Supporting Information

C-N and C-P bond formation *via* cross dehydrative coupling reaction: an efficient synthesis of novel 3,4-dihydroquinazolines

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1. General Information

All the other chemicals and solvents were obtained from commercial sources, and purified by using standard methods. Silica gel (100–200 mesh) was used for column chromatography and thin-layer chromatography was performed on pre-coated silica gel 60-F_{254} plates and visualized by UV-light and developed by iodine. The IR values are reported in reciprocal centimeters (cm^{-1}). All ^{1}H, $^{13}C\{^{1}H\}$, ^{31}P NMR spectras were recorded on a 300, 400, and 500 MHz spectrometer. Chemical shifts (δ) are reported in ppm, using TMS (δ =0) as an internal standard in $CDCl_3$. The peak patterns are indicated as follows: bs, broad singlet; s, singlet; d, doublet; t, triplet; dd, doublet of doublet; sep, septet; m, multiplet. The coupling constants (*J*) are reported in Hertz (Hz). Mass spectral data was compiled using MS (ESI), HRMS mass spectrometers and the orbitrap mass analyzer was used for the HRMS measurement. N-(2-aminobenzyl)anilines (**2**) were prepared by the literature method.[3]

2. Experimental section

(i) General procedure for the preparation of 3,4-diaryl-dihydroquinazolin-4-ol using KI/TBHP:

To a solution of *N*-(2-aminobenzyl) substituted anilines **1** (1,3-diamine) (3 mmol) in 6 mL of ethanol, aldehyde **2** (3 mmol) was added and stirred at room temperature for 3 hours. To the same solution, KI (20 mol%) and 1.5 mL of 70 wt% TBHP in H_2O (4 equivalent) was added drop wise for 5 minutes and stirred at room temperature for overnight. The solvent (EtOH) was removed under reduced pressure. The residue was diluted with 6 mL of dimethoxy ethane (DME). The mixture was stirred at 100 ^{o}C for 5-6 hours. The progress of the reaction was monitored by TLC. After completion of reaction, the reaction mixture allowed to cool RT, the solvent (DME) was removed under vacumm. The crude product was purified by column chromatography using petroleum ether/ethyl acetate mixture as an eluent and was analyzed by ^{1}H NMR, ^{13}C NMR, IR, ESI-MS and ESI-HRMS (Table S1).

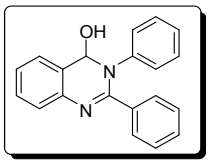
(ii) General procedure for synthesis of N-(2,3-diaryl-3,4-dihydroquinazolin-4-yl)amide derivatives *via* cross dehydrative coupling reaction.

To a solution of 3,4-diaryl-dihydroquinazolin-4-ol **(3)** (0.25 mmol) and amide (**4**) (0.5 mmol, 2 equiv.) in 2 mL of DCE, $FeCl_2$ (10 mol%) was added and the mixture was stirred magnetically at 75 ^oC for 2 hours. The progress of the reaction was monitored by TLC. After completion of reaction, the reaction mixture was allowed to cool to RT and filter through celite using chloroform/ethylacetate. The solution was concentrated under vacumm and afforded the crude product. The crude product was purified by SiO_2 column chromatography using petroleum ether/ethyl acetate mixture as an eluent and was analyzed by ^1H NMR, ^{13}C NMR, ESI-MS, ESI-HRMS.

(iii) General procedure for synthesis of dimethyl 2,3-diaryl-3,4-dihydroquinazolin-4-ylphosphonate derivatives *via* cross dehydrative coupling reaction.

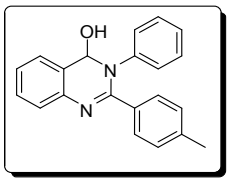
To a solution of 3,4-diaryl-dihydroquinazolin-4-ol **(3)** (0.25 mmol) in 2 mL of DCE dialkyl or diaryl phosphite (**6**) (0.5 mmol, 2 equiv.) was added and the mixture was stirred magnetically at 75 ^oC for 2 hours. The progress of the reaction was monitored by TLC. After completion of reaction, the reaction mixture was allowed to cool to RT and filter through celite using chloroform/ethylacetate. The solution was concentrated under vacumm and afforded the crude product. The crude product was purified by column chromatography using petroleum ether/ethyl acetate mixture as eluent and was analyzed by ^1H NMR, ^{13}C NMR, ^{31} PNMR, ESI-MS, ESI-HRMS.

3. Spectroscopic data for products



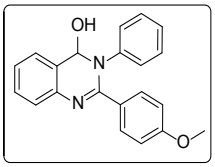
2,3-diphenyl-3,4-dihydroquinazolin-4-ol: (3a)

White solid. Isolated yield: 78% (Petroleum ether/Ethyl acetate = 1;1, Rf = 0.5). IR ν_{max} cm^{-1}: 3061, 2930, 1588, 1547, 1487, 1405, 1250, 1029, 763. ^{1}H NMR ($CDCl_3$, 300 MHz, ppm): δ 7.29-6.88 (m, 14 H), 5.89 (s, 1H). ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 144.9, 140.2, 134.1, 130.5, 129.3, 129.1, 128.5, 127.4, 126.0, 125.5, 125.1, 124.9, 124.2, 123.7. MS (ESI) m/z = 301 $(M + H)^+$; (ESI-HRMS) calculated for $C_{20}H_{17}ON_2$ $(M+H)^+$: 301.13354, found: 301.13411.



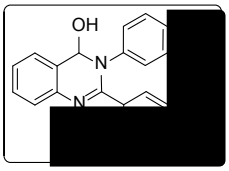
3-phenyl-2-p-tolyl-3,4-dihydroquinazolin-4-ol (3b).

White solid. Isolated yield: 84%. mp 188-190 ^{o}C. (Petroleum ether/ethyl acetate = 2:1, Rf = 0.5). IR ν_{max} (cm^{-1}): 3302, 2884, 1586, 1548, 1483, 1321, 1250, 1054, 994, 823, 629,560, 466. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.22 (d, J = 7.7 Hz, 1H), 7.16-7.09 (m, 7H), 7.03 (t, J = 7.1 Hz, 2H), 6.96 (d, J = 7.0 Hz, 1H), 6.88 (d, J = 7.7 Hz, 2H), 5.95 (s, 1H), 2.26 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 153.2, 145.1, 140.4, 139.3, 131.4, 130.4, 129.1, 128.4, 128.1, 126.0, 125.1, 125.0, 124.9, 124.1, 123.8, 82.5, 21.3. MS (ESI) m/z = 315 $(M + H)^+$; (ESI-HRMS) calculated for $C_{21}H_{19}ON_2$ $(M+H)^+$ = 315.14919, found 329.14995.



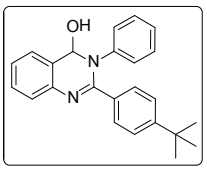
2-(4-methoxyphenyl)-3-phenyl-3,4-dihydroquinazolin-4-ol (3c).

White solid. Isolated yield: 58%. mp. 170-172 ^{o}C. (Petroleum ether/ethyl acetate = 2:1, Rf = 0.4). IR ν_{max} (cm^{-1}): 3073, 2889, 1586, 1546, 1483, 1291, 1250, 1035, 994, 837, 698, 523. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.19-7.18 (m, 3H), 7.14-7.10 (m, 5H), 7.03 (t, J = 7.0 Hz, 2H), 6.93-6.92 (m, 1H), 6.58 (d, J = 8.5 Hz, 2H), 5.93 (s, 1H), 3.76 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.3, 152.9,145.3, 140.4, 132.1, 128.9, 128.5, 126.4, 126.0, 125.0, 124.8, 124.3, 123.5, 112.7, 82.6, 55.1. MS (ESI) m/z = 331 $(M + H)^+$; (ESI-HRMS) calculated for $C_{21}H_{19}O_2N_2$ $(M+H)^+$ = 331.14410, found 331.14499.



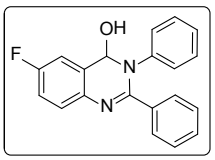
3-phenyl-2-(4-(trifluoromethyl)phenyl)-3,4-dihydroquinazolin-4-ol (3d).

White solid. Isolated yield: 67%. mp 188-190 ^{o}C. (Petroleum ether/ethyl acetate = 2:1, Rf = 0.5). IR ν_{max} (cm^{-1}): 3143, 2961, 2880, 1586, 1546, 1480, 1358, 1252, 1055, 970, 842, 698, 550, 520. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.38-7.29 (m, 6H), 7.24-7.14 (m, 3H), 7.11-7.06 (m, 2H), 6.95-6.90 (m, 2H), 5.96 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.7, 144.3, 139.9, 137.5, 130.5, 129.3, 128.9, 126.2, 125.7, 124.7, 124.4, 124.0, 82.4. MS (ESI) m/z = 369 $(M + H)^+$; (ESI-HRMS) calculated for $C_{21}H_{16}ON_2F_3$ $(M+H)^+$ = 369.12092, found 369.12226.



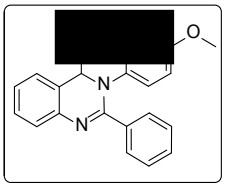
2-(4-tert-butylphenyl)-3-phenyl-3,4-dihydroquinazolin-4-ol (3e).

White solid. Isolated yield: 81%. mp 194-196 ^{o}C. (Petroleum ether/ethyl acetate = 2:1, Rf = 0.5). IR ν_{max} (cm^{-1}): 3464, 2964, 2872, 1579, 1544, 1482, 1361, 1251, 1054, 1014, 841, 697, 565, 468. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.23-7.05 (m, 11H), 6.99 (d, J = 7.3 Hz, 1H), 6.90 (t, J = 6.9 Hz, 1H), 5.93 (s, 1H), 1.26 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 153.1, 152.3, 145.2, 140.3, 130.8, 130.4, 128.9, 128.4, 125.8, 125.2, 125.0, 124.9, 124.2, 123.5, 82.7, 34.5, 31.1. MS (ESI) m/z = 357 $(M + H)^+$; (ESI-HRMS) calculated for $C_{24}H_{25}ON_2$ $(M+H)^+$ = 357.19614, found 357.19713.



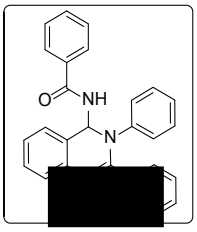
6-fluoro-2,3-diphenyl-3,4-dihydroquinazolin-4-ol (3f).

White solid. Isolated yield: 80%. mp 202-204 ^{o}C, (Petroleum ether/ethyl acetate = 2:1, Rf = 0.5). IR ν_{max} (cm^{-1}): 2946, 2828, 1590, 1550, 1489, 1398, 1243, 1038, 943, 831, 698, 555, 504. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.23-7.17 (m, 4H), 7.13-7.02 (m, 7H), 6.83 (t, J = 8.6 Hz, 1H), 6.57 (d, J = 8.2 Hz, 1H), 5.85 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.1, 159.2, 152.8, 144.8, 136.5, 133.2, 130.5, 129.5, 128.6, 127.3, 125.5, 125.2, 125.0, 124.7, 116.5, 116.3, 112.1, 112.0, 82.2. MS (ESI) m/z = 319 $(M + H)^+$; (ESI-HRMS) calculated for $C_{20}H_{16}ON_2F$ $(M+H)^+$ = 319.12412, found 319.12489.



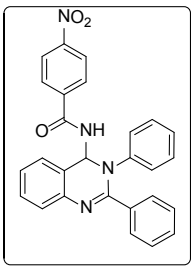
3-(4-methoxyphenyl)-2-phenyl-3,4-dihydroquinazolin-4-ol (3g).

White solid. Isolated yield: 63%. mp 208-210 ^{o}C. (Petroleum ether/ethyl acetate = 2:1, Rf = 0.4). IR ν_{max} (cm^{-1}): 3061, 2891, 1587, 1551, 1508, 1357, 1290, 1054, 998, 834, 661, 576, 497.^{1}H NMR (500 MHz, $CDCl_3$) δ 7.29-7.25 (m, 4H), 7.20 (t, *J* = 8.0 Hz, 2H), 7.12-7.07 (m, 3H), 7.00 (t, *J* = 8.2 Hz, 2H), 6.65 (d, *J* = 8.6 Hz, 2H), 5.93 (s, 1H), 3.71 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.1, 153.2, 140.5, 138.2, 134.5, 130.4, 129.1, 127.4, 126.3, 126.1, 125.3, 124.0, 123.9, 113.7, 82.7, 55.3. MS (ESI) m/z = 331 $(M + H)^+$; (ESI-HRMS) calculated for $C_{21}H_{19}O_2N_2$ $(M+H)^+$ = 331.14410, found 331.14475.



N-(2,3-diphenyl-3,4-dihydroquinazolin-4-yl)benzamide (5a).

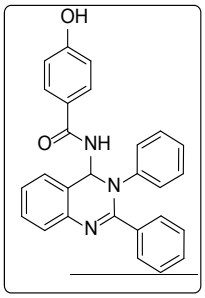
White solid. Isolated yield: 93%. mp 185-187 ^{o}C. (Petroleum ether/ethyl acetate = 2:1, Rf = 0.6). IR ν_{max} (cm^{-1}): 3107, 3033, 2927, 1654, 1547, 1486, 1336, 1244, 1040, 765, 696, 560, 517. ^{1}H NMR (300 MHz, DMSO-d_6) δ 9.78 (bs, 1H), 8.20-8.07 (m, 1H), 7.92 (d, *J* = 8.3, 2H), 7.60 (d, *J* = 7.7 Hz, 2H), 7.48-7.46 (m, 1H), 7.42-7.37 (m, 3H), 7.32 (d, *J* = 7.5 Hz, 1H), 7.24-7.12 (m, 8H), 7.06 (d, *J* = 8.4 Hz, 1H), 7.01-6.97 (m, 1H). ^{13}C NMR (75 MHz, DMSO-d_6) δ 165.0, 153.4, 144.6, 141.2, 136.4, 133.6, 131.6, 129.3, 128.8, 128.1, 127.7, 125.9, 125.7, 124.8, 124.5, 123.7, 79.0, 64.2. MS (ESI) m/z = 404 $(M + H)^+$; (ESI-HRMS) calculated for $C_{27}H_{22}ON_3$ $(M+H)^+$ = 404.1757, found 404.1755.



N-(2,3-diphenyl-3,4-dihydroquinazolin-4-yl)-4-nitrobenzamide (5b).

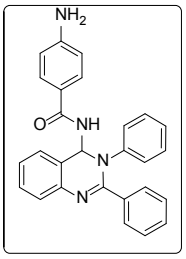
Yellow solid. Isolated yield: 89%. mp 216-218 ^{o}C. (Petroleum ether/ethyl acetate = 2:1, Rf = 0.3). IR ν_{max} (cm^{-1}): 3404, 3280, 3150, 1655, 1551, 1526, 1343, 1049, 1024, 997, 824, 560, 522. ^{1}H NMR (500 MHz, $CDCl_3$ + DMSO-d_6) δ 10.02 (bs, 1H), 8.20-8.14 (m, 4H), 7.60 (d, *J* = 7.0, 2H), 7.39 (d, *J* = 7.7 Hz, 1H), 7.35-7.31 (m, 2H), 7.22-7.15 (m, 4H), 7.09-7.07 (m, 5H), 6.97-6.95 (m, 1H). ^{13}C NMR (125

MHz, $CDCl_3$ + DMSO-d_6) δ 162.0, 152.1, 147.7, 143.1, 139.7, 137.9, 134.8, 128.1, 128.0, 127.9, 127.8, 127.4, 127.2, 126.2, 124.4, 124.3, 123.3, 123.1, 123.0, 122.0, 121.5, 63.1. MS (ESI) m/z = 449 $(M + H)^+$; (ESI-HRMS) calculated for $C_{27}H_{21}O_3N_4$ $(M+H)^+$ = 449.1608, found 449.1599.



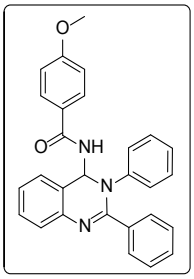
N-(2,3-diphenyl-3,4-dihydroquinazolin-4-yl)-4-hydroxybenzamide (5c).

White solid. Isolated yield: 55%. mp 190-192 ^oC. (Petroleum ether/ethyl acetate = 2:1, Rf = 0.5). IR ν_{max} (cm^{-1}): 3249, 2926, 1643, 1546, 1492, 1331, 1236, 1046, 970, 764, 689, 544, 474. ^1H NMR (300 MHz, $CDCl_3$ + DMSO-d_6) δ 9.51 (bs, 1H), 8.77 (bs, 1H), 7.74 (d, *J* = 8.6 Hz, 2H), 7.59-7.55 (m, 2H), 7.38 (d, *J* = 8.4 Hz, 1H), 7.31-7.27 (m, 2H), 7.18-7.02 (m, 9H), 6.90 (t, *J* = 6.9 Hz, 1H), 6.72 (d, *J* = 8.6 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$ + DMSO-d_6) δ 164.3, 159.7, 152.9, 143.7, 140.3, 135.5, 128.9, 128.7, 128.6, 128.3, 127.8, 127.6, 126.7, 125.0, 124.7, 123.6, 123.5, 123.2, 113.9, 63.3. MS (ESI) m/z = 420 $(M + H)^+$; (ESI-HRMS) calculated for $C_{27}H_{22}O_2N_3$ $(M+H)^+$ = 420.1706, found 420.1704.



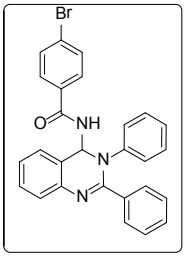
4-amino-N-(2,3-diphenyl-3,4-dihydroquinazolin-4-yl)benzamide (5d).

White solid. Isolated yield: 65%. mp 165-167^oC. (Petroleum ether/ethyl acetate = 2:1, Rf = 0.4). IR ν_{max} (cm^{-1}): 3360, 2931, 2856, 1606, 1545, 1490, 1322, 1243, 1027, 843, 764, 696, 556, 506. ^1H NMR (300 MHz, $CDCl_3$) δ 7.69 (d, *J* = 9.2 Hz, 2H), 7.59-7.56 (m, 3H), 7.46-7.40 (m, 1H), 7.34-7.26 (m, 7H), 7.20-7.12 (m, 3H), 7.03-6.98 (m, 1H) 6.72 (d, *J* = 9.2 Hz, 1H), 6.61 (d, *J* = 8.4 Hz, 2H), 3.98 (s, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.1, 154.4, 150.0, 144.1, 141.3, 135.9, 129.9, 129.7, 129.3, 129.1, 128.8, 128.2, 126.2, 125.7, 124.8, 124.7, 124.3, 123.9, 122.8, 114.0, 64.4. MS (ESI) m/z = 419 $(M + H)^+$; (ESI-HRMS) calculated for $C_{27}H_{23}ON_4$ $(M+H)^+$ = 419.1866, found 419.1867.



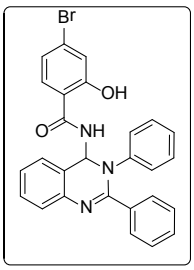
N-(2,3-diphenyl-3,4-dihydroquinazolin-4-yl)-4-methoxybenzamide (5e).

White solid. Isolated yield: 94%. mp 160-162 ^{o}C. (Petroleum ether/ethyl acetate = 2:1, Rf = 0.5). IR ν_{max} (cm^{-1}): 3372, 3249, 2924, 1648, 1545, 1490, 1392, 1250, 1033, 968, 846, 568, 466. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.84 (d, *J* = 8.6 Hz, 2H), 7.59-7.51 (m, 3H), 7.39-7.12 (m, 12H), 6.99 (t, *J* = 7.3 Hz, 1H), 6.90 (d, *J* = 8.8 Hz, 2H), 3.81 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.0, 162.6, 154.4, 144.1, 141.2, 135.7, 129.9, 129.7, 129.3, 129.2, 128.8, 128.1, 126.3, 125.7, 124.8, 124.7, 124.4, 123.7, 113.7, 64.6, 55.3. MS (ESI) m/z = 434 $(M + H)^+$; (ESI-HRMS) calculated for $C_{28}H_{24}O_2N_3$ $(M+H)^+$ = 434.1863, found 434.1862.



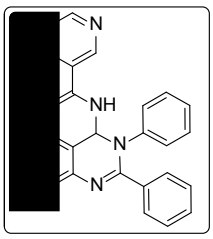
4-bromo-N-(2,3-diphenyl-3,4-dihydroquinazolin-4-yl)benzamide (5f).

White solid. Isolated yield: 84%. mp 190-192 ^{o}C. (Petroleum ether/ethyl acetate = 2:1, Rf = 0.6). IR ν_{max} (cm^{-1}): 3306, 2930, 2857, 1657, 1544, 1483, 1326, 1243, 1019, 951, 844, 762, 697, 533, 477. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.67 (d, *J* = 8.5 Hz, 2H), 7.61 (d, *J* = 8.5 Hz, 2H), 7.56-7.54 (m, 2H), 7.42 (t, *J* = 8.6 Hz, 1H), 7.32-7.13 (m, 12H), 7.02 (t, *J* = 7.3 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 164.7, 154.4, 144.0, 141.3, 135.6, 132.5, 131.8, 130.0, 129.7, 129.5, 128.9, 128.1, 126.8, 126.4, 125.7, 124.9, 124.7, 124.4, 123.3, 64.8. MS (ESI) m/z = 482 $(M + H)^+$; (ESI-HRMS) calculated for $C_{27}H_{21}ON_3Br$ $(M+H)^+$ = 482.0862, found 482.0865.



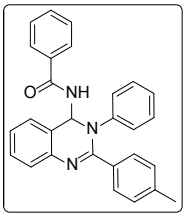
4-bromo-N-(2,3-diphenyl-3,4-dihydroquinazolin-4-yl)-2-hydroxybenzamide (5g).

White solid. Isolated yield: 76%. mp 203-205 ^{o}C. (Petroleum ether/ethyl acetate = 2:1, Rf = 0.7). IR ν_{max} (cm^{-1}): 2929, 2380, 1655, 1545, 1485, 1288, 1153, 1052, 959, 698, 563, 451. ^{1}H NMR (400 MHz, $CDCl_3$ + DMSO-d_6) δ 9.78 (d, *J* = 8.6 Hz, 1H), 8.25 (d, *J* = 2.3 Hz, 1H), 7.66 (d, *J* = 7.8 Hz, 1H), 7.52-7.48 (m, 1H), 7.41-7.36 (m, 3H), 7.25-7.14 (m, 11H), 7.04-7.00 (m, 1H), 6.82 (d, *J* = 8.6 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$ + DMSO-d_6) δ 165.0, 158.4, 153.1, 143.7, 140.3, 135.3, 130.4, 128.9, 128.7, 128.3, 127.9, 127.0, 125.2, 125.1, 124.1, 123.9, 123.7, 122.7, 118.6, 116.4, 109.6, 63.4. MS (ESI) m/z = 498 $(M + H)^+$; (ESI-HRMS) calculated for $C_{27}H_{21}O_2N_3Br$ $(M+H)^+$ = 498.0811, found 498.0813.



N-(2,3-diphenyl-3,4-dihydroquinazolin-4-yl)nicotinamide (5h).

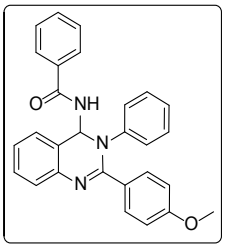
White solid. Isolated yield: 83%. mp 173-175 ^{o}C. (Petroleum ether/ethyl acetate = 2:1, Rf = 0.2). IR ν_{max} (cm^{-1}): 2932, 2856, 1660, 1588, 1485, 1324, 1241, 1032, 964, 765, 699, 533, 467. ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.04 (bs, 1H), 8.61 (d, *J* = 3.5 Hz, 1H), 8.44-8.41 (m, 1H), 8.16 (d, *J* = 7.9 Hz, 1H), 7.45-7.38 (m, 3H), 7.33-7.30 (m, 3H), 7.22-7.17 (m, 3H), 7.14 (d, *J* = 4.3 Hz, 4H), 7.11-7.05 (m, 2H), 7.03-6.97 (m, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 164.1, 152.4, 148.6, 144.1, 141.2, 135.3, 129.8, 129.6, 128.9, 128.0, 126.3, 125.9, 125.0, 124.8, 124.4, 123.3, 64.8. MS (ESI) m/z = 405 $(M + H)^+$; (ESI-HRMS) calculated for $C_{26}H_{21}ON_4(M+H)^+$ = 405.1709, found 405.1705.



N-(3-phenyl-2-p-tolyl-3,4-dihydroquinazolin-4-yl)benzamide (5i).

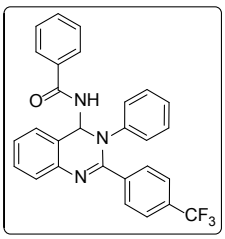
White solid. Isolated yield: 87%. mp 206-208 ^{o}C. (Petroleum ether/ethyl acetate = 2:1, Rf = 0.5). IR ν_{max} (cm^{-1}): 2926, 2855, 2313, 1686, 1584, 1548, 1483, 1389, 1276, 1184, 1044, 955, 825, 760, 696,

553, 456. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.77 (d, *J* = 7.5 Hz, 2H), 7.56 (d, *J* = 8.3 Hz, 3H), 7.49 (d, *J* = 7.5 Hz, 1H), 7.44-7.37 (m, 3H), 7.33-7.11 (m, 8H), 7.03 (d, *J* = 7.5 Hz, 3H), 2.28 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.6, 154.3, 144.3, 141.5, 140.2, 133.7, 132.9, 132.0, 129.6, 129.4, 128.6, 127.2, 126.1, 125.7, 124.8, 124.6, 124.3, 123.6, 64.7, 21.3. MS (ESI) m/z = 418 $(M + H)^+$; (ESI-HRMS) calculated for $C_{28}H_{24}ON_3$ $(M+H)^+$ = 418.1903, found 418.1903.



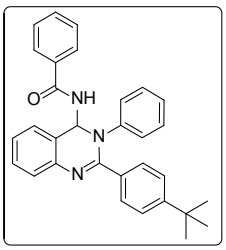
N-(2-(4-methoxyphenyl)-3-phenyl-3,4-dihydroquinazolin-4-yl)benzamide (5j).

White solid. Isolated yield: 82%. mp 223-224 ^{o}C, (Petroleum ether/ethyl acetate = 2:1, Rf = 0.5). IR ν_{max} (cm^{-1}): 2925, 2853, 2312, 1683, 1546, 1512, 1391, 1250, 1175, 1032, 962, 837, 761, 697, 546, 499. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8.0 Hz, 2H), 7.62 (d, *J* = 8.8 Hz, 2H), 7.54 (d, *J* = 7.9 Hz, 1H), 7.49 (t, *J* = 8.2 Hz, 1H), 7.43-7.39 (m, 3H), 7.32-7.28 (m, 3H), 7.22-7.17 (m, 3H), 7.11 (d, *J* = 9.0 Hz, 1H), 7.03-6.97 (m, 2H), 6.74 (d, *J* = 8.8 Hz, 2H), 3.75 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.6, 160.9, 154.0, 144.4, 141.5, 133.7, 132.0, 131.3, 129.3, 128.9, 128.5, 127.2, 125.9, 125.7, 124.6, 124.2, 123.6, 113.5, 64.8, 55.1. MS (ESI) m/z = 434 $(M + H)^+$; (ESI-HRMS) calculated for $C_{28}H_{24}O_2N_3$ $(M+H)^+$ = 434.1863, found 434.1858.



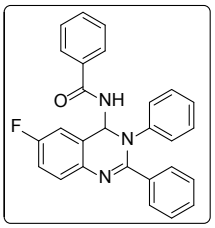
N-(3-phenyl-2-(4-(trifluoromethyl)phenyl)-3,4-dihydroquinazolin-4-yl)benzamide (5k).

Plae yellow solid. Isolated yield: 71%. mp 208-210 ^{o}C. (Petroleum ether/ethyl acetate = 2:1, Rf = 0.6). IR ν_{max} (cm^{-1}): 2932, 2886, 2311, 1658, 1548, 1403, 1324, 1238, 1129, 1065, 969, 845, 762, 699, 548, 499. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.78 (d, *J* = 7.5 Hz, 4H), 7.58 (d, *J* = 7.5 Hz, 1H), 7.51-7.39 (m, 6H), 7.35-7.14 (m, 8H), 7.09-6.97 (m, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.7, 153.0, 143.6, 141.0, 139.2, 133.5, 132.2, 129.9, 129.6, 129.2, 128.7, 127.2, 126.9, 125.9, 125.3, 125.0, 124.4, 123.3, 64.7. MS (ESI) m/z = 472 $(M + H)^+$; (ESI-HRMS) calculated for $C_{28}H_{21}ON_3F_3$ $(M+H)^+$ = 472.1631, found 472.1628.



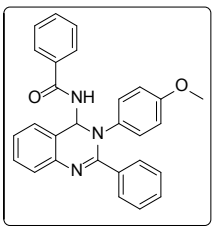
N-(2-(4-tert-butylphenyl)-3-phenyl-3,4-dihydroquinazolin-4-yl)benzamide (5l).

White solid. Isolated yield: 83%. mp 258-260 ^{o}C. (Petroleum ether/ethyl acetate = 2:1, Rf = 0.6). IR ν_{max} (cm^{-1}): 2938, 2385, 2310, 1661, 1542, 1492, 1392, 1233, 1054, 944, 844, 761, 699, 635, 545.^{1}H NMR (500 MHz, DMSO-d$_6$) δ 9.77 (d, *J* = 8.3 Hz, 1H), 8.30 (s, 1H), 7.92 (d, *J* = 7.1 Hz, 2H), 7.55 (d, *J* = 8.1 Hz, 2H), 7.46-7.39 (m, 4H), 7.32-7.29 (m, 3H), 7.23-7.18 (m, 5H), 7.05-6.99 (m, 2H), 1.21 (s, 9H). ^{13}C NMR (75 MHz, DMSO-d$_6$) δ 165.2, 153.2, 152.2, 144.8, 141.3, 133.5, 131.6, 129.2, 128.9, 128.1, 127.8, 125.6, 124.6, 124.2, 79.1, 64.4, 34.4, 30.9. MS (ESI) m/z = 460 (M + H)$^{+}$; (ESI-HRMS) calculated for $C_{31}H_{30}ON_3$ (M+H)$^{+}$ = 460.2383, found 460.2370.



N-(6-fluoro-2,3-diphenyl-3,4-dihydroquinazolin-4-yl)benzamide (5m).

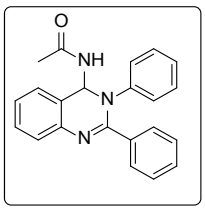
White solid. Isolated yield: 85%. mp 234-236 ^{o}C. (Petroleum ether/ethyl acetate = 2:1, Rf = 0.5). IR ν_{max} (cm^{-1}): 2925, 2855, 1739, 1655, 1554, 1521, 1487, 1379, 1321, 1245, 1136, 1071, 948, 830, 754, 697, 546, 520.^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (d, *J* = 7.3 Hz, 2H), 7.57 (d, *J* = 8.2 Hz, 2H), 7.54-7.48 (m, 2H), 7.44 (t, *J* = 7.4 Hz, 2H), 7.31-7.25 (m, 2H), 7.21-7.07 (m, 8H), 7.03 (d, *J* = 7.1 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.7, 161.7, 159.7, 153.8, 144.0, 137.7, 135.3, 133.6, 132.1, 129.9, 129.6, 128.9, 128.6, 128.1, 127.4, 126.2, 125.0, 124.6, 124.3, 116.7, 116.5, 112.2, 64.3. MS (ESI) m/z = 329 (M + H)$^{+}$; (ESI-HRMS) calculated for $C_{27}H_{21}ON_3F$ (M+H)$^{+}$ = 422.1654, found 422.1655.



N-(3-(4-methoxyphenyl)-2-phenyl-3,4-dihydroquinazolin-4-yl)benzamide (5n).

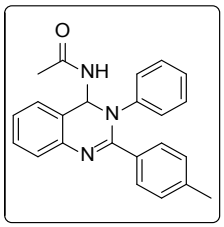
White solid. Isolated yield: 73%. mp 206-208 ^{o}C. (Petroleum ether/ethyl acetate = 2:1, Rf = 0.5). IR ν_{max} (cm^{-1}): 2958, 2927, 1647, 1547, 1510, 1483, 1394, 1324, 1245, 1178, 1125, 1033, 833, 766, 697, 558, 542, 494, 462. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.82 (d, *J* = 7.5 Hz, 2H), 7.62 (d, *J* = 6.7 Hz, 2H),

7.55-7.48 (m, 2H), 7.46 (d, J = 7.5 Hz, 3H), 7.34-7.27 (m, 3H), 7.24-7.09 (m, 7H), 6.70 (d, J = 9.0 Hz, 1H), 3.70 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.6, 156.9, 154.6, 141.3, 137.3, 135.7, 133.7, 132.0, 129.7, 128.5, 128.0, 127.3, 126.1, 125.8, 124.6, 123.2, 114.1, 65.0, 55.2. MS (ESI) m/z = 434 $(M + H)^+$; (ESI-HRMS) calculated for $C_{28}H_{24}O_2N_2$ $(M+H)^+$ = 434.1849, found 434.1851.



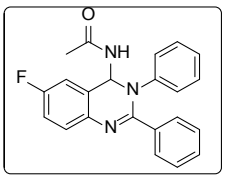
N-(2,3-diphenyl-3,4-dihydroquinazolin-4-yl)acetamide (5o).

White solid. Isolated yield: 76%. mp 240-242 ^{o}C, (Petroleum ether/ethyl acetate = 1:2, Rf = 0.2). IR ν_{max} (cm^{-1}): 3418, 2963, 2892, 1703, 1583, 1547, 1398, 1359, 1252, 1197, 1150, 1056, 969, 894, 843, 611, 557. ^{1}H NMR (300 MHz, DMSO-d_6) δ 9.17 (d, J = 8.6 Hz, 1H), 7.59 (d, J = 7.7 Hz, 2H), 7.42 (d, J = 3.7 Hz, 2H), 7.32-7.29 (m, 3H), 7.25-7.12 (m, 6H), 7.02 (t, J = 6.7 Hz, 1H), 6.71 (d, J = 8.6 Hz, 1H), 1.88 (s, 3H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 168.4, 153.4, 144.4, 136.1, 129.8, 129.4, 129.0, 128.0, 126.0, 125.9, 124.7, 124.4, 124.2, 124.1, 63.5, 22.6. MS (ESI) m/z = 342 $(M + H)^+$; (ESI-HRMS) calculated for $C_{22}H_{20}ON_3$ $(M+H)^+$ = 342.1600, found 342.1597.



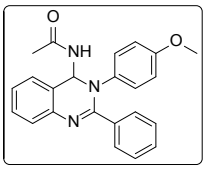
N-(3-phenyl-2-(p-tolyl)-3,4-dihydroquinazolin-4-yl)acetamide (5p).

White solid. Isolated yield: 78%. mp 238-240 ^{o}C. (Petroleum ether/ethyl acetate = 1:2, Rf = 0.4). IR ν_{max} (cm^{-1}): 3207, 2931, 1659, 1540, 1395, 1286, 1237, 1063, 836, 696, 550, 496. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.19 (bs, 1H), 7.28-7.26 (m, 3H), 7.23-7.20 (m, 1H), 7.13-7.02 (m, 6H), 6.99-6.95 (m, 1H), 6.91-6.85 (m, 3H), 2.26 (s, 3H), 2.21 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 168.4, 154.6, 144.3, 140.9, 139.8, 132.2, 129.6, 129.0, 128.7, 128.6, 125.8, 125.5, 124.6, 124.3, 123.6, 63.8, 23.6, 21.3. MS (ESI) m/z = 356 $(M + H)^+$; (ESI-HRMS) calculated for $C_{23}H_{22}ON_3$ $(M+H)^+$ = 356.1746, found 356.1747.



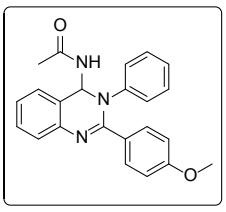
N-(6-fluoro-2,3-diphenyl-3,4-dihydroquinazolin-4-yl)acetamide (5q).

White solid. Isolated yield: 78%. mp 264-266 ^{o}C. (Petroleum ether/ethyl acetate = 1:2, Rf = 0.3). IR ν_{max} (cm^{-1}): 3395, 3269, 1637, 1547, 1488, 1365, 1237, 1033, 754, 692, 524, 485, 449. ^{1}H NMR (300 MHz, $CDCl_3$ + DMSO-d_6) δ 9.15 (bs, 1H), 7.86-7.75 (m, 1H), 7.55 (d, *J* = 7.1 Hz, 2H), 7.38-7.34 (m, 1H), 7.21-7.17 (m, 2H), 7.09-7.03 (m, 5H), 6.94 (d, *J* = 6.0 Hz, 2H), 6.71 (d, *J* = 8.6 Hz, 1H), 1.90 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$ + DMSO-d_6) δ 167.3, 159.7, 157.7, 151.7, 142.9, 136.2, 134.5, 128.1, 127.2, 126.4, 124.7, 124.0, 123.2, 122.7, 114.5, 114.3, 61.9, 21.3. MS (ESI) m/z = 360 (M + H)$^{+}$; (ESI-HRMS) calculated for $C_{22}H_{19}ON_3F$ $(M+H)^{+}$ = 360.1506, found 360.1507.



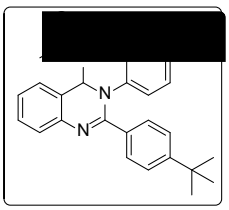
N-(3-(4-methoxyphenyl)-2-phenyl-3,4-dihydroquinazolin-4-yl)acetamide (5r).

White solid. Isolated yield: 68%. mp 220-222 ^{o}C. (Petroleum ether/ethyl acetate = 1:2, Rf = 0.2). IR ν_{max} (cm^{-1}): 3064, 2931, 1653, 1542, 1509, 1369, 1245, 1179, 1144, 1068, 1033, 833, 765, 696, 519, 458. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43 (d, *J* = 6.8 Hz, 1H), 7.38-7.33 (m, 1H), 7.30-7.07 (m, 8H), 7.02 (d, *J* = 8.2 Hz, 2H), 6.81 (d, *J* = 9.4 Hz, 1H), 6.64 (t, *J* = 8.0 Hz, 2H), 3.68 (s, 3H), 2.16 (bs, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 168.4, 156.9, 154.8, 140.9, 137.3, 135.2, 129.7, 129.4, 129.0, 127.8, 126.1, 125.9, 125.6, 123.6, 123.2, 113.9, 64.0, 55.2. MS (ESI) m/z = 372 (M + H)$^{+}$; (ESI-HRMS) calculated for $C_{23}H_{22}O_2N_3$ $(M+H)^{+}$ = 372.1705, found 372.1705.



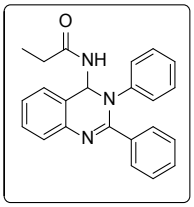
N-(2-(4-methoxyphenyl)-3-phenyl-3,4-dihydroquinazolin-4-yl)acetamide (5s).

White solid. Isolated yield: 69%. mp 240-242 ^{o}C, (Petroleum ether/ethyl acetate = 1:2, Rf = 0.4). IR ν_{max} (cm^{-1}): 2938, 2382, 1677, 1544, 1512, 1388, 1285, 1241, 1175, 1063, 985, 842, 698, 533, 498. ^{1}H NMR (500 MHz, $CDCl_3$ + DMSO-d_6) δ 9.09 (d, *J* = 9.0 Hz, 1H), 7.54 (d, *J* = 9.0 Hz, 2H), 7.37 (bs, 2H), 7.20-7.10 (m, 6H), 6.99 (t, *J* = 6.7 Hz, 1H), 6.83 (d, *J* = 8.3 Hz, 2H), 6.67 (d, *J* = 8.3 Hz, 1H), 3.71 (s, 3H), 1.87(s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$ + DMSO-d_6) δ 166.3, 158.4, 151.0, 142.8, 139.4, 129.2, 126.8, 126.3, 123.8, 123.5, 122.3, 121.8, 111.4, 61.6, 53.2, 20.6. MS (ESI) m/z = 372 (M + H)$^{+}$; (ESI-HRMS) calculated for $C_{23}H_{22}O_2N_3$ $(M+H)^{+}$ = 372.1706, found 372.1705.



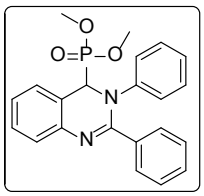
N-(2-(4-tert-butylphenyl)-3-phenyl-3,4-dihydroquinazolin-4-yl)acetamide (5t).

White solid. Isolated yield: 77%. mp 258-260 ^{o}C. (Petroleum ether/ethyl acetate = 1:2, Rf = 0.4). IR ν_{max} (cm^{-1}): 2966, 2936, 2379, 1676, 1540, 1398, 1328, 1239, 1066, 984, 841, 697, 629, 548, 461. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.48 (d, J = 8.2 Hz, 1H), 7.44-7.26 (m, 4H), 7.21-7.11 (m, 8H), 7.01-6.97 (m, 1H), 6.86 (d, J = 9.3 Hz, 1H), 2.10 (bs, 3H), 1.25 (s, 9H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 168.4, 154.5, 152.9, 144.3, 140.9, 132.1, 129.4, 129.0, 128.7, 125.9, 125.4, 124.7, 124.5, 124.3, 123.6, 63.8, 34.6, 31.0, 23.6. MS (ESI) m/z = 398 $(M + H)^+$; (ESI-HRMS) calculated for $C_{26}H_{28}ON_3$ $(M+H)^+$ = 398.2226, found 398.2223.



N-(2,3-diphenyl-3,4-dihydroquinazolin-4-yl)propionamide (5u).

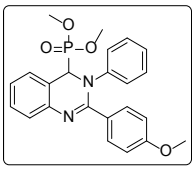
White solid. Isolated yield: 81%. mp 238-240 ^{o}C. (Petroleum ether/ethyl acetate = 2:1, Rf = 0.5). IR ν_{max} (cm^{-1}): 3420, 3328, 2946, 2892, 1682, 1582, 1545, 1389, 1365, 1242, 1197, 1145, 1065, 968, 879, 843, 693, 545. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.49 (d, J = 6.9 Hz, 2H), 7.37 (d, J = 7.5 Hz, 1H), 7.32-7.22 (m, 3H), 7.19-7.09 (m, 8H), 7.00-6.95 (m, 1H), 6.89 (t, J = 9.2 Hz, 1H), 2.36 (q, J = 7.5 Hz, 2H), 2.36 (t, J = 7.5 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 172.2, 154.4, 144.0, 141.0, 135.4, 129.7, 129.6, 129.1, 128.8, 128.0, 126.1, 125.6, 124.7, 124.3, 124.1, 123.6, 63.9, 29.7, 9.6. MS (ESI) m/z = 356 $(M + H)^+$; (ESI-HRMS) calculated for $C_{23}H_{22}ON_3$ $(M+H)^+$ = 356.1757, found 356.1756.



Dimethyl 2,3-diphenyl-3,4-dihydroquinazolin-4-ylphosphonate (7a).

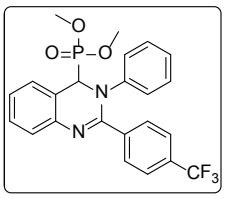
White solid. Isolated yield: 93%. mp 160-162 ^{o}C. (Petroleum ether/ethyl acetate = 1:4, Rf = 0.3). IR ν_{max} (cm^{-1}): 3061, 2955, 2854, 1584, 1547, 1510, 1489, 1455, 1364, 1310, 1255, 1145, 1029, 851, 767, 698, 532, 506, 406. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.78-7.76 (m, 2H), 7.45 (d, J = 7.7 Hz, 1H), 7.38-7.35 (m, 1H), 7.30-7.25 (m, 3H), 7.22-7.11 (m, 6H), 7.00 (t, J = 7.1 Hz, 1H), 5.34 (d, J = 13.4 Hz, 1H), 3.72-3.61 (m, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.4, 145.8, 142.4, 135.7, 130.0, 129.2,

128.7, 128.2, 126.7, 126.0, 124.6, 124.2, 120.0, 61.5, 60.1, 53.6, 53.5. ^{31}P NMR (202 MHz, $CDCl_3$): δ 21.9. MS (ESI) m/z = 393 $(M + H)^+$; (ESI-HRMS) calculated for $C_{22}H_{22}O_3N_2P$ $(M+H)^+$ = 393.1362, found 393.1362.



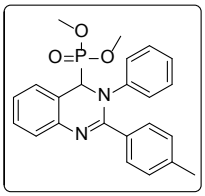
Dimethyl (2-(4-methoxyphenyl)-3-phenyl-3,4-dihydroquinazolin-4-yl)phosphonate (7b).

Yellow oil. Isolated yield: 83%. (Petroleum ether/ethyl acetate = 1:4, Rf = 0.2). IR ν_{max} (cm^{-1}): 2954, 2929, 2853, 1583, 1546, 1485, 1364, 1307, 1252, 1174, 1146, 1029, 840, 765, 696, 539, 445, 420. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.8 Hz, 2H), 7.46 (d, *J* = 7.9 Hz, 1H), 7.36 (t, *J* = 7.1 Hz, 1H), 7.23-7.09 (m, 6H), 7.01 (t, *J* = 6.9 Hz, 1H), 6.79 (d, *J* = 8.8 Hz, 2H), 5.31 (d, *J* = 13.9 Hz, 1H), 3.76 (s, 3H), 3.72-3.60 (m, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.2, 155.3, 146.0, 142.2, 131.5, 129.2, 128.8, 127.5, 126.6, 125.8, 124.3, 124.3, 120.0, 113.7, 61.6, 60.3, 55.2, 53.6, 29.6. ^{31}P NMR (202 MHz, $CDCl_3$): δ 21.4. MS (ESI) m/z = 423 $(M + H)^+$; (ESI-HRMS) calculated for $C_{23}H_{24}O_4N_2P$ $(M+H)^+$ = 423.1468, found 423.1461.



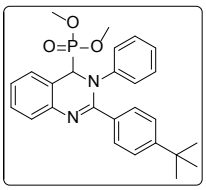
Dimethyl 3-phenyl-2-(4-(trifluoromethyl)phenyl)-3,4-dihydroquinazolin-4-ylphosphonate (7c).

Yellow oil. Isolated yield: 92%. (Petroleum ether/ethyl acetate = 1:4, Rf = 0.4). IR ν_{max} (cm^{-1}): 3453, 2927, 2855, 1586, 1550, 1486, 1457, 1368, 1322, 1254, 1231, 1168, 1125, 1031, 960, 847, 766, 696, 558, 534, 450. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.91 (d, *J* = 7.5 Hz, 2H), 7.53 (d, *J* = 8.3 Hz, 2H), 7.46 (d, *J* = 8.3 Hz, 1H), 7.38 (t, *J* = 7.5 Hz, 1H), 7.25-7.12 (m, 6H), 7.06-7.00 (m, 1H), 5.34 (d, *J* = 13.5 Hz, 1H), 3.71-3.62 (m, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 153.9, 145.2, 142.0, 139.3, 131.8, 131.3, 129.9, 129.4, 129.0, 126.6, 125.2, 124.9, 124.0, 119.9, 61.8, 59.6, 53.7, 53.6, 53.5, 53.4. ^{31}P NMR (202 MHz, $CDCl_3$): δ 22.0. MS (ESI) m/z = 461 $(M + H)^+$; (ESI-HRMS) calculated for $C_{23}H_{21}O_3N_2F_3P$ $(M+H)^+$ = 461.1236, found 461.1221.



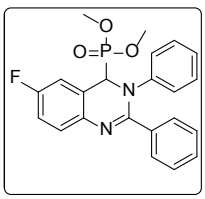
Dimethyl 3-phenyl-2-p-tolyl-3,4-dihydroquinazolin-4-ylphosphonate (7d).

Yellow oil. Isolated yield: 79%. (Petroleum ether/ethyl acetate = 1:4, Rf = 0.2). IR ν_{max} (cm^{-1}): 2954, 2926, 2854, 1583, 1546, 1483, 1455, 1365, 1280, 1254, 1230, 1181, 1145, 1030, 959, 827, 766, 696, 596, 536, 448. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.67 (d, *J* = 8.3 Hz, 2H), 7.44 (d, *J* = 8.3 Hz, 1H), 7.35 (t, *J* = 6.7 Hz, 1H), 7.22-7.05 (m, 8H), 6.99 (t, *J* = 6.7 Hz, 1H), 5.32 (d, *J* = 13.5 Hz, 1H), 3.72-3.59 (m, 6H), 2.29 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.4, 146.0, 142.5, 140.3, 132.8, 129.7, 129.2, 128.9, 128.7, 126.6, 125.8, 124.5, 124.3, 124.1, 120.0, 61.5, 60.2, 53.5, 21.3. ^{31}P NMR (202 MHz, $CDCl_3$): δ 21.6. MS (ESI) m/z = 407 $(M + H)^+$; (ESI-HRMS) calculated for $C_{23}H_{24}O_3N_2P$ $(M+H)^+$ = 407.1518, found 407.1518.



Dimethyl 2-(4-tert-butylphenyl)-3-phenyl-3,4-dihydroquinazolin-4-ylphosphonate (7e).

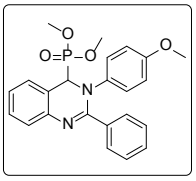
Yellow oil. Isolated yield: 89%. (Petroleum ether/ethyl acetate = 1:4, Rf = 0.5). IR ν_{max} (cm^{-1}): 2980, 2932, 2312, 1551, 1487, 1364, 1234, 1157, 1136, 984, 766, 697, 587, 554, 462. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.5 Hz, 2H), 7.44 (d, *J* = 7.4 Hz, 1H), 7.34 (t, *J* = 7.4 Hz, 1H), 7.27 (d, *J* = 8.2 Hz, 2H), 7.21 (d, *J* = 7.7 Hz, 2H), 7.18-7.10 (m, 4H), 6.98 (t, *J* = 7.1 Hz, 1H), 5.32 (d, *J* = 13.7 Hz, 1H), 3.72-3.58 (m, 6H), 1.24 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.4, 153.3, 146.0, 142.5, 132.7, 129.3, 128.7, 126.6, 125.8, 124.5, 124.2, 124.0, 119.9, 61.5, 60.2, 53.6, 53.5, 53.4, 34.6, 31.0. ^{31}P NMR (202 MHz, $CDCl_3$): δ 22.0. MS (ESI) m/z = 449 $(M + H)^+$; (ESI-HRMS) calculated for $C_{26}H_{30}O_3N_2P$ $(M+H)^+$ = 449.1975, found 449.1975.



Dimethyl 6-fluoro-2,3-diphenyl-3,4-dihydroquinazolin-4-ylphosphonate (7f).

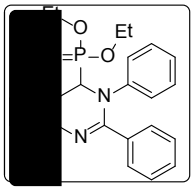
Yellow oil. Isolated yield: 90%. (Petroleum ether/ethyl acetate = 1:4, Rf = 0.5). IR ν_{max} (cm^{-1}): 3439, 2955, 2927, 2855, 1590, 1552, 1487, 1364, 1239, 1181, 1030, 943, 876, 754, 699, 575, 534. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8.2 Hz, 2H), 7.42-7.39 (m, 1H), 7.30-7.25 (m, 3H), 7.20 (d, *J* = 8.3 Hz, 2H), 7.15 (t, *J* = 7.4 Hz, 2H), 7.08-6.99 (m, 2H), 6.85-6.82 (m, 1H), 5.28 (d, *J* = 14.3 Hz, 1H),

3.72-3.67 (m, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.7, 159.8, 154.9, 145.7, 138.9, 135.5, 130.1, 129.6, 128.8, 128.3, 126.1, 124.6, 124.2, 121.5, 116.2, 116.0, 113.5, 113.3, 61.3, 60.0, 53.7, 53.6, 53.5. ^{31}P NMR (202 MHz, $CDCl_3$): δ 21.3. MS (ESI) m/z = 411 $(M + H)^+$; (ESI-HRMS) calculated for $C_{22}H_{21}O_3N_2FP$ $(M+H)^+$ = 411.1264, found 411.1264.



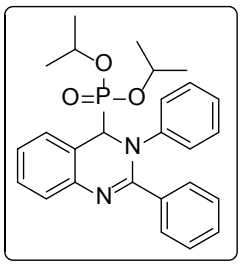
Dimethyl 3-(4-methoxyphenyl)-2-phenyl-3,4-dihydroquinazolin-4-ylphosphonate (7g).

Yellow oil. Isolated yield: 71%. (Petroleum ether/ethyl acetate = 1:4, Rf = 0.2). IR ν_{max} (cm^{-1}): 3746, 3368, 2929, 2376, 1646, 1546, 1509, 1369, 1246, 1179, 1033, 831, 765, 620, 522. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.75 (d, *J* = 7.9 Hz, 2H), 7.43 (d, *J* = 7.0 Hz, 1H), 7.37-7.34 (m, 1H), 7.29-7.26 (m, 3H), 7.20-7.17 (m, 3H), 7.10-7.08 (m, 1H), 6.67 (d, *J* = 9.1 Hz, 2H), 5.24 (d, *J* = 13.4 Hz, 1H), 3.72-3.61 (m, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.7, 155.7, 142.6, 139.3, 135.8, 129.9, 129.8, 129.2, 128.2, 126.6, 126.0, 125.9, 124.6, 119.6, 114.0, 62.0, 60.7, 55.3, 53.6, 53.5. ^{31}P NMR (202 MHz, $CDCl_3$): δ 21.7. MS (ESI) m/z = 423 $(M + H)^+$; (ESI-HRMS) calculated for $C_{23}H_{24}O_4N_2P$ $(M+H)^+$ = 423.1468, found 423.1461.



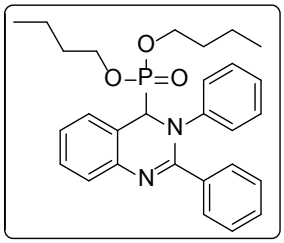
Diethyl 2,3-diphenyl-3,4-dihydroquinazolin-4-ylphosphonate (7h).

Yellow oil. Isolated yield: 92%. (Petroleum ether/ethyl acetate = 1:4, Rf = 0.4). IR ν_{max} (cm^{-1}): 2985, 2380, 1587, 1548, 1487, 1364, 1249, 1151, 1023, 963, 837, 766, 698, 635, 543, 460. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.78 (d, *J* = 7.7 Hz, 2H), 7.44 (d, *J* = 7.7 Hz, 1H), 7.35 (t, *J* = 7.4 Hz, 1H), 7.29-7.22 (m, 5H), 7.19-7.11 (m, 4H), 6.99 (t, *J* = 7.3 Hz, 1H), 5.30 (d, *J* = 13.7 Hz, 1H), 4.15-3.92 (m, 4H), 1.23-1.19 (m, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 146.0, 142.5, 135.9, 129.9, 129.7, 129.1, 128.7, 128.1, 126.7, 125.9, 124.5, 124.3, 124.2, 120.2, 63.2, 63.1, 63.0, 62.9, 62.2, 60.0, 16.4, 16.3. ^{31}P NMR (202 MHz, $CDCl_3$): δ 19.8. MS (ESI) m/z = 421 $(M + H)^+$; (ESI-HRMS) calculated for $C_{24}H_{26}O_3N_2P$ $(M+H)^+$ = 421.1675, found 421.1667.



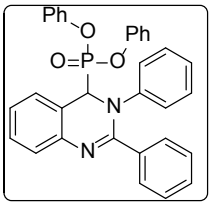
Diisopropyl 2,3-diphenyl-3,4-dihydroquinazolin-4-ylphosphonate (7i).

