Electronic Supplementary Material (ESI) for RSC Advances.

Synthesis of 2-hydroxy-3-alkyl-2-phenyl-2, 3-dihydroquinazolin-4(1*H*)-one via molybdenum hexacarbonyl mediated CO gas-and ligand free carbonylative reactions.

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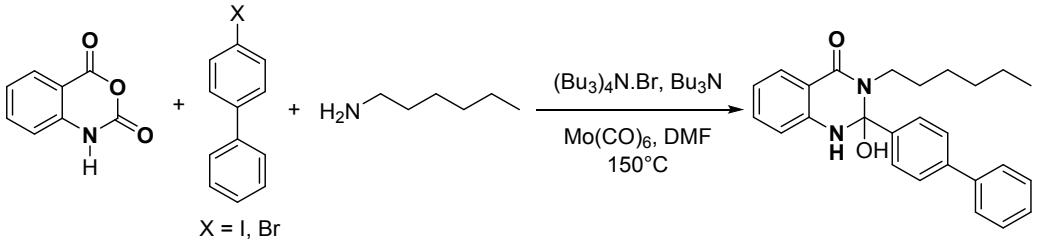
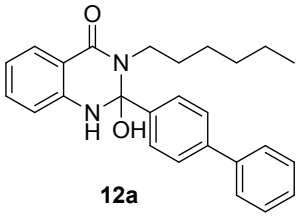
Supporting Information **P. No**

General methods: Unless stated otherwise, reactions were performed under nitrogen atmosphere using oven dried glassware. Reactions were monitored by thin layer chromatography (TLC) on silica gel plates (60 F254), visualizing with ultraviolet light or iodine spray. Flash chromatography was performed on silica gel (100-200 mesh) using distilled hexane, ethyl acetate, dichloromethane. ^{1}H NMR and 13C NMR spectra were determined in $CDCl_3$ or DMSO-d_6 solution by using 400 or 100 MHz spectrometers, respectively. Proton chemical shifts (δ) are relative to tetramethylsilane (TMS, δ = 0.00) as internal standard and expressed in ppm. Spin multiplicities are given as s (singlet), d (doublet), t (triplet) and m (multiplet) as well as b (broad). Coupling constants (*J*) are given in hertz. Melting points were determined using melting point B-540 apparatus and are uncorrected. HRMS was determined using waters LCT premier XETOF ARE-047 apparatus.

General process for the synthesisof substituted2-hydroxy-2, 3-dihydroquinazolin-4-(1*H*)-one:

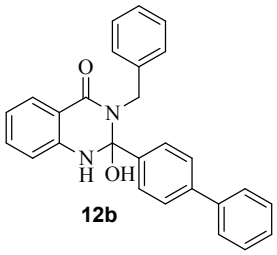


General procedure: A mixture of Isatoic anhydride (500 mg, 3.0 mmol), aryl halides (868 mg, 3.0 mmol), amine (344 mg, 3.4 mmol), Mo $(CO)_6$ (820 mg, 3.0 mmol), $Et_4N.Br$ (200 mg, 0.6 mmol), and Bu_3N (689 mg, 3.7 mmol), in DMF (5 mL) was heated to 150°C under argon balloon. Maintained the reaction mass for 15 to 18 hours and check the progress of reaction as indicated by TLC. The reaction mixture was cooled to room temperature and added water (20 mL) and ethyl acetate (20 mL), total reaction mixture was filtered through celite bed and bed washed with Ethyl acetate (3*20 mL) and both layers were separated and aqueous layer was back extracted with ethyl acetate (20 mL) and then combined organic layers was washed with water (20 mL) and dry over anhydrous Na_2SO_4 and the total organic layer was concentrated under reduced pressure to afford the crude hydroxy compounds. The above crude was purified by (100-200 mesh silica gel) gravity column purification and product was eluted at 8 to 10 % of EtOAc/Hexanes to give pure hydroxy compounds of 10a to 15o.



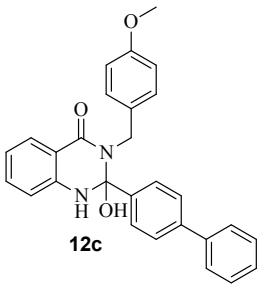
12a

2-([1, 1'-biphenyl]-4-yl)-3-hexyl-2-hydroxy-2, 3-dihydroquinazolin-4(1*H*)-one (12a): White solid, Yield-72 %, mp: 97-105°C, IR (KBr) = 3325, 2922, 1672, 1548, 1310, 1076, 984, 858, 797, 745, 692, 450 cm^{-1}, ^1H NMR (400 MHz, $CDCl_3$): δ=12.16 (s, 1H), 8.84 (d, *J* = 8.4 Hz, 1H), 8.12 (d, *J*= 8.4 Hz, 2H), 7.74 (d, *J* = 8.4 Hz, 2H), 7.65 (d, *J* = 7.6 Hz, 2H), 7.55 – 7.26 (m, 5H), 7.13 (t, *J* = 7.6 Hz, 1H). 6.28 (s, br, 1H), 3.50 – 3.43 (m, 2H), 1.68 – 1.56 (m, 2H), 1.40 – 1.25 (m, 6H), 0.91 – 0.89 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ =169.2, 144.54, 140.10, 139.83, 133.55, 132.51, 128.91-(2C), 127.97-(2C), 127.92- (2C), 127.42-(2C), 127.23- (2C), 126.4, 122.8, 121.6, 120.8, 40.1, 31.4, 29.4, 26.6, 22.5, 13.9; HRMS: m/z calcd for $C_{26}H_{29}N_2O_2$ (M+H) 401.2249, found 401.2241.



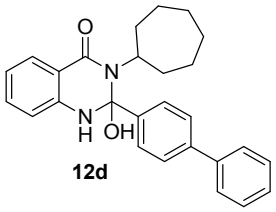
12b

2-([1, 1'- biphenyl]-4-yl)-3-benzyl-2-hydroxy-2, 3-dihydroquinazolin-4(1*H*)-one (12b): White solid, Yield- 67 %, mp:154-158°C , IR (KBr) = 3325, 2922, 1672, 1548, 1310, 1076, 984, 745, 692, 450 cm^{-1}, ^1H NMR (400 MHz, $CDCl_3$): δ =12.20 (s, 1H), 8.86 (d, *J*=, 8.4 Hz, 1H), 8.13 (d, *J*= 8.4 Hz, 2H), 7.75 (d, *J*= 8.0 Hz, 2H), 7.56 -7.32 (m, 12H), 7.12 (t, *J*= 7.6 Hz, 1H), 6.56 (s, 1H), 4.68 (d, *J*= 5.6 Hz, 2H), ^{13}C NMR (100 MHz, $CDCl_3$): δ = 167.0, 144.3, 139.9, 138.1, 132.9, 132.8, 128.8, 128.7, 128.6, 127.97-(2C), 127.93-(2C), 127.90-(2C), 127.83, 127.81, 127.77, 127.60, 127.48, 127.40, 127.21, 127.17, 126.5, 122.8, 121.6, 44.0; HRMS: m/z calcd for $C_{27}H_{23}N_2O_2$ (M+H) 406.1760, found 406.1757.



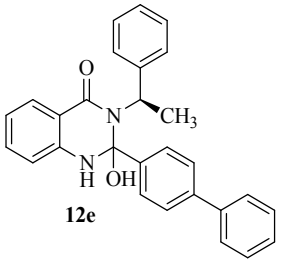
12c

2-([1, 1'-biphenyl]-4-yl)-2-hydroxy-3-(4-methoxybenzyl)-2, 3-dihydroquinazolin-4(1*H*)-one (12c): Brown solid, Yield-58 %, mp : 168-172°C, IR (KBr) = 3328, 2926, 1638, 1512, 1428, 1249, 1027, 809, 746, 580, 520 cm^{-1}, ^1H NMR (400 MHz, $CDCl_3$): δ= 12.22 (s, 1H), 8.86 (d, *J*= 8.4 Hz, 1H), 8.14 (d, *J*= 8.4 Hz, 1H), 7.86 (d, *J*= 8.4 Hz, 2H), 7.75 (d, *J*= 8.4 Hz, 1H), 7.66 (d, *J*= 6.4 Hz, 2H), 7.56-7.49 (m, 5H), 7.44-7.38 (m, 1H), 7.38-7.26 (m, 2H), 6.91-6.85 (m, 2H), 6.36 (s, 1H), 4.61 (d, *J*= 4.8 Hz, 2H), 3.80 (s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$): δ = 169.00, 166.30, 159.10, 144.27, 140.05, 133.51, 133.05, 132.76, 130.25, 129.27, 129.24, 128.88, 128.87, 127.95, 127.92, 127.45, 127.39, 127.20, 127.17, 127.14,126.56, 122.78, 121.57, 120.26, 114.24, 114.14, 55.28, 43.6; HRMS: m/z calcd for $C_{28}H_{25}N_2O_3$ (M+H) 437.1865, found 437.1865.



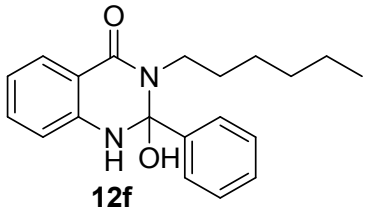
12d

2-([1, 1'- biphenyl]-4-yl)-3-cycloheptyl-2-hydroxy-2, 3-dihydroquinazilin-4 (1*H*)-one (12d): White solid, Yield- 70 %, mp: 139-142°C , IR (KBr) = 3337, 2923, 1628, 1512, 1446, 1278, 1006, 901, 743, 662, 546 cm^{-1}, ^1H NMR (400 MHz, $CDCl_3$): δ= 12.09 (s, 1H), 8.82 (d, *J*= 8.4 Hz, 1H), 8.12 (d, *J*= 8.4 Hz, 2H), 7.74 (d, *J*= 8.4 Hz, 2H), 7.59-7.41 (m, 7H), 7.10 (t, *J*= 7.2 Hz, 1H), 6.23 (s, br, 1H), 4.19-4.17 (m, 1H), 2.08-2.02 (m, 2H), 1.67-1.56 (m, 10H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 168.02, 144.44, 143.97, 140.04, 140.01, 139.81, 133.70, 132.43, 128.86-(2C), 128.85-(2C), 127.92-(2C), 127.89-(2C), 127.30-(2C), 127.12, 50.95, 50.88, 35.16, 35.00, 27.99, 27.96, 24.11, 24.00; HRMS: m/z calcd for $C_{27}H_{29}N_2O_2$ (M+H) 413.2229, found 413.2228.



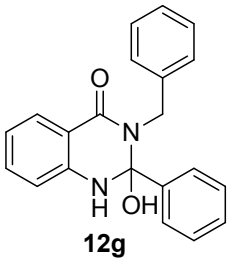
12e

2-([1, 1'-biphenyl]-4-yl)-2-hydroxy-3-(R) -1-phenylethyl)-2, 3-dihydroquinazolin-4 (1*H*)-one, (12e): Colorless solid, Yield-62 %, mp = 205-211°C, IR (KBr) = 3334, 2969, 1670, 1591, 1259, 1160, 883, 753, 558 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ= 12.10 (s, 1H), 8.84 (d, *J*= 8.4 Hz, 1H), 8.09 (d, *J*= 8.0 Hz, 2H), 7.73 (d, *J*= 8.4 Hz, 2H), 7.65 (d, *J*= 7.2 Hz, 2H), 7.56-7.48 (m, 4H), 7.46-7.38 (m, 5H), 7.36-7.30 (m, 1H), 7.13 (t, *J*= 7.6 Hz, 1H), 6.48 (d, *J*= 7.2 Hz, 1H), 5.37-5.30 (m, 1H), 1.65 (d, *J*= 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ= 166.24, 144.31, 143.11, 140.01, 133.22, 128.89-(2C), 128.76-(2C), 127.97-(3C), 127.48-(3C), 127.43-(3C), 127.22-(3C), 127.19-(3C), 126.26-(2H), 49.24, 21.72, HRMS: m/z calcd for $C_{28}H_{25}N_2O_2$ (M+H) 421.1898 found 421.1896.



12f

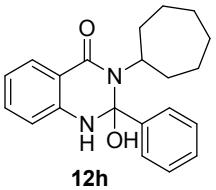
3-hexyl-2-hydroxy-2-phenyl-2, 3-dihydroquinazilin-4 (1*H*)-one (12f): Syrupy liquid, Yield- 68 %, IR (KBr) = 3345, 2928, 1642, 1525, 1449, 1302, 1159, 1029, 758, 26 cm^{-1}, ^1H NMR (400 MHz, $CDCl_3$): δ= 12.09 (s, 1H), 8.82 (d, *J*= 8.4 Hz, 1H), 8.05 (d, *J*= 7.6 Hz, 2H), 7.54-7.42 (m, 5H), 7.13 (t, *J*= 7.6 Hz, 1H), 6.2 (s, 1H), 3.48-3.43 (m, 2H), 1.66-1.59 (m, 2H), 1.40-1.31 (m, 6H), 0.93-0.89 (m, 3H), $^{13}CNMR$ (100 MHz, $CDCl_3$): δ = 169.18, 139.77, 134.82, 132.48, 131.77, 131.27, 128.73, 128.52, 127.37, 126.78, 126.45, 122.80, 121.60, 120.86, 40.11, 31.44, 29.40, 26.64, 22.53, 13.97, HRMS: m/z calcd for $C_{20}H_{25}N_2O_2$ (M+H) 325.1916, found 325.1911.



12g

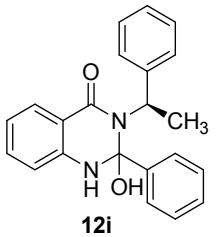
3-benzyl-2-hydroxy-2-phenyl-2, 3-dihydroquinazolin-4 (1*H*)-one: (12g): Syrupy liquid, Yield- 68 %, IR (KBr) = 3294, 2925, 1680, 1525, 1157, 1044, 796, 755, 580 cm^{-1}, ^1H NMR

(400 MHz, $CDCl_3$): δ= 12.10 (s, 1H), 8.83 (d, *J*= 8.4 Hz, 1H), 8.05 (d, *J*= 6.8 Hz, 2H), 7.57-7.50 (m, 5H), 7.39-7.31 (m, 5H), 7.10 (t, *J*= 7.6Hz, 1H), 6.60 (s, br, 1H), 4.66 (d, *J*= 5.6 Hz, 2H), ^{13}C NMR (100 MHz, $CDCl_3$): δ = 169.06, 139.88, 137.43, 134.73, 132.75, 131.82, 131.53, 128.85, 128.74, 128.65, 128.56, 127.82, 127.78, 127.71, 127.59, 127.35, 126.90, 126.58, 122.82, 121.56, 44.02, HRMS: m/z calcd for $C_{21}H_{19}N_2O_2$ (M+H) 331.1447 found 331.1440.



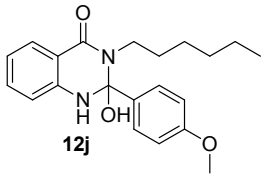
12h

3-cycloheptyl-2-hydroxy-2-phenyl-2, 3-dihydroquinazolin-4 (1*H*)-one (12h): Brown solid, Yield-65 %, mp: 89-94°C **,** IR (KBr) = 3327, 2856, 1630, 1491, 1073, 887, 752, 671 cm^{-1}, ^1H NMR (400 MHz, $CDCl_3$): δ= 12.10 (s, 1H), 8.80 (d, *J*= 8.0 Hz, 1H), 8.05 (d, *J*= 7.2 Hz, 2H), 7.46-7.40 (m, 5H), 7.12 (t, *J*= 7.6 Hz, 1H), 6.20 (s, 1H), 4.16 (s, 1H), 2.04-2.03 (m, 2H), 1.66-1.54 (m, 10H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 168.50, 132.52, 131.76, 131.20, 128.75, 128.50-(2C), 127.41- (2C), 126.78- (2C), 126.33, 122.79, 50.93, 50.86, 35.20, 35.08. 28.05, 28.01, 24.15, 24.04, HRMS: m/z calcd for $C_{21}H_{25}N_2O_2$ (M+H) 337.1916 found 337.1890.



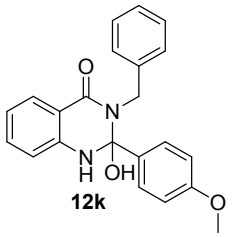
12i

2-hydroxy-2-phenyl-3-((R) -1-phenylethyl)-2, 3-dihydroquinazolin-4 (1H)-one (12i): White solid, Yield-60 %, mp: 101-106°C, IR (KBr) = 3305, 2927, 1634, 1446, 1209, 1028, 928, 754, 700, 551 cm^{-1}, ^1H NMR (400 MHz, $CDCl_3$): δ= 12.04 (s, 1H), 8.81 (d, J= 8.8 Hz, 1H), 8.01 (d, J= 7.6 Hz, 1H), 7.78 (d, J= 7.6 Hz, 2H), 7.54-7.47 (m, 2H), 7.43-7.36 (m, 6H), 7.31-7.25 (m, 2H), 6.34 (s, br, 1H), 5.37-5.30 (m, 1H), 1.61 (d, J= 6.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.53, 143.09, 134.59, 132.75, 131.76, 131.44, 128.85, 128.74-(2C), 128.54-(2C), 127.66, 127.46, 127.40, 126.88, 126.43, 126.23, 126.16, 122.80, 121.67, 49.20, 21.69, HRMS: m/z calcd for $C_{22}H_{21}N_2O_2$ (M+H) 345.1503 found 345.1595.



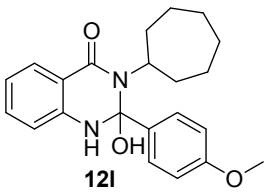
12j

3-hexyl-2-hydroxy-2-(4-methoxyphenyl)-2, 3- dihydroquinazolin-4 (1*H*)-one, (12j); Brown solid, Yield-48 %, mp:68-72°C, IR (KBr) = 3337, 2923, 1682, 1512, 1446, 1278, 1006, 901, 662, 546 cm^{-1}, ^1H NMR (400 MHz, $CDCl_3$): δ = 12.10 (s, 1H), 8.79 (d, *J*= 8.4 Hz, 1H), 8.01 (d, *J*= 8.4 Hz, 2H), 7.52-7.47 (m, 2H), 7.05-6.91 (m, 2H), 6.69-6.63 (m, s, 1H), 6.32 (s, 1H), 3.87 (s, 3H), 3.48-3.40 (m, 2H), 1.66-1.56 (m, 2H), 1.41-1.27 (m, 6H), 0.91-0.88 (m, 3H), ^{13}C NMR (100 MHz, $CDCl_3$): δ= 169.18, 165.59, 139.77, 134.82, 132.48, 131.77, 131.27, 128.73, 127.37, 126.8, 126.45, 122.80, 121.60, 120.86, 55.42, 40.11, 31.44, 29.40, 26.64, 22.53, 13.97; HRMS: m/z calcd for $C_{21}H_{27}N_2O_3$ (M+H) 355.2022 found 355.2007.



12k

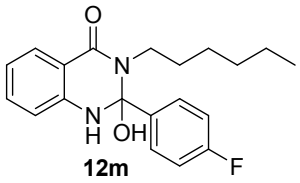
3-benzyl-2-hydroxy-2-(4-methoxyphenyl)-2, 3-dihydroquinazolin-4- (1*H*)-one, (12k): White solid, Yield-48 %, mp: 115-119°C, IR (KBr) =3327, 2856, 1630, 1556, 1073, 887, 752, 671, 585 cm^{-1}, ^1H NMR (400 MHz, $CDCl_3$): δ= 12.04 (s, 1H), 8.81 (d, *J*= 8.4 Hz, 1H), 8.03 (d, *J*= 8.8 Hz, 2H), 7.56-7.49 (m, 3H), 7.39-7.29 (m, 5H), 7.01 (d, *J*= 8.4 Hz, 2H), 6.32 (s, 1H), 4.61 (d, *J*= 5.2 Hz, 2H), 3.87 (s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$): δ= 169.14, 162.51, 140.30, 137.45, 135.03, 132.86, 132.40, 129.32, 128.77, 128.42, 127.85, 127.79, 127.55, 127.05, 126.42, 122.57, 121.61, 120.10, 117.35, 116.59,55.42, 44.11;HRMS: m/z calcd for $C_{22}H_{21}N_2O_2$ (M+H) 361.1552 found 361.1537.



12l

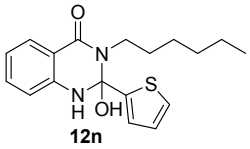
3-cycloheptyl-2-hydroxy-2-(4-methoxyphenyl)-2, 3-dihydroquinqzolin-4(1*H*)-one, (12l): Syrupy liquid, Yield-52 %, IR (KBr) = 3314, 2856, 1678, 1591, 1412, 1173, 1022, 834, 755, 666, 573, 528 cm^{-1}, ^1H NMR (400 MHz, $CDCl_3$): δ = 11.99 (s, 1H), 8.78 (d, *J*= 8.4 Hz, 1H), 8.02 (d, *J*= 8.8 Hz, 2H), 7.54-7.45 (m, 2H), 7.10 (t, *J*= 8.0 Hz, 1H), 7.01 (d, *J*= 8.8 Hz, 2H),

6.18 (s, br, 1H), 4.17-4.15 (m, 1H), 3.87 (s, 3H), 2.07-2.01 (m, 2H), 1.68-1.53 (m, 10 H), ^{13}C NMR (100 MHz, $CDCl_3$): δ= 168.07, 162.42, 140.00, 132.45, 129.28-(2C), 127.15-(2C), 126.36, 122.52-(2C), 121.52, 120.90, 113.92, 55.41, 50.90, 35.03-(2C), 27.98-(2C), 23.99-(2C), HRMS: m/z calcd for $C_{22}H_{27}N_2O_3$ (M+H) 367.2022 found 367.2030.



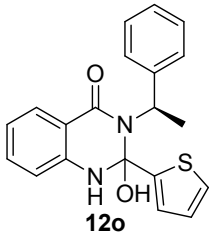
12m

2-(4-fluorophenyl)-3-hexyl-2-hydroxy-2, 3-dihydroquinazolin-4 (1*H*)-one, (12m): White solid, Yield-26 %, mp:170-176°C, IR (KBr) = 3327, 2856, 1681, 1525, 1491, 1073, 887, 671, 585, 527 cm^{-1}, ^{1}H NMR (400 MHz, $CDCl_3$): δ = 12.10 (s, 1H), 8.82 (d, *J*= 8.8 Hz, 1H), 8.07-8.06 (m, 2H), 7.55-7.49 (m, 2H), 7.20-7.08 (m, 3H), 6.21 (s, br, 1H), 3.49-3.42 (m, 2H), 1.67-1.63 (m, 2H), 1.41-1.33 (m, 6H), 0.91-0.88 (m, 3H), ^{13}C NMR (100 MHz, $CDCl_3$): δ= 169.7, 165.8 (C-F), 129.83, 129.75 (2C), 126.33, 122.90 (2C), 121.55 (2C), 115.88 (2C), 115.66 (2C), 40.12, 31.42, 29.38, 26.63, 22.53, 13.99, HRMS: m/z calcd for $C_{20}H_{24}FN_2O_2$ (M+H) 343.1803 found 343.1822.



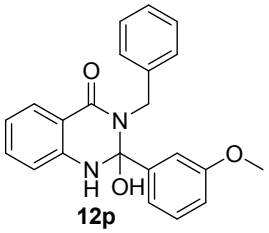
12n

3-hexyl-2-hydroxy-2-(thiophen-2-yl)-2, 3-dihydroquinazolin-4-(1*H*)-one, (12n): Syrupy liquid, Yield-80 %, IR (KBr) = 3334, 2868, 1670, 1591, 1259, 1160, 883, 753, 558 cm^{-1}; ^{1}H NMR (400MHz, $CDCl_3$): δ= 12.16 (s, 1H), 8.73 (d, J= 8.4 Hz, 1H), 7.77 (d, J= 3.2 Hz, 1H), 7.54-7.47 (m, 3H), 7.14-7.07 (m, 2H), 6.28 (s, br, 1H), 3.49-3.41 (m, 2H), 1.70-1.60 (m, 2H), 1.42-1.32 (m, 6H), 0.94-0.86 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ= 169.14, 160.32, 139.73, 132.63 (2C), 130.97, 128.53, 127.91, 126.38, 122.72, 121.37, 120.23, 40.13, 31.45, 29.39, 26.65, 22.53, 13.98; HRMS: m/z calcd for $C_{18}H_{23}SN_2O_2$ (M+H) 331.1469 found 331.1480.



