163.08
1124.50
1080.14
1047.35
1024.20
975.98
837.11
804.32
Cl
O
OCH3
N
OCH3
Chemical Formula: C27H22ClNO3
Molecular Weight: 443.92
4000 3000 2000 1500 1000 500
1DMB
1/cm

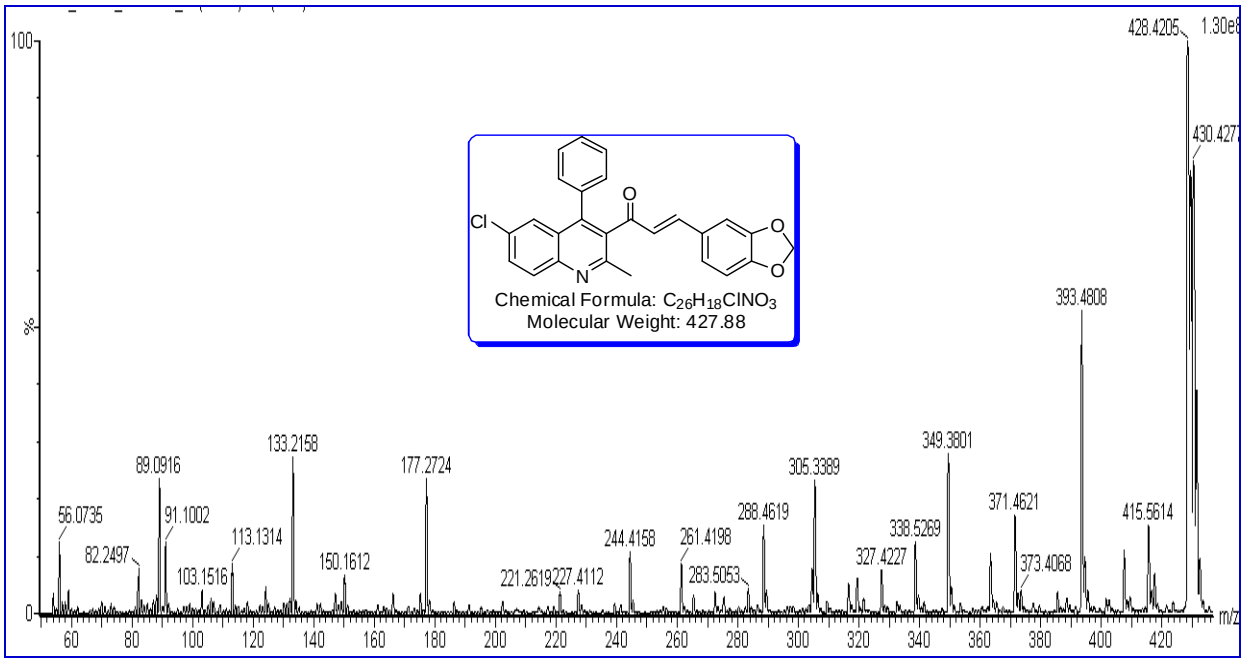

2M3A5CPDMAB
8.065
8.043
7.680
7.674
7.658
7.652
7.559
7.553
7.403
7.394
7.379
7.377
7.367
7.300
7.293
7.281
7.276
7.246
7.223
7.021
6.981
6.606
6.584
6.469
6.429
3.014
2.698
Cl
O
N
N
Chemical Formula: C27H23ClN2O
Molecular Weight: 426.94
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
1.00 1.07 1.03 2.96 1.05 1.05 1.08 1.05 1.02 2.03 1.03 1.12 6.05 3.01

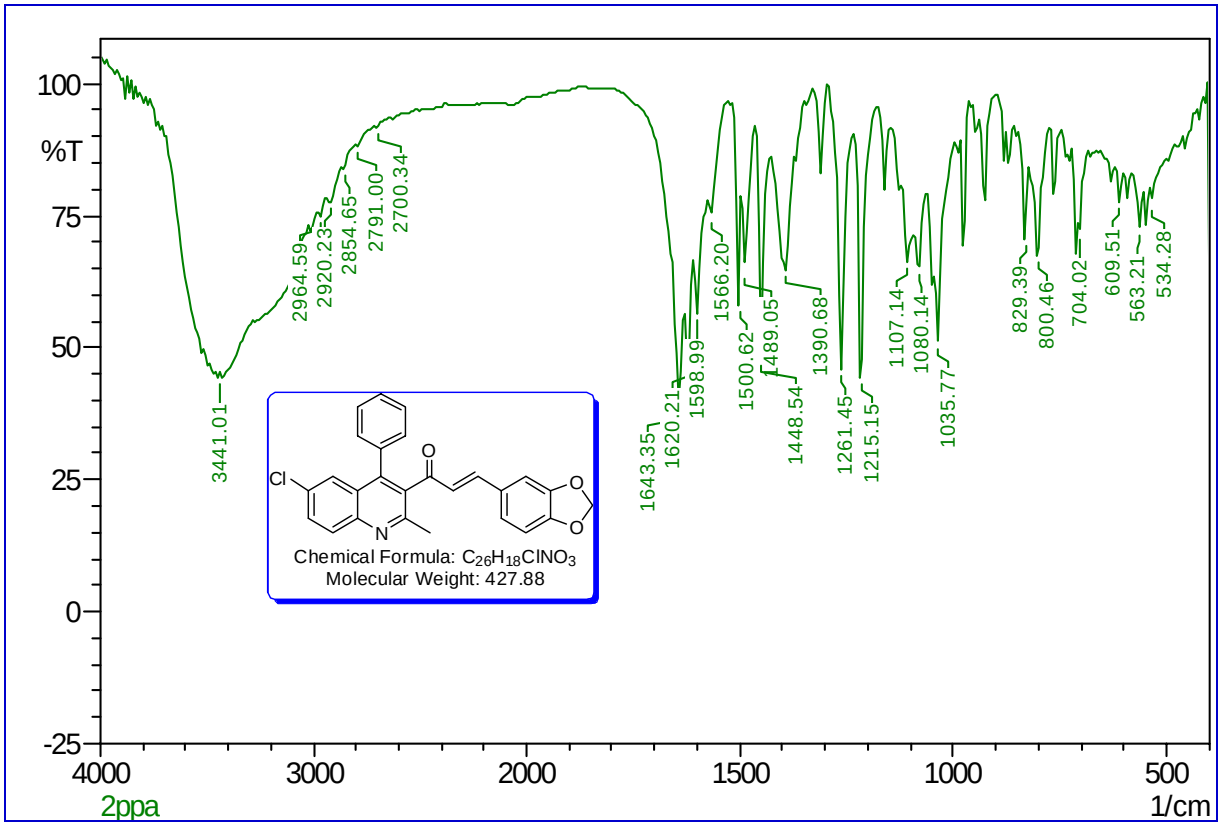

1-NNDMB
191.80
150.21
146.66
144.03
142.04
140.87
139.28
129.36
128.23
127.16
125.70
125.30
124.64
123.30
121.62
120.50
119.87
118.17
105.78
104.47
72.12
72.01
71.80
71.49
50.77
18.72
Cl
O
N
N
C27H23ClN2O
Mol. Wt.: 426.94
200 180 160 140 120 100 80 60 40 20 0 ppm

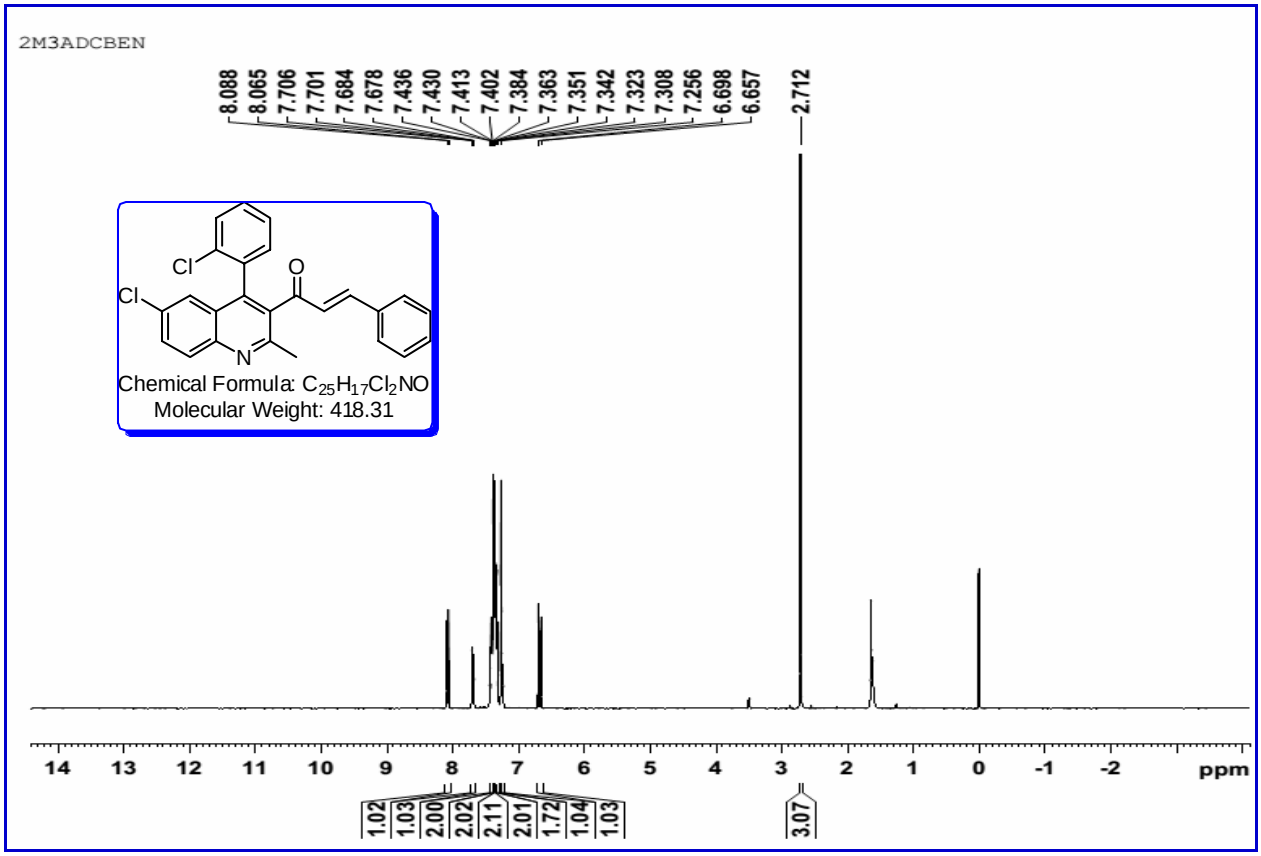

Cl
O
N
N
C27H23ClN2O
Mol. Wt.: 426.94
427.3541
1.23e8
393.4808
429.4868
349.4428
206.4528
206.9548
206.2645
296.3044
305.3389
133.2158
160.2026
252.3218
89.0916
89.2799
120.1611
207.4568
306.4055
407.5321
113.1314
177.2724
363.4324
254.2042
218.3126
227.2858
280.2428
134.1572
319.3296
417.5059
58.0823
82.1242
338.5269
373.4068
%
m/z

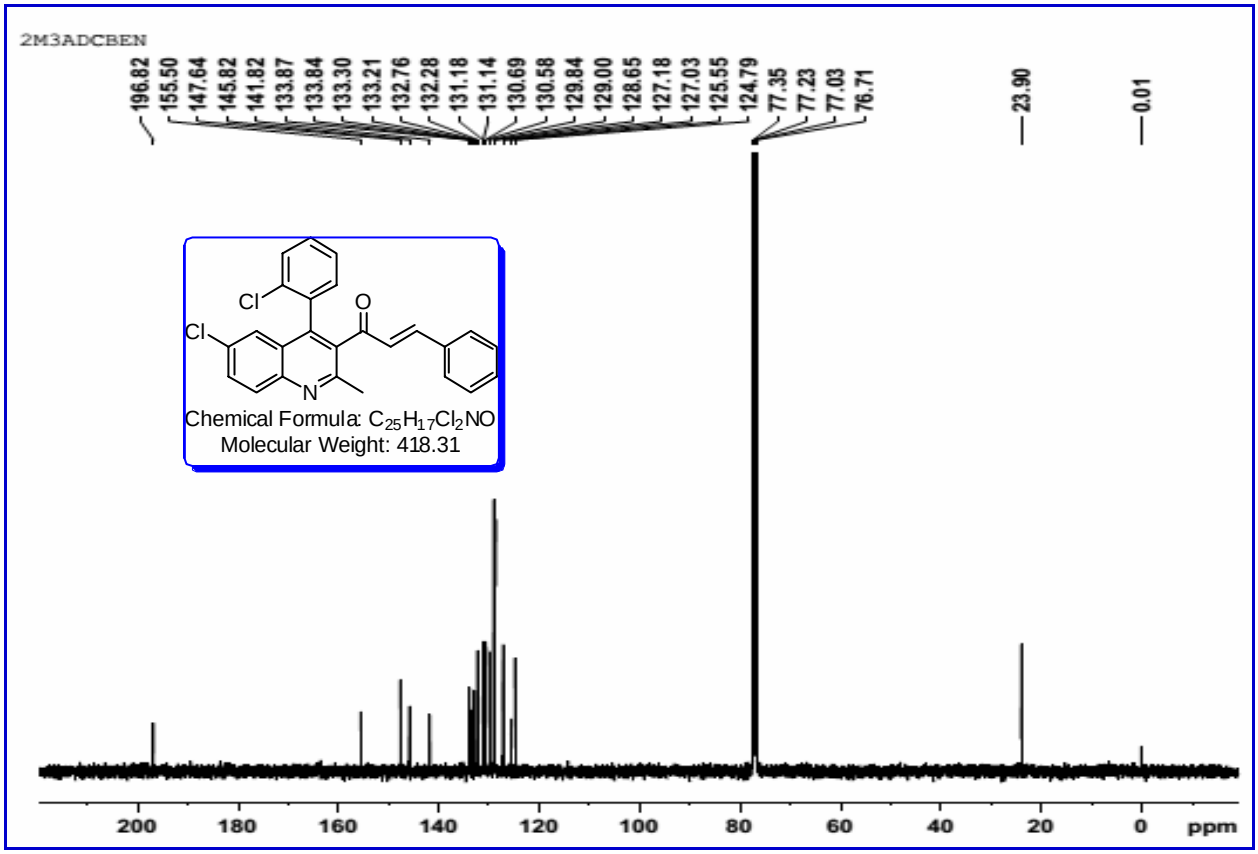

2M3A5CPPA
8.065
8.043
7.689
7.666
7.574
7.413
7.398
7.288
7.272
7.260
7.017
6.976
6.819
6.794
6.755
6.735
6.440
6.400
5.986
2.687
-0.003
Cl
O
O
O
N
Chemical Formula: C26H18ClNO3
Molecular Weight: 427.88
ppm
1.00
0.96
0.98
3.05
2.07
1.01
3.04
1.00
2.01
3.05

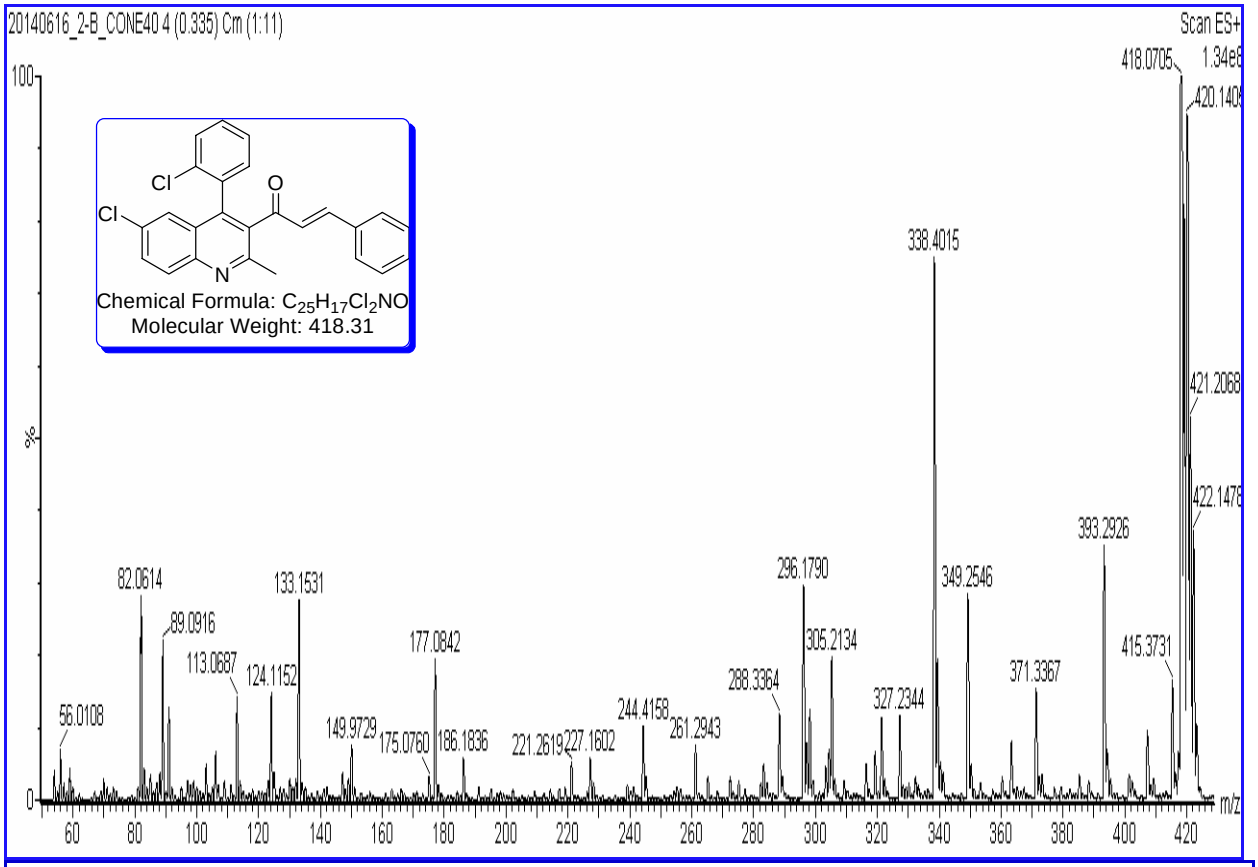

2M3A5CPPA
196.99
155.42
150.40
148.47
146.80
146.13
144.49
134.59
133.50
132.42
130.97
130.57
129.88
128.86
128.58
128.38
126.17
125.75
125.37
125.10
108.64
106.53
101.74
77.34
77.03
76.71
23.96
Cl
O
O
O
N
Chemical Formula: C26H18ClNO3
Molecular Weight: 427.88
200
180
160
140
120
100
80
60
40
20
0
ppm

