Revised supplementary information with track change:

SUPPLEMENTARY INFORMATION

Unexplored Reactivity of 2-Oxoaldehydes towards Pictet-Spengler condition in different directions: Concise approach to *β*-carbolines based marine natural Products

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1. General

All purchased chemicals were used without further purification. Thin Layer chromatography (TLC) was performed using per-coated Silica gel 60 F254 MERCK.TLC plates were visualized by exposing UV light or by iodine vapours. All experiments were carried out under air atmosphere. Melting points of solid compounds were determined on BUCHI-B-545-Switzerland melting point apparatus. and ^{1}H NMR and ^{13}C spectra were recorded on BUCKER 500 and 400 MHz instruments. Proton and carbon magnetic resonance spectra (^{1}H NMR and ^{13}C NMR) were recorded using tetramethylsilane (TMS) in the solvent of $CDCl_3$ as the internal standard (1H NMR: TMS at 0.00 ppm, $CDCl_3$: at 7.26 ppm: 13C NMR: $CDCl_3$ at 77.0ppm).All the NMR spectra were processed in MestReNova. HRMS spectra recoded with LCMS-QTOF Module No.G654A(UHD)

2.General Experimental Procedure

General procedure for preparation of 3a-3w:
Acetophenone (1a, 82mg, 0.458 mmol.) and iodine (58mg, 0.458 mmol) were added to 2ml of DMSO and the resulting solution was heated at 90^{o}C for 1h. Tryptophan methyl ester (2, 100mg, 0.458 mmol) was added and the solution was stirred at same temperature for 2-3 h till completion of reaction (monitored by TLC). The reaction mixture was then cooled to room temperature followed by addition of water (25ml) and extracted with EtOAc (2x25ml). The extract was washed with 10% $Na_2S_2O_3$, dried over Na_2SO_4, filtered and evaporated under reduced pressure. The residue was purified by chromatography on a silica gel (#100-200) using acetone: DCM (0.1: 9.9) as eluent to give the desired product 3a as a yellow solid (152 mg, 85% yield).

General procedure for preparation of 6a-7m:
Tyrptophanmethylester hydrochloride (2a, 500mg, 1.96 mmol) and glyoxal monohydrate (5a, 381mg, 1.96 mmol) were added to 20mL of acetonitrile and the reaction mixture was stirred at 85 ^{o}C for 3 h till completion of reaction. The reaction mixture was slowly cooled to ambient temperature and the precipitate / crude mixture was treated with EtOAc (50ml) and10% $NaHCO_3$ (50ml). Later the extract was dried over Na_2SO_4, filtered and evaporated under reduced pressure.The residue was purified by chromatography on a silica gel (#100-200) column chromatography using EtOAc: Hexane (2:8) as eluent to give the desired product 6a as a white solid (703mg, 95% yield).

Procedure for synthesis of:
Marinacarbolines A,B
Acetone (1w, 67µl, 0.91 mmol) and iodine (58mg, 0.458 mmol) in DMSO (2ml) was stirred at 90 ^{o}C for 1 h. To this was added tryptophan methyl ester (2, 100mg, 0.458 mmol). The reaction was stirred further for 2 h at 90 ^{o}C till completion of reaction (monitored by TLC). Later the reaction mixture was cooled to room temperature and water (25ml) was added. The mixture was then extracted with EtOAc (2x25ml). The extract was washed with 10% $Na_2S_2O_3$ solution, dried with anhydrous Na_2SO_4 and evaporated. The residue was purified by chromatography on a silica gel (#100-200) column chromatography using acetone: DCM (0.1: 9.9) as eluent to give the desired product 3w as a yellow solid in 80% yield (98mg). Compound 3w (100mg, 0.373 mmol) was treated with respective amine (4-Methoxy phenyl ethylamine) (328 µl, 2.24mmol) under neat conditions (6equiv.concentration) at 85 ^{o}C for 4 h. After complition of reaction (monitored by TLC), the reaction was cooled to room temperature and residue was extracted in EtOAc. The organic extract was dried over Na_2SO_4 and concentrated in vaccuum. Resulting crude product

was purified by silica gel (#100-200) column chromatography eluted with EtOAc: Hexane (3:7) produced Marinacarbolines A (132mg 92%) and Same procedure was followed for synthesis of Marinacarbolines B (125mg 90%) respectively.

1-(1H-indole-3-carbonyl)-9H-β-carboline-3-carboxylic acid (Pityriacitrin B)

2N NaOH was added drop wise to the reaction mixture of compound 3i (100 mg, 0.271 mmol) taken in 5ml MeOH to maintain the basic pH and stirred at room temperature for 24 h. After complete conversion of reaction (monitored by TLC), crude mixture was concentrated and acidified (pH 7) by drop wise addition of 1N HCl to afford us crude product. Later crude product was extracted in EtOAc. The organic extract was dried over Na_2SO_4, filtrate and concentrated in vaccuum to afford desired carboxylic acid (Pityriacitrin B, 86mg, 90% yield) as a yellow solid.

Eudistomin Y1 / Pityriacitrin:

4-Hydroxy acetophenone (85mg, 0.625 mmol) and iodine (79mg, 0.625 mmol) were added to 2ml of DMSO and the resulting solution was heated at 90 ^oC for 1hr. Tryptamine (12a ,100mg, 0.625 mmol) was added and the solution was stirred at same temperature for 2 h till completion of reaction (monitored by TLC). The reaction mixture was then cooled to room temperature followed by addition of water (25ml) and extracted with EtOAc (2x25ml). The extract was washed with 10% $Na_2S_2O_3$, dried over Na_2SO_4, filtered and evaporated under reduced pressure. The residue was purified by chromatography on a silica gel (#100-200) using acetone: DCM (0.1: 9.9) as eluent to give the desired product 14 (Eudistomin Y1) as a yellow solid (72mg, 40% yield).

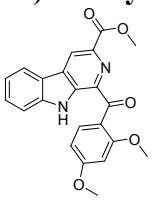
Same procedure was followed for synthesis of Pityriacitrin (11, 42% yield).

Fascaplysin:

To a stirred solution of 2-Chloro acetophenone (96mg, 0.625 mmol) and iodine (79mg, 0.625 mmol) in DMSO (2ml) at 90 ^oC for 1 h was added tryptamine (12a ,100mg, 0.625 mmol). The reaction mixture was continued stirring at same temperature for 2 h. After completion of reaction (monitored by TLC), water (25ml) was added, which was then extracted with EtOAc (2x25ml). The extract was washed with 10% $Na_2S_2O_3$ solution, dride with anhydrous Na2SO4, and evaporated. The residue was purified by chromatography on a silica gel column (Acetone: DCM/ 0.1: 9.9) to afford the desired product 13 as light yellow solid (143mg, 75%). Compound 13 (100 mg, 0.326 mmol) taken in sealed tube and heated at 220 ^oC for 15 min. Reaction was cooled and the product was recrystallized from DCM/diethyl ether producing brick-red colored powder of fascaplysin (15, 82 mg) in 82% yield.

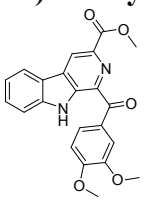
3. Characterization of the Compounds

3a) Methyl 1-(2,4- dimethoxybenzoyl)- *β*-carboline-3-carboxylate:



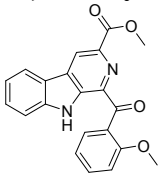
85% yield; Yellow solid; mp 221-223 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.68 (s, 1H), 8.99 (s, 1H), 8.21 (d, *J* = 7.8 Hz, 1H), 7.91 (d, *J* = 8.5 Hz, 1H), 7.61 (s, 2H), 7.38 (t, *J* = 5.9 Hz, 1H), 6.62 – 6.57 (m, 2H), 3.99 (s, 3H), 3.89 (s, 3H), 3.77 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 195.15, 166.31, 164.06, 161.36, 141.36, 137.82, 136.40, 136.27, 134.67, 131.83, 129.60, 121.97, 121.46, 121.15, 120.42, 120.03, 112.38, 104.39, 99.27, 55.86, 55.57, 52.67. IR ($CHCl_3$): v_{max} (cm^{-1}) 3360, 2948, 1715, 1646, 1622, 1603, 1577, 1495, 1459, 1334, 1287, 1224, 1161, 1128, 1028, ESI-MS: m/z 391.10 $(M+H)^+$; HRMS: m/z 391.1292 calcd for $C_{22}H_{18}N_2O_5+H^+$ (391.1288).

3b) Methyl 1-(3,4- dimethoxybenzoyl)- *β*-carboline-3-carboxylate:



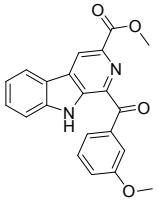
83% yield; Yellow solid; mp 200-202 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.76 (s, 1H), 9.05 (s, 1H), 8.67 (s, 1H), 8.41 (d, *J* = 8.5 Hz, 1H), 8.24 (d, *J* = 7.8 Hz, 1H), 7.65 (d, *J* = 5.7 Hz, 2H), 7.41 (t, *J* = 6.8 Hz, 1H), 7.04 (d, *J* = 8.5 Hz, 1H), 4.08 (s, 3H), 4.07 (s, 3H), 4.01 (s, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 190.93, 166.15, 153.42, 148.29, 141.22, 138.33, 136.30, 136.07, 131.98, 129.71, 129.65, 126.68, 121.99, 121.56, 121.19, 120.39, 114.96, 112.35, 110.31, 56.06, 55.94, 52.64. IR ($CHCl_3$): v_{max} (cm^{-1}) 3435, 2922, 1620, 1590, 1513, 1460, 1431, 1359, 1262, 1215, 1135, 1032, 1018. ESI-MS: m/z 391 $(M+H)^+$; HRMS: m/z 391.1293 calcd for $C_{22}H_{18}N_2O_5+H^+$ (391.1288).

3c) Methyl 1-(2-methoxybenzoyl)- *β*-carboline-3-carboxylate:



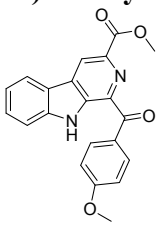
83% yield; yellow solid; mp 219-221 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.65 (brs, 1H), 9.01 (s, 1H), 8.23 (d, *J* = 7.9 Hz, 1H), 7.75 (d, *J* = 7.3 Hz, 1H), 7.64 (s, 2H), 7.54 (t, *J* = 7.3 Hz, 1H), 7.41 (d, *J* = 5.4 Hz, 1H), 7.13-7.01 (m, 2H), 3.97 (s, 3H), 3.78 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 197.42, 166.23, 158.94, 141.41, 137.65, 136.74, 135.66, 132.87, 131.99, 131.64, 129.73, 127.34, 122.05, 121.61, 121.13, 120.75, 120.22, 112.40, 112.10, 55.94, 52.65. IR ($CHCl_3$): v_{max} (cm^{-1}) 3368, 2921, 2851, 1696, 1600, 1652, 1492, 1458, 1432, 1262, 1222, 120. ESI-MS: m/z 361 $(M+H)^+$; HRMS: m/z 361.1189 calcd for $C_{21}H_{16}N_2O_4+H^+$ (361.1183).

3d) Methyl 1-(3-methoxybenzoyl)- *β*-carboline-3-carboxylate:



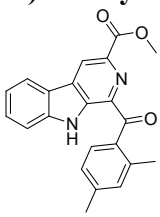
80%yield; Yellow solid; mp 195-197 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.72 (s, 1H), 9.05 (s, 1H), 8.44 (dd, *J* = 2.4, 1.5 Hz, 1H), 8.20 (dd, *J* = 22.1, 7.7 Hz, 2H), 7.68 – 7.63 (m, 2H), 7.48 – 7.41 (m, 2H), 7.21 – 7.18 (m, 1H), 4.06 (s, 3H), 3.96 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.92, 166.14, 159.28, 141.29, 138.34, 137.89, 136.34, 135.69, 132.14, 129.80, 129.16, 124.36, 122.03, 121.68, 121.19, 120.64, 120.31, 116.26, 112.38, 55.44, 52.68. IR ($CHCl_3$): v_{max} (cm^{-1}); 3434, 2919, 1711, 1620, 1580, 1492, 1455, 1432, 1361, 1336,1263, 1203, 1180, 1017, 1033. ESI-MS: m/z 361 $(M+H)^+$; HRMS: m/z 361.1182 calcd for $C_{21}H_{16}N_2O_4+H^+$ (361.1183).

3e) Methyl 1-(4-methoxybenzoyl)- *β*-carboline-3-carboxylate:[(1)]



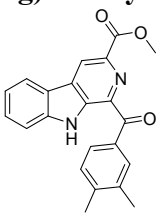
85%yield; Yellow solid; mp 185-187 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.71 (s, 1H), 9.04 (s, 1H), 8.75 (d, *J* = 8.8 Hz, 2H), 8.24 (d, *J* = 7.9 Hz, 1H), 7.64 (s, 2H), 7.42 (d, *J* = 5.7 Hz, 1H), 7.06 (d, *J* = 8.8 Hz, 2H), 4.08 (s, 3H), 3.93 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 191.69, 166.26, 163.69, 141.25, 138.29, 136.19, 134.46, 131.95, 129.70, 122.02, 121.56, 121.23, 120.41, 120.38, 113.59, 112.37, 55.54, 52.79. IR ($CHCl_3$): v_{max} (cm^{-1}); 3416, 3074, 2820, 2850, 1705, 1628, 1618,1596,1564,1454,1434, 1361, 1256, 1172, 1024. ESI-MS: m/z 361.10$(M+H)^+$; HRMS: m/z 361.1182 calcd for $C_{21}H_{16}N_2O_4+H^+$(361.1183).

3f) Methyl 1-(2,4-dimethyl benzoyl)- *β*-carboline-3-carboxylate:



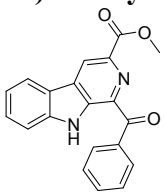
72%yield; Yellow solid; mp 245-247 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.73 (s, 1H), 9.03 (s, 1H), 8.23 (d, *J* = 7.9 Hz, 1H), 7.89 (d, *J* = 8.3 Hz, 1H), 7.68 – 7.62 (m, 2H), 7.43 – 7.39 (m, 1H), 7.14 (d, *J* = 6.0 Hz, 2H), 4.00 (s, 3H), 2.48 (s, 3H), 2.41 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.09, 166.21, 141.63, 141.37, 139.06, 138.15, 136.73, 135.85, 133.80, 132.55, 132.20, 132.05, 129.74, 125.60, 122.06, 121.63, 121.18, 120.57, 112.34, 52.68, 21.51, 21.00. IR ($CHCl_3$): v_{max} (cm^{-1}) 3369, 2921, 2851, 1711, 1637, 1624, 1611, 1455, 1495, 1360, 1258, 1121, 1015. ESI-MS: m/z 359 $(M+H)^+$; HRMS: m/z 359.1386 calcd for $C_{22}H_{18}N_2O_3+H^+$(359.1390).

3g) Methyl 1-(3,4-dimethyl benzoyl)- *β*-carboline-3-carboxylate:



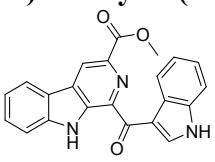
75%yield; Yellow solid; mp 209-211 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.71 (s, 1H), 9.05 (s, 1H), 8.52 (s, 1H), 8.38 (d, *J* = 7.8 Hz, 1H), 8.24 (d, *J* = 7.9 Hz, 1H), 7.65 (s, 2H), 7.43 – 7.39 (m, 1H), 7.32 (d, *J* = 7.9 Hz, 1H), 4.08 (s, 3H), 2.41 (s, 3H), 2.38 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 193.29, 166.35, 142.67, 141.25, 138.26, 136.41, 136.24, 135.92, 134.54, 133.18, 131.96, 129.74, 129.70, 129.52, 122.03, 121.58, 121.21, 120.45, 112.38, 52.79, 20.16, 19.93. IR ($CHCl_3$): v_{max} (cm^{-1}) 3399, 2920, 1715, 1619, 1601, 1493, 1455, 1431, 1362, 1337, 1260, 1235, 1212, 1121, 1019. ESI-MS: m/z 359 $(M+H)^+$; HRMS: m/z 359.1392 calcd for $C_{22}H_{18}N_2O_3+H^+$(359.1390).

3h) Methyl 1- (benzoyl)- *β*-carboline-3-carboxylate:[2]



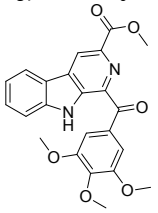
70% yield; Yellow solid; mp 237-239 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.71 (s, 1H), 9.06 (s, 1H), 8.62 (d, *J* = 7.5 Hz, 2H), 8.24 (d, *J* = 7.8 Hz, 1H), 7.64 (d, *J* = 11.3 Hz, 3H), 7.57 (t, *J* = 7.4 Hz, 2H), 7.42 (d, *J* = 5.2 Hz, 1H), 4.07 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 193.77, 166.22, 141.29, 138.31, 136.77, 136.38, 135.57, 133.04, 132.12, 131.97, 129.83, 128.21, 122.08, 121.70, 121.18, 120.69, 112.41, 52.87. IR ($CHCl_3$): v_{max} (cm^{-1}) 3436, 2919, 1700, 1620, 1595,1455, 1433, 1336, 1293, 1263,1124,1015.ESI-MS: m/z 331.00$(M+H)^+$; HRMS: m/z 331.1082 calcd for $C_{20}H_{14}N_2O_3+H^+$(331.1077).

3i) Methyl 1-(1H-indole-3-carbonyl)- *β*-carboline-3-carboxylate:



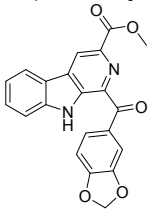
78%yield; Yellow solid; mp 254-256 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.00 (s, 1H), 9.85 (d, *J* = 3.0 Hz, 1H), 9.02 (s, 1H), 8.85 (s, 1H), 8.71 (d, *J* = 7.6 Hz, 1H), 8.24 (d, *J* = 8.0 Hz, 1H), 7.66 (d, *J* = 3.7 Hz, 2H), 7.49 (d, *J* = 7.9 Hz, 1H), 7.44 – 7.30 (m, 3H), 4.12 (s, 3H). ^{13}C NMR (125 MHz, DMSO) δ 186.25, 165.58, 142.04, 138.36, 137.30, 135.99, 135.85, 134.74, 131.23, 129.17, 127.23, 123.00, 122.20, 122.07, 121.64, 120.78, 120.42, 119.83, 114.11, 113.41, 112.28, 52.37. IR ($CHCl_3$): v_{max} (cm^{-1}) 3409, 2922, 2851, 1715, 1600, 1493, 1456, 1433, 1305, 1245, 1159, 1125, 1019. ESI-MS: m/z 370 $(M+H)^+$; HRMS: m/z 370.1184 calcd for $C_{22}H_{15}N_3O_3+H^+$(370.1186).

3j) Methyl 1-(3,4,5- trimethoxybenzoyl)- *β*-carboline-3-carboxylate:



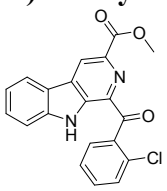
81%yield; Yellow solid; mp 203-205 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.76 (s, 1H), 9.07 (s, 1H), 8.26 – 8.24 (m, 3H), 7.70 – 7.65 (m, 2H), 7.45-7.41 (m, 1H), 4.06 (s, 3H), 4.05 (s, 6H), 4.00 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.08, 166.06, 152.69, 141.27, 138.46, 136.16, 135.97, 132.21, 131.58, 129.85, 122.06, 121.71,121.20,120.60,112.39, 107.28, 105.57, 60.99, 56.20, 53.43, 52.60. IR ($CHCl_3$): v_{max} (cm^{-1}) 3427, 2923, 1715, 1619, 1502, 1461, 1431, 1415, 1360, 1131, 1259, 1240, 1126, 1020. ESI-MS: m/z 421 $(M+H)^+$; HRMS: m/z 421.1392 calcd for $C_{23}H_{20}N_2O_6+H^+$(421.1394).

3k) Methyl 1-(benzo[d][1,3]dioxole-5-carbonyl)- *β*-carboline-3-carboxylate:



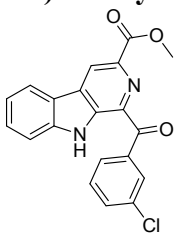
84%yield; Yellow solid; mp 199-201 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.68 (s, 1H), 9.03 (s, 1H), 8.47 (dd, *J* = 8.3, 1.6 Hz, 1H), 8.27 – 8.18 (m, 2H), 7.72 – 7.60 (m, 2H), 7.41 (ddd, *J* = 8.0, 5.9, 2.2 Hz, 1H), 6.98 (d, *J* = 8.3 Hz, 1H), 6.09 (s, 2H), 4.08 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 191.04, 166.24, 151.93, 147.71, 141.22, 138.28, 136.11, 135.93, 132.01, 131.14, 129.76, 129.07, 122.04, 121.60,121.19, 120.46, 112.37, 111.66, 107.98, 101.78, 52.88, IR ($CHCl_3$): v_{max} (cm^{-1}) 3391, 2922, 1714, 1637, 1599, 1434, 1362, 1338, 1218, 1263, 1106, 1071, 1040. ESI-MS:m/z 375$(M+H)^+$; HRMS: m/z375.0980 calcd for $C_{21}H_{14}N_2O_5+H^+$(375.0975).

3l) Methyl 1-(2- chlorobenzoyl)- *β*-carboline-3-carboxylate:



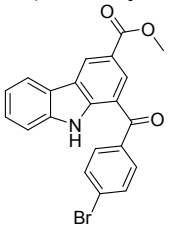
75%yield; Yellow solid; mp 232-234 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.65 (s, 1H), 9.04 (s, 1H), 8.24 (d, *J* = 7.9 Hz, 1H), 7.81 (dd, *J* = 7.4, 1.5 Hz, 1H), 7.68– 7.65 (m, 2H), 7.51 – 7.41 (m, 4H), 3.97 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.34, 165.96, 141.45, 137.87, 137.16, 136.83, 134.69, 132.83, 132.28, 131.65, 131.61, 130.32, 129.95, 126.02, 122.13, 121.86, 121.12, 121.10, 112.44, 52.68, IR ($CHCl_3$): v_{max} (cm^{-1}) 3368, 2949, 2922, 1701, 1651, 1625, 1591, 1496, 1454, 1432, 1361, 1294, 1266, 1222, 1125, 1107, 1055, 1014. ESI-MS: m/z 365 $(M+H)^+$; HRMS: m/z 365.0688 calcd for $C_{20}H_{13}ClN_2O_3+H^+$(365.0687).

3m) Methyl 1-(3- chlorobenzoyl)- *β*-carboline-3-carboxylate:



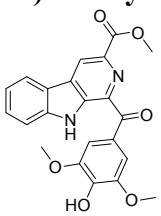
66%yield; Yellow solid; mp 214-216 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.67 (s, 1H), 9.07 (s, 1H), 8.80 (t, *J* = 1.8 Hz, 1H), 8.55 – 8.46 (m, 1H), 8.25 (d, *J* = 7.8 Hz, 1H), 7.68 – 7.66 (m, 2H), 7.63-7.60 (m, 1H), 7.51 (t, *J* = 7.9 Hz, 1H), 7.45-7.42 (m, 1H), 4.09 (s, 3H).^{13}C NMR (125 MHz, $CDCl_3$) δ 191.94, 166.11, 141.30, 138.27, 138.19, 136.45, 135.01, 134.29, 132.86, 132.35, 132.29, 129.97, 129.94, 129.47, 122.14, 121.79, 121.15, 120.85, 112.44, 52.88.IR ($CHCl_3$): v_{max} (cm^{-1}) 3400,2922, 2852, 1710, 1648,1456, 1363, 1268,1217,1033, 1018. ESI-MS:m/z 364.90 $(M+H)^+$; HRMS:m/z 365.0686 calcd for $C_{20}H_{13}ClN_2O_3+H^+$(365.0687).

3n) Methyl 1-(4-Bromobenzoyl)- *β*-carboline-3-carboxylate:



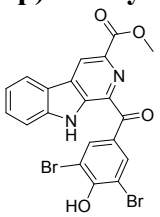
65%yield; Yellow solid; mp 216-218 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.64 (s, 1H), 9.00 (s, 1H), 8.49 (d, *J* = 8.5 Hz, 2H), 8.19 (d, *J* = 7.9 Hz, 1H), 7.72 – 7.56 (m, 4H), 7.44 – 7.34 (m, 1H), 4.07 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 192.38, 166.06, 141.26, 138.17, 136.33, 135.43, 135.18, 133.47, 132.17, 131.44, 129.89, 128.45, 122.06, 121.77, 121.08, 120.77, 112.41, 52.88. IR ($CHCl_3$): v_{max} (cm^{-1}) ;3436, 2919, 1711, 1586, 1430, 1363, 1337, 1267, 1018. ESI-MS: m/z 409.0 $(M+H)^+$; HRMS :m/z 409.0195 calcd for $C_{20}H_{13}BrN_2O_3+H^+$(409.012).

3o) Methyl 1-(4-hydroxy-3, 5-dimethoxybenzoyl)- *β*-carboline-3-carboxylate:



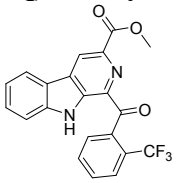
64% yield; Yellow solid; mp 226-228 ^{o}C ; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.77 (s, 1H), 9.06 (s, 1H), 8.39 (s, 2H), 8.25 (d, *J* = 7.9 Hz, 1H), 7.69 – 7.64 (m, 2H), 7.42-7.41(m, 1H), 6.08 (s, 1H), 4.08 (s, 6H), 4.05 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 190.22, 166.11, 146.49, 141.20, 139.95, 138.38, 136.27, 135.90, 132.07, 129.77, 127.90, 122.02, 121.62, 121.16, 120.45, 112.38, 109.64, 56.36, 52.63. IR ($CHCl_3$): v_{max} (cm^{-1}) 3625, 3418, 2923, 1657, 1650, 1633, 1622, 1709, 1517, 1494, 1458, 1431, 1362, 1340, 1270, 1217, 1171, 1120, 1042, 1021. ESI-MS: m/z 407.00 $(M+H)^+$; HRMS: m/z 407.1239 calcd for $C_{22}H_{19}N_2O_6+H^+$(407.1238).

3p) Methyl 1-(3, 5- dibromo-4-hydroxybenzoyl)- *β*-carboline-3-carboxylate:



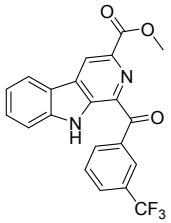
84% yield; Yellow solid; mp 297-299 ^{o}C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.42 (s, 1H), 9.15 (s, 1H), 8.97 (s, 2H), 8.47-8.29 (m, 2H), 7.85 (d, *J* = 8.1 Hz, 1H), 7.64 (t, *J* = 7.6 Hz, 1H), 7.36 (t, *J* = 7.4 Hz, 1H), 3.98 (s, 3H), ^{13}C NMR (125 MHz, DMSO) δ 186.75, 165.28, 155.00, 142.02, 136.74, 136.14, 135.28, 134.70, 131.69, 130.15, 129.48, 122.20, 121.12, 120.59, 120.40, 113.38, 110.89, 79.11, 52.36. IR ($CHCl_3$): v_{max} (cm^{-1}); 3433, 2920, 1712, 1633, 1456, 1431, 1365, 1303, 1268, 1209, 1149, 1019. ESI-MS: m/z 504.80$(M+2)^+$; HRMS: m/z 504.921 calcd for $C_{20}H_{12}Br_2N_2O_4+H^+$(502.9237).

3q) Methyl 1-(2-(trifluoromethyl)benzoyl)- *β*-carboline-3-carboxylate:



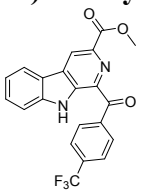
76% yield; Yellow solid; mp 238-240 ^{o}C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.60 (s, 1H), 9.18 (s, 1H), 8.50 (d, *J* = 7.7 Hz, 1H), 7.94 – 7.90 (m, 2H),7.81(d, *J* = 6.0 Hz, 3H), 7.69 (t, *J* = 7.5 Hz, 1H), 7.40 (t, *J* = 7.4 Hz, 1H), 3.84 (s, 3H).^{13}C NMR (100 MHz, DMSO) δ 195.96, 164.95, 142.36, 137.52, 136.22, 135.84, 134.74, 131.71, 131.60, 130.37, 129.96, 129.64, 127.01, 126.36, 122.34, 121.36, 121.30, 120.26, 113.47, 52.21, IR ($CHCl_3$): v_{max} (cm^{-1}) 3347, 2922, 1740, 1690, 1623, 1653, 1580, 1494, 1432, 1333, 1312, 1262, 1163,1106, 1056, 1087. ESI-MS: m/z 398.90$(M+H)^+$; HRMS: m/z 421.0767 (M+Na) calcd for $C_{21}H_{13}F_3N_2NaO_3^+$(421.0770).

3r) Methyl 1-(3-(trifluoromethyl)benzoyl)- *β*-carboline-3-carboxylate:



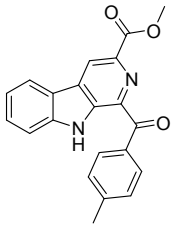
75% yield; Yellow solid; mp 219-221 ^{o}C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.53 (s, 1H), 9.19 (d, *J* = 15.1 Hz, 2H), 8.58 (d, *J* = 7.8 Hz, 1H), 8.50 (d, *J* = 7.9 Hz, 1H), 8.08 (d, *J* = 7.8 Hz, 1H), 7.87 (dd, *J* = 13.5, 8.0 Hz, 2H), 7.72 – 7.63 (m, 1H), 7.40 (t, *J* = 7.5 Hz, 1H), 3.94 (s, 3H). ^{13}C NMR (125 MHz, DMSO) δ 190.26, 165.31, 142.15, 137.35, 136.84, 135.05, 134.92, 134.52, 131.81, 129.57, 129.36, 128.98, 122.34, 121.21, 120.90, 120.42, 113.42, 79.13, 52.25, IR ($CHCl_3$): v_{max} (cm^{-1}) 3380, 3341, 2921, 2851, 1709, 1641, 1623, 1590, 1494, 1456, 1433, 1364, 1283, 1267, 1170, 1119, 1072. ESI-MS: m/z 398.9$(M+H)^+$; HRMS: m/z 399.0954 calcd for $C_{21}H_{13}F_3N_2O_3+H^+$(399.0952).

3s) Methyl 1-(4-(trifluoromethyl)benzoyl)- *β*-carboline-3-carboxylate:



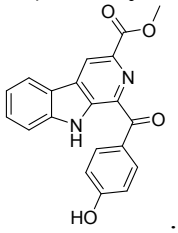
76% yield; Yellow solid; mp 214-216 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.65 (s, 1H), 9.03 (s, 1H), 8.68 (d, *J* = 8.0 Hz, 2H), 8.21 (d, *J* = 7.8 Hz, 1H), 7.80 (d, *J* = 8.1 Hz, 2H), 7.65 (q, *J* = 8.1 Hz, 2H), 7.42 (t, *J* = 7.2 Hz, 1H), 4.07 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 192.70, 165.97, 141.30, 139.52, 138.23, 136.52, 134.81, 132.34, 132.18, 130.02, 125.06, 122.11, 121.90, 121.06, 120.98, 112.44, 52.91. IR (CHCl3): v_{max} (cm^{-1}) 3395, 2922, 2851, 1707, 1653, 1627, 1590, 1498, 1457, 1433, 1364, 1332, 1298, 1270, 1189, 1125, 1105, 1091, 1067, 1015.ESI-MS:m/z 399$(M+H)^+$; HRMS: m/z 399.0946 calcd for $C_{21}H_{13}F_3N_2O_3+H^+$(399.0951).

3t) Methyl 1-(4-methylbenzoyl)- *β*-carboline-3-carboxylate:



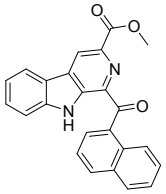
78% yield; Yellow solid; mp 214-216 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.70 (s, 1H), 9.04 (s, 1H), 8.55 (d, *J* = 8.2 Hz, 2H), 8.23 (d, *J* = 7.8 Hz, 1H), 7.68 – 7.62 (m, 2H), 7.41 – 7.35 (m, 3H), 4.07 (s, 3H), 2.47 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 193.25, 166.25, 143.88, 141.24, 138.24, 136.27, 135.83, 134.15, 132.07, 131.98, 129.71, 128.93, 122.01, 121.58, 121.17, 120.51, 112.35, 52.81, 21.79. IR ($CHCl_3$): v_{max} (cm^{-1}) 3390, 2952, 2921, 1713, 1621, 1604, 1493, 1455, 1430, 1360, 1336, 1260, 1180, 1126, 1105, ESI-MS: m/z 345.00$(M+H)^+$; HRMS: m/z 345.1221 calcd for $C_{21}H_{16}N_2O_3+H^+$(345.1234).

3u) Methyl 1-(4-hydroxybenzoyl)- *β*-carboline-3-carboxylate:



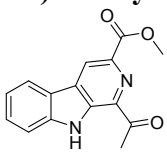
65% yield; Yellow solid; mp 268-270 ^{o}C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.34 (s, 1H), 9.14 (s, 1H), 8.44 (dd, *J* = 18.9, 8.3 Hz, 3H), 7.83 (d, *J* = 8.2 Hz, 1H), 7.64 (t, *J* = 7.6 Hz, 1H), 7.36 (t, *J* = 7.5 Hz, 1H), 6.96 (d, *J* = 8.7 Hz, 2H), 3.96 (s, 3H). ^{13}C NMR (125MHz, DMSO) δ 190.14, 165.44, 162.24, 141.88, 136.89, 136.53, 134.84, 134.03, 130.99, 129.28, 127.80, 122.18, 120.86, 120.46, 120.07, 114.99, 113.19, 52.29, IR ($CHCl_3$): v_{max} (cm^{-1}) 3424, 2920, 1712, 1598, 1568, 1463, 1352, 1290, 1250, 1224, 1163, 1019. ESI-MS: m/z 346.90$(M+H)^+$; HRMS: m/z 347.1022 calcd for $C_{20}H_{14}N_2O_4+H^+$(347.1026).

3v) Methyl 1-(1-naphthoyl)- *β*-carboline-3-carboxylate:



80% yield; Yellow solid; mp 283-285 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.61 (s, 1H), 9.21 (s, 1H), 8.54 (d, *J* = 7.9 Hz, 1H), 8.27 – 8.18 (m, 2H), 8.11 (dd, *J* = 6.2, 3.2 Hz, 1H), 7.93 (dd, *J* = 14.4, 7.7 Hz, 2H), 7.74 – 7.57 (m, 4H), 7.42 (t, *J* = 7.5 Hz, 1H), 3.82 (s, 3H).^{13}C NMR (125 MHz, DMSO) δ 196.66, 165.20, 142.23, 136.78, 136.38, 135.56, 134.64, 133.32, 131.50, 130.66, 130.42, 129.53, 128.55, 127.35, 126.25, 125.10, 124.46, 122.35, 121.14, 120.94, 120.44, 113.37, 52.17. IR ($CHCl_3$): v_{max} (cm^{-1}) 3410, 1714, 1632, 1625, 1508, 1496, 1454, 1431, 1333, 1361, 1295, 1259, 1235, 1212, 1176, 1047, 1066, 1039. ESI-MS: m/z 381 $(M+H)^+$; HRMS: m/z 381.1229 calcd for $C_{24}H_{16}N_2O_3$+H^+(381.1234).

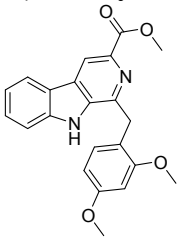
3w) Methyl 1-acetyl- *β*-carboline-3-carboxylate:



80% yield; lightYellow solid; mp 222-224°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.50 (s, 1H), 9.04 (s, 1H), 8.22 (d, *J* = 7.9 Hz, 1H), 7.68 – 7.62 (m, 2H), 7.43-7.39 (m, 1H), 4.09 (s, 3H), 2.97 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.21, 166.10, 141.44, 136.84, 136.46, 135.29, 131.91, 129.76, 122.05, 121.64, 121.26, 120.93, 112.35, 52.78, 25.69. IR ($CHCl_3$): v_{max} (cm^{-1}) 3436, 2924, 1712, 1670, 1632,1498, 1434, 1365, 1334, 1292, 1265, 1207, 1181, 1148, 1120, 1062, ESI-MS: m/z 269.1 $(M+H)^+$; HRMS: m/z 269.0920 calcd for $C_{15}H_{12}N_2O_3$+H^+(269.0921).

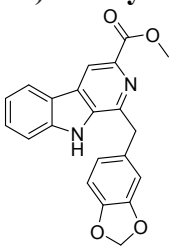
Spectral data of compound 6a-7m:]

6a) Methyl 1-(2, 4-dimethoxybenzyl)-9H-pyrido[3,4-b]indole-3-carboxylate:



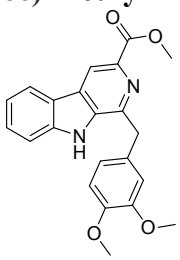
95% yield; White solid; mp 172-174 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.36 (s, 1H), 8.76 (s, 1H), 8.11 (d, *J* = 7.9 Hz, 1H), 7.55 – 7.51 (m, 1H), 7.45 (d, *J* = 8.2 Hz, 1H), 7.30 – 7.23 (m, 2H), 6.54 (d, *J* = 2.3 Hz, 1H), 6.43 (dd, *J* = 8.4, 2.4 Hz, 1H), 4.51 (s, 2H), 4.05 (s, 3H), 4.04 (s, 3H), 3.74 (s, 3H). ^{13} C NMR (125 MHz $CDCl_3$) δ 167.07, 159.81, 156.65, 145.08, 140.18, 137.14, 136.05, 131.71, 128.47, 128.29, 122.08, 121.85, 120.66, 118.53, 116.90, 111.88, 105.71, 99.24, 56.05, 55.40, 52.70, 34.32, IR ($CHCl_3$) v_{max} (cm^{-1}): 3368, 2923, 1713, 1588, 1505, 1433, 1350, 1257, 1208, 1155, 1118, 1037. ESI-MS: m/z 377 $(M+H)^+$; HRMS: m/z 377.1504 calcd for $C_{22}H_{20}N_2O_4$+H+(377.1496).

6b) Methyl 1-(benzo[d][1,3]dioxol-5-ylmethyl)-9H-pyrido[3,4-b]indole-3-carboxylate:



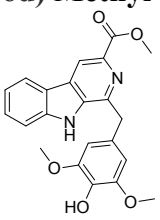
90% yield; Orange solid; mp 140-142 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.83 (s, 1H), 8.24 (s, 1H), 8.15 (d, *J* = 7.9 Hz, 1H), 7.58 – 7.49 (m, 1H), 7.42 (d, *J* = 8.2 Hz, 1H), 7.32 (t, *J* = 7.5 Hz, 1H), 6.83 – 6.69 (m, 3H), 5.90 (s, 2H), 4.53 (s, 2H), 4.06 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.86, 148.24, 146.64, 143.93, 140.34, 137.36, 136.24, 131.53, 129.24, 128.77, 121.83, 121.54, 121.01, 117.08, 112.00, 109.24, 108.52, 101.09, 52.75, 41.72.IR ($CHCl_3$) v_{max} (cm^{-1}) ; 3270, 2950, 2922, 1713, 1626, 1598, 1566, 1501, 1434, 1384, 1349, 1217, 1137, 1105, 1039, 1002, ESI-MS: m/z 361.10 $(M+H)^{+}$; HRMS: m/z 361.1191calcd for $C_{21}H_{16}N_2O_4$+H^{+}(361.1183).

6c) Methyl 1-(3,4-dimethoxybenzyl)-9H-pyrido[3,4-b]indole-3-carboxylate:



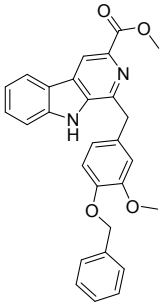
89%yield; Orange solid; mp 176-178 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.83 (s, 1H), 8.56 (s, 1H), 8.13 (d, *J* = 7.9 Hz, 1H), 7.50 (t, *J* = 7.3 Hz, 1H), 7.39 (d, *J* = 8.2 Hz, 1H), 7.29 (dd, *J* = 13.6, 6.3 Hz, 2H), 6.84 – 6.72 (m, 3H), 4.54 (s, 2H), 4.04 (s, 3H), 3.81 (s, 3H), 3.69 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.88, 149.43, 148.10, 144.13, 140.38, 137.25, 136.34, 130.32, 129.19, 128.74, 121.75, 120.93, 120.67, 117.00, 112.11, 112.05, 111.42, 55.87, 52.71, 41.69. IR ($CHCl_3$) v_{max} (cm^{-1}) : 3436, 2075, 1633, 1458, 1433, 1365, 1334, 1292, 1265, 1219, 1181, 1119, 1017.ESI-MS: m/z 377 $(M+H)^{+}$; HRMS: m/z 377.1499 calcd for $C_{22}H_{20}N_2O_4$+H+(377.1496).

6d) Methyl 1-(4- hydroxy-3, 5-dimethoxybenzyl)-9H-pyrido[3,4-b]indole-3-carboxylate:



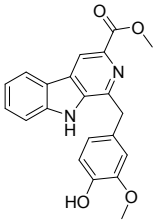
88% yield; White solid; mp 184-186 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.84 (s, 1H), 8.15 (d, *J* = 8.2 Hz, 2H), 7.53 (t, *J* = 7.6 Hz, 1H), 7.44 – 7.28 (m, 2H), 6.55 (s, 2H), 5.51 (s, 1H), 4.57 (s, 2H), 4.08 (s, 3H), 3.78 (s, 6H).^{13}C NMR (100 MHz, CDCl3) δ 166.86, 147.48, 143.98, 140.30, 137.27, 136.34, 133.82, 129.25, 128.81, 121.75, 121.69, 121.00, 117.05, 112.10, 105.66, 56.38, 52.77, 42.48. IR ($CHCl_3$) v_{max} (cm^{-1}) : 3436, 2921, 1619, 1416, 1021. ESI-MS: m/z 393 $(M+H)^{+}$; HRMS: m/z 393.1443 calcd for $C_{22}H_{20}N_2O_5$+H^{+}(393.1445).

6e) Methyl 1-(4-(benzyloxy)-3-methoxybenzyl)-9H-pyrido[3,4-b]indole-3-carboxylate:



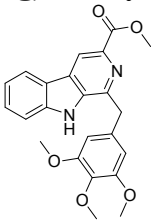
86%yield; light yellow solid; mp 117-119 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.83 (s, 1H), 8.13 (d, *J* = 7.9 Hz, 1H), 7.50 (t, *J* = 7.7 Hz, 1H), 7.42 – 7.23 (m, 8H), 6.77 (dd, *J* = 11.5, 7.7 Hz, 3H), 5.09 (s, 2H), 4.52 (s, 2H), 4.05 (s, 3H), 3.69 (s, 3H).. ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.92, 149.98, 147.07, 144.10, 140.38, 137.10, 136.89, 136.34, 130.89, 129.15, 128.75, 128.54, 127.90, 127.33, 121.76, 121.68, 120.92, 120.59, 117.06, 114.01, 112.48, 112.12, 70.96, 55.88, 52.80, 41.65, IR ($CHCl_3$) v_{max} (cm^{-1}): 3325, 3032, 2924, 2856, 1712, 1625, 1599, 1565, 1512 1433, 1382, 1256, 1220, 1139, 1106, 1080, 1032. ESI-MS: m/z 453.10 $(M+H)^+$; HRMS: m/z 453.1800 calcd for $C_{28}H_{25}N_2O_4^+$(453.1809).

6f) Methyl 1-(4-hydroxy-3-methoxybenzyl)-9H-pyrido[3,4-b]indole-3-carboxylate:



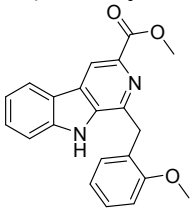
85%yield; light yellow solid; 117-119 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.83 (s, 1H), 8.14 (d, *J* = 8.0 Hz, 1H), 8.01 (s, 1H), 7.52 (t, *J* = 7.7 Hz, 1H), 7.43 – 7.28 (m, 2H), 6.93 (s, 2H), 6.77 (s, 1H), 5.61 (s, 1H), 4.58 (s, 2H), 4.08 (s, 3H), 3.74 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.88, 147.23, 144.89, 144.21, 140.20, 136.31, 129.66, 129.27, 128.80, 121.80, 121.36, 121.03, 117.07, 114.63, 112.00, 111.43, 55.94, 52.86, 42.32.IR ($CHCl_3$) v_{max} (cm^{-1}) :3327, 2925, 2849,1712, 1625, 1599, 1513, 1433, 1350, 1256, 1125, 1033. ESI-MS: m/z 363.10 $(M+H)^+$; HRMS: m/z 363.1339 calcd for $C_{21}H_{18}N_2O_4$+H^+(363.1339).

6g) Methyl 1-(3,4,5-trimethoxybenzyl)-9H-pyrido[3,4-b]indole-3-carboxylate:



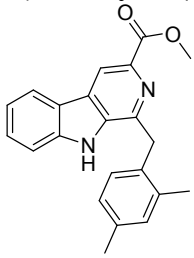
84%yield; yellow solid; mp 110-112 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.85 (s, 1H), 8.16 (d, *J* = 7.7 Hz, 2H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.41 (d, *J* = 8.1 Hz, 1H), 7.33 (t, *J* = 7.3 Hz, 1H), 6.55 (s, 2H), 4.59 (s, 2H), 4.08 (s, 3H), 3.84 (s, 3H), 3.76 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.84, 153.66, 143.68, 140.28, 137.30, 136.91, 136.33,133.53, 129.28, 128.90, 121.83, 121.71,121.07,117.15, 112.09, 105.82, 60.95, 56.17, 52.87, 42.61. IR ($CHCl_3$) v_{max} (cm^{-1}) : 3305, 2922, 2852, 1712, 1590, 1504, 1457, 1432, 1250, 1126, 1014. ESI-MS: m/z 407 $(M+H)^+$; HRMS: m/z 407.1598 calcd for $C_{23}H_{22}N_2O_5$+H^+(407.1601).

6h) Methyl 1-(2-methoxybenzyl)-9H-pyrido[3,4-b]indole-3-carboxylate:



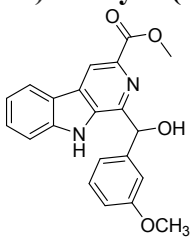
55%Yield; White solid; mp 212-214 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.42 (s, 1H), 8.78 (s, 1H), 8.12 (d, *J* = 7.8 Hz, 1H), 7.56 – 7.52 (m, 1H), 7.47 – 7.42 (m, 2H), 7.32 – 7.26 (m, 1H), 7.23 – 7.19 (m, 1H), 6.99 (d, *J* = 8.1 Hz, 1H), 6.95 – 6.86 (m, 1H), 4.61 (s, 2H), 4.10 (s, 3H), 4.06 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 167.05, 155.73, 144.69, 140.17, 137.24, 136.11, 131.45, 128.50, 128.31, 128.26, 126.28, 122.10, 122.03, 121.89, 120.69, 116.98, 111.86, 111.52, 56.15, 52.73, 34.92. IR ($CHCl_3$) v_{max} (cm^{-1}) : 3233, 2945, 1718, 1625, 1598, 1492, 1457, 1431, 1351, 1259, 1219, 1133, 1106, 1030. ESI-MS: m/z 347$(M+H)^+$; HRMS: m/z 347.1402 calcd for $C_{21}H_{18}N_2O_3$+H^+(347.1390).

6i) Methyl 1-(2,4-dimethylbenzyl)-9H-pyrido[3,4-b]indole-3-carboxylate:



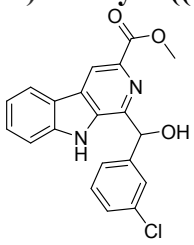
40% Yield; White solid; mp 232-234 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.81 (s, 1H), 8.14 (d, *J* = 7.6 Hz, 1H), 7.86 (s, 1H), 7.50 (td, *J* = 7.5, 1.0 Hz, 1H), 7.30 (dd, *J* = 7.5, 6.8 Hz, 2H), 7.08 (d, *J* = 7.6 Hz, 1H), 7.03 (s, 1H), 7.00 (d, *J* = 7.7 Hz, 1H), 4.60 (s, 2H), 4.06 (s, 3H), 2.33 (s, 3H), 2.19 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.91, 143.62, 140.10, 137.50, 137.48, 137.21, 136.31, 132.82, 131.80, 129.22, 129.16, 128.69, 127.21, 121.79, 121.58, 120.89, 116.74, 111.91, 52.81, 40.72, 21.03, 19.90. IR ($CHCl_3$) : v_{max} (cm^{-1}) 3270, 2949, 2920, 2852, 2349, 1714, 1626, 1596, 1566, 1502, 1456, 1433, 1384, 1350, 1307, 1254, 1217, 1154, 1134, 1105, 1015. ESI-MS: m/z 345.10 $(M+H)^+$; HRMS: m/z 345.1598 calcd for $C_{22}H_{20}N_2O_2$+H^+(345.1598).

7k)Methyl1-(hydroxyl(3-methoxyphenyl)methyl)-9H-pyrido[3,4-b]indole-3-carboxylate:



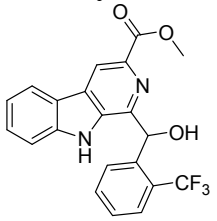
60% Yield, light yellow solid;m.p 176-178 ^{o}C; ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.67 (s, 1H), 8.84 (s, 1H), 8.36 (d, *J* = 7.8 Hz, 1H), 7.80 (d, *J* = 8.2 Hz, 1H), 7.58 (t, *J* = 7.6 Hz, 1H), 7.32 – 7.25 (m, 2H), 7.19 (t, *J* = 7.9 Hz, 1H), 7.10 (d, *J* = 7.6 Hz, 1H), 6.77 (d, *J* = 4.1 Hz, 1H), 6.16 (s, 1H), 6.15 (s, 1H), 3.92 (s, 3H), 3.72 (s, 3H). ^{13}C NMR (125 MHz, DMSO) δ 165.97, 159.08, 147.32, 144.43, 141.03, 135.16, 133.69, 129.10, 128.66, 128.46, 121.70, 120.56, 120.06, 118.39, 116.75, 112.98, 112.05, 75.89, 54.95, 51.94. IR ($CHCl_3$) : v_{max} (cm^{-1}) 3735, 3435, 2918, 1713, 1598, 1489, 1434, 1350, 1257, 1019. ESI-MS: m/z 363 $(M+1)^+$; HRMS: m/z 363.1336 calcd for $C_{21}H_{18}N_2O_4$+H^+(363.1339).

7l) Methyl1-((3-chlorophenyl(hydroxyl)methyl)-9H-pyrido[3,4-b]indole-3-carboxylate:



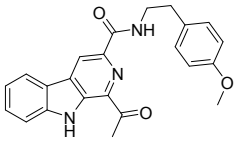
55%Yield; yellow solid; mp 115-117 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.49 (s, 1H), 8.59 (s, 1H), 8.08 (d, *J* = 7.9 Hz, 1H), 7.54 (dd, *J* = 11.3, 4.0 Hz, 1H), 7.46 – 7.44 (m, 2H), 7.32 – 7.2 (m, 2H), 7.09 (dt, *J* = 15.5, 7.9 Hz, 2H), 6.33 (s, 1H), 3.89 (s, 3H).^{13}C NMR (125 MHz, $CDCl_3$) δ 166.41, 144.90, 143.41, 140.68, 135.74, 134.44, 129.97, 129.75, 129.04, 127.97, 126.54, 124.67, 121.63, 121.30, 120.95, 117.44, 112.24, 75.41, 52.53.IR ($CHCl_3$) : v_{max} (cm^{-1}) : 3901, 3735, 3648, 3436, 2923, 1713, 1626, 1595, 1502, 1434, 1251, 1019. ESI-MS: m/z 366.90 $(M+H)^+$; HRMS: m/z 367.0841 calcd for $C_{20}H_{15}ClN_2O_3+H^+$(367.0844).

7m) Methyl1-(hydroxyl(2-(trifluoromethyl)phenyl)methyl)-9H-pyrido[3,4-b]indole-3-carboxylate



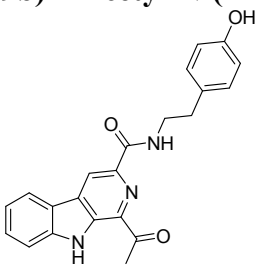
42%Yield; light yellow solid; mp 197-198 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.85 (s, 1H), 8.40 (s, 1H), 8.16 (d, *J* = 7.9 Hz, 1H), 7.80 – 7.77 (m, 1H), 7.56 (t, *J* = 7.6 Hz, 1H),7.45 -7.38 (m, 4H), 7.26 – 7.24 (m, 1H), 6.58 (s, 1H), 5.30 (s, 1H), 4.06 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.27, 142.92, 140.44, 136.23, 133.91, 132.89, 130.41, 130.16, 129.21, 128.58, 125.96, 125.90, 121.82, 121.50, 121.35, 117.69, 112.14, 68.75, 53.40, 52.59. IR ($CHCl_3$) : 3432, 2925, 2850, 1717, 1625, 1566, 1496, 1456, 1434, 1350, 1312, 1260, 1158, 1124,1061,1036, ESI-MS: m/z 401.00 $(M+H)^+$; HRMS: m/z 401.1104 calcd for $C_{21}H_{15}F_3N_2O_3+H^+$(401.1108).

9a) 1-Acetyl-N-(4-methoxy phenethyl)-*β*-carboline-3-carboxamide (marinacarbolines A)[3]



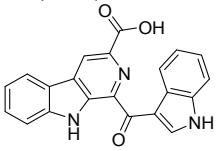
92% yield; Light yellow solid; mp 177-178 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.39 (s, 1H), 9.07 (s, 1H), 8.20 (d, *J* = 7.8 Hz, 1H), 8.06 (t, *J* = 5.5 Hz, 1H), 7.64 – 7.57 (m, 2H), 7.39 – 7.36 (m, 1H), 7.25 (d, *J* = 8.6 Hz, 2H), 6.90 (d, *J* = 8.5 Hz, 2H), 3.84 – 3.79 (m, 5H), 2.96 (t, *J* = 6.8 Hz, 2H), 2.77 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 202.27, 164.51, 158.38, 141.51, 139.25, 136.26, 133.47, 132.60, 131.01, 129.90, 129.73, 122.31, 121.53, 121.04, 118.35, 114.15, 112.19, 55.30, 40.70, 34.98, 25.73.IR ($CHCl_3$): v_{max} (cm^{-1}) : 3391, 3249, 2922, 2852, 1660, 1529,1512, 1493, 1462, 1452, 1383, 1330, 1288, 1245, 1150, 1037. ESI-MS: m/z 388.10 $(M+H)^+$; HRMS: m/z 410.1477 $[M+Na^+]$ calcd for $C_{23}H_{21}N_3O_3+Na^+$ (410.1475).

9b) 1-Acetyl-N-(4-Hydroxy phenethyl)-β-carboline-3-carboxamide(marinacarbolines B)[3]



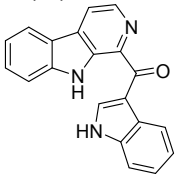
90% yield; yellow solid; mp 260-262 °C; ^{1}H NMR (400 MHz, DMSO) δ 12.18 (s, 1H), 9.09 (s, 1H), 8.69 (t, *J* = 5.7 Hz, 1H), 8.45 (d, *J* = 7.8 Hz, 1H), 7.84 (d, *J* = 8.2 Hz, 1H), 7.63 (t, *J* = 7.6 Hz, 1H), 7.34 (t, *J* = 7.5 Hz, 1H), 7.12 (d, *J* = 8.2 Hz, 2H), 6.72 (d, *J* = 8.2 Hz, 2H), 5.76 (s, 1H), 3.59 (dd, *J* = 13.4, 6.6 Hz, 2H), 2.88 (s, 3H), 2.84–2.75 (m, 2H).^{13}C NMR (125 MHz, DMSO) δ 200.95, 163.93, 155.70, 142.31, 138.61, 134.77, 133.86, 131.92, 129.54, 129.39, 129.27, 122.21, 120.76, 120.24, 117.77, 115.22, 113.26, 54.86, 34.50, 25.95. IR ($CHCl_3$) : v_{max} (cm^{-1}): 3360, 3335, 2922, 2851, 2677, 1742, 1673, 1644, 1610, 1592, 1515,1376, 1334, 1286, 1266, 1233, 1205, 1183,1159,1019. ESI-MS: m/z 374.00 $(M+H)^+$; HRMS: m/z 374.1496 (M+H) calcd for $C_{22}H_{19}N_3O_3+H^+$ (374.1499).

10) 1-(1H-indole-3-carbonyl)-9H-*β*-carboline-3-carboxylic acid (Pityriacitrin B)[4]



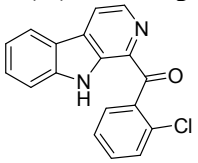
90%yield; yellow solid; mp 256-258 °C; ^{1}H NMR (400 MHz, DMSO) δ 12.41 (s, 1H), 12.27 (s, 1H), 9.75 (s, 1H), 9.15 (s, 1H), 8.61 (d, *J* = 7.2 Hz, 1H), 8.47 (d, *J* = 7.8 Hz, 1H), 7.91 (d, *J* = 8.1 Hz, 1H), 7.67 – 7.57 (m, 2H), 7.42 – 7.25 (m, 3H), 5.75 (s, 1H). ^{13}C NMR (125 MHz, DMSO) δ 186.36, 166.81, 142.03, 138.34, 137.08, 135.94, 135.80, 135.76, 131.29, 129.09, 127.27, 122.93, 122.18, 122.05, 121.65, 120.68, 120.44, 119.84, 114.14, 113.38, 112.24. IR ($CHCl_3$): v_{max} (cm^{-1}): 3436, 2071, 1633, 1355, 1017. ESI-MS: m/z 356 $(M+H)^+$; HRMS: m/z 356.1029 calcd for $C_{21}H_{13}N_3O_3+H^+$(356.1030)

11) (9H-carbazol-1-yl)(1H-indole-3-yl) methanone) (Pityriacitrin)[4]



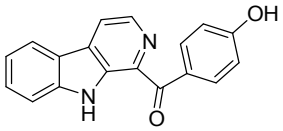
42%yield; yellow solid; mp 231-233 °C; ^{1}H NMR (400 MHz, Acetone) δ 11.48 (brs, 1H), 11.17 (brs, 1H), 9.56 (d, *J* = 2.5 Hz, 1H), 8.69 (d, *J* = 8.2 Hz, 1H), 8.60 (d, *J* = 4.9 Hz, 1H), 8.34 (dd, *J* = 15.7, 6.3 Hz, 2H), 7.97 (d, *J* = 8.2 Hz, 1H), 7.70 – 7.56 (m, 2H), 7.39 – 7.26 (m, 3H).^{13}C NMR (100 MHz, Acetone) δ 188.95, 142.63, 139.65, 138.54, 138.11, 137.12, 136.92, 132.13, 129.67, 128.73, 124.93, 123.87, 123.24, 122.91, 122.44, 121.64, 120.99, 118.54, 116.03, 113.58, 112.76. IR ($CHCl_3$): v_{max} (cm^{-1}) :3413, 2921,2851, 1597, 1491, 1443, 1384, 1318,1286, 1233,1216 1134, 1020.ESI-MS:m/z 312 $(M+H)^+$; HRMS: m/z 312.1130 calcd for $C_{20}H_{13}N_3O+H^+$(312.1131).

13) (2-chlorophenyl)(9H-pyrido[3,4-b]indol-1-yl)methanone:[5]



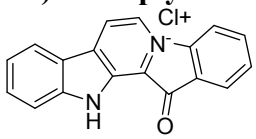
75%yield; yellow solid; mp 204-206 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.44 (s, 1H), 8.56 (d, *J* = 4.9 Hz, 1H), 8.25 – 8.11 (m, 2H), 7.68 – 7.56 (m, 3H), 7.54 – 7.33 (m, 4H), ^{13}C NMR (125 MHz, $CDCl_3$) δ 197.59, 141.22, 138.84, 138.40, 136.82, 135.50, 131.85, 131.20,130.05, 129.91, 129.49, 126.36, 121.92, 121.03, 120.73, 119.19, 112.11.IR (CHCl3): ν_{max} (cm^{-1}) : 3436, 2078, 1643, 1464, 1430, 1285, 1208, 1117, 1018.ESI-MS: m/z 307 $(M+H)^+$; HRMS: m/z 307.0635 calcd for $C_{18}H_{11}ClN_2O+H^+$(307.0633).

14) (4-Hydroxyphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone (Eudistomin-Y1)[6]



40%yield; Yellow solid; mp 217-219 °C; ^{1}H NMR (400 MHz, Acetone-d_6) δ 11.30 (s, 1H), 8.56 (d, *J* = 4.9 Hz, 1H), 8.48 (d, *J* = 8.7 Hz, 2H), 8.35 (d, *J* = 4.9 Hz, 1H), 8.30 (d, *J* = 7.9 Hz, 1H), 7.88 (d, *J* = 8.2 Hz, 1H), 7.63 (t, *J* = 7.7 Hz, 1H), 7.34 (t, *J* = 7.5 Hz, 1H), 7.00 (d, *J* = 8.7 Hz, 3H). ^{13}C NMR (125 MHz, Acetone) δ 191.73, 161.61, 141.67, 141.53, 137.57, 137.21, 136.66, 136.50, 134.08, 131.28, 131.23, 129.41, 128.93, 121.63, 120.77, 120.73, 120.31, 118.07, 114.61, 112.64, 112.59. IR ($CHCl_3$): ν_{max} (cm^{-1}) : 3400, 2921, 1600, 1384, 1317, 1245, 1216, 1164, 1045. ESI-MS: m/z 289 $(M+H)^+$; HRMS: m/z 289.0977 calcd for $C_{18}H_{12}N_2O_2+H^+$(289.0972).

15) Fascaplysin:[5]



82% yield; Brick red solid; m.p. 230-232 °C; ^{1}H NMR (400 MHz, MeOD) δ 9.27 (d, *J* = 6.2 Hz, 1H), 8.86 (d, *J* = 6.2 Hz, 1H), 8.39 (d, *J* = 8.0 Hz, 1H), 8.24 (d, *J* = 8.1 Hz, 1H), 7.97 (d, *J* = 7.4 Hz, 1H), 7.89 (t, *J* = 7.8 Hz, 1H), 7.81 (t, *J* = 7.7 Hz, 1H), 7.72 (d, *J* = 8.3 Hz, 1H), 7.66 (t, *J* = 7.5 Hz, 1H), 7.45 (t, *J* = 7.4 Hz, 1H). ^{13}C NMR (100 MHz, MeOD) δ 183.30, 148.94, 148.79, 142.96, 138.26, 135.90, 133.16, 132.72, 127.49, 126.84, 125.61, 125.21, 124.64, 123.76, 121.29, 121.11, 116.40, 114.66. IR ($CHCl_3$): ν_{max} (cm^{-1}) 3437, 2921, 1637, 1018 cm^{-1}; ESI-MS: *m/z* 271.00$[M-Cl]^+$; HRMS: *m/z* 271.0865 calcd for $C_{18}H_{11}N_2O^+$ (271.0877).

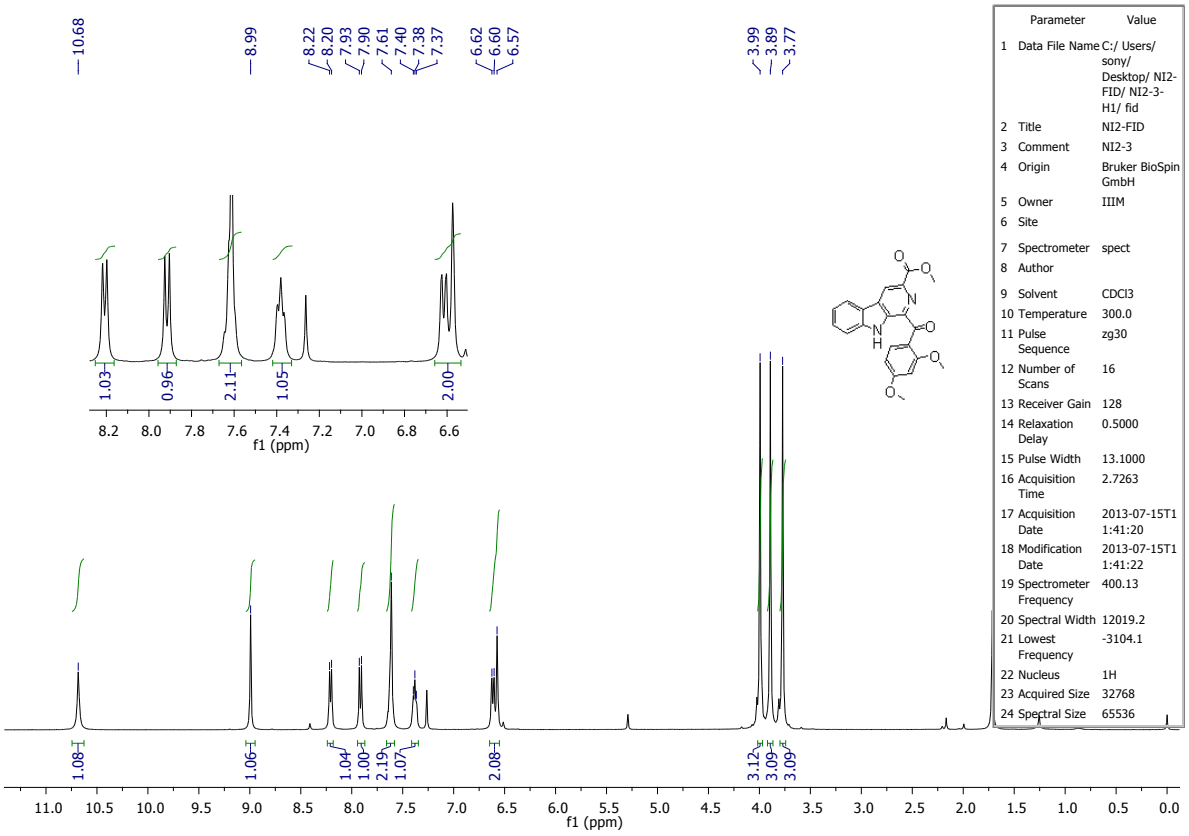
4. References:

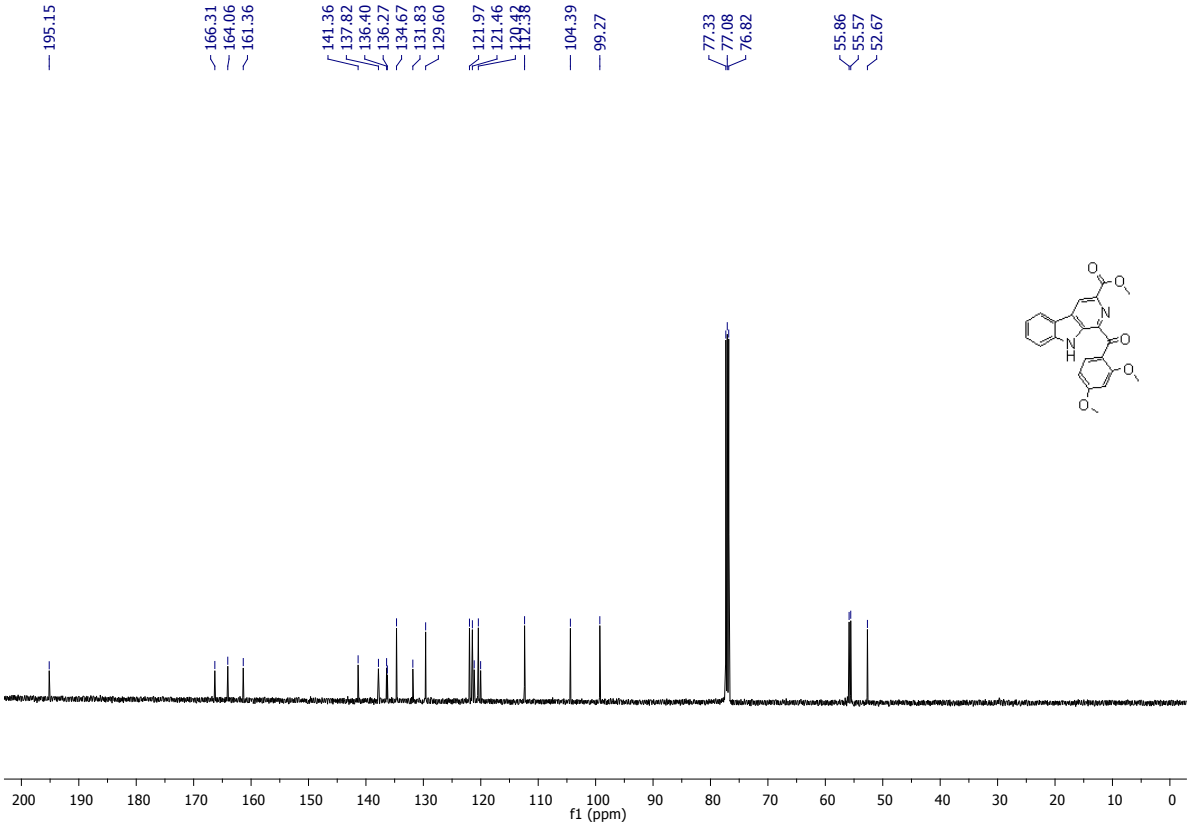
1) Yang, M. L.; Kuo, P. C.; Hwang, T. L.; Chiou, W. F.; Qian, K.; Lai, C. Y.; Lee, K. H.; Wu, T. S., *Bioorg. Med. Chem.* 2011, **19**, 1674-1682
2) Panarese, J. D.; Waters, S. P., *Org. Biomol. Chem.* 2013, **11**, 3428–3431.
3) Huang, H.; Yao, Y.; He, Z.; Yang, T.; Ma, J.; Tian, X.; Li, Y.; Huang, C.; Chen, X.; Li, W.; Zhang, S.; Zhang, C.; Ju, J., *J. Nat. Prod.* 2011, **74**, 2122-2127.
4) Zhang, P.; Sun, X.; Xu, B.; Bijian, K.; Wan, S.; Li, G.; Jamali, M. A.; Jiang, T., *Eur. J Med. Chem.* 2011, **46**, 6089-6097.
5) Bharate, S. B.; Manda, S.; Joshi, P.; Singh, B.; Vishwakarma, R. A., *Med. Chem. Commun.* 2012, **3**, 1098-1103.

6) Jin, H.; Zhang, P.; Bijian, K.; Ren, S.; Wan, S.; Jamali, M. A. A.; Jiang, T., *Mar. Drugs* 2013, **11**, 1427-1439.

5. Copies of ^{1}H NMR and ^{13}C NMR Spectra of Products:

3a) Methyl 1-(2,4-dimethoxybenzoyl)-9H-*β*-carboline-3-carboxylate:

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99.27
77.33
77.08
76.82
55.86
55.57
52.67
200
190
180
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130
120
110
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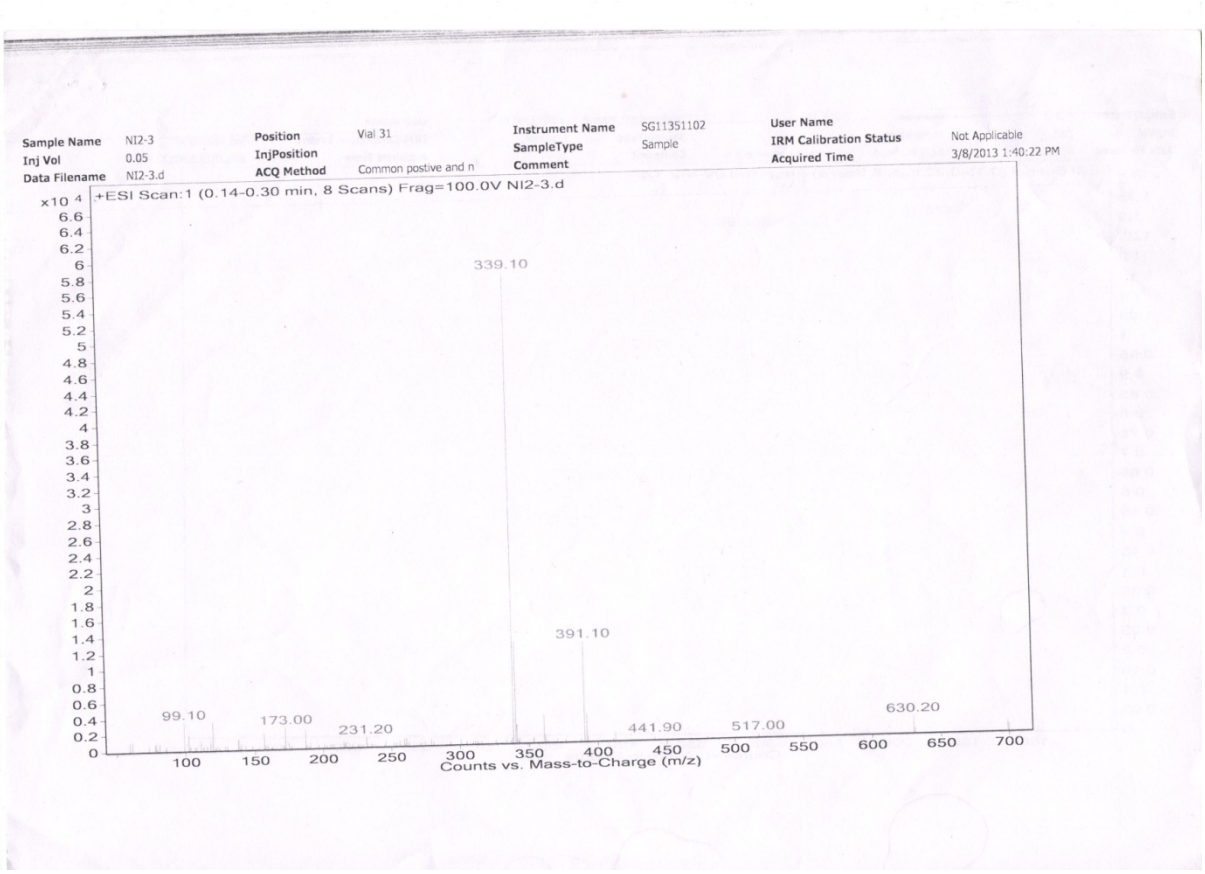
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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SampleType Sample
Comment
User Name
IRM Calibration Status Not Applicable
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Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

Data File	NI2-3.d	**Sample Name**	NI2-3
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IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			

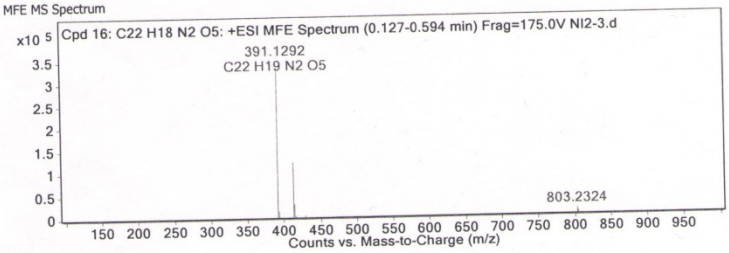
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 16: C22 H18 N2 O5	0.188	390.1218	C22 H18 N2 O5	C22 H18 N2 O5	-0.49	C22 H18 N2 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 16: C22 H18 N2 O5	391.1292	0.188	Find by Molecular Feature	390.1218

MFE MS Spectrum



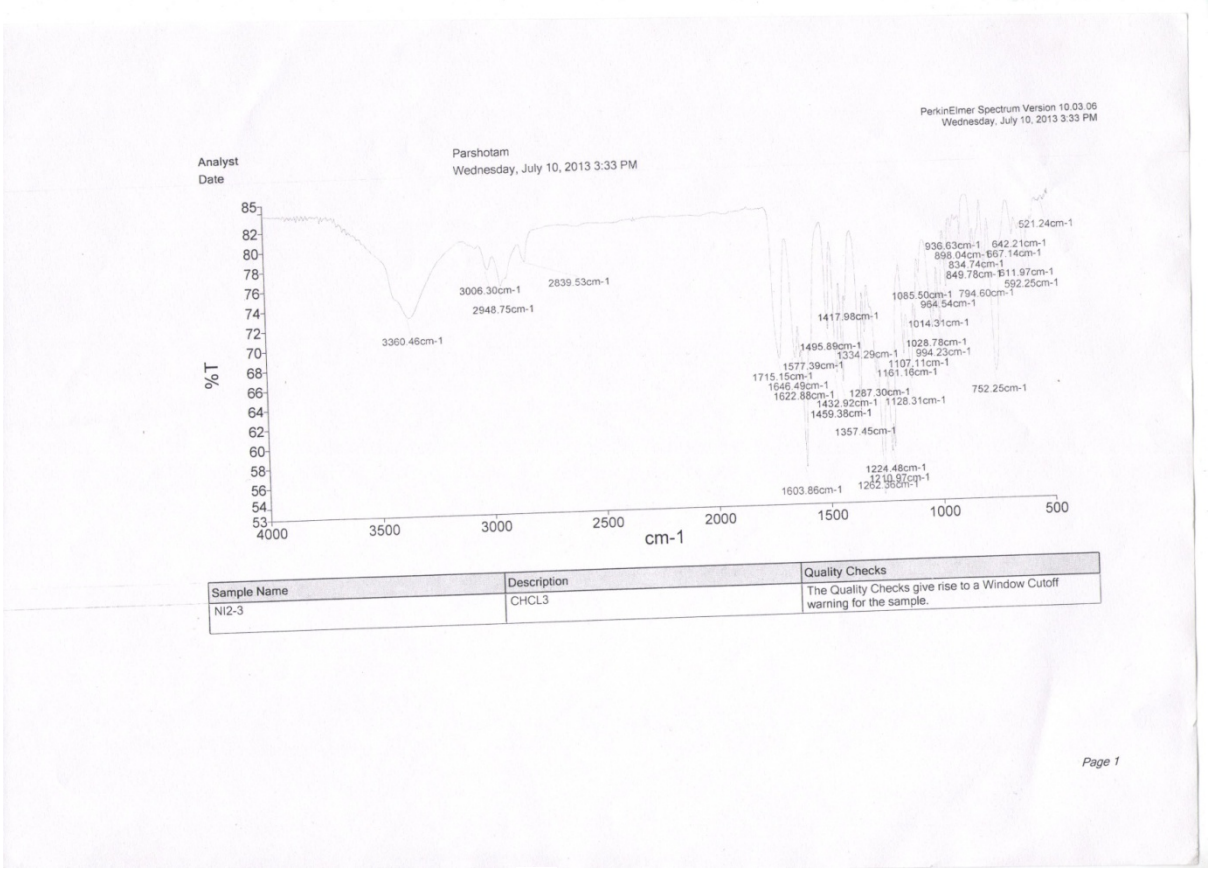
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
391.1292	1	333531.09	C22 H19 N2 O5	(M+H)+
392.1318	1	78993.43	C22 H19 N2 O5	(M+H)+
393.134	1	14013.15	C22 H19 N2 O5	(M+H)+
394.1376	1	2051.48	C22 H19 N2 O5	(M+H)+
413.1105	1	121681.12	C22 H18 N2 Na O5	(M+Na)+
414.1133	1	30095.73	C22 H18 N2 Na O5	(M+Na)+
415.1154	1	4438.8	C22 H18 N2 Na O5	(M+Na)+
429.0841	1	4886.82	C22 H18 K N2 O5	(M+K)+
803.2324	1	12582.04		(2M+Na)+
804.2355	1	5579.91		(2M+Na)+

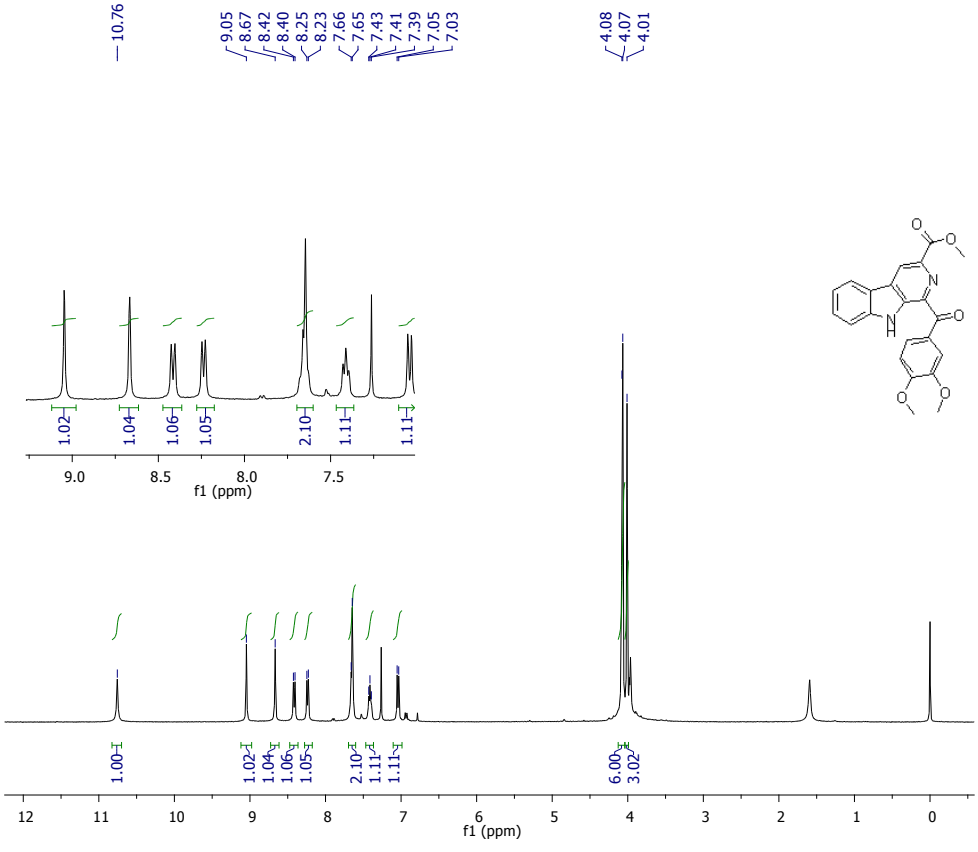
Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	391.1292	391.1288	-0.88	100	100	77.82	77.27
2	392.1318	392.132	0.73	23.68	24.93	18.43	19.27
3	393.134	393.1347	1.84	4.2	4.01	3.27	3.1
4	394.1376	394.1373	-0.67	0.62	0.48	0.48	0.37

--- End Of Report ---



3b) Methyl 1-(3,4-dimethoxybenzoyl)-9H-*β*-carboline-3-carboxylate:



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6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
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11	Pulse Sequence	zg30
12	Number of Scans	10
13	Receiver Gain	181
14	Relaxation Delay	0.5000
15	Pulse Width	13.1000
16	Acquisition Time	2.7263
17	Acquisition Date	2014-04-23T11:48:11
18	Modification Date	2014-04-23T11:48:14
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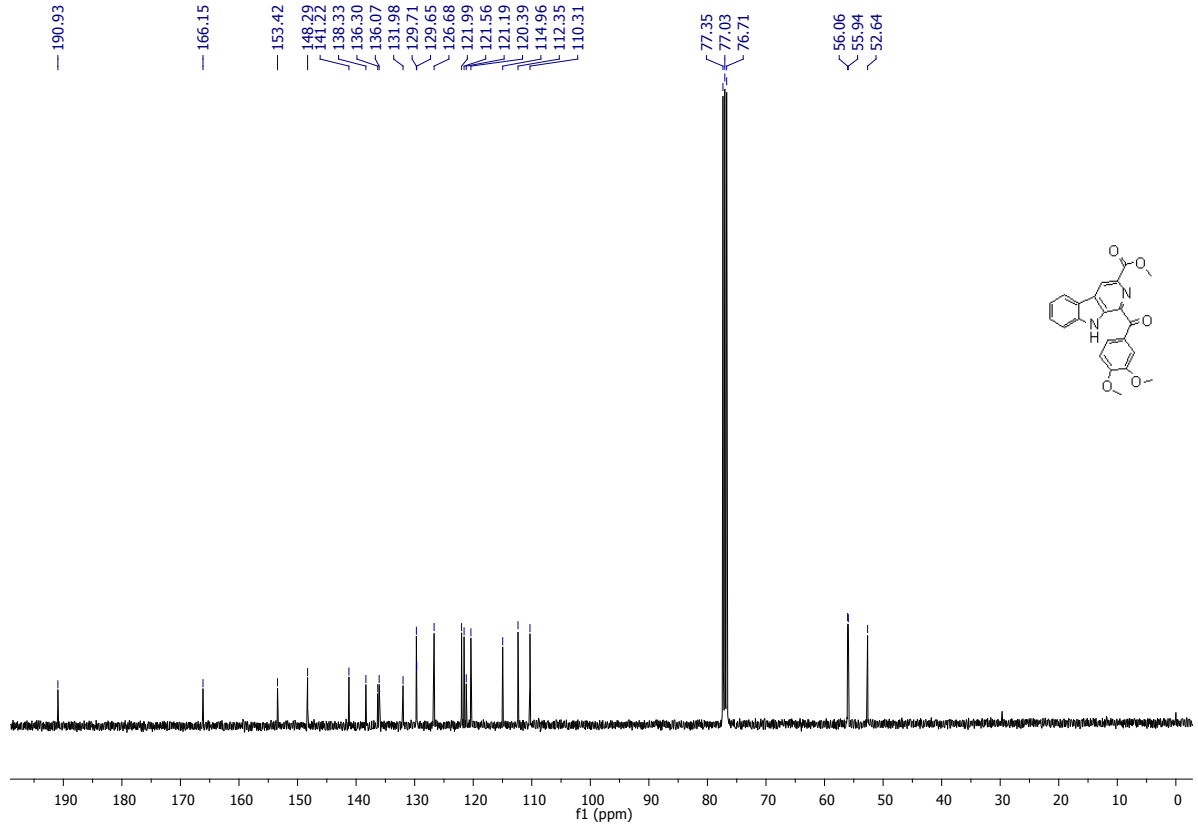
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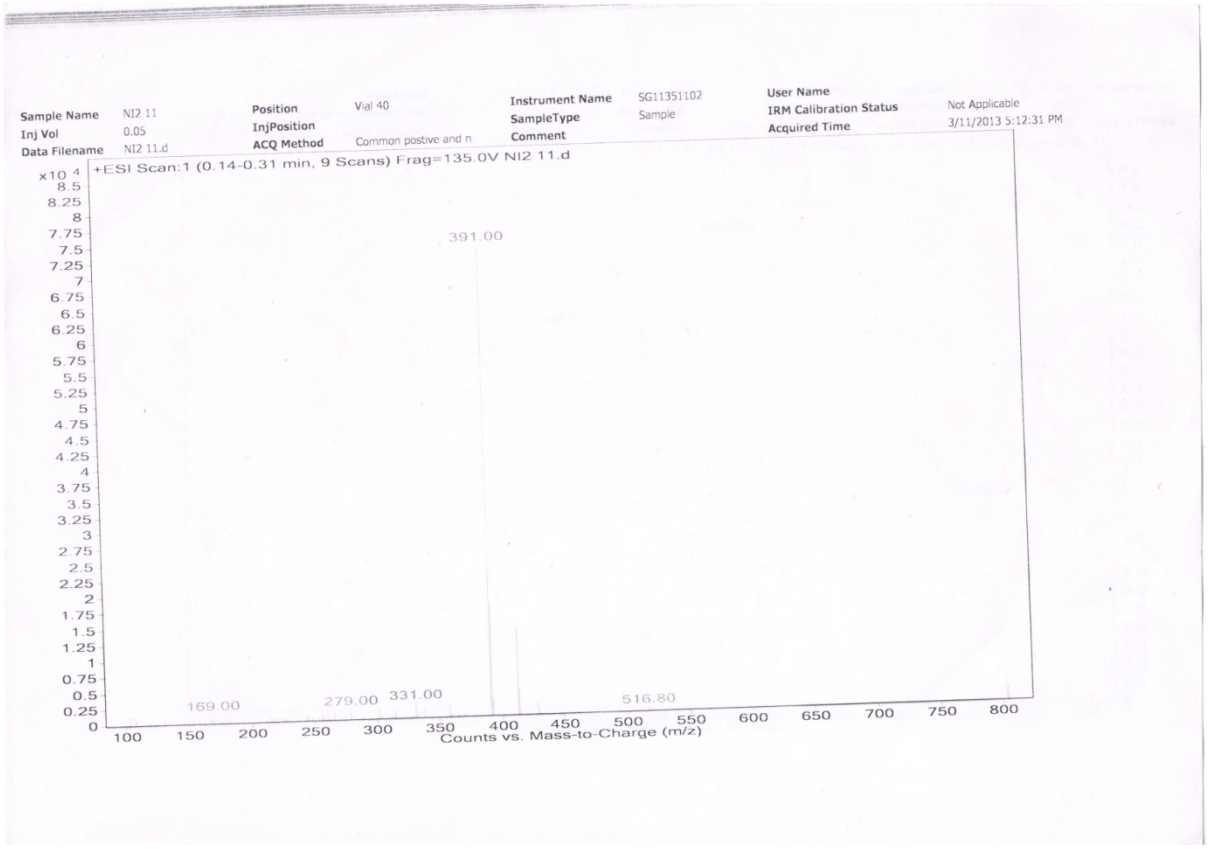
f1 (ppm)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Comment
User Name
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Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

Data File	NI2-11.d	**Sample Name**	NI2-11
Sample Type	Sample	**Position**	Vial 15
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	13-03-2013 PM 7:51:08
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			

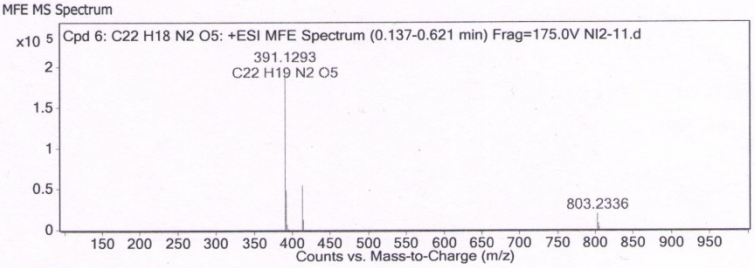
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 6: C22 H18 N2 O5	0.19	390.122	C22 H18 N2 O5	C22 H18 N2 O5	-0.98	C22 H18 N2 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 6: C22 H18 N2 O5	391.1293	0.19	Find by Molecular Feature	390.122

MFE MS Spectrum



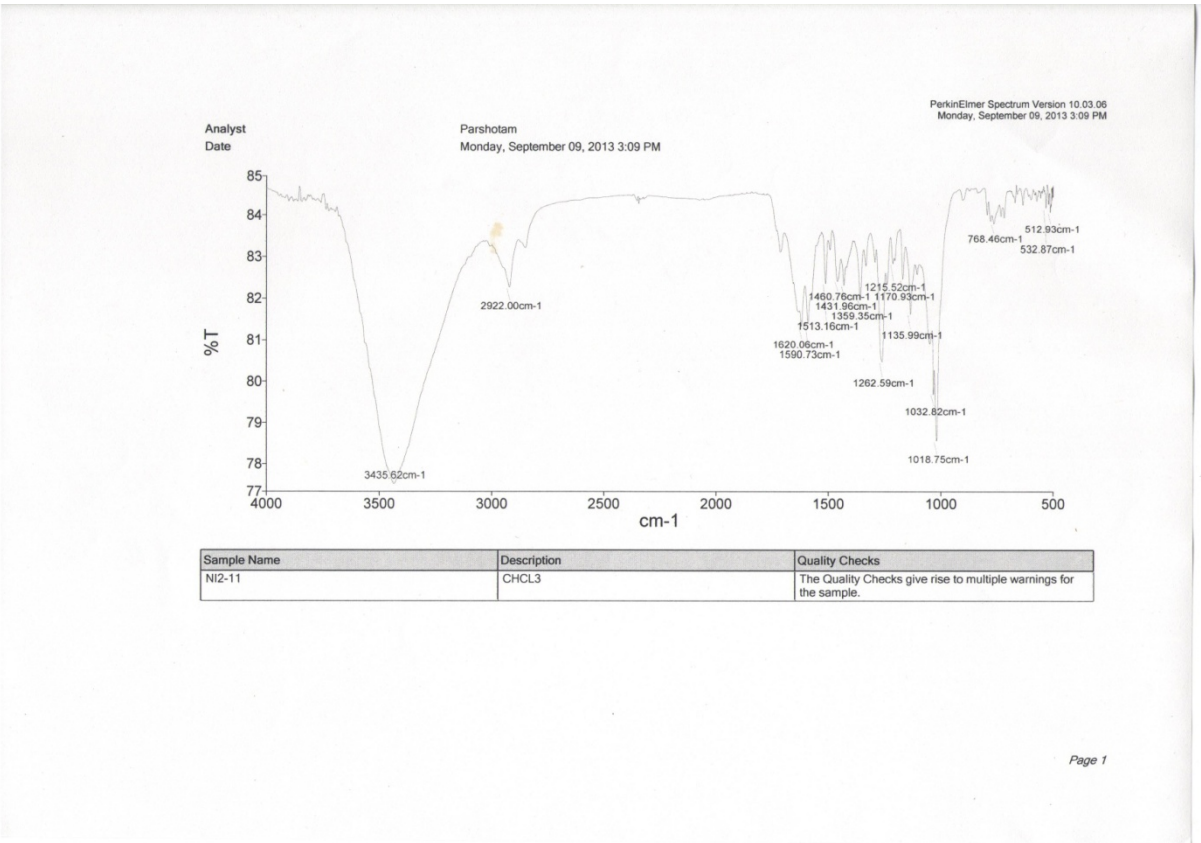
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
391.1293	1	191486.5	C22 H19 N2 O5	(M+H)+
392.1321	1	48023.76	C22 H19 N2 O5	(M+H)+
393.1352	1	7321.17	C22 H19 N2 O5	(M+H)+
394.1383	1	874.13	C22 H19 N2 O5	(M+H)+
413.1109	1	54469.64	C22 H18 N2 Na O5	(M+Na)+
414.1141	1	12238.9	C22 H18 N2 Na O5	(M+Na)+
415.1171	1	2558.84	C22 H18 N2 Na O5	(M+Na)+
803.2336	1	18940.7		(2M+Na)+
804.2371	1	8231.94		(2M+Na)+
805.2378	1	3425.42		(2M+Na)+