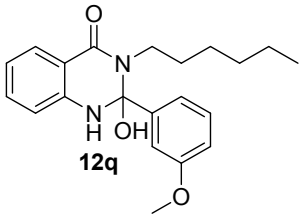
12o

2-hydroxy-3-((R)-1-Phenylethyl)-2-(thiophen-2-yl)-2, 3-dihydroquinqzolin-4 (1*H*)-one, (18):Brown solid, Yield-77 %, mp: 143-149°C, IR (KBr) = 3334, 2969, 1626, 1591, 1259, 1160, 1090, 883, 753 cm^{-1}, ^1H NMR (400 MHz, $CDCl_3$): δ= 12.1 (s, 1H), 8.72 (d, *J*= 8.0 Hz, 1H), 7.73 (d, *J*=4 Hz, 1H), 7.41-7.25 (m, 8H), 7.13-7.05 (m, 2H), 6.52 (s, br, 1H), 5.38-5.29 (m, 1H), 1.68-1.64 (d, *J*= 16.8 Hz, 3H), ^{13}C NMR (100 MHz, $CDCl_3$): δ= 168.32, 142.47, 140.43, 139.91, 132.86, 131.01, 129.88, 128.88, 128.75, 128.55, 128.00, 127.90, 127.71, 127.55, 126.42, 126.19, 122.71, 121.42, 49.33, 21.60, HRMS: m/z calcd for $C_{20}H_{19}SN_2O_2$ (M+H) 351.1167 found 351.1176.



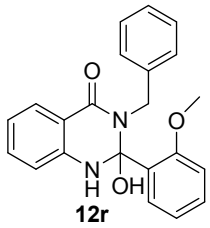
12p

3-Benzyl-2-hydroxy-2-(3-methoxy phenyl)-2, 3-dihydro quinazolin-4(1*H*) one (12p): White solid, Yield-49 %, ^1H NMR (400 MHz, $CDCl_3$): δ = 12.13 (s, 1H), 8.78 (d, *J*= 8.4 Hz, 1H), 7.59-7.58 (m, 2H), 7.50-7.49 (m, 2H), 7.41-7.25 (m, 6H), 7.07-7.05 (m, 2H), 6.75 (s, br, 1H), 4.65-4.62 (m, 2H), 3.87 (s, 3H);^{13}C NMR (100 MHz, $CDCl_3$): δ= 169.2, 167.3, 165.4, 159.9, 159.7, 139.7, 136.3, 132.4, 129.7, 129.4, 126.4, 122.8, 121.5, 120.8, 119.1, 118.5, 118.3, 117.4, 112.4, 112.2, 53.4, 41.1; HRMS: m/z calcd for $C_{22}H_{21}N_2O_3$ (M+H) 361.1552 found 361.1533.



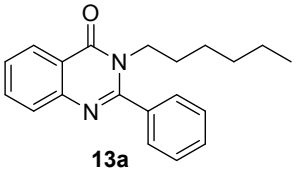
12q

3-Hexyl-2-hydroxy-2-(3-methoxy phenyl)-2, 3-dihydro quinazolin-4(1*H*) one (12q): white solid, Yield-52 %, ^{1}H NMR (400 MHz, $CDCl_3$): δ = 12.10 (s, 1H), 8.78 (d, *J*= 8.4 Hz, 1H), 7.49-7.47 (m, 2H), 7.42-7.38 (m, 2H), 7.34-7.28 (m, 1H), 7.08-7.05 (m, 2H), 6.51 (s, br, 1H), 3.87 (s, 3H), 3.44-3.41 (m, 2H), 1.63-1.60 (m, 2H), 1.38-1.24 (m, 6H), 0.89-0.86, (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ= 169.9, 165.4, 139.7, 136.3, 132.4, 129.7, 129.4, 126.4, 122.8, 120.8, 120.8, 119.1, 118.5, 112.4, 112.2, 53.4, 40.1, 31.4, 29.4, 26.6, 22.5, 13.9; MS (EI) *m/z*:186.26, 355.20$(M+H)^+$, 731.30.



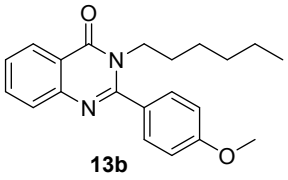
12r

3-Benzyl-2-hydroxy-2-(2-methoxy phenyl)-2,3-dihydro quinazolin-4(1*H*) one (12r): Light green color solid, Yield-35 %, ^{1}H NMR (400 MHz, $CDCl_3$): δ = 11.72 (s, 1H), 8.69 (d, *J*= 8.4 Hz, 1H), 7.50-7.44 (m, 3H), 7.35-7.25 (m, 7H), 7.18 (d, *J*= 1.2 Hz, 1H), 7.0 (d, *J*= 16Hz, 1H), 6.49 (s, br, 1H), 4.64-4.59 (m, 2H), 4.01 (s, 3H);^{13}C NMR (100 MHz, $CDCl_3$): δ= 169.1, 167.3, 165.4, 159.9, 159.7, 139.7, 136.3, 132.4, 129.7, 129.4, 126.4, 122.8, 121.5, 120.8, 119.1, 118.5, 118.3, 117.4, 112.4, 112.2, 55.4, 40.1; HRMS: m/z calcd for $C_{22}H_{21}N_2O_3$ (M+H) 361.1552 found 361.1537.



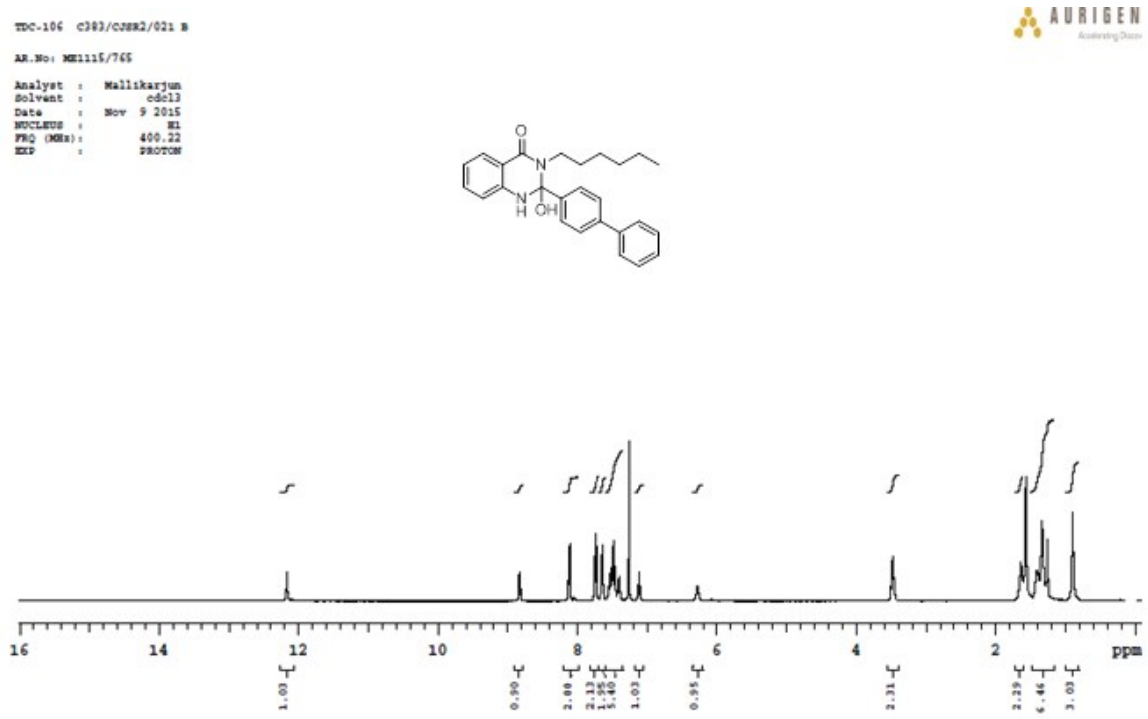
13a

3-Hexyl-2-phenyl quinazolin-4-(3*H*)-one (13a): Syrupy liquid,^{1}H NMR (400MHz, $CDCl_3$): δ=8.34 (d, *J* = 7.6 Hz, 1H), 8.11-8.09 (m, 1H), 7.78-7.72 (m, 2H), 7.54-7.49 (m, 5H), 3.99-3.95 (m, 2H), 1.63-1.56 (m, 2H), 1.20-1.07 (m, 6H), 0.84-0.78 (m, 3H); ^{13}C NMR (100 MHz, CDCl3): δ =162.16, 156.29, 147.15, 135.51, 134.29, 133.61, 130.15, 129.79, 128.74, 128.45, 127.79, 127.39, 126.97, 126.77, 45.94, 30.97, 28.55, 26.28, 22.30, 13.87;HRMS: m/z calcd for $C_{20}H_{23}N_2O$ (M+H) 307.1810, found 307.1805.



13b

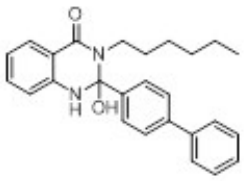
3-Hexyl-2-(4-methoxyphenyl) quinazolin-4 (3*H*)-one (22): Syrupy liquid,^{1}H NMR (400MHz, $CDCl_3$):8.32 (d, J= 7.2 Hz, 1H), 7.74 – 7.72 (m, 1H), 7.50-7.49 (m, 2H), 7.31-7.26 (m, 2H), 7.04-7.01 (m, 1H), 6.87-6.83 (m, 1H), 4.02-3.98 (m, 2H), 3.88 (s, 3H), 1.62-1.54 (m, 2H), 1.25-1.14 (m, 6H), 0.86-0.79 (m, 3H);^{13}C NMR (100 MHz, CDCl3): δ= 162.33, 160.64, 156.18, 147.25, 134.19, 133.22, 134.19, 133.22, 128.04, 127.36, 126.76, 126.72, 120.83, 119.18, 114.16, 114.10, 55.43, 45.97, 31.04, 27.51, 26.31, 22.33, 13.89; HRMS: m/z calcd for $C_{21}H_{25}N_2O_2$ (M+H) 337.1916, found 337.1916.

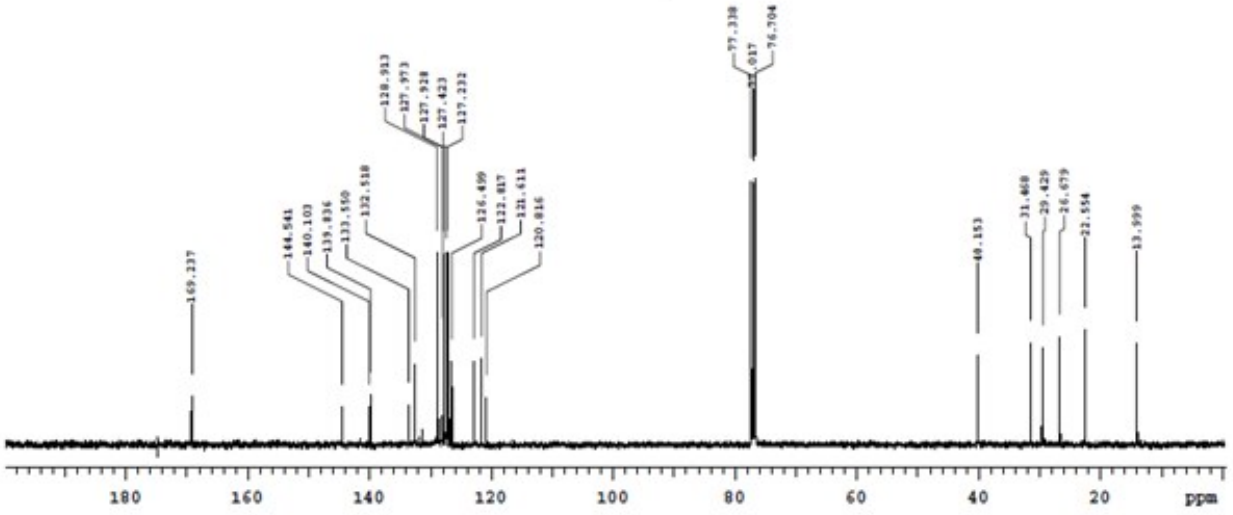


TDC-106 C383/CJSR1/021

AR.No: MK1115/1930

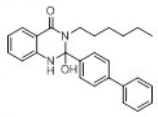
Analyst	:	Mallikarjun
Solvent	:	cdcl3
Date	:	Nov 22 2015
NUCLEUS	:	C13
FRQ (MHz)	:	100.65
EXP	:	CARBON



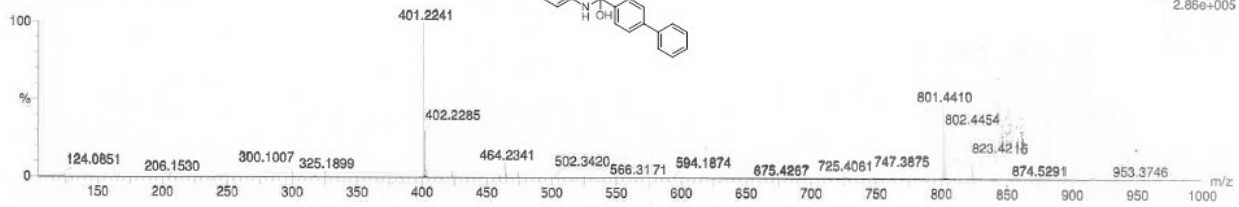


Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
42 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 0-30 H: 0-35 N: 0-3 O: 0-3
C383/CJSR1/021 A
151119008 34 (0.635) Cm (34:38)



TOF MS ES+
2.86e+005

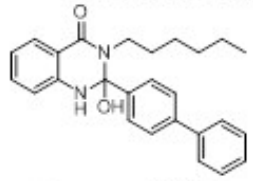


Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
401.2241	401.2229	1.2	3.0	13.5	33.6	C26 H29 N2 O2

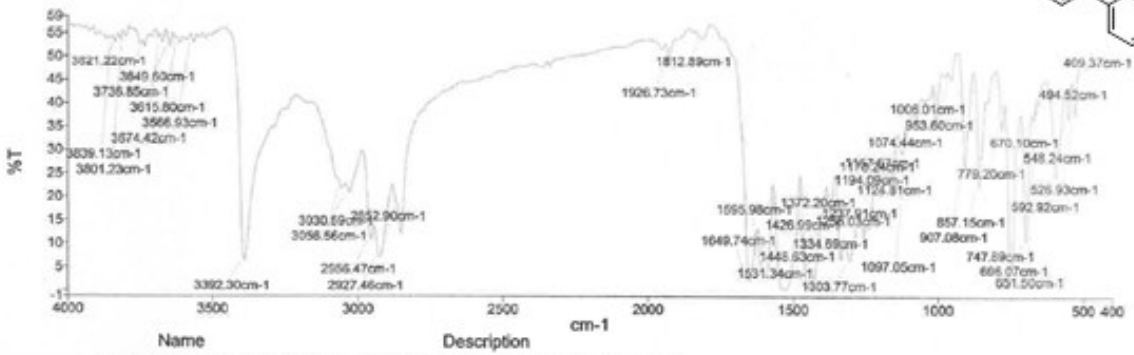
Friday, February 05, 2016 8:01 PM

DR.REDDY'S LABORATORIES LIMITED,CPS

Analytical Research Department



Peak Table Graph



Name Description

C383-CJSR2-021_1_1 Sample 016 By pet2 Date Friday, February 05 2016

Analyzed By: pet2

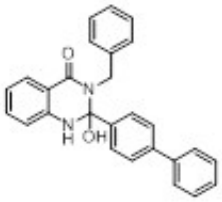
Analyzed Date: 2/5/2016 8:00:55 PM

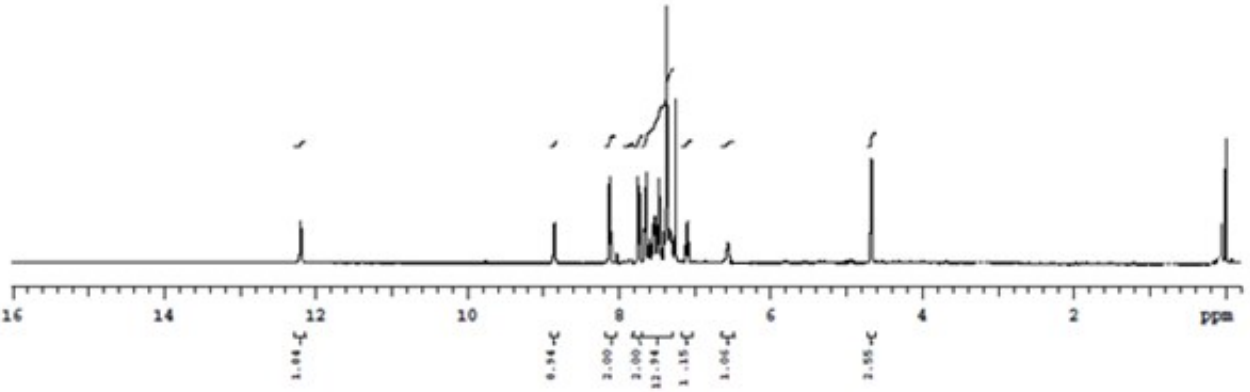
TDC-106 C383/CJSR1/041 Fr-2

A.R.No: MR0116/2276

Analyst : Mallikarjun
Solvent : cdcl3
Date : Jan 30 2016
NUCLEUS : H1
FRQ (MHz): 400.22
EXP : PROTON

AURIGENE

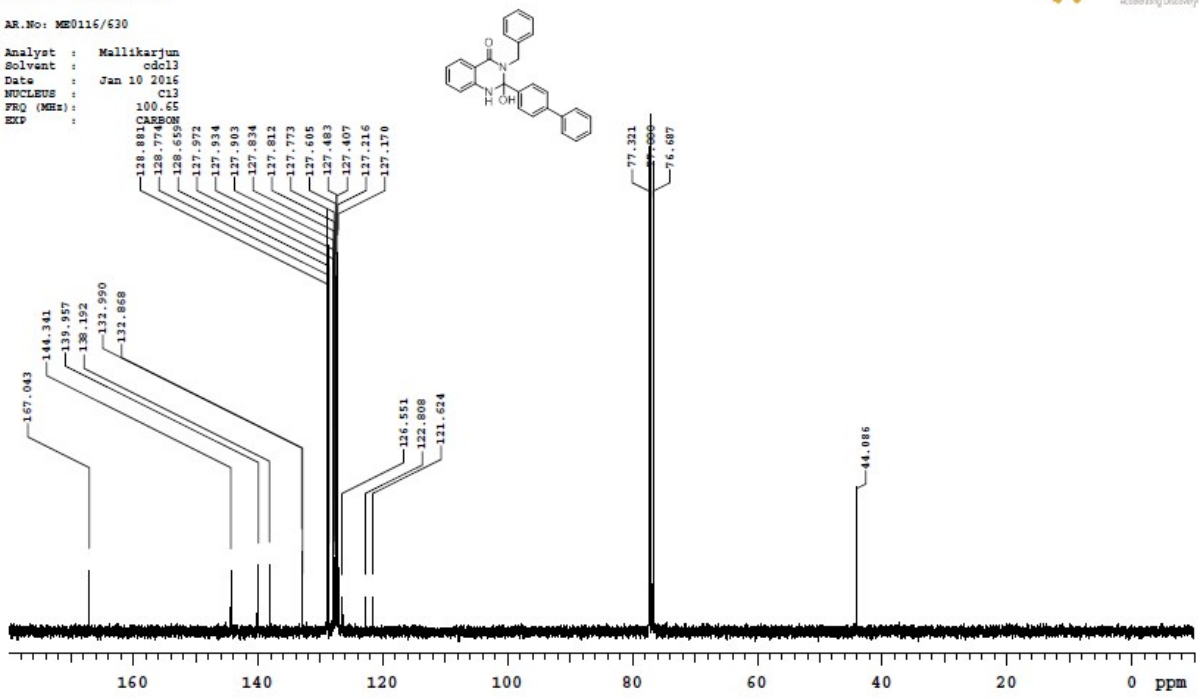




TDC-106 C383/CJSR1/041

AR.No: ME0116/630

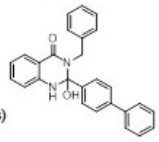
Analyst : Mallikarjun
Solvent : cdcl3
Date : Jan 10 2016
NUCLEUS : C13
FRQ (MHz): 100.65
EXP : CARBON



Elemental Composition Report

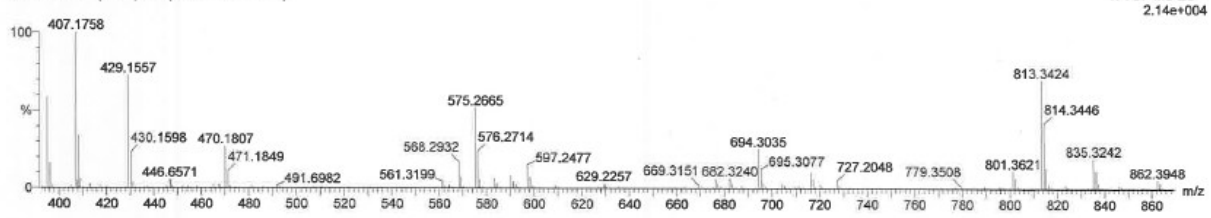
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2



Monoisotopic Mass, Even Electron Ions
32 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 0-30 H: 0-30 N: 0-3 O: 0-3
C383/CJSR1/041
151215015 19 (0.352) Cm (17:21-64:69x0.500)

1: TOF MS ES+
2.14e+004



Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
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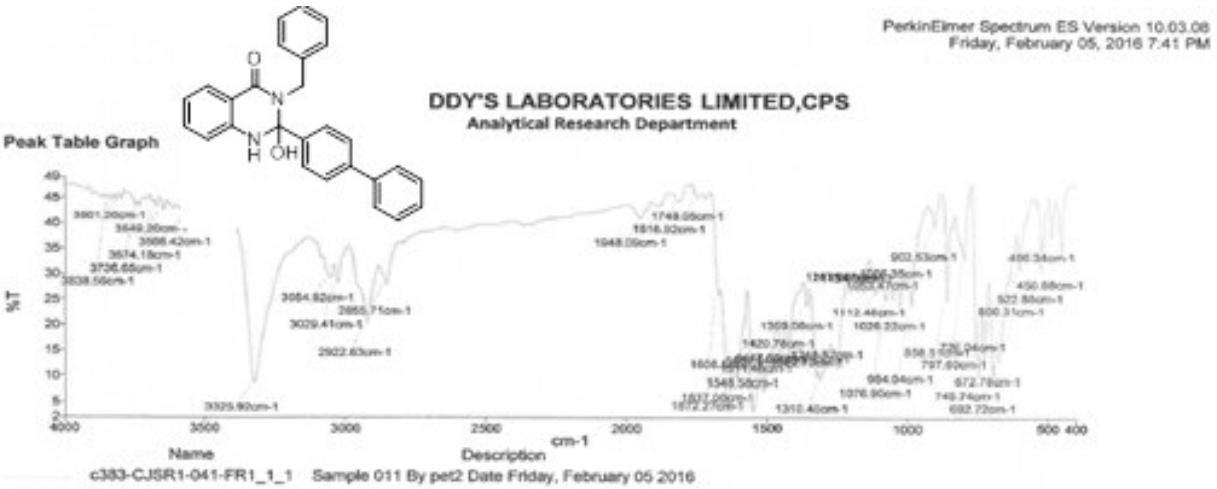
R. Mallikarjun 09/03/2016