Yellow oil. Isolated yield: 87%. (Petroleum ether/ethyl acetate = 1:1, Rf = 0.4). IR ν_{max} (cm^{-1}): 2982, 2932, 2312, 1549, 1488, 1367, 1244, 1145, 1106, 986, 765, 697, 633, 588, 547, 467. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.79 (d, *J* = 7.6 Hz, 2H), 7.43 (d, *J* = 7.9 Hz, 1H), 7.34 (t, *J* = 7.4 Hz, 1H), 7.29-7.23 (m, 5H), 7.18-7.12 (m, 4H), 6.97 (t, *J* = 7.1 Hz, 1H), 5.23 (d, *J* = 13.7 Hz, 1H), 4.68 (q, *J* = 6.2 Hz, 1H), 4.57 (q, *J* = 6.2 Hz, 1H), 1.27-1.24 (m, 6H), 1.19-1.18 (m, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.3, 146.2, 142.5, 136.1, 129.8, 129.7, 128.9, 128.6, 128.0, 126.9, 125.7, 124.6, 124.2, 120.5, 72.2, 71.9, 62.3, 61.0, 24.2, 24.1, 23.8, 23.7. ^{31}P NMR (202 MHz, $CDCl_3$): δ 17.3. MS (ESI) m/z = 449 $(M + H)^+$; (ESI-HRMS) calculated for $C_{26}H_{30}O_3N_2P$ $(M+H)^+$ = 449.1988, found 449.1976.



Dibutyl (2,3-diphenyl-3,4-dihydroquinazolin-4-yl)phosphonate (7j).

Yellow oil. Isolated yield: 90%. (Petroleum ether/ethyl acetate = 1:1, Rf = 0.4). IR ν_{max} (cm^{-1}): 2955, 2874, 2380, 2310, 1549, 1487, 1364, 1243, 1148, 981, 902, 844, 764, 697, 544, 466, 440. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.2 Hz, 2H), 7.44 (d, *J* = 7.6 Hz, 1H), 7.35 (t, *J* = 9.1 Hz, 1H), 7.29-7.22 (m, 5H), 7.19-7.10 (m, 4H), 6.98 (t, *J* = 7.3 Hz, 1H), 5.30 (d, *J* = 13.7 Hz, 1H), 4.60-3.86 (m, 4H), 1.58-1.50 (m, 4H), 1.31-1.22 (m, 4H), 0.85-0.78 (m, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.3, 146.0, 142.5, 135.9, 129.9, 129.7, 129.0, 128.6, 128.1, 126.7, 125.8, 124.5, 124.3, 124.1, 120.3, 66.8, 66.5, 65.4, 61.7, 60.4, 32.4, 32.3, 18.6, 18.5, 13.4. ^{31}P NMR (202 MHz, $CDCl_3$): δ 20.0. MS (ESI) m/z = 477 $(M + H)^+$; (ESI-HRMS) calculated for $C_{28}H_{34}O_3N_2P$ $(M+H)^+$ = 477.2277, found 477.2286.

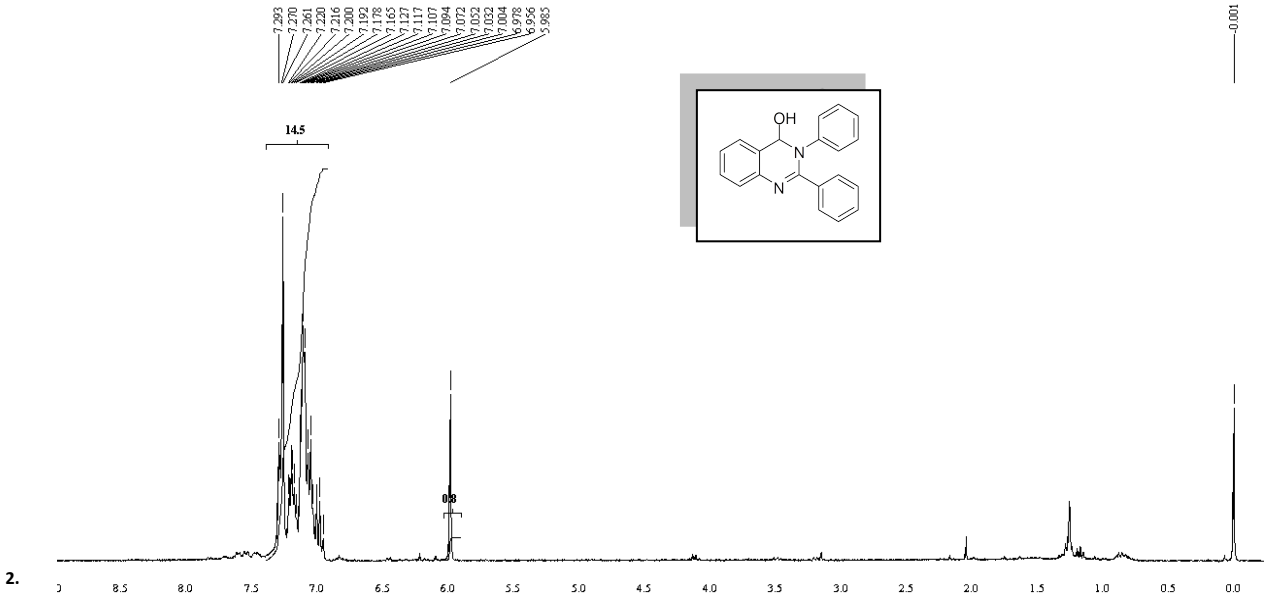


Diphenyl 2,3-diphenyl-3,4-dihydroquinazolin-4-ylphosphonate (7k).

Yellow oil. Isolated yield: 51%. (Petroleum ether/ethyl acetate = 1:1, Rf = 0.6). IR ν_{max} (cm^{-1}): 2930, 2378, 1741, 1589, 1550, 1487, 1363, 1234, 1204, 1070, 937, 837, 762, 692, 564, 466. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.0 Hz, 2H), 7.51 (d, *J* = 7.7 Hz, 1H), 7.41 (t, *J* = 7.7 Hz, 1H), 7.31-7.24 (m, 6H), 7.23-7.12 (m, 8H), 7.09-6.98 (m, 4H), 6.88 (d, *J* = 8.6 Hz, 2H), 5.70 (d, *J* = 12.3 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.3, 150.3, 150.2, 150.0, 149.9, 146.0, 142.7, 135.7, 130.0, 129.8, 129.5, 129.4, 128.9, 128.1, 127.0, 126.2, 125.1, 124.7, 124.3, 120.6, 119.1, 62.3, 60.9. ^{31}P NMR (202 MHz, $CDCl_3$): δ 11.9. MS (ESI) m/z = 517 $(M + H)^+$; (ESI-HRMS) calculated for $C_{32}H_{26}O_3N_2P$ $(M+H)^+$ = 517.1675, found 517.1663.

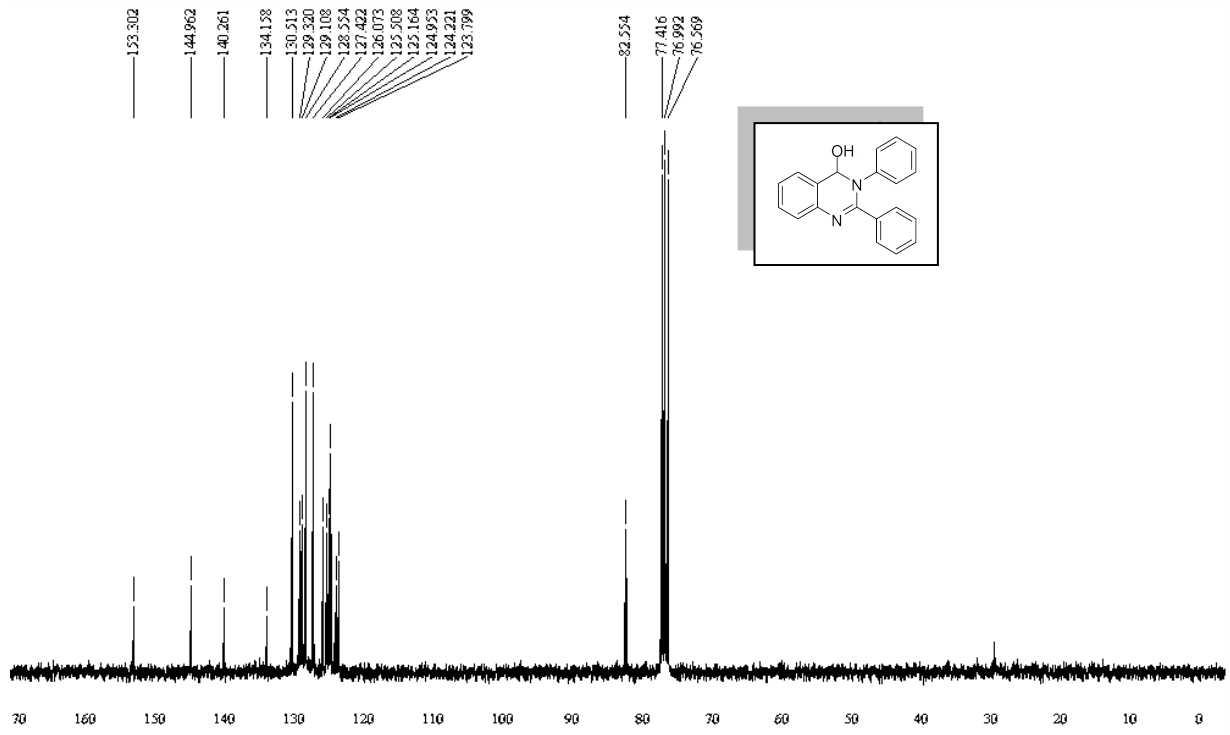
1. Copies of ^{1}H NMR, ^{13}C NMR, ^{31}P NMR HRMS spectra for products

^{1}H NMR (300 MHz, $CDCl_3$): (Table S1, 3a)



2.

^{13}C NMR (75 MHz, $CDCl_3$): (Table S1, 3a)

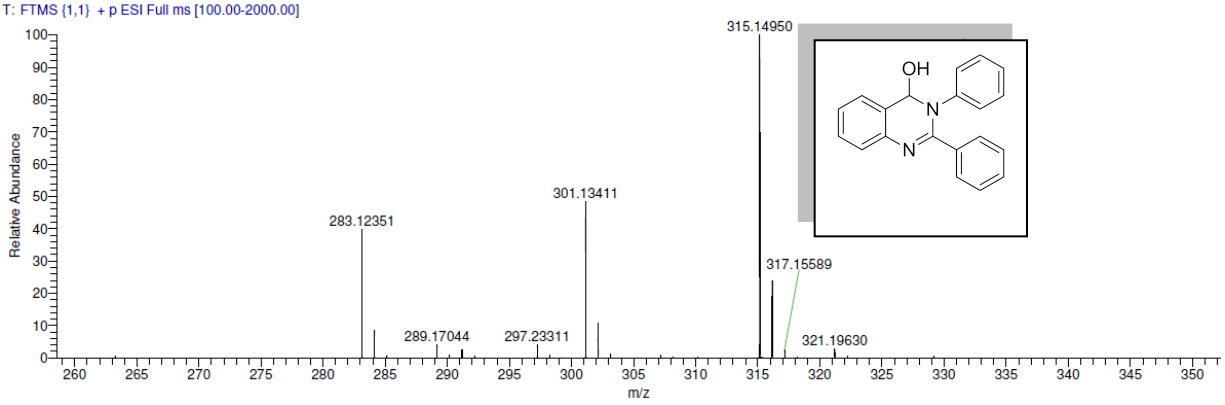


HIGH RESOLUTION MASS SPECTRA of compound 3a in MeOH: (Table S1, 3a)

National Centre for Mass Spectrometry
CSIR-Indian Institute of Chemical Technology

File Name C:\IICT-HRMS\...\KRR-3-71
Sample Name
Sample ID G SAIDULU
Date and Time 08-09-14 23:01:07

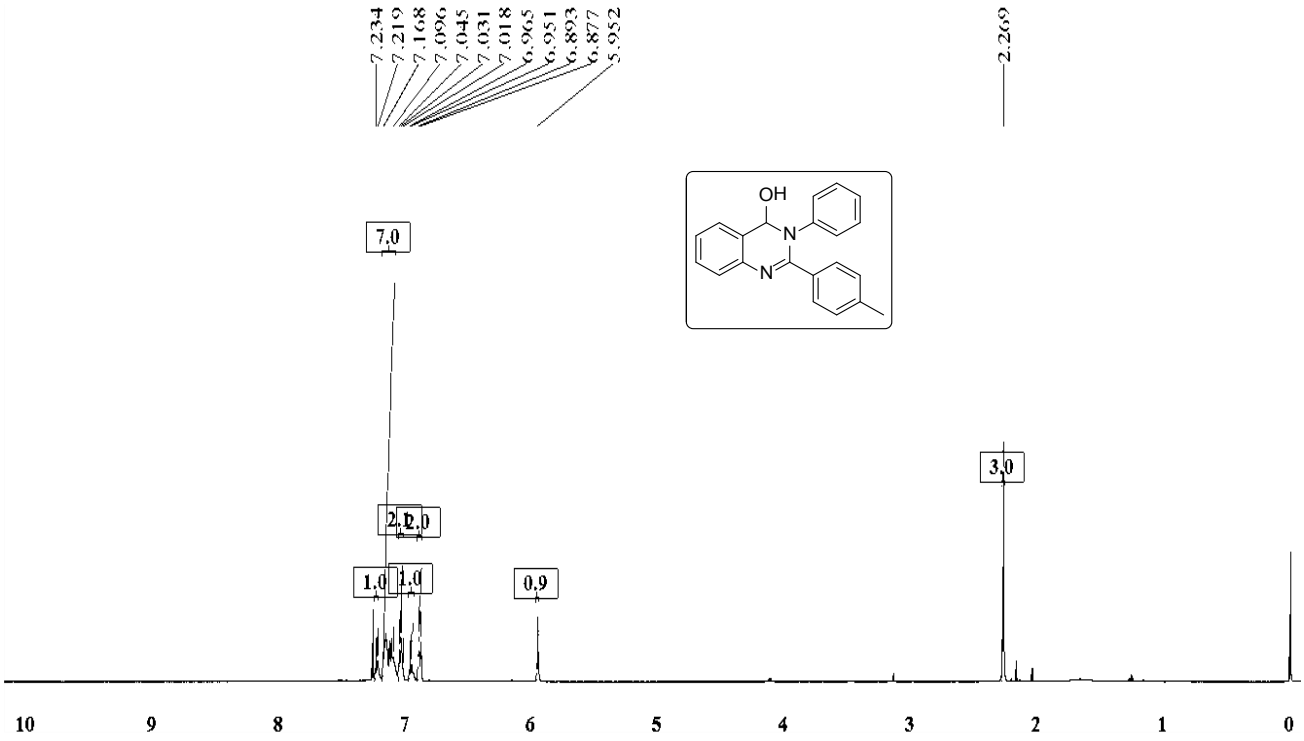
KRR-3-71 #6-89 RT: 0.02-0.30 AV: 84 SB: 326 0.80-1.90 NL: 1.95E8
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]



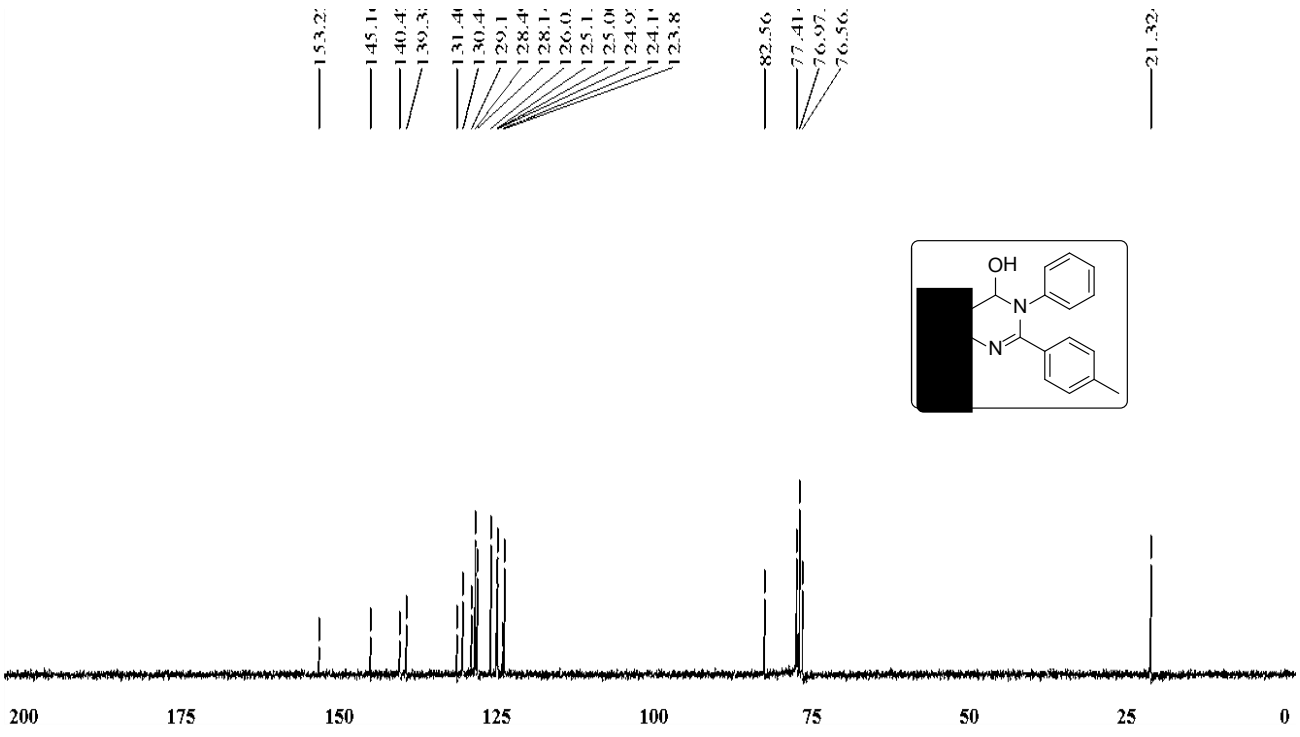
KRR-3-71#8-30 RT: 0.03-0.10 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]
m/z= 298.46-303.73

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
301.13408	121940112.0	100.00	301.13354	0.54	13.5	$C_{20}H_{17}ON_2$

^{1}H NMR (500 MHz, $CDCl_3$): (Table S1, 3b)



^{13}C NMR (75 MHz, $CDCl_3$): (Table S1, 3b)

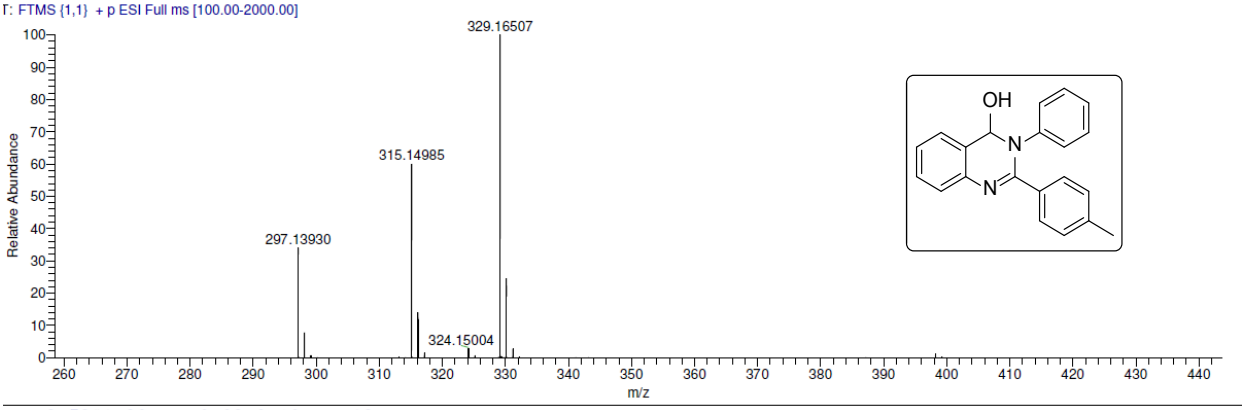


HIGH RESOLUTION MASS SPECTRA: (Table S1, 3b)

National Centre for Mass Spectrometry
CSIR-Indian Institute of Chemical Technology

File Name C:\IICT-HRMS\...\KRR-3-73
Sample Name
Sample ID G SAIDULU
Date and Time 08-09-14 23:03:47

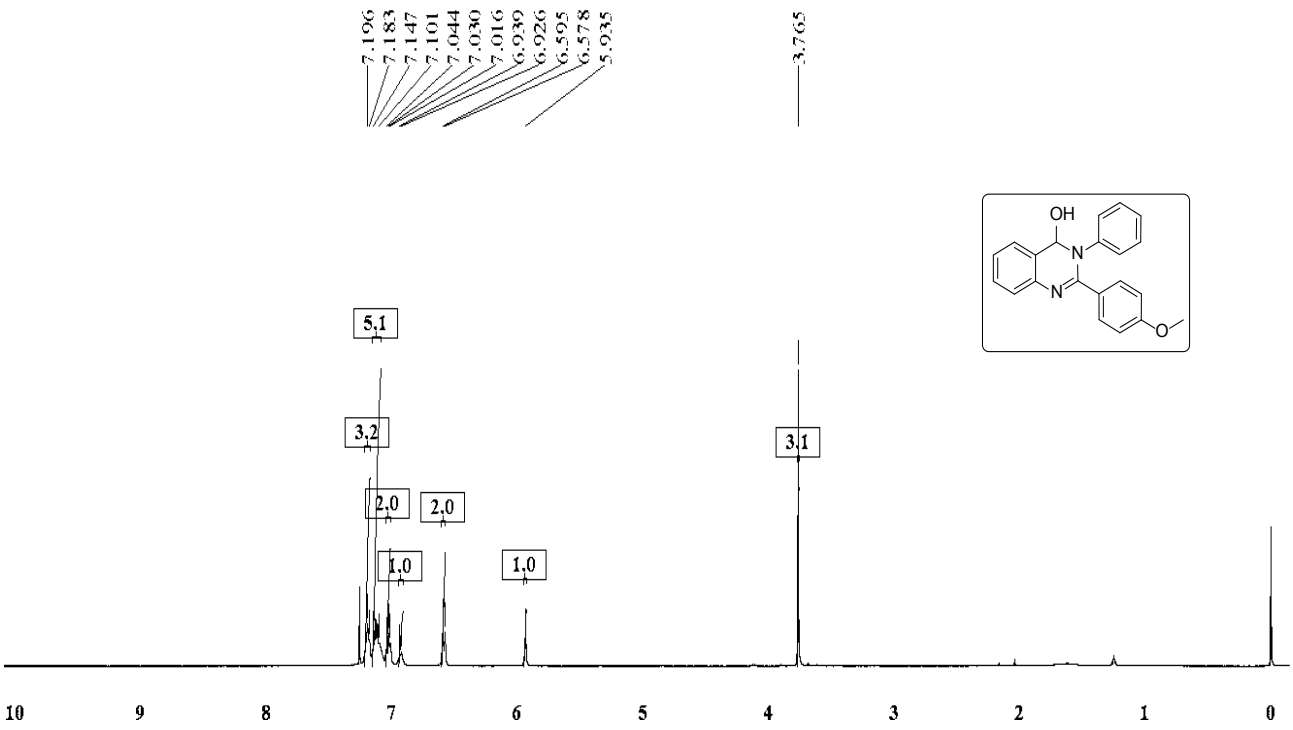
KRR-3-73 #6-89 RT: 0.02-0.30 AV: 84 SB: 326 0.80-1.90 NL: 2.28E8
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]



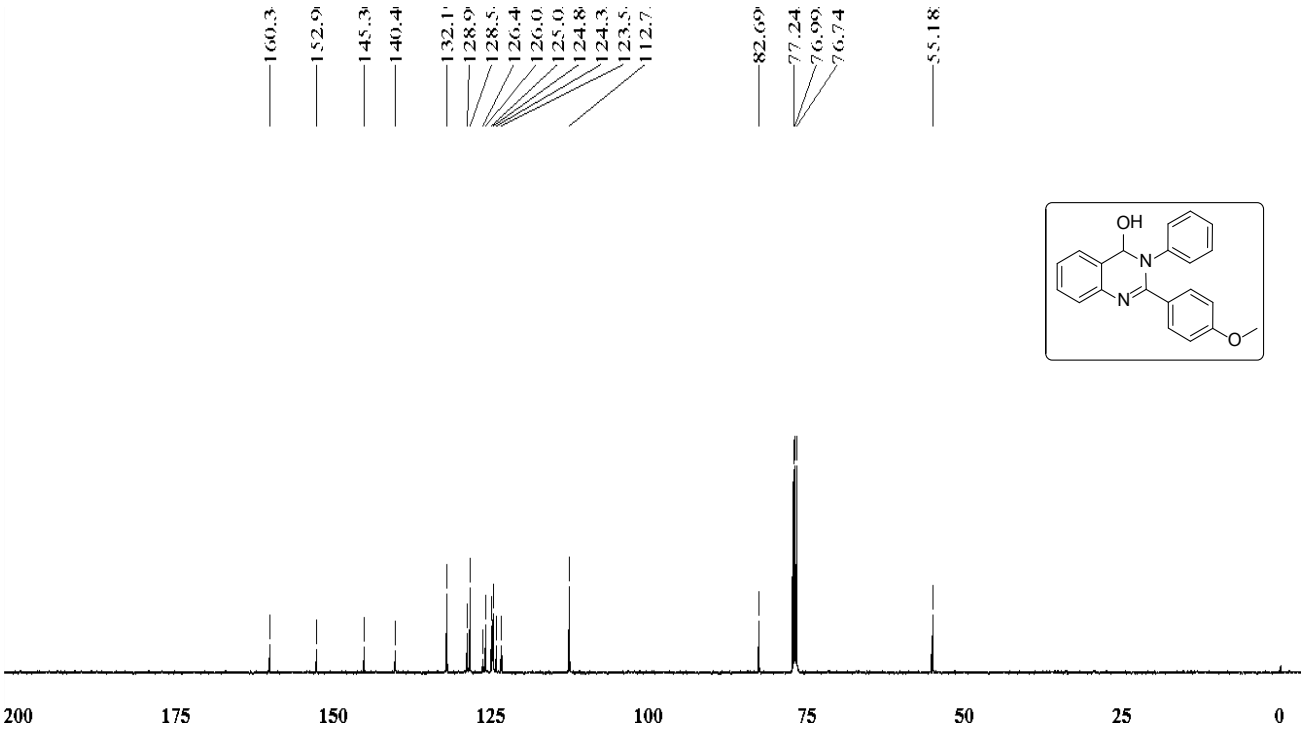
KRR-3-73#8-30 RT: 0.03-0.10 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]
m/z= 311.63-317.02

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
315.14973	189787408.0	100.00	315.14919	0.54	13.5	$C_{21}H_{19}ON_2$

^{1}H NMR (500 MHz, $CDCl_3$): (Table S1, 3c)



^{13}C NMR (125 MHz, $CDCl_3$): (Table S1, 3c)

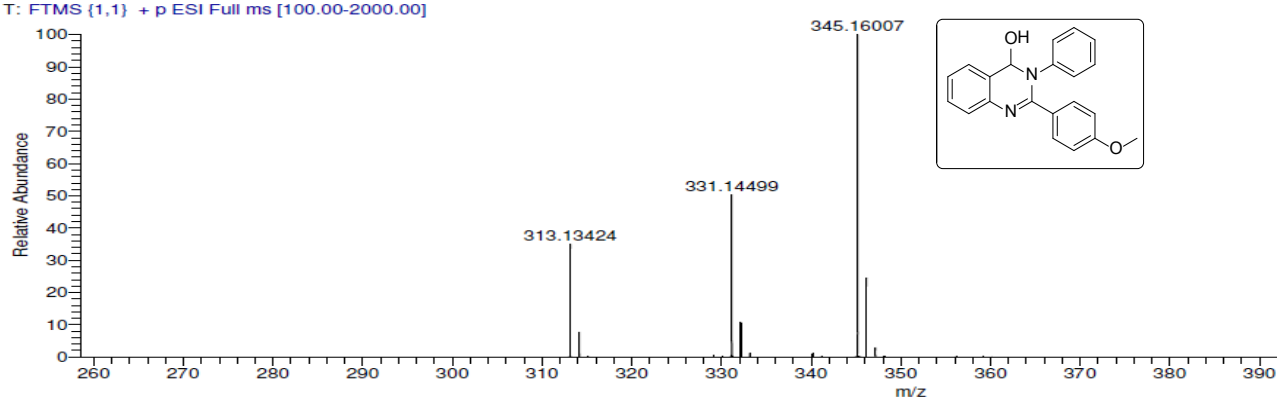


HIGH RESOLUTION MASS SPECTRA: (Table S1, 3c)

National Centre for Mass Spectrometry
CSIR-Indian Institute of Chemical Technology

File Name C:\IICT-HRMS\...\KRR-3-74
Sample Name
Sample ID G SAIDULU
Date and Time 08-09-14 23:06:27

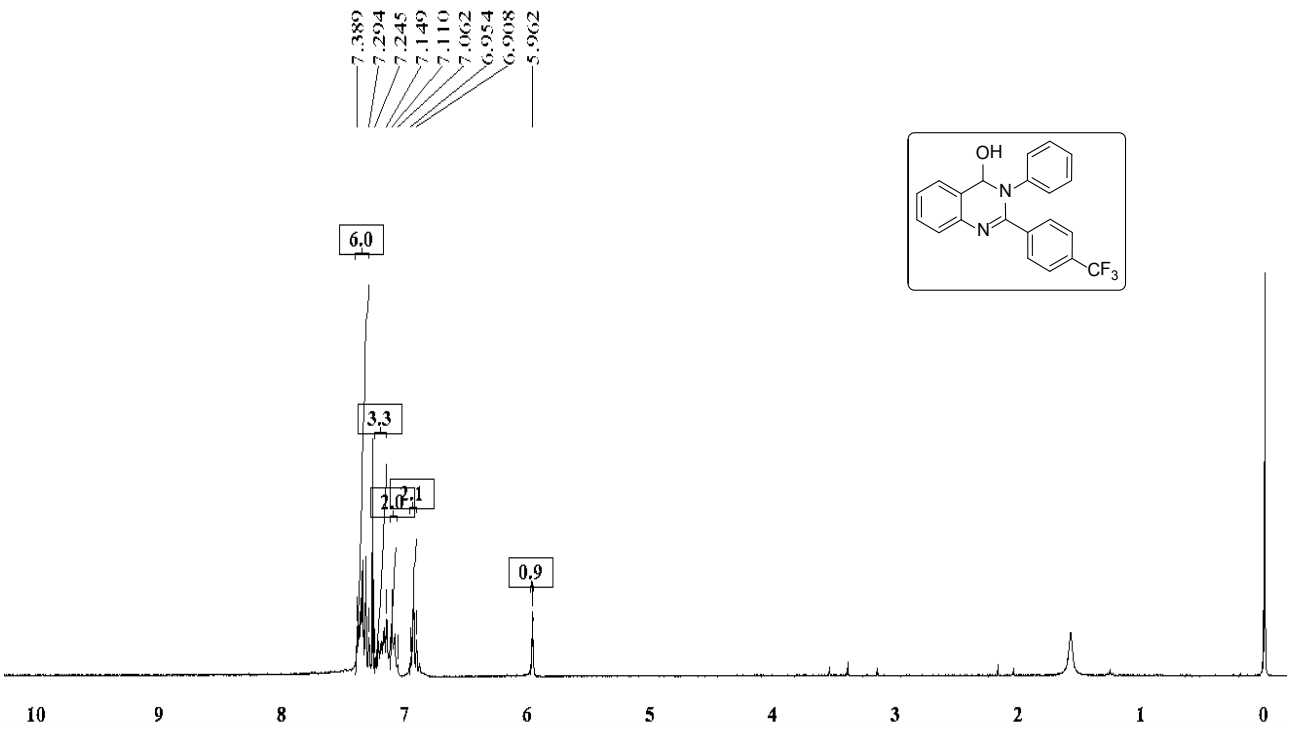
KRR-3-74 #6-89 RT: 0.02-0.30 AV: 84 SB: 326 0.80-1.90 NL: 2.45E8
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]



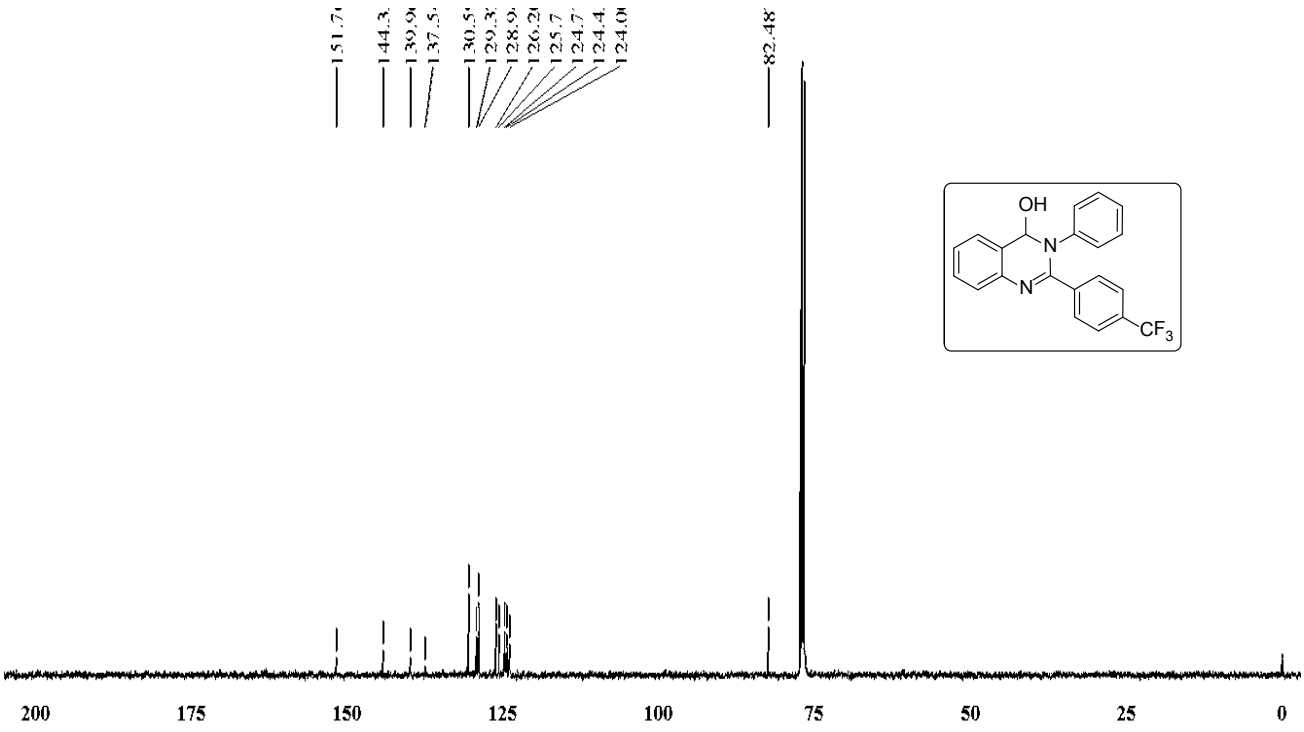
KRR-3-74#8-30 RT: 0.03-0.10 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]
m/z= 327.57-334.63

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
331.14486	131950568.0	100.00	331.14410	0.76	13.5	$C_{21}H_{19}O_2N_2$

^{1}H NMR (300 MHz, $CDCl_3$): (Table S1, 3d)



^{13}C NMR (125 MHz, CDCl$_3$): (Table S1, 3d)

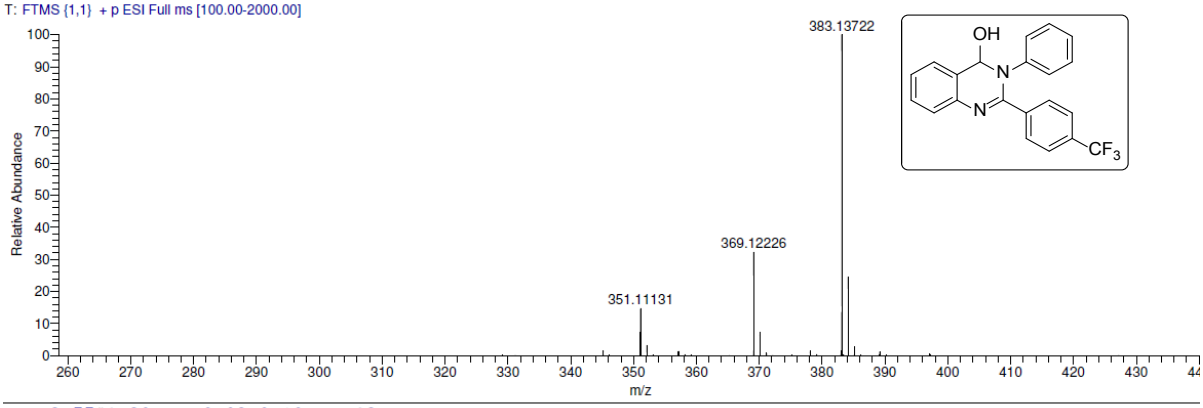


HIGH RESOLUTION MASS SPECTRA: (Table S1, 3d)

National Centre for Mass Spectrometry
CSIR-Indian Institute of Chemical Technology

File Name C:\IICT-HRMS\...\KRR-3-77
Sample Name
Sample ID G SAIDULU
Date and Time 08-09-14 23:09:07

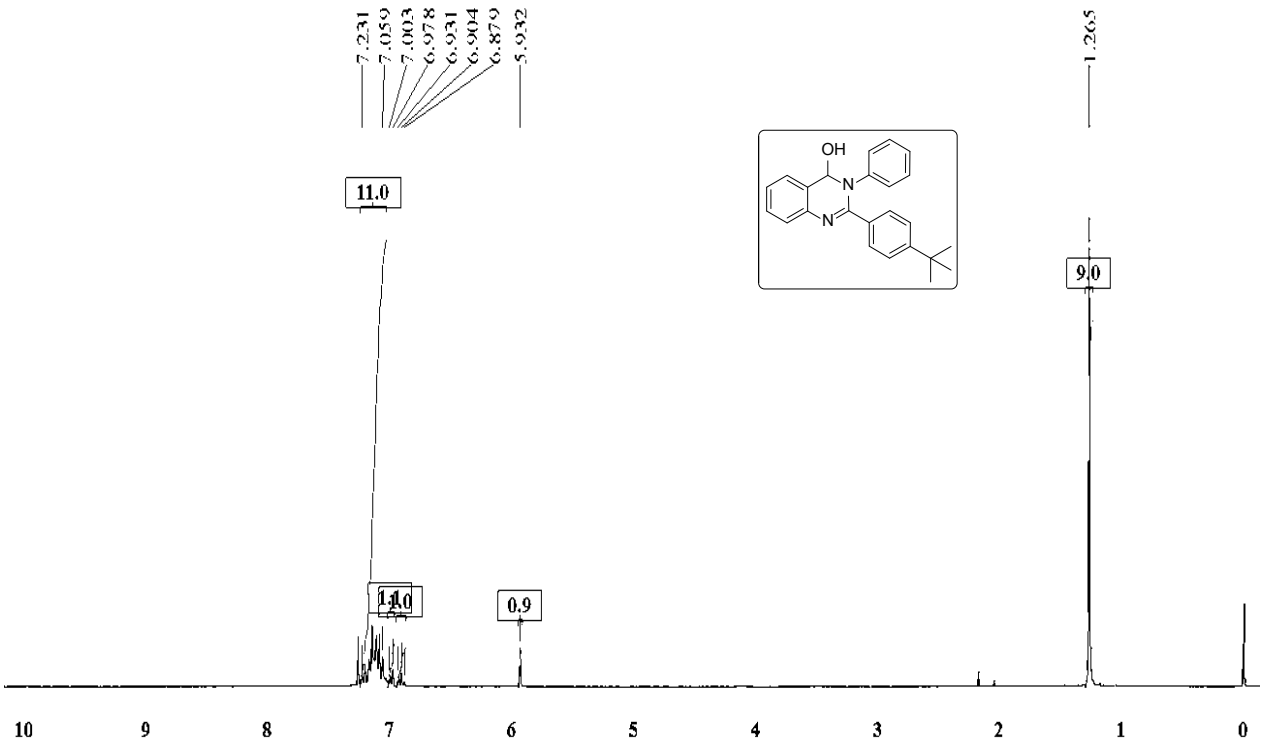
KRR-3-77 #6-89 RT: 0.02-0.30 AV: 84 SB: 326 0.80-1.90 NL: 2.81E8
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]



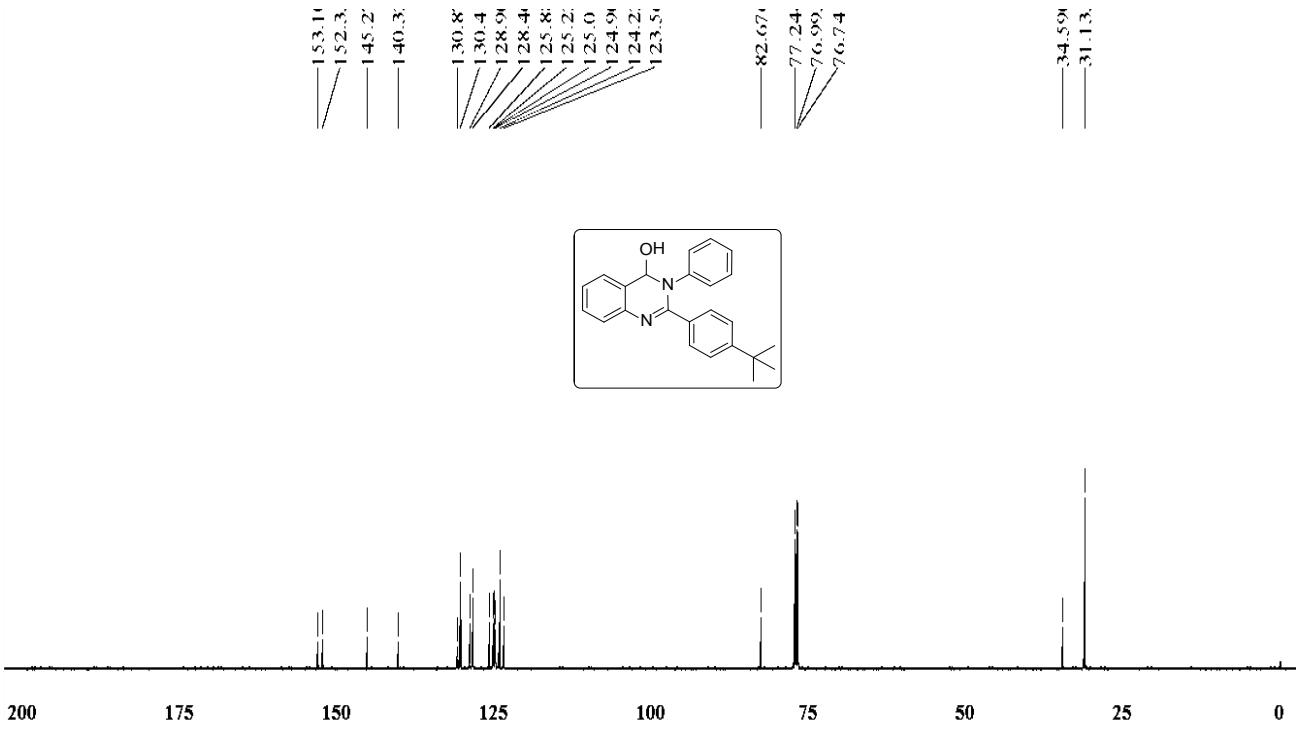
KRR-3-77#8-30 RT: 0.03-0.10 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]
m/z= 367.34-372.37

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
369.12204	114809248.0	100.00	369.12092	1.12	13.5	$C_{21}H_{16}ON_2F_3$

^{1}H NMR (300 MHz, $CDCl_3$): (Table S1, 3e)



^{13}C NMR (125 MHz, $CDCl_3$): (Table S1, 3e)

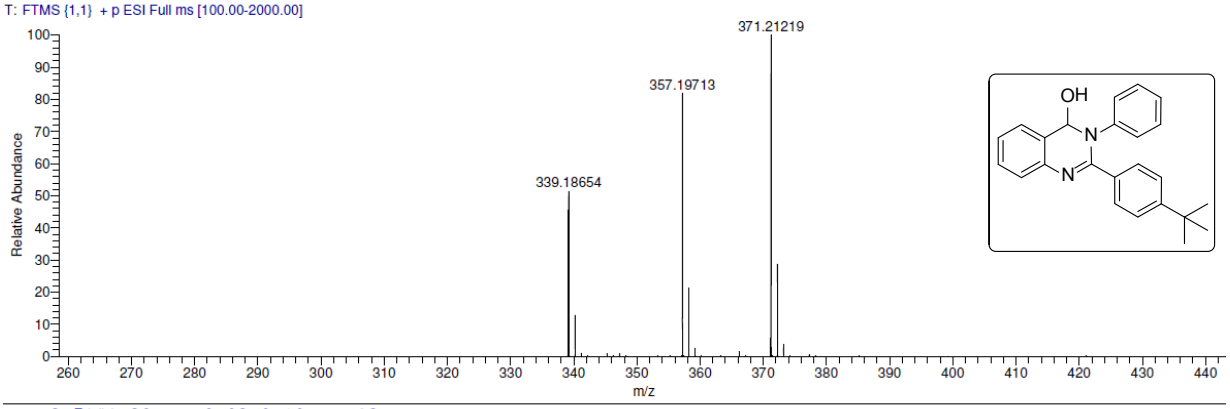


HIGH RESOLUTION MASS SPECTRA: (Table S1, 3e)

National Centre for Mass Spectrometry
CSIR-Indian Institute of Chemical Technology

File Name C:\IICT-HRMS\...\KRR-3-79
Sample Name
Sample ID G SAIDULU
Date and Time 08-09-14 23:11:48

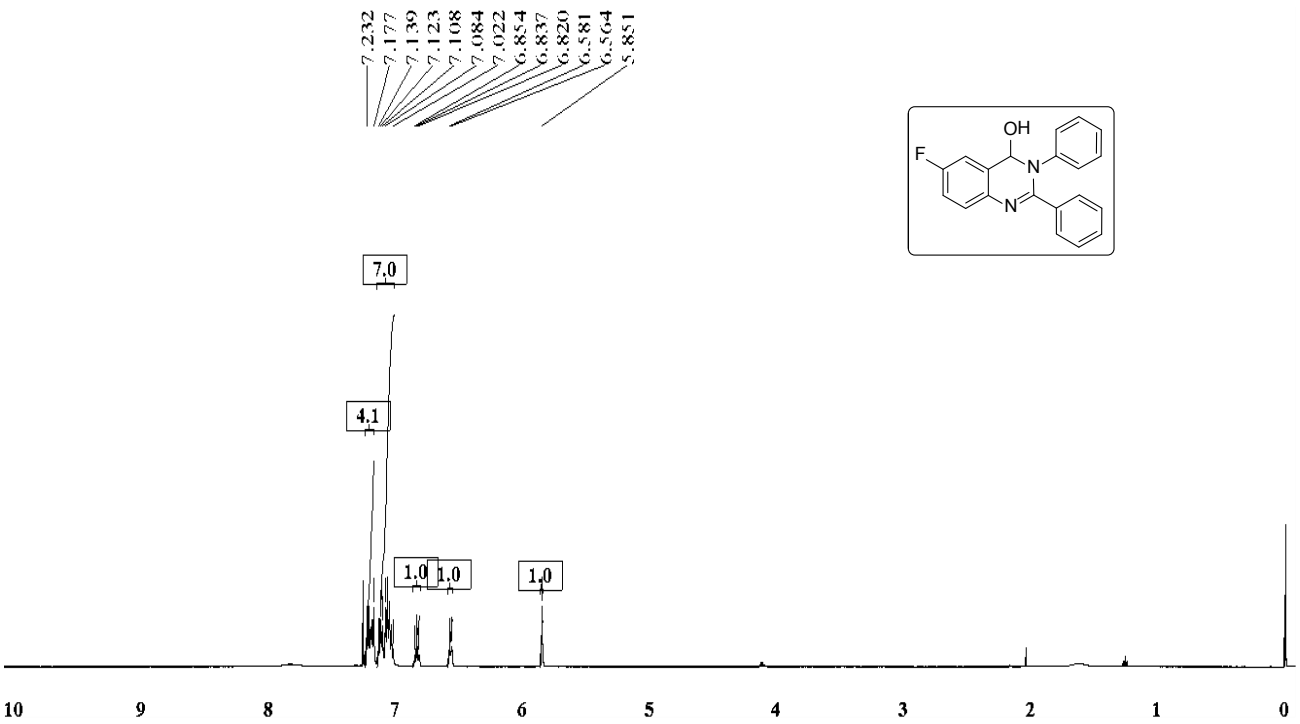
KRR-3-79 #6-89 RT: 0.02-0.30 AV: 84 SB: 326 0.80-1.90 NL: 2.35E8
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]



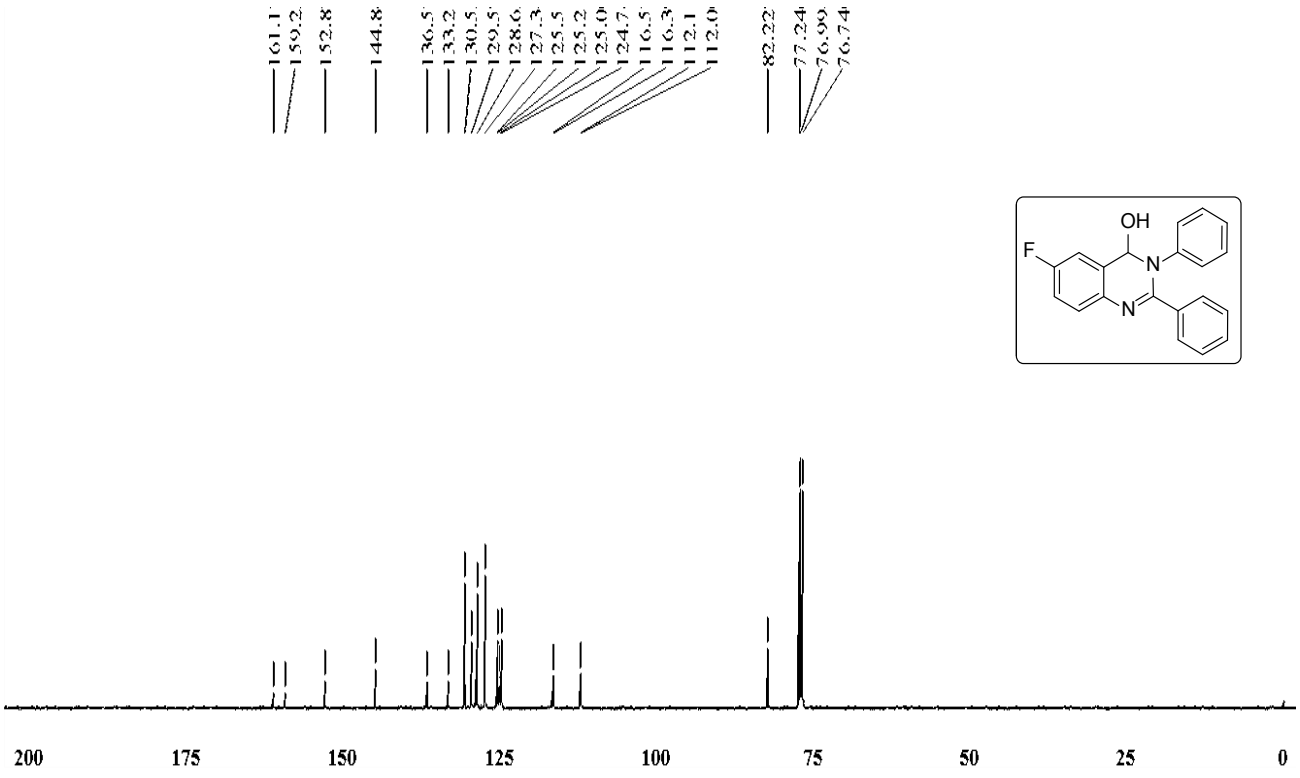
KRR-3-79#8-30 RT: 0.03-0.10 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]
m/z= 354.04-361.47

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
357.19671	207134192.0	100.00	357.19614	0.57	13.5	$C_{24}H_{25}ON_2$

^{1}H NMR (500 MHz, $CDCl_3$): (Table S1, 3f)



^{13}C NMR (125 MHz, $CDCl_3$): (Table S1, 3f)

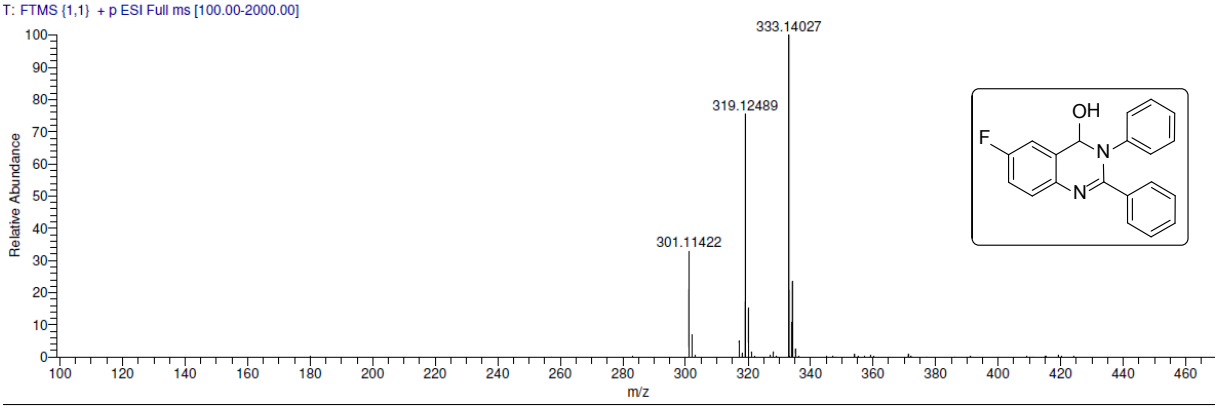


HIGH RESOLUTION MASS SPECTRA: (Table S1, 3f)

National Centre for Mass Spectrometry
CSIR-Indian Institute of Chemical Technology

File Name C:\IICT-HRMS\...\KRR-3-89
Sample Name
Sample ID G SAIDULU
Date and Time 08-09-14 23:14:29