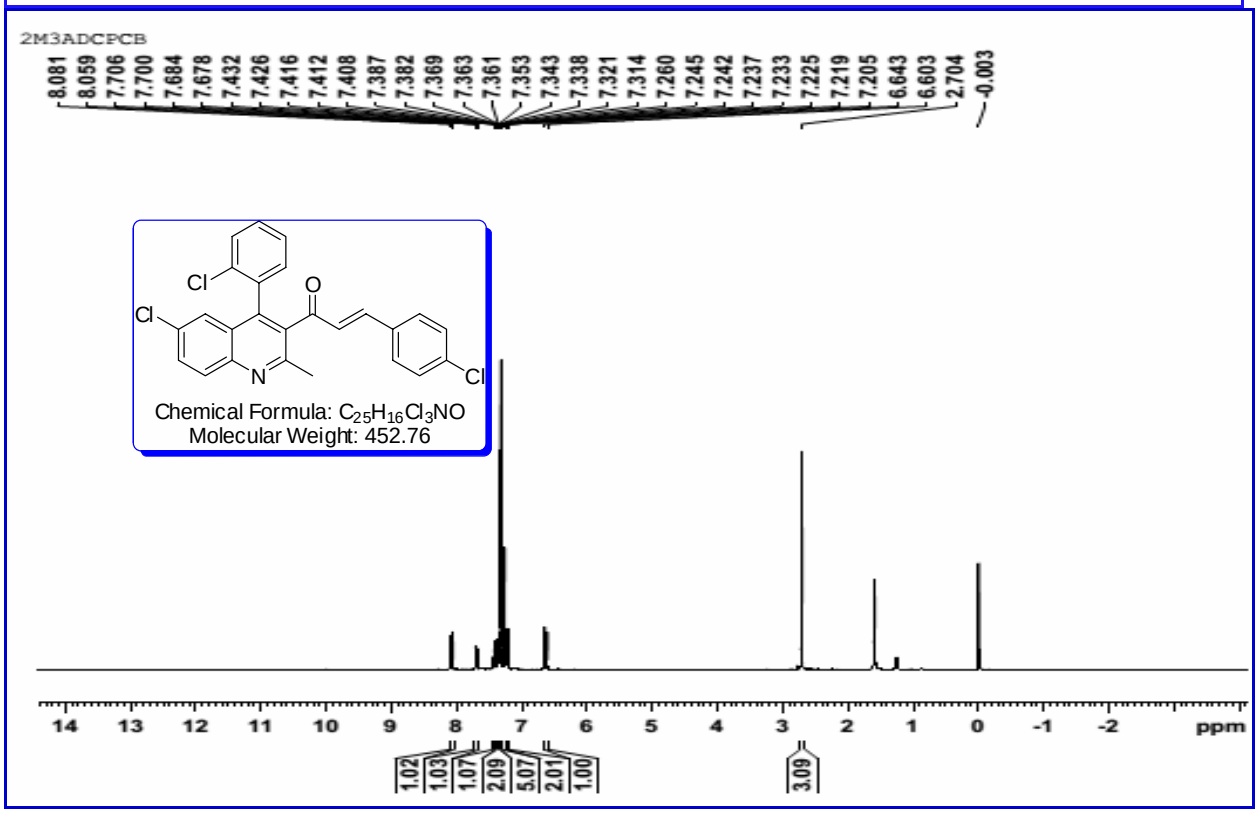

100
%
0
428.4205
1.30e8
430.4277
393.4808
349.3801
305.3389
371.4621
415.5614
338.5269
327.4227
373.4068
288.4619
261.4198
244.4158
283.5053
177.2724
133.2158
89.0916
91.1002
113.1314
56.0735
82.2497
103.1516
150.1612
221.2619
227.4112
Cl
O
O
O
N
Chemical Formula: C26H18ClNO3
Molecular Weight: 427.88
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
400
420
m/z

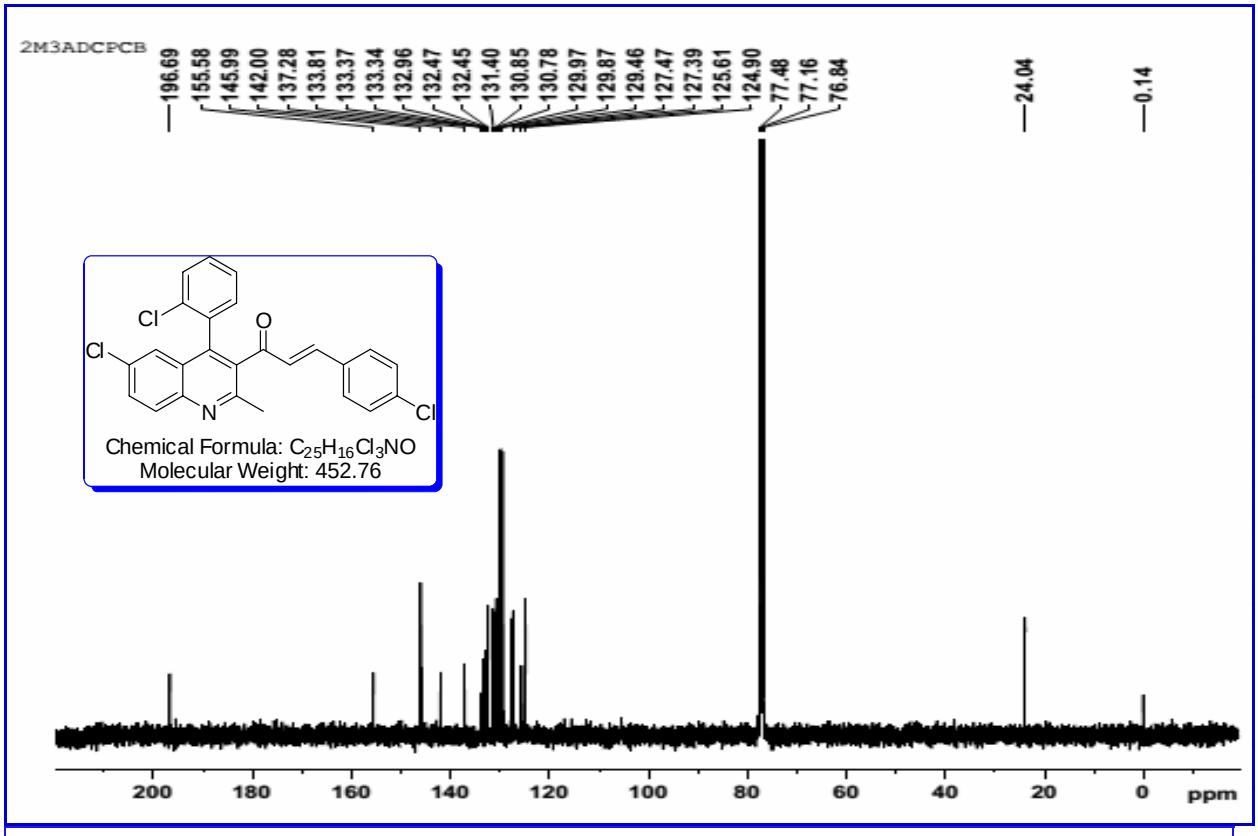

100
%T
75
50
25
0
-25
4000
3000
2000
1500
1000
500
1/cm
2ppa
3441.01
2964.59
2920.23
2854.65
2791.00
2700.34
1643.35
1620.21
1598.99
1566.20
1500.62
1489.05
1448.54
1390.68
1261.45
1215.15
1107.14
1080.14
1035.77
829.39
800.46
704.02
609.51
563.21
534.28
Cl
O
N
O
O
Chemical Formula: C26H18ClNO3
Molecular Weight: 427.88

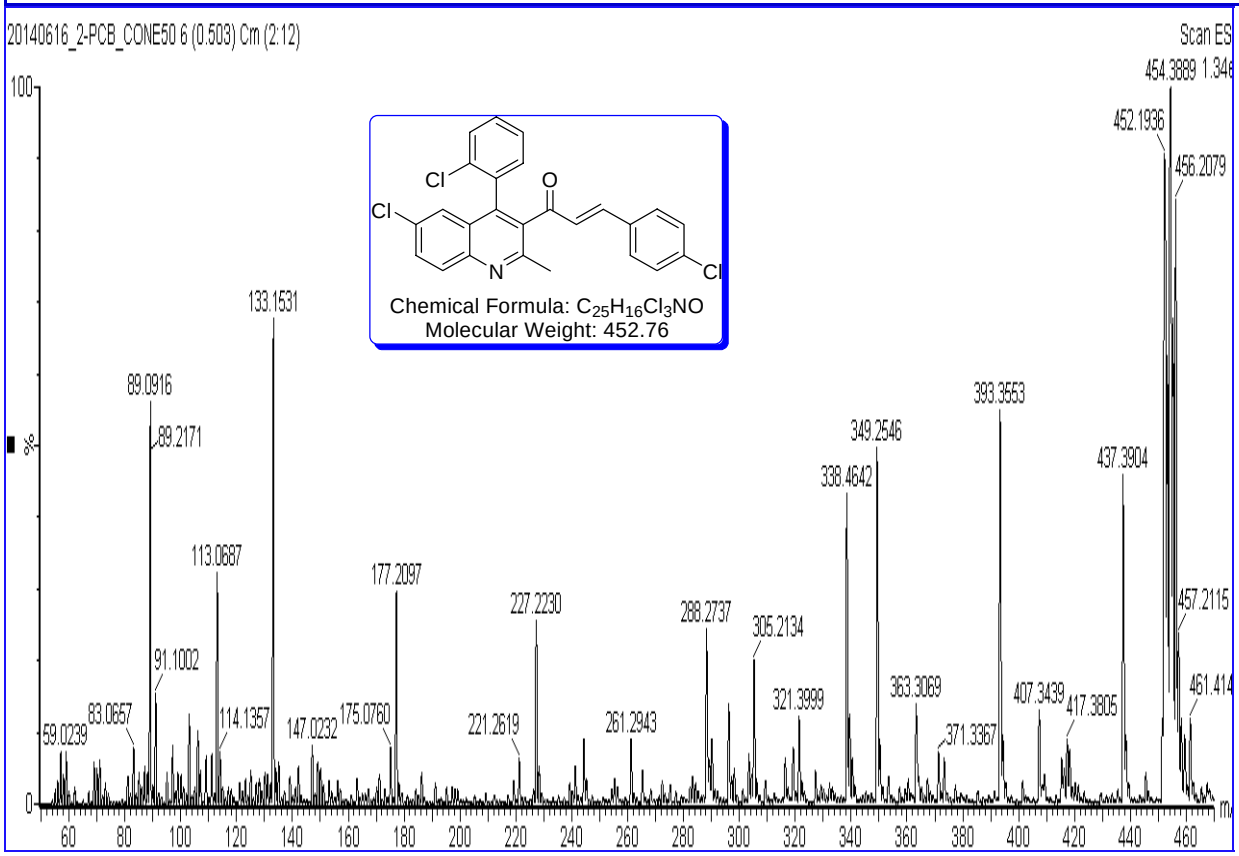

2M3ADCBEN
8.088
8.065
7.706
7.701
7.684
7.678
7.436
7.430
7.413
7.402
7.384
7.363
7.351
7.342
7.323
7.308
7.256
6.698
6.657
2.712
Cl
Cl
O
N
Chemical Formula: C25H17Cl2NO
Molecular Weight: 418.31
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
ppm
1.02
1.03
2.00
2.02
2.11
2.01
1.72
1.04
1.03
3.07

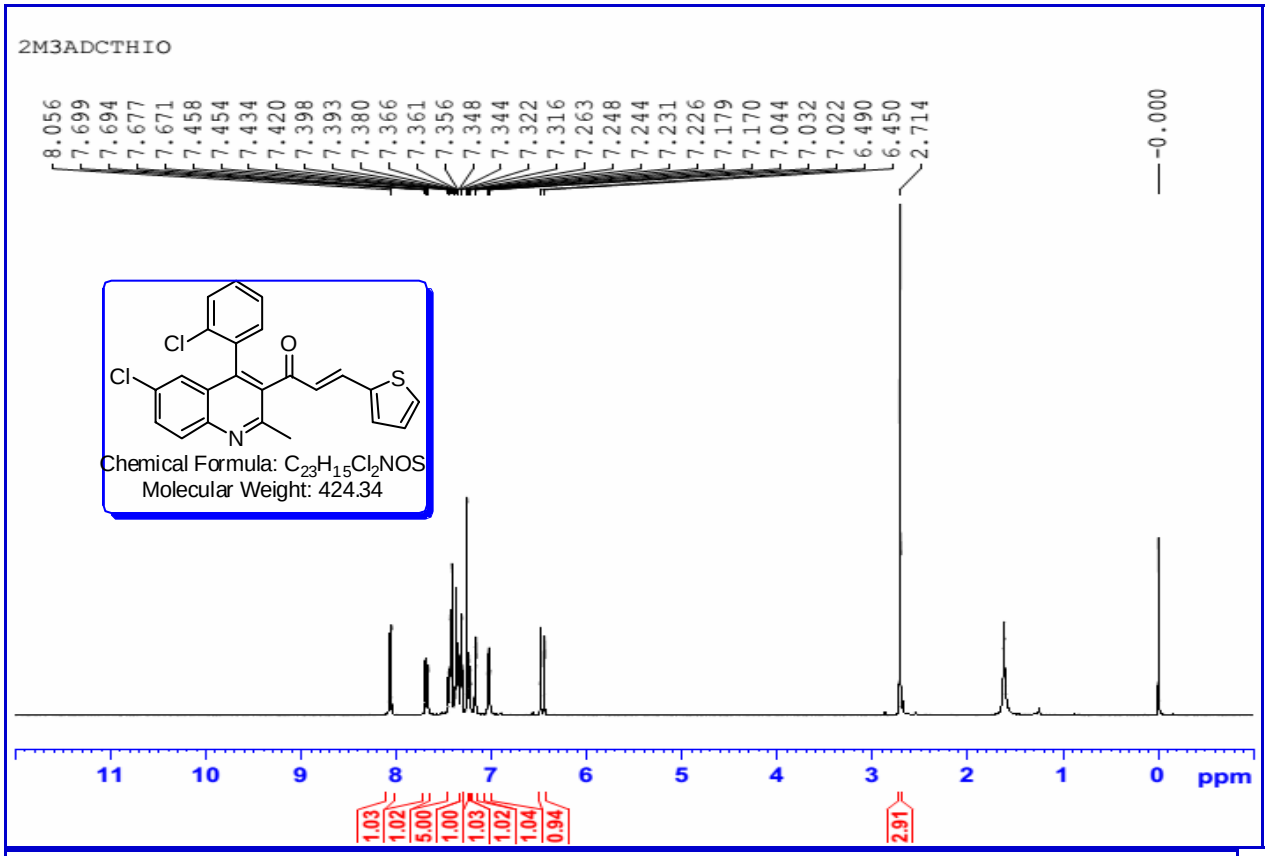

2M3ADCBEN
196.82
155.50
147.64
145.82
141.82
133.87
133.84
133.30
133.21
132.76
132.28
131.18
131.14
130.69
130.58
129.84
129.00
128.65
127.18
127.03
125.55
124.79
77.35
77.23
77.03
76.71
23.90
0.01
Cl
Cl
O
N
Chemical Formula: C25H17Cl2NO
Molecular Weight: 418.31
200
180
160
140
120
100
80
60
40
20
0
ppm

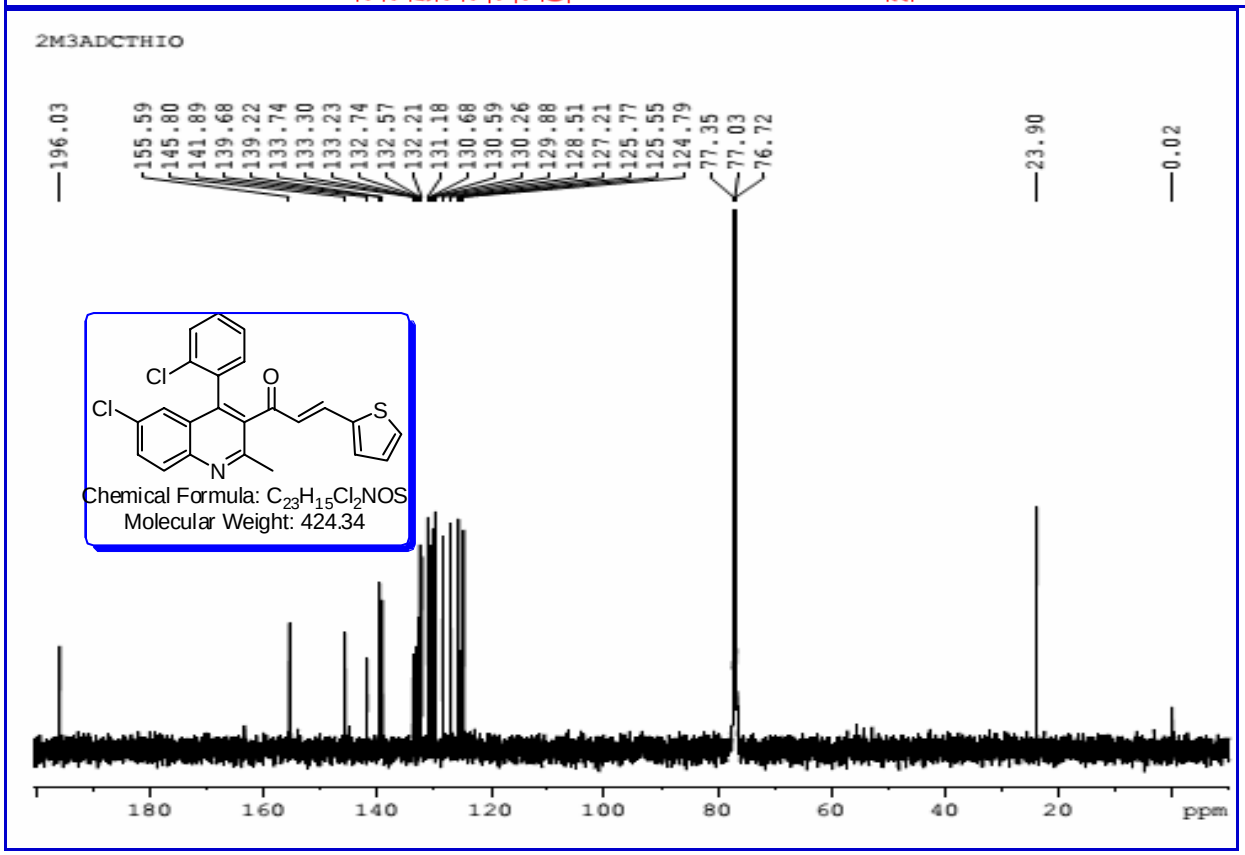

20140616_2-B_CONE40 4 (0.335) Cm (1:11)
Scan ES+
1.34e8
Cl
Cl
O
N
Chemical Formula: C25H17Cl2NO
Molecular Weight: 418.31
418.0705
420.1409
421.2068
422.1478
338.4015
393.2926
296.1790
349.2546
305.2134
82.0614
89.0916
133.1531
113.0687
124.1152
177.0842
56.0108
149.9729
175.0760
186.1836
221.2619
227.1602
244.4158
261.2943
288.3364
327.2344
371.3367
415.3731
%
m/z