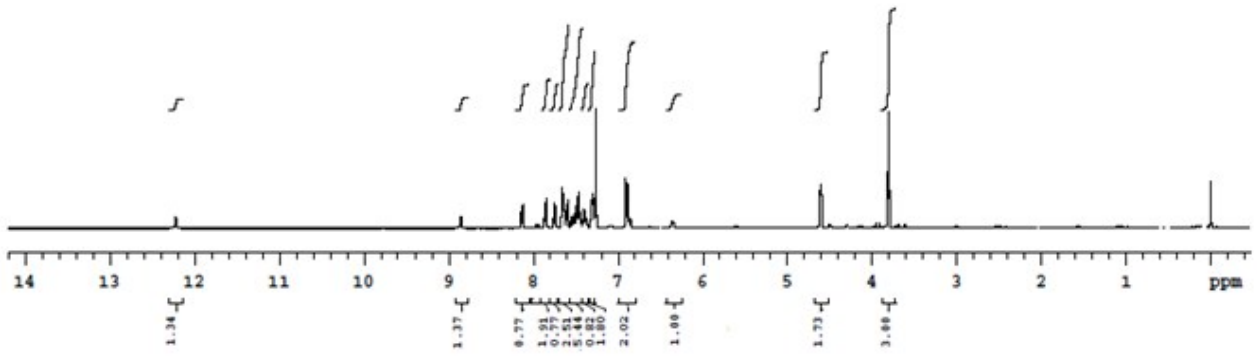
Analyzed By: pet2
Analyzed Date: 2/5/2016 7:40:24 PM

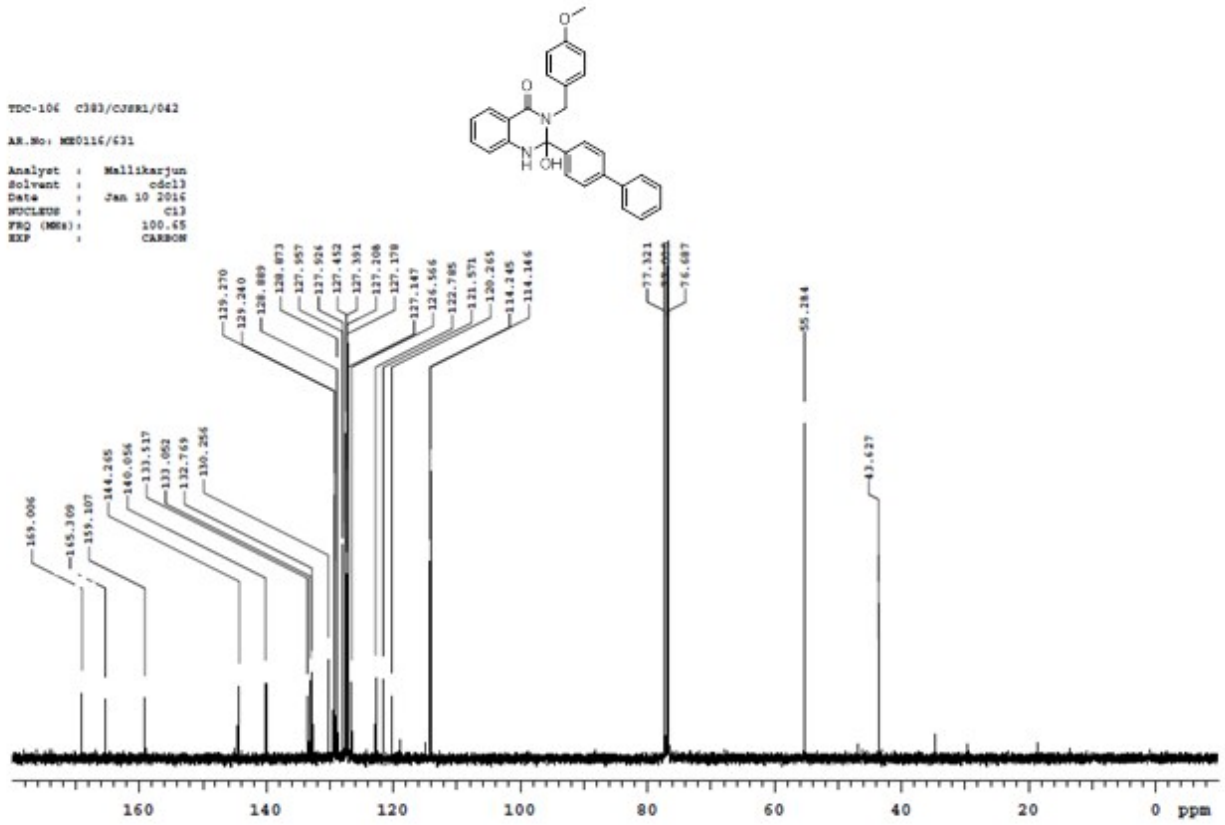
Checked By:
Checked Date:

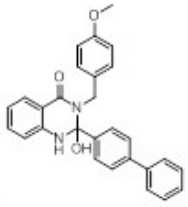
TDC-106 C383/CJSR1/042(Fr-1)

A.R.No: ME0116/2325

Analyst	:	Mallikarjun
Solvent	:	cdcl3
Date	:	Feb 1 2016
NUCLEUS	:	H1
FRQ (MHz)	:	400.22
EXP	:	PROTON





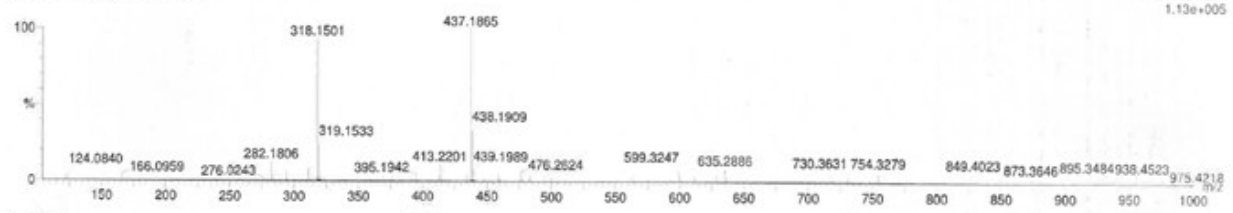


Elemental Composition Report

Page 1

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
61 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 0-32 H: 0-35 N: 0-3 O: 0-5
C383/CJSR1/042
151222009 25 (0.472) Cm (25:28)



Minimum:		5.0	5.0	-1.5		
Maximum:				100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
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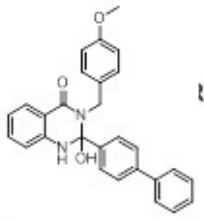
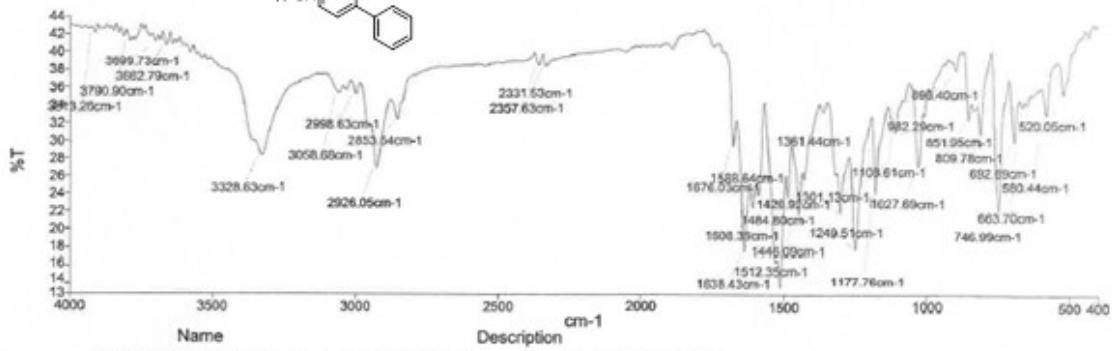
PerkinElmer Spectrum ES Version 10.03.08
Friday, February 05, 2016 7:55 PM



EDDY'S LABORATORIES LIMITED,CPS
Analytical Research Department

Peak Table Graph



Name Description

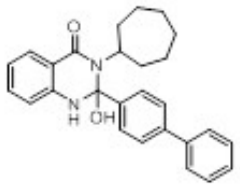
C383-CJSR1-042-FR2_1_1 Sample 014 By pet2 Date Friday, February 05 2016

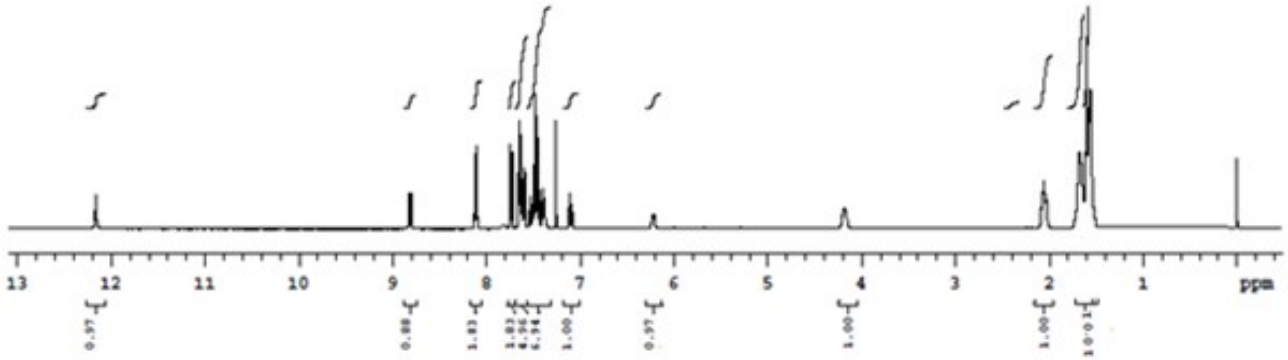
Analyzed By: pet2
Analyzed Date: 2/5/2016 7:54:57 PM

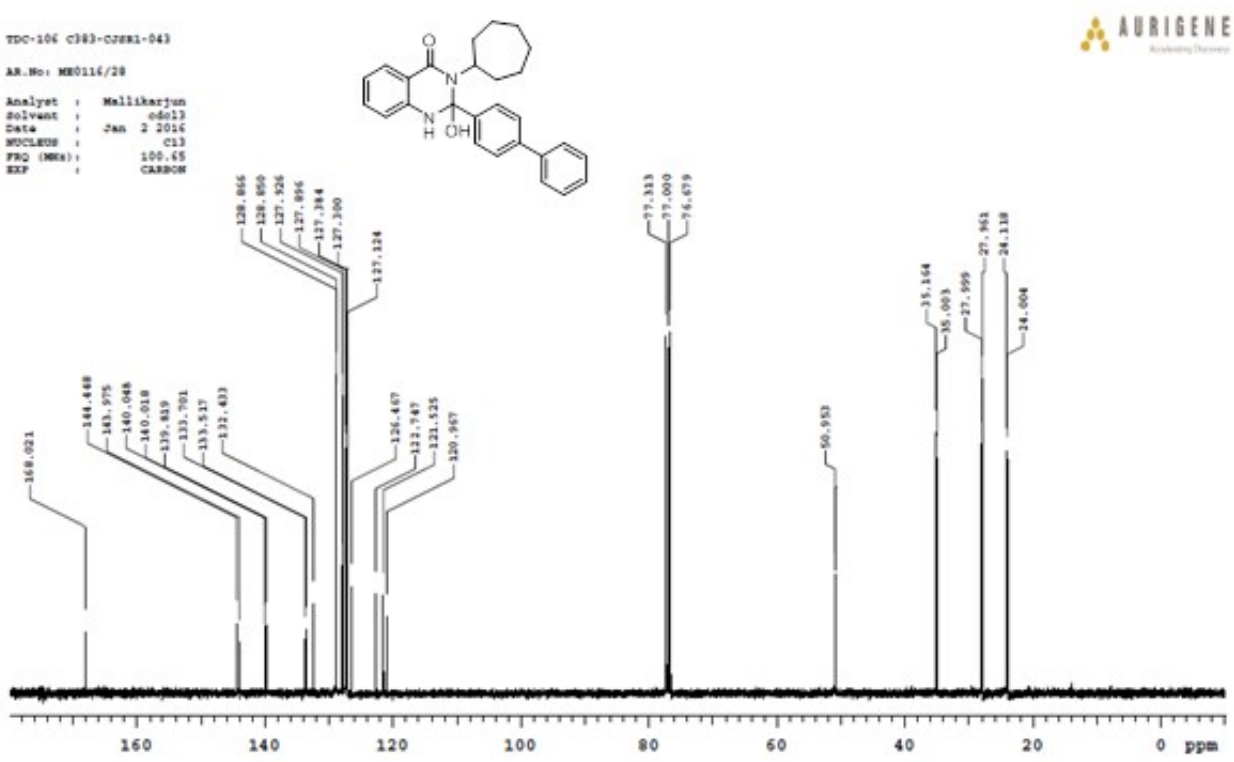
TDC-106 C383/CJSR1/043

AR.No: MK1215/1714

Analyst : Mallikarjun
Solvent : cdcl3
Date : Dec 17 2015
NUCLEUS : H1
FRQ (MHz): 400.22
EXP : PROTON

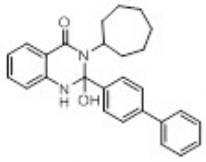


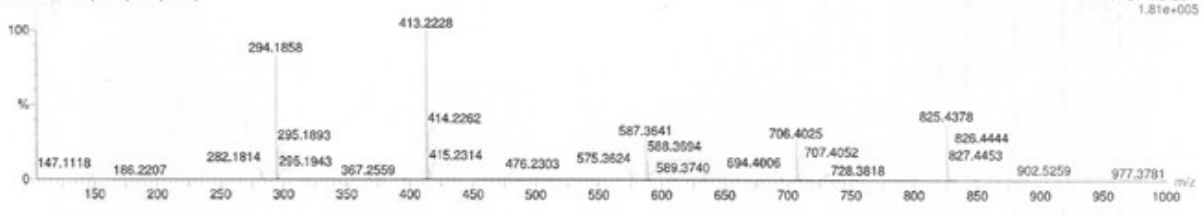




Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

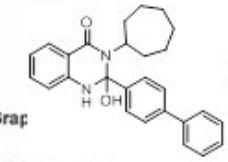
Monoisotopic Mass, Even Electron Ions
72 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 0-32 H: 0-35 N: 0-3 O: 0-5
C383/CJSR1/043
151222008 20 (0.365) Cm (18:20)





Minimum:		5.0	5.0	-1.5		
Maximum:				100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
413.2228	413.2229	-0.1	-0.2	14.5	1.5	C27 H29 N2 O2

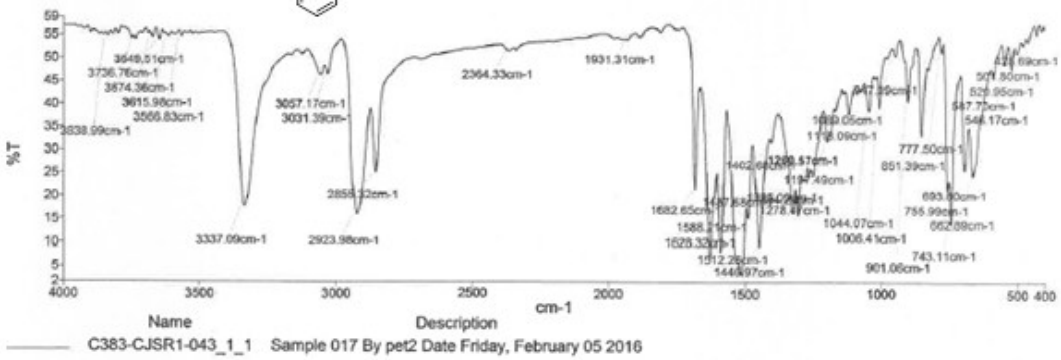
PerkinElmer Spectrum ES Version 10.03.08
Friday, February 05, 2016 8:04 PM



DR.REDDY'S LABORATORIES LIMITED,CPS

Analytical Research Department

Peak Table Grap



Name Description

C383-CJSR1-043_1_1 Sample 017 By pet2 Date Friday, February 05 2016

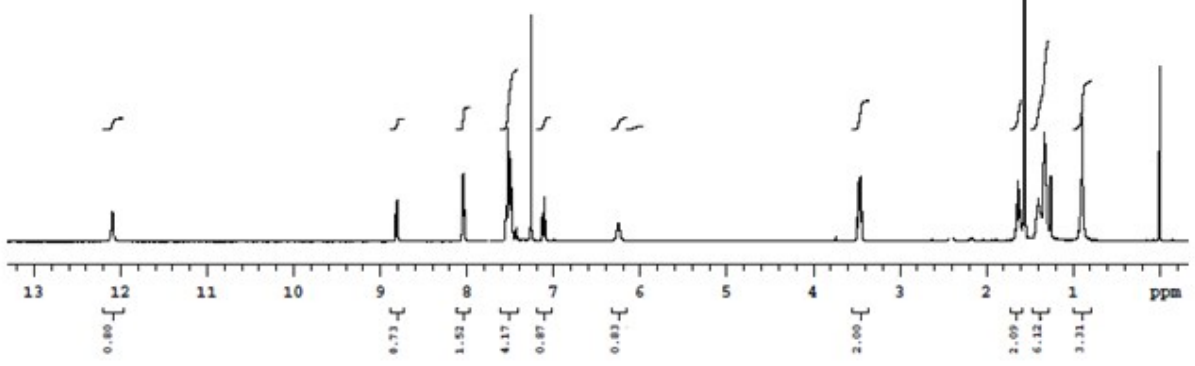
Analyzed By: pet2
Analyzed Date: 2/5/2016 8:03:39 PM

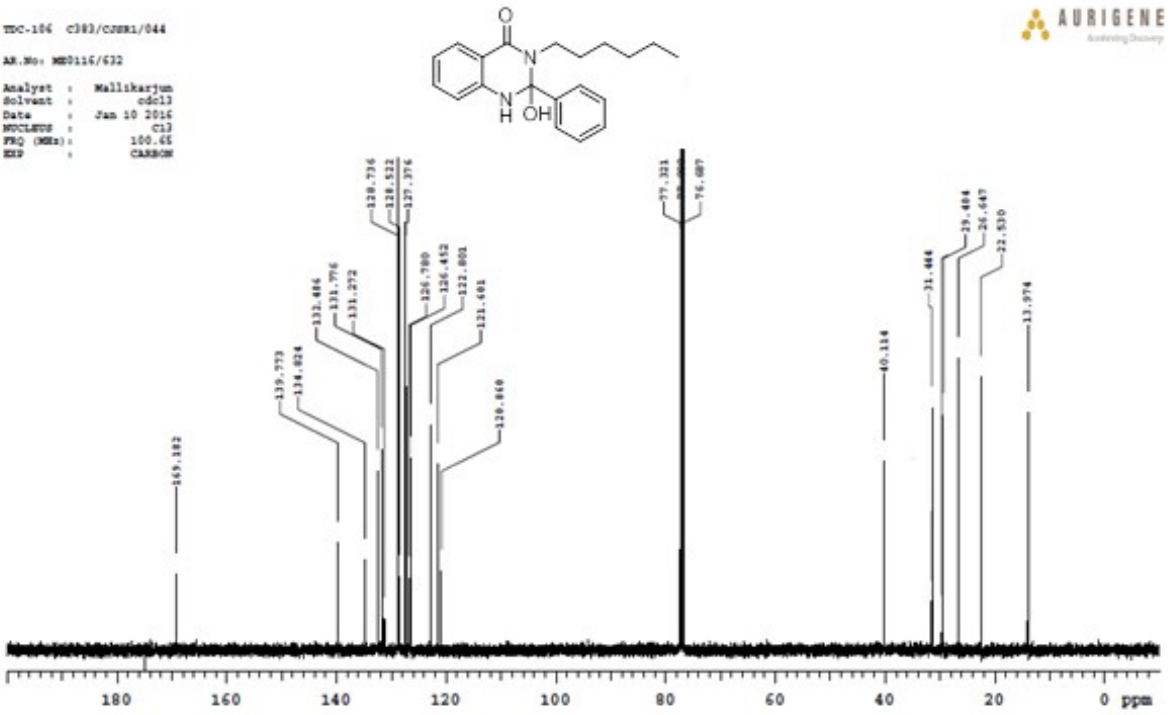
TDC-106 C383/CSJR1/044

AR.No: MK1215/2201

Analyst : Mallikarjun
Solvent : cdcl3
Date : Dec 24 2015
NUCLEUS : H1
FRQ (MHz): 400.22
EXP : PROTON

AURIGENI

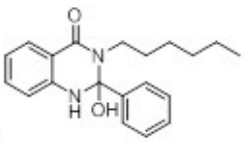




Elemental Composition Report

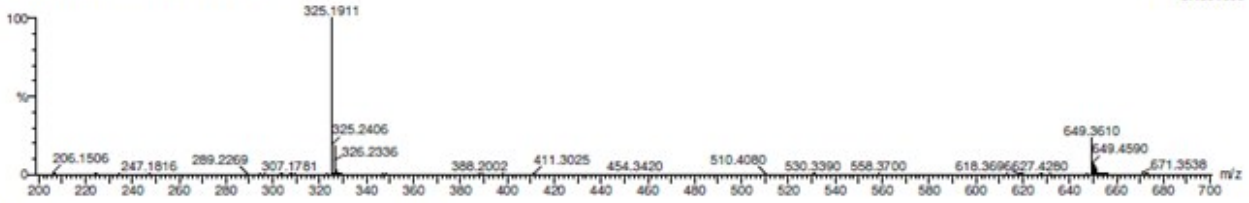
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

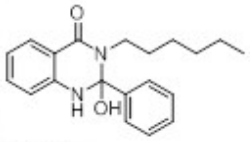


Monoisotopic Mass, Even Electron Ions
29 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 0-22 H: 0-26 N: 0-3 O: 0-4
C383/CJSR1/044
160204011 19 (0.352) Cm (19:20-47:53x0.500)

1: TOF MS ES+
8.48e+005



Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
325.1911	325.1916	-0.5	-1.5	9.5	5752.5	C20 H25 N2 O2



PerkinElmer Spectrum ES Version 10.03.08
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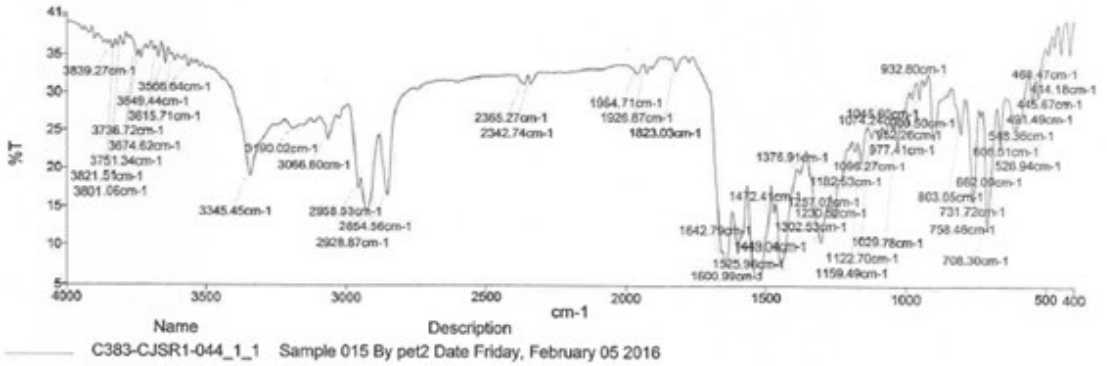
Analytical Research Department

Peak Table Graph



Name Description
C383-CJSR1-044_1_1 Sample 015 By pet2 Date Friday, February 05 2016

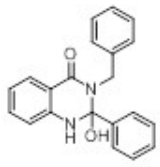
Analyzed By: pet2
Analyzed Date: 2/5/2016 7:57:43 PM