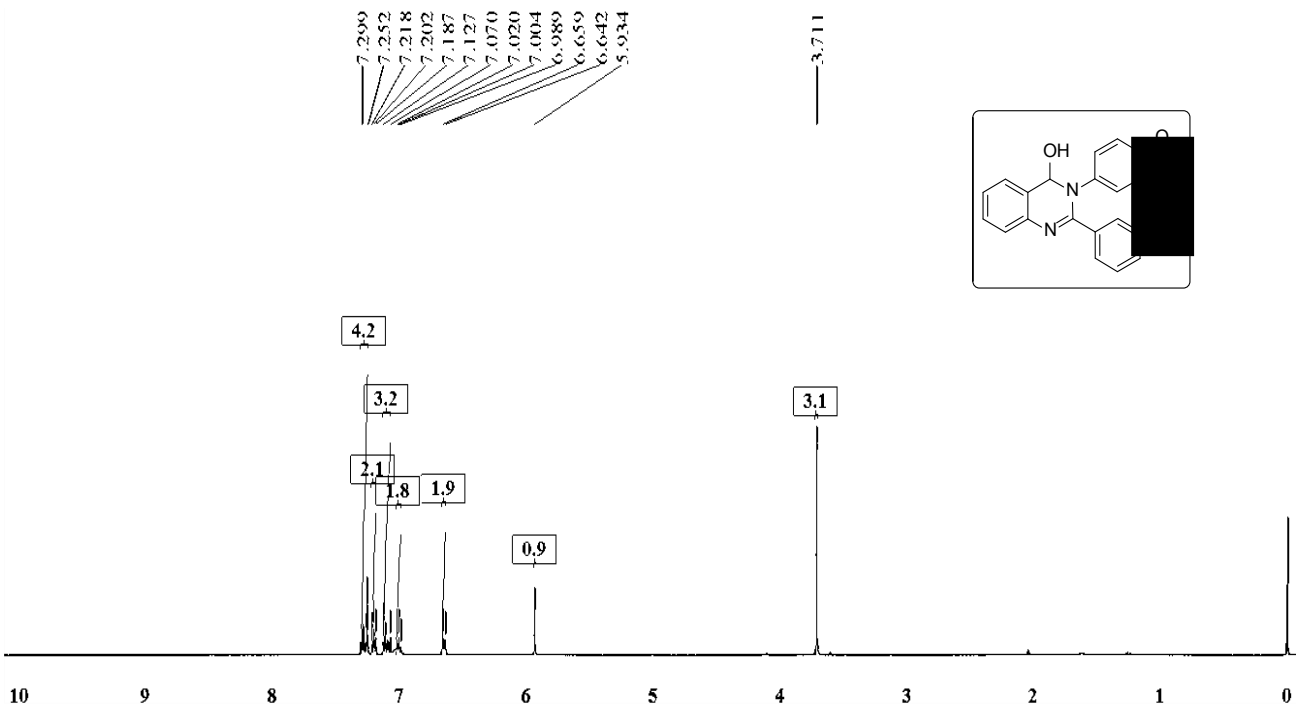
KRR-3-89 #6-89 RT: 0.02-0.30 AV: 84 SB: 326 0.80-1.90 NL: 1.78E8
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]



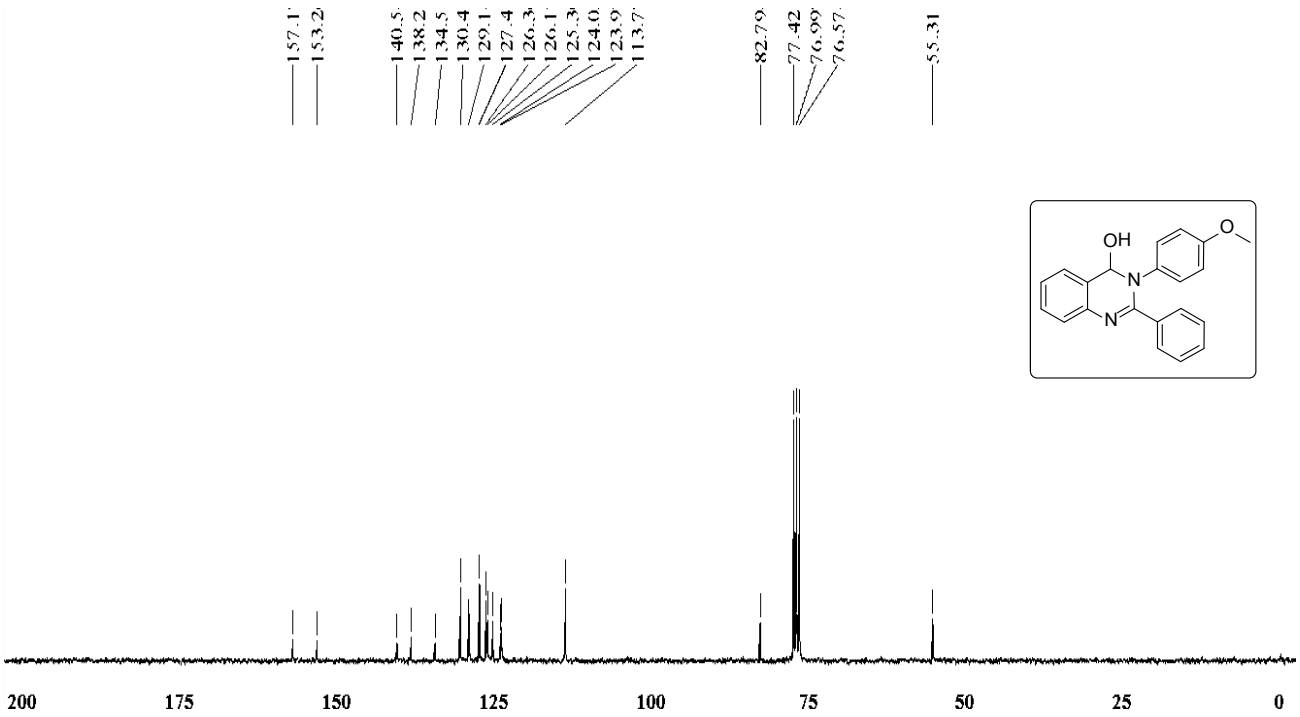
KRR-3-89#8-30 RT: 0.03-0.10 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]
m/z= 312.96-322.34

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
319.12477	163107584.0	100.00	319.12412	0.66	13.5	$C_{20}H_{16}ON_2F$

^{1}H NMR (500 MHz, $CDCl_3$): (Table S1, 3g)



^{13}C NMR (125 MHz, $CDCl_3$): (Table S1, 3g)

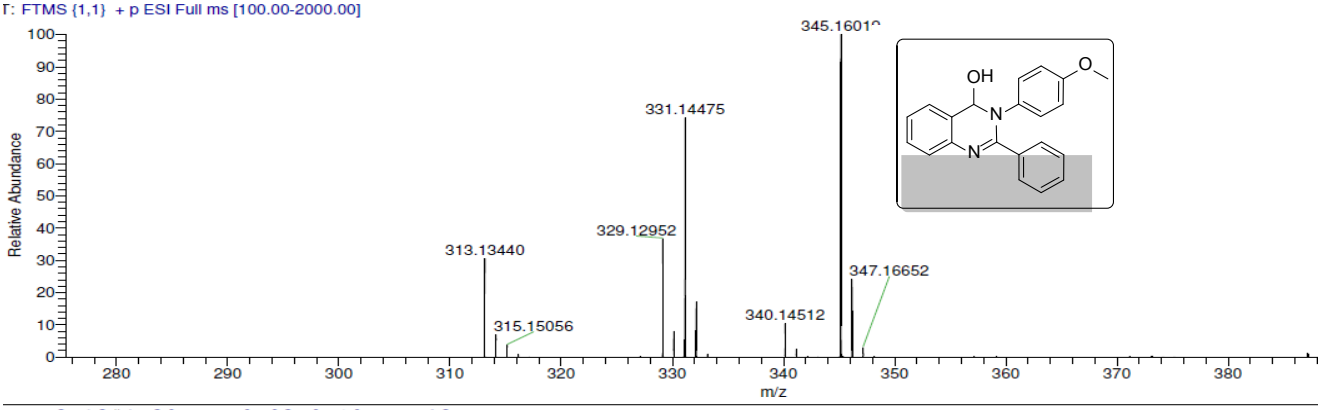


HIGH RESOLUTION MASS SPECTRA: (Table S1, 3g)

National Centre for Mass Spectrometry
CSIR-Indian Institute of Chemical Technology

File Name C:\IICT-HRMS\...\KRR-3-93
Sample Name
Sample ID G SAIDULU
Date and Time 08-09-14 23:17:10

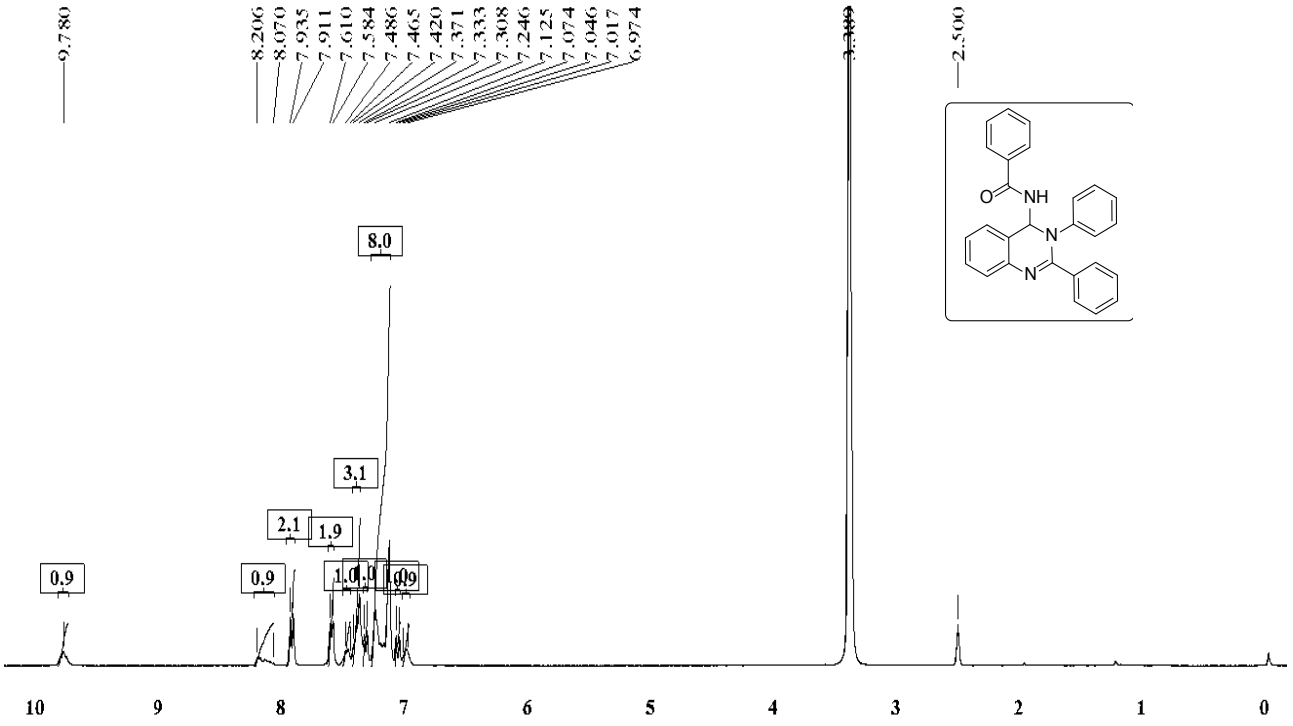
<RR-3-93 #6-89 RT: 0.02-0.30 AV: 84 SB: 326 0.80-1.90 NL: 9.72E7
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]



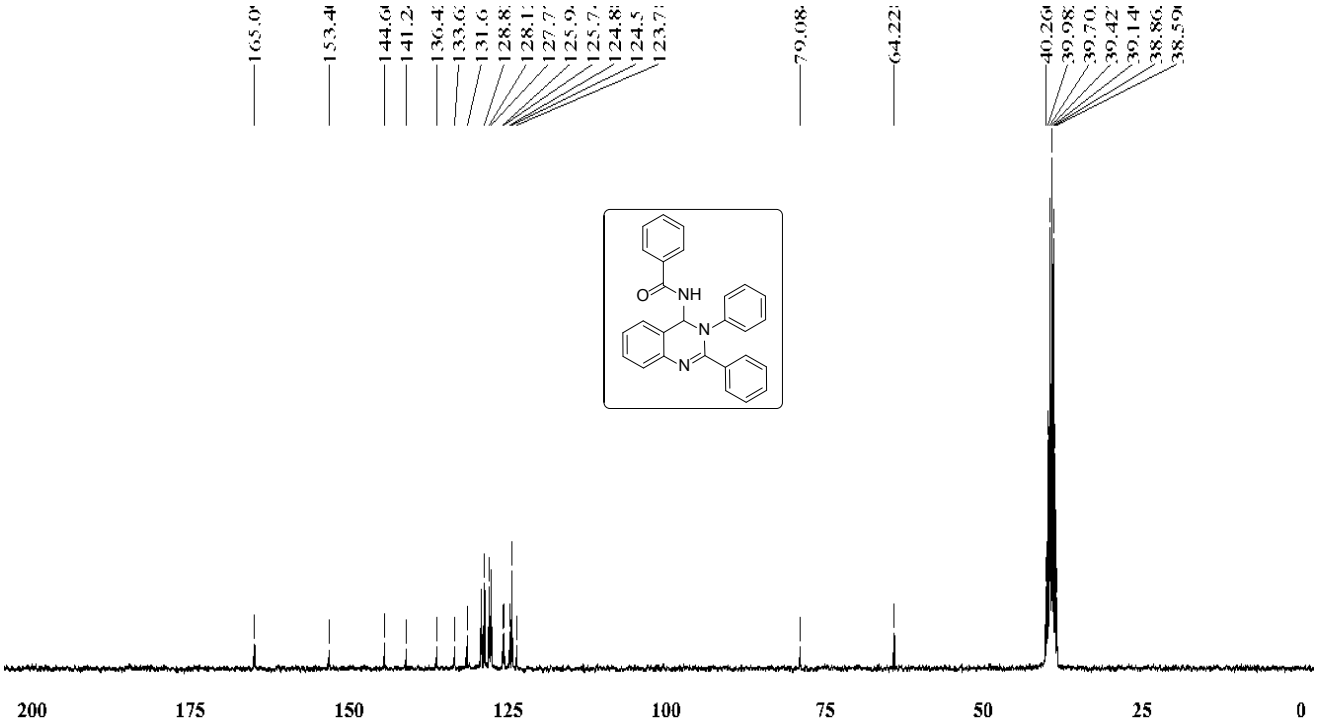
KRR-3-93#8-30 RT: 0.03-0.10 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
331.14466	93258624.0	100.00	331.14410	0.55	13.5	$C_{21}H_{19}O_2N_2$

^{1}H NMR (300 MHz, DMSO-d$_6$): (Table 2, 5a)



^{13}C NMR (75 MHz, DMSO-d$_6$): (Table 2, 5a)

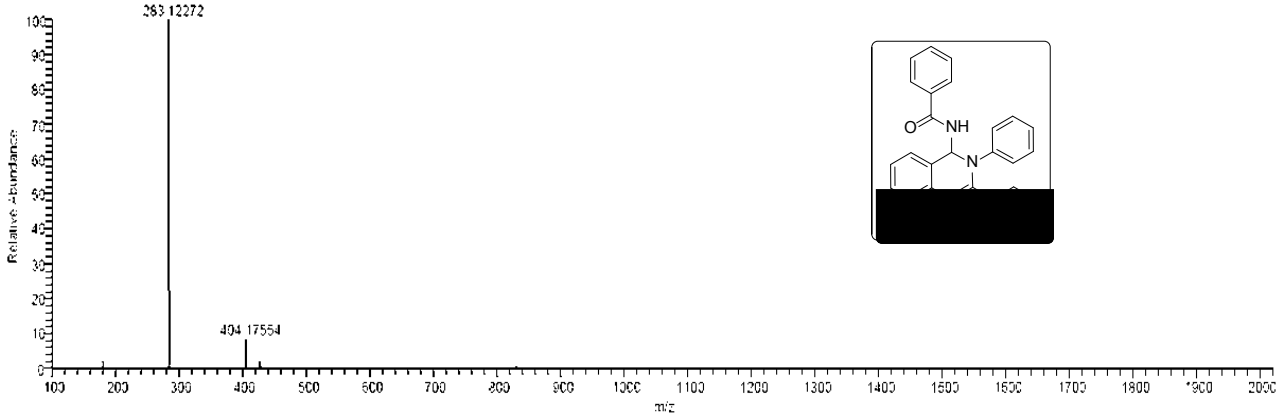


HIGH RESOLUTION MASS SPECTRA: (Table 2, 5a)

National Centre for Mass Spectrometry
CSIR-Indian Institute of Chemical Technology

File Name C:\IICT-HRMS\31.12.2013\KRR-SAI-64
Sample Name
Sample ID G-SAIDULU
Date and Time 01-01-14 01:50:59

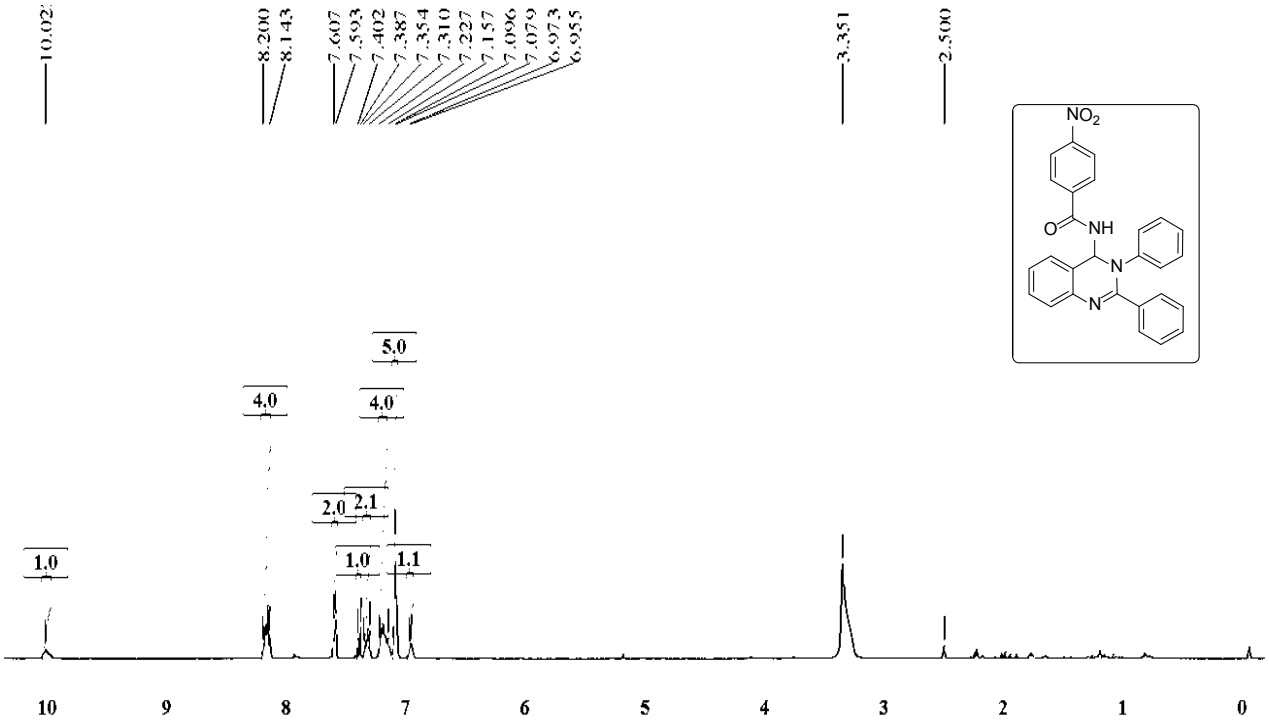
KRR-SAI-64 #1-94 RT: 0.01-0.34 AV: 94 NL: 2.24E8
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]



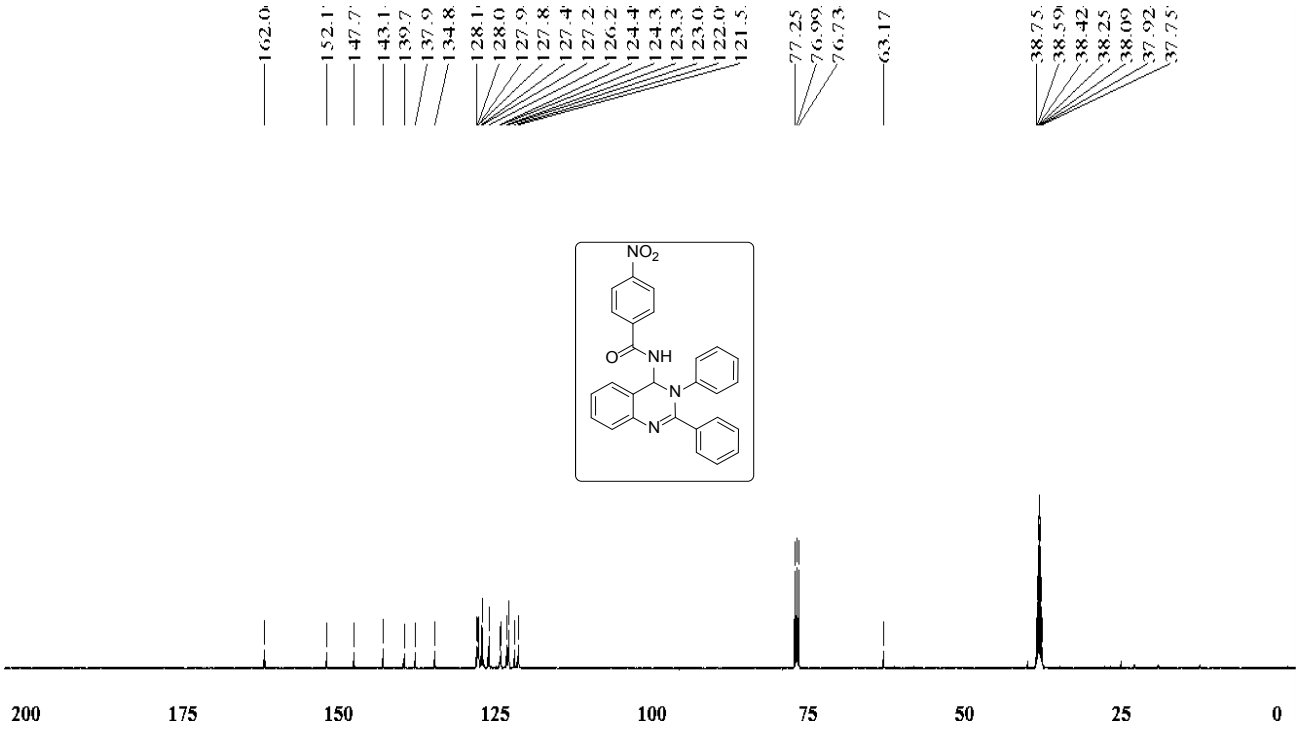
KRR-SAI-64#8-30 RT: 0.05-0.12 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]
m/z= 362.84-434.80

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
404.17551	34625132.0	100.00	404.17574	-0.56	18.5	$C_{27}H_{22}ON_3$
426.15787	12725434.0	36.75	426.15768	0.43	18.5	$C_{27}H_{21}ON_3Na$

^{1}H NMR (500 MHz, $CDCl_3$ + DMSO-d_6): (Table 2, 5b)



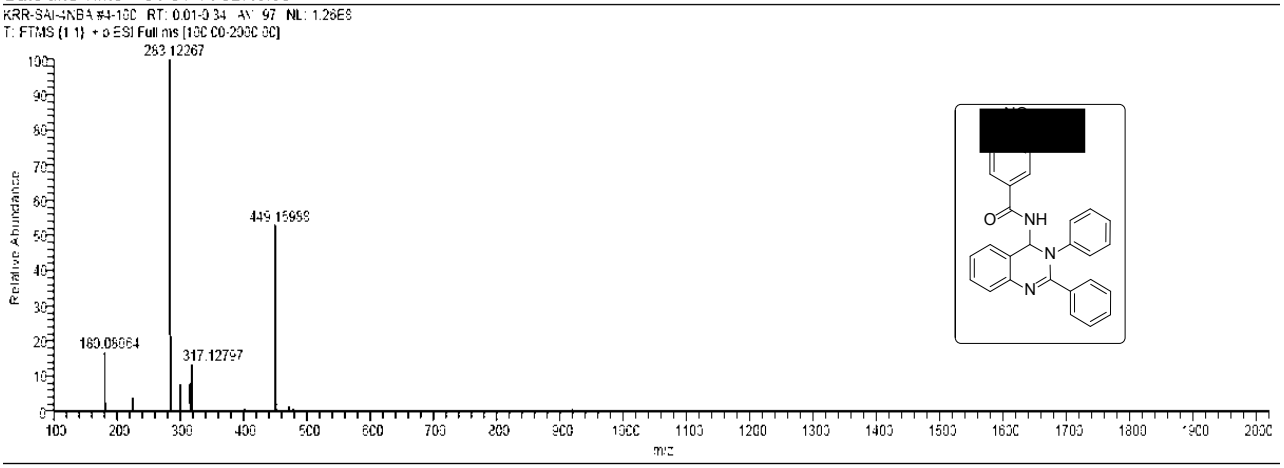
^{13}C NMR (125 MHz, $CDCl_3$ + DMSO-d_6): (Table 2, 5b)



HIGH RESOLUTION MASS SPECTRA: (Table 2, 5b)

National Centre for Mass Spectrometry
CSIR-Indian Institute of Chemical Technology

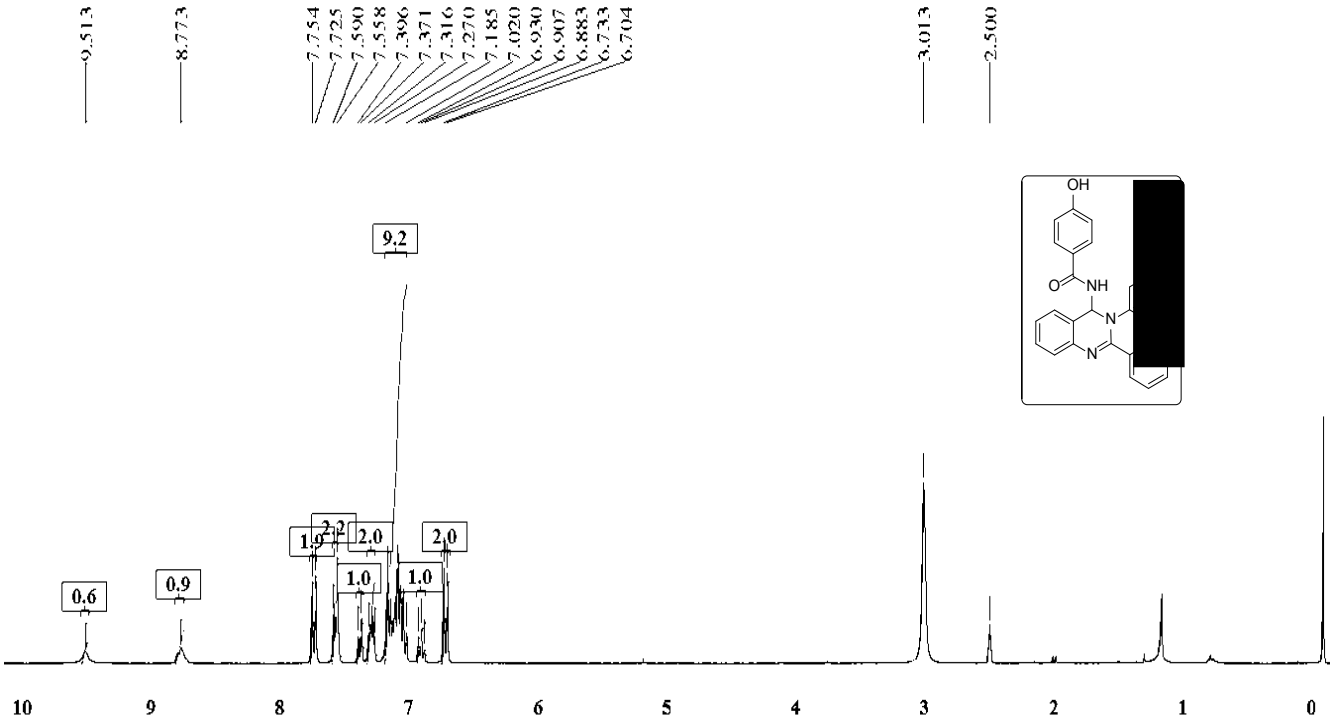
File Name C:\IICT-HRMS\31.12.2013\KRR-SAI-4NBA
Sample Name
Sample ID G-SAIDULU
Date and Time 01-01-14 02:43:30



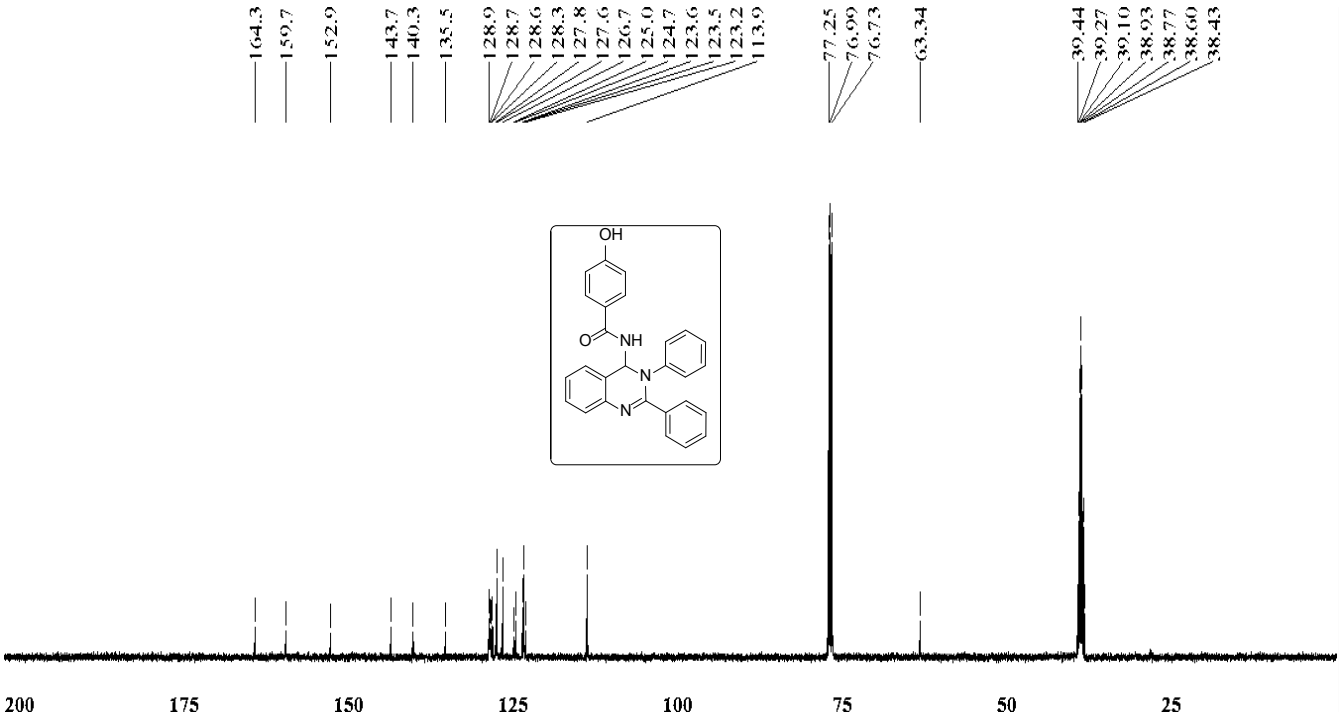
KRR-SAI-4NBA#8-30 RT: 0.03-0.10 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]
m/z= 417.12-476.46

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
449.15990	62629820.0	100.00	449.16082	-2.04	19.5	$C_{27}H_{21}O_3N_4$
450.16379	17995474.0	28.73				

^{1}H NMR (300 MHz, $CDCl_3$ + DMSO-d_6): (Table 2, 5c)



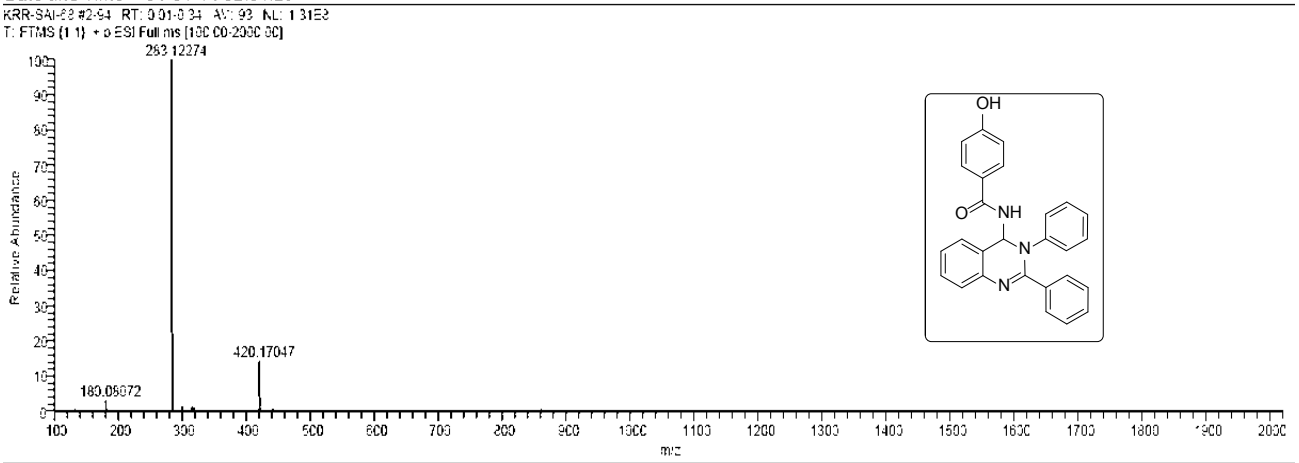
^{13}C NMR (125 MHz, $CDCl_3$ + DMSO-d_6): (Table 2, 5c)



HIGH RESOLUTION MASS SPECTRA: (Table 2, 5c)

National Centre for Mass Spectrometry
CSIR-Indian Institute of Chemical Technology

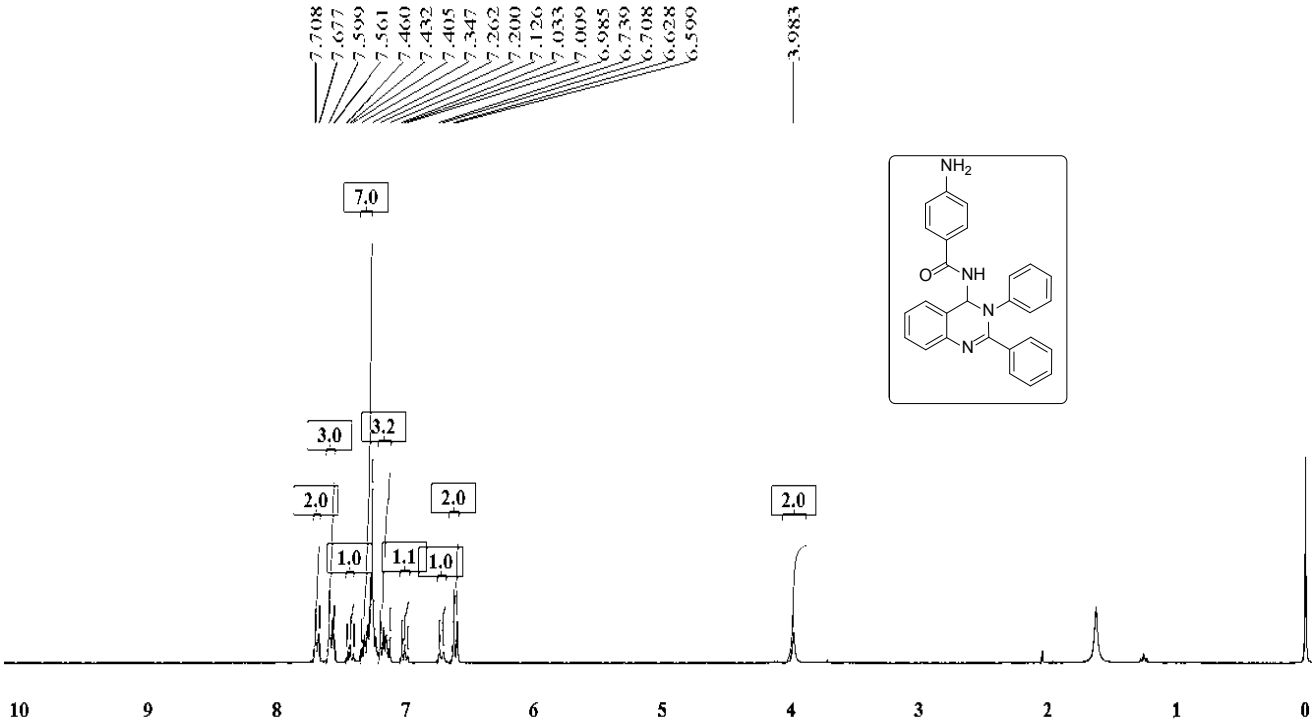
File Name C:\IICT-HRMS\31.12.2013 KRR-SAI-68
Sample Name
Sample ID G-SAIDULU
Date and Time 01-01-14 02:01:29



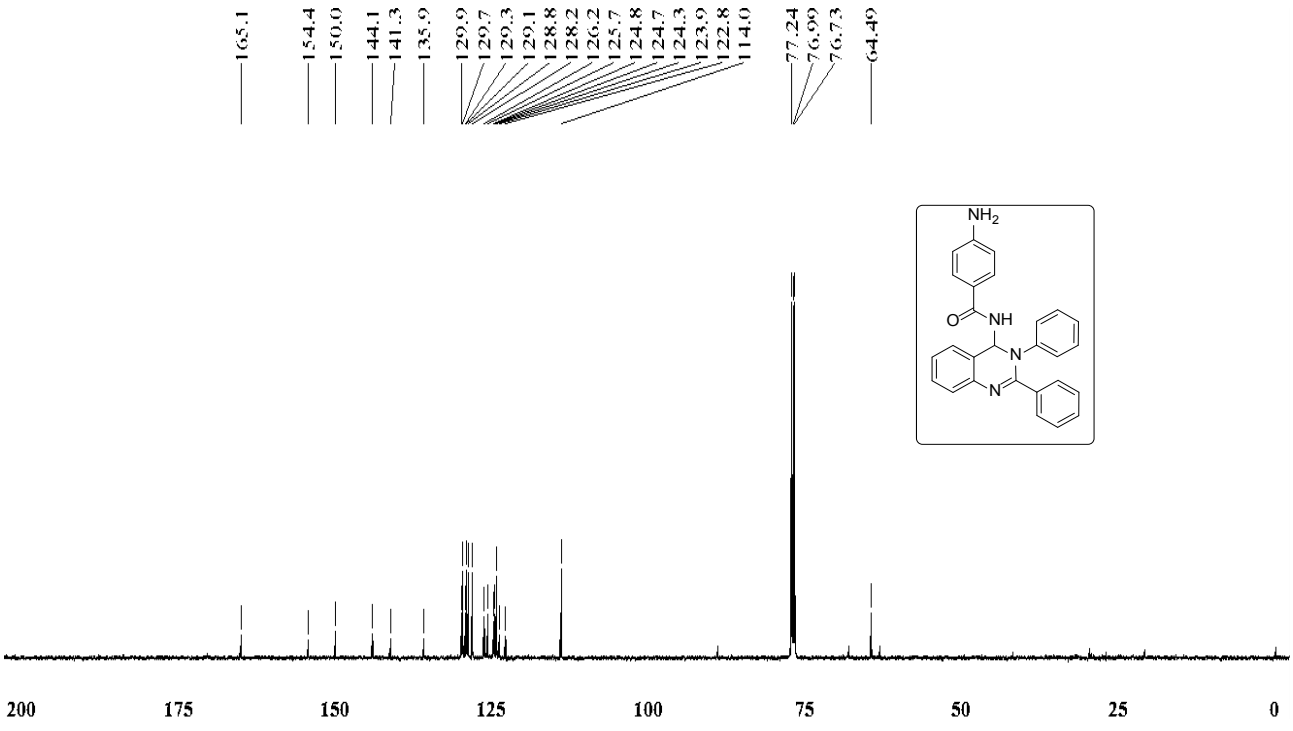
KRR-SAI-68#8-30 RT: 0.05-0.12 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]
m/z= 400.71-447.42

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
420.17042	41431880.0	100.00	420.17065	-0.56	18.5	$C_{27}H_{22}O_2N_3$
421.17397	11544743.0	27.86				

^{1}H NMR (300 MHz, $CDCl_3$): (Table 2, 5d)



^{13}C NMR (125 MHz, $CDCl_3$): (Table 2, 5d)

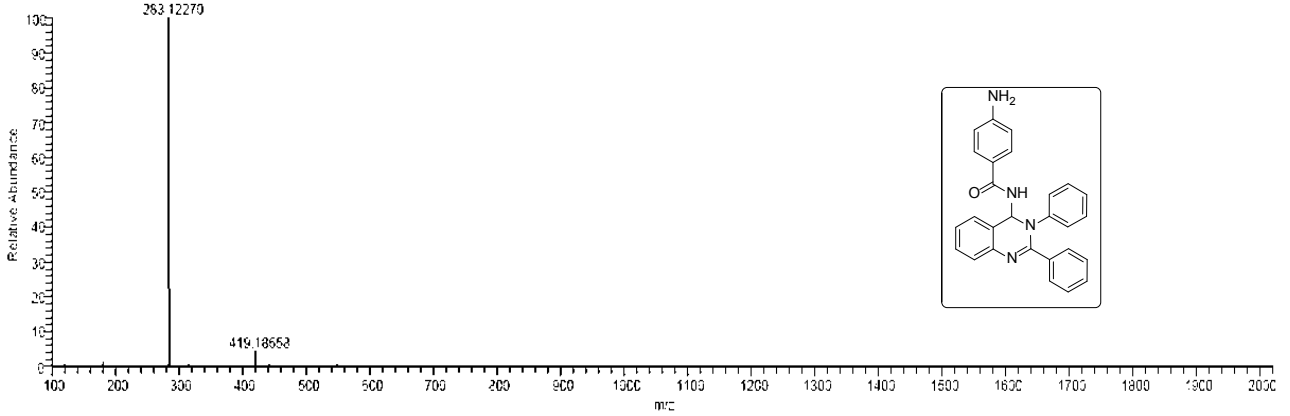


HIGH RESOLUTION MASS SPECTRA: (Table 2, 5d)

National Centre for Mass Spectrometry
CSIR-Indian Institute of Chemical Technology

File Name C:\IICT-HRMS\31 12 2013 KRR-SAI-69
Sample Name
Sample ID G-SAIDULU
Date and Time 01-01-14 02:04:09

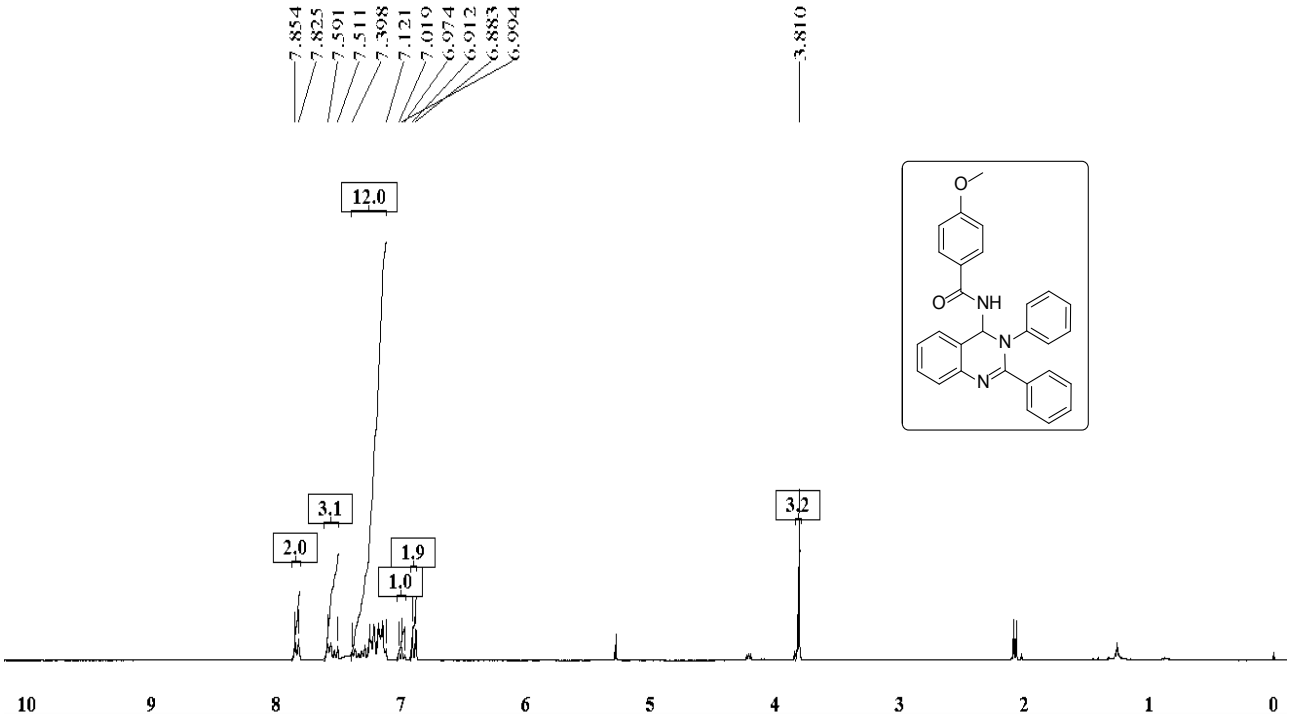
KRR-SAI-69#1-93 RT: 0.01-0.34 AV: 93 NL: 2.58E8
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]



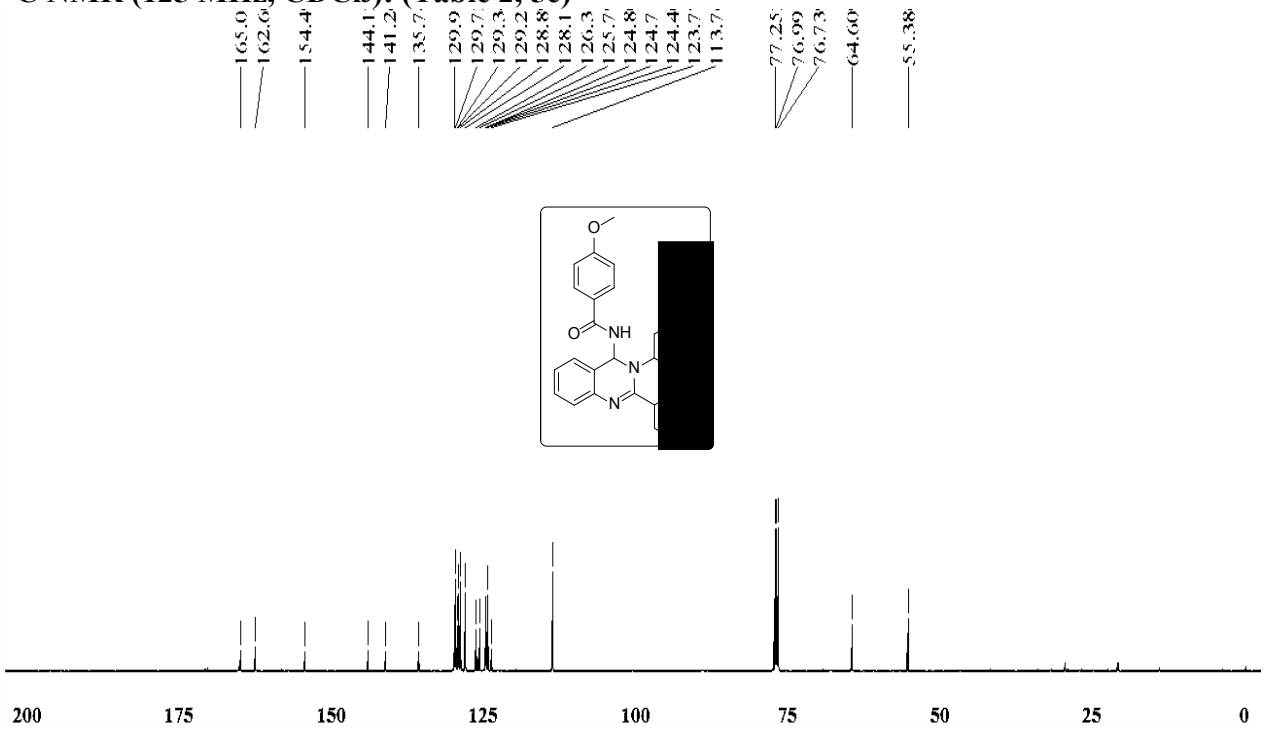
KRR-SAI-69#8-30 RT: 0.05-0.12 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]
m/z= 377.99-467.62

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
419.18677	18091240.0	100.00	419.18664	0.32	18.5	$C_{27}H_{23}ON_4$
420.19018	5141609.5	28.42				

^{1}H NMR (300 MHz, $CDCl_3$): (Table 2, 5e)



^{13}C NMR (125 MHz, $CDCl_3$): (Table 2, 5e)

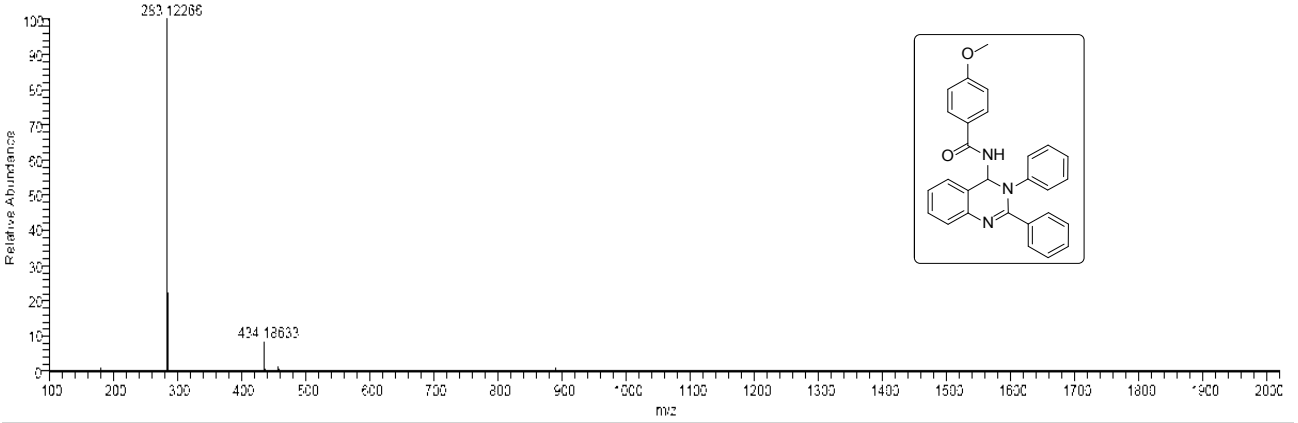


HIGH RESOLUTION MASS SPECTRA: (Table 2, 5e)

National Centre for Mass Spectrometry
CSIR-Indian Institute of Chemical Technology

File Name C:\IICT-HRMS\31.12.2013\KRR-SAI-66
Sample Name
Sample ID G-SAIDULU
Date and Time 01-01-14 01:56:21

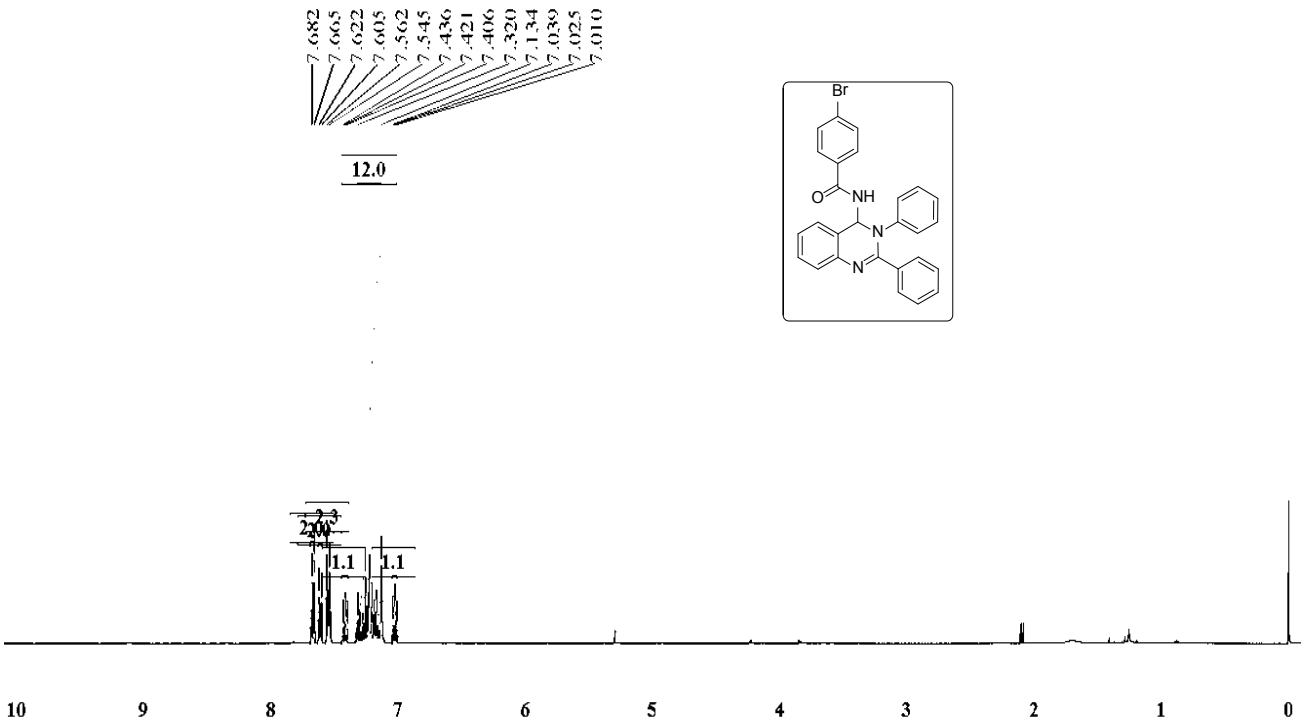
(KRR-SAI-66 #2-56 RT: 0.01-0.34 AV: 55 NL: 1.95E8
F: FTMS {1,1} + p ESI Full ms [100.00-2000.00]