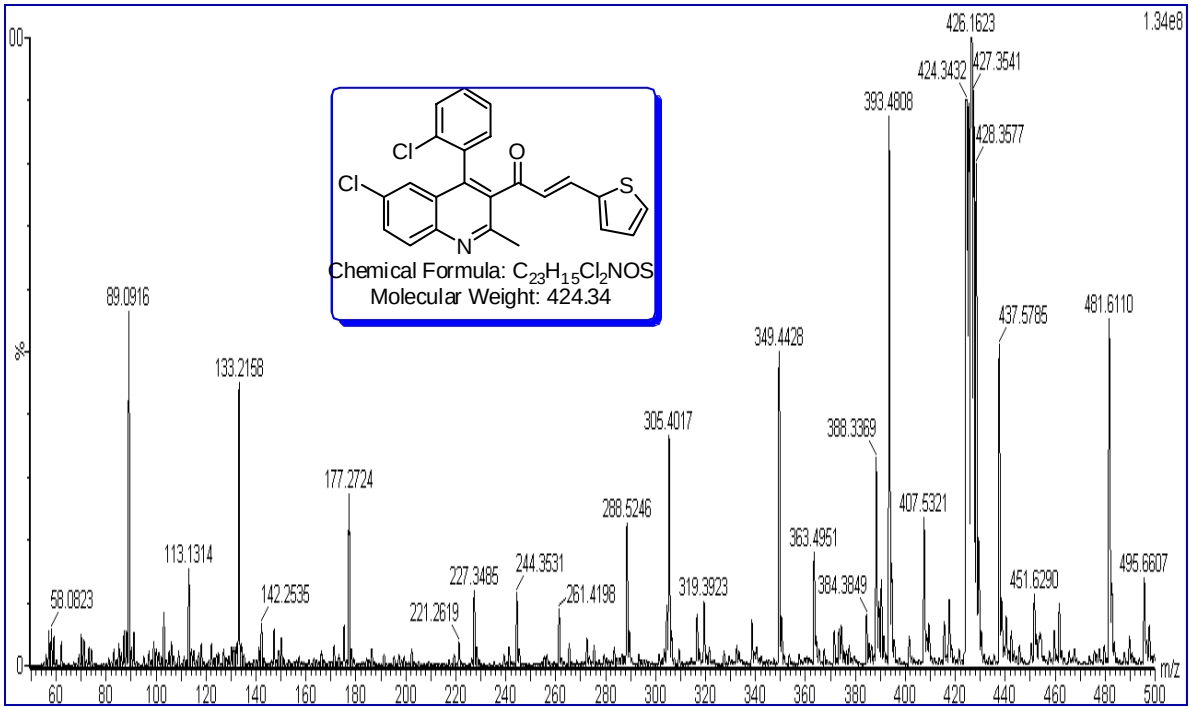

2M3ADCPCB
8.081
8.059
7.706
7.700
7.684
7.678
7.432
7.426
7.416
7.412
7.408
7.387
7.382
7.369
7.363
7.361
7.353
7.343
7.338
7.321
7.314
7.260
7.245
7.242
7.237
7.233
7.225
7.219
7.205
6.643
6.603
2.704
-0.003
Cl
Cl
O
N
Cl
Chemical Formula: C25H16Cl3NO
Molecular Weight: 452.76
ppm
1.02
1.03
1.07
2.09
5.07
2.01
1.00
3.09

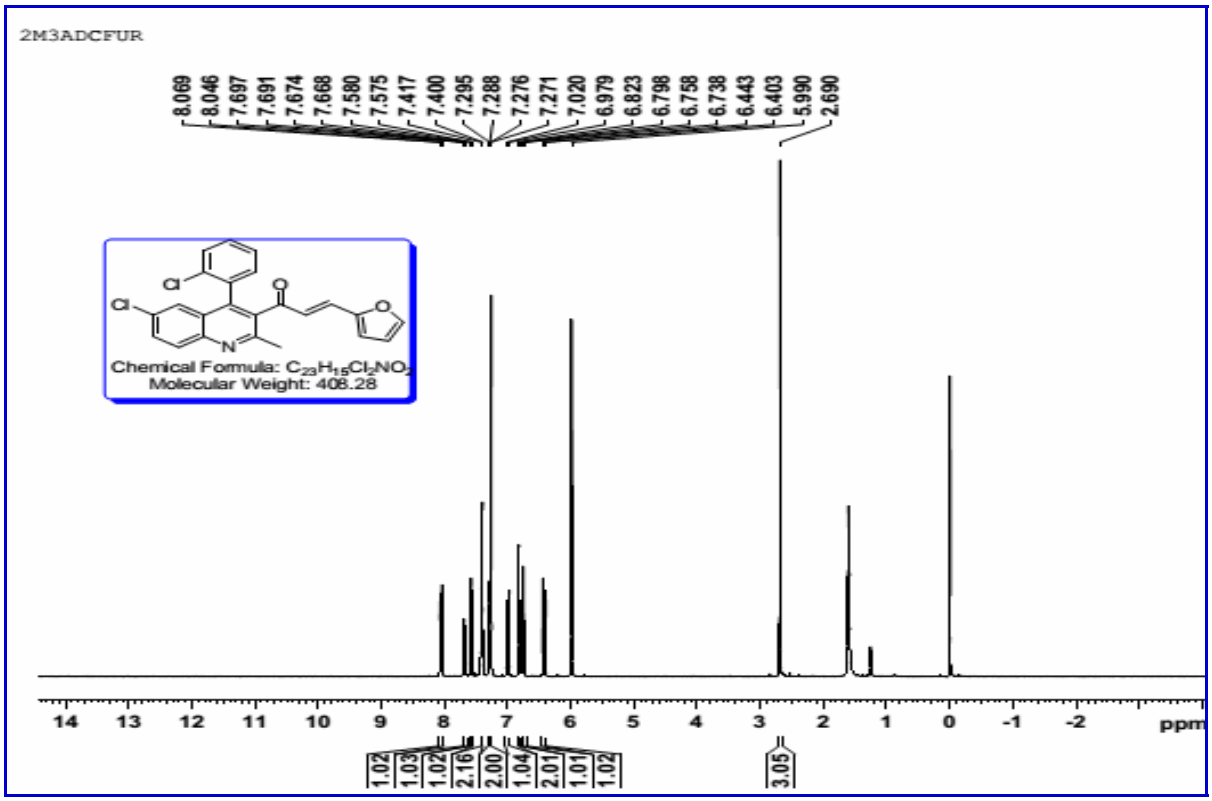

2M3ADCPCB
196.69
155.58
145.99
142.00
137.28
133.81
133.37
133.34
132.96
132.47
132.45
131.40
130.85
130.78
129.97
129.87
129.46
127.47
127.39
125.61
124.90
77.48
77.16
76.84
24.04
0.14
Cl
Cl
O
N
Cl
Chemical Formula: C25H16Cl3NO
Molecular Weight: 452.76
200
180
160
140
120
100
80
60
40
20
0
ppm

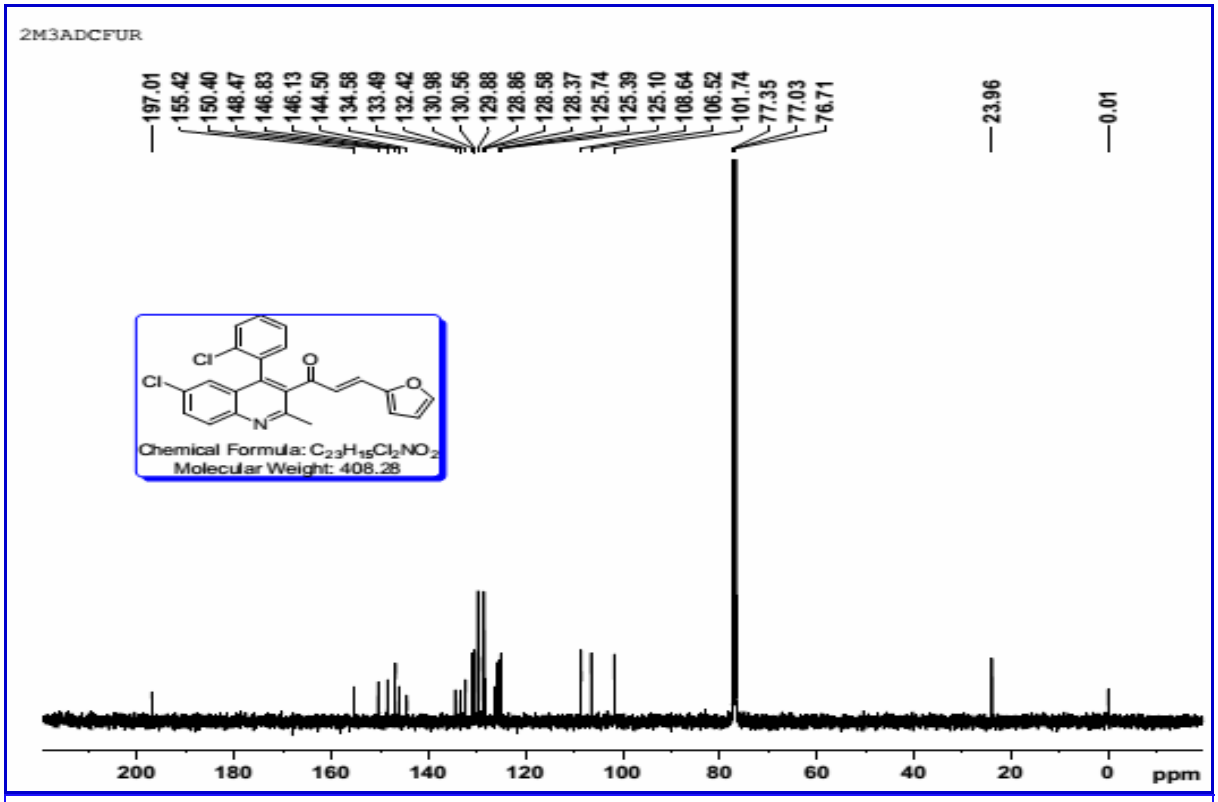

20140616_2-PCB_CONE50 6 (0.503) Cm (2:12)
Scan ES
100
%
0
454.3889
452.1936
456.2079
457.2115
461.414
437.3904
393.3653
349.2546
338.4642
305.2134
288.2737
227.2230
177.2097
133.1531
113.0687
89.0916
89.2171
91.1002
83.0657
59.0239
114.1357
147.0232
175.0760
221.2619
261.2943
321.3999
363.3069
371.3367
407.3439
417.3805
Cl
Cl
O
N
Cl
Chemical Formula: C25H16Cl3NO
Molecular Weight: 452.76
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
400
420
440
460
m/z

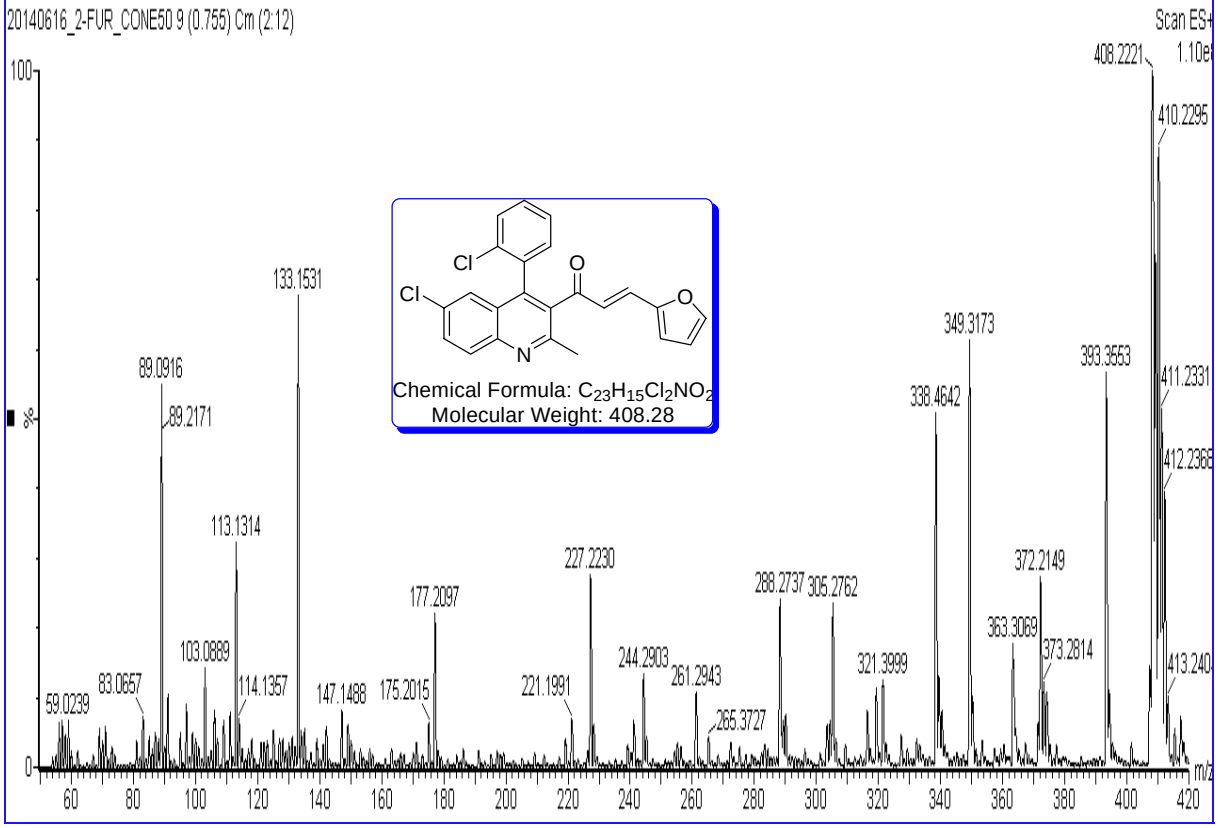

2M3ADCTHIO
8.056
7.699
7.694
7.677
7.671
7.458
7.454
7.434
7.420
7.398
7.393
7.380
7.366
7.361
7.356
7.348
7.344
7.322
7.316
7.263
7.248
7.244
7.231
7.226
7.179
7.170
7.044
7.032
7.022
6.490
6.450
2.714
0.000
Cl
Cl
O
S
N
Chemical Formula: C23H15Cl2NOS
Molecular Weight: 424.34
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.03
1.02
5.00
1.00
1.03
1.02
1.04
0.94
2.91

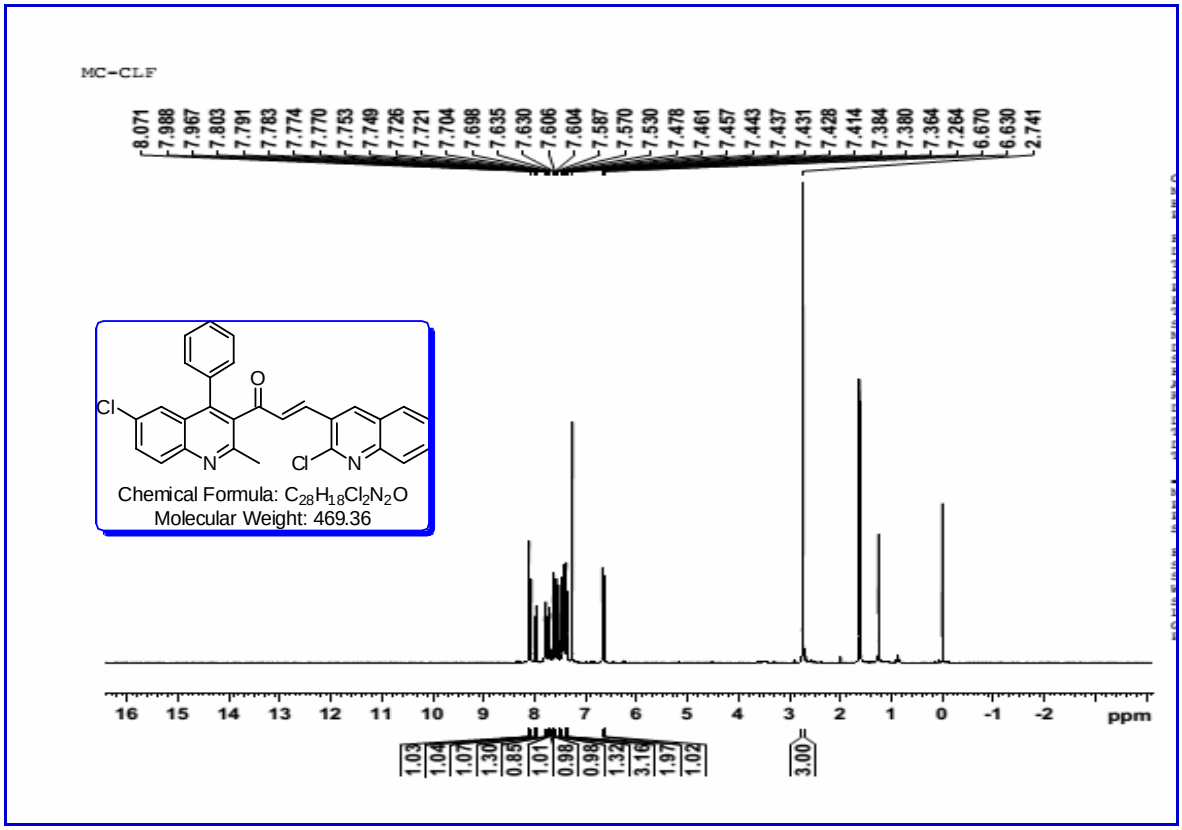

2M3ADCTHIO
196.03
155.59
145.80
141.89
139.68
139.22
133.74
133.30
133.23
132.74
132.57
132.21
131.18
130.68
130.59
130.26
129.88
128.51
127.21
125.77
125.55
124.79
77.35
77.03
76.72
23.90
0.02
Cl
Cl
O
S
N
Chemical Formula: C23H15Cl2NOS
Molecular Weight: 424.34
180
160
140
120
100
80
60
40
20
ppm