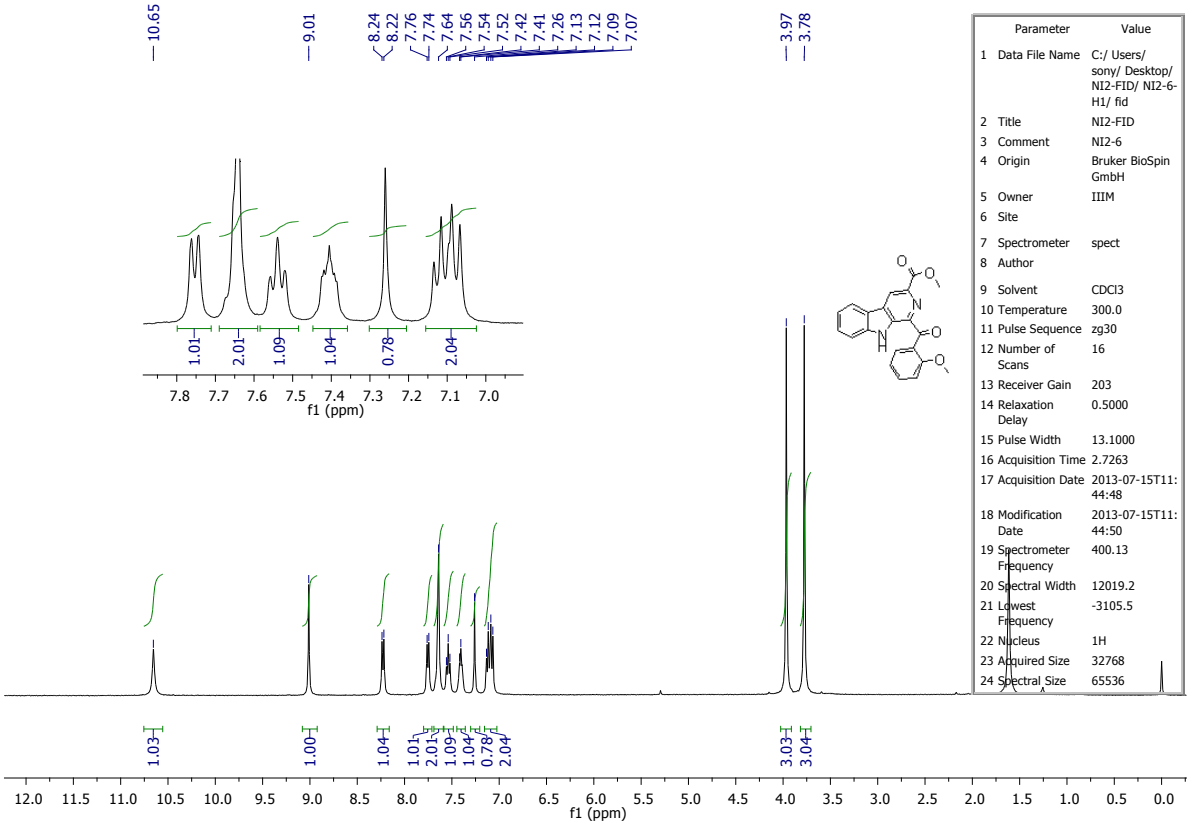
Predicted Isotope Match Table

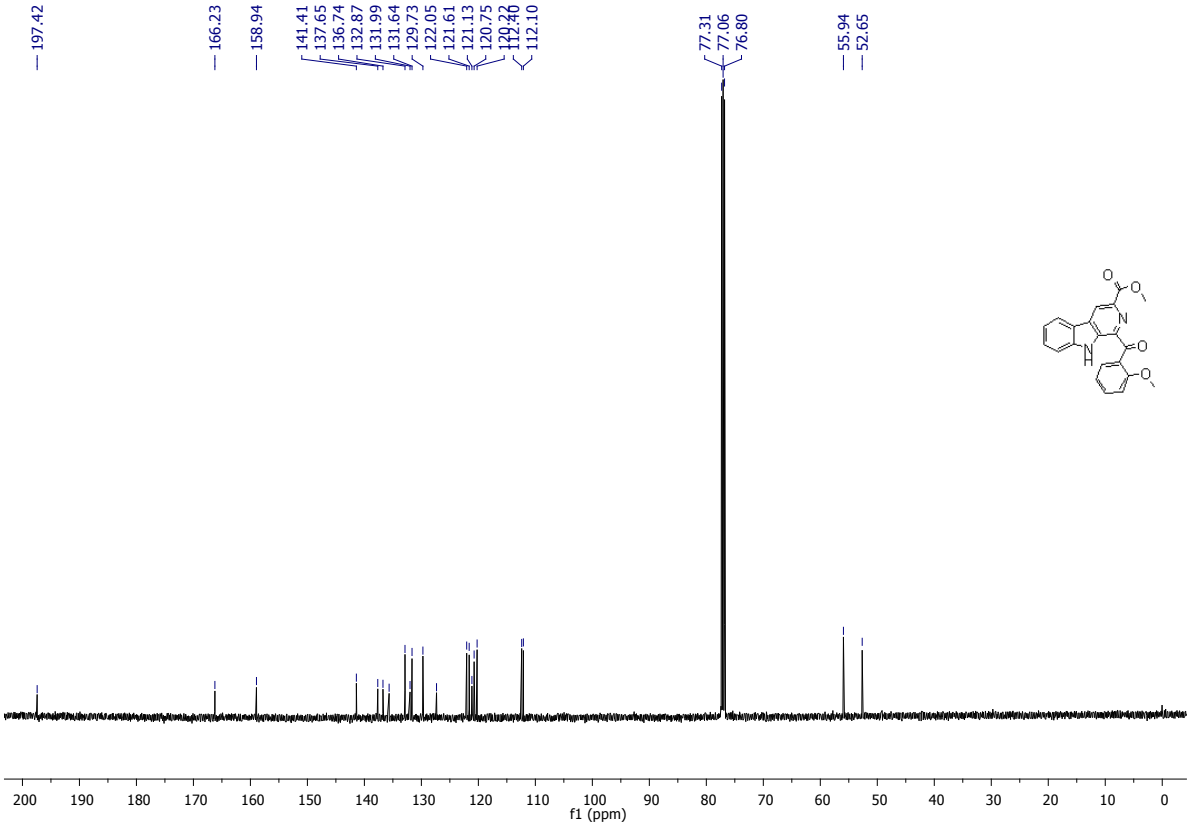
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	391.1293	391.1288	-1.15	100	100	77.3	77.27
2	392.1321	392.132	-0.2	25.08	24.93	19.39	19.27
3	393.1352	393.1347	-1.26	3.82	4.01	2.96	3.1
4	394.1383	394.1373	-2.46	0.46	0.48	0.35	0.37

--- End Of Report ---



3c) Methyl 1-(2-methoxybenzoyl)-9H -*β*-carboline-3-carboxylate:

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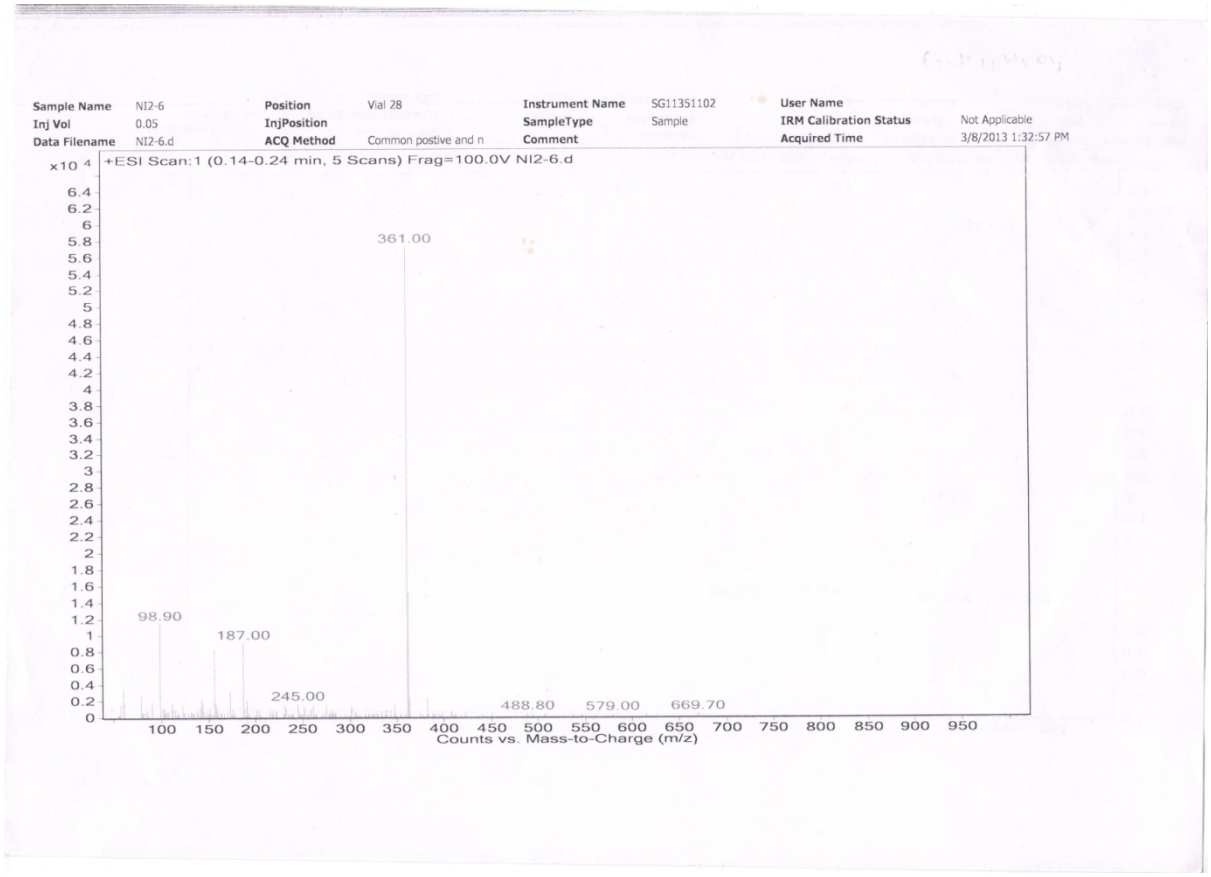
f1 (ppm)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SampleType Sample
Comment
User Name
IRM Calibration Status Not Applicable
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Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

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Comment			

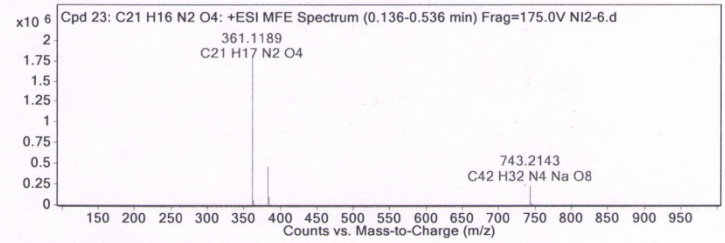
Sample Group		**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)	

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 23: C21 H16 N2 O4	0.19	360.1117	C21 H16 N2 O4	C21 H16 N2 O4	-1.82	C21 H16 N2 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 23: C21 H16 N2 O4	361.1189	0.19	Find by Molecular Feature	360.1117

MFE MS Spectrum



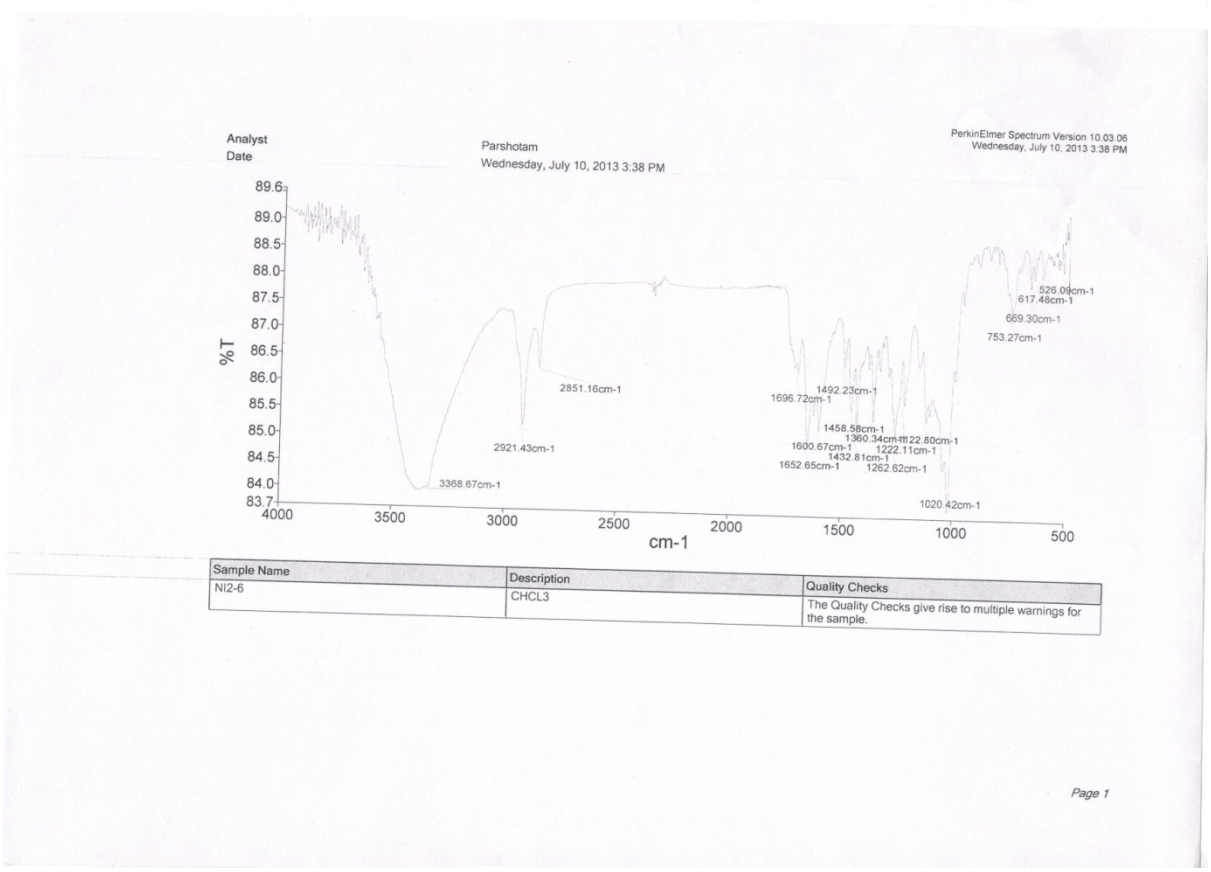
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
361.1189	1	1823820.13	C21 H17 N2 O4	(M+H)+
362.1225	1	379544.5	C21 H17 N2 O4	(M+H)+
363.1247	1	51118.58	C21 H17 N2 O4	(M+H)+
364.1272	1	5937	C21 H17 N2 O4	(M+H)+
383.1013	1	460787.91	C21 H16 N2 Na O4	(M+Na)+
384.104	1	103345.23	C21 H16 N2 Na O4	(M+Na)+
385.1062	1	15190.69	C21 H16 N2 Na O4	(M+Na)+
743.2143	1	234470.06	C42 H32 N4 Na O8	(2M+Na)+
744.217	1	109741.46	C42 H32 N4 Na O8	(2M+Na)+
745.2188	1	27185.73	C42 H32 N4 Na O8	(2M+Na)+

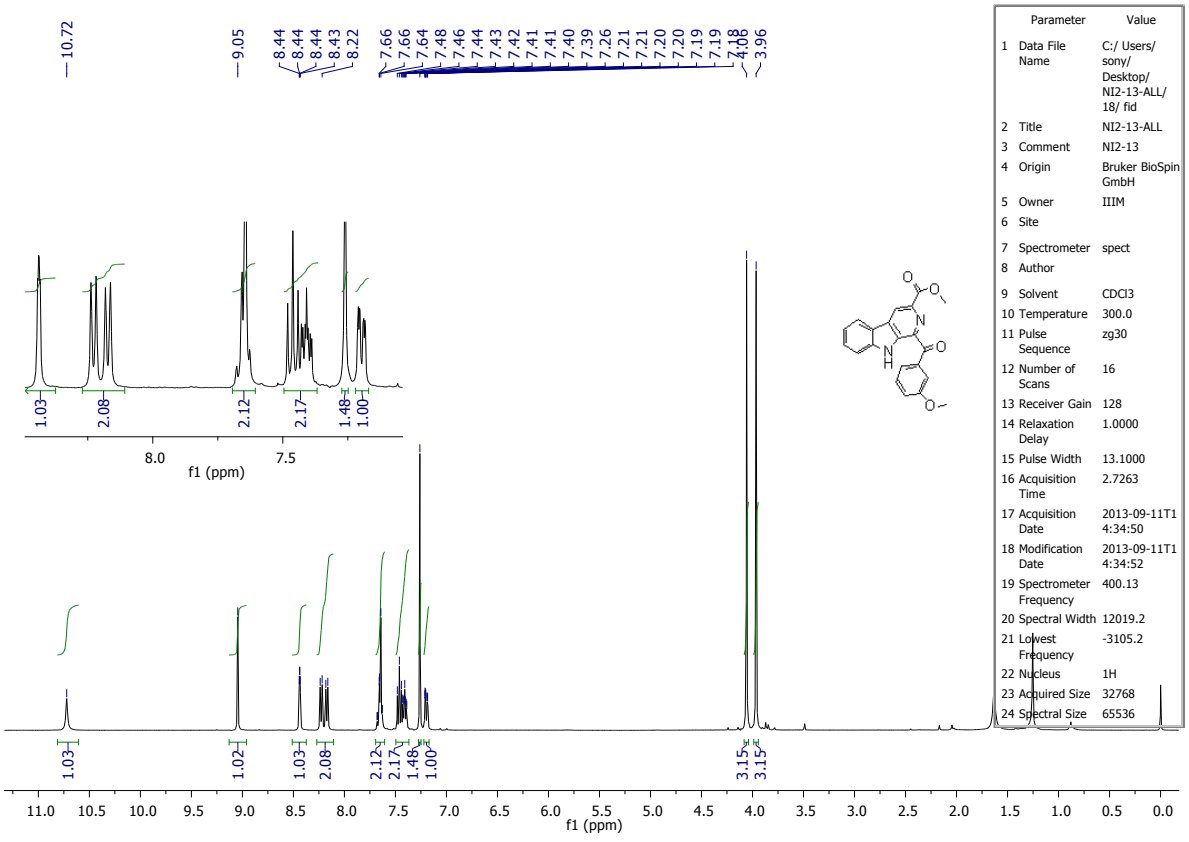
Predicted Isotope Match Table

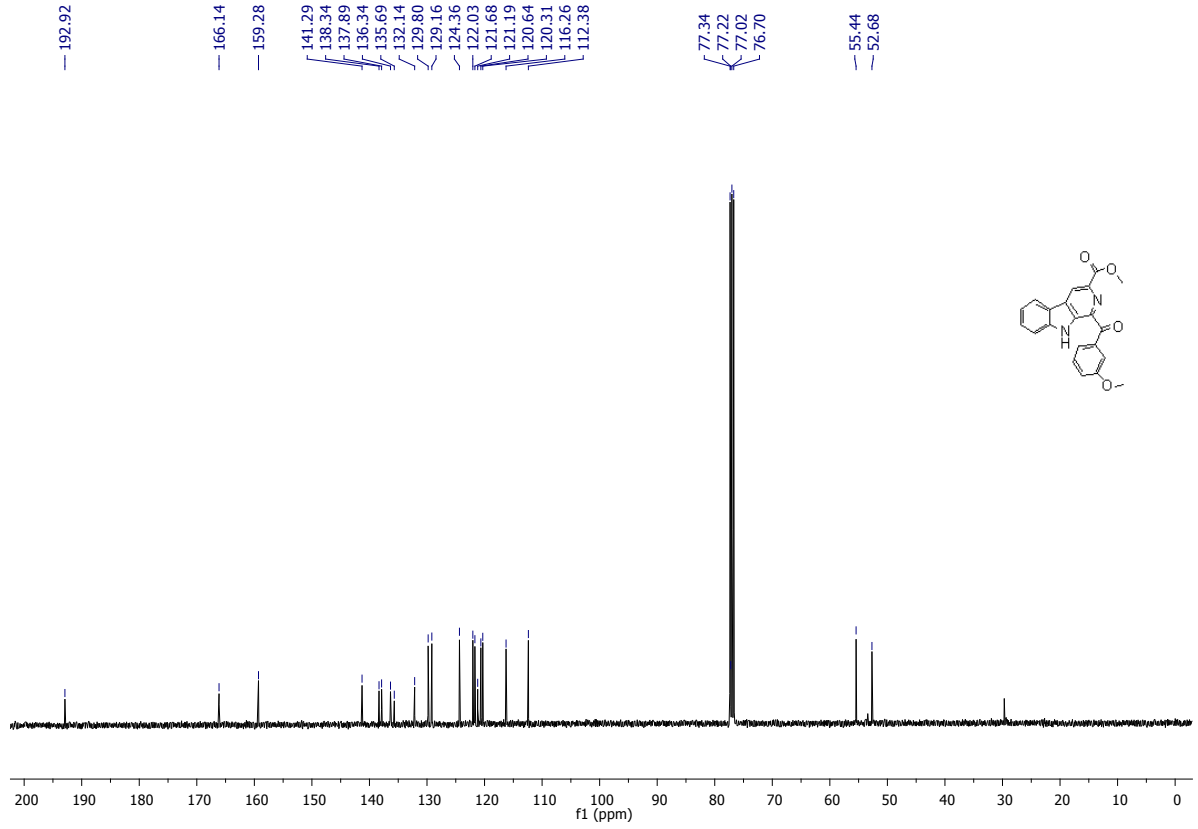
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	361.1189	361.1183	-1.59	100	100	80.66	78.28
2	362.1225	362.1215	-2.93	20.81	23.79	16.79	18.62
3	363.1247	363.1242	-1.49	2.8	3.53	2.26	2.76
4	364.1272	364.1268	-1.27	0.33	0.39	0.26	0.31
5	365.131	365.1294	-4.62	0.03	0.03	0.03	0.03

--- End Of Report ---



3d) Methyl 1-(3-methoxybenzoyl)- 9H- *β*-carboline-3-carboxylate:

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122.03
121.68
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77.02
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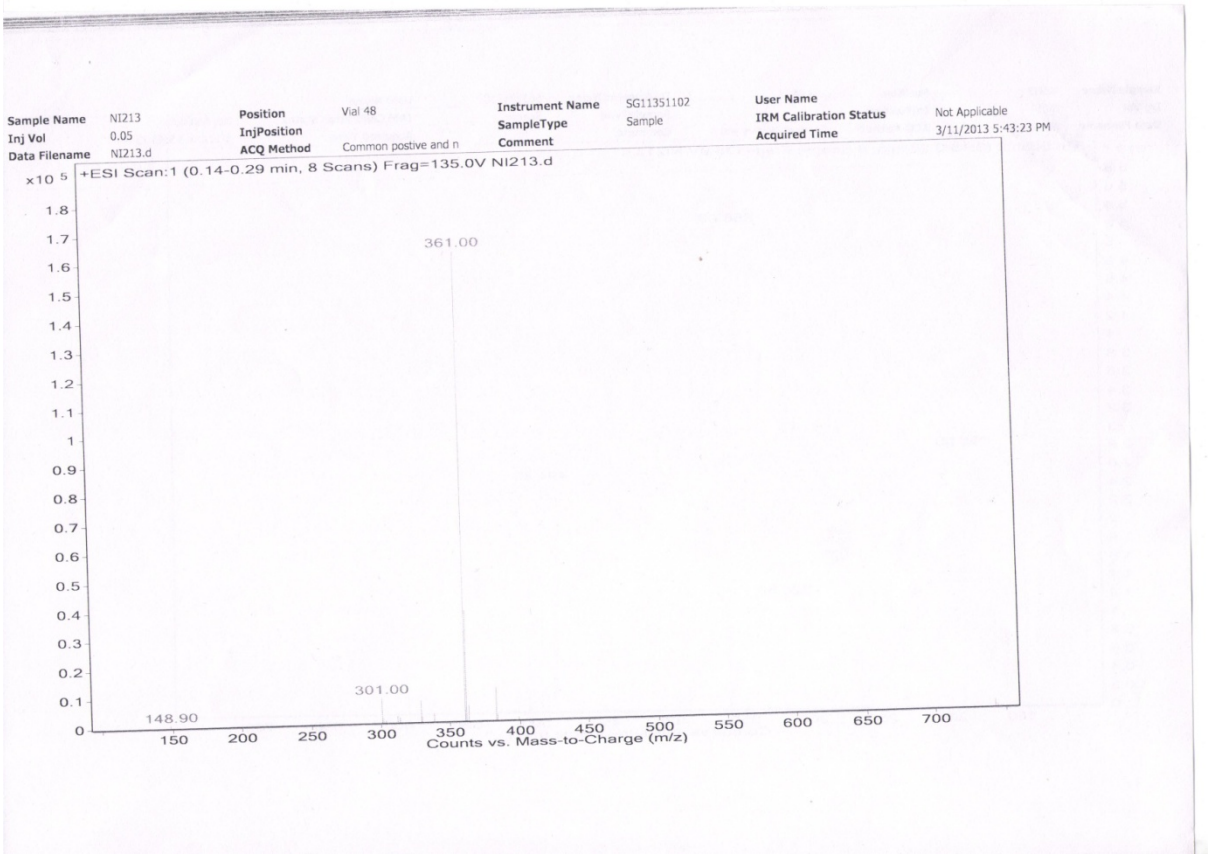
52.68
f1 (ppm)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Comment
User Name
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Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

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Comment			

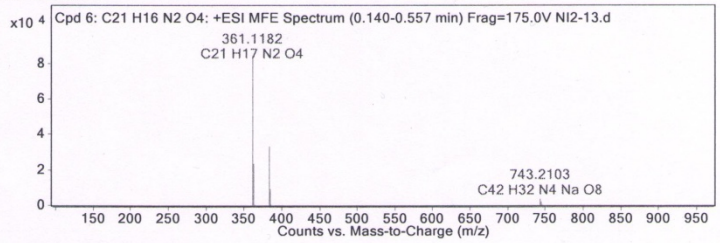
Sample Group		**Info.**	65:25(ACN:H20)
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 6: C21 H16 N2 O4	0.19	360.1109	C21 H16 N2 O4	C21 H16 N2 O4	0.29	C21 H16 N2 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 6: C21 H16 N2 O4	361.1182	0.19	Find by Molecular Feature	360.1109

MFE MS Spectrum



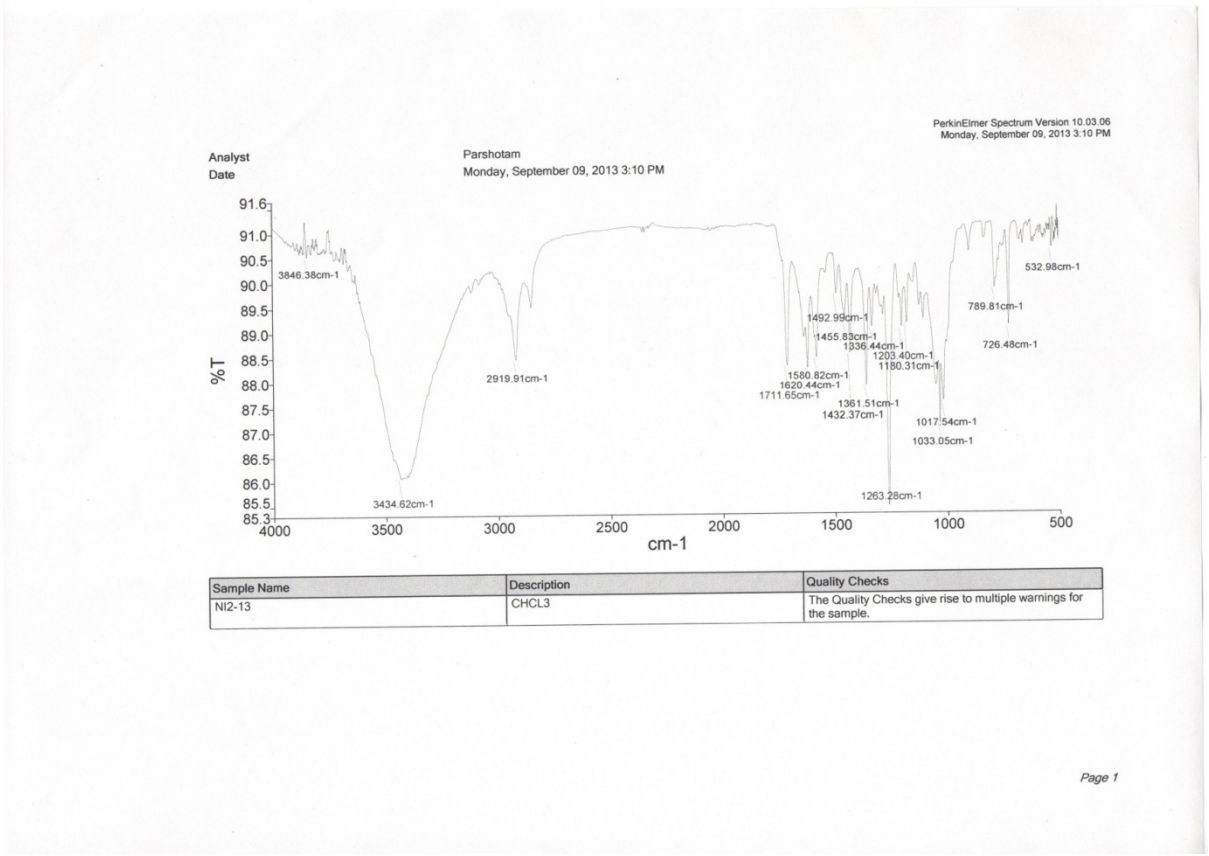
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
361.1182	1	84781.13	C21 H17 N2 O4	(M+H)+
362.1212	1	23536.27	C21 H17 N2 O4	(M+H)+
363.1238	1	3804.35	C21 H17 N2 O4	(M+H)+
364.1289	1	373.68	C21 H17 N2 O4	(M+H)+
383.0997	1	33070.25	C21 H16 N2 Na O4	(M+Na)+
384.1036	1	8941.5	C21 H16 N2 Na O4	(M+Na)+
385.1055	1	1308.98	C21 H16 N2 Na O4	(M+Na)+
743.2103	1	3584.38	C42 H32 N4 Na O8	(2M+Na)+
744.2139	1	1834.63	C42 H32 N4 Na O8	(2M+Na)+
745.2189	1	543.91	C42 H32 N4 Na O8	(2M+Na)+

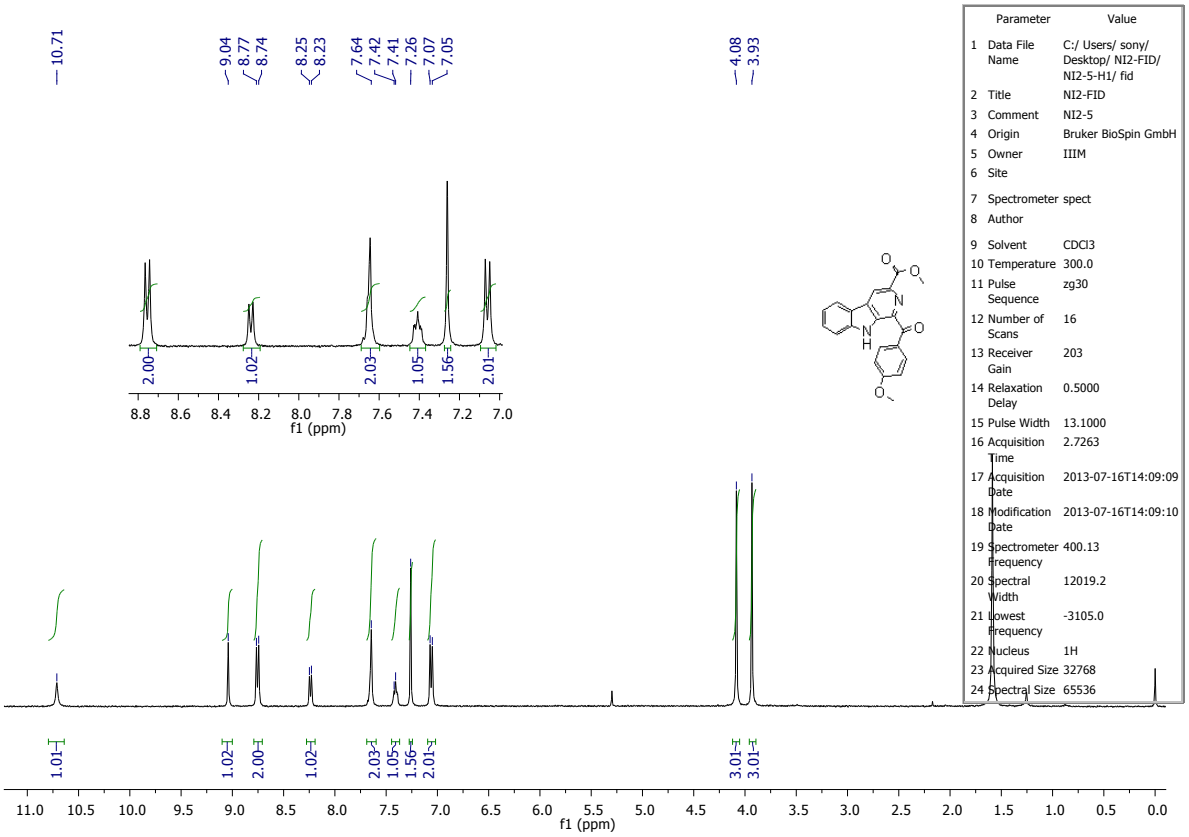
Predicted Isotope Match Table

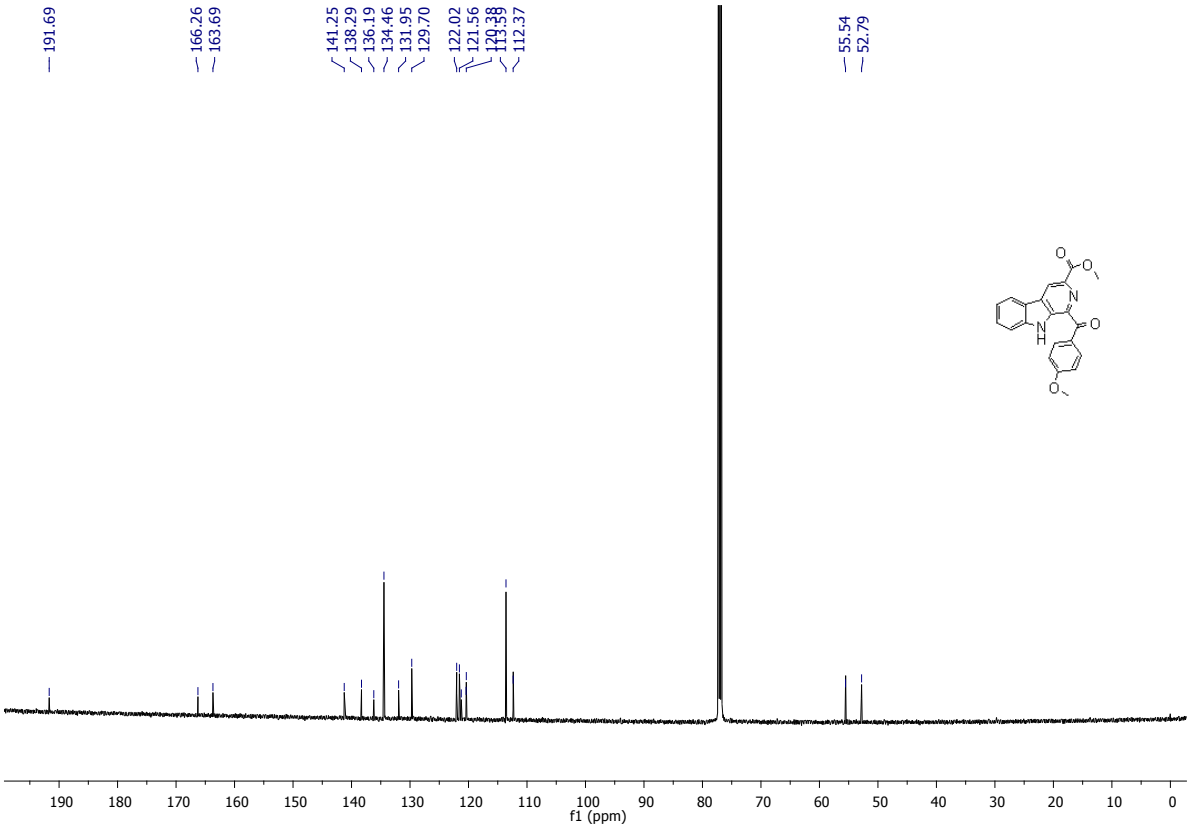
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	361.1182	361.1183	0.15	100	100	75.36	78.3
2	362.1212	362.1215	0.79	27.76	23.79	20.92	18.63
3	363.1238	363.1242	0.87	4.49	3.53	3.38	2.76
4	364.1289	364.1268	-5.92	0.44	0.39	0.33	0.31

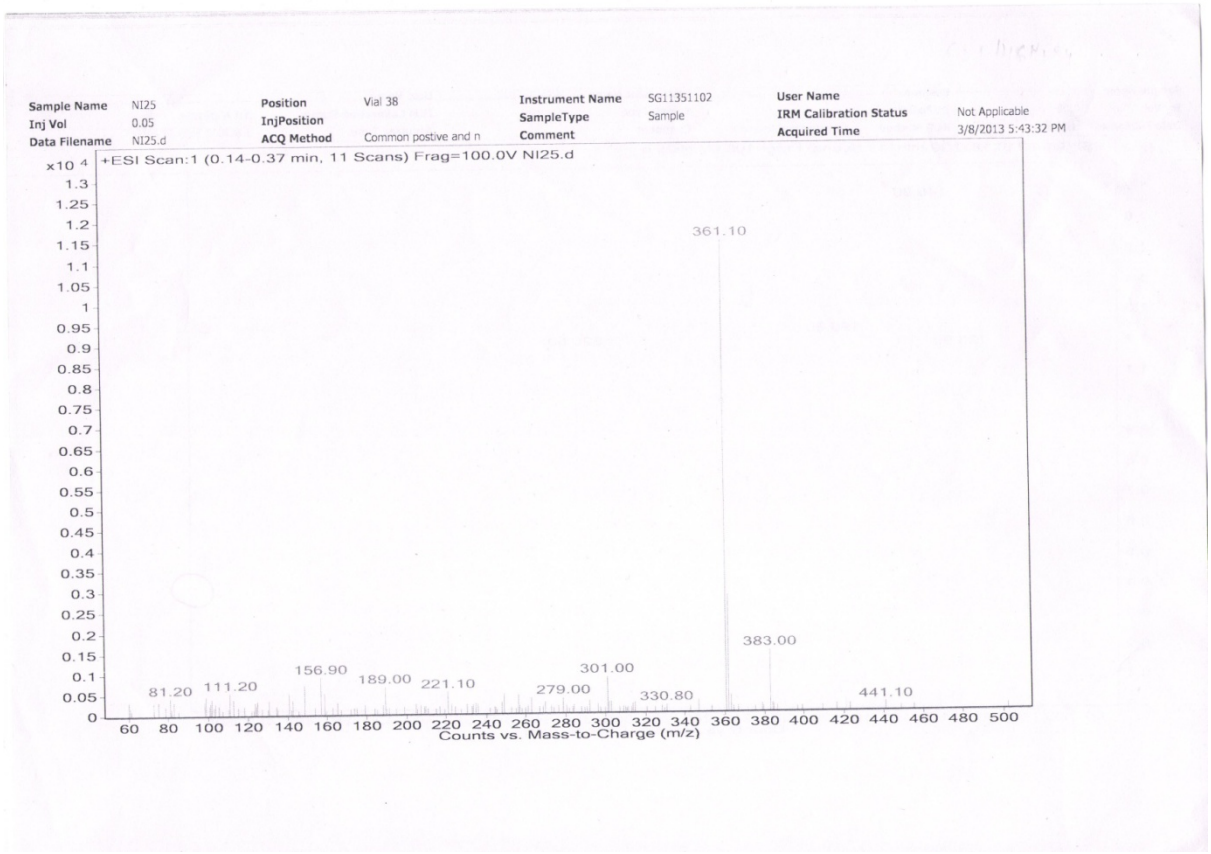
--- End Of Report ---



3e) Methyl 1-(4-methoxybenzoyl)-9H-*β*-carboline-3-carboxylate:




191.69
166.26
163.69
141.25
138.29
136.19
134.46
131.95
129.70
122.02
121.56
120.38
113.59
112.37
55.54
52.79
O
O
N
H
O
O
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


Sample Name NI25
Inj Vol 0.05
Data Filename NI25.d
Position Vial 38
InjPosition
ACQ Method Common postive and n
Instrument Name SG11351102
SampleType Sample
Comment
User Name
IRM Calibration Status Not Applicable
Acquired Time 3/8/2013 5:43:32 PM
+ESI Scan:1 (0.14-0.37 min, 11 Scans) Frag=100.0V NI25.d
x10 4
361.10
383.00
301.00
156.90
189.00
221.10
279.00
330.80
441.10
81.20
111.20
Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

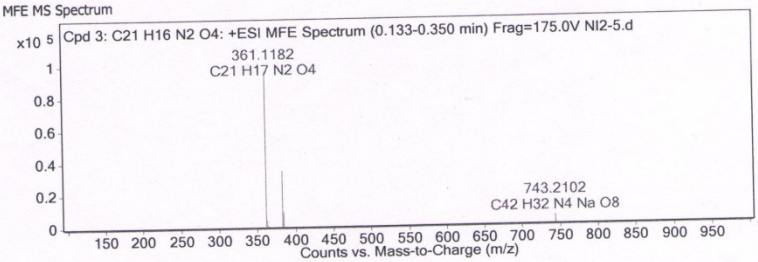
Data File	NI2-5.d	**Sample Name**	NI2-5
Sample Type	Sample	**Position**	Vial 10
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	13-03-2013 PM 7:28:26
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			
Sample Group		**Info.**	65:25(ACN:H20)
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 3: C21 H16 N2 O4	0.189	360.111	C21 H16 N2 O4	C21 H16 N2 O4	0.1	C21 H16 N2 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 3: C21 H16 N2 O4	361.1182	0.189	Find by Molecular Feature	360.111

MFE MS Spectrum



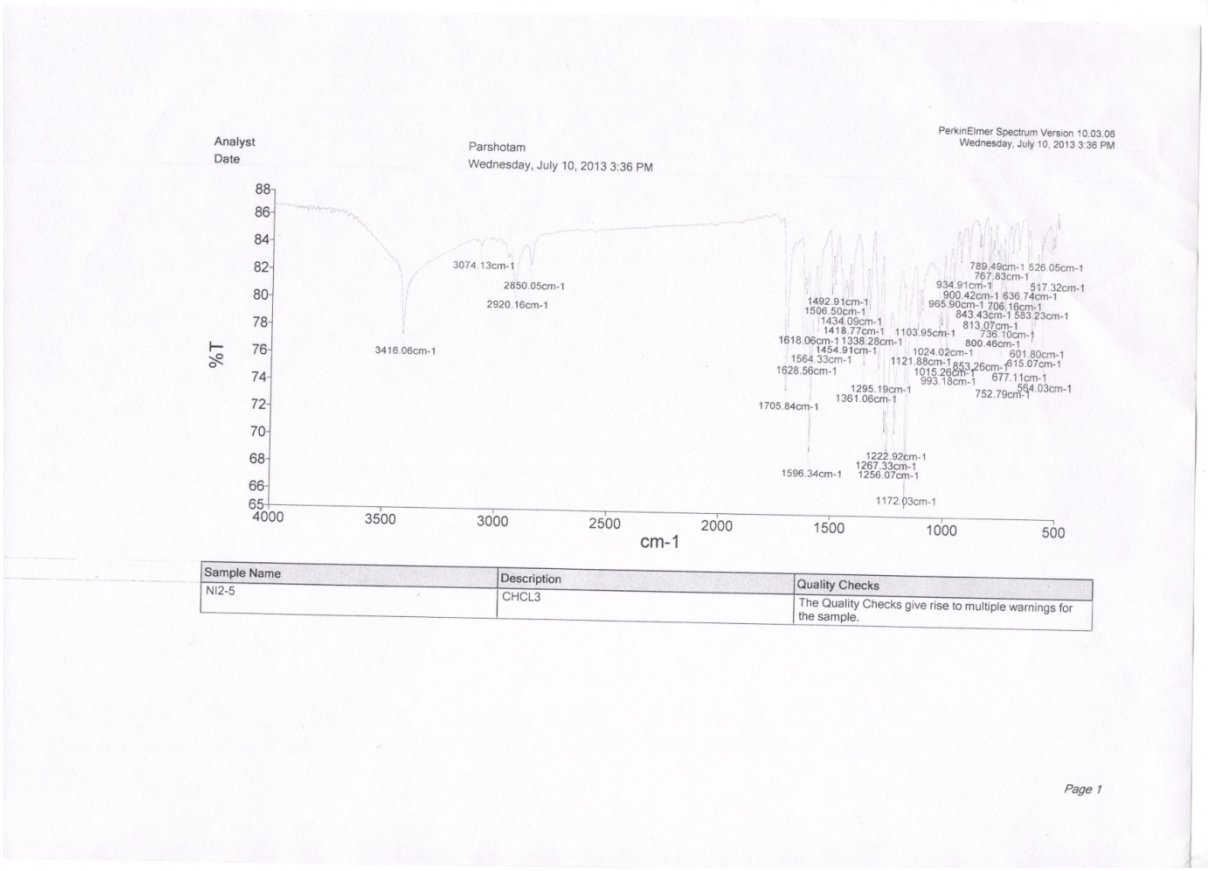
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
361.1182	1	96375.27	C21 H17 N2 O4	(M+H)+
362.1215	1	21838.33	C21 H17 N2 O4	(M+H)+
363.1242	1	3782.32	C21 H17 N2 O4	(M+H)+
364.126	1	502.02	C21 H17 N2 O4	(M+H)+
383.1001	1	34746.69	C21 H16 N2 Na O4	(M+Na)+
384.1028	1	8991.07	C21 H16 N2 Na O4	(M+Na)+
385.1064	1	1363.96	C21 H16 N2 Na O4	(M+Na)+
743.2102	1	5045.41	C42 H32 N4 Na O8	(2M+Na)+
744.2129	1	2557.92	C42 H32 N4 Na O8	(2M+Na)+
745.2168	1	538.51	C42 H32 N4 Na O8	(2M+Na)+

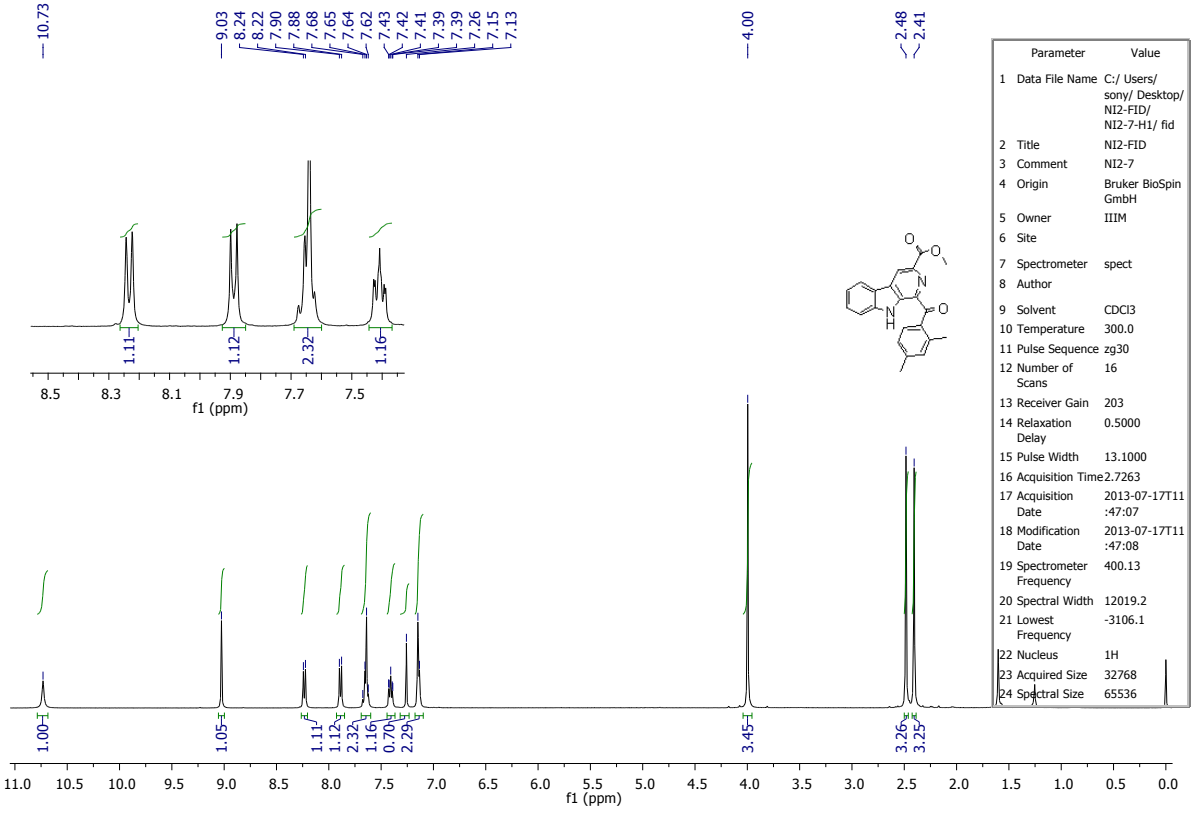
Predicted Isotope Match Table

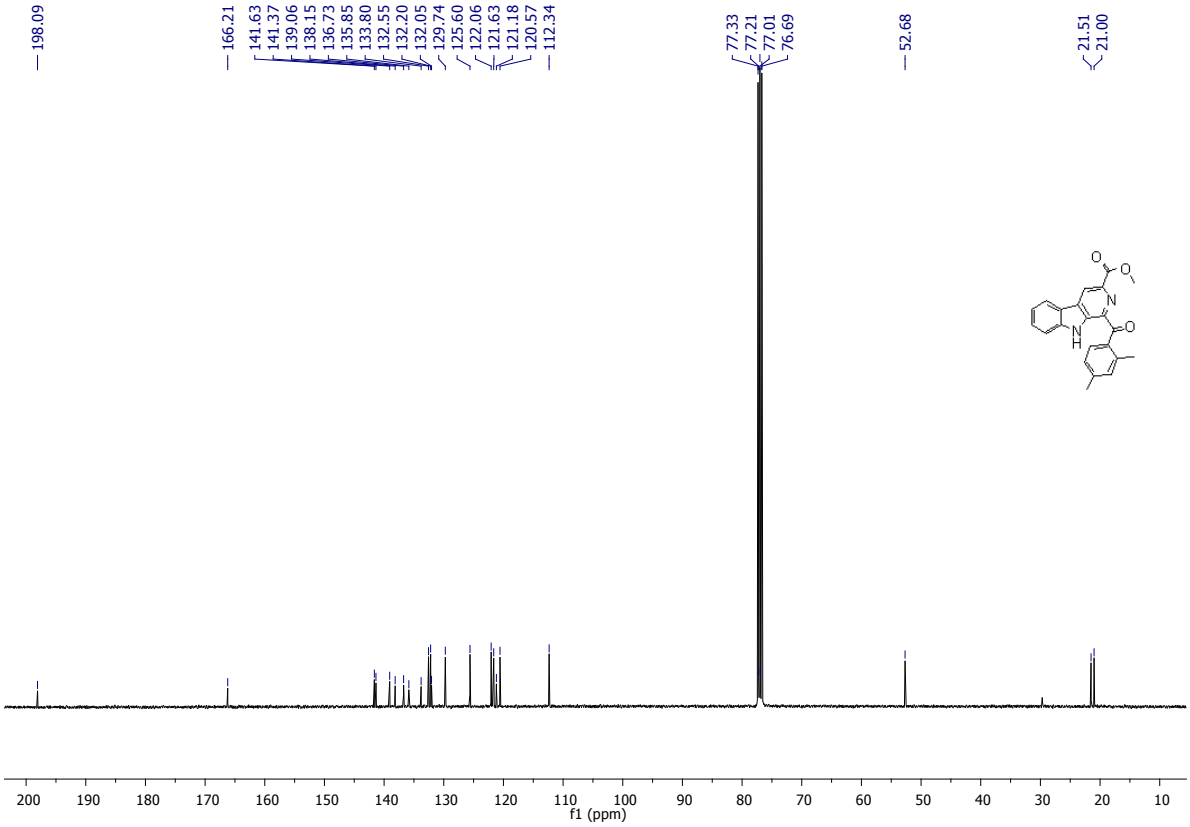
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	361.1182	361.1183	0.16	100	100	78.68	78.3
2	362.1215	362.1215	-0.18	22.66	23.79	17.83	18.63
3	363.1242	363.1242	-0.07	3.92	3.53	3.09	2.76
4	364.126	364.1268	2.21	0.52	0.39	0.41	0.31

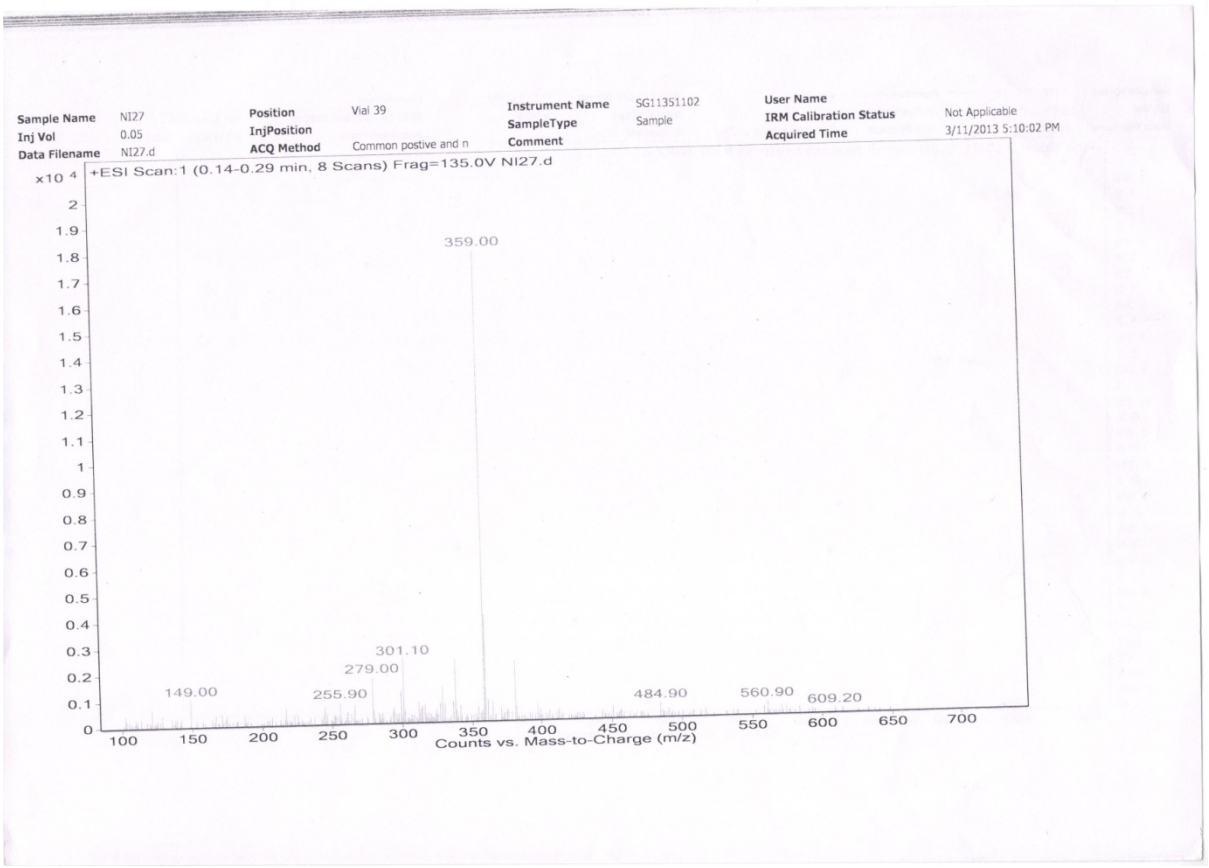
--- End Of Report ---



3f) Methyl 1-(2,4-dimethyl benzoyl)-9H-*β*-carboline-3-carboxylate:




198.09
166.21
141.63
141.37
139.06
138.15
136.73
135.85
133.80
132.55
132.20
132.05
129.74
125.60
122.06
121.63
121.18
120.57
112.34
77.33
77.21
77.01
76.69
52.68
21.51
21.00
O
O
N
N
H
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


Sample Name NI27
Inj Vol 0.05
Data Filename NI27.d
Position Vial 39
InjPosition
ACQ Method Common postive and n
Instrument Name SG11351102
SampleType Sample
Comment
User Name
IRM Calibration Status Not Applicable
Acquired Time 3/11/2013 5:10:02 PM
+ESI Scan:1 (0.14-0.29 min, 8 Scans) Frag=135.0V NI27.d
x10 4
359.00
301.10
279.00
149.00
255.90
484.90
560.90
609.20
Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

Data File	NI2-7.d	**Sample Name**	NI2-7
Sample Type	Sample	**Position**	Vial 14
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	13-03-2013 PM 7:49:32
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			

Info.

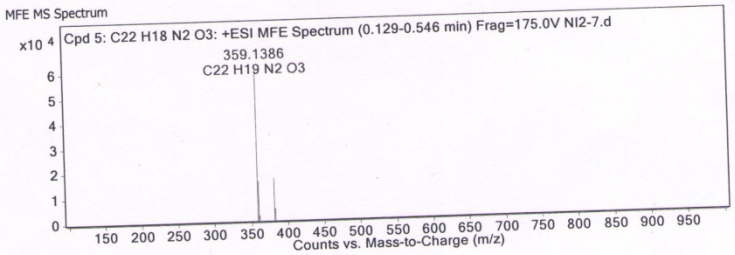
Sample Group	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 5: C22 H18 N2 O3	0.188	358.1312	C22 H18 N2 O3	C22 H18 N2 O3	1.39	C22 H18 N2 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 5: C22 H18 N2 O3	359.1386	0.188	Find by Molecular Feature	358.1312

MFE MS Spectrum



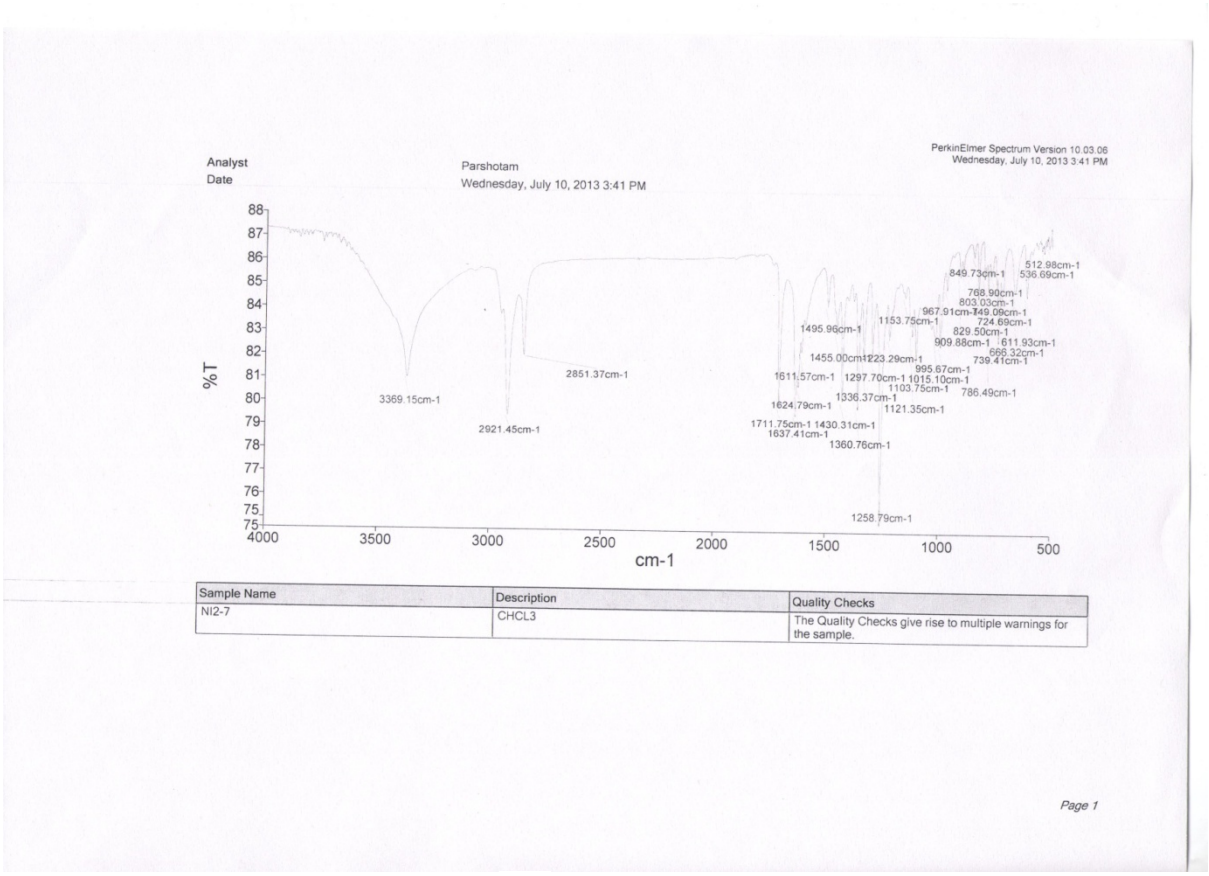
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
359.1386	1	60236.83	C22 H19 N2 O3	(M+H)+
360.1414	1	15948.56	C22 H19 N2 O3	(M+H)+
361.1436	1	2129.97	C22 H19 N2 O3	(M+H)+
381.1205	1	16770.99	C22 H18 N2 Na O3	(M+Na)+
382.1239	1	4690.01	C22 H18 N2 Na O3	(M+Na)+
383.1253	1	699.72	C22 H18 N2 Na O3	(M+Na)+

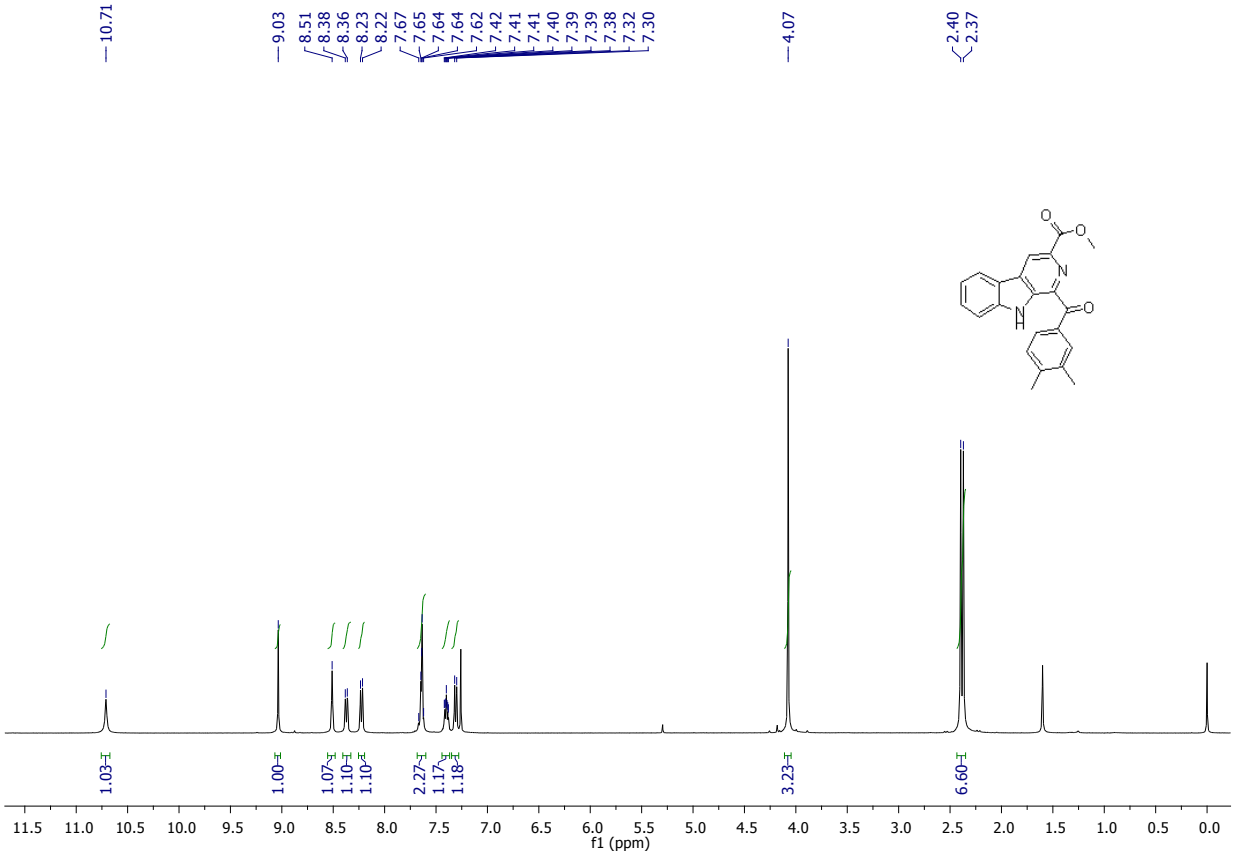
Predicted Isotope Match Table

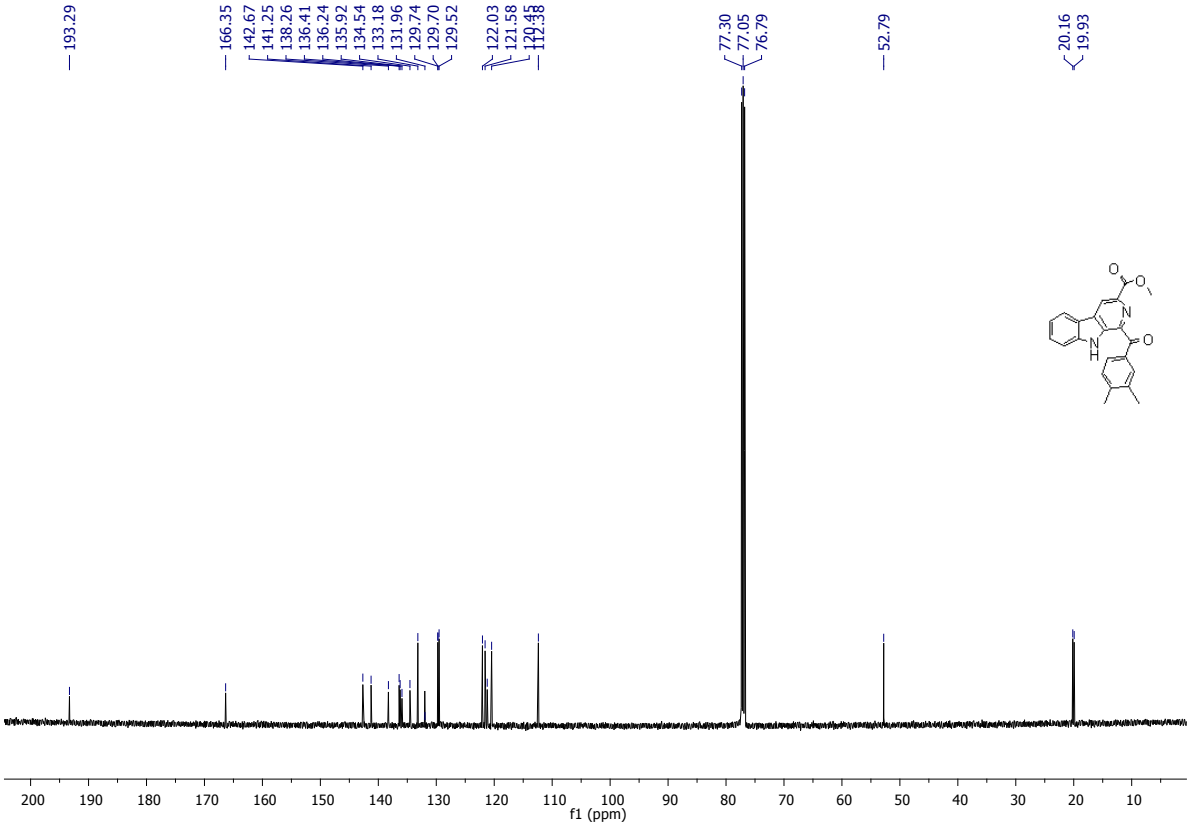
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	359.1386	359.139	1.05	100	100	76.92	77.86
2	360.1414	360.1422	2.29	26.48	24.86	20.36	19.35
3	361.1436	361.145	3.96	3.54	3.58	2.72	2.78

--- End Of Report ---



3g) Methyl 1-(3,4-dimethyl benzoyl)-9H- *β*-carboline-3-carboxylate:




193.29
166.35
142.67
141.25
138.26
136.41
136.24
135.92
134.54
133.18
131.96
129.74
129.70
129.52
122.03
121.58
77.30
77.05
76.79
52.79
20.16
19.93
O
O
N
H
O
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

Qualitative Compound Report

Data File	NI2-35.d	**Sample Name**	NI2-35
Sample Type	Sample	**Position**	Vial 3
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	17-07-2013 AM 11:38:24
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

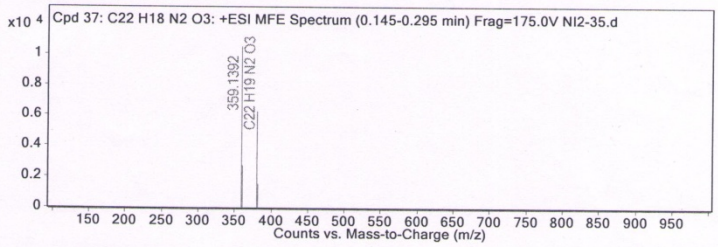
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 37: C22 H18 N2 O3	0.198	358.1319	C22 H18 N2 O3	C22 H18 N2 O3	-0.39	C22 H18 N2 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 37: C22 H18 N2 O3	359.1392	0.198	Find by Molecular Feature	358.1319

MFE MS Spectrum



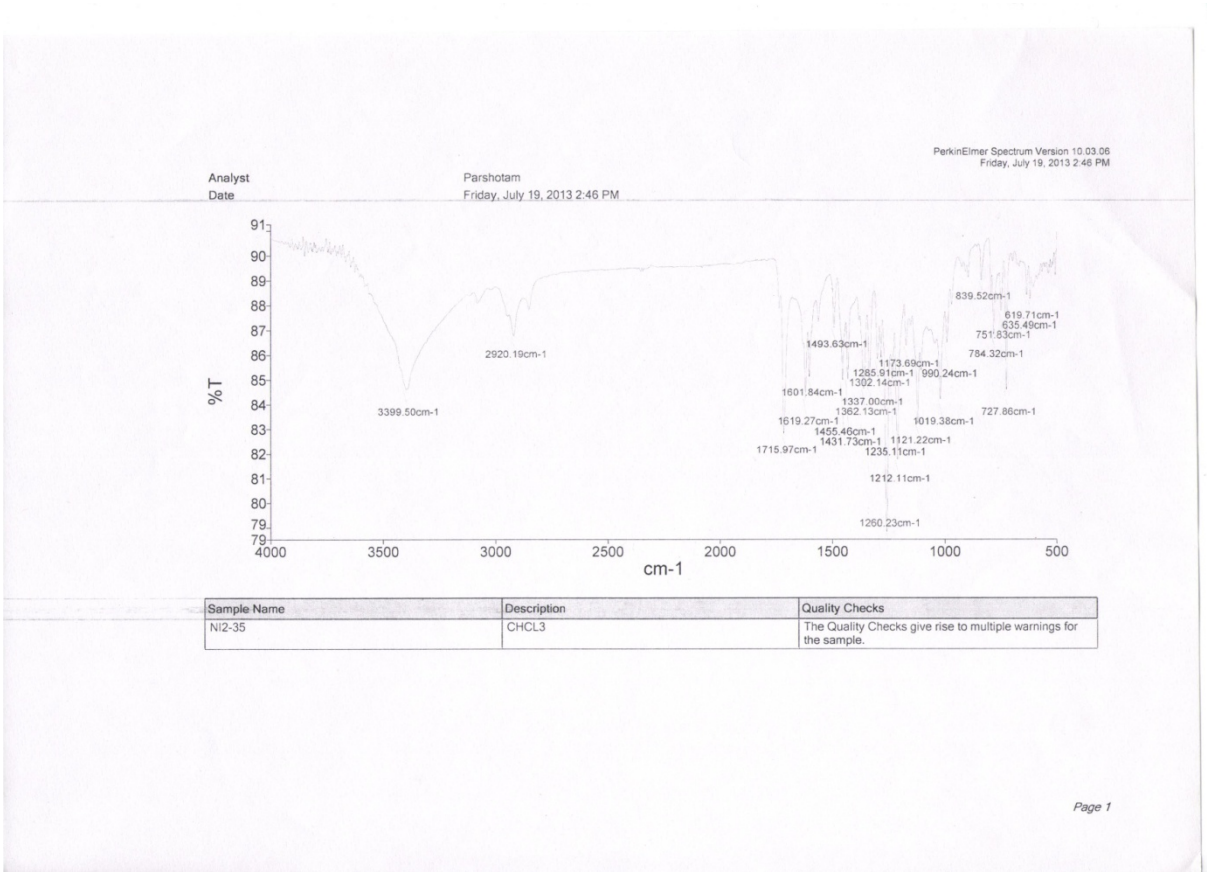
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
359.1392	1	10528.21	C22 H19 N2 O3	(M+H)+
360.1423	1	2721.06	C22 H19 N2 O3	(M+H)+
381.12	1	6228.8	C22 H18 N2 Na O3	(M+Na)+
382.1252	1	1522.5	C22 H18 N2 Na O3	(M+Na)+

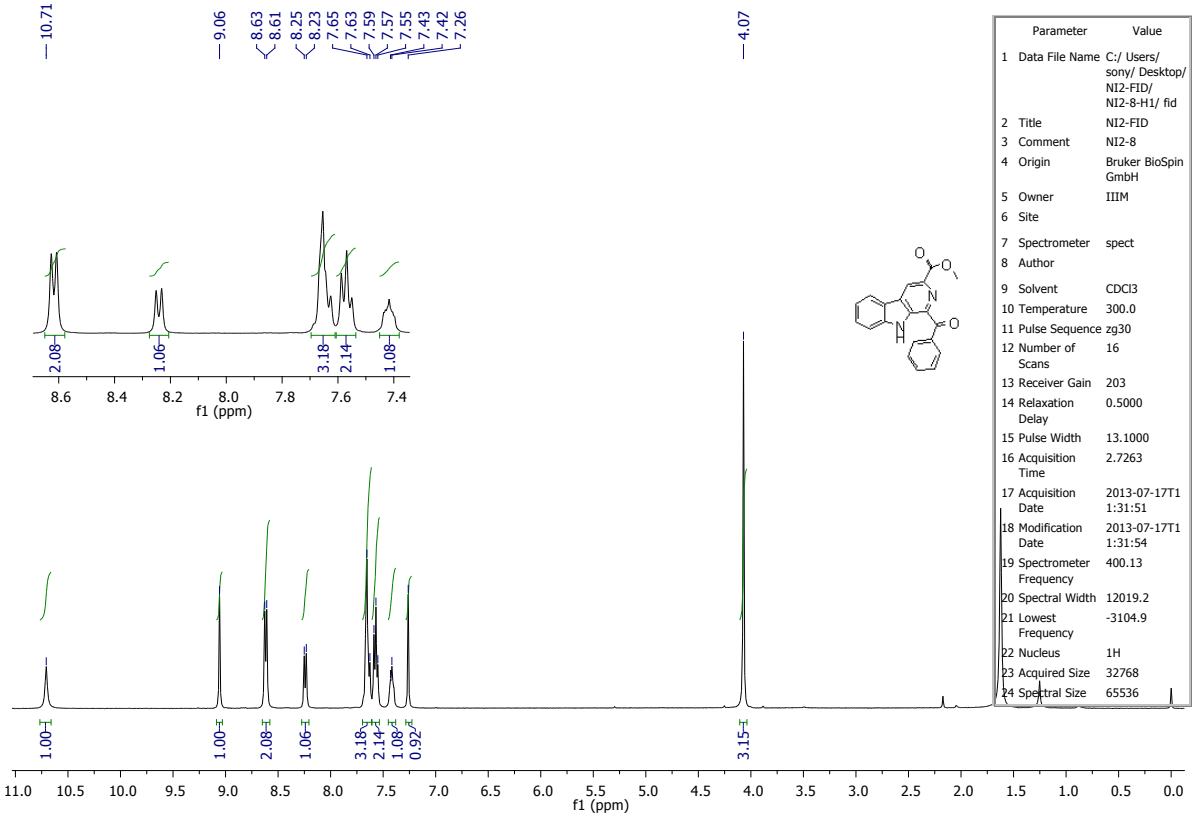
Predicted Isotope Match Table

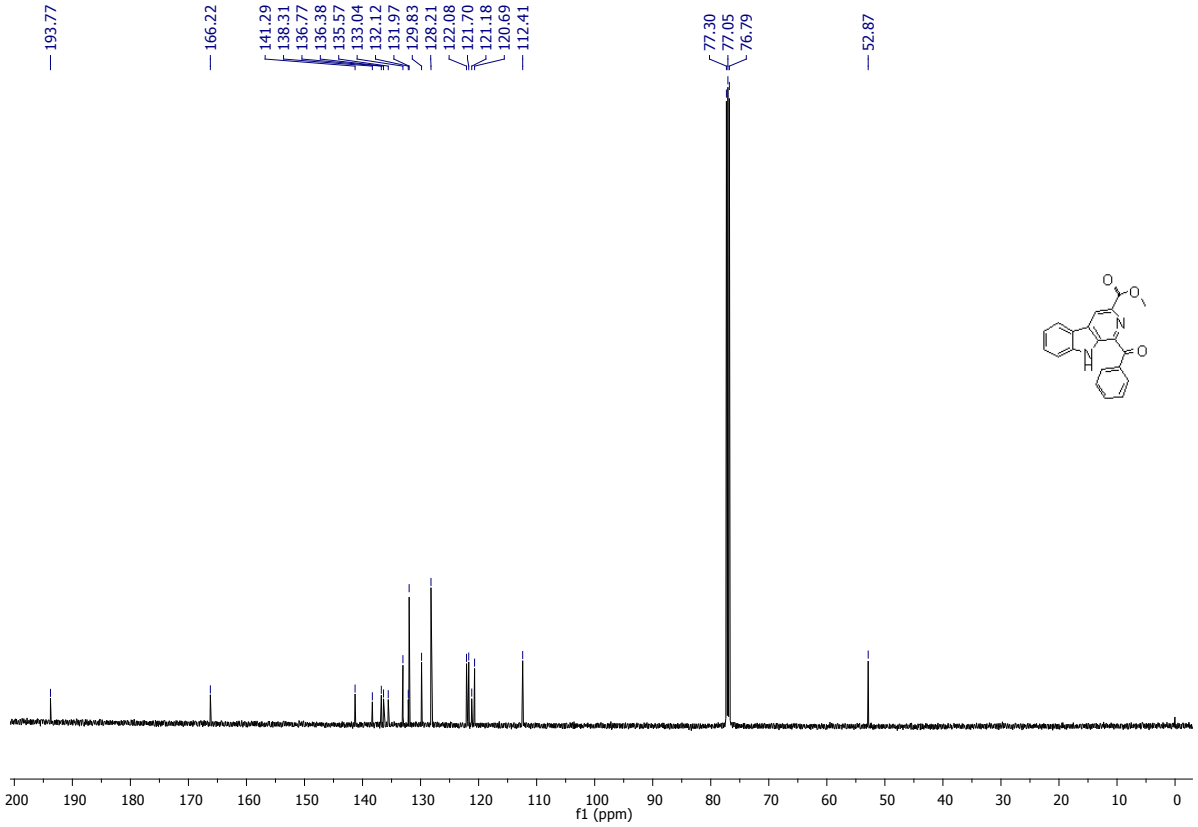
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	359.1392	359.139	-0.44	100	100	79.46	80.09
2	360.1423	360.1422	-0.19	25.85	24.86	20.54	19.91

--- End Of Report ---



3h) Methyl 1- (benzoyl)-9H- *β*-carboline-3-carboxylate:




193.77
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136.77
136.38
135.57
133.04
132.12
131.97
129.83
128.21
122.08
121.70
121.18
120.69
112.41
77.30
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N
H
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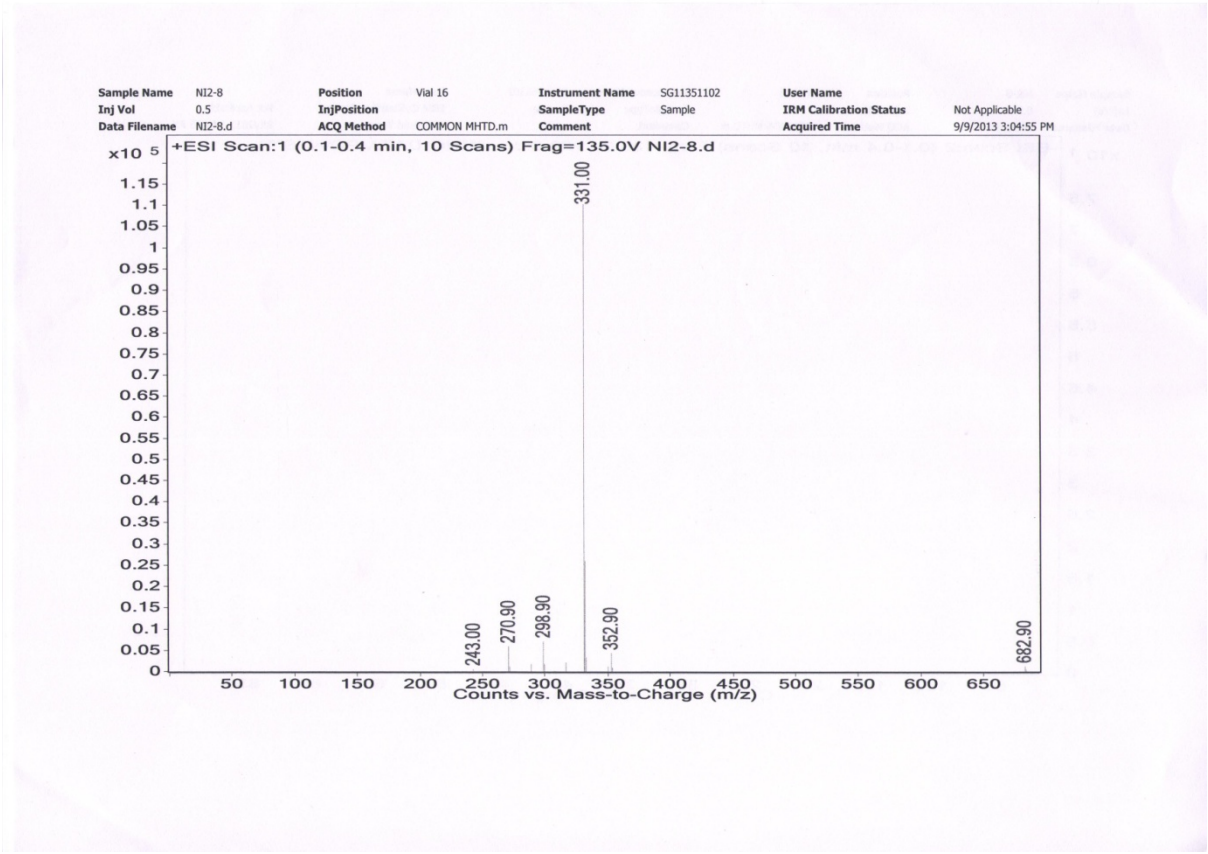
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


Sample Name NI2-8
Position Vial 16
Instrument Name SG11351102
User Name
Inj Vol 0.5
InjPosition
SampleType Sample
IRM Calibration Status Not Applicable
Data Filename NI2-8.d
ACQ Method COMMON MHTD.m
Comment
Acquired Time 9/9/2013 3:04:55 PM
+ESI Scan:1 (0.1-0.4 min, 10 Scans) Frag=135.0V NI2-8.d
x10 5
1.15
1.1
1.05
1
0.95
0.9
0.85
0.8
0.75
0.7
0.65
0.6
0.55
0.5
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
331.00
243.00
270.90
298.90
352.90
682.90
50 100 150 200 250 300 350 400 450 500 550 600 650
Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

Data File	NI2-8.d	**Sample Name**	NI2-8
Sample Type	Sample	**Position**	Vial 13
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	13-03-2013 PM 7:42:02
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			

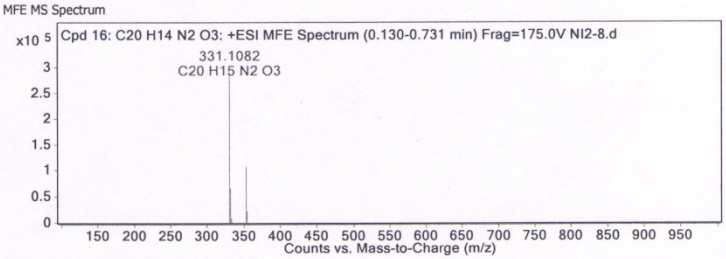
Sample Group		**Info.**	65:25(ACN:H20)
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 16: C20 H14 N2 O3	0.189	330.1009	C20 H14 N2 O3	C20 H14 N2 O3	-1.35	C20 H14 N2 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 16: C20 H14 N2 O3	331.1082	0.189	Find by Molecular Feature	330.1009

MFE MS Spectrum



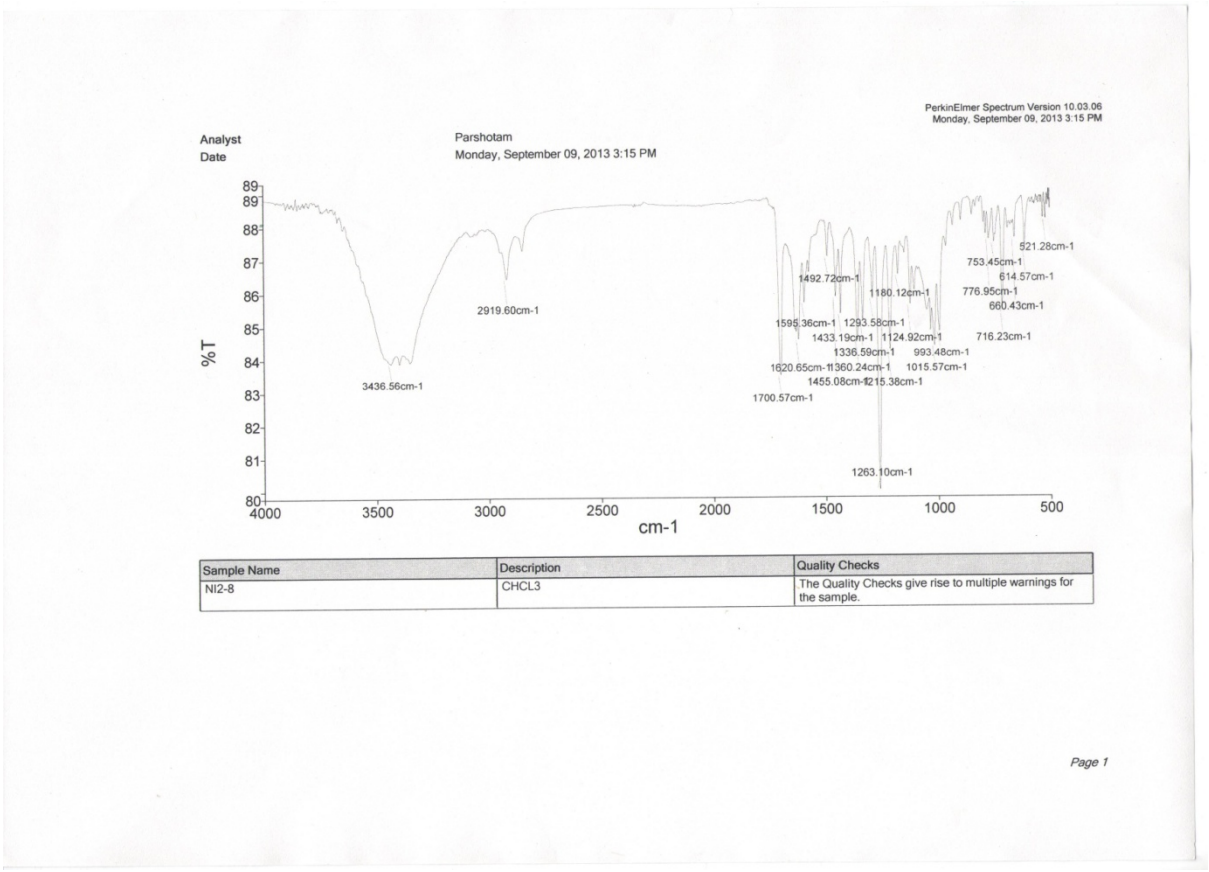
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
331.1082	1	290273.63	C20 H15 N2 O3	(M+H)+
332.111	1	66369.91	C20 H15 N2 O3	(M+H)+
333.1155	1	8995.54	C20 H15 N2 O3	(M+H)+
334.1195	1	1015.52	C20 H15 N2 O3	(M+H)+
353.0898	1	106949.66	C20 H14 N2 Na O3	(M+Na)+
354.093	1	22558.94	C20 H14 N2 Na O3	(M+Na)+
355.0953	1	3360.5	C20 H14 N2 Na O3	(M+Na)+
356.0986	1	484.3	C20 H14 N2 Na O3	(M+Na)+

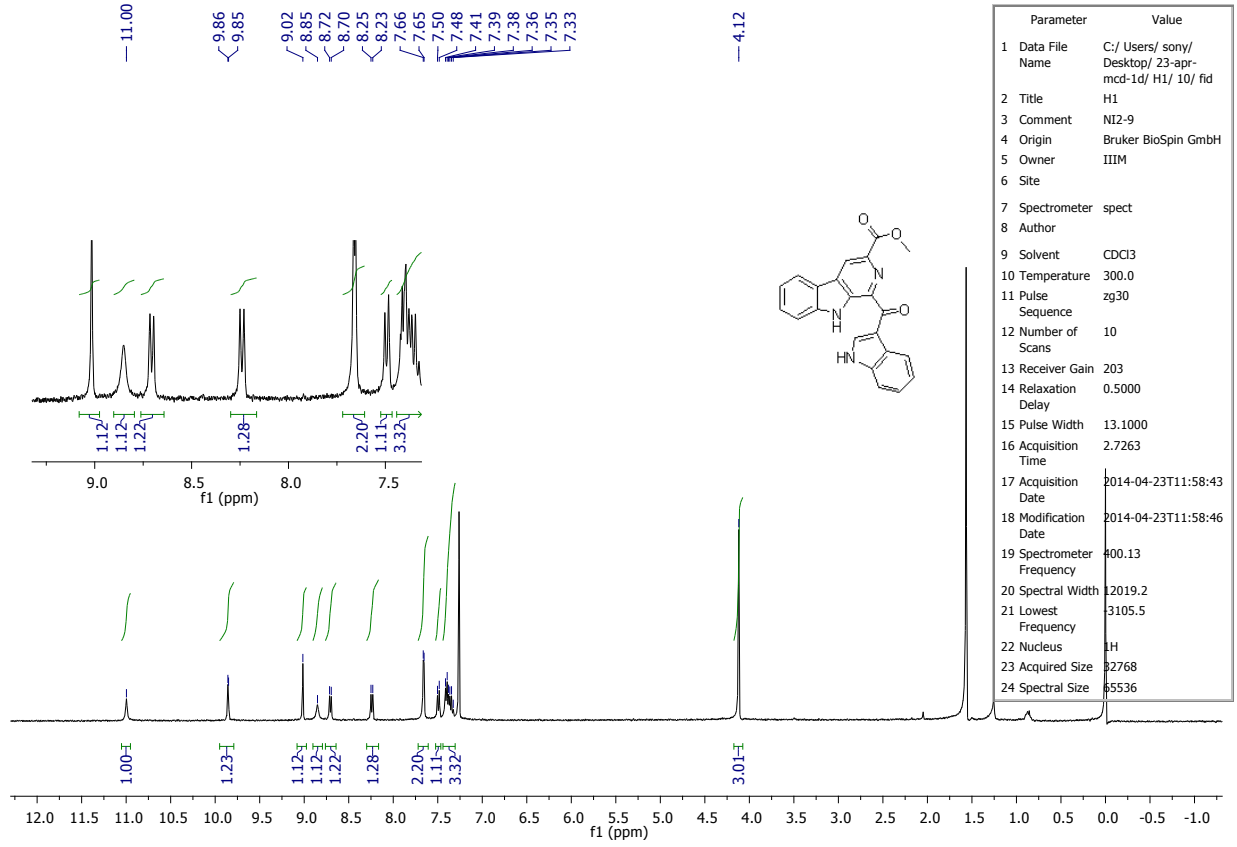
Predicted Isotope Match Table

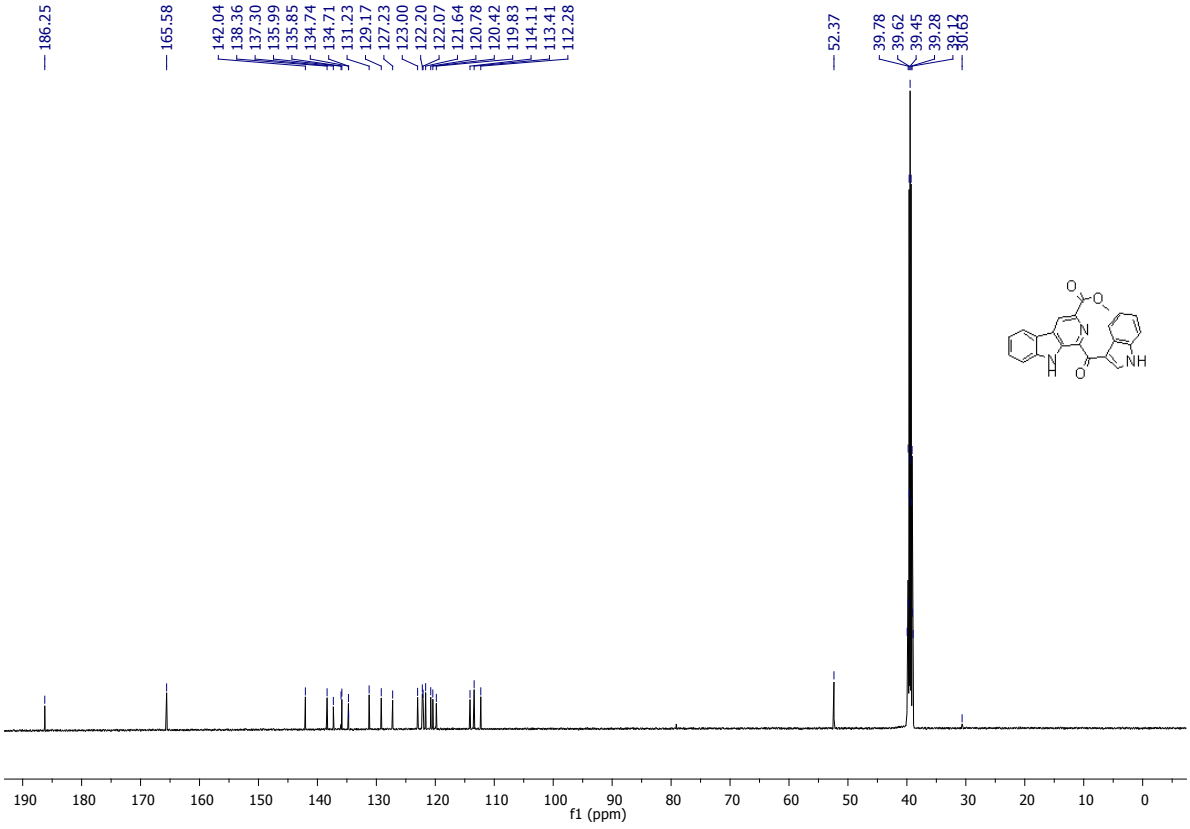
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	331.1082	331.1077	-1.42	100	100	79.17	79.35
2	332.111	332.1109	-0.31	22.86	22.65	18.1	17.97
3	333.1155	333.1136	-5.47	3.1	3.06	2.45	2.43
4	334.1195	334.1163	-9.77	0.35	0.31	0.28	0.24