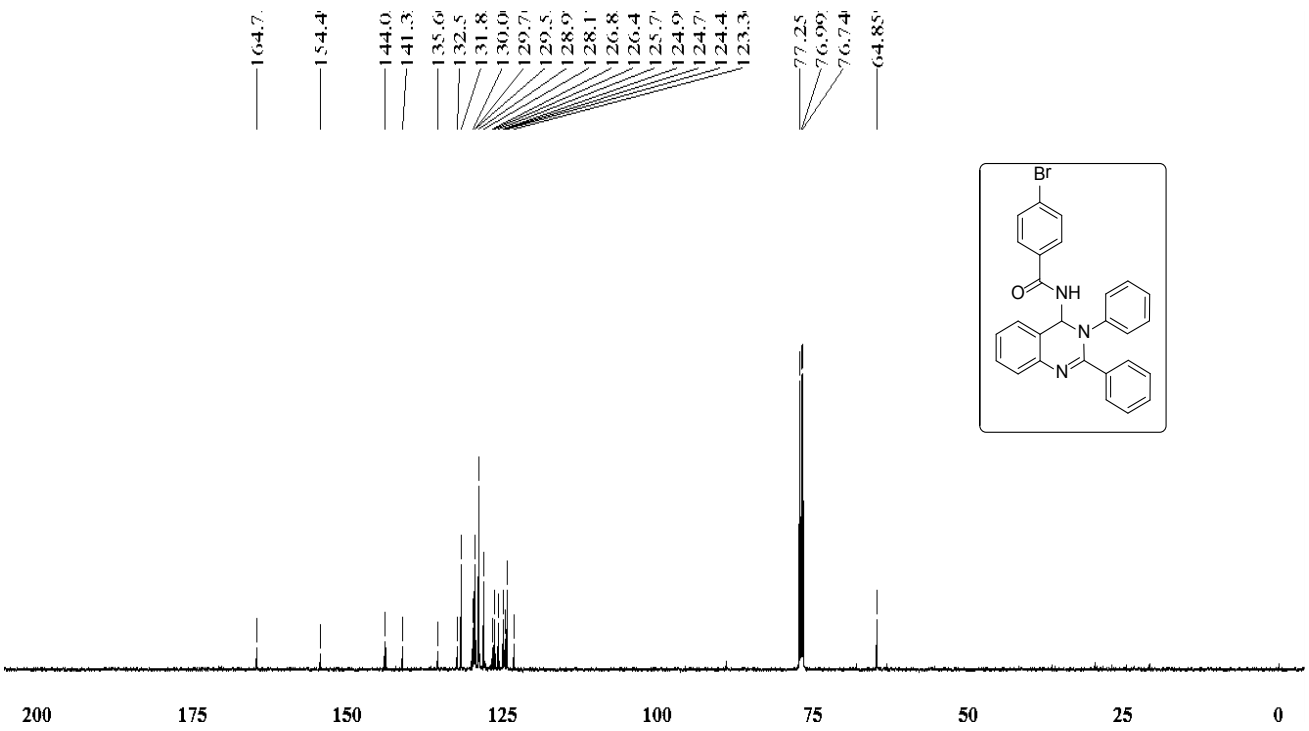
KRR-SAI-66#8-30 RT: 0.04-0.11 AV: 23
F: FTMS {1,1} + p ESI Full ms [100.00-2000.00]
m/z= 412.08-453.73

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
434.18623	33117368.0	100.00	434.18630	-0.17	18.5	$C_{28}H_{24}O_2N_3$
435.18966	9972754.0	30.11	435.19172	-4.74	15.0	$C_{26}H_{26}O_2N_3Na$

^{1}H NMR (500 MHz, $CDCl_3$): (Table 2, 5f)



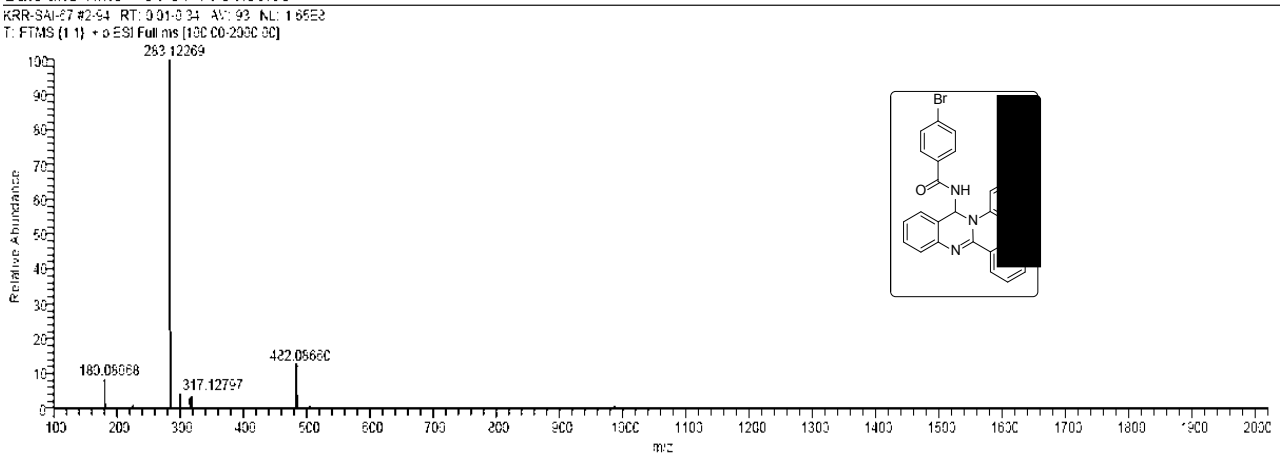
^{13}C NMR (125 MHz, $CDCl_3$): (Table 2, 5f)



HIGH RESOLUTION MASS SPECTRA: (Table 2, 5f)

National Centre for Mass Spectrometry
CSIR-Indian Institute of Chemical Technology

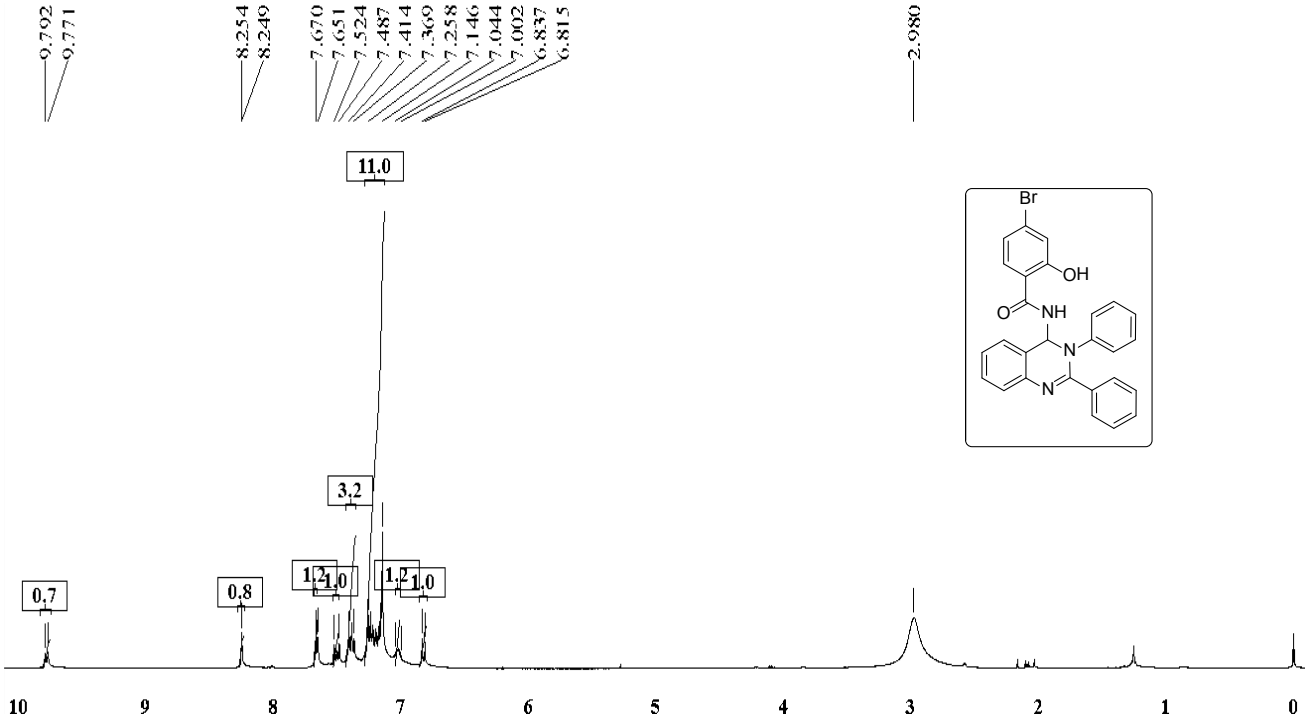
File Name C:\IICT-HRMS\31.12.2013\KRR-SAI-67
Sample Name
Sample ID G-SAIDULU
Date and Time 01-01-14 01:58:53



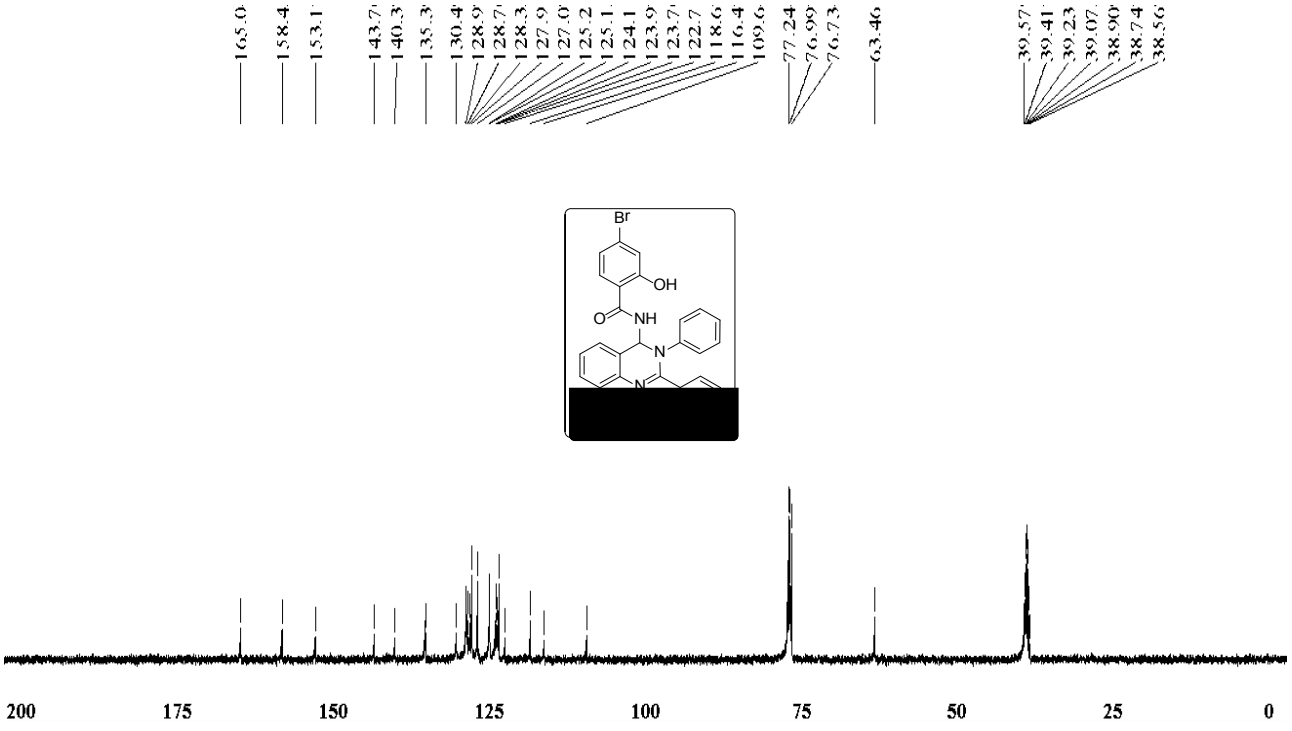
KRR-SAI-67#8-30 RT: 0.05-0.12 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]
m/z= 452.47-518.11

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
482.08659	36968744.0	100.00	482.08625	0.71	18.5	$C_{27}H_{21}ON_3Br$
			482.08519	2.92	15.0	$C_{27}H_{24}O_2BrNa$

^{1}H NMR (400 MHz, $CDCl_3$ + DMSO-d_6): (Table 2, 5g)

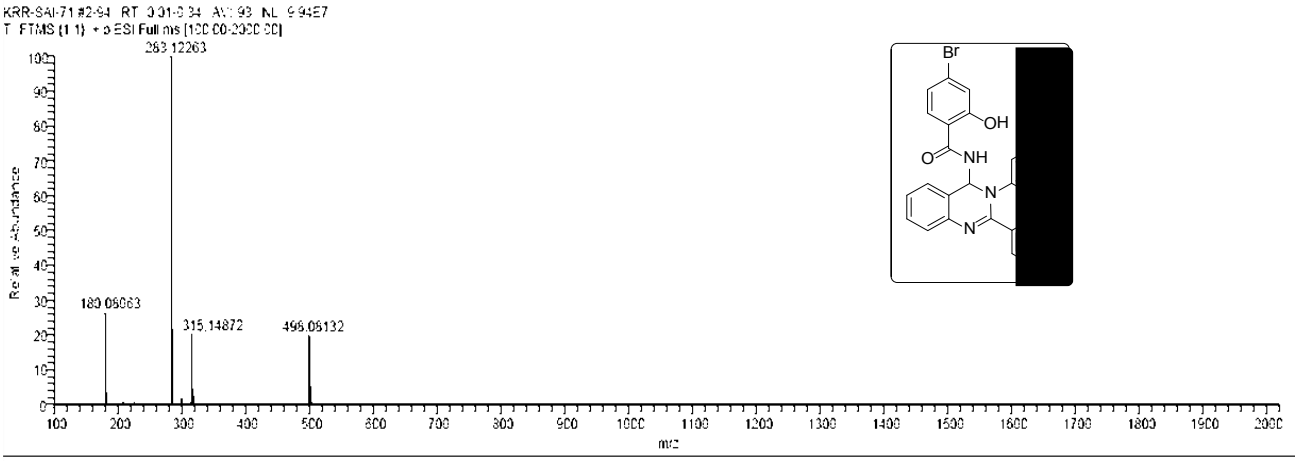


^{13}C NMR (125 MHz, $CDCl_3$ + DMSO-d_6): (Table 2, 5g)



HIGH RESOLUTION MASS SPECTRA: (Table 2, 5g)

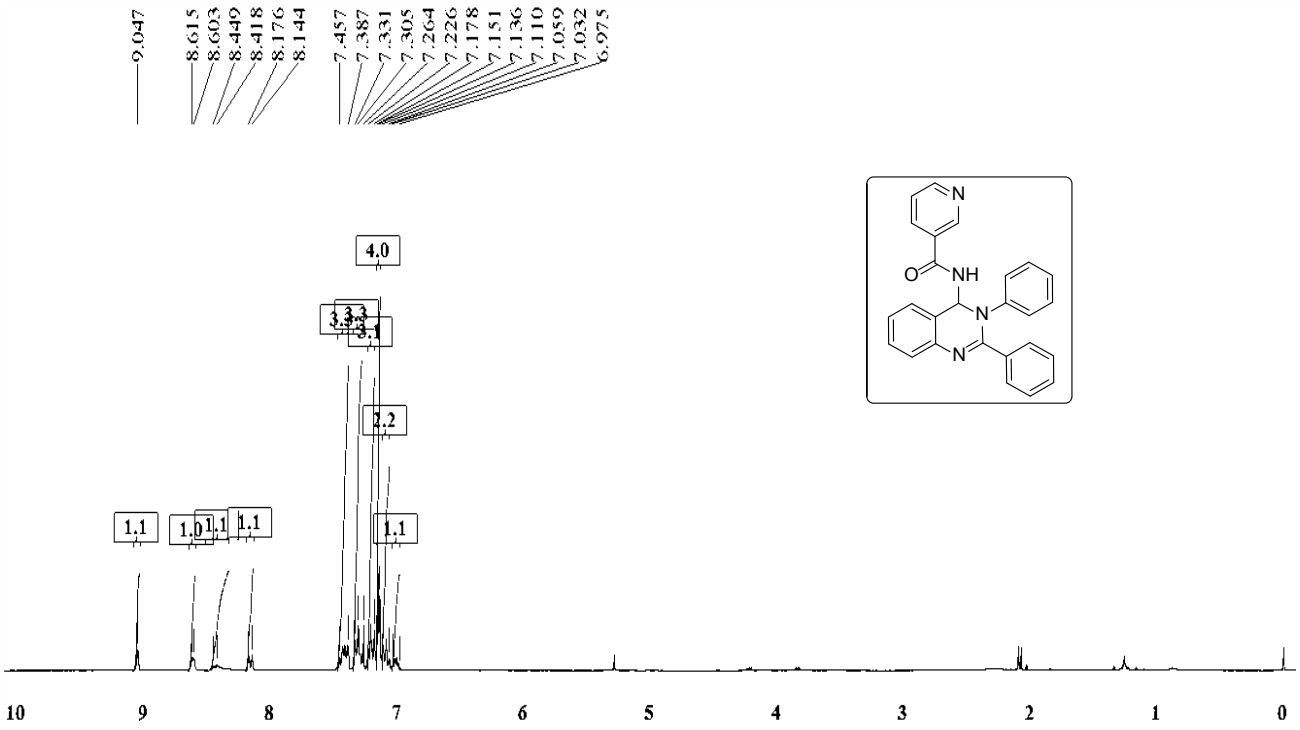
National Centre for Mass Spectrometry



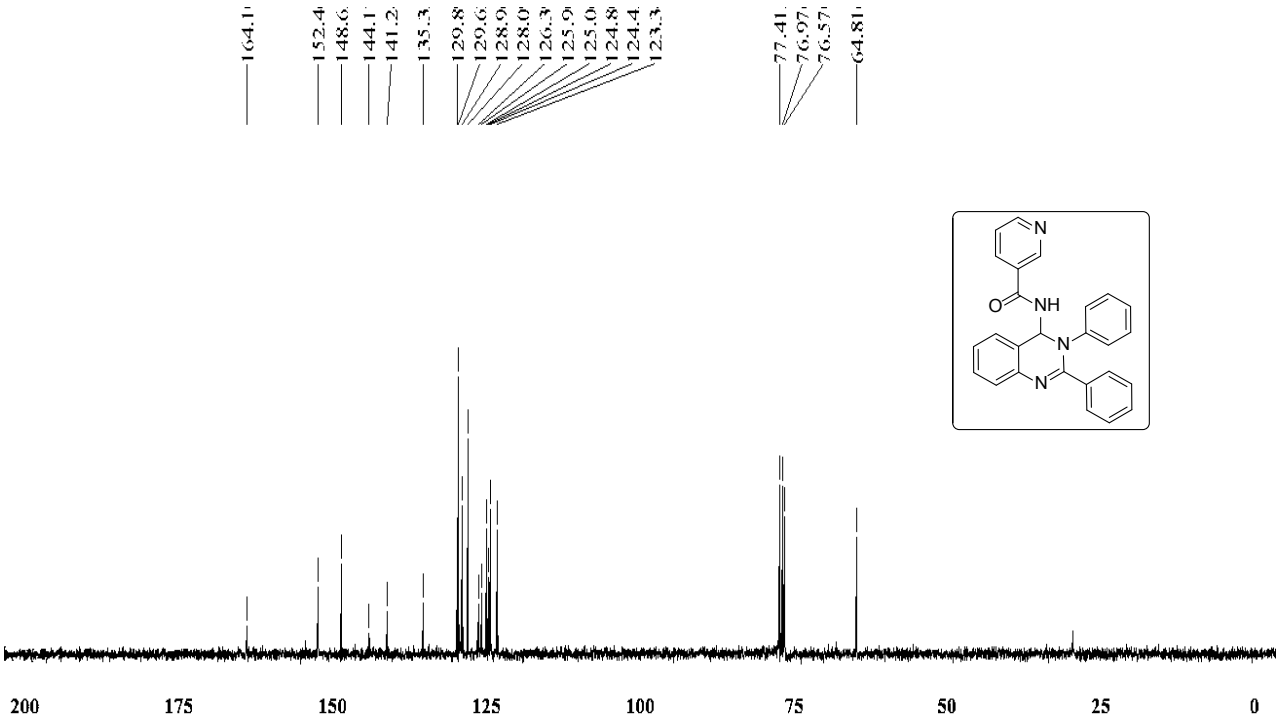
KRR-SAI-71#8-30 RT: 0.05-0.12 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]
m/z= 472.67-514.33

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
498.08135	36953036.0	100.00	498.08117	0.37	18.5	$C_{27}H_{21}O_2N_3Br$
500.07938	36720308.0	99.37				

^{1}H NMR (300 MHz, $CDCl_3$): (Table 2, 5h)



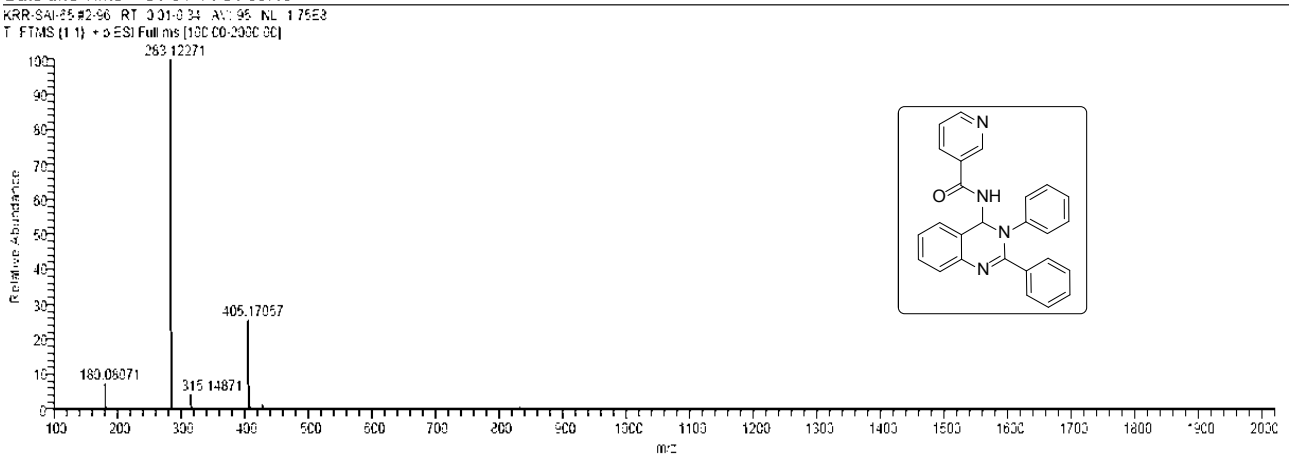
^{13}C NMR (75 MHz, $CDCl_3$): (Table 2, 5h)



HIGH RESOLUTION MASS SPECTRA: (Table 2, 5h)

National Centre for Mass Spectrometry
CSIR-Indian Institute of Chemical Technology

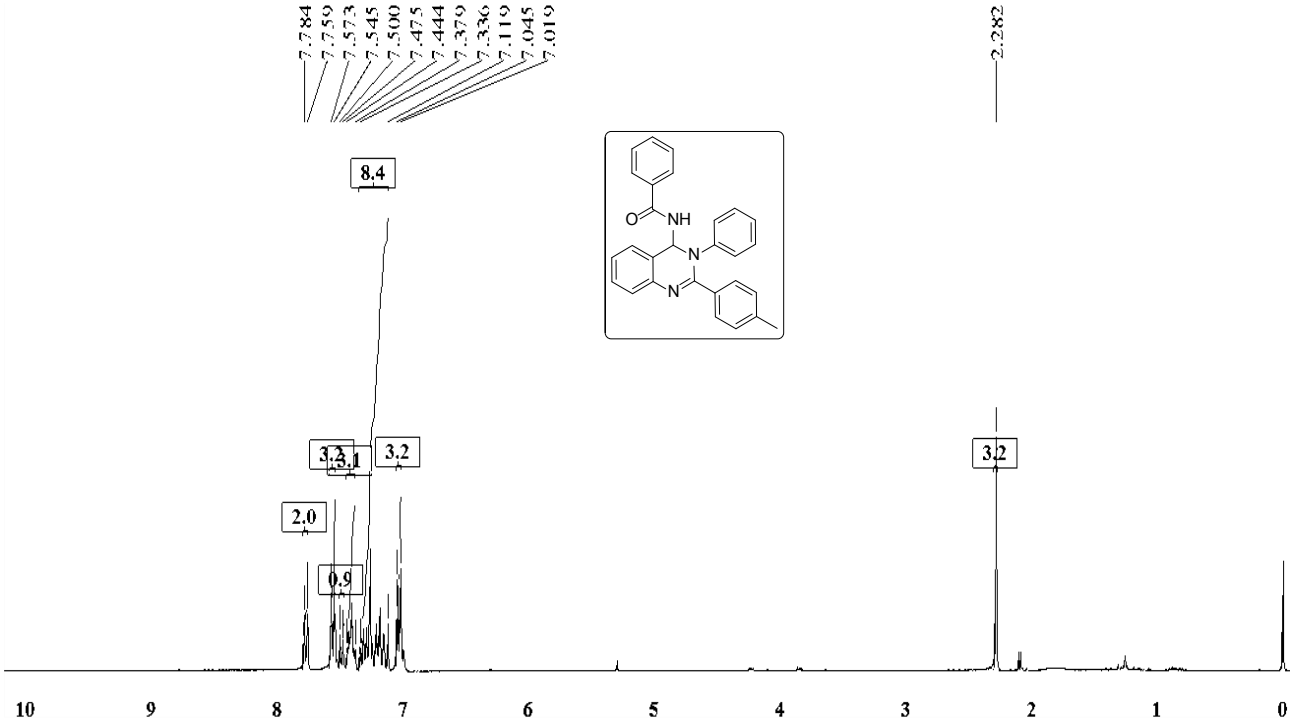
File Name C:\IICT-HRMS\31.12.2013\KRR-SAI-65
Sample Name
Sample ID G-SAIDULU
Date and Time 01-01-14 01:53:40



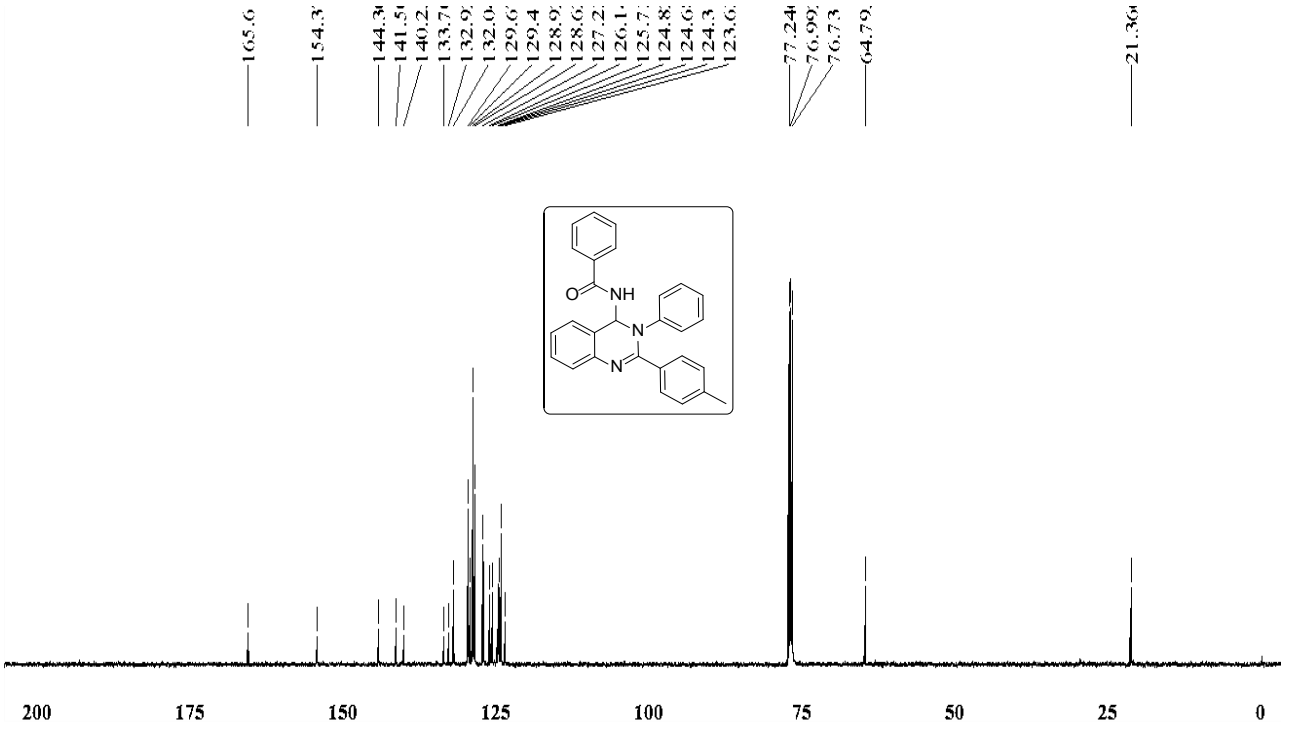
KRR-SAI-65#8-30 RT: 0.04-0.12 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]
m/z= 374.20-429.75

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
405.17055	65943060.0	100.00	405.17099	-1.08	18.5	$C_{26}H_{21}ON_4$
406.17381	17320384.0	26.27				

^{1}H NMR (300 MHz, $CDCl_3$): (Table 2, 5i)

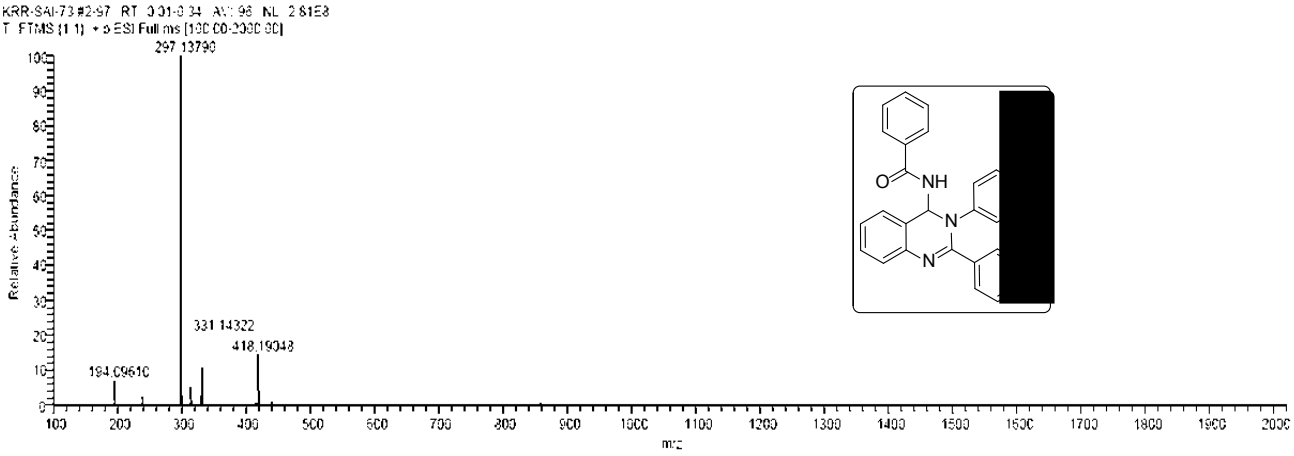


^{13}C NMR (125 MHz, $CDCl_3$): (Table 2, 5i)



HIGH RESOLUTION MASS SPECTRA: (Table 2, 5i)

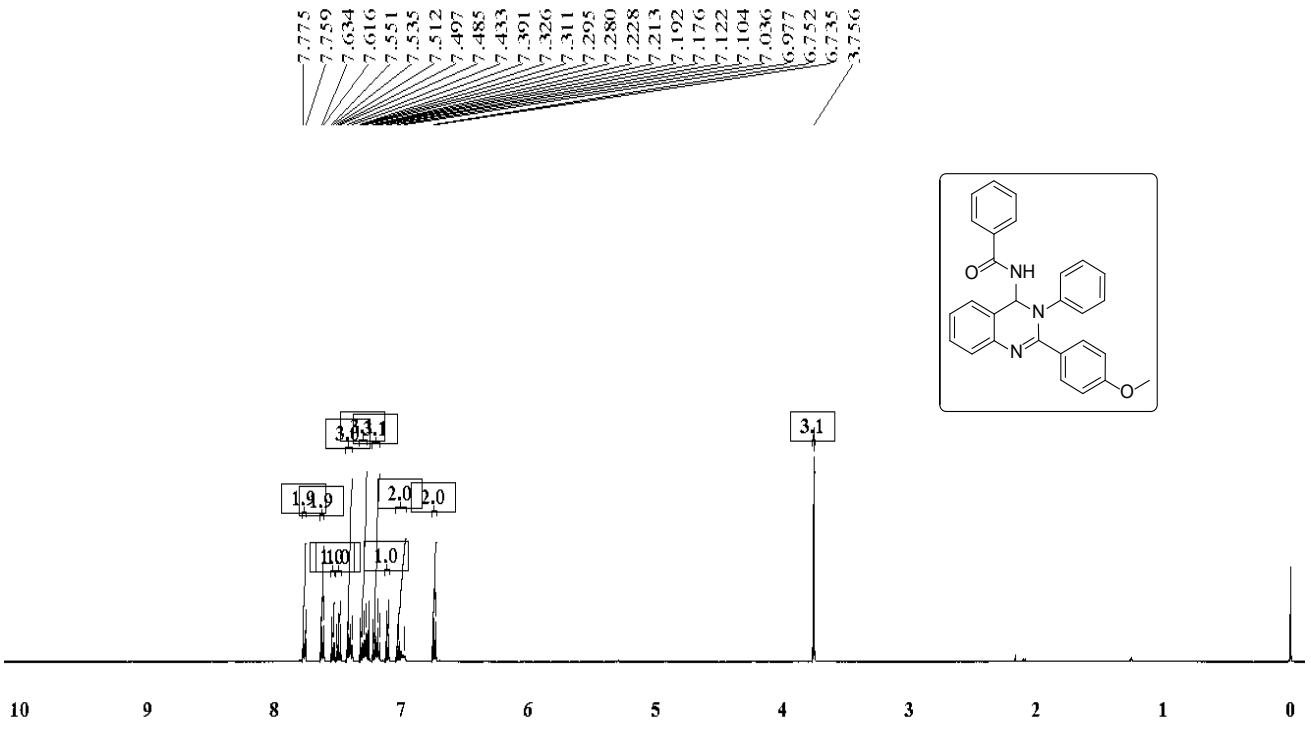
National Centre for Mass Spectrometry



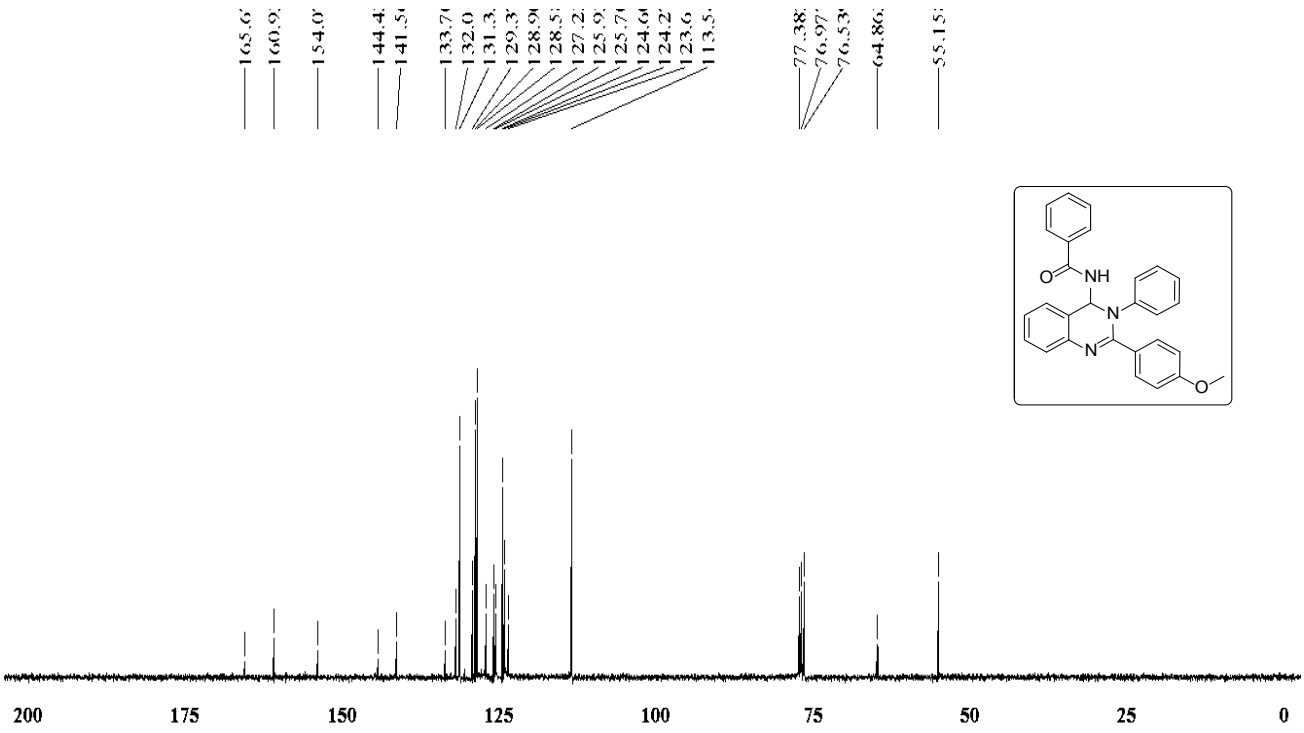
KRR-SAI-73#8-30 RT: 0.04-0.11 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]
m/z= 381.78-444.90

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
418.19039	47566736.0	100.00	418.19033	0.16	15.0	$C_{28}H_{27}O_2Na$
			418.19139	-2.38	18.5	$C_{28}H_{24}ON_3$

^{1}H NMR (500 MHz, $CDCl_3$): (Table 2, 5j)

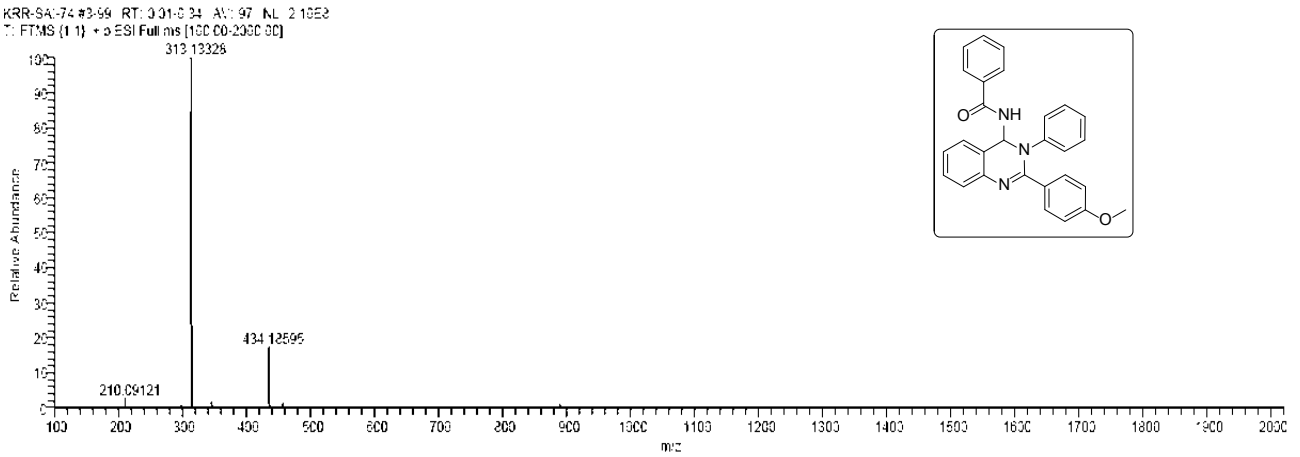


^{13}C NMR (75 MHz, $CDCl_3$): (Table 2, 5j)



HIGH RESOLUTION MASS SPECTRA: (Table 2, 5j)

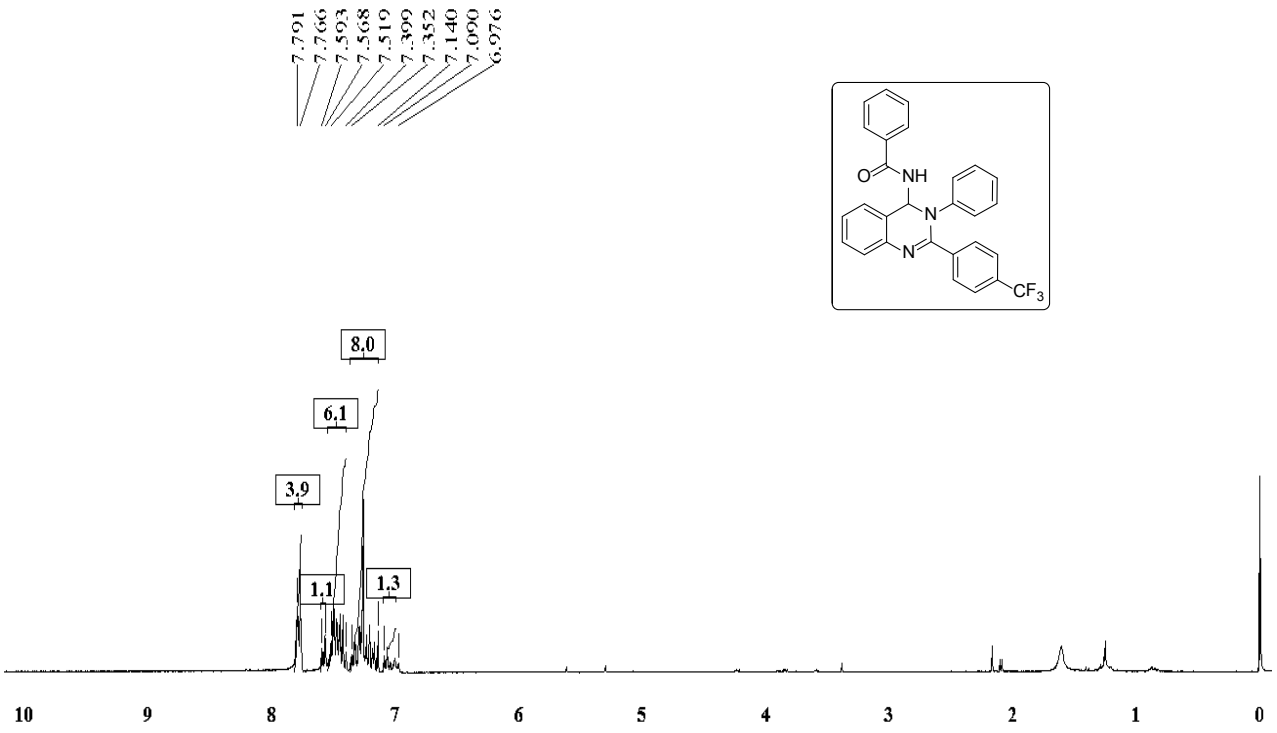
National Centre for Mass Spectrometry



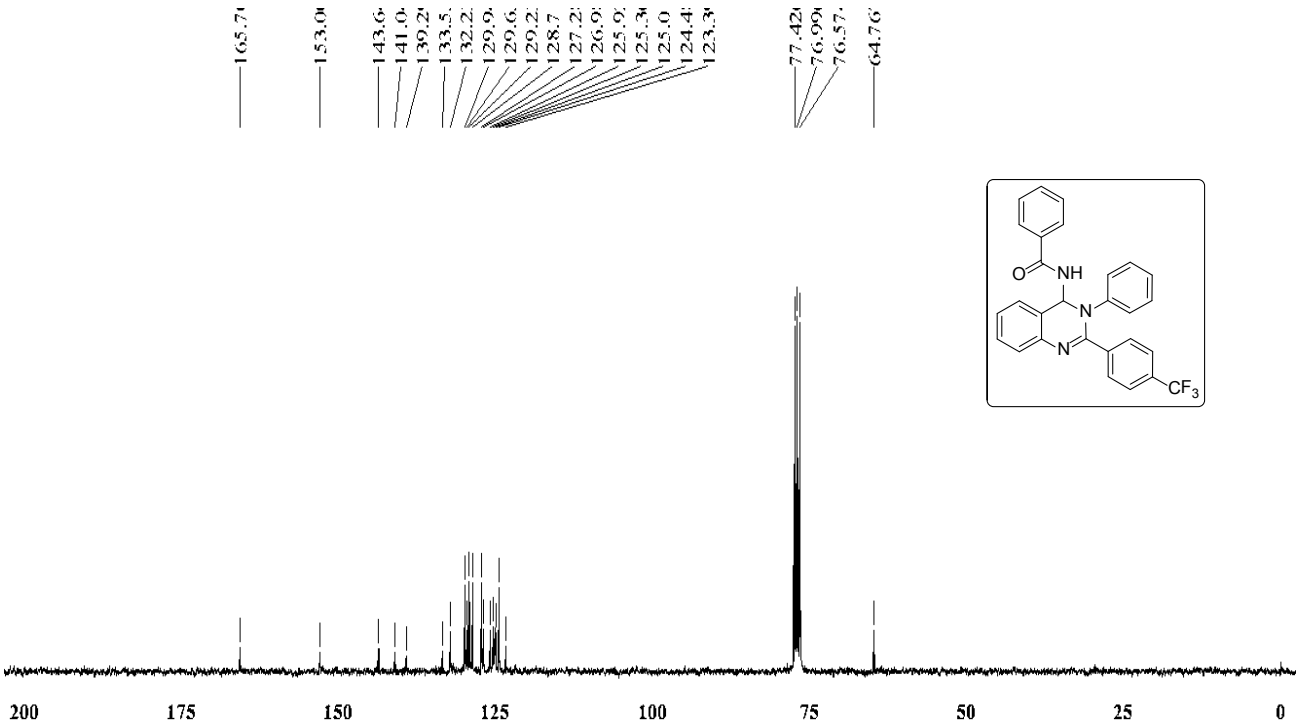
KRR-SAI-74#8-30 RT: 0.03-0.11 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]
m/z= 400.71-478.98

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
434.18580	55150060.0	100.00	434.18630	-1.16	18.5	$C_{28}H_{24}O_2N_3$
435.18950	16283793.0	29.53				

^{1}H NMR (300 MHz, $CDCl_3$): (Table 2, 5k)

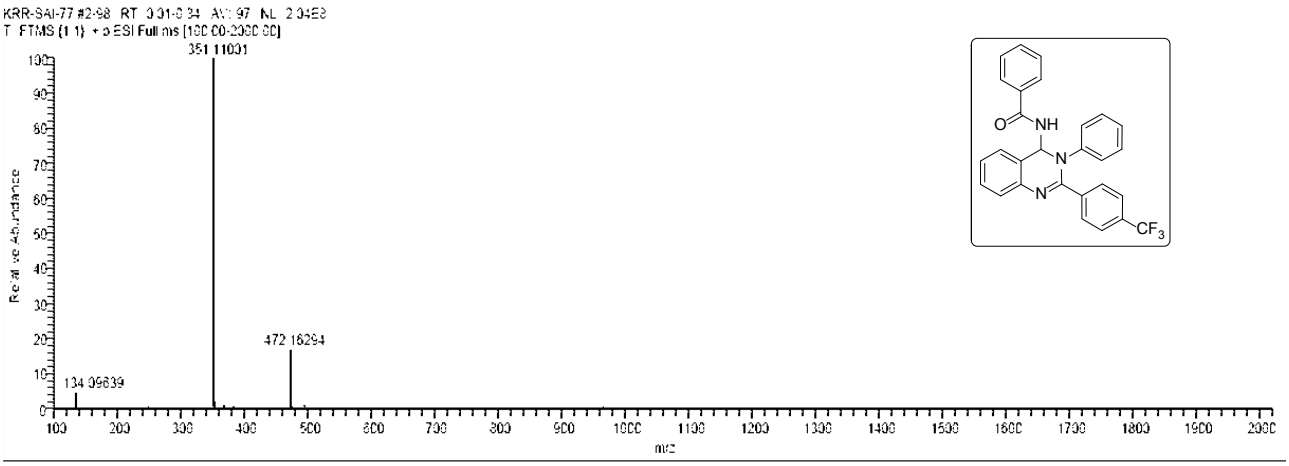


^{13}C NMR (75 MHz, $CDCl_3$): (Table 2, 5k)



HIGH RESOLUTION MASS SPECTRA: (Table 2, 5k)

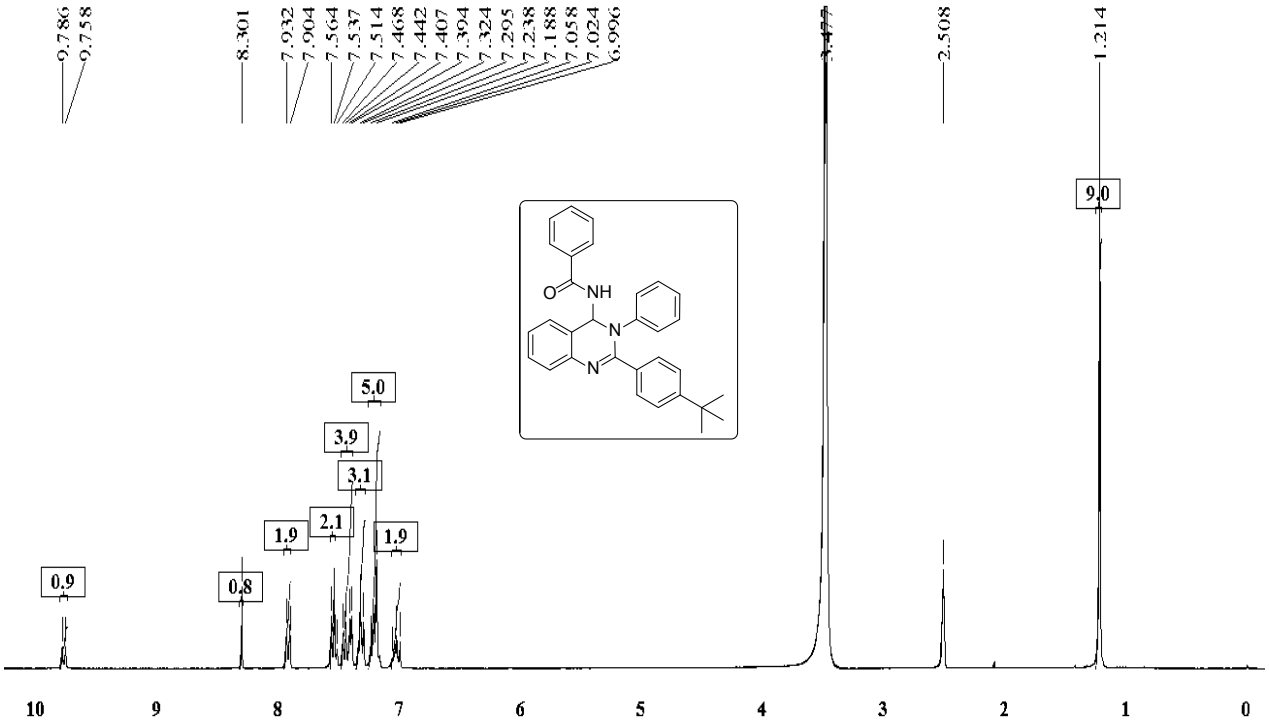
National Centre for Mass Spectrometry



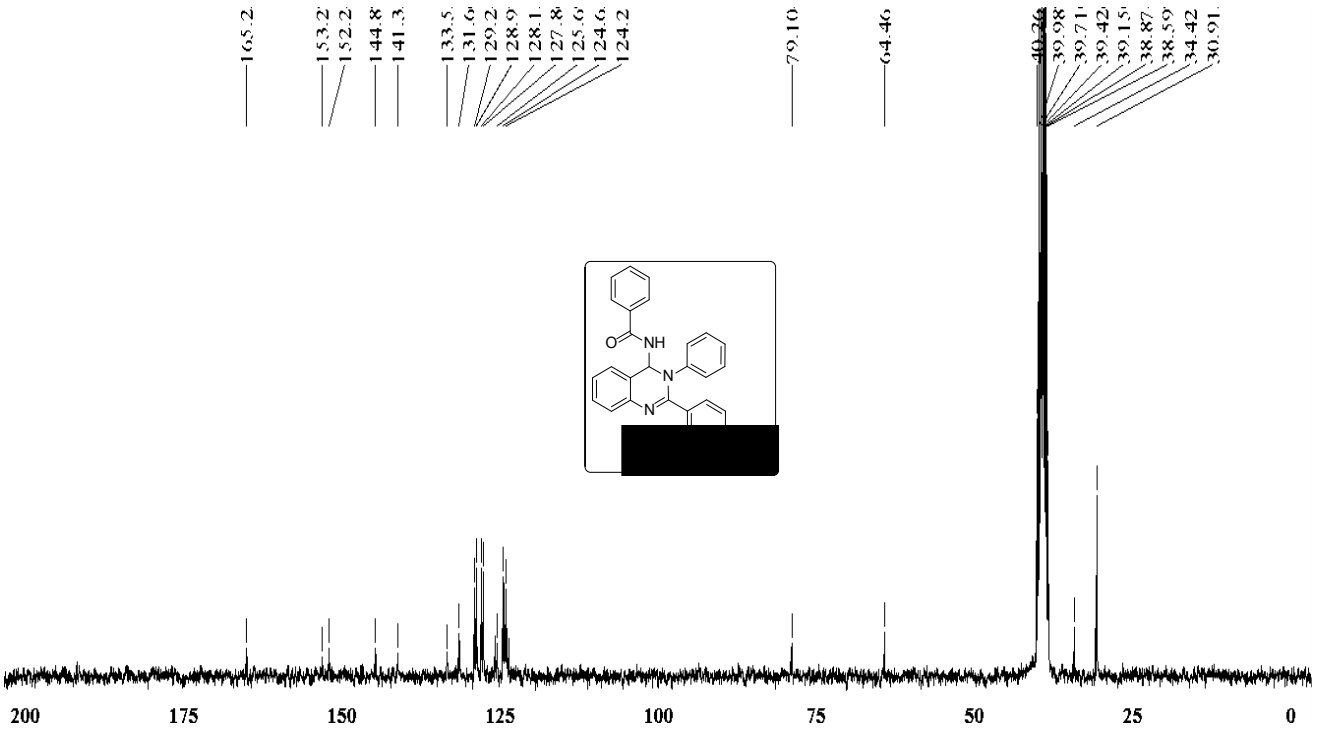
KRR-SAI-77#8-30 RT: 0.03-0.11 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]
m/z= 444.90-489.08

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
472.16281	49721168.0	100.00	472.16312	-0.67	18.5	$C_{28}H_{21}ON_3F_3$
473.16601	15238817.0	30.65				

^{1}H NMR (500 MHz, DMSO-d_6): (Table 2, 5l)

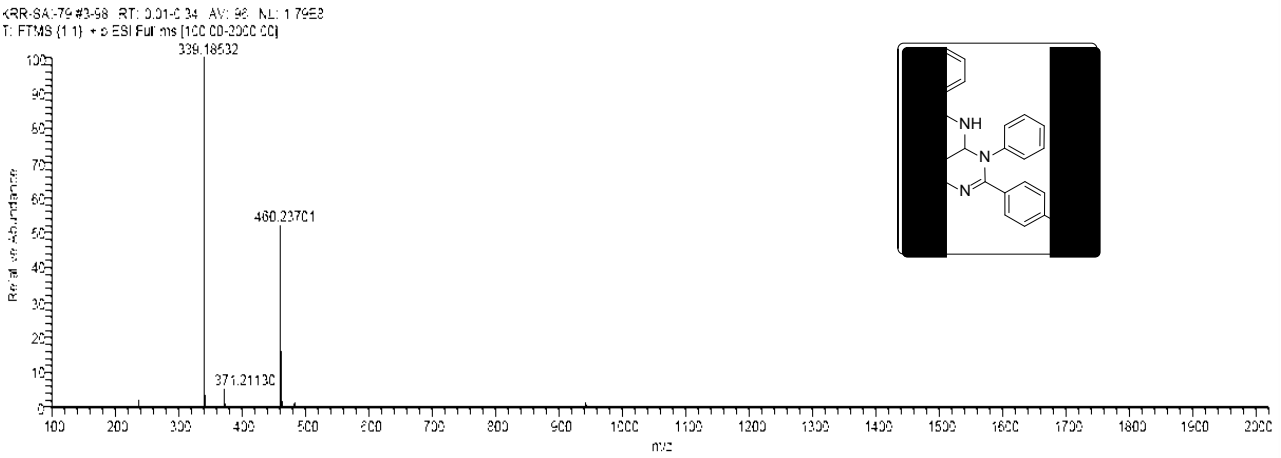


^{13}C NMR (75 MHz, DMSO-d_6): (Table 2, 5l)