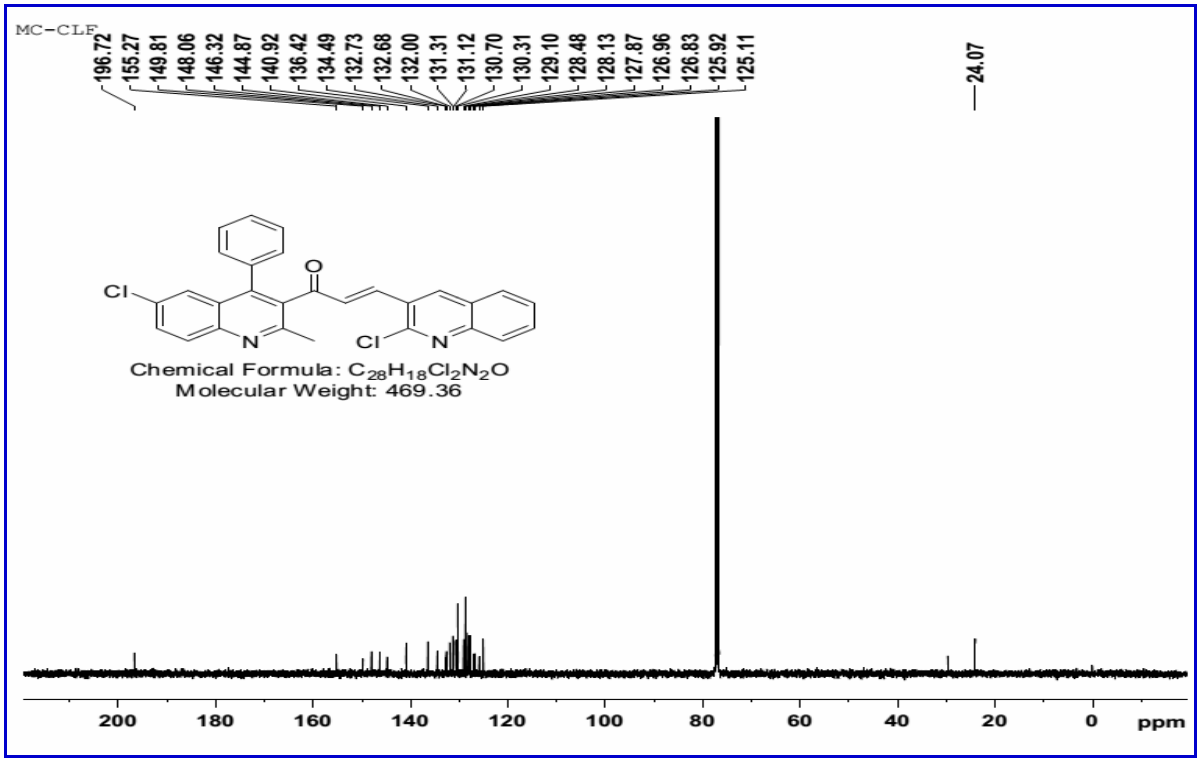

1.34e8
426.1623
427.3541
424.3432
393.4808
428.3577
Chemical Formula: C23H15Cl2NOS
Molecular Weight: 424.34
89.0916
133.2158
349.4428
437.5785
481.6110
305.4017
388.3369
177.2724
407.5321
288.5246
363.4951
113.1314
244.3531
227.3485
261.4198
319.3923
384.3849
451.6290
495.6607
58.0823
142.2535
221.2619
%
m/z

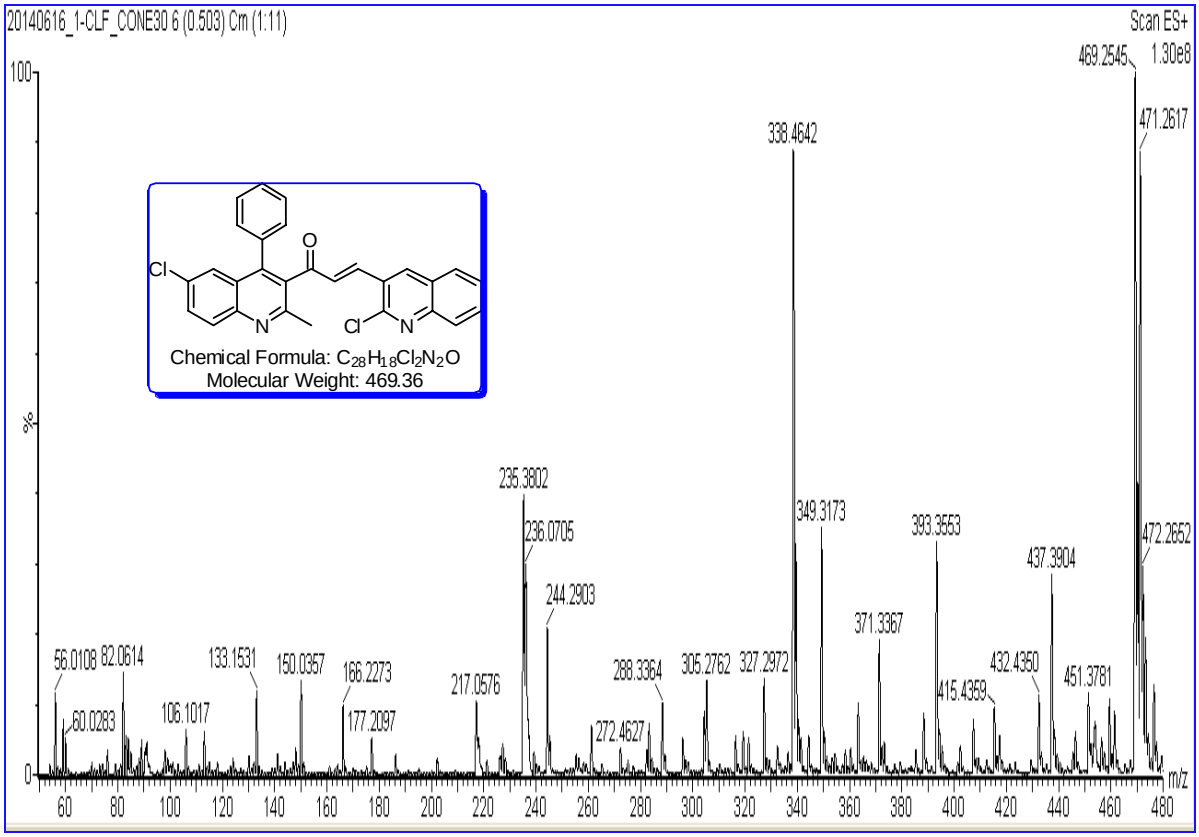

2M3ADCFUR
8.069
8.046
7.697
7.691
7.674
7.668
7.580
7.575
7.417
7.400
7.295
7.288
7.276
7.271
7.020
6.979
6.823
6.798
6.758
6.738
6.443
6.403
5.990
2.690
Chemical Formula: C23H15Cl2NO2
Molecular Weight: 408.28
ppm
1.02
1.03
1.02
2.16
2.00
1.04
2.01
1.01
1.02
3.05

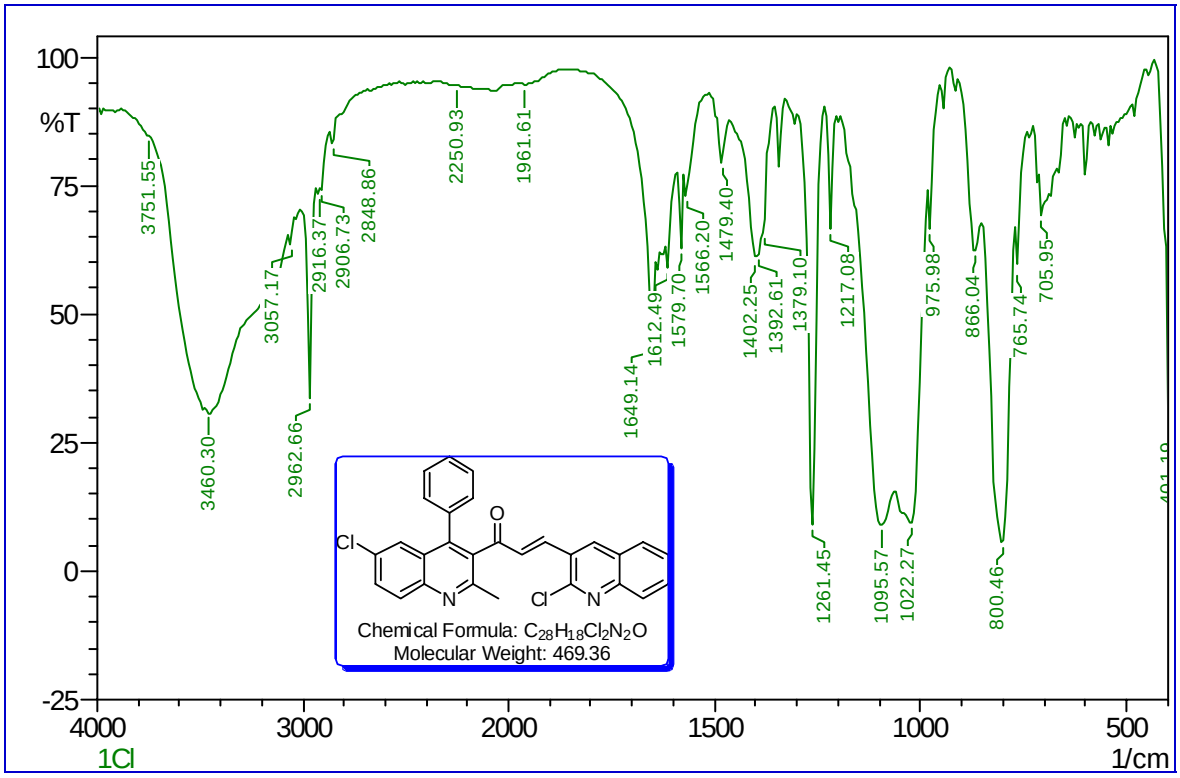

2M3ADCFUR
197.01
155.42
150.40
148.47
146.83
146.13
144.50
134.58
133.49
132.42
130.98
130.56
129.88
128.86
128.58
128.37
125.74
125.39
125.10
108.64
106.52
101.74
77.35
77.03
76.71
23.96
0.01
Cl
Cl
O
O
N
Chemical Formula: C23H15Cl2NO2
Molecular Weight: 408.28
200
180
160
140
120
100
80
60
40
20
0
ppm

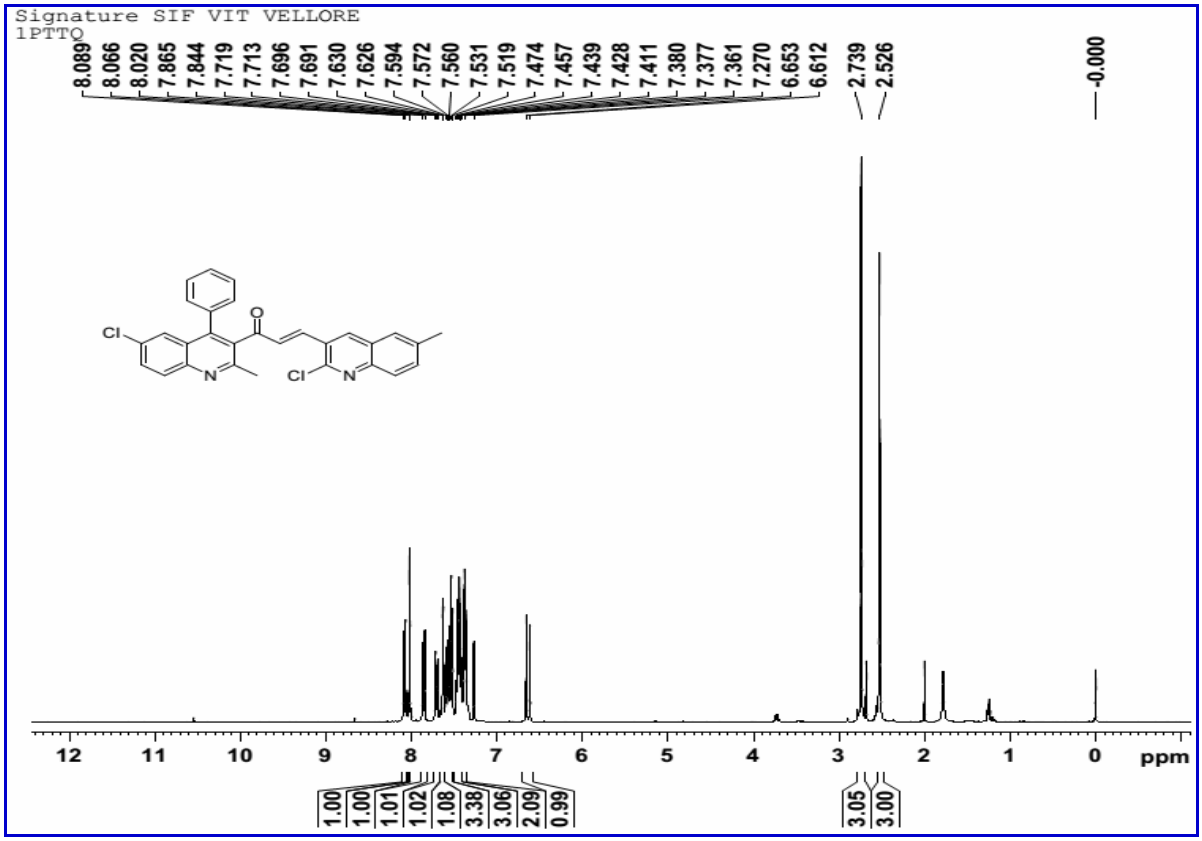

20140616_2-FUR_CONE50 9 (0.755) Cm (2:12)
Scan ES+
100
%
0
408.2221
410.2295
411.2331
412.2366
413.240
393.3553
349.3173
338.4642
372.2149
363.3069
373.2814
321.3999
305.2762
288.2737
227.2230
177.2097
133.1531
113.1314
89.0916
89.2171
103.0889
114.1357
83.0657
59.0239
147.1488
175.2015
221.1991
244.2903
261.2943
265.3727
Cl
Cl
O
O
N
Chemical Formula: C23H15Cl2NO2
Molecular Weight: 408.28
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
400
420
m/z

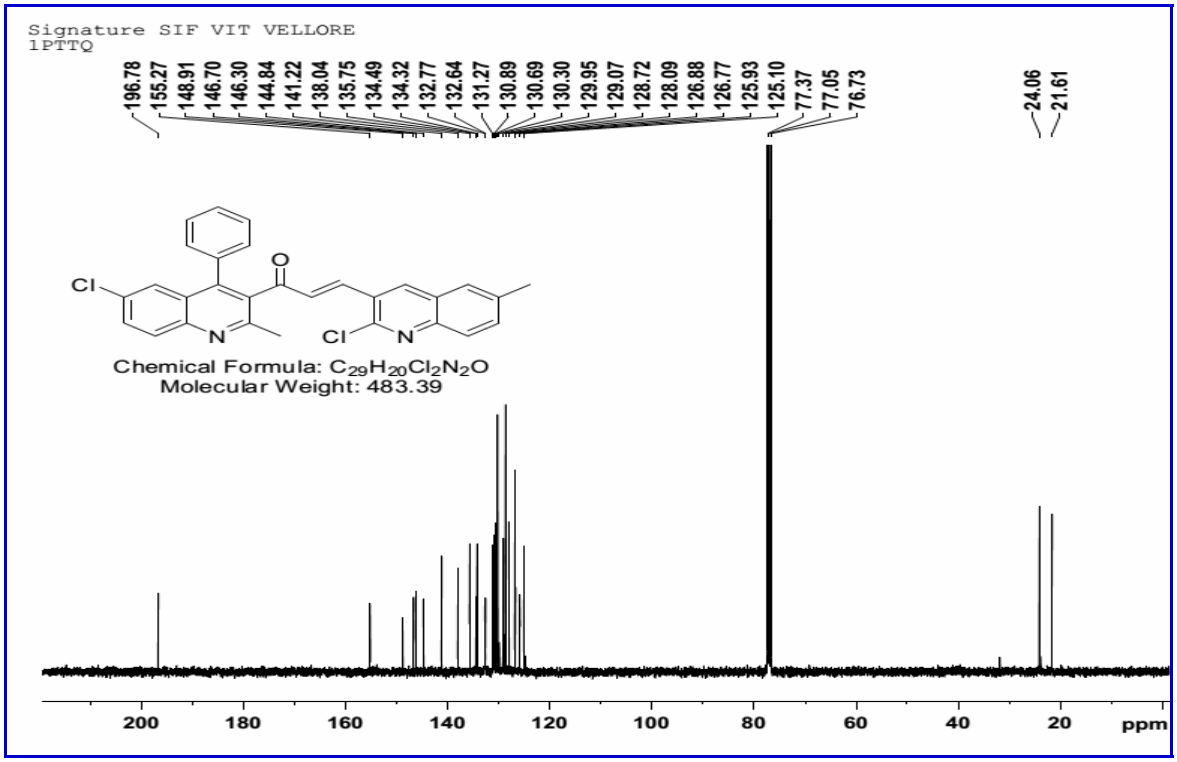

MC-CLF
8.071
7.988
7.967
7.803
7.791
7.783
7.774
7.770
7.753
7.749
7.726
7.721
7.704
7.698
7.635
7.630
7.606
7.604
7.587
7.570
7.530
7.478
7.461
7.457
7.443
7.437
7.431
7.428
7.414
7.384
7.380
7.364
7.264
6.670
6.630
2.741
Cl
O
N
Cl
N
Chemical Formula: C28H18Cl2N2O
Molecular Weight: 469.36
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
1.03
1.04
1.07
1.30
0.85
1.01
0.98
0.98
1.32
3.16
1.97
1.02
3.00

