Supporting Information

Synthesis of functionalized isoxazole-oxindole hybrids *via* on water, catalyst free vinylogous Henry and 1,6-Michael addition reactions†

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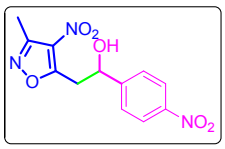
2-(3-methyl-4-nitroisoxazol-5-yl)-1-(4-nitrophenyl) ethanol:

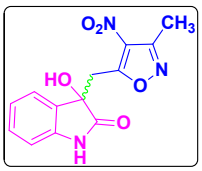


Yield = 80% (White solid); M.P. 128-129 °C;

^{1}H-NMR (500 MHz, $CDCl_3$): δ 8.25 (d, *J* = 15 Hz, 2H), 7.64 (s, 2H), 5.42 (s, 1H), 3.64 (s, 2H), 2.74 (s, 1H), 2.59 (s, 3H).

IR (KBr) ν_{max}: 3498 (O-H), 1141 (O-H), 1522 (NO_2) cm^{-1}

3-hydroxy-3-((3-methyl-4-nitroisoxazol-5-yl) methyl) indolin-2-one:

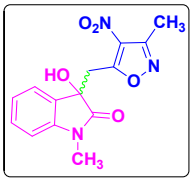


Yield = 99% (White solid); M.P. 78-80 °C;

^{1}H-NMR (500 MHz, MeOD): δ 7.28-7.24 (m, 1H), 7.02 (t, *J* = 5 Hz, 1H), 6.89 (d, *J* = 5 Hz, 1H), 3.97 (d, *J* = 15 Hz, 1H), 3.71 (d, *J* = 15 Hz, 1H), 3.34 (s, 1H), 2.47 (s, 3H); Mass (ESI-MS): m/z Calculated: 289; Observed: 312 (M+Na)

IR (KBr) ν_{max}: 3238 (N-H), 3233 (OH), 1707 (C=O), 1183 (O-H), 1522 (NO_2) cm^{-1}

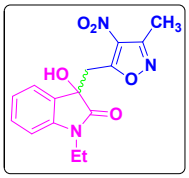
3-hydroxy-1-methyl-3-((3-methyl-4-nitroisoxazol-5-yl)methyl)indolin-2-one



Yield = 98% (pale yellow solid); M.P.: 99-101 °C;

^{1}H-NMR (500 MHz, $CDCl_3$): δ 7.36 – 7.22 (m, 3H), 6.86 (d, *J* = 5 Hz, 1H), 4.02 (d, *J* = 15 Hz, 1H), 3.60 (m, 2H), 3.21 (s, 3H), 2.52 (s, 3H).

1-ethyl-3-hydroxy-3-((3-methyl-4-nitroisoxazol-5-yl)methyl)indolin-2-one:



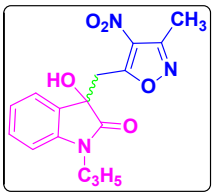
Yield = 92% (White solid); M.P.: 137-139 °C;

^{1}H- NMR (500 MHz, MeOD): δ 7.35 (d, *J* = 10 Hz, 2H), 7.09 (d, *J* = 10 Hz, 1H), 7.01 (d, *J* = 10 Hz, 1H), 3.99 (d, *J* = 15 Hz, 1H), 3.88 – 3.79 (m, 1H), 3.77 – 3.63 (m, 2H), 3.34 (s, 1H), 2.45 (s, 3H), 1.25 (s, 3H). ^{13}C- NMR (126 MHz, MeOD): δ 176.25, 168.81, 155.24, 141.78, 129.97, 129.60, 123.60, 122.73, 108.76, 74.61, 34.68, 34.34, 11.09, 10.03

Mass (ESI-MS); m/z Calculated: 317; Observed: 335 (M+ H_2O)

IR (KBr) ν_{max}: 3346 (OH), 1710 (C=O), 1220 (O-H), 1518 (NO_2) cm^{-1}

1-allyl-3-hydroxy-3-((3-methyl-4-nitroisoxazol-5-yl)methyl)indolin-2-one:



Yield = 93% (White solid), M.P.: 149-150 °C;

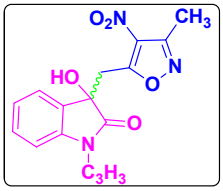
^{1}H NMR (500 MHz, MeOD): δ 7.34 (t, *J* = 5 Hz, 2H), 7.10 (t, *J* = 5 Hz, 1H), 6.96 (d, *J* = 5 Hz, 1H), 5.91-5.84 (m,1H), 5.25 (t, *J* = 15 Hz, 2H), 4.40 (t, *J* = 5 Hz, 1H), 4.27 (dd, *J* = 5, 5, Hz, 1H), 3.99 (d, *J* = 15 Hz, 1H), 3.77 (d, *J* = 15 Hz, 1H), 3.34 (s, 1H), 2.47 (s, 3H).

^{13}C NMR (126 MHz, MeOD): δ 176.26, 168.92, 155.32, 142.03, 131.06, 129.88, 129.47, 123.54, 122.85, 116.73, 109.54, 74.55, 38.60, 38.45, 37.93, 34.75, 10.16.

Mass (ESI-MS): m/z Calculated: 329; Observed: 328(M-1)

IR (KBr) ν_{max}: 3412 (OH), 1712 (C=O), 1177 (O-H), 1517 (NO_2) cm^{-1}

3-hydroxy-3-((3-methyl-4-nitroisoxazol-5-yl)methyl)-1-(prop-2-yn-1-yl)indolin-2-one:



Yield = 95% (White solid); M.P.: 132-133 °C;

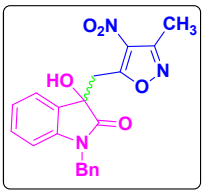
^{1}H-NMR (500 MHz, $CDCl_3$): δ 7.39-7.09 (m, 4H), 4.49 (d, *J* = 15 Hz, 2H), 4.04 (d, *J* = 15 Hz, 1H), 3.60 (d, *J* = 15 Hz, 1H), 3.33 (s, 1H), 2.54 (s, 3H), 2.28 (s, 1H).

^{13}C- NMR (126 MHz, $CDCl_3$): δ 174.80, 168.49, 155.59, 141.04, 130.68, 127.93, 124.10, 123.86, 110.03, 75.95, 75.05, 73.02, 35.66, 29.67, 11.63.

Mass (ESI-MS): m/z Calculated: 327; Observed: 328 (M+1).

IR (KBr) ν_{max}: 3289 (OH), 1715 (C=O), 1175 (O-H), 1518 (NO_2) cm^{-1}

3-hydroxy-3-((3-methyl-4-nitroisoxazol-5-yl)methyl)-1-phenethylindolin-2-one:



Yield = 90% (White solid), M.P.: 98-99 °C;

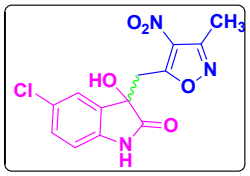
^{1}H- NMR (500 MHz, $CDCl_3$): δ 7.36 –7.31 (m, 2H), 7.29 (d, *J* = 10 Hz, 3H), 7.26-7.22 (m, *J* = 9.0 Hz, 2H), 7.05 (t, *J* = 5 Hz, 1H), 6.74 (d, *J* = 10 Hz, 1H), 4.97 (d, *J* = 15Hz, 1H), 4.80 (d, *J* = 15 Hz, 1H), 4.10 (d, *J* = 15 Hz, 1H), 3.65 (d, *J* = 10 Hz, 1H), 2.55 (s, 3H).

^{13}C-NMR (126 MHz, $CDCl_3$): δ 175.84, 168.68, 155.62, 142.21, 134.93, 130.63, 128.96, 127.99, 127.33, 124.06, 123.53, 110.09, 74.99, 44.23, 35.60, 11.65

IR (KBr) ν_{max}: 3325 (OH), 1709 (C=O), 1173 (O-H), 1517 (NO_2) cm^{-1}

5-chloro-3-hydroxy-3-((3-methyl-4-nitroisoxazol-5-yl)methyl)indolin-2-one:

Yield = 96% (White solid), M.P: 98-100 °C;



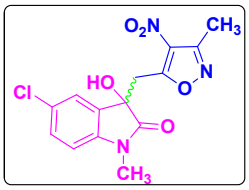
^{1}H-NMR (500 MHz, MeOD): δ 7.28 (t, *J* = 5 Hz, 2H), 6.88 (d, *J* = 5 Hz, 1H), 3.95 (d, *J* = 15 Hz, 1H), 3.73 (d, *J* = 15 Hz, 1H), 3.34 (s, 1H), 2.49 (s, 3H). ^{13}C- NMR (126 MHz, MeOD): δ 178.16, 168.67, 155.34, 139.84, 131.89, 131.17, 129.68, 127.54, 124.19, 111.29, 74.81, 34.50, 10.08.

Mass (ESI-MS): m/z Calculated: 323; Observed: 346 (M+ Na)

IR (KBr) ν_{max}: 3415 (N-H), 3168 (OH), 1719 (C=O), 1183 (O-H), 1521 (NO_2) cm^{-1}

5-chloro-3-hydroxy-1-methyl-3-((3-methyl-4-nitroisoxazol-5-yl) methyl)indolin-2-one:

Yield = 93% (gray solid); M.P.: 181-182 °C;

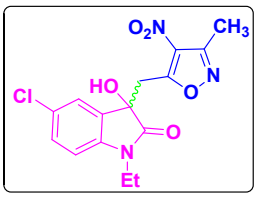


1H- NMR (500 MHz, $CDCl_3$): δ 7.36 (s, 1H), 7.08 (s, 1H), 6.86 (d, *J* = 5 Hz, 1H), 4.02 (d, *J* = 15 Hz, 1H), 3.59 (t, *J* = 10 Hz, 2H), 3.21 (s, 3H), 2.52 (s, 3H).

Mass (ESI-MS): m/z Calculated: 337; Observed: 336 (M-1)

5-chloro-1-ethyl-3-hydroxy-3-((3-methyl-4-nitroisoxazol-5-yl)methyl)indolin-2-one:

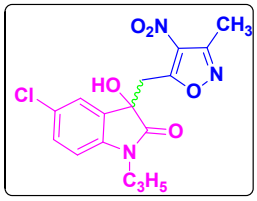
Yield = 90% (gray solid), M.P : 159-160 °C, ^{1}H-NMR (500 MHz, $CDCl_3$): δ 7.34-7.26 (M, 2H), 6.81 (d, *J* = 5 Hz, 1H), 3.99 (d, *J* = 15 Hz, 1H), 3.83-3,78 (M,1H), 3.71 – 3.60(m, 3H), 2.53 (s, 3H), 1.28 (s, 3H). ^{13}C- NMR (126 MHz, $CDCl_3$) δ 175.00, 169.45, 155.67, 141.10, 132.52, 130.08, 126.96, 124.67, 110.90, 74.89, 35.24, 34.64, 12.43, 11.55



IR (KBr) ν_{max}: 3289 (OH), 1713 (C=O), 1217 (O-H), 1518 (NO_2) cm^{-1}

1-allyl-5-chloro-3-hydroxy-3-((3-methyl-4-nitroisoxazol-5-yl)methyl)indolin-2-one:

Yield = 95% (gray solid); M.P.: 126-127 °C;



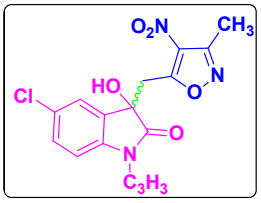
^{1}H- NMR (500 MHz, $CDCl_3$): δ 7.30-7.27 (m, Hz, 2H), 6.79 (d, *J* = 10 Hz, 1H), 5.83-5.5.75 (m, 1H), 5.27-5.23 (m, 2H), 4.40 (dd, *J* = 5.5, Hz, 1H), 4.29 – 4.16 (m, 2H), 3.99 (d, *J* = 15 Hz, 1H), 3.66 (d, *J* = 15 Hz, 1H), 2.51 (s, 3H).

^{13}C- NMR (126 MHz, $CDCl_3$): δ 175.43, 168.22, 155.64, 140.61, 131.55, 130.37, 130.04, 129.02, 124.62, 118.56, 111.03, 74.89, 42.85, 35.65, 11.60.

Mass (ESI-MS Spectrum); m/z Calculated: 363; Observed: 363 (m/z)

IR (KBr) ν_{max}: 3376 (OH), 1716 (C=O), 1174 (O-H), 1523 (NO_2) cm^{-1}

5-chloro-3-hydroxy-3-((3-methyl-4-nitroisoxazol-5-yl)methyl)-1-(prop-2-yn-1-yl)indolin-2-one:



Yield = 95% (gray solid); M.P.: 148-149 °C;

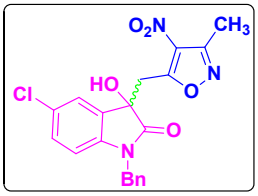
^{1}H- NMR (500 MHz, MeOD): δ 7.41-7.36 (m, 2H), 7.13 (d, *J* = 10Hz, 1H), 4.52 (s, 2H), 3.94 (d, *J* = 15 Hz, 1H), 3.77 (d, *J* = 10 Hz, 1H), 2.74 (s, 1H), 2.48 (s, 3H).

^{13}C- NMR (126 MHz, MeOD): δ 175.19, 168.31, 155.30, 139.68, 131.33, 129.66, 128.52, 124.08, 110.88, 34.67, 28.74, 10.08

Mass (ESI-MS): m/z Calculated: 361; Observed: 362 (M+1).

IR (KBr) ν_{max}: 3363 (OH), 1725 (C=O), 1172 (O-H), 1521 (NO_2) cm^{-1}

1-benzyl-5-chloro-3-hydroxy-3-((3-methyl-4-nitroisoxazol-5-yl)methyl)indolin-2-one:



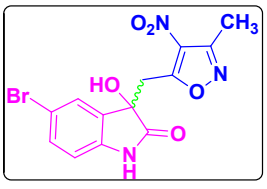
Yield = 93% (gray solid), M.P.: 130-131 °C;

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.32 – 7.26 (m, 6H), 7.05 (s, 1H), 6.74 (s, 1H), 4.97 (d, *J* = 15 Hz, 1H), 4.80 (d, *J* = 15 Hz, 1H), 4.11 (d, *J* = 15 Hz, 1H), 3.66 (d, *J* = 15 Hz, 1H), 3.42 (s, 1H), 2.54 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$): δ 175.88, 168.68, 155.62, 142.18, 134.92, 130.62, 128.95, 127.99, 127.33, 124.06, 123.54, 110.09, 75.00, 44.22, 35.58, 11.65.

Mass (ESI-MS): m/z Calculated: 413; Observed: 412 (M-1).

IR (KBr) ν_{max}: 3317 (OH), 1708 (C=O), 1168 (O-H), 1523 (NO_2) cm^{-1}

5-bromo-3-hydroxy-3-((3-methyl-4-nitroisoxazol-5-yl)methyl)indolin-2-one:

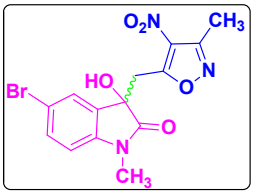


Yield = 90% (gray solid), M.P.: 198-199 °C;

^{1}H-NMR (500 MHz, MeOD): δ 7.53 (s, 2H), 7.17 (s, 2H), 3.92(s, 1H), 3.63 (s, 1H), 2.80 (s, 3H).

Mass (ESI-MS): m/z Calculated: 366; Observed: 349 (M- H_2O)

5-bromo-3-hydroxy-1-methyl-3-((3-methyl-4-nitroisoxazol-5-yl)methyl)indolin-2-one:



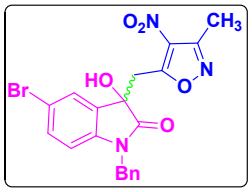
Yield = 92% (gray solid), M.P.: 151-152^{o}C;

^{1}H NMR (500 MHz, MeOD, DMSO-d_6): δ 7.50 (d, J = 10 Hz, 1H), 7.42 (s, 1H), 6.94 (d, J = 10 Hz, 1H), 3.88 (d, J = 10 Hz, 1H), 3.69 (d, J = 15 Hz, 1H), 3.29 (s, 1H), 3.15 (s, 3H), 2.46 (s, 3H).

^{13}C-NMR (126 MHz, MeOD): δ 175.85, 168.83, 155.42, 151.75, 142.18, 132.78, 131.94, 131.31, 126.75, 115.13, 110.56, 74.38, 38.39, 34.73, 25.46, 10.29

Mass (ESI-MS Spectrum): m/z Calculated: 381; Observed: 364 (M- H_2O).

1-benzyl-5-bromo-3-hydroxy-3-((3-methyl-4-nitroisoxazol-5-l)methyl)indolin-2-one:

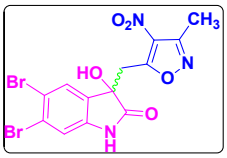


Yield = 87% (gray solid), M.P: 116-117 ^{o}C;

Mass (ESI-MS): m/z Calculated: 458; Observed: 456 (M-2).

IR (KBr) ν_{max}: 3314 (OH), 1707 (C=O), 1170 (O-H), 1524 (NO_2) cm^{-1}

5,6-dibromo-3-hydroxy-3-((3-methyl-4-nitroisoxazol-5-yl)methyl)indolin-2-one:



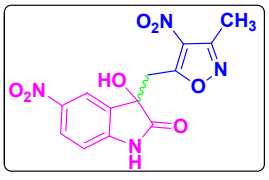
Yield = 89% (White solid), M.P.; 148-149 ^{o}C;

^{1}H-NMR (500 MHz, $CDCl_3$): δ 8.23 (s, 1H), 7.52 (s, 1H), 3.90-3.76 (m, 2H), 1.25 (s, 3H).

^{13}C-NMR (126 MHz, CDCl3): δ 175.43, 168.22, 155.64, 140.61, 130.38, 130.04, 129.02, 124.62, 118.56, 111.03, 42.85, 35.65, 11.60

IR (KBr) ν_{max}: 3429 (N-H), 3207 (OH), 1728 (C=O), 1181 (O-H), 1454 (NO_2) cm^{-1}

3-hydroxy-3-((3-methyl-4-nitroisoxazol-5-yl)methyl)-5-nitroindolin-2-one:



Yield = 82% (gray solid), M.P.: 149-150 ^{o}C;

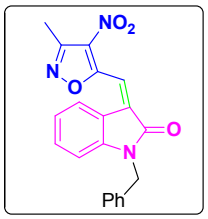
^{1}H-NMR (500 MHz, $CDCl_3$): δ 10.32 (s, 1H), 7.63 – 6.33 (m, 3H), 3.91 – 3.67 (m, 2H), 3.04 (s, 3H).

^{13}C-NMR (126 MHz, $CDCl_3$): δ 189.45, 182.51, 176.82, 174.32, 164.42, 160.16, 159.79, 155.82, 146.15, 143.34, 135.93, 134.86, 134.59, 129.83, 128.70, 127.87, 126.92, 122.55, 117.42, 115.16, 18.68, 16.33

Mass (ESI-MS): m/z Calculated: 334; Observed: 236 (M+1)

IR (KBr) ν_{max}: 3344 (N-H), 3243 (OH), 1710 (C=O), 1185 (O-H), 1523 (NO_2) cm^{-1}

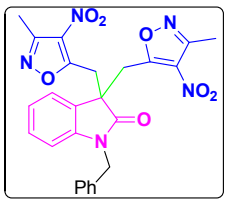
(E)-1-benzyl-3-((3-methyl-4-nitroisoxazol-5-yl)methylene)indolin-2-one:



Yield = 90% (brick red solid), M.P.: 73-74 °C;

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.36 (d, *J* = 10 Hz, 1H), 8.16 (s, 1H), 7.37 – 7.04 (m, 6H), 7.08-704 (m, 1H), 6.75 (d, *J* = 10 Hz, 1H), 4.98 (s, 2H), 2.68 (s, 3H). Mass (ESI-MS): m/z Calculated: 361; Observed: 362 (M+1)

1-benzyl-3,3-bis((3-methyl-4-nitroisoxazol-5-yl)methyl)indolin-2-one:



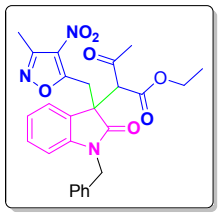
Yield = 90% (gray color semi solid), M.P.: 73-74 °C;

^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.39–7.26 (m, 5H), 7.15–7.03 (m, 2H), 6.91 (t, *J* = 7.2 Hz, 1H), 6.63 (d, *J* = 7.9 Hz, 1H), 4.91 (s, 2H), 4.19 (d, *J* = 16 Hz, 2H), 3.81 (d, *J* = 16 Hz, 2H), 2.45 (s, 6H).

^{13}C-NMR (101 MHz, $CDCl_3$): δ 175.71, 168.90, 155.42, 142.42, 135.32, 130.06, 129.36, 127.89, 127.31, 123.07, 110.11, 50.39, 44.54, 33.73, 11.41

Mass: m/z Calculated: 502; Observed: 503 (M+1)

ethyl 2-(1-benzyl-3-((3-methyl-4-nitroisoxazol-5-yl)methyl)-2-oxoindolin-3-yl)-3-oxobutanoate

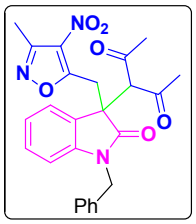


Yield = 87% (Black semi solid), M.P: 73-74 °C;

^{1}H- NMR (500 MHz, $CDCl_3$): δ 7.75 (d, *J* = 5 Hz, 1H), 7.47 – 7.35 (m, 3H), 7.19 – 7.13 (m, 2H), 7.00 – 6.93 (m, 2H), 6.75-6.69 (m, 1H), 5.92 (s, 1H), 4.92 (d, *J* = 10 Hz, 2H), 4.04 (dd, *J* = 5, 10 Hz, 2H), 3.77 (dd, *J* = 5, 10 Hz, 2H), 2.36 (s, 3H), 2.27 (s, 3H), 1.15 (s, 3H).