HIGH RESOLUTION MASS SPECTRA: (Table 2, 5l)

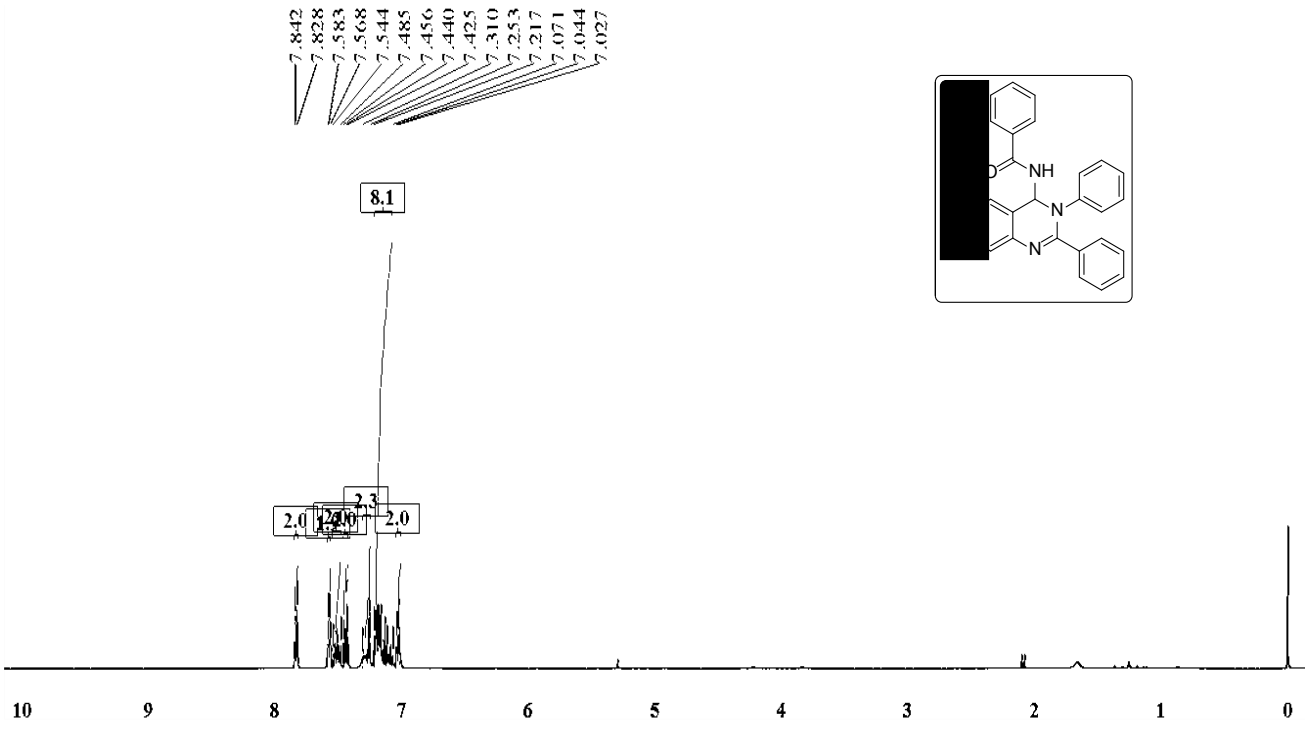
National Centre for Mass Spectrometry



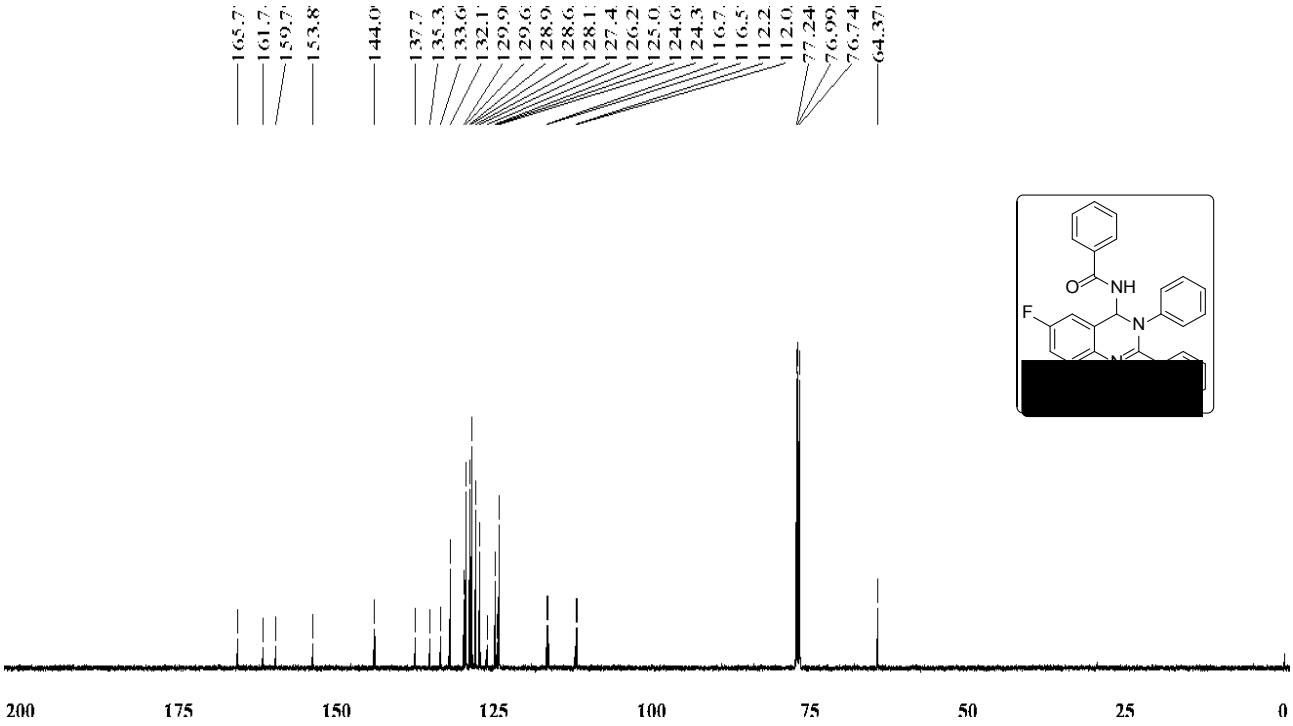
KRR-SAI-79#8-30 RT: 0.03-0.11 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]
m/z= 437.32-477.72

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
460.23700	146705488.0	100.00	460.23834	-2.90	18.5	$C_{31}H_{30}ON_3$
461.24119	46438476.0	31.65				

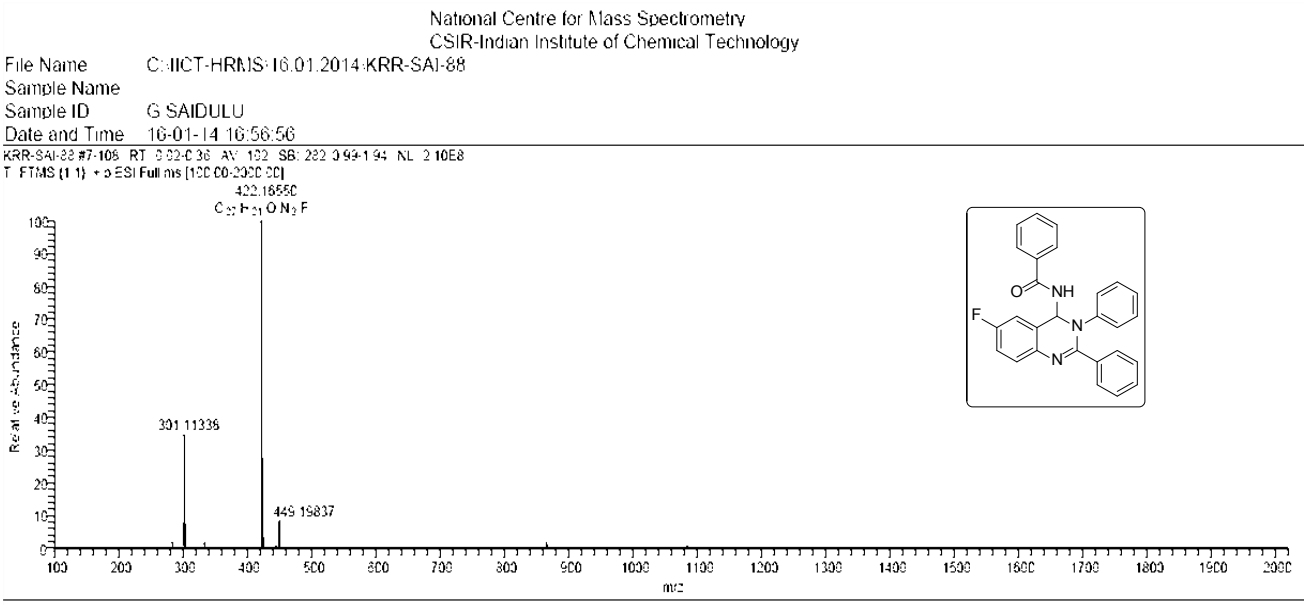
^{1}H NMR (500 MHz, $CDCl_3$): (Table 2, 5m)



^{13}C NMR (125 MHz, $CDCl_3$): (Table 2, 5m)



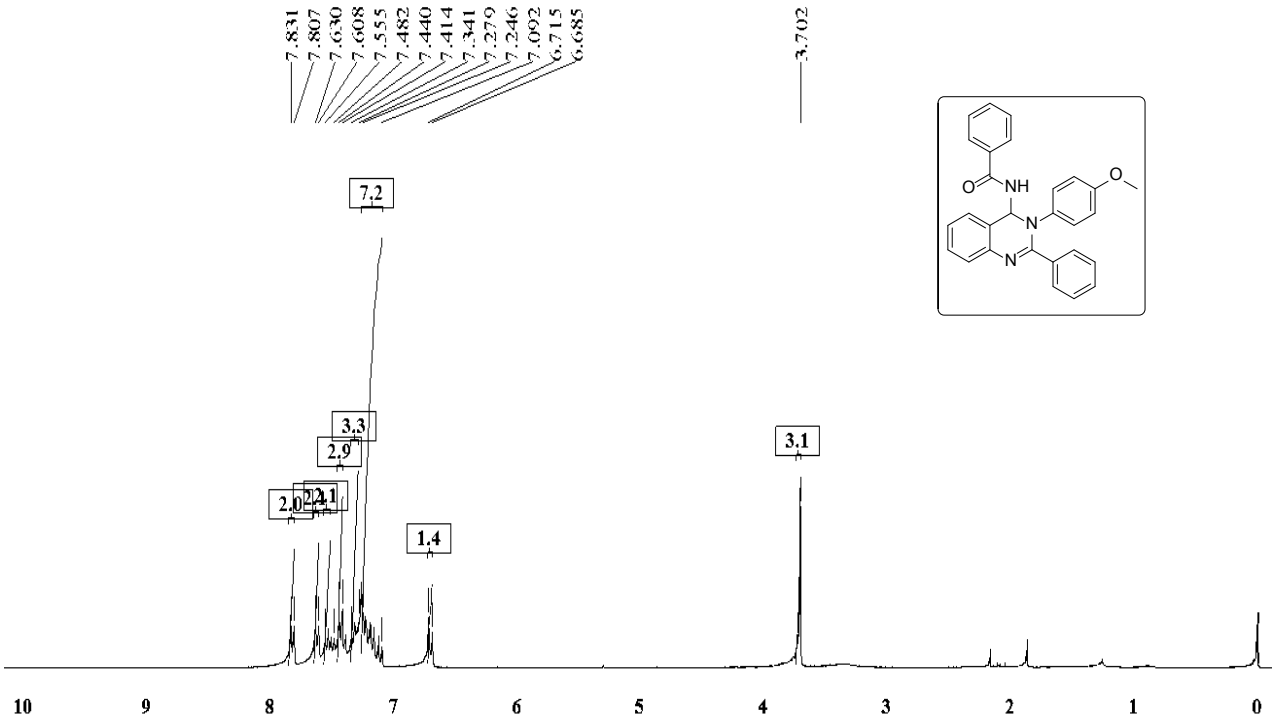
HIGH RESOLUTION MASS SPECTRA: (Table 2, 5m)



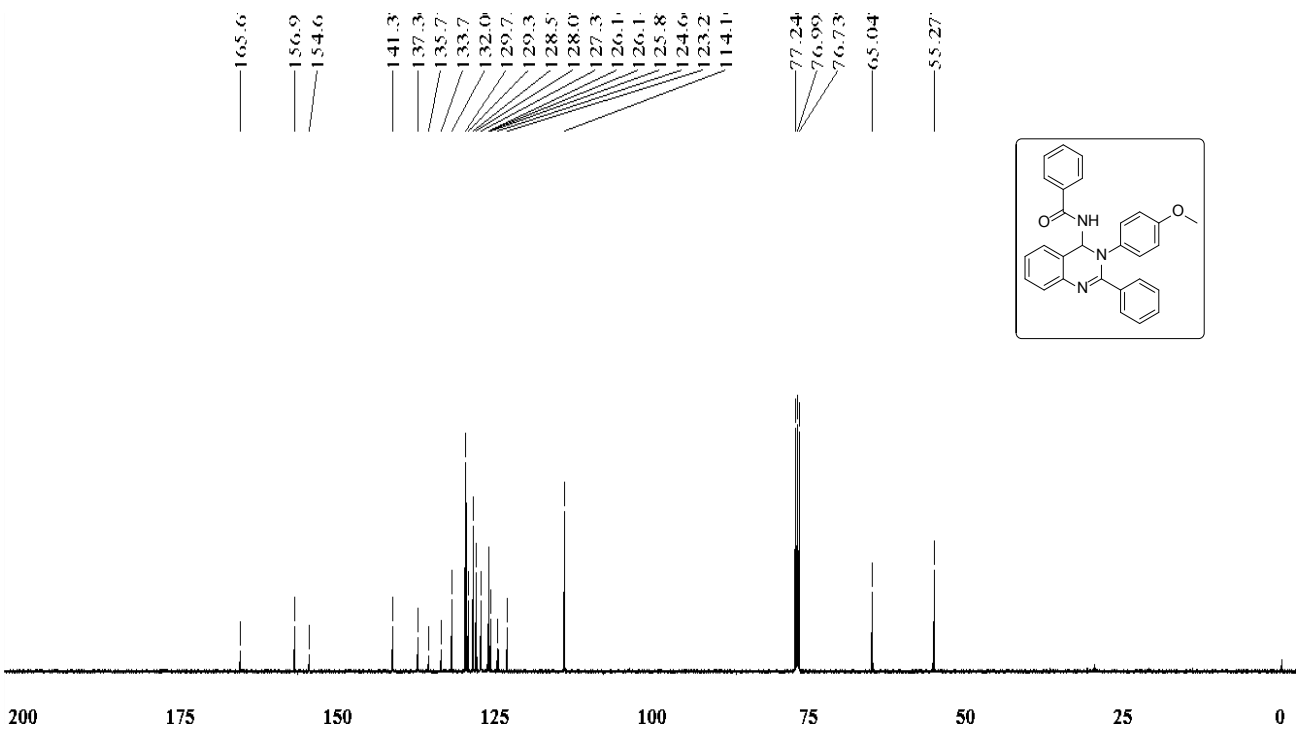
KRR-SAI-88#8-30 RT: 0.03-0.10 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
301.11328	85417728.0	36.55				
422.16542	233691344.0	100.00				

^{1}H NMR (300 MHz, $CDCl_3$): (Table 2, 5n)



^{13}C NMR (125 MHz, $CDCl_3$): (Table 2, 5n)

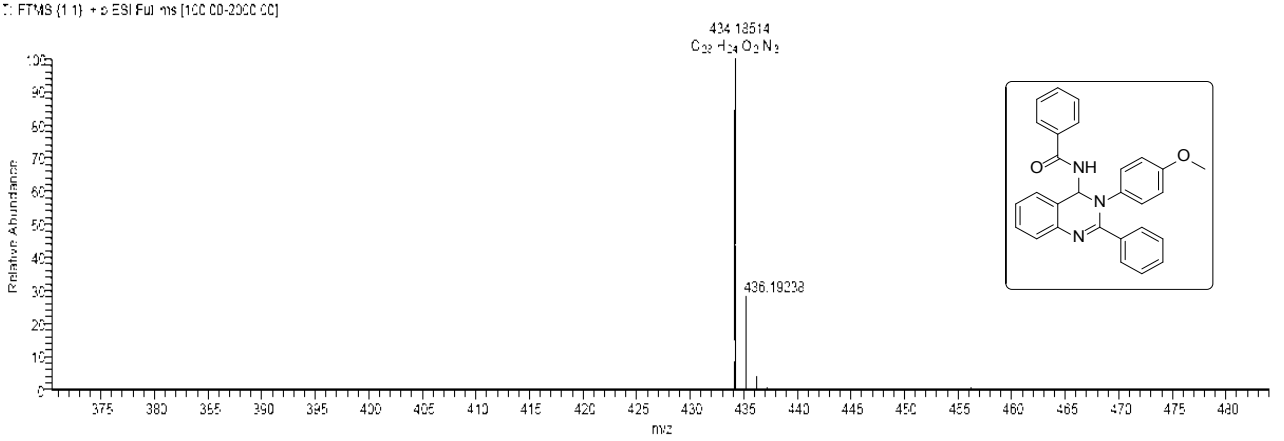


HIGH RESOLUTION MASS SPECTRA: (Table 2, 5n)

National Centre for Mass Spectrometry
CSIR-Indian Institute of Chemical Technology

File Name C:\IICT-HRMS\16.01.2014\KRR-SAI-93
Sample Name
Sample ID G SAIDULU
Date and Time 16-01-14 17:07:24

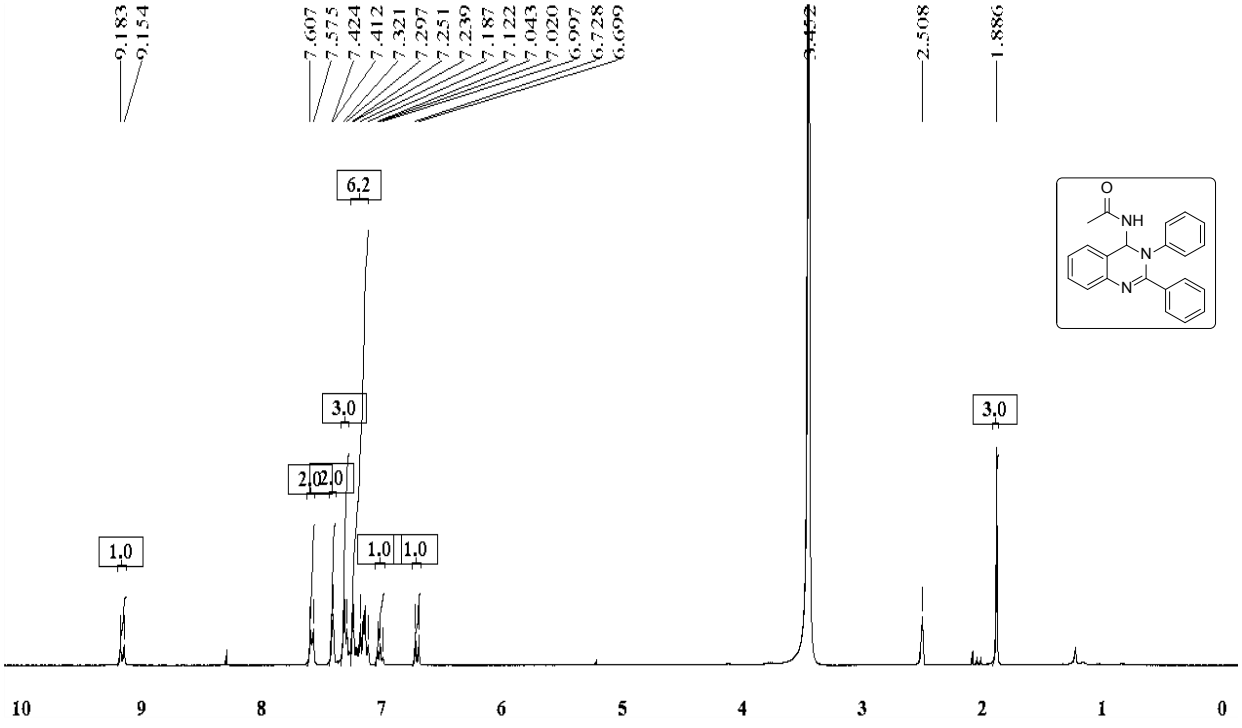
KRR-SAI-93#8-105 RT: 0.02-0.36 AV: 103 SB: 282 0.99-1.94 NL: 2.29E8
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]



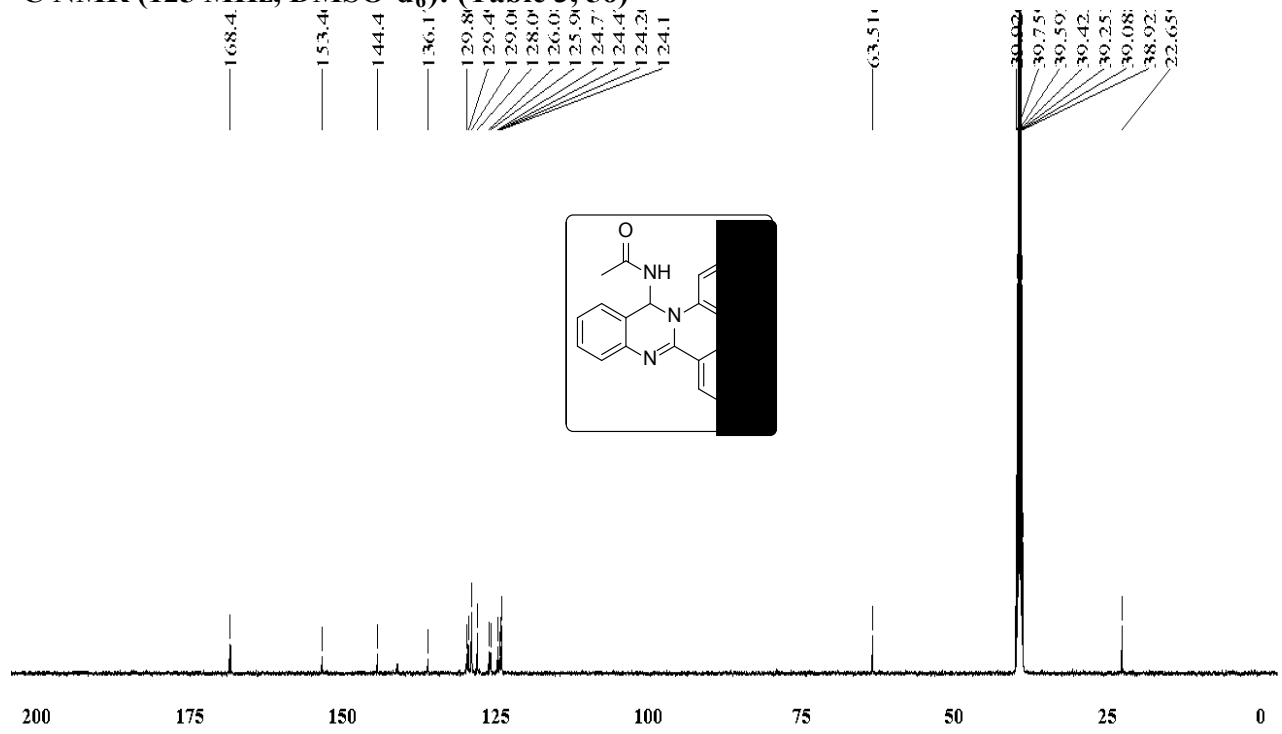
KRR-SAI-93#8-30 RT: 0.03-0.10 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
313.13315	95680376.0	34.24				
434.18497	279455904.0	100.00				

^{1}H NMR ((300 MHz, DMSO-d$_6$): (Table 2, 5o)

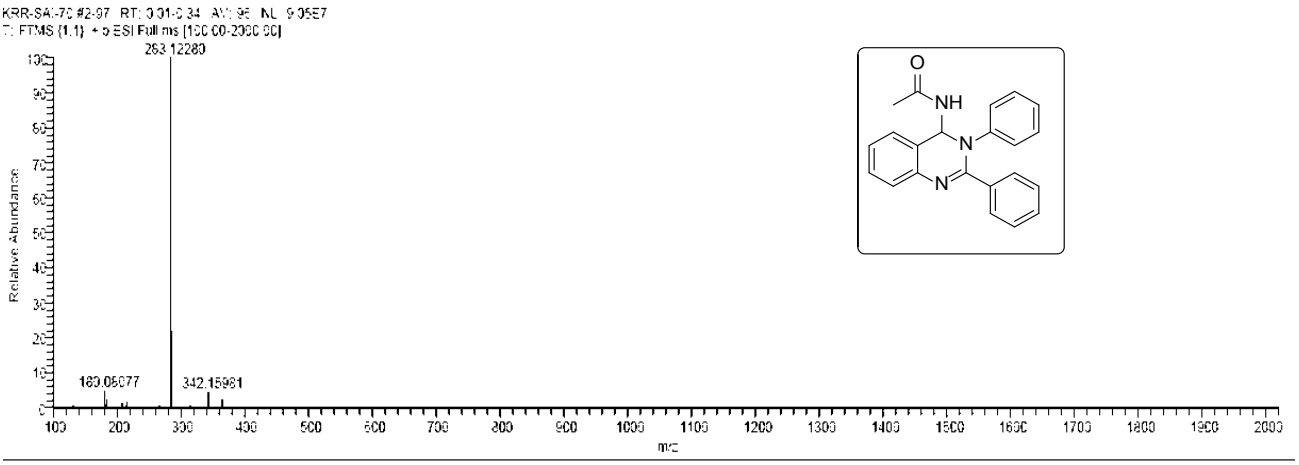


^{13}C NMR (125 MHz, DMSO-d$_6$): (Table 3, 5o)



HIGH RESOLUTION MASS SPECTRA: (Table 2, 5o)

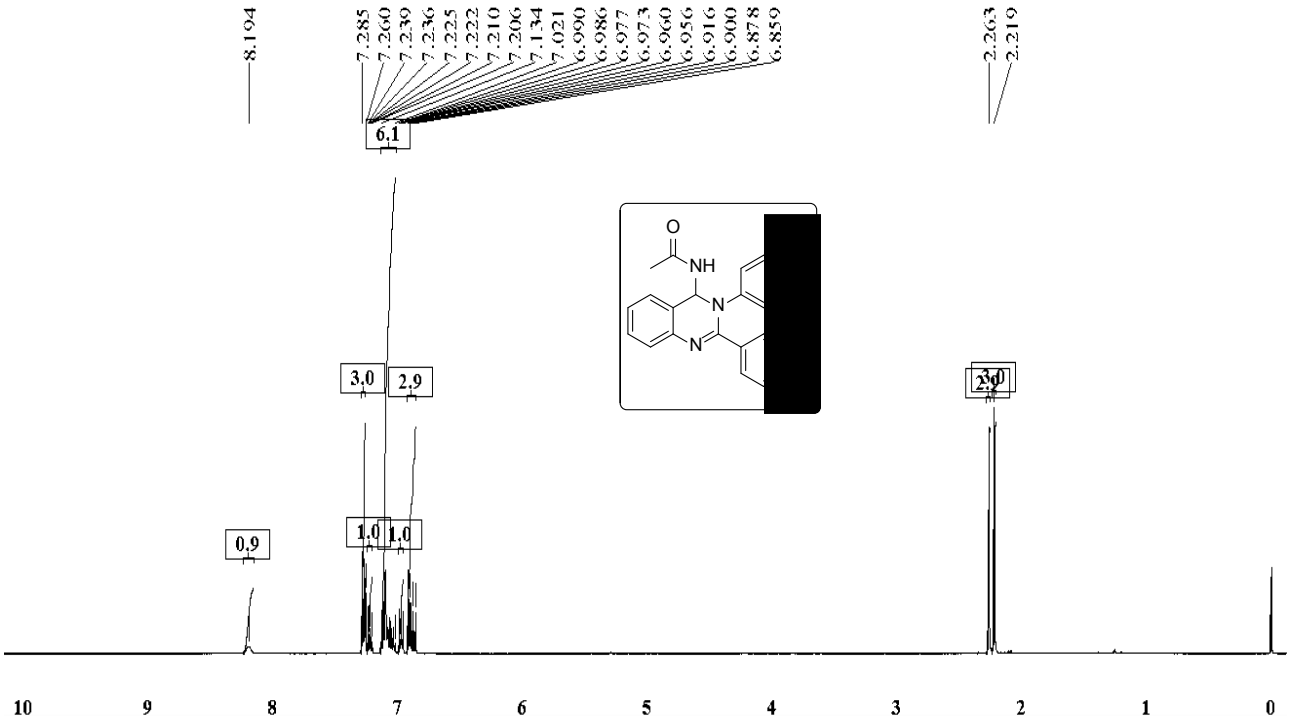
National Centre for Mass Spectrometry



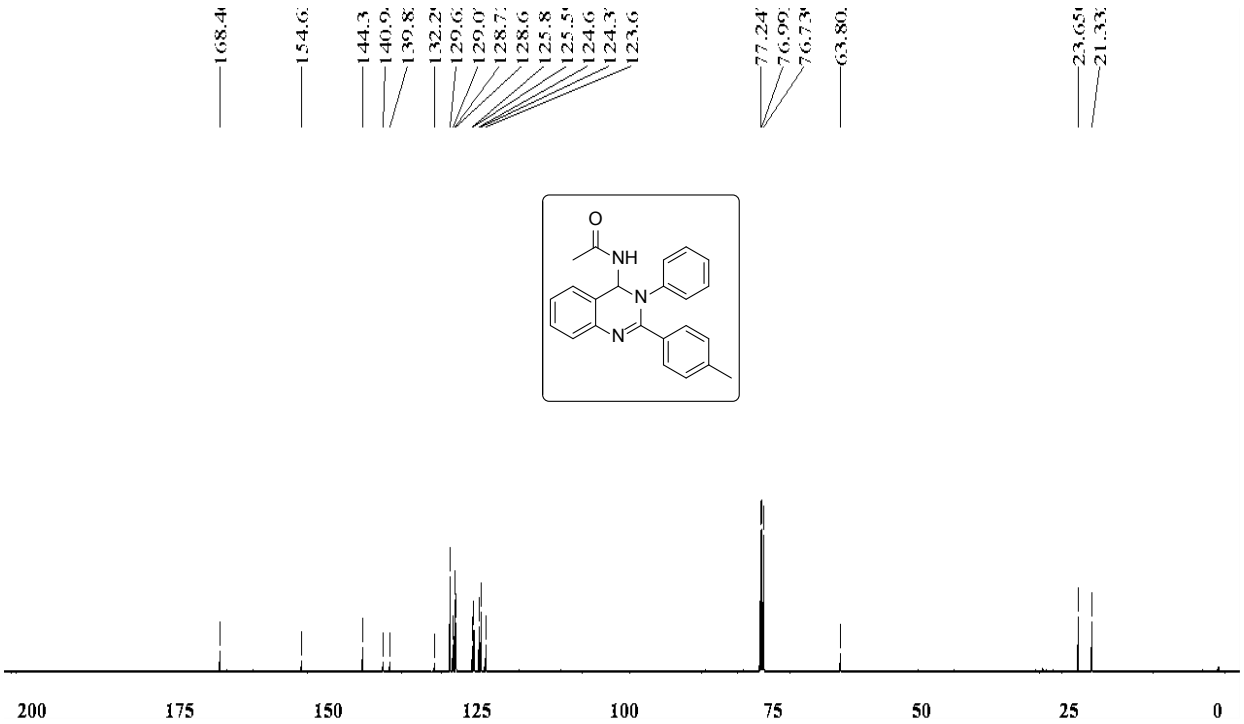
KRR-SAI-70#8-30 RT: 0.04-0.11 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]
m/z= 319.92-389.35

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
342.15975	9139558.0	100.00	342.16009	-0.98	14.5	$C_{22}H_{20}ON_3$
364.14200	7256361.5	79.40	364.14203	-0.08	14.5	$C_{22}H_{19}ON_3Na$

^{1}H NMR (500 MHz, $CDCl_3$): (Table 2, 5p)

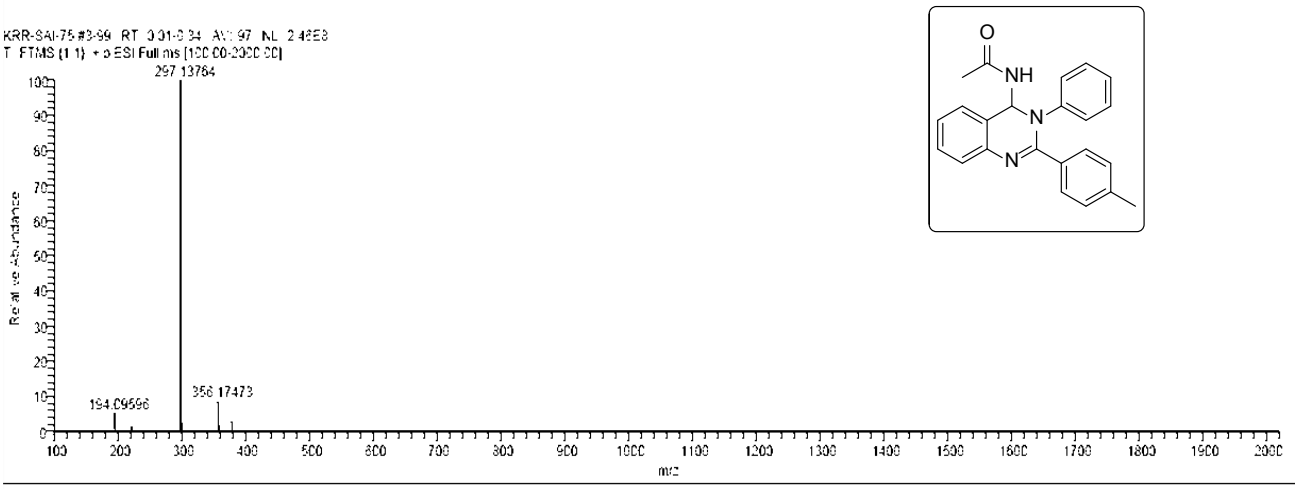


^{13}C NMR (125 MHz, $CDCl_3$): (Table 2, 5p)



HIGH RESOLUTION MASS SPECTRA: (Table 2, 5p)

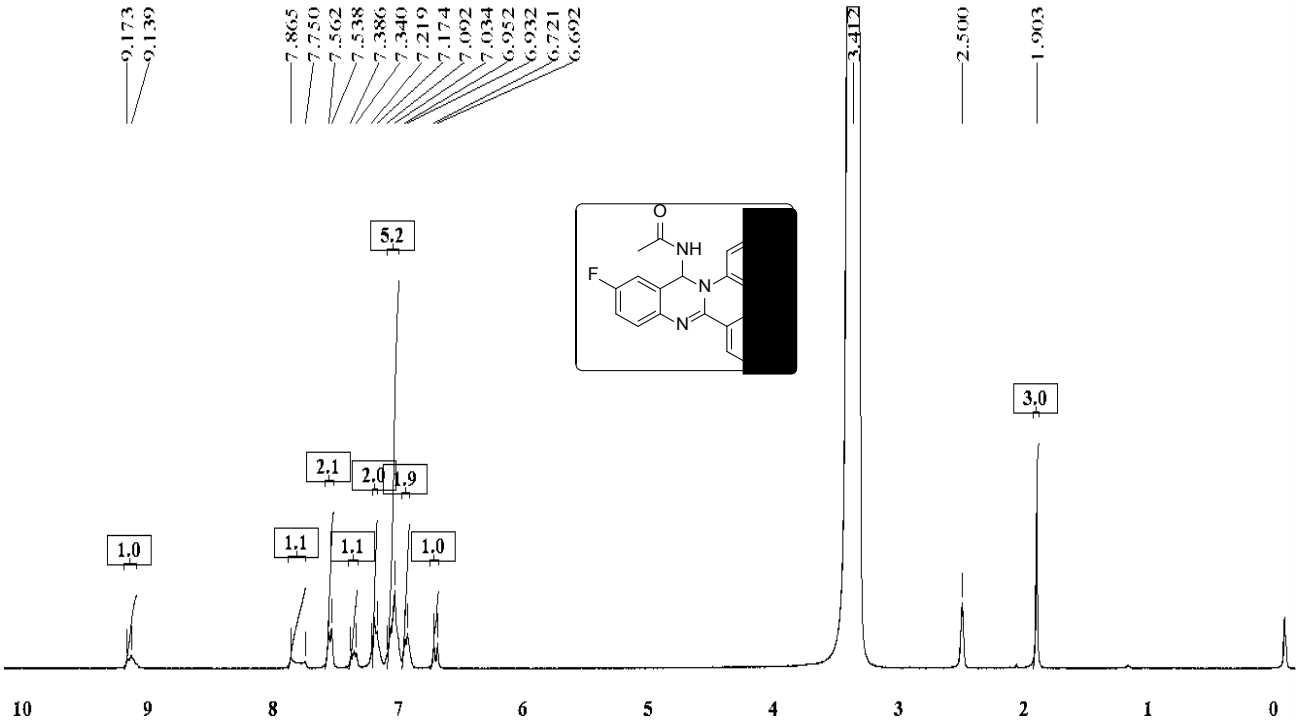
National Centre for Mass Spectrometry



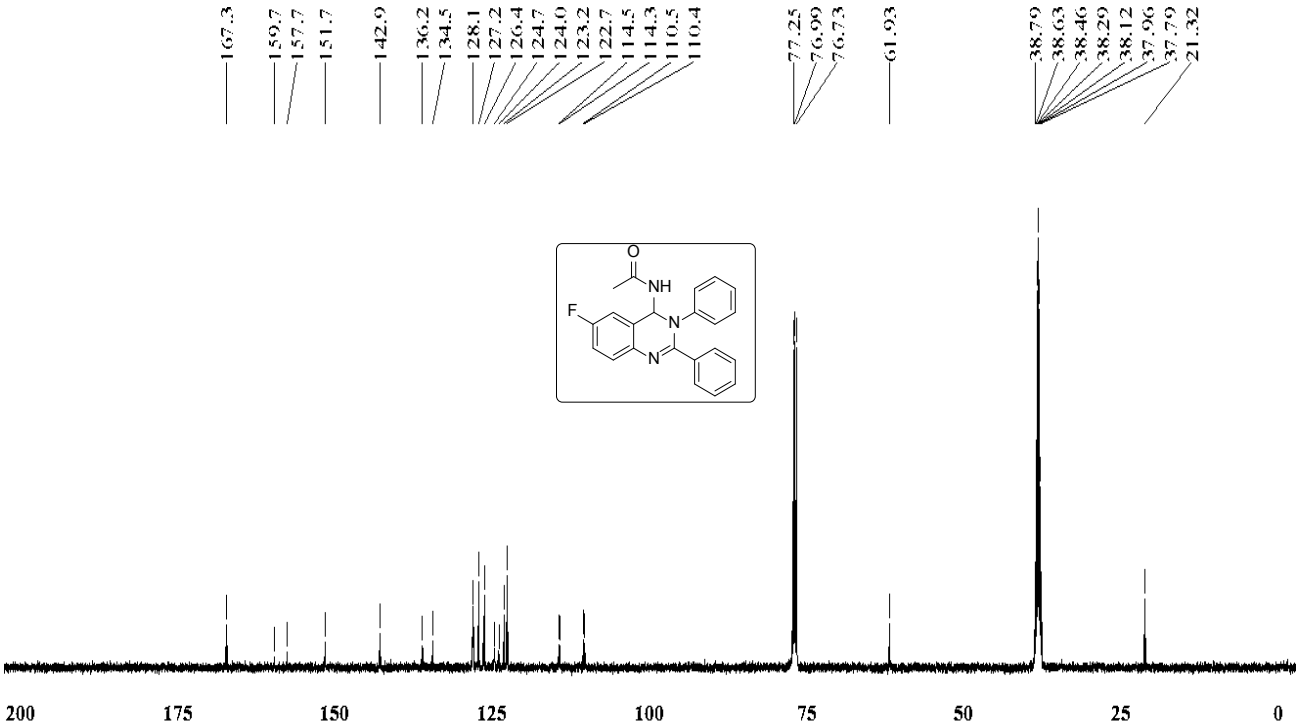
KRR-SAI-75#8-30 RT: 0.03-0.11 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]
m/z= 338.86-375.47

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
356.17473	34735476.0	100.00	356.17468	0.15	11.0	$C_{23}H_{25}O_2Na$
			356.17574	-2.84	14.5	$C_{23}H_{22}ON_3$

^{1}H NMR (300 MHz, $CDCl_3$ + DMSO-d_6): (Table 2, 5q)



^{13}C NMR (125 MHz, $CDCl_3$ + DMSO-d_6): (Table 2, 5q)

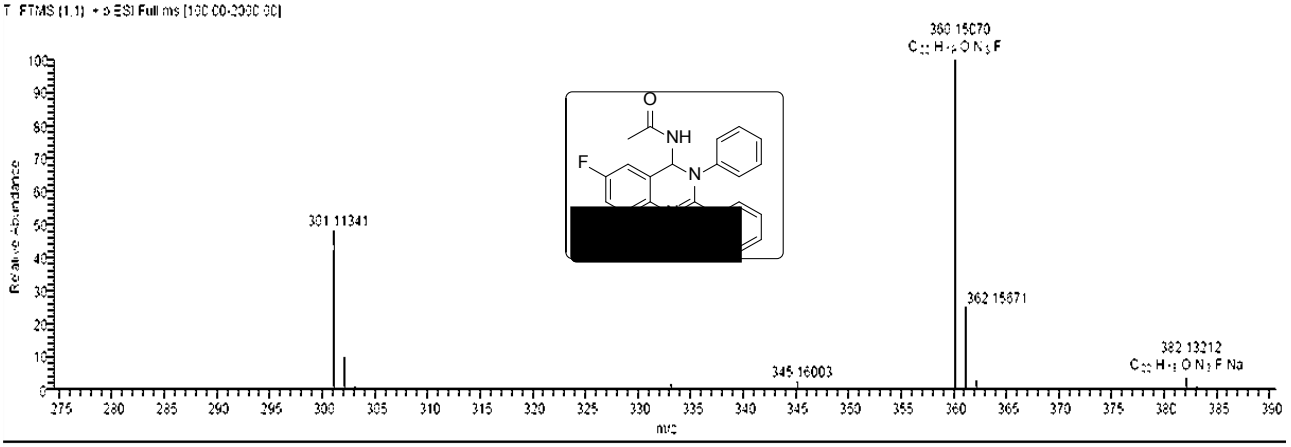


HIGH RESOLUTION MASS SPECTRA: (Table 2, 5q)

National Centre for Mass Spectrometry
CSIR-Indian Institute of Chemical Technology

File Name C:\IICT-HRMS\16.01.2014\KRR-SAI-89
Sample Name
Sample ID G SAIDULU
Date and Time 16-01-14 16:59:29

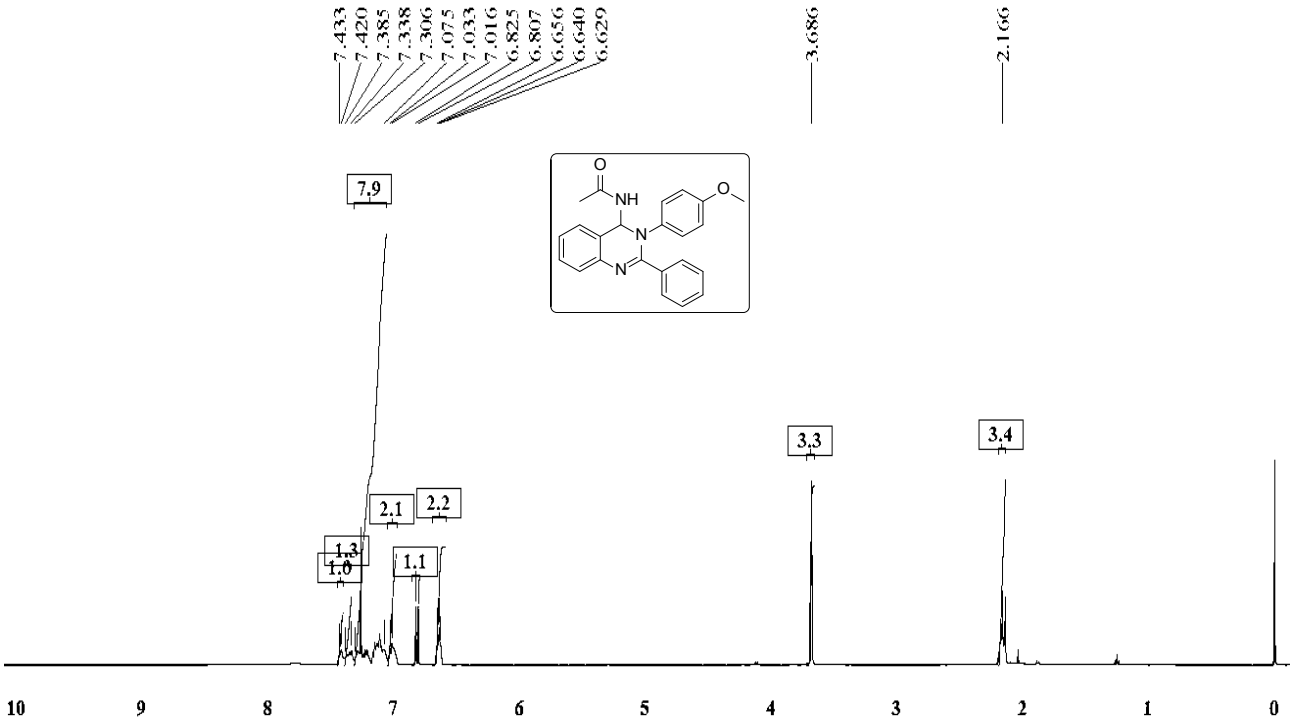
KRR-SAI-89 #7-105 RT: 0.02-0.36 AV: 102 SB: 282 0.99-1.94 NL: 1.53E8
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]



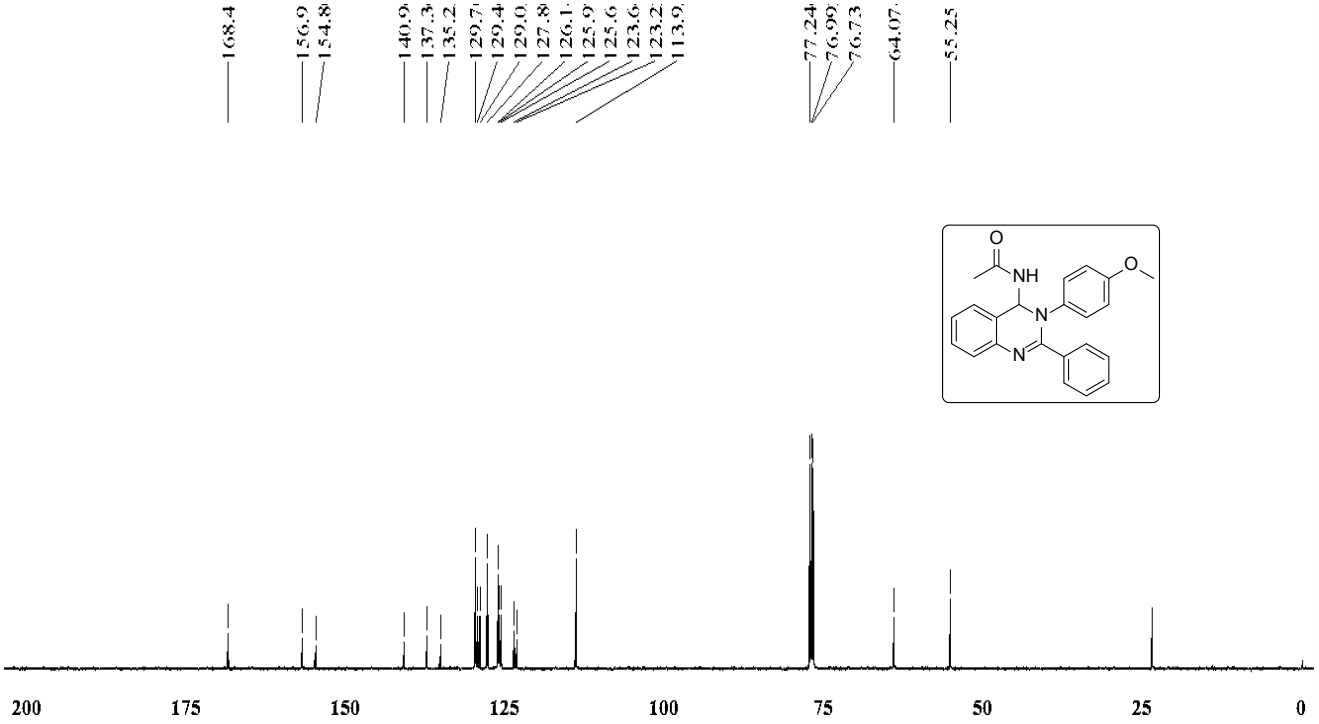
KRR-SAI-89#8-30 RT: 0.03-0.10 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
301.11338	125247360.0	48.96				
360.15065	255824528.0	100.00				

^{1}H NMR (500 MHz, $CDCl_3$): (Table 2, 5r)



^{13}C NMR (75 MHz, $CDCl_3$): (Table 2, 5r)

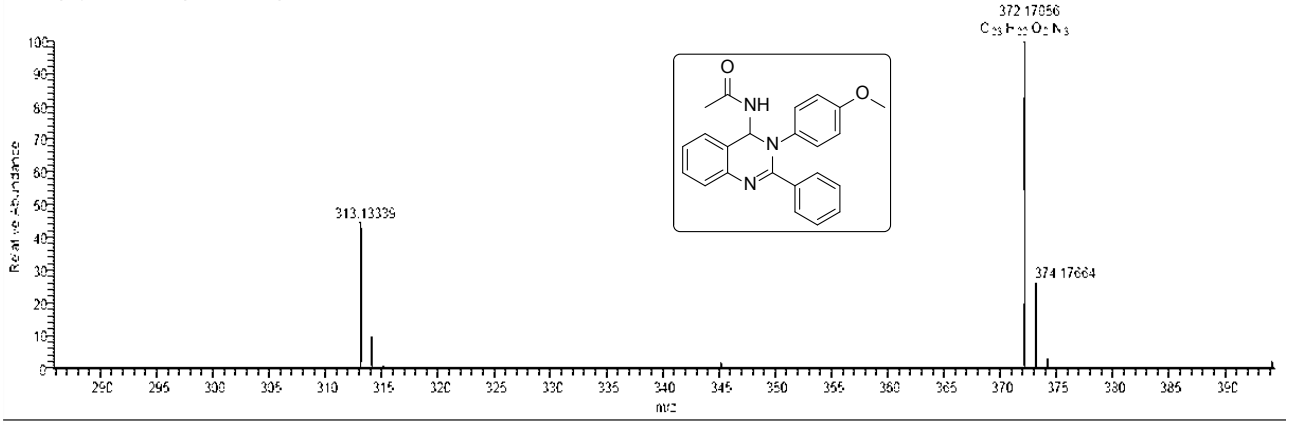


HIGH RESOLUTION MASS SPECTRA: (Table 2, 5r)

National Centre for Mass Spectrometry
CSIR-Indian Institute of Chemical Technology

File Name C:\IICT-HRMS\16.01.2014\KRR-SAI-94
Sample Name
Sample ID G SAIDULU
Date and Time 16-01-14 17:09:59

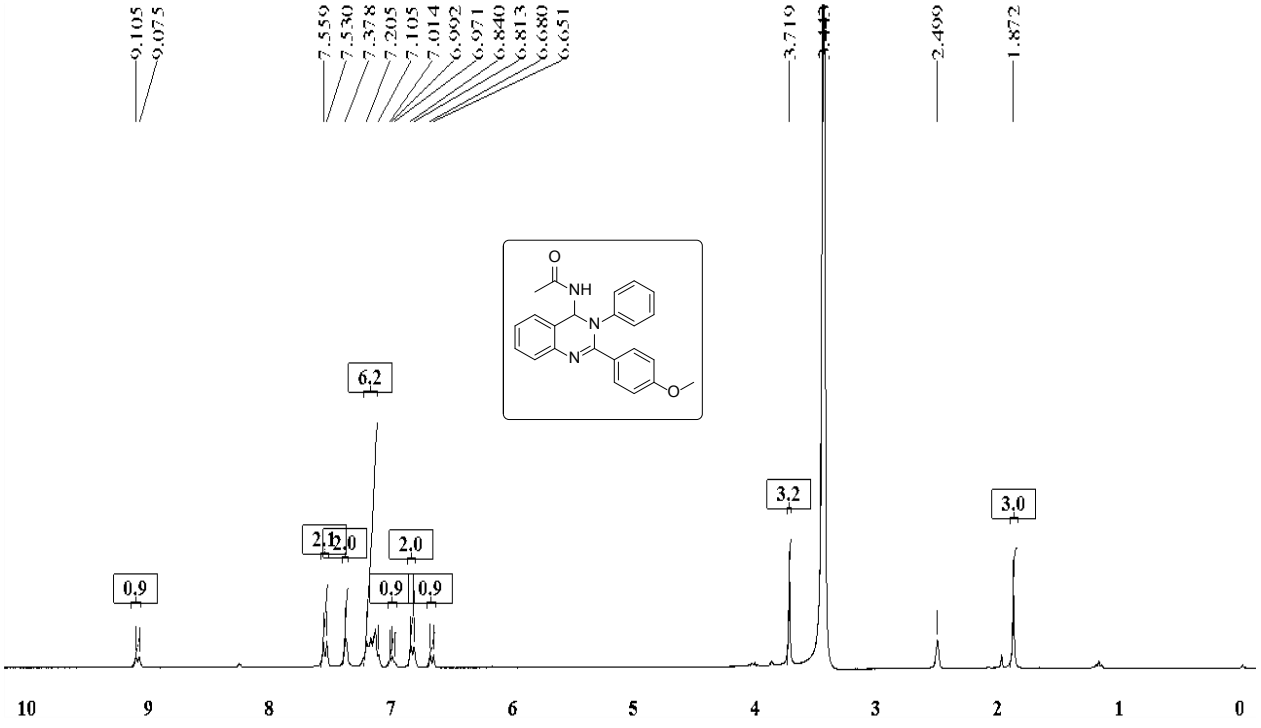
KRR-SAI-94 #8-108 RT: 0.02-0.36 AV: 103 SB: 282 0.99-1.94 NL: 2.17E8
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]