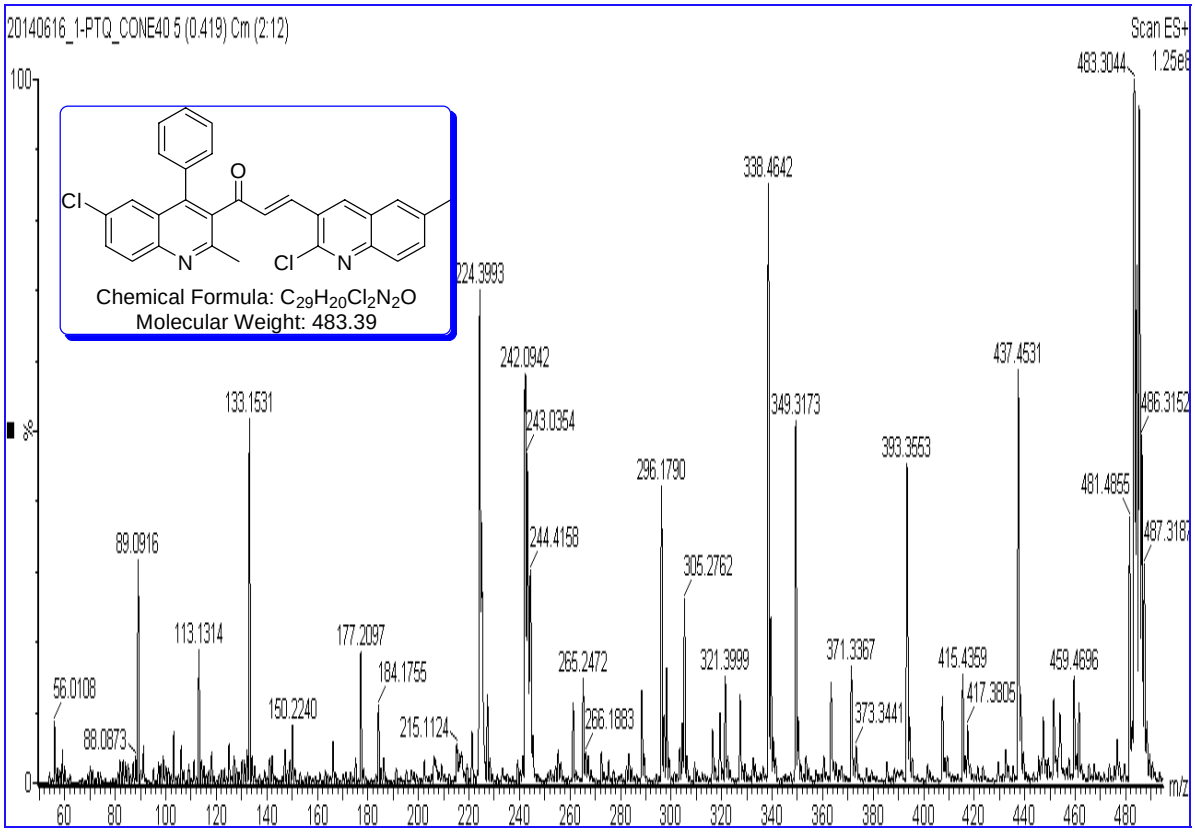

MC-CLF
196.72
155.27
149.81
148.06
146.32
144.87
140.92
136.42
134.49
132.73
132.68
132.00
131.31
131.12
130.70
130.31
129.10
128.48
128.13
127.87
126.96
126.83
125.92
125.11
24.07
Cl
O
N
Cl
N
Chemical Formula: C28H18Cl2N2O
Molecular Weight: 469.36
200 180 160 140 120 100 80 60 40 20 0 ppm

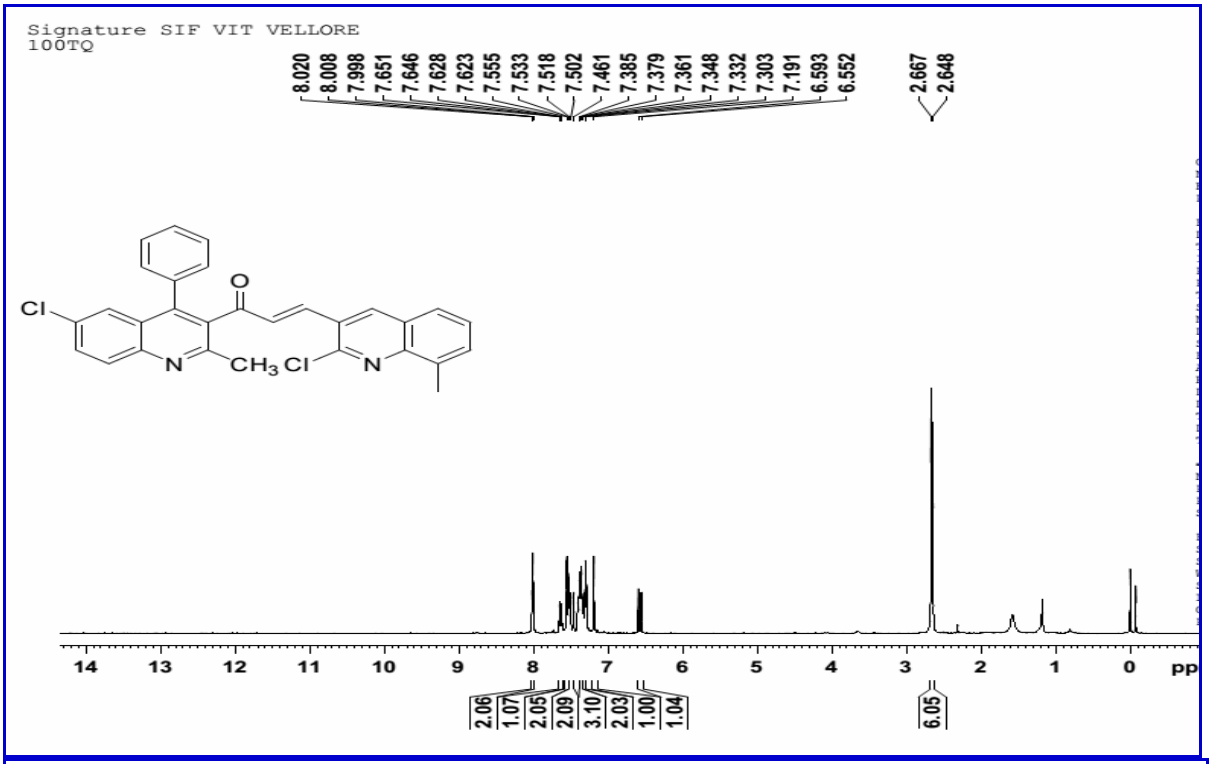

20140616_1-CLF_CONE30 6 (0.503) Cm (1:11)
Scan ES+
469.2545
1.30e8
471.2617
338.4642
349.3173
235.3802
236.0705
244.2903
393.3553
437.3904
472.2652
371.3367
56.0108
82.0614
133.1531
150.0357
166.2273
217.0576
288.3364
305.2762
327.2972
432.4350
451.3781
415.4359
60.0283
106.1017
177.2097
272.4627
Chemical Formula: C28H18Cl2N2O
Molecular Weight: 469.36
%
m/z

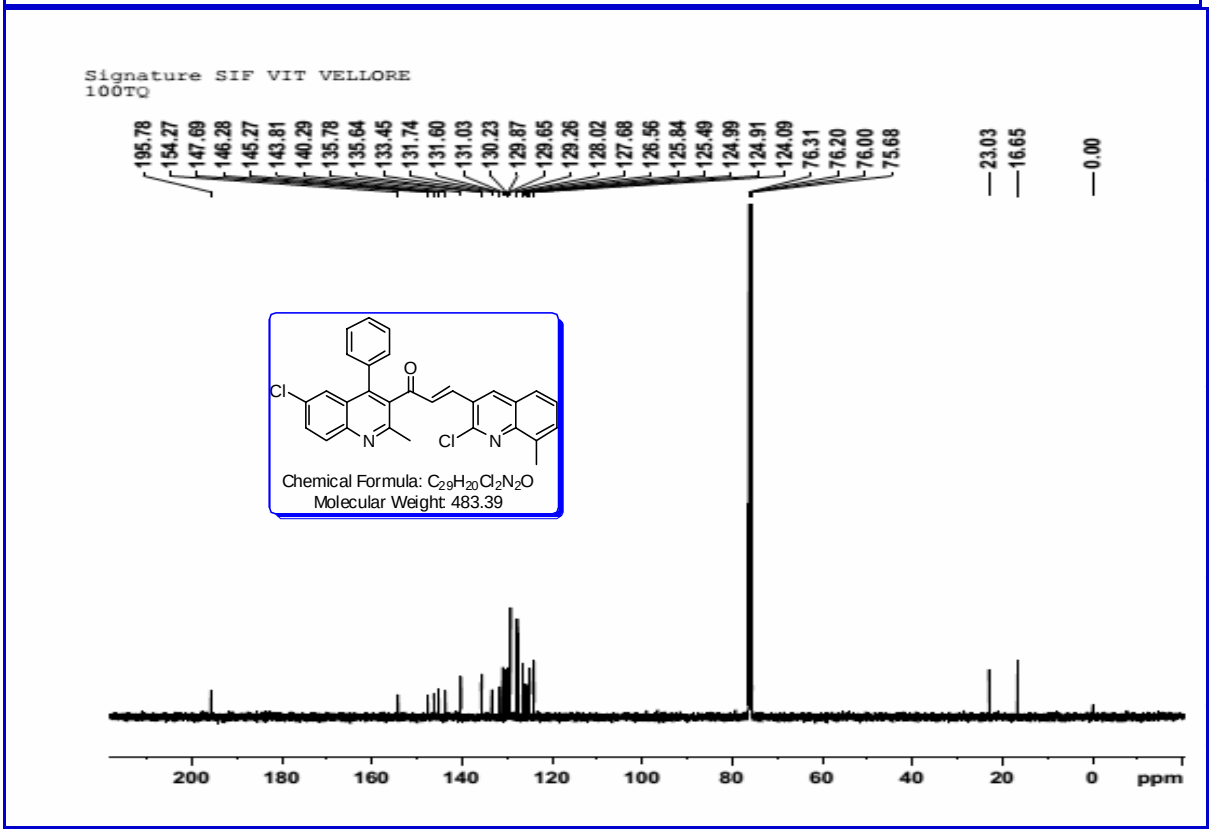

%T
3751.55
3460.30
3057.17
2962.66
2916.37
2906.73
2848.86
2250.93
1961.61
1649.14
1612.49
1579.70
1566.20
1479.40
1402.25
1392.61
1379.10
1261.45
1217.08
1095.57
1022.27
975.98
866.04
800.46
765.74
705.95
Chemical Formula: C28H18Cl2N2O
Molecular Weight: 469.36
1Cl
1/cm

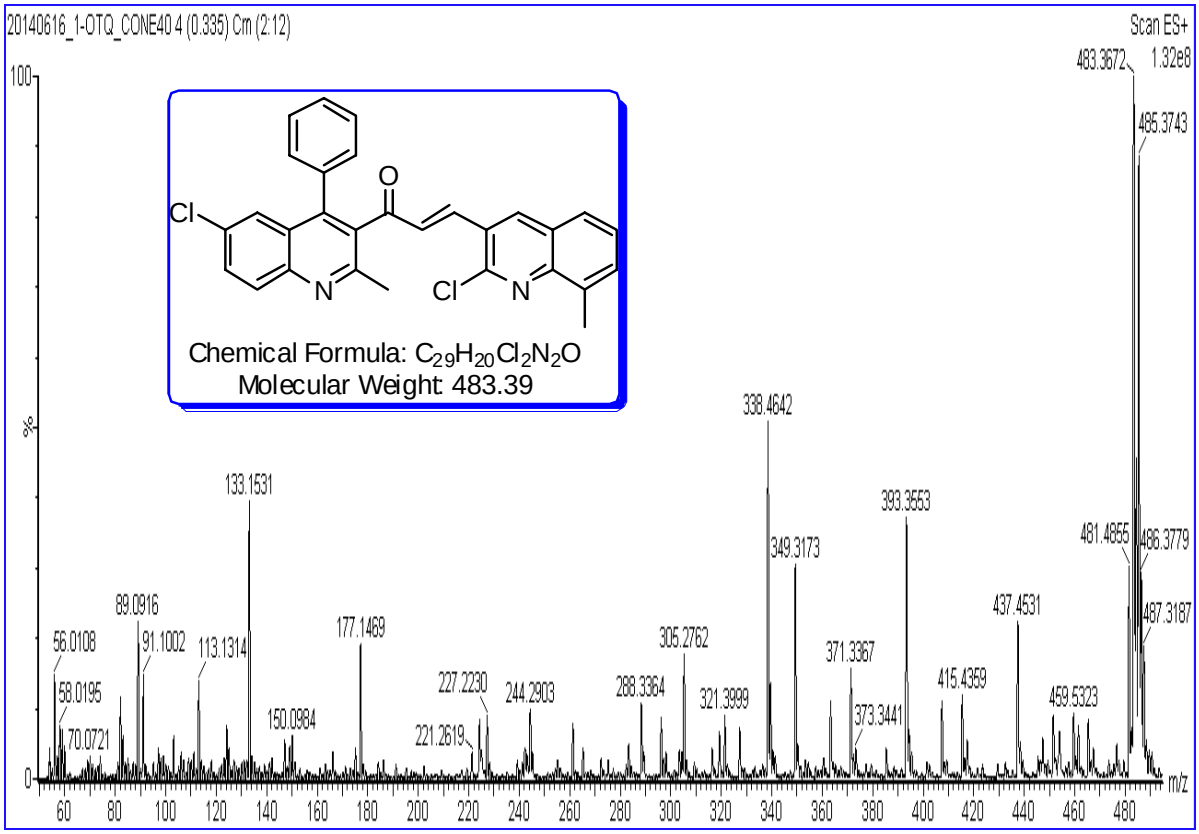

Signature SIF VIT VELLORE
1PTTQ
8.089
8.066
8.020
7.865
7.844
7.719
7.713
7.696
7.691
7.630
7.626
7.594
7.572
7.560
7.531
7.519
7.474
7.457
7.439
7.428
7.411
7.380
7.377
7.361
7.270
6.653
6.612
2.739
2.526
-0.000
Cl
O
N
Cl
N
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.00
1.01
1.02
1.08
3.38
3.06
2.09
0.99
3.05
3.00

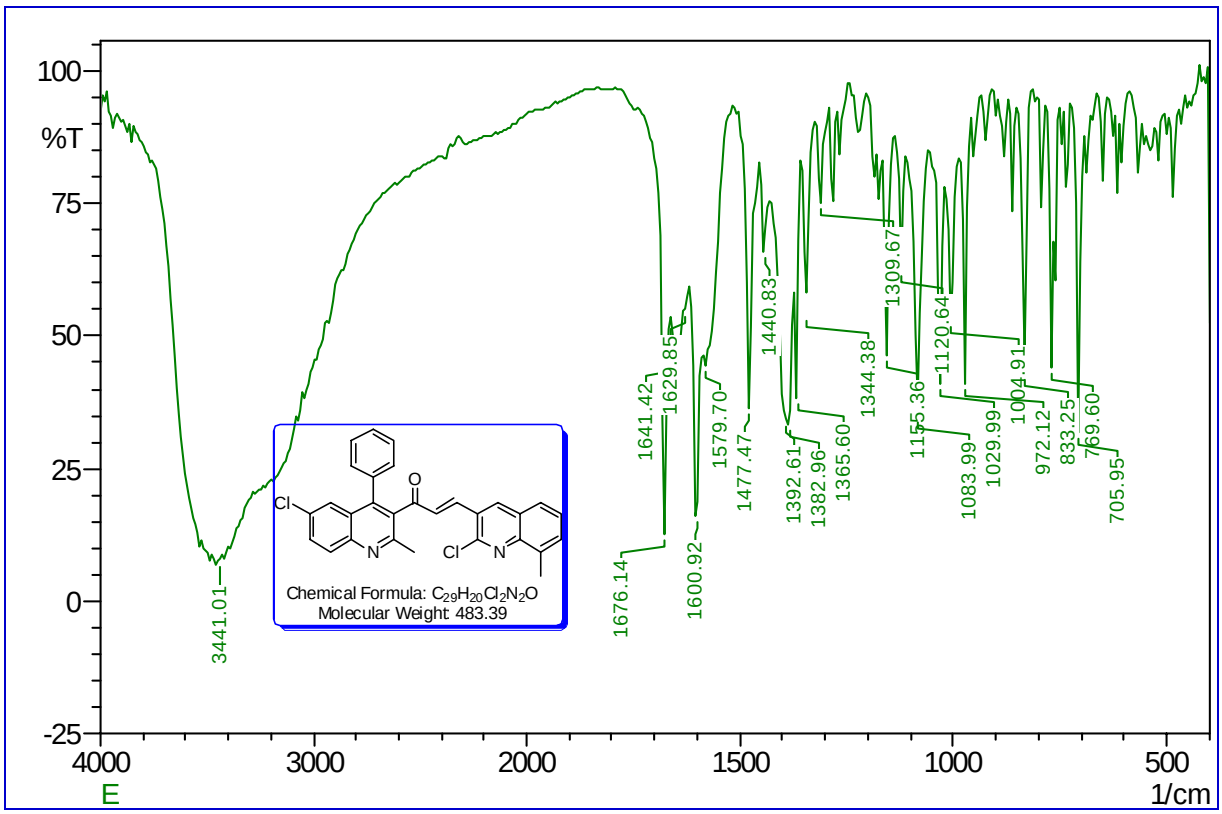

Signature SIF VIT VELLORE
1PTTQ
196.78
155.27
148.91
146.70
146.30
144.84
141.22
138.04
135.75
134.49
134.32
132.77
132.64
131.27
130.89
130.69
130.30
129.95
129.07
128.72
128.09
126.88
126.77
125.93
125.10
77.37
77.05
76.73
24.06
21.61
Cl
O
N
Cl
N
Chemical Formula: C29H20Cl2N2O
Molecular Weight: 483.39
200
180
160
140
120
100
80
60
40
20
ppm

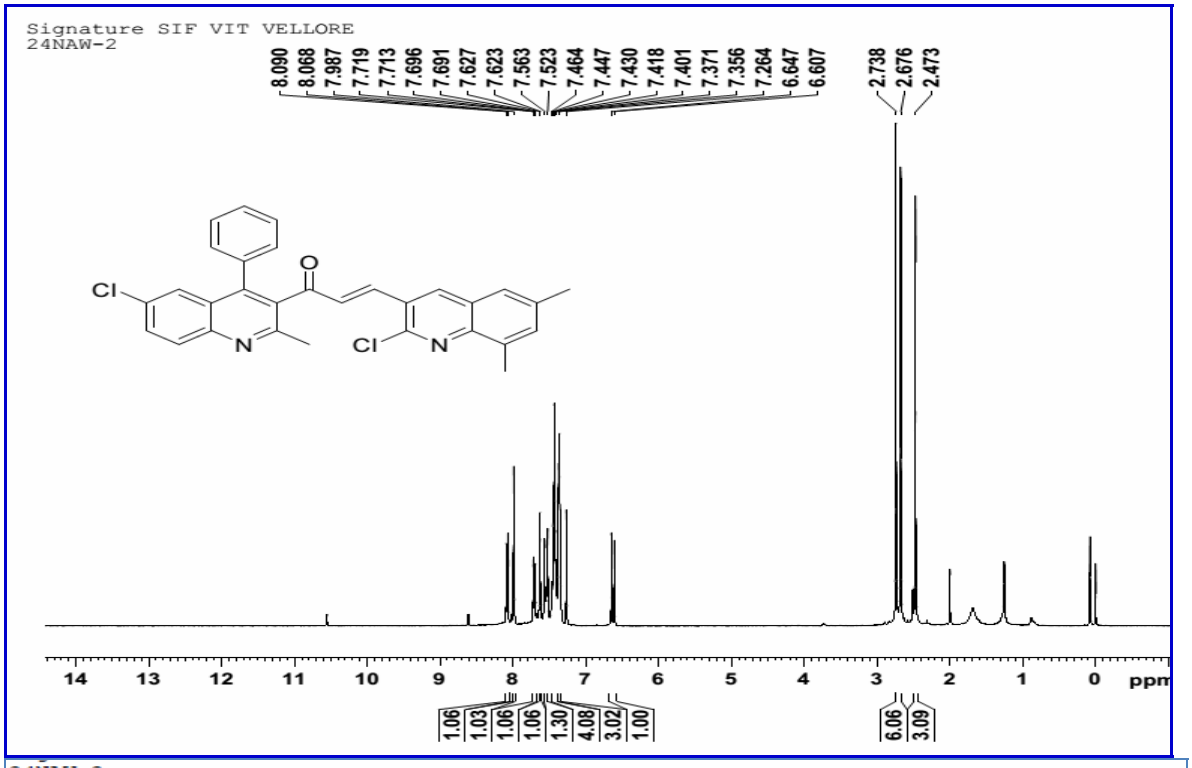

20140616_1-PTQ_CONE40 5 (0.419) Cm (2:12)
Scan ES+
1.25e8
100
%
0
m/z
Cl
O
N
Cl
N
Chemical Formula: C29H20Cl2N2O
Molecular Weight: 483.39
483.3044
338.4642
224.3993
242.0942
437.4531
133.1531
243.0354
349.3173
486.3152
393.3553
296.1790
481.4855
89.0916
244.4158
305.2762
487.3187
113.1314
177.2097
371.3367
415.4359
459.4696
56.0108
184.1755
265.2472
321.3999
417.3805
150.2240
373.3441
215.1124
266.1883
88.0873
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
400
420
440
460
480