--- End Of Report ---



3i) Methyl 1-(1H-indole-3-carbonyl)-9H-*β*-carboline-3-carboxylate:




186.25
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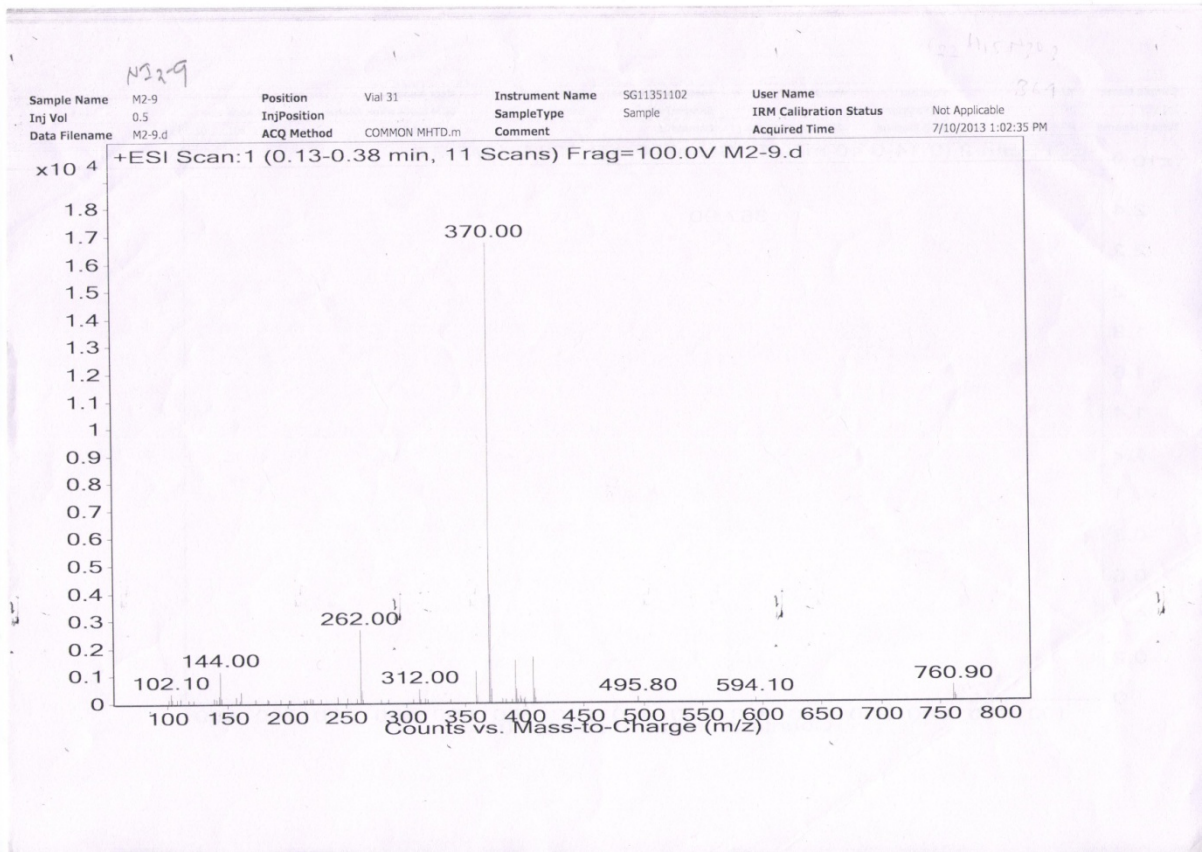
142.04
138.36
137.30
135.99
135.85
134.74
134.71
131.23
129.17
127.23
123.00
122.20
122.07
121.64
120.78
120.42
119.83
114.11
113.41
112.28
52.37
39.78
39.62
39.45
39.28
39.12
30.63
O
O
N
NH
O
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


M2-9
Sample Name M2-9
Inj Vol 0.5
Data Filename M2-9.d
Position Vial 31
InjPosition
ACQ Method COMMON MHTD.m
Instrument Name SG11351102
SampleType Sample
Comment
User Name
IRM Calibration Status Not Applicable
Acquired Time 7/10/2013 1:02:35 PM
+ESI Scan:1 (0.13-0.38 min, 11 Scans) Frag=100.0V M2-9.d
x10 4
1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
370.00
262.00
144.00
102.10
312.00
495.80
594.10
760.90
100 150 200 250 300 350 400 450 500 550 600 650 700 750 800
Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

Data File	NI2-9.d	**Sample Name**	NI2-9
Sample Type	Sample	**Position**	Vial 36
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	11-07-2013 PM 3:41:36
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

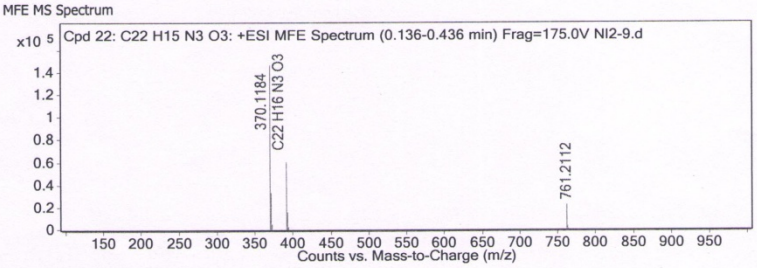
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 22: C22 H15 N3 O3	0.197	369.111	C22 H15 N3 O3	C22 H15 N3 O3	0.8	C22 H15 N3 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 22: C22 H15 N3 O3	370.1184	0.197	Find by Molecular Feature	369.111

MFE MS Spectrum



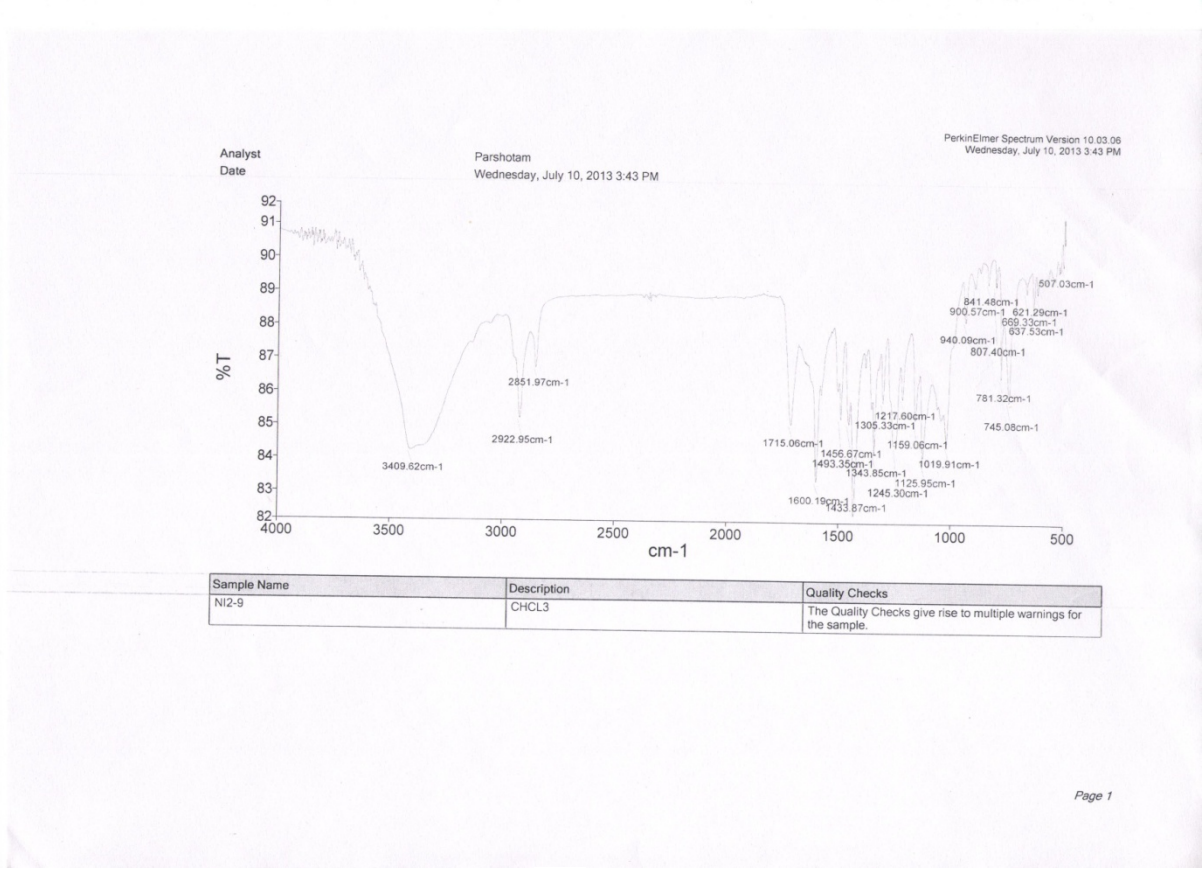
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
370.1184	1	146597.08	C22 H16 N3 O3	(M+H)+
371.1214	1	32817.45	C22 H16 N3 O3	(M+H)+
372.124	1	5306.75	C22 H16 N3 O3	(M+H)+
373.125	1	843.04	C22 H16 N3 O3	(M+H)+
392.1	1	60600.2	C22 H15 N3 Na O3	(M+Na)+
393.1032	1	15910.22	C22 H15 N3 Na O3	(M+Na)+
394.1049	1	2609.06	C22 H15 N3 Na O3	(M+Na)+
761.2112	1	22654.78		(2M+Na)+
762.2149	1	12998.13		(2M+Na)+
763.2153	1	3265.26		(2M+Na)+

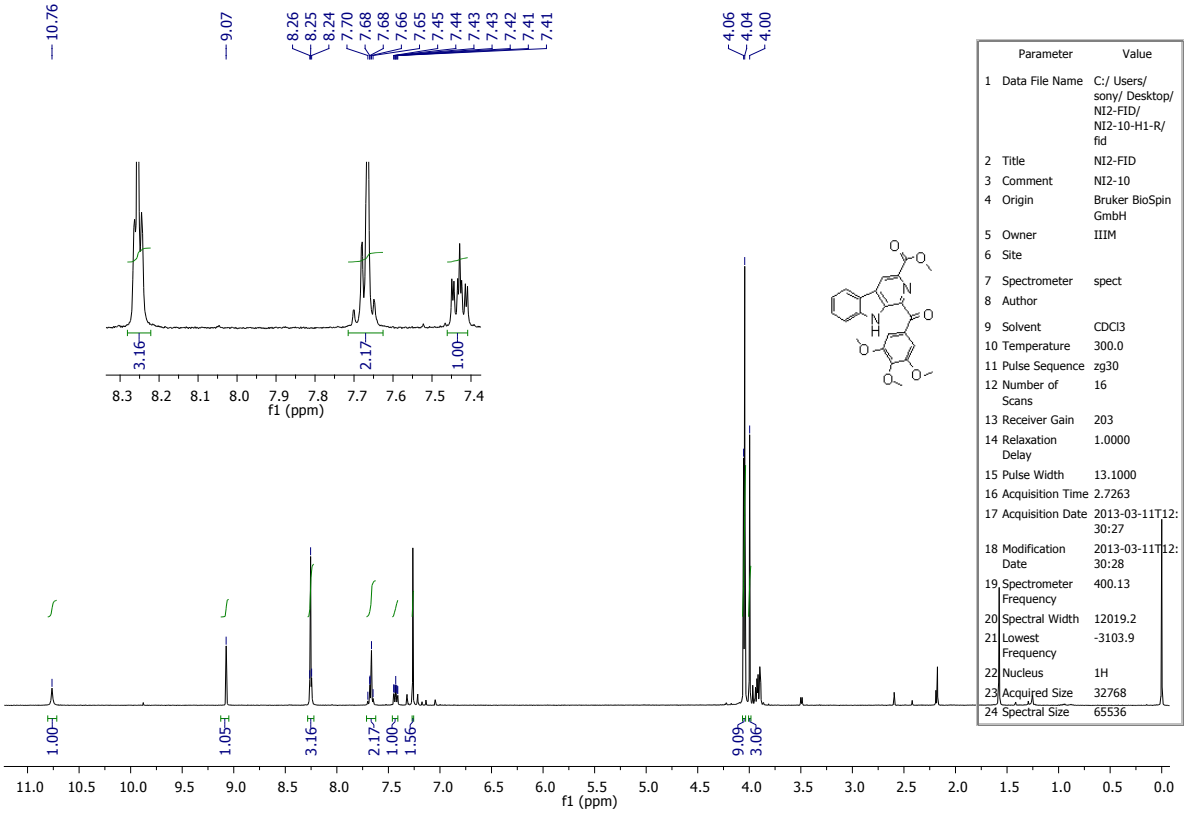
Predicted Isotope Match Table

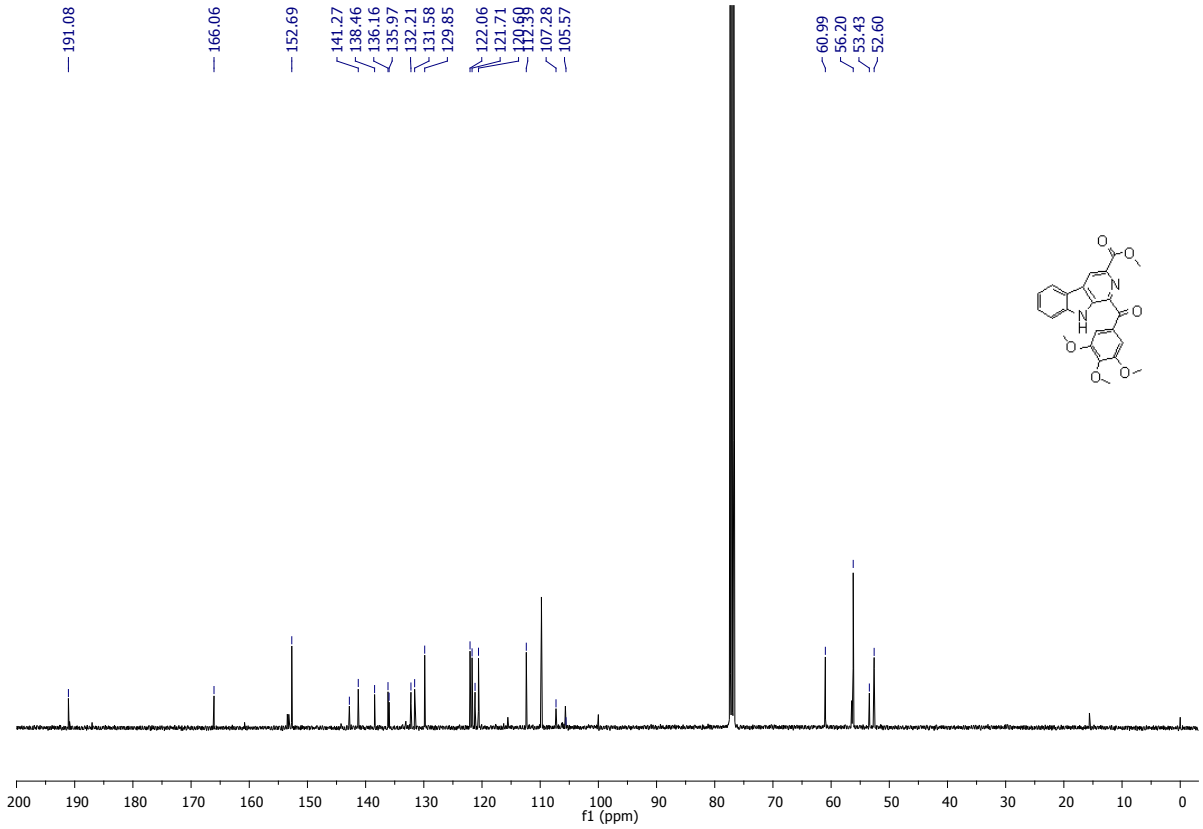
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	370.1184	370.1186	0.72	100	100	79	77.38
2	371.1214	371.1217	0.94	22.39	25.19	17.69	19.49
3	372.124	372.1245	1.4	3.62	3.66	2.86	2.83
4	373.125	373.1271	5.74	0.58	0.39	0.45	0.3

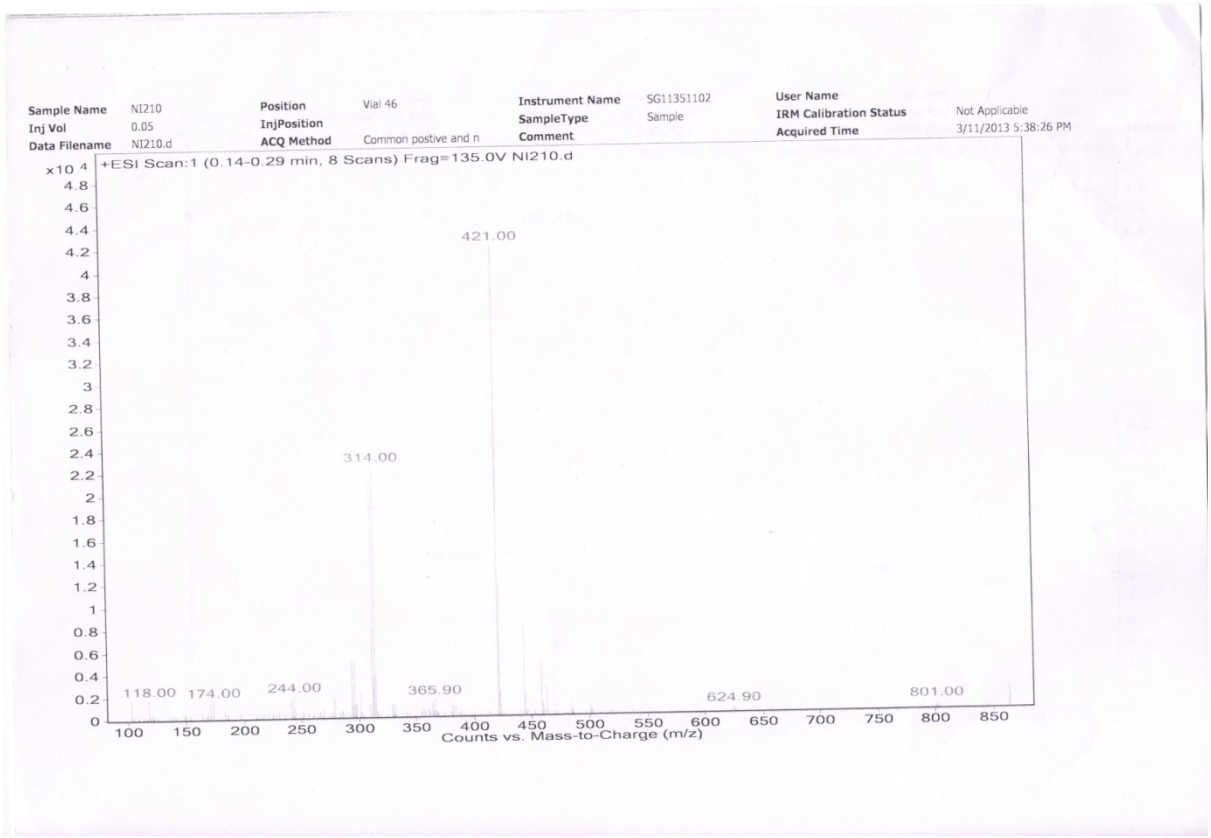
--- End Of Report ---



3j) Methyl 1-(3,4,5-trimethoxybenzoyl)-9H-*β*-carboline-3-carboxylate:




191.08
166.06
152.69
141.27
138.46
136.16
135.97
132.21
131.58
129.85
122.06
121.71
107.28
105.57
60.99
56.20
53.43
52.60
f1 (ppm)


Sample Name NI210
Inj Vol 0.05
Data Filename NI210.d
Position Vial 46
InjPosition
ACQ Method Common postive and n
Instrument Name SG11351102
SampleType Sample
Comment
User Name
IRM Calibration Status Not Applicable
Acquired Time 3/11/2013 5:38:26 PM
+ESI Scan:1 (0.14-0.29 min, 8 Scans) Frag=135.0V NI210.d
421.00
314.00
118.00
174.00
244.00
365.90
624.90
801.00
Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

Data File	NI2-10.d	**Sample Name**	NI2-10
Sample Type	Sample	**Position**	Vial 40
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	12-03-2013 PM 4:11:20
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			

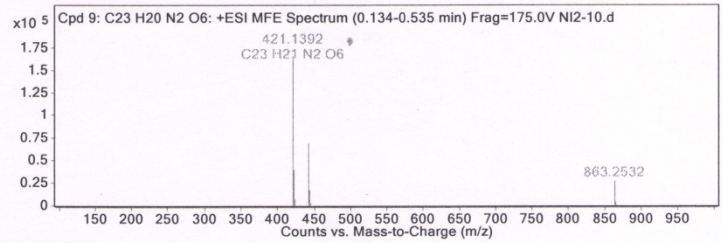
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 9: C23 H20 N2 O6	0.191	420.1319	C23 H20 N2 O6	C23 H20 N2 O6	0.56	C23 H20 N2 O6

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 9: C23 H20 N2 O6	421.1392	0.191	Find by Molecular Feature	420.1319

MFE MS Spectrum



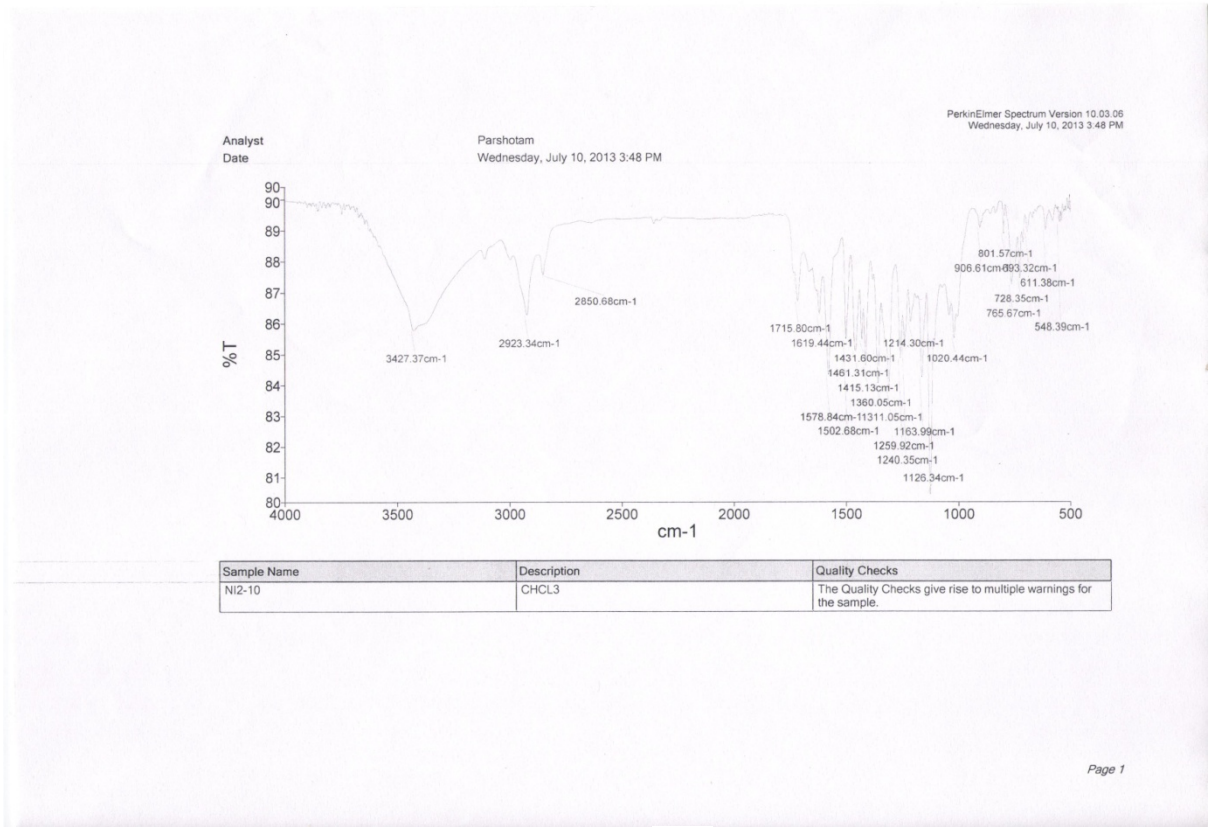
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
421.1392	1	166426.06	C23 H21 N2 O6	(M+H)+
422.1421	1	39932.81	C23 H21 N2 O6	(M+H)+
423.1448	1	7197.14	C23 H21 N2 O6	(M+H)+
424.1491	1	1272.4	C23 H21 N2 O6	(M+H)+
443.1211	1	68938.02	C23 H20 N2 Na O6	(M+Na)+
444.1245	1	16542.27	C23 H20 N2 Na O6	(M+Na)+
445.1267	1	3108.77	C23 H20 N2 Na O6	(M+Na)+
863.2532	1	26643.17		(2M+Na)+
864.2556	1	13493.43		(2M+Na)+
865.2587	1	4265.18		(2M+Na)+

Predicted Isotope Match Table

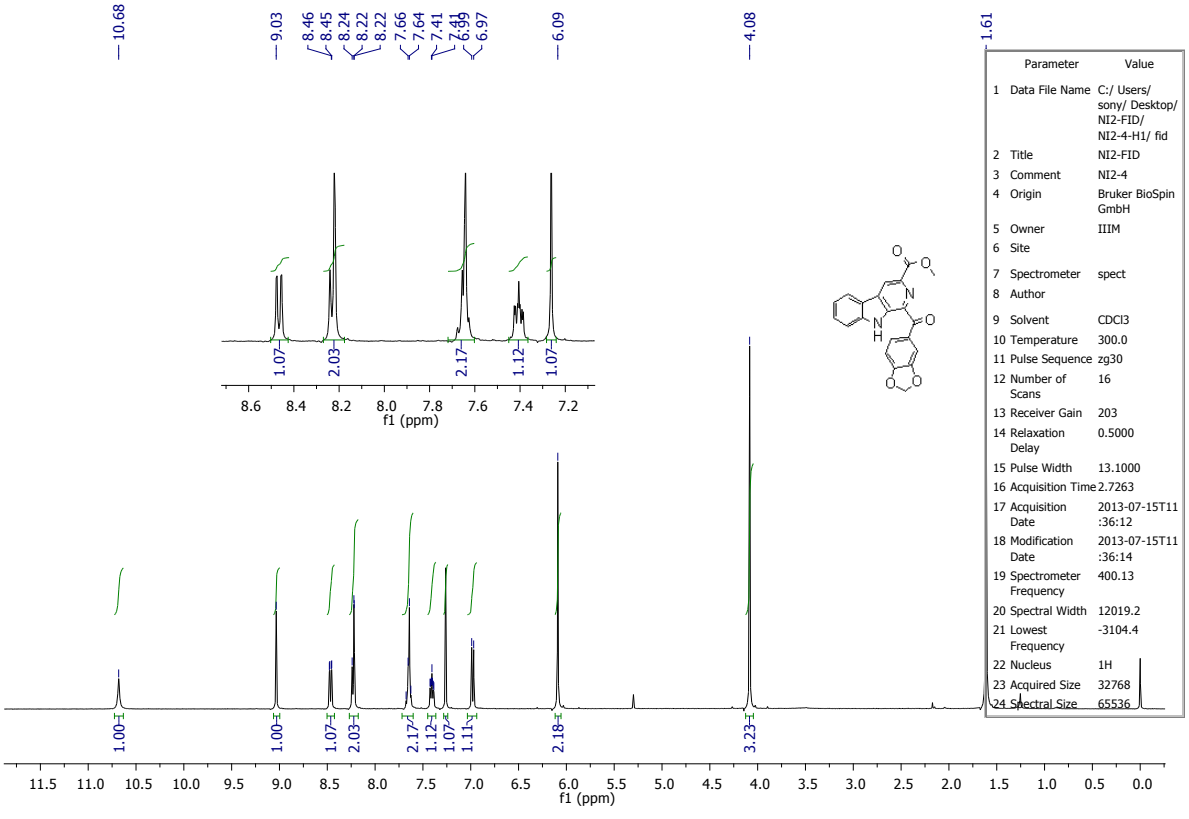
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	421.1392	421.1394	0.42	100	100	77.47	76.24
2	422.1421	422.1426	1.15	23.99	26.08	18.59	19.88
3	423.1448	423.1452	0.97	4.32	4.5	3.35	3.43
4	424.1491	424.1478	-2.87	0.76	0.58	0.59	0.44

--- End Of Report ---

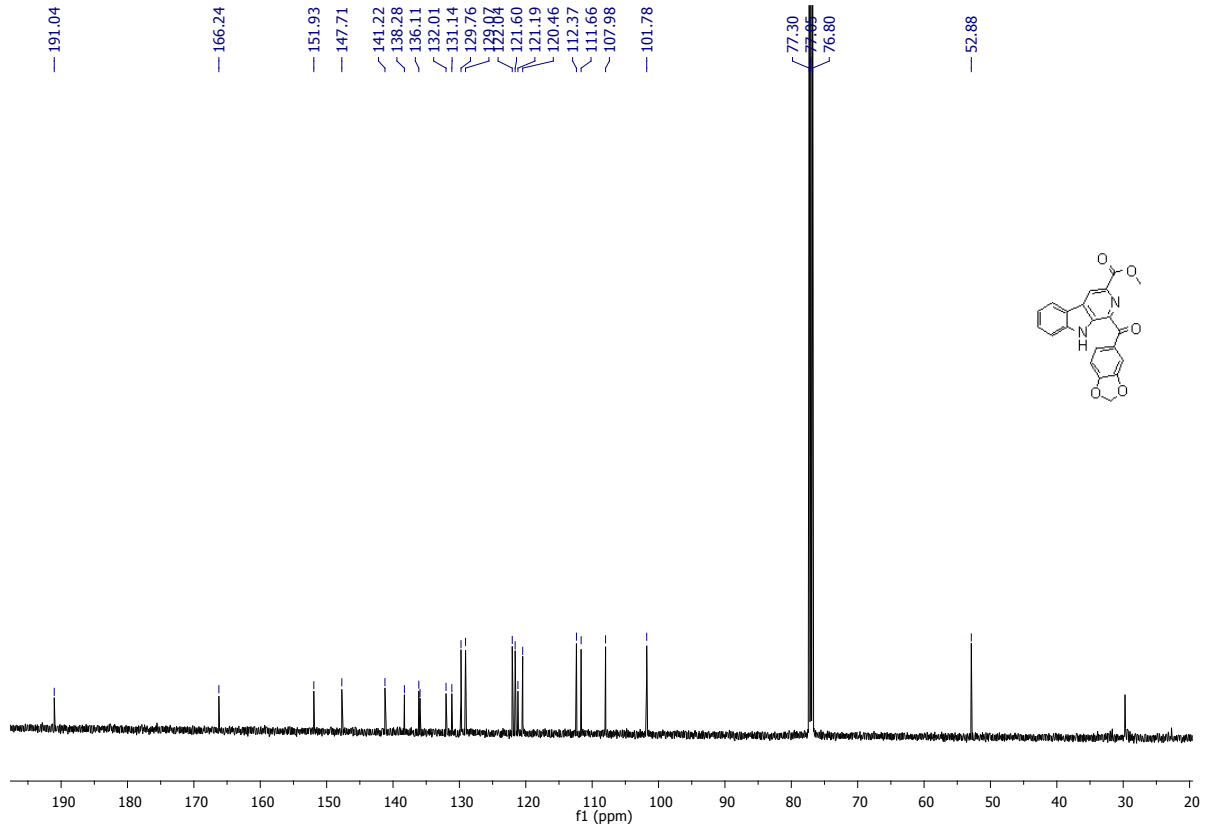


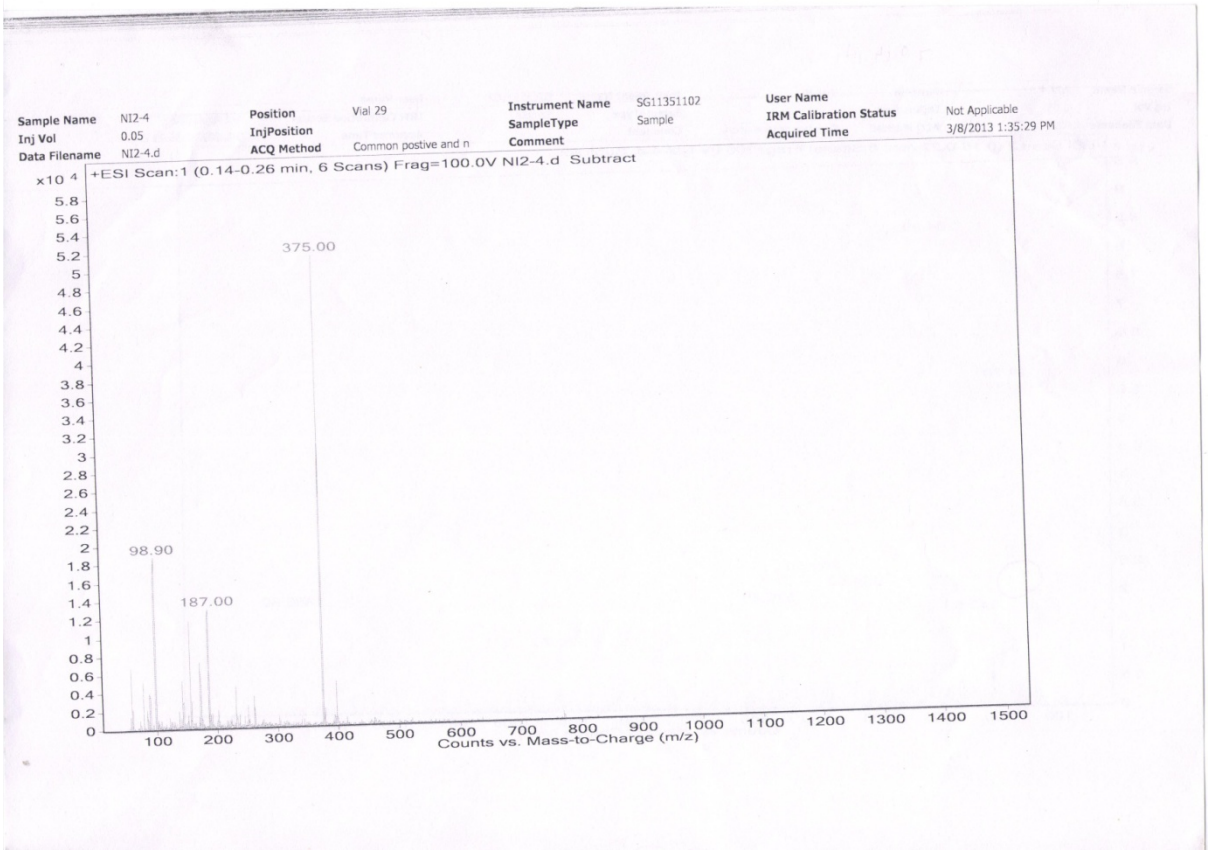
Sample Name	Description	Quality Checks
NI2-10	CHCL3	The Quality Checks give rise to multiple warnings for the sample.

3k) Methyl 1-(benzo[d][1,3]dioxole-5-carbonyl)- 9H- *β*-carboline-3-carboxylate:



	Parameter	Value
1	Data File Name	C:/ Users/ sony/ Desktop/ NI2-FID/ NI2-4-H1/ fid
2	Title	NI2-FID
3	Comment	NI2-4
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	203
14	Relaxation Delay	0.5000
15	Pulse Width	13.1000
16	Acquisition Time	2.7263
17	Acquisition Date	2013-07-15T11 :36:12
18	Modification Date	2013-07-15T11 :36:14
19	Spectrometer Frequency	400.13
20	Spectral Width	12019.2
21	Lowest Frequency	-3104.4
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536


191.04
166.24
151.93
147.71
141.22
138.28
136.11
132.01
131.14
129.76
121.60
121.19
120.46
112.37
111.66
107.98
101.78
77.30
77.05
76.80
52.88
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20
f1 (ppm)


Sample Name NI2-4
Inj Vol 0.05
Data Filename NI2-4.d
Position Vial 29
InjPosition
ACQ Method Common postive and n
Instrument Name SG11351102
SampleType Sample
Comment
User Name
IRM Calibration Status Not Applicable
Acquired Time 3/8/2013 1:35:29 PM
+ESI Scan:1 (0.14-0.26 min, 6 Scans) Frag=100.0V NI2-4.d Subtract
x10 4
375.00
98.90
187.00
Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

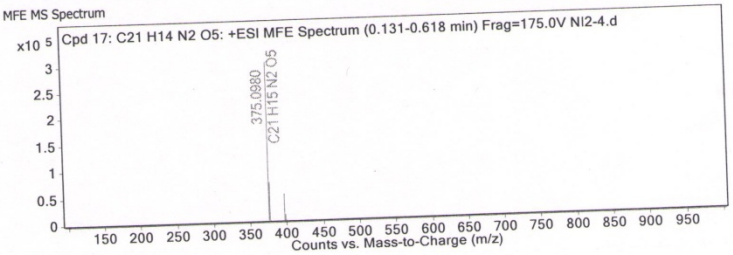
Data File	NI2-4.d	**Sample Name**	NI2-4
Sample Type	Sample	**Position**	Vial 42
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	19-03-2013 PM 12:48:53
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			
Sample Group		**Info.**	65:25(ACN:H20)
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 17: C21 H14 N2 O5	0.187	374.0906	C21 H14 N2 O5	C21 H14 N2 O5	-0.86	C21 H14 N2 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 17: C21 H14 N2 O5	375.098	0.187	Find by Molecular Feature	374.0906

MFE MS Spectrum



MS Spectrum Peak List

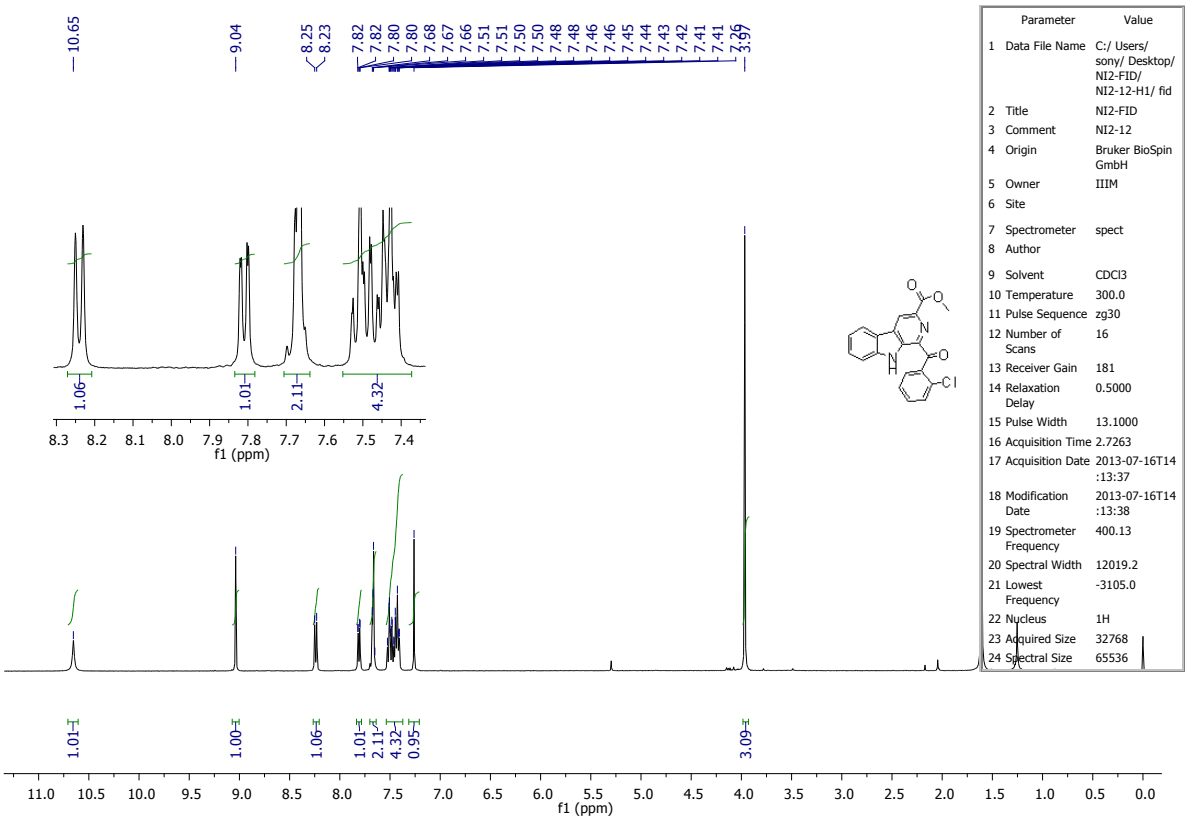
m/z	z	Abund	Formula	Ion
375.098	1	300747.13	C21 H15 N2 O5	(M+H)+
376.1007	1	73065.72	C21 H15 N2 O5	(M+H)+
377.1034	1	9085.42	C21 H15 N2 O5	(M+H)+
378.1059	1	1062.78	C21 H15 N2 O5	(M+H)+
397.0795	1	51497.28	C21 H14 N2 Na O5	(M+Na)+
398.0825	1	12614.31	C21 H14 N2 Na O5	(M+Na)+
399.0864	1	1994.45	C21 H14 N2 Na O5	(M+Na)+

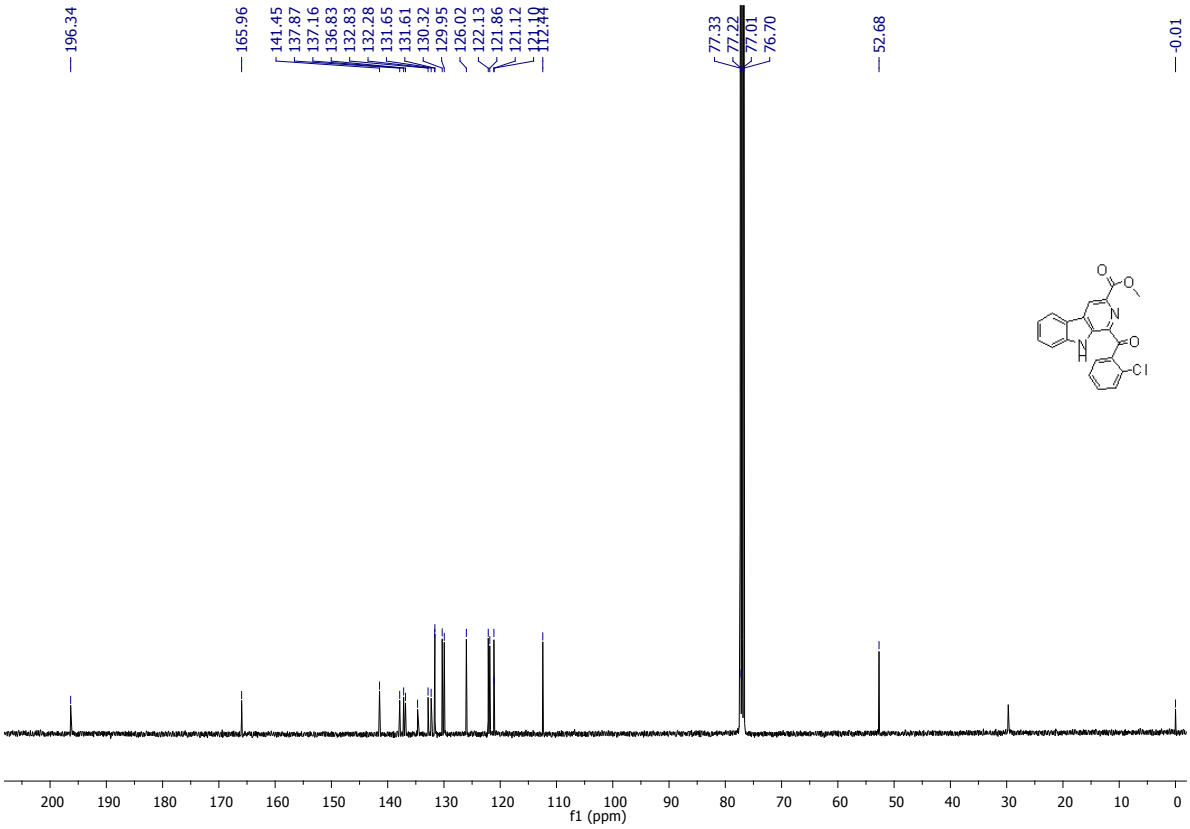
Predicted Isotope Match Table

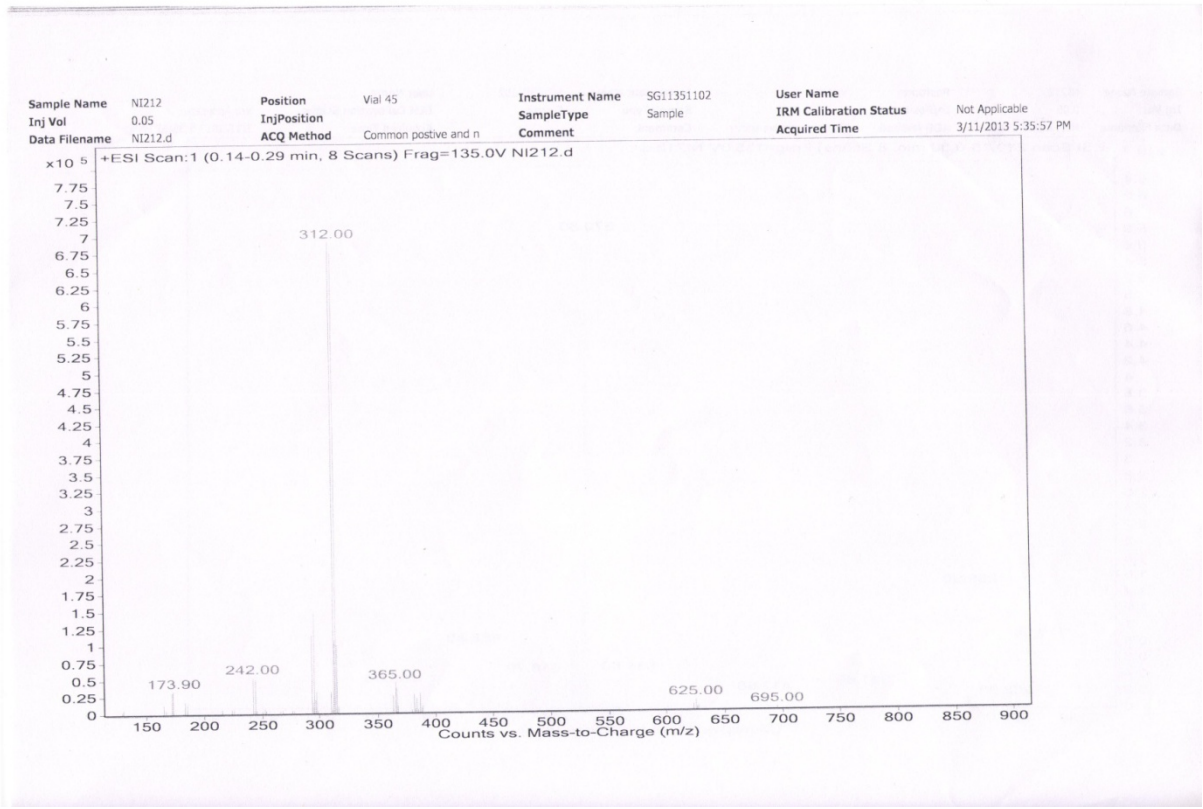
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	375.098	375.0975	-1.09	100	100	78.33	78.13
2	376.1007	376.1007	0	24.29	23.81	19.03	18.6
3	377.1034	377.1033	-0.23	3.02	3.74	2.37	2.92
4	378.1059	378.1059	0.1	0.35	0.44	0.28	0.34

--- End Of Report ---

3l) Methyl 1-(2-chlorobenzoyl)-9H-*β*-carboline-3-carboxylate:


10.65
9.04
8.25
8.23
7.82
7.82
7.80
7.80
7.68
7.67
7.66
7.51
7.51
7.50
7.50
7.48
7.48
7.46
7.46
7.45
7.44
7.43
7.42
7.41
7.41
7.39
3.97
1.06
1.01
2.11
4.32
f1 (ppm)
1.01
1.00
1.06
1.01
2.11
4.32
0.95
3.09
f1 (ppm)
Parameter Value
1 Data File Name C:/ Users/ sony/ Desktop/ NI2-FID/ NI2-12-H1/ fid
2 Title NI2-FID
3 Comment NI2-12
4 Origin Bruker BioSpin GmbH
5 Owner IIIM
6 Site
7 Spectrometer spect
8 Author
9 Solvent CDCl3
10 Temperature 300.0
11 Pulse Sequence zg30
12 Number of Scans 16
13 Receiver Gain 181
14 Relaxation Delay 0.5000
15 Pulse Width 13.1000
16 Acquisition Time 2.7263
17 Acquisition Date 2013-07-16T14:13:37
18 Modification Date 2013-07-16T14:13:38
19 Spectrometer Frequency 400.13
20 Spectral Width 12019.2
21 Lowest Frequency -3105.0
22 Nucleus 1H
23 Acquired Size 32768
24 Spectral Size 65536


196.34
165.96
141.45
137.87
137.16
136.83
132.28
131.65
131.61
130.32
129.95
126.02
122.13
121.86
121.12
77.33
77.22
77.01
76.70
52.68
-0.01
O
O
N
H
O
Cl
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


Sample Name NI212
Inj Vol 0.05
Data Filename NI212.d
Position Vial 45
InjPosition
ACQ Method Common postive and n
Instrument Name SG11351102
SampleType Sample
Comment
User Name
IRM Calibration Status Not Applicable
Acquired Time 3/11/2013 5:35:57 PM
+ESI Scan:1 (0.14-0.29 min, 8 Scans) Frag=135.0V NI212.d
x10 5
312.00
173.90
242.00
365.00
625.00
695.00
Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

Data File	NI2-12.d	**Sample Name**	NI2-12
Sample Type	Sample	**Position**	Vial 38
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	12-03-2013 PM 4:02:18
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			

Info.

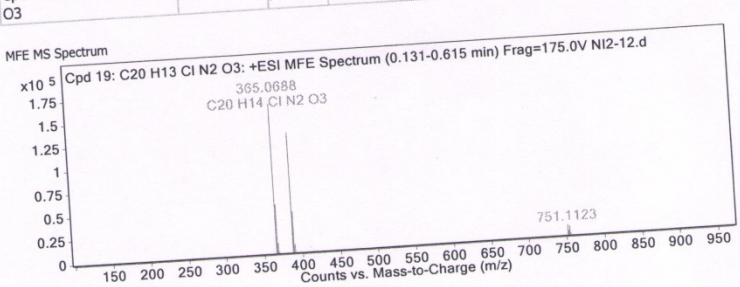
Sample Group	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 19: C20 H13 Cl N2 O3	0.19	364.0615	C20 H13 Cl N2 O3	C20 H13 Cl N2 O3	-0.08	C20 H13 Cl N2 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 19: C20 H13 Cl N2 O3	365.0688	0.19	Find by Molecular Feature	364.0615

MFE MS Spectrum



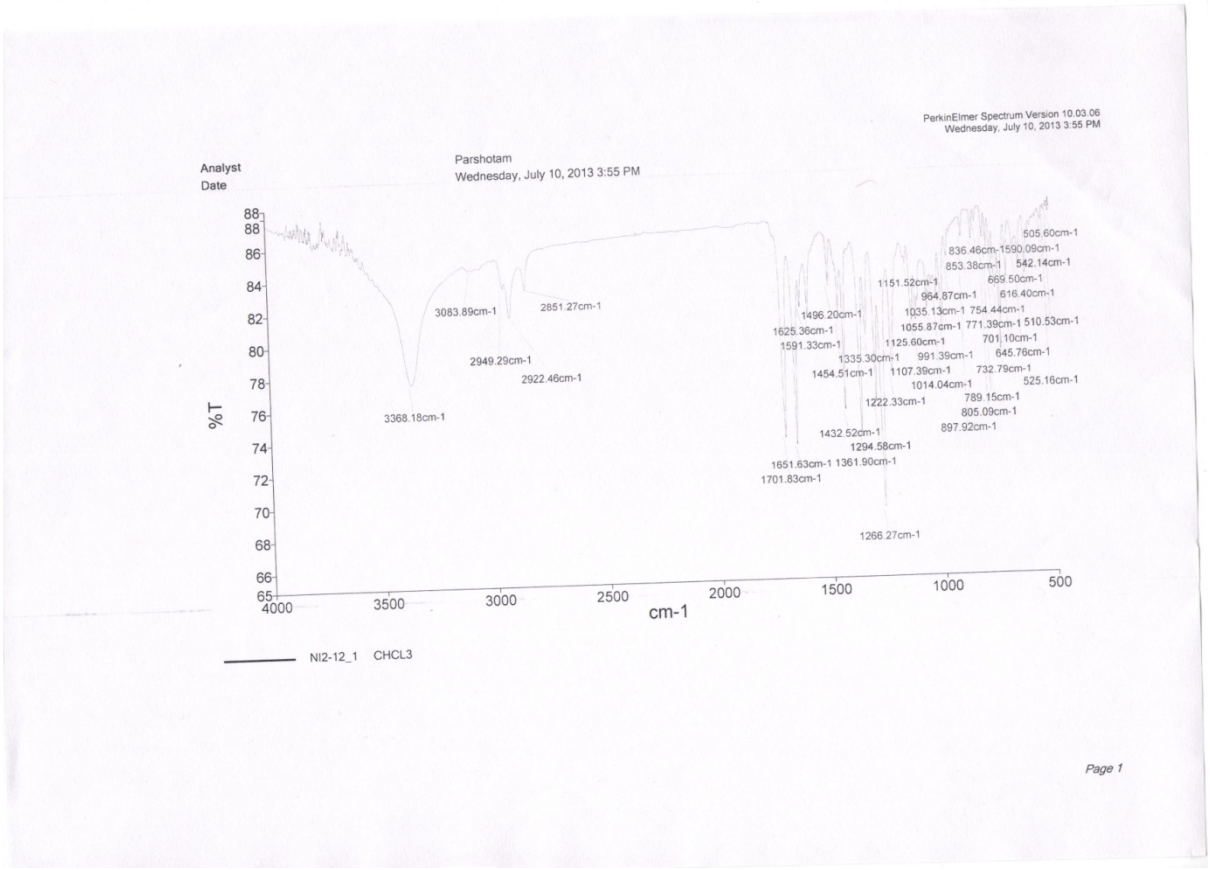
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
365.0688	1	160417.3	C20 H14 Cl N2 O3	(M+H)+
366.0716	1	34211.36	C20 H14 Cl N2 O3	(M+H)+
367.0667	1	51696.98	C20 H14 Cl N2 O3	(M+H)+
368.0695	1	10503.08	C20 H14 Cl N2 O3	(M+H)+
387.0507	1	128660.2	C20 H13 Cl N2 Na O3	(M+Na)+
388.0536	1	27533.55	C20 H13 Cl N2 Na O3	(M+Na)+
389.0482	1	43306.07	C20 H13 Cl N2 Na O3	(M+Na)+
390.051	1	8635.03	C20 H13 Cl N2 Na O3	(M+Na)+
751.1123	1	10216.72		(2M+Na)+
753.1112	1	9208.93		(2M+Na)+

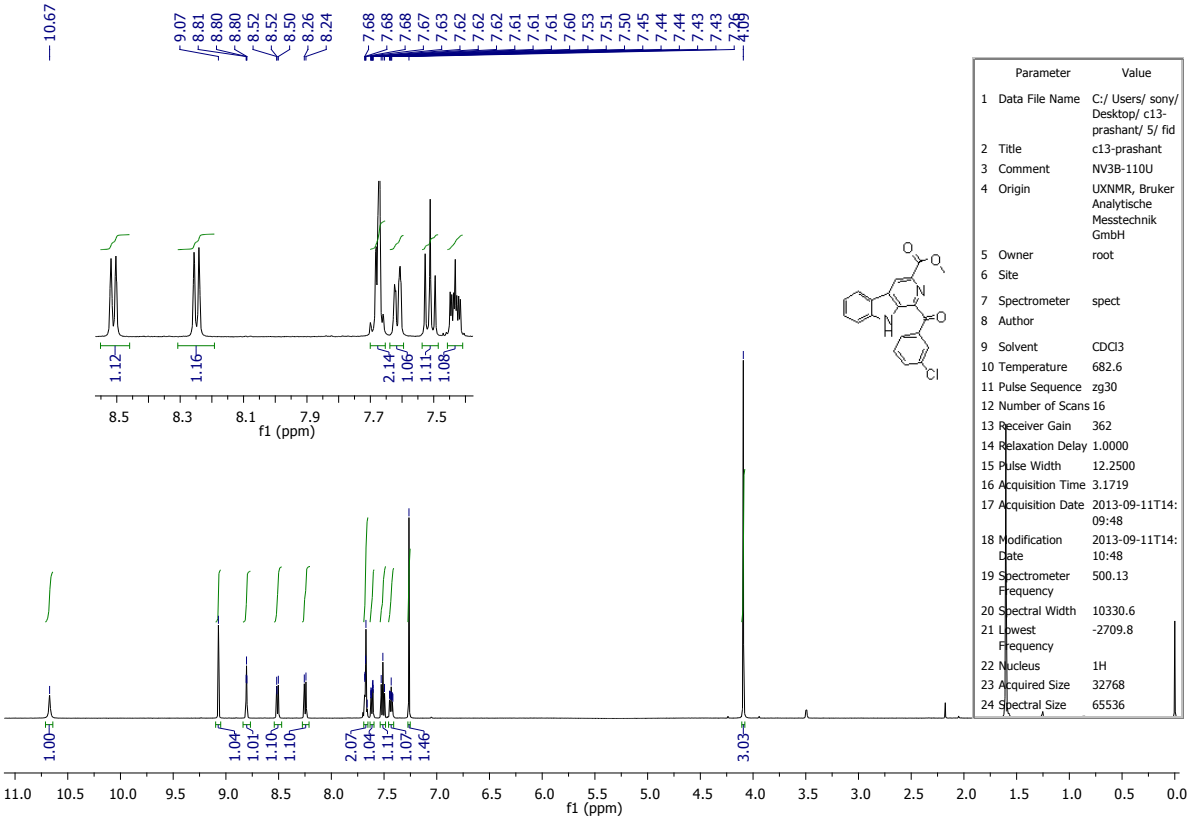
Predicted Isotope Match Table

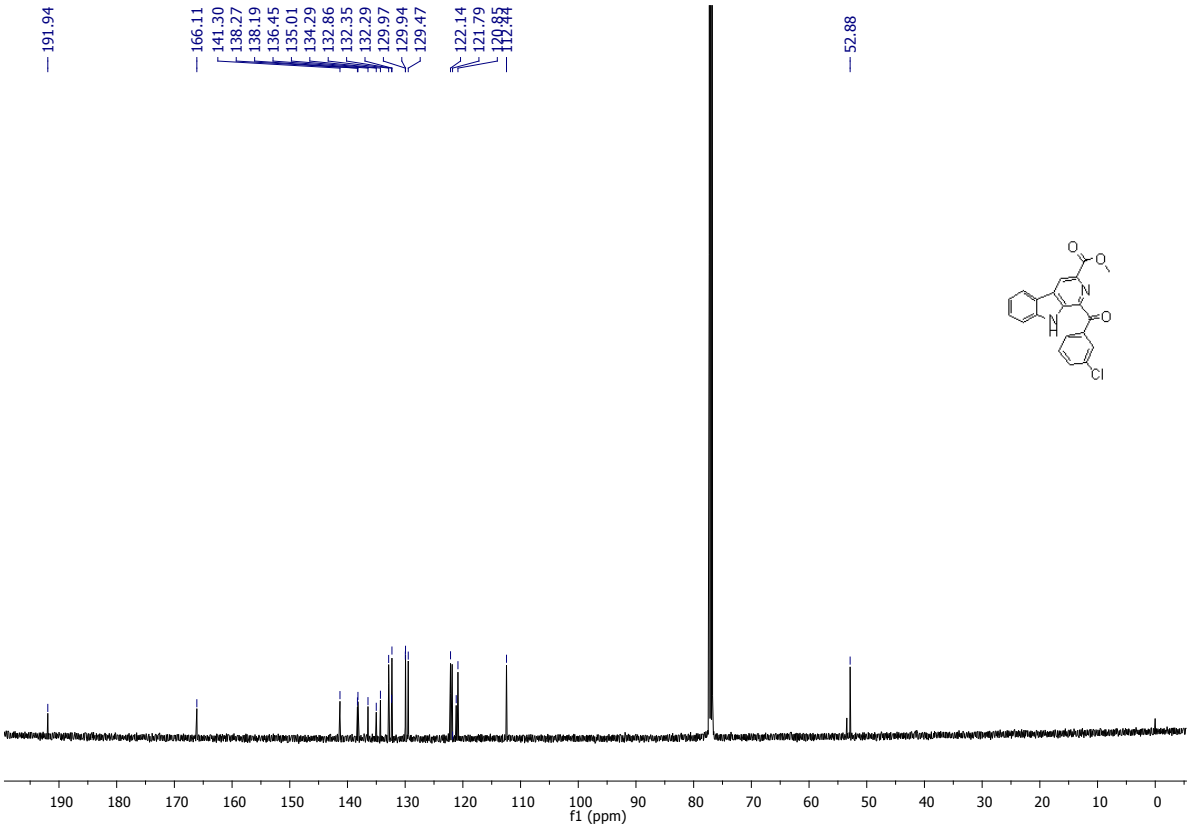
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	365.0688	365.0687	-0.25	100	100	61.91	60.12
2	366.0716	366.0719	1	21.33	22.64	13.2	13.61
3	367.0667	367.0666	-0.27	32.23	35.06	19.95	21.07
4	368.0695	368.0693	-0.38	6.55	7.55	4.05	4.54
5	369.072	369.0719	-0.1	1.19	1	0.74	0.6
6	370.0705	370.0745	10.8	0.23	0.1	0.14	0.06

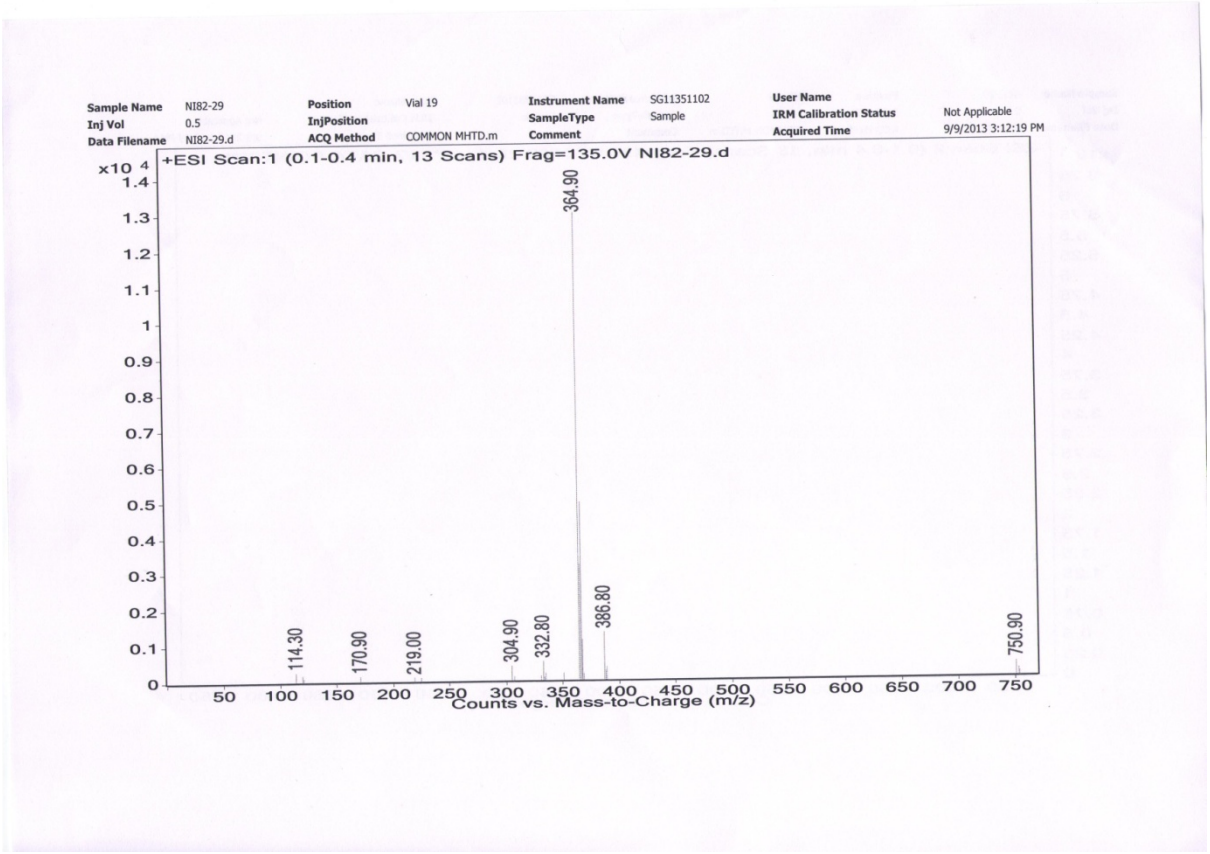
--- End Of Report ---



3m) Methyl 1-(3-chlorobenzoyl)-9H-*β*-carboline-3-carboxylate:




191.94
166.11
141.30
138.27
138.19
136.45
135.01
134.29
132.86
132.35
132.29
129.97
129.94
129.47
122.14
121.79
120.85
112.44
52.88
O
O
N
N
H
O
Cl
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


Sample Name NI82-29
Inj Vol 0.5
Data Filename NI82-29.d
Position Vial 19
InjPosition
ACQ Method COMMON MHTD.m
Instrument Name SG11351102
SampleType Sample
Comment
User Name
IRM Calibration Status Not Applicable
Acquired Time 9/9/2013 3:12:19 PM
+ESI Scan:1 (0.1-0.4 min, 13 Scans) Frag=135.0V NI82-29.d
x10 4
1.4
1.3
1.2
1.1
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
364.90
386.80
114.30
170.90
219.00
304.90
332.80
750.90
50 100 150 200 250 300 350 400 450 500 550 600 650 700 750
Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

Data File	NI2-29.d	**Sample Name**	NI2-29
Sample Type	Sample	**Position**	Vial 5
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	09-09-2013 PM 12:05:40
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

Info.

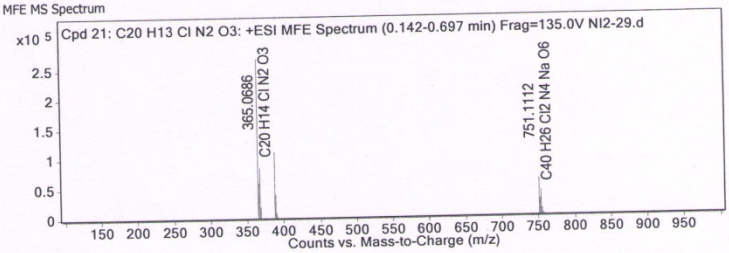
Sample Group	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 21: C20 H13 Cl N2 O3	0.194	364.0613	C20 H13 Cl N2 O3	C20 H13 Cl N2 O3	0.44	C20 H13 Cl N2 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 21: C20 H13 Cl N2 O3	365.0686	0.194	Find by Molecular Feature	364.0613

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
365.0686	1	268688.72	C20 H14 Cl N2 O3	(M+H)+
366.0716	1	59193.41	C20 H14 Cl N2 O3	(M+H)+
367.0665	1	84267.04	C20 H14 Cl N2 O3	(M+H)+
387.0502	1	110225.02	C20 H13 Cl N2 Na O3	(M+Na)+
388.0536	1	24455.3	C20 H13 Cl N2 Na O3	(M+Na)+
389.0481	1	38827.7	C20 H13 Cl N2 Na O3	(M+Na)+
751.1112	1	60813.67	C40 H26 Cl2 N4 Na O6	(2M+Na)+
752.1139	1	26644.06	C40 H26 Cl2 N4 Na O6	(2M+Na)+
753.1103	1	41003.48	C40 H26 Cl2 N4 Na O6	(2M+Na)+
754.1118	1	18317.71	C40 H26 Cl2 N4 Na O6	(2M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	365.0686	365.0687	0.4	100	100	62.09	60.15
2	366.0716	366.0719	0.93	22.03	22.64	13.68	13.62
3	367.0665	367.0666	0.22	31.36	35.06	19.47	21.09
4	368.0693	368.0693	0.01	6.74	7.55	4.19	4.54
5	369.0706	369.0719	3.5	0.92	1	0.57	0.6

--- End Of Report ---

Qualitative Compound Report

Data File	NI2-29.d	**Sample Name**	NI2-29
Sample Type	Sample	**Position**	Vial 5
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	09-09-2013 PM 12:05:40
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

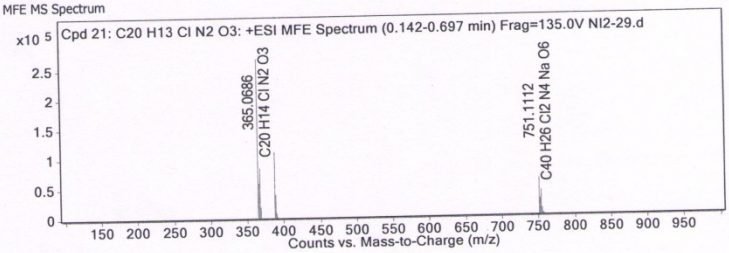
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 21: C20 H13 Cl N2 O3	0.194	364.0613	C20 H13 Cl N2 O3	C20 H13 Cl N2 O3	0.44	C20 H13 Cl N2 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 21: C20 H13 Cl N2 O3	365.0686	0.194	Find by Molecular Feature	364.0613

MFE MS Spectrum



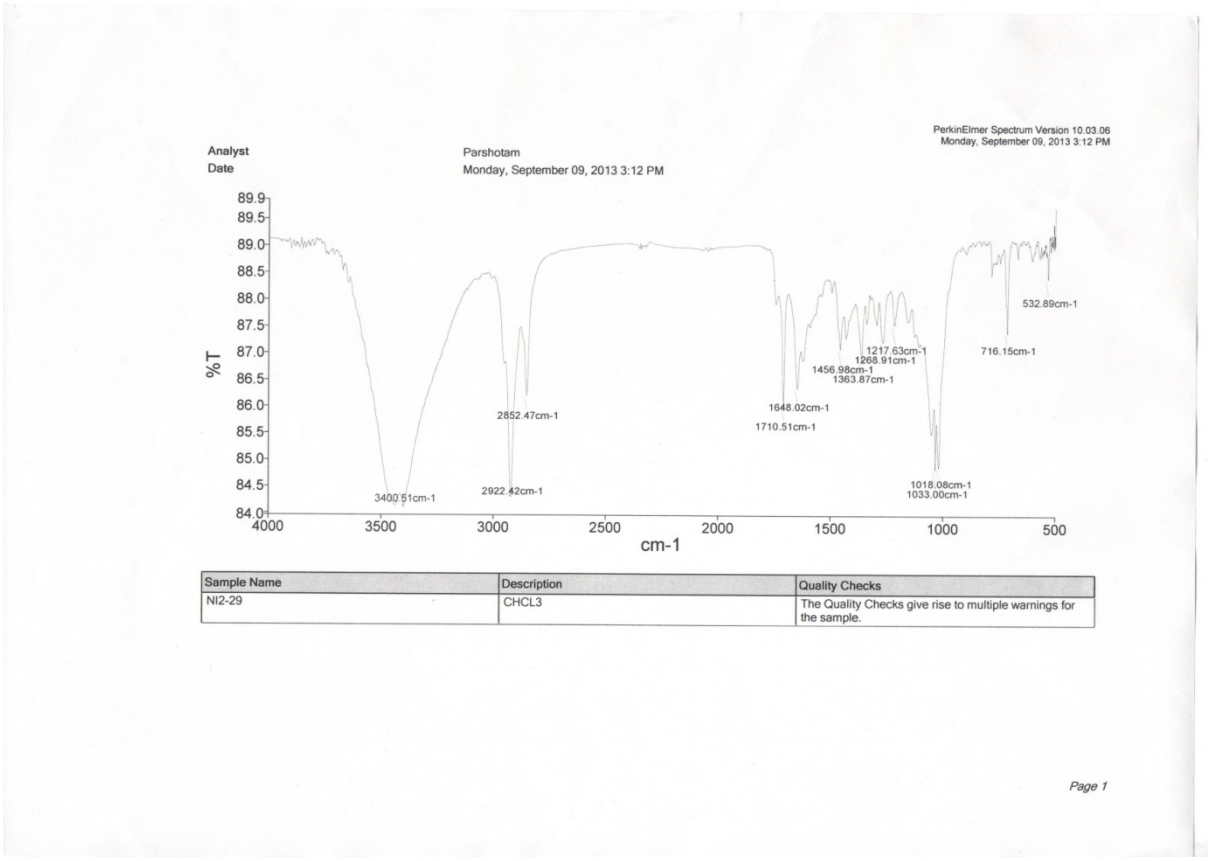
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
365.0686	1	268688.72	C20 H14 Cl N2 O3	(M+H)+
366.0716	1	59193.41	C20 H14 Cl N2 O3	(M+H)+
367.0665	1	84267.04	C20 H14 Cl N2 O3	(M+H)+
387.0502	1	110225.02	C20 H13 Cl N2 Na O3	(M+Na)+
388.0536	1	24455.3	C20 H13 Cl N2 Na O3	(M+Na)+
389.0481	1	38827.7	C20 H13 Cl N2 Na O3	(M+Na)+
751.1112	1	60813.67	C40 H26 Cl2 N4 Na O6	(2M+Na)+
752.1139	1	26644.06	C40 H26 Cl2 N4 Na O6	(2M+Na)+
753.1103	1	41003.48	C40 H26 Cl2 N4 Na O6	(2M+Na)+
754.1118	1	18317.71	C40 H26 Cl2 N4 Na O6	(2M+Na)+

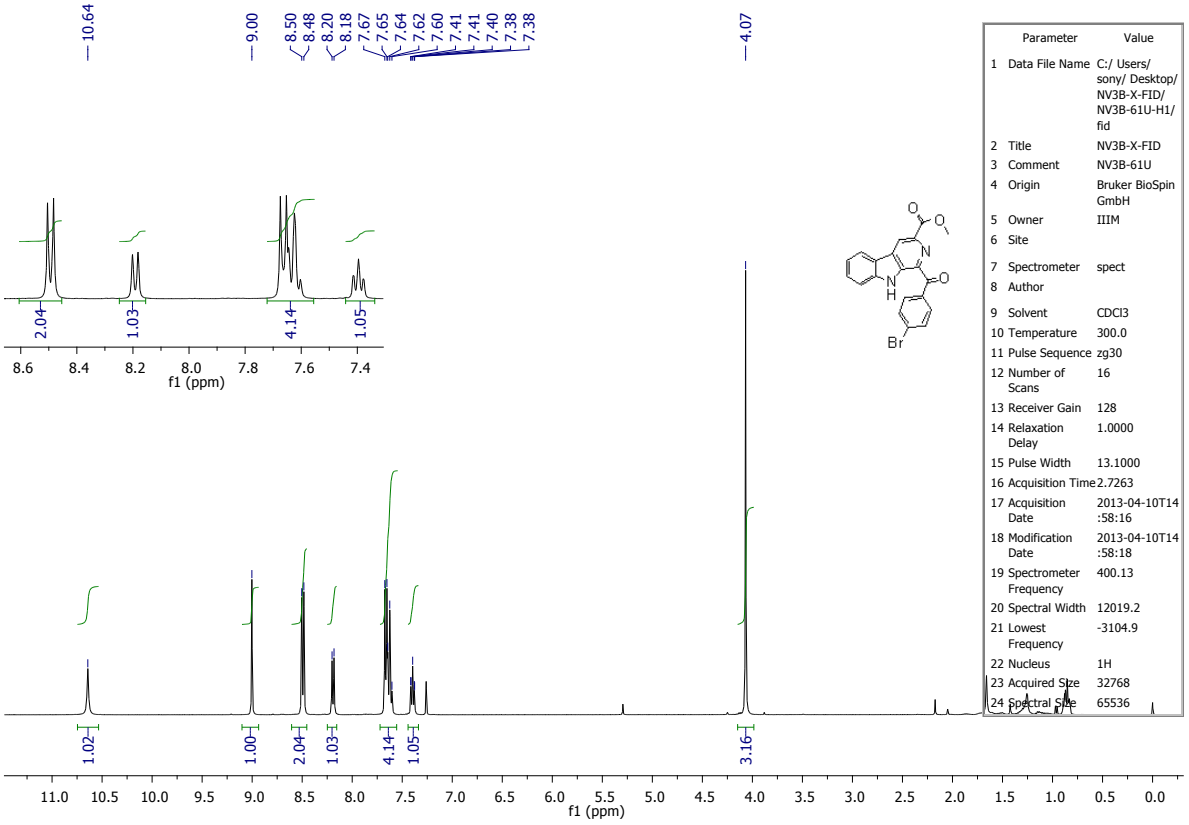
Predicted Isotope Match Table

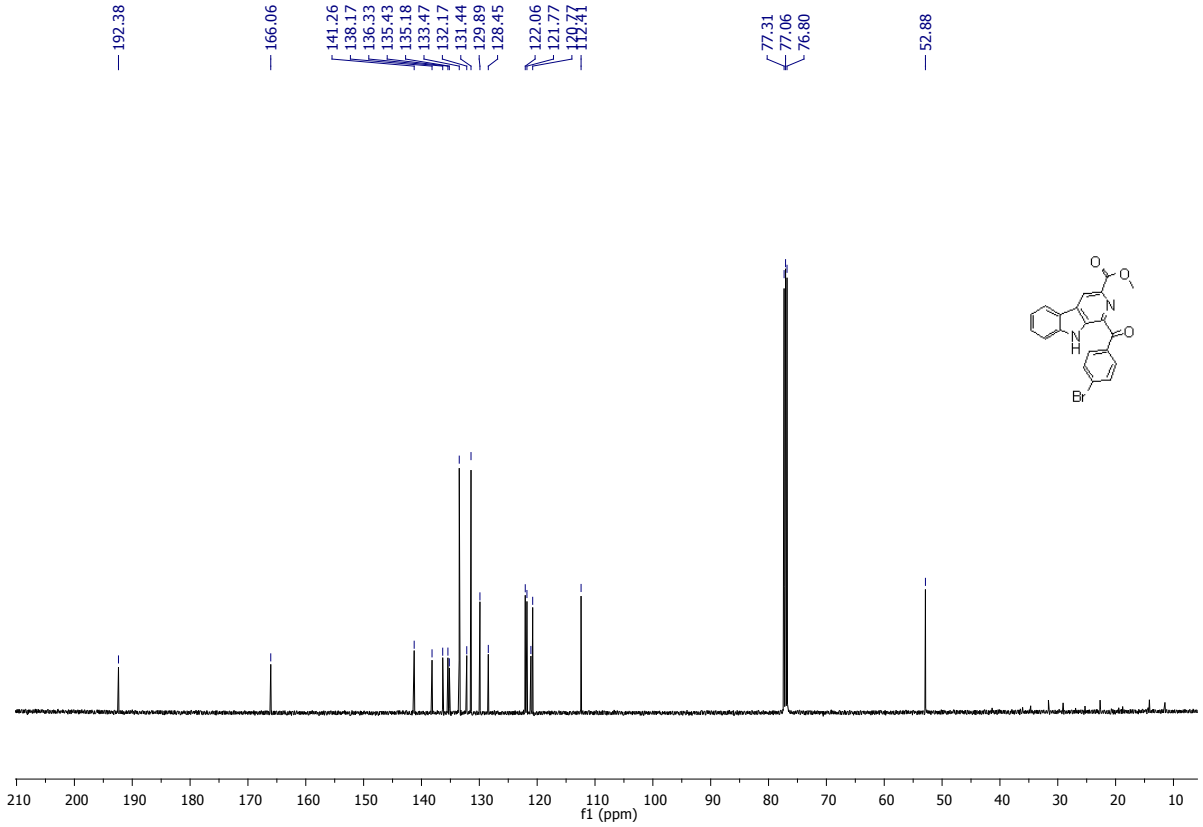
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	365.0686	365.0687	0.4	100	100	62.09	60.15
2	366.0716	366.0719	0.93	22.03	22.64	13.68	13.62
3	367.0665	367.0666	0.22	31.36	35.06	19.47	21.09
4	368.0693	368.0693	0.01	6.74	7.55	4.19	4.54
5	369.0706	369.0719	3.5	0.92	1	0.57	0.6

--- End Of Report ---



3n) Methyl 1-(4-Bromobenzoyl)-9H-*β*-carboline-3-carboxylate:

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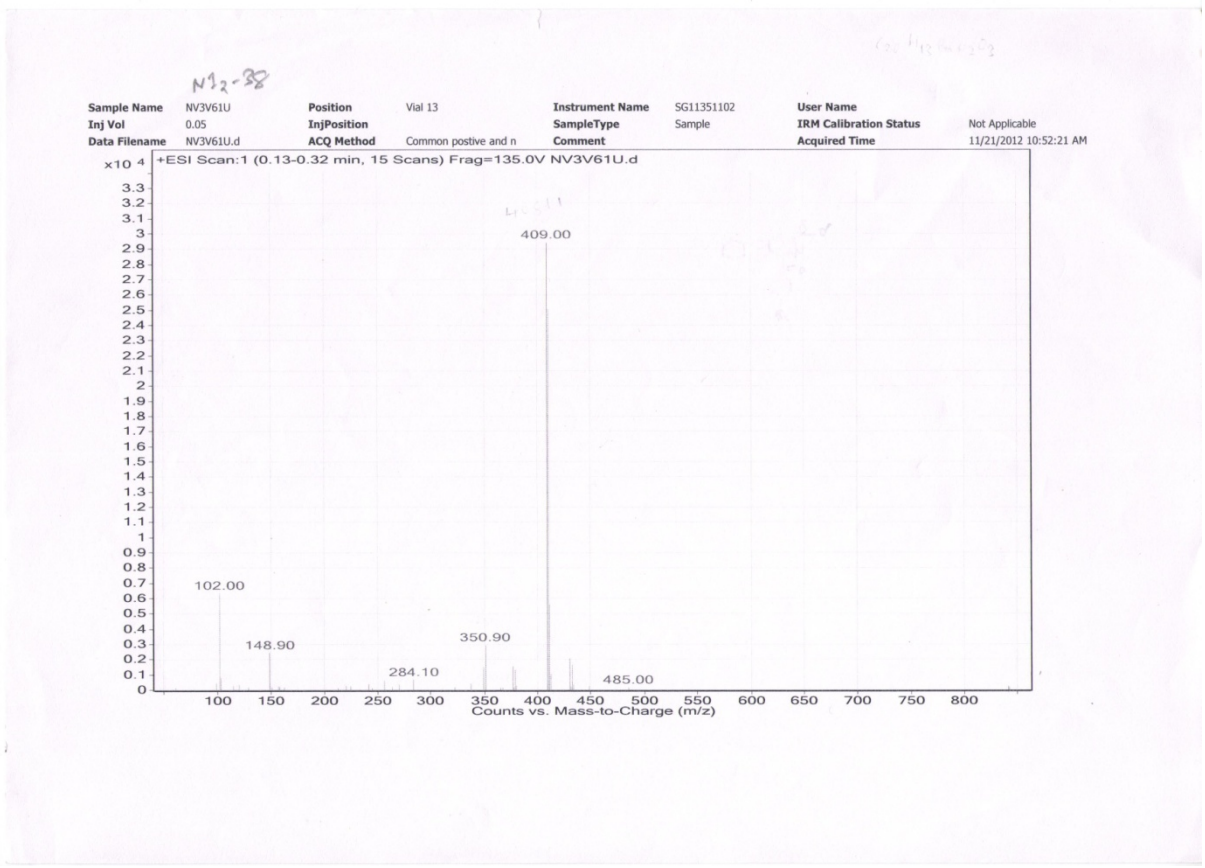
141.26
138.17
136.33
135.43
135.18
133.47
132.17
131.44
129.89
128.45
122.06
121.77
120.77
112.41
77.31
77.06
76.80
52.88
O
O
N
N
H
O
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


NV2-38
Sample Name NV3V61U
Position Vial 13
Instrument Name SG11351102
User Name
Inj Vol 0.05
InjPosition
SampleType Sample
IRM Calibration Status Not Applicable
Data Filename NV3V61U.d
ACQ Method Common postive and n
Comment
Acquired Time 11/21/2012 10:52:21 AM
+ESI Scan:1 (0.13-0.32 min, 15 Scans) Frag=135.0V NV3V61U.d
x10 4
409.00
102.00
148.90
284.10
350.90
485.00
Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

Data File	NV3B-61U.d	**Sample Name**	NV3B-61U
Sample Type	Sample	**Position**	Vial 6
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	13-09-2013 PM 12:13:47
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

Sample Group **Info.**

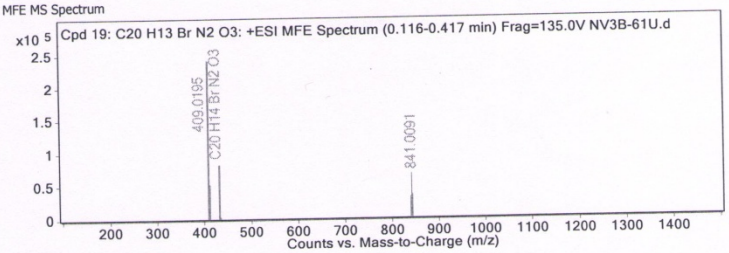
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 19: C20 H13 Br N2 O3	0.196	408.0124	C20 H13 Br N2 O3	C20 H13 Br N2 O3	-3.58	C20 H13 Br N2 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 19: C20 H13 Br N2 O3	409.0195	0.196	Find by Molecular Feature	408.0124

MFE MS Spectrum



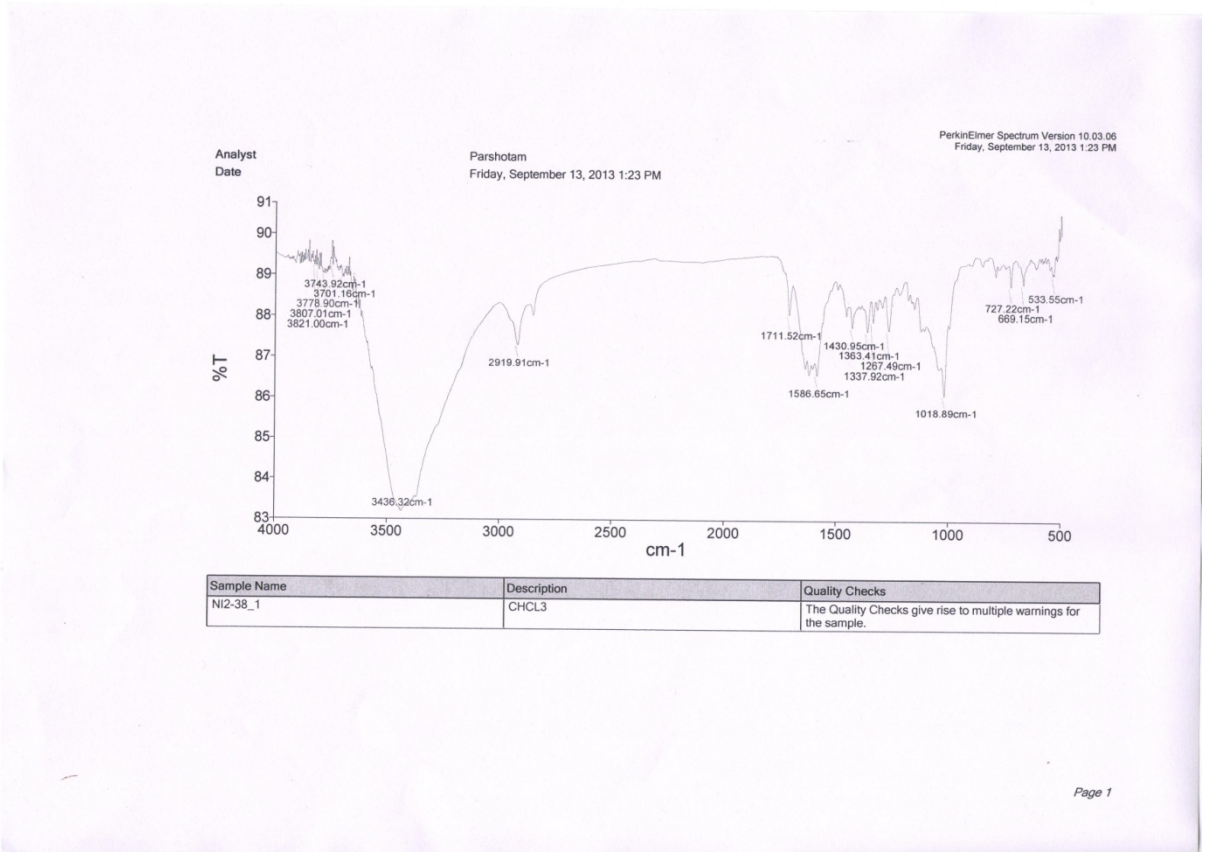
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
409.0195	1	242097.78	C20 H14 Br N2 O3	(M+H)+
410.0229	1	59460.74	C20 H14 Br N2 O3	(M+H)+
411.018	1	241353.08	C20 H14 Br N2 O3	(M+H)+
412.0211	1	52650.13	C20 H14 Br N2 O3	(M+H)+
431.0017	1	82429.76	C20 H13 Br N2 Na O3	(M+Na)+
433.0001	1	81490.95	C20 H13 Br N2 Na O3	(M+Na)+
839.0106	1	31416.47		(2M+Na)+
841.0091	1	67003.68		(2M+Na)+
842.0115	1	30487.85		(2M+Na)+
843.008	1	35573.8		(2M+Na)+

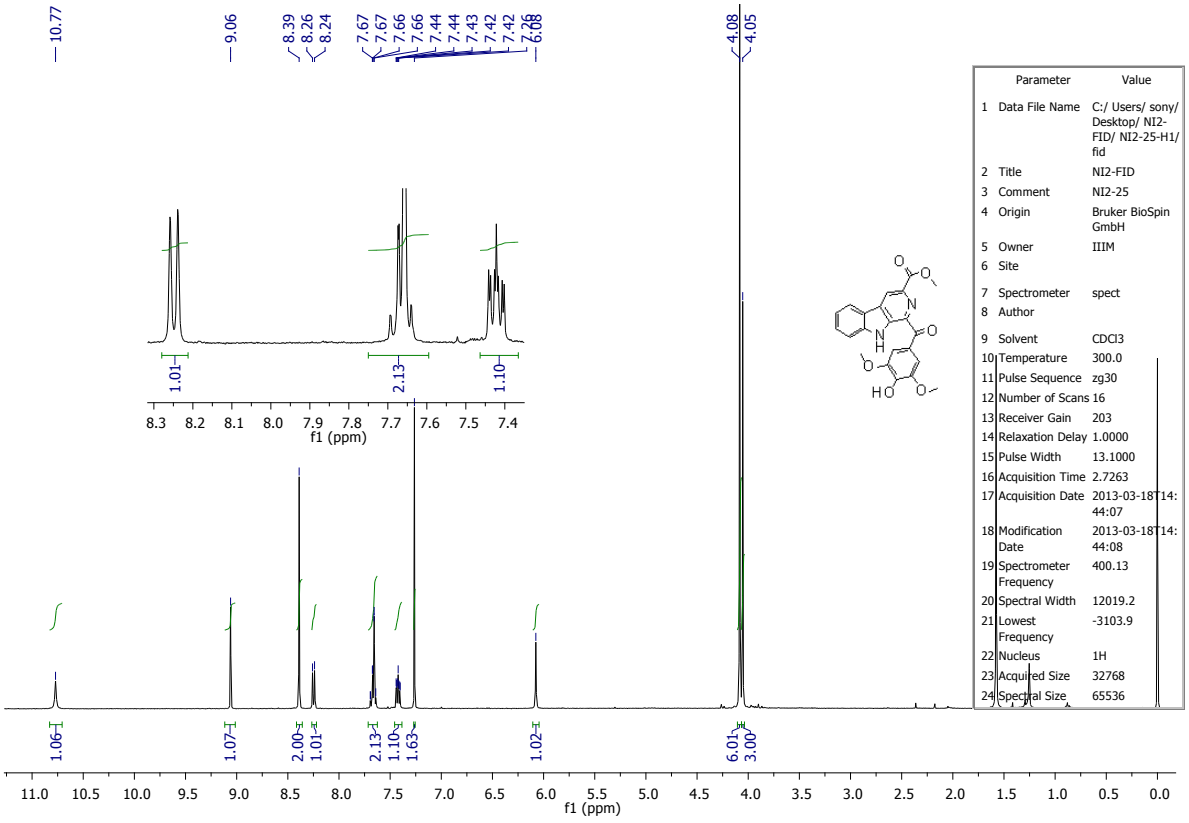
Predicted Isotope Match Table

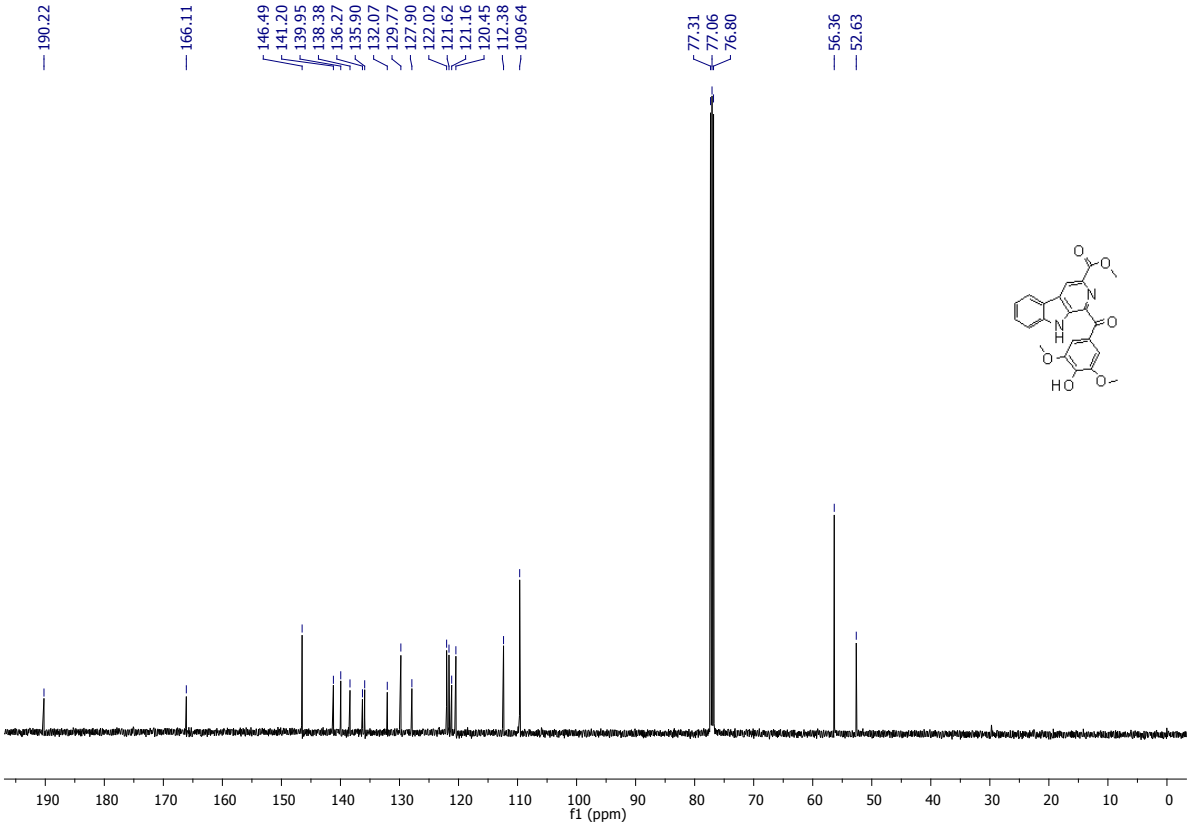
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	409.0195	409.0182	-3.19	100	99.66	39.96	40.22
2	410.0229	410.0214	-3.66	24.56	22.56	9.81	9.1
3	411.018	411.0164	-3.81	99.69	100	39.84	40.36
4	412.0211	412.0195	-3.87	21.75	22.25	8.69	8.98
5	413.0238	413.0222	-3.88	3.78	2.99	1.51	1.21
6	414.0251	414.0248	-0.78	0.33	0.3	0.13	0.12
7	415.038	415.0274	-25.54	0.15	0.02	0.06	0.01