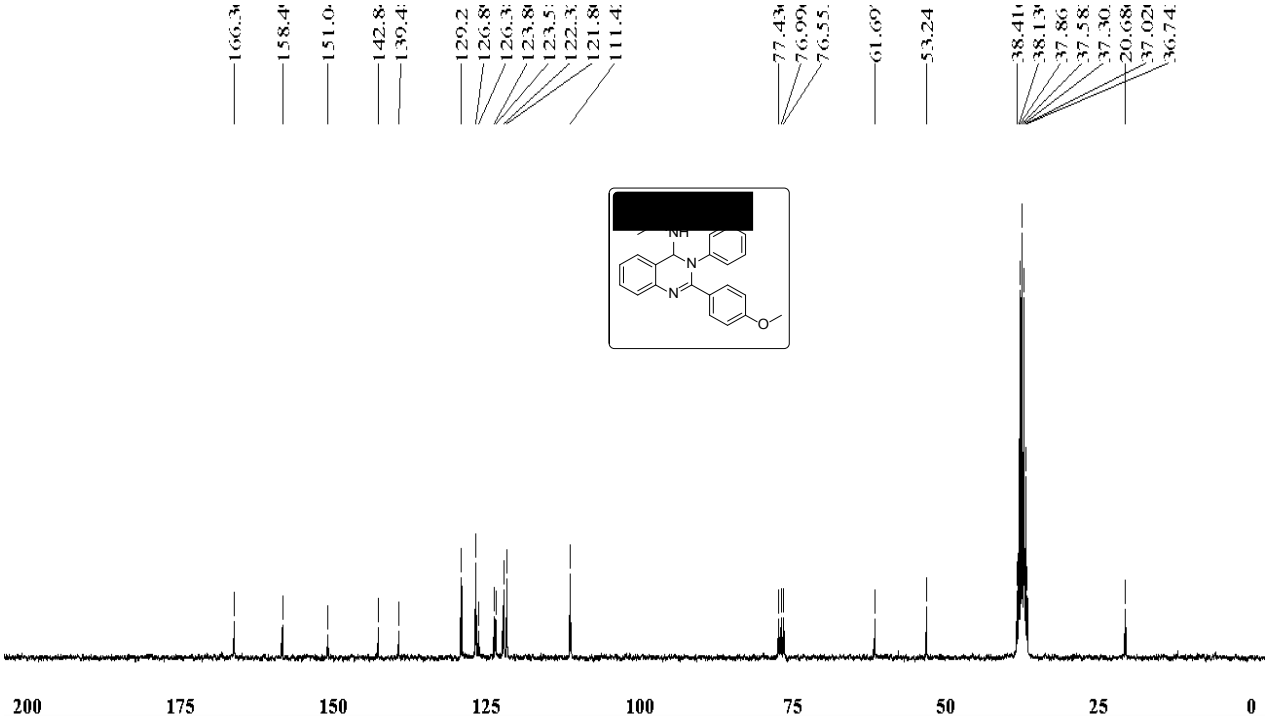
KRR-SAI-94#8-30 RT: 0.03-0.10 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
313.13333	100293880.0	43.61				
372.17052	229982784.0	100.00				

^{1}H NMR (500 MHz, $CDCl_3$ + DMSO-d_6): (Table 2, 5s)

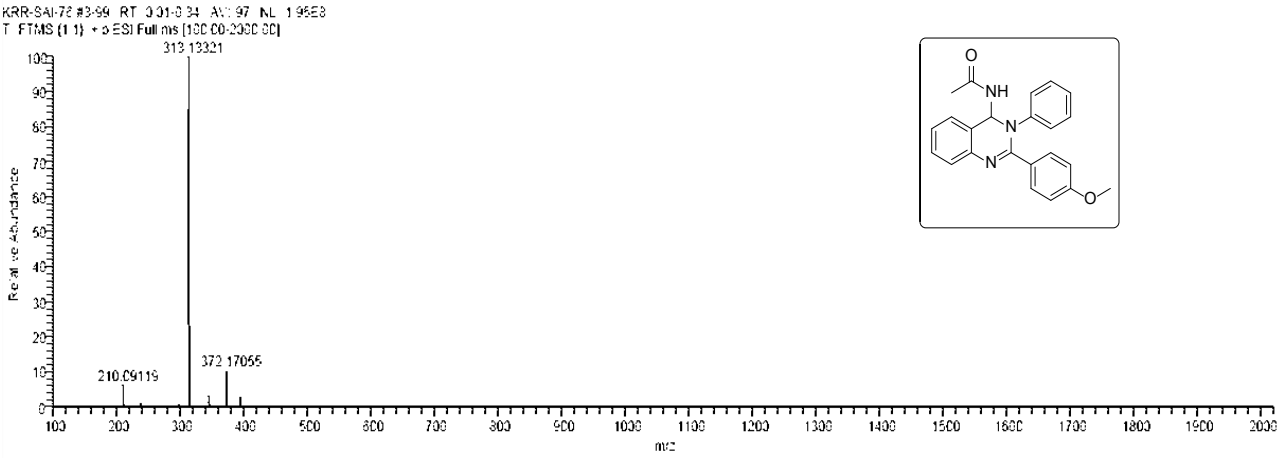


^{13}C NMR (125 MHz, $CDCl_3$ + DMSO-d_6): (Table 2, 5s)



HIGH RESOLUTION MASS SPECTRA: (Table 2, 5s)

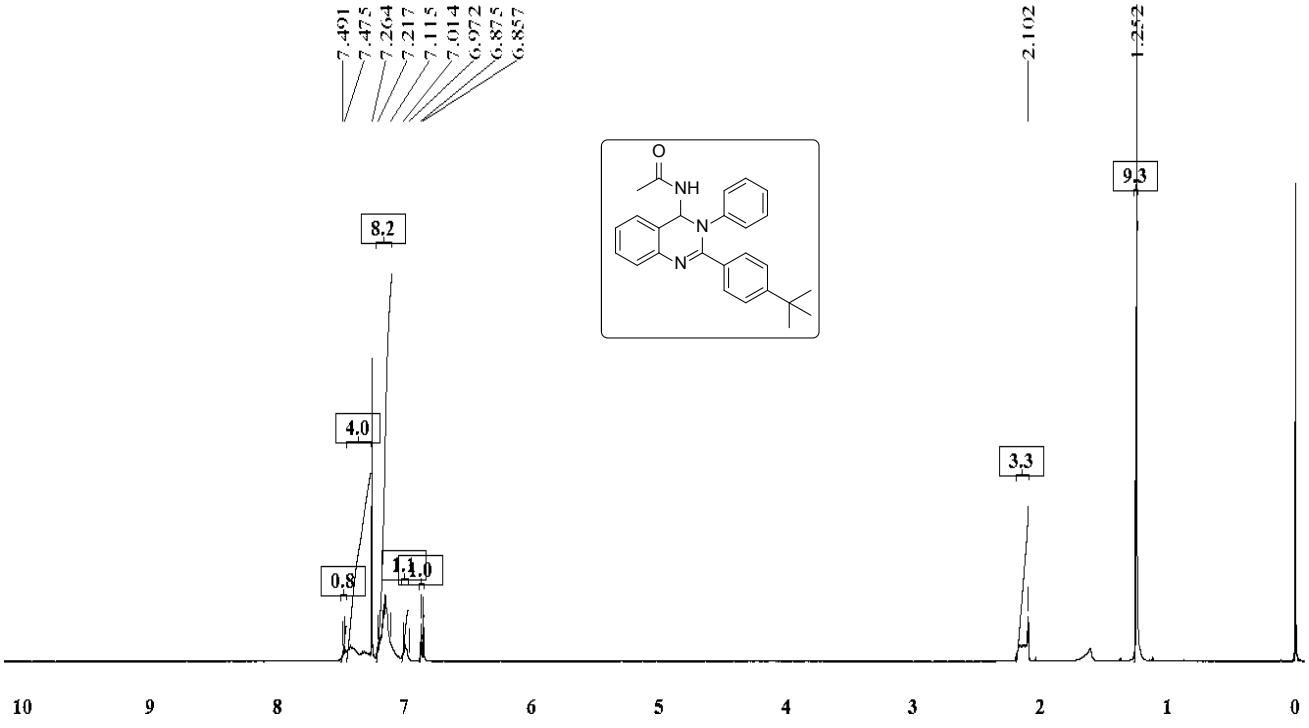
National Centre for Mass Spectrometry



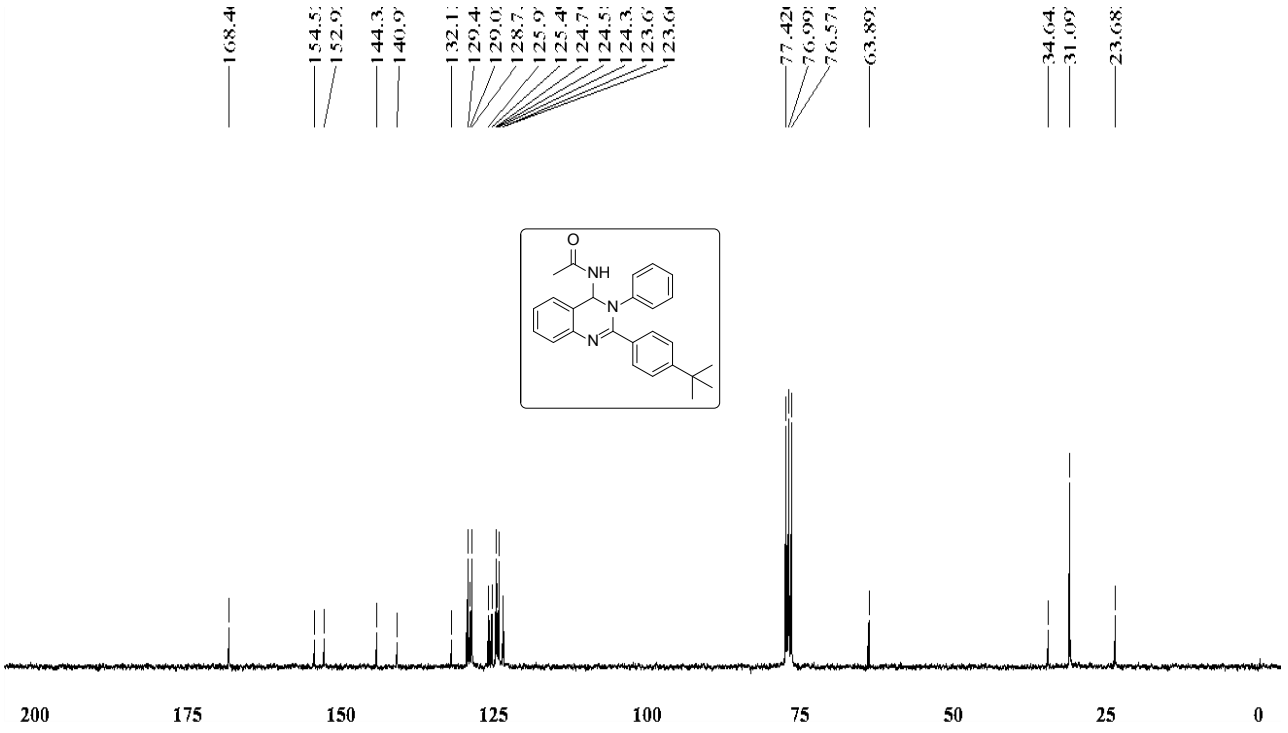
KRR-SAI-76#8-30 RT: 0.03-0.11 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]
m/z= 352.74-389.35

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
372.17051	28083474.0	100.00	372.17065	-0.39	14.5	$C_{23}H_{22}O_2N_3$
373.17357	6645891.5	23.66				

^{1}H NMR (500 MHz, $CDCl_3$): (Table 2, 5t)



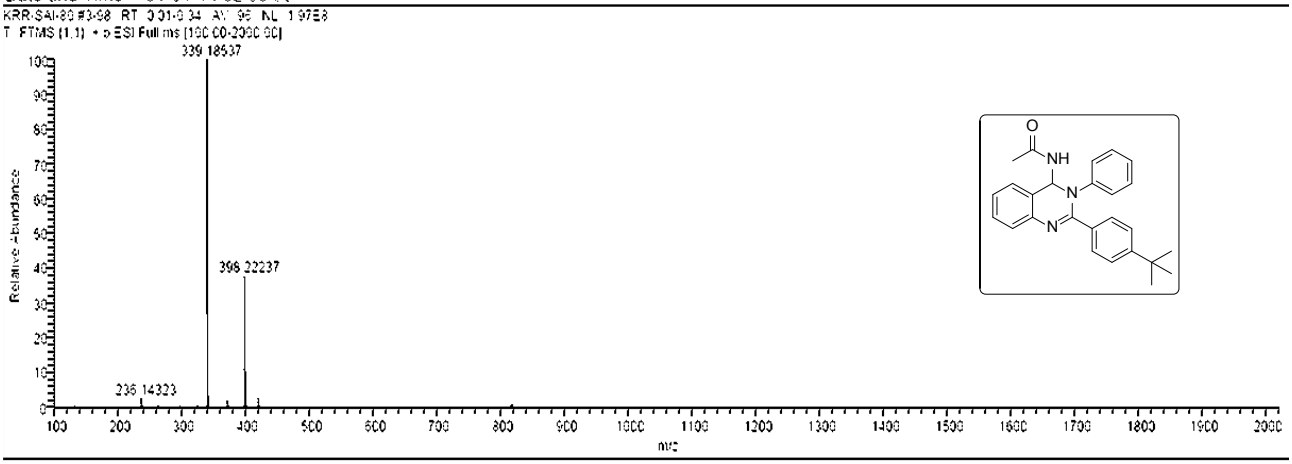
^{13}C NMR (75 MHz, $CDCl_3$): (Table 2, 5t)



HIGH RESOLUTION MASS SPECTRA: (Table 2, 5t)

National Centre for Mass Spectrometry
CSIR-Indian Institute of Chemical Technology

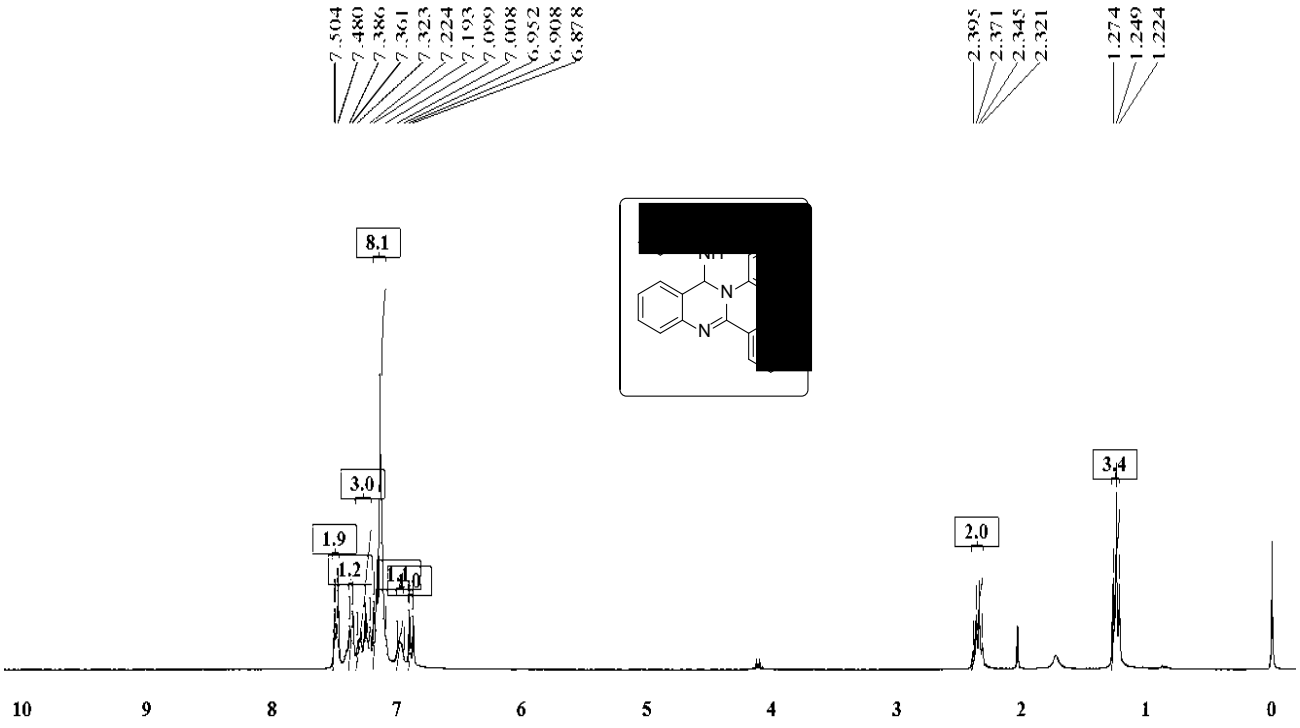
File Name C:\IICT-HRMS\31.12.2013\KRR-SAI-80
Sample Name
Sample ID G-SAIDULU
Date and Time 01-01-14 02:30:39



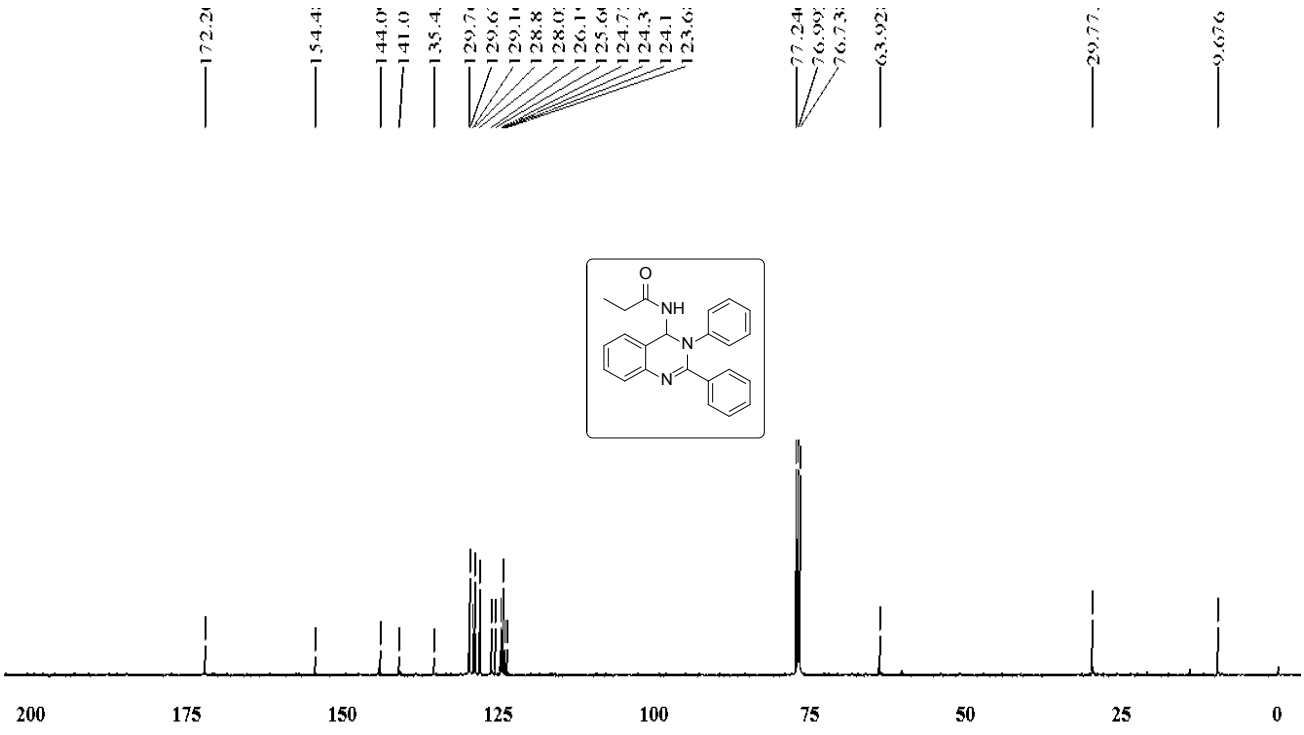
KRR-SAI-80#8-30 RT: 0.03-0.11 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
339.18534	330307648.0	100.00				
398.22237	114875960.0	34.78	398.22269	-0.81	14.5	$C_{26}H_{28}ON_3$

^{1}H NMR (300 MHz, $CDCl_3$): (Table 2, 5u)



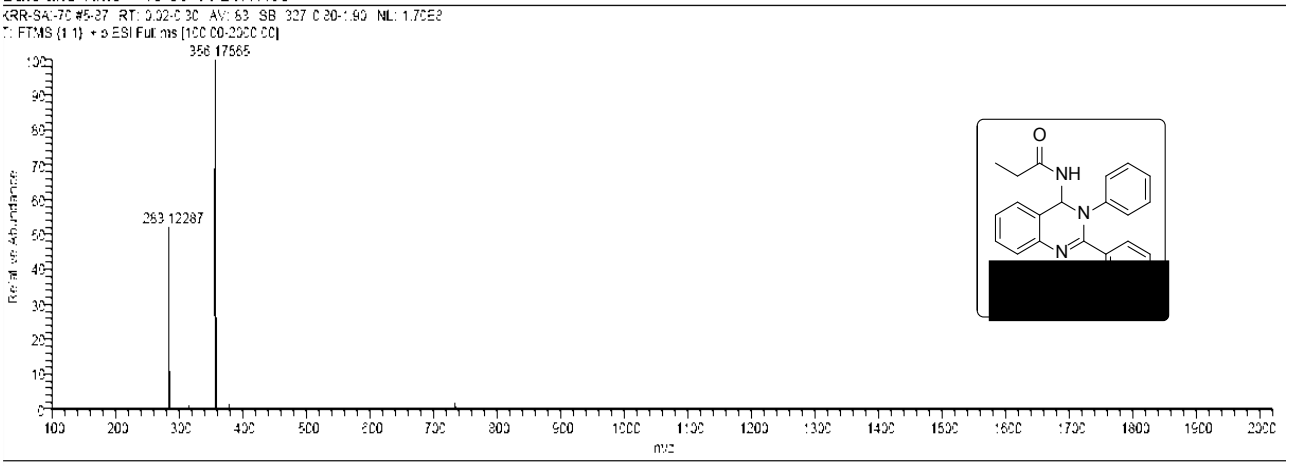
^{13}C NMR (125 MHz, $CDCl_3$): (Table 2, 5u)



HIGH RESOLUTION MASS SPECTRA: (Table 2, 5u)

National Centre for Mass Spectrometry
CSIR-Indian Institute of Chemical Technology

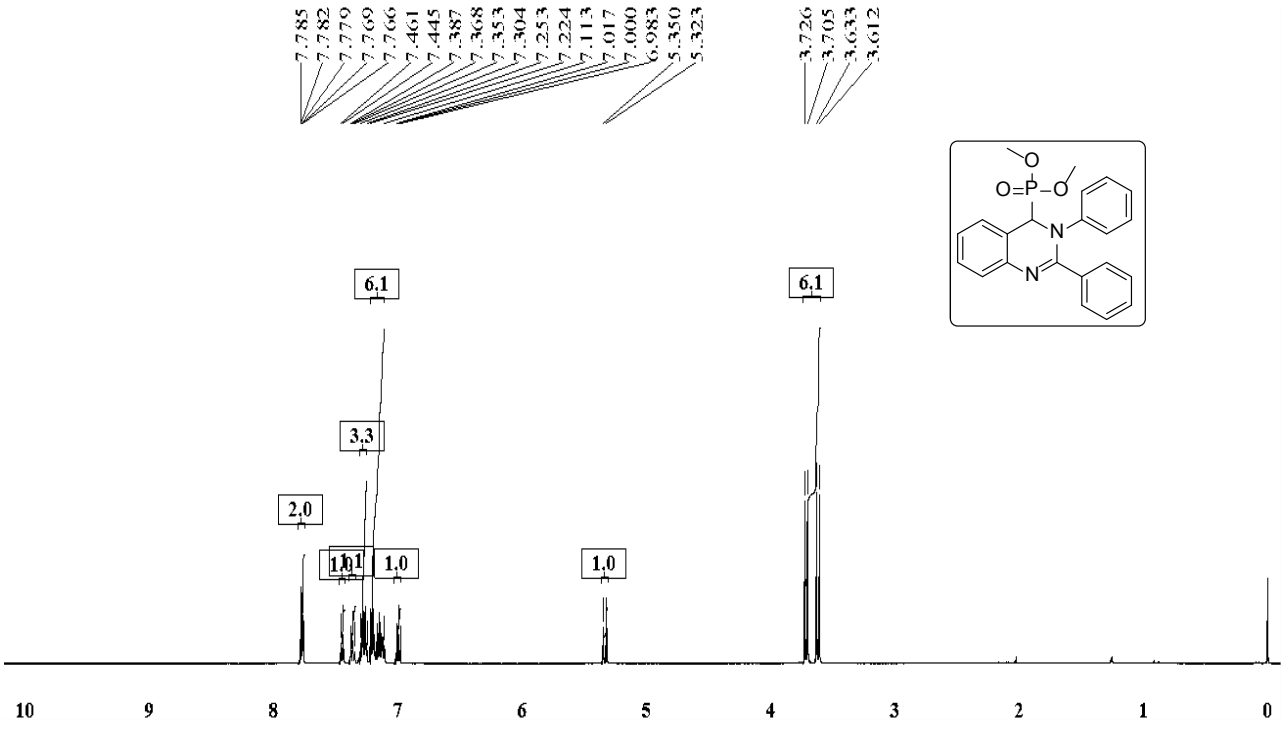
File Name C:\IICT-HRMS\10.03.2014\KRR-SAI-70
Sample Name G SAIDULU
Sample ID 1
Date and Time 10-03-14 21:17:30



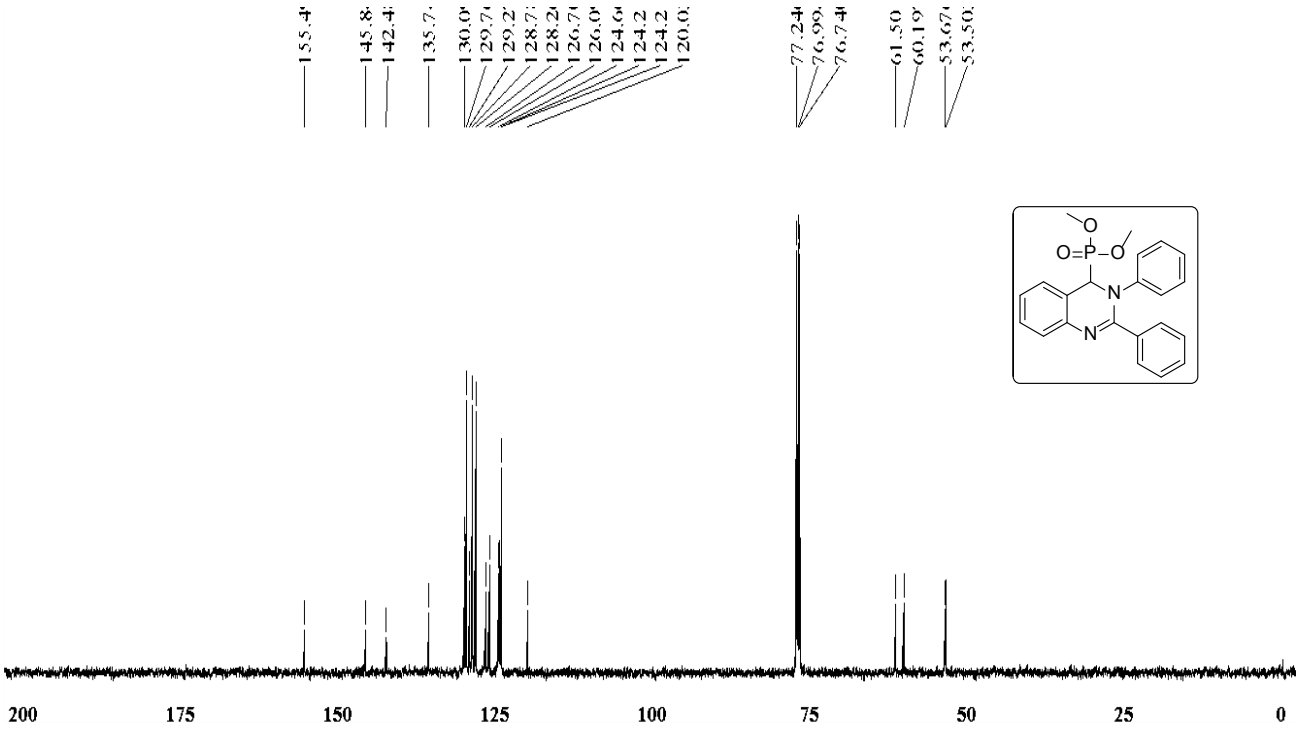
KRR-SAI-70#8-30 RT: 0.03-0.11 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
356.17561	224874336.0	100.00	356.17574	-0.35	14.5	$C_{23}H_{22}ON_3$

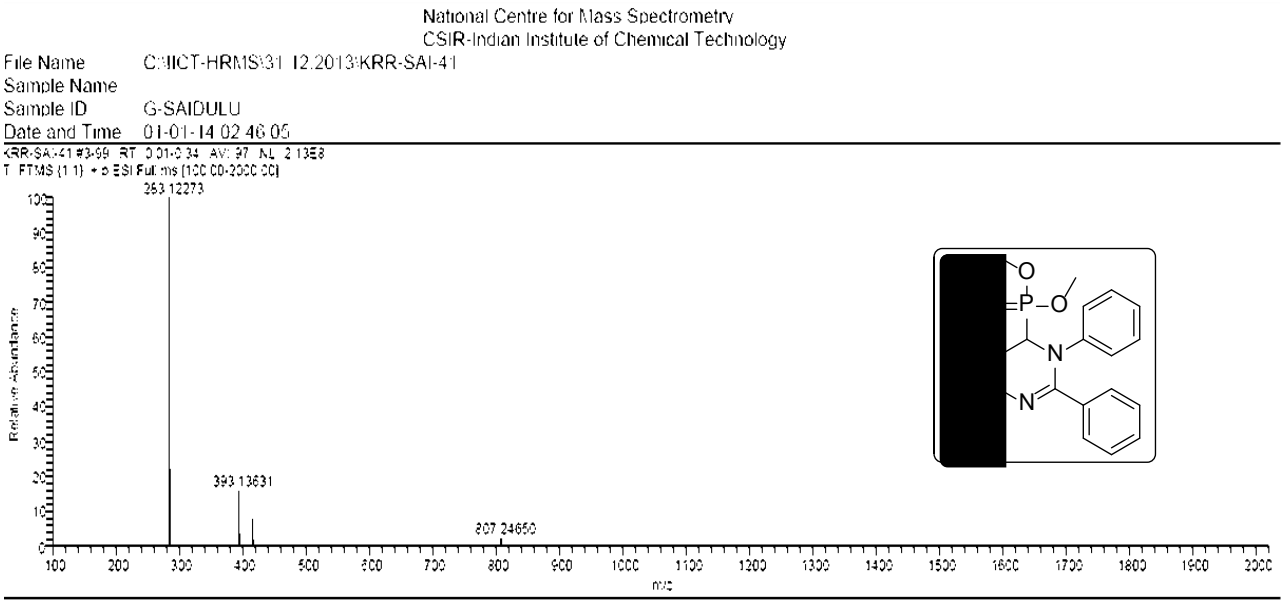
^{1}H NMR (500 MHz, $CDCl_3$): (Table 3, 7a)



^{13}C NMR (125 MHz, $CDCl_3$): (Table 3, 7a)



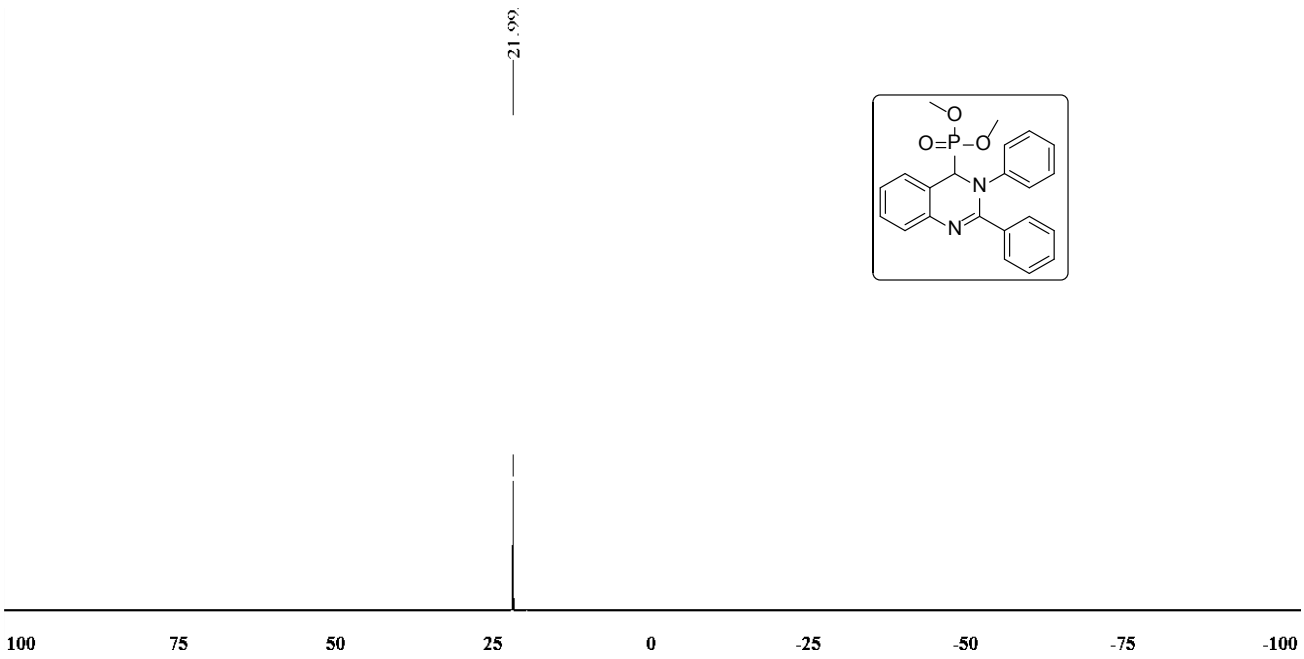
HIGH RESOLUTION MASS SPECTRA: (Table 3, 7a)



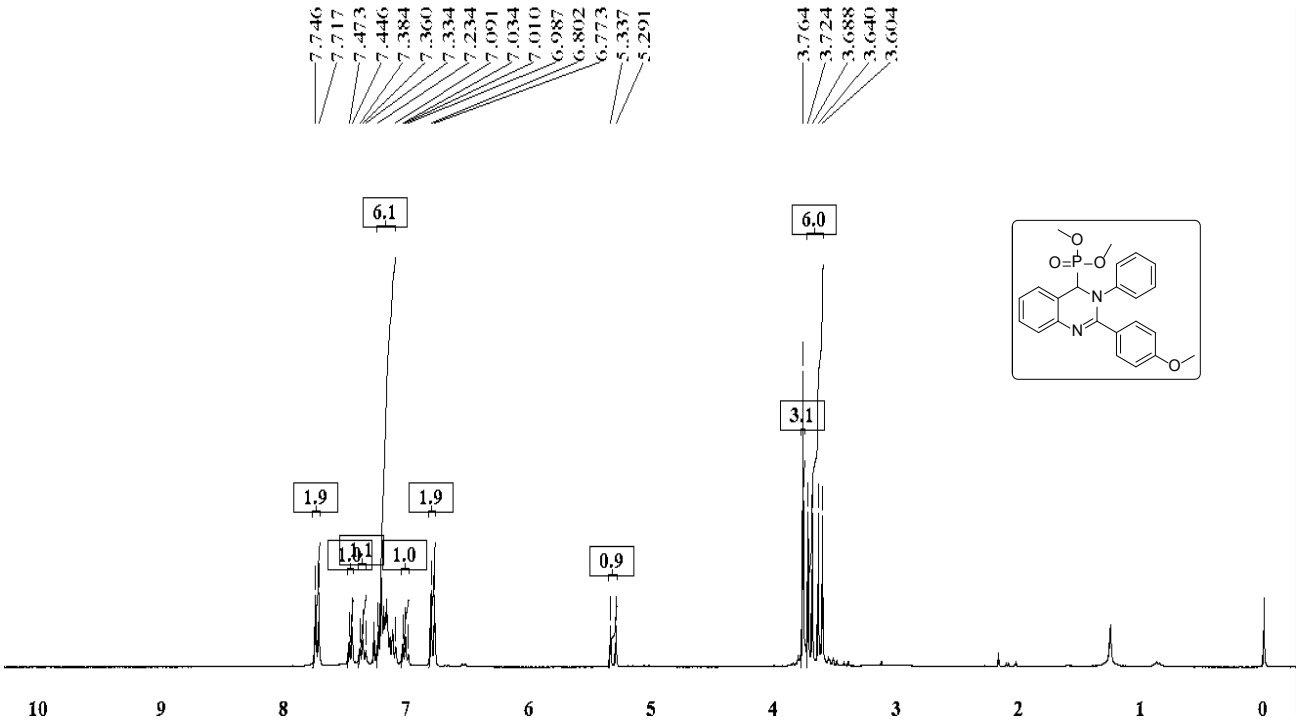
KRR-SAI-41#8-30 RT: 0.03-0.10 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]
m/z= 364.10-470.14

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
393.13627	60560948.0	100.00	393.13626	0.05	13.5	$C_{22}H_{22}O_3N_2P$
415.11772	54026884.0	89.21	415.11820	-1.16	13.5	$C_{22}H_{21}O_3N_2NaP$

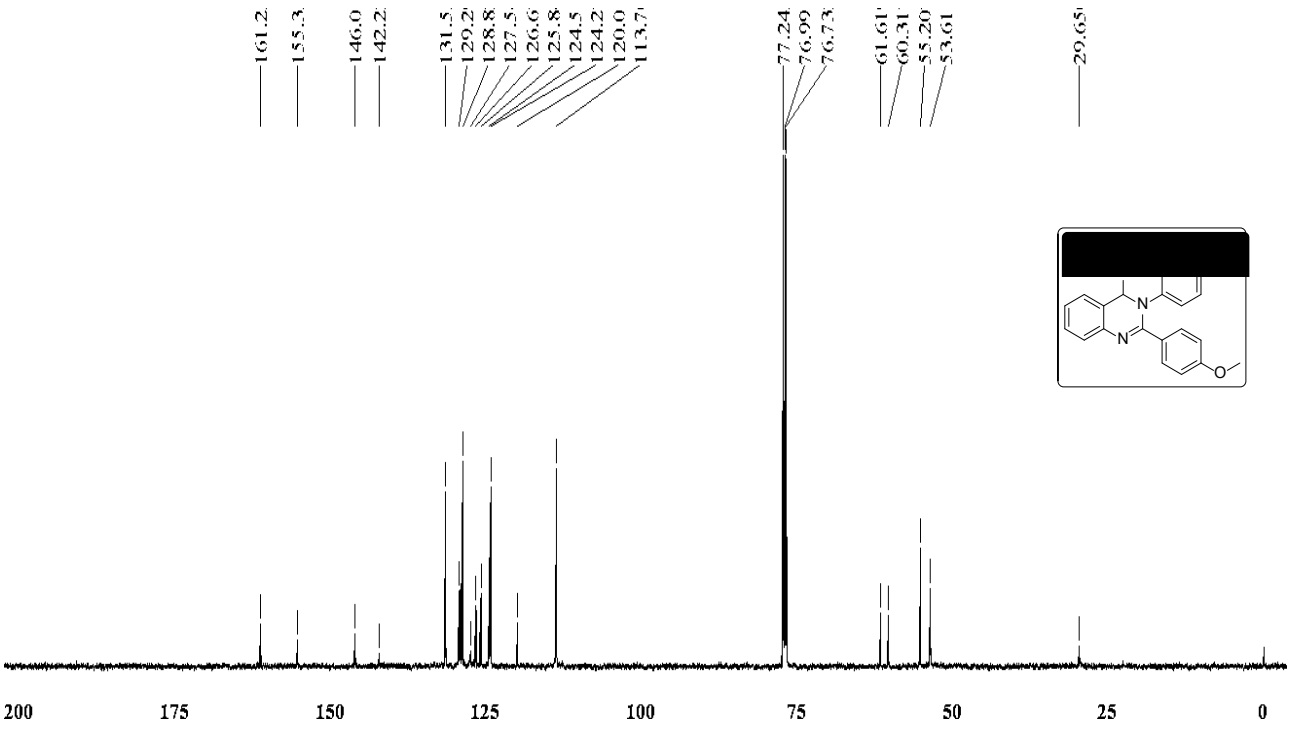
^{31}P NMR (202 MHz, $CDCl_3$): (Table 3, 7a)



^{1}H NMR (300 MHz, $CDCl_3$): (Table 3, 7b)



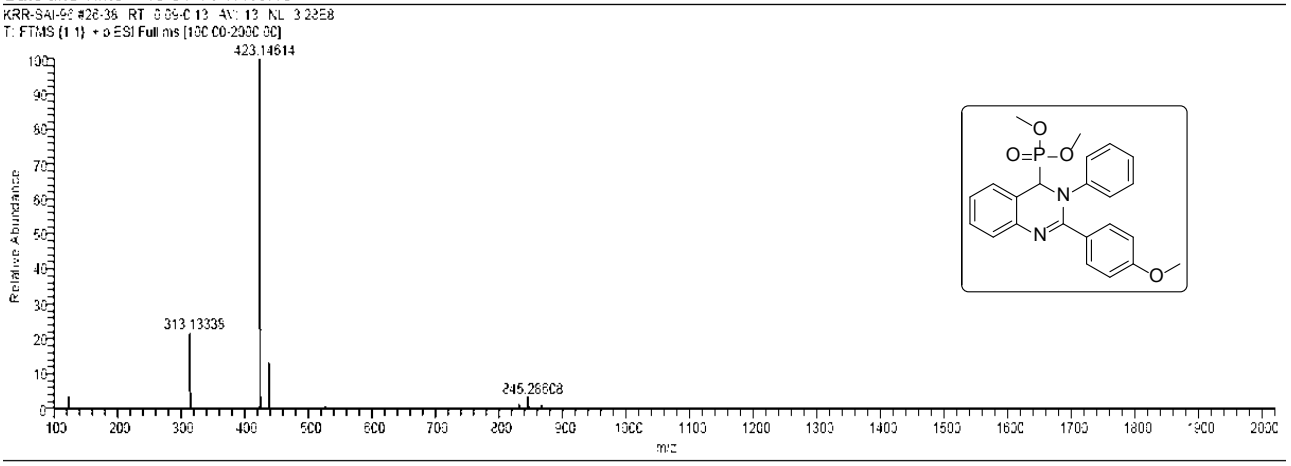
^{13}C NMR (125 MHz, $CDCl_3$): (Table 3, 7b)



HIGH RESOLUTION MASS SPECTRA: (Table 3, 7b)

National Centre for Mass Spectrometry
CSIR-Indian Institute of Chemical Technology

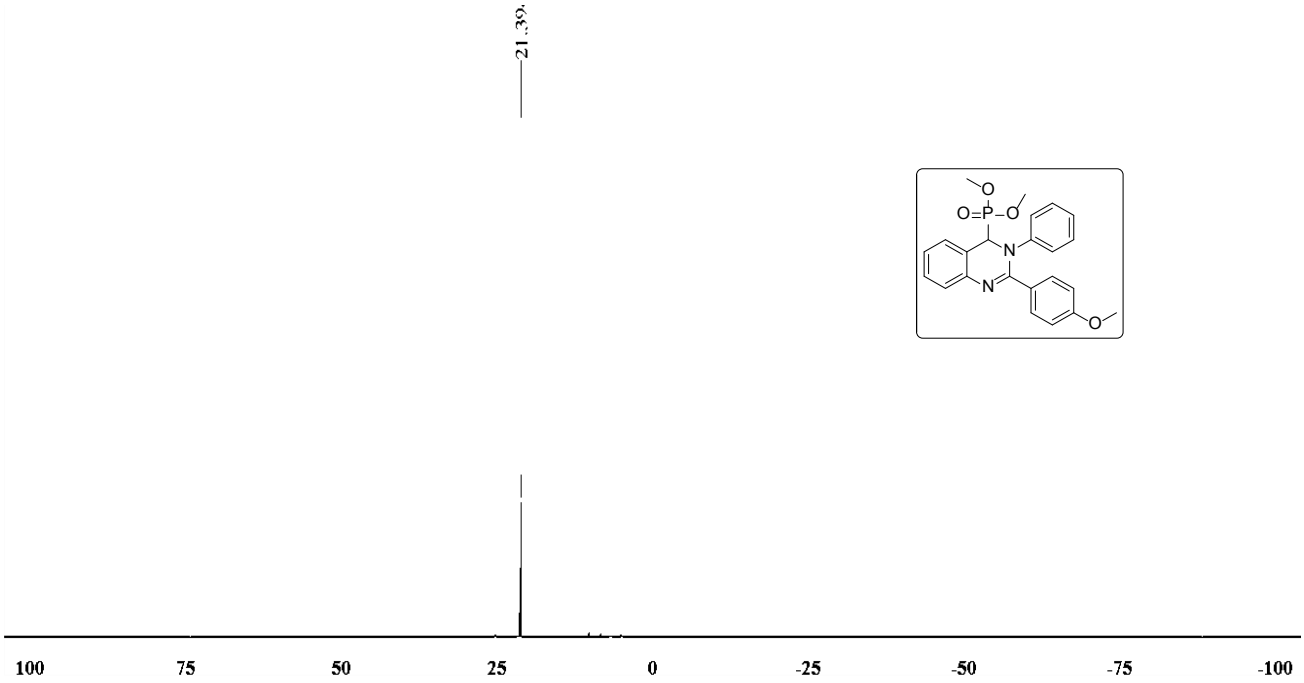
File Name C:\IICT-HRMS\16.01.2014\KRR-SAI-96
Sample Name
Sample ID G SAIDULU
Date and Time 16-01-14 17:15:13



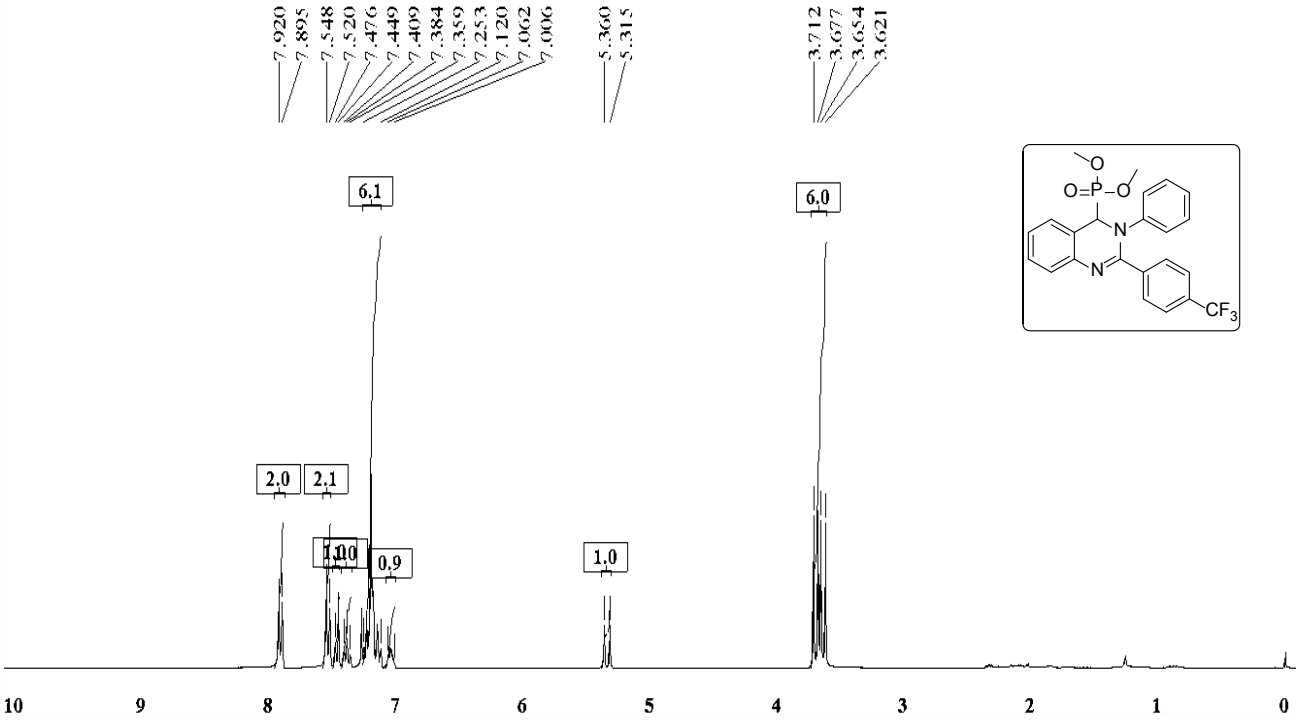
KRR-SAI-96#8-30 RT: 0.03-0.10 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
423.14615	256755584.0	100.00	423.14682	-1.59	13.5	$C_{23}H_{24}O_4N_2P$
424.14940	60567468.0	23.59				

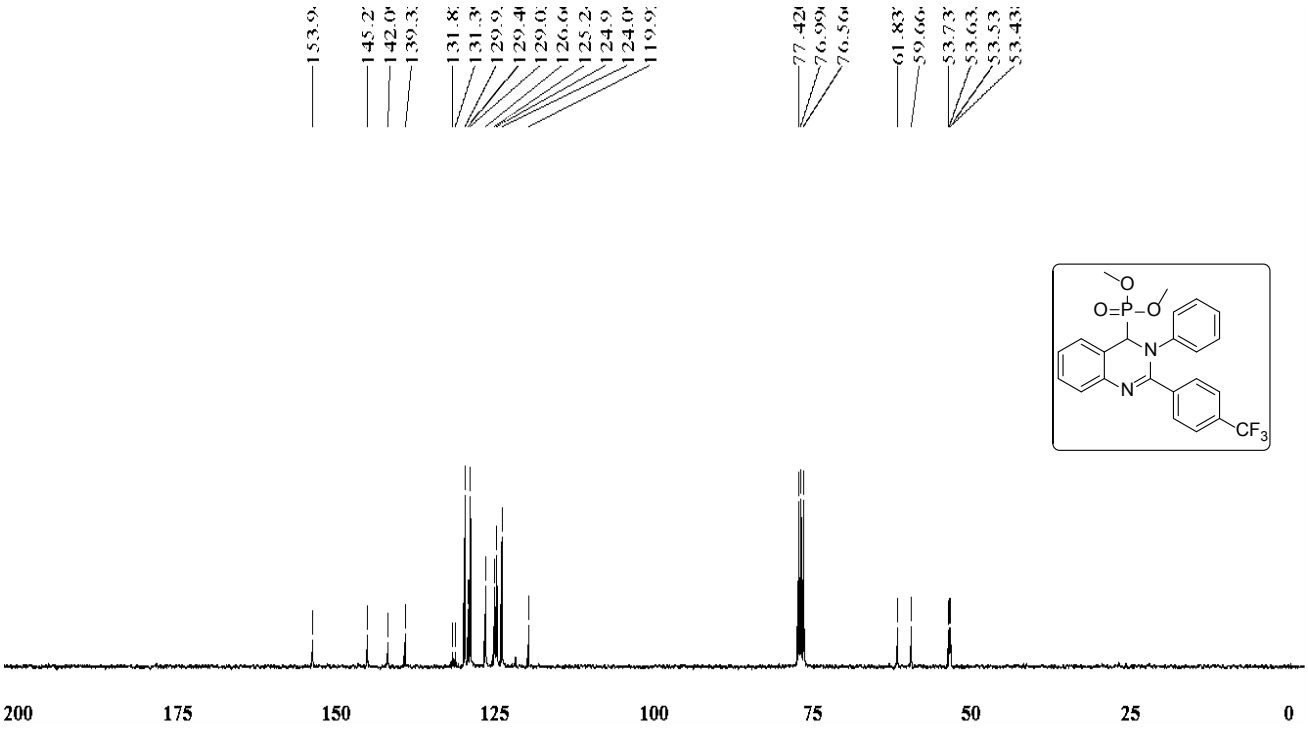
^{31}P NMR (202 MHz, $CDCl_3$): (Table 3, 7b)



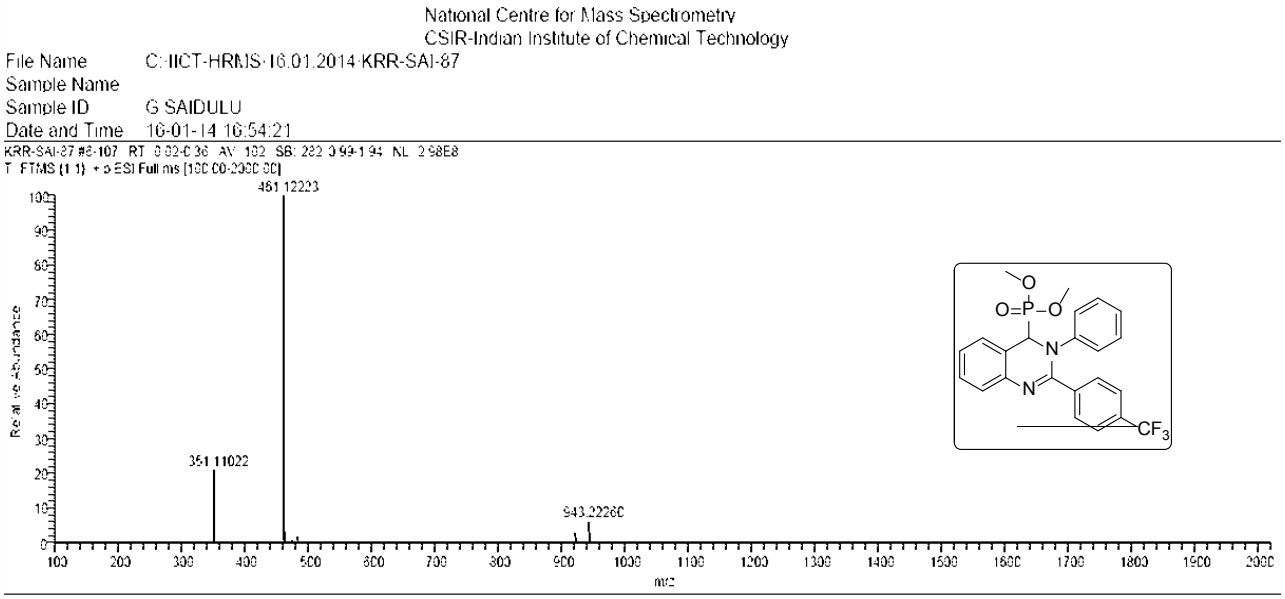
^{1}H NMR (300 MHz, $CDCl_3$): (Table 3, 7c)



^{13}C NMR (75 MHz, $CDCl_3$): (Table 3, 7c)