^{13}C-NMR (126 MHz, $CDCl_3$): δ 201.41, 176.34, 167.24, 160.63, 145.88, 143.73, 135.82, 128.58, 127.70, 127.55, 127.07, 123.10, 122.75, 108.86, 61.33, 51.92, 50.14, 44.73, 30.22, 14.08, 13.40, 9.74

3-(1-benzyl-3-((3-methyl-4-nitroisoxazol-5-yl)methyl)-2-oxoindolin-3-yl)pentane-2,4-dione:



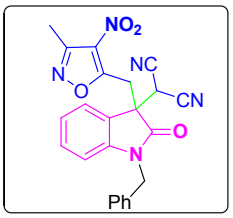
Yield = 95% (semi solid), M.P.: 73-74 °C;

^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.56 (d, *J* = 8 Hz, 1H), 7.43 (d, *J* = 8 Hz, 2H), 7.35 (t, *J* = 8 Hz, 2H), 7.29 (d, *J* =8 Hz, 1H), 7.15 (t, *J* = 8Hz, 1H), 6.95 (t, *J* = 4 Hz, 1H), 6.73 (d, *J* = 8 Hz, 1H), 5.3 (d, *J* = 8 Hz, 2H,) 5.28 (s, 1H), 5.19 (d, *J* = 16 Hz, 1H), 4.78 (d, *J* = 16 Hz, 1H), 2.35 (s, 3H), 2.25 (s, 3H), 2.00 (s, 3H).

^{13}C-NMR (100 MHz, $CDCl_3$): δ 201.39, 201.08, 190.39, 177.76, 160.66, 146.66, 144.37, 135.36, 128.80, 127.67, 126.53, 124.13, 123.22, 109.18, 107.26, 71.74, 53.40, 45.30, 30.98, 30.74, 29.73, 26.98, 9.72

Mass: m/z Calculated: 461; Observed: 484(M+Na).

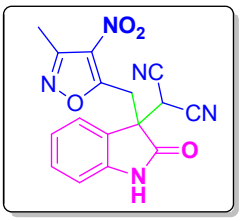
2-(1-benzyl-3-((3-methyl-4-nitroisoxazol-5-yl)methyl)-2-oxoindolin-3-yl)malononitrile:



Yield = 99% (black solid), M.P: 73-74 ^{o}C;

^{1}H-NMR (400 MHz, $CDCl_3$): δ 8.13 (d, *J* = 8 Hz, 1H), 7.48 – 7.09 (m, 7H), 7.11 (t, *J* = 8 Hz, 1H), 6.78 (d, *J* = 8.0 Hz, 4H), 4.92 (s, 2H), 1.57 (s, 3H)

2-(3-((3-methyl-4-5-yl)methyl)-2-oxoindolin-3-yl)malononitrile:

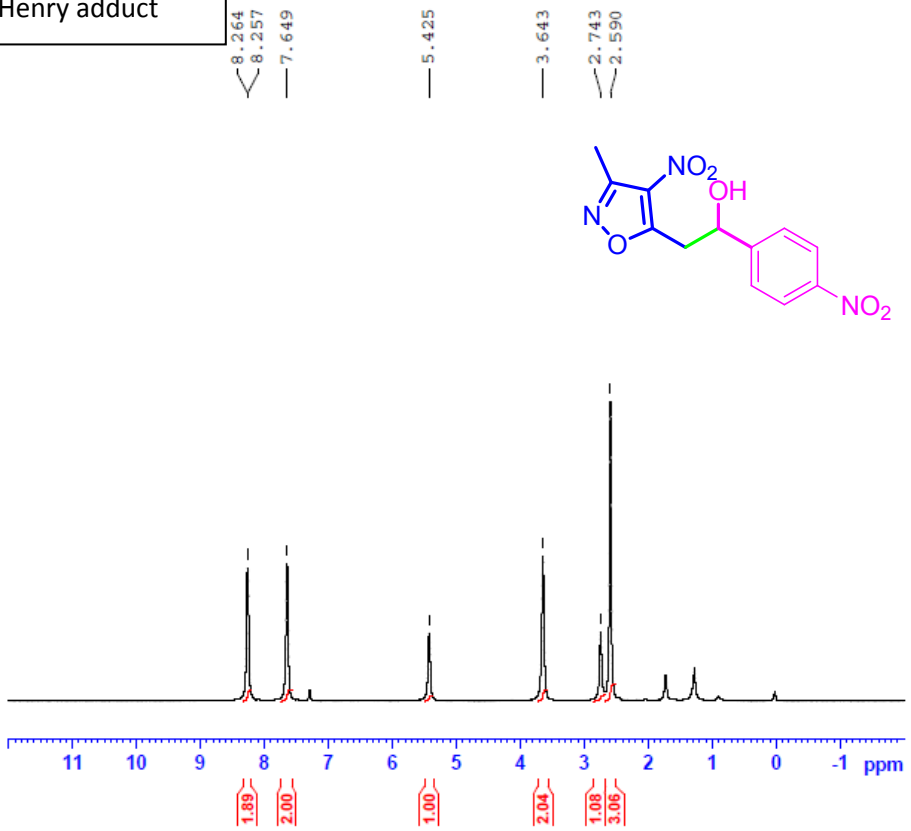


Yield = 99% (black solid), M.P.: 73-74 ^{o}C;

^{1}H-NMR (500 MHz, $CDCl_3$): δ 8.37 (d, *J* = 5 Hz 1H), 8.08 (t, *J* = 15 Hz1H), 7.69 (d, *J* = 30.8 Hz, 2H), 7.38 (s, 1H), 7.11 (s,1H), 5.33 (s, 1H), 4.15 (d, *J* = 15 Hz, 1H), 3.76 (d, *J* = 15 Hz, 1H), 2.68 (t, *J* = 15 Hz, 3H).

^{13}C-NMR (126 MHz, $CDCl_3$): δ 174.27, 170.75, 167.26, 155.07, 143.07, 135.36, 129.00, 128.81, 127.69, 127.37, 124.25, 122.66, 109.31, 50.79, 44.82, 37.51, 11.48

Henry adduct

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EXPNO                   1113
PROCNO                     1

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RG                    137.26
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DE                     6.50 usec
TE                    296.8 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
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NUC1                       1H
P1                      12.15 usec
PLW1             17.00000000 W

F2 - Processing parameters
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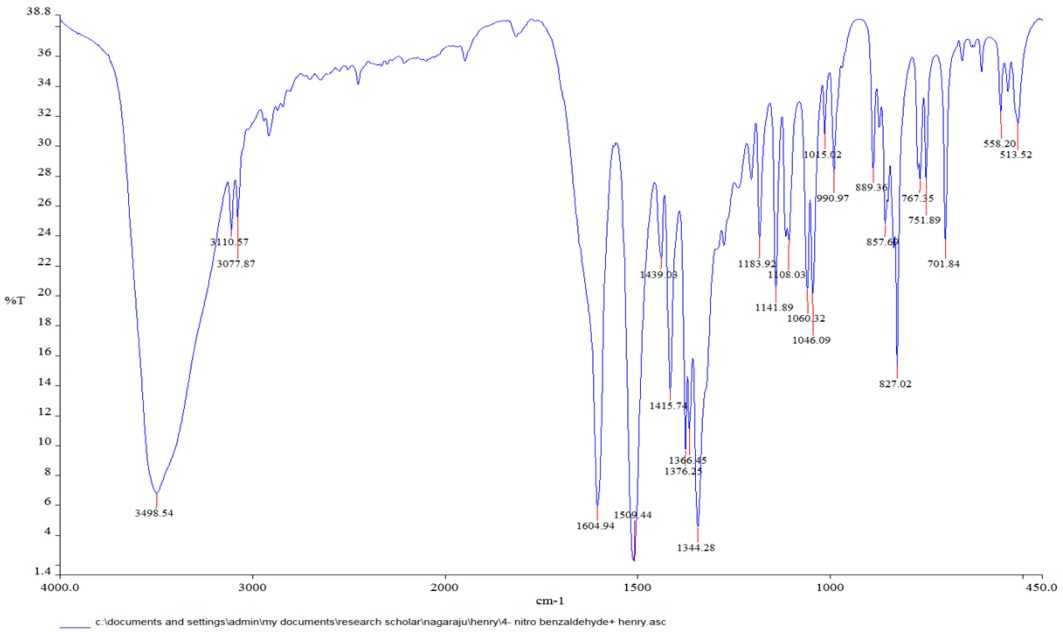

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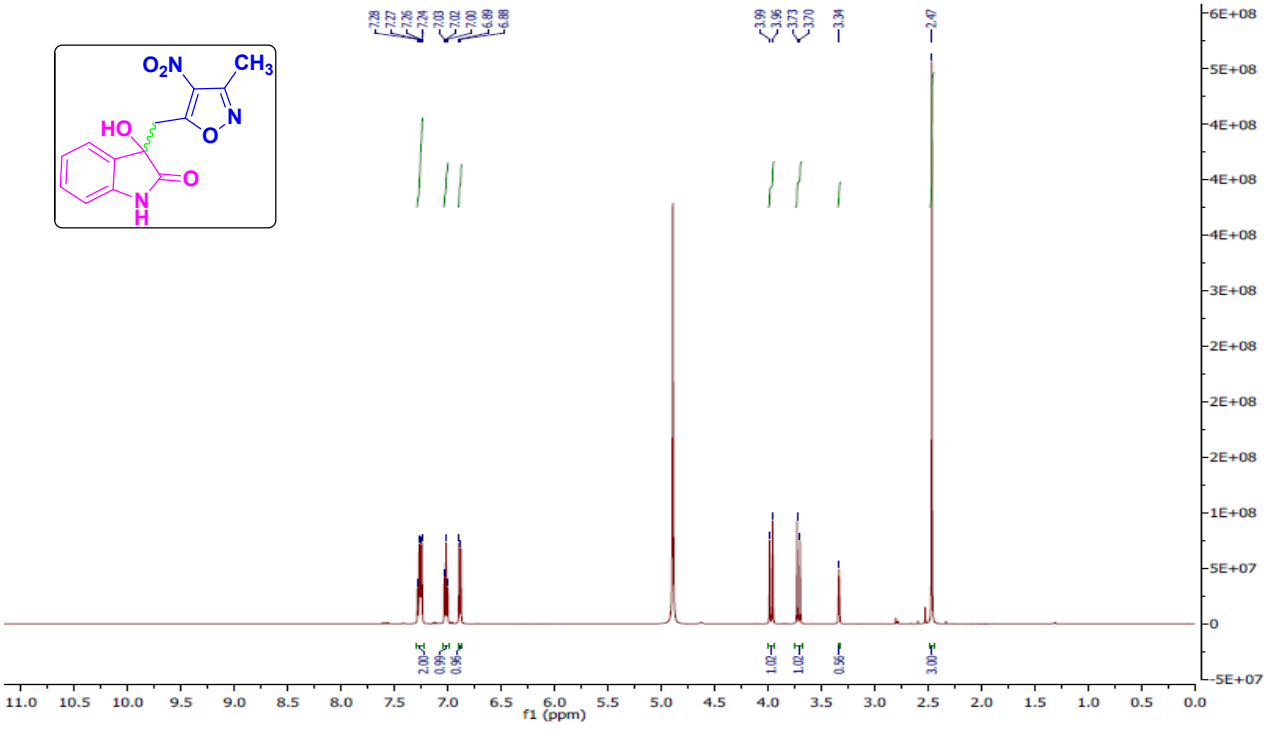

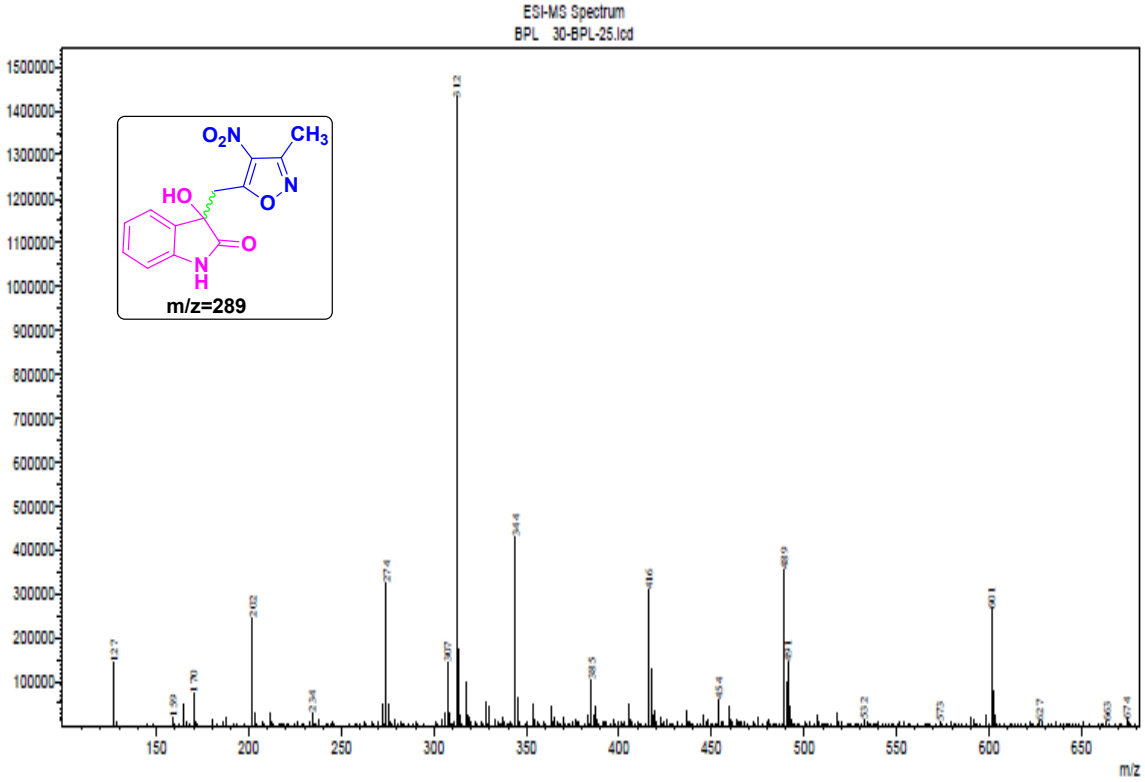

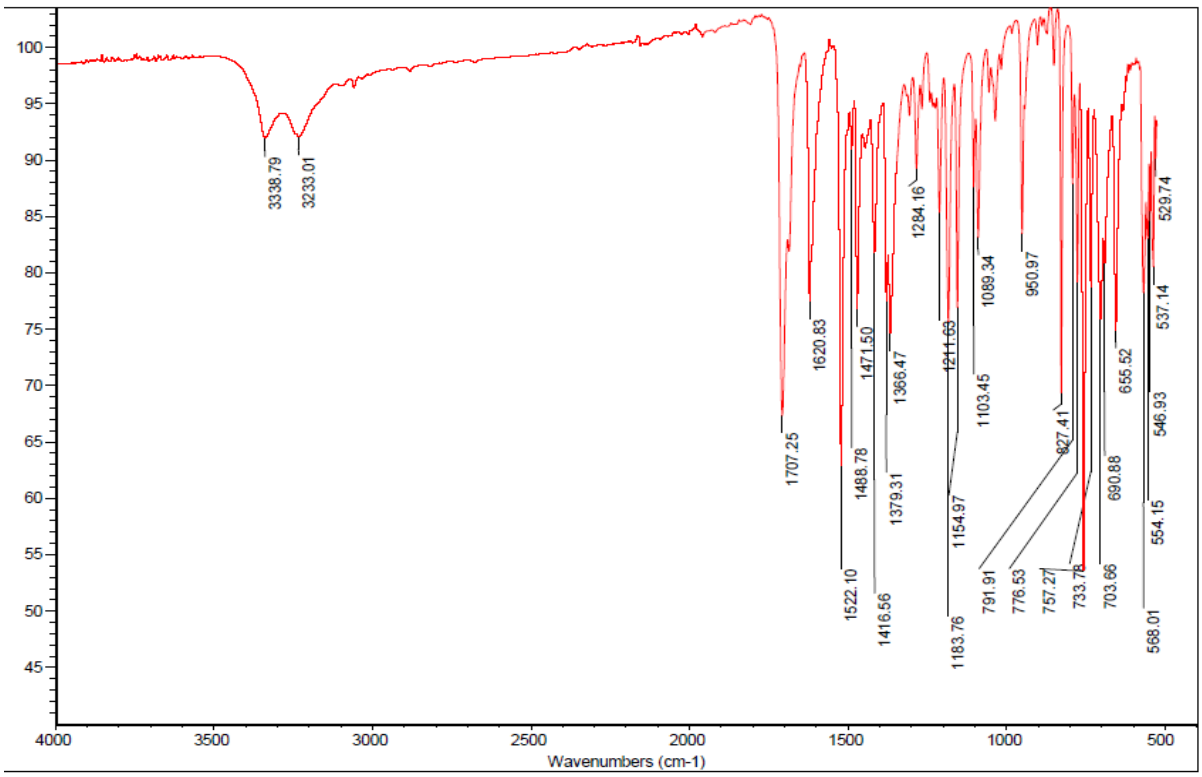

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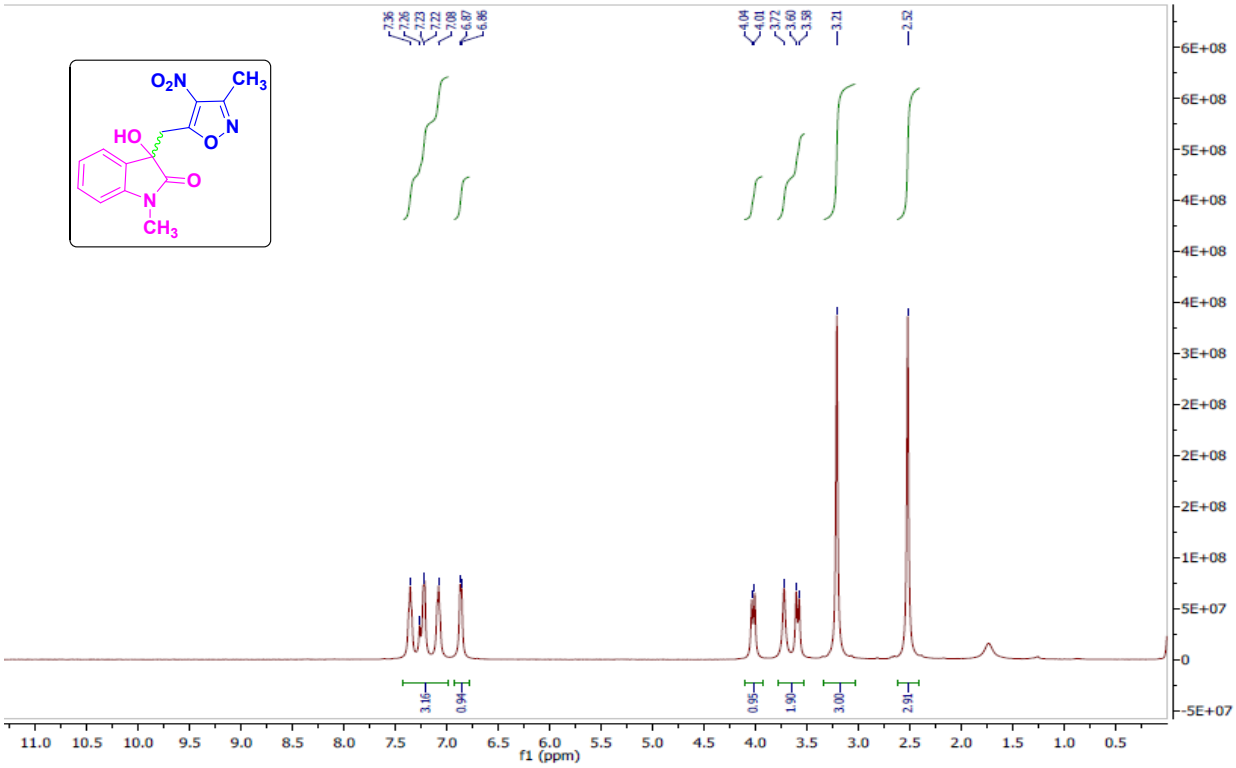