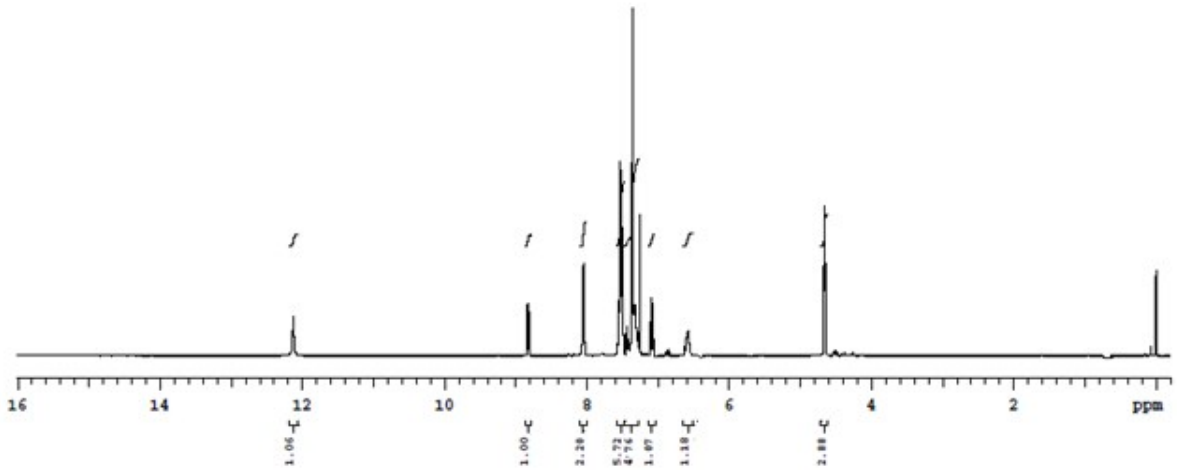
AURIGENE

TDC-106 C383/CSJR1/045(Fr-2)

AR.No: ME1215/2465

Analyst	:	Mallikarjun
Solvent	:	cdcl3
Date	:	Dec 29 2015
NUCLEUS	:	H1
FRQ (MHz)	:	400.22
EXP	:	PROTON

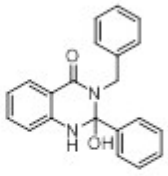




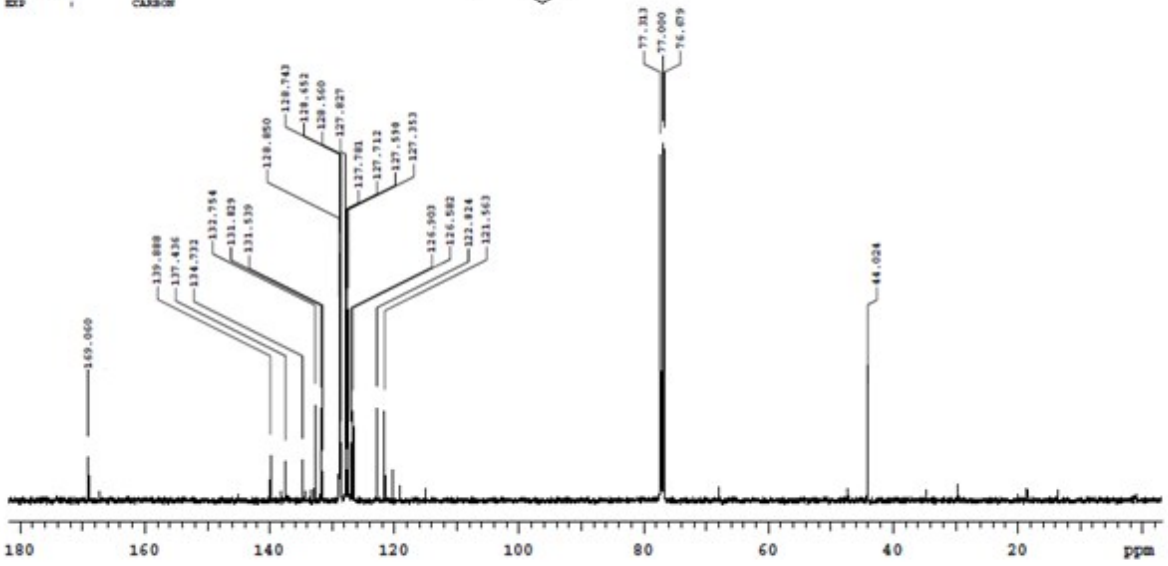
TDC-186 C383/CDSR1/045

A.R.No: MR0216/527

Analyst	:	Mallikarjun
Solvent	:	cdcl3
Date	:	Feb 7 2016
NUCLEUS	:	C13
FRQ (MHz)	:	100.65
EXP	:	CARBON



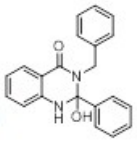
AURIGENE



Elemental Composition Report

Single Mass Analysis

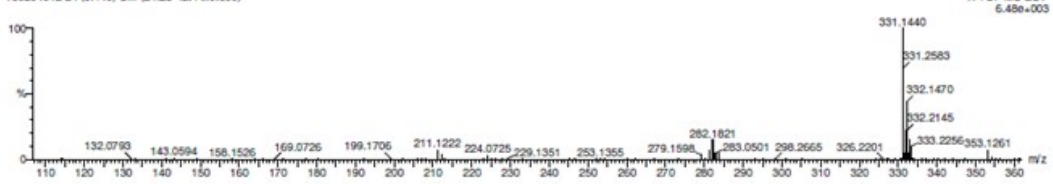
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2



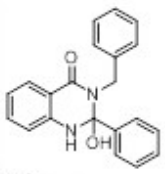
Monoisotopic Mass, Even Electron Ions
28 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 0-22 H: 0-26 N: 0-3 O: 0-4

C383/CJSR1/045
160204012 24 (0.440) Cm (24:25-42:44x0.500)

1: TOF MS ES+
6.48e+003



Minimum:		5.0	5.0	-1.5		
Maximum:				100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
331.1440	331.1447	-0.7	-2.1	13.5	240.4	C21 H19 N2 O2



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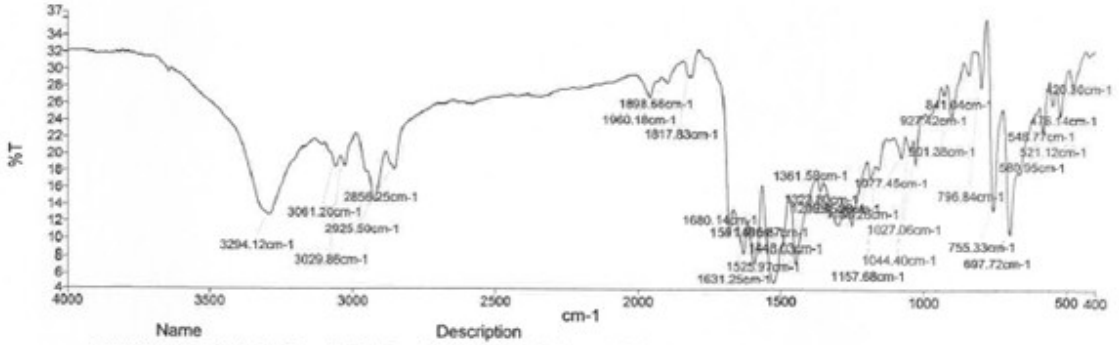
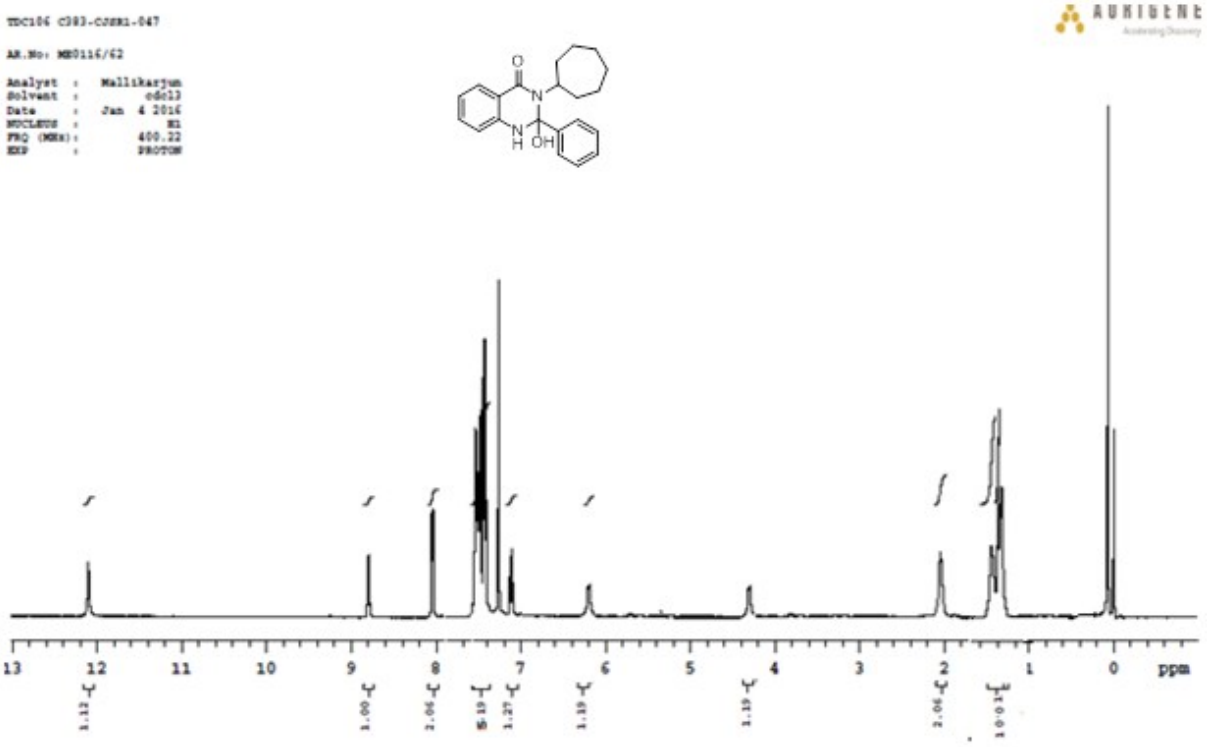
Analytical Research Department

Peak Table Graph



Name Description
C383-CJSR1-045_1_1 Sample 020 By pet2 Date Friday, February 05 2016

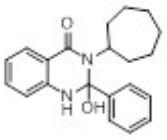
Analyzed By: pet2
Analyzed Date: 2/5/2016 8:19:12 PM

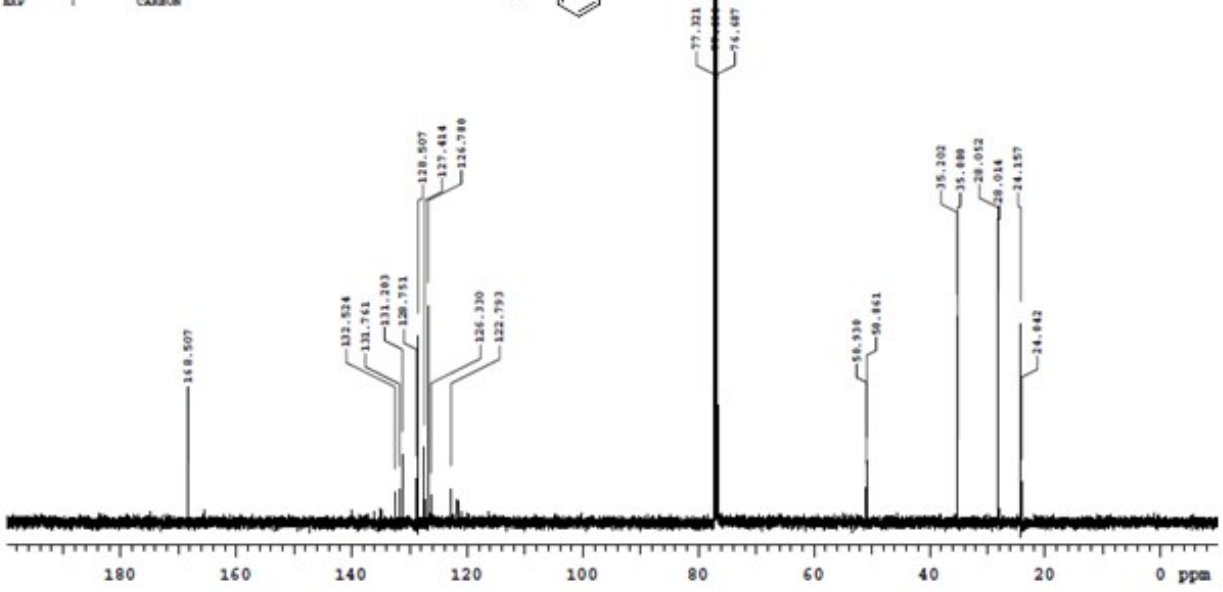


TDC-106 C383/CJSR1/047

AR.No: MS0116/633

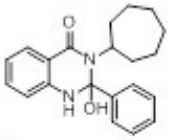
Analyst	:	Mallikarjun
Solvent	:	cdcl3
Date	:	Jan 10 2016
NUCLEUS	:	C13
FRQ (MHz)	:	100.65
EXP	:	CARBON





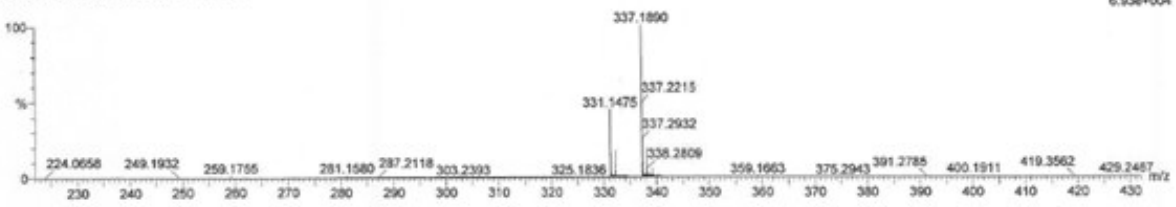
Elemental Composition Report

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2



Monoisotopic Mass, Even Electron Ions
46 formula(e) evaluated with 1 results within limits (up to 5 closest results for each mass)
Elements Used:
C: 0-25 H: 0-30 N: 0-3 O: 0-4
C383/CJSR1/047
160204003 25 (0.472) Cm (25-53x0.500)

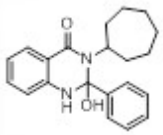
1: TOF MS ES+
6.93e+004



Minimum:		5.0	10.0	-1.5		
Maximum:				100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
337.1890	337.1916	-2.6	-7.7	10.5	507.1	C21 H25 N2 O2

R. Nagaraju
24/01/2016.

PerkinElmer Spectrum ES Version 10.03.08
Friday, February 05, 2016 8:13 PM



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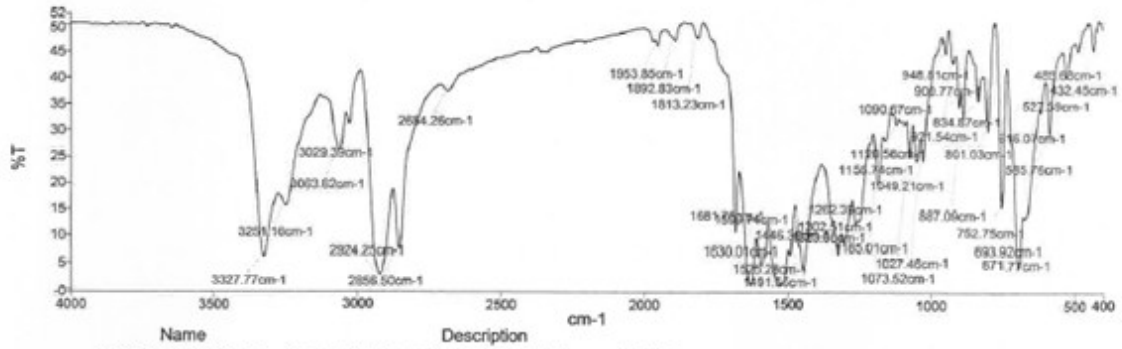
Analytical Research Department

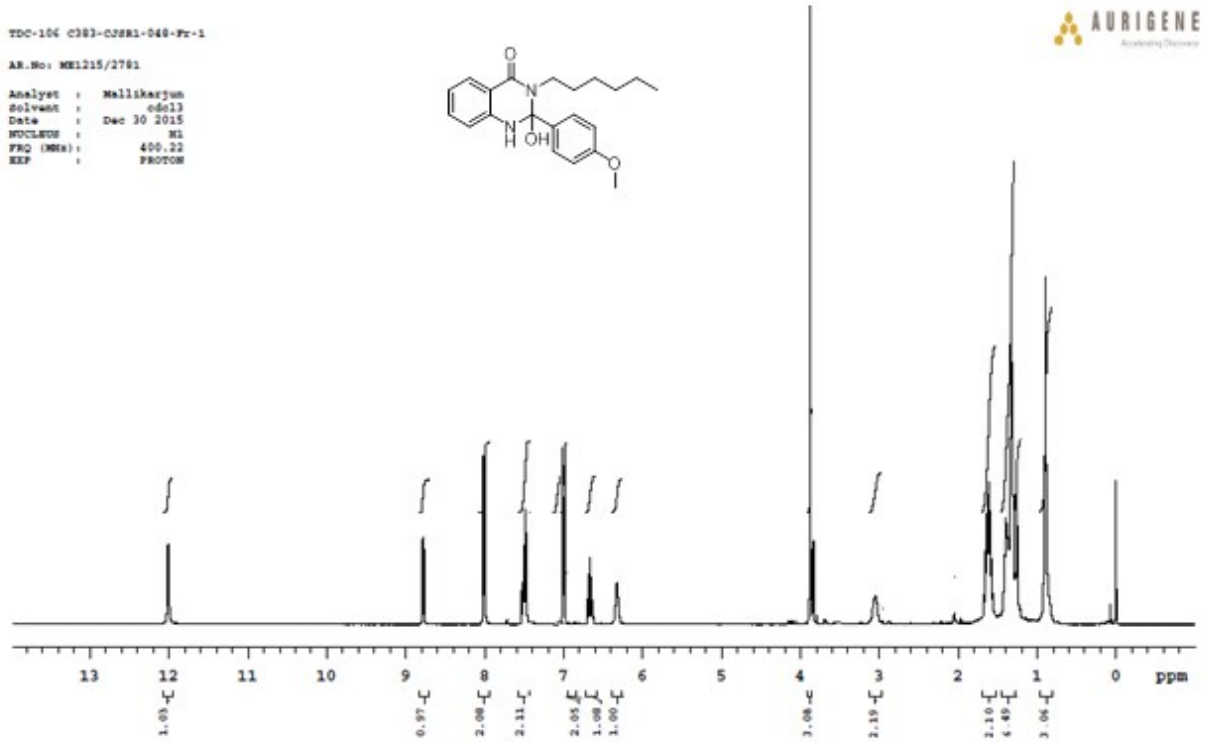
Peak Table Graph

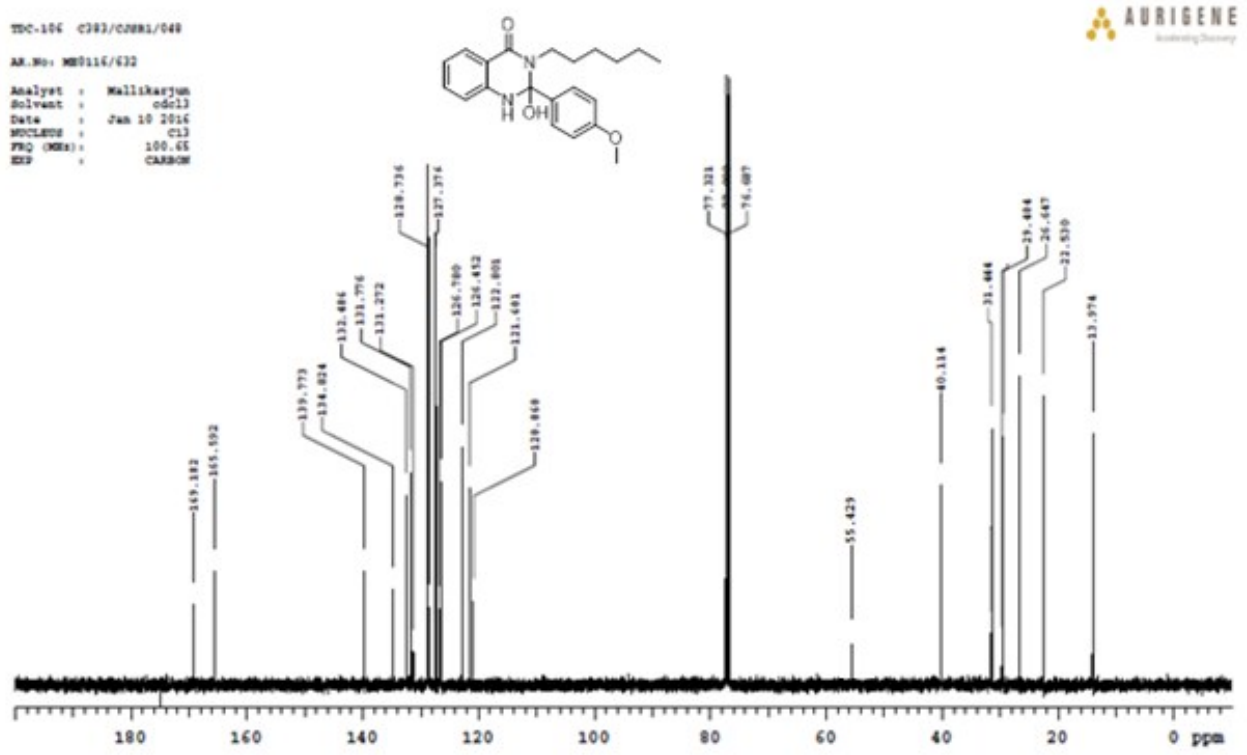


Name Description

C383-CJSR1-047_1_1 Sample 018 By pet2 Date Friday, February 05 2016

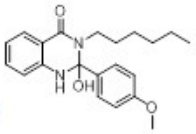
Analyzed By: pet2
Analyzed Date: 2/5/2016 8:12:08 PM


TDC-106 C383-CJSR1-048-Fr-1
AR.No: MH1215/2791
Analyst : Mallikarjun
Solvent : cdcl3
Date : Dec 30 2015
NUCLEUS : H1
FRQ (MHz): 400.22
EXP : PROTON
AURIGENE
ppm


TDC-106 C383/CJSR1/048
AR.No: MH0116/632
Analyst : Mallikarjun
Solvent : cdcl3
Date : Jan 10 2016
NUCLEUS : C13
FRQ (MHz): 100.65
EXP : CARBON
AURIGENE
ppm

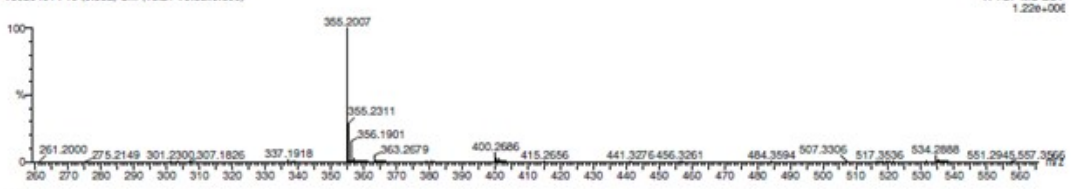
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

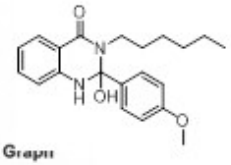


Monoisotopic Mass, Even Electron Ions
22 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 0-22 H: 0-29 N: 0-3 O: 0-4
C383/CJSR1/048
160204014 19 (0.352) Cm (18:21-73:80x0.500)

1: TOF MS ES+
1.22e+006



Minimum:		5.0	5.0	-1.5		
Maximum:				100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
355.2007	355.2022	-1.5	-4.2	9.5	328435.5	C21 H27 N2 O3