--- End Of Report ---



30) Methyl 1-(4-hydroxy-3,5-dimethoxybenzoyl)-9H-*β*-carboline-3-carboxylate:




190.22
166.11
146.49
141.20
139.95
138.38
136.27
135.90
132.07
129.77
127.90
122.02
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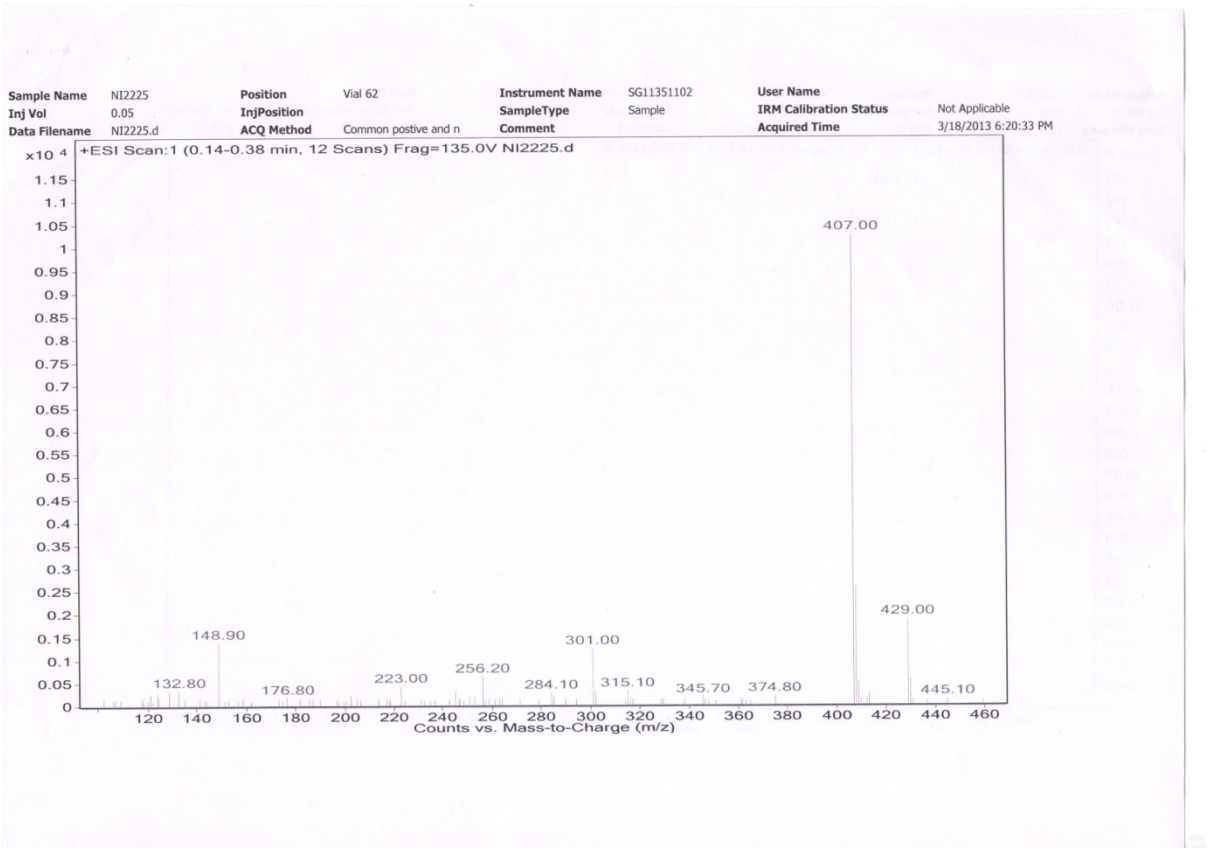
77.06
76.80
56.36
52.63
f1 (ppm)


Sample Name NI2225
Inj Vol 0.05
Data Filename NI2225.d
Position Vial 62
InjPosition
ACQ Method Common postive and n
Instrument Name SG11351102
SampleType Sample
Comment
User Name
IRM Calibration Status Not Applicable
Acquired Time 3/18/2013 6:20:33 PM
+ESI Scan:1 (0.14-0.38 min, 12 Scans) Frag=135.0V NI2225.d
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429.00
148.90
301.00
256.20
132.80
176.80
223.00
284.10
315.10
345.70
374.80
445.10
Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

Data File	NI2-25.d	**Sample Name**	NI2-25
Sample Type	Sample	**Position**	Vial 37
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	19-03-2013 PM 12:21:37
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			

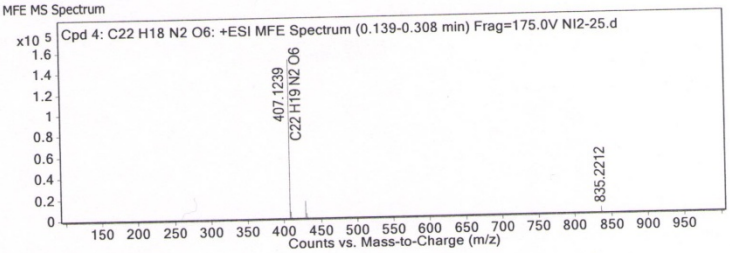
Sample Group		**Info.**	65:25(ACN:H20)
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C22 H18 N2 O6	0.185	406.1166	C22 H18 N2 O6	C22 H18 N2 O6	-0.24	C22 H18 N2 O6

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 4: C22 H18 N2 O6	407.1239	0.185	Find by Molecular Feature	406.1166

MFE MS Spectrum



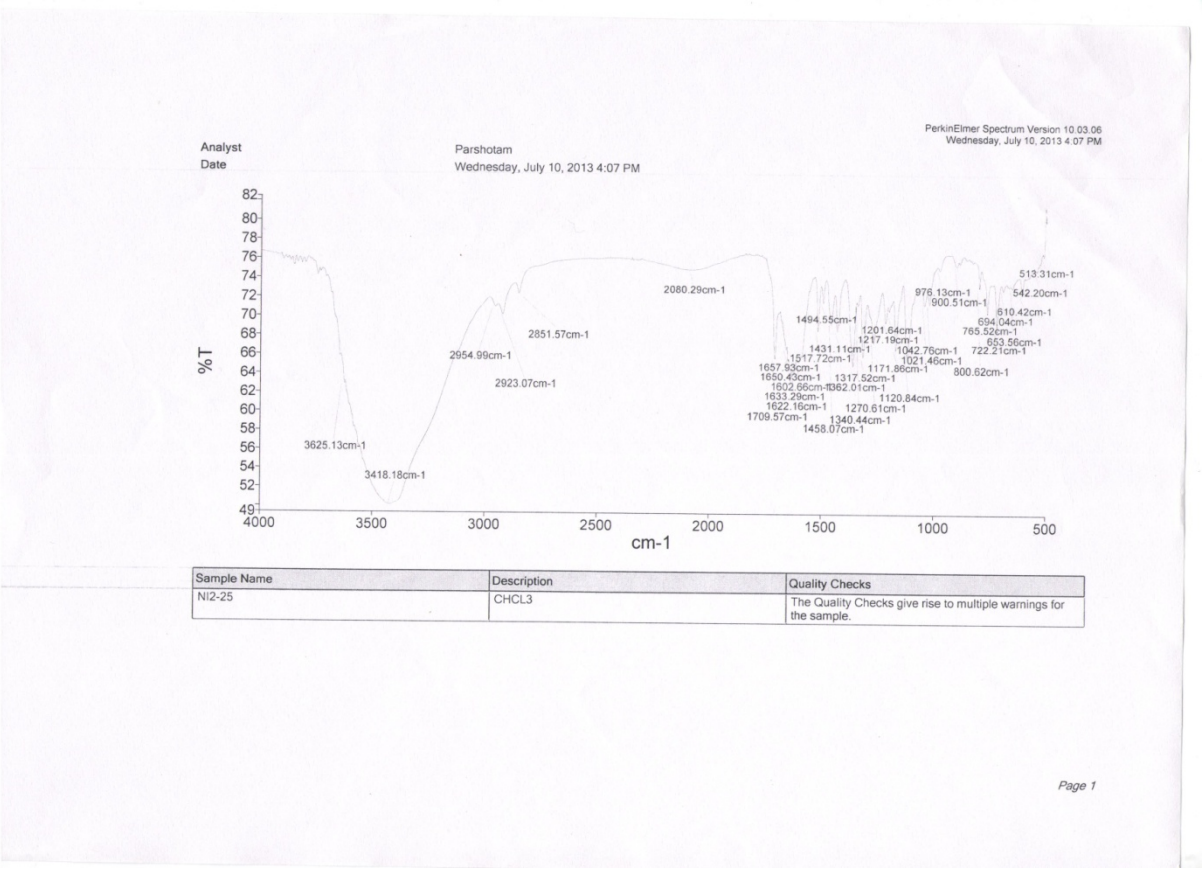
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
407.1239	1	151254.63	C22 H19 N2 O6	(M+H)+
408.1269	1	37879.96	C22 H19 N2 O6	(M+H)+
409.1297	1	6320.96	C22 H19 N2 O6	(M+H)+
410.1313	1	1020.56	C22 H19 N2 O6	(M+H)+
429.1059	1	16620.46	C22 H18 N2 Na O6	(M+Na)+
430.1084	1	4231.2	C22 H18 N2 Na O6	(M+Na)+
431.1113	1	789.23	C22 H18 N2 Na O6	(M+Na)+
835.2212	1	5374.36		(2M+Na)+
836.2251	1	2905.04		(2M+Na)+
837.2281	1	894.8		(2M+Na)+

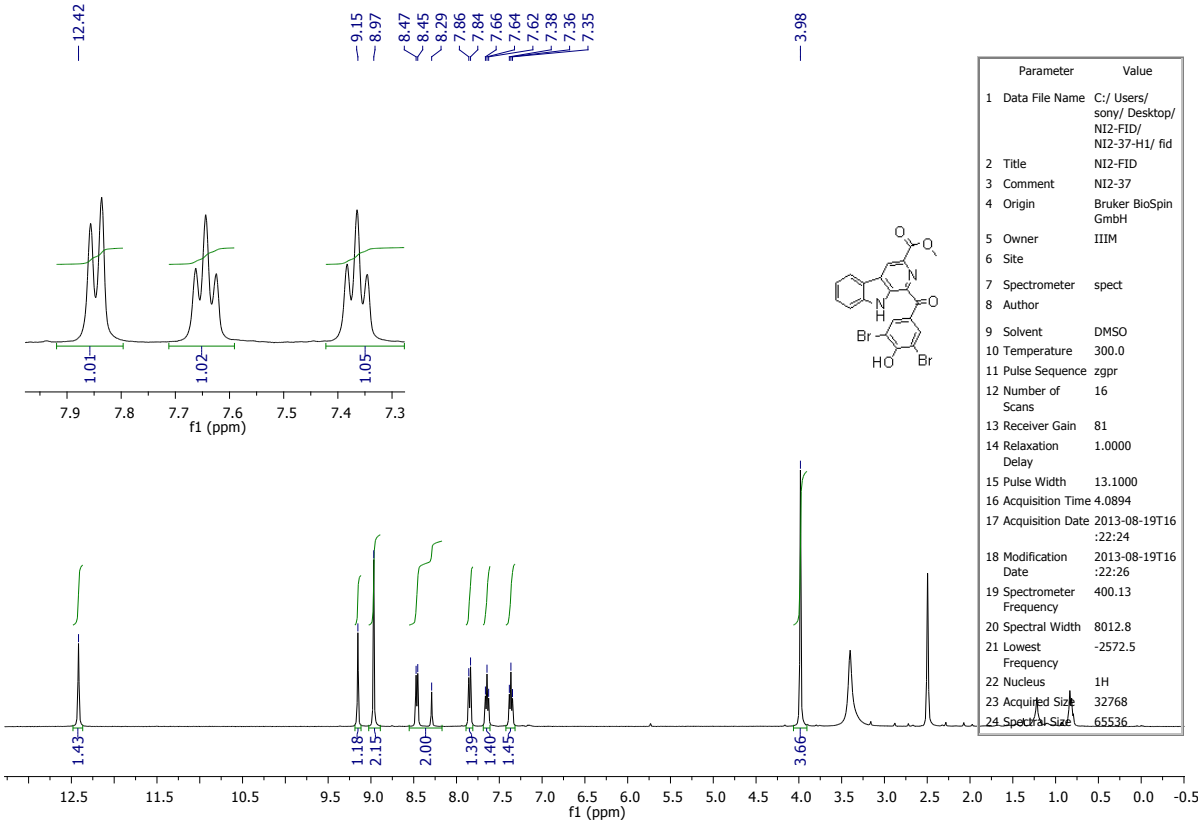
Predicted Isotope Match Table

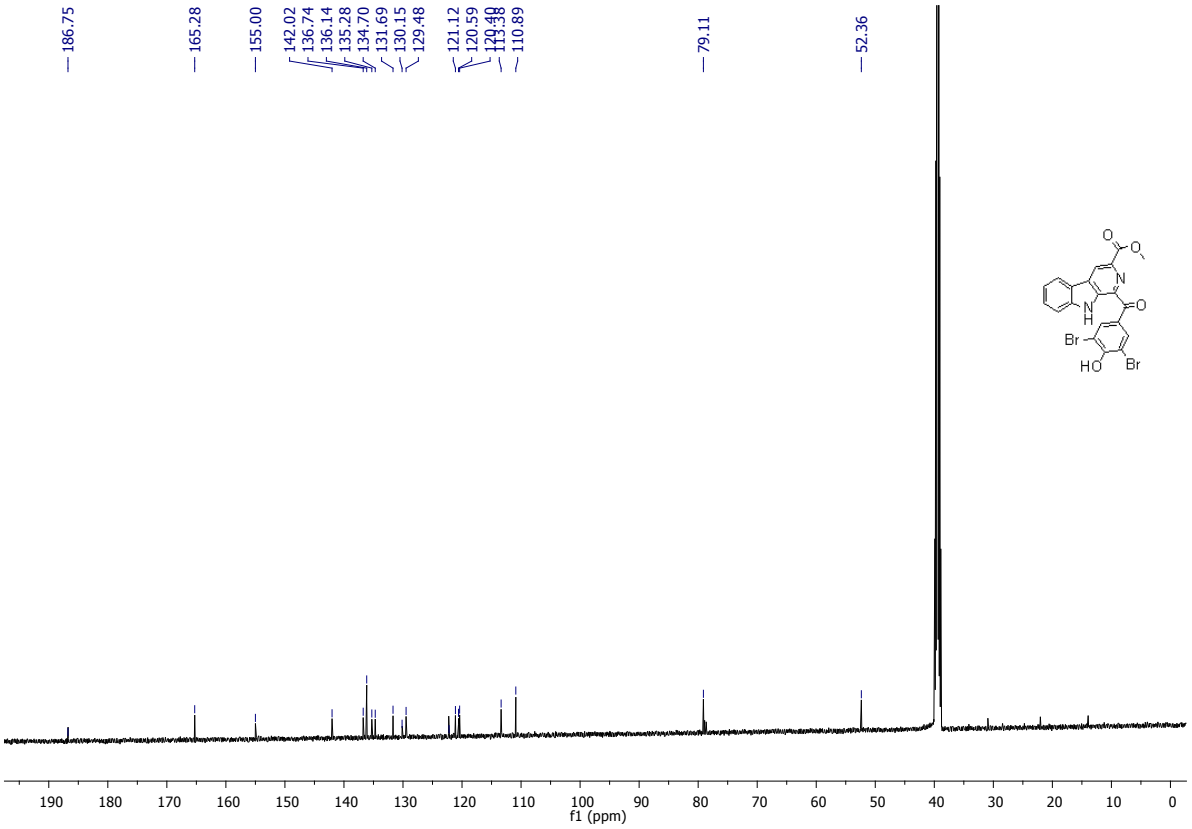
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	407.1239	407.1238	-0.34	100	100	76.98	77.08
2	408.1269	408.127	0.16	25.04	24.97	19.28	19.25
3	409.1297	409.1295	-0.51	4.18	4.22	3.22	3.25
4	410.1313	410.1321	1.91	0.67	0.54	0.52	0.41

--- End Of Report ---



3p) Methyl 1-(3, 5-dibromo-4-hydroxybenzoyl)-9H-*β*-carboline-3-carboxylate:

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165.28
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136.74
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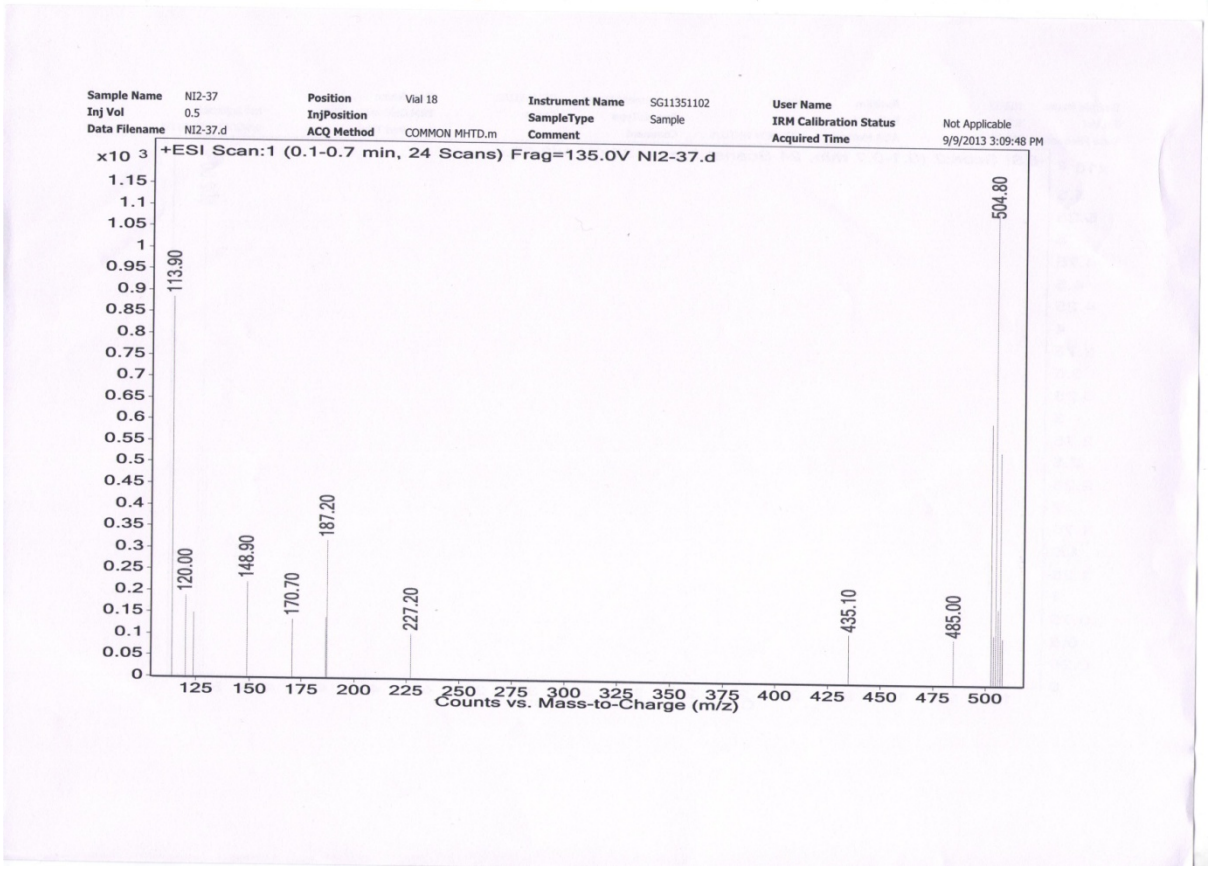
110.89
79.11
52.36
f1 (ppm)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Inj Vol 0.5
Data Filename NI2-37.d
Position Vial 18
InjPosition
ACQ Method COMMON MHTD.m
Instrument Name SG11351102
SampleType Sample
Comment
User Name
IRM Calibration Status Not Applicable
Acquired Time 9/9/2013 3:09:48 PM
+ESI Scan:1 (0.1-0.7 min, 24 Scans) Frag=135.0V NI2-37.d
x10 3
113.90
120.00
148.90
170.70
187.20
227.20
435.10
485.00
504.80
Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

Data File	NI2-37.d	**Sample Name**	NI2-37
Sample Type	Sample	**Position**	Vial 6
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	09-09-2013 PM 12:09:58
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

Info.

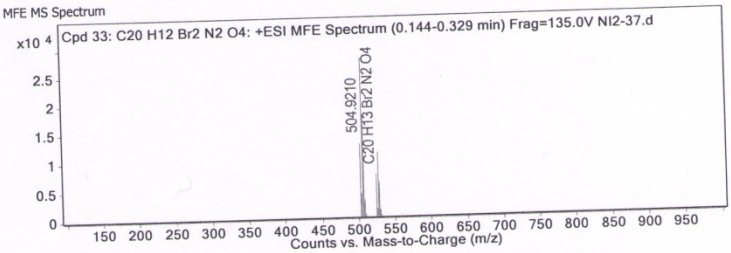
Sample Group	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 33: C20 H12 Br2 N2 O4	0.195	501.9158	C20 H12 Br2 N2 O4	C20 H12 Br2 N2 O4	1.08	C20 H12 Br2 N2 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 33: C20 H12 Br2 N2 O4	502.9233	0.195	Find by Molecular Feature	501.9158

MFE MS Spectrum



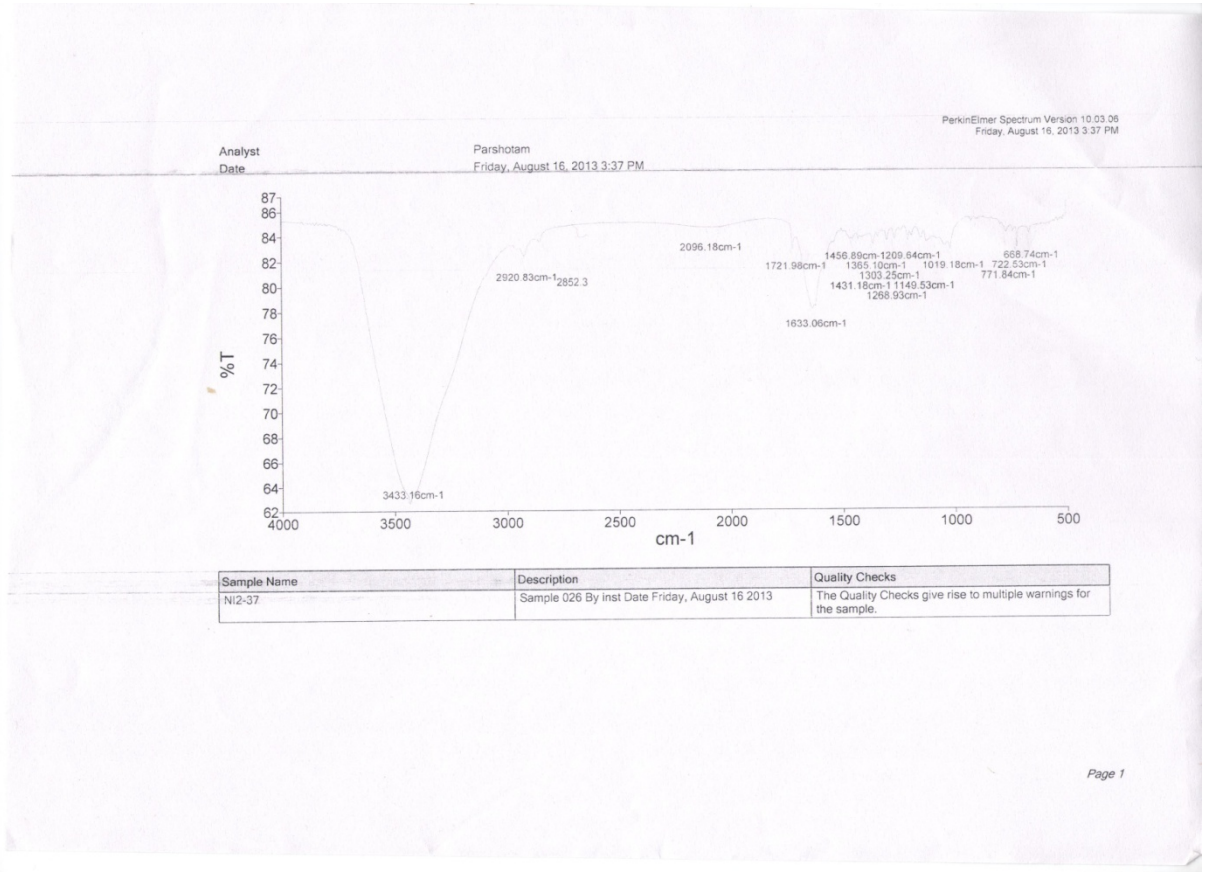
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
502.9233	1	12748.17	C20 H13 Br2 N2 O4	(M+H)+
503.9259	1	4018.93	C20 H13 Br2 N2 O4	(M+H)+
504.921	1	27735.06	C20 H13 Br2 N2 O4	(M+H)+
505.9242	1	5780.68	C20 H13 Br2 N2 O4	(M+H)+
506.9199	1	17635.32	C20 H13 Br2 N2 O4	(M+H)+
507.9218	1	2932.32	C20 H13 Br2 N2 O4	(M+H)+
524.9047	1	7380.06		(M+Na)+
526.9031	1	11083.71		(M+Na)+
527.9064	1	2589.94		(M+Na)+
528.901	1	5975.29		(M+Na)+

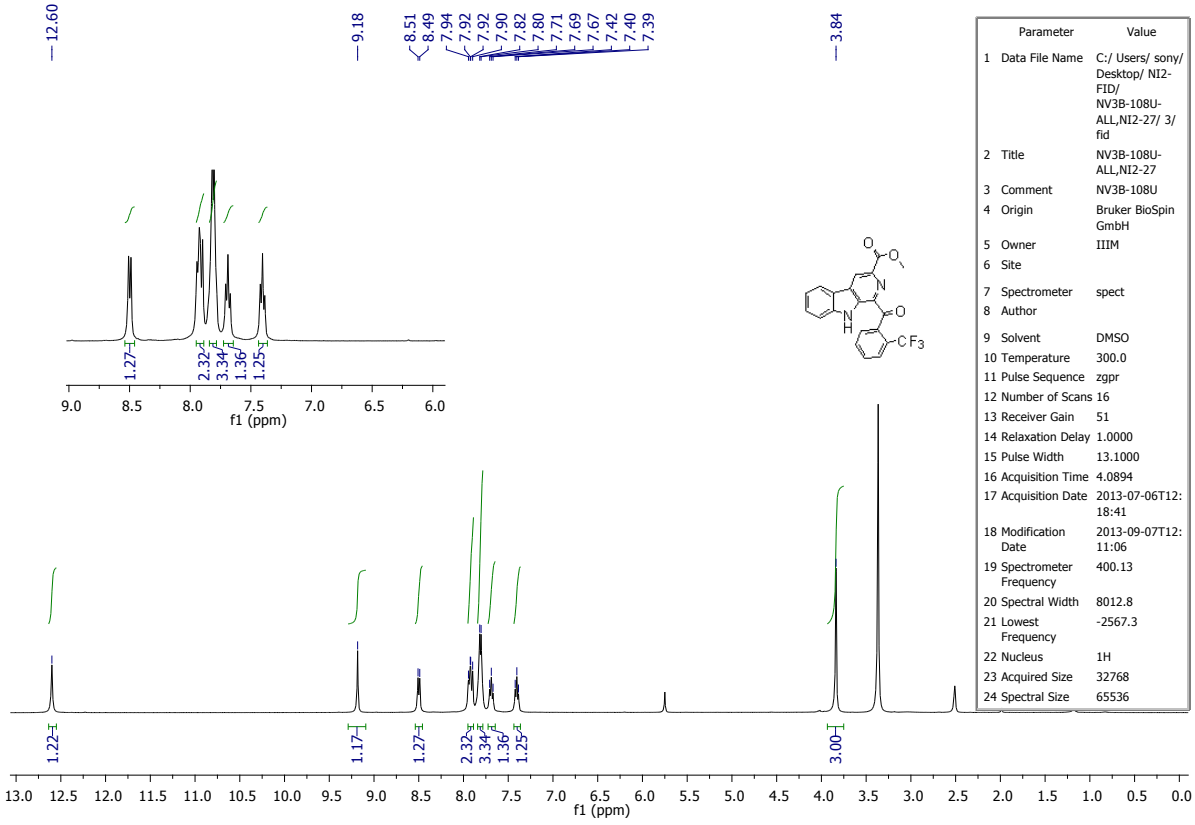
Predicted Isotope Match Table

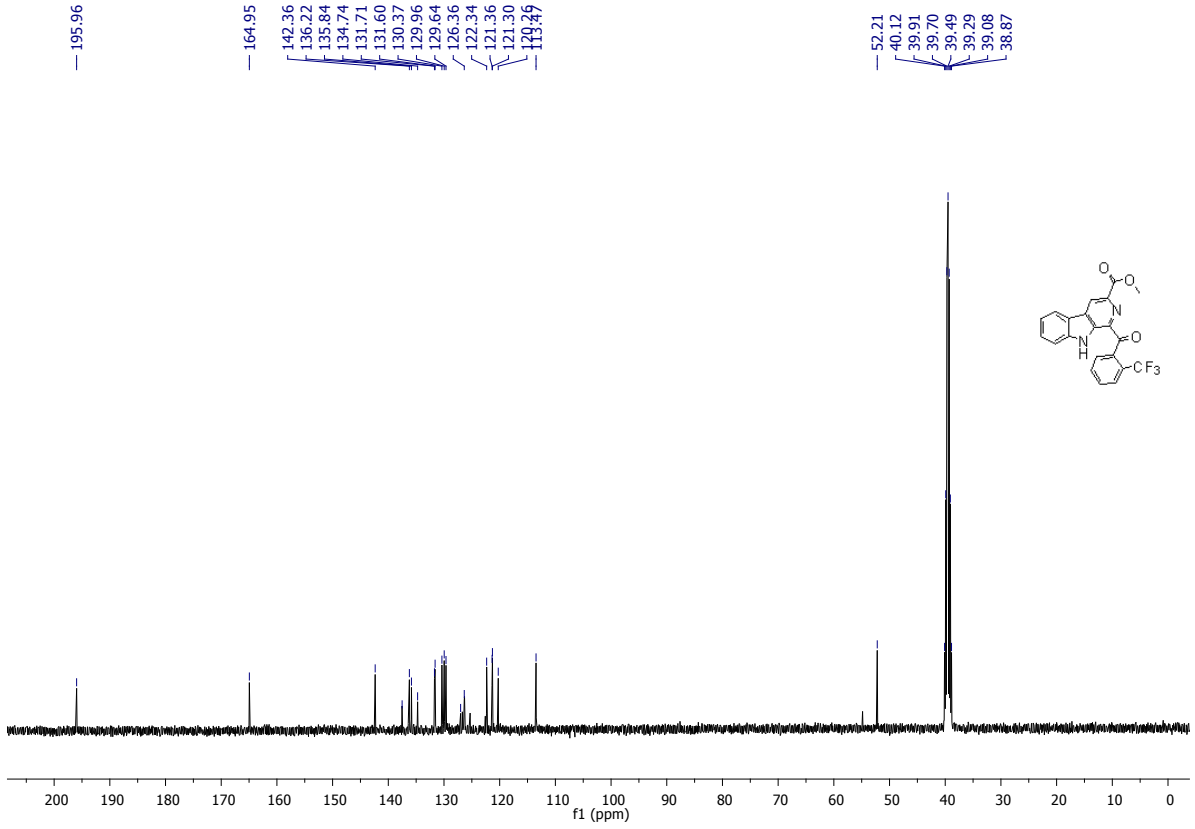
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	502.9233	502.9237	0.7	45.96	50.55	17.88	20.36
2	503.9259	503.9268	1.88	14.49	11.46	5.64	4.61
3	504.921	504.9217	1.52	100	100	38.91	40.27
4	505.9242	505.9248	1.27	20.84	22.47	8.11	9.05
5	506.9199	506.9201	0.3	63.58	51.07	24.74	20.56
6	507.9218	507.923	2.32	10.57	11.19	4.11	4.51
7	508.9271	508.9255	-3.1	1.57	1.6	0.61	0.64

--- End Of Report ---



3q) Methyl 1-(2-(trifluoromethyl)benzoyl)-9H-*β*-carboline-3-carboxylate:

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142.36
136.22
135.84
134.74
131.71
131.60
130.37
129.96
129.64
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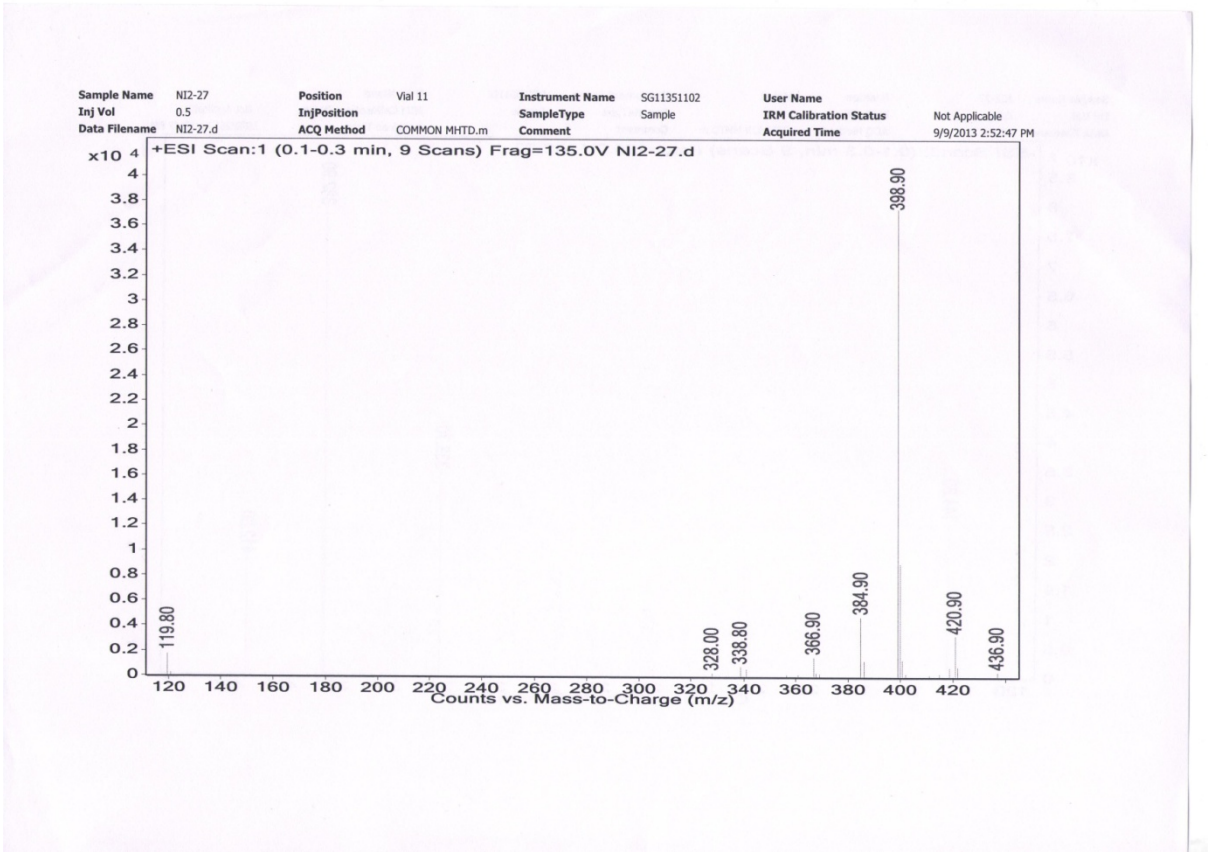
121.36
121.30
52.21
40.12
39.91
39.70
39.49
39.29
39.08
38.87
f1 (ppm)


Sample Name NI2-27
Position Vial 11
Instrument Name SG11351102
User Name
Inj Vol 0.5
InjPosition
SampleType Sample
IRM Calibration Status Not Applicable
Data Filename NI2-27.d
ACQ Method COMMON MHTD.m
Comment
Acquired Time 9/9/2013 2:52:47 PM
+ESI Scan:1 (0.1-0.3 min, 9 Scans) Frag=135.0V NI2-27.d
x10 4
398.90
384.90
119.80
328.00
338.80
366.90
420.90
436.90
Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

Data File	NV3B-108U.d	**Sample Name**	NV3B-108U
Sample Type	Sample	**Position**	Vial 42
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	16-07-2013 PM 1:36:43
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

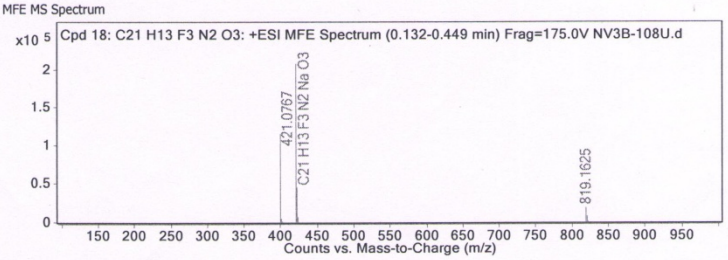
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 18: C21 H13 F3 N2 O3	0.196	398.0875	C21 H13 F3 N2 O3	C21 H13 F3 N2 O3	0.88	C21 H13 F3 N2 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 18: C21 H13 F3 N2 O3	421.0767	0.196	Find by Molecular Feature	398.0875

MFE MS Spectrum



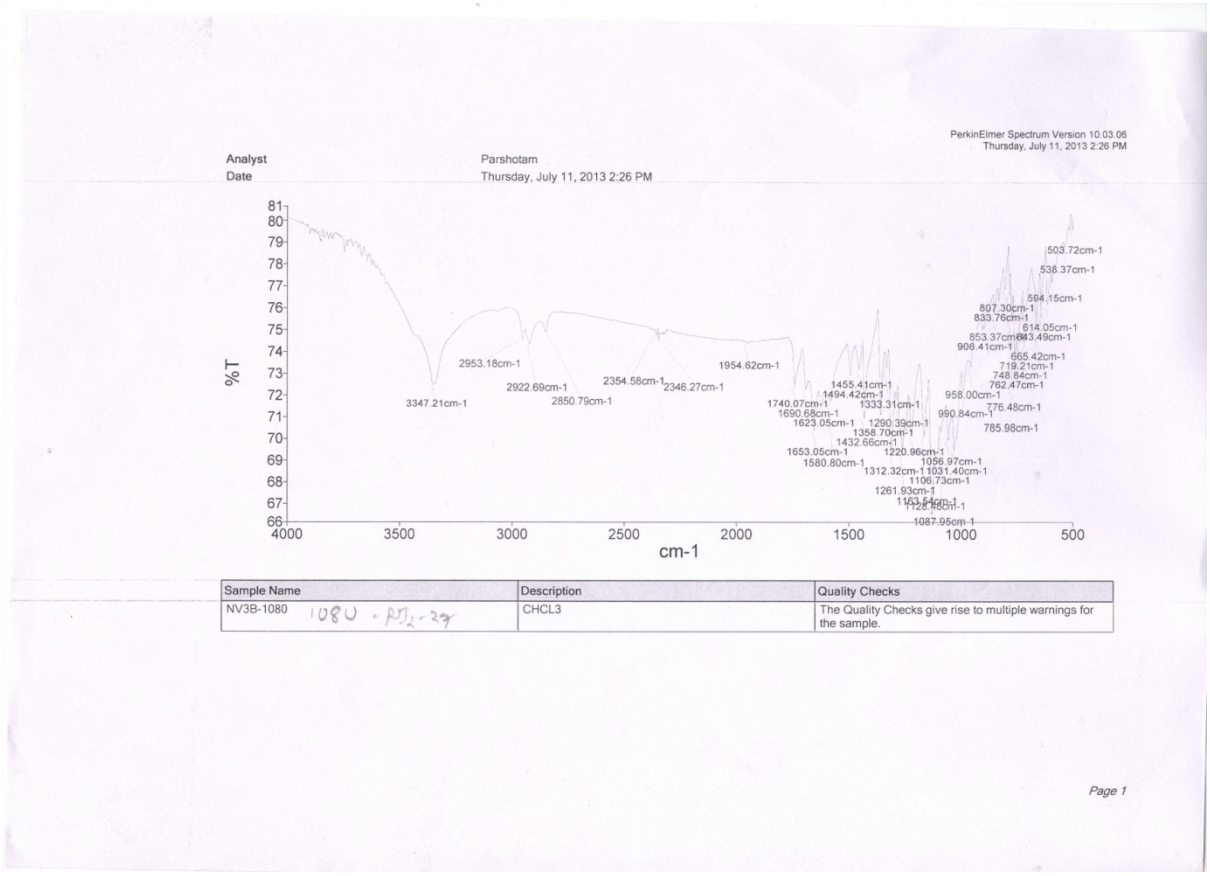
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
399.0947	1	115125.55	C21 H14 F3 N2 O3	(M+H)+
400.098	1	24854.56	C21 H14 F3 N2 O3	(M+H)+
401.1028	1	4389.9	C21 H14 F3 N2 O3	(M+H)+
402.1078	1	876.4	C21 H14 F3 N2 O3	(M+H)+
421.0767	1	208010.16	C21 H13 F3 N2 Na O3	(M+Na)+
422.0797	1	46307.66	C21 H13 F3 N2 Na O3	(M+Na)+
423.0833	1	6868.61	C21 H13 F3 N2 Na O3	(M+Na)+
819.1625	1	18275.43		(2M+Na)+
820.1668	1	8148.3		(2M+Na)+
821.166	1	3227.28		(2M+Na)+

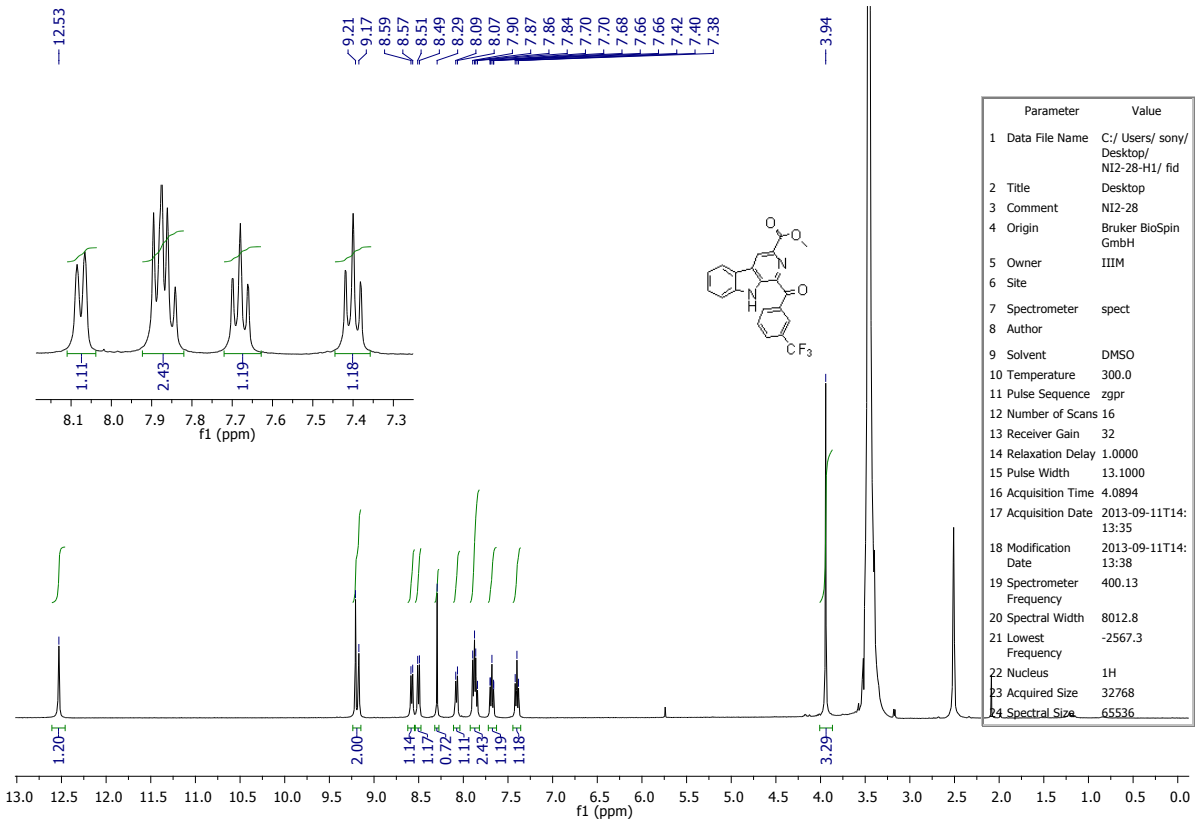
Predicted Isotope Match Table

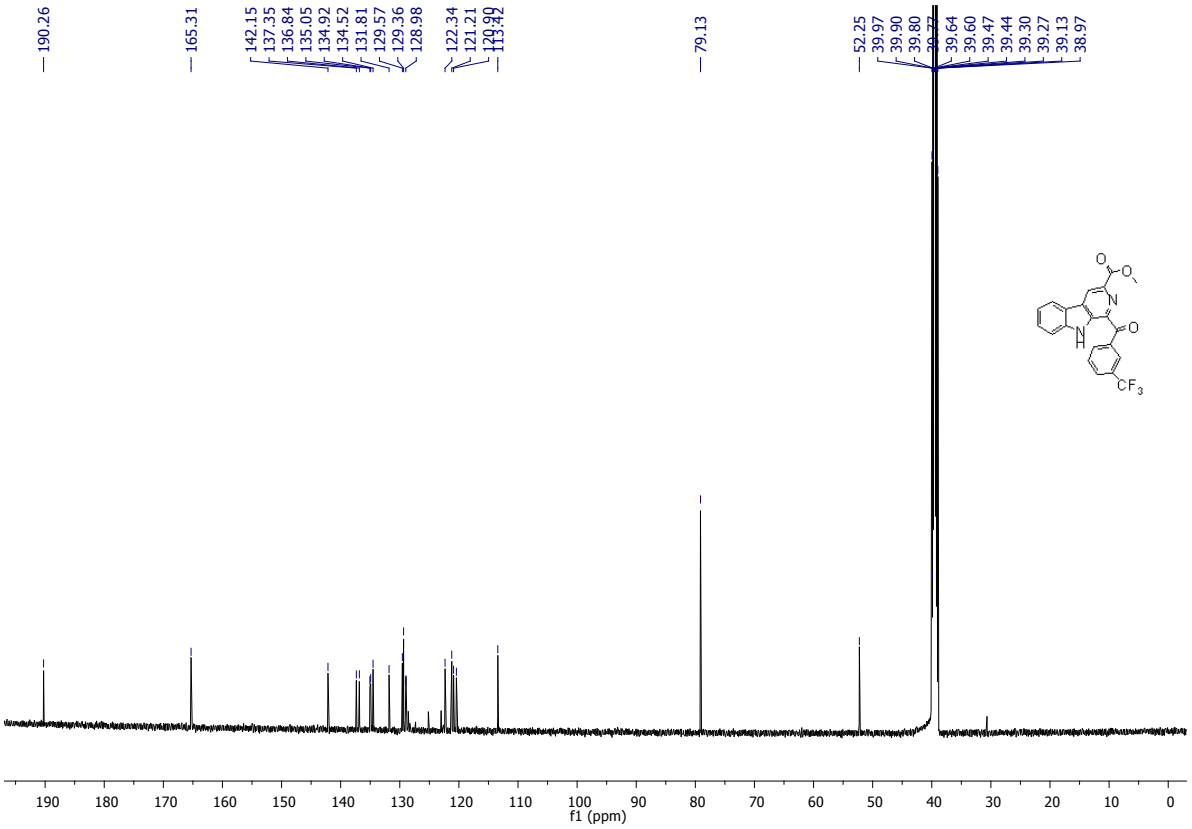
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	399.0947	399.0951	1.05	100	100	79.26	78.52
2	400.098	400.0983	0.61	21.59	23.72	17.11	18.62
3	401.1028	401.1011	-4.36	3.81	3.31	3.02	2.6
4	402.1078	402.1037	-10.13	0.76	0.34	0.6	0.27

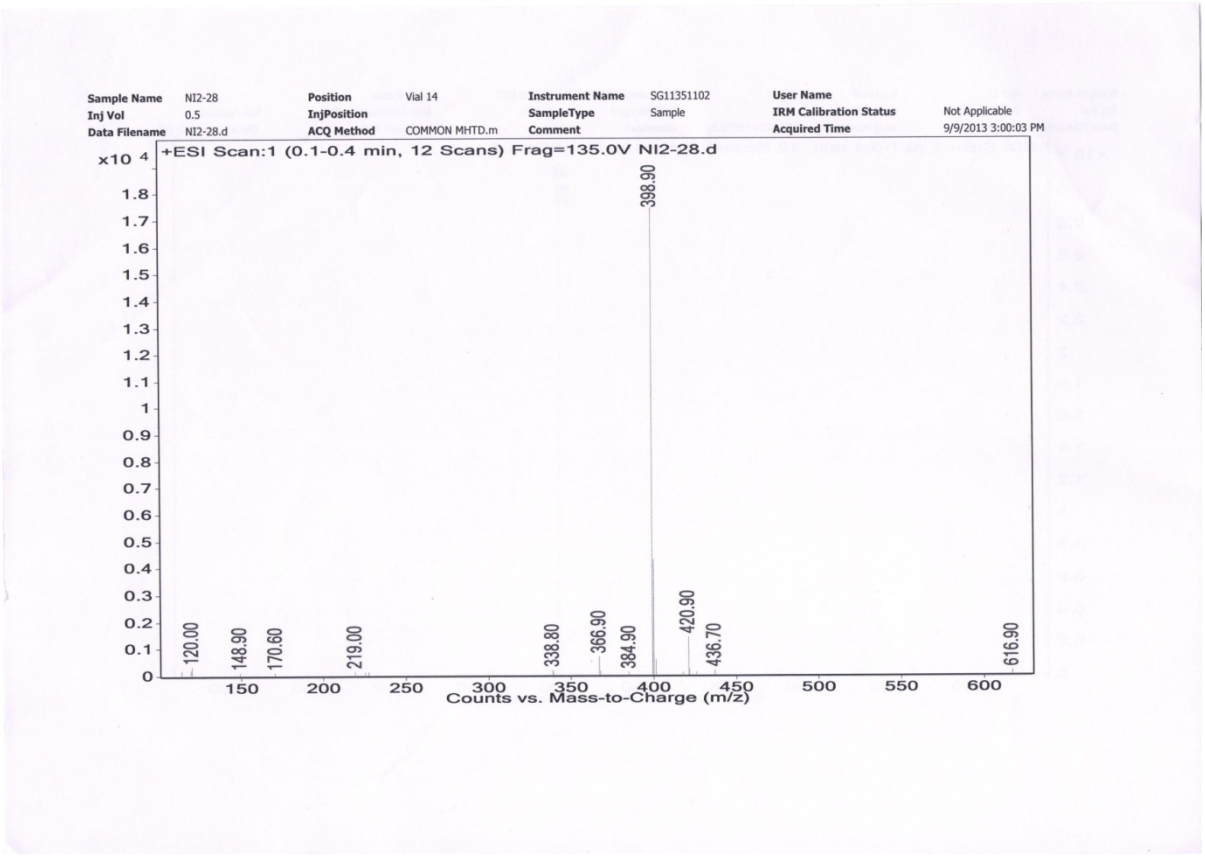
--- End Of Report ---



3r) Methyl 1-(3-(trifluoromethyl)benzoyl)-9H-*β*-carboline-3-carboxylate:




190.26
165.31
142.15
137.35
136.84
135.05
134.92
134.52
131.81
129.57
129.36
128.98
122.34
121.21
120.90
113.42
79.13
52.25
39.97
39.90
39.80
39.64
39.60
39.47
39.44
39.30
39.27
39.13
38.97
O
O
N
H
O
CF3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


Sample Name NI2-28
Position Vial 14
Instrument Name SG11351102
User Name
Inj Vol 0.5
InjPosition
SampleType Sample
IRM Calibration Status Not Applicable
Data Filename NI2-28.d
ACQ Method COMMON MHTD.m
Comment
Acquired Time 9/9/2013 3:00:03 PM
+ESI Scan:1 (0.1-0.4 min, 12 Scans) Frag=135.0V NI2-28.d
x10 4
1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
398.90
420.90
120.00
148.90
170.60
219.00
338.80
366.90
384.90
436.70
616.90
150 200 250 300 350 400 450 500 550 600
Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

Data File	NI2-28.d	**Sample Name**	NI2-28
Sample Type	Sample	**Position**	Vial 3
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	09-09-2013 AM 11:41:03
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

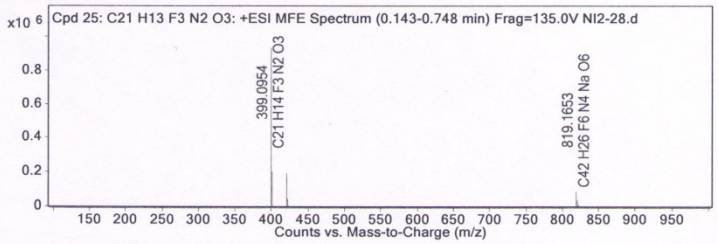
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 25: C21 H13 F3 N2 O3	0.195	398.0881	C21 H13 F3 N2 O3	C21 H13 F3 N2 O3	-0.76	C21 H13 F3 N2 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 25: C21 H13 F3 N2 O3	399.0954	0.195	Find by Molecular Feature	398.0881

MFE MS Spectrum



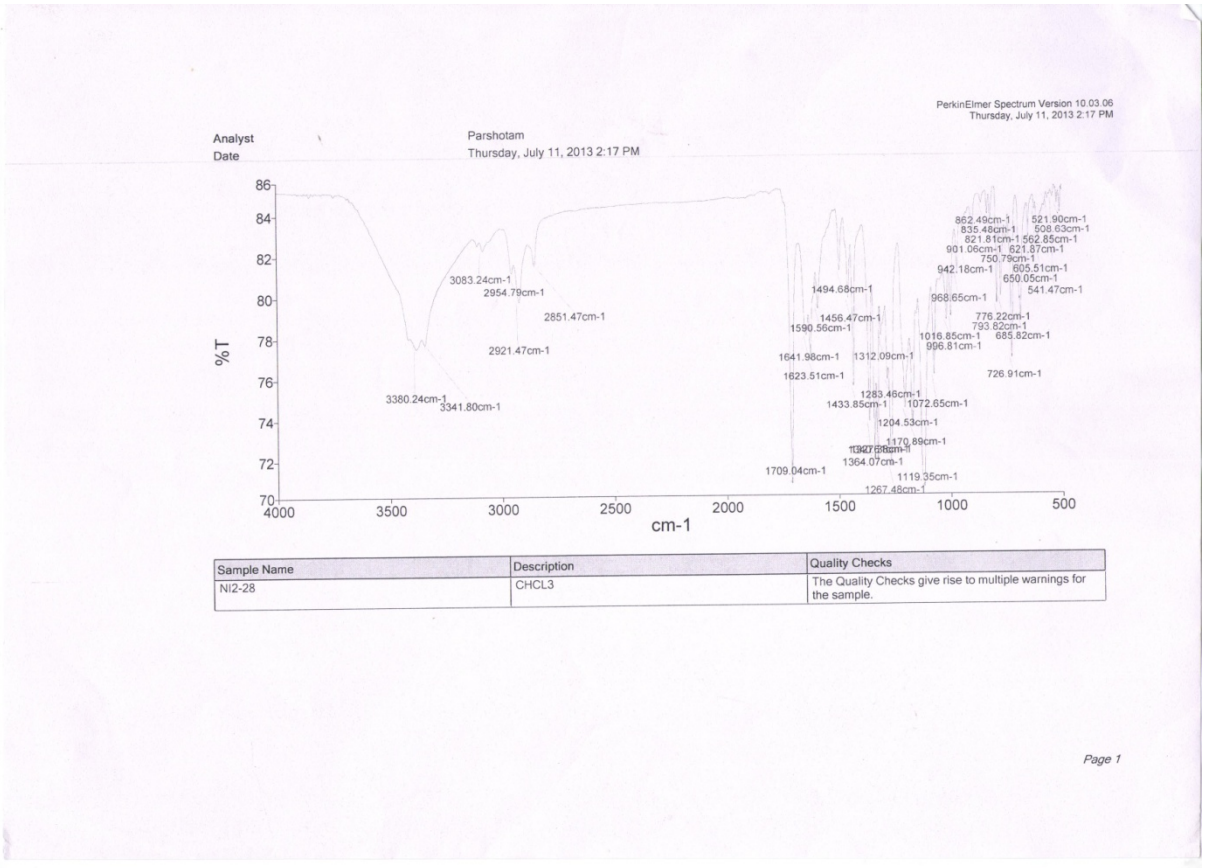
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
399.0954	1	935851.56	C21 H14 F3 N2 O3	(M+H)+
400.0985	1	200702.89	C21 H14 F3 N2 O3	(M+H)+
401.1011	1	27222.68	C21 H14 F3 N2 O3	(M+H)+
402.104	1	4262.1	C21 H14 F3 N2 O3	(M+H)+
421.0772	1	191706.66	C21 H13 F3 N2 Na O3	(M+Na)+
422.0803	1	41597.26	C21 H13 F3 N2 Na O3	(M+Na)+
423.0829	1	6923.52	C21 H13 F3 N2 Na O3	(M+Na)+
819.1653	1	84361.56	C42 H26 F6 N4 Na O6	(2M+Na)+
820.1684	1	36561.13	C42 H26 F6 N4 Na O6	(2M+Na)+
821.1705	1	10565.38	C42 H26 F6 N4 Na O6	(2M+Na)+

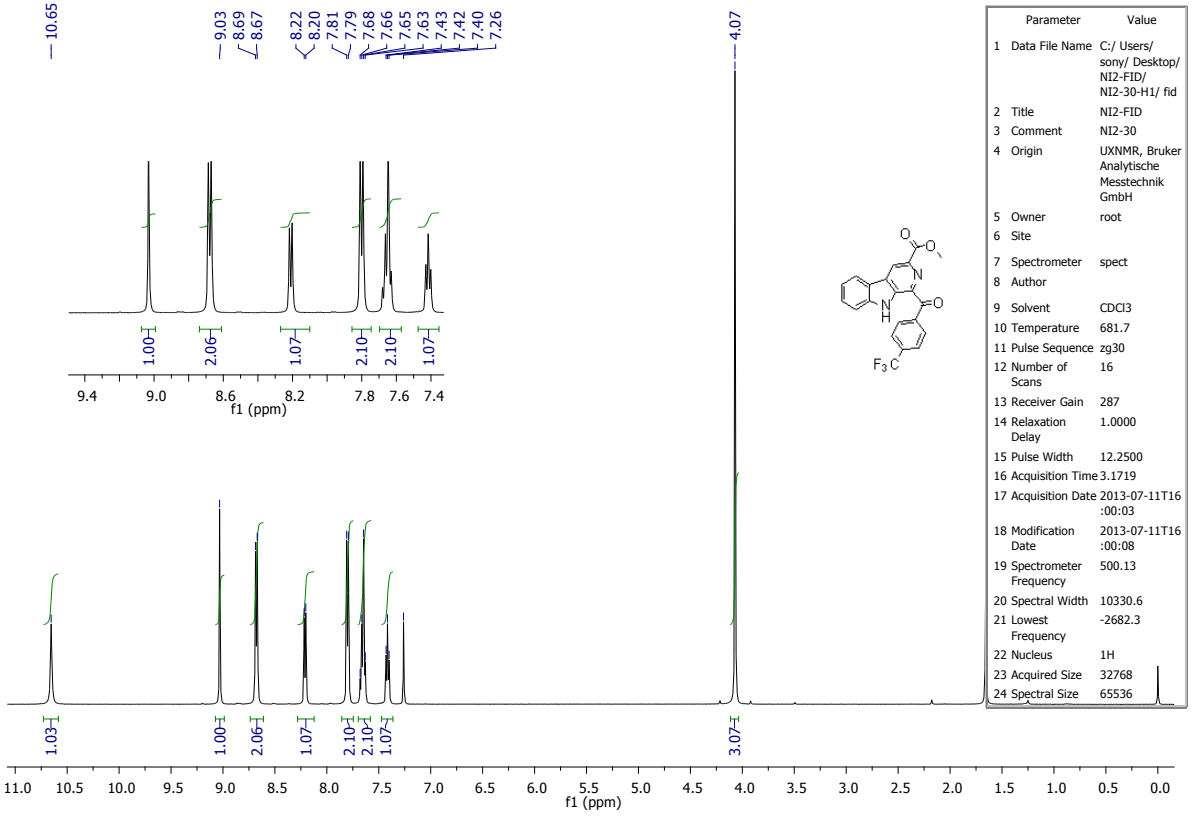
Predicted Isotope Match Table

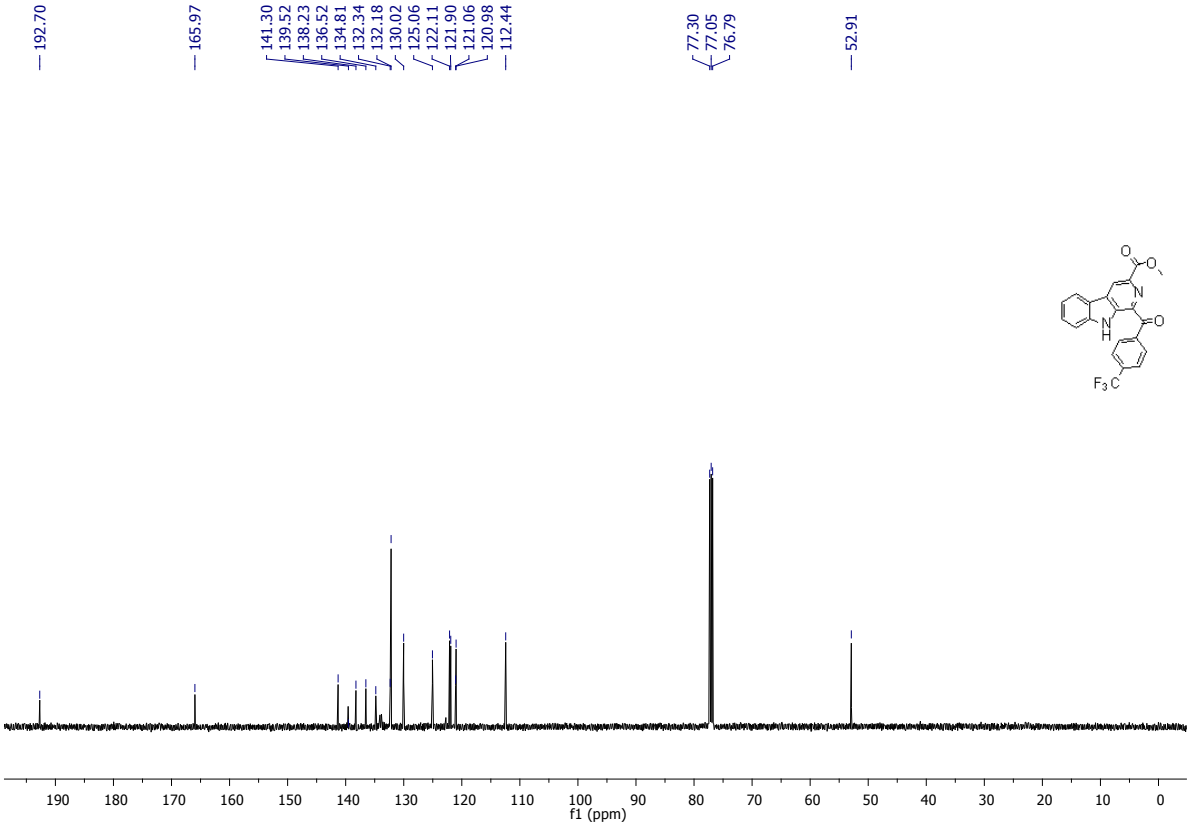
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	399.0954	399.0951	-0.82	100	100	80.09	78.5
2	400.0985	400.0983	-0.6	21.45	23.72	17.18	18.62
3	401.1011	401.1011	0	2.91	3.31	2.33	2.59
4	402.104	402.1037	-0.69	0.46	0.34	0.36	0.27
5	403.1029	403.1064	8.61	0.04	0.03	0.03	0.02

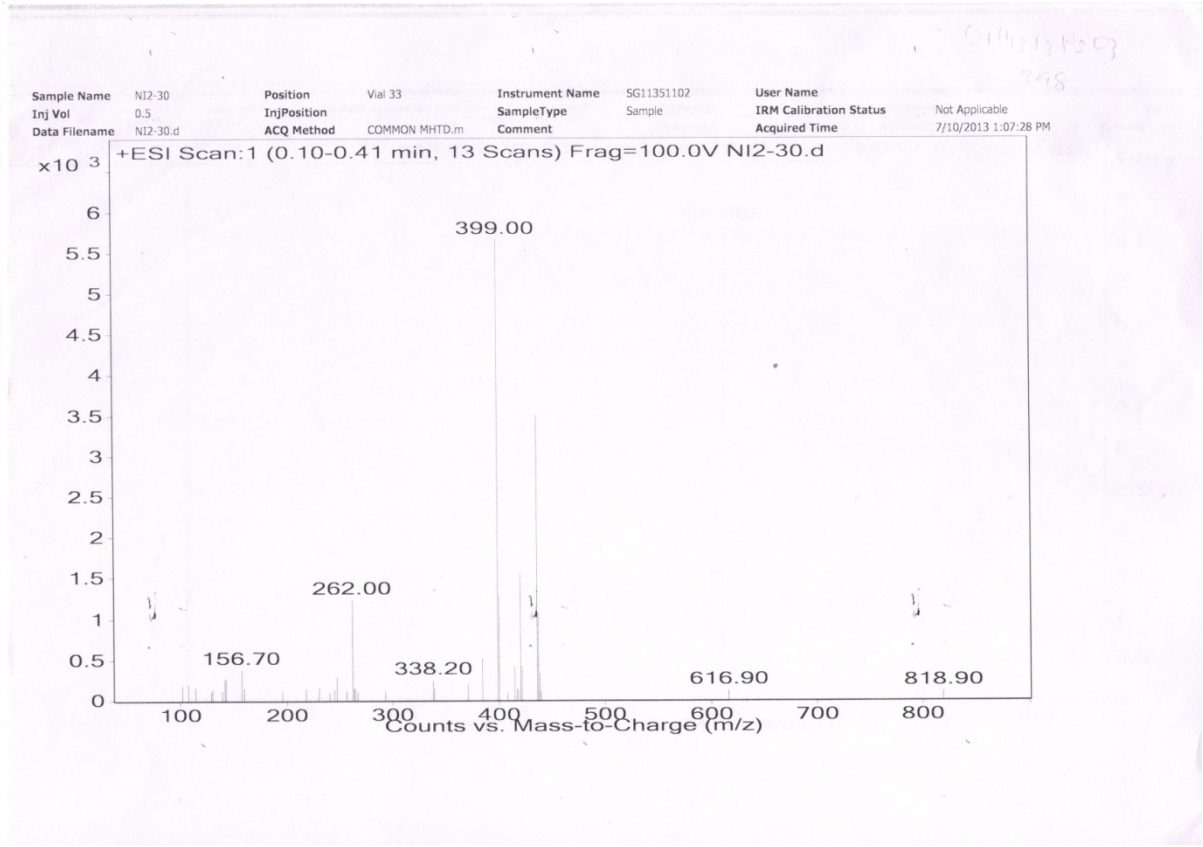
--- End Of Report ---



3s) Methyl 1-(4-(trifluoromethyl)benzoyl)- 9H-*β*-carboline-3-carboxylate:




192.70
165.97
141.30
139.52
138.23
136.52
134.81
132.34
132.18
130.02
125.06
122.11
121.90
121.06
120.98
112.44
77.30
77.05
76.79
52.91
O
O
N
H
O
F3C
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Sample Name NI2-30
Inj Vol 0.5
Data Filename NI2-30.d
Position Vial 33
InjPosition
ACQ Method COMMON MHTD.m
Instrument Name SG11351102
SampleType Sample
Comment
User Name
IRM Calibration Status Not Applicable
Acquired Time 7/10/2013 1:07:28 PM
+ESI Scan:1 (0.10-0.41 min, 13 Scans) Frag=100.0V NI2-30.d
x10 3
399.00
262.00
156.70
338.20
616.90
818.90
Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

Data File	NI2-30.d	**Sample Name**	NI2-30
Sample Type	Sample	**Position**	Vial 35
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	11-07-2013 PM 3:40:05
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

Sample Group **Info.**

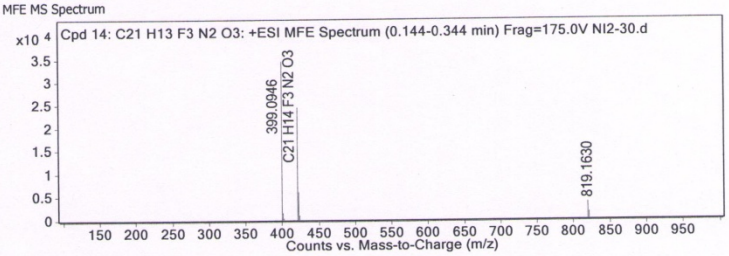
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 14: C21 H13 F3 N2 O3	0.196	398.0876	C21 H13 F3 N2 O3	C21 H13 F3 N2 O3	0.56	C21 H13 F3 N2 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 14: C21 H13 F3 N2 O3	399.0946	0.196	Find by Molecular Feature	398.0876

MFE MS Spectrum



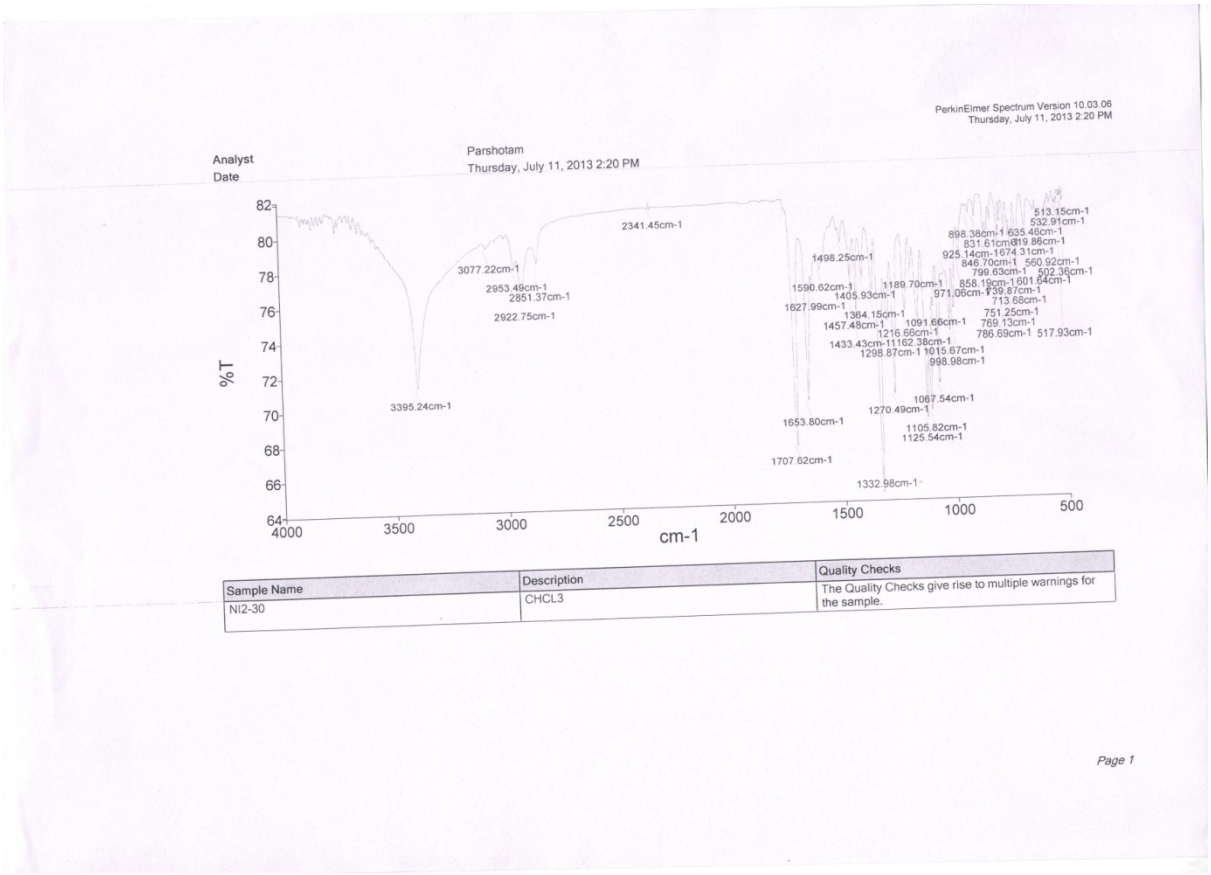
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
399.0946	1	34564.29	C21 H14 F3 N2 O3	(M+H)+
400.0987	1	7225.81	C21 H14 F3 N2 O3	(M+H)+
401.1022	1	1645.52	C21 H14 F3 N2 O3	(M+H)+
402.1096	1	312.49	C21 H14 F3 N2 O3	(M+H)+
421.0765	1	24435.17	C21 H13 F3 N2 Na O3	(M+Na)+
422.0802	1	6034.57	C21 H13 F3 N2 Na O3	(M+Na)+
423.0825	1	959.37	C21 H13 F3 N2 Na O3	(M+Na)+
819.163	1	3615.62		(2M+Na)+
820.1678	1	1570.52		(2M+Na)+
821.1719	1	534.81		(2M+Na)+

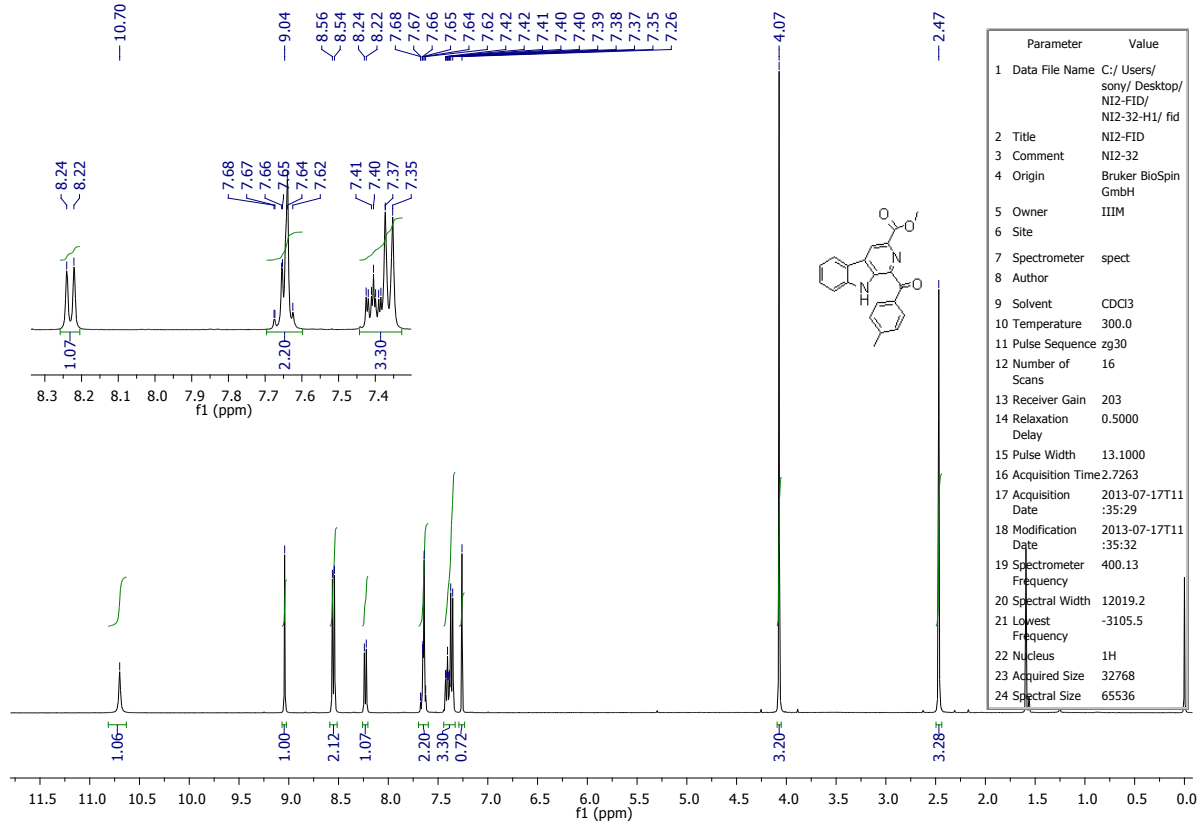
Predicted Isotope Match Table

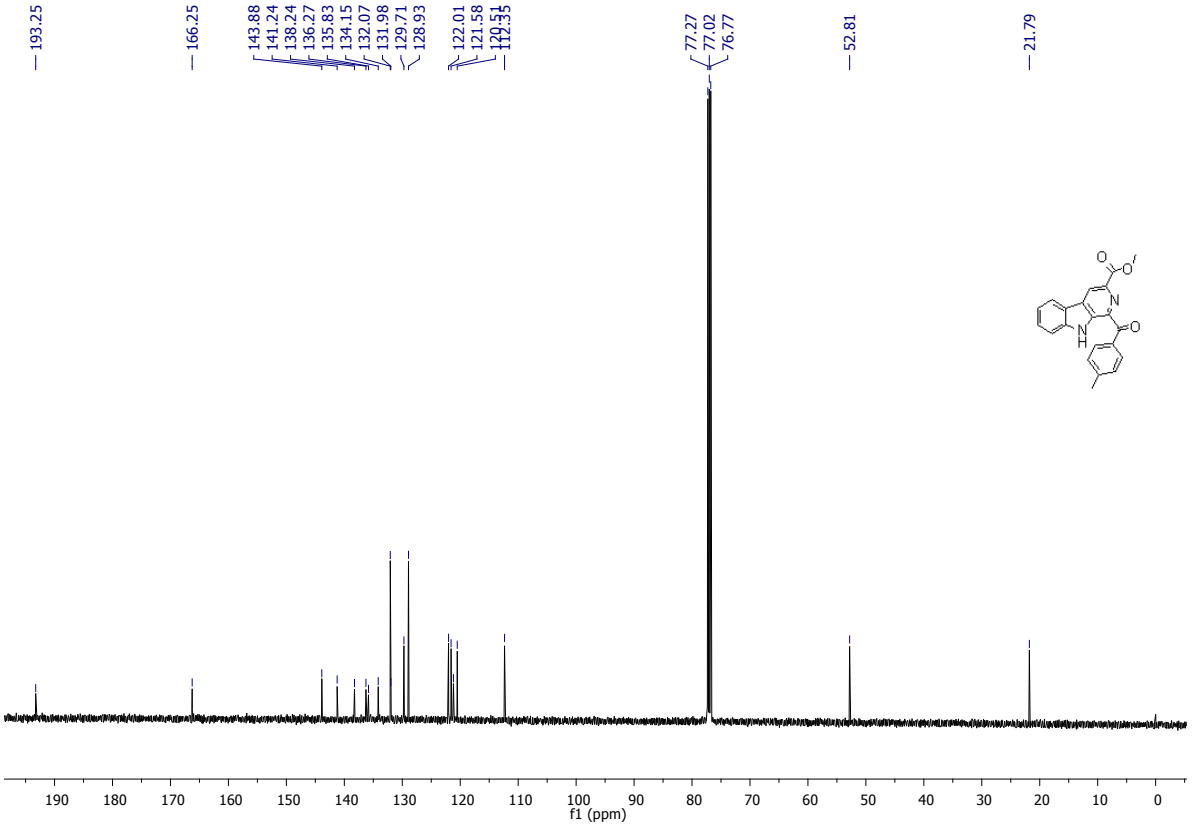
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	399.0946	399.0951	1.19	100	100	79.01	78.52
2	400.0987	400.0983	-1.04	20.91	23.72	16.52	18.62
3	401.1022	401.1011	-2.8	4.76	3.31	3.76	2.6
4	402.1096	402.1037	-14.66	0.9	0.34	0.71	0.27

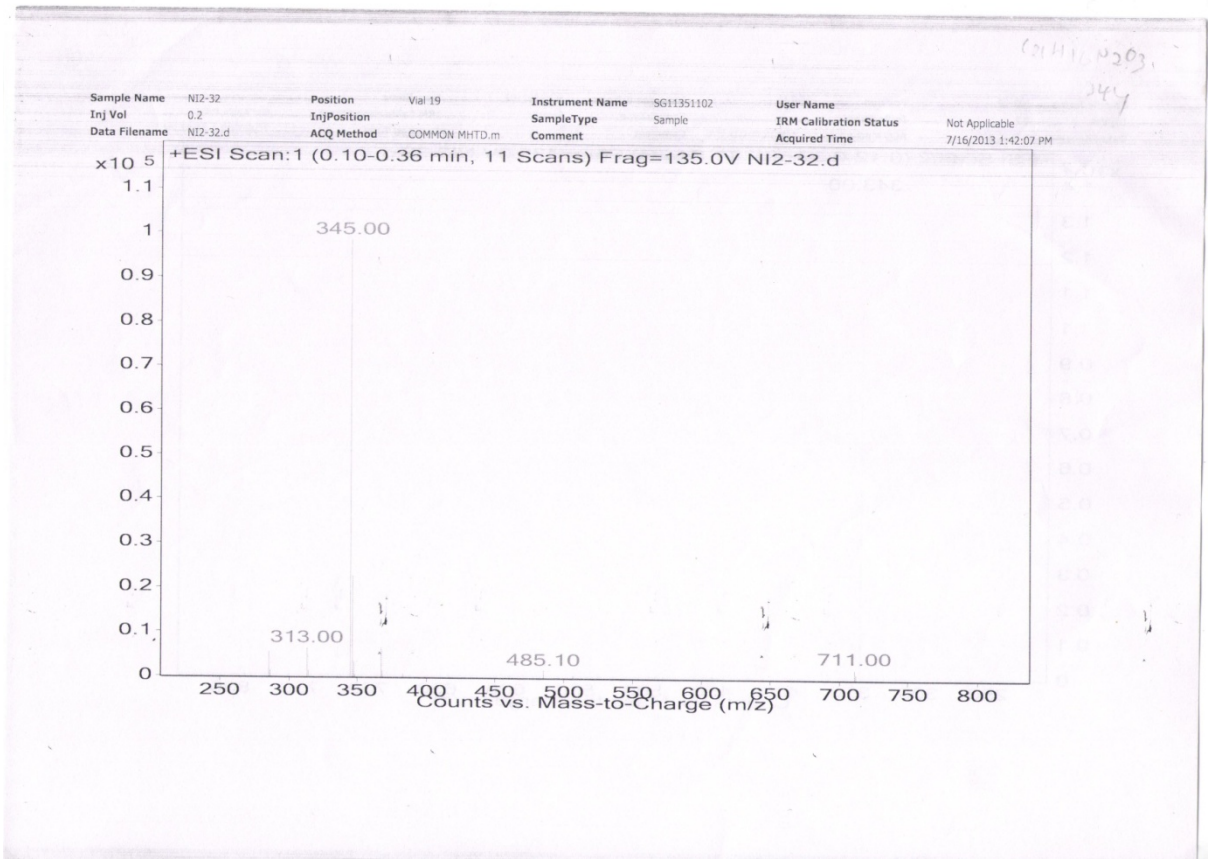
--- End Of Report ---



3t) Methyl 1-(4-methylbenzoyl)-9H-*β*-carboline-3-carboxylate:




193.25
166.25
143.88
141.24
138.24
136.27
135.83
134.15
132.07
131.98
129.71
128.93
122.01
121.58
120.51
112.35
77.27
77.02
76.77
52.81
21.79
O
O
N
N
H
O
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


Sample Name NI2-32
Inj Vol 0.2
Data Filename NI2-32.d
Position Vial 19
InjPosition
ACQ Method COMMON MHTD.m
Instrument Name SG11351102
SampleType Sample
Comment
User Name
IRM Calibration Status Not Applicable
Acquired Time 7/16/2013 1:42:07 PM
+ESI Scan:1 (0.10-0.36 min, 11 Scans) Frag=135.0V NI2-32.d
x10 5
345.00
313.00
485.10
711.00
Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

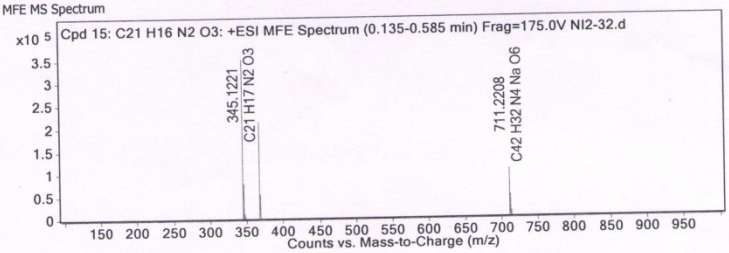
Data File	NI2-32.d	**Sample Name**	Unavailable
Sample Type	Unavailable	**Position**	Unavailable
Instrument Name	Unavailable	**User Name**	Unavailable
Acq Method		**Acquired Time**	Unavailable
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment	Sample information is unavailable		

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 15: C21 H16 N2 O3	0.195	344.1148	C21 H16 N2 O3	C21 H16 N2 O3	3.77	C21 H16 N2 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 15: C21 H16 N2 O3	345.1221	0.195	Find by Molecular Feature	344.1148

MFE MS Spectrum



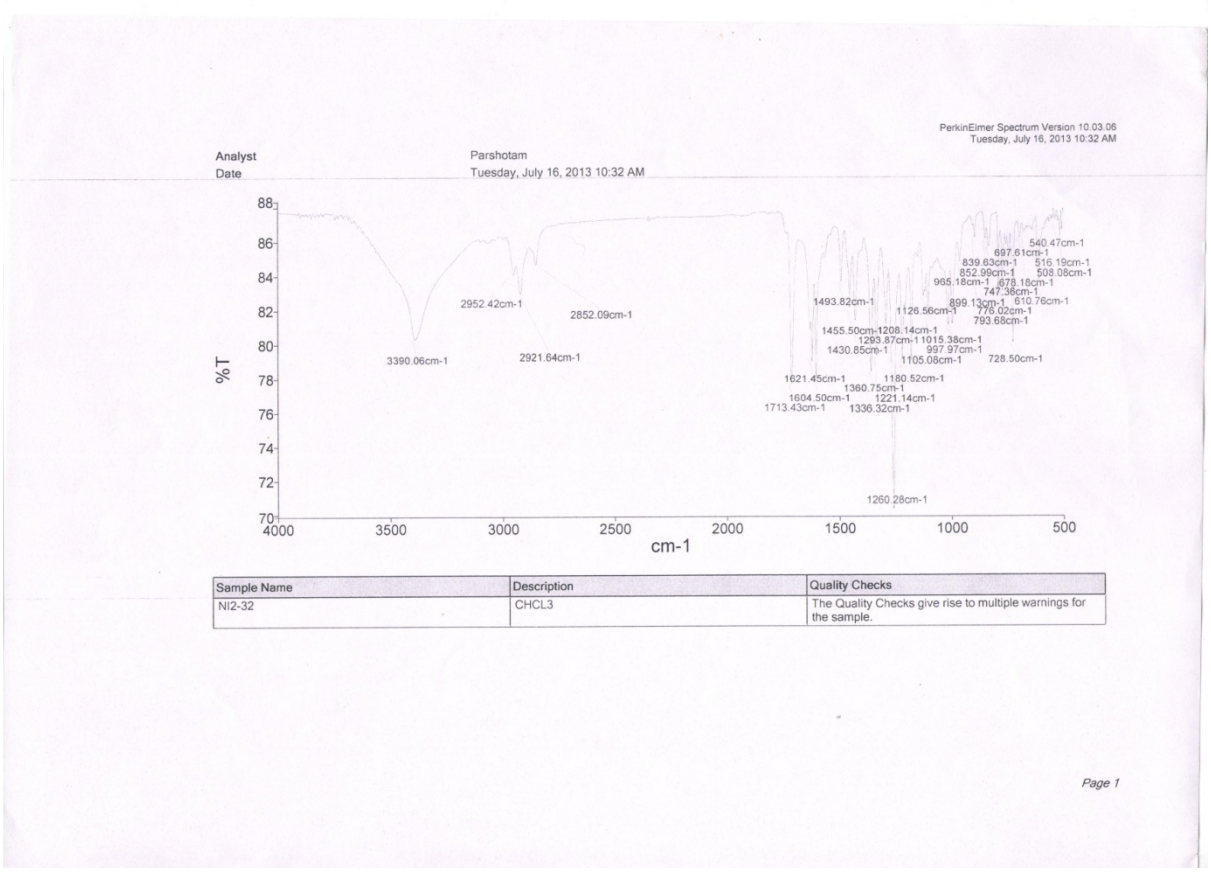
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
345.1221	1	352047.44	C21 H17 N2 O3	(M+H)+
346.125	1	78272.8	C21 H17 N2 O3	(M+H)+
347.1274	1	10790.16	C21 H17 N2 O3	(M+H)+
367.1037	1	213320.33	C21 H16 N2 Na O3	(M+Na)+
368.1068	1	53848.11	C21 H16 N2 Na O3	(M+Na)+
369.1097	1	6764.57	C21 H16 N2 Na O3	(M+Na)+
711.2208	1	106376.54	C42 H32 N4 Na O6	(2M+Na)+
712.2234	1	48771.91	C42 H32 N4 Na O6	(2M+Na)+
713.2269	1	12482	C42 H32 N4 Na O6	(2M+Na)+
714.2285	1	2365.49	C42 H32 N4 Na O6	(2M+Na)+

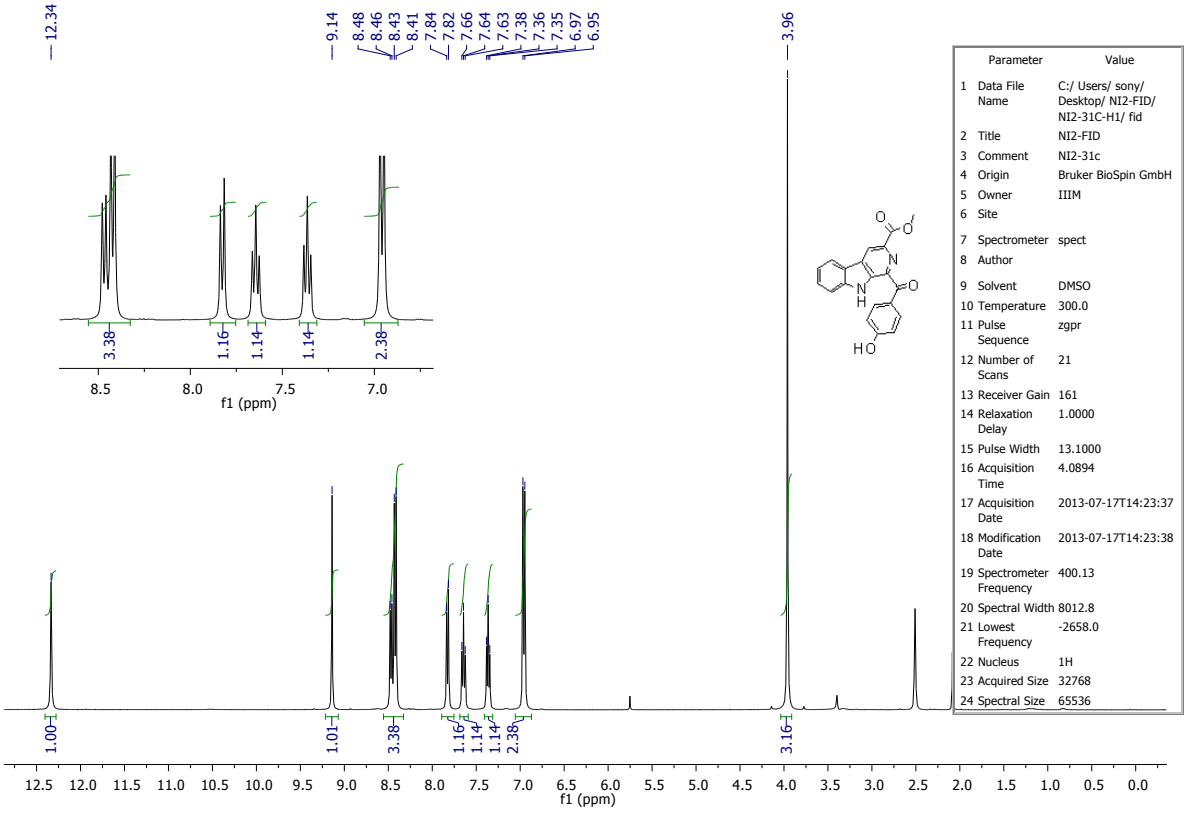
Predicted Isotope Match Table

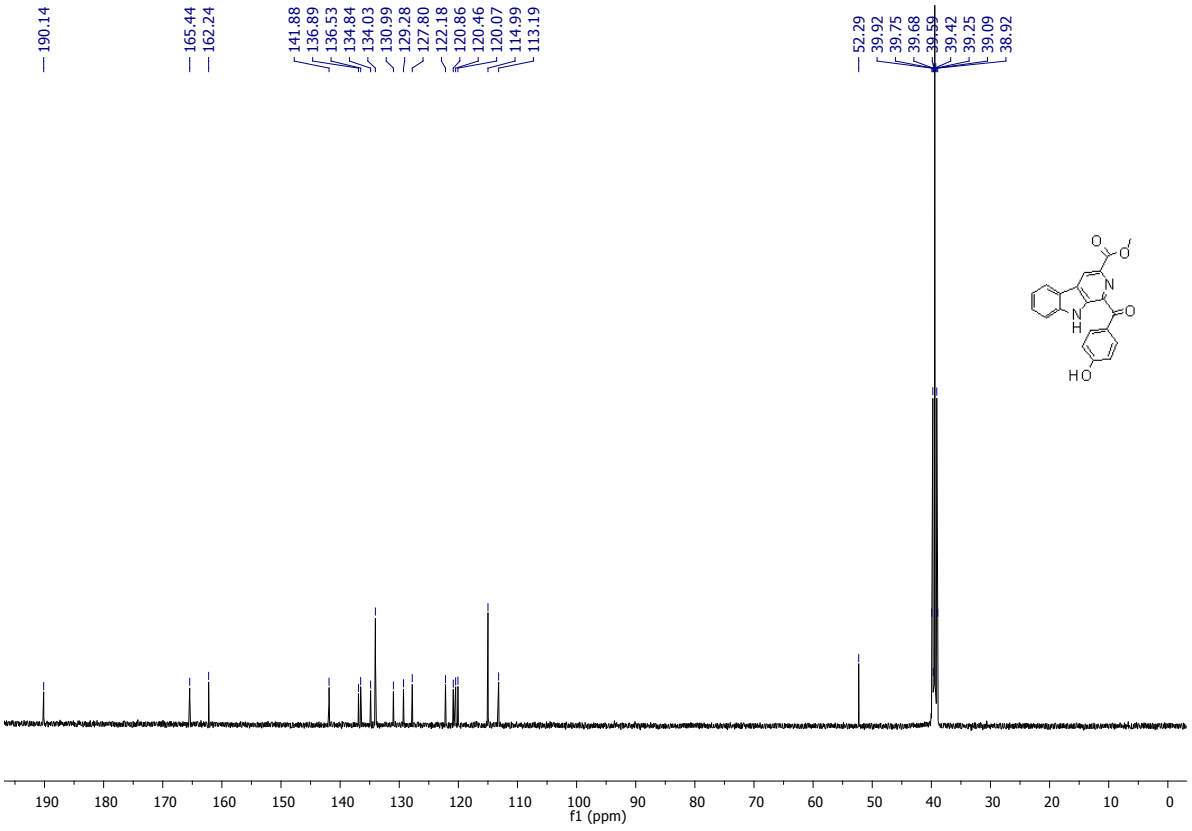
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	345.1221	345.1234	3.54	100	100	79.49	78.49
2	346.125	346.1266	4.38	22.23	23.75	17.67	18.64
3	347.1274	347.1293	5.47	3.06	3.31	2.44	2.6
4	348.1289	348.132	9.05	0.51	0.34	0.4	0.27

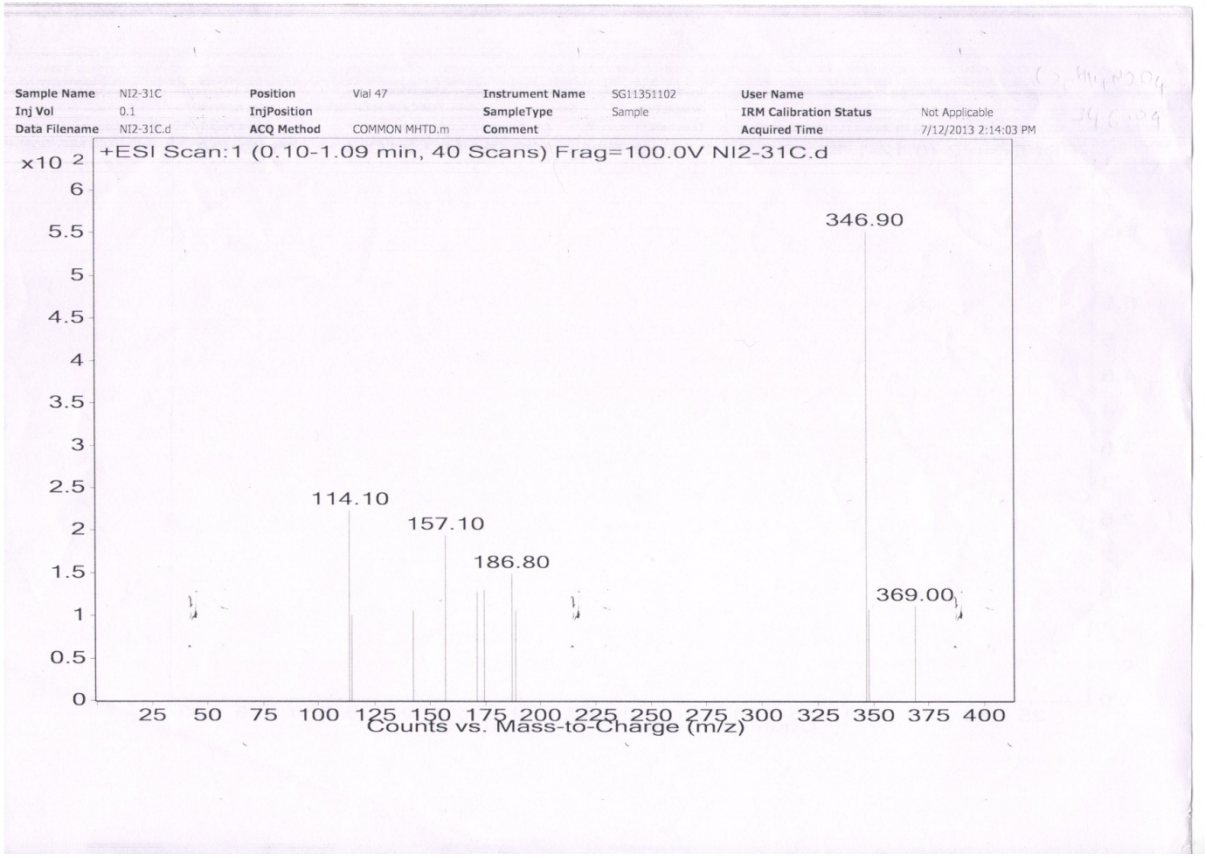
--- End Of Report ---



3u) Methyl 1-(4-hydroxybenzoyl)-9H-*β*-carboline-3-carboxylate:




190.14
165.44
162.24
141.88
136.89
136.53
134.84
134.03
130.99
129.28
127.80
122.18
120.86
120.46
120.07
114.99
113.19
52.29
39.92
39.75
39.68
39.59
39.42
39.25
39.09
38.92
O
O
N
N
H
O
HO
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


Sample Name NI2-31C
Position Vial 47
Instrument Name SG11351102
User Name
Inj Vol 0.1
InjPosition
SampleType Sample
IRM Calibration Status Not Applicable
Data Filename NI2-31C.d
ACQ Method COMMON MHTD.m
Comment
Acquired Time 7/12/2013 2:14:03 PM
+ESI Scan:1 (0.10-1.09 min, 40 Scans) Frag=100.0V NI2-31C.d
x10 2
6
5.5
5
4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
346.90
114.10
157.10
186.80
369.00
25 50 75 100 125 150 175 200 225 250 275 300 325 350 375 400
Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

Data File	NI2-31C.d	**Sample Name**	NI2-31C
Sample Type	Sample	**Position**	Vial 41
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	16-07-2013 PM 1:32:13
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

Info.