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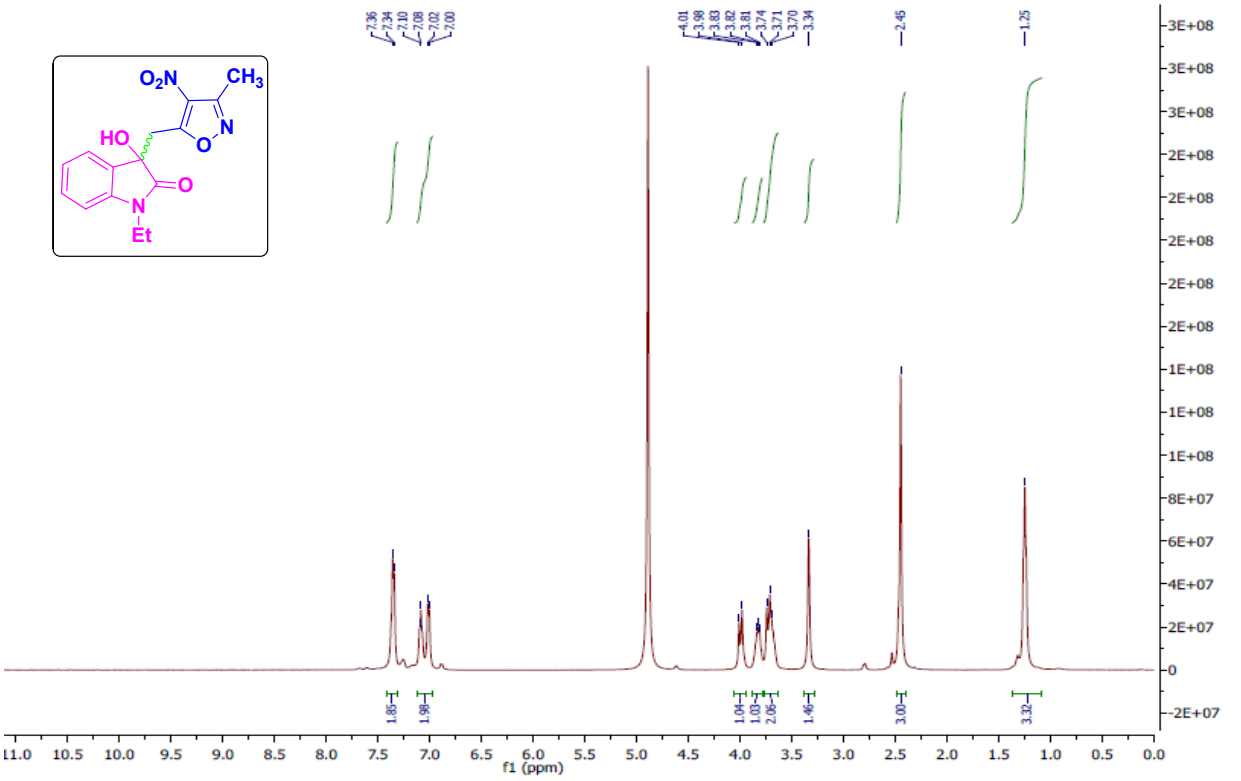
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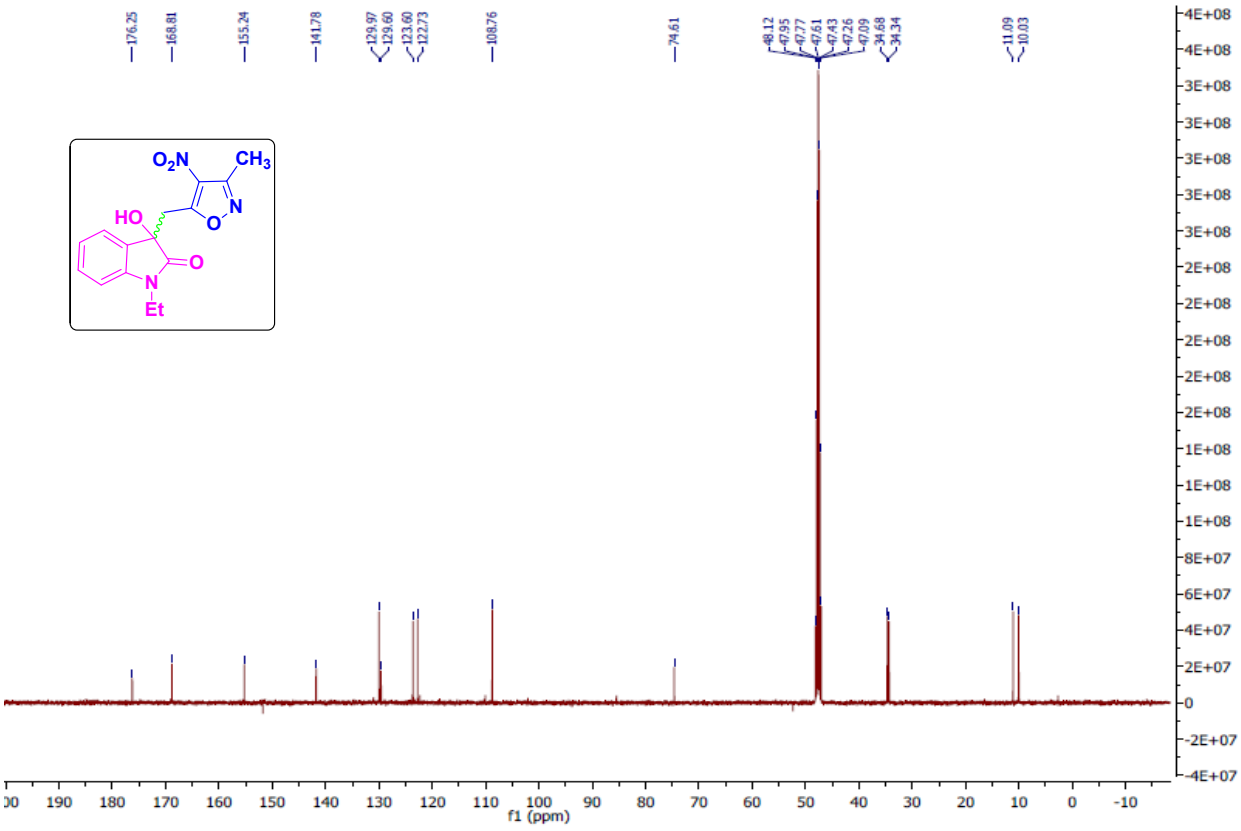
f1 (ppm)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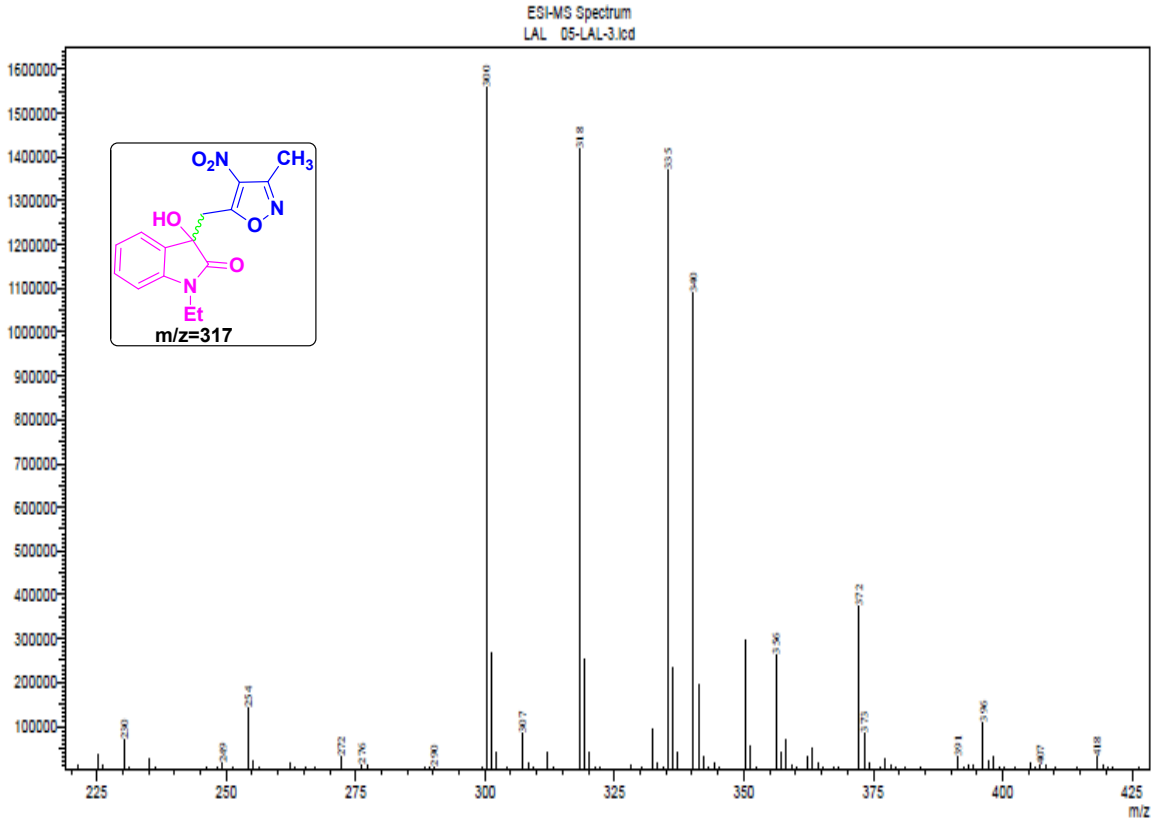
f1 (ppm)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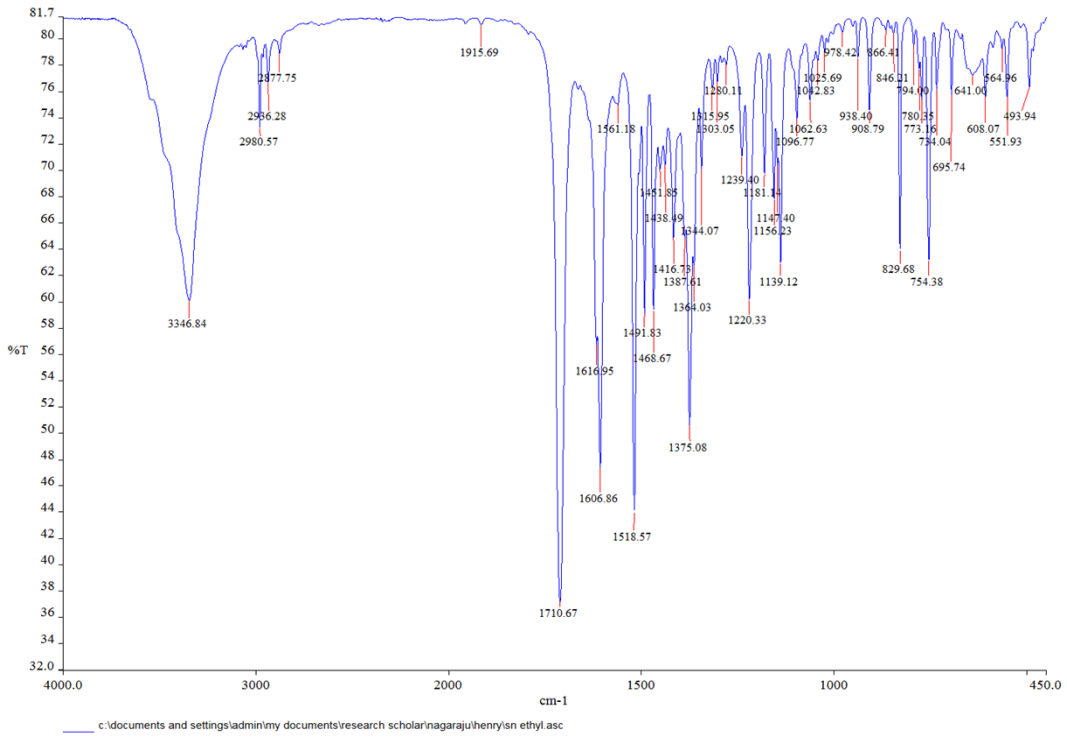
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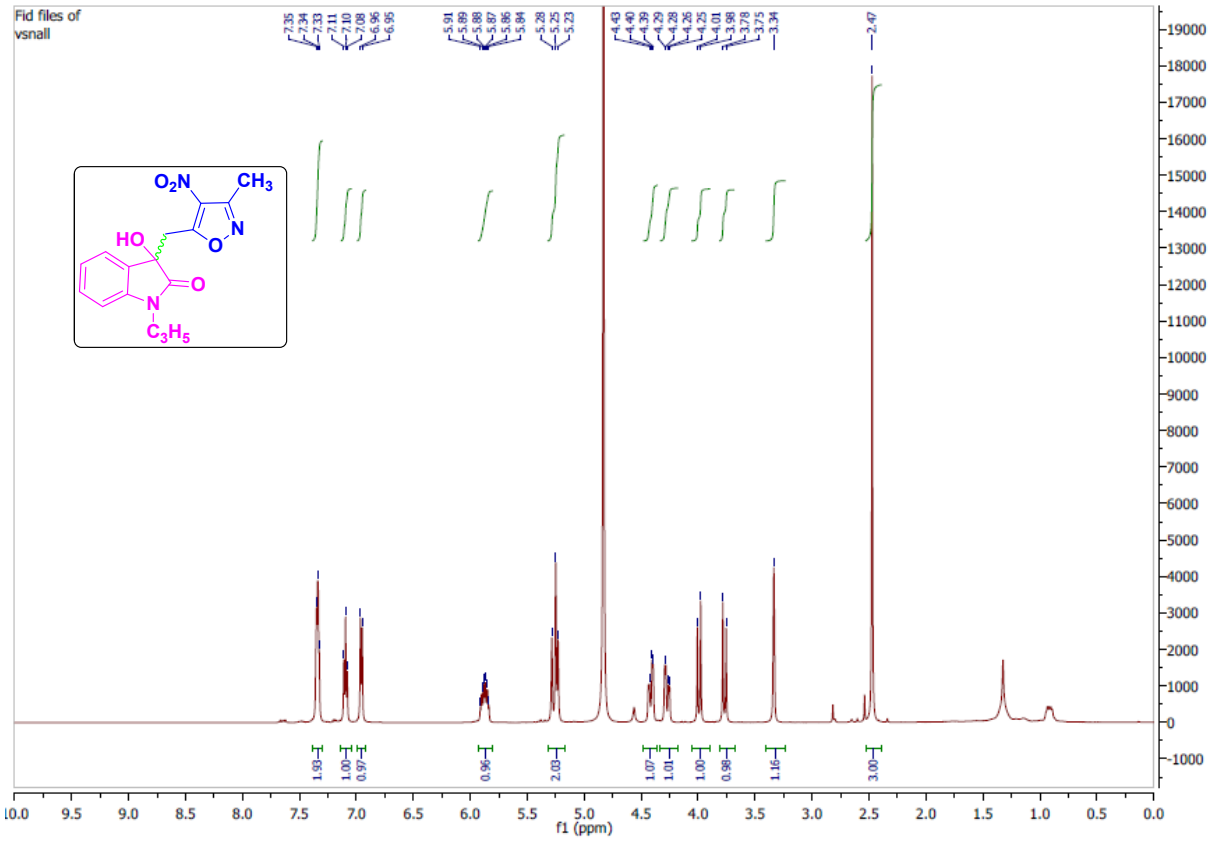
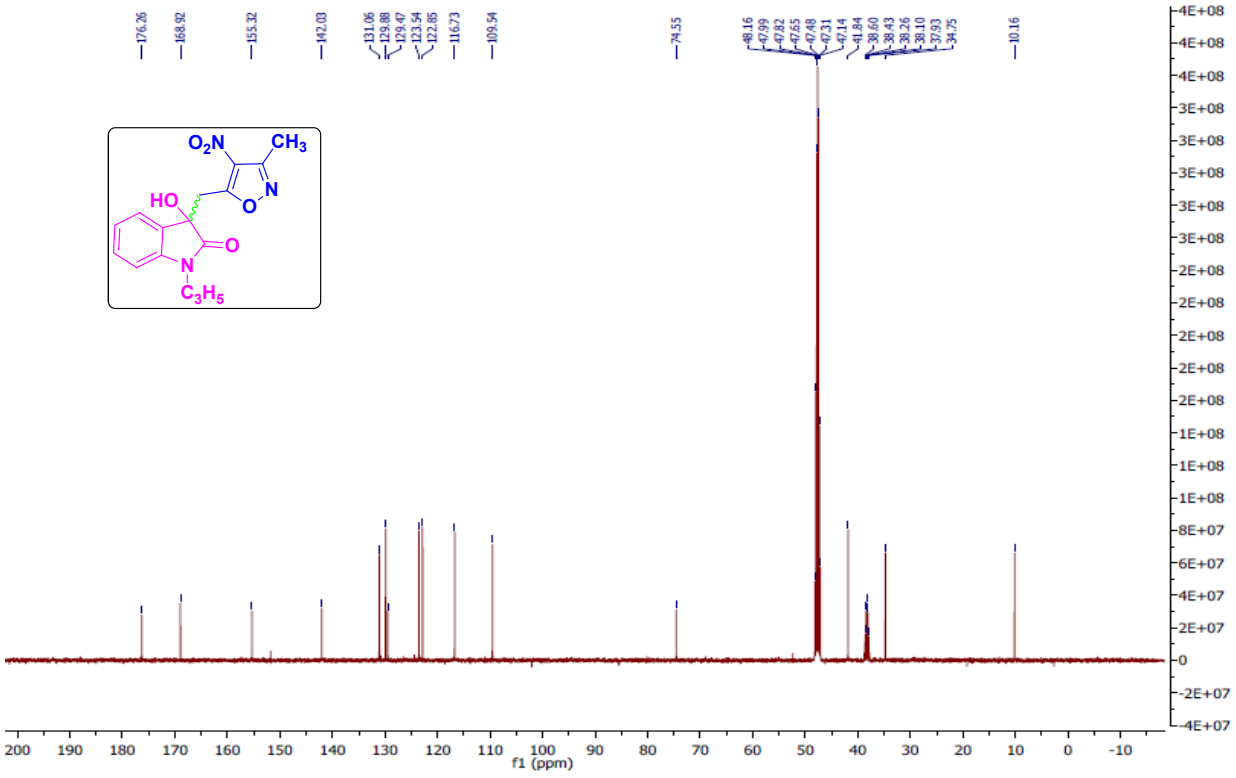
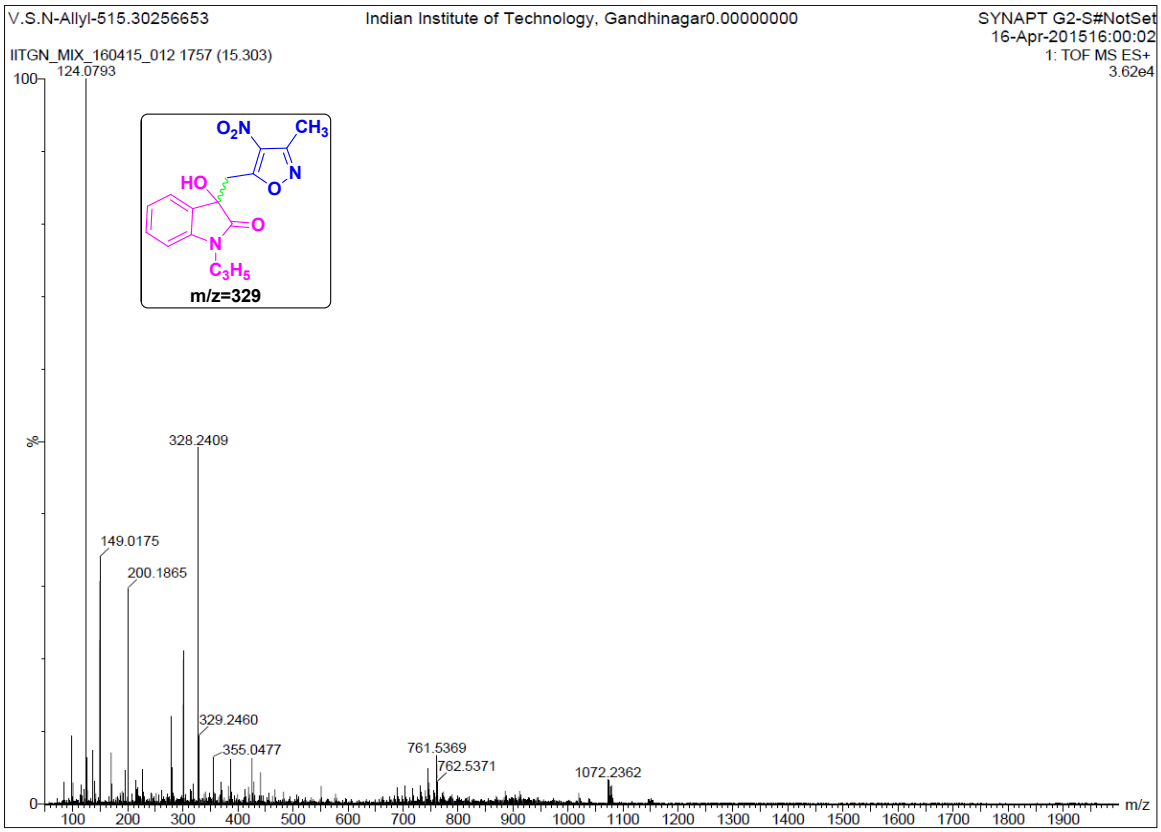
1-allyl-3-hydroxy-3-((3-methyl-4-nitroisoxazol-5-yl)methyl)indolin-2-one:



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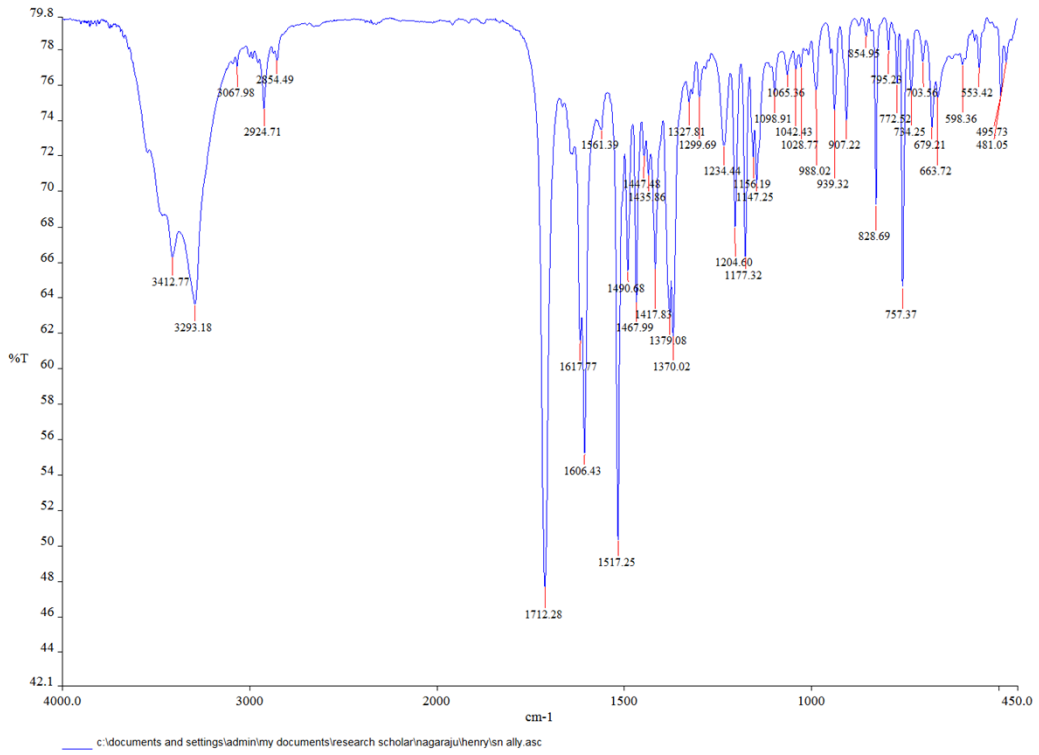
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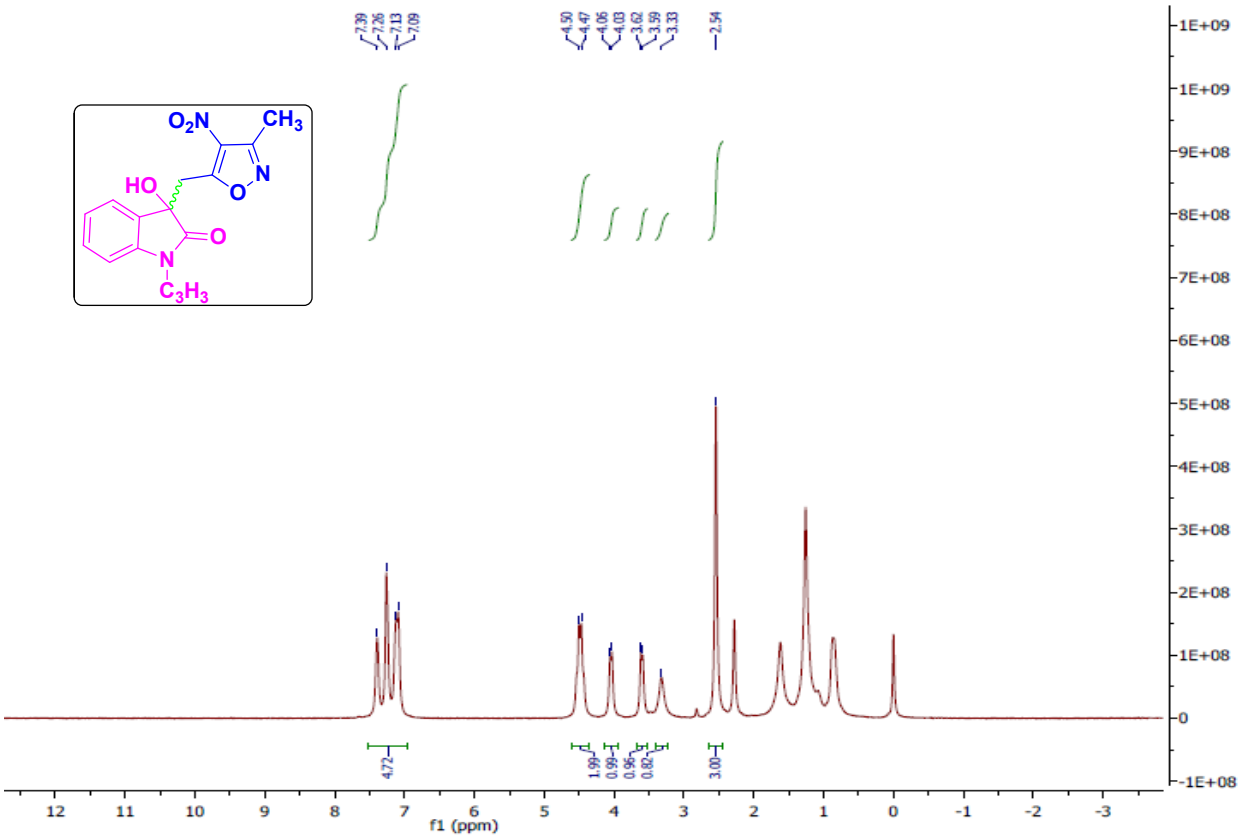
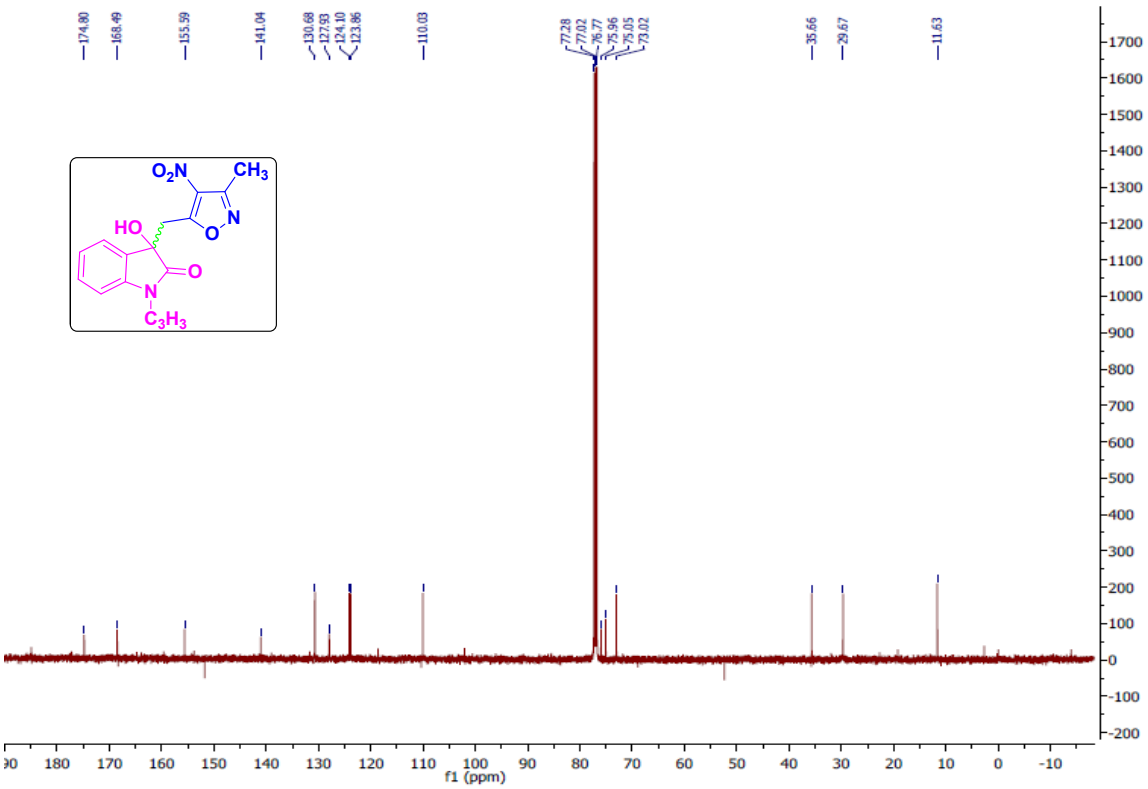
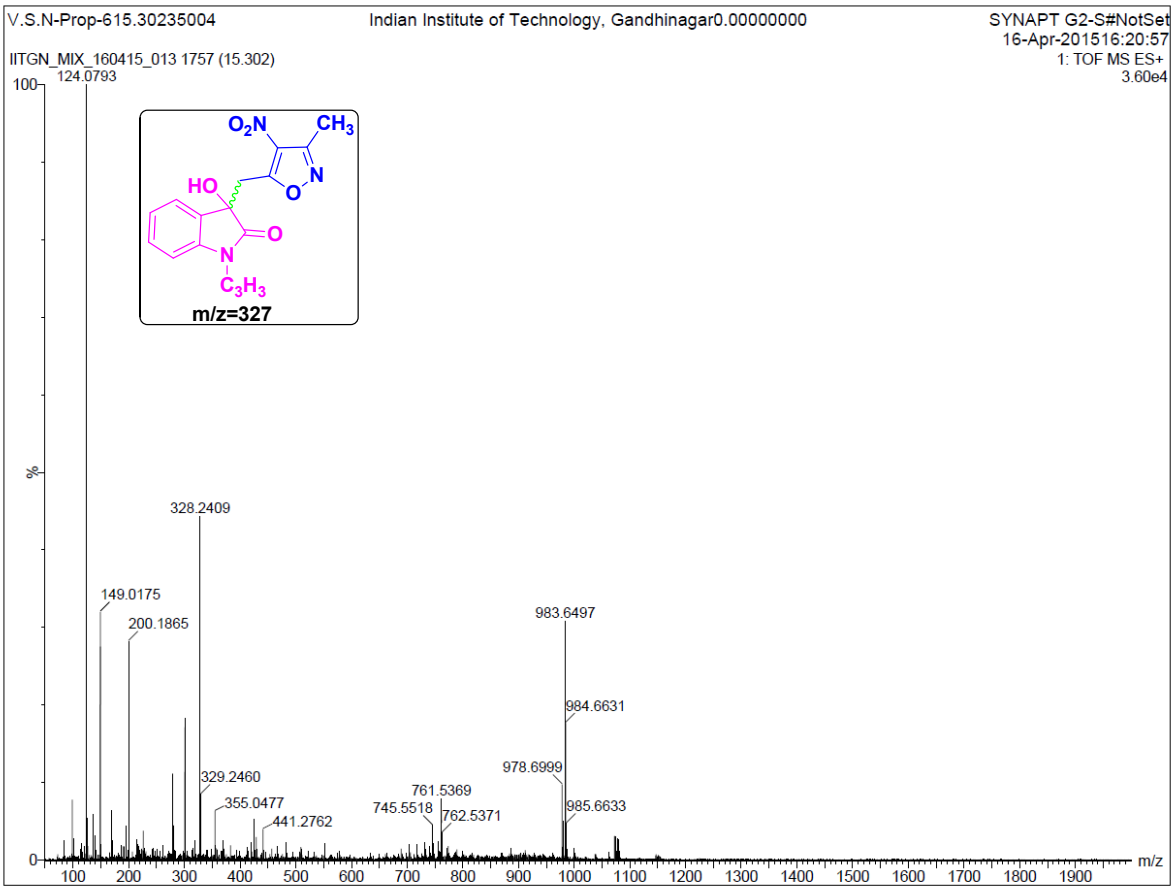
3-hydroxy-3-((3-methyl-4-nitroisoxazol-5-yl)methyl)-1-(prop-2-yn-1-yl)indolin-2-one:



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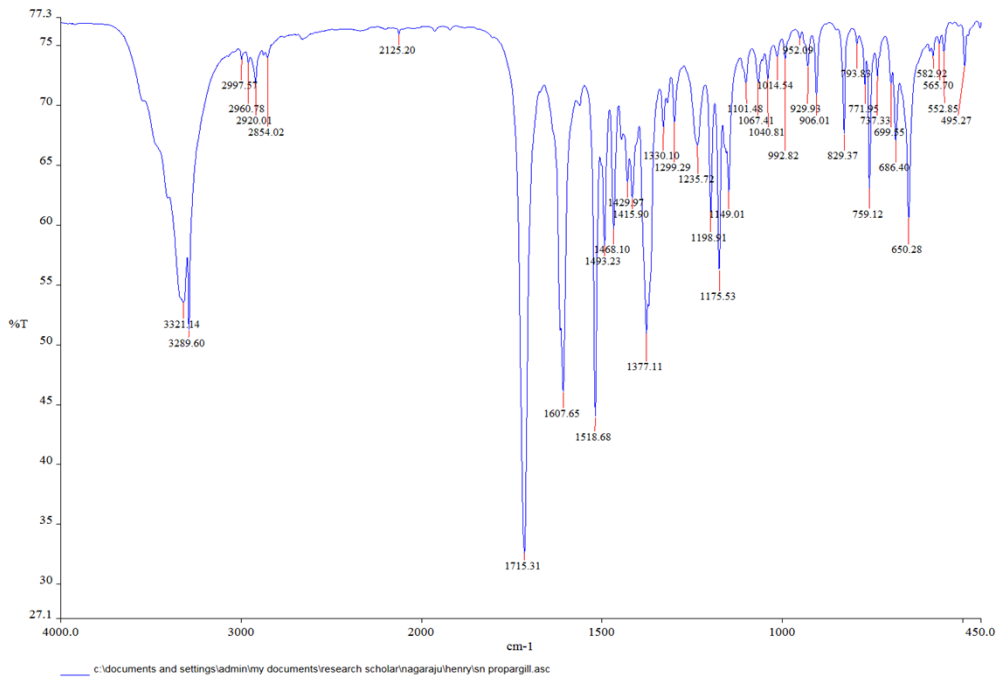
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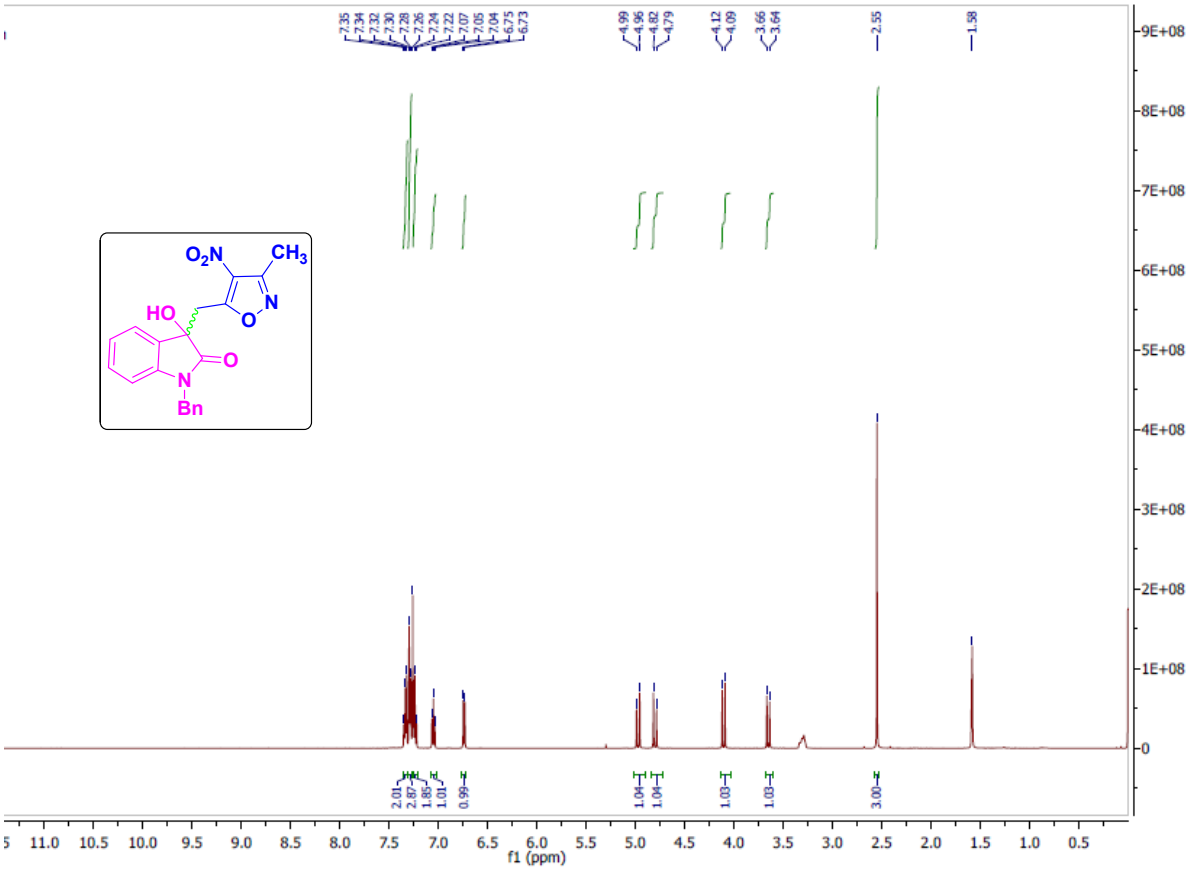
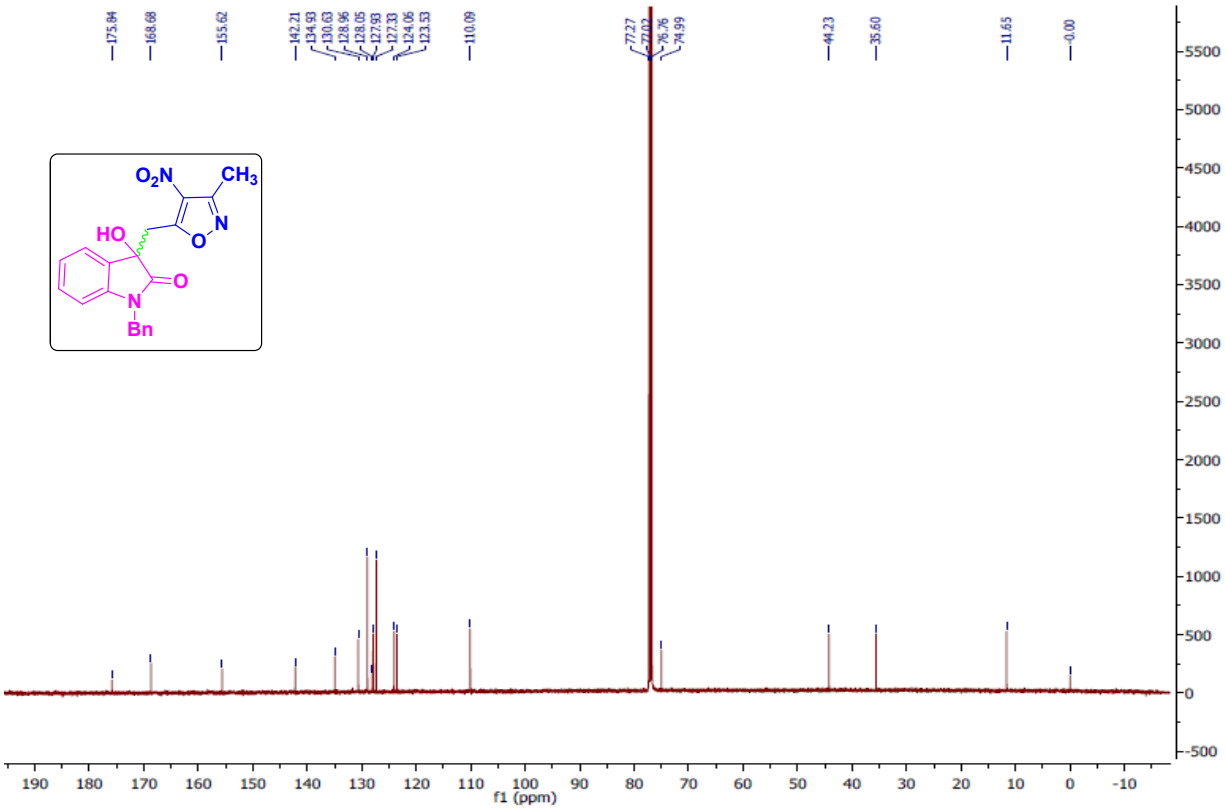
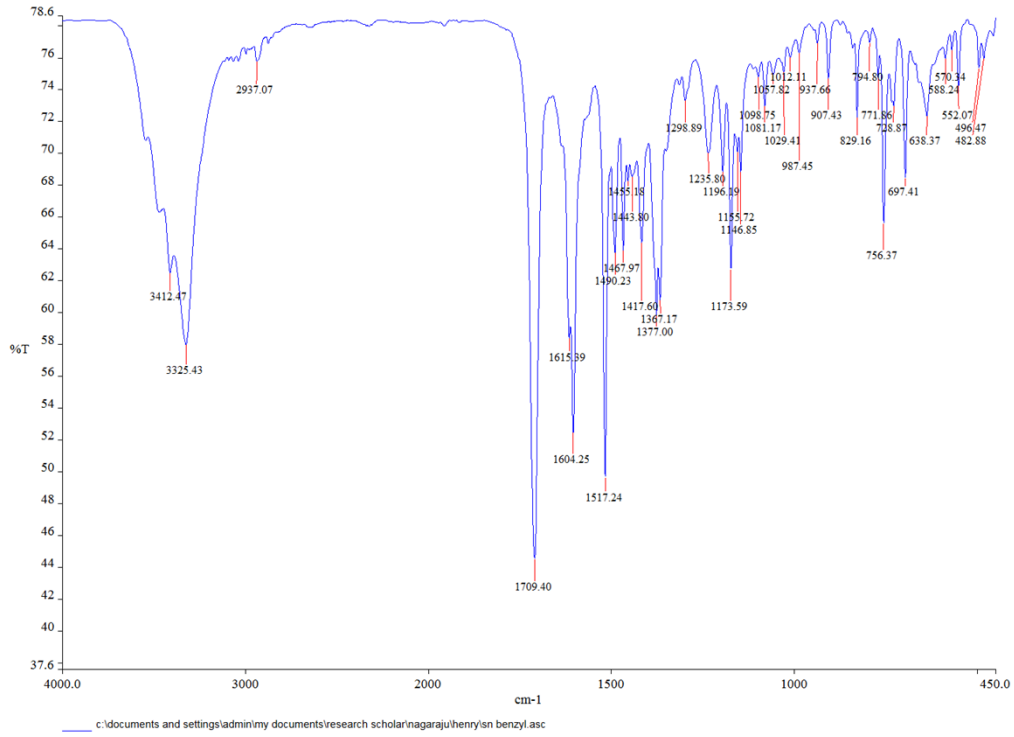
3-hydroxy-3-((3-methyl-4-nitroisoxazol-5-yl)methyl)-1-phenethylindolin-2-one:







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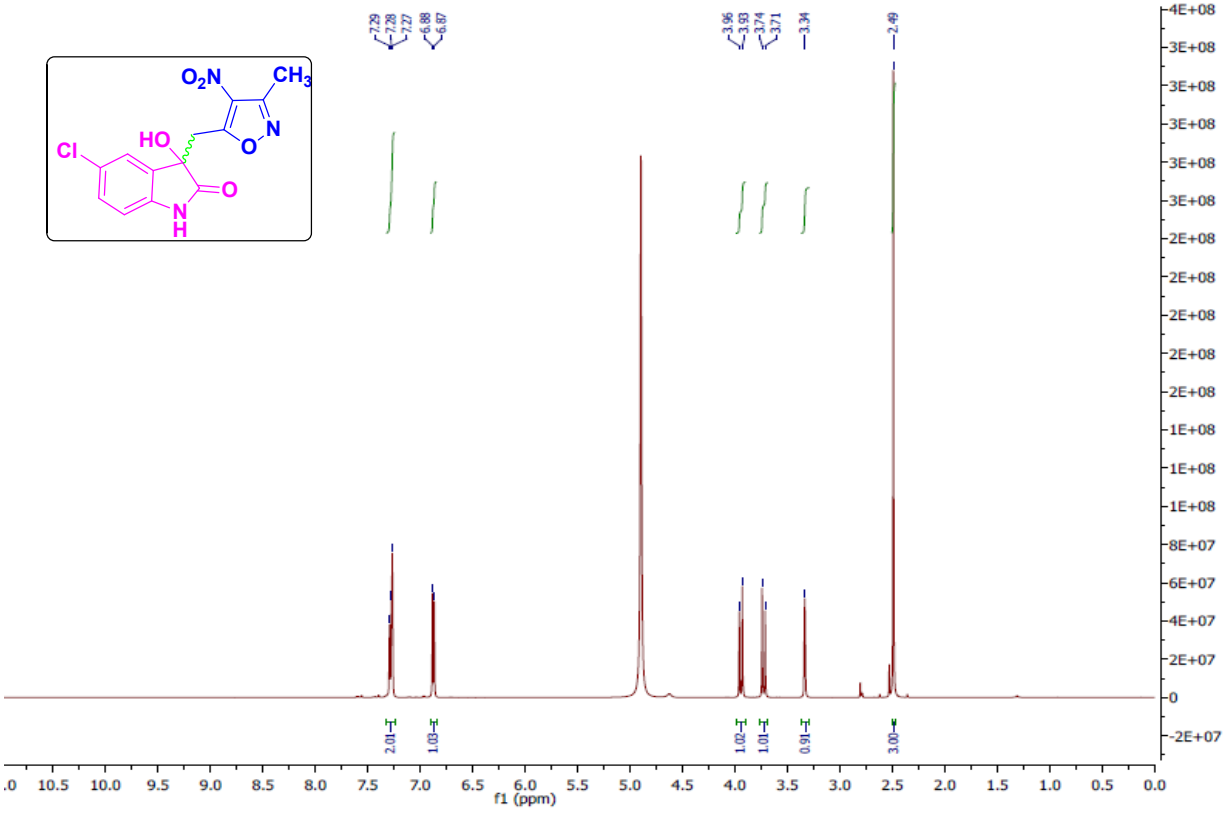

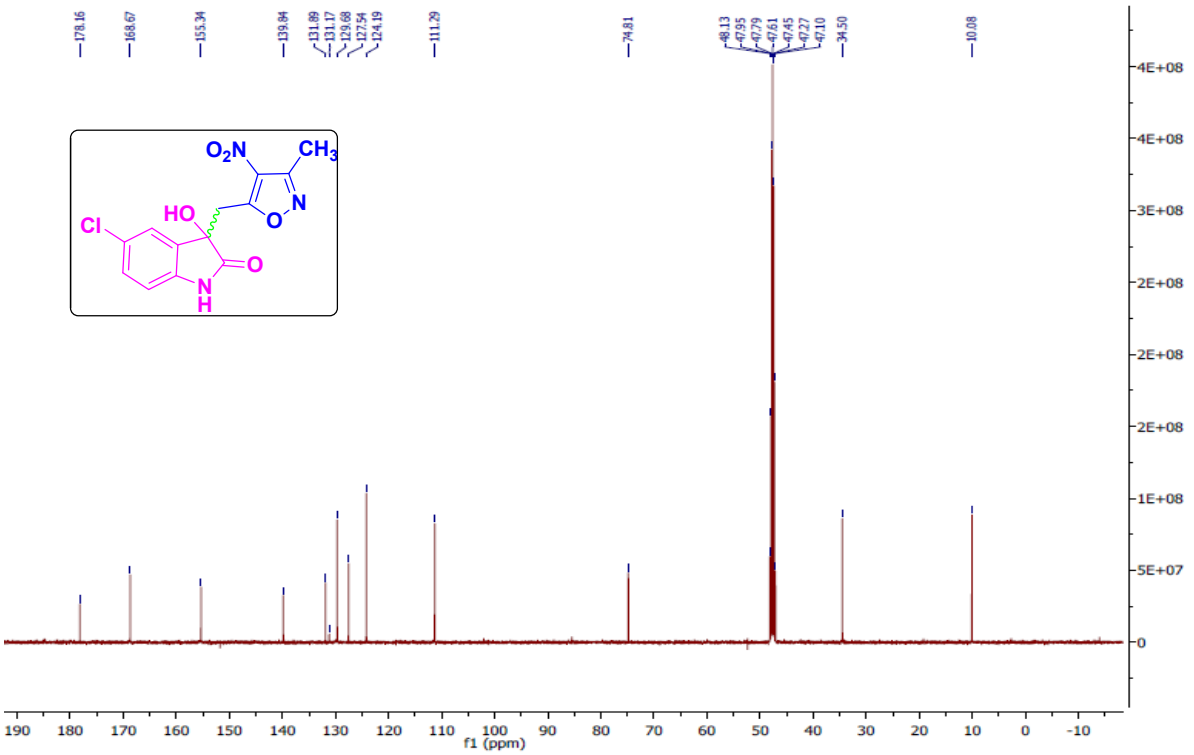
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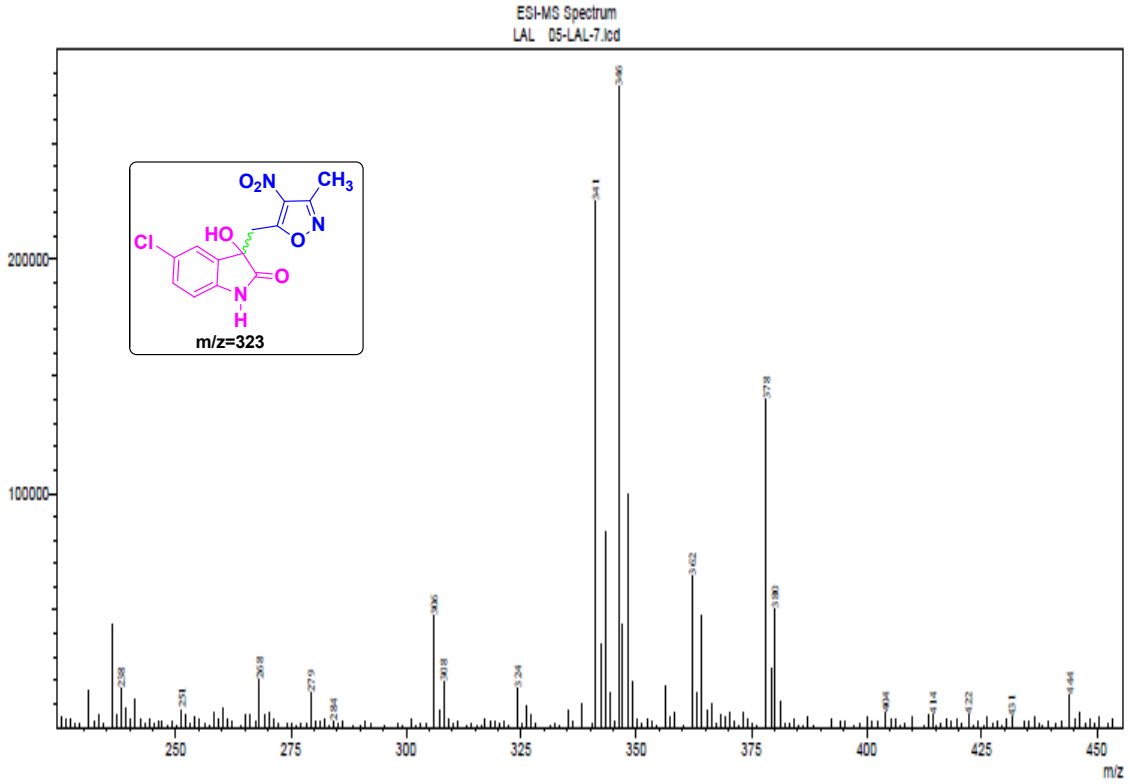
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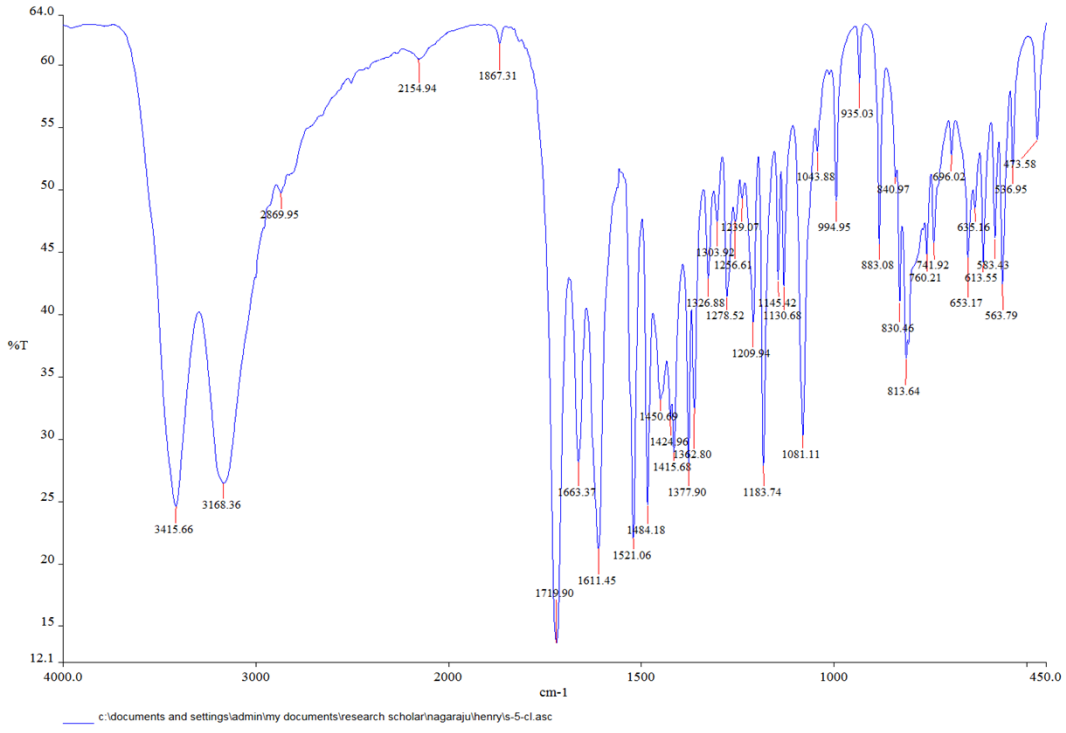

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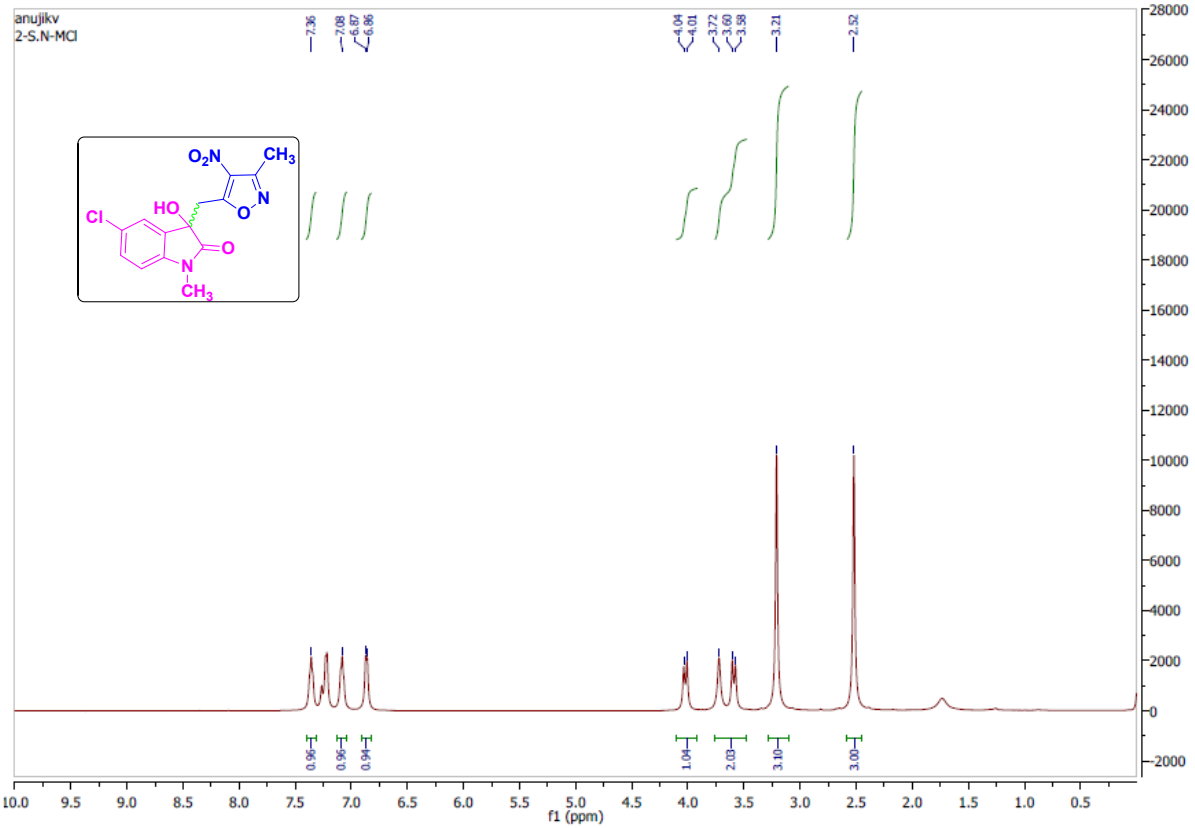
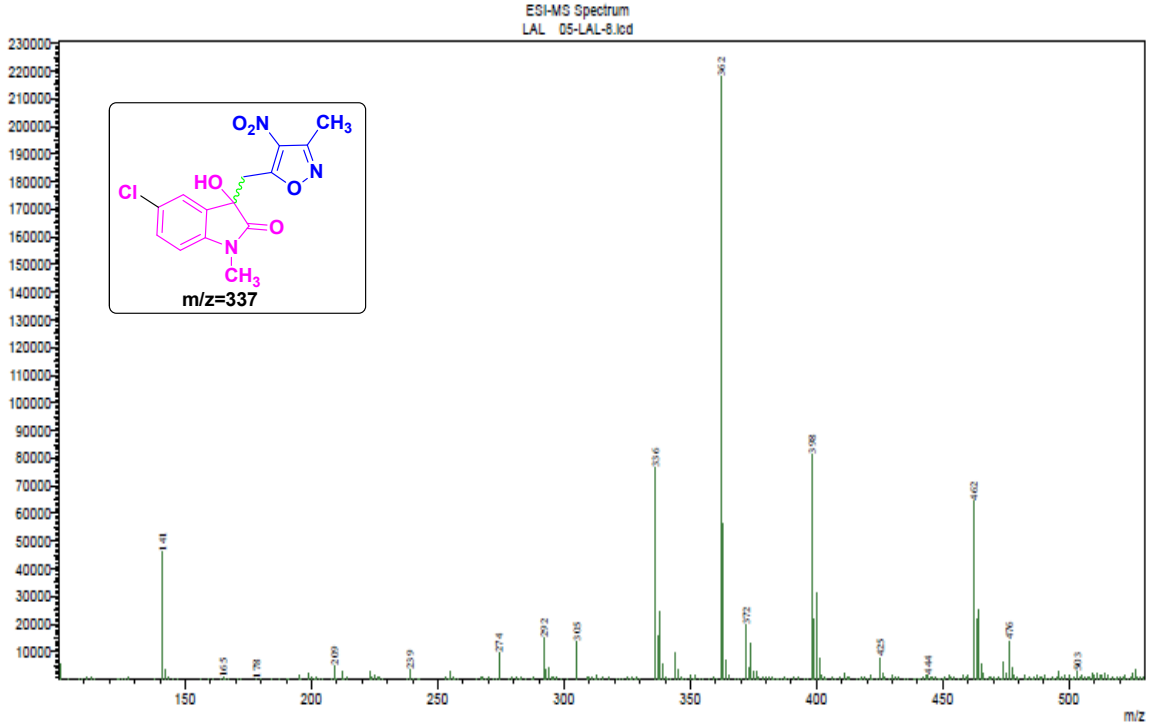
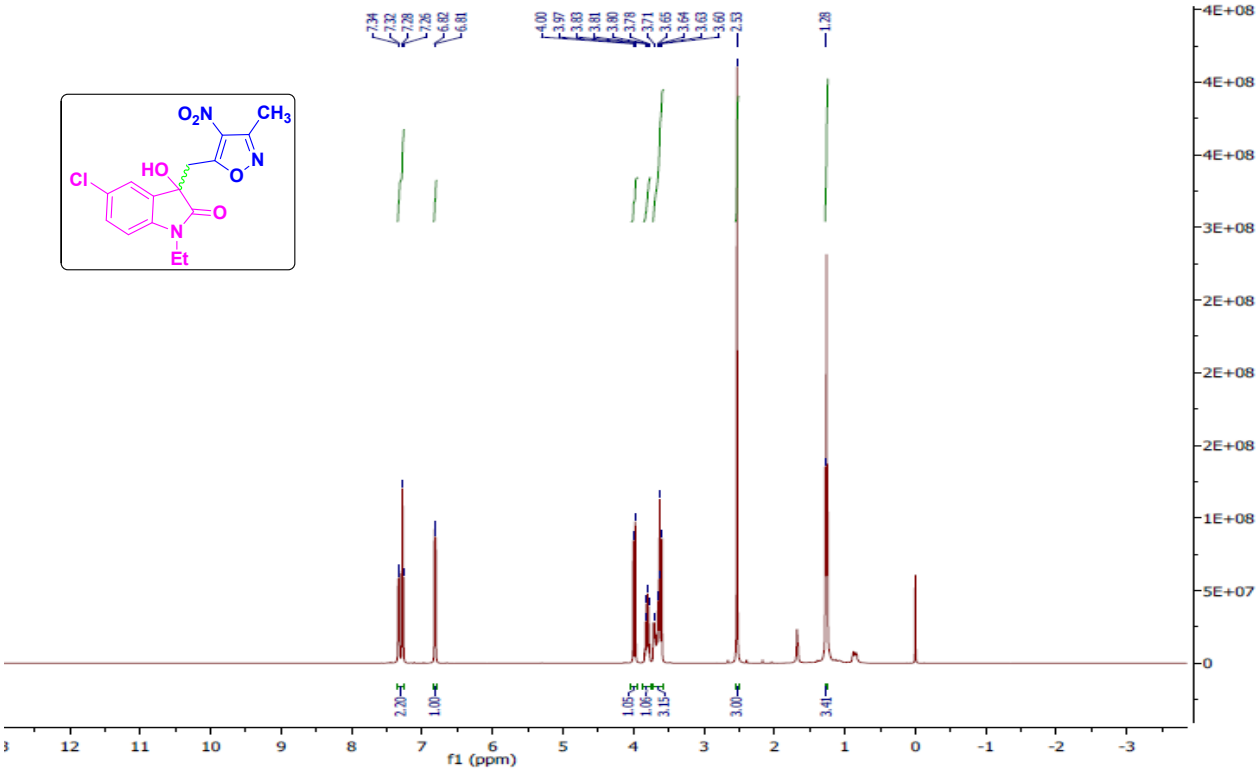
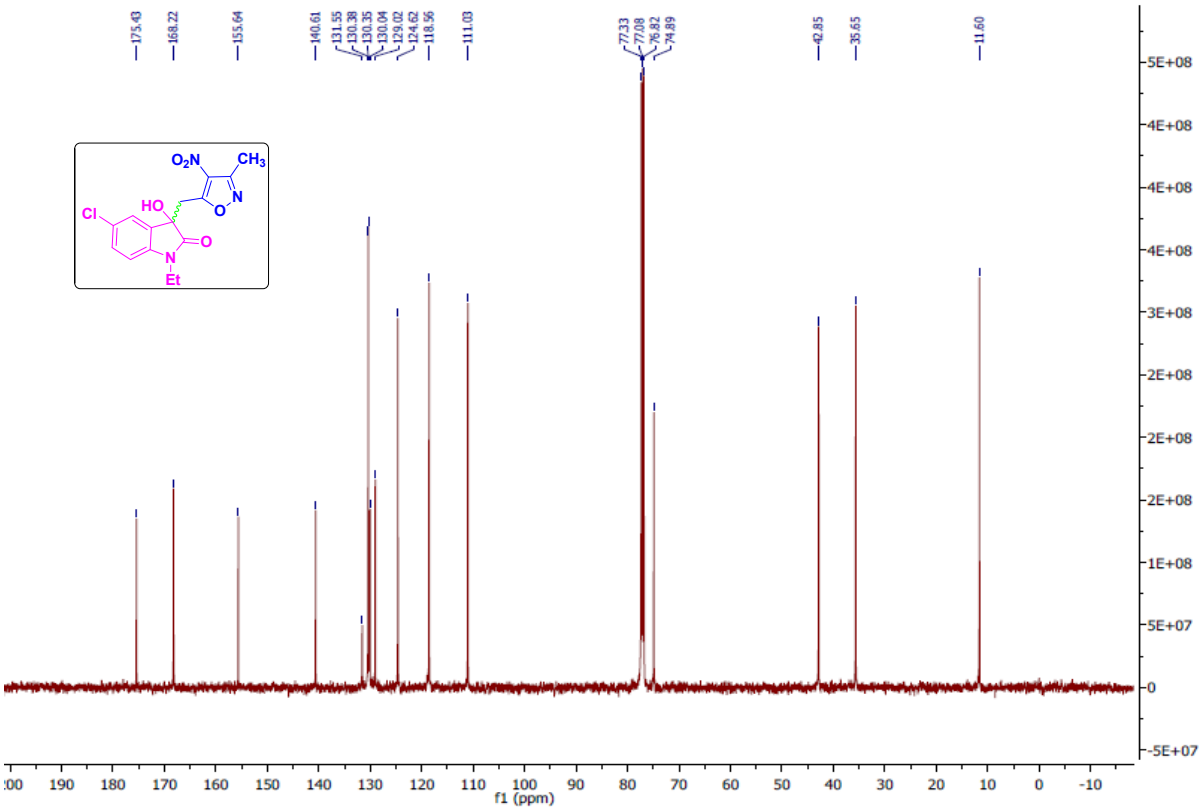