PerkinElmer Spectrum ES Version 10.03.08
Friday, February 05, 2016 8:04 PM

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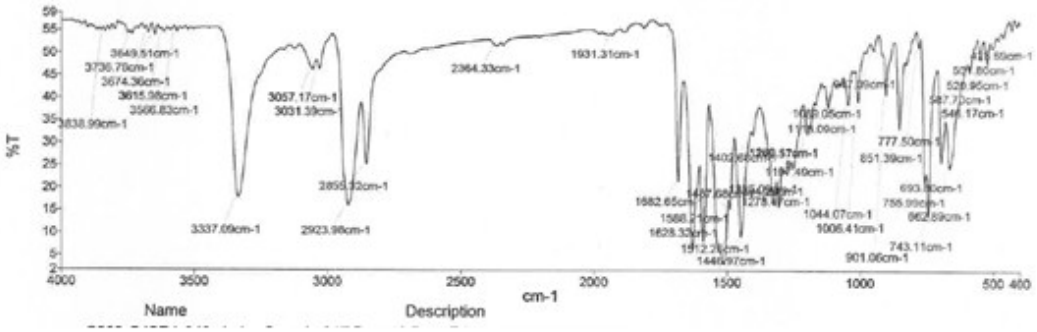
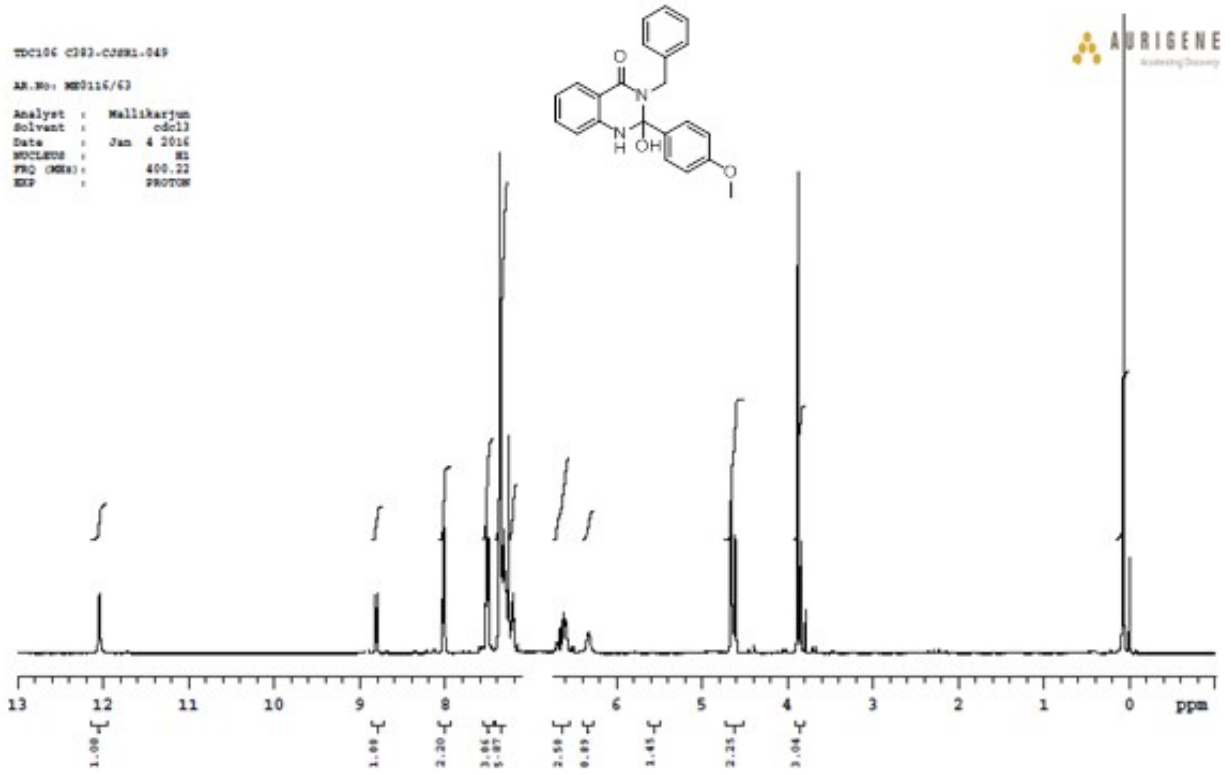
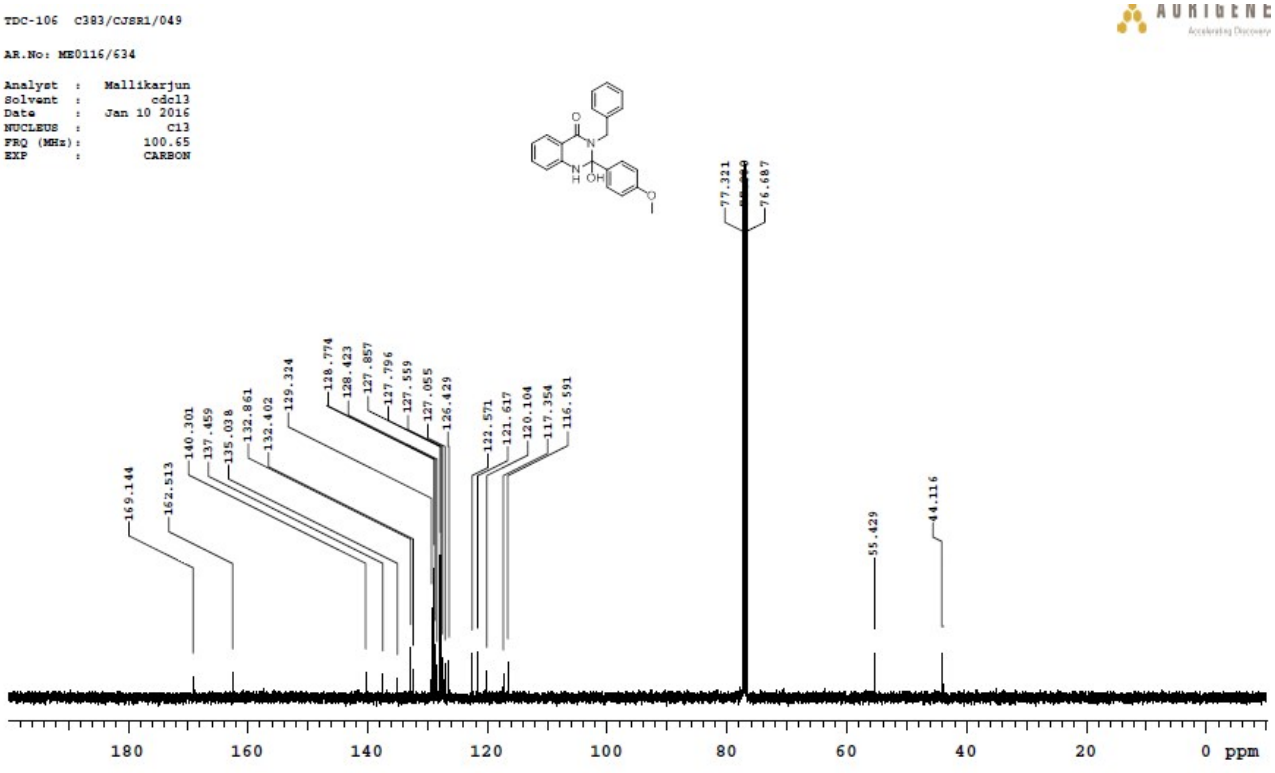
Analytical Research Department

Peak Table Graph

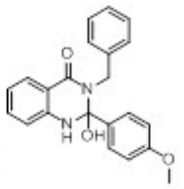


Name Description


TDC106 C383.CJSR1.049
AR.No: ME0116/63
Analyst : Mallikarjun
Solvent : cdcl3
Date : Jan 4 2016
NUCLEUS : H1
FRQ (MHz): 400.22
EXP : PROTON
AURIGENE
13 12 11 10 9 8 6 5 4 3 2 1 0 ppm
1.00 1.08 2.20 3.06 5.87 2.58 0.89 1.45 2.25 3.04


TDC-106 C383/CJSR1/049
AR.No: ME0116/634
Analyst : Mallikarjun
Solvent : cdcl3
Date : Jan 10 2016
NUCLEUS : C13
FRQ (MHz): 100.65
EXP : CARBON
AURIGENE
169.144
162.513
140.301
137.459
135.038
132.861
132.402
129.324
128.774
128.423
127.857
127.796
127.559
127.055
126.429
122.571
121.617
120.104
117.354
116.591
77.321
76.687
55.429
44.116
180 160 140 120 100 80 60 40 20 0 ppm

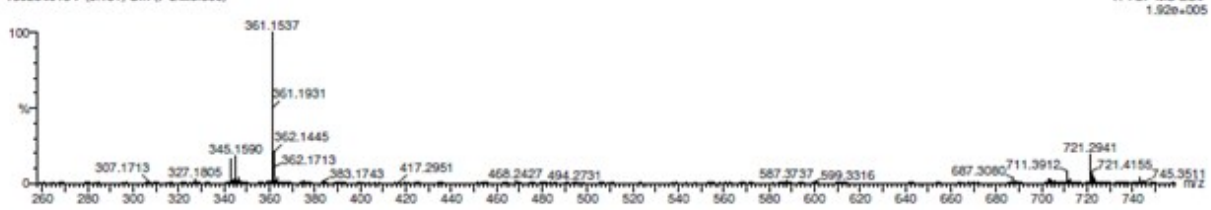
Elemental Composition Report



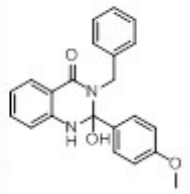
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
34 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 0-25 H: 0-29 N: 0-3 O: 0-4
C383/CJSR1/049
160204015 7 (0.131) Cm (7-24x0.500)

1: TOF MS ES+
1.92e+005



Minimum:		5.0	5.0	-1.5		
Maximum:				100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
361.1537	361.1552	-1.5	-4.2	13.5	12316.0	C22 H21 N2 O3



PerkinElmer Spectrum ES Version 10.03.08
Friday, February 05, 2016 8:13 PM

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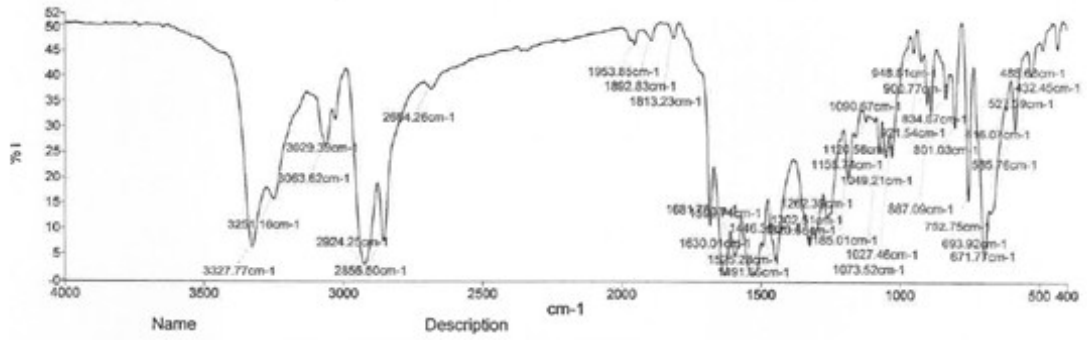
Analytical Research Department

Peak Table Graph

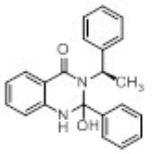


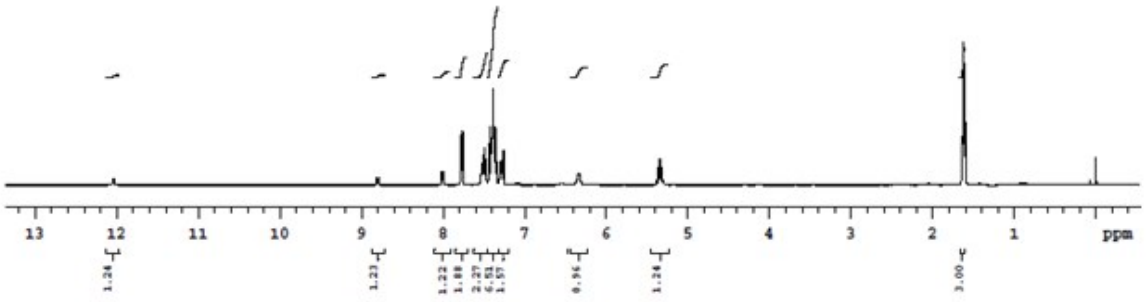
Name Description

TDC-106 C303/CJSR1/050 Fr-2

AR.No: MR0116/335

Analyst	:	Mallikarjun
Solvent	:	cdcl3
Date	:	Jan 6 2016
NUCLEUS	:	H1
FRQ (MHz)	:	400.22
EXP	:	PROTON

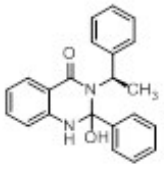


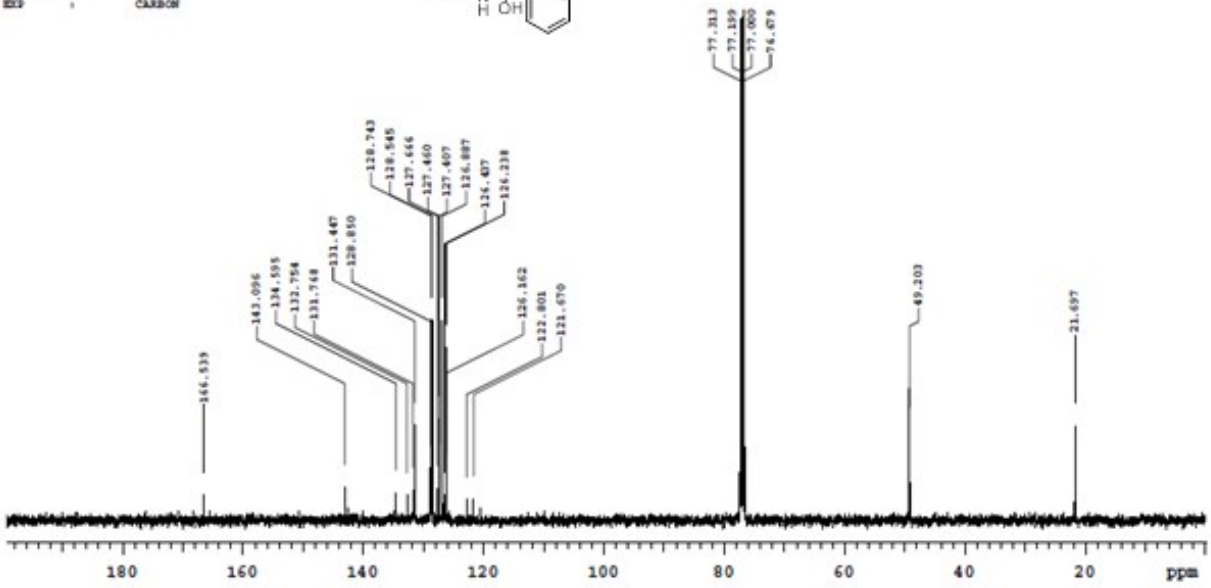


TDC-106 C303/CJSR1/050

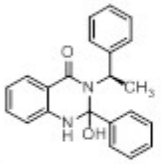
A.R.No: MR0216/962

Analyst	:	Mallikarjun
Solvent	:	cdcl3
Date	:	Feb 10 2016
NUCLEUS	:	C13
FRQ (MHz)	:	100.65
EXP	:	CARBON





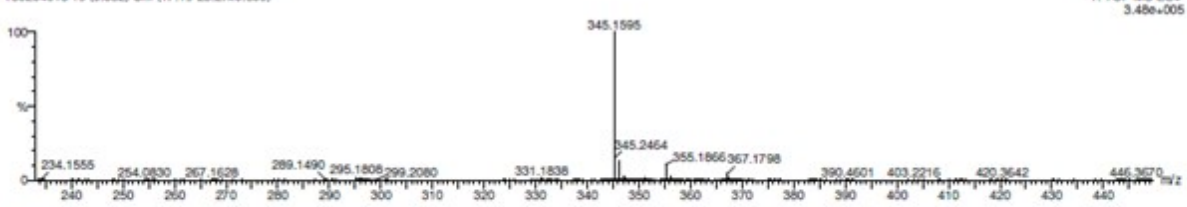
Elemental Composition Report



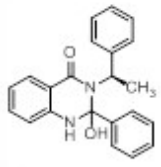
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
80 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 0-24 H: 0-29 N: 0-5 O: 0-5
C383/CJSR1/050
160204018 19 (0.352) Cm (17:19-25:27x0.500)

1: TOF MS ES+
3.48e+005



Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
345.1595	345.1603	-0.8	-2.3	13.5	14251.7	C22 H21 N2 O2



PerkinElmer Spectrum ES Version 10.03.08
Friday, February 05, 2016 8:24 PM

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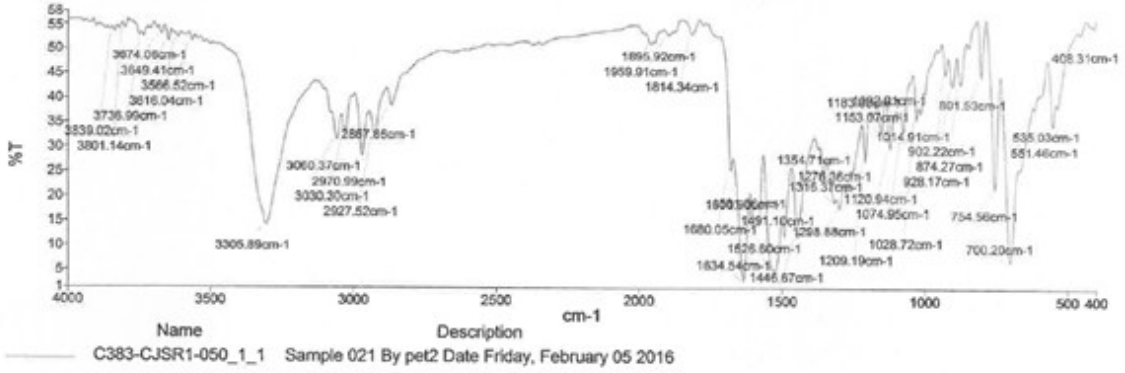
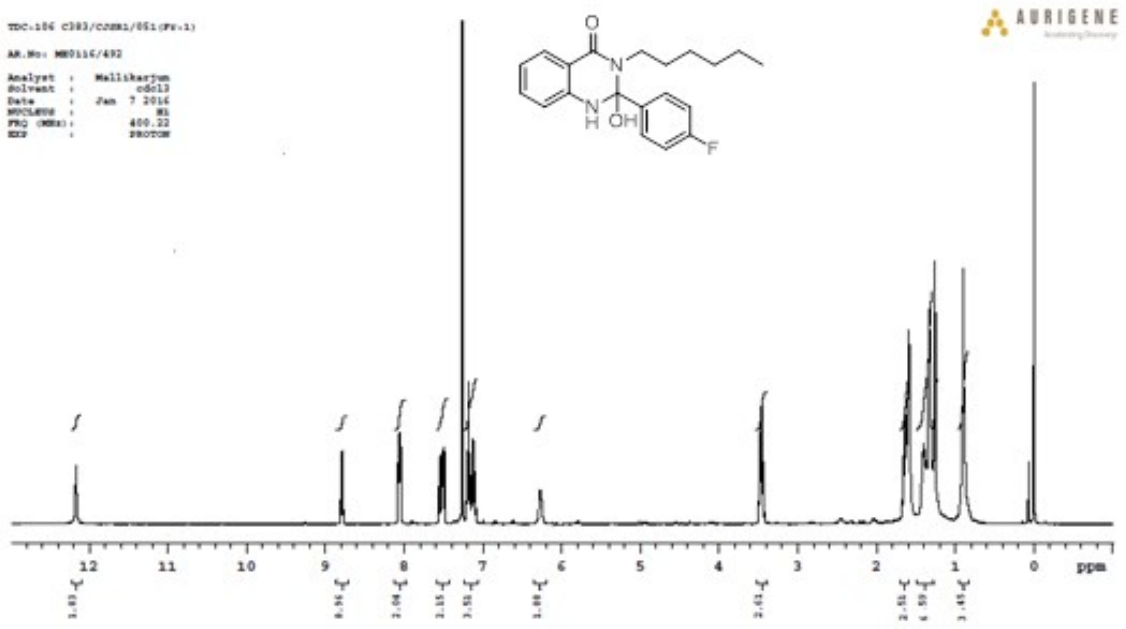
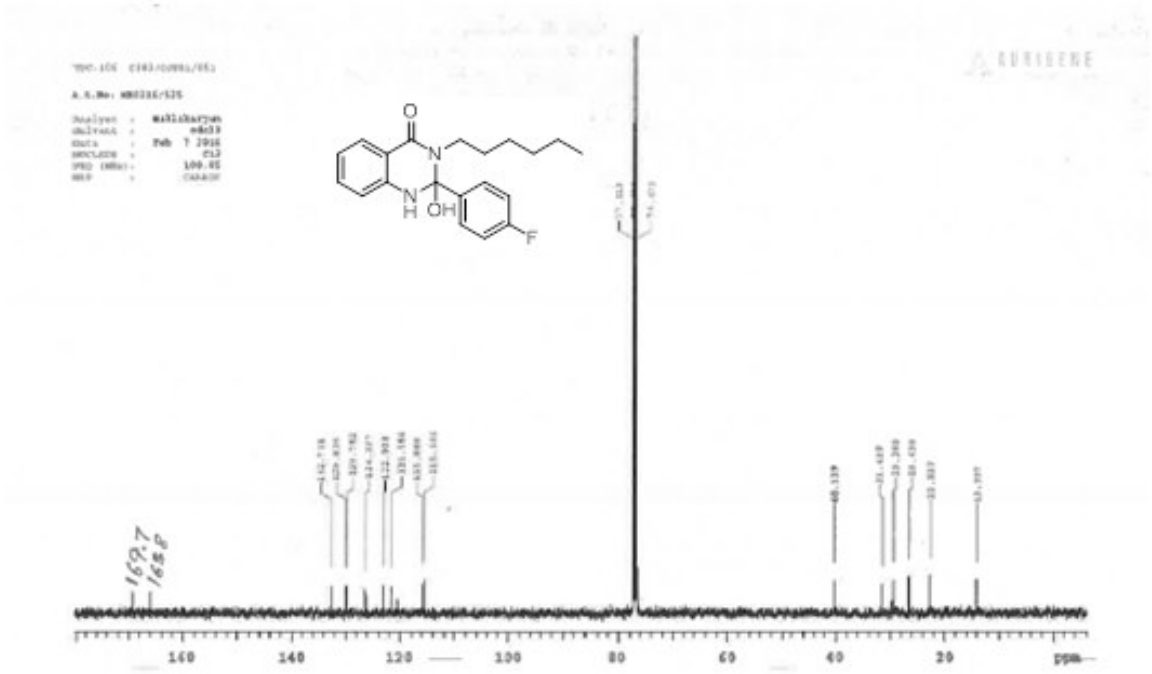
Analytical Research Department

Peak Table Graph



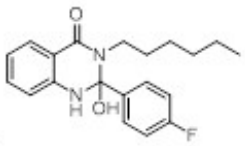
Name Description
C383-CJSR1-050_1_1 Sample 021 By pet2 Date Friday, February 05 2016


TDC-106 C303/C2SN1/051(Fr-1)
AR.No: MM0116/492
Analyst : Mallikarjun
Solvent : cdcl3
Date : Jan 7 2016
NUCLEUS : H1
FRQ (MHz): 400.22
EXP : PROTON
AURIGENE
O
N
H
OH
F
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm



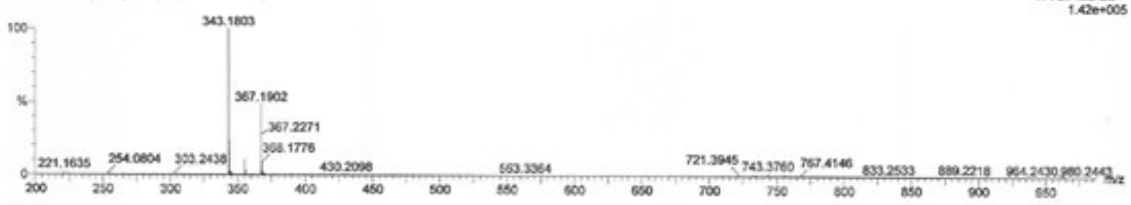
Elemental Composition Report

Single Mass Analysis
Tolerance = 6.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2



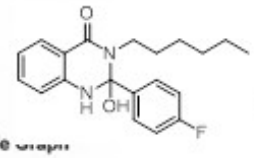
Monoisotopic Mass, Even Electron Ions
88 formula(e) evaluated with 1 results within limits (up to 5 closest results for each mass)
Elements Used:
C: 0-22 H: 0-30 N: 0-4 O: 0-4 F: 0-1
C383/CJSR1/051
160204007 30 (0.560) Cm (29:32-52:56x0.500)

1: TOF MS ES+
1.42e+005



Minimum:				-1.5		
Maximum:		5.0	6.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
343.1803	343.1822	-1.9	-5.5	9.5	245.7	C20 H24 N2 O2 F