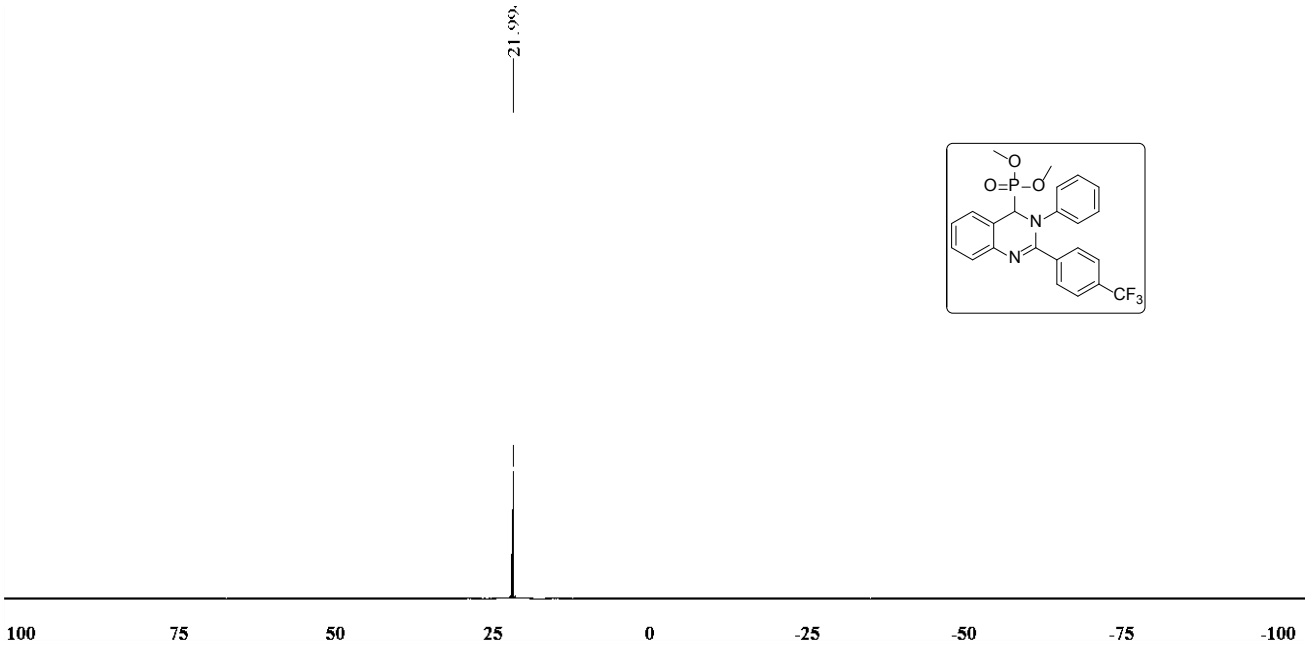
HIGH RESOLUTION MASS SPECTRA: (Table 3, 7c)



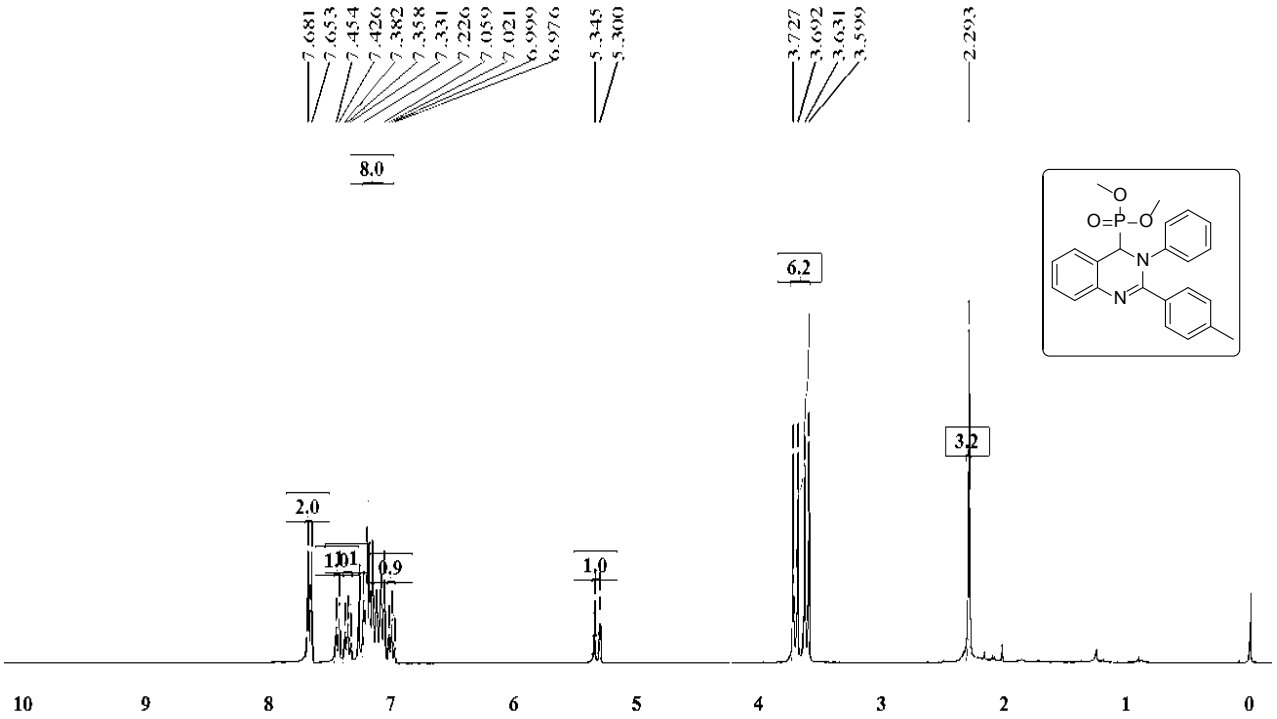
KRR-SAI-87#8-30 RT: 0.03-0.10 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
461.12219	357058752.0	100.00	461.12364	-3.14	13.5	$C_{23}H_{21}O_3N_2F_3P$
462.12617	80502408.0	22.55				

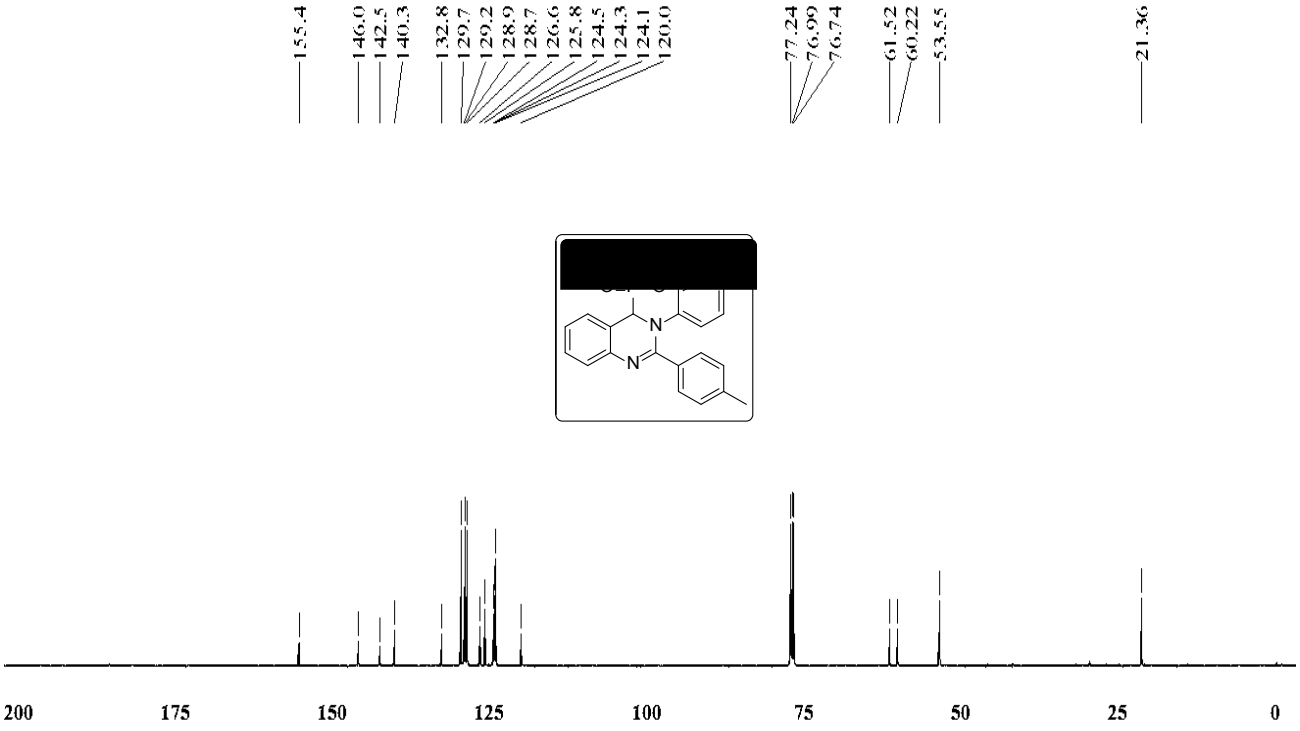
^{31}P NMR (202 MHz, $CDCl_3$): (Table 3, 7c)



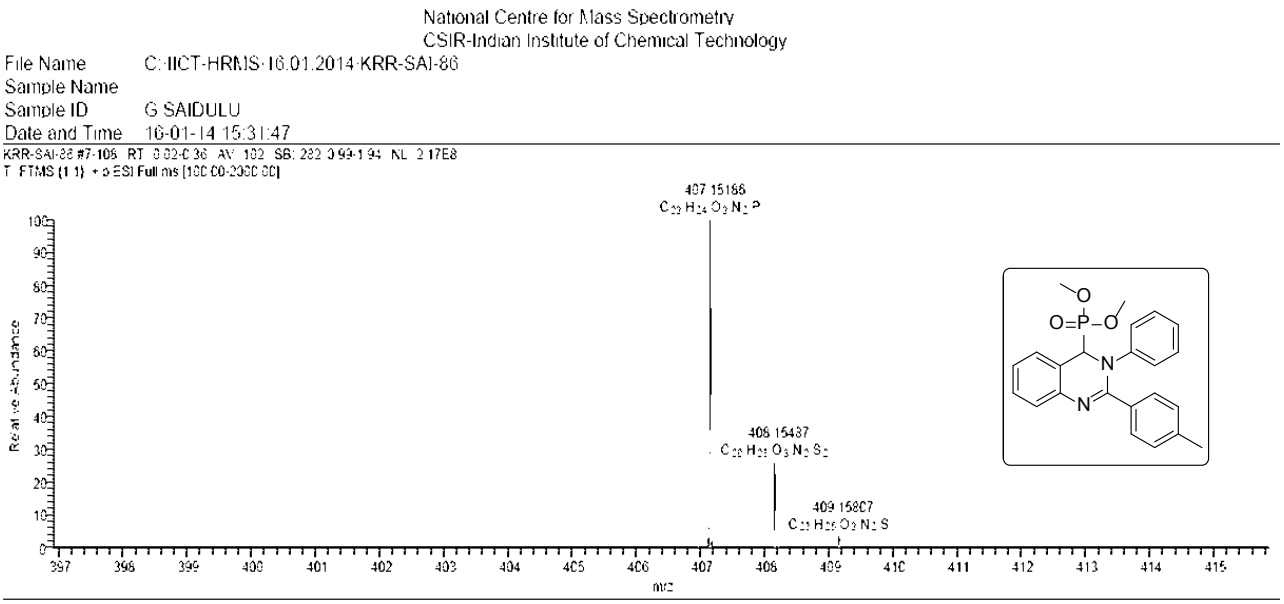
^{1}H NMR (300 MHz, $CDCl_3$): (Table 3, 7d)



^{13}C NMR (125 MHz, $CDCl_3$): (Table 3, 7d)



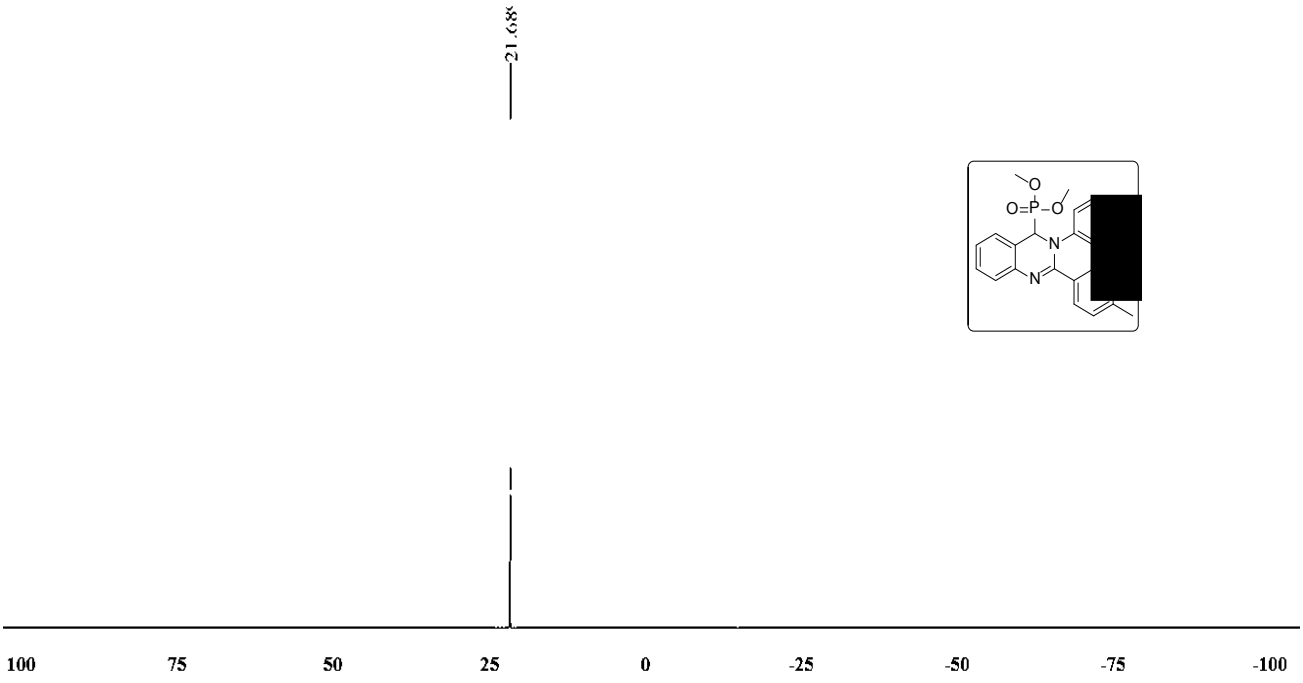
HIGH RESOLUTION MASS SPECTRA: (Table 3, 7d)



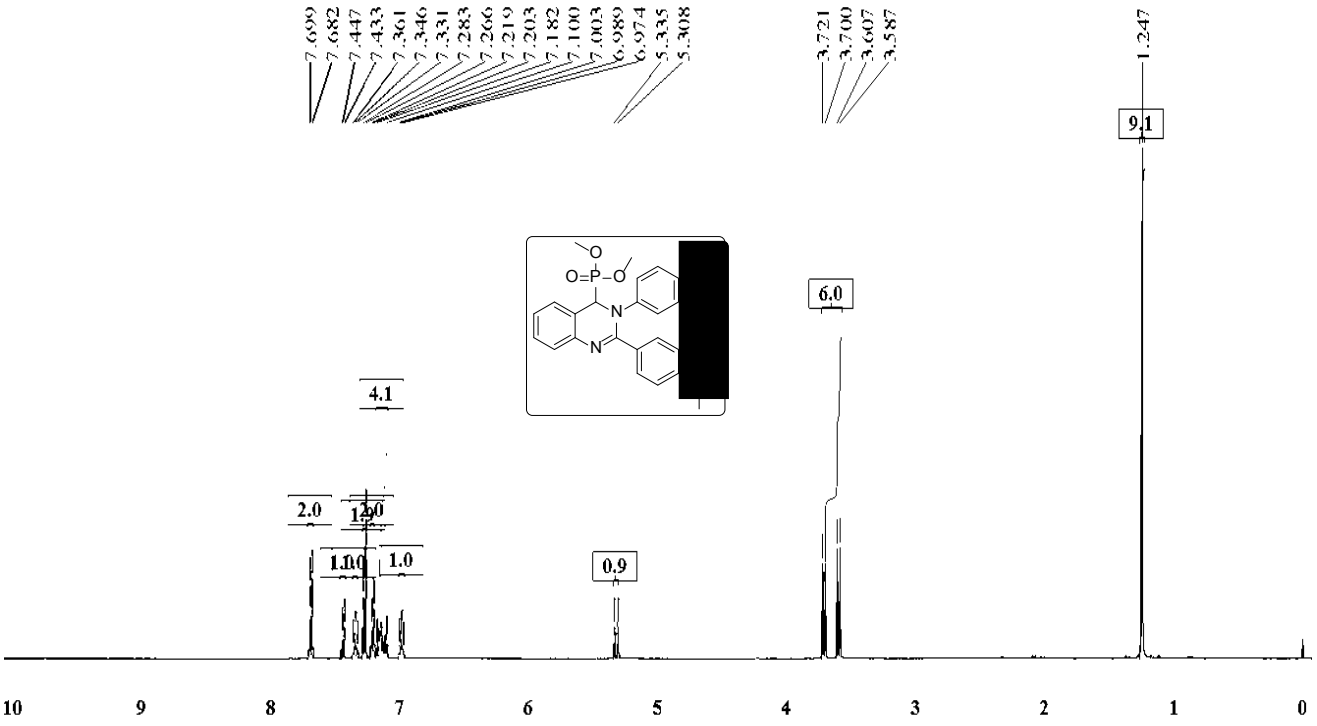
KRR-SAI-86#8-30 RT: 0.03-0.10 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
297.13862	104728592.0	29.78				
407.15186	351704000.0	100.00				

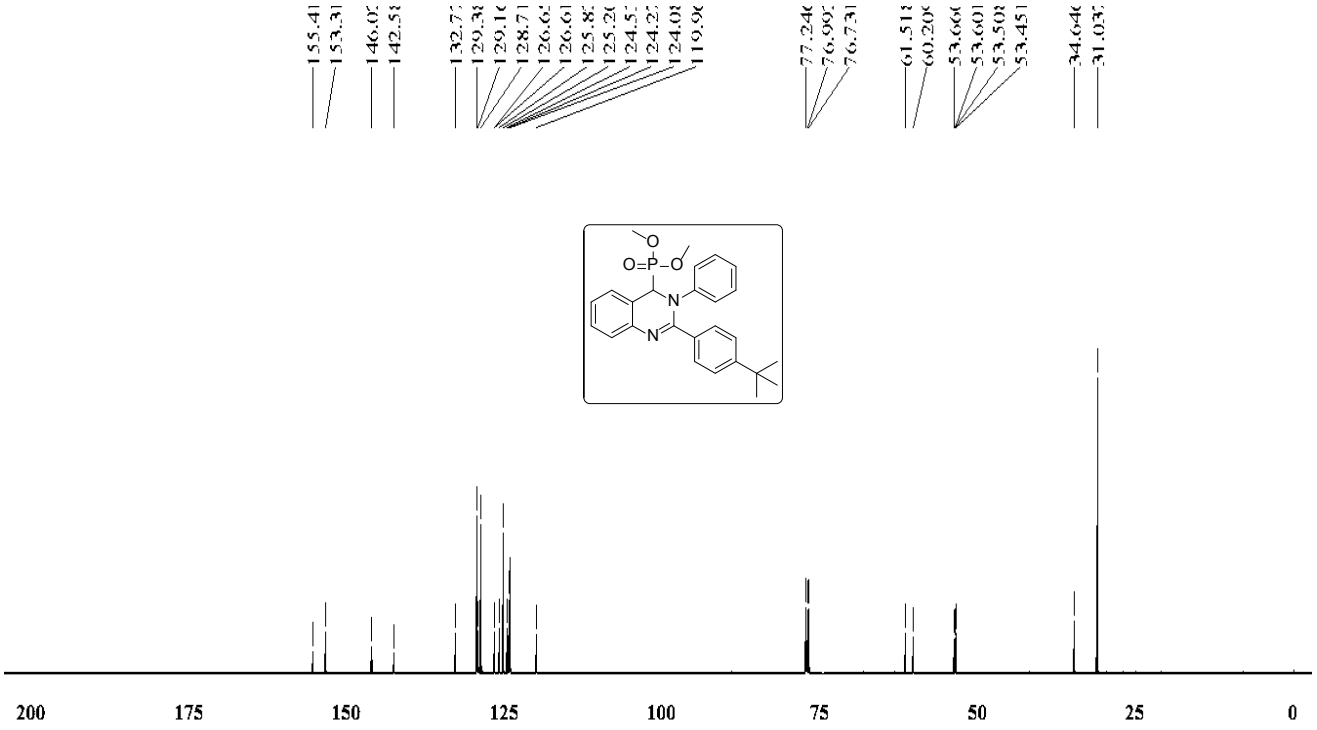
^{31}P NMR (202 MHz, $CDCl_3$): (Table 3, 7d)



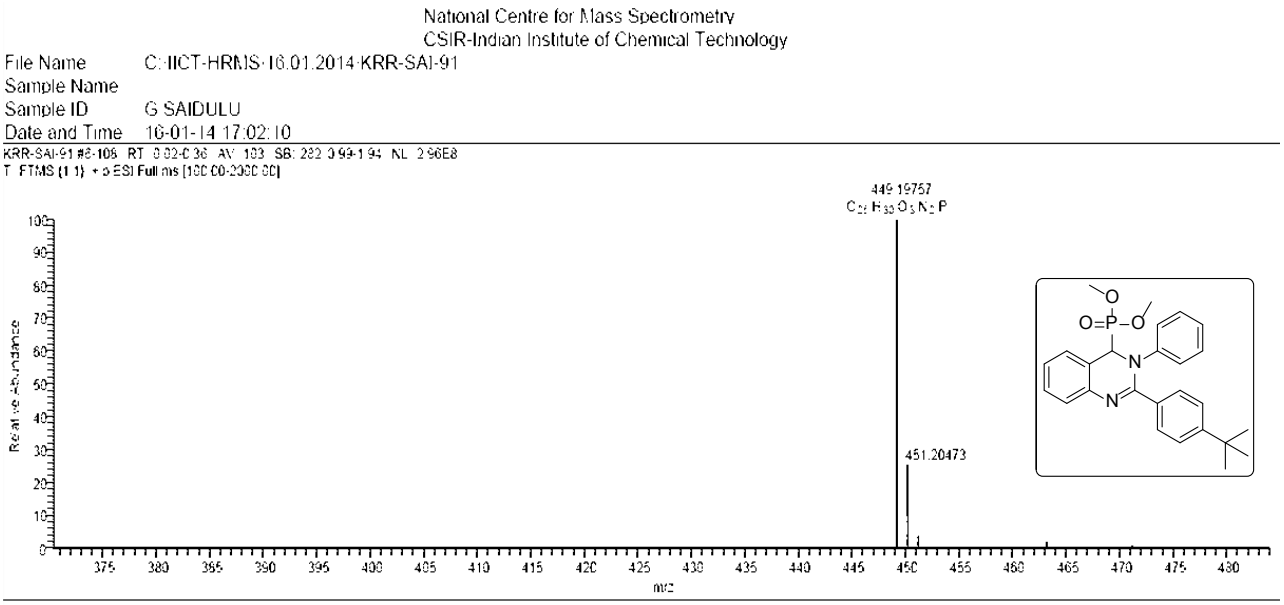
^{1}H NMR (500 MHz, $CDCl_3$): (Table 3, 7e)



^{13}C NMR (125 MHz, $CDCl_3$): (Table 3, 7e)



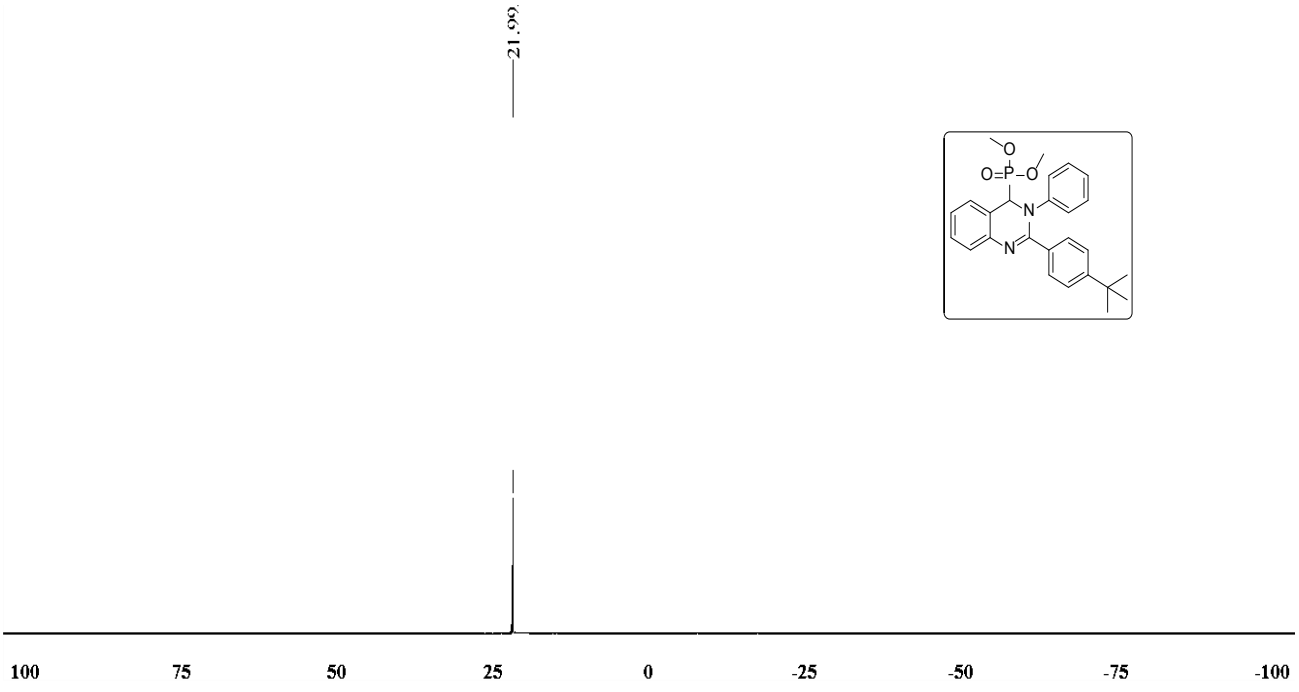
HIGH RESOLUTION MASS SPECTRA: (Table 3, 7e)



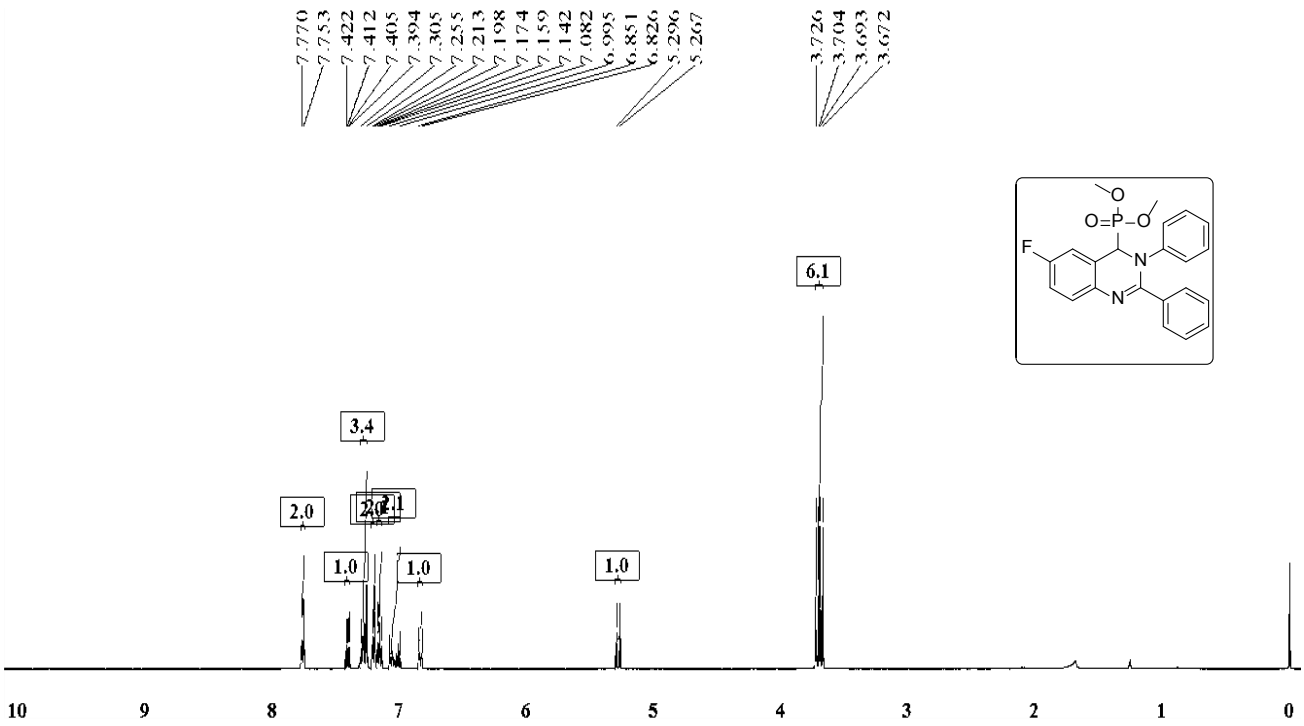
KRR-SAI-91#8-30 RT: 0.03-0.10 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
449.19751	386733952.0	100.00				
450.20126	99731704.0	25.79				

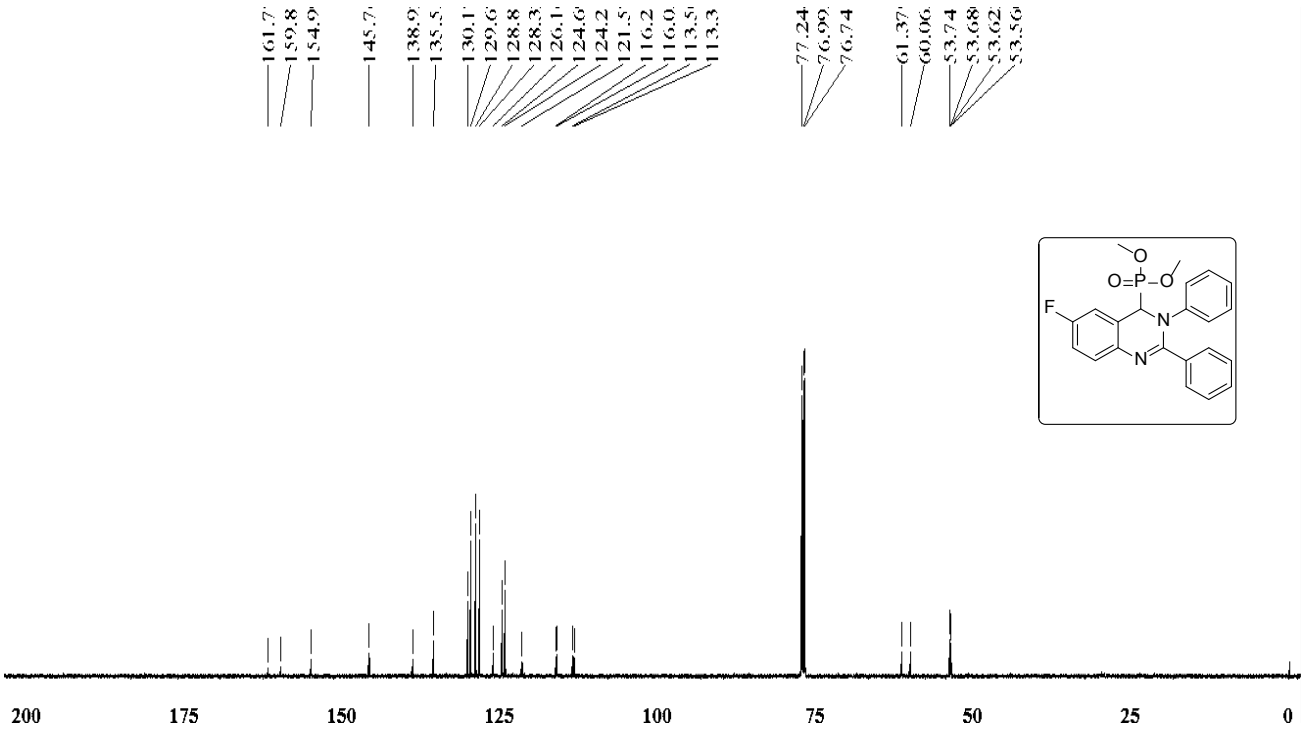
^{31}P NMR (202 MHz, $CDCl_3$): (Table 3, 7e)



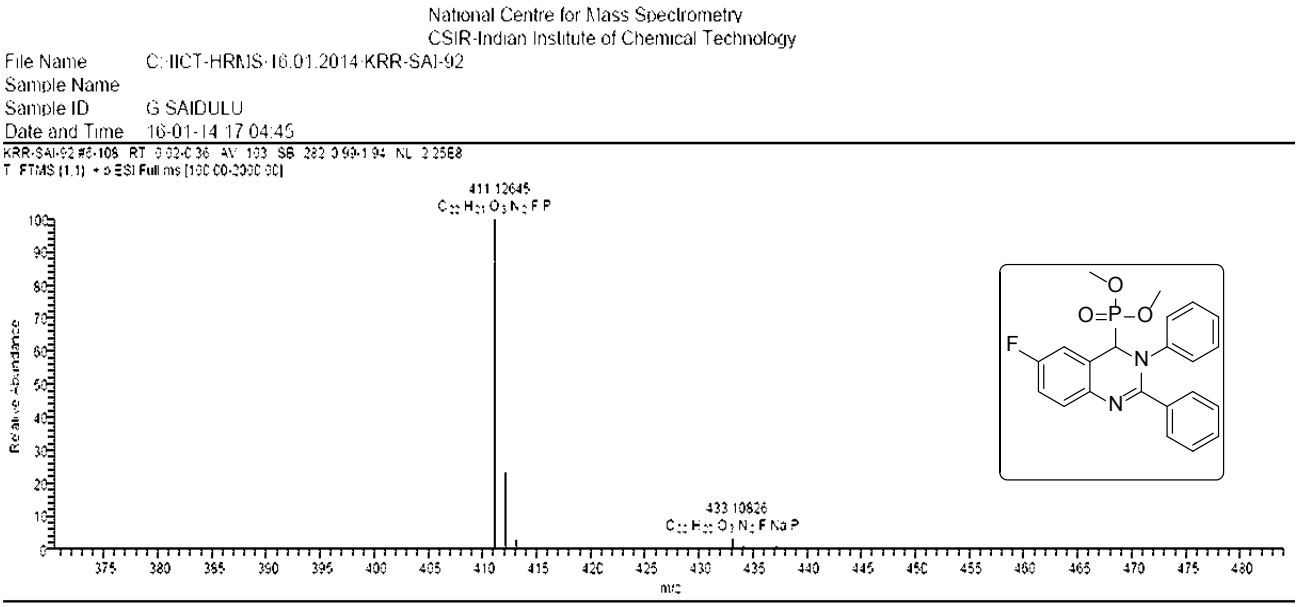
^{1}H NMR (500 MHz, $CDCl_3$): (Table 3, 7f)



^{13}C NMR (125 MHz, $CDCl_3$): (Table 3, 7f)



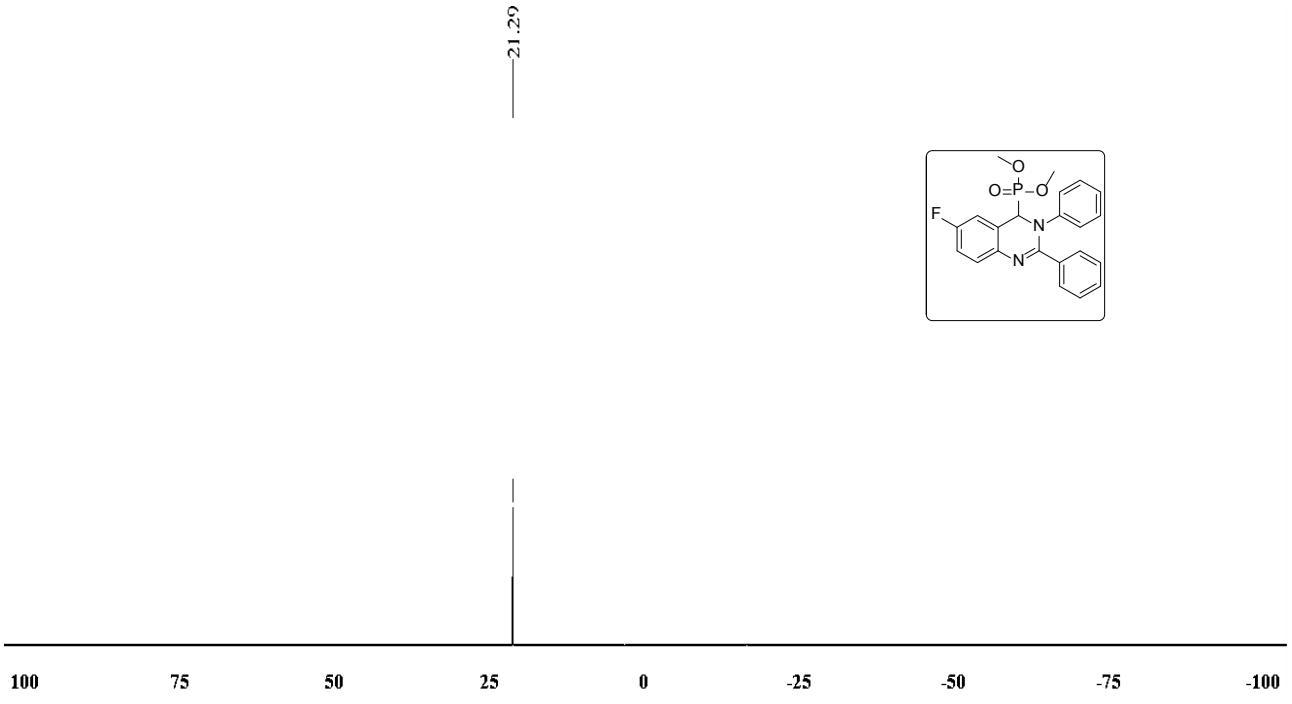
HIGH RESOLUTION MASS SPECTRA: (Table 3, 7f)



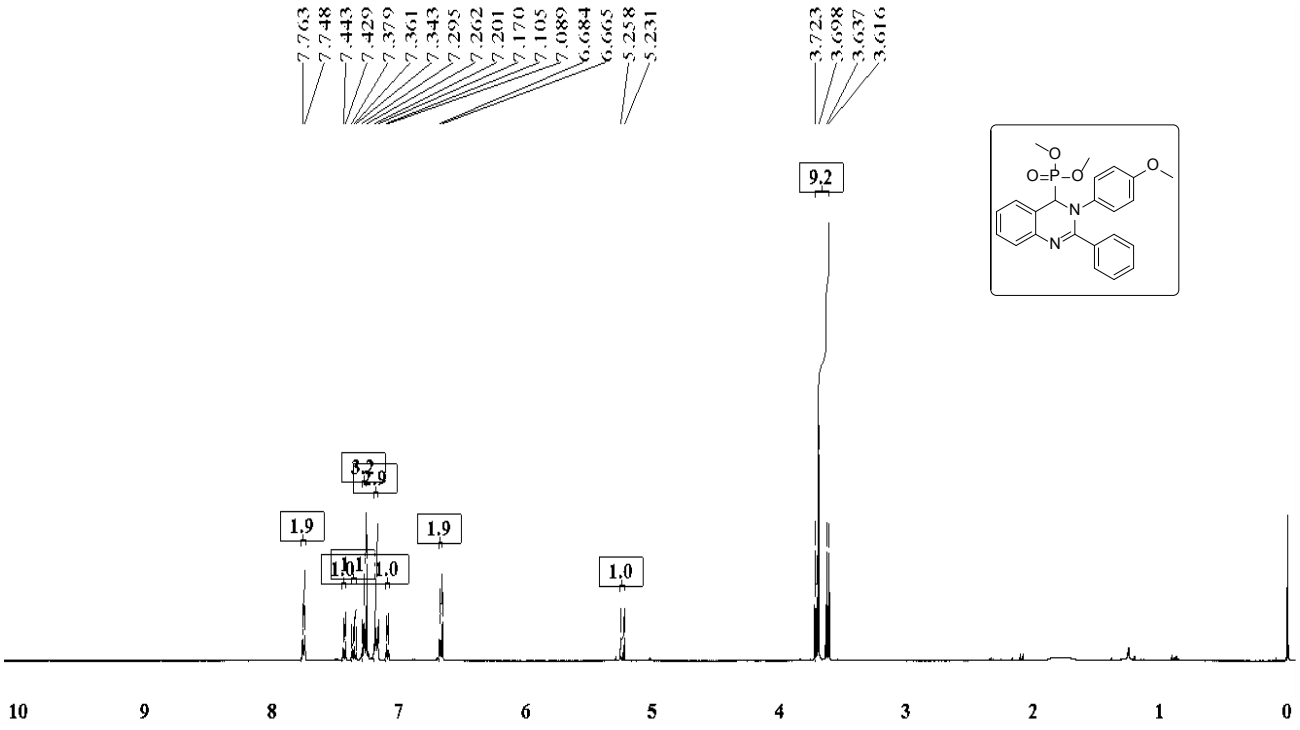
KRR-SAI-92#8-30 RT: 0.03-0.10 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
301.11343	105868544.0	34.30				
411.12646	308653088.0	100.00				

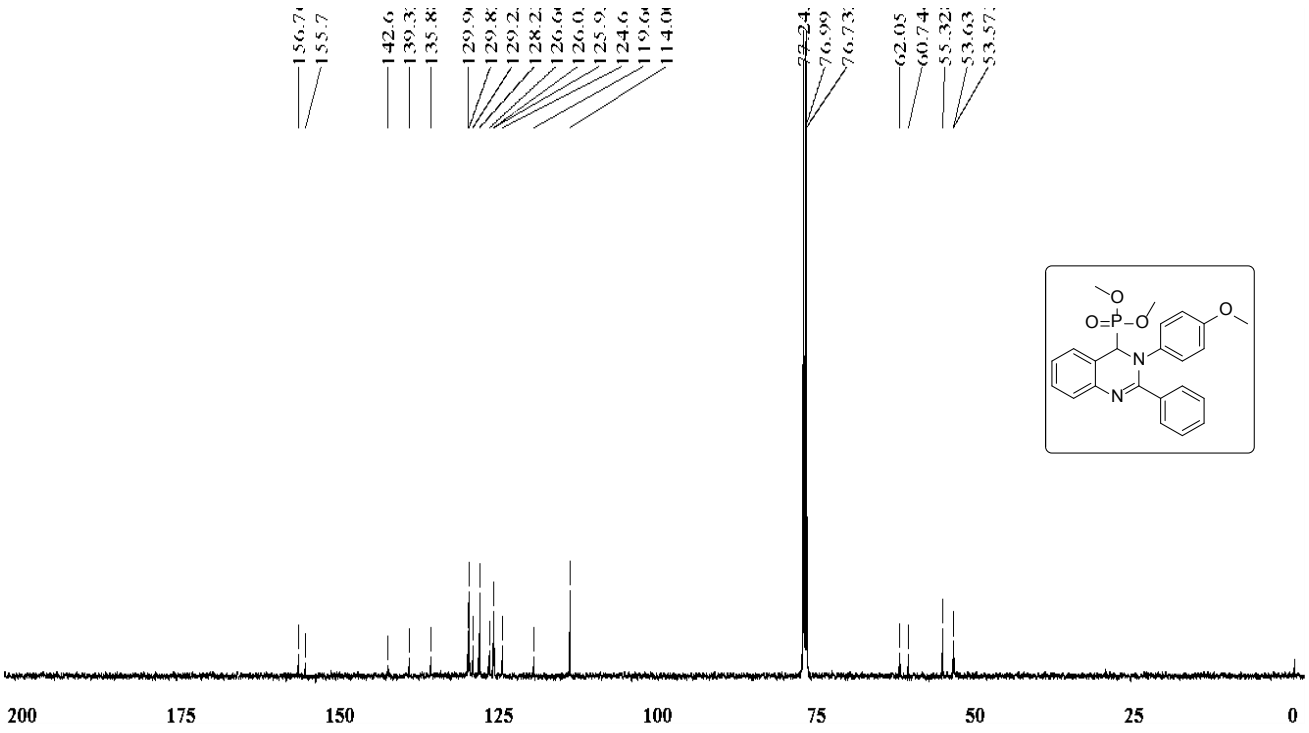
^{31}P NMR (202 MHz, $CDCl_3$): (Table 3, 7f)



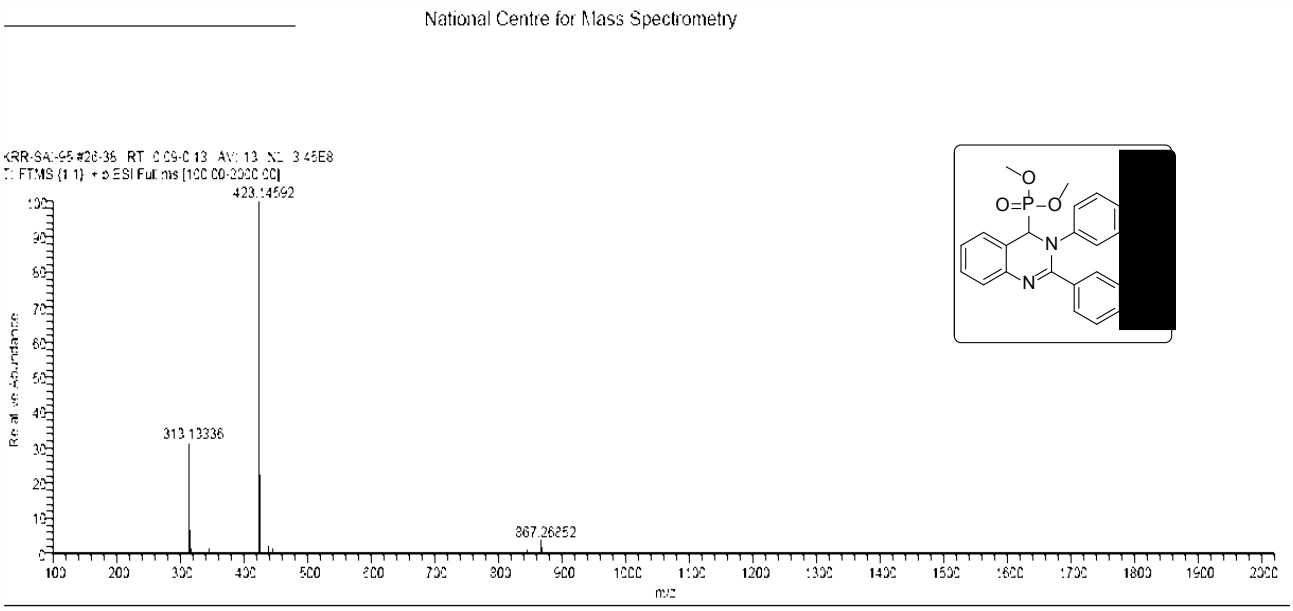
^{1}H NMR (500 MHz, $CDCl_3$): (Table 1, 7g)



^{13}C NMR (125 MHz, $CDCl_3$): (Table 1, 7g)



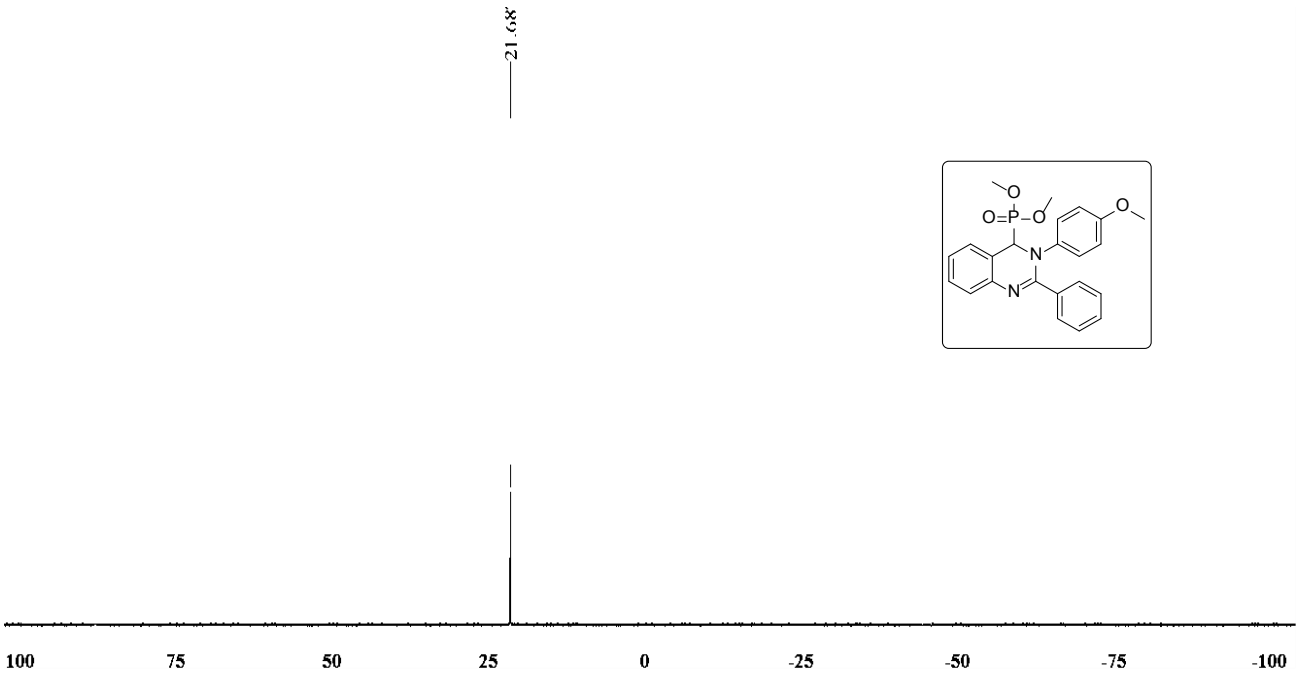
HIGH RESOLUTION MASS SPECTRA: (Table 1, 7g)



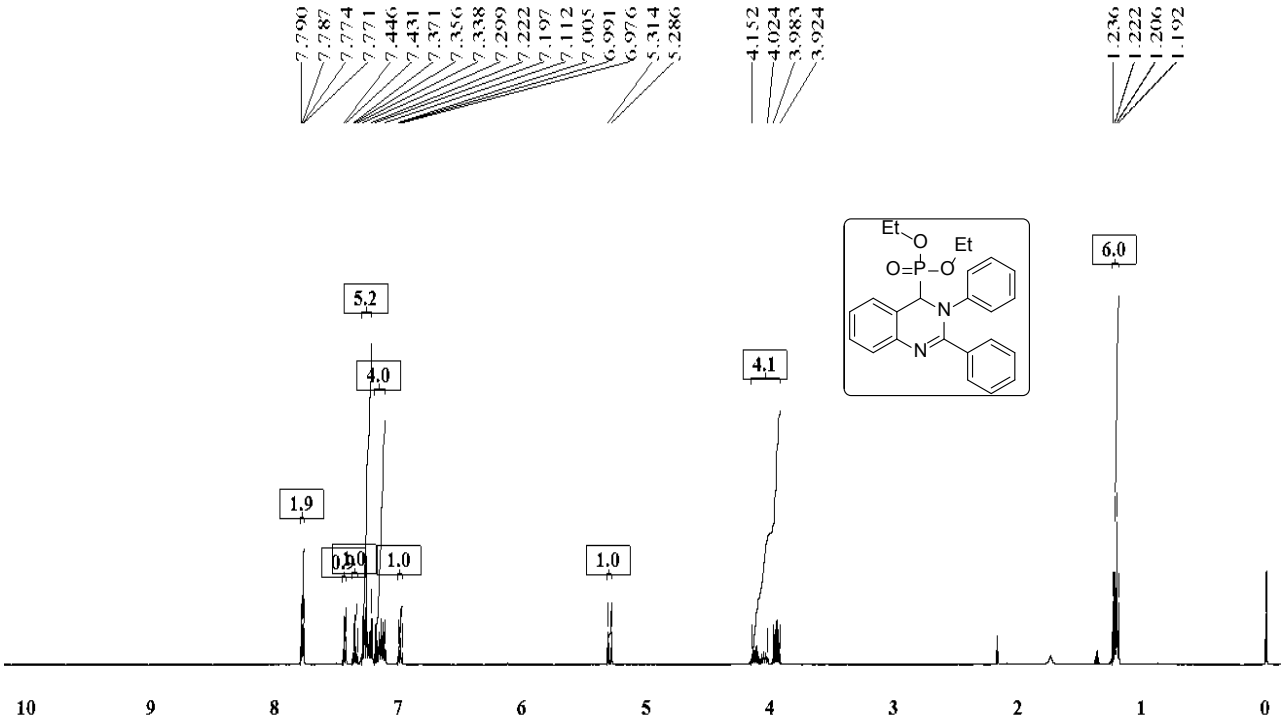
KRR-SAI-95#8-30 RT: 0.03-0.10 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]
m/z= 343.91-596.38

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
423.14615	252058624.0	100.00	423.14682	-1.58	13.5	$C_{23}H_{24}O_4N_2P$
424.14945	60046328.0	23.82				

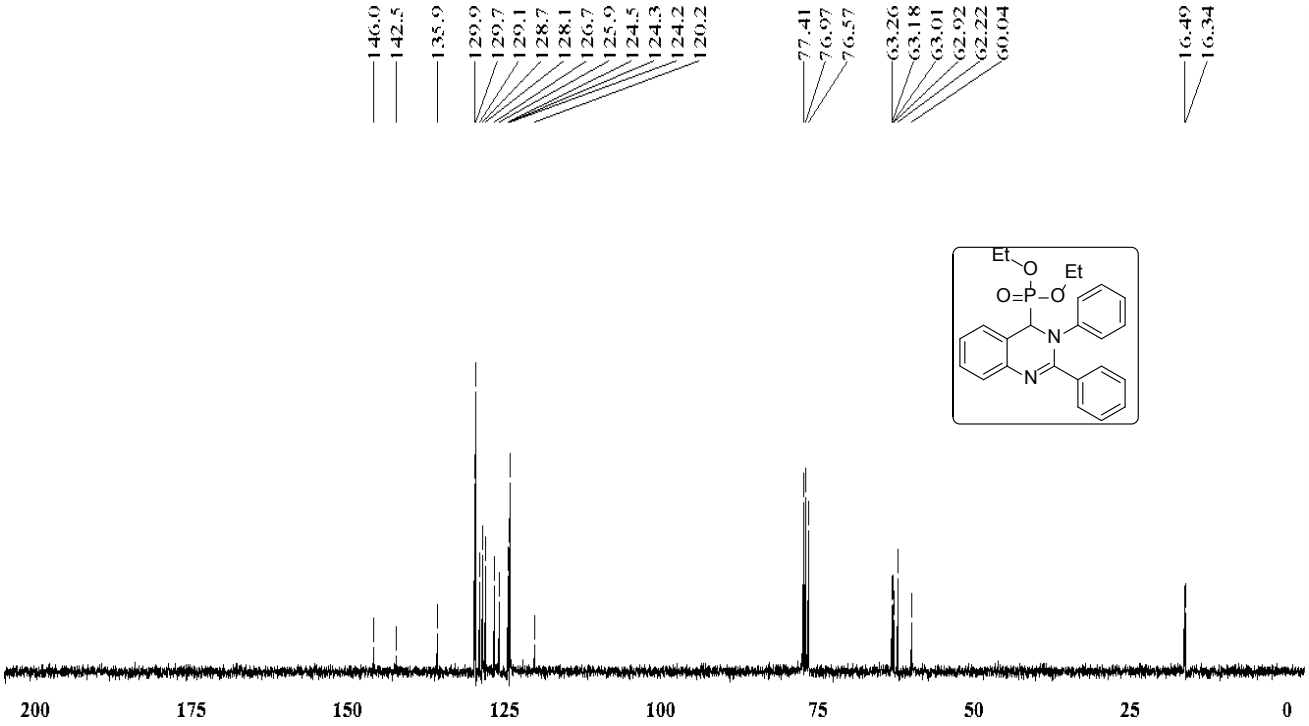
^{31}P NMR (500 MHz, $CDCl_3$): (Table 1, 7g)