6-chloro-1-ethyl-3-hydroxy-3-((3-methyl-4-nitroisoxazol-5-yl)methyl)indolin-2-one:

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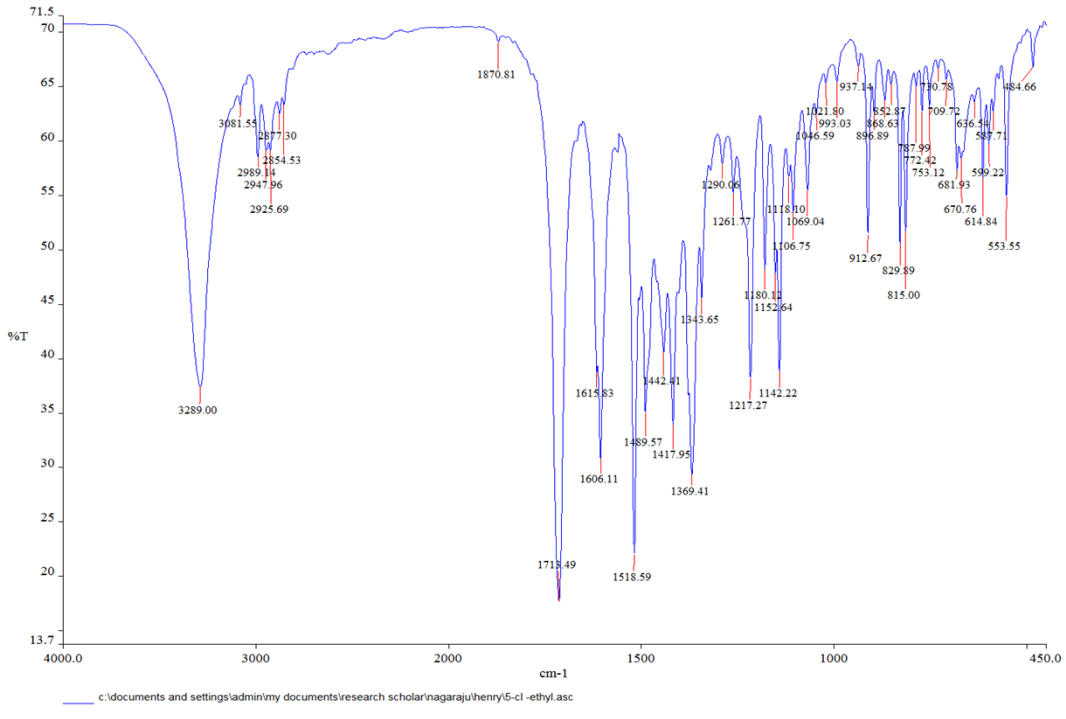
f1 (ppm)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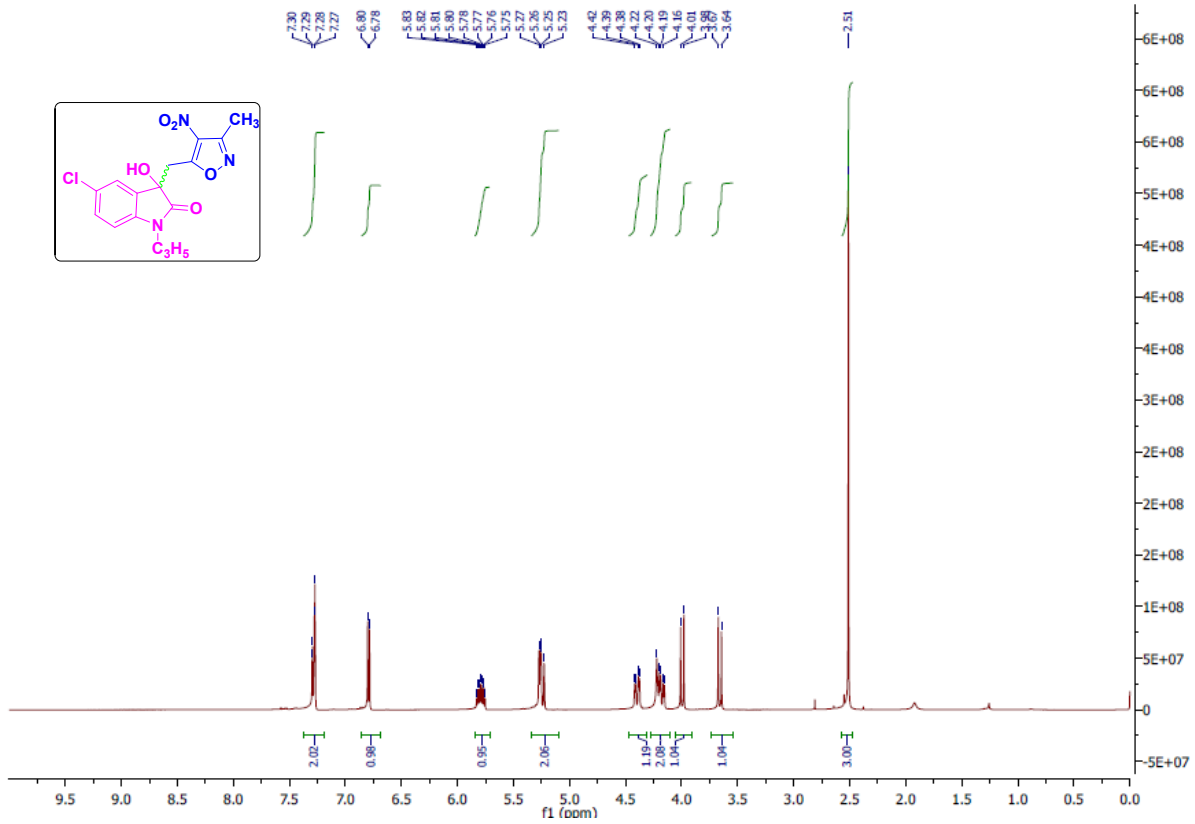
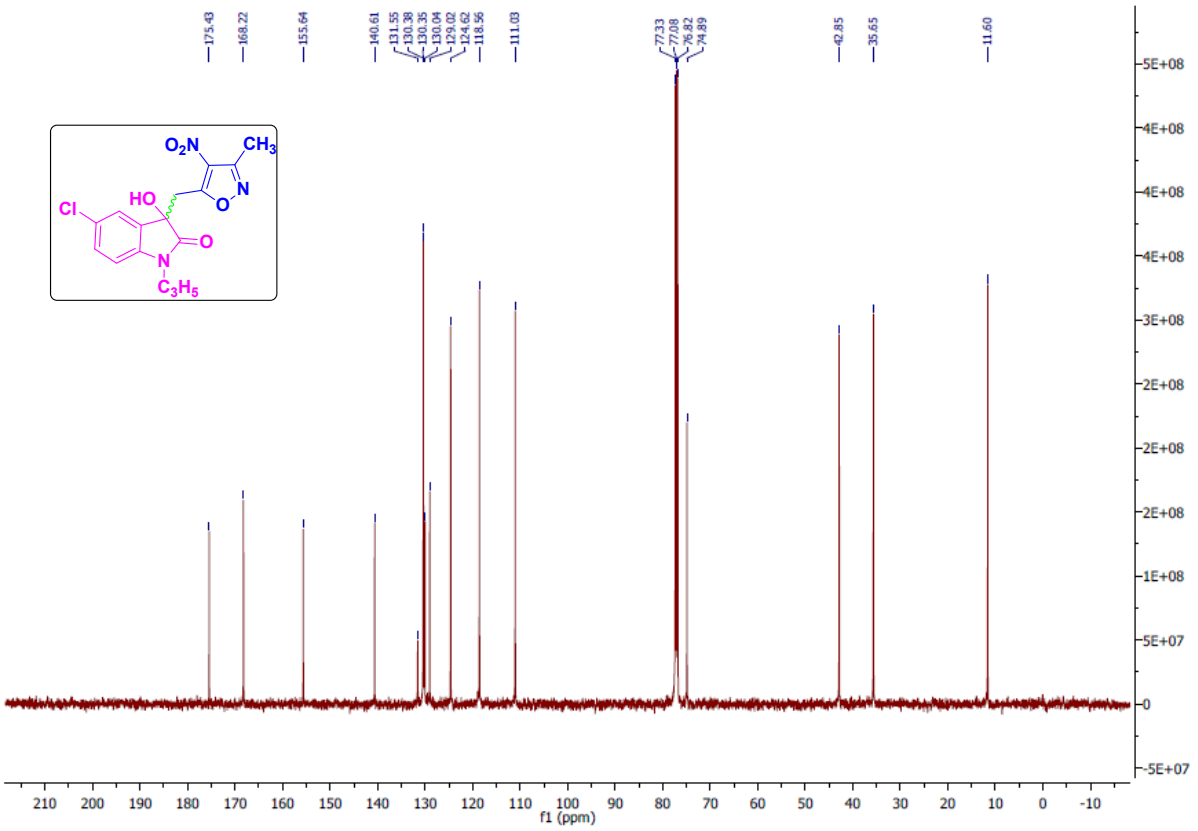
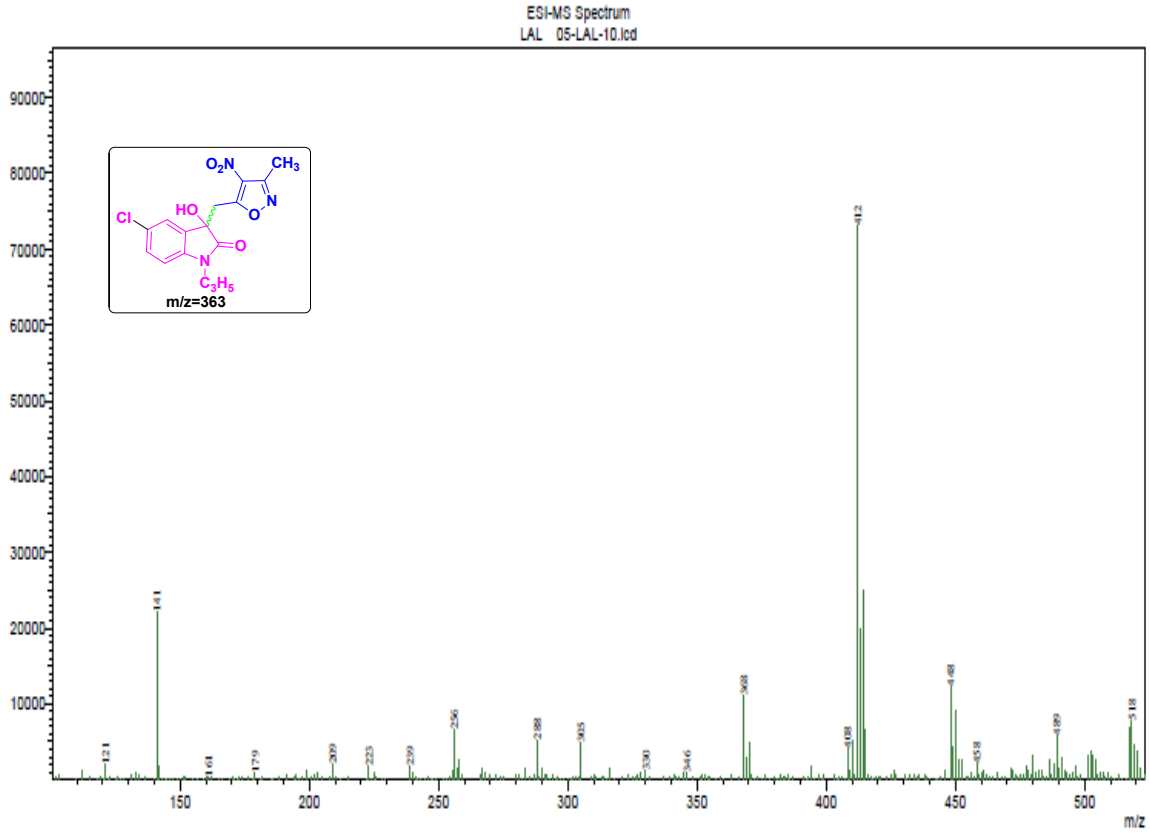
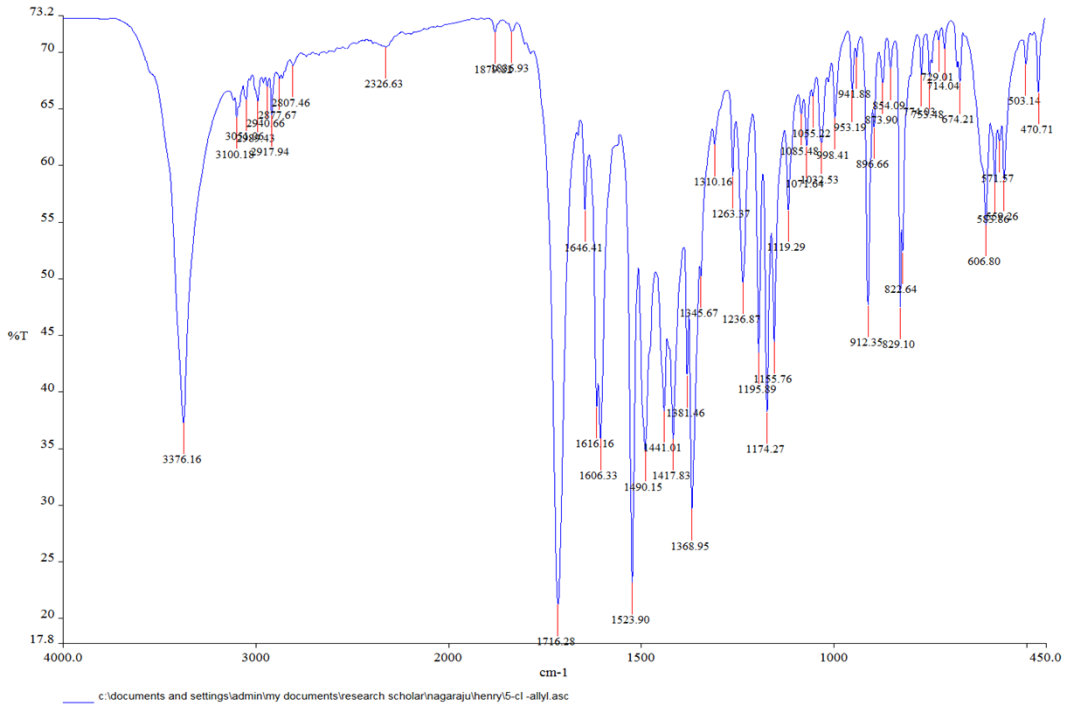
1142.22
1118.10
1106.75
1069.04
1046.59
1021.80
993.03
937.14
912.67
896.89
868.63
852.87
829.89
815.00
787.99
772.42
753.12
730.78
709.72
681.93
670.76
636.50
614.84
599.22
587.71
553.55
484.66
c:\documents and settings\admin\my documents\research scholar\nagaraju\henry\5-cl -ethyl.asc

1-allyl-5-chloro-3-hydroxy-3-((3-methyl-4-nitroisoxazol-5-yl)methyl)indolin-2-one