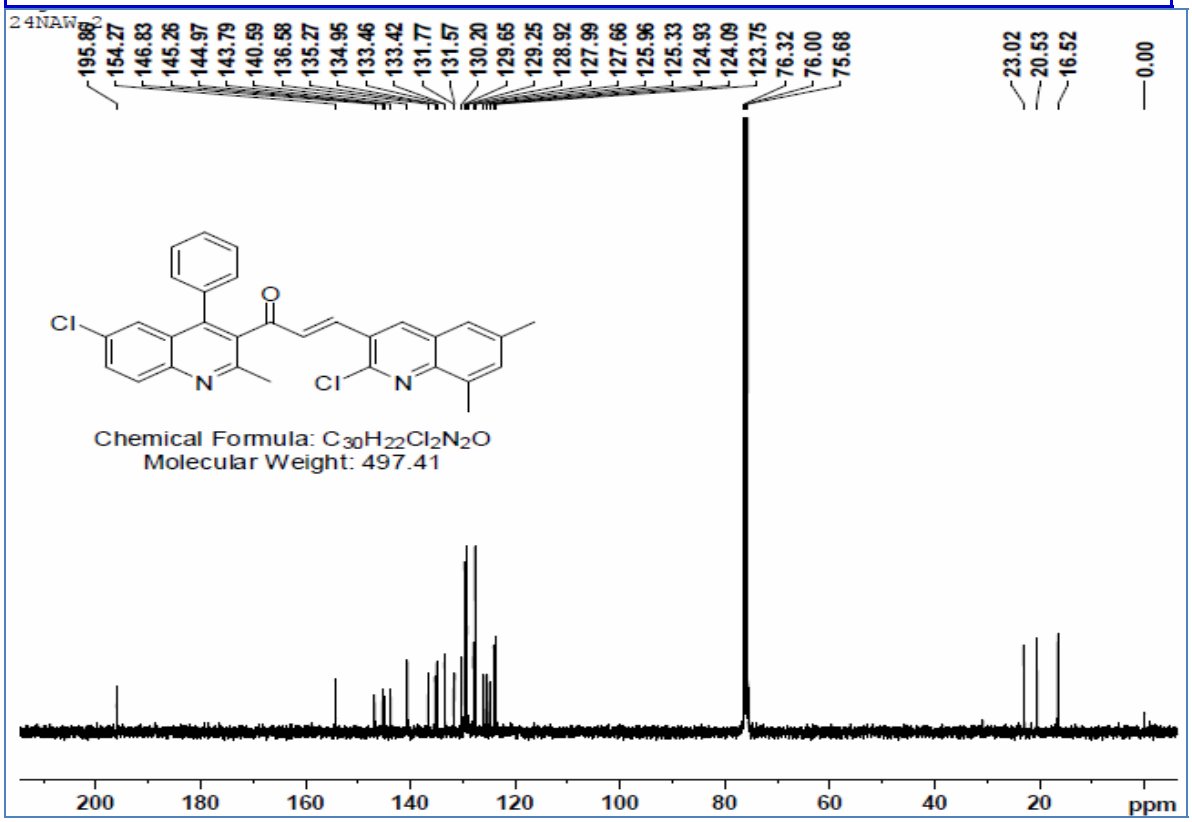

Signature SIF VIT VELLORE
100TQ
8.020
8.008
7.998
7.651
7.646
7.628
7.623
7.555
7.533
7.518
7.502
7.461
7.385
7.379
7.361
7.348
7.332
7.303
7.191
6.593
6.552
2.667
2.648
Cl
O
N
CH3 Cl
N
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.06
1.07
2.05
2.09
3.10
2.03
1.00
1.04
6.05

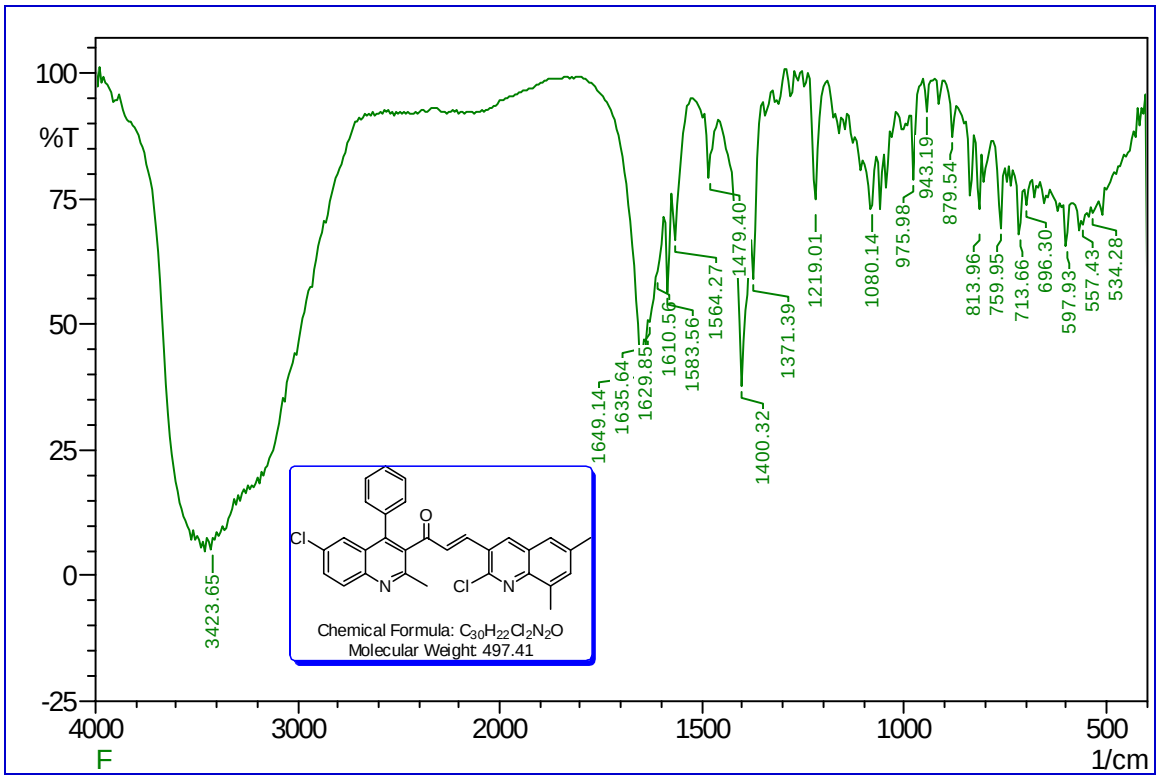

Signature SIF VIT VELLORE
100TQ
195.78
154.27
147.69
146.28
145.27
143.81
140.29
135.78
135.64
133.45
131.74
131.60
131.03
130.23
129.87
129.65
129.26
128.02
127.68
126.56
125.84
125.49
124.99
124.91
124.09
76.31
76.20
76.00
75.68
23.03
16.65
0.00
Cl
O
N
Cl
N
Chemical Formula: C29H20Cl2N2O
Molecular Weight: 483.39
200
180
160
140
120
100
80
60
40
20
0
ppm

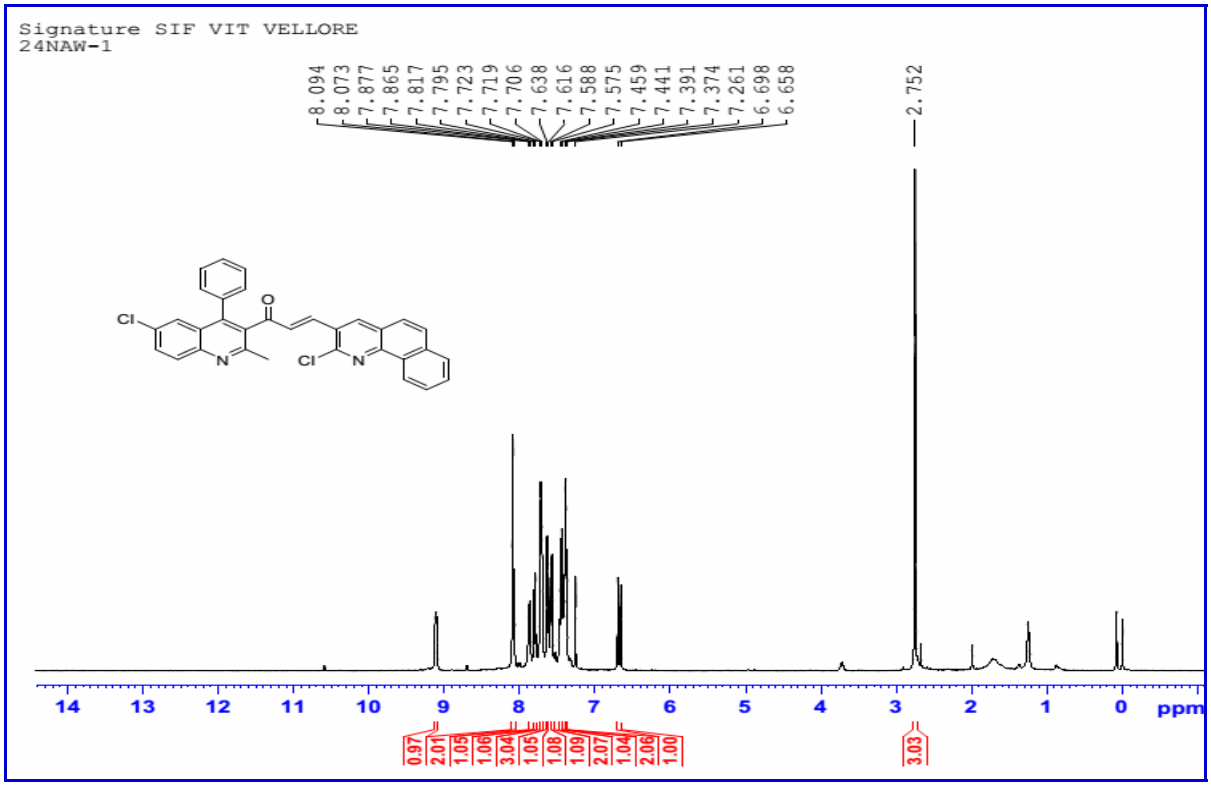

20140616_1-OTQ_CONE40 4 (0.335) Cm (2:12)
Scan ES+
1.32e8
Chemical Formula: C29H20Cl2N2O
Molecular Weight: 483.39
483.3672
485.3743
338.4642
133.1531
393.3553
349.3173
481.4855
486.3779
89.0916
487.3187
437.4531
177.1469
56.0108
91.1002
113.1314
305.2762
371.3367
227.2230
244.2903
288.3364
321.3999
415.4359
58.0195
373.3441
459.5323
150.0984
221.2619
70.0721
%
m/z

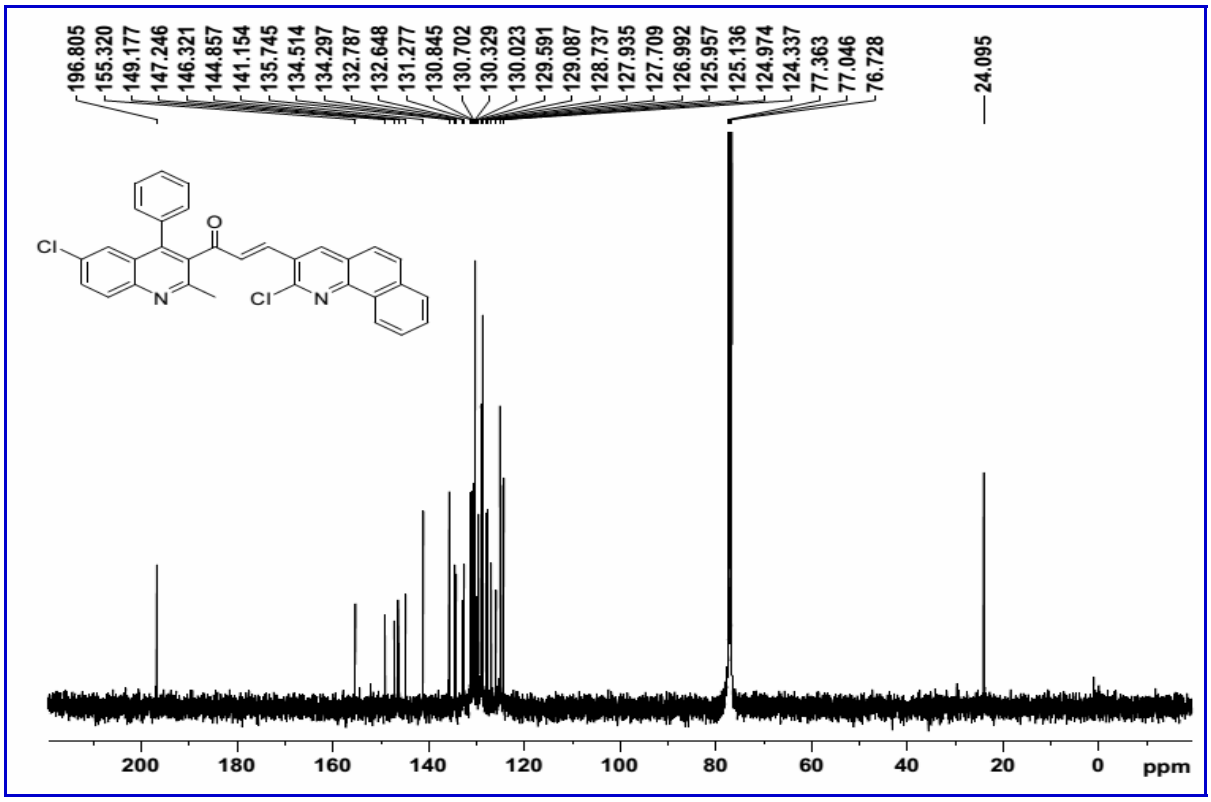

%T
Chemical Formula: C29H20Cl2N2O
Molecular Weight: 483.39
3441.01
1676.14
1641.42
1629.85
1600.92
1579.70
1477.47
1440.83
1392.61
1382.96
1365.60
1344.38
1309.67
1155.36
1120.64
1083.99
1029.99
1004.91
972.12
833.25
769.60
705.95
E
1/cm

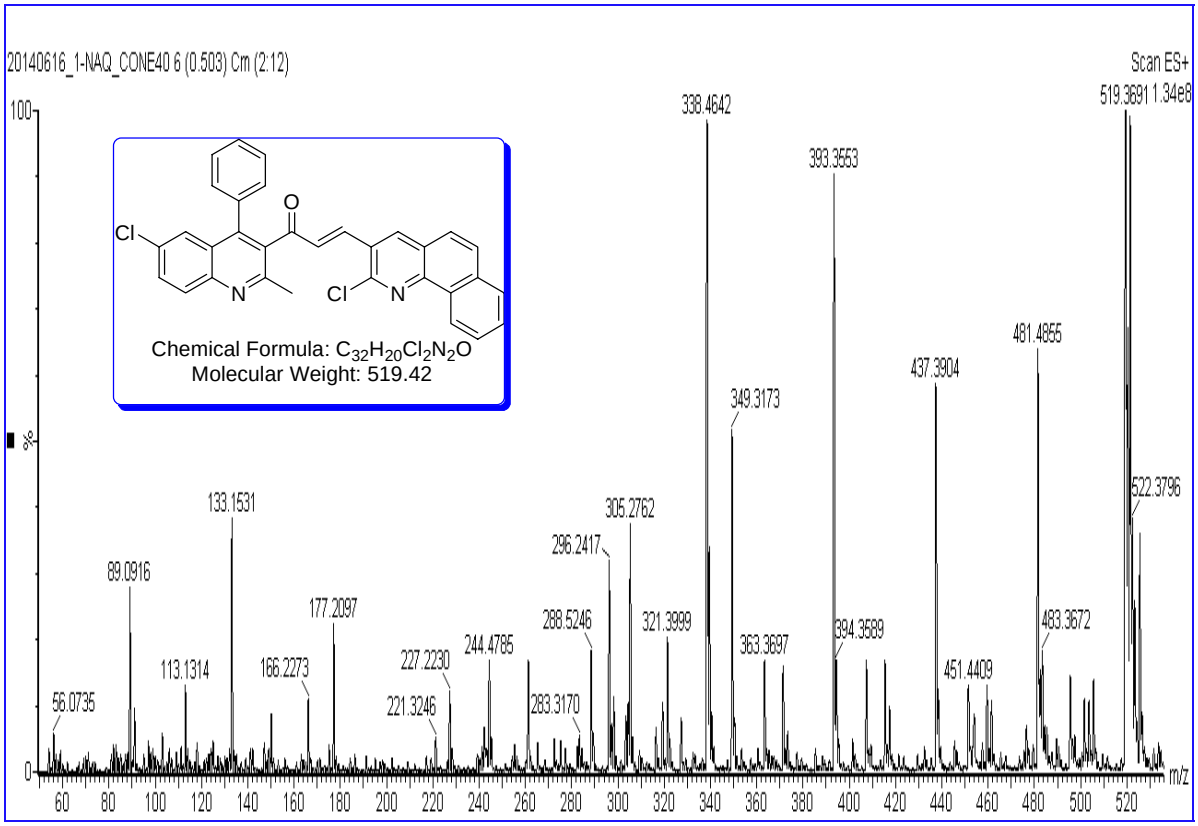

Signature SIF VIT VELLORE
24NAW-2
8.090
8.068
7.987
7.719
7.713
7.696
7.691
7.627
7.623
7.563
7.523
7.464
7.447
7.430
7.418
7.401
7.371
7.356
7.264
6.647
6.607
2.738
2.676
2.473
Cl
O
N
Cl
N
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.06
1.03
1.06
1.06
1.30
4.08
3.02
1.00
6.06
3.09