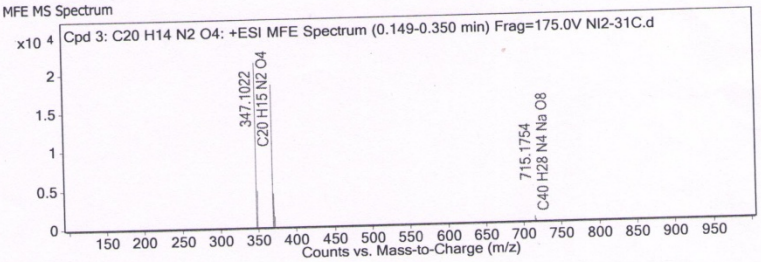
Sample Group	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 3: C20 H14 N2 O4	0.194	346.095	C20 H14 N2 O4	C20 H14 N2 O4	1.11	C20 H14 N2 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 3: C20 H14 N2 O4	347.1022	0.194	Find by Molecular Feature	346.095

MFE MS Spectrum



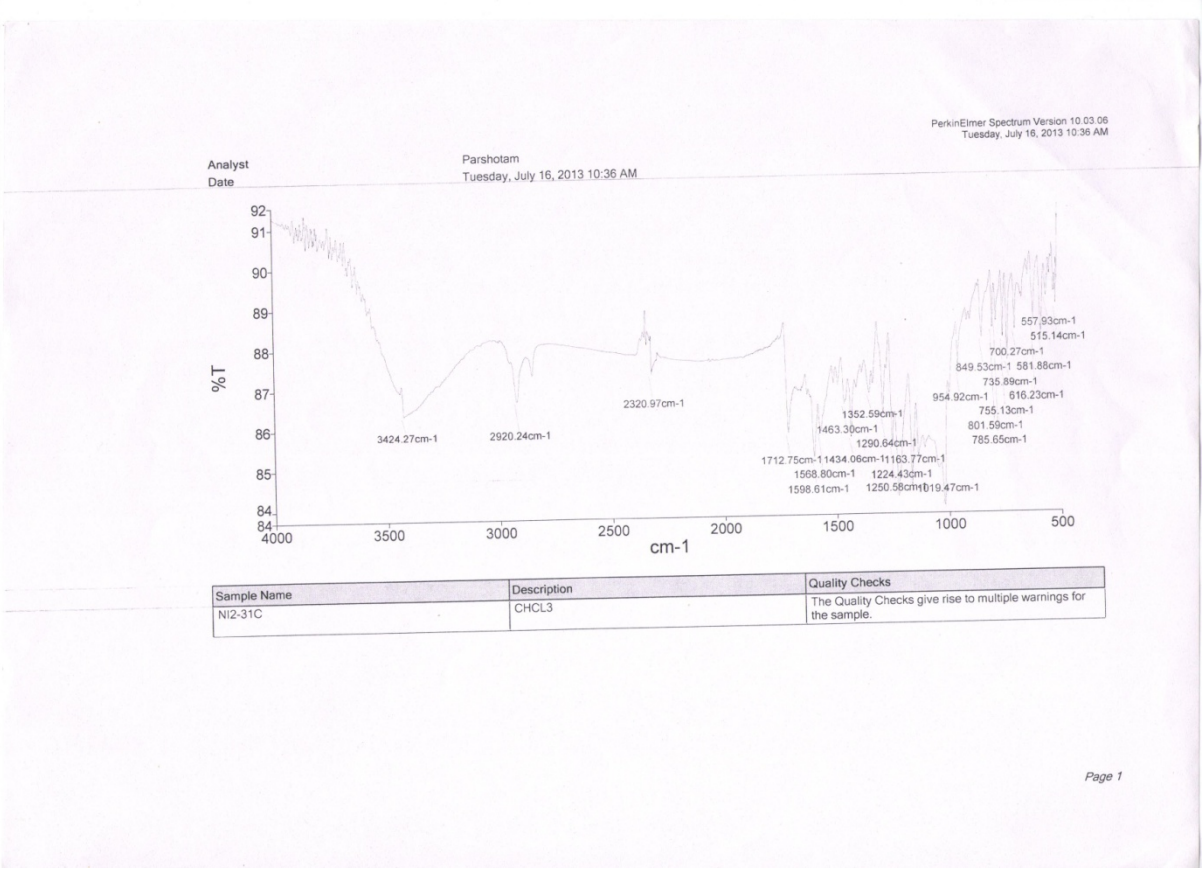
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
347.1022	1	21388.99	C20 H15 N2 O4	(M+H)+
348.1056	1	4732.7	C20 H15 N2 O4	(M+H)+
349.109	1	1111.43	C20 H15 N2 O4	(M+H)+
369.0845	1	18445.39	C20 H14 N2 Na O4	(M+Na)+
370.0878	1	4346.04	C20 H14 N2 Na O4	(M+Na)+
371.0933	1	1275.32	C20 H14 N2 Na O4	(M+Na)+
715.1754	1	578.75	C40 H28 N4 Na O8	(2M+Na)+
716.1872	1	301.32	C40 H28 N4 Na O8	(2M+Na)+

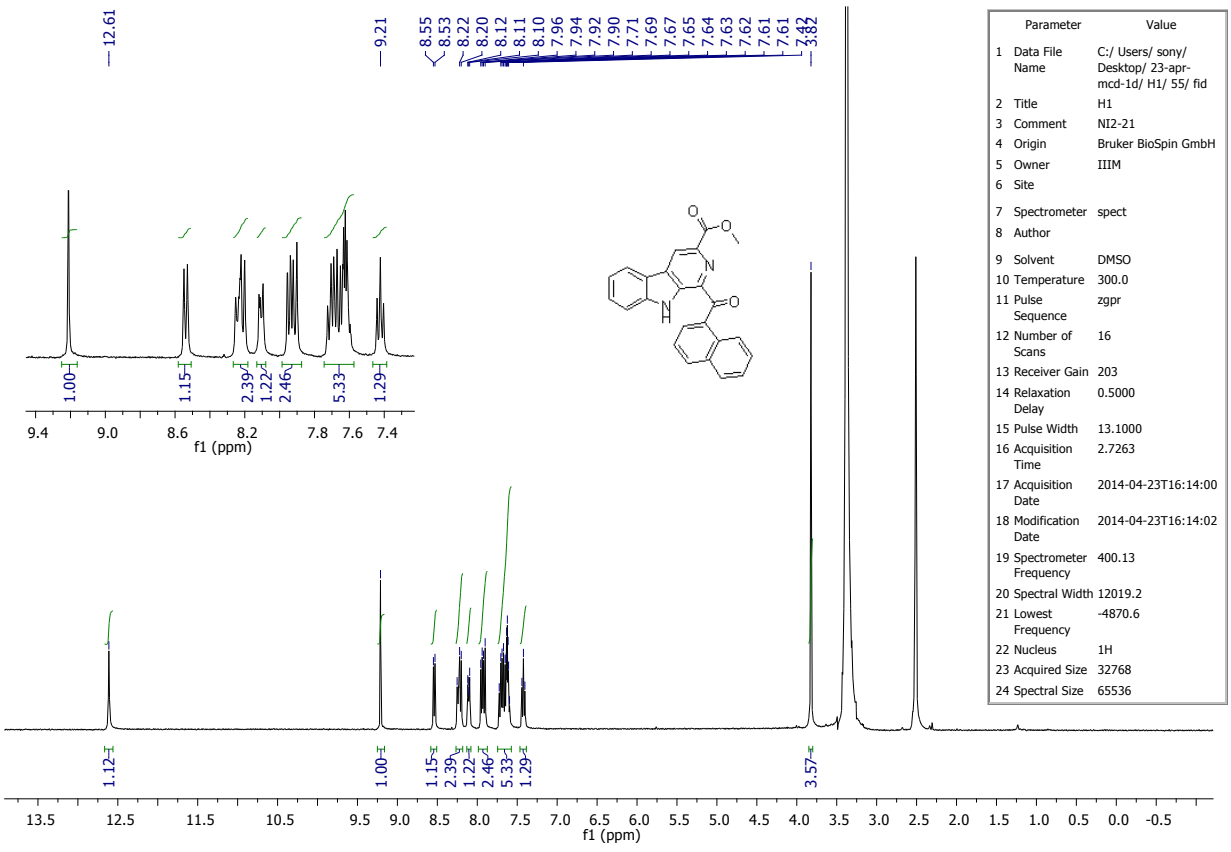
Predicted Isotope Match Table

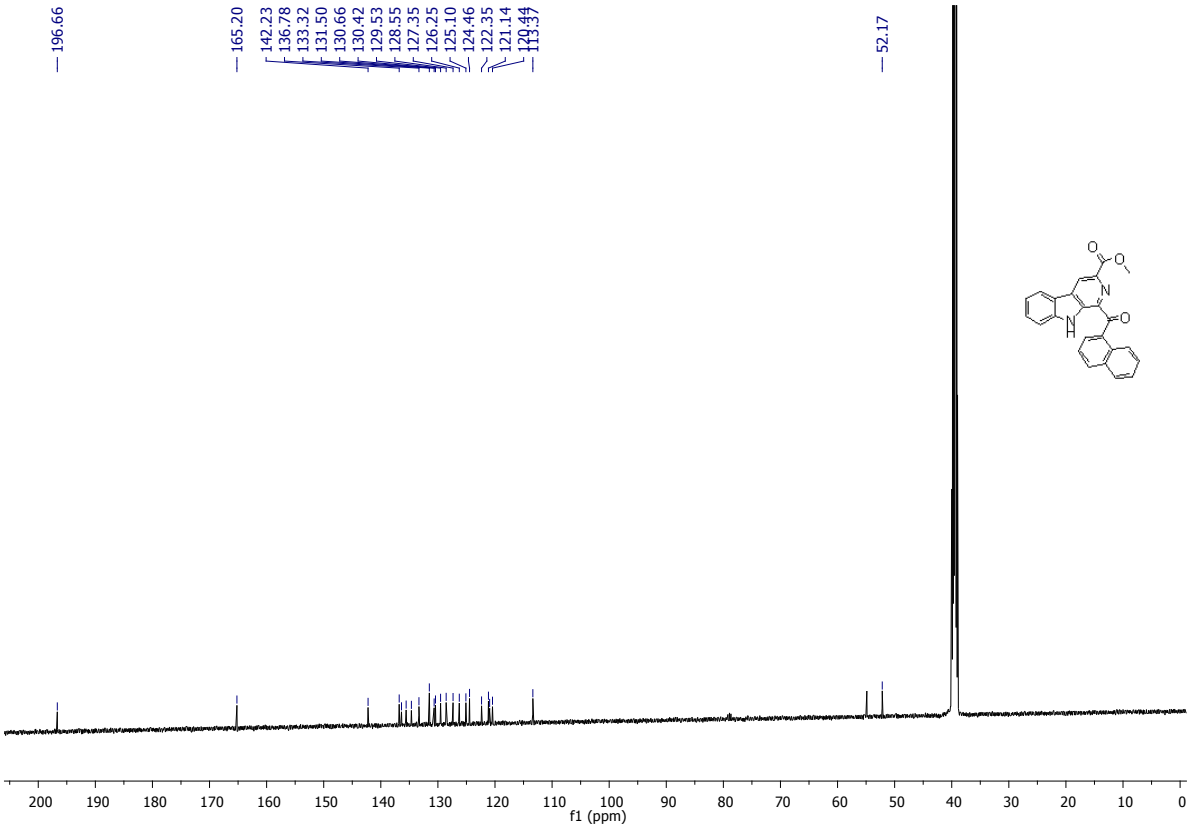
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	347.1022	347.1026	1.35	100	100	78.54	79.39
2	348.1056	348.1058	0.59	22.13	22.69	17.38	18.01
3	349.109	349.1085	-1.52	5.2	3.28	4.08	2.6

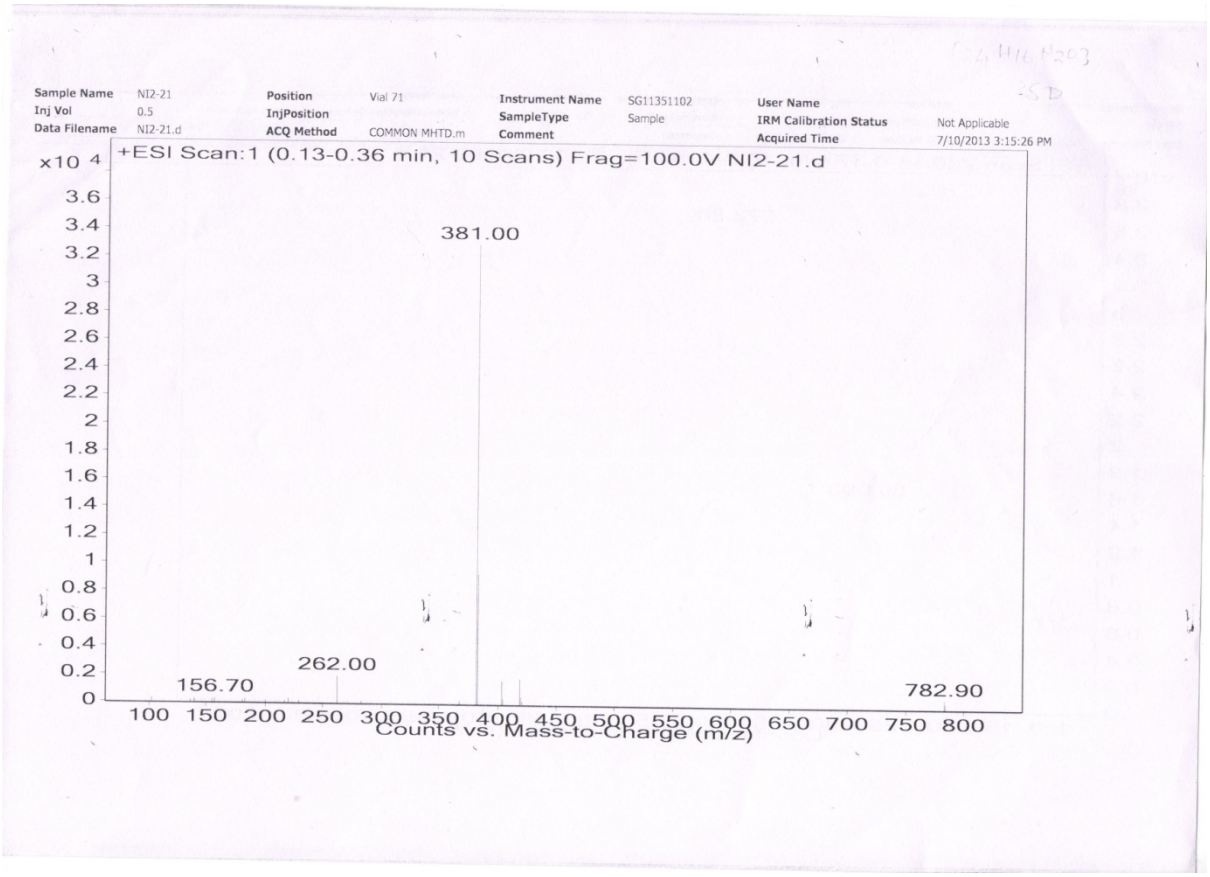
--- End Of Report ---



3v) Methyl 1-(1-naphthoyl)-9H-*β*-carboline-3-carboxylate:




196.66
165.20
142.23
136.78
133.32
131.50
130.66
130.42
129.53
128.55
127.35
126.25
125.10
124.46
122.35
121.14
120.44
113.37
52.17
O
O
N
H
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


Sample Name NI2-21
Inj Vol 0.5
Data Filename NI2-21.d
Position Vial 71
InjPosition
ACQ Method COMMON MHTD.m
Instrument Name SG11351102
SampleType Sample
Comment
User Name
IRM Calibration Status Not Applicable
Acquired Time 7/10/2013 3:15:26 PM
+ESI Scan:1 (0.13-0.36 min, 10 Scans) Frag=100.0V NI2-21.d
x10 4
3.6
3.4
3.2
3
2.8
2.6
2.4
2.2
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
381.00
262.00
156.70
782.90
100 150 200 250 300 350 400 450 500 550 600 650 700 750 800
Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

Data File	NI2-21.d	**Sample Name**	NI2-21
Sample Type	Sample	**Position**	Vial 38
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	11-07-2013 PM 3:50:40
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

Info.

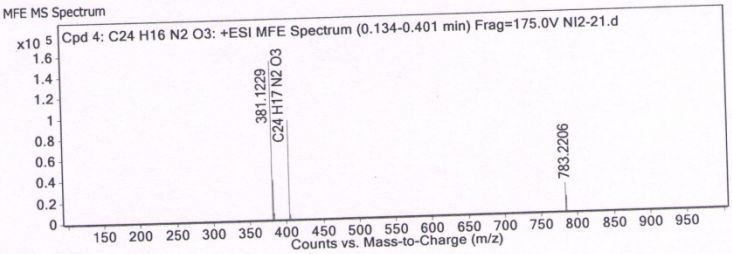
Sample Group	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C24 H16 N2 O3	0.195	380.1156	C24 H16 N2 O3	C24 H16 N2 O3	1.4	C24 H16 N2 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 4: C24 H16 N2 O3	381.1229	0.195	Find by Molecular Feature	380.1156

MFE MS Spectrum



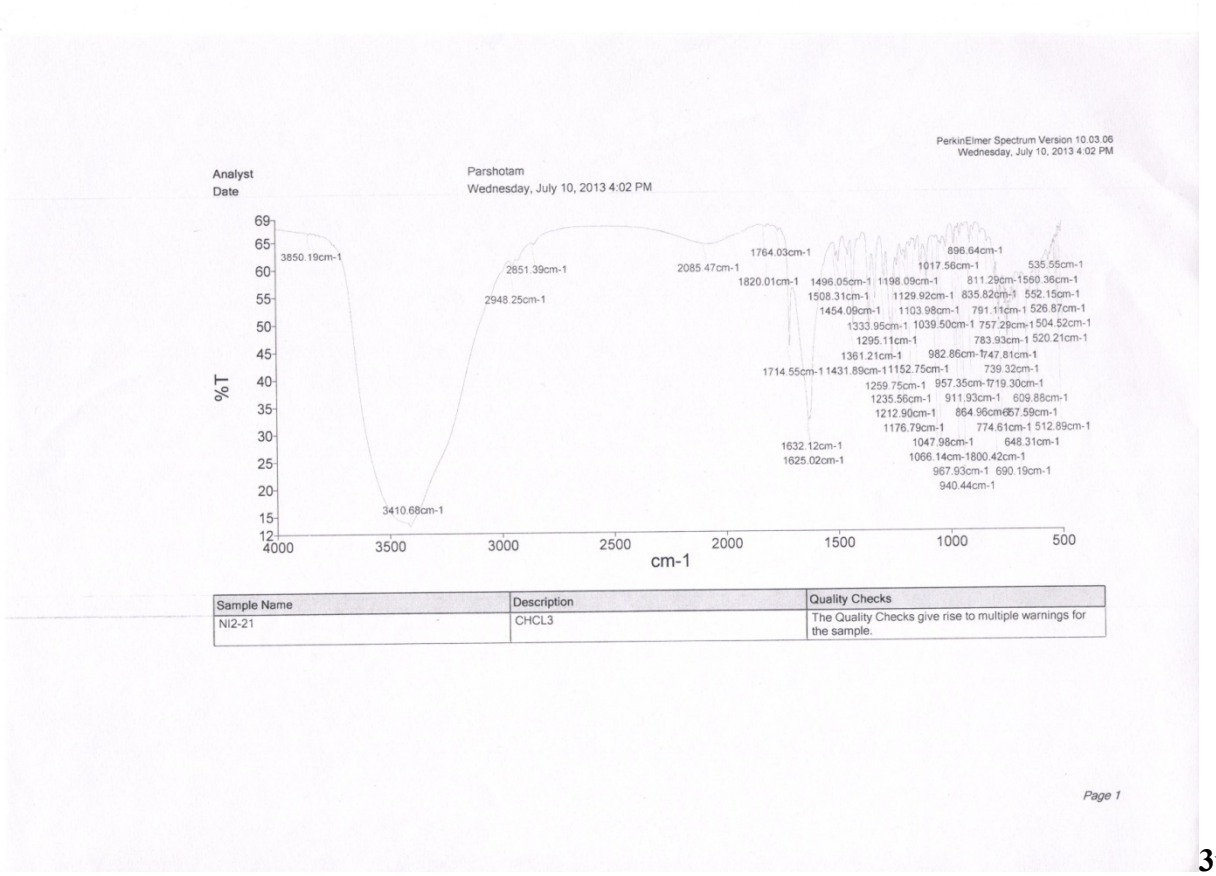
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
381.1229	1	152075.69	C24 H17 N2 O3	(M+H)+
382.126	1	37499.38	C24 H17 N2 O3	(M+H)+
383.1283	1	6311.75	C24 H17 N2 O3	(M+H)+
403.1048	1	94302.7	C24 H16 N2 Na O3	(M+Na)+
404.1079	1	27594.26	C24 H16 N2 Na O3	(M+Na)+
405.1113	1	4267.79	C24 H16 N2 Na O3	(M+Na)+
783.2206	1	26672.13		(2M+Na)+
784.2227	1	14668.57		(2M+Na)+
785.2261	1	4559.12		(2M+Na)+
786.2327	1	881.01		(2M+Na)+

Predicted Isotope Match Table

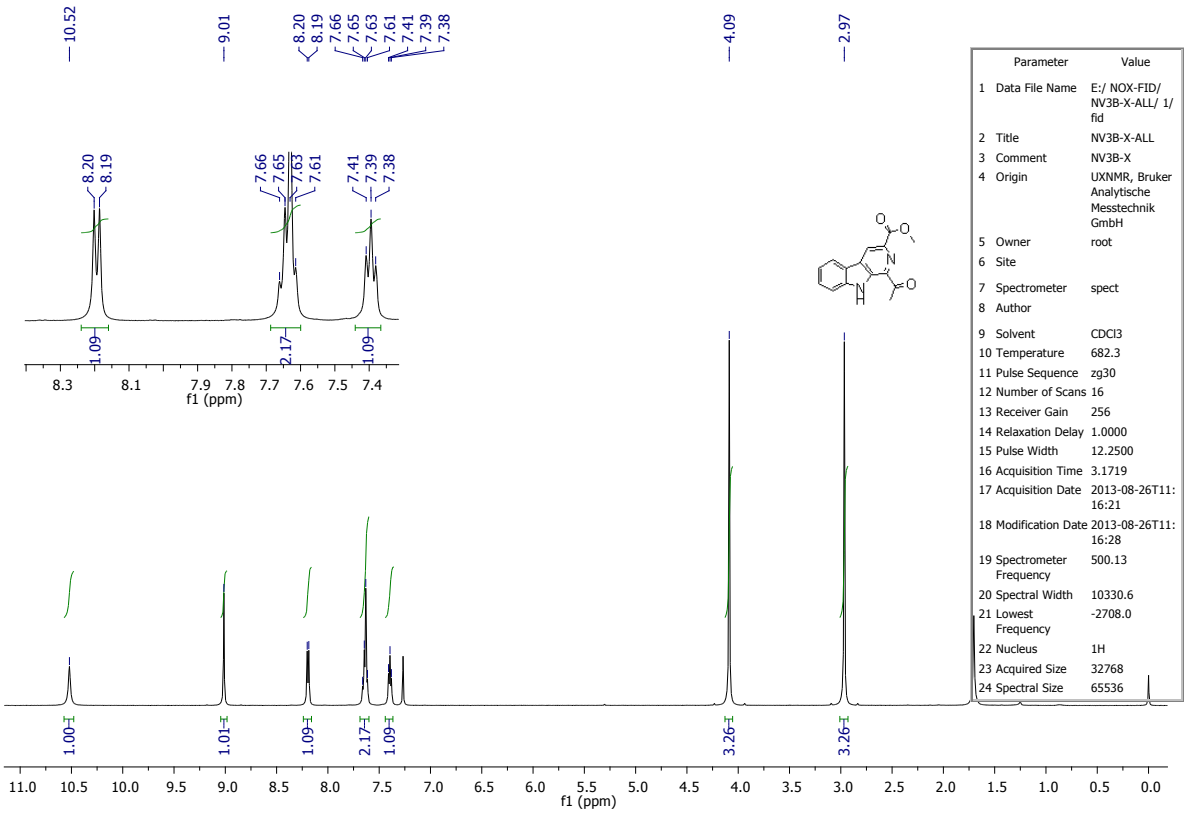
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	381.1229	381.1234	1.32	100	100	77.41	76
2	382.126	382.1266	1.42	24.66	27	19.09	20.52
3	383.1283	383.1295	2.9	4.15	4.12	3.21	3.13
4	384.1306	384.1322	4.18	0.37	0.46	0.29	0.35

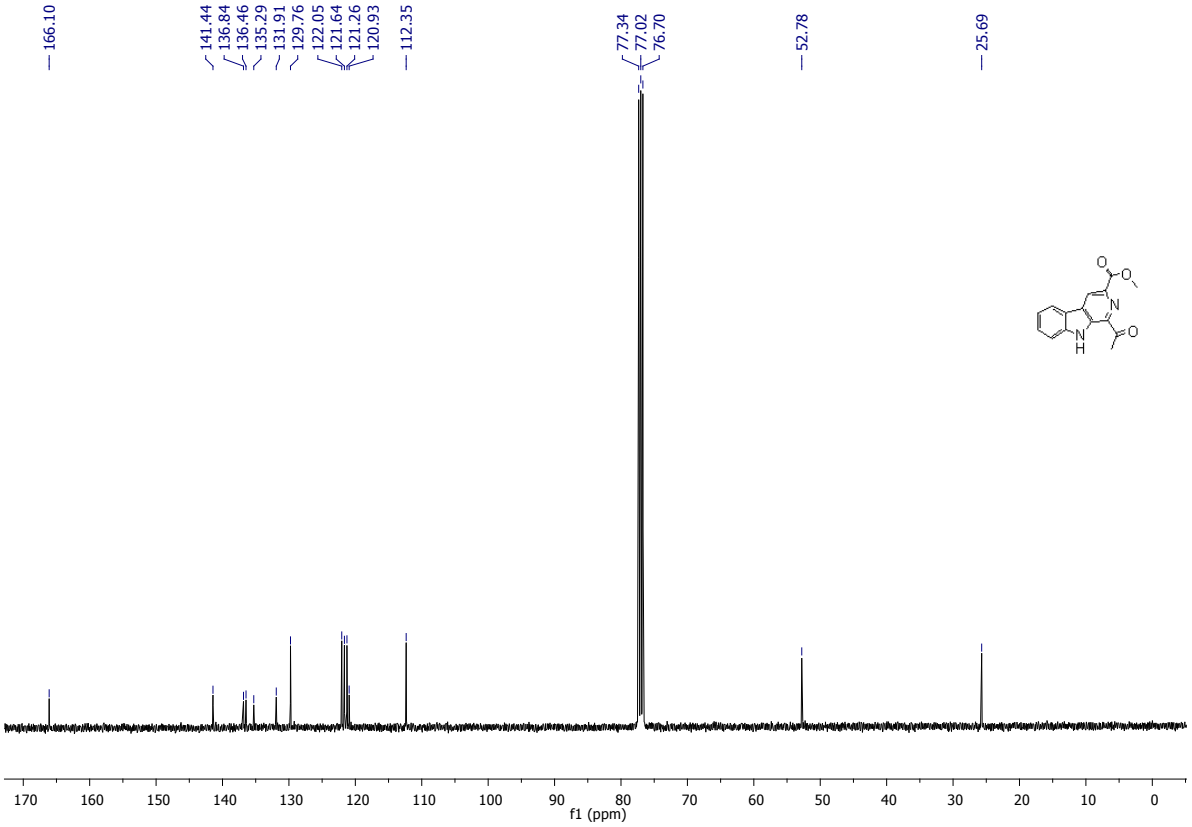
--- End Of Report ---

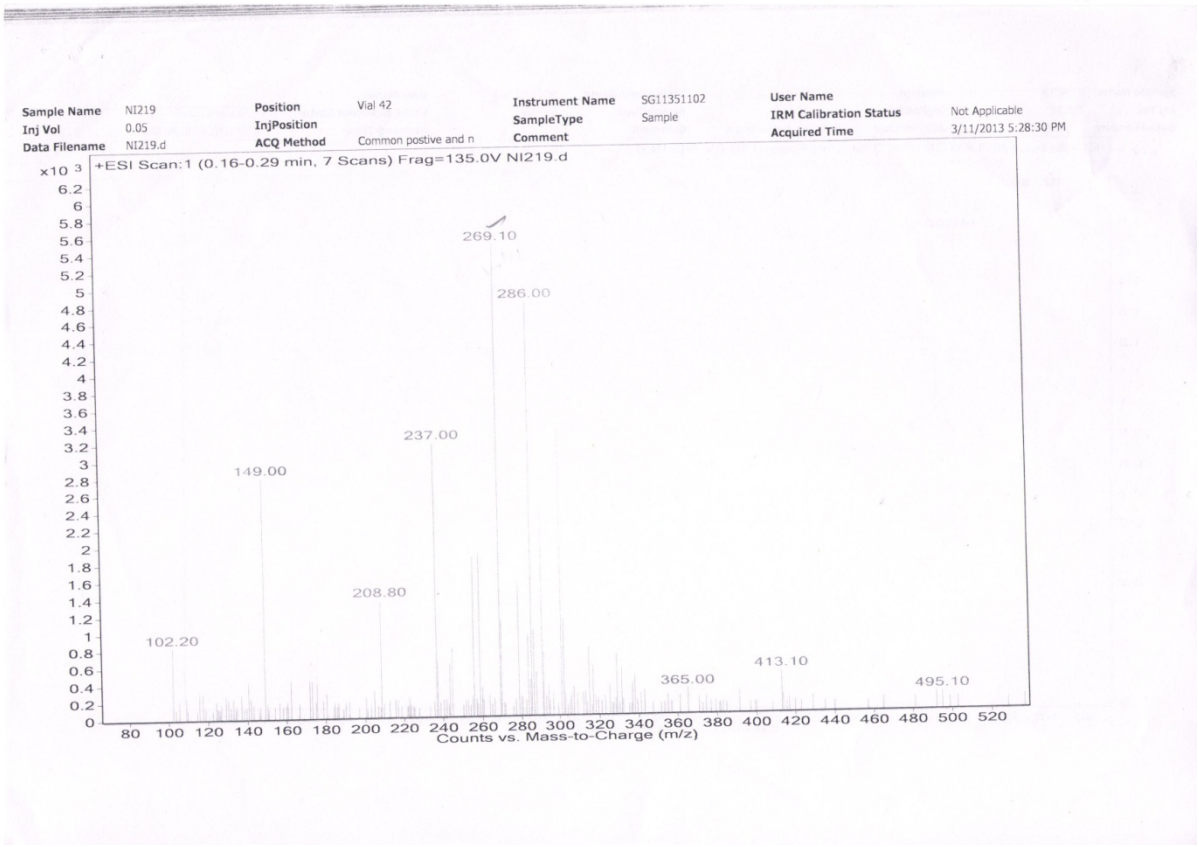


3w

) Methyl 1-acetyl-9H-*β*-carboline-3-carboxylate:




166.10
141.44
136.84
136.46
135.29
131.91
129.76
122.05
121.64
121.26
120.93
112.35
77.34
77.02
76.70
52.78
25.69
f1 (ppm)


Sample Name NI219
Inj Vol 0.05
Data Filename NI219.d
Position Vial 42
InjPosition
ACQ Method Common postive and n
Instrument Name SG11351102
SampleType Sample
Comment
User Name
IRM Calibration Status Not Applicable
Acquired Time 3/11/2013 5:28:30 PM
+ESI Scan:1 (0.16-0.29 min, 7 Scans) Frag=135.0V NI219.d
269.10
286.00
237.00
149.00
208.80
102.20
365.00
413.10
495.10
Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

Data File	NI2-19.d	**Sample Name**	NI2-19
Sample Type	Sample	**Position**	Vial 45
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	19-03-2013 PM 1:07:02
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			

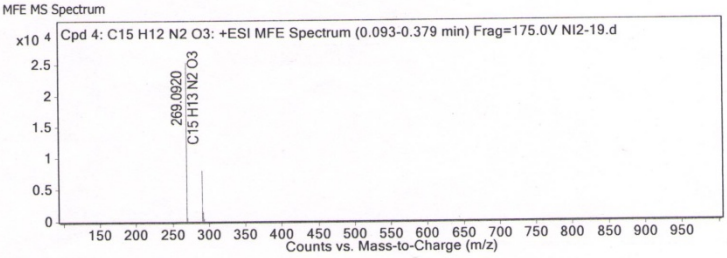
Sample Group		**Info.**	65:25(ACN:H20)
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C15 H12 N2 O3	0.185	268.0847	C15 H12 N2 O3	C15 H12 N2 O3	0.38	C15 H12 N2 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 4: C15 H12 N2 O3	269.092	0.185	Find by Molecular Feature	268.0847

MFE MS Spectrum



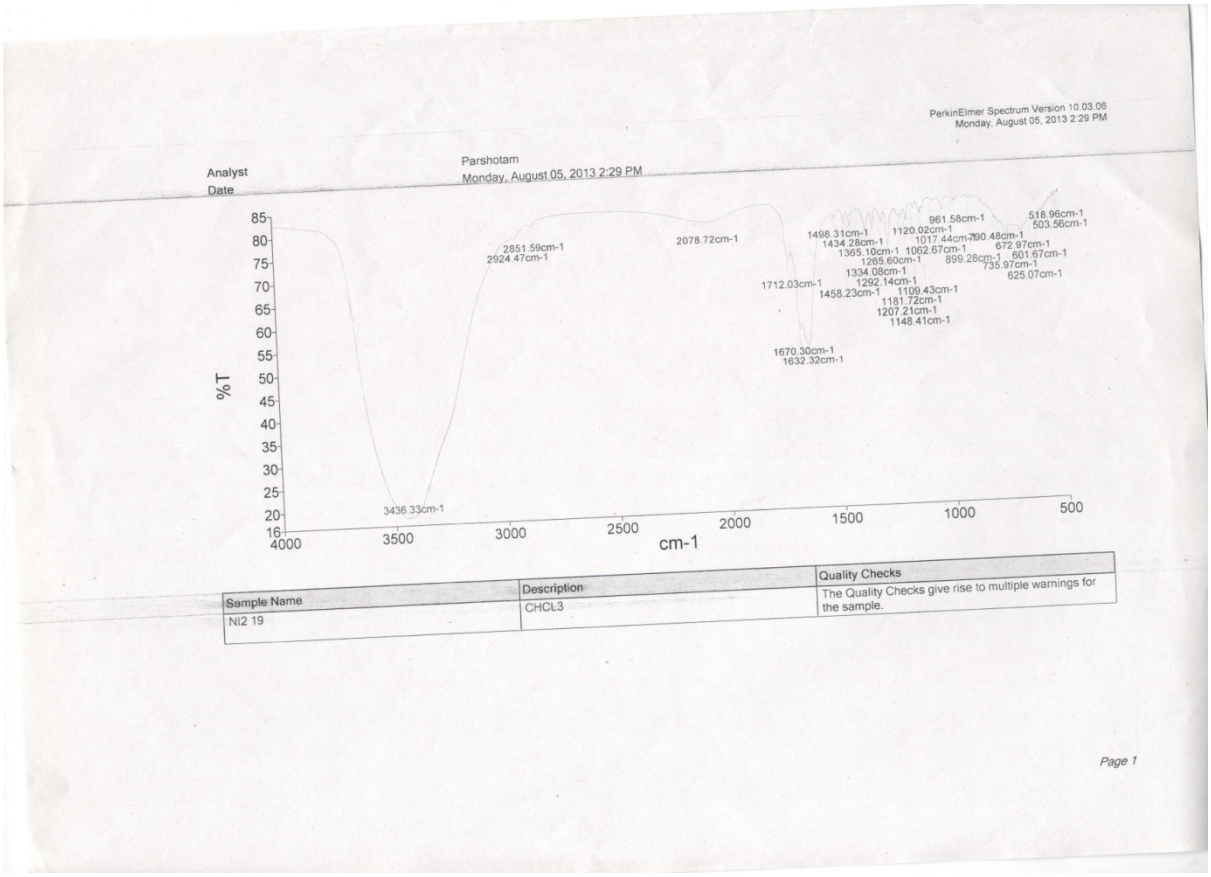
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
269.092	1	25247.01	C15 H13 N2 O3	(M+H)+
270.0954	1	3714.75	C15 H13 N2 O3	(M+H)+
271.0958	1	599.55	C15 H13 N2 O3	(M+H)+
291.0739	1	8048.49	C15 H12 N2 Na O3	(M+Na)+
292.0762	1	1616.05	C15 H12 N2 Na O3	(M+Na)+
293.0763	1	358.34	C15 H12 N2 Na O3	(M+Na)+

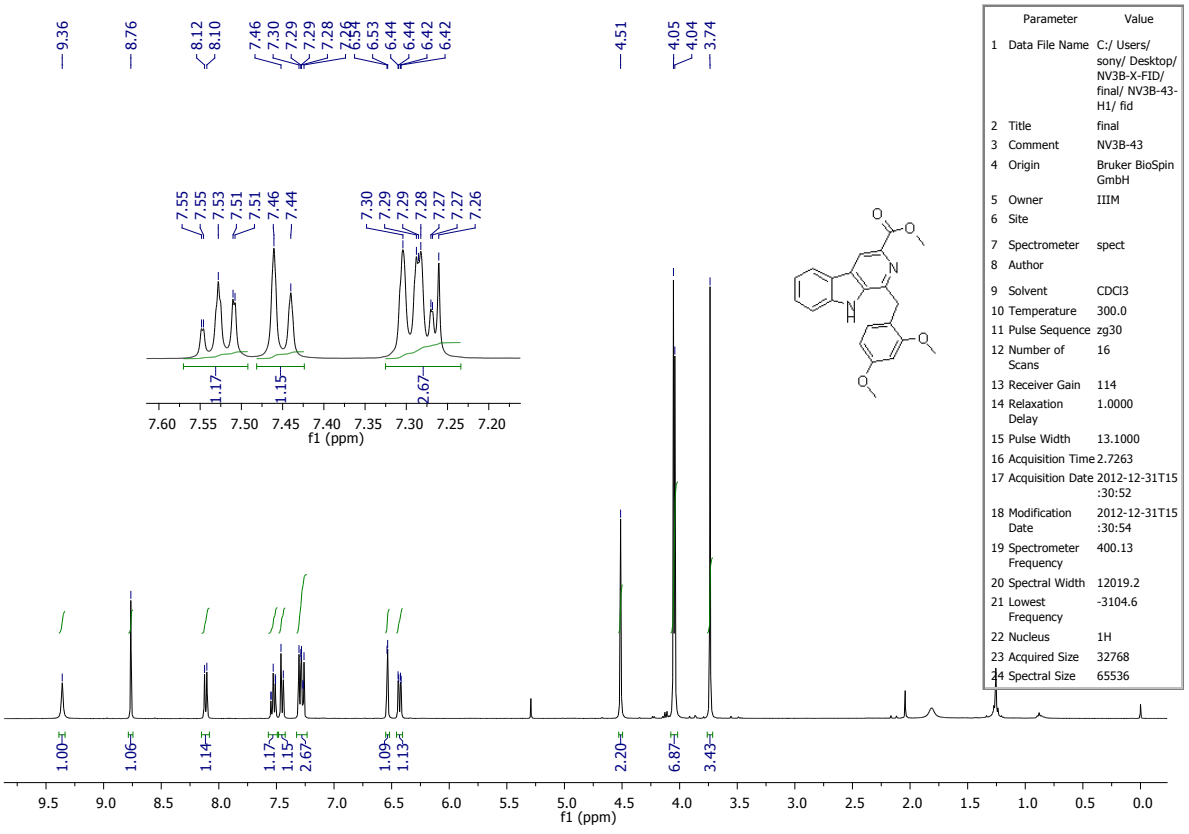
Predicted Isotope Match Table

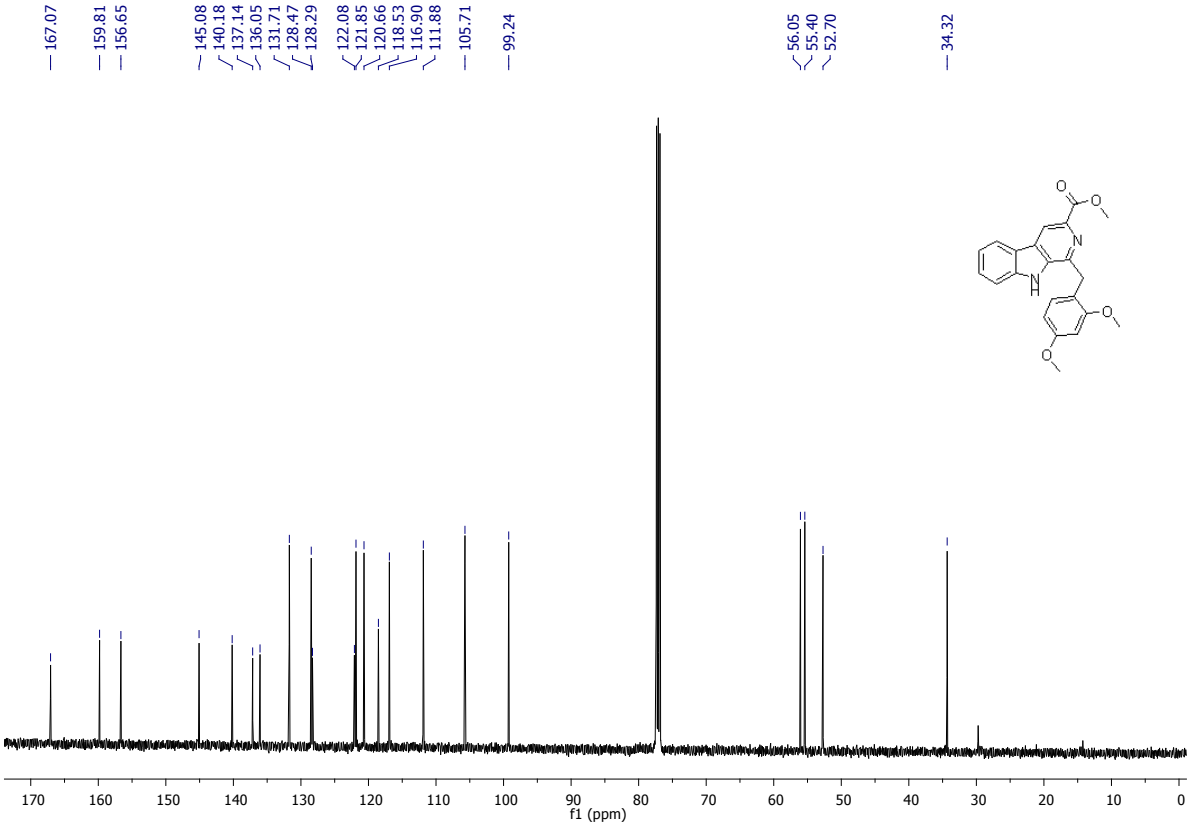
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	269.092	269.0921	0.38	100	100	85.41	83.87
2	270.0954	270.0952	-0.65	14.71	17.22	12.57	14.44
3	271.0958	271.0977	6.86	2.37	2.01	2.03	1.69

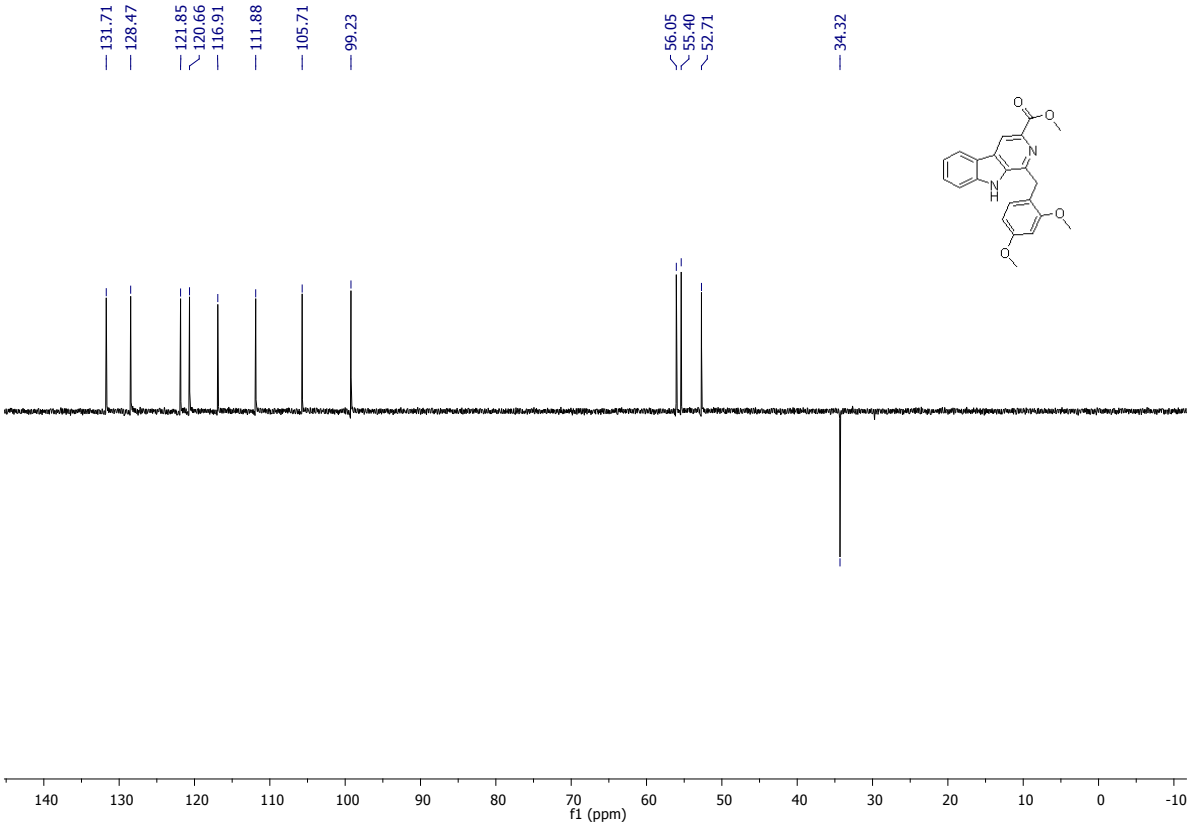
--- End Of Report ---

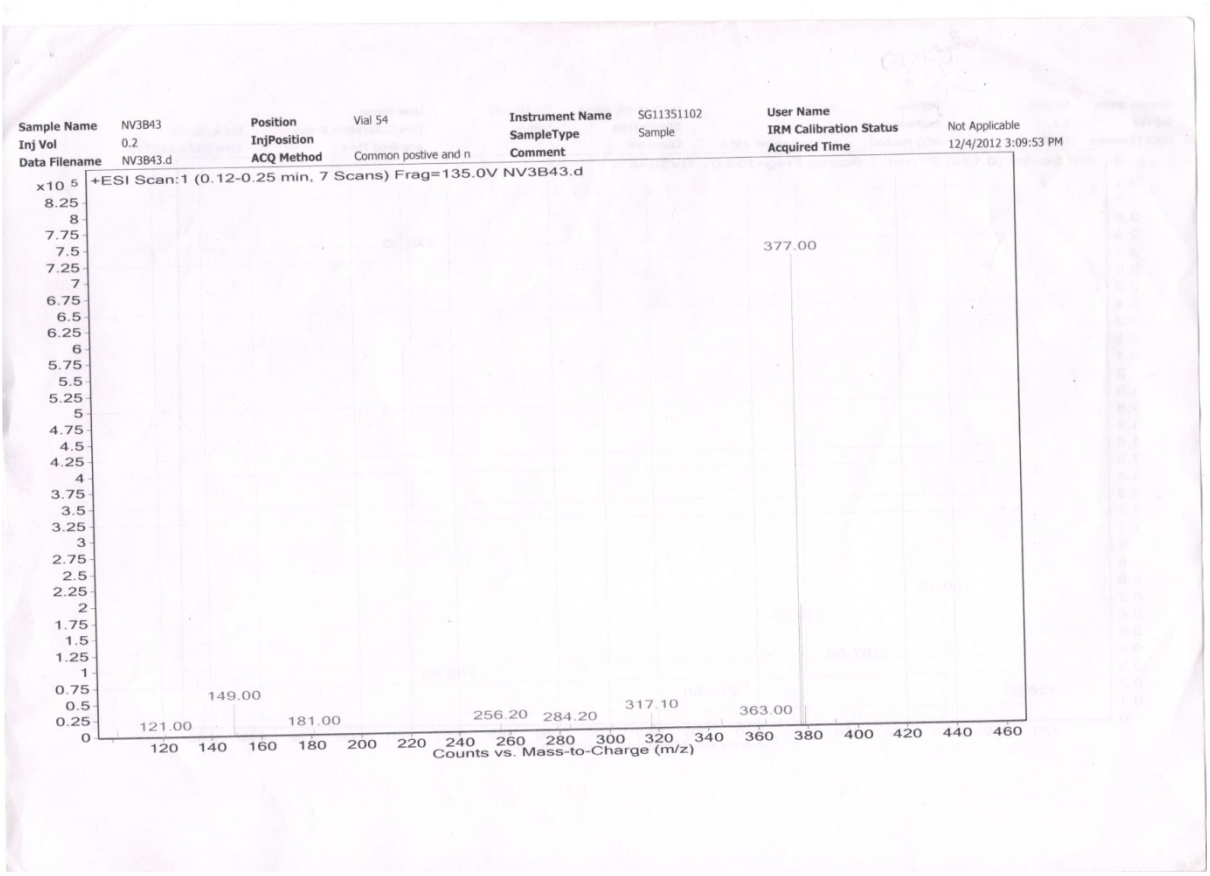


6a) Methyl 1-(2, 4-dimethoxybenzyl)-9H-pyrido[3,4-b]indole-3-carboxylate:




167.07
159.81
156.65
145.08
140.18
137.14
136.05
131.71
128.47
128.29
122.08
121.85
120.66
118.53
116.90
111.88
105.71
99.24
56.05
55.40
52.70
34.32
f1 (ppm)


131.71
128.47
121.85
120.66
116.91
111.88
105.71
99.23
56.05
55.40
52.71
34.32
f1 (ppm)


Sample Name NV3B43
Inj Vol 0.2
Data Filename NV3B43.d
Position Vial 54
InjPosition
ACQ Method Common postive and n
Instrument Name SG11351102
SampleType Sample
Comment
User Name
IRM Calibration Status Not Applicable
Acquired Time 12/4/2012 3:09:53 PM
+ESI Scan:1 (0.12-0.25 min, 7 Scans) Frag=135.0V NV3B43.d
x10 5
377.00
149.00
121.00
181.00
256.20
284.20
317.10
363.00
Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

Data File	NV3B-43.d	**Sample Name**	NV3B-43
Sample Type	Sample	**Position**	Vial 18
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	05-03-2013 PM 2:13:30
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			

Info.

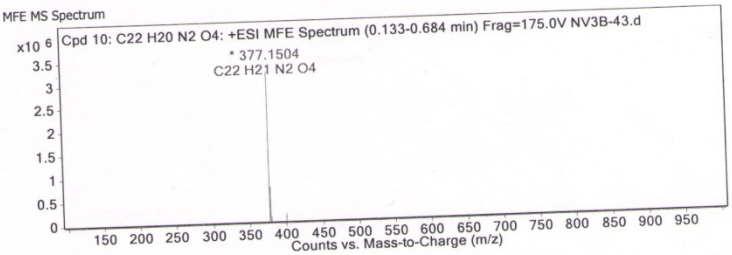
Sample Group	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 10: C22 H20 N2 O4	0.193	376.1434	C22 H20 N2 O4	C22 H20 N2 O4	-2.78	C22 H20 N2 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 10: C22 H20 N2 O4	377.1504	0.193	Find by Molecular Feature	376.1434

MFE MS Spectrum



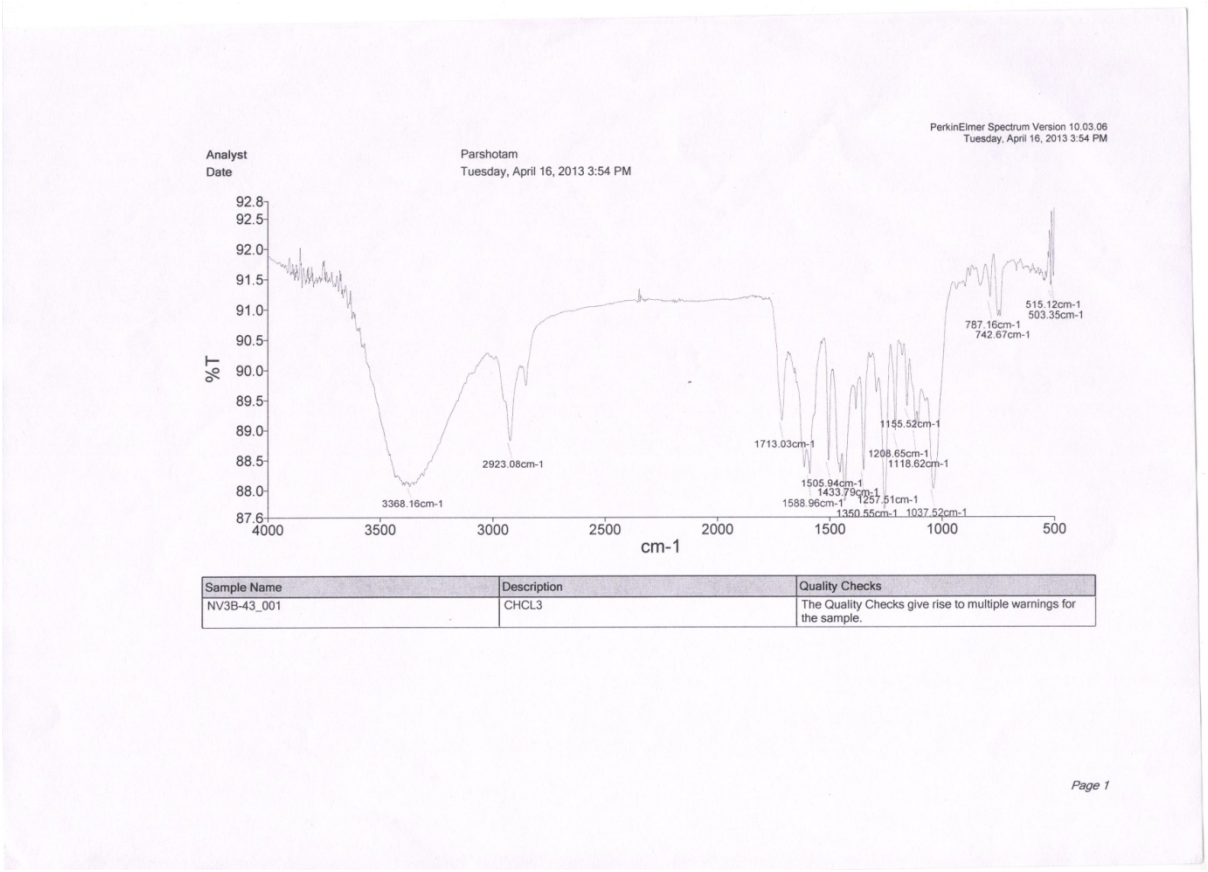
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
377.1504	1	3226680.25	C22 H21 N2 O4	(M+H)+
378.1548	1	761267.44	C22 H21 N2 O4	(M+H)+
379.1563	1	109653.34	C22 H21 N2 O4	(M+H)+
380.1581	1	10270.54	C22 H21 N2 O4	(M+H)+
381.1593	1	1068.27	C22 H21 N2 O4	(M+H)+
399.1323	1	164534.38	C22 H20 N2 Na O4	(M+Na)+
400.1348	1	41163.12	C22 H20 N2 Na O4	(M+Na)+
401.1379	1	6046.31	C22 H20 N2 Na O4	(M+Na)+
402.1398	1	736.12	C22 H20 N2 Na O4	(M+Na)+

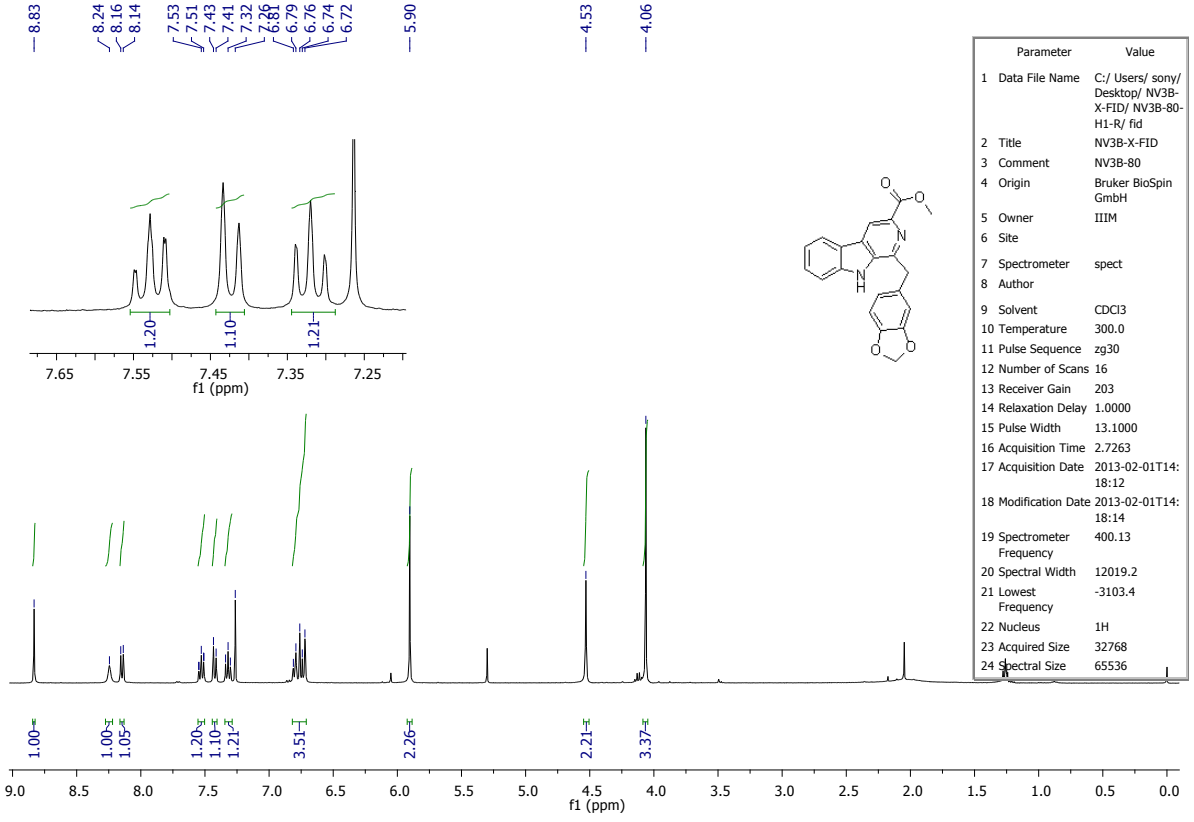
Predicted Isotope Match Table

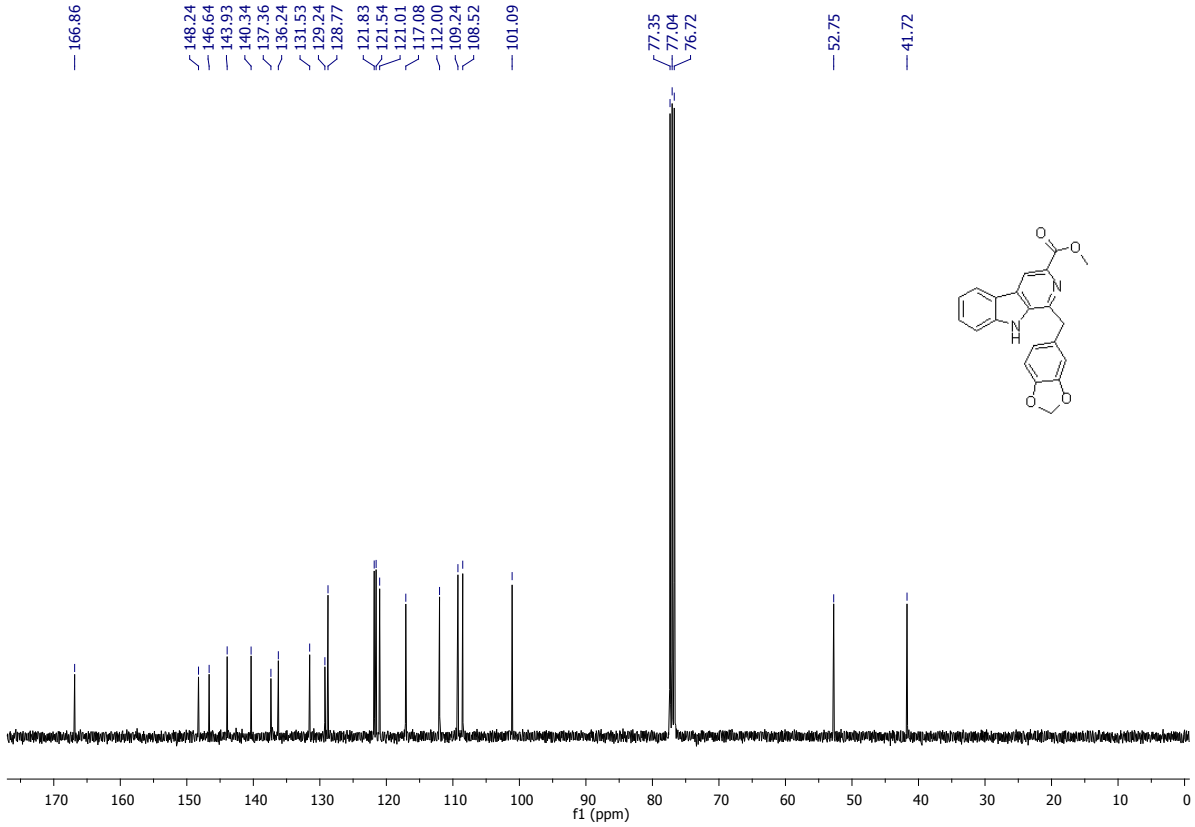
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	377.1504	377.1496	-2.22	100	100	78.53	77.41
2	378.1548	378.1528	-5.21	23.59	24.92	18.53	19.29
3	379.1563	379.1555	-2.13	3.4	3.8	2.67	2.94
4	380.1581	380.1582	0.02	0.32	0.43	0.25	0.33
5	381.1593	381.1608	3.75	0.03	0.04	0.03	0.03

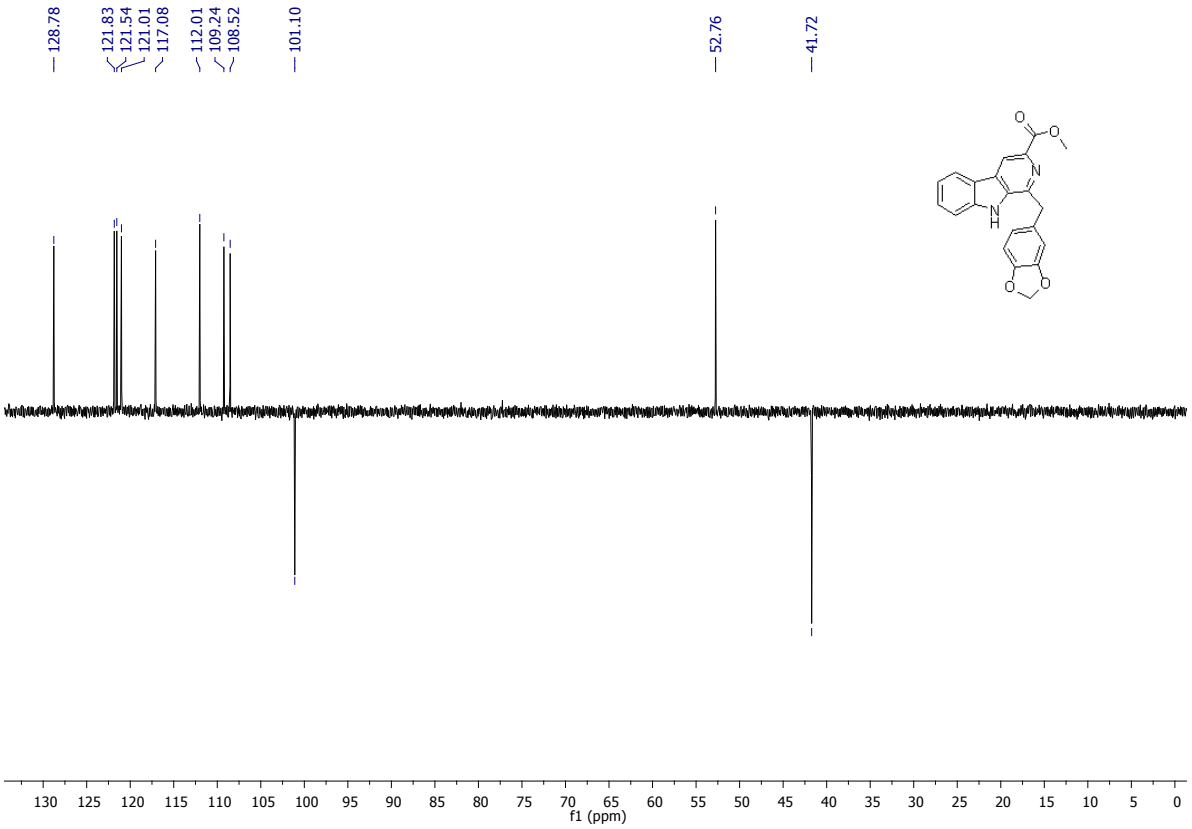
--- End Of Report ---

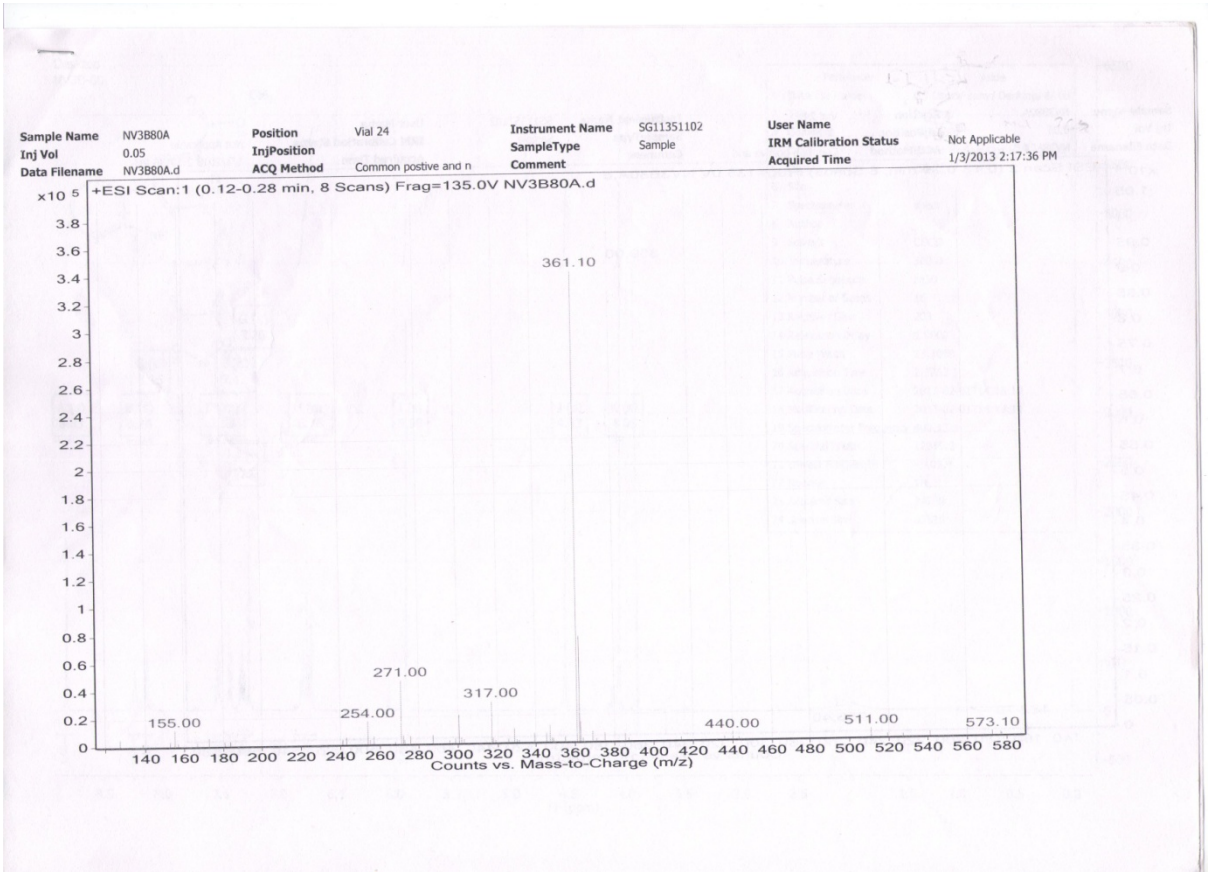


6b) Methyl 1-(benzo[d][1,3]dioxol-5-ylmethyl)-9H-pyrido[3,4-b]indole-3-carboxylate:




166.86
148.24
146.64
143.93
140.34
137.36
136.24
131.53
129.24
128.77
121.83
121.54
121.01
117.08
112.00
109.24
108.52
101.09
77.35
77.04
76.72
52.75
41.72
O
O
N
N
H
O
O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


128.78
121.83
121.54
121.01
117.08
112.01
109.24
108.52
101.10
52.76
41.72
O
O
N
N
H
O
O
130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)


Sample Name NV3B80A
Inj Vol 0.05
Data Filename NV3B80A.d
Position Vial 24
InjPosition
ACQ Method Common postive and n
Instrument Name SG11351102
SampleType Sample
Comment
User Name
IRM Calibration Status Not Applicable
Acquired Time 1/3/2013 2:17:36 PM
+ESI Scan:1 (0.12-0.28 min, 8 Scans) Frag=135.0V NV3B80A.d
x10 5
361.10
271.00
317.00
254.00
155.00
440.00
511.00
573.10
Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

Data File	NV3B-80.d	**Sample Name**	NV3B-80
Sample Type	Sample	**Position**	Vial 22
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	05-03-2013 PM 2:37:21
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			

Info.

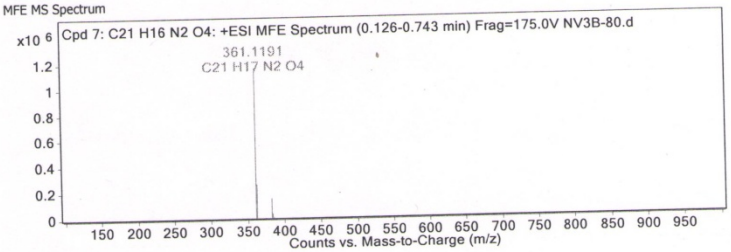
Sample Group	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 7: C21 H16 N2 O4	0.193	360.1118	C21 H16 N2 O4	C21 H16 N2 O4	-2.28	C21 H16 N2 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 7: C21 H16 N2 O4	361.1191	0.193	Find by Molecular Feature	360.1118

MFE MS Spectrum



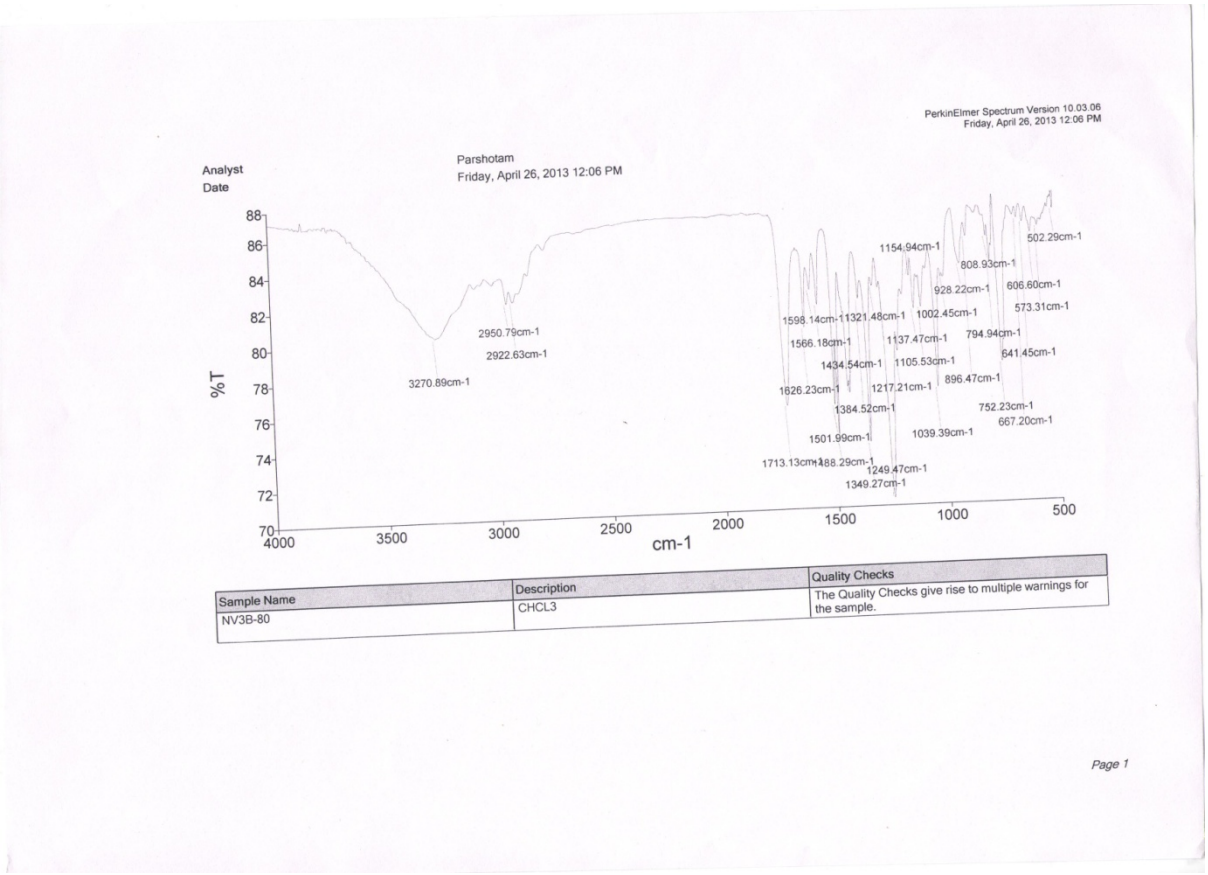
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
361.1191	1	1159489.88	C21 H17 N2 O4	(M+H)+
362.1223	1	255856.77	C21 H17 N2 O4	(M+H)+
363.1243	1	33993.12	C21 H17 N2 O4	(M+H)+
364.1263	1	3354.56	C21 H17 N2 O4	(M+H)+
383.1007	1	152528.78	C21 H16 N2 Na O4	(M+Na)+
384.1034	1	34425.18	C21 H16 N2 Na O4	(M+Na)+
385.1053	1	5176	C21 H16 N2 Na O4	(M+Na)+
386.1076	1	643.72	C21 H16 N2 Na O4	(M+Na)+

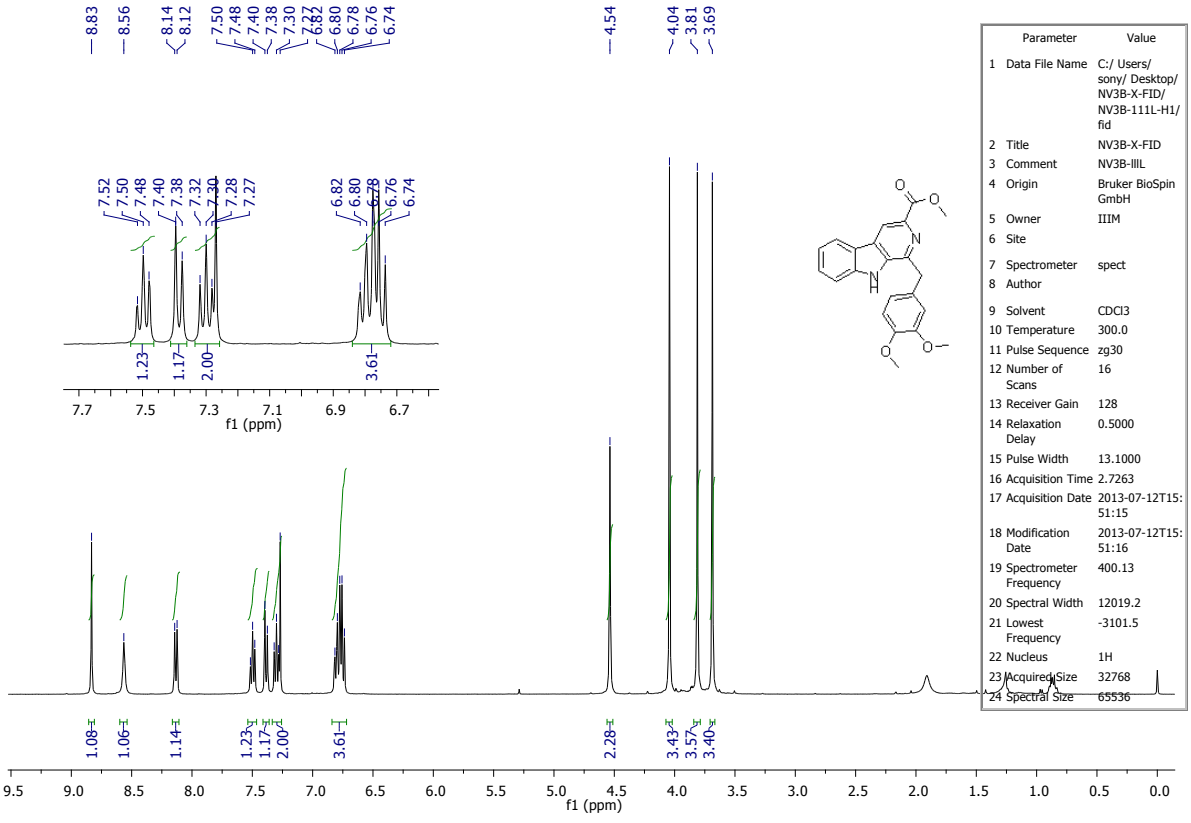
Predicted Isotope Match Table

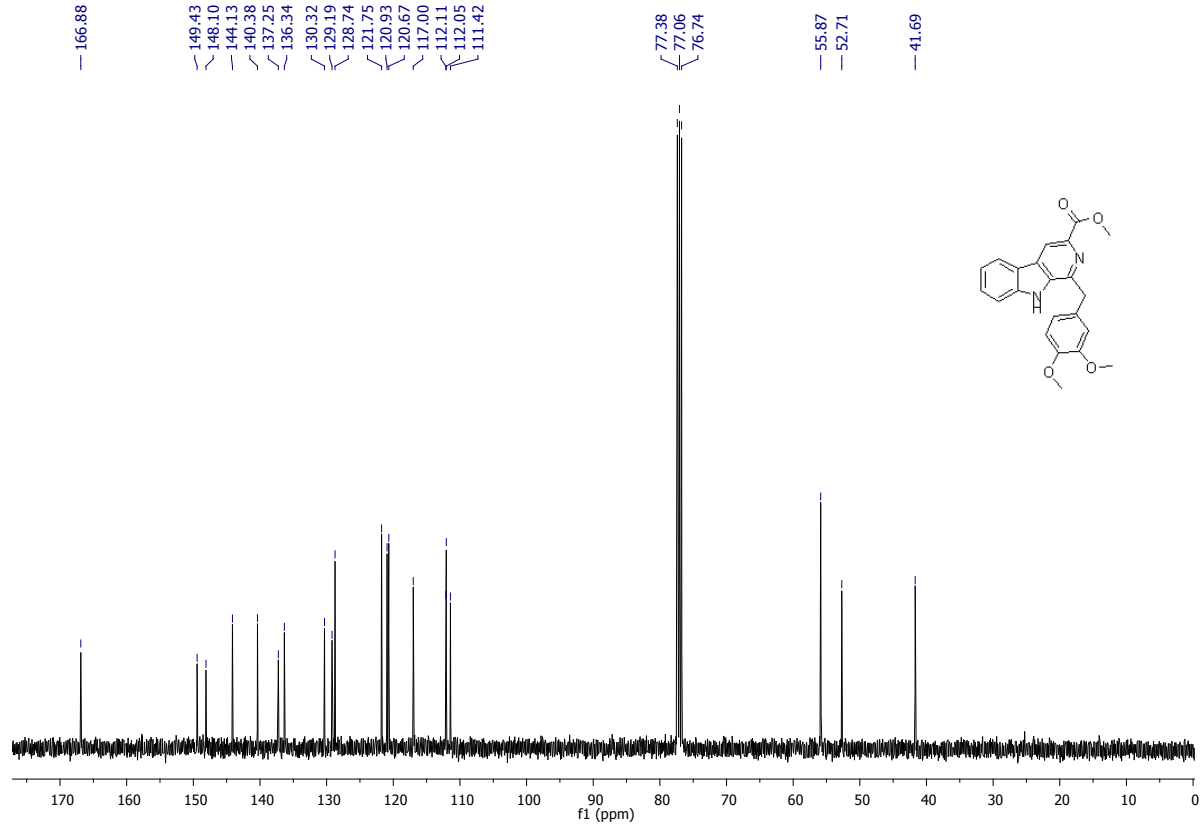
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	361.1191	361.1183	-2.36	100	100	79.82	78.3
2	362.1223	362.1215	-2.16	22.07	23.79	17.61	18.63
3	363.1243	363.1242	-0.38	2.93	3.53	2.34	2.76
4	364.1263	364.1268	1.21	0.29	0.39	0.23	0.31

--- End Of Report ---



6c) Methyl 1-(3,4-dimethoxybenzyl)-9H-pyrido[3,4-b]indole-3-carboxylate:

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149.43
148.10
144.13
140.38
137.25
136.34
130.32
129.19
128.74
121.75
120.93
120.67
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112.05
111.42
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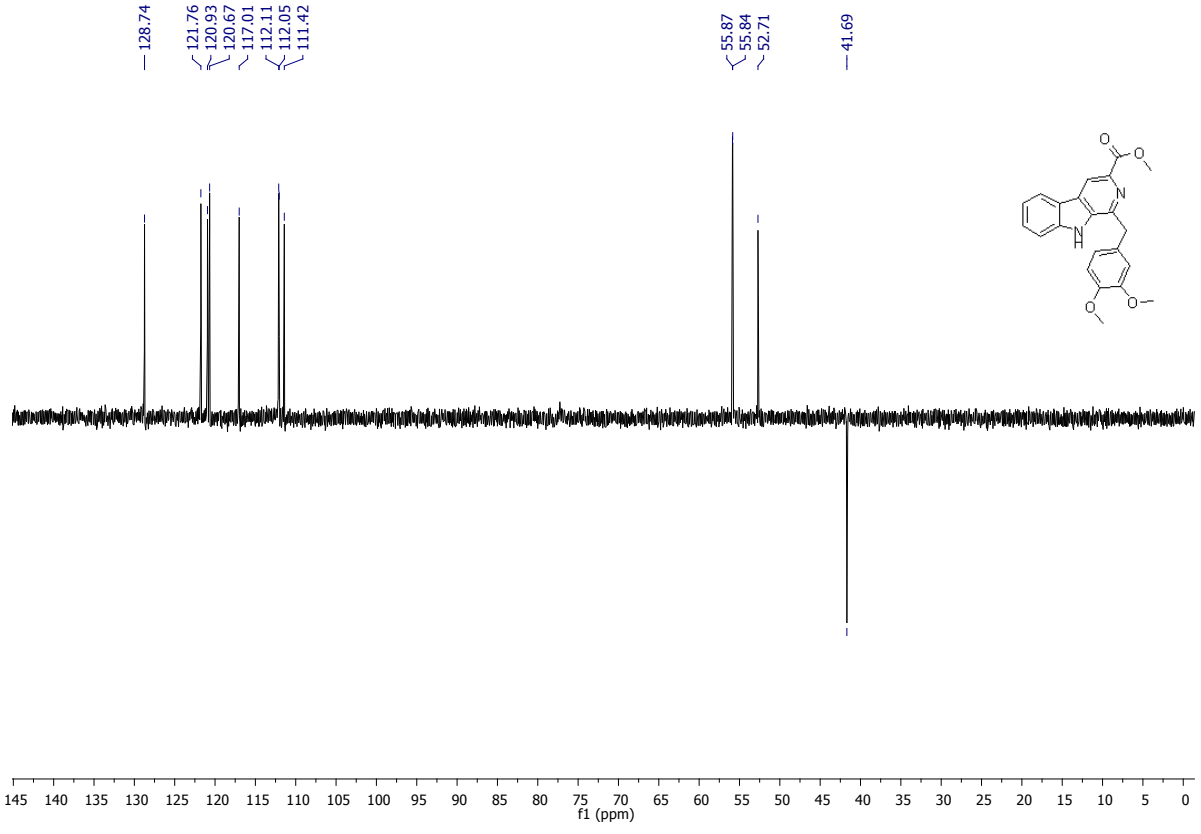
76.74
55.87
52.71
41.69
f1 (ppm)


128.74
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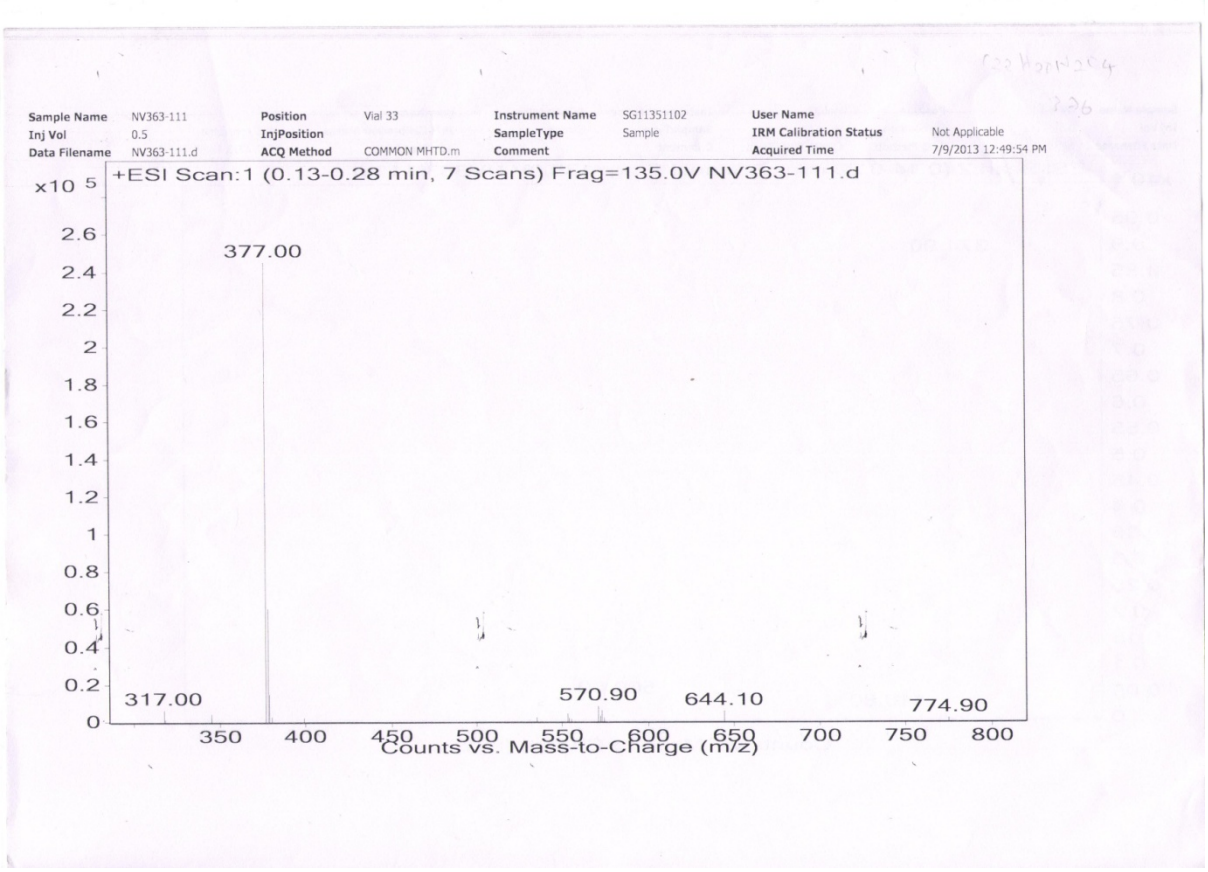
112.05
111.42
55.87
55.84
52.71
41.69
f1 (ppm)


Sample Name NV363-111
Position Vial 33
Instrument Name SG11351102
User Name
Inj Vol 0.5
InjPosition
SampleType Sample
IRM Calibration Status Not Applicable
Data Filename NV363-111.d
ACQ Method COMMON MHTD.m
Comment
Acquired Time 7/9/2013 12:49:54 PM
+ESI Scan:1 (0.13-0.28 min, 7 Scans) Frag=135.0V NV363-111.d
x10 5
377.00
317.00
570.90
644.10
774.90
Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

Data File	NV3B-111.d	**Sample Name**	NV3B-111
Sample Type	Sample	**Position**	Vial 14
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	12-07-2013 PM 1:00:12
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

Info.