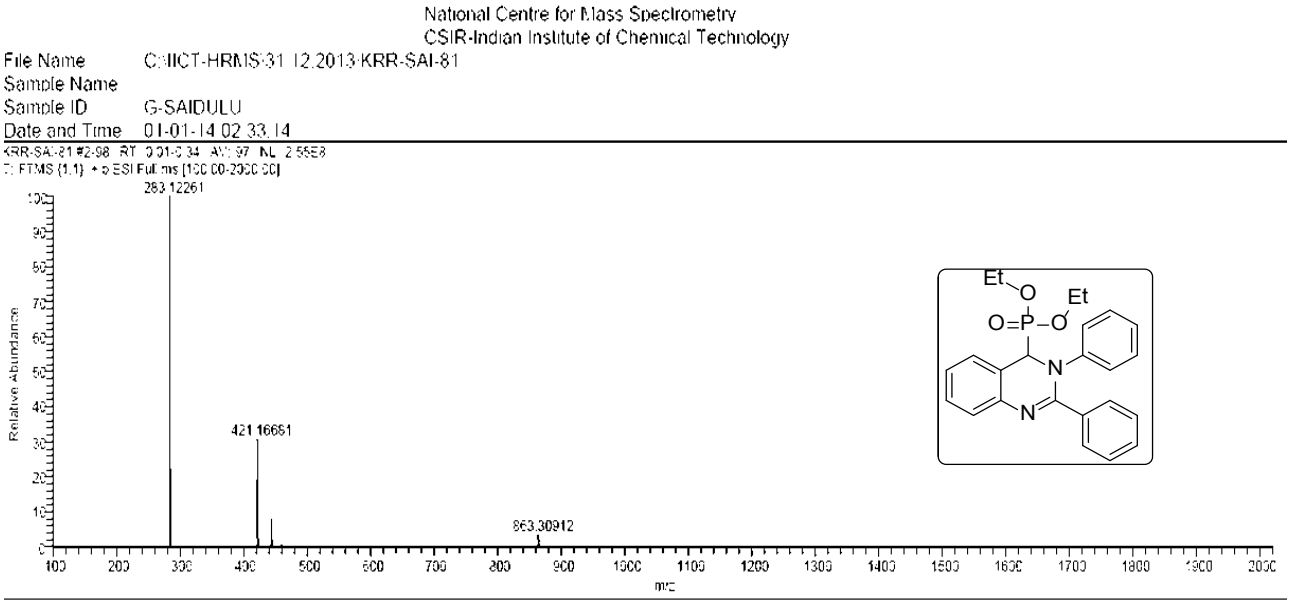
^{1}H NMR (500 MHz, $CDCl_3$): (Table 3, 7h)



^{13}C NMR (75 MHz, $CDCl_3$): (Table 3, 7h)



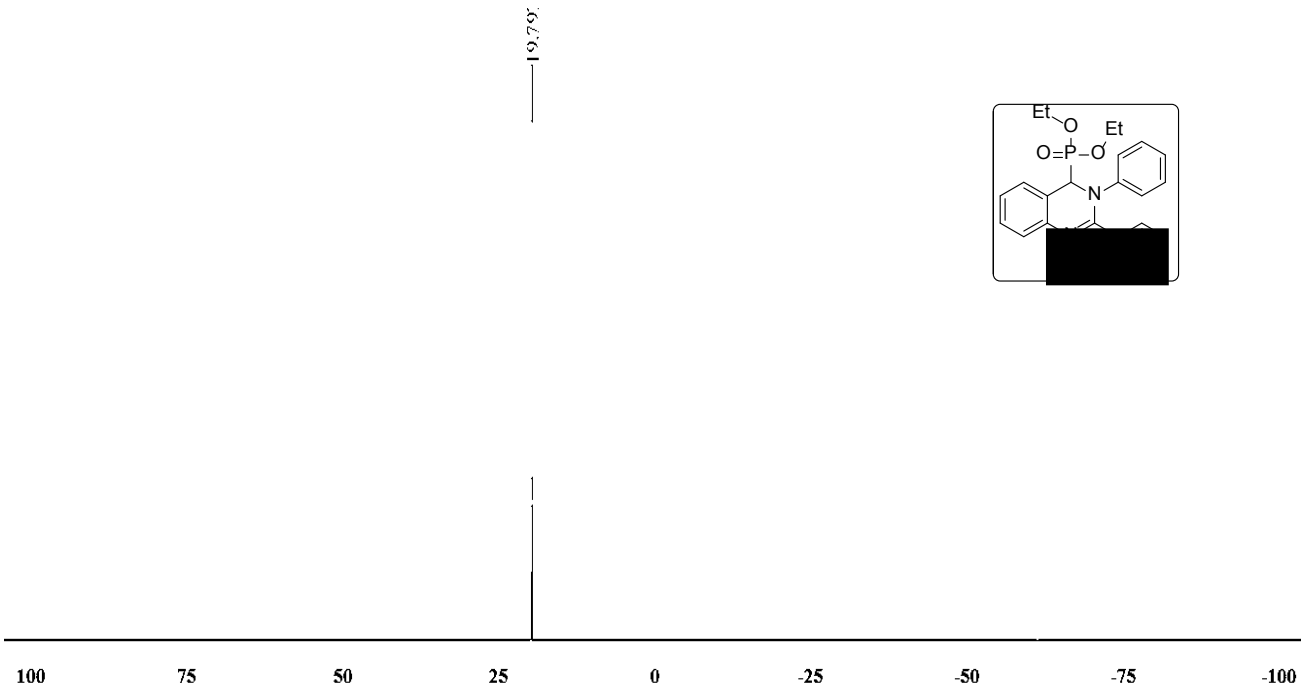
HIGH RESOLUTION MASS SPECTRA: (Table 3, 7h)



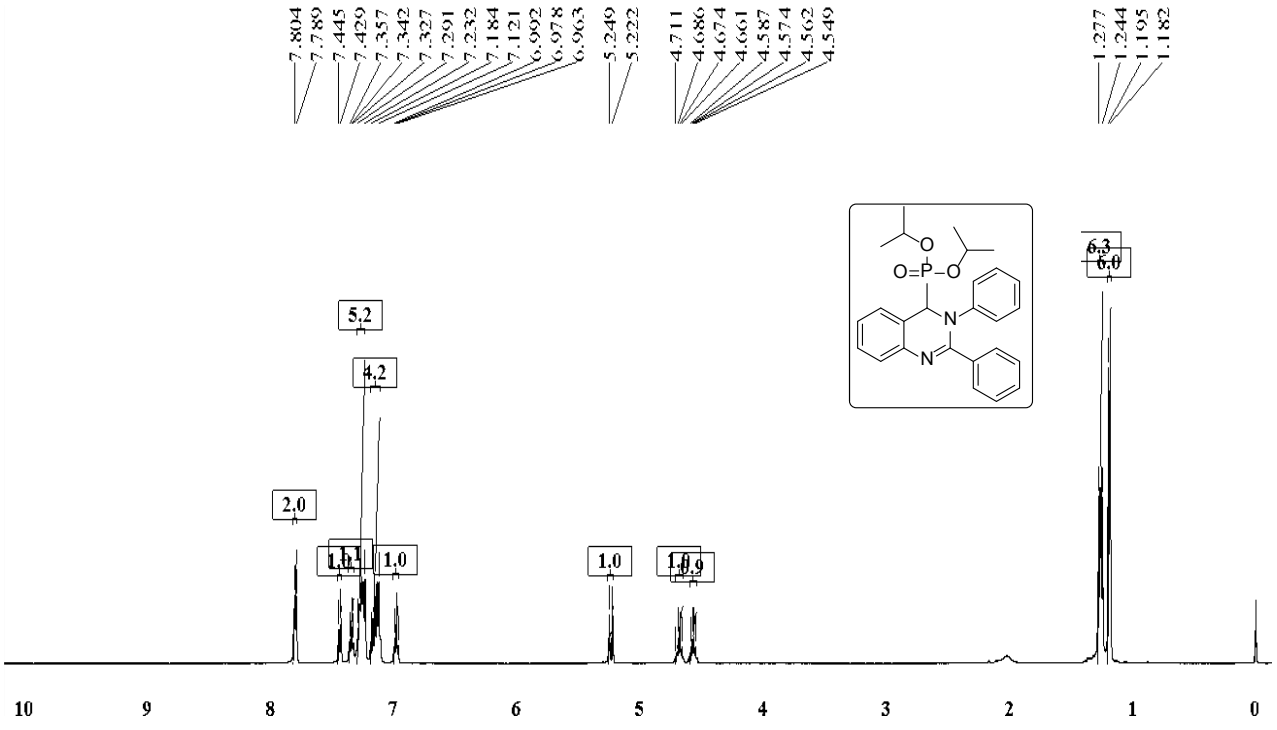
KRR-SAI-81#8-30 RT: 0.03-0.11 AV: 23
I: FTMS {1,1} + p ESI Full ms [100.00-2000.00]
m/z= 399.45-448.68

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
421.16671	133806960.0	100.00	421.16756	-2.01	13.5	$C_{24}H_{26}O_3N_2P$
443.14885	54426320.0	40.68	443.14950	-1.48	13.5	$C_{24}H_{25}O_3N_2NaP$

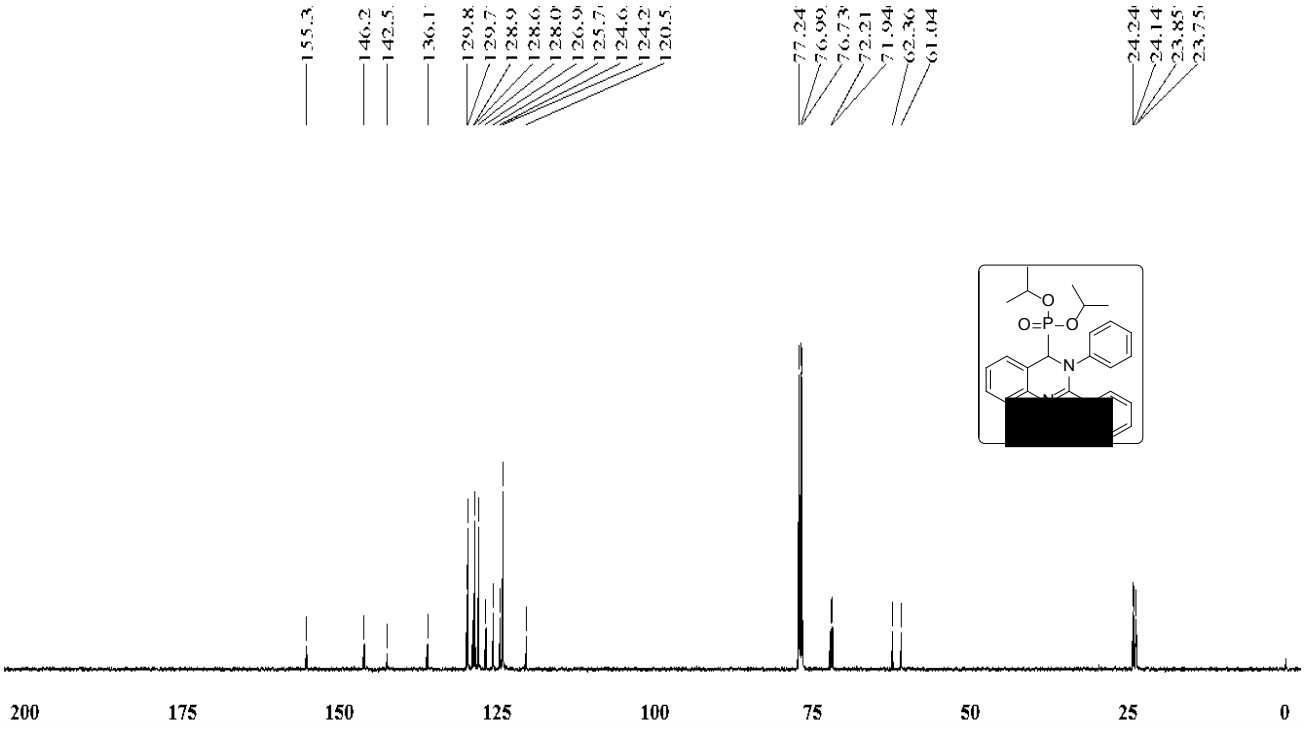
^{31}P NMR (202 MHz, $CDCl_3$): (Table 3, 7h)



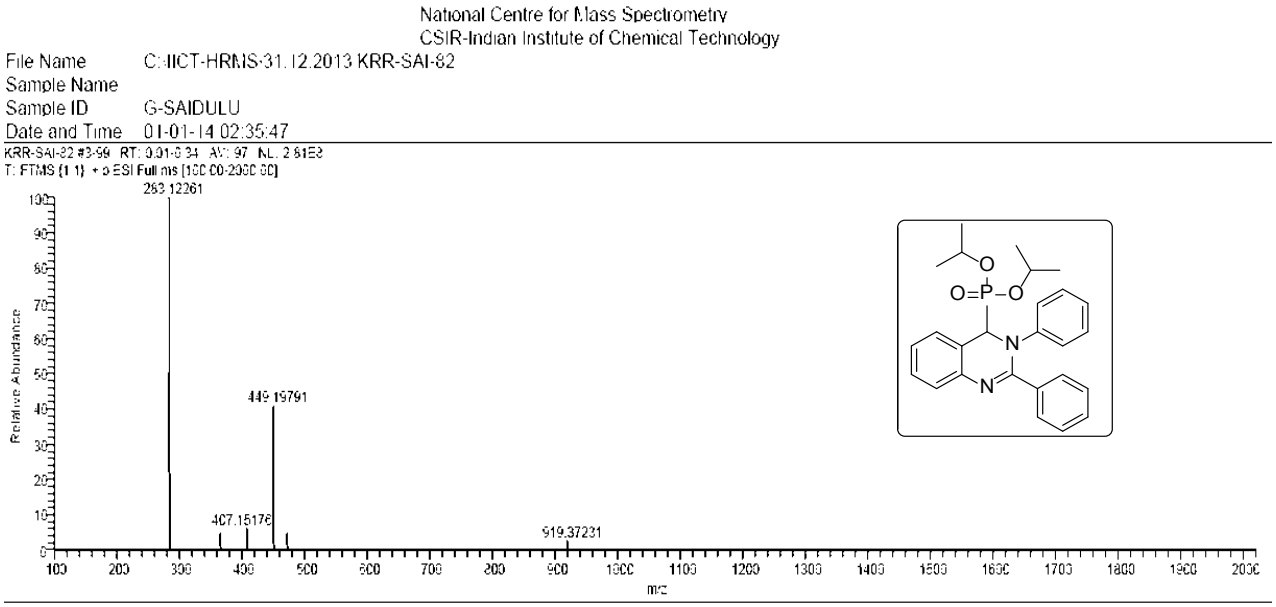
^{1}H NMR (500 MHz, $CDCl_3$): (Table 3, 7i)



^{13}C NMR (125 MHz, $CDCl_3$): (Table 3, 7i)



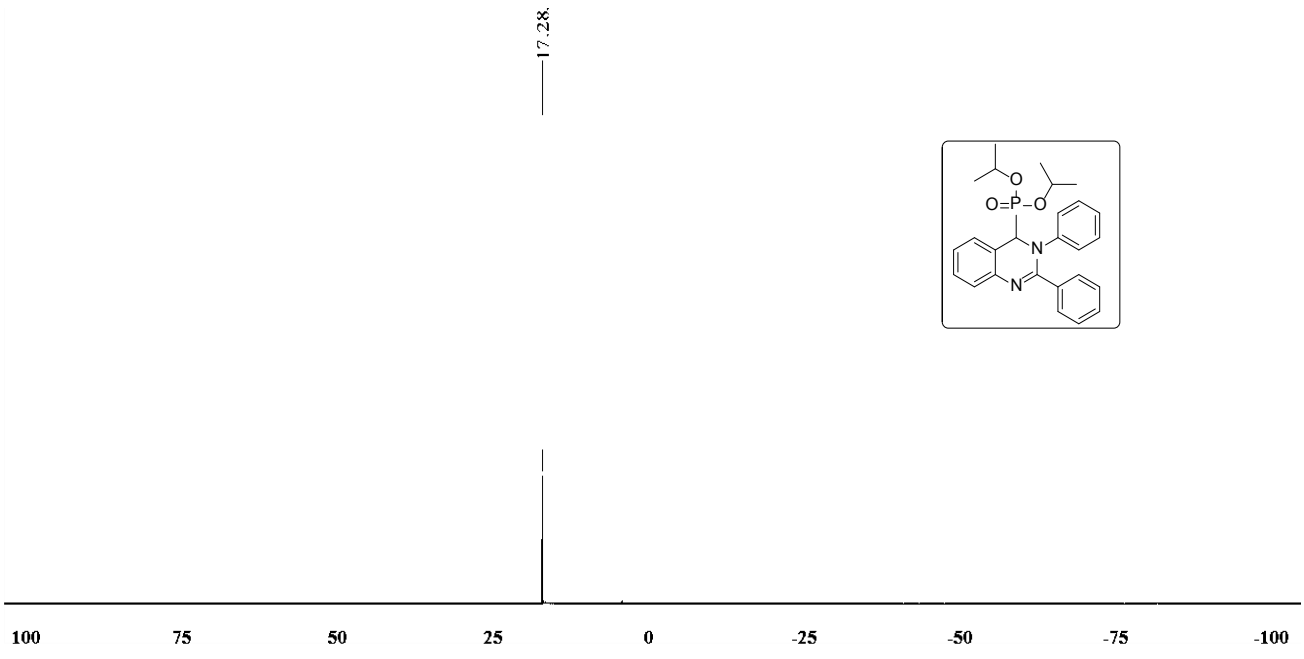
HIGH RESOLUTION MASS SPECTRA: (Table 3, 7i)



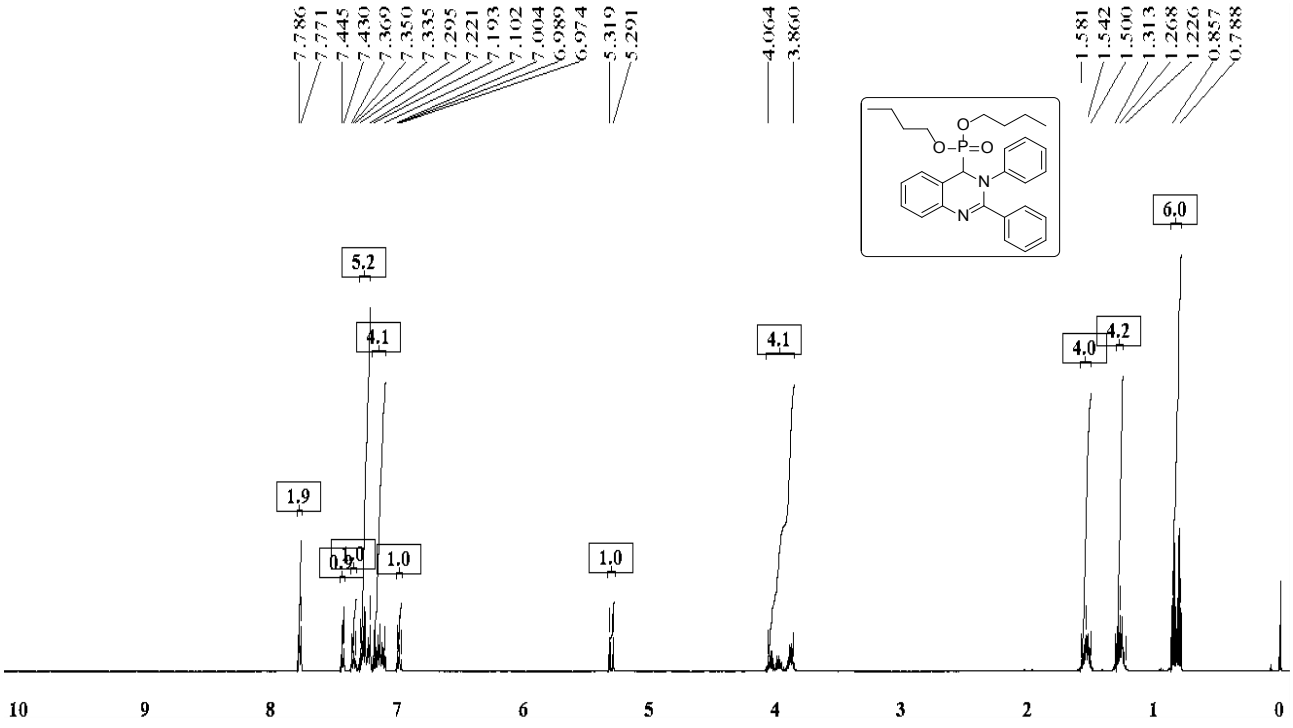
KRR-SAI-82#8-30 RT: 0.03-0.11 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]
m/z= 417.12-484.03

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
449.19767	170649056.0	100.00	449.19886	-2.64	13.5	$C_{26}H_{30}O_3N_2P$
450.20179	45042236.0	26.39				

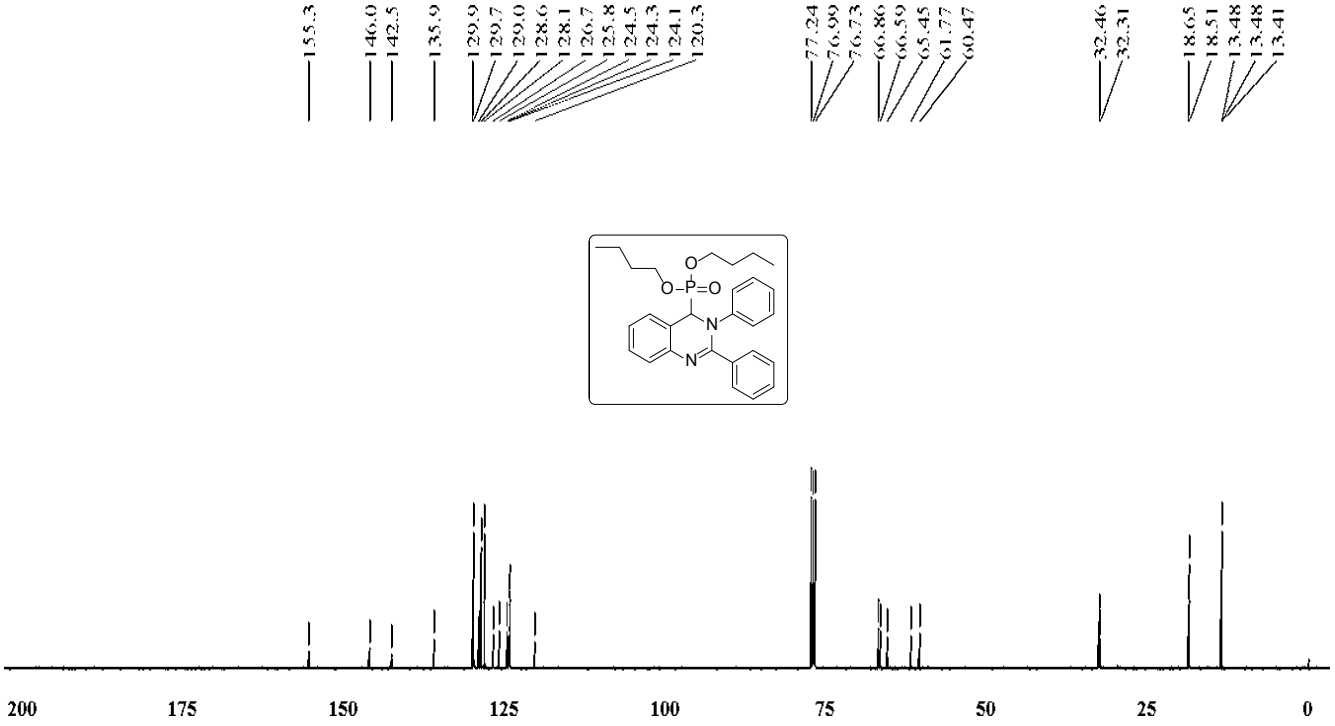
^{31}P NMR (202 MHz, $CDCl_3$): (Table 3, 7i)



^{1}H NMR (500 MHz, $CDCl_3$): (Table 3, 7j)



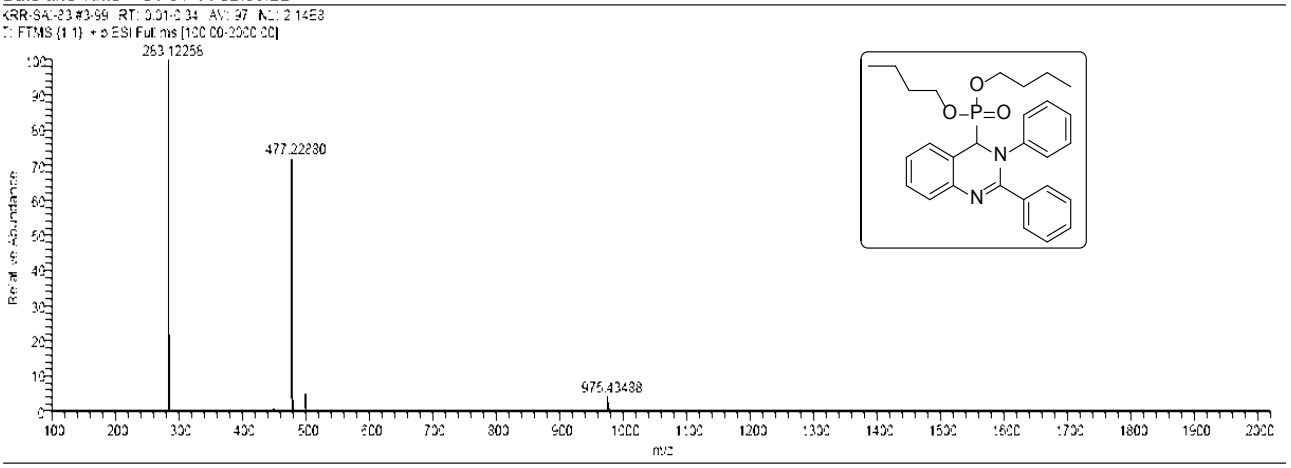
^{13}C NMR (125 MHz, $CDCl_3$): (Table 3, 7j)



HIGH RESOLUTION MASS SPECTRA: (Table 3, 7j)

National Centre for Mass Spectrometry
CSIR-Indian Institute of Chemical Technology

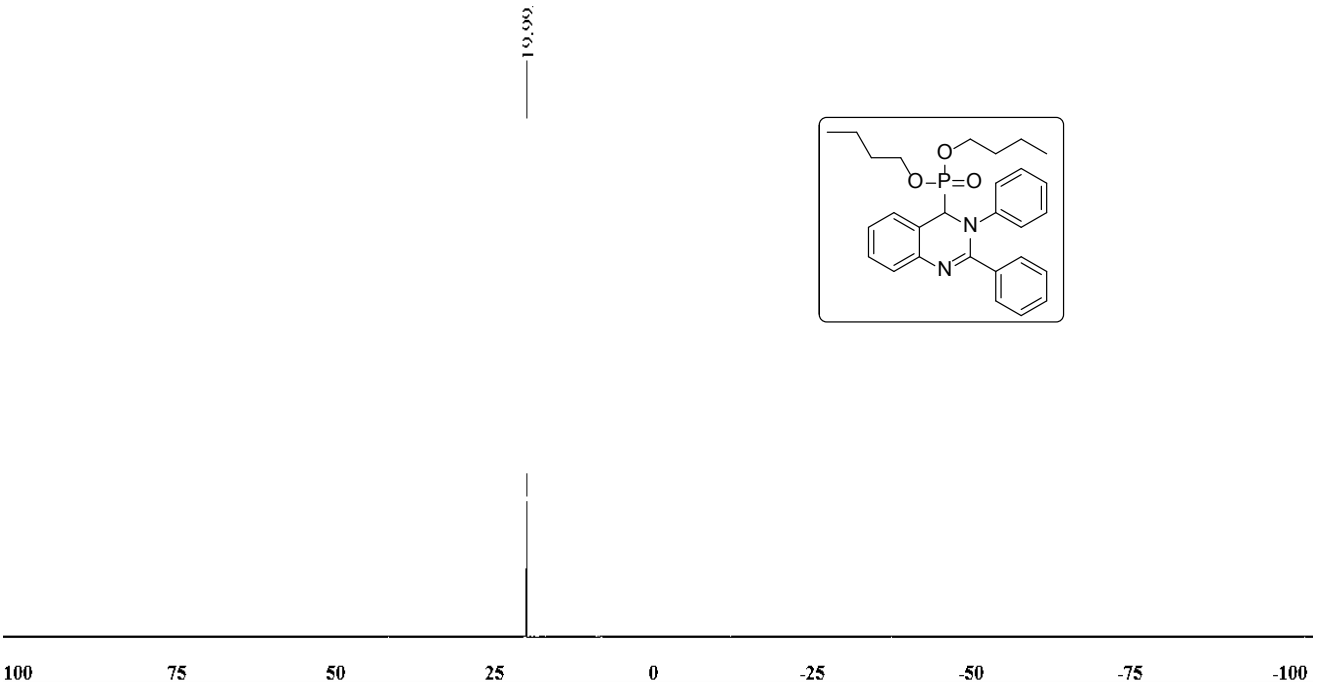
File Name C:\IICT-HRMS\31.12.2013\KRR-SAI-83
Sample Name
Sample ID G-SAIDULU
Date and Time 01-01-14 02:38:22



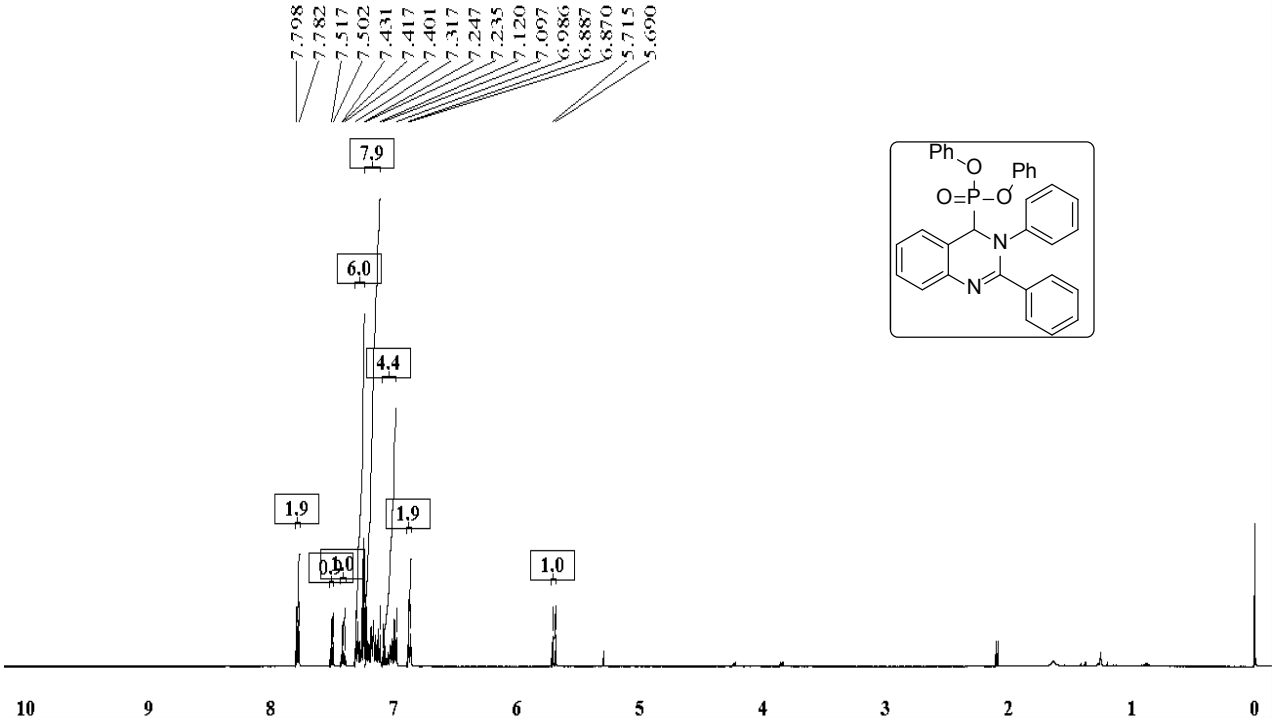
KRR-SAI-83#8-30 RT: 0.03-0.10 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]
m/z= 443.83-502.96

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
477.22861	187288384.0	100.00	477.22775	1.79	10.5	$C_{26}H_{35}O_3N_2NaP$
			477.23016	-3.25	13.5	$C_{29}H_{34}O_3N_2P$

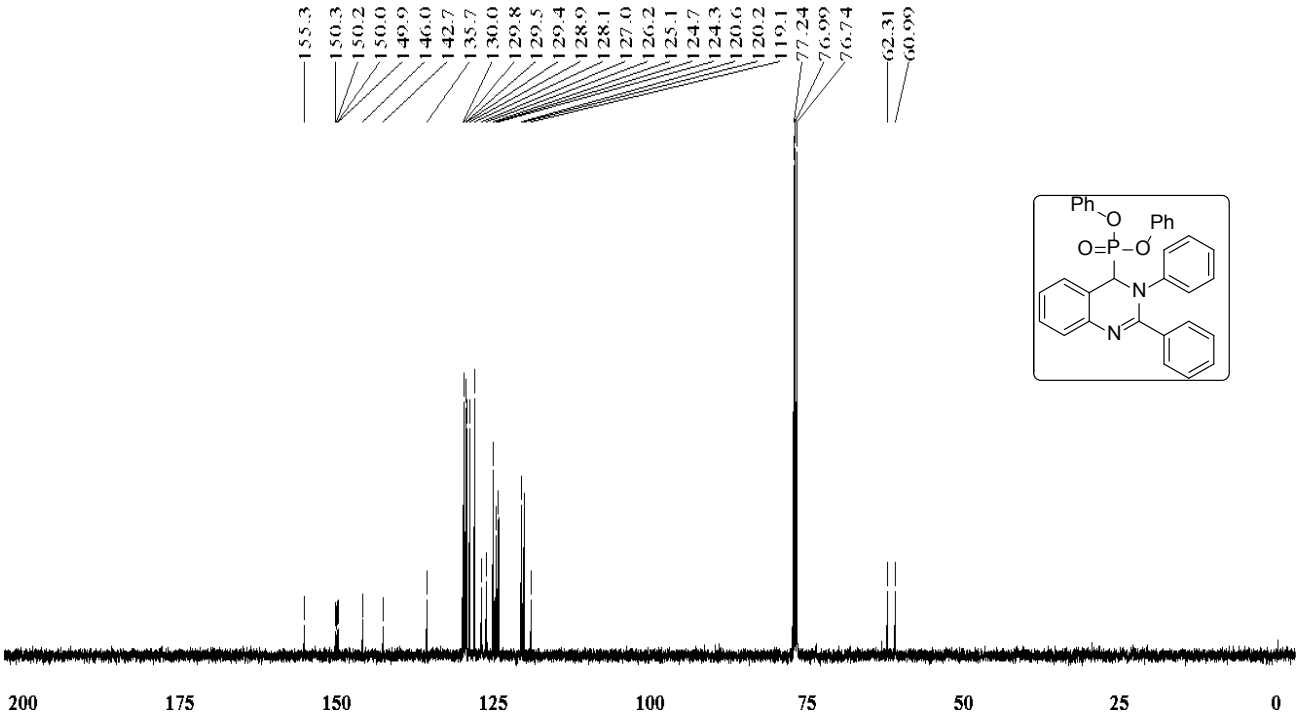
^{31}P NMR (202 MHz, $CDCl_3$): (Table 3, 7j)



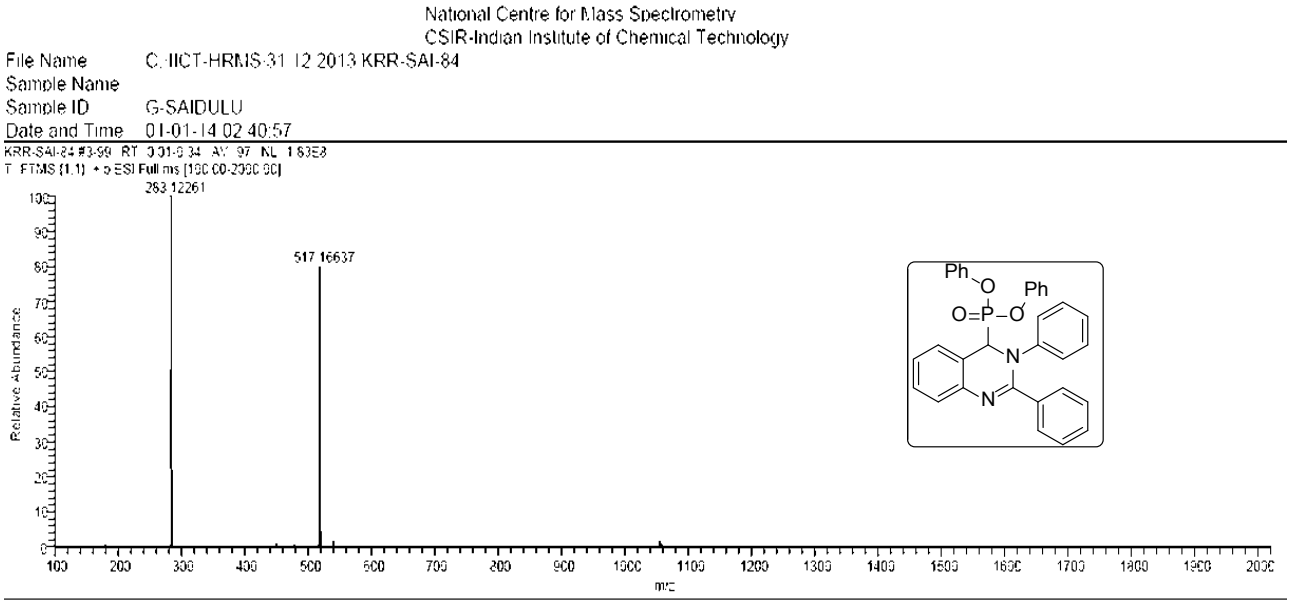
^{1}H NMR (300 MHz, $CDCl_3$): (Table 3, 7k)



^{13}C NMR (125 MHz, $CDCl_3$): (Table 3, 7k)



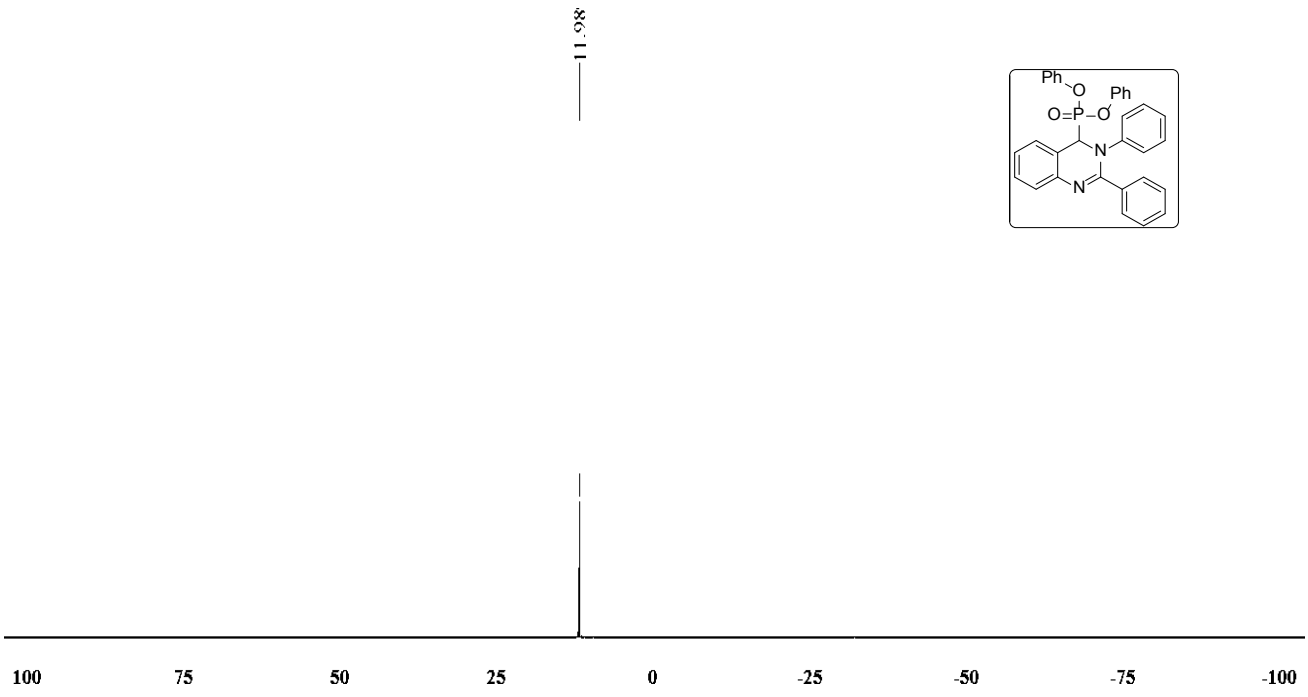
HIGH RESOLUTION MASS SPECTRA: (Table 3, 7k)



KRR-SAI-84#8-30 RT: 0.03-0.10 AV: 23
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
283.12258	173280048.0	100.00				
517.16636	159955920.0	92.31	517.16756	-2.30	21.5	$C_{32}H_{26}O_3N_2P$

^{31}P NMR (202 MHz, $CDCl_3$): (Table 3, 7k)



X-ray Studies:

X-ray data for compounds **5i**, **5p** and **7e** were collected at room temperature using a Bruker Smart Apex CCD diffractometer with graphite monochromated MoKα radiation (λ=0.71073 Å) with ω-scan method.[1] Preliminary lattice parameters and orientation matrices were obtained from four sets of frames.

Integration and scaling of intensity data were accomplished using SAINT program.[1] The structures were solved by Direct Methods using SHELXS97[2] and refinement was carried out by full-matrix least-squares technique using SHELXL97.[2] Anisotropic displacement parameters were included for all non-hydrogen atoms. The hydrogen atom attached to nitrogen atom of compounds was located in a difference density map and refined isotropically. All other H atoms were located in a difference density map but were positioned geometrically and included as riding atoms, with C-H = 0.93-0.98 Å and $U_{iso}(H) = 1.2U_{eq}(c)$.

Crystal data for compound 5i (CCDC 996992):

Compound **5i** was crystallized by slow evaporation method chloroform as a solvent. MF = $C_{28}H_{23}N_3O$, M = 417.49, colorless block, 0.18 x 0.15 x 0.04 mm^3, triclinic, space group P-1 (No. 2), a = 10.6039(8), b = 10.7930(8), c = 11.0137(8) Å, α = 100.245(1), β = 111.738(1), γ = 101.524(1)°, V = 1102.46(14) $Å^3$, Z = 2, D_c = 1.258 g/cm^3, F_{000} = 440, Bruker SMART APEX CCD area-detector, MoKα radiation, λ = 0.71073 Å, T = 294(2)K, $2\theta_{max}$ = 50.0º, 10635 reflections collected, 3869 unique (R_{int} = 0.0167). Final *GooF* = 1.026, *R1* = 0.0373, *wR2* = 0.1001, *R* indices based on 3334 reflections with I>2σ(I) (refinement on F^2), 294 parameters, 0 restraints, μ = 0.078 mm^{-1}. CCDC 996992 contains supplementary Crystallographic data for the structure.

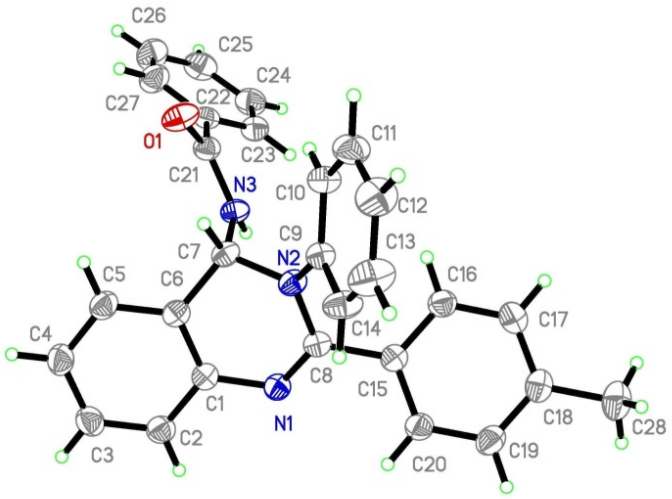


Fig.1.A view of compound **5i**, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are represented by circles of arbitrary radii.

Crystal data for compound 5p (CCDC 996993):

Compound **5p** was crystallized by slow evaporation method using chloroform as a solvent. MF = $C_{23}H_{21}N_3O$, M = 355.43, colorless needle, 0.18 x 0.09 x 0.07 mm^3, monoclinic, space group $P2_1/c$ (No. 14), a = 9.3171(12), b = 15.390(2), c = 13.1098(17) Å, β = 92.604(2)°, V = 1877.9(4) $Å^3$, Z = 4, D_c = 1.257 g/cm^3, F_{000} = 752, Bruker SMART APEX CCD area-detector, MoKα radiation, λ = 0.71073 Å, T = 294(2)K, $2\theta_{max}$ = 50.0º, 17388 reflections collected, 3305 unique (R_{int} = 0.0265). Final *GooF* = 1.080, *R1* = 0.0361, *wR2* = 0.0914, *R* indices based on 2647 reflections with I>2σ(I) (refinement on F^2), 250 parameters, 0 restraints, μ = 0.079 mm^{-1}. CCDC 996993 contains supplementary Crystallographic data for the structure.

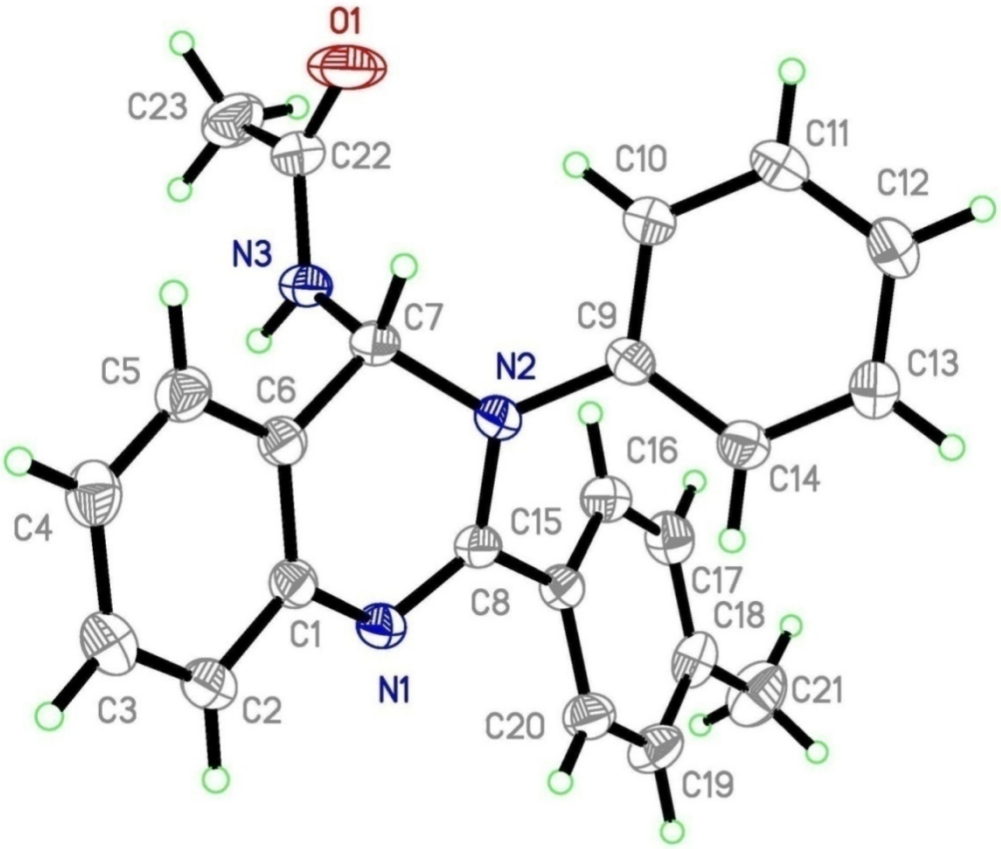


Fig. 2. A view of compound **5p**, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are represented by circles of arbitrary radii.

Crystal data for compound 7e (CCDC 996994):

Compound **5i** was crystallized by slow evaporation method using ethylacetate as solvent. MF:$C_{26}H_{29}N_2O_3P$, M = 448.48, colorless plate, 0.16 x 0.14 x 0.07 mm^3, monoclinic, space group $P2_1/c$ (No. 14), a = 14.6985(13), b = 11.7586(10), c = 13.8686(12) Å, β = 103.257(1)°, V = 2333.1(4) $Å^3$, Z = 4, D_c = 1.277 g/cm^3, F_{000} = 952, Bruker SMART APEX CCD area-detector, MoKα radiation, λ = 0.71073 Å, T = 294(2)K, $2\theta_{max}$ = 50.0º, 22035 reflections collected, 4110 unique (R_{int} = 0.0214). Final *GooF* = 1.038, *R1* = 0.0365, *wR2* = 0.0995, *R* indices based on 3707 reflections with I>2σ(I) (refinement on F^2), 294 parameters, 0 restraints, μ = 0.148 mm^{-1}. CCDC 996994 contains supplementary Crystallographic data for the structure. These data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html [or from the Cambridge Crystallographic Data Centre (CCDC), 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44(0) 1223 336 033; email: deposit@ccdc.cam.ac.uk].

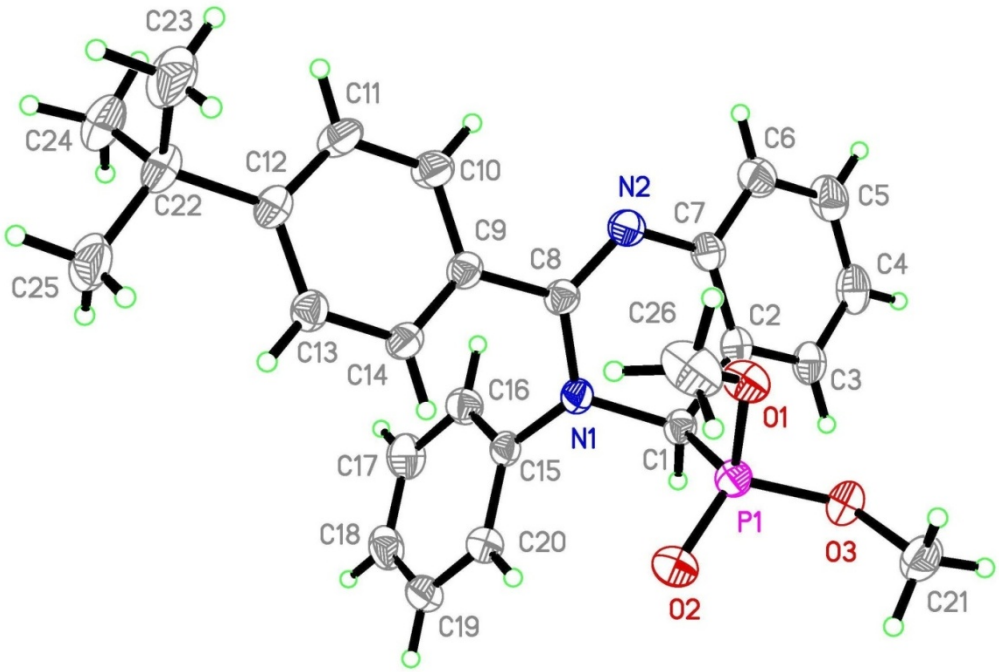
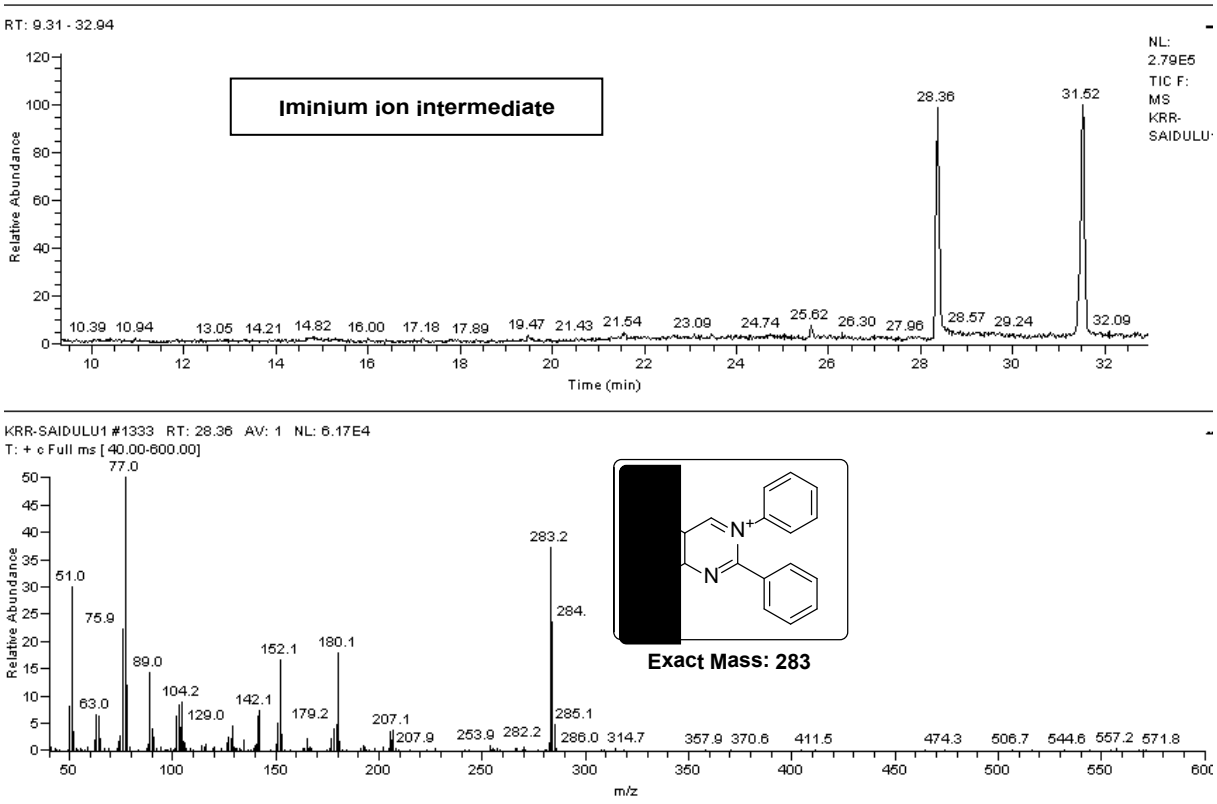


Fig.3.A view of compound **7e**, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are represented by circles of arbitrary radii.

Experiment the formation of iminium ion:

A reaction was performed with 3,4-diaryl-dihydroquinazolin-4-ol (**3a**) in DCE solvent at 75 ^{o}C in the absence of nucleophile and the reaction mixture is subjected to GC-MS analysis after 12 hrs. The recorded GC-MS spectra clearly shows the formation of iminium ion species.



References:

1. SMART & SAINT. Software Reference manuals. Versions 6.28a & 5.625, Bruker Analytical X-ray Systems Inc., Madison, Wisconsin, U.S.A., 2001.
2. G. M. Sheldrick, *Acta Cryst.* 2008, **A64**, 112-122.
3. F. Ishikawa, Y. Watanabe and J. Saegusa, *Chemical & Pharmaceutical Bulletin*; 1980, **28**, 1357.