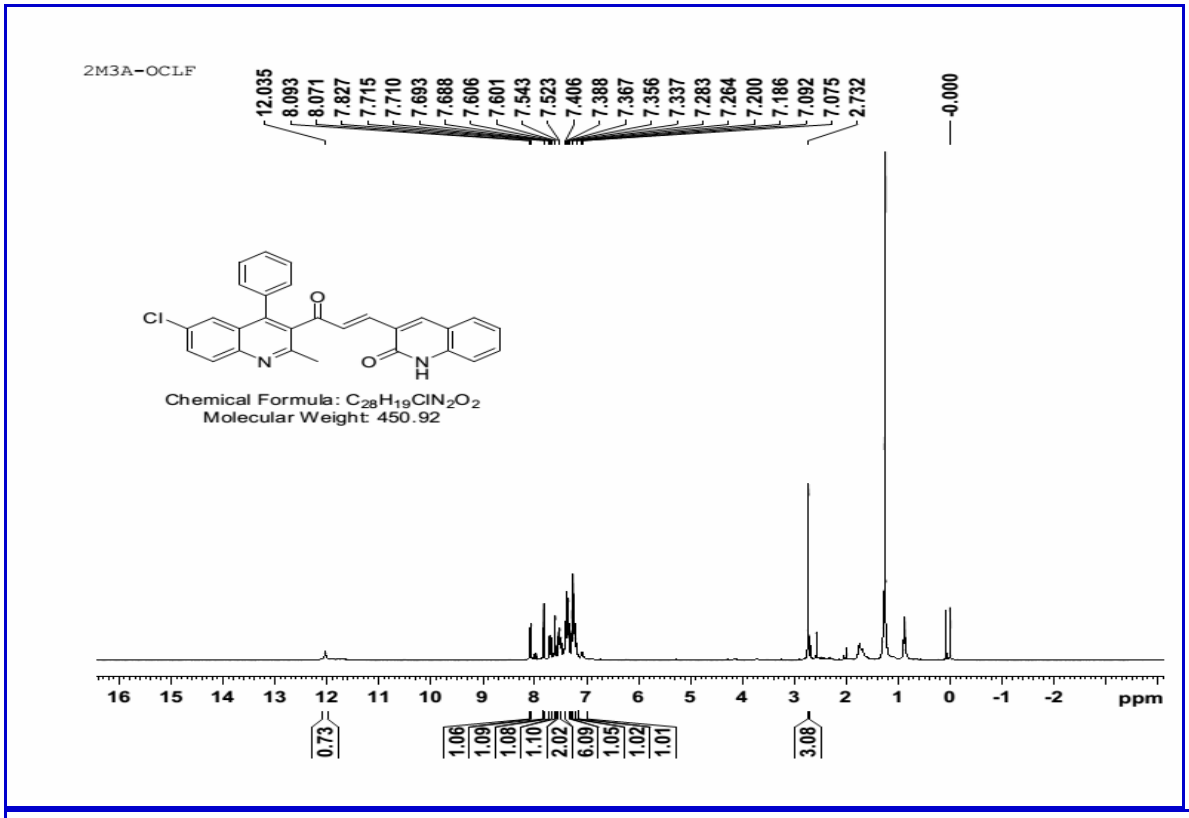

24NAW-2
195.88
154.27
146.83
145.26
144.97
143.79
140.59
136.58
135.27
134.95
133.46
133.42
131.77
131.57
130.20
129.65
129.25
128.92
127.99
127.66
125.96
125.33
124.93
124.09
123.75
76.32
76.00
75.68
23.02
20.53
16.52
0.00
Cl
O
N
Cl
N
Chemical Formula: C30H22Cl2N2O
Molecular Weight: 497.41
200 180 160 140 120 100 80 60 40 20 ppm

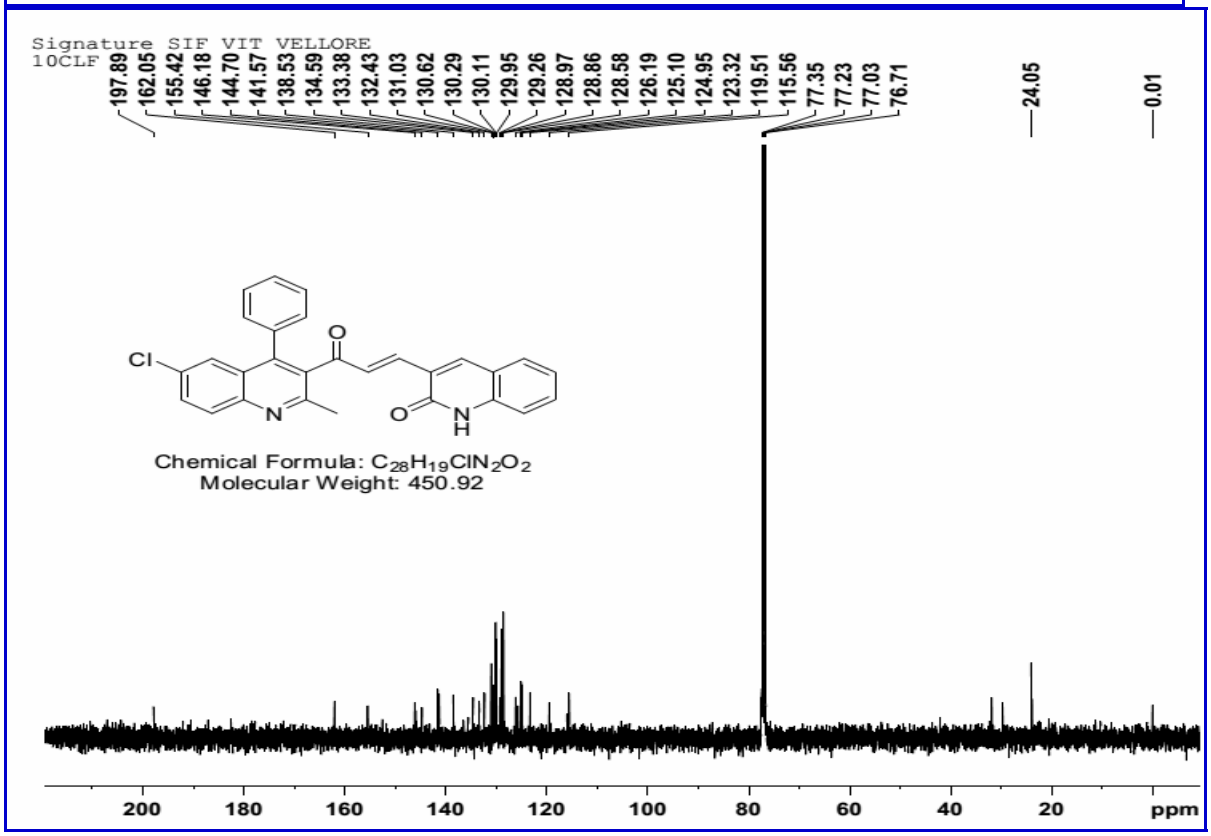

100
%T
75
50
25
0
-25
4000
3000
2000
1500
1000
500
1/cm
F
3423.65
1649.14
1635.64
1629.85
1610.56
1583.56
1564.27
1479.40
1400.32
1371.39
1219.01
1080.14
975.98
943.19
879.54
813.96
759.95
713.66
696.30
597.93
557.43
534.28
Cl
O
N
Cl
N
Chemical Formula: C30H22Cl2N2O
Molecular Weight: 497.41

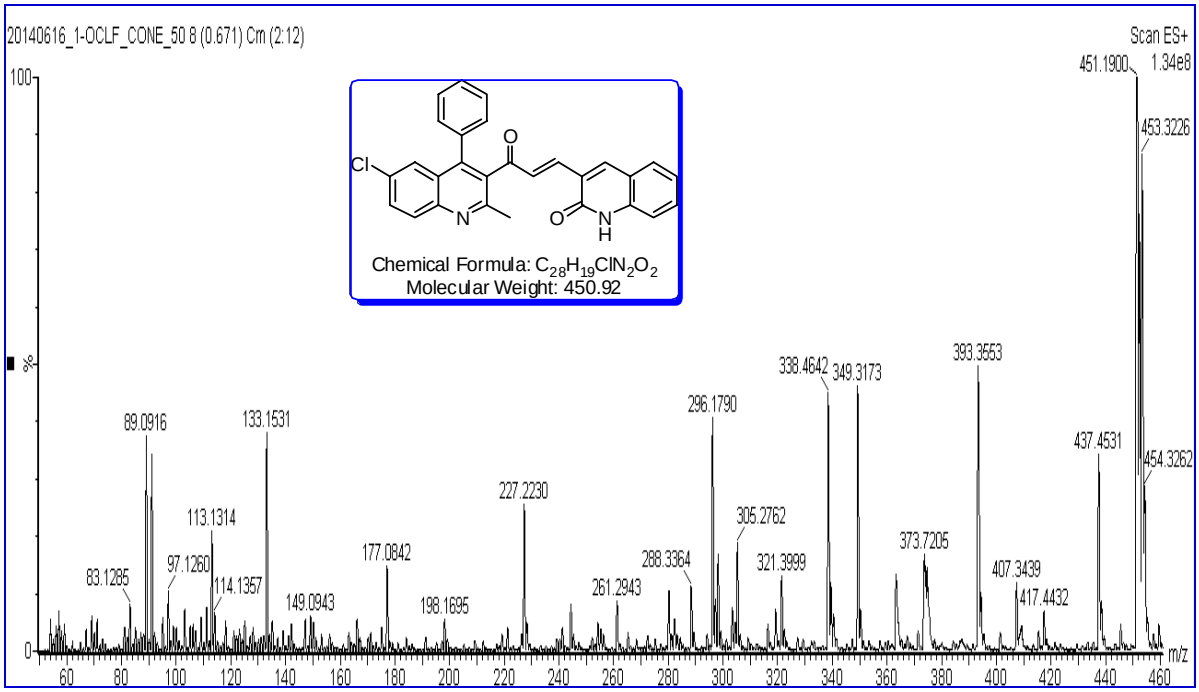

Signature SIF VIT VELLORE
24NAW-1
8.094
8.073
7.877
7.865
7.817
7.795
7.723
7.719
7.706
7.638
7.616
7.588
7.575
7.459
7.441
7.391
7.374
7.261
6.698
6.658
2.752
Cl
O
N
Cl
N
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.97
2.01
1.05
1.06
3.04
1.05
1.08
1.09
2.07
1.04
2.06
1.00
3.03

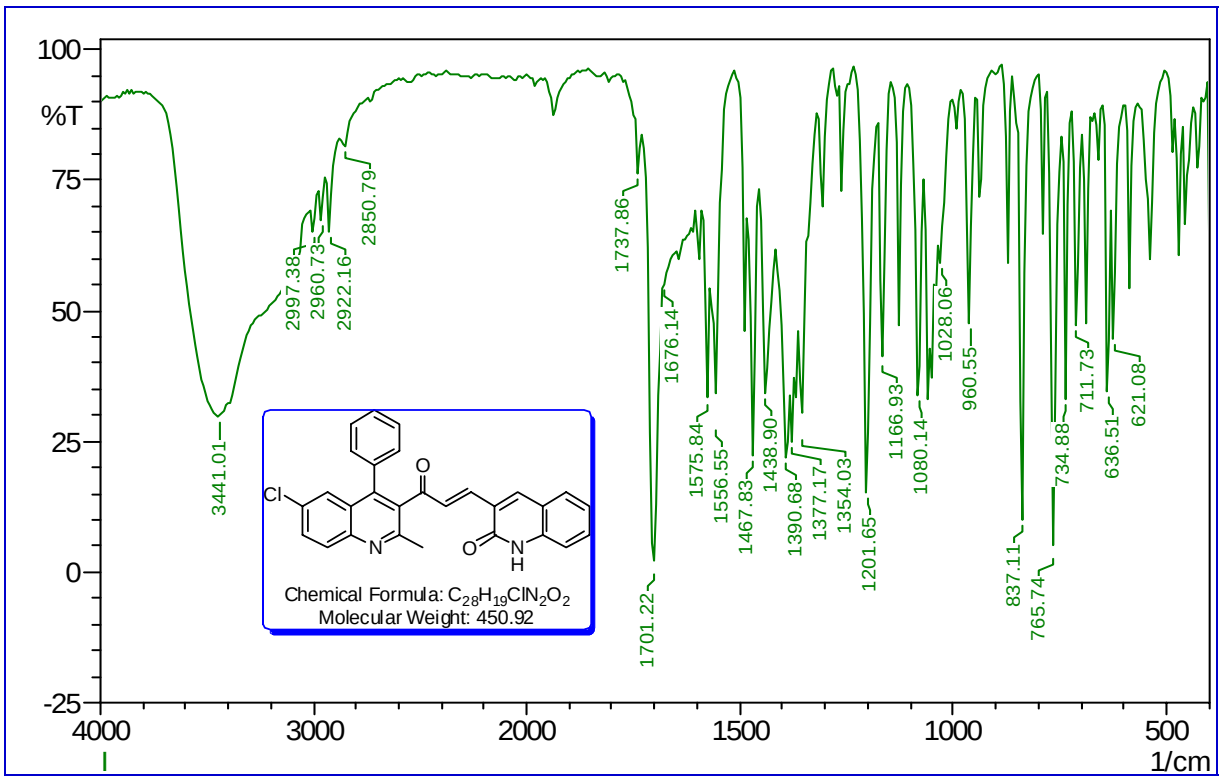

196.805
155.320
149.177
147.246
146.321
144.857
141.154
135.745
134.514
134.297
132.787
132.648
131.277
130.845
130.702
130.329
130.023
129.591
129.087
128.737
127.935
127.709
126.992
125.957
125.136
124.974
124.337
77.363
77.046
76.728
24.095
Cl
O
N
Cl
N
200
180
160
140
120
100
80
60
40
20
0
ppm

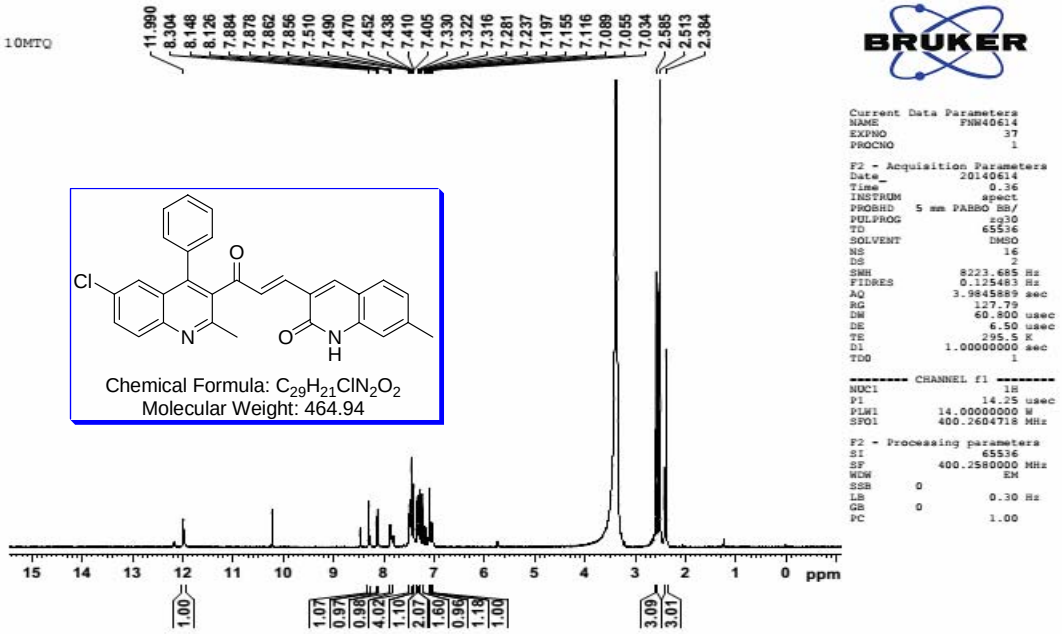

20140616_1-NAQ_CONE40 6 (0.503) Cm (2:12)
Scan ES+
519.3691 1.34e8
100
%
0
O
Cl
N
Cl
N
Chemical Formula: C32H20Cl2N2O
Molecular Weight: 519.42
338.4642
393.3553
481.4855
437.3904
349.3173
522.3796
305.2762
296.2417
133.1531
89.0916
177.2097
288.5246
321.3999
244.4785
227.2230
363.3697
394.3589
483.3672
113.1314
166.2273
451.4409
56.0735
221.3246
283.3170
m/z
60 80 100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500 520

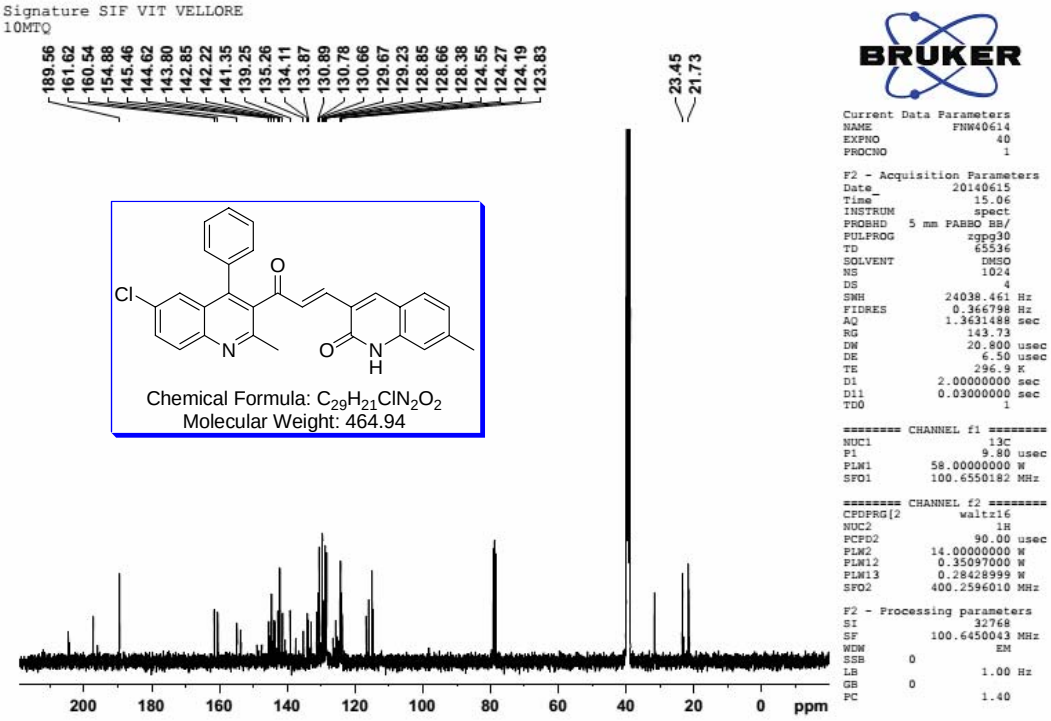

2M3A-OCLF
12.035
8.093
8.071
7.827
7.715
7.710
7.693
7.688
7.606
7.601
7.543
7.523
7.406
7.388
7.367
7.356
7.337
7.283
7.264
7.200
7.186
7.092
7.075
2.732
0.000
Cl
O
N
O
N
H
Chemical Formula: C28H19ClN2O2
Molecular Weight: 450.92
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
0.73
1.06
1.09
1.08
1.10
2.02
6.09
1.05
1.02
1.01
3.08