R. Murugan 22/02/2016



PerkinElmer Spectrum ES Version 10.03.08
Friday, February 05, 2016 8:13 PM

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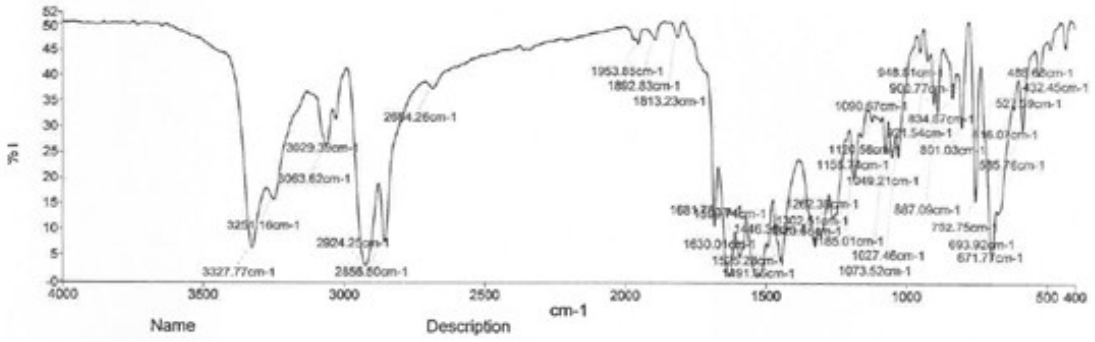
Analytical Research Department

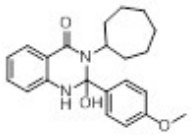
Peak Table Graph



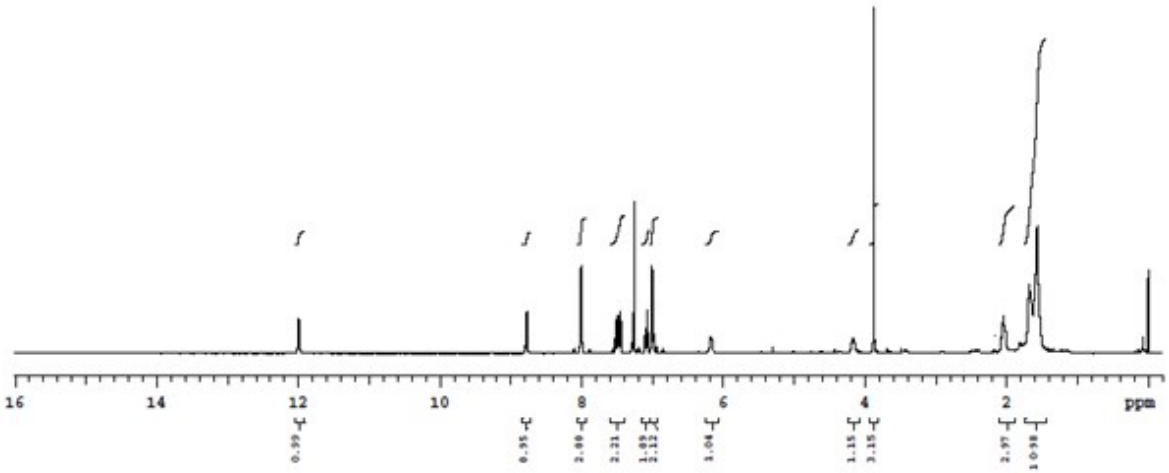
TDC-106 C383/CJSR1/052 Fr-1

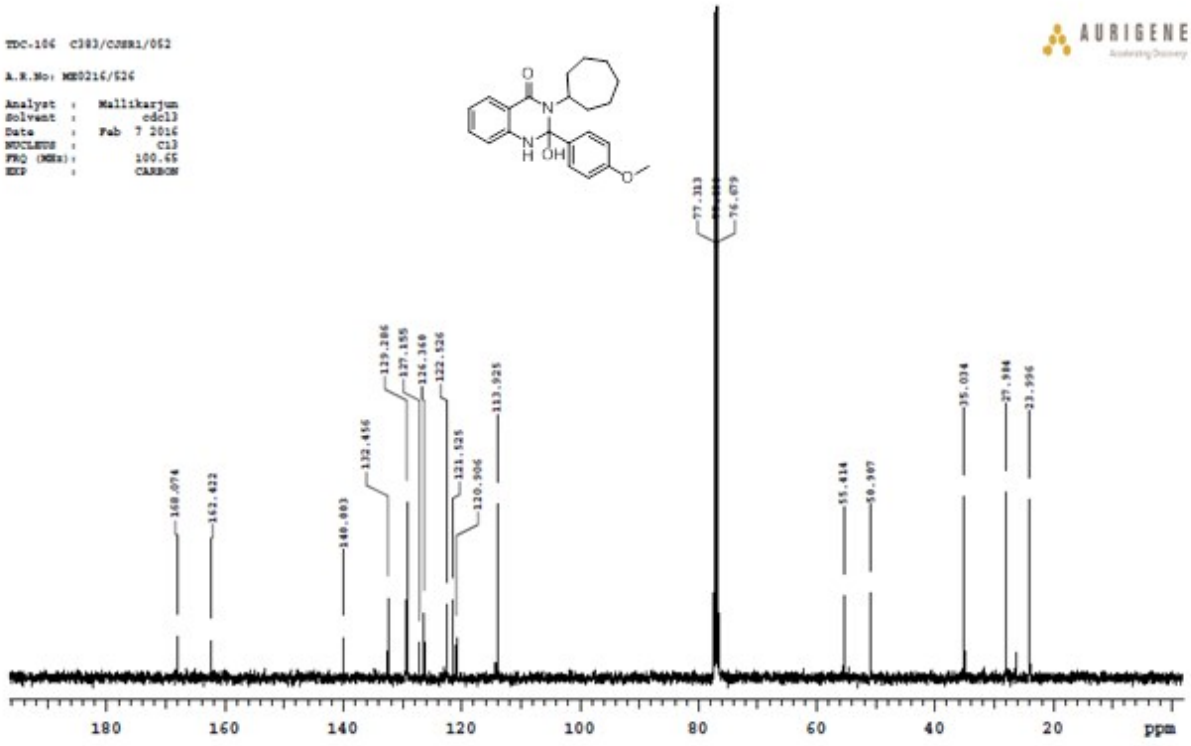
AR.No: MR0116/816

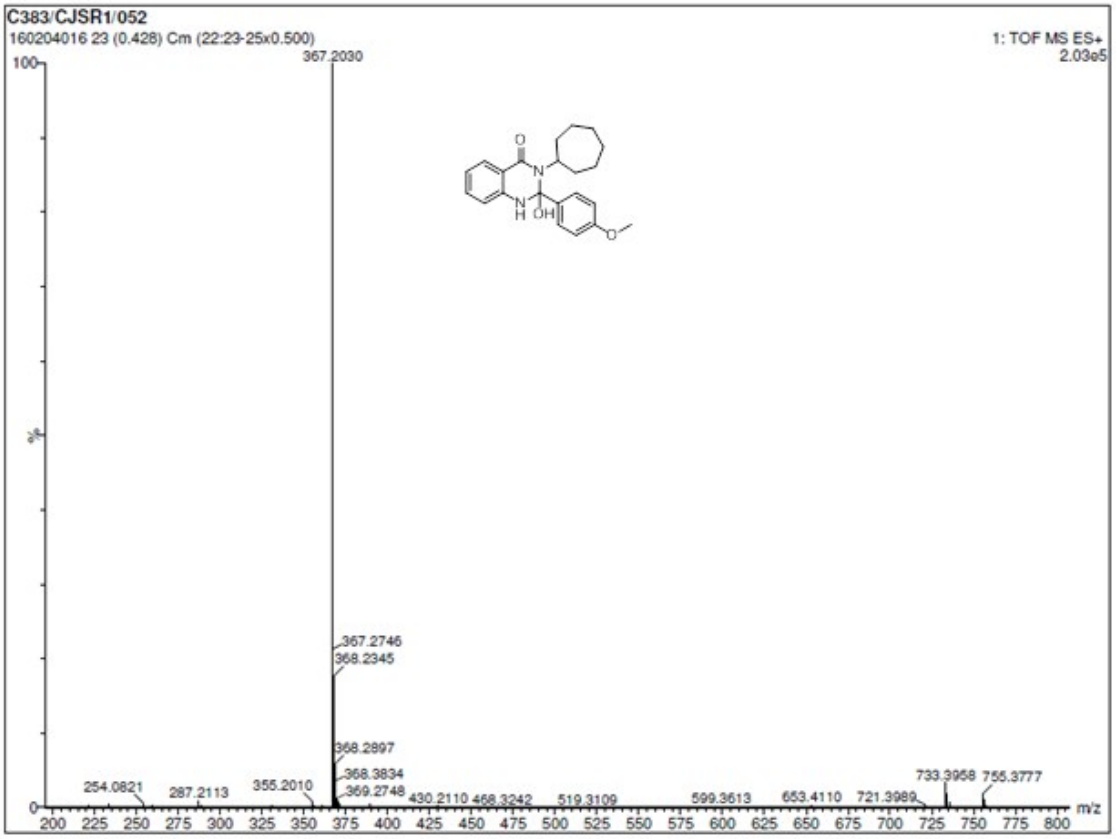
Analyst : Mallikarjun
Solvent : cdcl3
Date : Jan 12 2016
NUCLEUS : H1
FRQ (MHz) : 400.22
EXP : PROTON

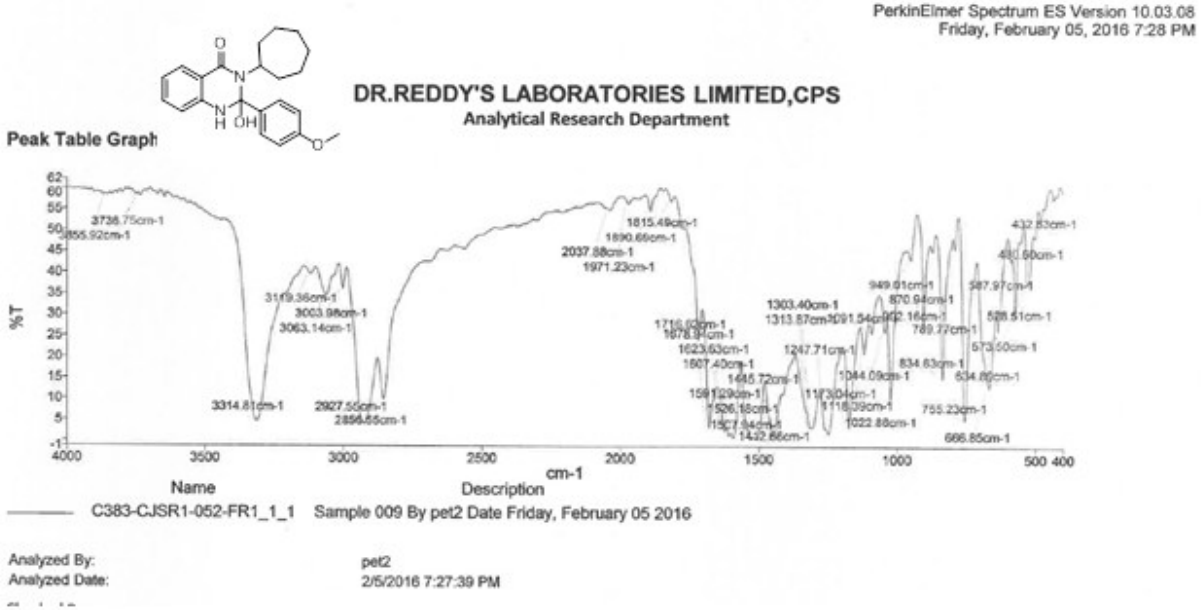


AURIGENE




TDC-106 C303/CONBR1/052
A.R.No: MR0216/526
Analyst : Mallikarjun
Solvent : cdcl3
Date : Feb 7 2016
NUCLEUS : C13
FRQ (MHz): 100.65
EXP : CARBON
AURIGENE
O
N
H
N
OH
O
77.333
76.679
160.074
152.422
140.603
132.456
129.286
127.155
126.349
122.526
121.525
120.506
113.925
55.414
50.597
35.034
27.984
23.996
180
160
140
120
100
80
60
40
20
ppm


C383/CJSR1/052
160204016 23 (0.428) Cm (22:23-25x0.500)
1: TOF MS ES+
2.03e5
367.2030
367.2746
368.2345
368.2897
368.3834
369.2748
254.0821
287.2113
355.2010
430.2110
468.3242
519.3109
599.3613
653.4110
721.3989
733.3958
755.3777
%
m/z


PerkinElmer Spectrum ES Version 10.03.08
Friday, February 05, 2016 7:28 PM
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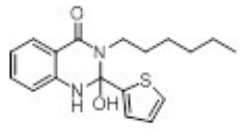
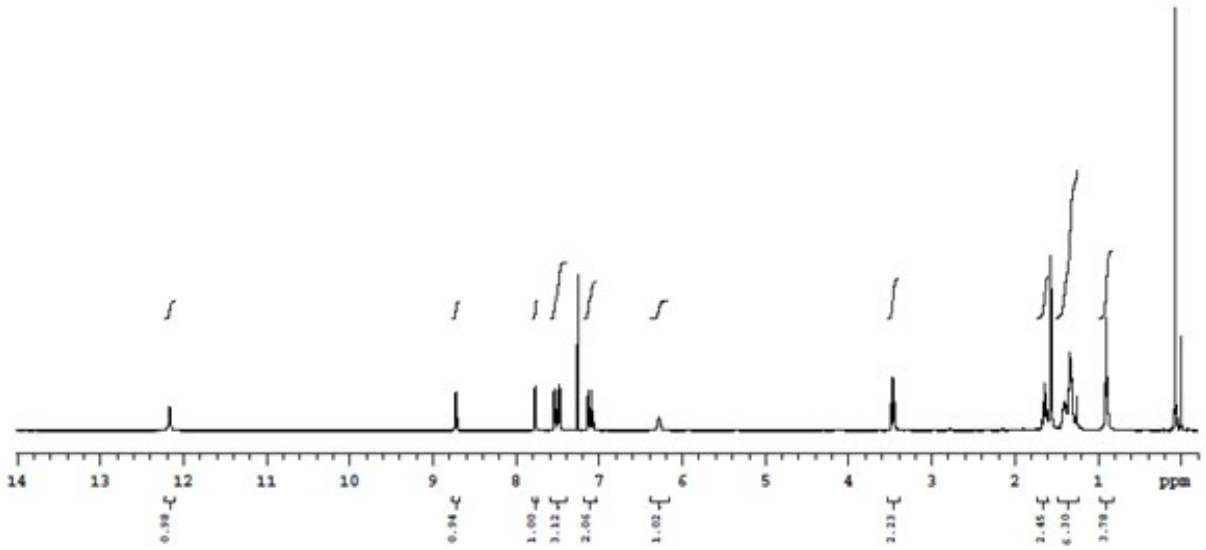
Analytical Research Department
Peak Table Graph
%T
cm-1
3738.75cm-1
3655.92cm-1
3119.36cm-1
3063.14cm-1
3003.98cm-1
3314.81cm-1
2927.55cm-1
2856.55cm-1
2037.88cm-1
1971.23cm-1
1815.49cm-1
1890.66cm-1
1716.63cm-1
1678.34cm-1
1623.63cm-1
1607.40cm-1
1495.72cm-1
1303.40cm-1
1313.87cm-1
1247.71cm-1
1044.09cm-1
949.01cm-1
870.94cm-1
834.63cm-1
789.77cm-1
755.23cm-1
666.85cm-1
Name
Description
C383-CJSR1-052-FR1_1_1 Sample 009 By pet2 Date Friday, February 05 2016
Analyzed By: pet2
Analyzed Date: 2/5/2016 7:27:39 PM

TDC-106 C383-CDER1-055-Pr-2

A.R.No: MR0116/2095
Analyst : Mallikarjun
Solvent : cdcl3
Date : Jan 29 2016
NUCLEUS : H1
FRQ (MHz): 400.22
EXP : PROTON

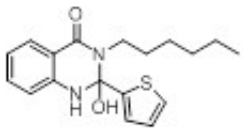


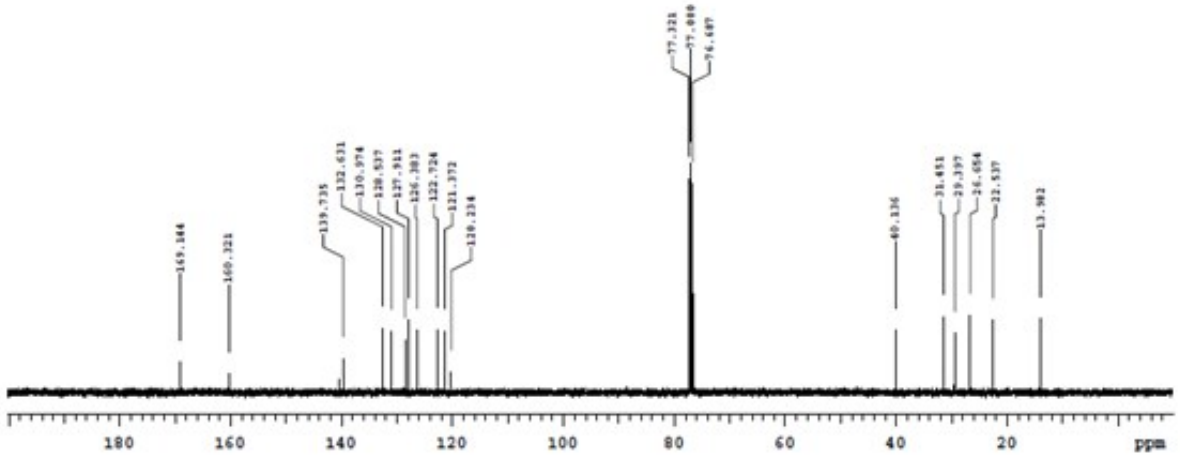


TDC-106 C383/CDER1/055

A.R.No: MR0216/2106

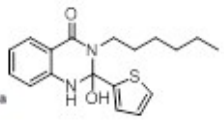
Analyst : Mallikarjun
Solvent : cdcl3
Date : Feb 24 2016
NUCLEUS : C13
FRQ (MHz): 100.65
EXP : CARBON





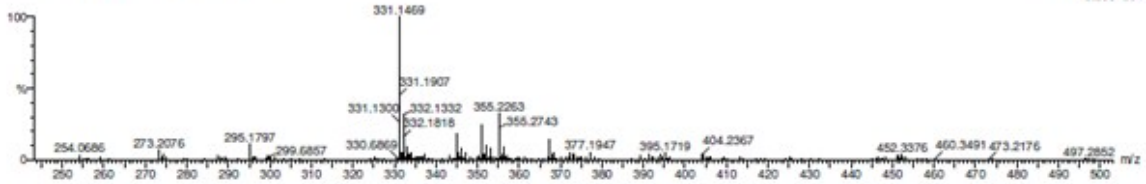
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

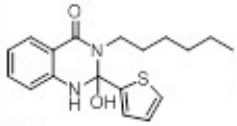


Monoisotopic Mass, Even Electron Ions
139 formula(e) evaluated with 1 results within limits (up to 10 closest results for each ma
Elements Used:
C: 0-20 H: 0-29 N: 0-3 O: 0-5 S: 0-2
C383/CJSR1/055
160204020 34 (0.634) Cm (34:36-68:70x0.500)

1: TOF MS ES+
3.89e+004



Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
331.1469	331.1480	-1.1	-3.3	8.5	6848.4	C18 H23 N2 O2 S



PerkinElmer Spectrum ES Version 10.03.
Friday, February 05, 2016 7:16 I

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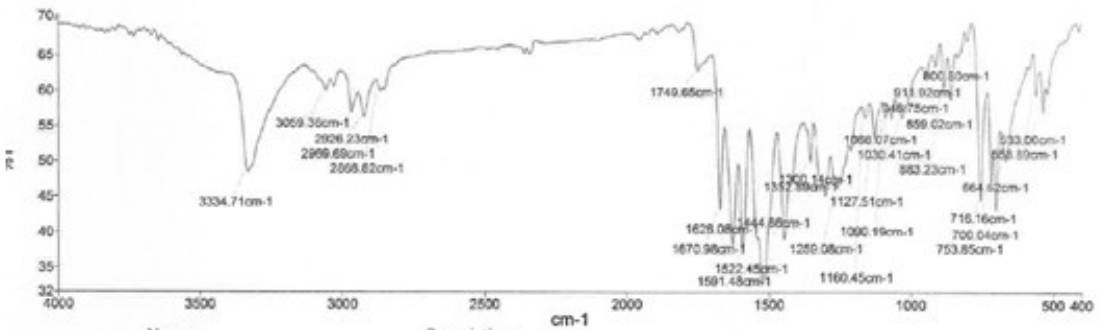
Analytical Research Department

eak Table Graph

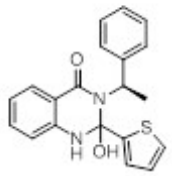


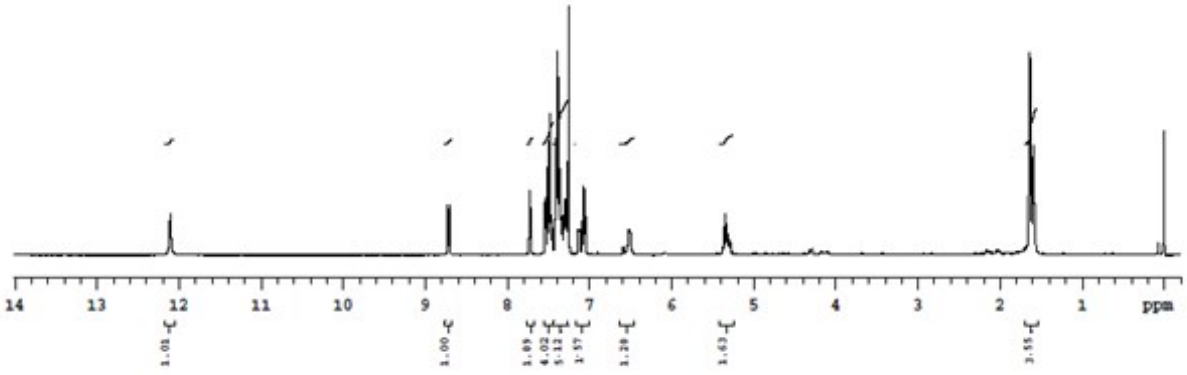
Name	Description
C383-CJSR1-055	Sample 007 By pet2 Date Friday, February 05 2016

TDC-106 C303-CDSR1-056

A.R.No: MK0216/305

Analyst : Mallikarjun
Solvent : cdcl3
Date : Feb 4 2016
NUCLEUS : H1
FRQ (MHz): 400.22
EXP : PROTON

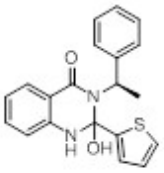




TDC.106 C303/CDSR1/056

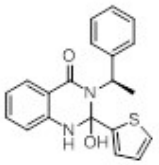
A.R.No: MK0216/1071

Analyst : Mallikarjun
Solvent : cdcl3
Date : Feb 12 2016
NUCLEUS : C13
FRQ (MHz): 100.65
EXP : CARBON



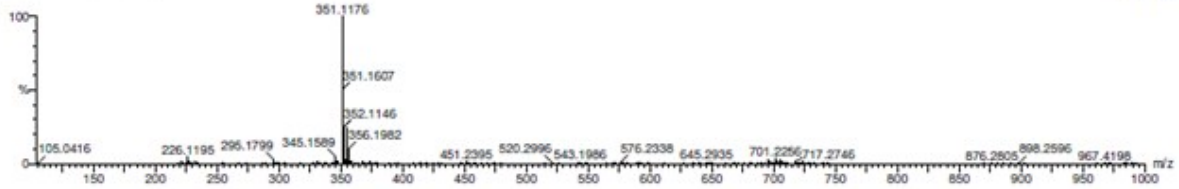
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

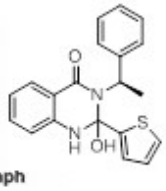


Monoisotopic Mass, Even Electron Ions
169 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 0-24 H: 0-29 N: 0-3 O: 0-5 S: 0-2
C383/CJSR1/056
160204019 37 (0.692) Cm (37:38-56:60x0.500)