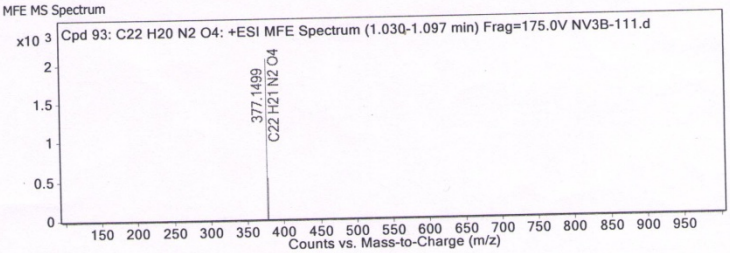
Sample Group	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 93: C22 H20 N2 O4	1.084	376.1423	C22 H20 N2 O4	C22 H20 N2 O4	0.08	C22 H20 N2 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 93: C22 H20 N2 O4	377.1499	1.084	Find by Molecular Feature	376.1423

MFE MS Spectrum



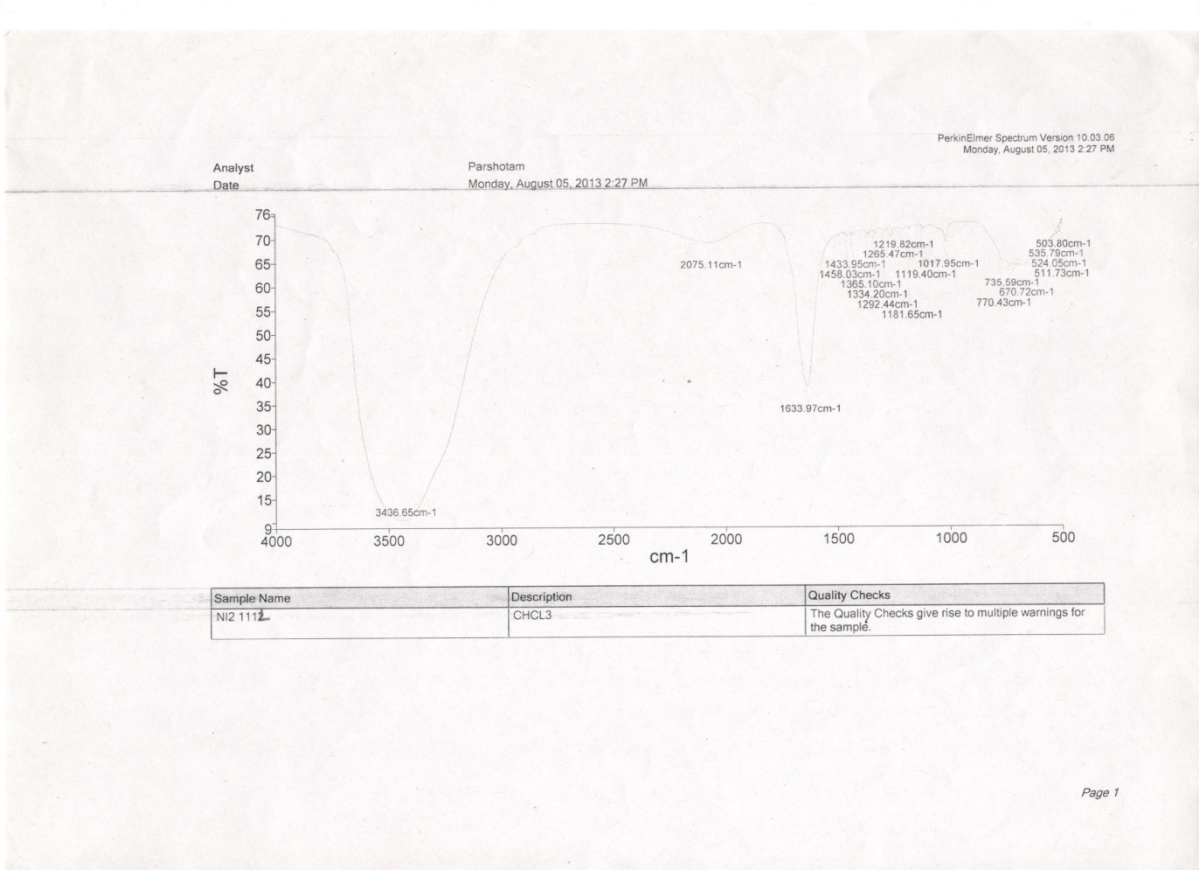
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
377.1499	1	2069.12	C22 H21 N2 O4	(M+H)+
378.1514	1	534.52	C22 H21 N2 O4	(M+H)+

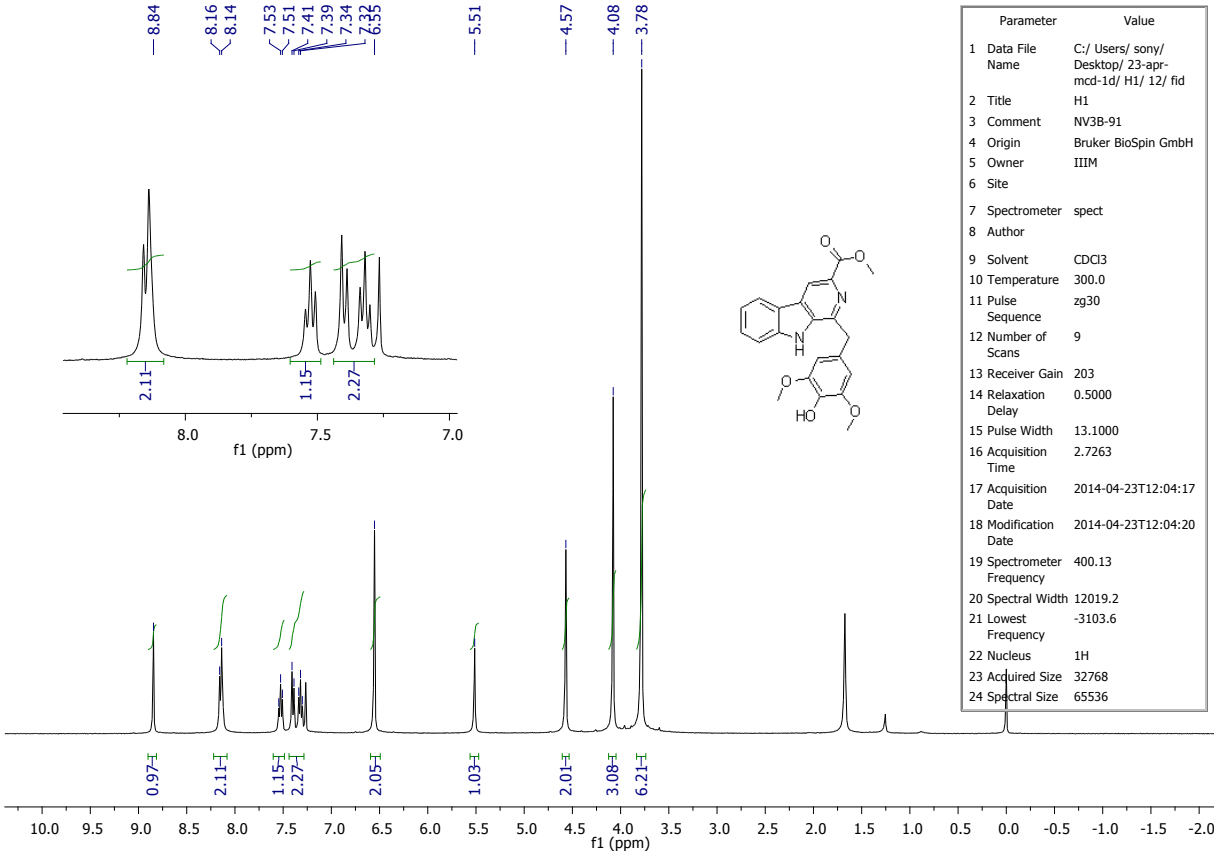
Predicted Isotope Match Table

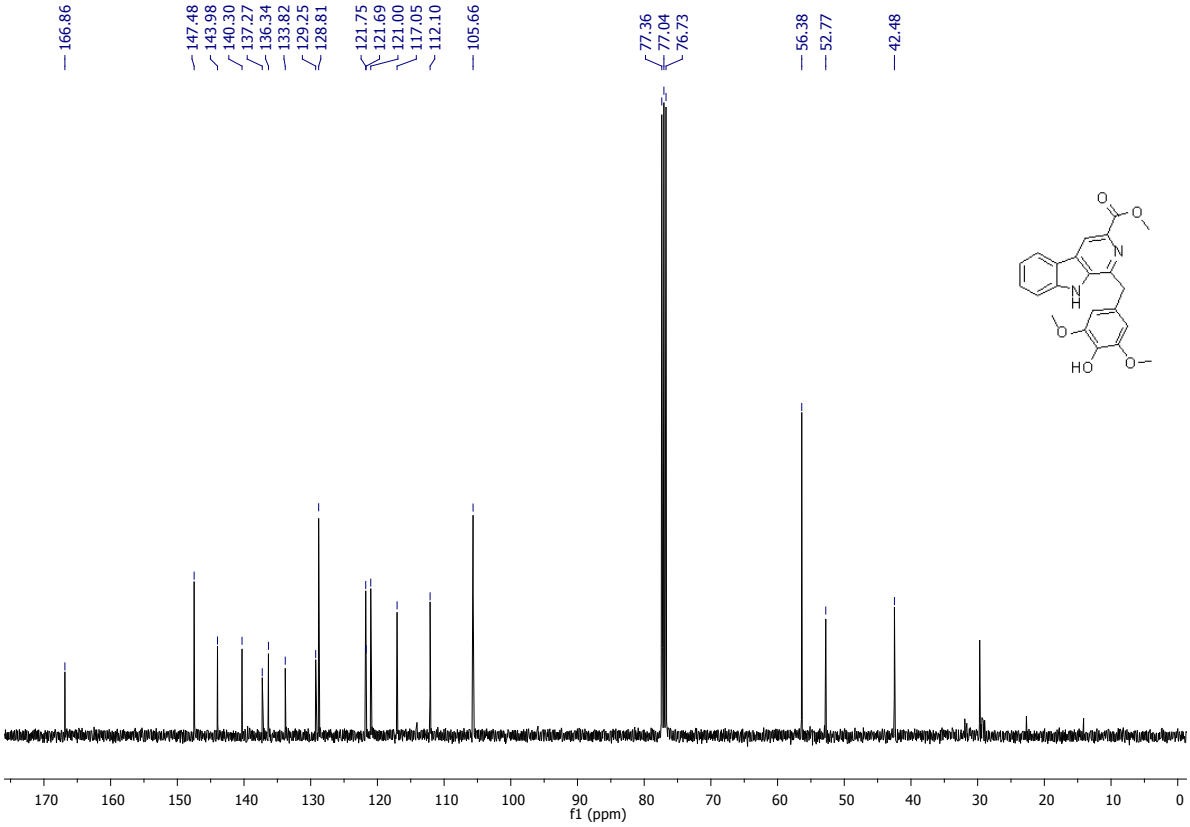
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	377.1499	377.1496	-0.88	100	100	79.47	80.05
2	378.1514	378.1528	3.78	25.83	24.92	20.53	19.95

--- End Of Report ---



6d) Methyl 1-(4- hydroxy-3,5-dimethoxybenzyl)-9H-pyrido[3,4-b]indole-3-carboxylate:

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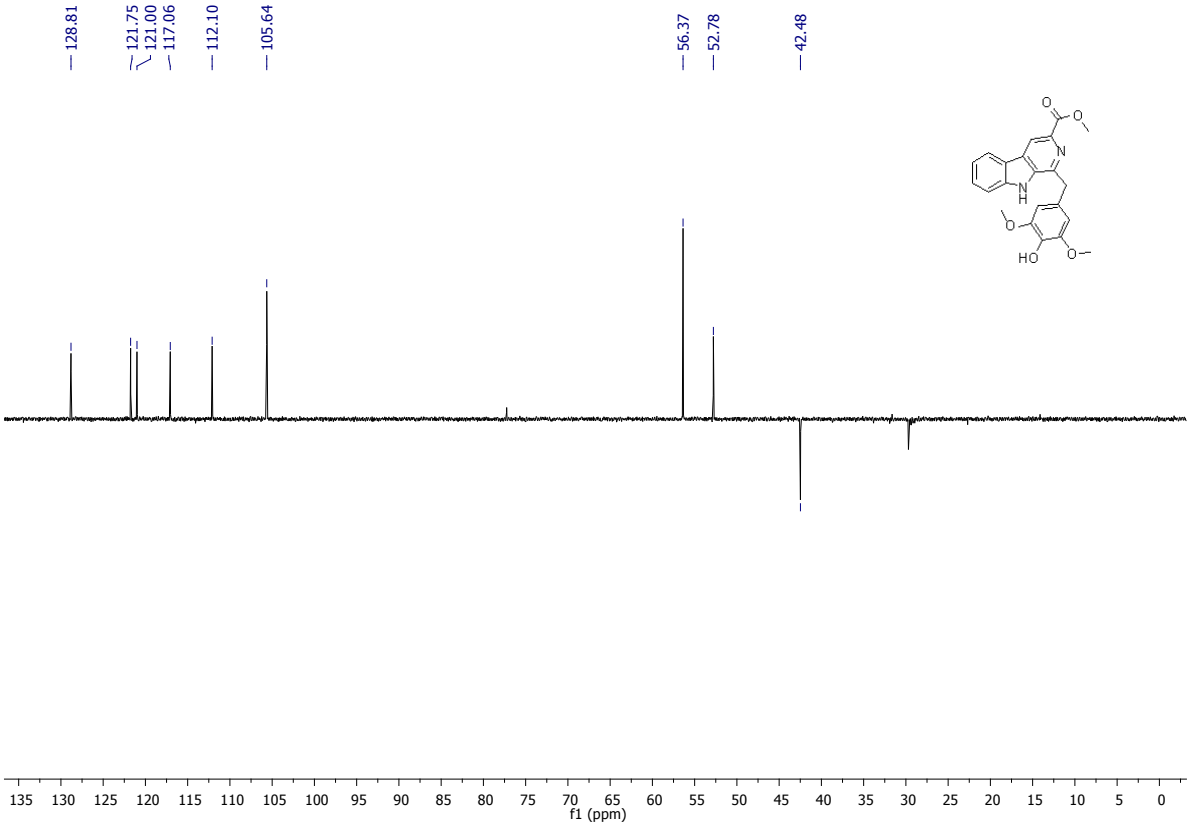
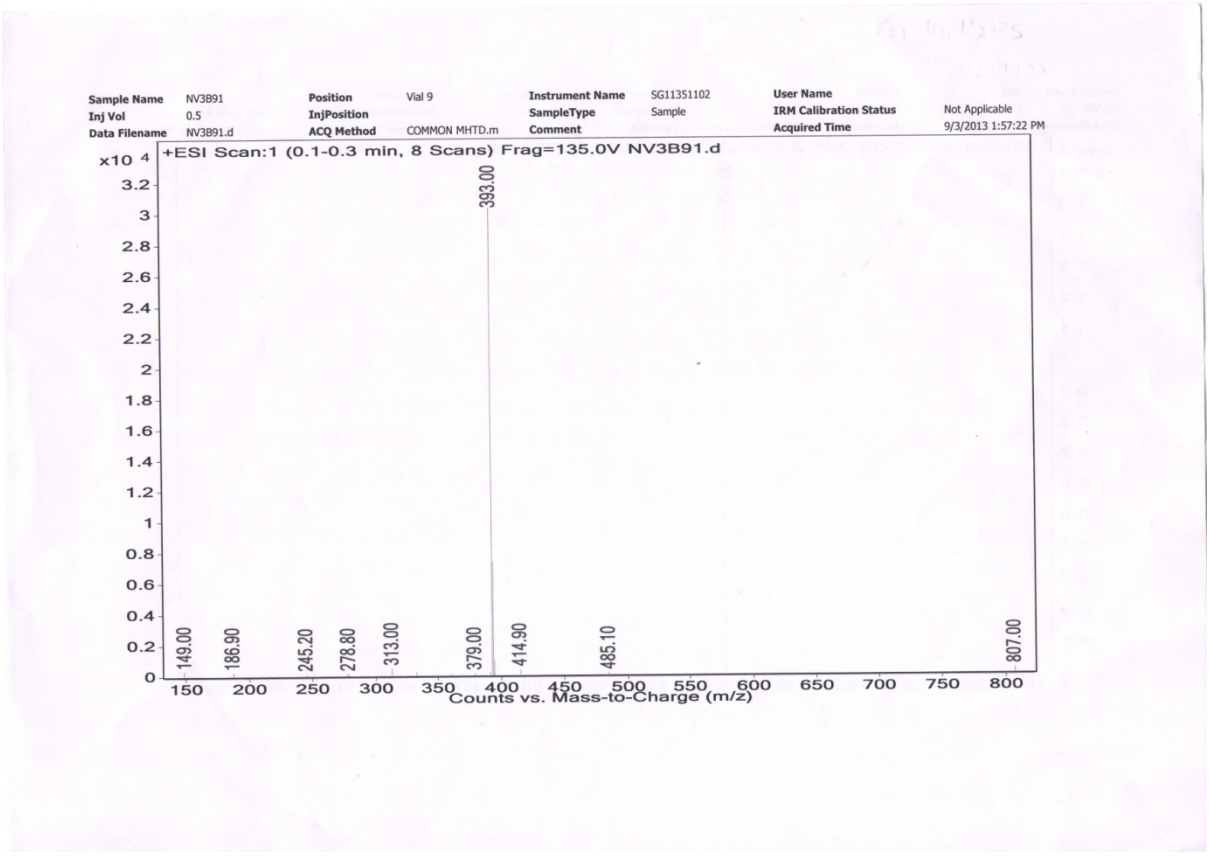
140.30
137.27
136.34
133.82
129.25
128.81
121.75
121.69
121.00
117.05
112.10
105.66
77.36
77.04
76.73
56.38
52.77
42.48
O
O
N
H
O
HO
O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


128.81
121.75
121.00
117.06
112.10
105.64
56.37
52.78
42.48
O
O
N
N
H
O
HO
O
135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)


Sample Name NV3B91
Inj Vol 0.5
Data Filename NV3B91.d
Position Vial 9
InjPosition
ACQ Method COMMON MHTD.m
Instrument Name SG11351102
SampleType Sample
Comment
User Name
IRM Calibration Status Not Applicable
Acquired Time 9/3/2013 1:57:22 PM
+ESI Scan:1 (0.1-0.3 min, 8 Scans) Frag=135.0V NV3B91.d
x10 4
3.2
3
2.8
2.6
2.4
2.2
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
393.00
149.00
186.90
245.20
278.80
313.00
379.00
414.90
485.10
807.00
150 200 250 300 350 400 450 500 550 600 650 700 750 800
Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

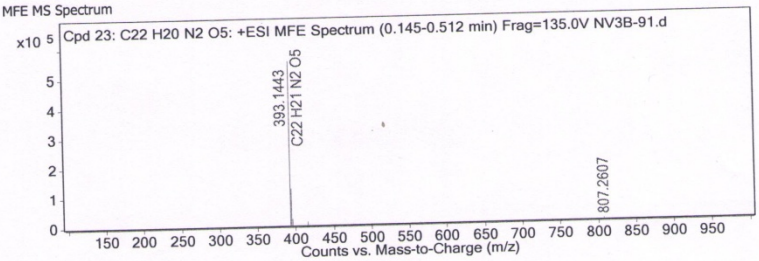
Data File	NV3B-91.d	**Sample Name**	Unavailable
Sample Type	Unavailable	**Position**	Unavailable
Instrument Name	Unavailable	**User Name**	Unavailable
Acq Method		**Acquired Time**	Unavailable
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment	Sample information is unavailable		

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 23: C22 H20 N2 O5	0.192	392.137	C22 H20 N2 O5	C22 H20 N2 O5	0.67	C22 H20 N2 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 23: C22 H20 N2 O5	393.1443	0.192	Find by Molecular Feature	392.137

MFE MS Spectrum



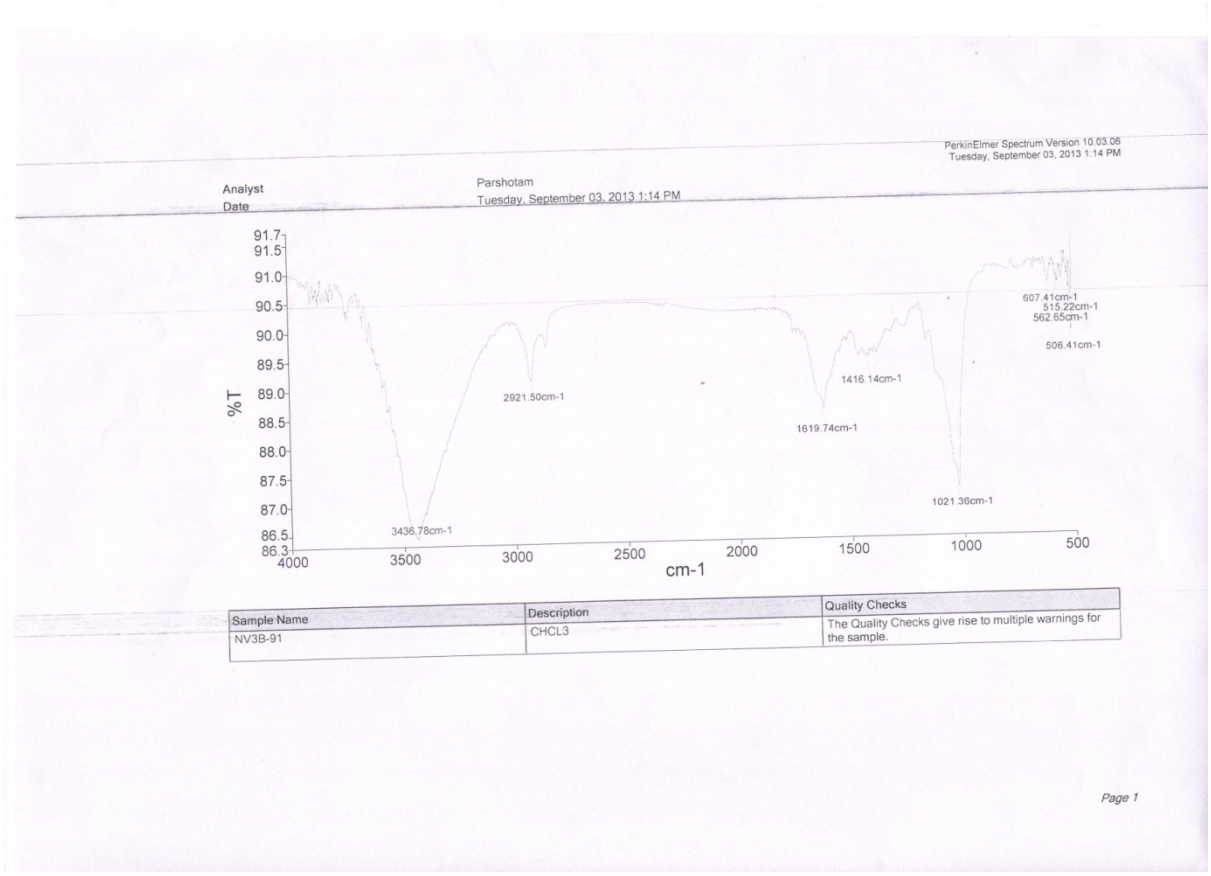
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
393.1443	1	553716.44	C22 H21 N2 O5	(M+H)+
394.1473	1	125690.59	C22 H21 N2 O5	(M+H)+
395.1505	1	23072.12	C22 H21 N2 O5	(M+H)+
396.1514	1	2773.05	C22 H21 N2 O5	(M+H)+
397.1607	1	355.69	C22 H21 N2 O5	(M+H)+
415.1254	1	12300.1	C22 H20 N2 Na O5	(M+Na)+
416.128	1	2886.59	C22 H20 N2 Na O5	(M+Na)+
417.1318	1	566.84	C22 H20 N2 Na O5	(M+Na)+
807.2607	1	1918.39		(2M+Na)+
808.2622	1	1130.32		(2M+Na)+

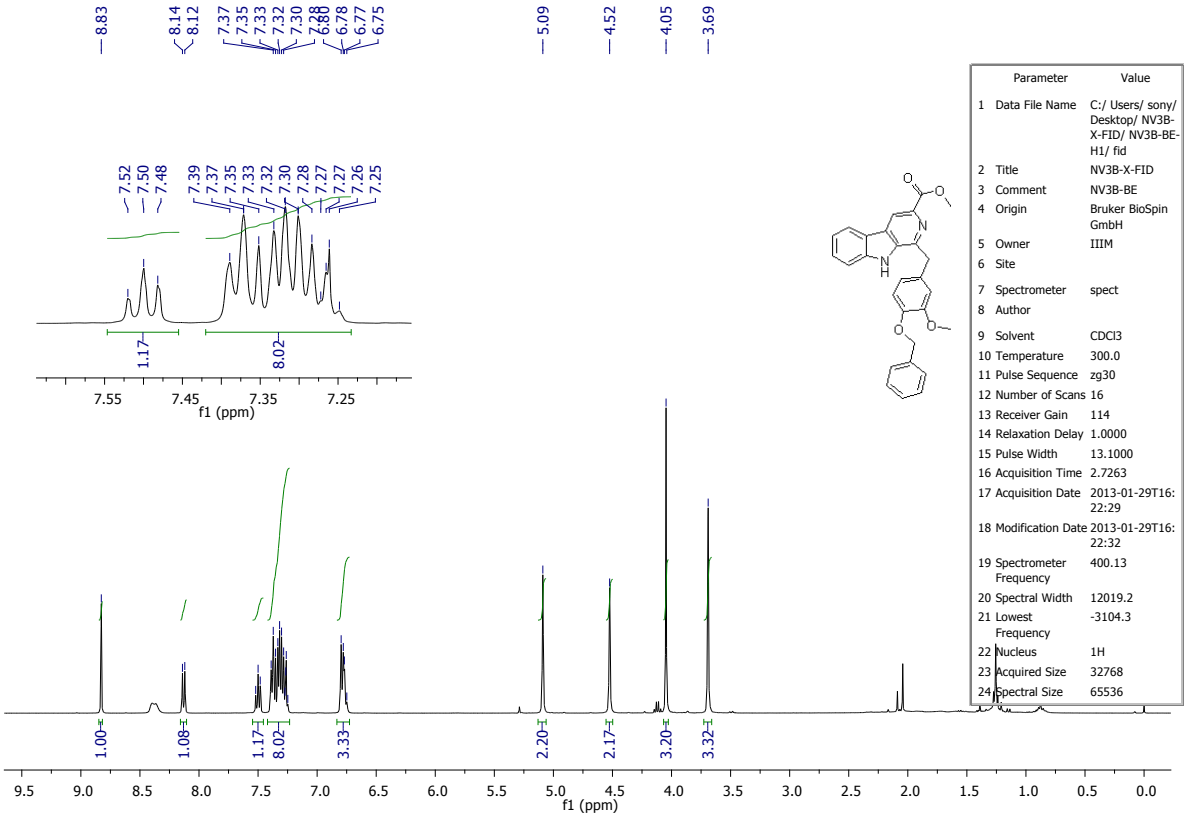
Predicted Isotope Match Table

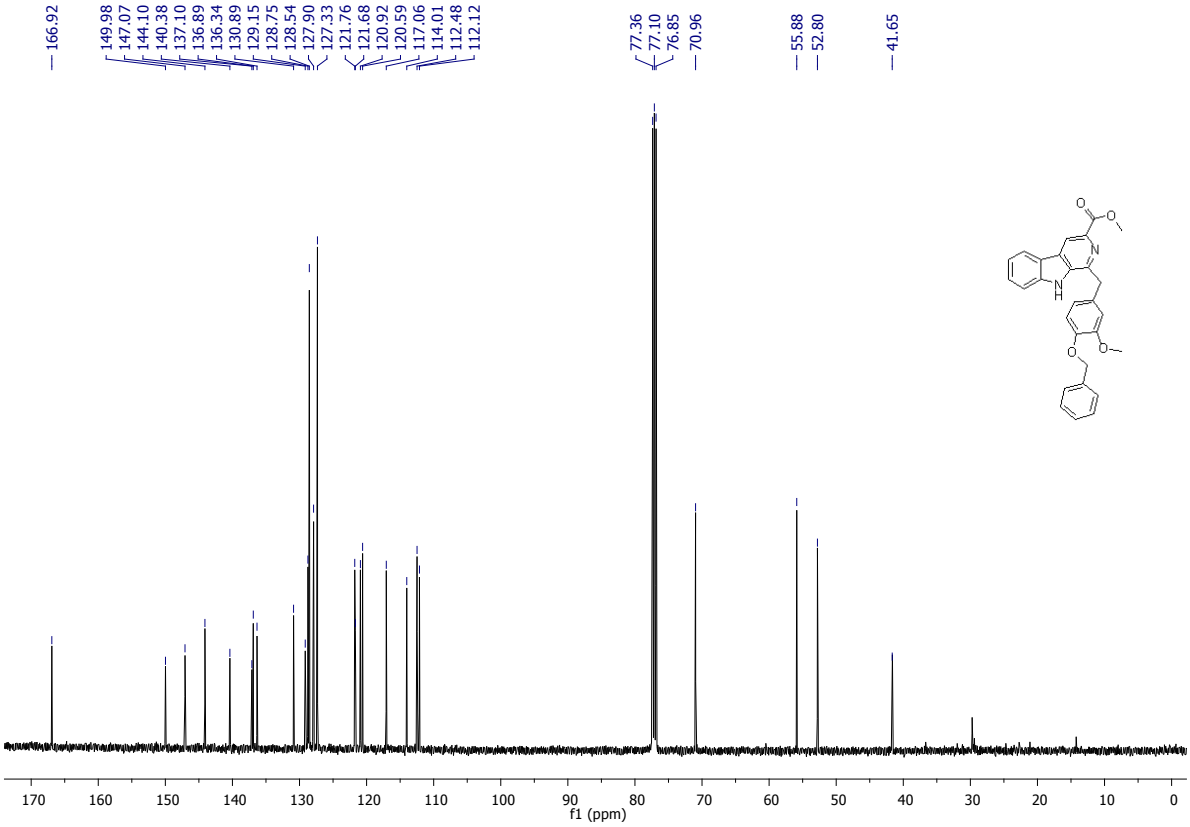
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	393.1443	393.1445	0.6	100	100	78.47	77.22
2	394.1473	394.1477	1.11	22.7	24.96	17.81	19.27
3	395.1505	395.1503	-0.31	4.17	4.01	3.27	3.1
4	396.1514	396.153	3.89	0.5	0.48	0.39	0.37
5	397.1607	397.1555	-13.02	0.06	0.05	0.05	0.04

--- End Of Report ---



6e) Methyl 1-(4-(benzyloxy)-3-methoxybenzyl)-9H-pyrido[3,4-b]indole-3-carboxylate:

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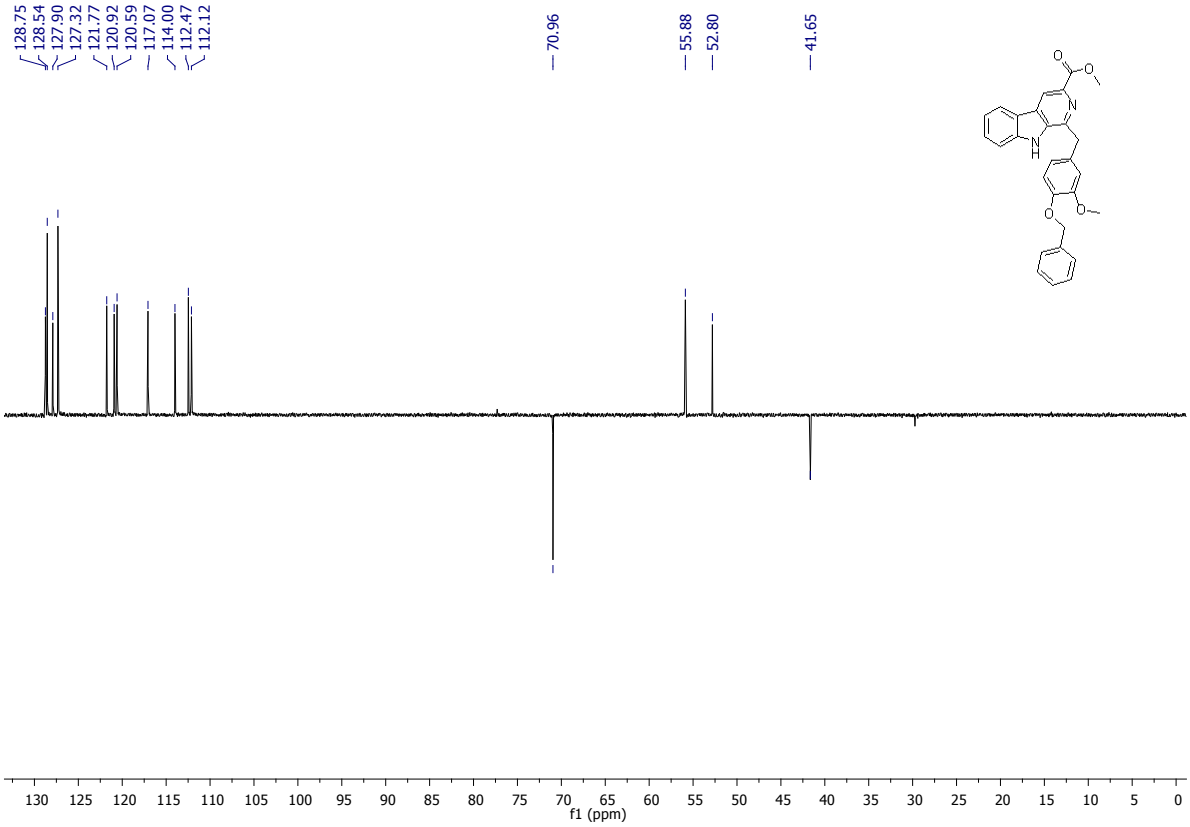
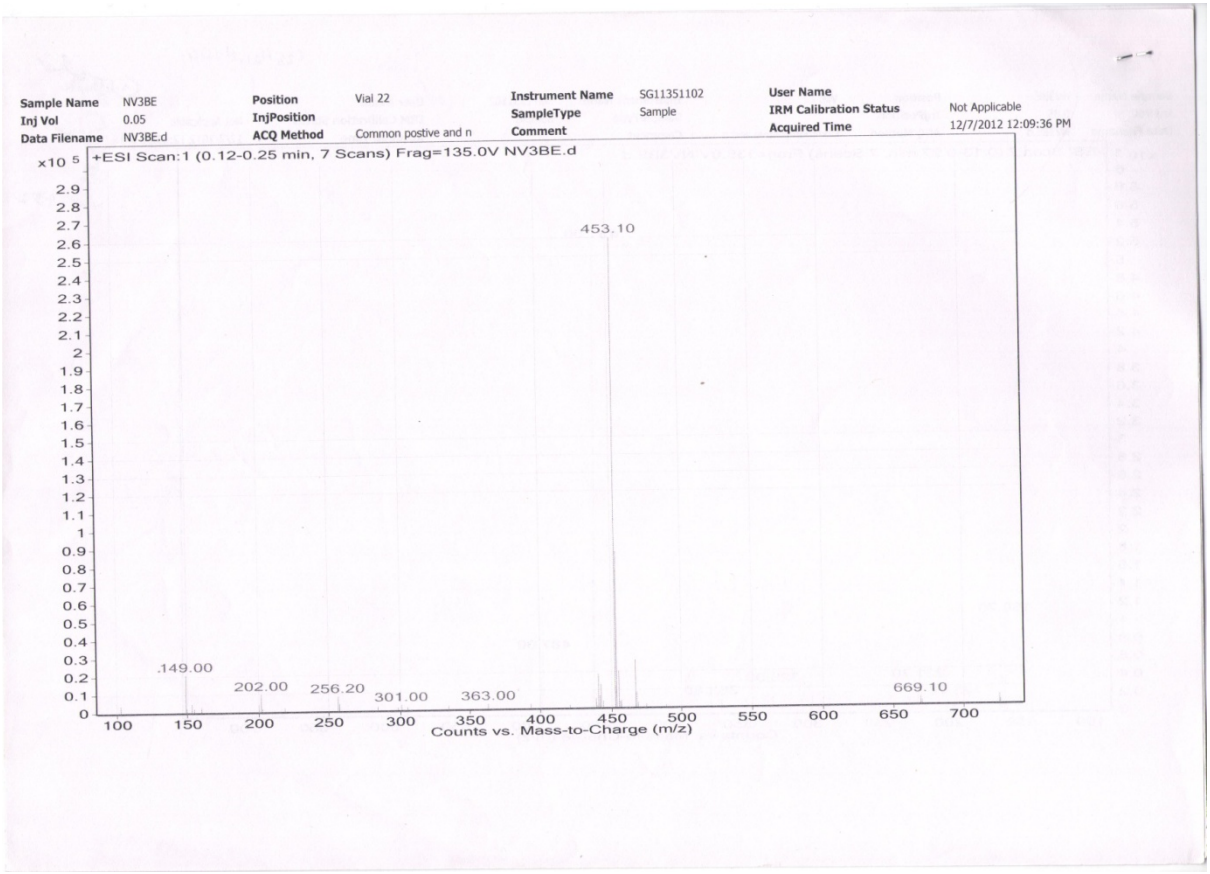
147.07
144.10
140.38
137.10
136.89
136.34
130.89
129.15
128.75
128.54
127.90
127.33
121.76
121.68
120.92
120.59
117.06
114.01
112.48
112.12
77.36
77.10
76.85
70.96
55.88
52.80
41.65
O
O
N
H
O
O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


128.75
128.54
127.90
127.32
121.77
120.92
120.59
117.07
114.00
112.47
112.12
70.96
55.88
52.80
41.65
130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)


Sample Name NV3BE
Inj Vol 0.05
Data Filename NV3BE.d
Position Vial 22
InjPosition
ACQ Method Common postive and n
Instrument Name SG11351102
SampleType Sample
Comment
User Name
IRM Calibration Status Not Applicable
Acquired Time 12/7/2012 12:09:36 PM
+ESI Scan:1 (0.12-0.25 min, 7 Scans) Frag=135.0V NV3BE.d
x10 5
453.10
149.00
202.00
256.20
301.00
363.00
669.10
Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

Data File	NV3B-BE.d	**Sample Name**	NV3B-BE
Sample Type	Sample	**Position**	Vial 3
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	06-09-2013 AM 11:46:44
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

Info.

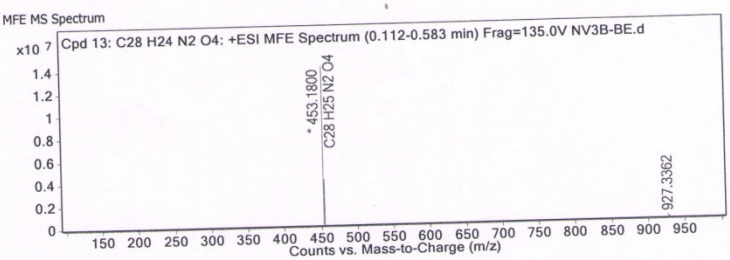
Sample Group	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 13: C28 H24 N2 O4	0.193	452.1731	C28 H24 N2 O4	C28 H24 N2 O4	1.19	C28 H24 N2 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 13: C28 H24 N2 O4	453.18	0.193	Find by Molecular Feature	452.1731

MFE MS Spectrum



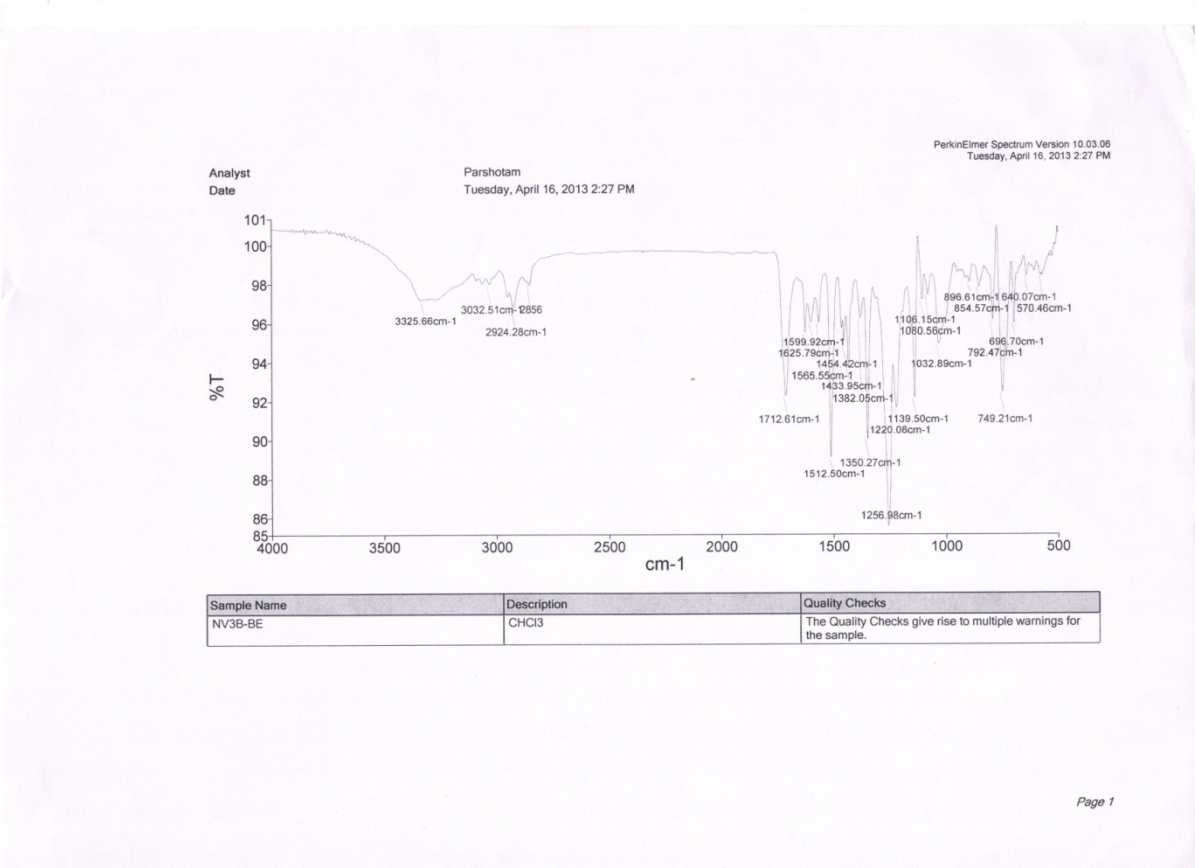
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
453.18	1	14156268	C28 H25 N2 O4	(M+H)+
454.1836	1	4173447.25	C28 H25 N2 O4	(M+H)+
455.1915	1	766174.75	C28 H25 N2 O4	(M+H)+
456.1939	1	93032.05	C28 H25 N2 O4	(M+H)+
457.1958	1	8733.57	C28 H25 N2 O4	(M+H)+
927.3362	1	229249.22		(2M+Na)+
928.3387	1	143515.58		(2M+Na)+
929.3419	1	44726.77		(2M+Na)+
930.344	1	10932.51		(2M+Na)+
931.3477	1	1930.98		(2M+Na)+

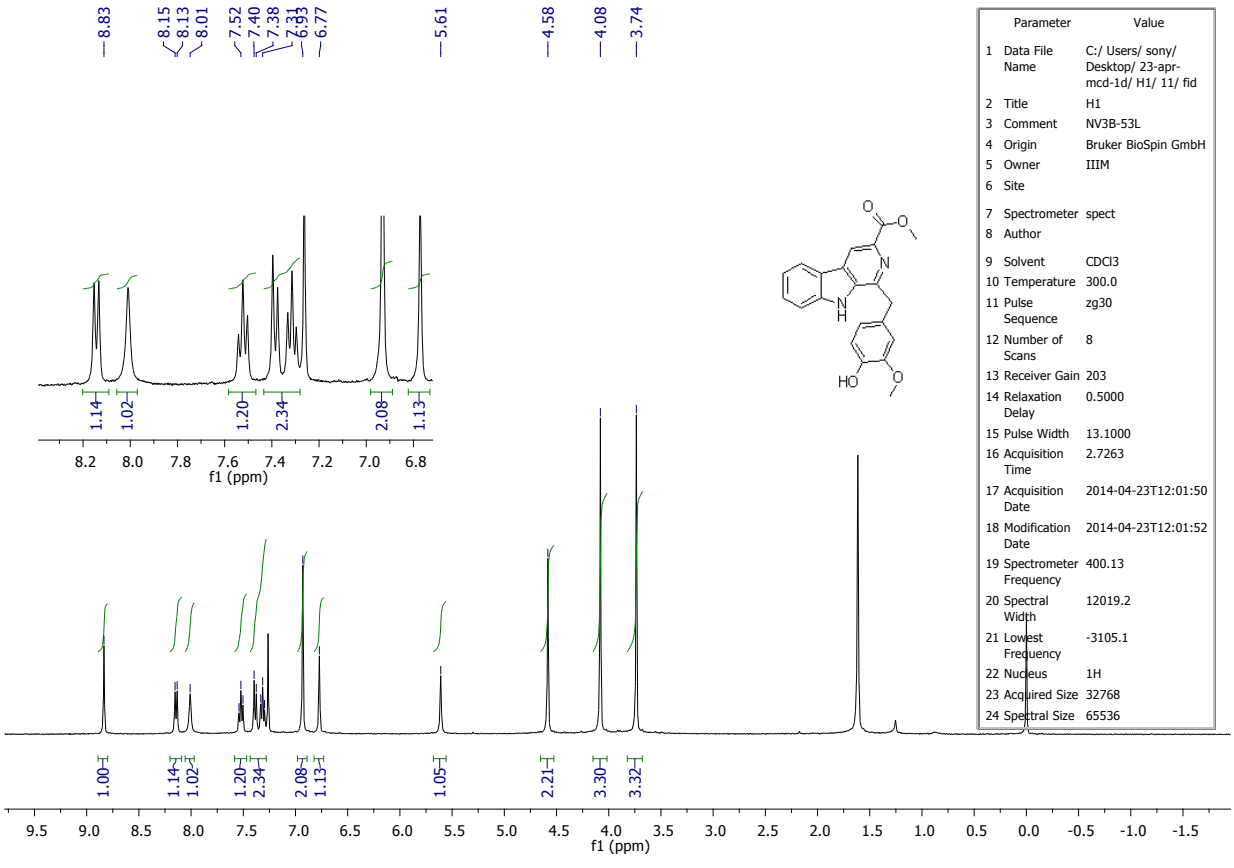
Predicted Isotope Match Table

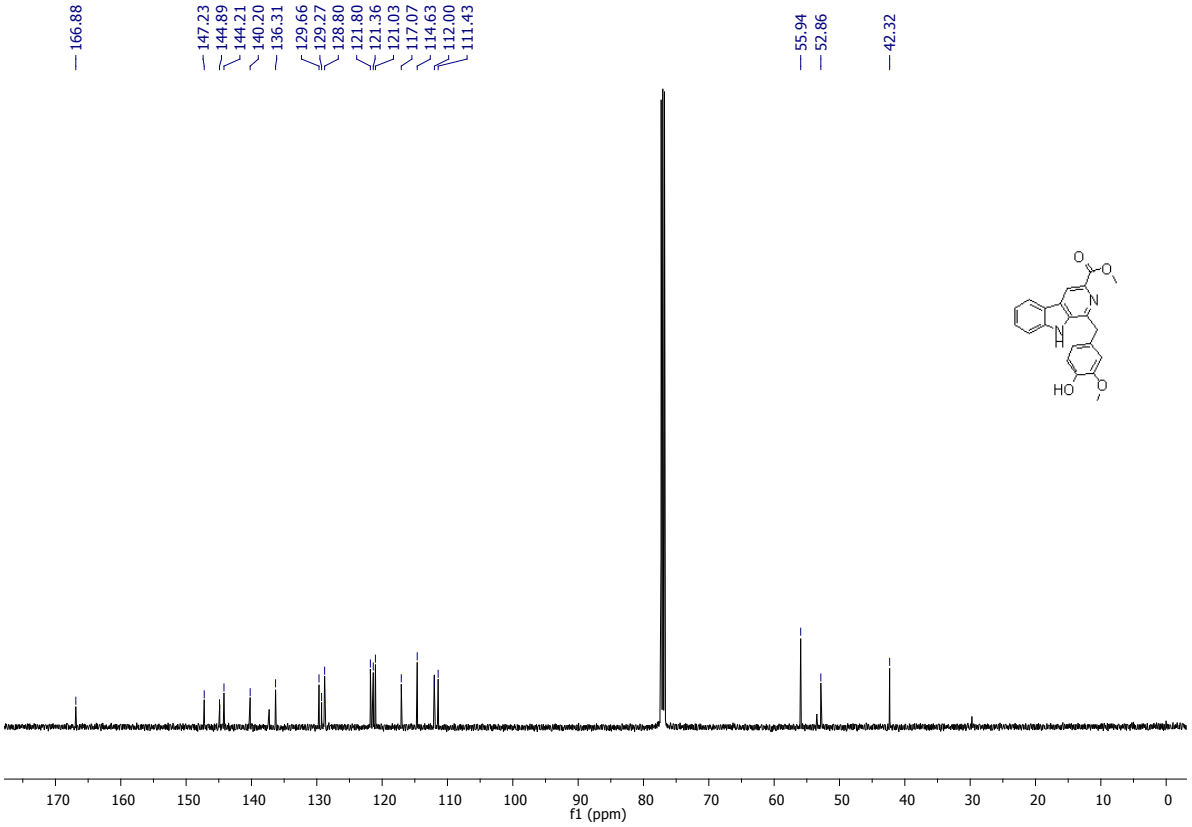
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	453.18	453.1809	1.88	100	100	73.74	72.54
2	454.1836	454.1841	1.08	29.48	31.45	21.74	22.82
3	455.1915	455.187	-9.83	5.41	5.6	3.99	4.06
4	456.1939	456.1898	-9.02	0.66	0.73	0.48	0.53
5	457.1958	457.1925	-7.29	0.06	0.07	0.05	0.05

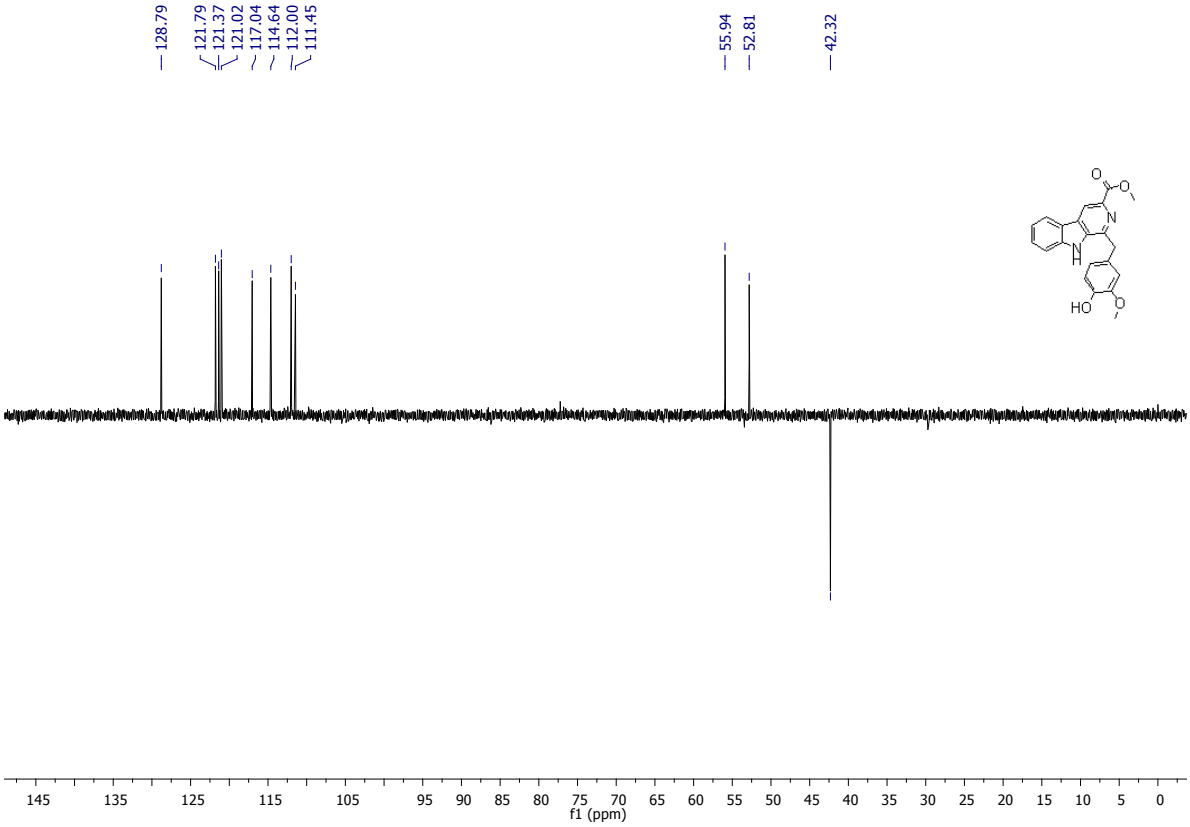
--- End Of Report ---



6f) Methyl 1-(4-hydroxy-3-methoxybenzyl)-9H-pyrido[3,4-b]indole-3-carboxylate:




166.88
147.23
144.89
144.21
140.20
136.31
129.66
129.27
128.80
121.80
121.36
121.03
117.07
114.63
112.00
111.43
55.94
52.86
42.32
O
O
N
H
HO
O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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121.02
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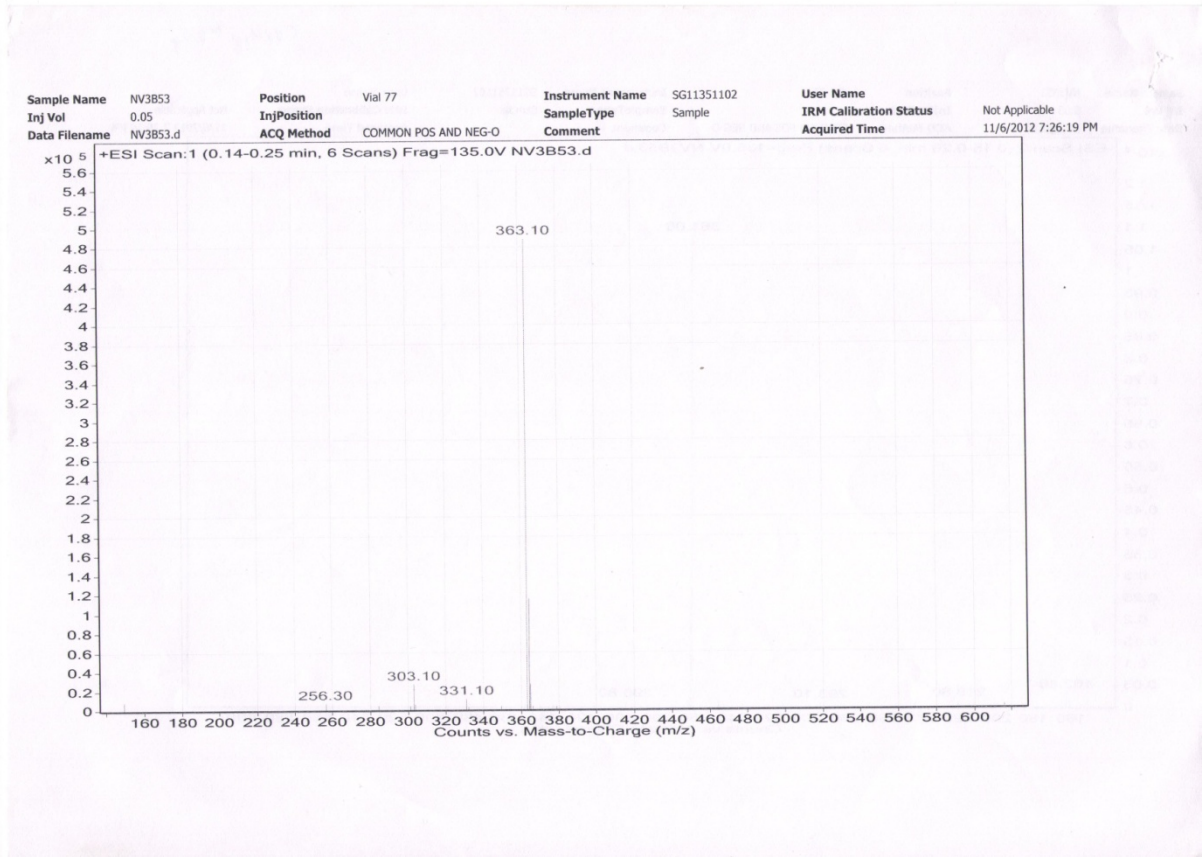
f1 (ppm)


Sample Name NV3B53
Inj Vol 0.05
Data Filename NV3B53.d
Position Vial 77
InjPosition
ACQ Method COMMON POS AND NEG-O
Instrument Name SG11351102
SampleType Sample
Comment
User Name
IRM Calibration Status Not Applicable
Acquired Time 11/6/2012 7:26:19 PM
+ESI Scan:1 (0.14-0.25 min, 6 Scans) Frag=135.0V NV3B53.d
x10 5
363.10
303.10
331.10
256.30
160 180 200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500 520 540 560 580 600
Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

Data File	NV3B-53.d	**Sample Name**	NV3B-53
Sample Type	Sample	**Position**	Vial 41
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	11/7/2012 1:55:34 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

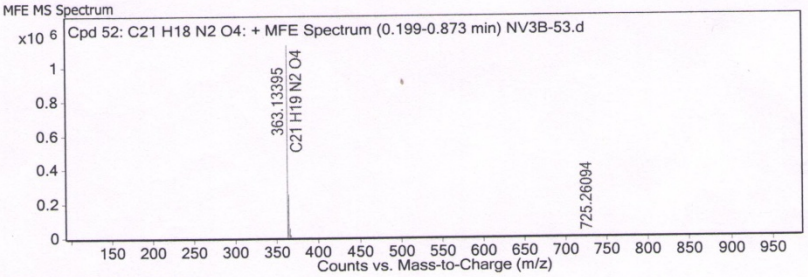
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 52: C21 H18 N2 O4	0.289	362.12667	C21 H18 N2 O4	C21 H18 N2 O4	-0.04	C21 H18 N2 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 52: C21 H18 N2 O4	363.13395	0.289	Find by Molecular Feature	362.12667

MFE MS Spectrum



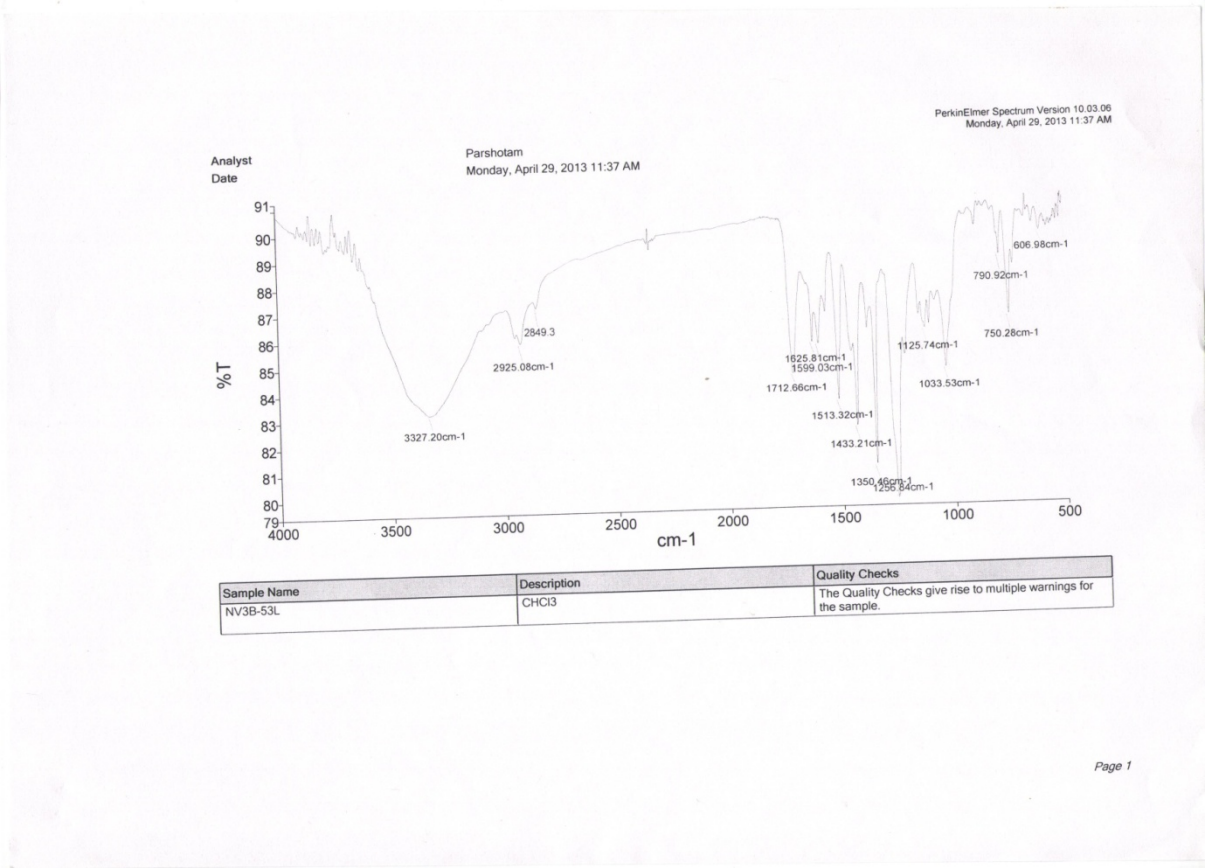
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
363.13395	1	1126750.8	C21 H19 N2 O4	(M+H)+
364.1367	1	248058.3	C21 H19 N2 O4	(M+H)+
365.14343	1	54018.2	C21 H19 N2 O4	(M+H)+
366.14896	1	9800	C21 H19 N2 O4	(M+H)+
367.15308	1	1811.6	C21 H19 N2 O4	(M+H)+
725.26094	1	1377.6		(2M+H)+
726.2583	1	1075.5		(2M+H)+

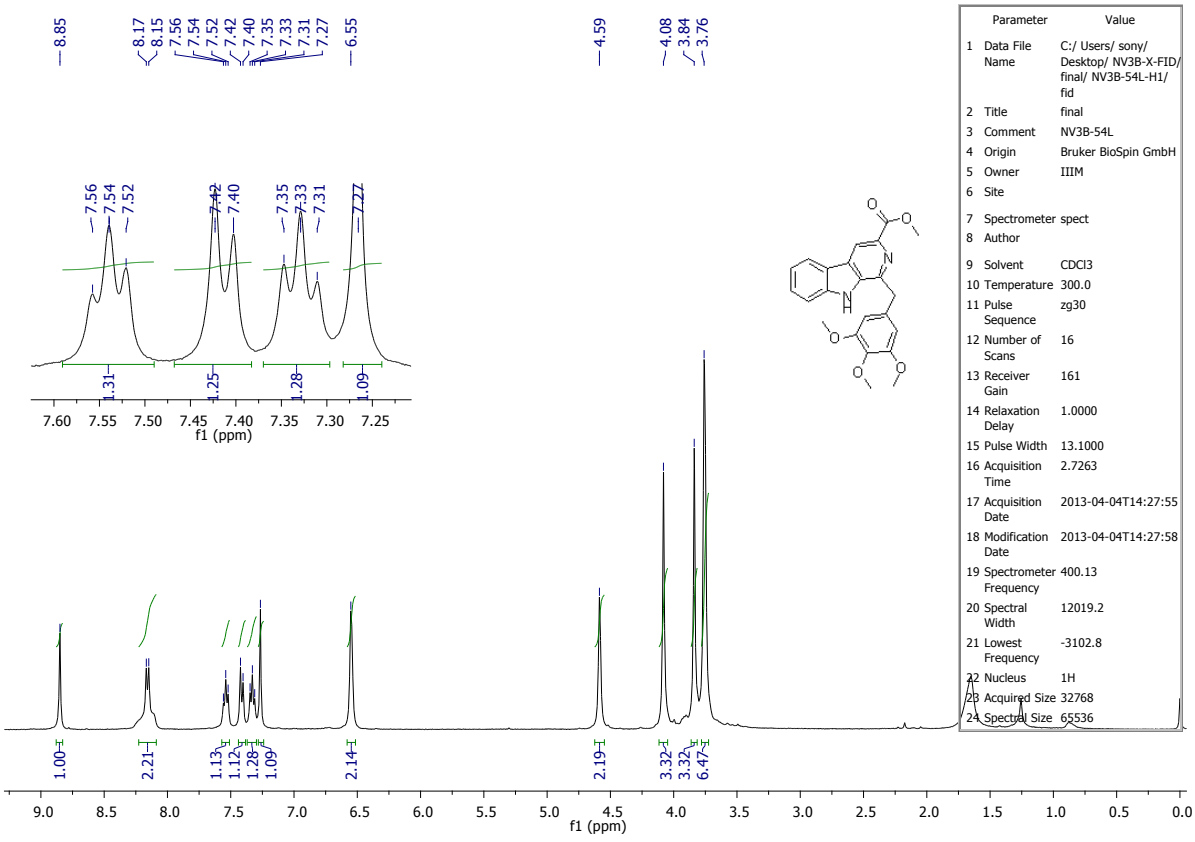
Predicted Isotope Match Table

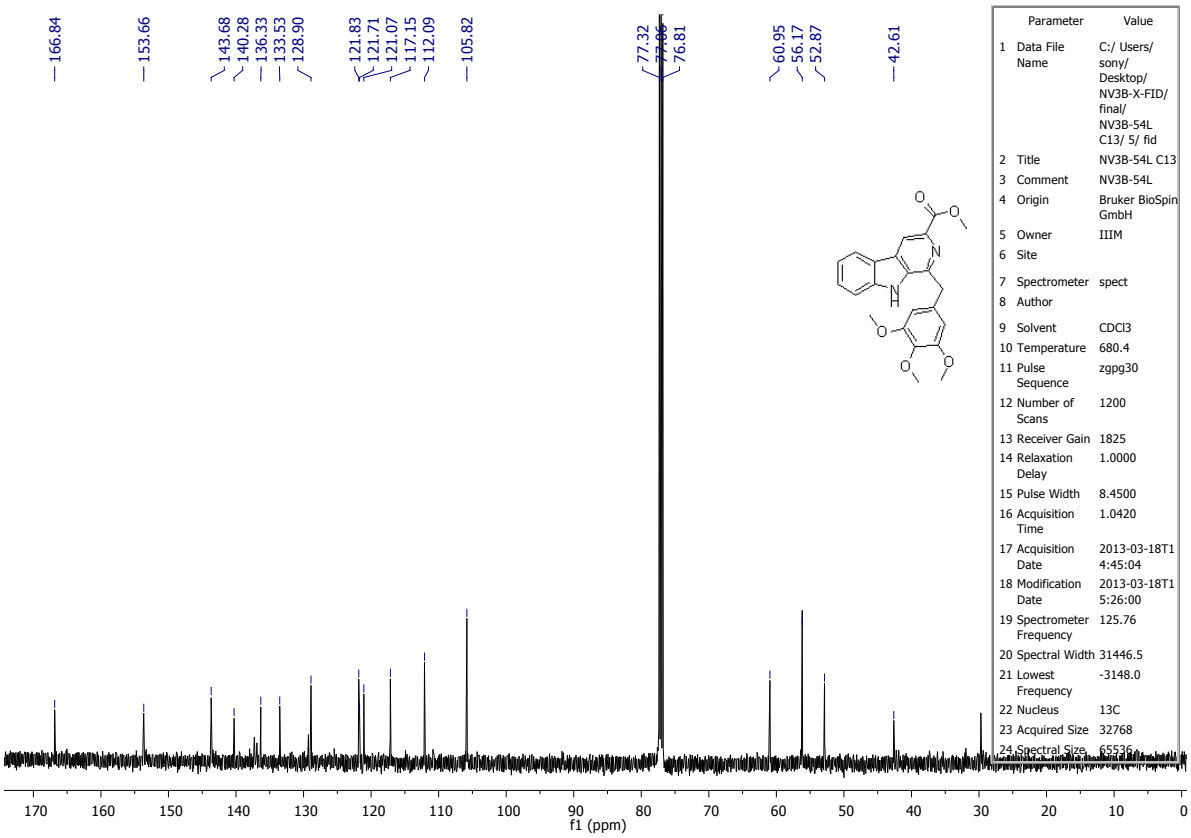
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	363.13395	363.13393	-0.06	100	100	78.22	78.26
2	364.1367	364.13713	1.17	22.02	23.81	17.22	18.64
3	365.14343	365.13982	-9.89	4.79	3.53	3.75	2.77
4	366.14896	366.14243	-17.83	0.87	0.39	0.68	0.31
5	367.15308	367.14501	-21.99	0.16	0.03	0.13	0.03

--- End Of Report ---

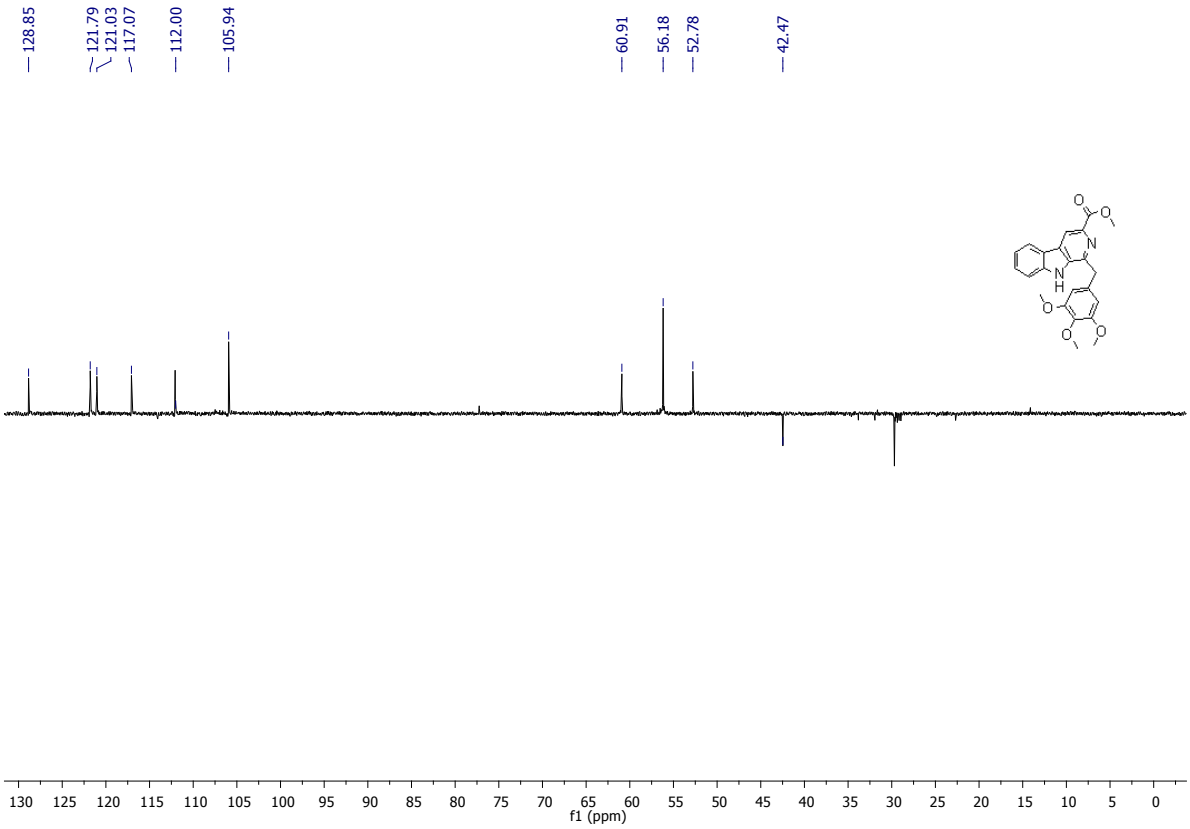


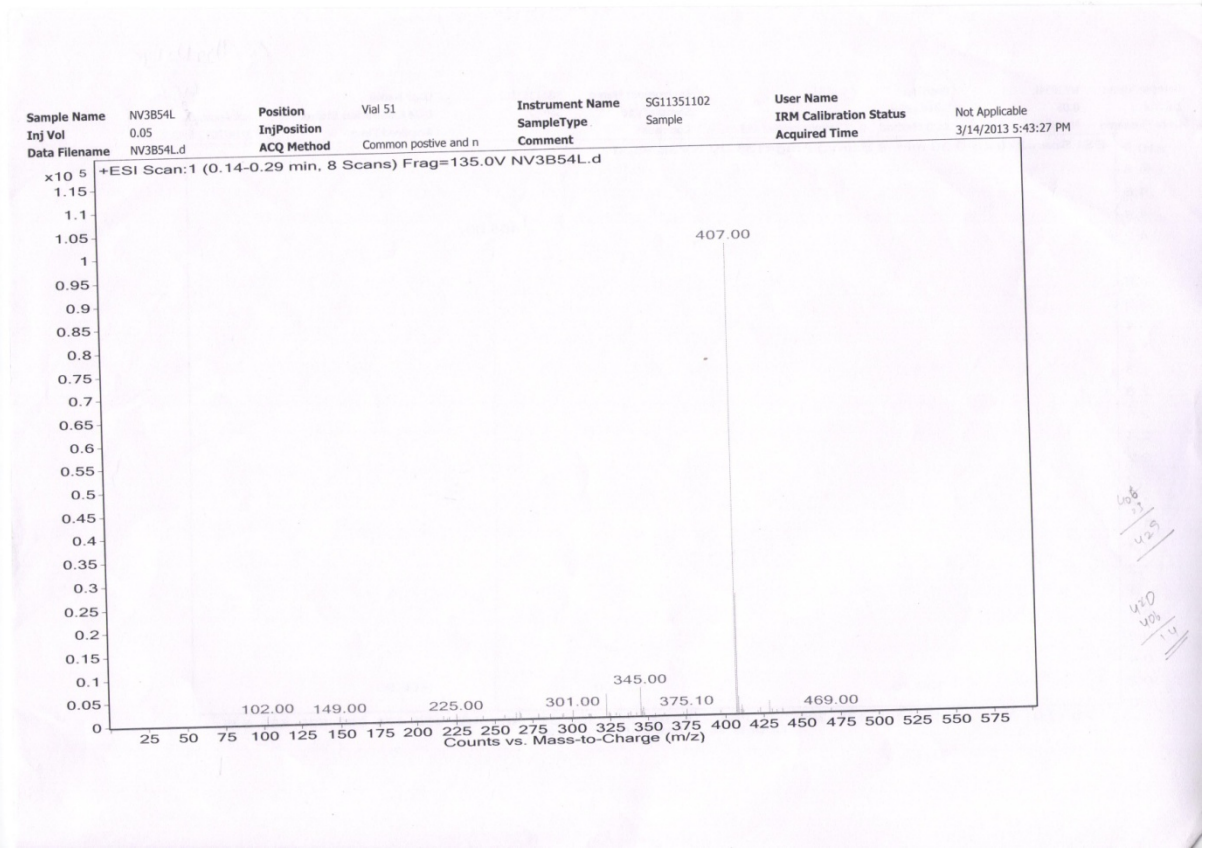
6g) Methyl 1-(3,4,5-trimethoxybenzyl)-9H-pyrido[3,4-b]indole-3-carboxylate:





	Parameter	Value
1	Data File Name	C:/ Users/ sony/ Desktop/ NV3B-X-FID/ final/ NV3B-54L C13/ 5/ fid
2	Title	NV3B-54L C13
3	Comment	NV3B-54L
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	680.4
11	Pulse Sequence	zgpg30
12	Number of Scans	1200
13	Receiver Gain	1825
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0420
17	Acquisition Date	2013-03-18T14:45:04
18	Modification Date	2013-03-18T15:26:00
19	Spectrometer Frequency	125.76
20	Spectral Width	31446.5
21	Lowest Frequency	-3148.0
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536


128.85
121.79
121.03
117.07
112.00
105.94
60.91
56.18
52.78
42.47
130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)


Sample Name NV3B54L
Inj Vol 0.05
Data Filename NV3B54L.d
Position Vial 51
InjPosition
ACQ Method Common postive and n
Instrument Name SG11351102
SampleType Sample
Comment
User Name
IRM Calibration Status Not Applicable
Acquired Time 3/14/2013 5:43:27 PM
+ESI Scan:1 (0.14-0.29 min, 8 Scans) Frag=135.0V NV3B54L.d
x10 5
407.00
345.00
102.00
149.00
225.00
301.00
375.10
469.00
Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

Data File	NV3B-54L.d	**Sample Name**	NV3B-54L
Sample Type	Sample	**Position**	Vial 2
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	06-09-2013 AM 11:42:23
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

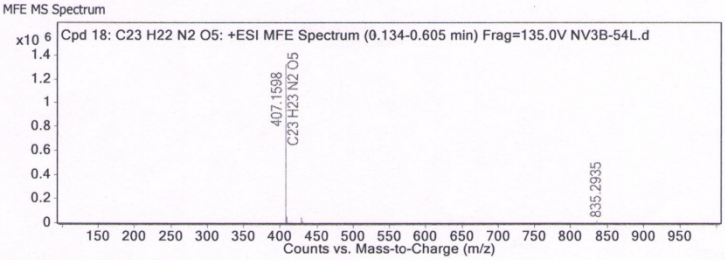
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 18: C23 H22 N2 O5	0.193	406.1526	C23 H22 N2 O5	C23 H22 N2 O5	0.69	C23 H22 N2 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 18: C23 H22 N2 O5	407.1598	0.193	Find by Molecular Feature	406.1526

MFE MS Spectrum



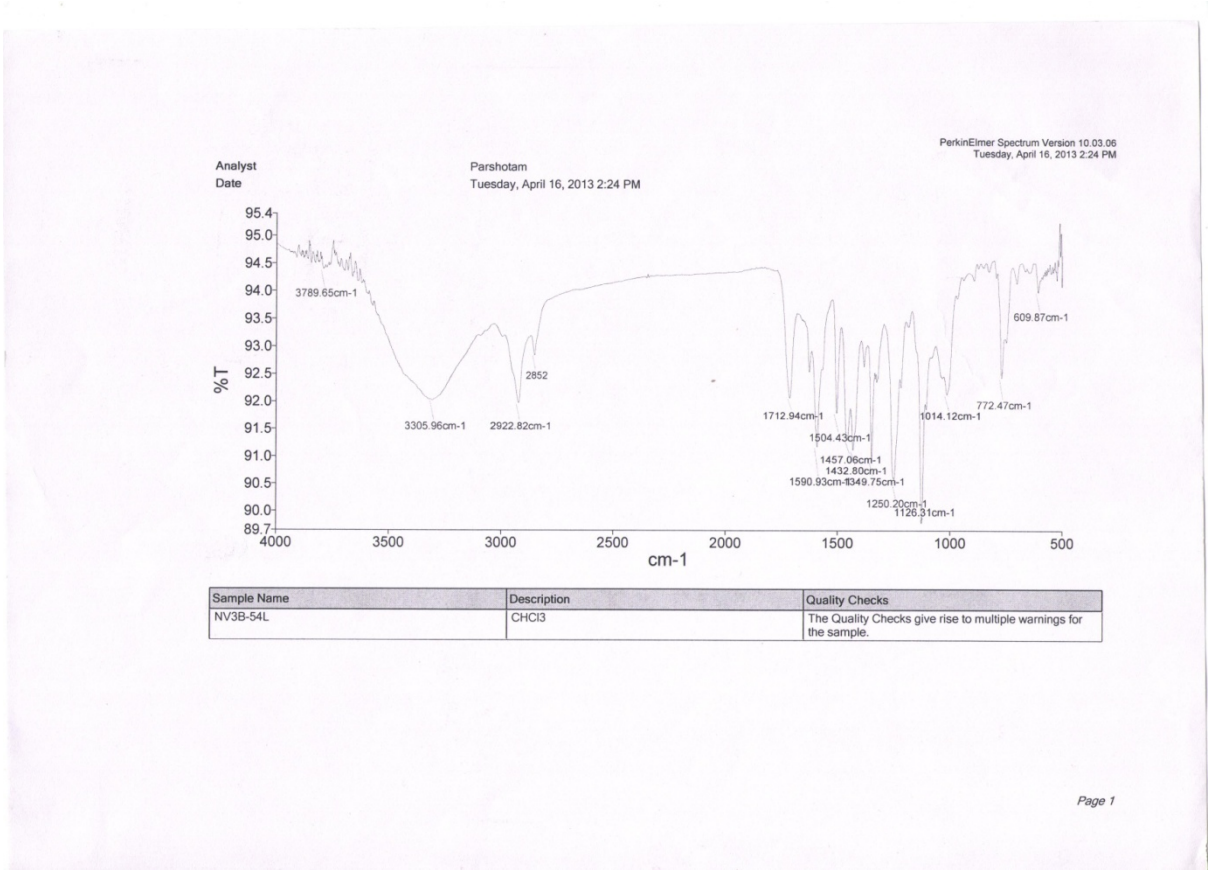
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
407.1598	1	1323387.38	C23 H23 N2 O5	(M+H)+
408.1634	1	320527.78	C23 H23 N2 O5	(M+H)+
409.1657	1	51522.08	C23 H23 N2 O5	(M+H)+
410.1679	1	6680.48	C23 H23 N2 O5	(M+H)+
429.1413	1	43063.52	C23 H22 N2 Na O5	(M+Na)+
430.1448	1	11433.1	C23 H22 N2 Na O5	(M+Na)+
431.1469	1	1758.17	C23 H22 N2 Na O5	(M+Na)+
835.2935	1	15240.44		(2M+Na)+
836.2967	1	8595.12		(2M+Na)+
837.2996	1	3073.66		(2M+Na)+

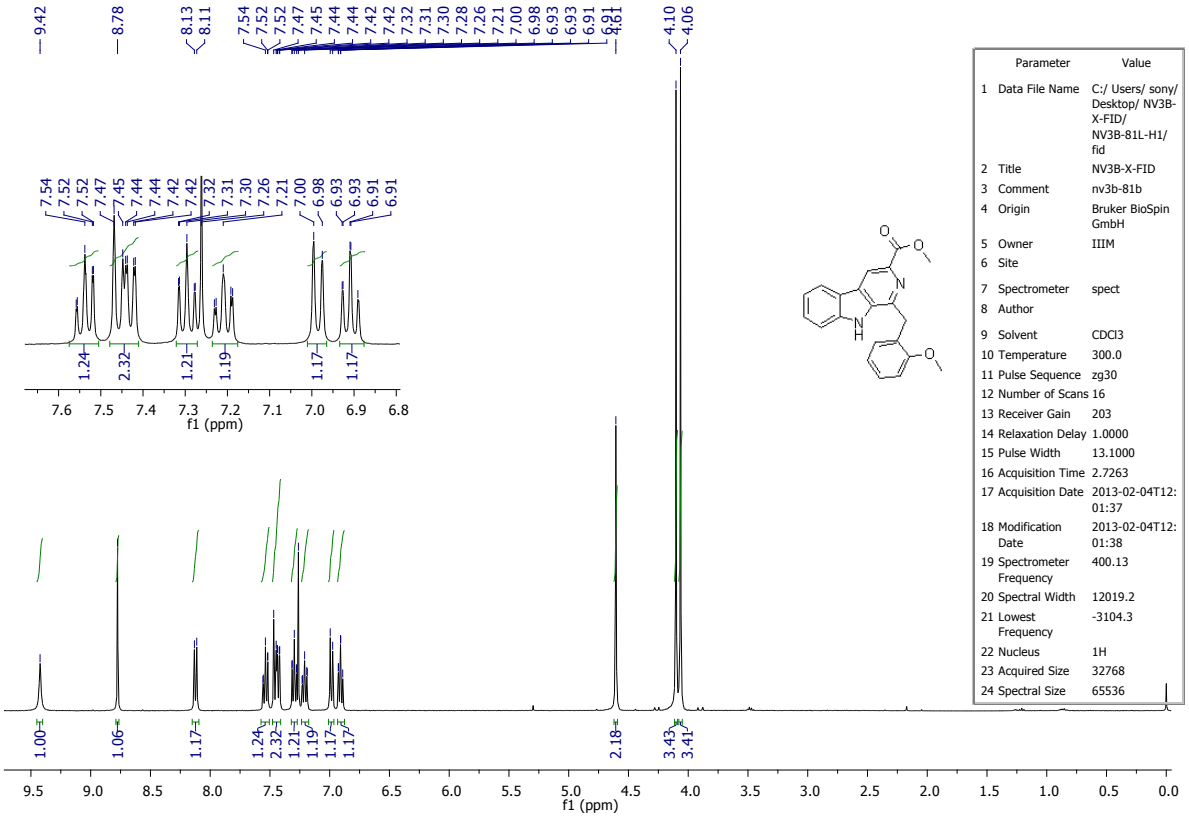
Predicted Isotope Match Table

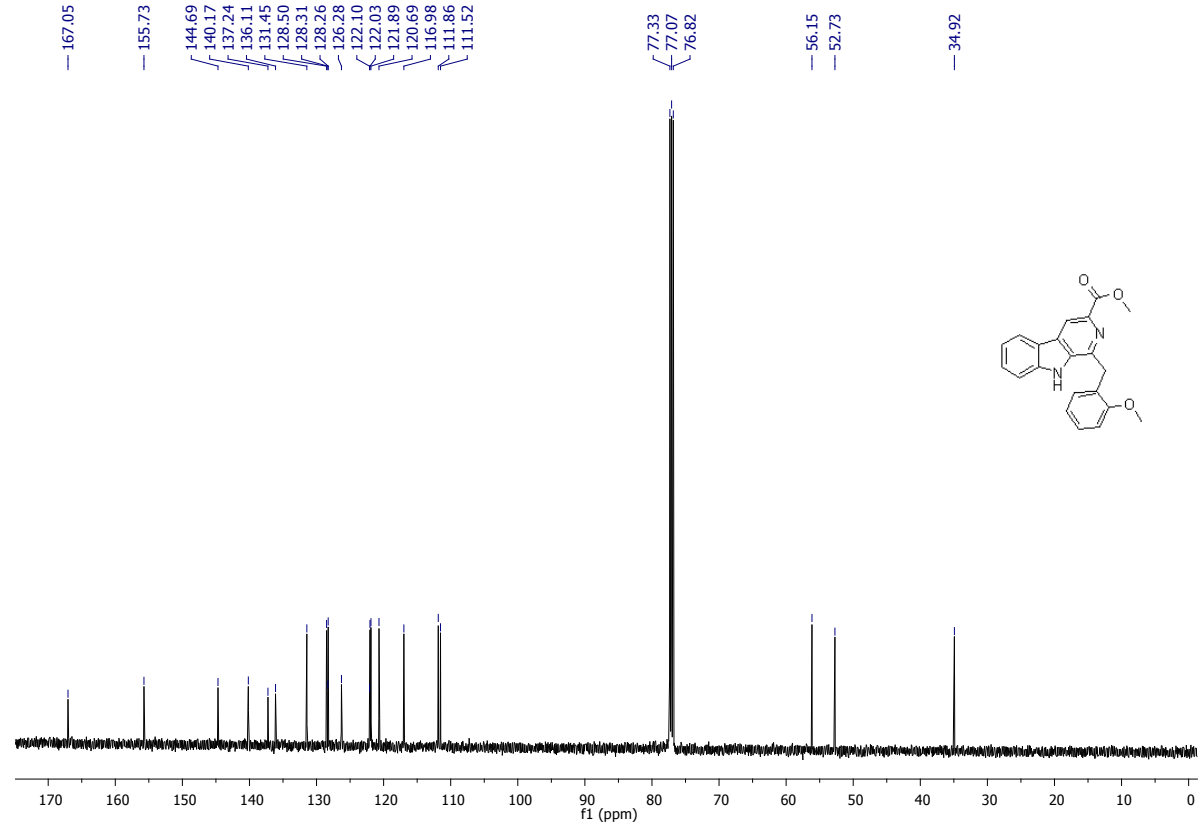
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	407.1598	407.1601	0.88	100	100	77.72	76.38
2	408.1634	408.1634	-0.09	24.22	26.06	18.82	19.91
3	409.1657	409.166	0.76	3.89	4.29	3.03	3.27
4	410.1679	410.1687	1.8	0.5	0.53	0.39	0.4
5	411.1756	411.1712	-10.7	0.05	0.05	0.04	0.04

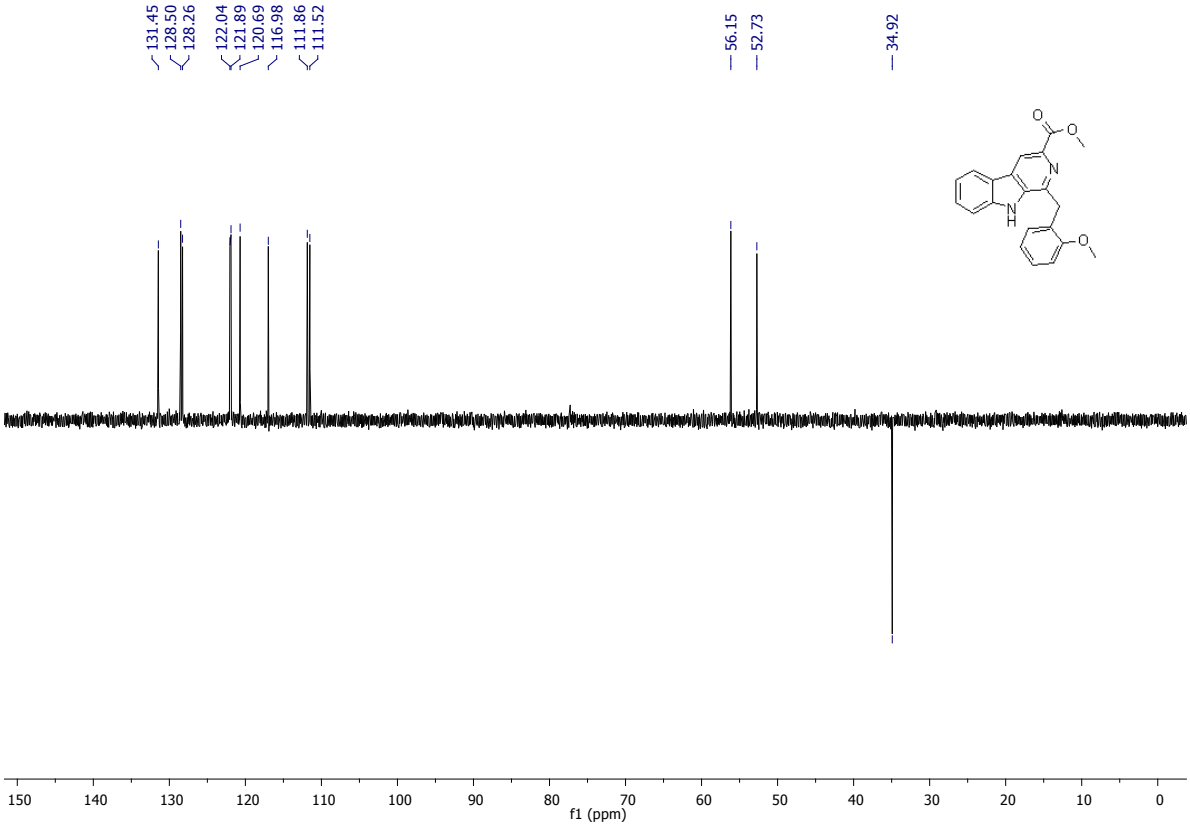
--- End Of Report ---

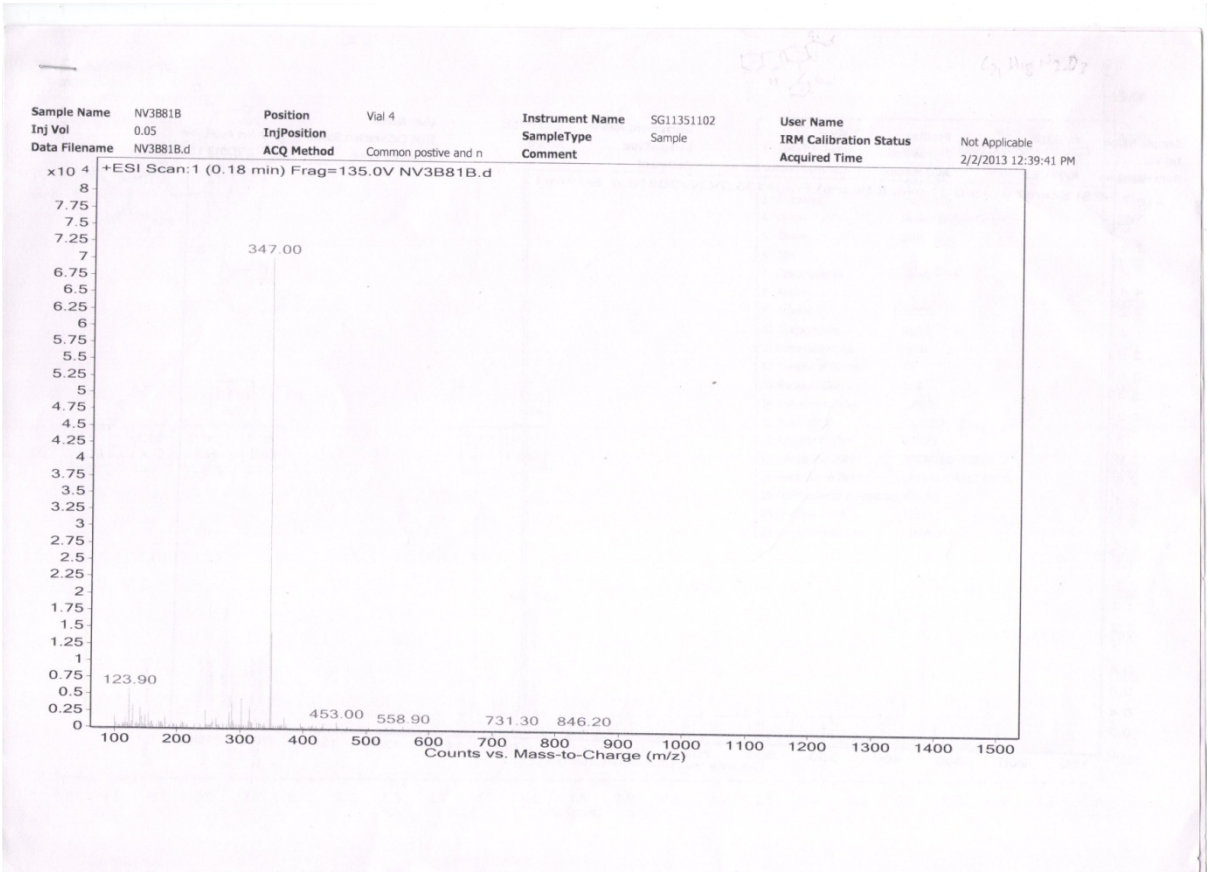


6h) Methyl 1-(2-methoxybenzyl)-9H-pyrido[3,4-b]indole-3-carboxylate:




167.05
155.73
144.69
140.17
137.24
136.11
131.45
128.50
128.31
128.26
126.28
122.10
122.03
121.89
120.69
116.98
111.86
111.52
77.33
77.07
76.82
56.15
52.73
34.92
O
O
N
N
H
O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


131.45
128.50
128.26
122.04
121.89
120.69
116.98
111.86
111.52
56.15
52.73
34.92
O
O
N
H
O
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


Sample Name NV3B81B
Inj Vol 0.05
Data Filename NV3B81B.d
Position Vial 4
InjPosition
ACQ Method Common postive and n
Instrument Name SG11351102
SampleType Sample
Comment
User Name
IRM Calibration Status Not Applicable
Acquired Time 2/2/2013 12:39:41 PM
x10 4
+ESI Scan:1 (0.18 min) Frag=135.0V NV3B81B.d
347.00
123.90
453.00
558.90
731.30
846.20
Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

Data File	NV3B-81B.d	**Sample Name**	NV3B-81B
Sample Type	Sample	**Position**	Vial 21
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	05-03-2013 PM 2:35:52
IRM Calibration Status	Success	**DA Method**	SamplePurity-Default.m
Comment			

Info.