Signature SIF VIT VELLORE
10CLF
197.89
162.05
155.42
146.18
144.70
141.57
138.53
134.59
133.38
132.43
131.03
130.62
130.29
130.11
129.95
129.26
128.97
128.86
128.58
126.19
125.10
124.95
123.32
119.51
115.56
77.35
77.23
77.03
76.71
24.05
0.01
Cl
O
N
O
N
H
Chemical Formula: C28H19ClN2O2
Molecular Weight: 450.92
200 180 160 140 120 100 80 60 40 20 ppm

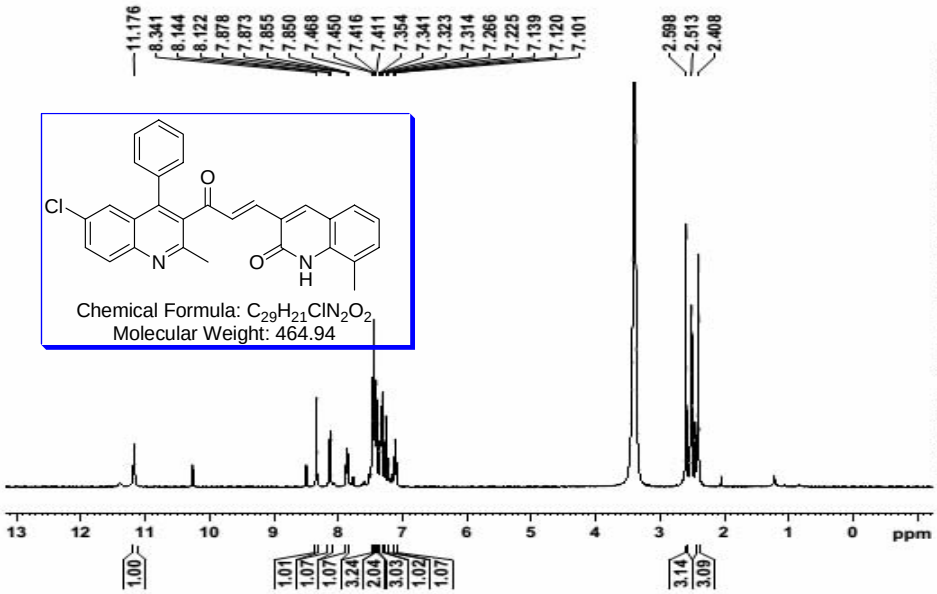

20140616_1-OCLF_CONE_50 8 (0.671) Cm (2:12)
Scan ES+
1.34e8
100
%
0
m/z
Chemical Formula: C28H19ClN2O2
Molecular Weight: 450.92
451.1900
453.3226
454.3262
437.4531
393.3553
338.4642
349.3173
296.1790
373.7205
305.2762
321.3999
288.3364
227.2230
261.2943
177.0842
133.1531
89.0916
113.1314
97.1260
114.1357
83.1285
149.0943
198.1695
407.3439
417.4432
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
400
420
440
460


100
%T
75
50
25
0
-25
4000
3000
2000
1500
1000
500
1/cm
Chemical Formula: C28H19ClN2O2
Molecular Weight: 450.92
3441.01
2997.38
2960.73
2922.16
2850.79
1737.86
1676.14
1701.22
1575.84
1556.55
1467.83
1438.90
1390.68
1377.17
1354.03
1201.65
1166.93
1080.14
1028.06
960.55
837.11
765.74
734.88
711.73
636.51
621.08


10MTQ
11.990
8.304
8.148
8.126
7.884
7.878
7.862
7.856
7.510
7.490
7.470
7.452
7.438
7.410
7.405
7.330
7.322
7.316
7.281
7.237
7.197
7.155
7.116
7.089
7.055
7.034
2.585
2.513
2.384
Cl
O
N
O
N
H
Chemical Formula: $C_{29}H_{21}ClN_2O_2$
Molecular Weight: 464.94
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.00
1.07
0.97
0.98
4.02
1.10
2.07
1.60
0.96
1.18
1.00
3.09
3.01
BRUKER
Current Data Parameters
NAME FNW40614
EXPNO 37
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140614
Time 0.36
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 127.79
DW 60.800 usec
DE 6.50 usec
TE 295.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.25 usec
PLW1 14.00000000 W
SFO1 400.2604718 MHz
F2 - Processing parameters
SI 65536
SF 400.2580000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


Signature SIF VIT VELLORE
10MTQ
189.56
161.62
160.54
154.88
145.46
144.62
143.80
142.85
142.22
141.35
139.25
135.26
134.11
133.87
130.89
130.78
130.66
129.67
129.23
128.85
128.66
128.38
124.55
124.27
124.19
123.83
23.45
21.73
Cl
O
N
O
N
H
Chemical Formula: $C_{29}H_{21}ClN_2O_2$
Molecular Weight: 464.94
200 180 160 140 120 100 80 60 40 20 0 ppm
BRUKER
Current Data Parameters
NAME FNW40614
EXPNO 40
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140615
Time 15.06
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 143.73
DW 20.800 usec
DE 6.50 usec
TE 296.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.80 usec
PLW1 58.00000000 W
SFO1 100.6550182 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.35097000 W
PLW13 0.28428999 W
SFO2 400.2596010 MHz
F2 - Processing parameters
SI 32768
SF 100.6450043 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Signature SIF VIT VELLORE
100TQ

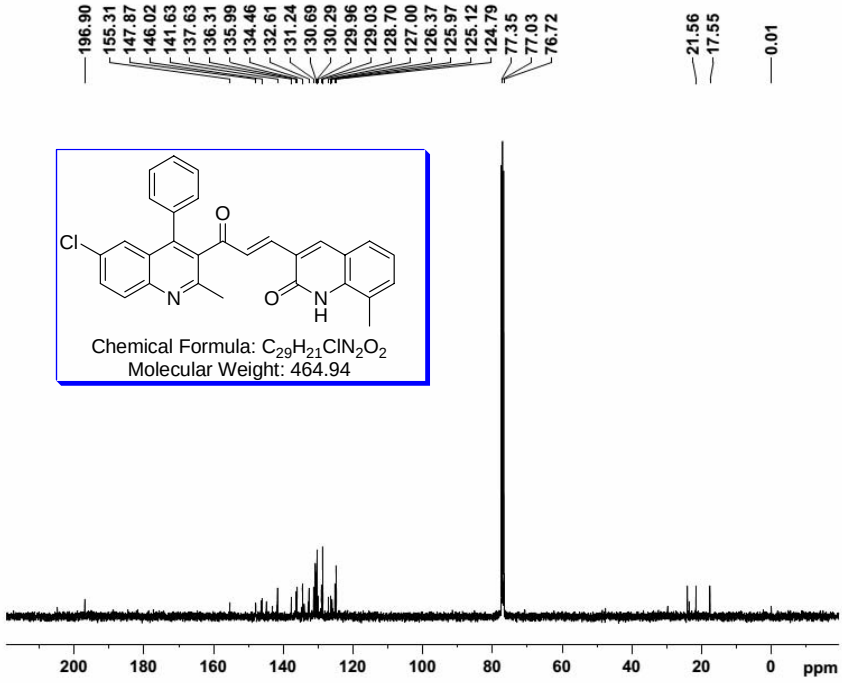


Chemical Formula: $C_{29}H_{21}ClN_2O_2$
Molecular Weight: 464.94

BRUKER

```
Current Data Parameters
NAME                  FNW40614
EXPNO                       43
PROCNO                       1

F2 - Acquisition Parameters
Date_               20140615
Time                   16.24
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                        16
DS                         2
SWH                 8223.685 Hz
FIDRES              0.125483 Hz
AQ                  3.9845889 sec
RG                      88.69
DW                     60.800 usec
DE                      6.50 usec
TE                     296.3 K
D1                  1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       1H
P1                      14.25 usec
PLW1               14.00000000 W
SFO1              400.2604718 MHz

F2 - Processing parameters
SI                        65536
SF                 400.2580000 MHz
WDW                          EM
SSB                 0
LB                          0.30 Hz
GB                  0
PC                          1.00
```

1007Q

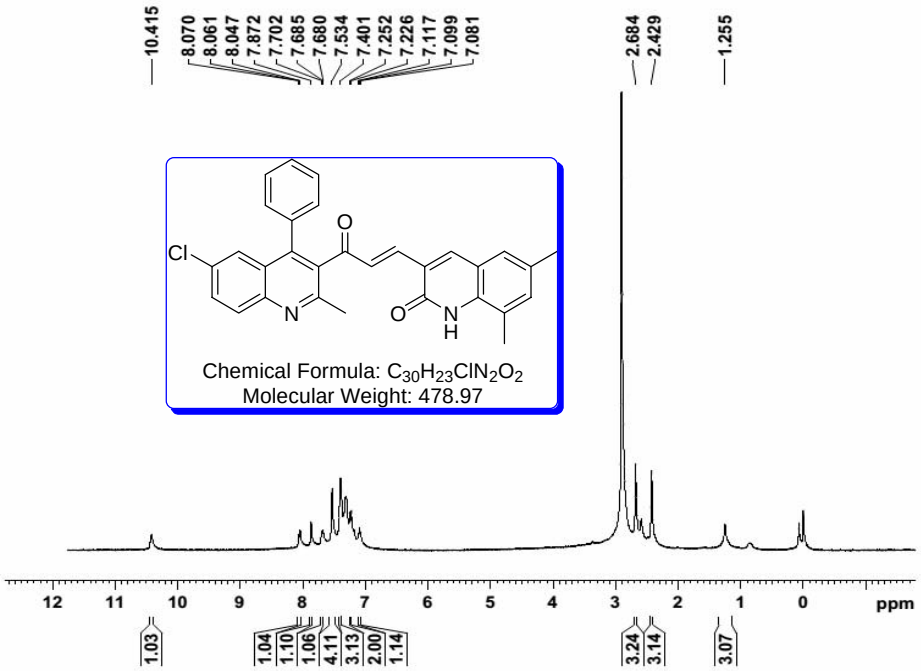


Chemical Formula: $C_{29}H_{21}ClN_2O_2$
Molecular Weight: 464.94

BRUKER

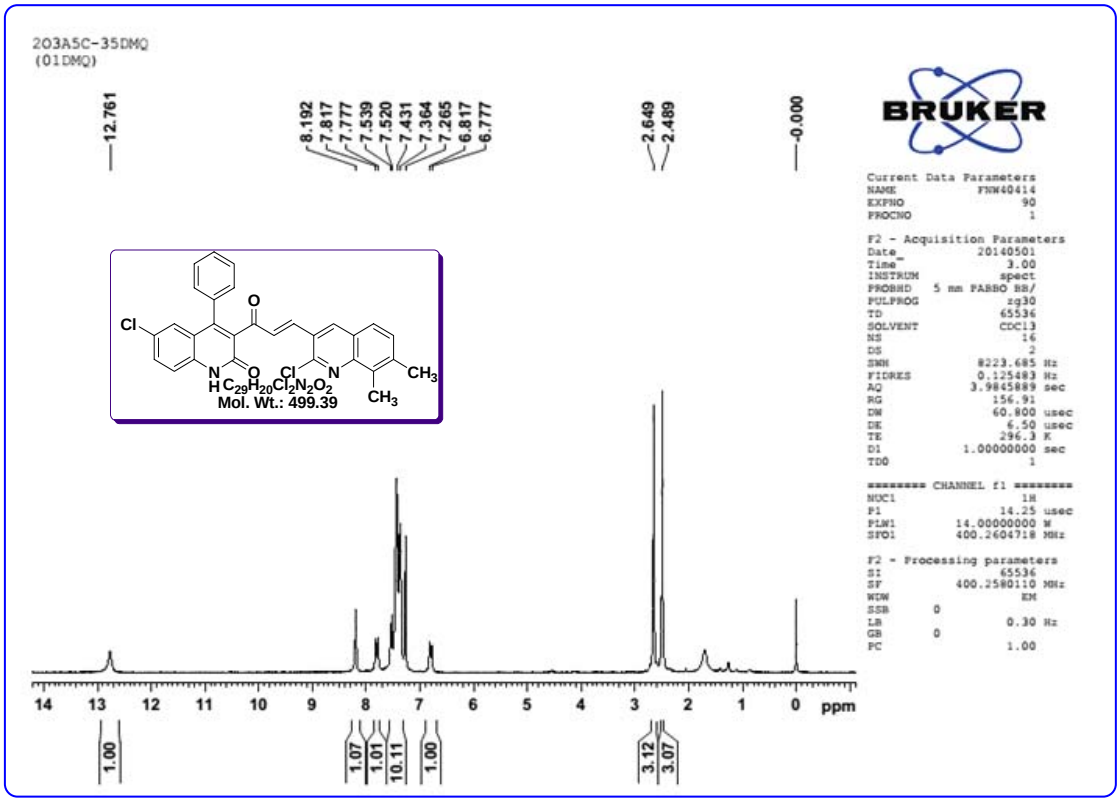
```
Current Data Parameters
NAME                  FNW40614
EXPNO                       28
PROCNO                       1

F2 - Acquisition Parameters
Date_               20140609
Time                   19.34
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG              zgpg30
TD                    65536
SOLVENT               CDC13
NS                      512
DS                        4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631488 sec
RG                     127.79
DW                     20.800 usec
DE                      6.50 usec
TE                     297.6 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                      13C
P1                       9.80 usec
PLW1               58.00000000 W
SFO1              100.6550182 MHz

======== CHANNEL f2 ========
CPDPRG[2              waltz16
NUC2                       1H
PCPD2                   90.00 usec
PLW2               14.00000000 W
PLW12               0.35097000 W
PLW13               0.28428999 W
SFO2              400.2596010 MHz

F2 - Processing parameters
SI                        32768
SF                 100.6449540 MHz
WDW                          EM
SSB                 0
LB                          1.00 Hz
GB                  0
PC                          1.40
```

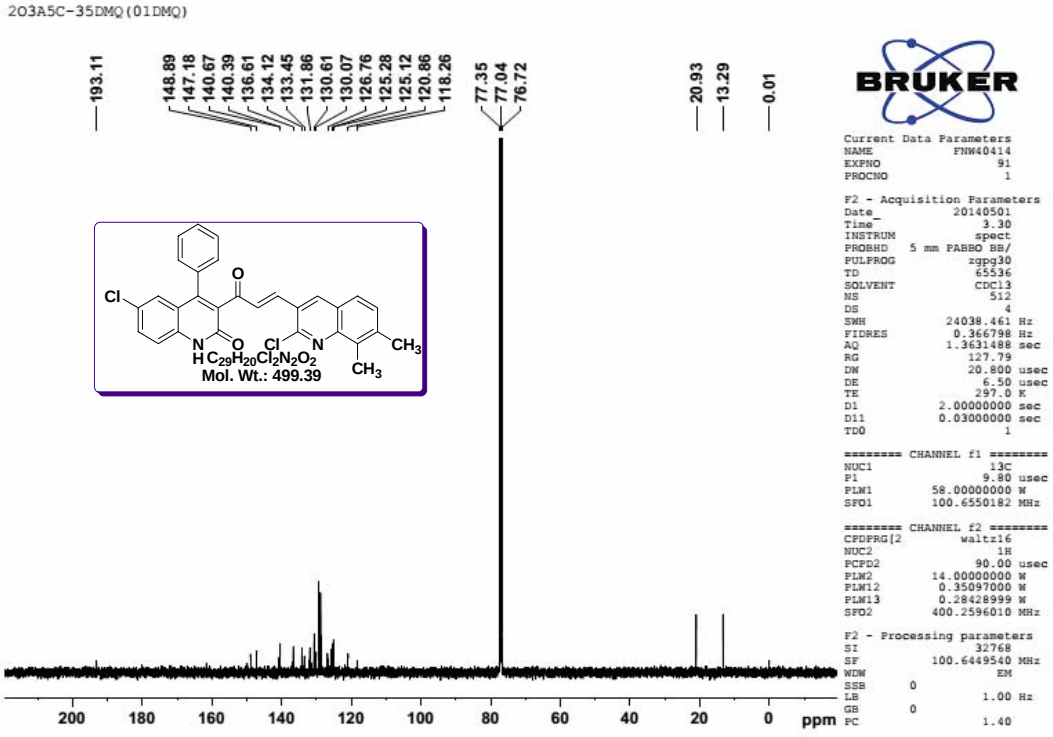
Signature SIF VIT VELLORE
124DMQ



BRUKER

```
Current Data Parameters
NAME                  FNW40614
EXPNO                       31
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20140609
Time                     20.13
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                         16
DS                          2
SWH                  8223.685 Hz
FIDRES               0.125483 Hz
AQ                   3.9845889 sec
RG                      175.97
DW                      60.800 usec
DE                       6.50 usec
TE                      297.1 K
D1                   1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                        1H
P1                       14.25 usec
PLW1                14.00000000 W
SFO1               400.2604718 MHz

F2 - Processing parameters
SI                      65536
SF                 400.2598783 MHz
WDW                        EM
SSB                 0
LB                       0.30 Hz
GB                  0
PC                       1.00
```


2O3A5C-35DMQ
(01DMQ)
12.761
8.192
7.817
7.777
7.539
7.520
7.431
7.364
7.265
6.817
6.777
2.649
2.489
-0.000
Cl
O
N
O
Cl
N
CH3
CH3
H C29H20Cl2N2O2
Mol. Wt.: 499.39
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.00
1.07
1.01
10.11
1.00
3.12
3.07
BRUKER
Current Data Parameters
NAME FNW40414
EXPNO 90
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140501
Time 3.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 156.91
DW 60.800 usec
DE 6.50 usec
TE 296.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.25 usec
PLW1 14.00000000 W
SFO1 400.2604718 MHz
F2 - Processing parameters
SI 65536
SF 400.2580110 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


2O3A5C-35DMQ(01DMQ)
193.11
148.89
147.18
140.67
140.39
136.61
134.12
133.45
131.86
130.61
130.07
126.76
125.28
125.12
120.86
118.26
77.35
77.04
76.72
20.93
13.29
0.01
Cl
O
N
O
Cl
N
CH3
CH3
H C29H20Cl2N2O2
Mol. Wt.: 499.39
200 180 160 140 120 100 80 60 40 20 0 ppm
BRUKER
Current Data Parameters
NAME FNW40414
EXPNO 91
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140501
Time 3.30
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 127.79
DW 20.800 usec
DE 6.50 usec
TE 297.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.80 usec
PLW1 58.00000000 W
SFO1 100.6550182 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.35097000 W
PLW13 0.28428999 W
SFO2 400.2596010 MHz
F2 - Processing parameters
SI 32768
SF 100.6449540 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40