1: TOF MS ES+
1.44e+005



Minimum:		5.0	5.0	-1.5		
Maximum:				100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
351.1176	351.1167	0.9	2.6	12.5	34.0	C20 H19 N2 O2 S



PerkinElmer Spectrum ES Version 10.03.08
Friday, February 05, 2016 7:16 PM

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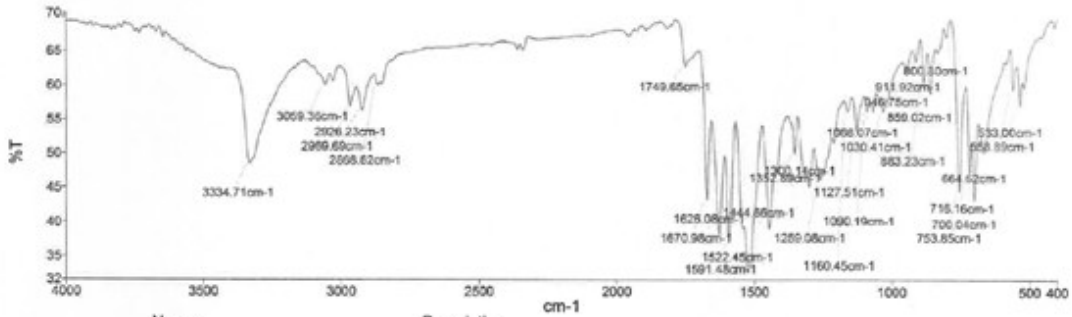
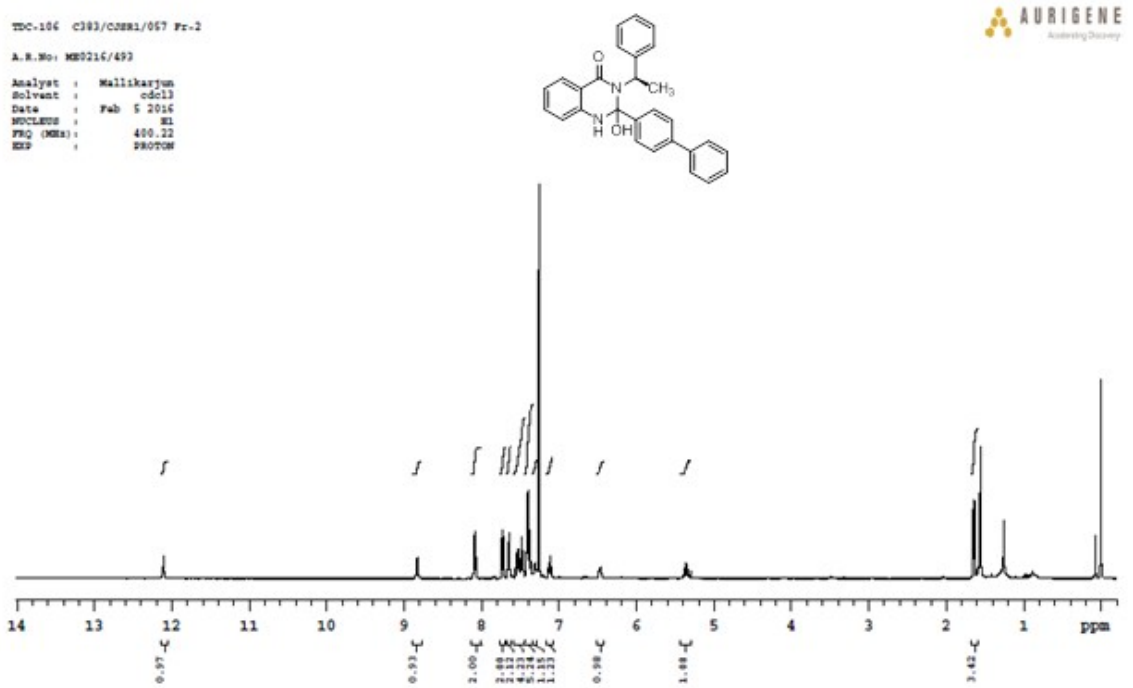
Analytical Research Department

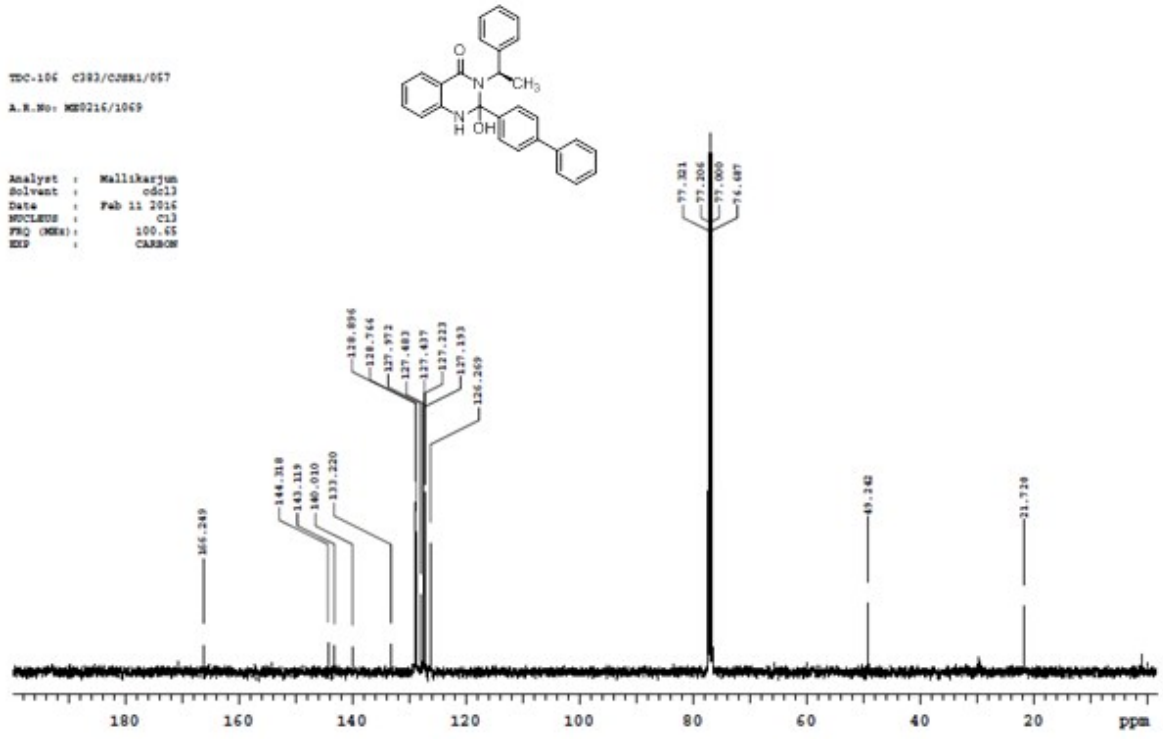
Peak Table Graph



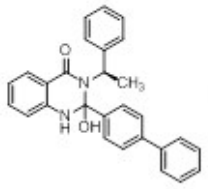
Name	Description
C383-CJSR1-056_1_1	Sample 007 By pet2 Date Friday, February 05 2016

Analyzed By: pet2
Analyzed Date: 2/5/2016 7:13:23 PM


TDC-106 C303/CJSR1/057 Fr-2
A.R.No: MH0216/493
Analyst : Mallikarjun
Solvent : cdcl3
Date : Feb 5 2016
NUCLEUS : H1
FRQ (MHz): 400.22
EXP : PROTON
AURIGENE
14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
0.97 0.93 2.00 3.42


TDC-106 C303/CJSR1/057
A.R.No: MH0216/1069
Analyst : Mallikarjun
Solvent : cdcl3
Date : Feb 11 2016
NUCLEUS : C13
FRQ (MHz): 100.65
EXP : CARBON
166.249
144.318
143.119
140.010
133.220
128.896
128.764
127.972
127.483
127.437
127.223
127.193
126.269
77.321
77.204
77.000
76.687
49.242
21.729
180 160 140 120 100 80 60 40 20 ppm

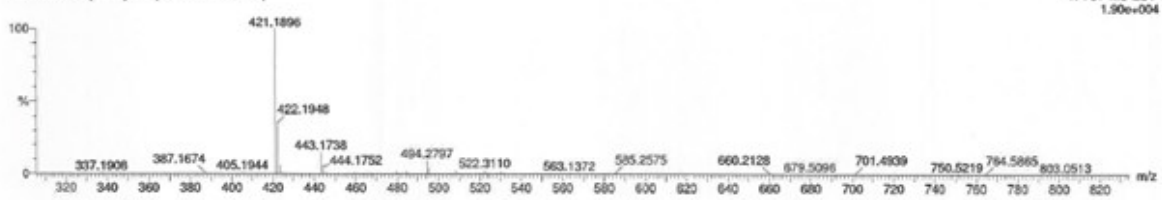
Elemental Composition Report



Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

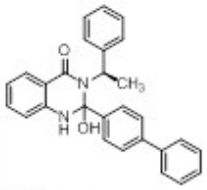
Monoisotopic Mass, Even Electron Ions
28 formula(e) evaluated with 1 results within limits (up to 2 closest results for each mass)
Elements Used:
C: 0-30 H: 0-26 N: 0-3 O: 0-4
C383/CJSR1/057
160209002 44 (0.812) Cm (44:51-79:92x0.500)

1: TOF MS ES+
1.90e+004



Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
421.1896	421.1916	-2.0	-4.7	17.5	13.8	C28 H25 N2 O2

R.Nagabath 22/01/2016



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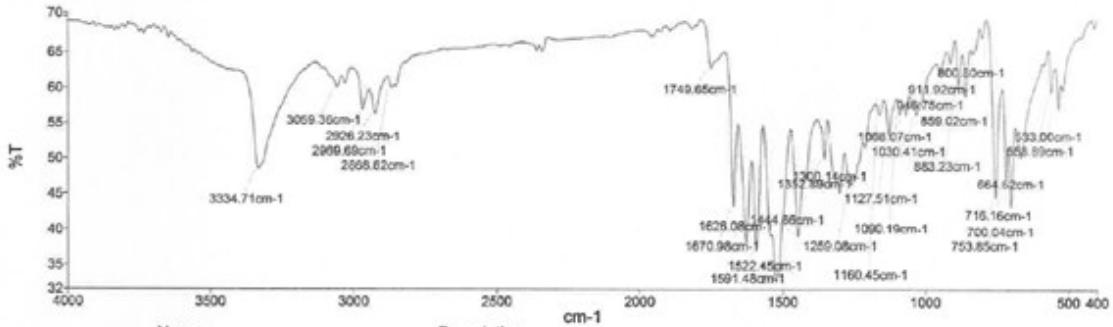
Analytical Research Department

Peak Table Graph



Name Description

C383-CJSR1-057_1_1 Sample 007 By pet2 Date Friday, February 05 2016

Analyzed By: pet2
Analyzed Date: 2/5/2016 7:13:23 PM

Checked By:
Checked Date:

CSIL/CSIL14/009-Fr-1 in CDCl3
A.R.No: NE16F215

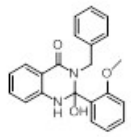
Sample Name:

Data Collected on:
DRILS-vnmrs400
Archive directory:

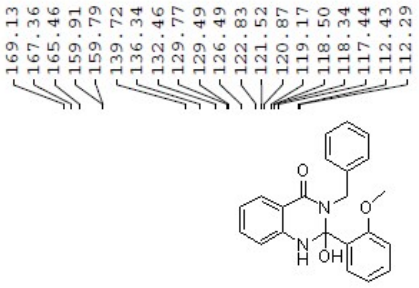
Sample directory:

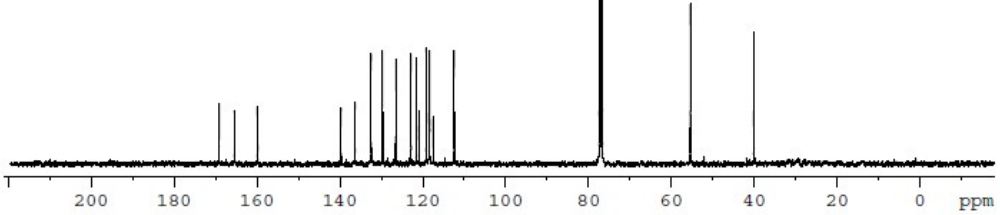
FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 17 2016



Dr.Reddy's
C383/CJSR1/066(Fr-2)
13C-NMR\CDCL3
21-06-2016
ANALYSED BY : KRP





Current Data Parameters
NAME QC11160621034
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160621
Time 22.46
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 24036
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 1.000102 Hz
AQ 0.4999488 sec
RG 195.98
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

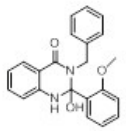
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
PLW1 52.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 13.00000000 W
PLW12 0.31457001 W
PLW13 0.25479999 W

F2 - Processing parameters
SI 32768
SF 100.6127715 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

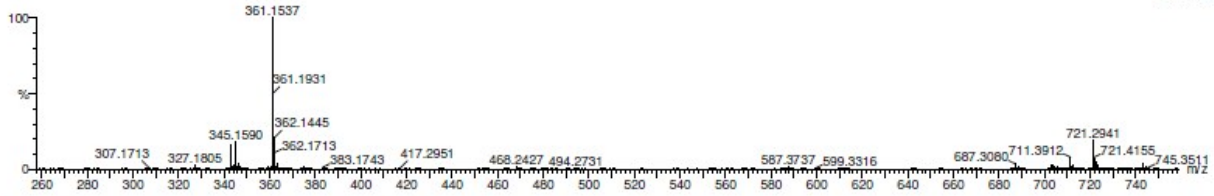
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2



Monoisotopic Mass, Even Electron Ions
34 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 0-25 H: 0-29 N: 0-3 O: 0-4
CSIL/CSIL14/009-Fr-1
160204015 7 (0.131) Cm (7-24x0.500)

1: TOF MS ES+
1.92e+005



Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
361.1537	361.1552	-1.5	-4.2	13.5	12316.0	C22 H21 N2 O3

CSIL/CSIL14/009-Fr-2 in CDCl3
A.R.No: NE16F216

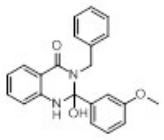
Sample Name:

Data Collected on:
DRILS-vnmrs400
Archive directory:

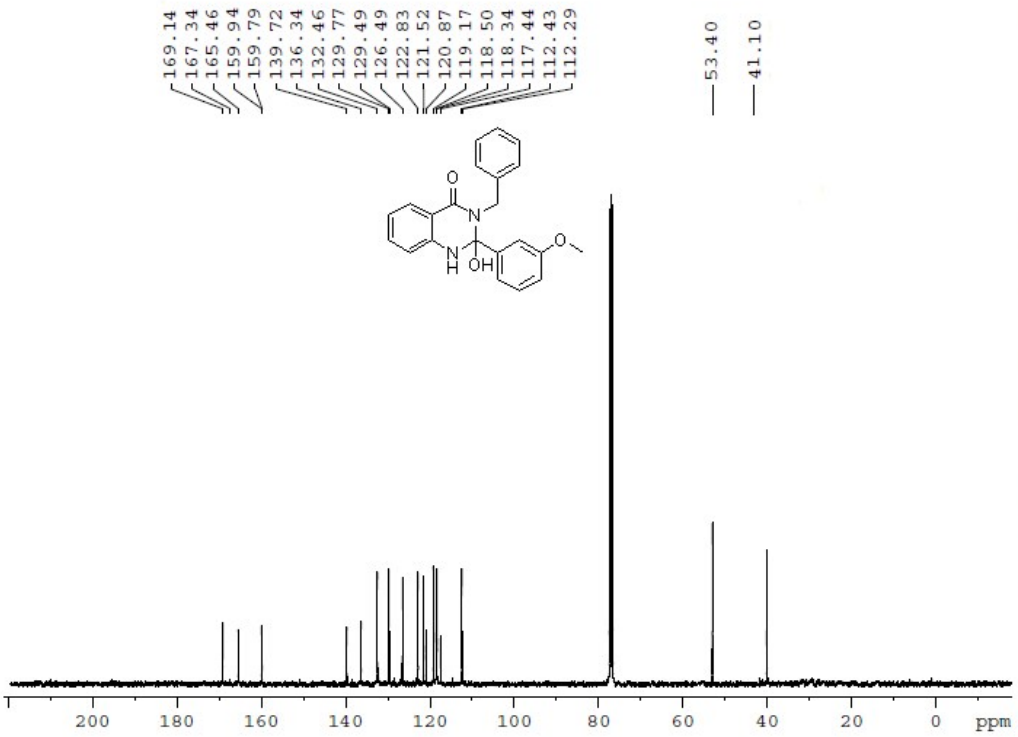
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 17 2016



Dr.Reddy's
C383/CJSR1/064
13C-NMR\CDCL3
21-06-2016
ANALYSED BY : KRP



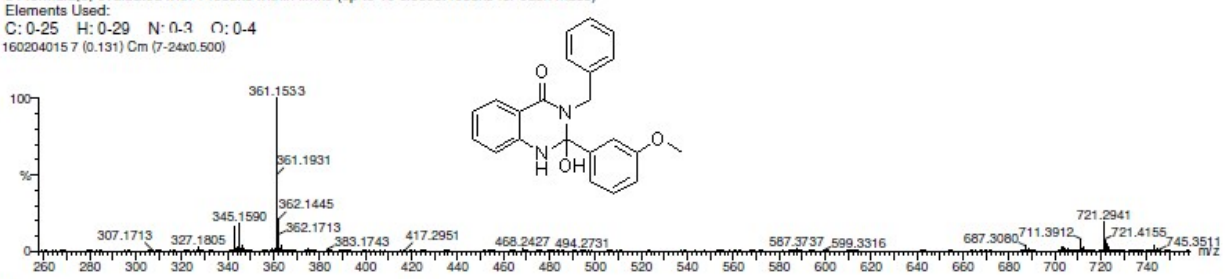

```
Current Data Parameters
NAME       QC11160621034
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20160621
Time               22.46
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               24036
SOLVENT          CDCl3
NS                1024
DS                   4
SWH          24038.461 Hz
FIDRES        1.000102 Hz
AQ            0.4999488 sec
RG               195.98
DW               20.800 usec
DE                6.50 usec
TE              298.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        100.6228293 MHz
NUC1               13C
P1               10.00 usec
PLW1        52.00000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            90.00 usec
PLW2        13.00000000 W
PLW12        0.31457001 W
PLW13        0.25479999 W

F2 - Processing parameters
SI                32768
SF          100.6127715 MHz
WDW                  EM
SSB       0
LB                3.00 Hz
GB        0
PC                1.40
```

Elemental Composition Report

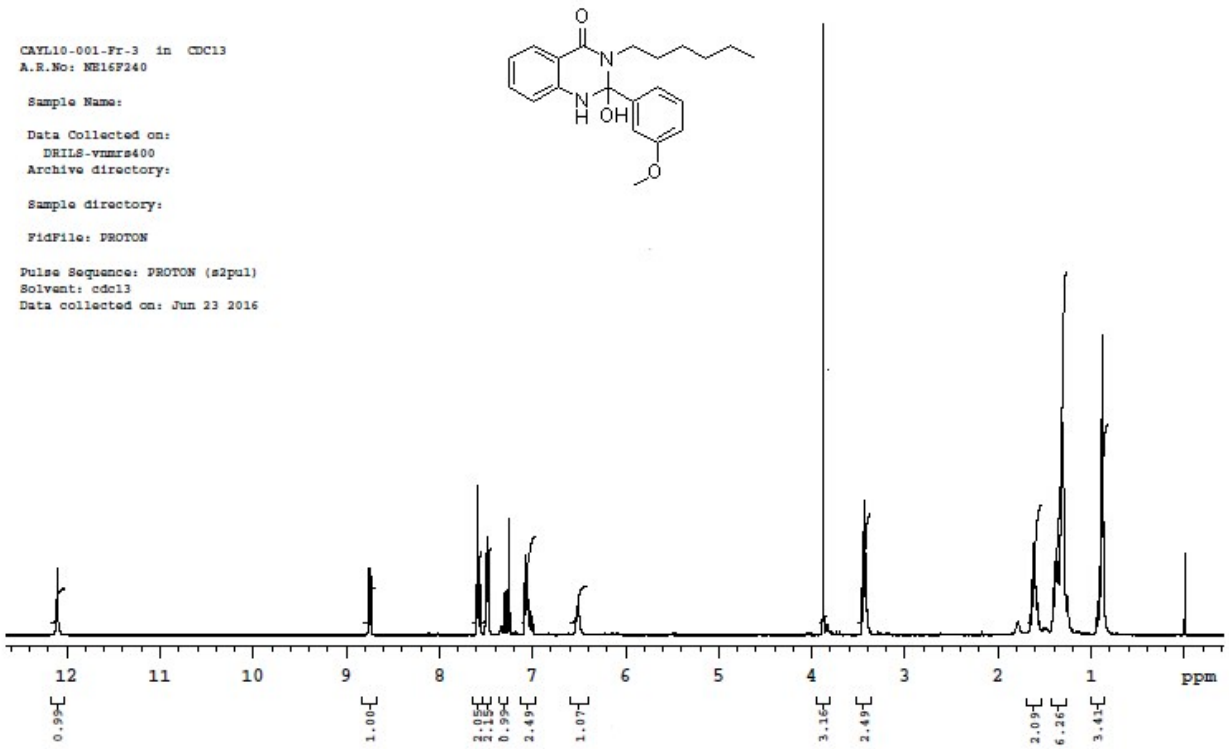
Single Mass Analysis

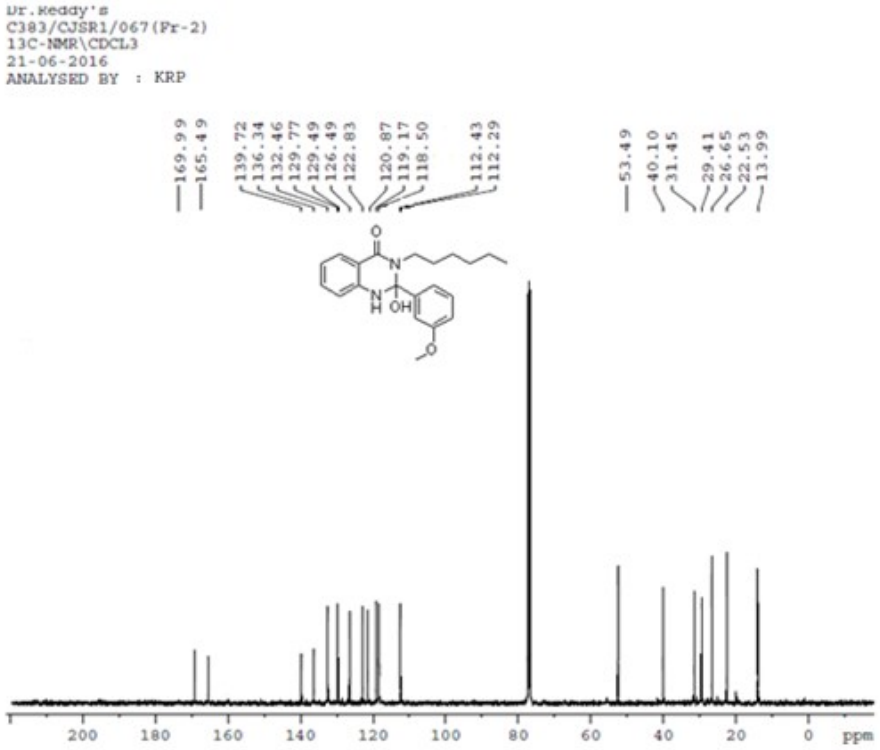
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
34 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 0-25 H: 0-29 N: 0-3 O: 0-4
1602040157 (0.131) Cm (7-24x0.500)



Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
361.1533	361.1552	-1.5	-4.2	13.5	12316.0	C22 H21 N2 O3