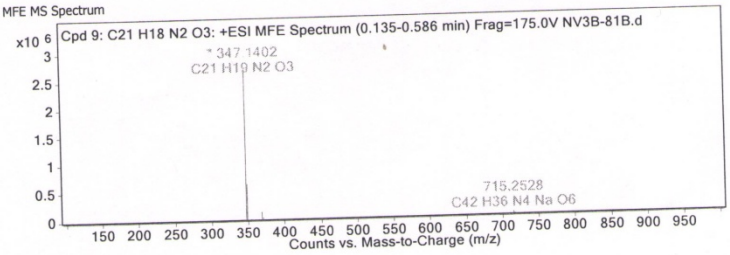
Sample Group	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 9: C21 H18 N2 O3	0.189	346.1329	C21 H18 N2 O3	C21 H18 N2 O3	-3.41	C21 H18 N2 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 9: C21 H18 N2 O3	347.1402	0.189	Find by Molecular Feature	346.1329

MFE MS Spectrum



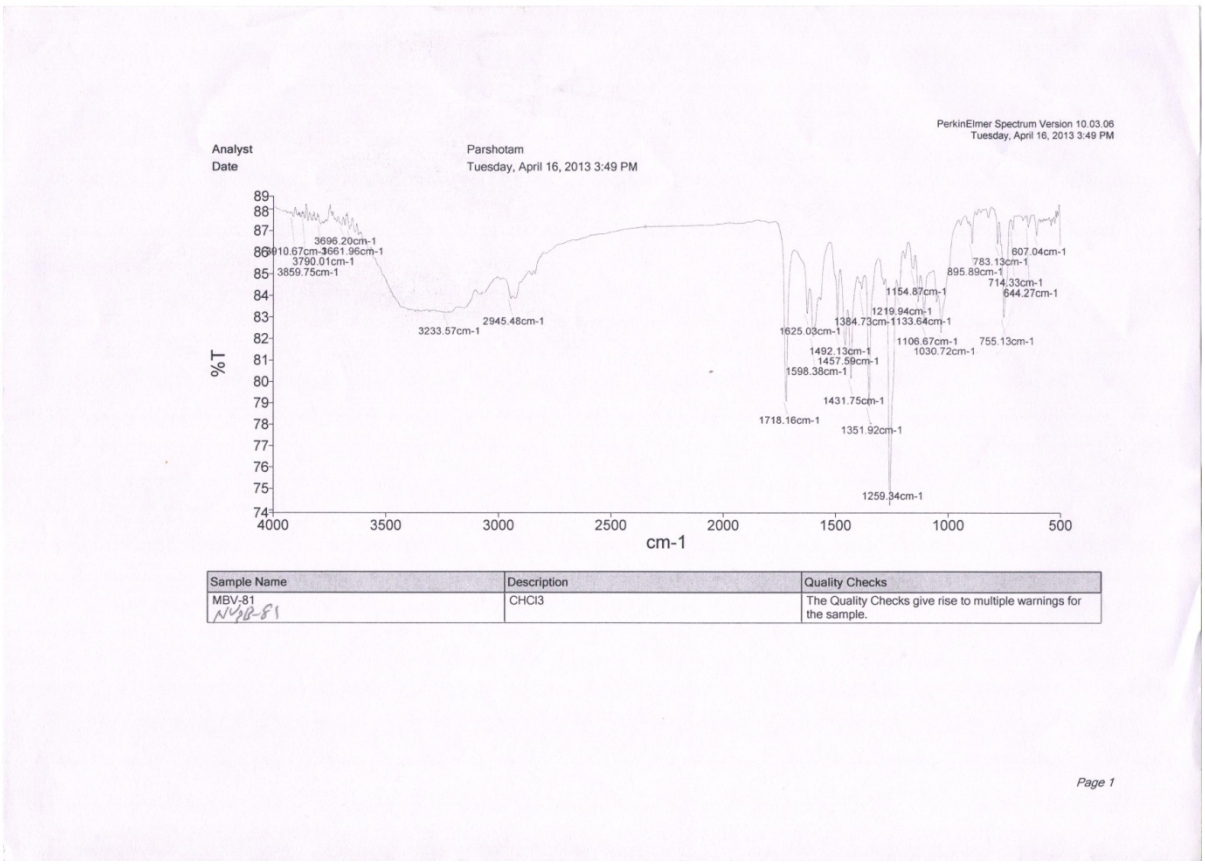
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
347.1402	1	2696448	C21 H19 N2 O3	(M+H)+
348.1436	1	624702.88	C21 H19 N2 O3	(M+H)+
349.1451	1	84869.91	C21 H19 N2 O3	(M+H)+
350.1476	1	7096.09	C21 H19 N2 O3	(M+H)+
369.1211	1	122056.3	C21 H18 N2 Na O3	(M+Na)+
370.1241	1	28274.41	C21 H18 N2 Na O3	(M+Na)+
371.1278	1	4299.05	C21 H18 N2 Na O3	(M+Na)+
715.2528	1	33629.79	C42 H36 N4 Na O6	(2M+Na)+
716.2562	1	15795.19	C42 H36 N4 Na O6	(2M+Na)+
717.2585	1	4902.11	C42 H36 N4 Na O6	(2M+Na)+

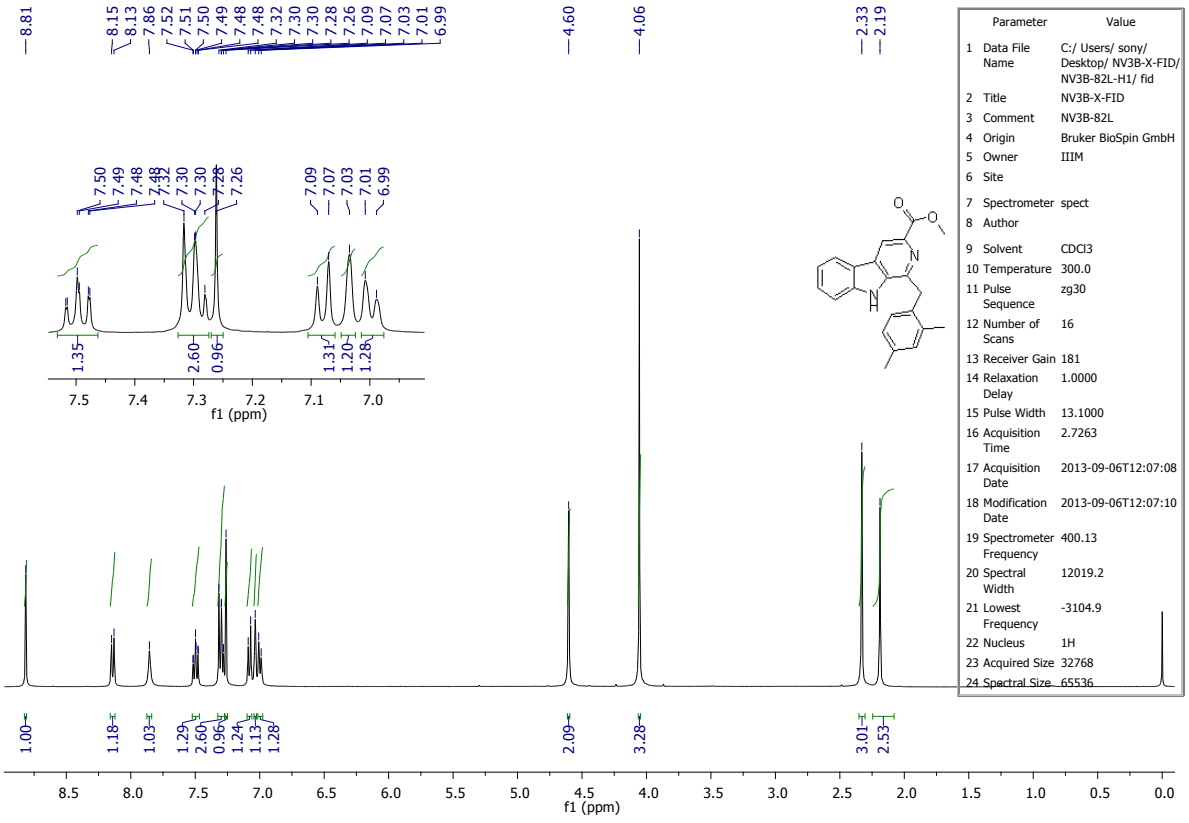
Predicted Isotope Match Table

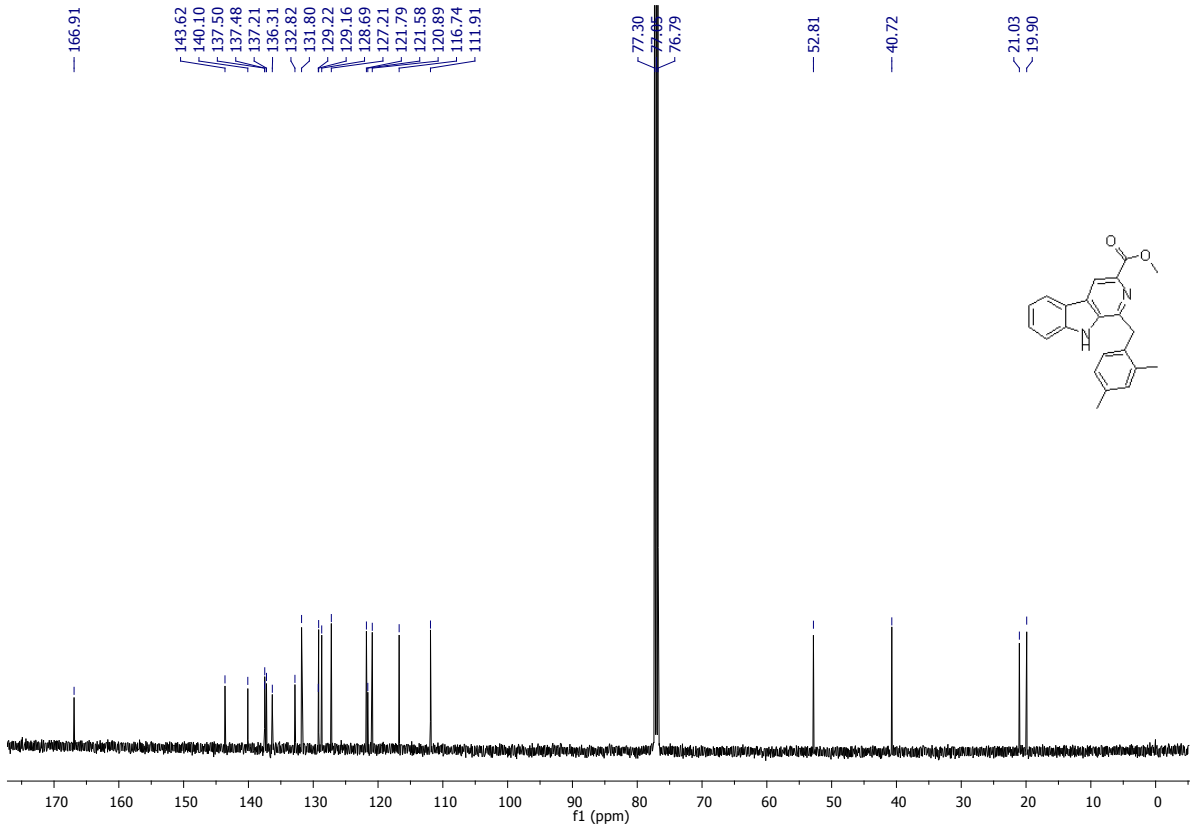
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	347.1402	347.139	-3.39	100	100	78.98	78.45
2	348.1436	348.1422	-3.88	23.17	23.78	18.3	18.65
3	349.1451	349.145	-0.43	3.15	3.32	2.49	2.6
4	350.1476	350.1477	0.09	0.26	0.34	0.21	0.27
5	351.1512	351.1503	-2.66	0.03	0.03	0.03	0.02

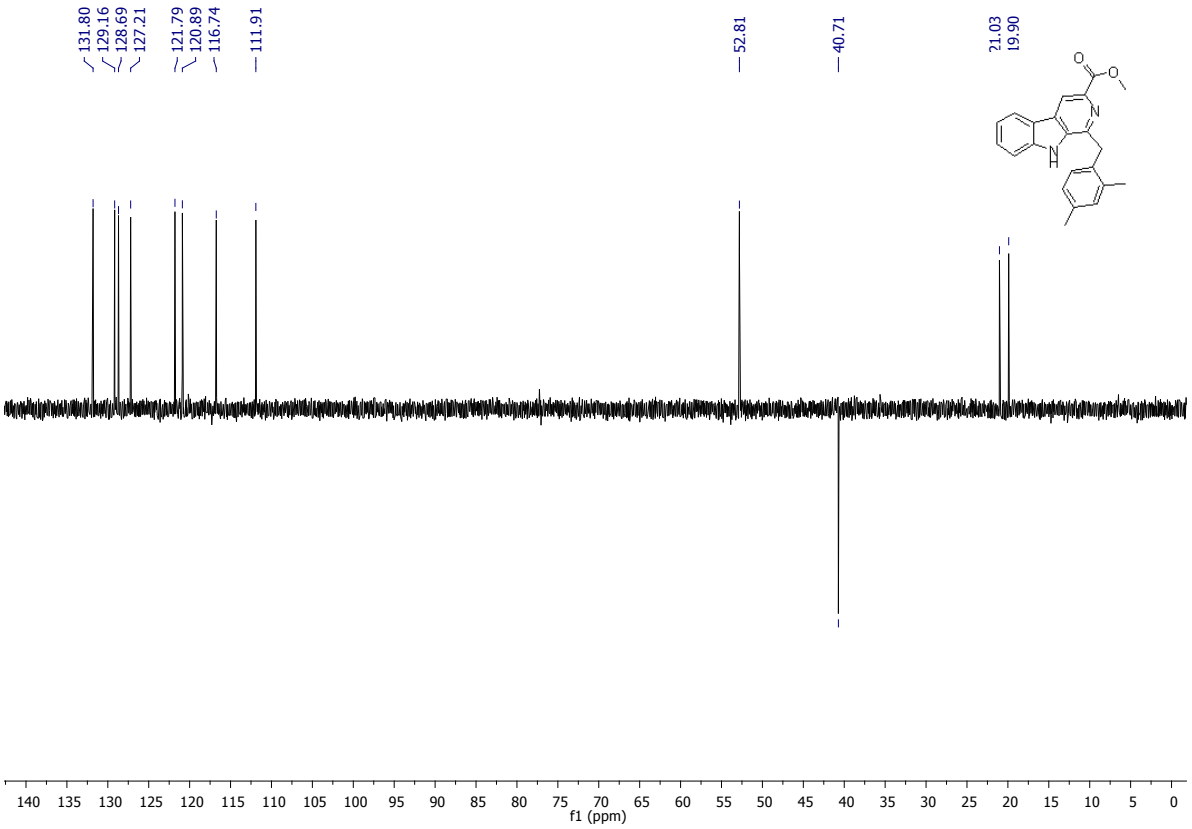
--- End Of Report ---

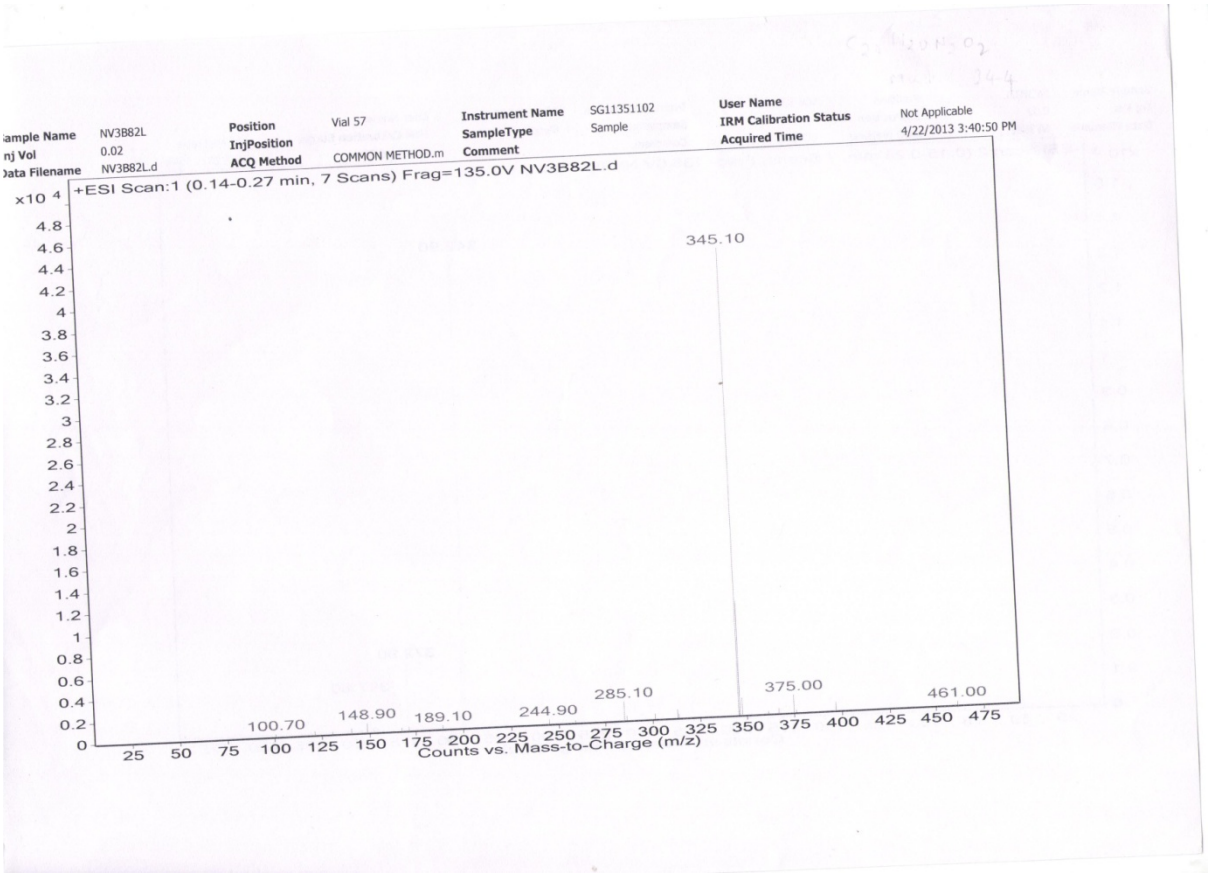


6i) Methyl 1-(2,4-dimethylbenzyl)-9H-pyrido[3,4-b]indole-3-carboxylate:




166.91
143.62
140.10
137.50
137.48
137.21
136.31
132.82
131.80
129.22
129.16
128.69
127.21
121.79
121.58
120.89
116.74
111.91
77.30
77.05
76.79
52.81
40.72
21.03
19.90
O
O
N
H
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


131.80
129.16
128.69
127.21
121.79
120.89
116.74
111.91
52.81
40.71
21.03
19.90
140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)


Sample Name NV3B82L
Inj Vol 0.02
Data Filename NV3B82L.d
Position Vial 57
InjPosition
ACQ Method COMMON METHOD.m
Instrument Name SG11351102
SampleType Sample
Comment
User Name
IRM Calibration Status Not Applicable
Acquired Time 4/22/2013 3:40:50 PM
+ESI Scan:1 (0.14-0.27 min, 7 Scans) Frag=135.0V NV3B82L.d
x10 4
345.10
285.10
375.00
461.00
100.70
148.90
189.10
244.90
Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

Data File	NV3B-82L.d	**Sample Name**	NV3B-82L
Sample Type	Sample	**Position**	Vial 15
Instrument Name	Instrument 1	**User Name**	vishal
Acq Method	vishal_12-01-13.m	**Acquired Time**	23-04-2013 PM 1:01:57
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

Sample Group **Info.**

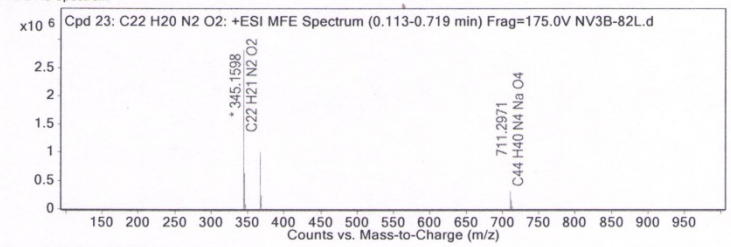
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 23: C22 H20 N2 O2	0.189	344.1527	C22 H20 N2 O2	C22 H20 N2 O2	-0.76	C22 H20 N2 O2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 23: C22 H20 N2 O2	345.1598	0.189	Find by Molecular Feature	344.1527

MFE MS Spectrum



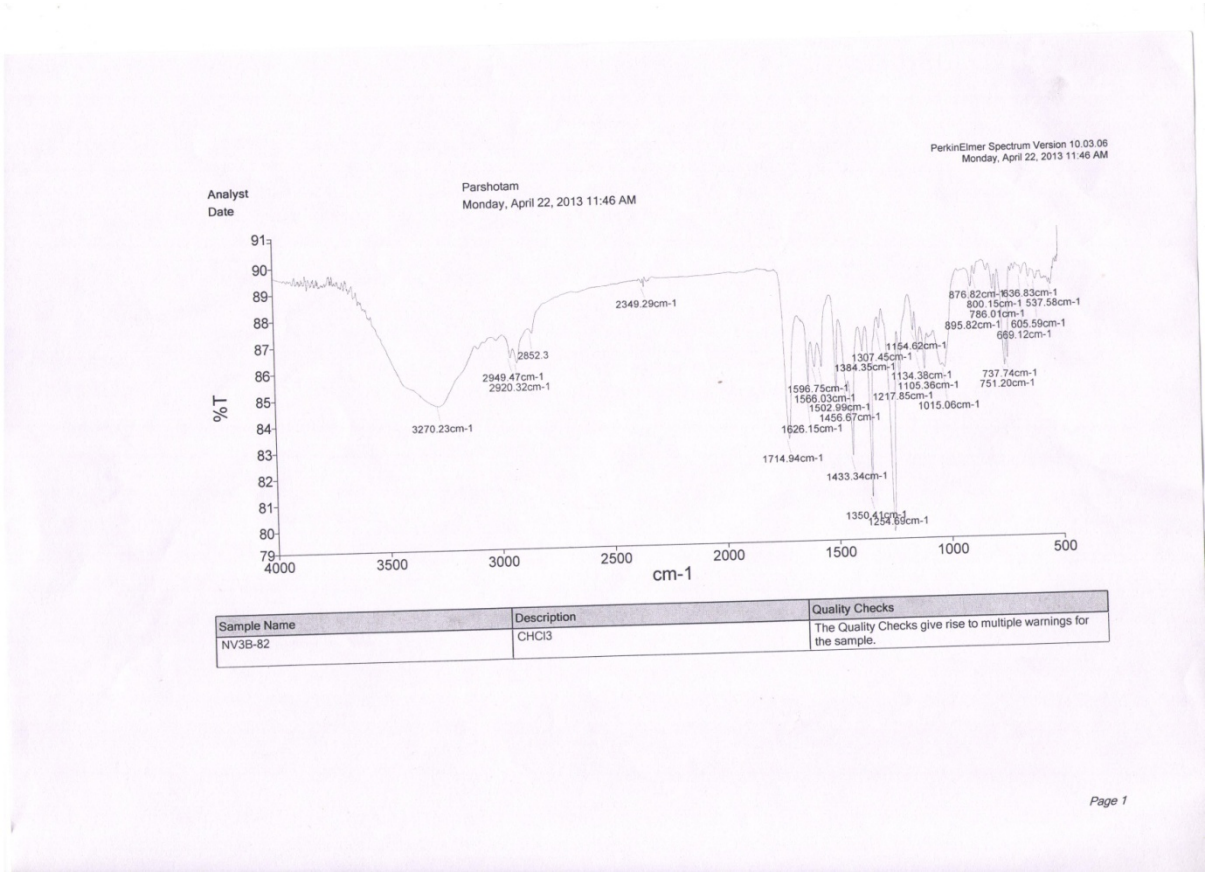
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
345.1598	1	2807460.25	C22 H21 N2 O2	(M+H)+
346.1643	1	637392.63	C22 H21 N2 O2	(M+H)+
347.1664	1	80521.94	C22 H21 N2 O2	(M+H)+
348.169	1	7868.49	C22 H21 N2 O2	(M+H)+
367.1428	1	1006526.75	C22 H20 N2 Na O2	(M+Na)+
368.1457	1	232279.86	C22 H20 N2 Na O2	(M+Na)+
369.1485	1	29741.38	C22 H20 N2 Na O2	(M+Na)+
711.2971	1	325387.97	C44 H40 N4 Na O4	(2M+Na)+
712.2995	1	155883.11	C44 H40 N4 Na O4	(2M+Na)+
713.3021	1	39890.18	C44 H40 N4 Na O4	(2M+Na)+

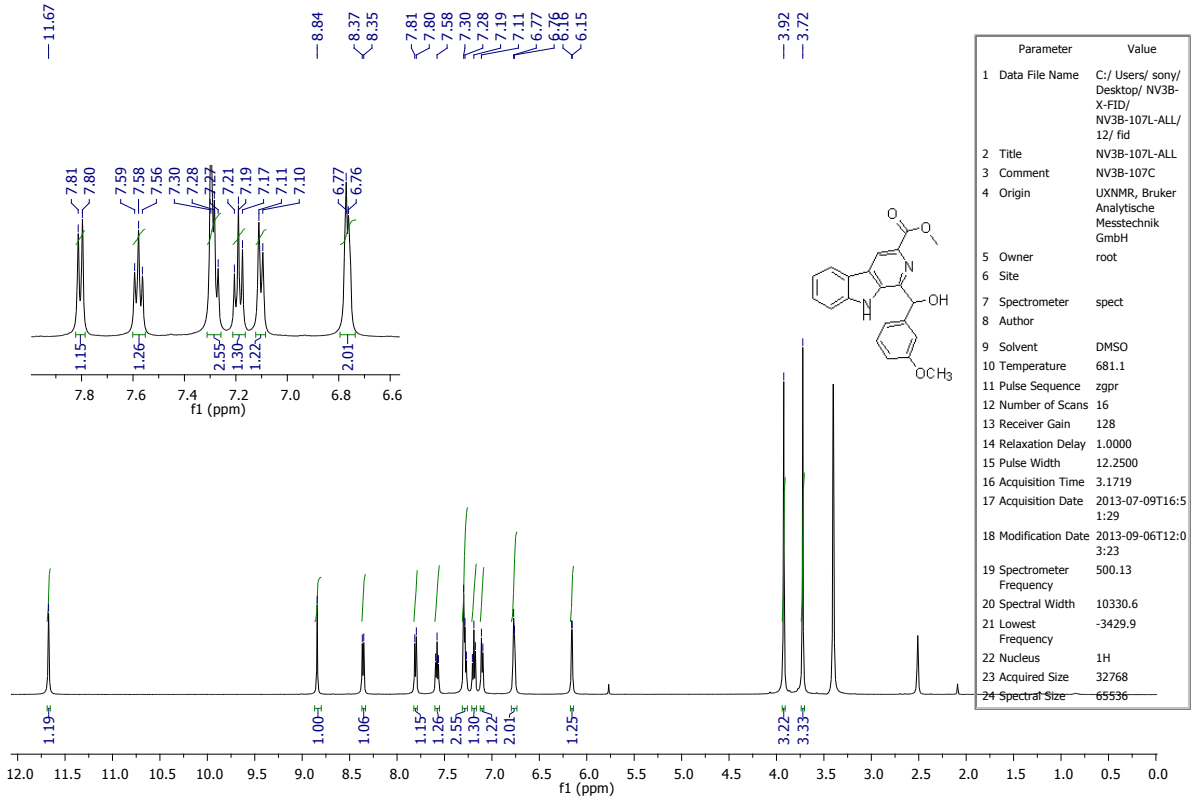
Predicted Isotope Match Table

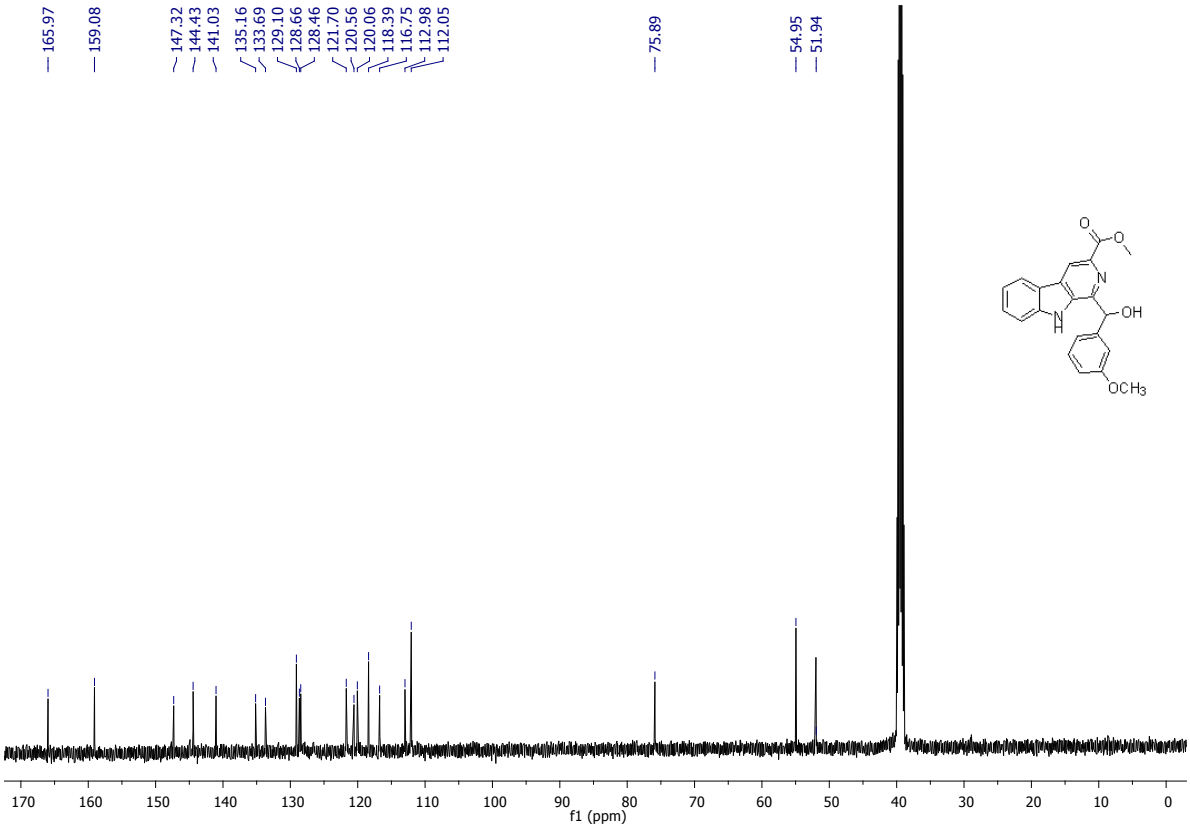
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	345.1598	345.1598	-0.03	100	100	79.43	77.78
2	346.1643	346.163	-3.8	22.7	24.84	18.03	19.32
3	347.1664	347.1659	-1.46	2.87	3.37	2.28	2.62
4	348.169	348.1687	-0.98	0.28	0.33	0.22	0.25
5	349.1797	349.1714	-23.67	0.04	0.02	0.03	0.02

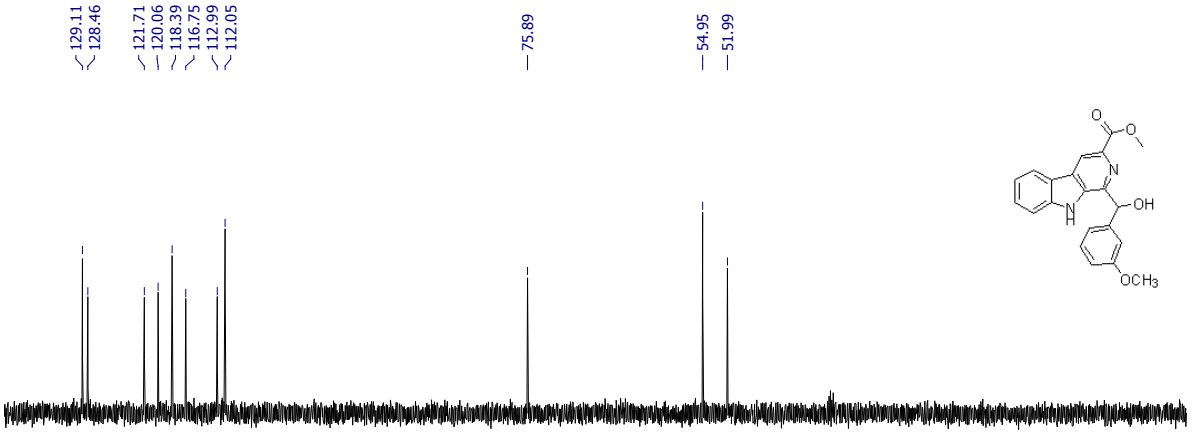
--- End Of Report ---



7k)Methyl1-(hydroxyl(3-methoxyphenyl)methyl)-9H-pyrido[3,4-b]indole-3-carboxylate:




165.97
159.08
147.32
144.43
141.03
135.16
133.69
129.10
128.66
128.46
121.70
120.56
120.06
118.39
116.75
112.98
112.05
75.89
54.95
51.94
O
O
N
H
OH
OCH3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


129.11
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118.39
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112.99
112.05
75.89
54.95
51.99
O
O
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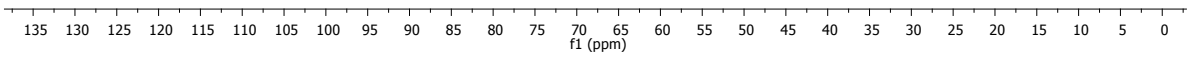
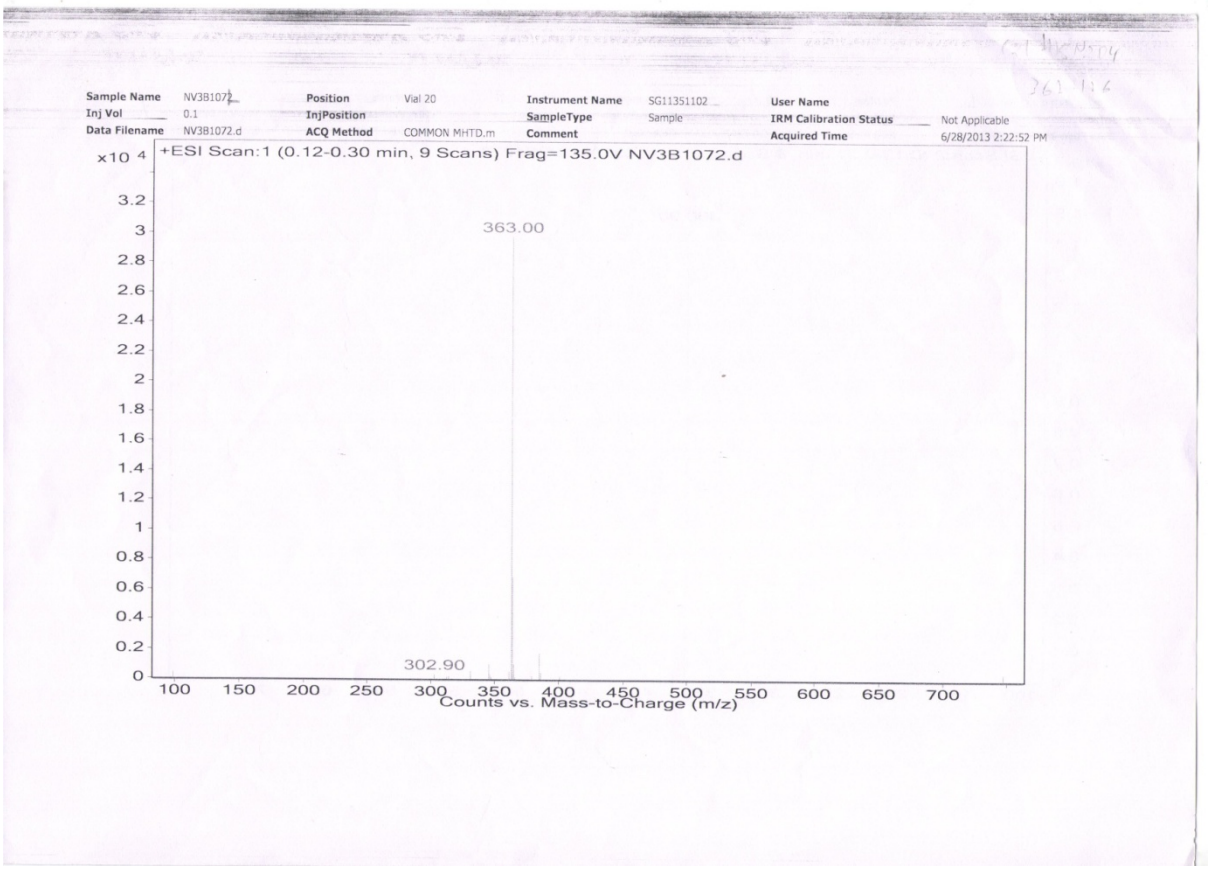
N
H
OH
OCH3


135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)


Sample Name NV3B1072
Position Vial 20
Instrument Name SG11351102
User Name
Inj Vol 0.1
InjPosition
SampleType Sample
IRM Calibration Status Not Applicable
Data Filename NV3B1072.d
ACQ Method COMMON MHTD.m
Comment
Acquired Time 6/28/2013 2:22:52 PM
+ESI Scan:1 (0.12-0.30 min, 9 Scans) Frag=135.0V NV3B1072.d
x10 4
363.00
302.90
Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

Data File	NV3B-107L.d	**Sample Name**	NV3B-107L
Sample Type	Sample	**Position**	Vial 3
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	03-09-2013 AM 10:52:14
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

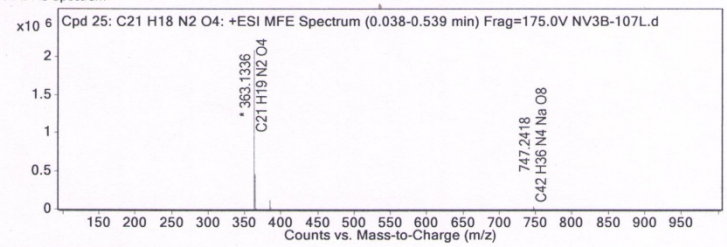
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 25: C21 H18 N2 O4	0.192	362.1265	C21 H18 N2 O4	C21 H18 N2 O4	0.5	C21 H18 N2 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 25: C21 H18 N2 O4	363.1336	0.192	Find by Molecular Feature	362.1265

MFE MS Spectrum



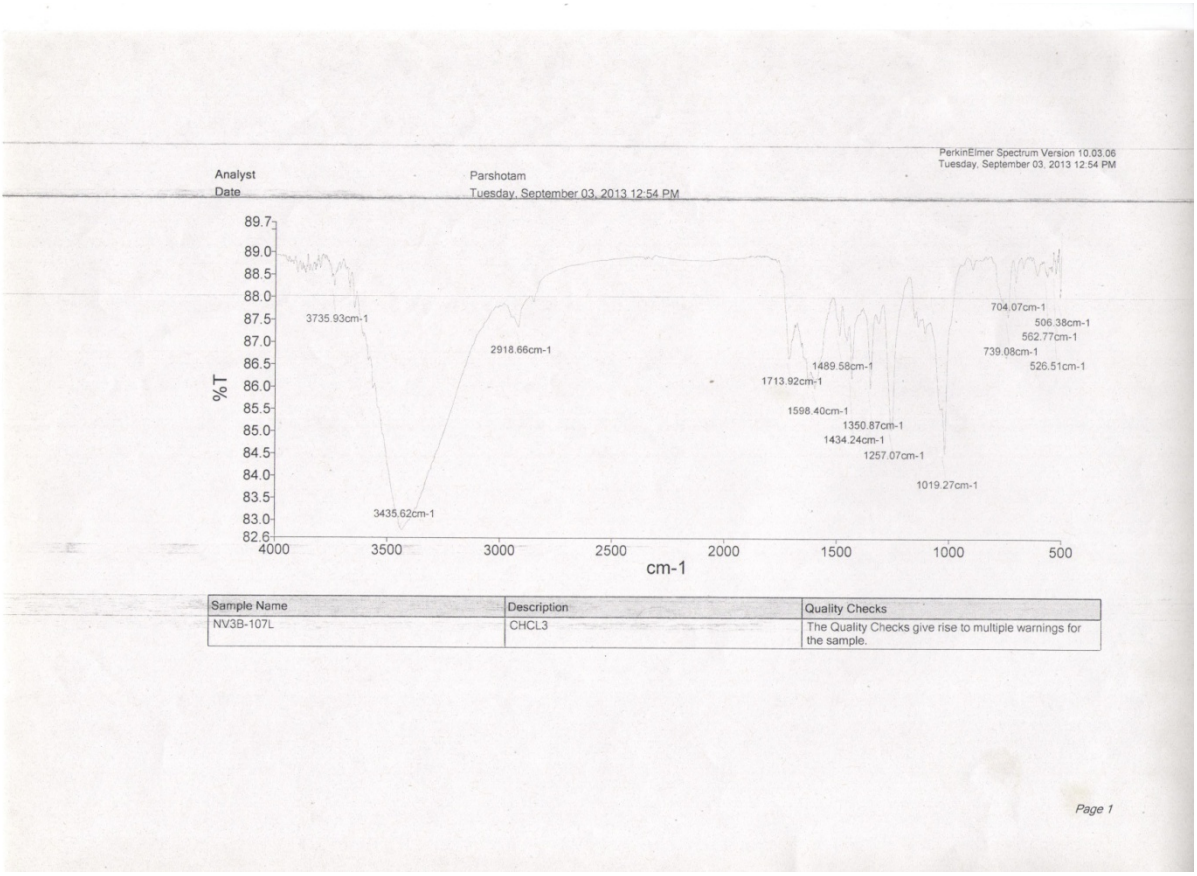
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
363.1336	1	2082372.38	C21 H19 N2 O4	(M+H)+
364.1376	1	459471.13	C21 H19 N2 O4	(M+H)+
365.1397	1	68970.91	C21 H19 N2 O4	(M+H)+
366.1428	1	7133.44	C21 H19 N2 O4	(M+H)+
385.1158	1	119297.59	C21 H18 N2 Na O4	(M+Na)+
386.119	1	28186.28	C21 H18 N2 Na O4	(M+Na)+
387.1209	1	4109.53	C21 H18 N2 Na O4	(M+Na)+
747.2418	1	37353.53	C42 H36 N4 Na O8	(2M+Na)+
748.2455	1	16711.87	C42 H36 N4 Na O8	(2M+Na)+
749.2493	1	5351.61	C42 H36 N4 Na O8	(2M+Na)+

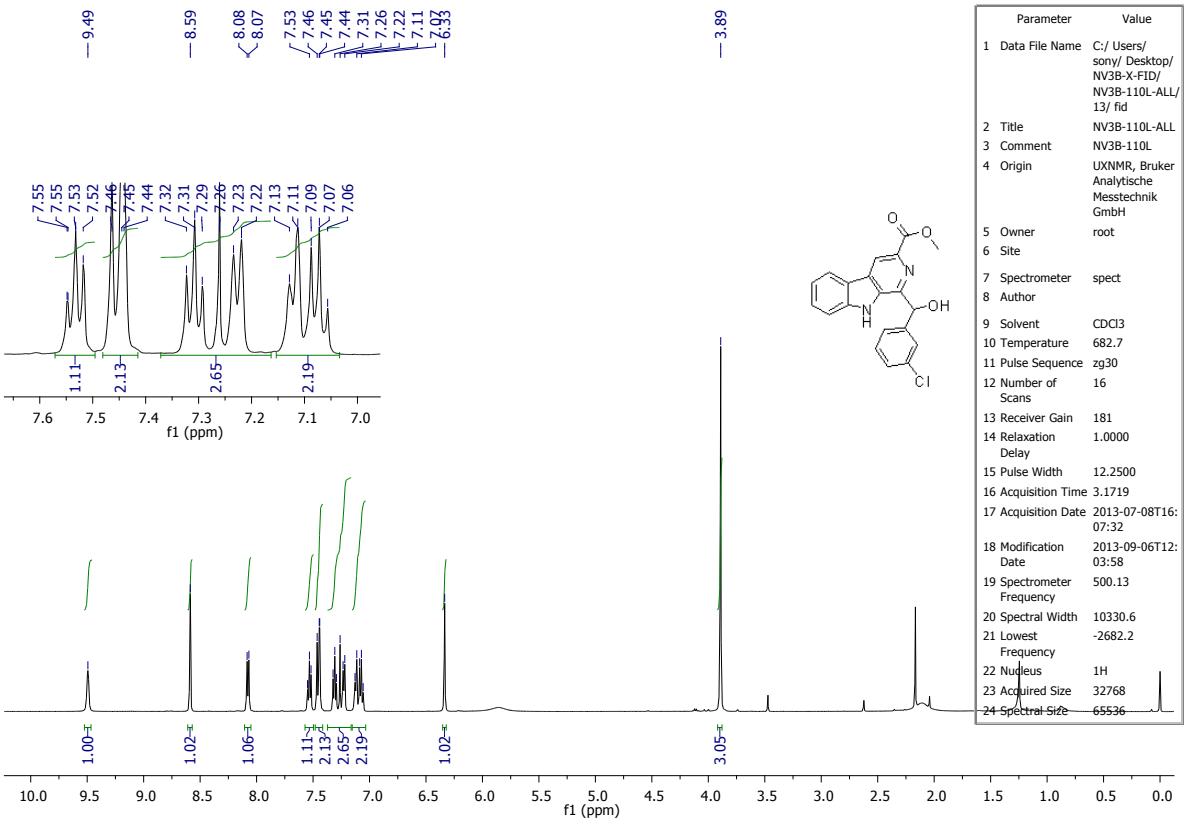
Predicted Isotope Match Table

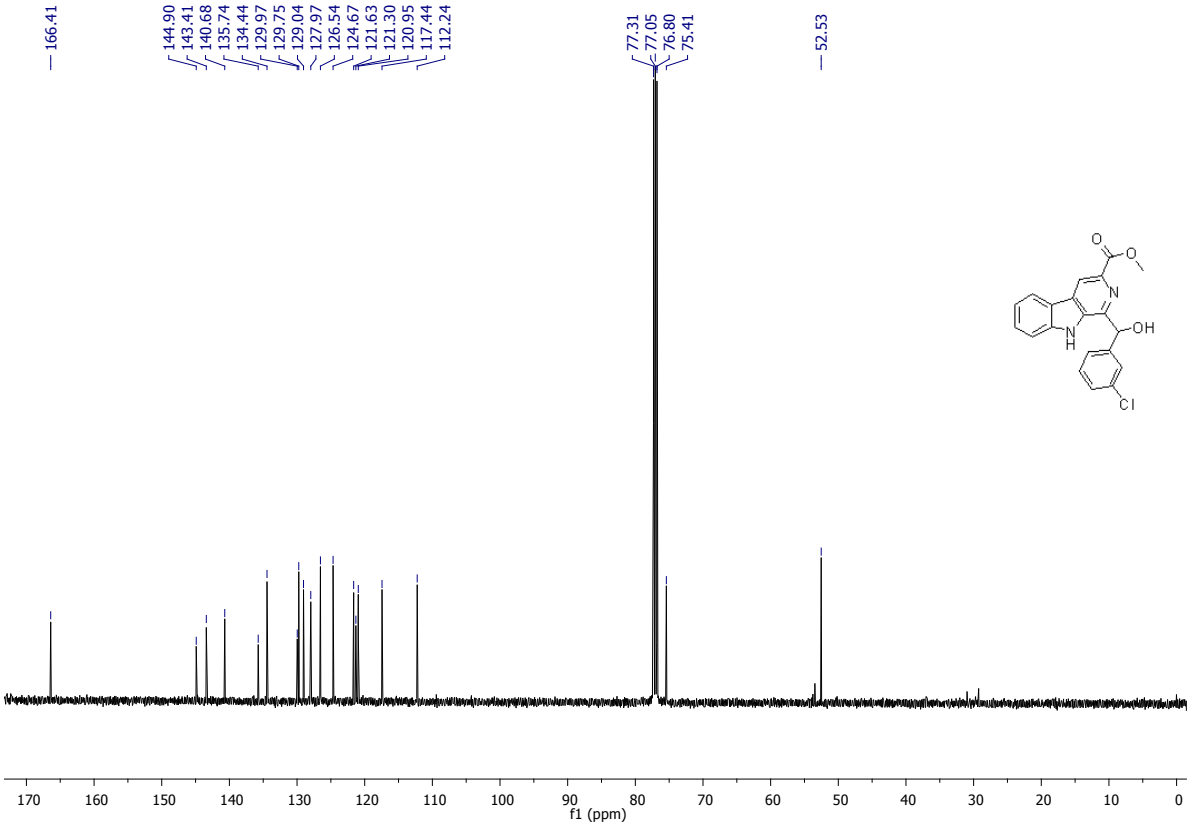
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	363.1336	363.1339	0.92	100	100	79.54	78.28
2	364.1376	364.1371	-1.38	22.06	23.81	17.55	18.64
3	365.1397	365.1398	0.35	3.31	3.53	2.63	2.77
4	366.1428	366.1424	-1.05	0.34	0.39	0.27	0.31

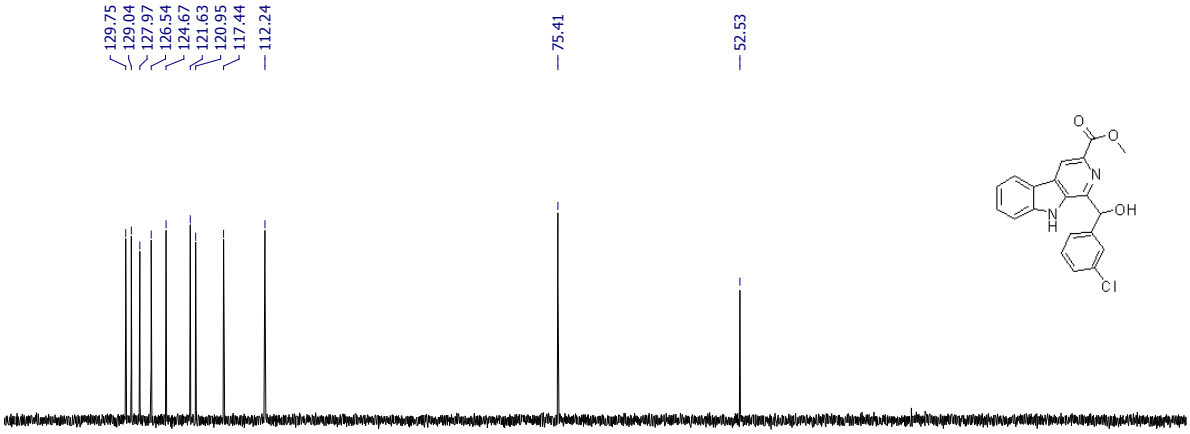
--- End Of Report ---

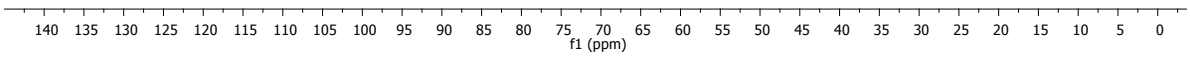


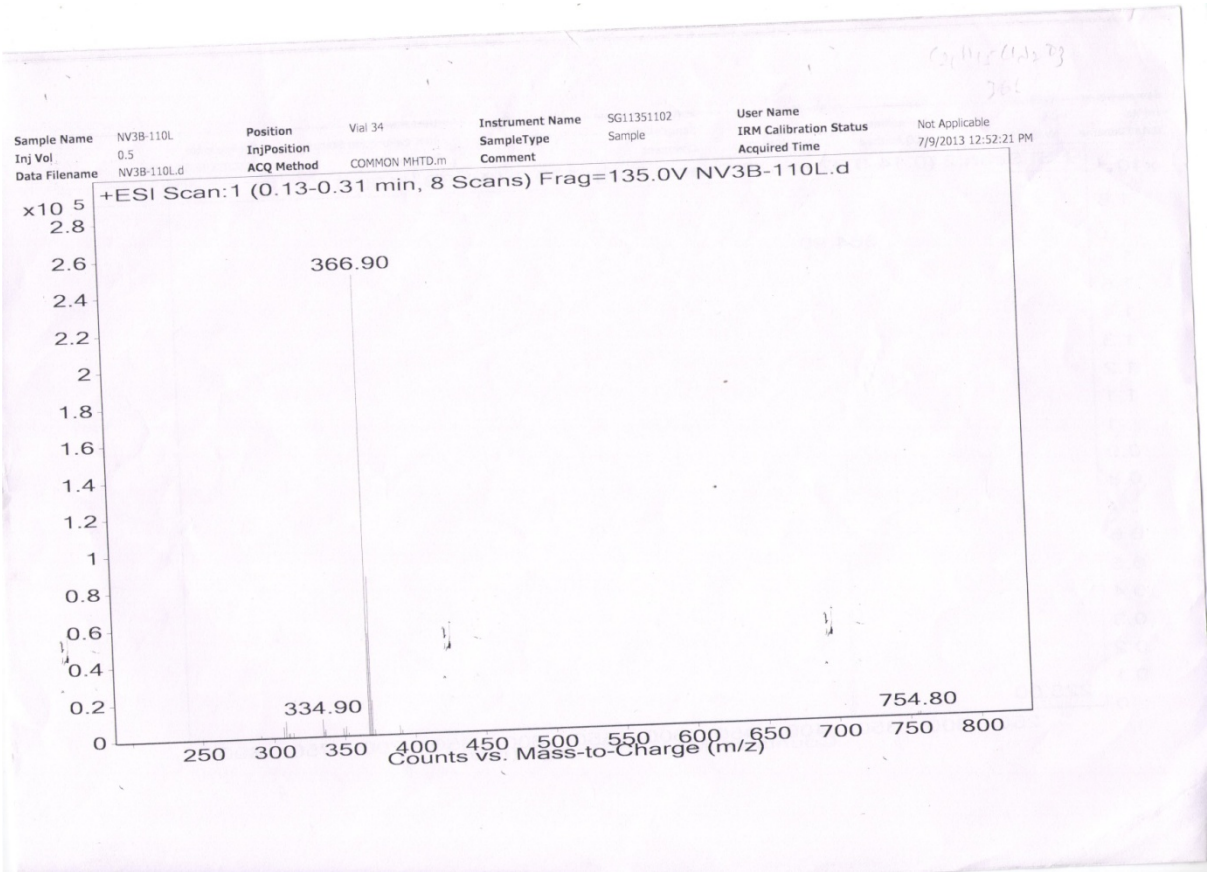
7l) Methyl1-((3-chlorophenyl(hydroxyl)methyl)-9H-pyrido[3,4-b]indole-3-carboxylate




166.41
144.90
143.41
140.68
135.74
134.44
129.97
129.75
129.04
127.97
126.54
124.67
121.63
121.30
120.95
117.44
112.24
77.31
77.05
76.80
75.41
52.53
O
O
N
N
H
OH
Cl
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


129.75
129.04
127.97
126.54
124.67
121.63
120.95
117.44
112.24
75.41
52.53
O
O
N
N
H
OH
Cl


140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)


Sample Name NV3B-110L
Inj Vol 0.5
Data Filename NV3B-110L.d
Position Vial 34
InjPosition
ACQ Method COMMON MHTD.m
Instrument Name SG11351102
SampleType Sample
Comment
User Name
IRM Calibration Status Not Applicable
Acquired Time 7/9/2013 12:52:21 PM
+ESI Scan:1 (0.13-0.31 min, 8 Scans) Frag=135.0V NV3B-110L.d
x10 5
366.90
334.90
754.80
Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

Data File	NV3B-110.d	**Sample Name**	NV3B-110
Sample Type	Sample	**Position**	Vial 11
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	12-07-2013 PM 12:46:40
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

Info.

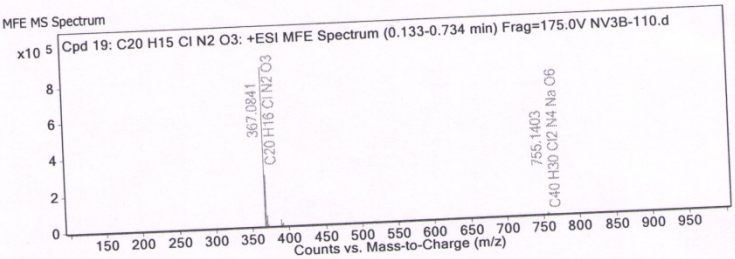
Sample Group	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 19: C20 H15 Cl N2 O3	0.194	366.0769	C20 H15 Cl N2 O3	C20 H15 Cl N2 O3	0.55	C20 H15 Cl N2 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 19: C20 H15 Cl N2 O3	367.0841	0.194	Find by Molecular Feature	366.0769

MFE MS Spectrum



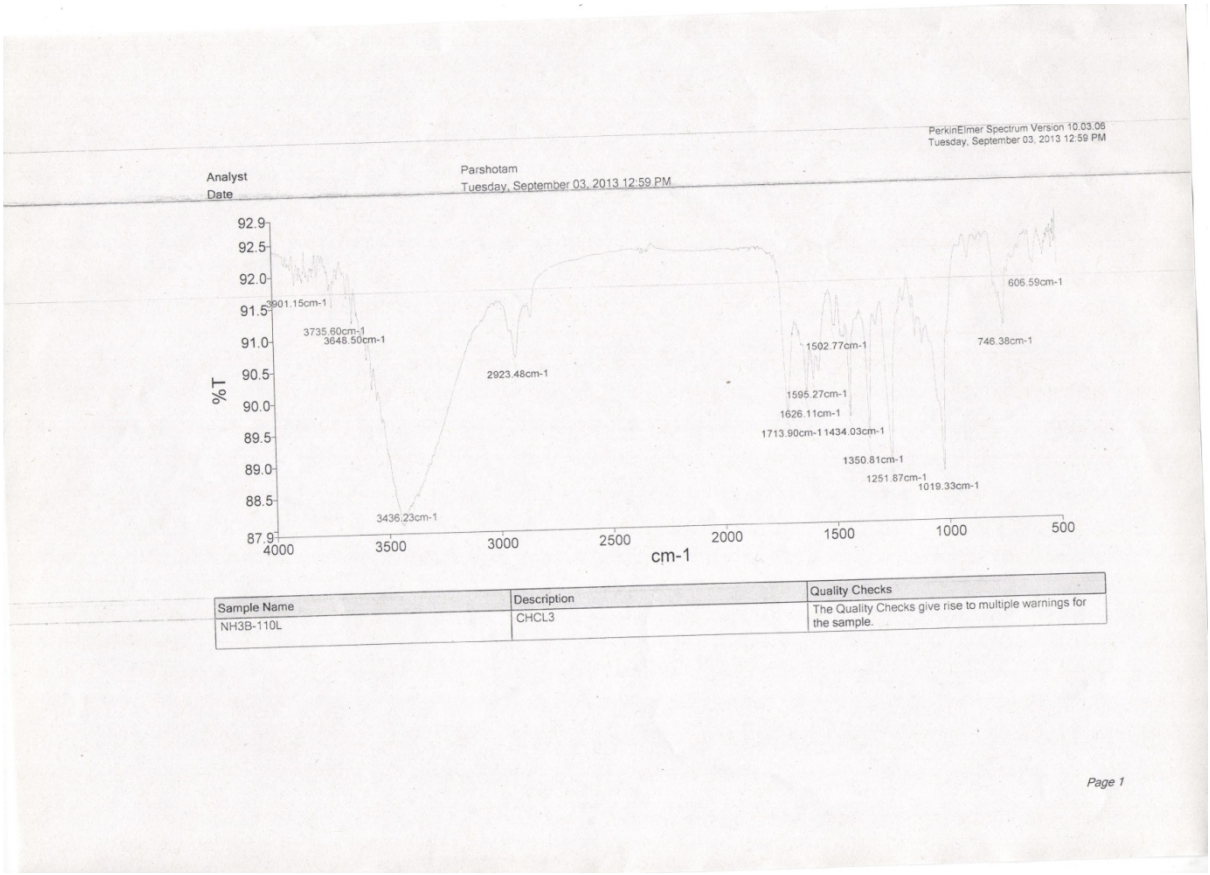
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
367.0841	1	877595.5	C20 H16 Cl N2 O3	(M+H)+
368.0874	1	184152.17	C20 H16 Cl N2 O3	(M+H)+
369.0824	1	284477.59	C20 H16 Cl N2 O3	(M+H)+
370.0847	1	60921.71	C20 H16 Cl N2 O3	(M+H)+
371.088	1	9738.43	C20 H16 Cl N2 O3	(M+H)+
389.0658	1	36573.13	C20 H15 Cl N2 Na O3	(M+Na)+
390.0689	1	9510.71	C20 H15 Cl N2 Na O3	(M+Na)+
391.0634	1	12573.15	C20 H15 Cl N2 Na O3	(M+Na)+
755.1403	1	7475.53	C40 H30 Cl2 N4 Na O6	(2M+Na)+
757.1392	1	5011.26	C40 H30 Cl2 N4 Na O6	(2M+Na)+

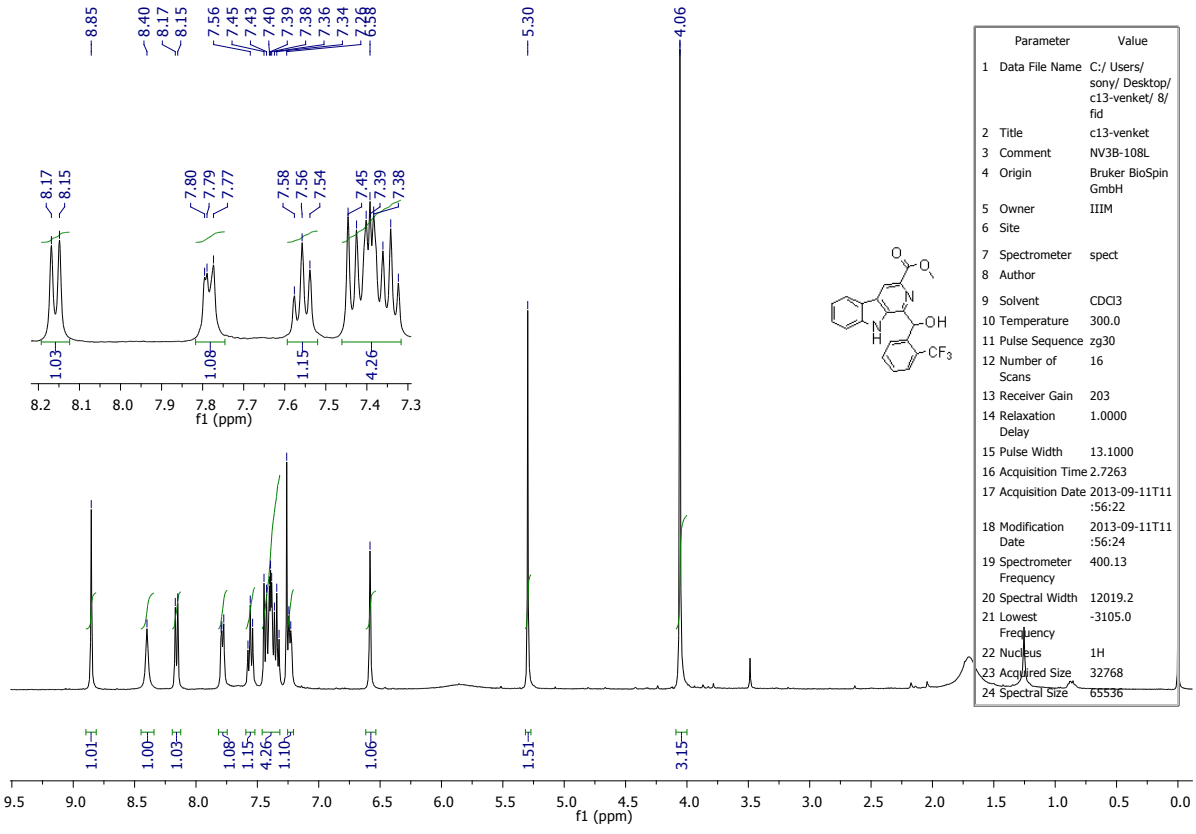
Predicted Isotope Match Table

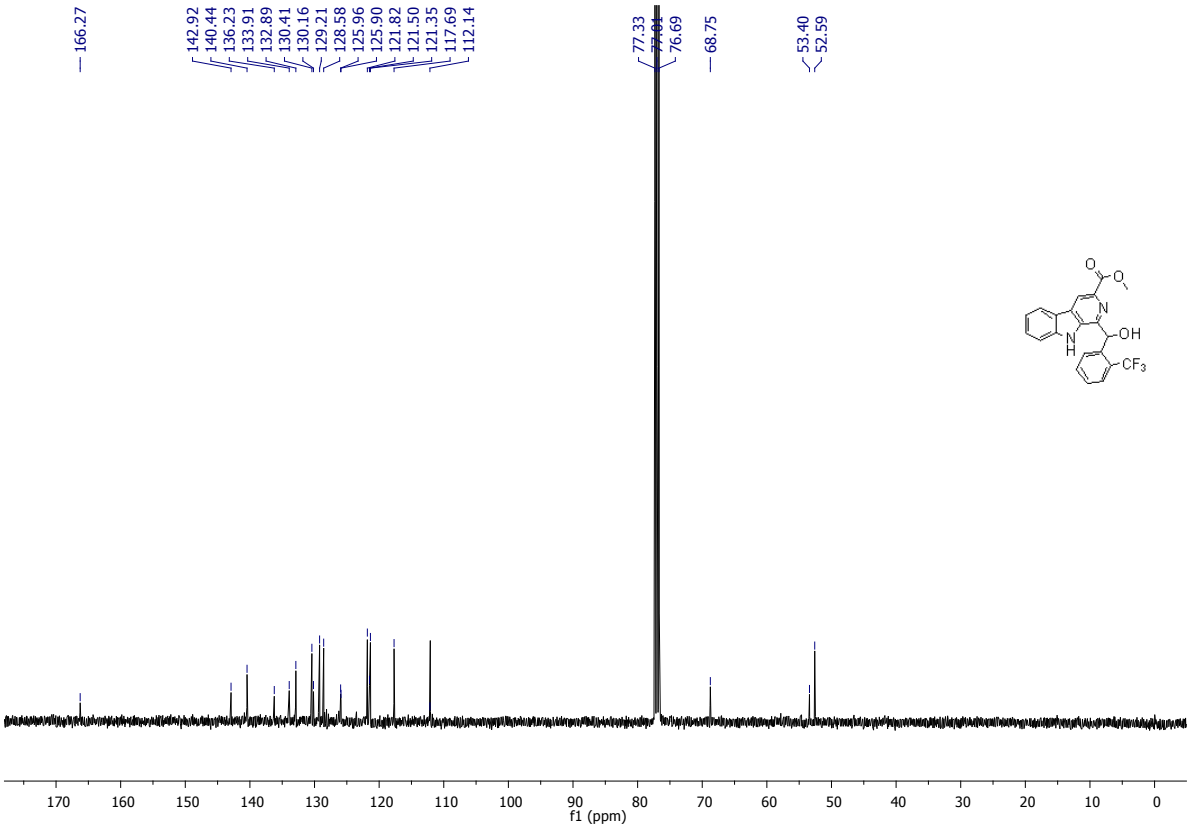
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	367.0841	367.0844	0.89	100	100	61.9	60.1
2	368.0874	368.0876	0.41	20.98	22.66	12.99	13.62
3	369.0824	369.0822	-0.35	32.42	35.06	20.06	21.07
4	370.0847	370.085	0.77	6.94	7.56	4.3	4.54
5	371.088	371.0876	-1.14	1.11	1.01	0.69	0.6
6	372.0951	372.0901	-13.45	0.11	0.1	0.07	0.06

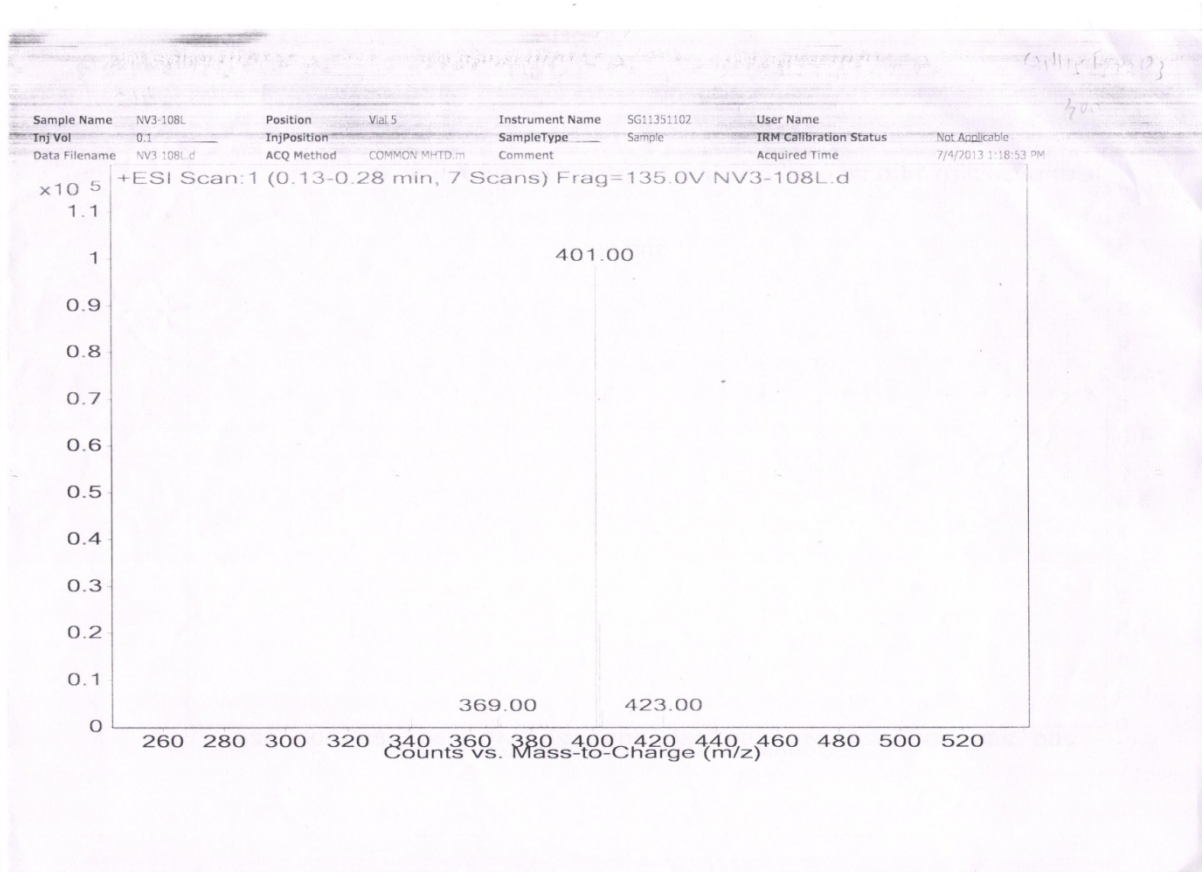
--- End Of Report ---



7m) Methyl1-(hydroxyl(2-(trifluoromethyl)phenyl)methyl)-9H-pyrido[3,4-b]indole-3-carboxylate:




166.27
142.92
140.44
136.23
133.91
132.89
130.41
130.16
129.21
128.58
125.96
125.90
121.82
121.50
121.35
117.69
112.14
77.33
77.01
76.69
68.75
53.40
52.59
O
O
N
H
OH
CF3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Sample Name NV3-108L
Position Vial 5
Instrument Name SG11351102
User Name
Inj Vol 0.1
InjPosition
SampleType Sample
IRM Calibration Status Not Applicable
Data Filename NV3-108L.d
ACQ Method COMMON MHTD.m
Comment
Acquired Time 7/4/2013 1:18:53 PM
+ESI Scan:1 (0.13-0.28 min, 7 Scans) Frag=135.0V NV3-108L.d
x10 5
401.00
369.00
423.00
Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

Data File	NV3-B-108.d	**Sample Name**	NV3-B-108
Sample Type	Sample	**Position**	Vial 39
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	12-09-2013 PM 1:05:13
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

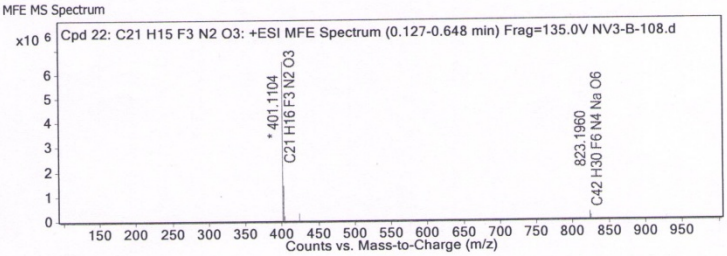
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 22: C21 H15 F3 N2 O3	0.194	400.1032	C21 H15 F3 N2 O3	C21 H15 F3 N2 O3	0.79	C21 H15 F3 N2 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 22: C21 H15 F3 N2 O3	401.1104	0.194	Find by Molecular Feature	400.1032

MFE MS Spectrum



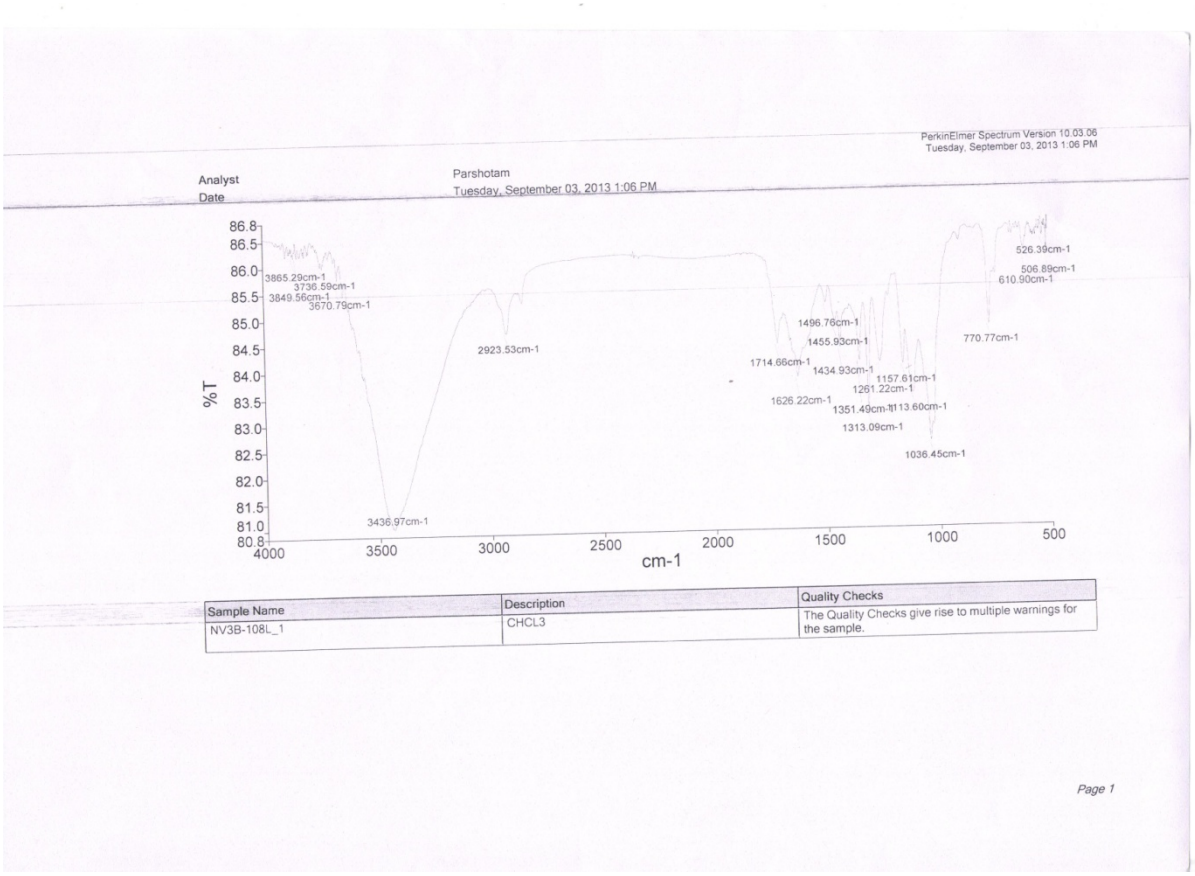
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
401.1104	1	6506811	C21 H16 F3 N2 O3	(M+H)+
402.1137	1	1450870.63	C21 H16 F3 N2 O3	(M+H)+
403.1168	1	193642.3	C21 H16 F3 N2 O3	(M+H)+
404.1191	1	20666.75	C21 H16 F3 N2 O3	(M+H)+
423.0925	1	277094.5	C21 H15 F3 N2 Na O3	(M+Na)+
424.0955	1	63094.83	C21 H15 F3 N2 Na O3	(M+Na)+
425.0986	1	11116.23	C21 H15 F3 N2 Na O3	(M+Na)+
823.196	1	286142.75	C42 H30 F6 N4 Na O6	(2M+Na)+
824.1988	1	137427.8	C42 H30 F6 N4 Na O6	(2M+Na)+
825.2018	1	31158.32	C42 H30 F6 N4 Na O6	(2M+Na)+

Predicted Isotope Match Table

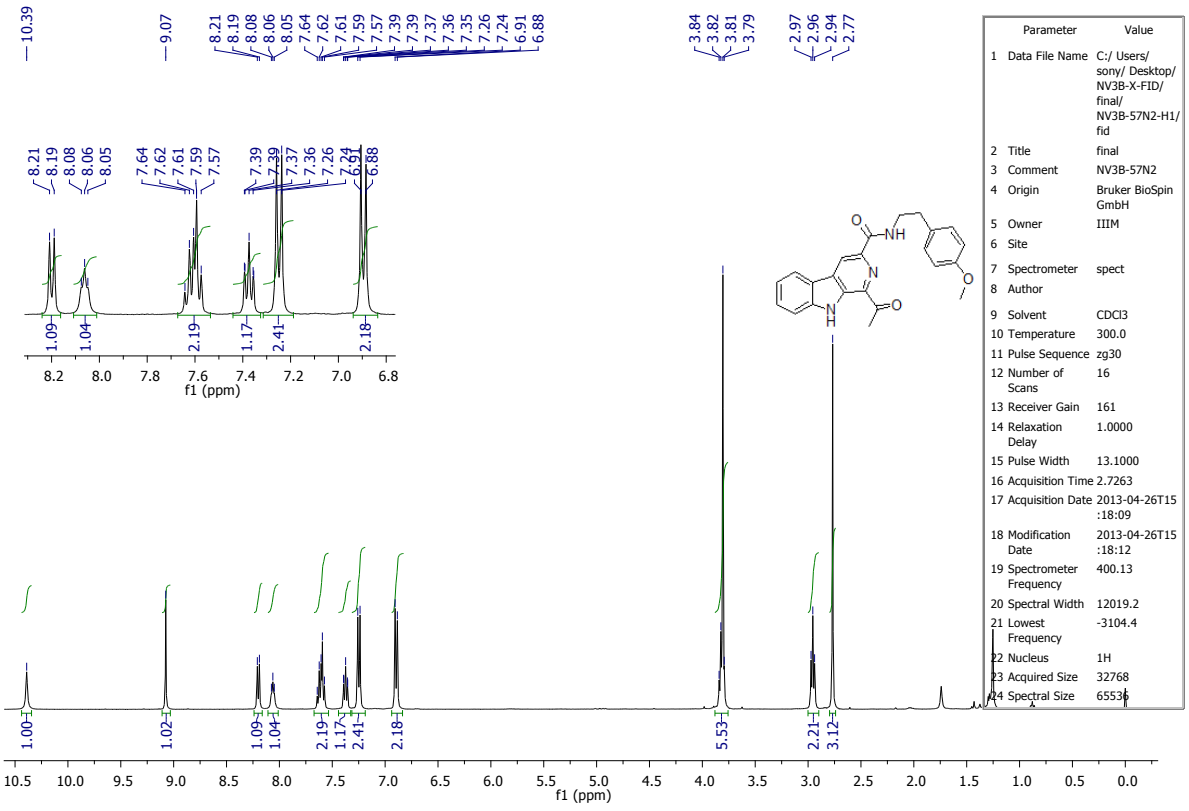
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	401.1104	401.1108	0.85	100	100	79.61	78.48
2	402.1137	402.1139	0.6	22.3	23.74	17.75	18.63
3	403.1168	403.1167	-0.12	2.98	3.31	2.37	2.6
4	404.1191	404.1194	0.61	0.32	0.34	0.25	0.27
5	405.123	405.122	-2.43	0.02	0.03	0.01	0.02

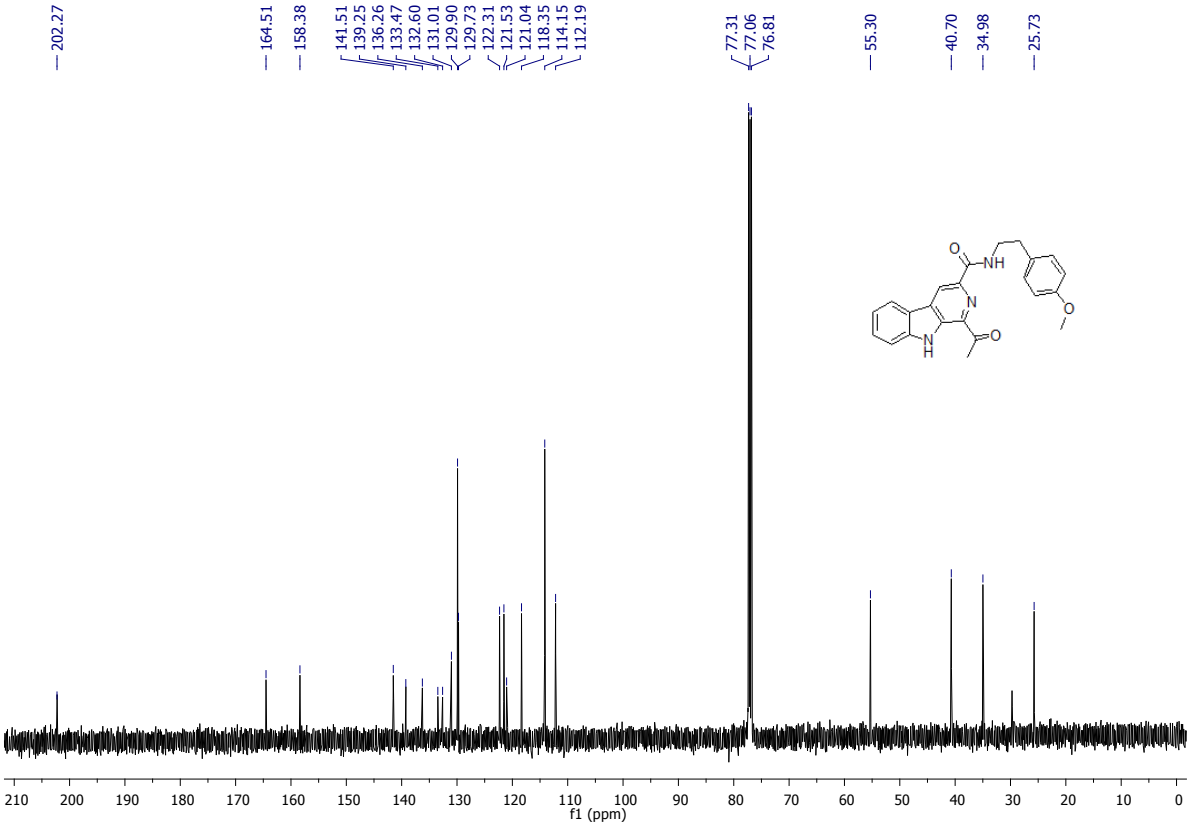
--- End Of Report ---

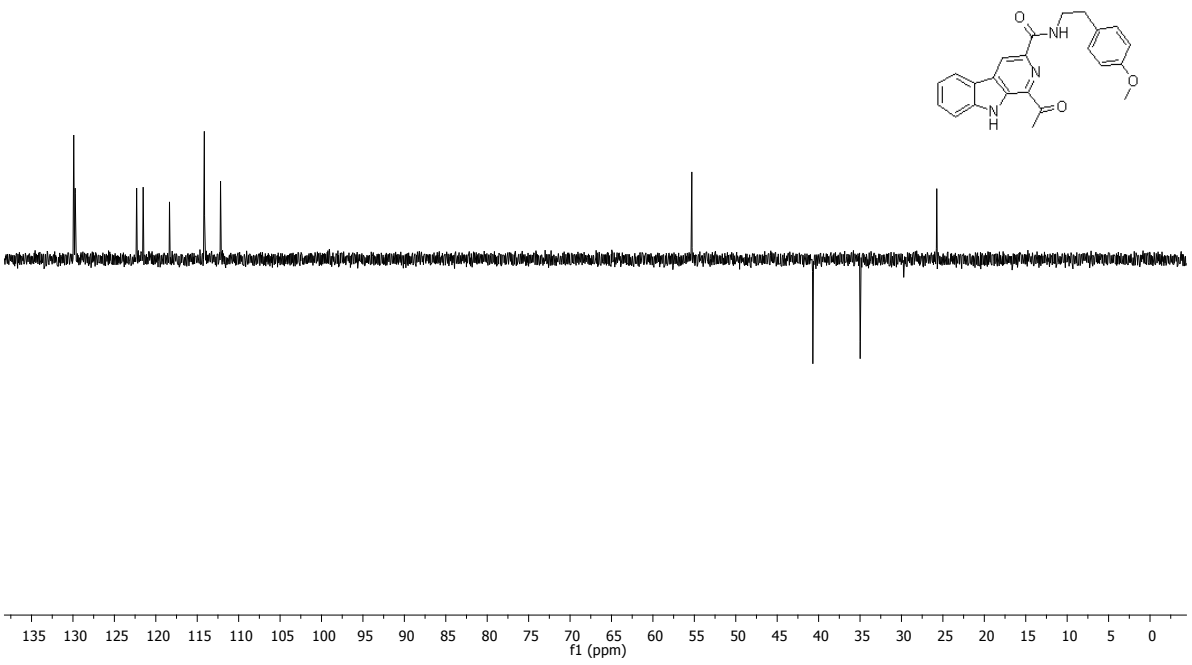


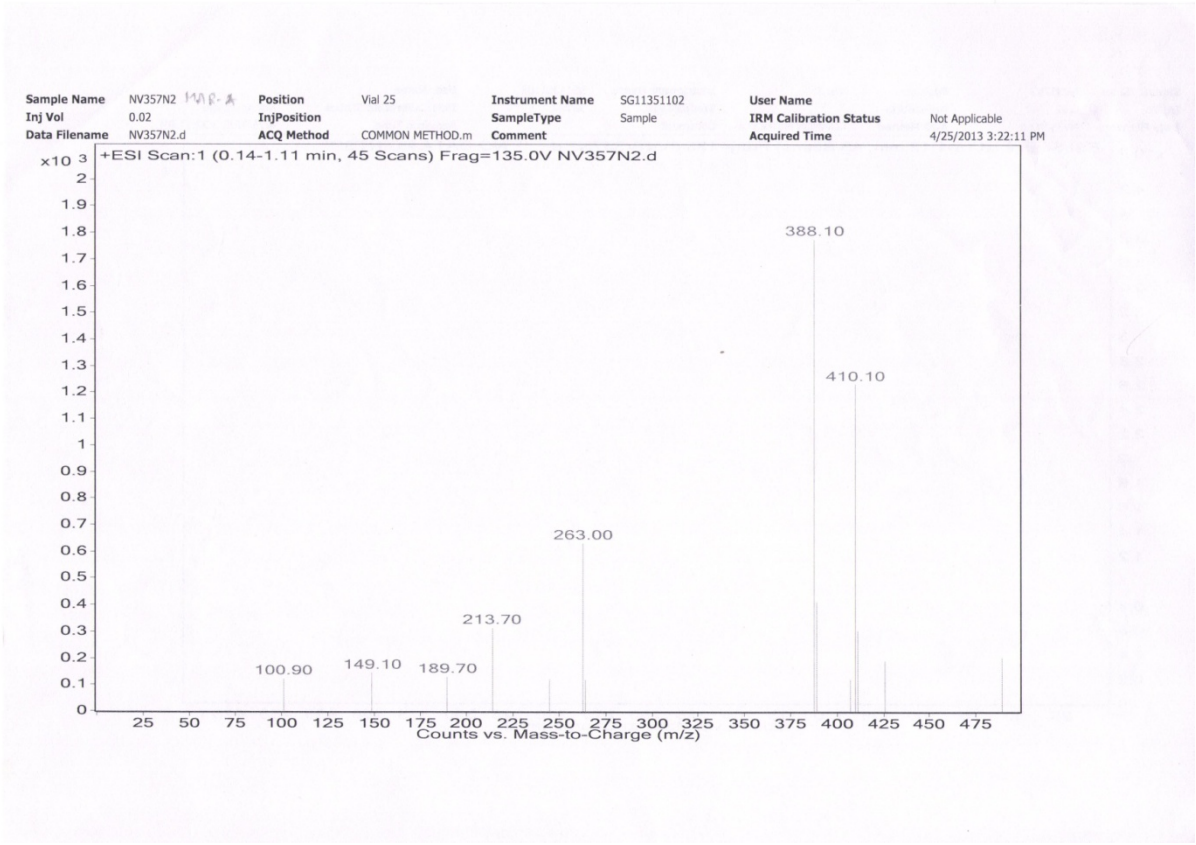
9a

)1-Acetyl-N-(4-methoxy phenethyl)- 9H -*β*-carboline-3-carboxamide,(Marinacarbolines-A)




202.27
164.51
158.38
141.51
139.25
136.26
133.47
132.60
131.01
129.90
129.73
122.31
121.53
121.04
118.35
114.15
112.19
77.31
77.06
76.81
55.30
40.70
34.98
25.73
O
NH
N
O
N
H
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


O
NH
N
O
O
N
H
135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)


Sample Name NV357N2
Inj Vol 0.02
Data Filename NV357N2.d
Position Vial 25
InjPosition
ACQ Method COMMON METHOD.m
Instrument Name SG11351102
SampleType Sample
Comment
User Name
IRM Calibration Status Not Applicable
Acquired Time 4/25/2013 3:22:11 PM
+ESI Scan:1 (0.14-1.11 min, 45 Scans) Frag=135.0V NV357N2.d
x10 3
388.10
410.10
263.00
213.70
100.90
149.10
189.70
Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

Data File	NV3B-57N2.d MAR-A	**Sample Name**	NV3B-57N2
Sample Type	Sample	**Position**	Vial 12
Instrument Name	Instrument 1	**User Name**	vishal
Acq Method	vishal_12-01-13.m	**Acquired Time**	26-04-2013 PM 2:44:10
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

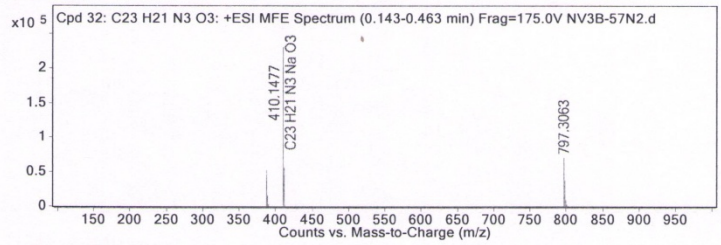
Sample Group **Info.**
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 32: C23 H21 N3 O3	0.19	387.1584	C23 H21 N3 O3	C23 H21 N3 O3	-0.35	C23 H21 N3 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 32: C23 H21 N3 O3	410.1477	0.19	Find by Molecular Feature	387.1584

MFE MS Spectrum



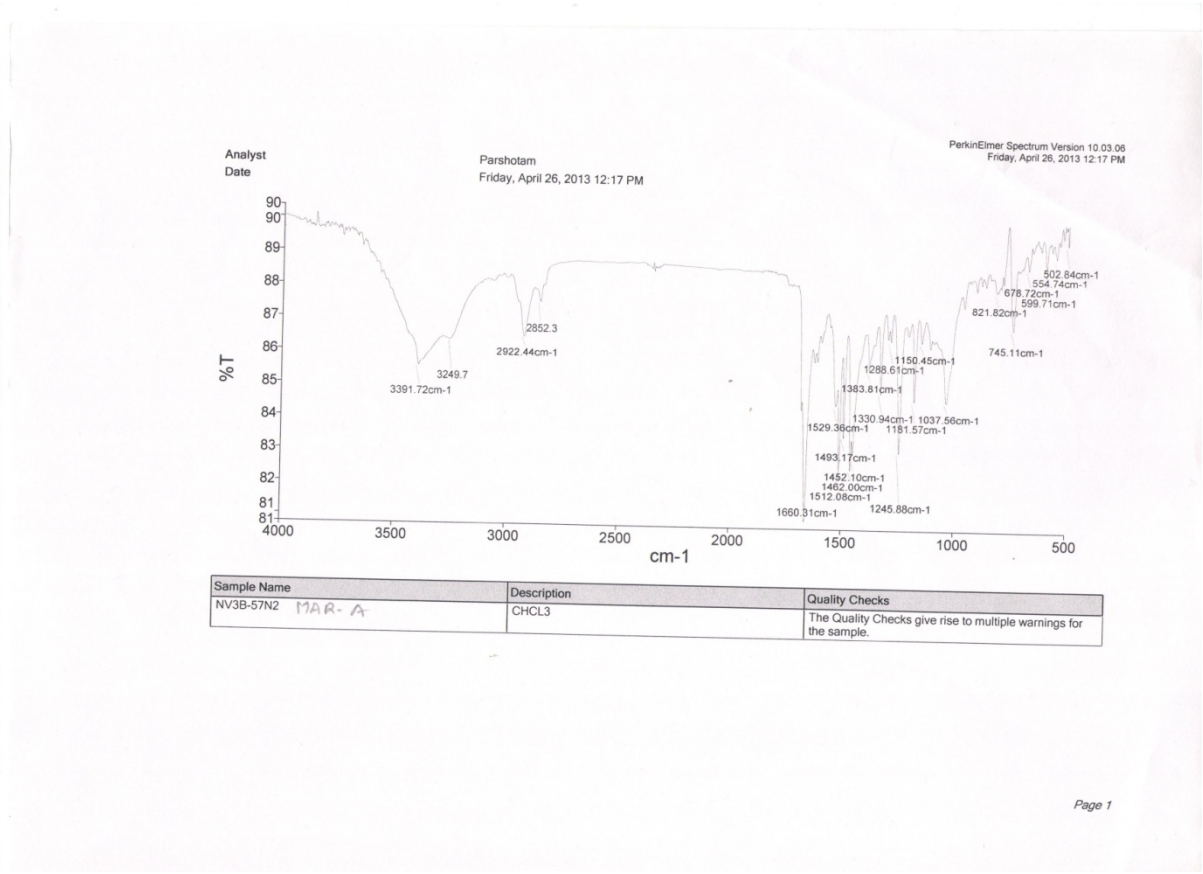
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
388.1655	1	52628.68	C23 H22 N3 O3	(M+H)+
389.1685	1	15646.81	C23 H22 N3 O3	(M+H)+
390.1722	1	2270.37	C23 H22 N3 O3	(M+H)+
410.1477	1	230045.98	C23 H21 N3 Na O3	(M+Na)+
411.1505	1	55421.39	C23 H21 N3 Na O3	(M+Na)+
412.1531	1	7345.83	C23 H21 N3 Na O3	(M+Na)+
797.3063	1	70238.97		(2M+Na)+
798.3087	1	36454.41		(2M+Na)+
799.3126	1	9579.08		(2M+Na)+
800.3132	1	2151.48		(2M+Na)+