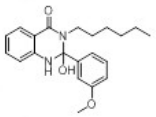



```
Current Data Parameters
NAME          gc51140421034
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20160421
Time                  22.46
INSTRUM               spect
PROBHD     5 mm PABBO BB/
PULPROG           zgpg30
TD                 24034
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH           24038.461 Hz
FIDRES         1.000102 Hz
AQ             0.4999488 sec
RG                 199.98
DW                20.800 usec
DE                 6.50 usec
TE                 298.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228293 MHz
NUC1                  13C
P1                 10.00 usec
PLW1        52.00000000 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2        13.00000000 W
PLW12        0.31457001 W
PLW13        0.25479999 W

F2 - Processing parameters
SI                 32768
SF          100.6127715 MHz
WDW                   EM
SSB        0
LB                 3.00 Hz
GB         0
PC                 1.40
```

CPS,MIYAPUR

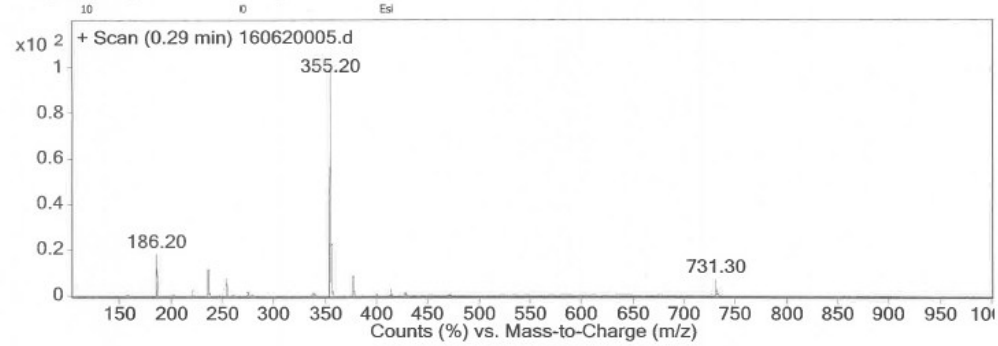
Mass Analysis Report

Data Filename	160620005.d	**Sample Name**	C383/CJSR1/067 Fr-2
Sample Type	Sample	**Position**	Vial 23
Instrument Name	Instrument 1	**User Name**	
Acq Method	ESI.m	**IRM Calibration Status**	Success
DA Method	CACH8.m	**Comment**	



User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
10	0	Esi

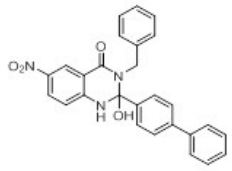


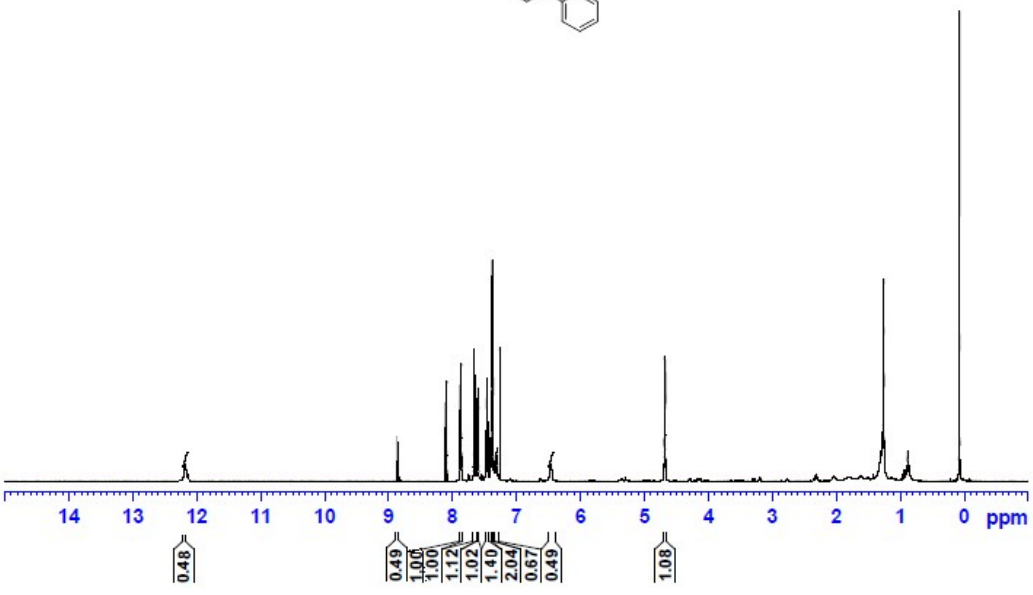
--- End Of Report ---

B Solicy
20/06/2016

Dr.Reddy's
C383/CJSR1/066(Fr-1)
1H-NMR\CDCL3
21-06-2016
ANALYSED BY : KRP

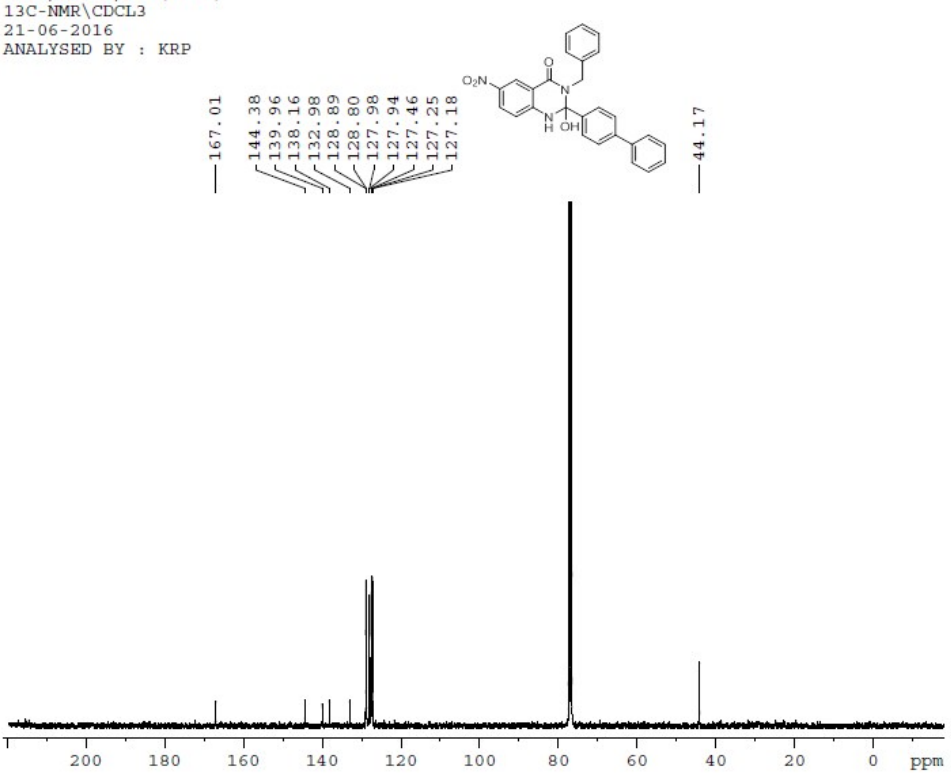
BRUKER






```
Current Data Parameters
NAME        QC11160621029
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20160621
Time                20.23
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 36056
SOLVENT             CDCl3
NS                     16
DS                      2
SWH             12019.230 Hz
FIDRES              0.333349 Hz
AQ              1.4999295 sec
RG                 195.98
DW                41.600 usec
DE                 6.50 usec
TE                298.1 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                    1H
P1                  14.00 usec
PLW1         13.47000027 W

F2 - Processing parameters
SI                  65536
SF            400.1300097 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

Dr.Reddy's
C383/CJSR1/066(Fr-1)
13C-NMR\CDCL3
21-06-2016
ANALYSED BY : KRP



Current Data Parameters
NAME QC11160621030
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160621
Time 21.08
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 24036
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 1.000102 Hz
AQ 0.4999488 sec
RG 195.98
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
PLW1 52.00000000 W

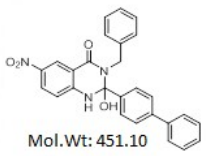
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 13.00000000 W
PLW12 0.31457001 W
PLW13 0.25479999 W

F2 - Processing parameters
SI 32768
SF 100.6127726 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

CPS,MIYAPUR

Mass Analysis Report

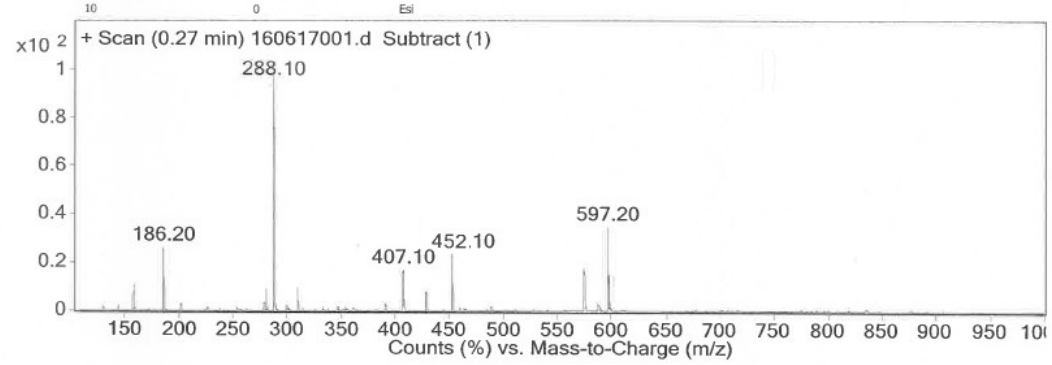
Data Filename	160617001.d	**Sample Name**	C383/CJSR1/066 Fr-1
Sample Type	Sample	**Position**	Vial 3
Instrument Name	Instrument 1	**User Name**	
Acq Method	ESI.m	**IRM Calibration Status**	Success
DA Method	CACH8.m	**Comment**	



Mol.Wt: 451.10

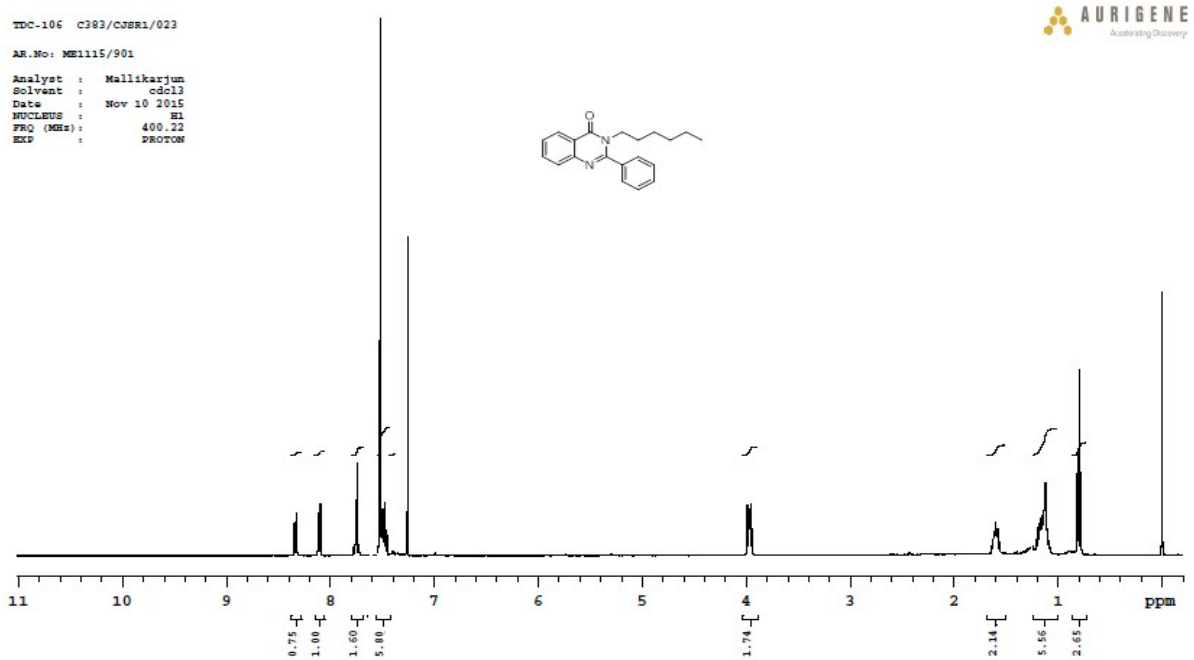
User Spectra

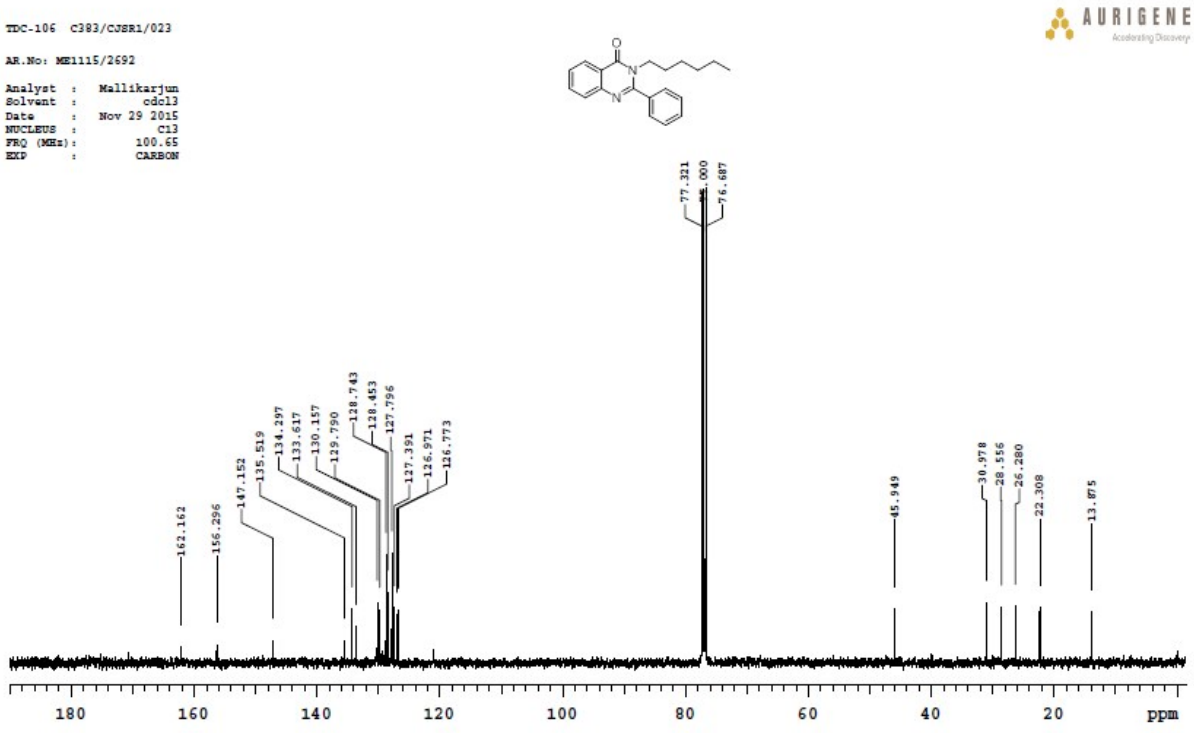
Fragmentor Voltage	Collision Energy	Ionization Mode
10	0	Esi



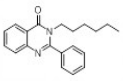
--- End Of Report ---

B.Sreenu
17/06/2016

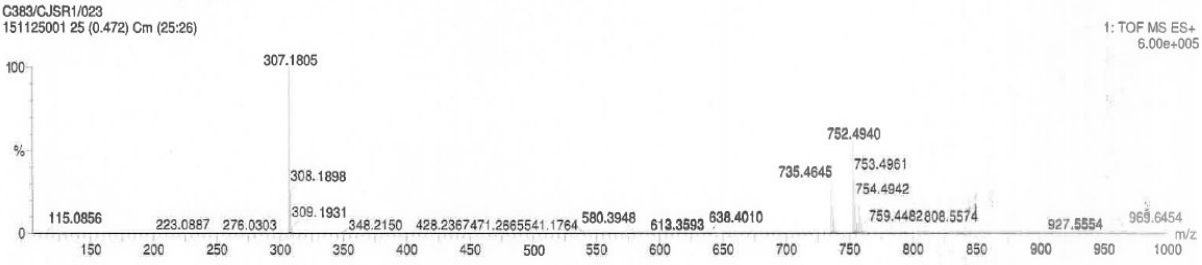

TDC-106 C383/CJSR1/023
AR.No: ME1115/901
Analyst : Mallikarjun
Solvent : cdcl3
Date : Nov 10 2015
NUCLEUS : H1
FRQ (MHz): 400.22
EXP : PROTON
AURIGENE
Accelerating Discovery
11 10 9 8 7 6 5 4 3 2 1 ppm
0.75 1.00 1.60 5.80 1.74 2.14 5.56 2.65


TDC-106 C383/CJSR1/023
AR.No: ME1115/2692
Analyst : Mallikarjun
Solvent : cdcl3
Date : Nov 29 2015
NUCLEUS : C13
FRQ (MHz): 100.65
EXP : CARBON
AURIGENE
Accelerating Discovery
77.321
77.000
76.687
162.162
156.296
147.152
135.519
134.297
133.617
130.157
129.790
128.743
128.453
127.796
127.391
126.971
126.773
45.949
30.978
28.556
26.280
22.308
13.875
180 160 140 120 100 80 60 40 20 ppm

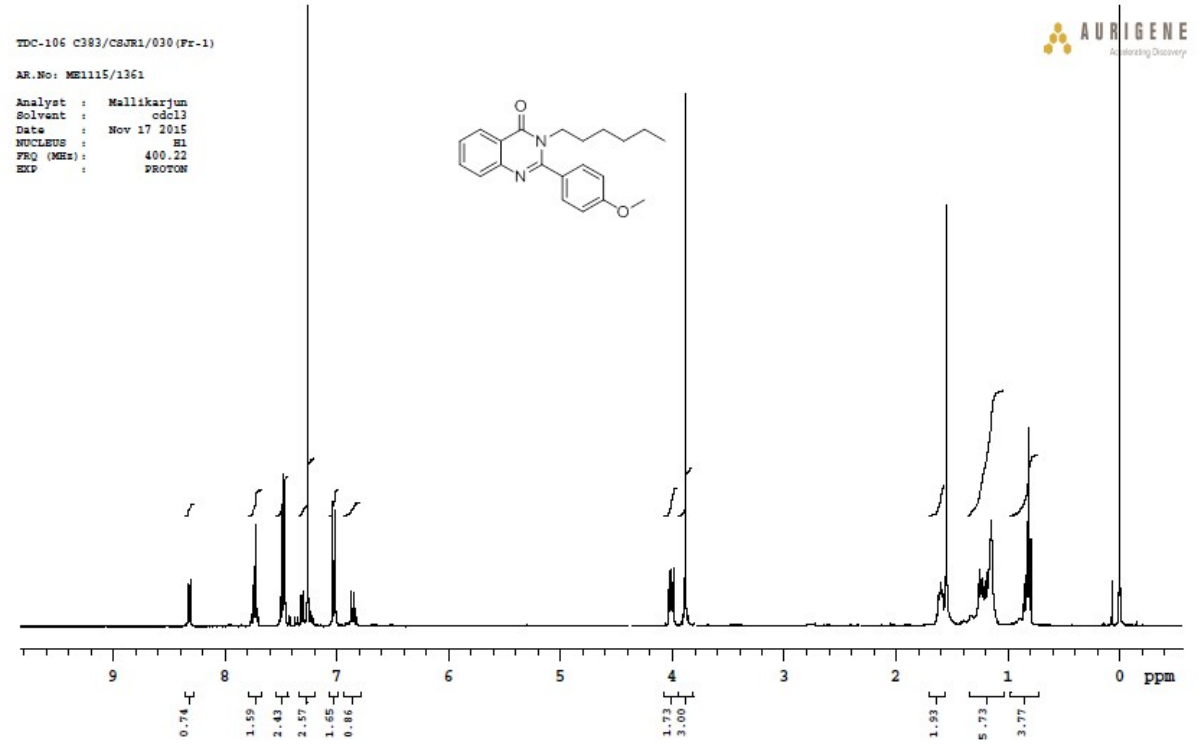
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2



Monoisotopic Mass, Even Electron Ions
70 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 0-25 H: 0-25 N: 0-5 O: 0-4
C383/CJSR1/023
151125001 25 (0.472) Cm (25:26)



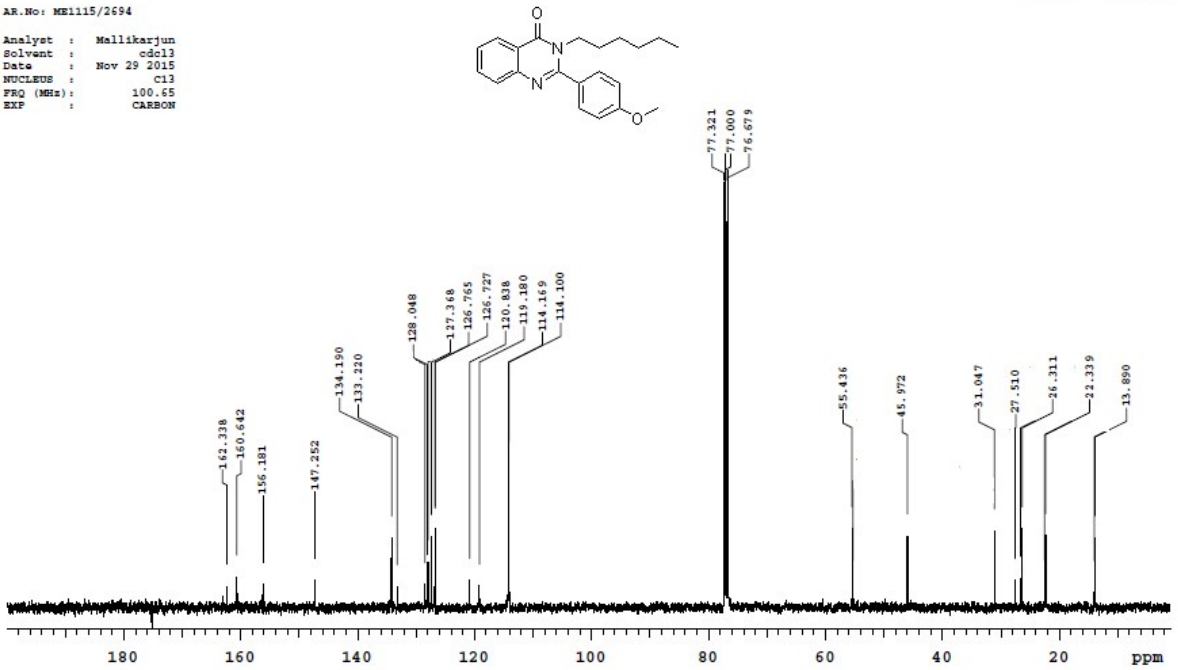
Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
307.1805	307.1810	-0.5	-1.6	10.5	545.9	C20 H23 N2 O



TDC-106 C383/CJSR1/030

AR.No: ME1115/2694

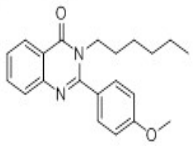
Analyst	:	Mallikarjun
Solvent	:	cdcl3
Date	:	Nov 29 2015
NUCLEUS	:	C13
FRQ (MHz)	:	100.65
EXP	:	CARBON



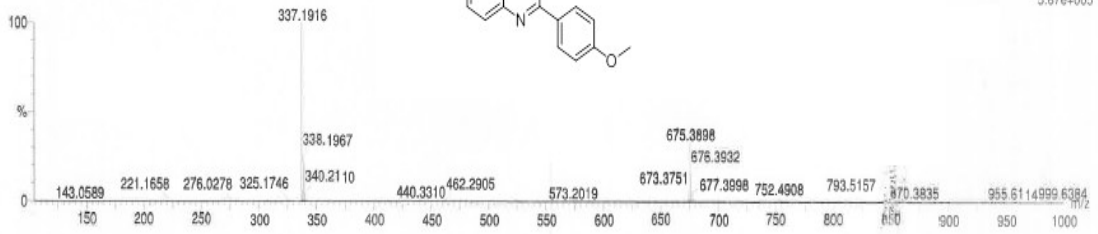
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
47 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 0-22 H: 0-25 N: 0-5 O: 0-4
C383/CJSR1/030
151125004 29 (0.545) Cm (29:31)



1: TOF MS ES+
5.67e+005



Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
337.1916	337.1916	0.0	0.0	10.5	53.9	C21 H25 N2 O2