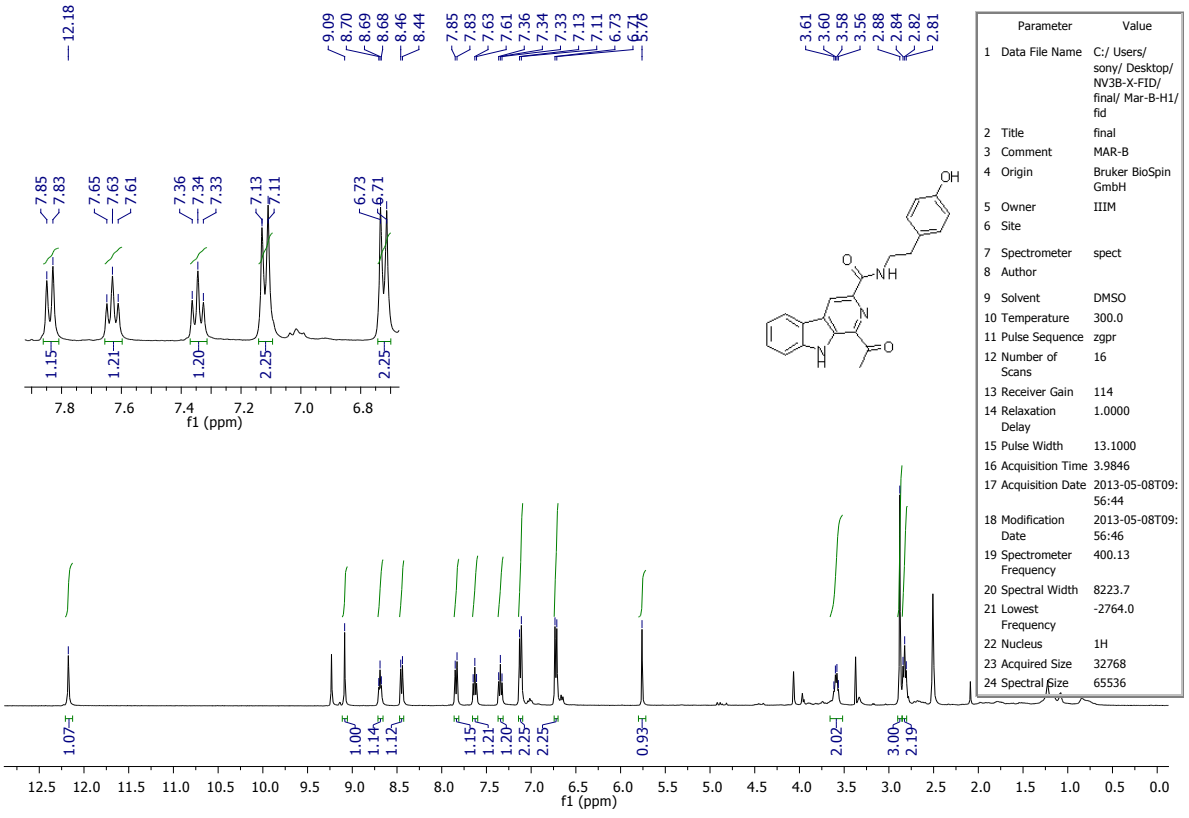
Predicted Isotope Match Table

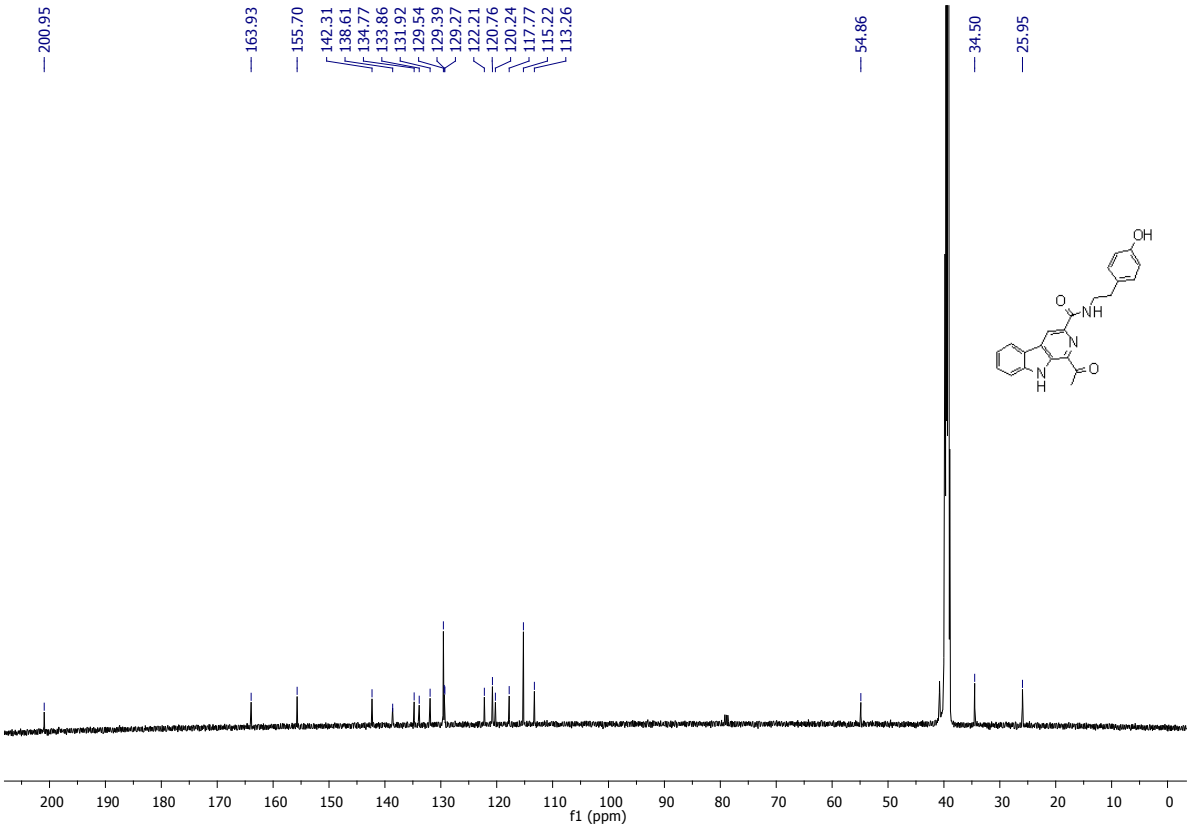
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	388.1655	388.1656	0.12	100	100	74.15	76.5
2	389.1685	389.1687	0.39	29.73	26.34	22.05	20.15
3	390.1722	390.1715	-1.71	4.31	3.95	3.2	3.02
4	391.1768	391.1742	-6.69	0.81	0.43	0.6	0.33

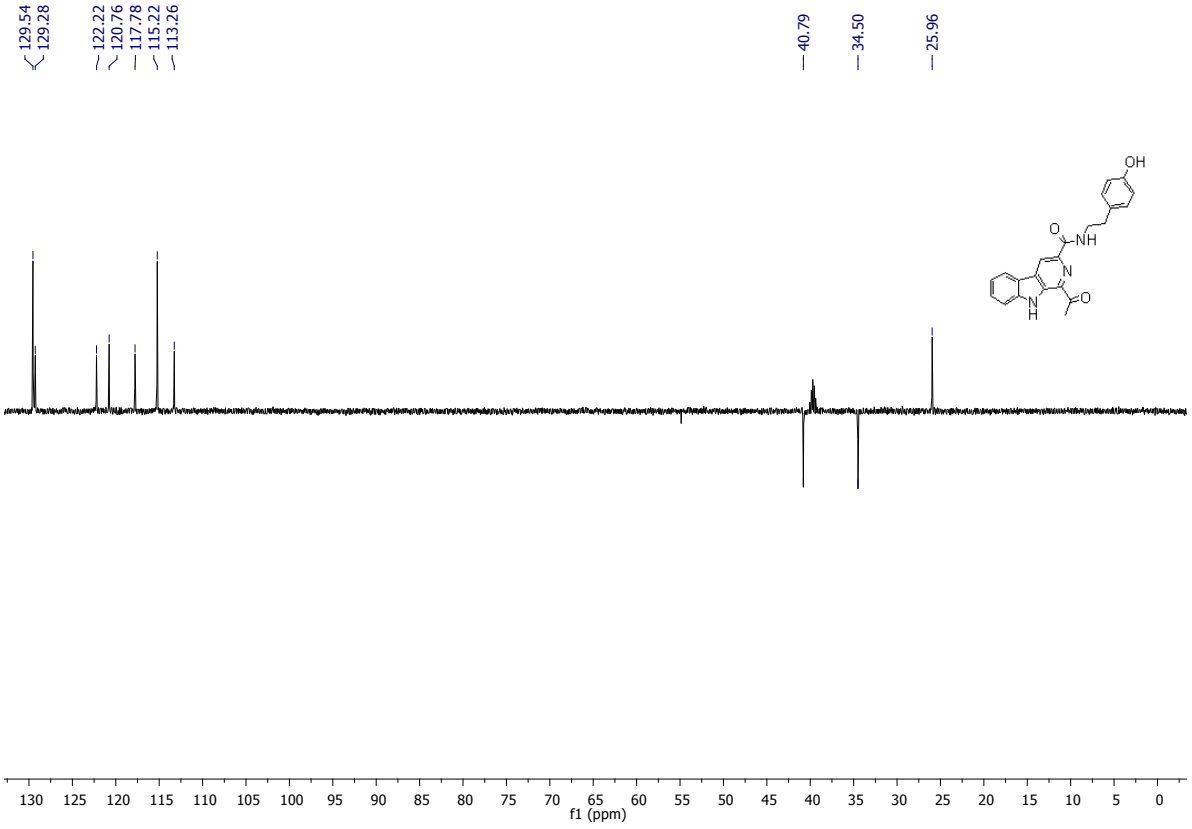
--- End Of Report ---



9b)1-Acetyl-N-(4-Hydroxy phenethyl)-9H-β-carboline-3-carboxamide: Marinacarbolines-B)




200.95
163.93
155.70
142.31
138.61
134.77
133.86
131.92
129.54
129.39
129.27
122.21
120.76
120.24
117.77
115.22
113.26
54.86
34.50
25.95
OH
O
NH
N
N
H
O
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


129.54
129.28
122.22
120.76
117.78
115.22
113.26
40.79
34.50
25.96
OH
O
NH
N
N
H
O
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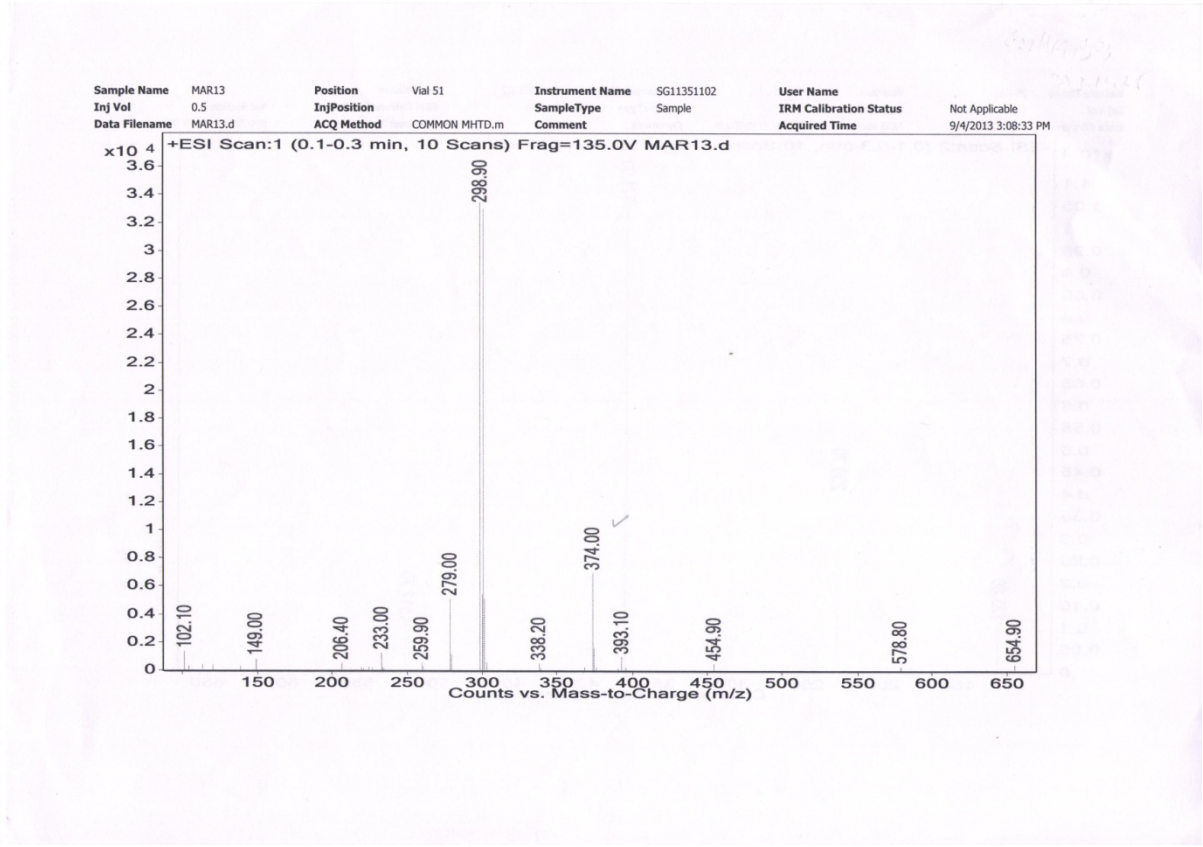
f1 (ppm)


Sample Name MAR13
Position Vial 51
Instrument Name SG11351102
User Name
Inj Vol 0.5
InjPosition
SampleType Sample
IRM Calibration Status Not Applicable
Data Filename MAR13.d
ACQ Method COMMON MHTD.m
Comment
Acquired Time 9/4/2013 3:08:33 PM
+ESI Scan:1 (0.1-0.3 min, 10 Scans) Frag=135.0V MAR13.d
x10 4
298.90
279.00
374.00
102.10
149.00
206.40
233.00
259.90
338.20
393.10
454.90
578.80
654.90
Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

Data File	MAR-B.d	**Sample Name**	MAR-B
Sample Type	Sample	**Position**	Vial 4
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	06-09-2013 AM 11:51:06
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

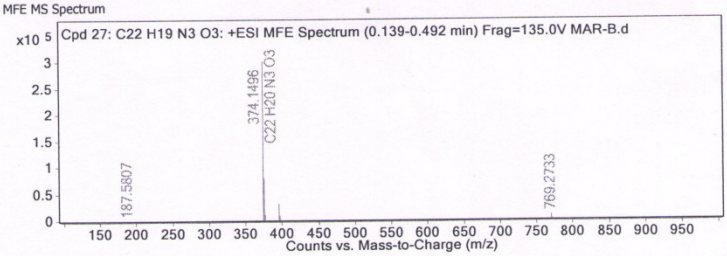
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 27: C22 H19 N3 O3	0.192	373.1423	C22 H19 N3 O3	C22 H19 N3 O3	0.81	C22 H19 N3 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 27: C22 H19 N3 O3	374.1496	0.192	Find by Molecular Feature	373.1423

MFE MS Spectrum



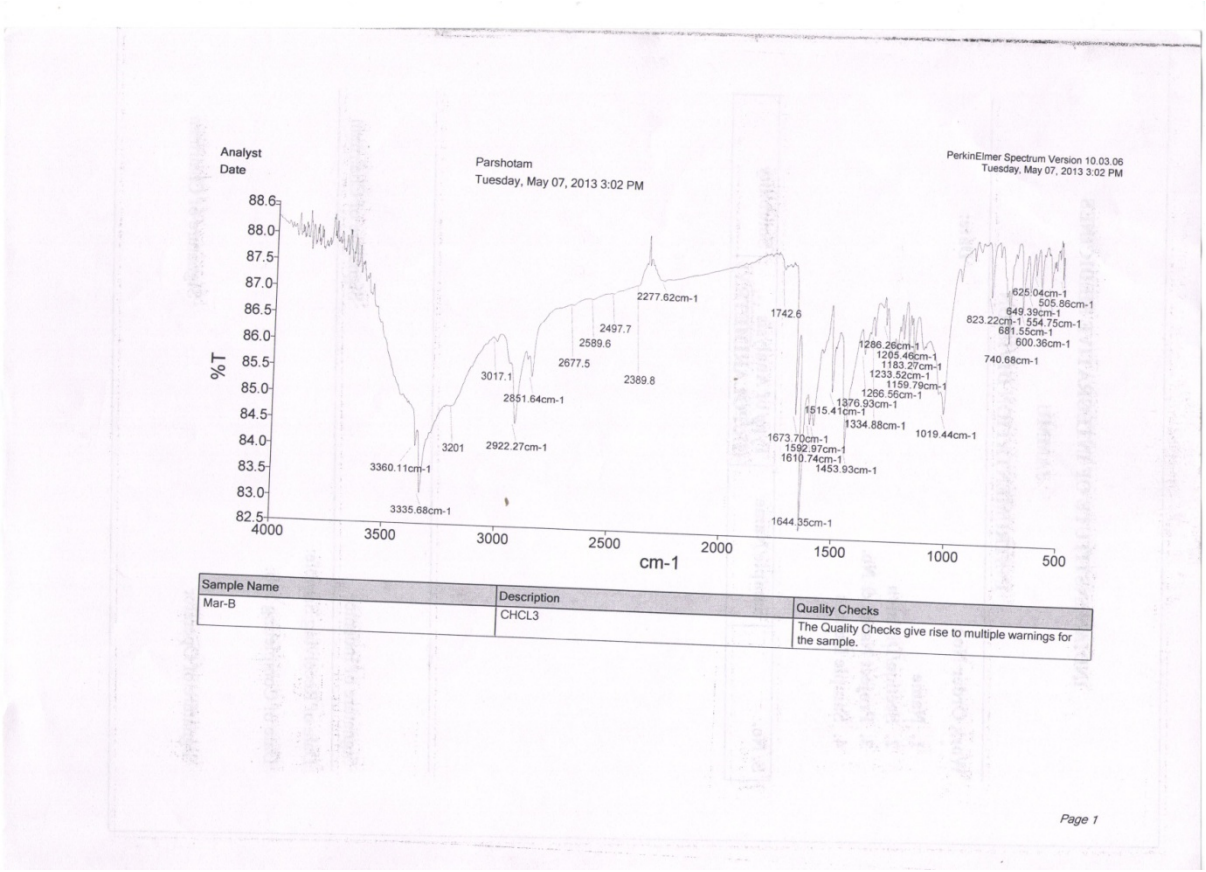
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
374.1496	1	299853.75	C22 H20 N3 O3	(M+H)+
375.1527	1	77960.38	C22 H20 N3 O3	(M+H)+
376.1557	1	10574.28	C22 H20 N3 O3	(M+H)+
377.159	1	1225.95	C22 H20 N3 O3	(M+H)+
396.1316	1	30533	C22 H19 N3 Na O3	(M+Na)+
397.1338	1	7851.57	C22 H19 N3 Na O3	(M+Na)+
398.1356	1	1339.05	C22 H19 N3 Na O3	(M+Na)+
769.2733	1	9032.73		(2M+Na)+
770.2768	1	4747.51		(2M+Na)+
771.2777	1	1072.51		(2M+Na)+

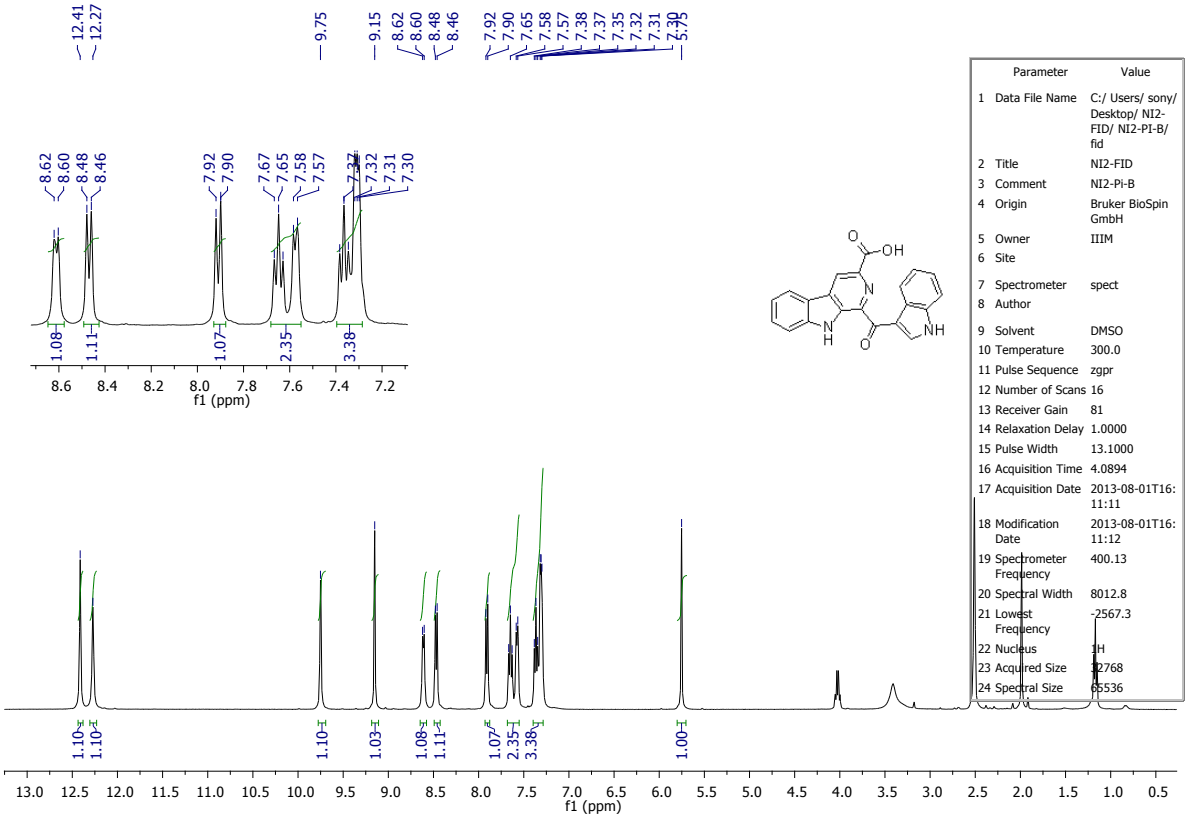
Predicted Isotope Match Table

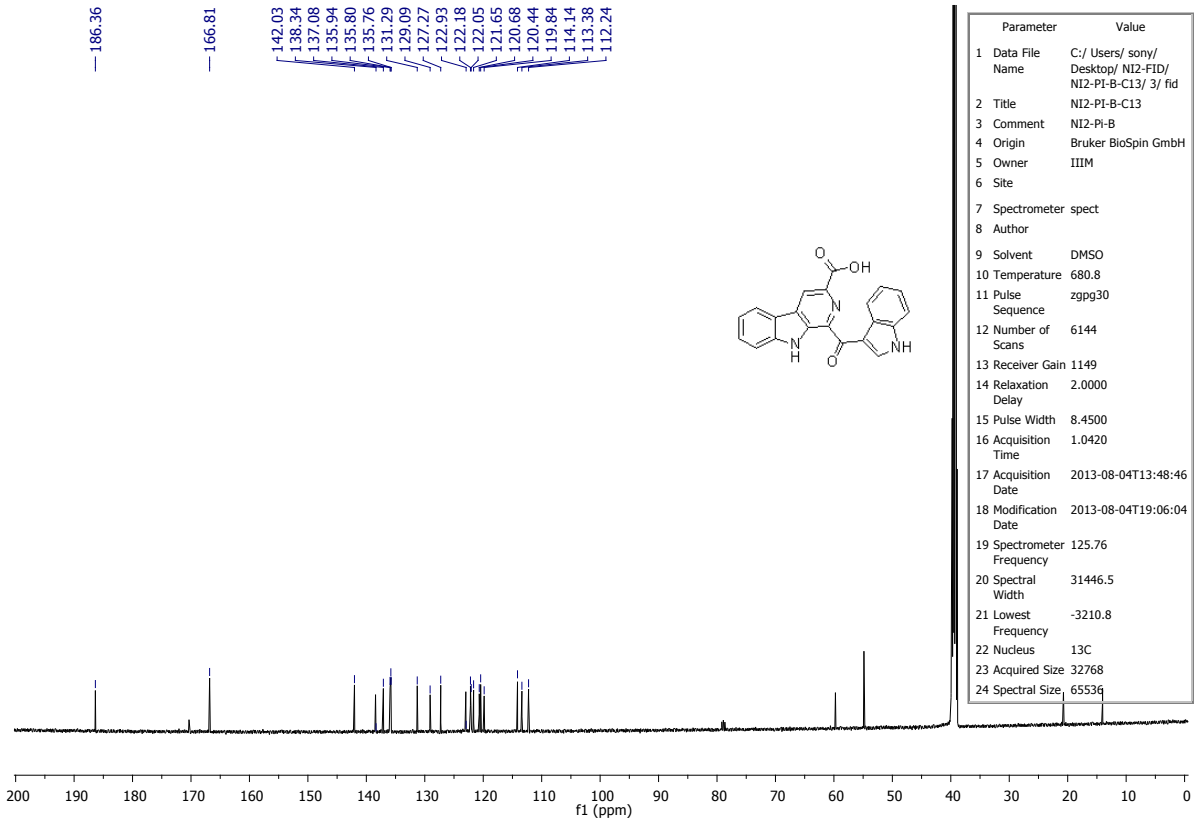
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	374.1496	374.1499	0.79	100	100	76.96	77.34
2	375.1527	375.153	0.95	26	25.23	20.01	19.52
3	376.1557	376.1558	0.39	3.53	3.67	2.71	2.84
4	377.159	377.1584	-1.49	0.41	0.39	0.31	0.3

--- End Of Report ---



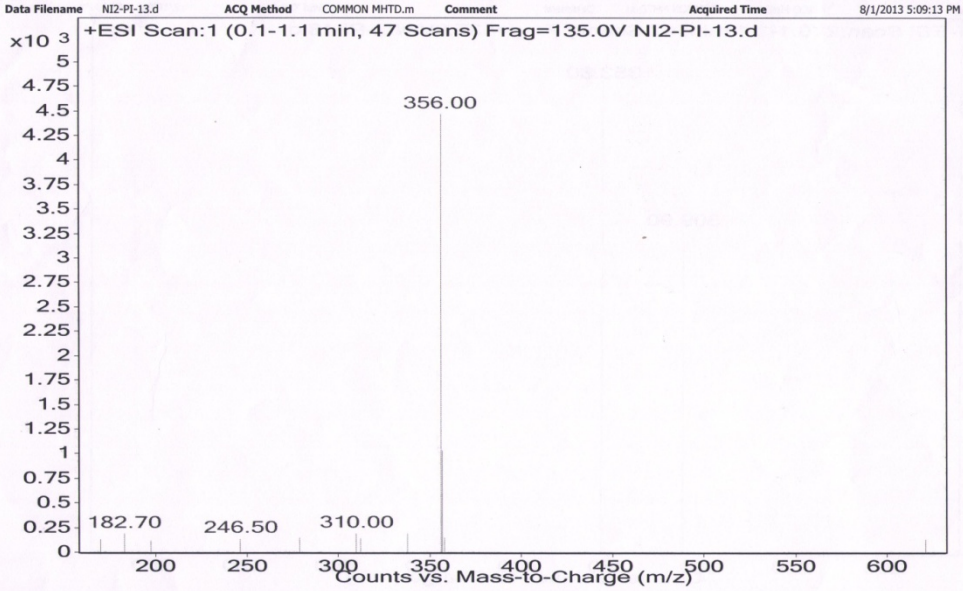
10) 1-(1H-indole-3-carbonyl)-9H-*β*-carboline-3-carboxylic acid (Pityriacitrin B)





	Parameter	Value
1	Data File Name	C:/ Users/ sony/ Desktop/ NI2-FID/ NI2-PI-B-C13/ 3/ fid
2	Title	NI2-PI-B-C13
3	Comment	NI2-Pi-B
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	680.8
11	Pulse Sequence	zgpg30
12	Number of Scans	6144
13	Receiver Gain	1149
14	Relaxation Delay	2.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0420
17	Acquisition Date	2013-08-04T13:48:46
18	Modification Date	2013-08-04T19:06:04
19	Spectrometer Frequency	125.76
20	Spectral Width	31446.5
21	Lowest Frequency	-3210.8
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

Sample Name	NI2-PI-B	**Position**	Vial 58	**Instrument Name**	SG11351102	**User Name**	
Inj Vol	0.5	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Not Applicable
Data Filename	NI2-PI-13.d	**ACQ Method**	COMMON MHTD.m	**Comment**		**Acquired Time**	8/1/2013 5:09:13 PM



Qualitative Compound Report

Data File	NI2-Pi-B.d	**Sample Name**	NI2-Pi-B
Sample Type	Sample	**Position**	Vial 8
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	02-08-2013 PM 12:47:17
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

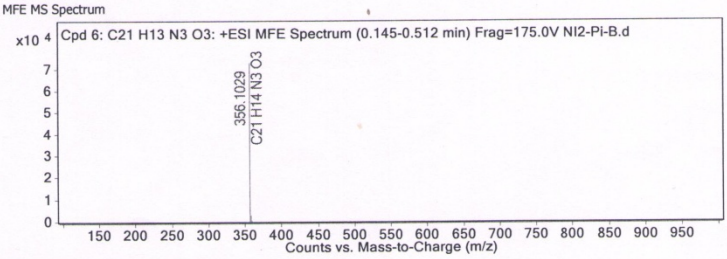
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 6: C21 H13 N3 O3	0.193	355.0956	C21 H13 N3 O3	C21 H13 N3 O3	0.19	C21 H13 N3 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 6: C21 H13 N3 O3	356.1029	0.193	Find by Molecular Feature	355.0956

MFE MS Spectrum



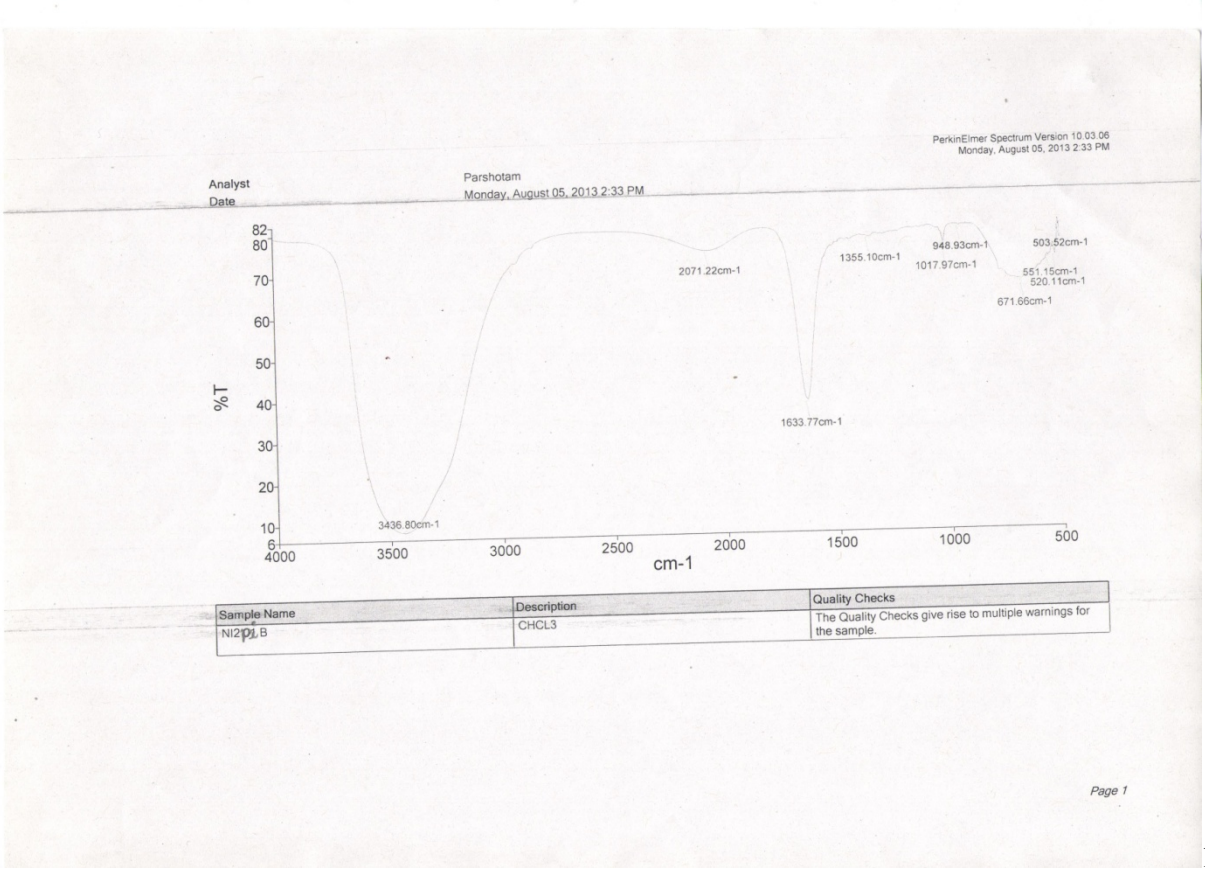
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
356.1029	1	72749.95	C21 H14 N3 O3	(M+H)+
357.1058	1	18118.63	C21 H14 N3 O3	(M+H)+
358.1084	1	2675.16	C21 H14 N3 O3	(M+H)+
359.1124	1	407.17	C21 H14 N3 O3	(M+H)+

Predicted Isotope Match Table

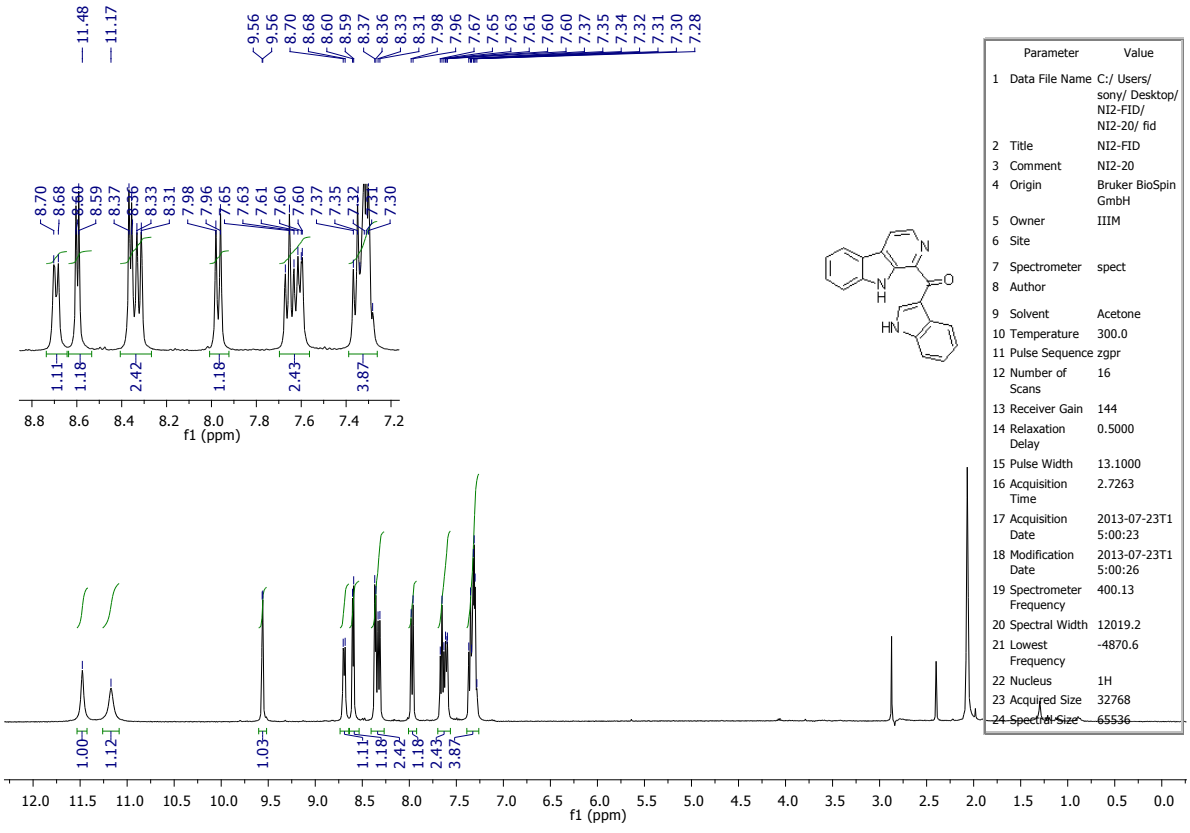
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	356.1029	356.103	0.07	100	100	77.43	78.23
2	357.1058	357.1061	0.63	24.91	24.08	19.29	18.84
3	358.1084	358.1088	1.01	3.68	3.39	2.85	2.65
4	359.1124	359.1114	-2.72	0.56	0.35	0.43	0.28

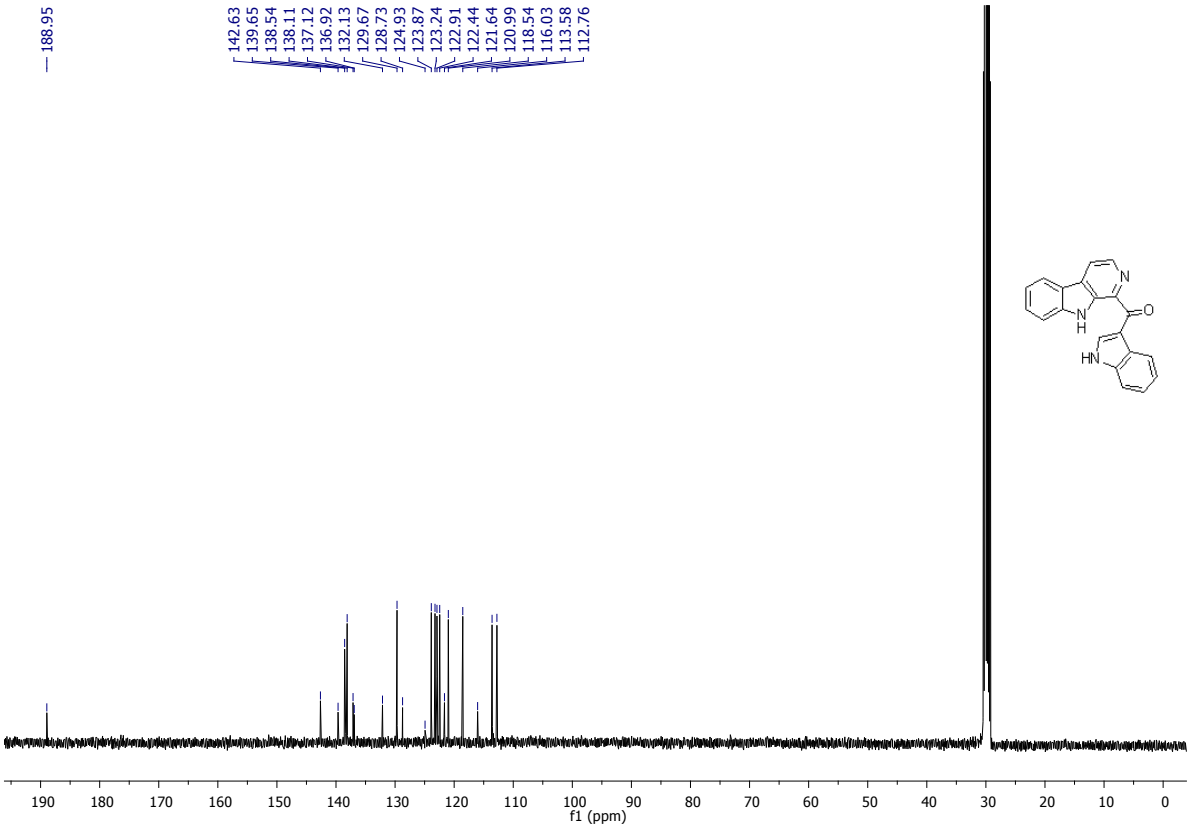
--- End Of Report ---



11

) (9H-carbazol-1-yl)(1H-indole-3-yl)methanone) (Pityriacitrin)




188.95
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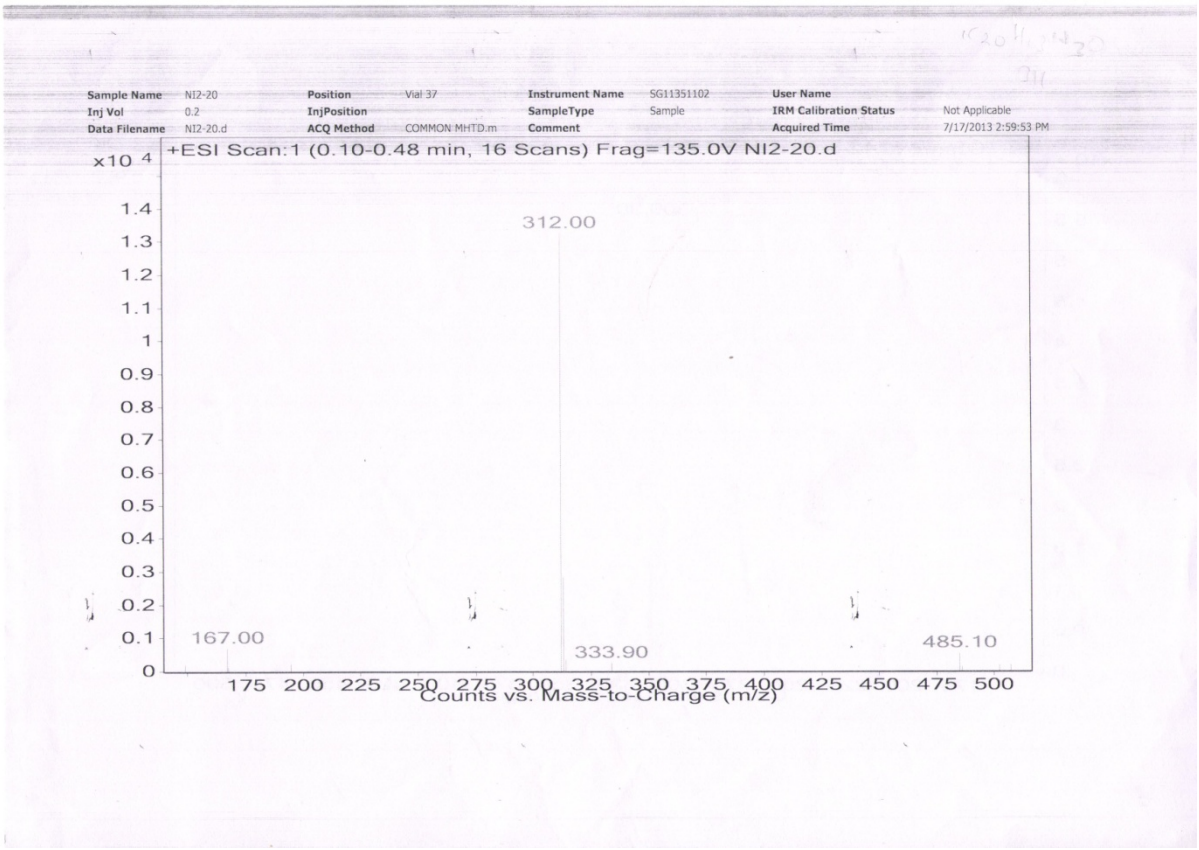
138.54
138.11
137.12
136.92
132.13
129.67
128.73
124.93
123.87
123.24
122.91
122.44
121.64
120.99
118.54
116.03
113.58
112.76
N
H
N
HN
O
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


Sample Name NI2-20
Position Vial 37
Instrument Name SG11351102
User Name
Inj Vol 0.2
InjPosition
SampleType Sample
IRM Calibration Status Not Applicable
Data Filename NI2-20.d
ACQ Method COMMON MHTD.m
Comment
Acquired Time 7/17/2013 2:59:53 PM
+ESI Scan:1 (0.10-0.48 min, 16 Scans) Frag=135.0V NI2-20.d
x10 4
1.4
1.3
1.2
1.1
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
312.00
167.00
333.90
485.10
175 200 225 250 275 300 325 350 375 400 425 450 475 500
Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

Data File	NI2-20.d	**Sample Name**	NI2-20
Sample Type	Sample	**Position**	Vial 33
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	18-07-2013 AM 11:52:33
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

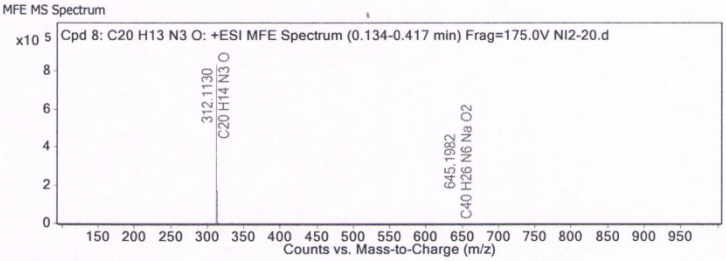
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 8: C20 H13 N3 O	0.193	311.1058	C20 H13 N3 O	C20 H13 N3 O	0.24	C20 H13 N3 O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 8: C20 H13 N3 O	312.113	0.193	Find by Molecular Feature	311.1058

MFE MS Spectrum



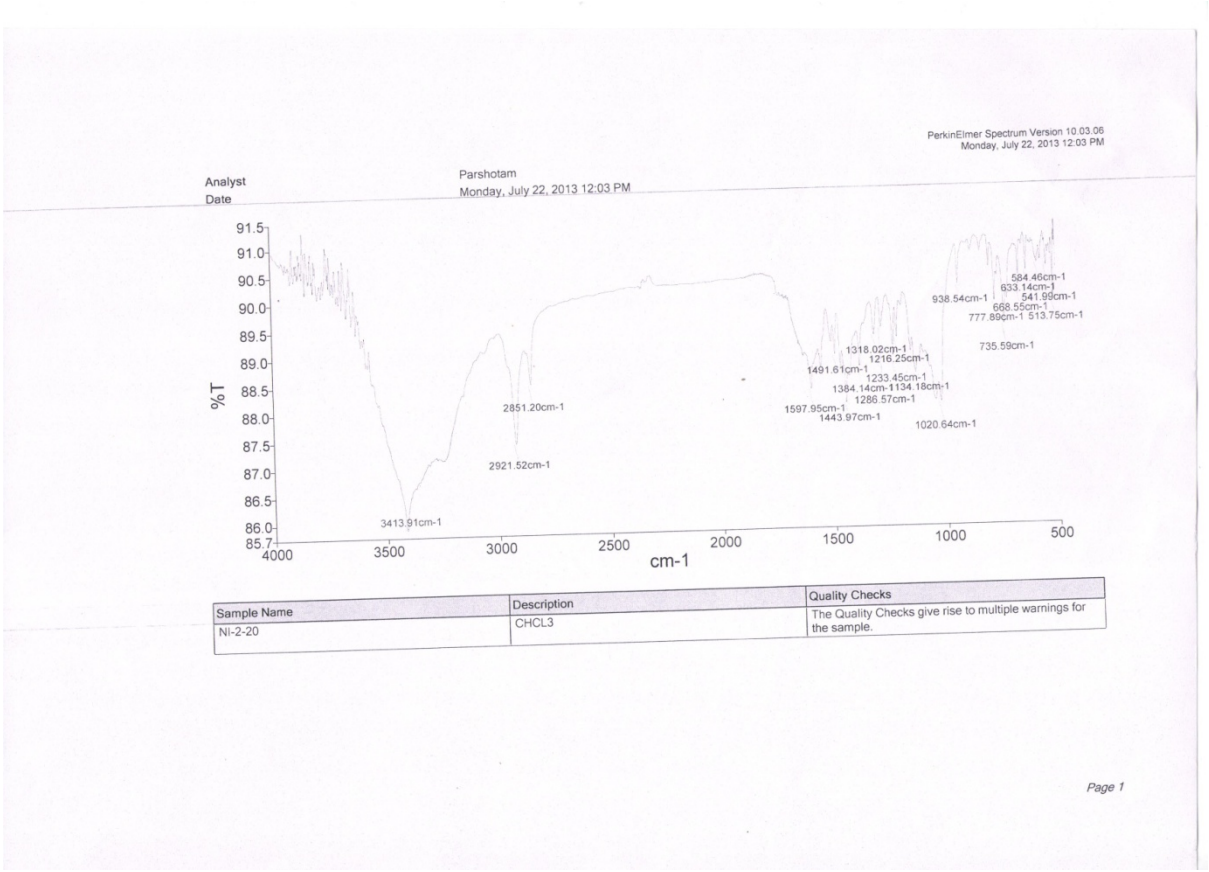
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
312.113	1	833087.38	C20 H14 N3 O	(M+H)+
313.1163	1	168770.94	C20 H14 N3 O	(M+H)+
314.1196	1	19281.89	C20 H14 N3 O	(M+H)+
315.1234	1	3008.61	C20 H14 N3 O	(M+H)+
334.0948	1	3135.46	C20 H13 N3 Na O	(M+Na)+
335.0971	1	767.67	C20 H13 N3 Na O	(M+Na)+
645.1982	1	451.84	C40 H26 N6 Na O2	(2M+Na)+

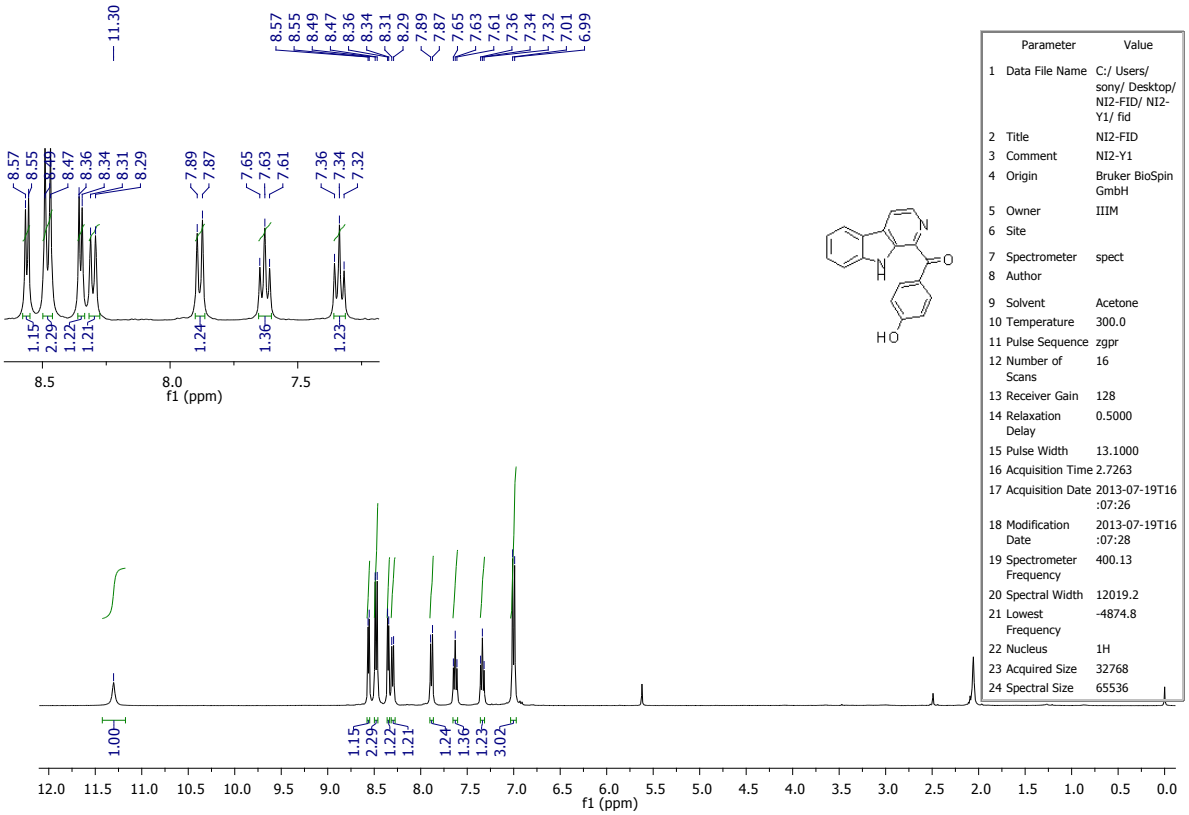
Predicted Isotope Match Table

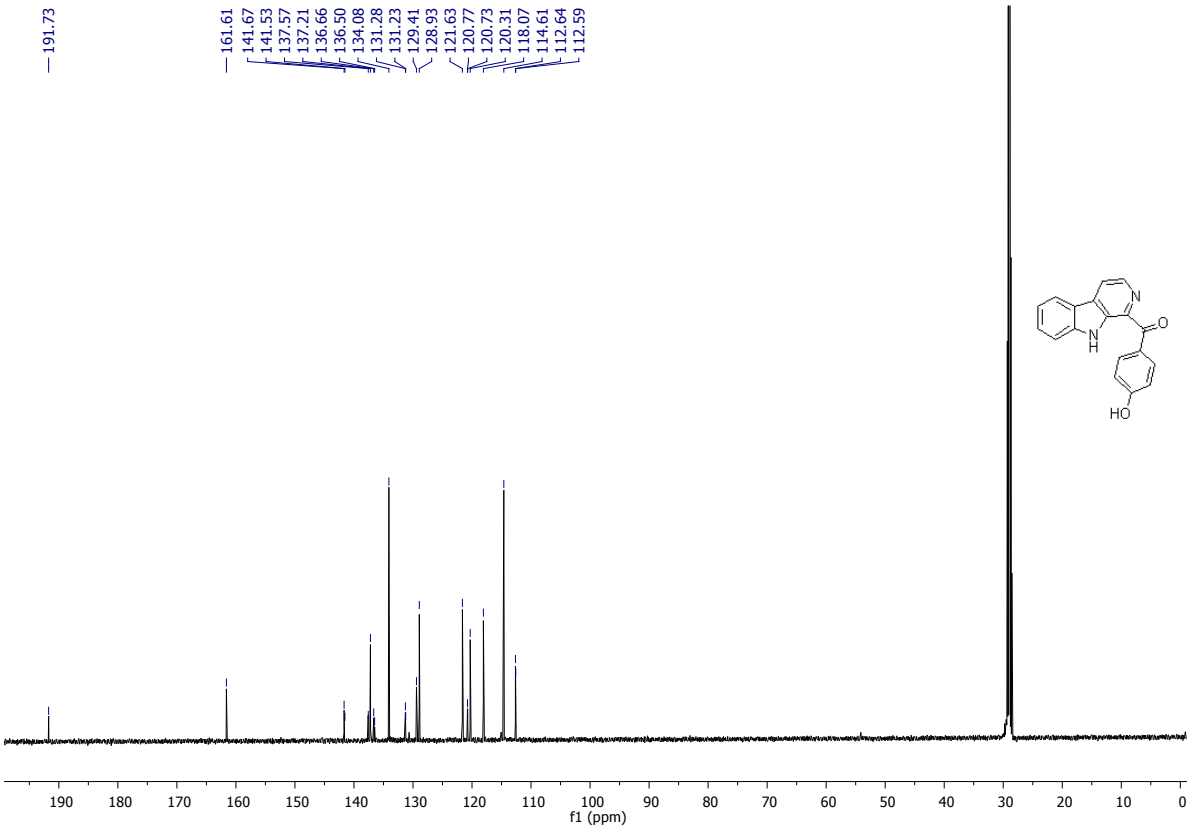
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	312.113	312.1131	0.42	100	100	81.34	79.45
2	313.1163	313.1162	-0.35	20.26	22.93	16.48	18.22
3	314.1196	314.1191	-1.53	2.31	2.71	1.88	2.16
4	315.1234	315.1219	-4.59	0.36	0.22	0.29	0.18

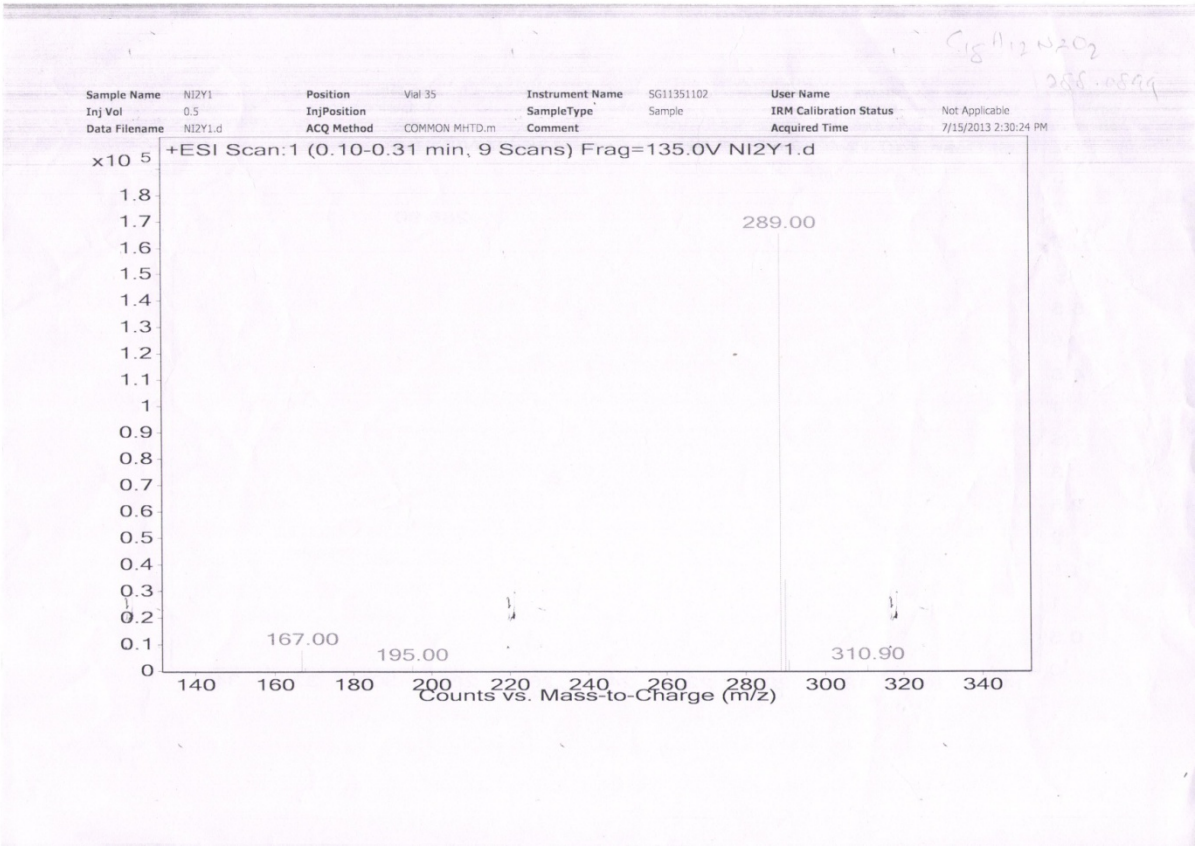
--- End Of Report ---



14) (4-Hydroxyphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone (Eudistomin-Y1)


11.30
8.57
8.55
8.49
8.47
8.36
8.34
8.31
8.29
7.89
7.87
7.65
7.63
7.61
7.36
7.34
7.32
7.01
6.99
1.15
2.29
1.22
1.21
1.24
1.36
1.23
8.5
8.0
7.5
f1 (ppm)
N
H
O
HO
Parameter Value
1 Data File Name C:/ Users/ sony/ Desktop/ NI2-FID/ NI2-Y1/ fid
2 Title NI2-FID
3 Comment NI2-Y1
4 Origin Bruker BioSpin GmbH
5 Owner IIIM
6 Site
7 Spectrometer spect
8 Author
9 Solvent Acetone
10 Temperature 300.0
11 Pulse Sequence zgpr
12 Number of Scans 16
13 Receiver Gain 128
14 Relaxation Delay 0.5000
15 Pulse Width 13.1000
16 Acquisition Time 2.7263
17 Acquisition Date 2013-07-19T16:07:26
18 Modification Date 2013-07-19T16:07:28
19 Spectrometer Frequency 400.13
20 Spectral Width 12019.2
21 Lowest Frequency -4874.8
22 Nucleus 1H
23 Acquired Size 32768
24 Spectral Size 65536
1.00
1.15
2.29
1.22
1.21
1.24
1.36
1.23
3.02
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


191.73
161.61
141.67
141.53
137.57
137.21
136.66
136.50
134.08
131.28
131.23
129.41
128.93
121.63
120.77
120.73
120.31
118.07
114.61
112.64
112.59
N
H
O
HO
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Sample Name NI2Y1
Position Vial 35
Instrument Name SG11351102
User Name
Inj Vol 0.5
InjPosition
SampleType Sample
IRM Calibration Status Not Applicable
Data Filename NI2Y1.d
ACQ Method COMMON MHTD.m
Comment
Acquired Time 7/15/2013 2:30:24 PM
+ESI Scan:1 (0.10-0.31 min, 9 Scans) Frag=135.0V NI2Y1.d
x10 5
289.00
167.00
195.00
310.90
Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

Data File	NI2-Y-1.d	**Sample Name**	NI2-Y-1
Sample Type	Sample	**Position**	Vial 40
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	16-07-2013 PM 1:27:39
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

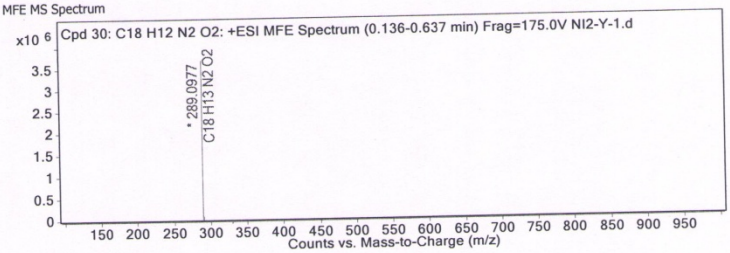
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 30: C18 H12 N2 O2	0.194	288.0924	C18 H12 N2 O2	C18 H12 N2 O2	-8.87	C18 H12 N2 O2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 30: C18 H12 N2 O2	289.0977	0.194	Find by Molecular Feature	288.0924

MFE MS Spectrum



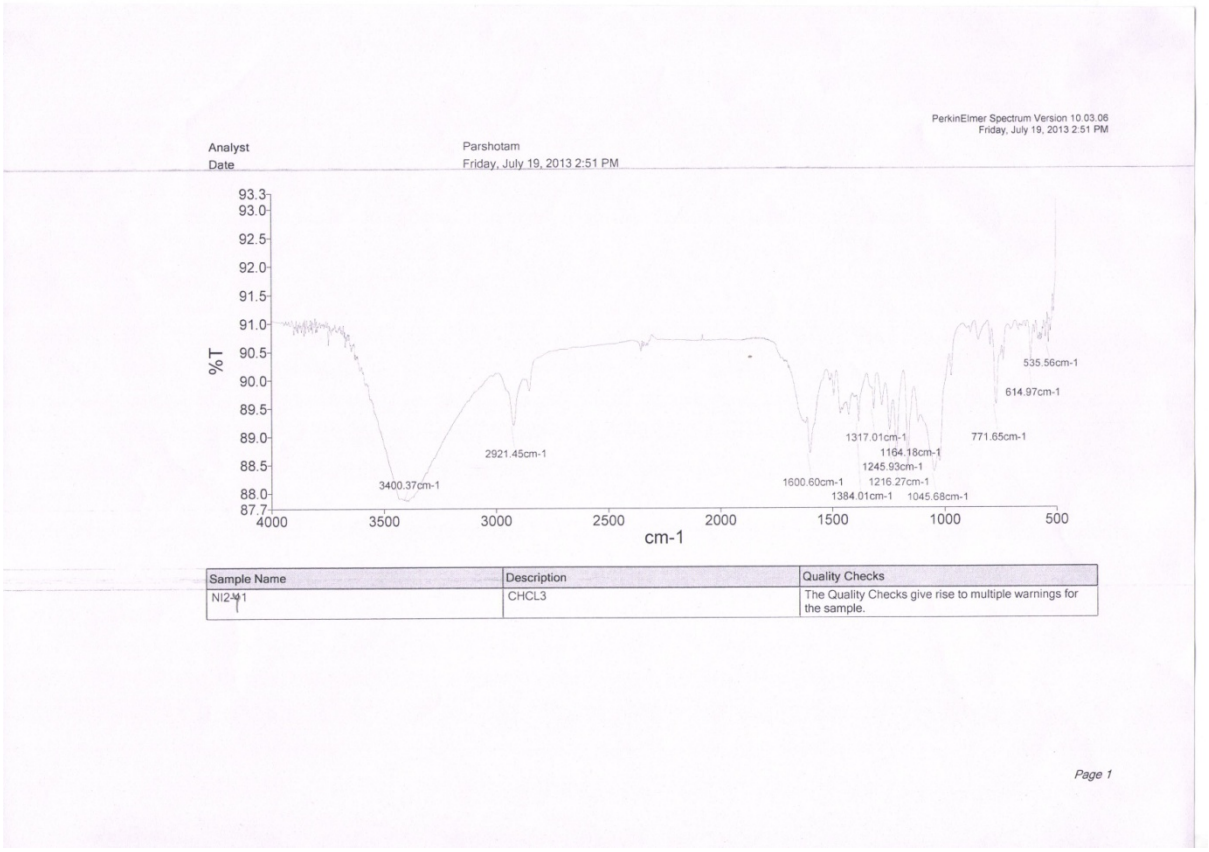
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
289.0977	1	3691099.75	C18 H13 N2 O2	(M+H)+
290.1119	1	730706.94	C18 H13 N2 O2	(M+H)+
291.1144	1	78486.31	C18 H13 N2 O2	(M+H)+
292.1175	1	4093.75	C18 H13 N2 O2	(M+H)+
293.1186	1	921.64	C18 H13 N2 O2	(M+H)+

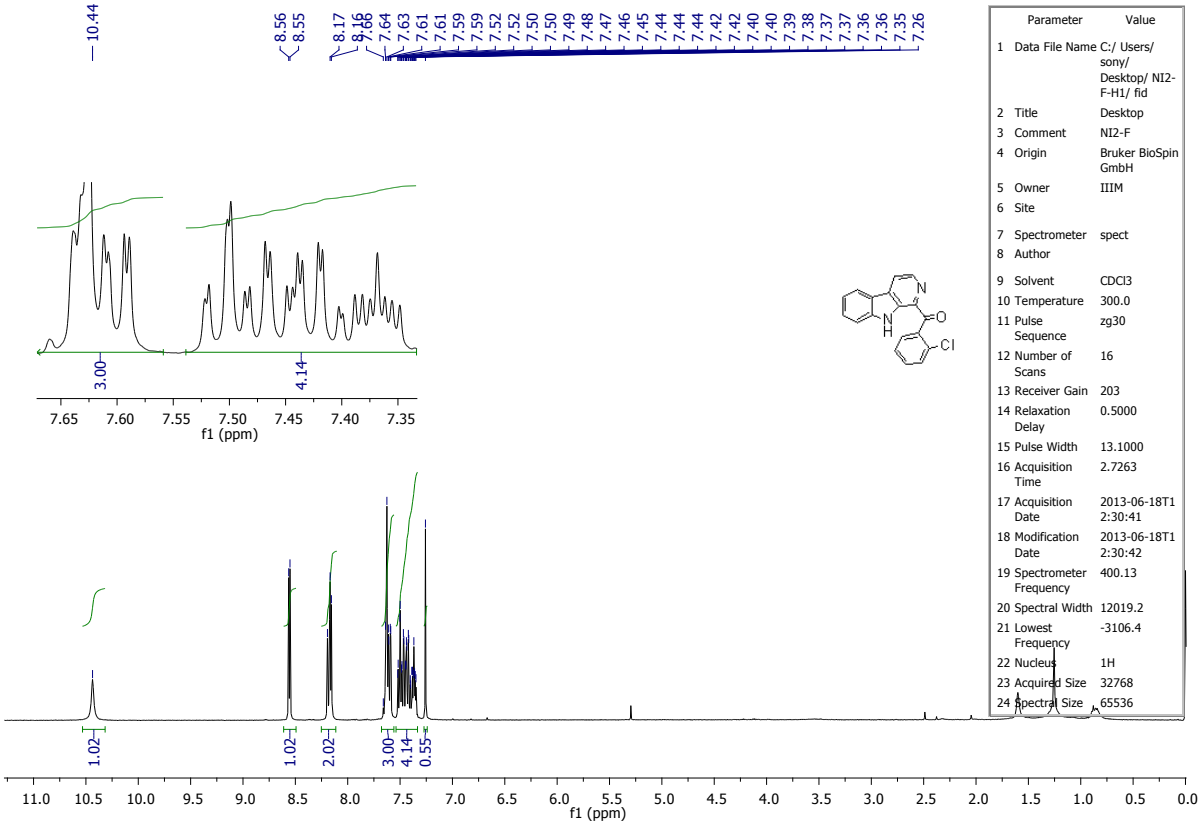
Predicted Isotope Match Table

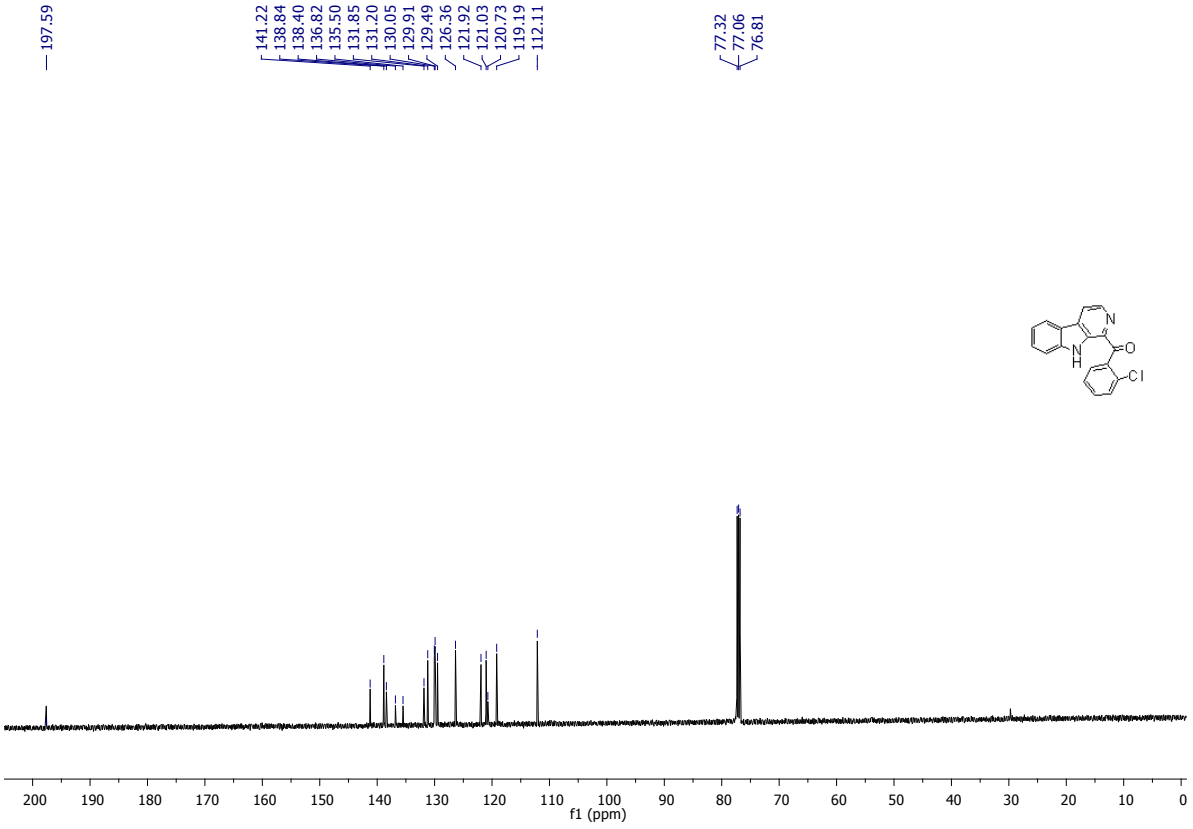
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	289.0977	289.0972	-2	100	100	81.93	81.28
2	290.1119	290.1003	-39.82	19.8	20.42	16.22	16.6
3	291.1144	291.1031	-38.67	2.13	2.39	1.74	1.94
4	292.1175	292.1057	-40.11	0.11	0.2	0.09	0.17
5	293.1186	293.1084	-34.83	0.02	0.01	0.02	0.01

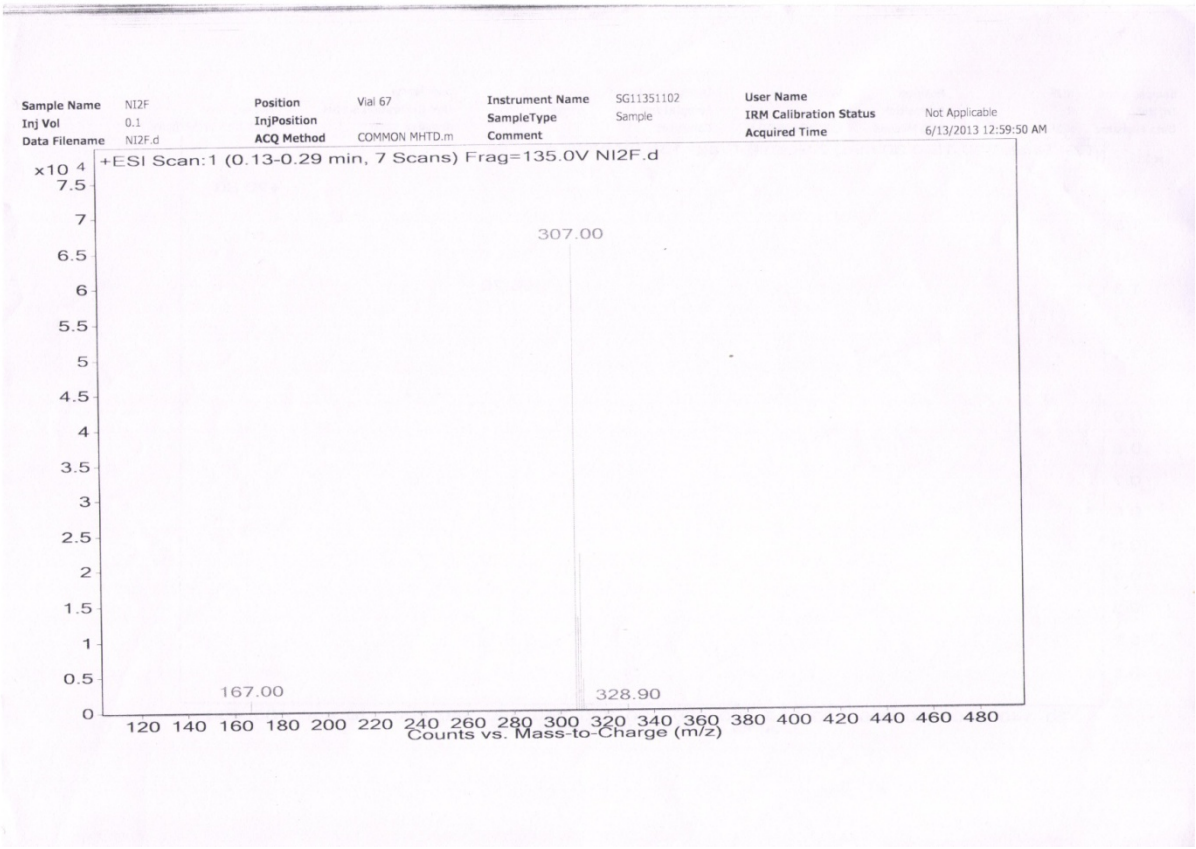
--- End Of Report ---



13) (2-chlorophenyl)(9H-pyrido[3,4-b]indol-1-yl)methanone




197.59
141.22
138.84
138.40
136.82
135.50
131.85
131.20
130.05
129.91
129.49
126.36
121.92
121.03
120.73
119.19
112.11
77.32
77.06
76.81
N
H
O
Cl
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


Sample Name NI2F
Inj Vol 0.1
Data Filename NI2F.d
Position Vial 67
InjPosition
ACQ Method COMMON MHTD.m
Instrument Name SG11351102
SampleType Sample
Comment
User Name
IRM Calibration Status Not Applicable
Acquired Time 6/13/2013 12:59:50 AM
+ESI Scan:1 (0.13-0.29 min, 7 Scans) Frag=135.0V NI2F.d
x10 4
307.00
167.00
328.90
Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

Data File	NI2-F.d	**Sample Name**	NI2-F
Sample Type	Sample	**Position**	Vial 42
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	26-06-2013 PM 5:43:58
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

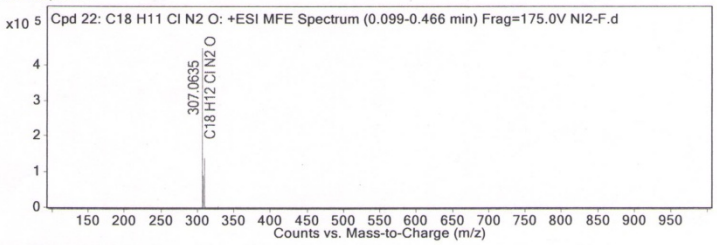
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 22: C18 H11 Cl N2 O	0.199	306.0561	C18 H11 Cl N2 O	C18 H11 Cl N2 O	-0.46	C18 H11 Cl N2 O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 22: C18 H11 Cl N2 O	307.0635	0.199	Find by Molecular Feature	306.0561

MFE MS Spectrum



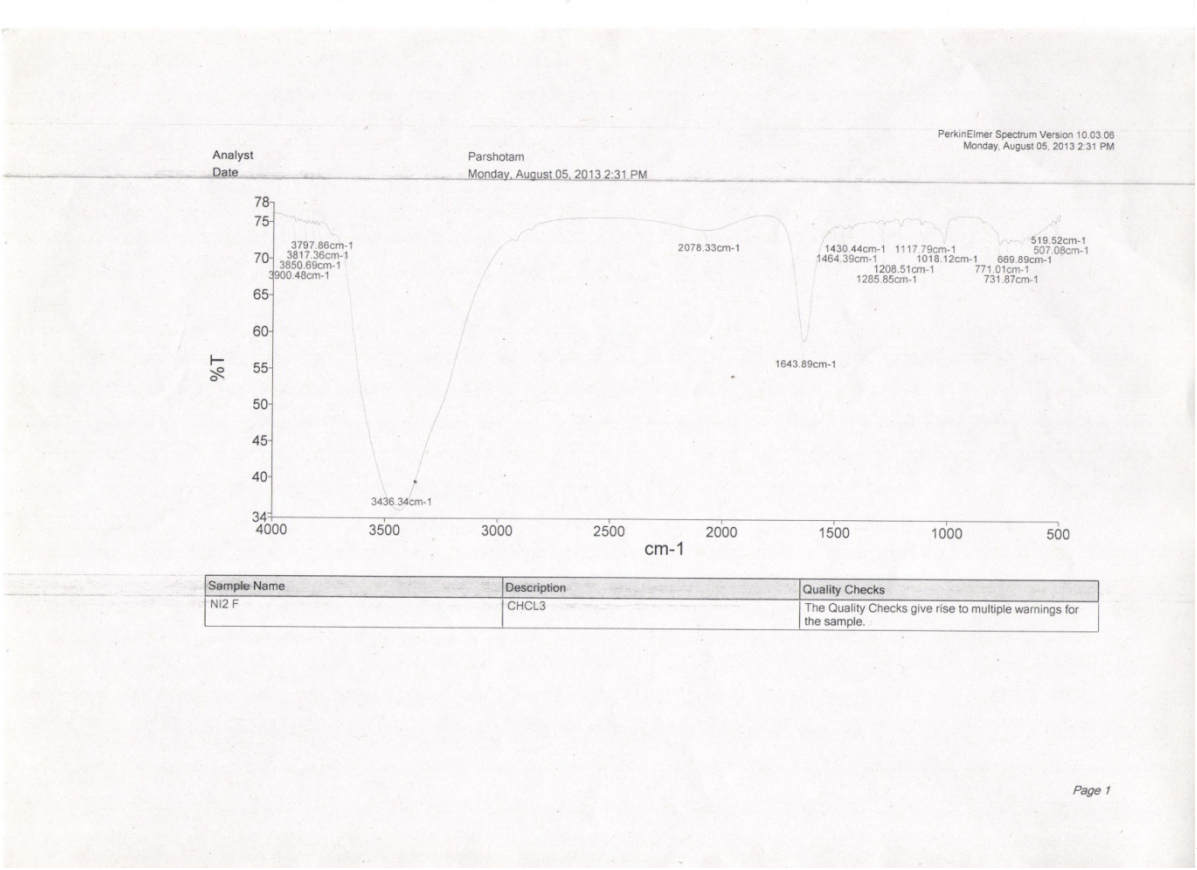
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
307.0635	1	447661.59	C18 H12 Cl N2 O	(M+H)+
308.0666	1	88647.37	C18 H12 Cl N2 O	(M+H)+
309.0608	1	137381.91	C18 H12 Cl N2 O	(M+H)+
310.0635	1	28267.65	C18 H12 Cl N2 O	(M+H)+
311.0662	1	3507.25	C18 H12 Cl N2 O	(M+H)+
312.069	1	269.08	C18 H12 Cl N2 O	(M+H)+
313.0651	1	359.09	C18 H12 Cl N2 O	(M+H)+
329.0448	1	1637.07	C18 H11 Cl N2 Na O	(M+Na)+

Predicted Isotope Match Table

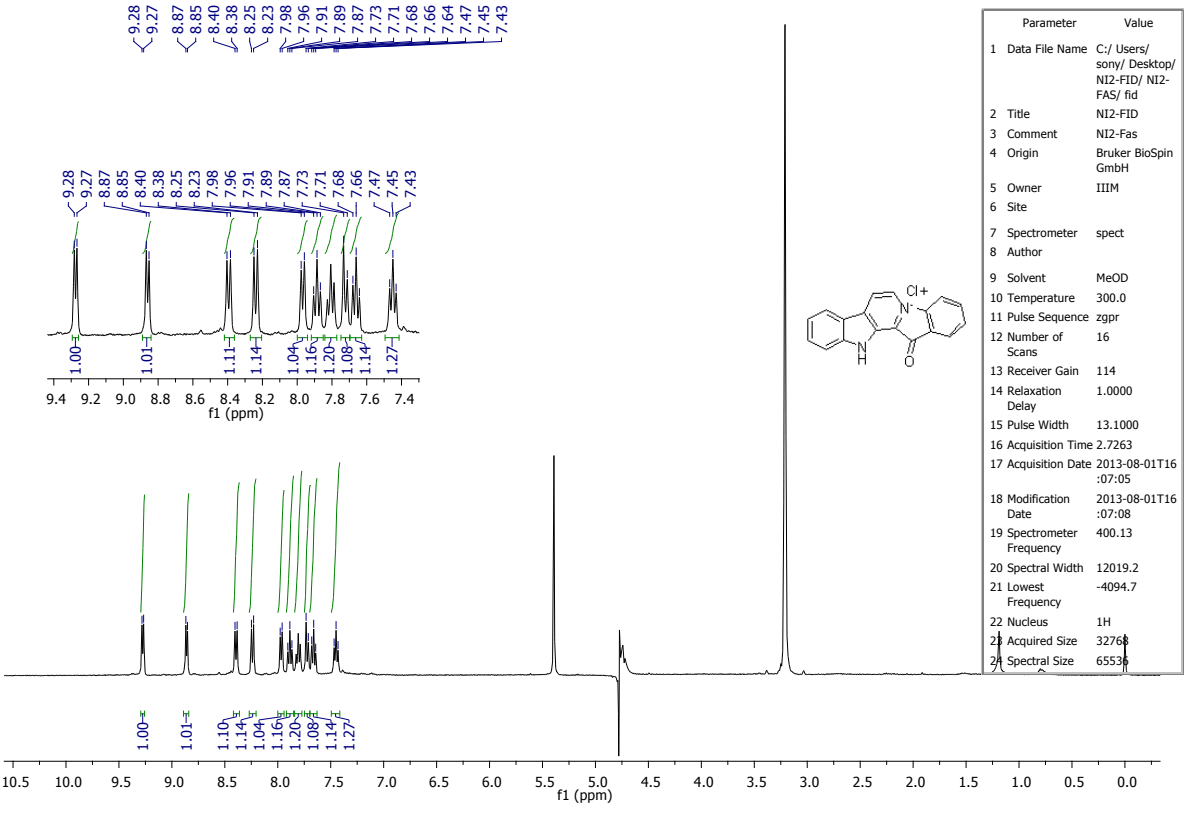
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	307.0635	307.0633	-0.8	100	100	63.4	61.73
2	308.0666	308.0664	-0.66	19.8	20.38	12.55	12.58
3	309.0608	309.0609	0.43	30.69	34.17	19.46	21.09
4	310.0635	310.0637	0.62	6.31	6.68	4	4.12
5	311.0662	311.0665	0.96	0.78	0.7	0.5	0.44
6	312.069	312.0693	0.71	0.06	0.05	0.04	0.03
7	313.0651	313.072	21.97	0.08	0	0.05	0

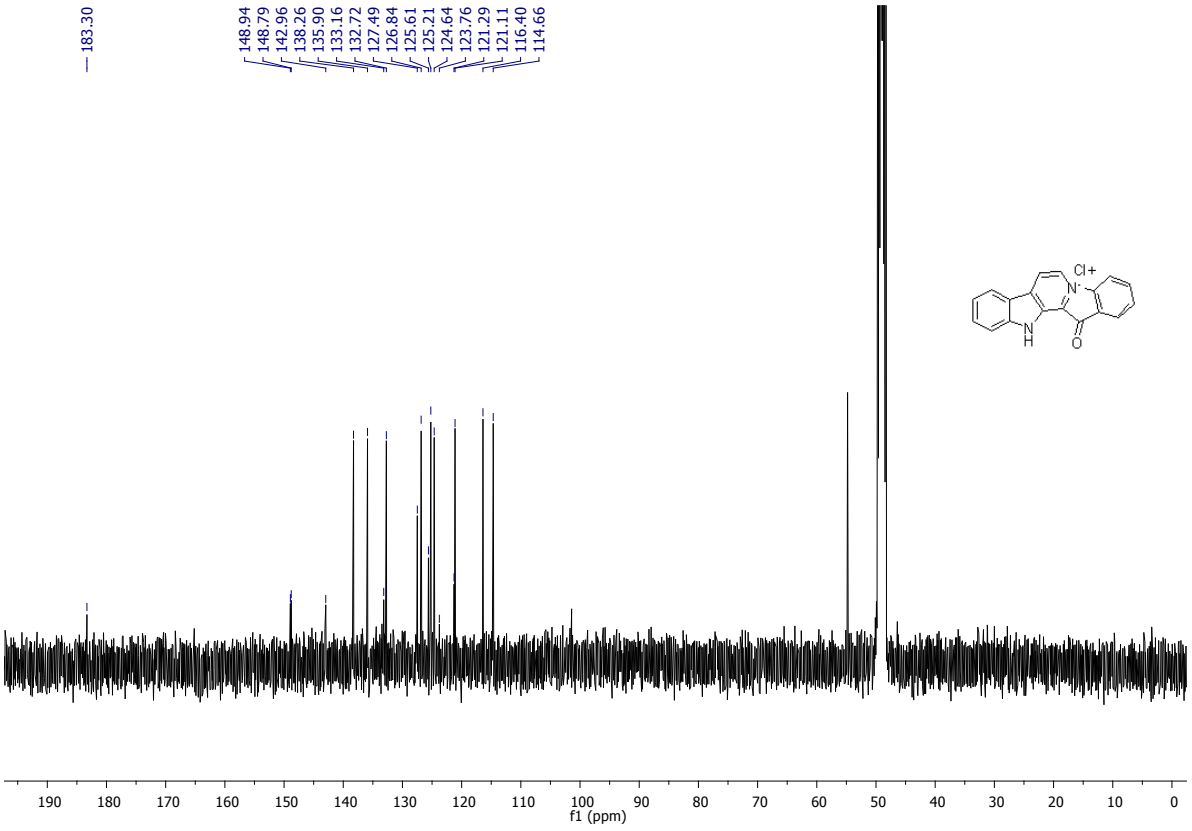
--- End Of Report ---



15

) Fascaplysin

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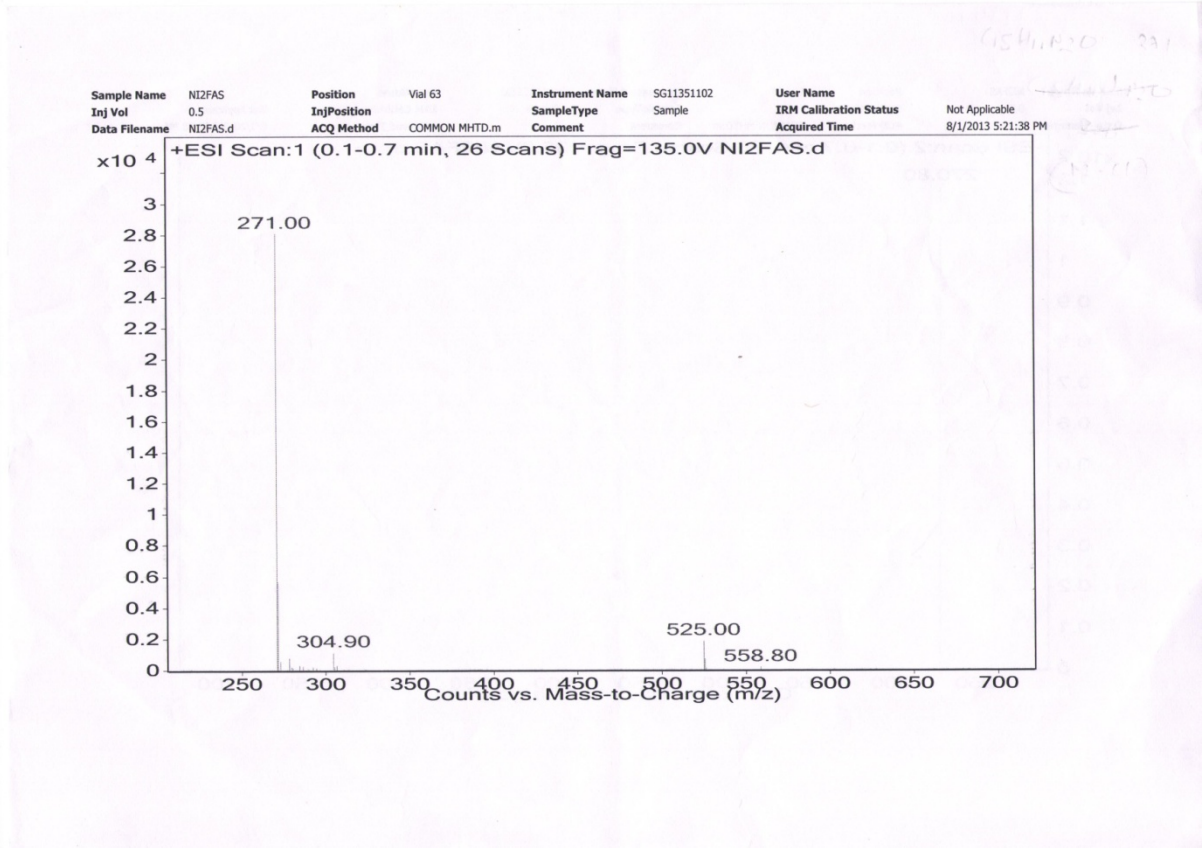
148.94
148.79
142.96
138.26
135.90
133.16
132.72
127.49
126.84
125.61
125.21
124.64
123.76
121.29
121.11
116.40
114.66
Cl+
N
H
O
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


Sample Name NI2FAS
Inj Vol 0.5
Data Filename NI2FAS.d
Position Vial 63
InjPosition
ACQ Method COMMON MHTD.m
Instrument Name SG11351102
SampleType Sample
Comment
User Name
IRM Calibration Status Not Applicable
Acquired Time 8/1/2013 5:21:38 PM
+ESI Scan:1 (0.1-0.7 min, 26 Scans) Frag=135.0V NI2FAS.d
x10 4
271.00
304.90
525.00
558.80
Counts vs. Mass-to-Charge (m/z)

Qualitative Compound Report

Data File	NI2-FAS.d	**Sample Name**	NI2-FAS
Sample Type	Sample	**Position**	Vial 2
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	10-09-2013 AM 10:54:38
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

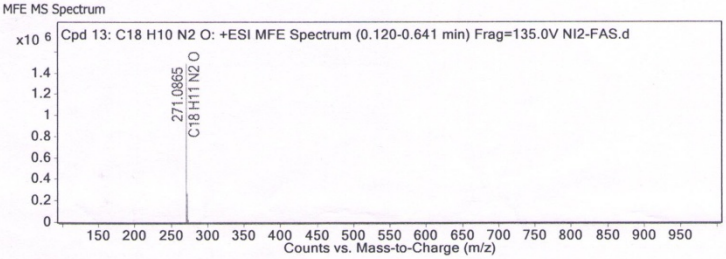
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 13: C18 H10 N2 O	0.196	270.0793	C18 H10 N2 O	C18 H10 N2 O	0.16	C18 H10 N2 O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 13: C18 H10 N2 O	271.0865	0.196	Find by Molecular Feature	270.0793

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
271.0865	1	1488100.88	C18 H11 N2 O	(M+H)+
272.0899	1	266393.78	C18 H11 N2 O	(M+H)+
273.0927	1	28140.96	C18 H11 N2 O	(M+H)+
274.0961	1	2836.29	C18 H11 N2 O	(M+H)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	271.0865	271.0866	0.31	100	100	83.34	81.5
2	272.0899	272.0897	-0.62	17.9	20.36	14.92	16.6
3	273.0927	273.0927	-0.25	1.89	2.17	1.58	1.77
4	274.0961	274.0955	-2.15	0.19	0.16	0.16	0.13

--- End Of Report ---