ESI-MS Spectrum
LAL 05-LAL-10.lcd
m/z=363
m/z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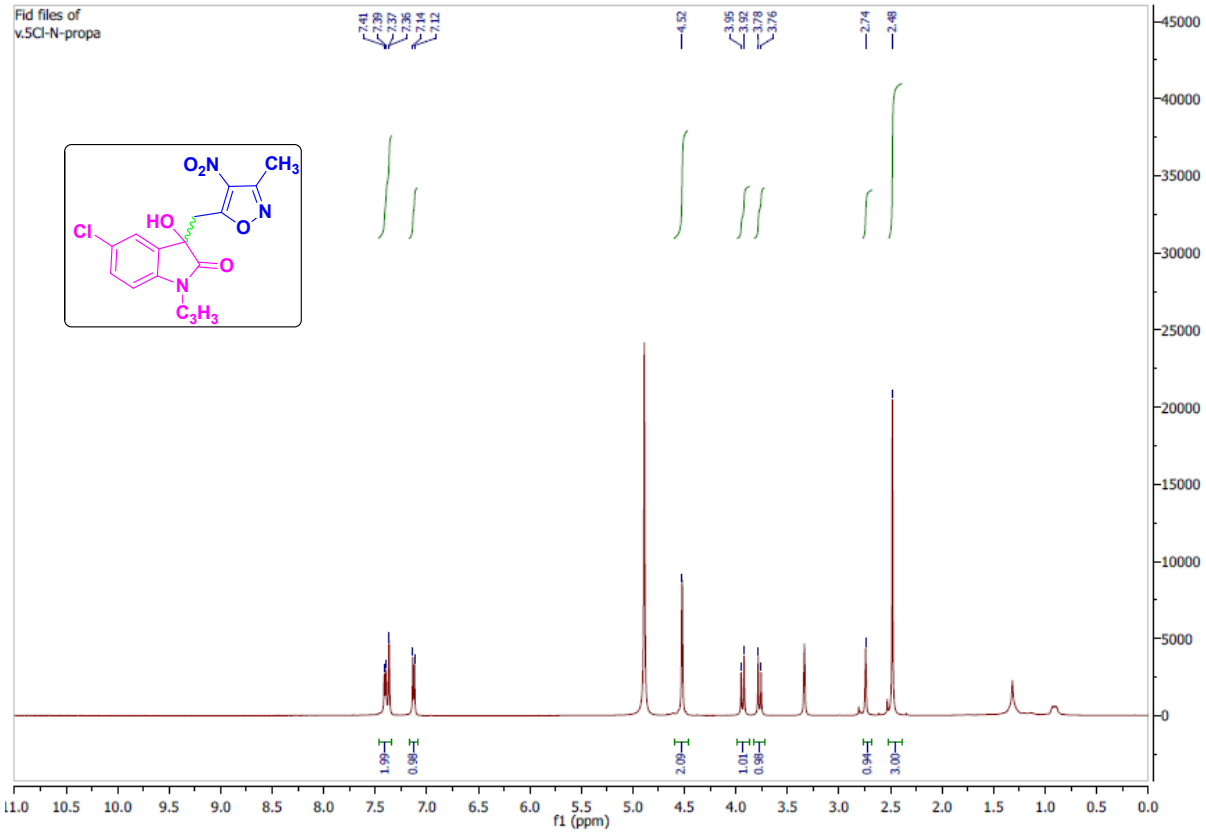
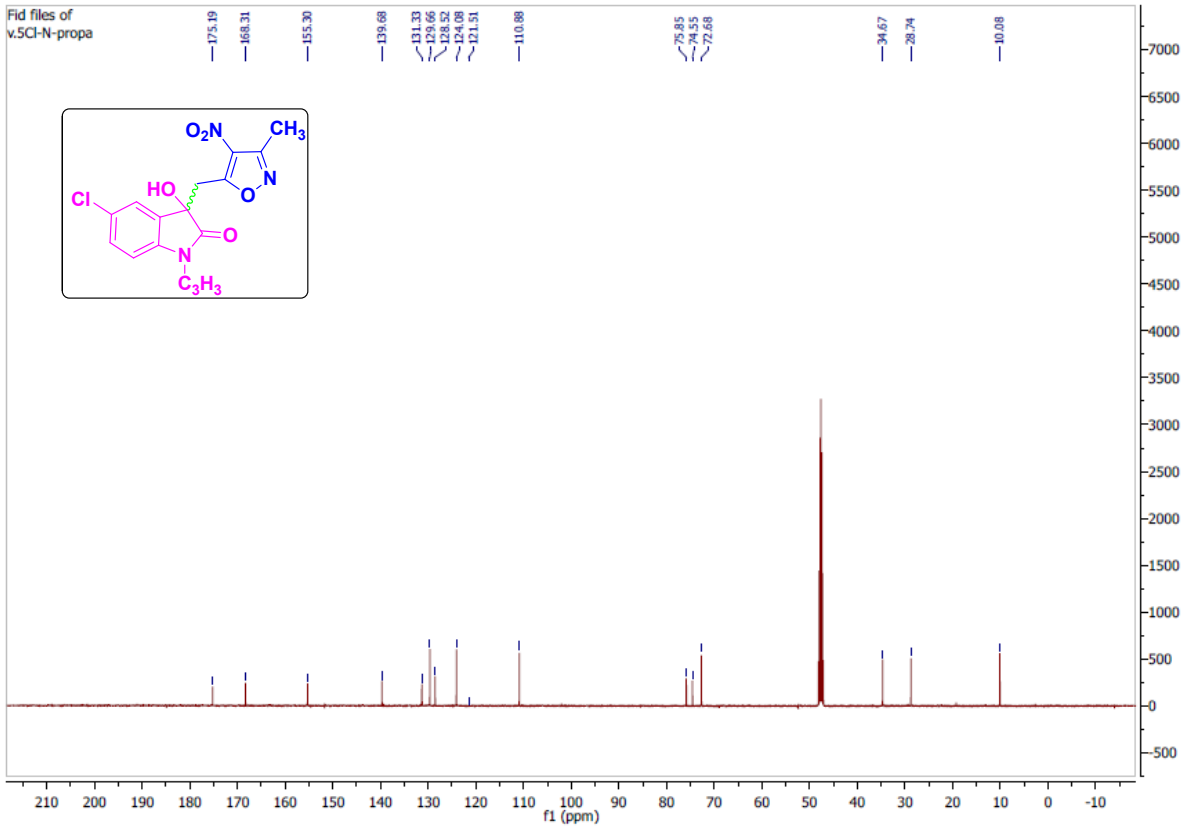
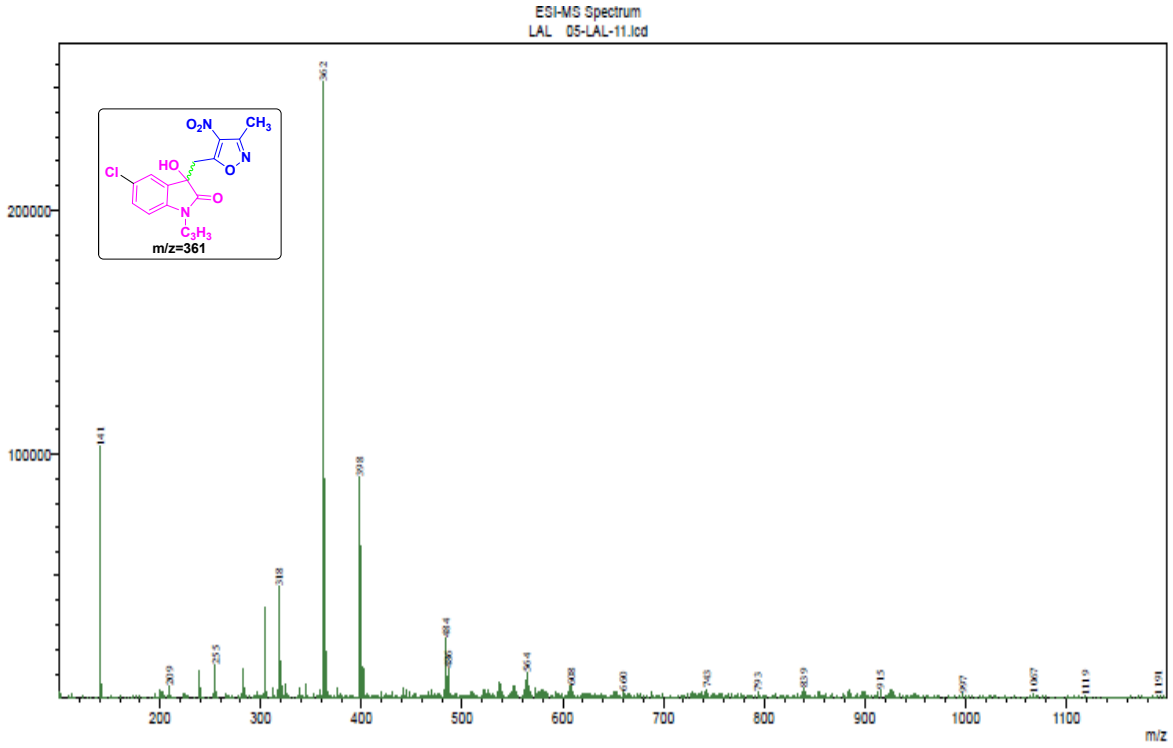
cm-1
c:\documents and settings\admin\my documents\research scholar\nagaraju\henry\5-cl -allyl.asc

5-chloro-3-hydroxy-3-((3-methyl-4-nitroisoxazol-5-yl)methyl)-1-(prop-2-yn-1-yl)indolin-2-one:






ESI-MS Spectrum
LAL 05-LAL-11.lcd
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100000
362
141
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318
484
255
309
364
488
560
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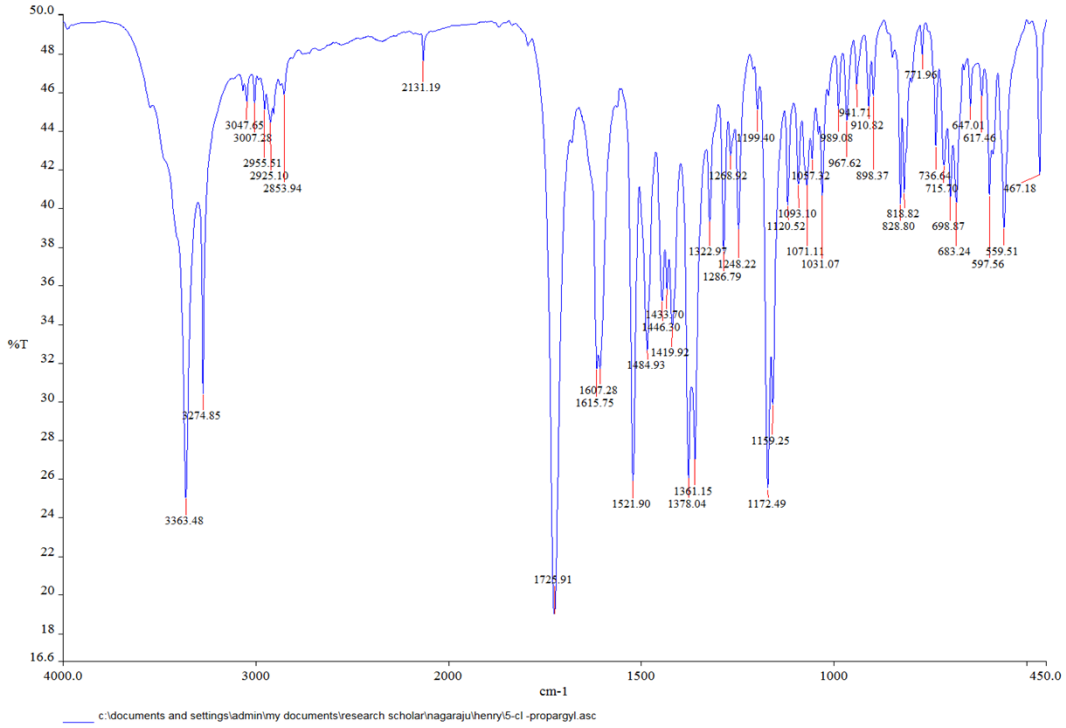
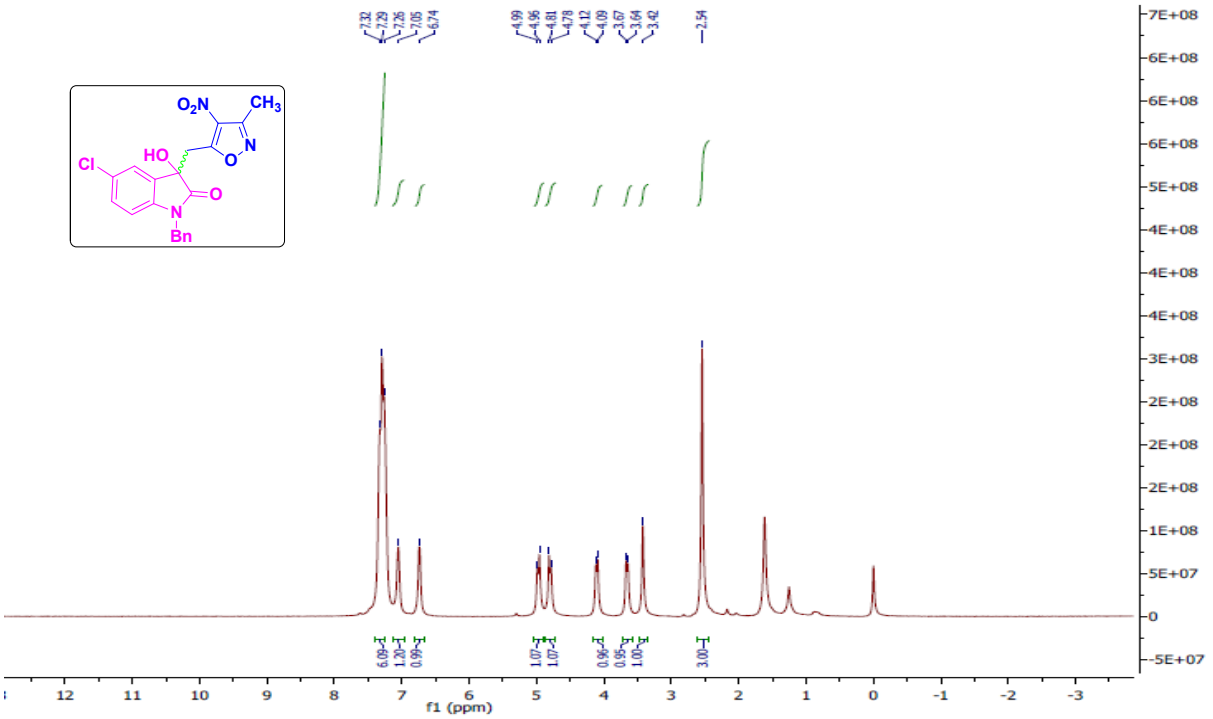
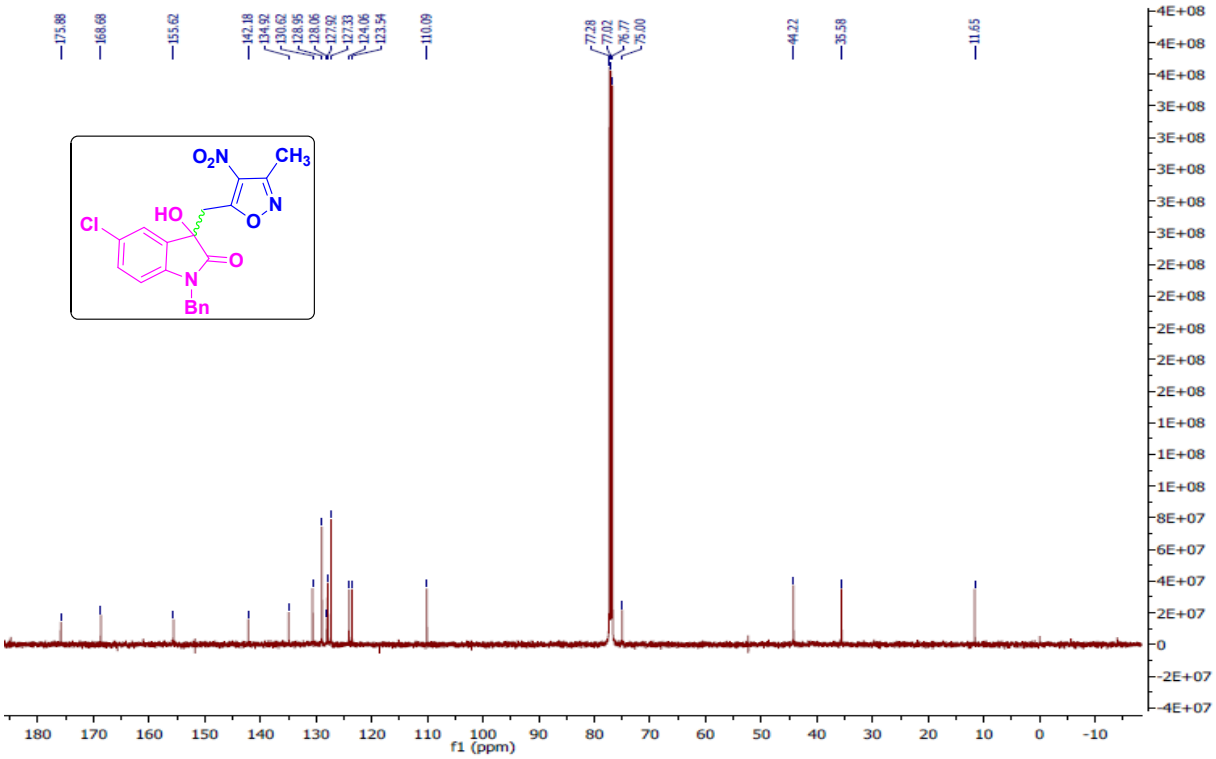
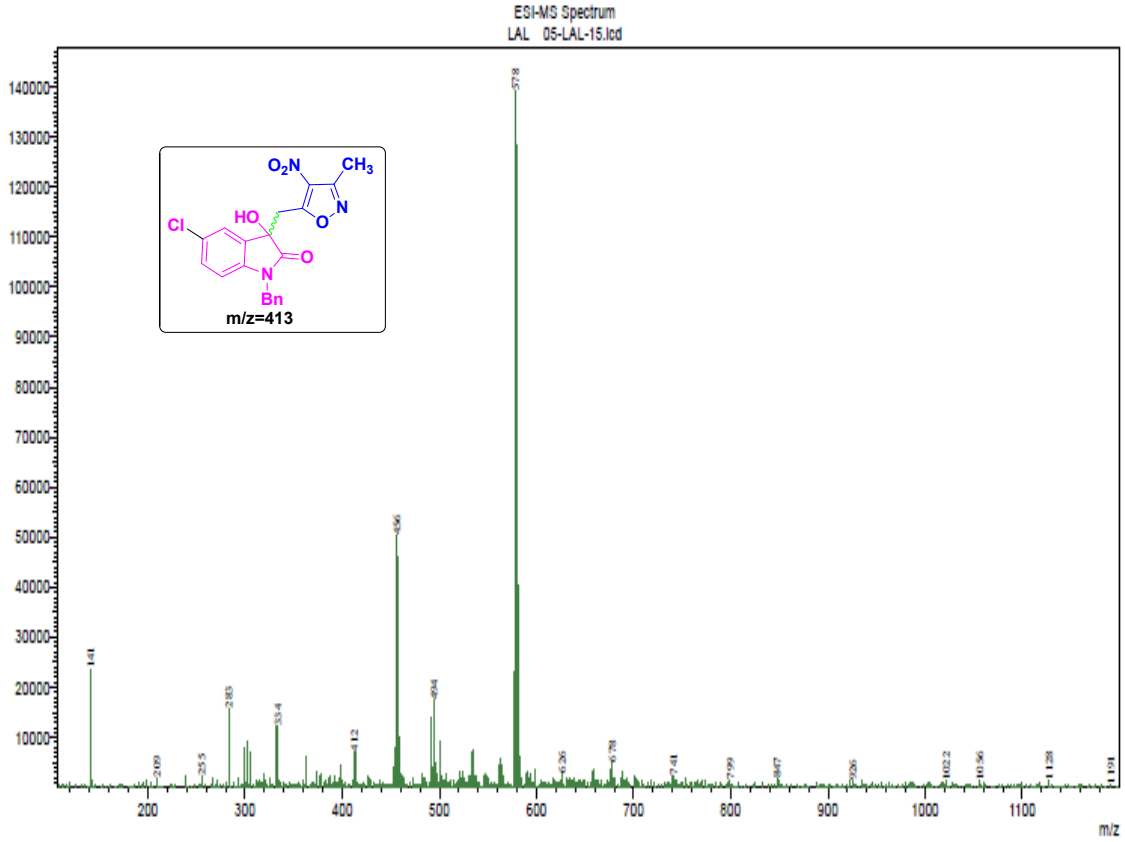
400
500
600
700
800
900
1000
1100
m/z


%T
50.0
48
46
44
42
40
38
36
34
32
30
28
26
24
22
20
18
16.6
4000.0
3000
2000
1500
1000
450.0
cm-1
3363.48
3274.85
3047.65
3007.28
2955.51
2925.10
2853.94
2131.19
1725.91
1607.28
1615.75
1521.90
1484.93
1446.30
1433.70
1419.92
1378.04
1361.15
1322.97
1286.79
1268.92
1248.22
1199.40
1172.49
1159.25
1120.52
1093.10
1071.11
1057.32
1031.07
989.08
967.62
941.71
910.82
898.37
828.80
818.82
771.96
736.64
715.70
698.87
683.24
647.01
617.46
597.56
559.51
467.18
c:\documents and settings\admin\my documents\research scholar\nagaraju\henry\5-cl -propargyl.asc

6-chloro-3-hydroxy-3-((3-methyl-4-nitroisoxazol-5-yl)methyl)-1-phenethylindolin-2-one:






ESI-MS Spectrum
LAL 05-LAL-15.lcd
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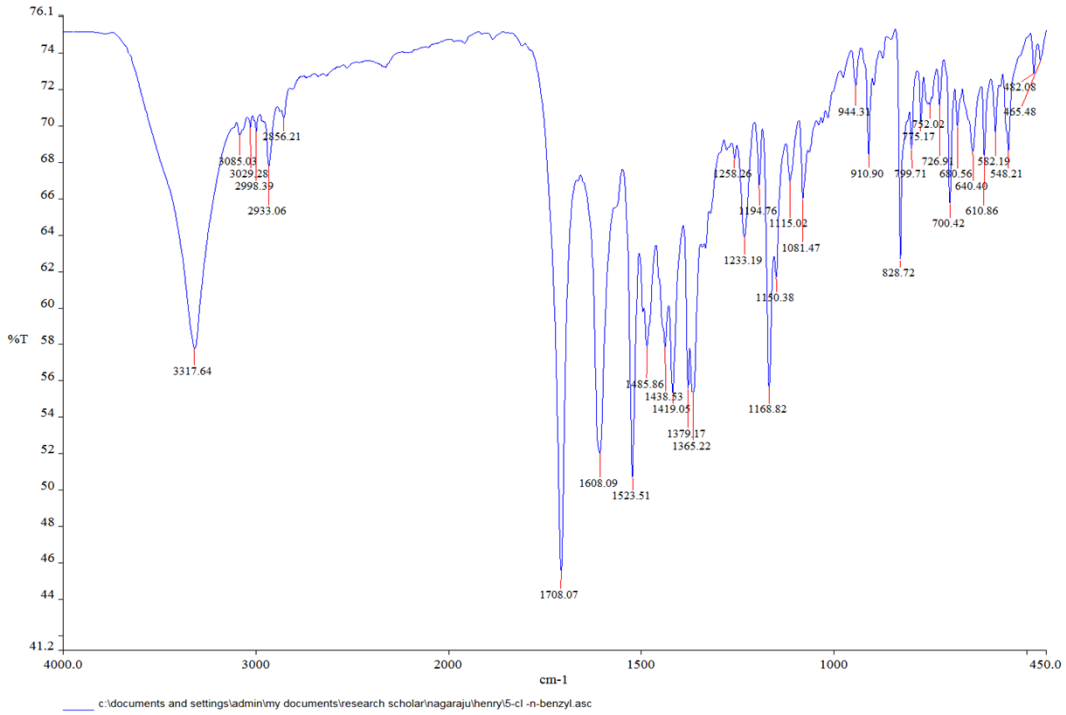
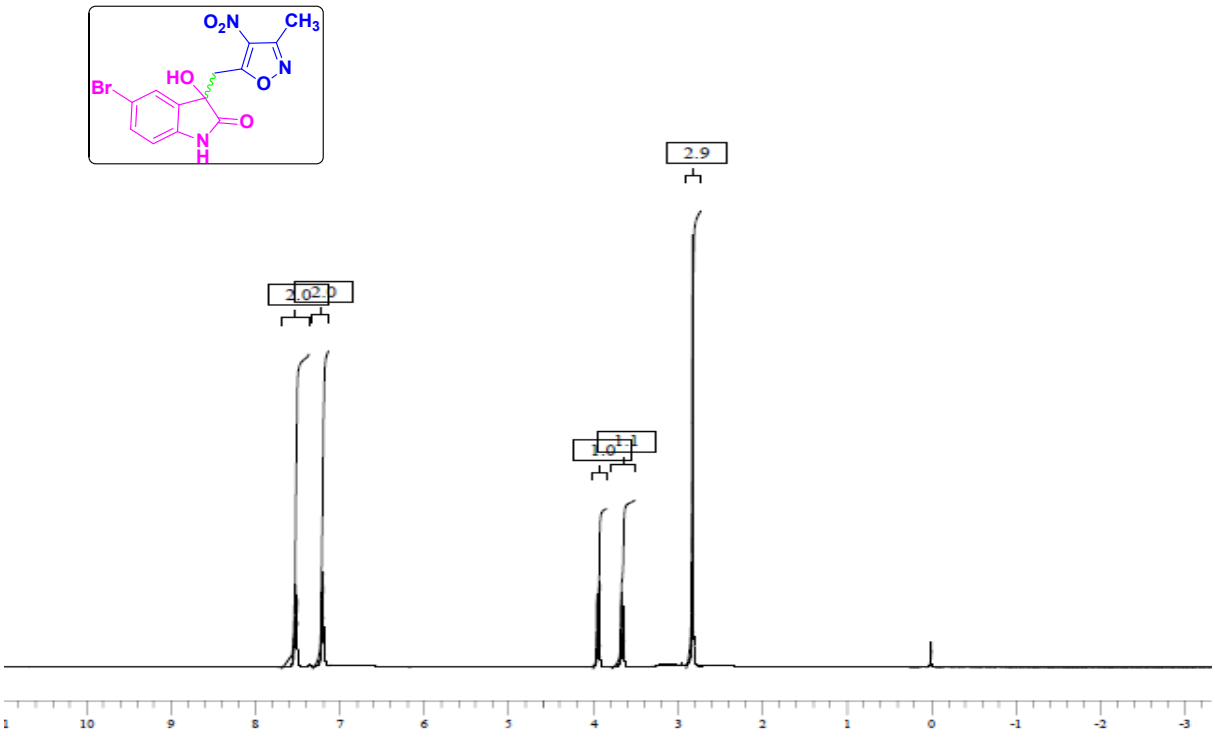
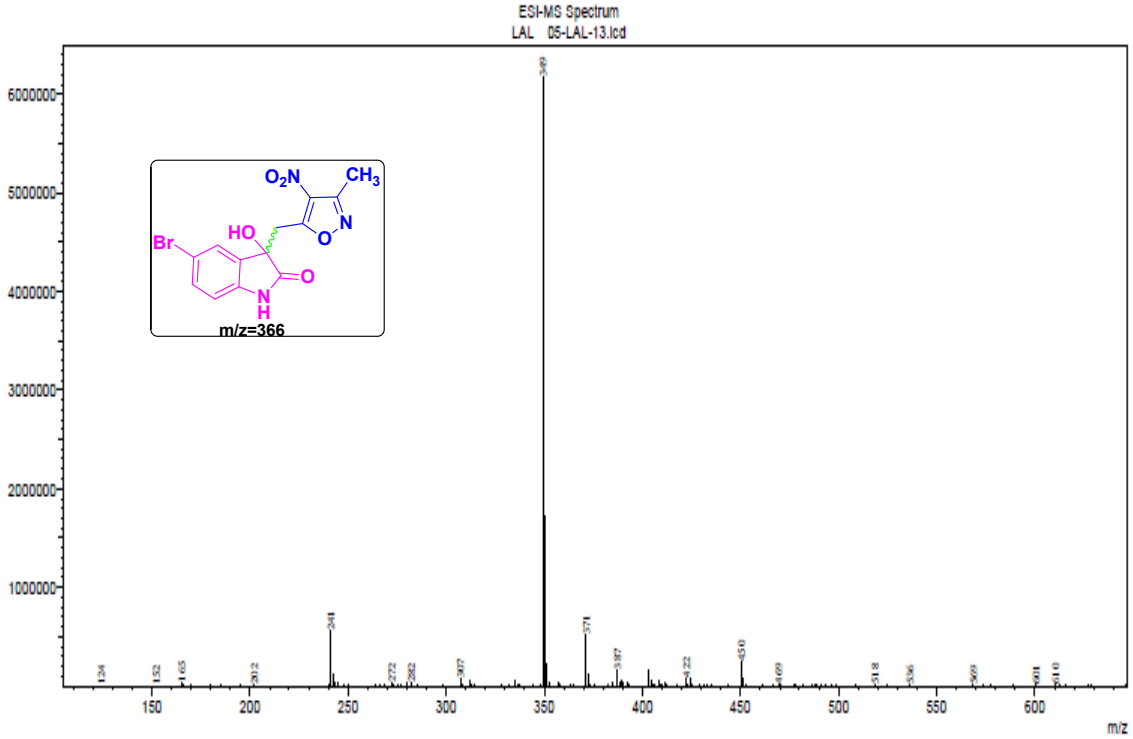
m/z

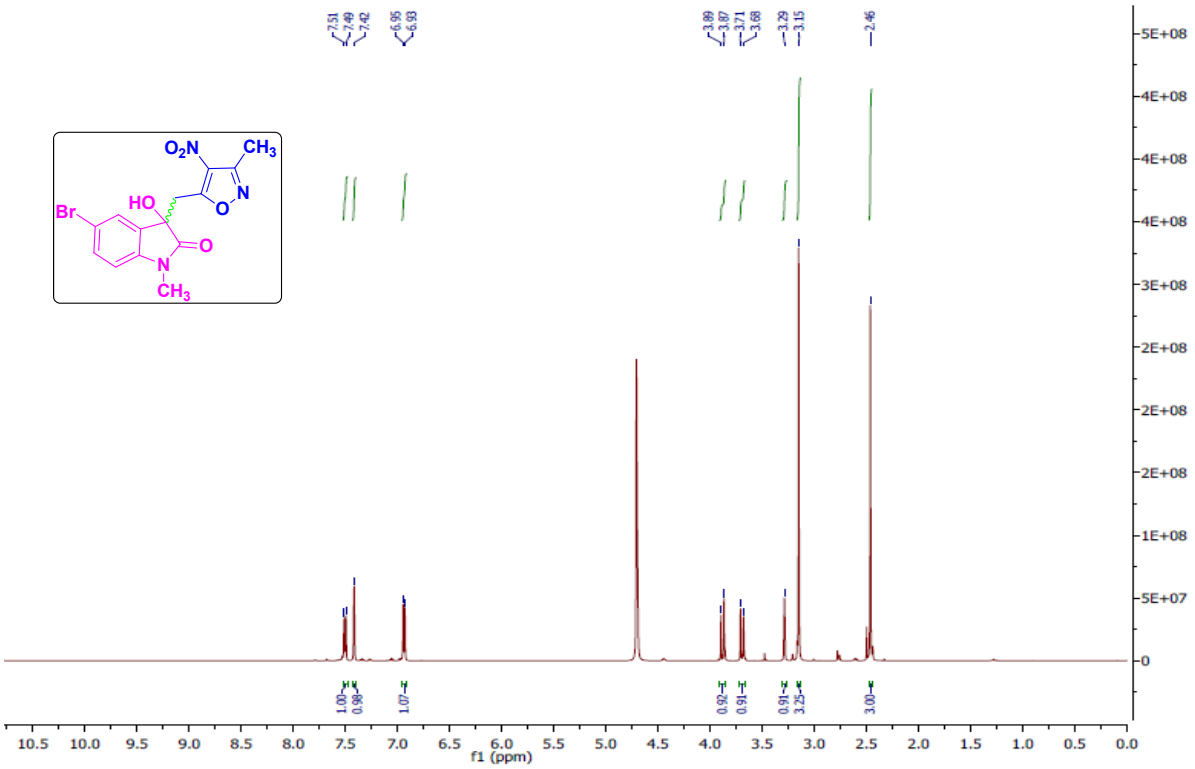

%T
cm-1
c:\documents and settings\admin\my documents\research scholar\nagaraju\henry\5-cl -n-benzyl.asc

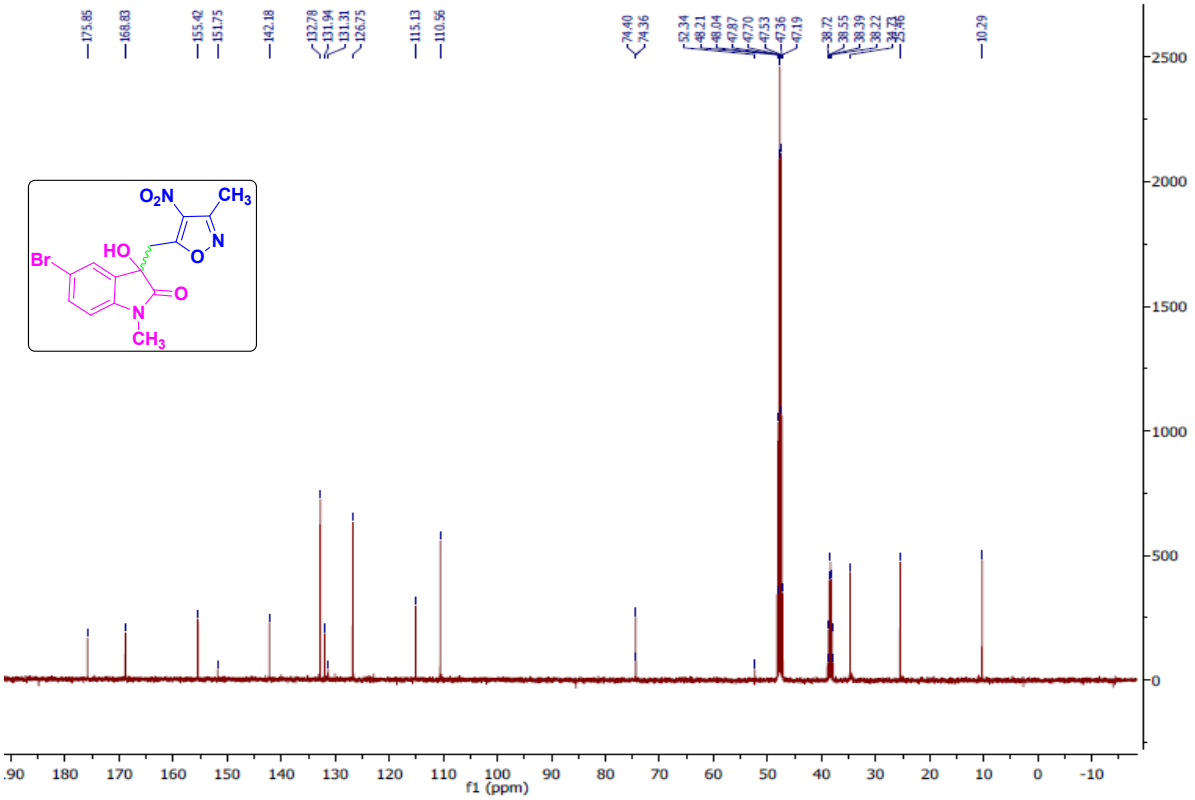
5-bromo-3-hydroxy-3-((3-methyl-4-nitroisoxazol-5-yl)methyl)indolin-2-one:

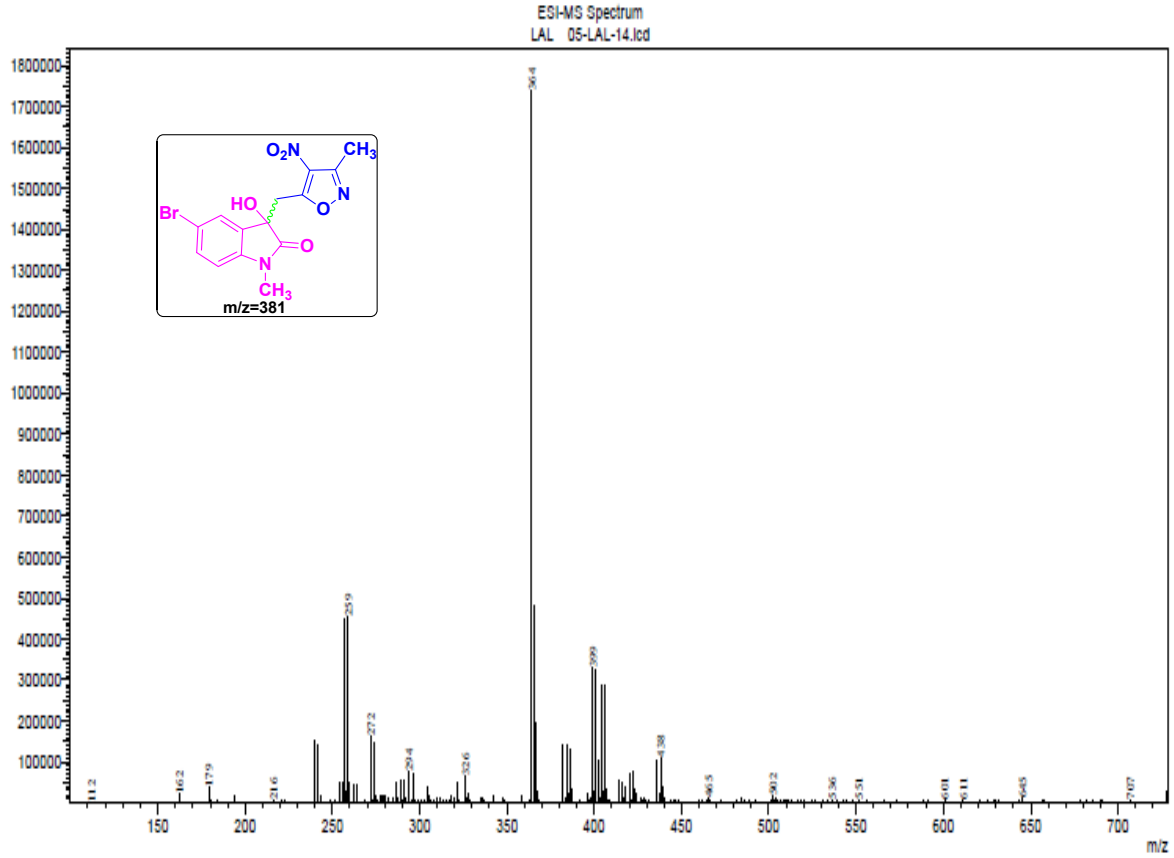




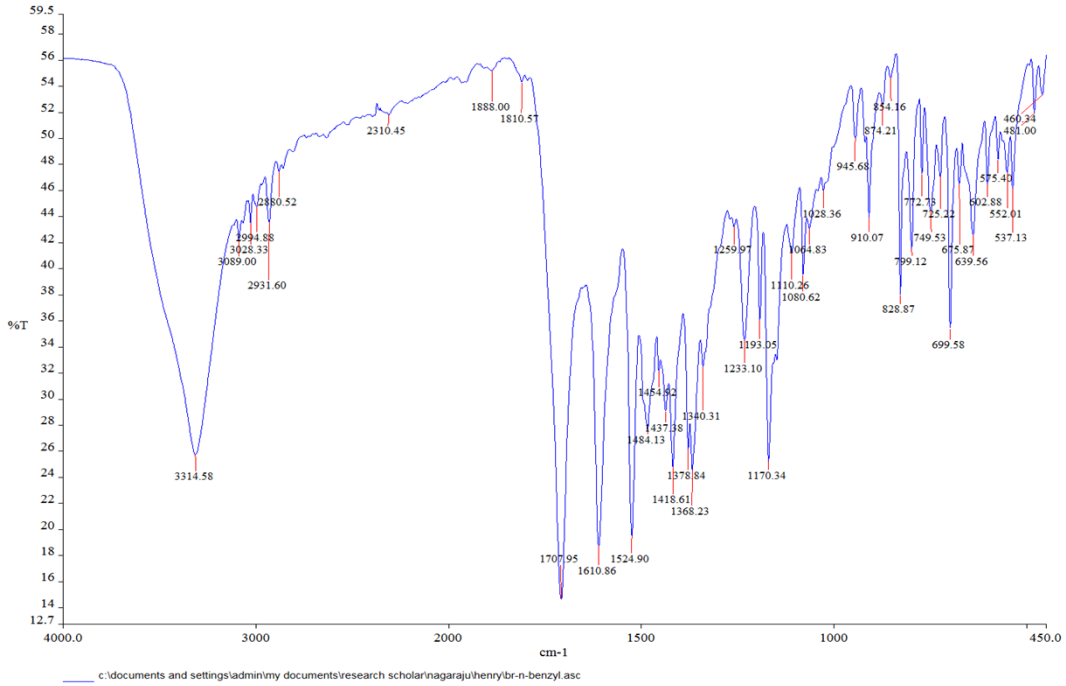
5-bromo-3-hydroxy-1-methyl-3-((3-methyl-4-nitroisoxazol-5-yl)methyl)indolin-2-one:



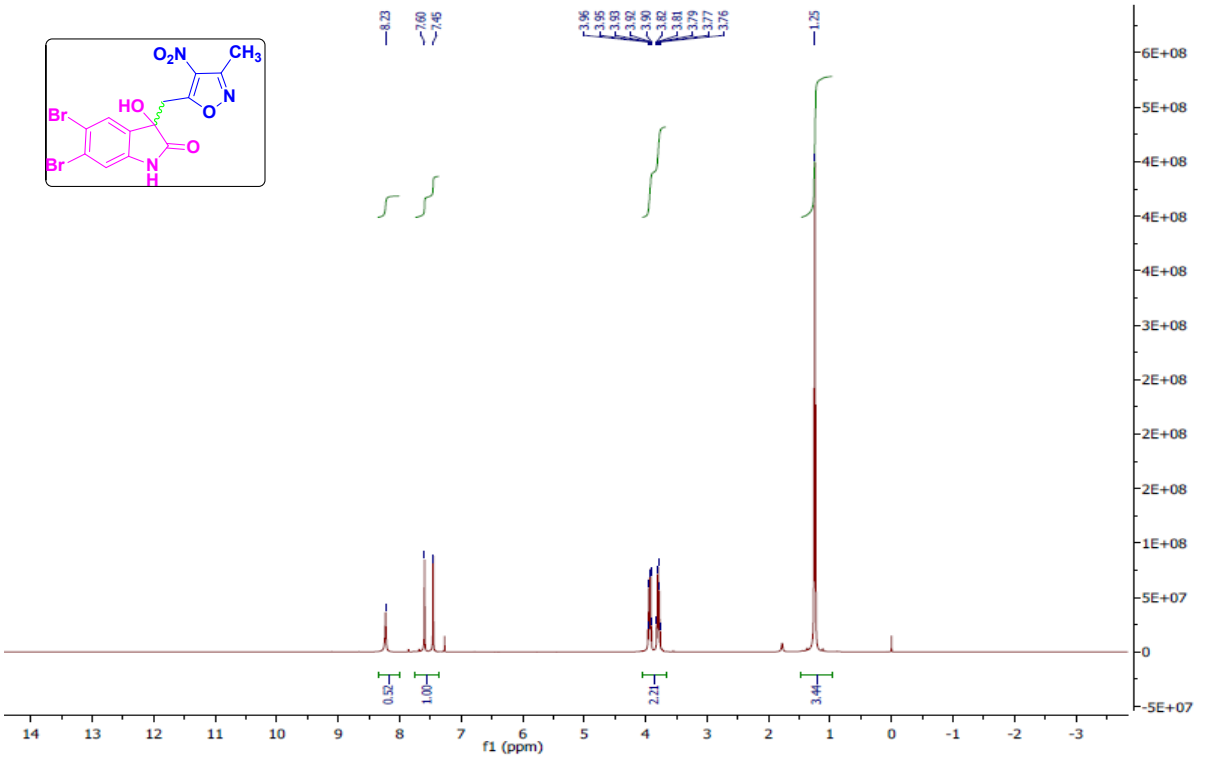


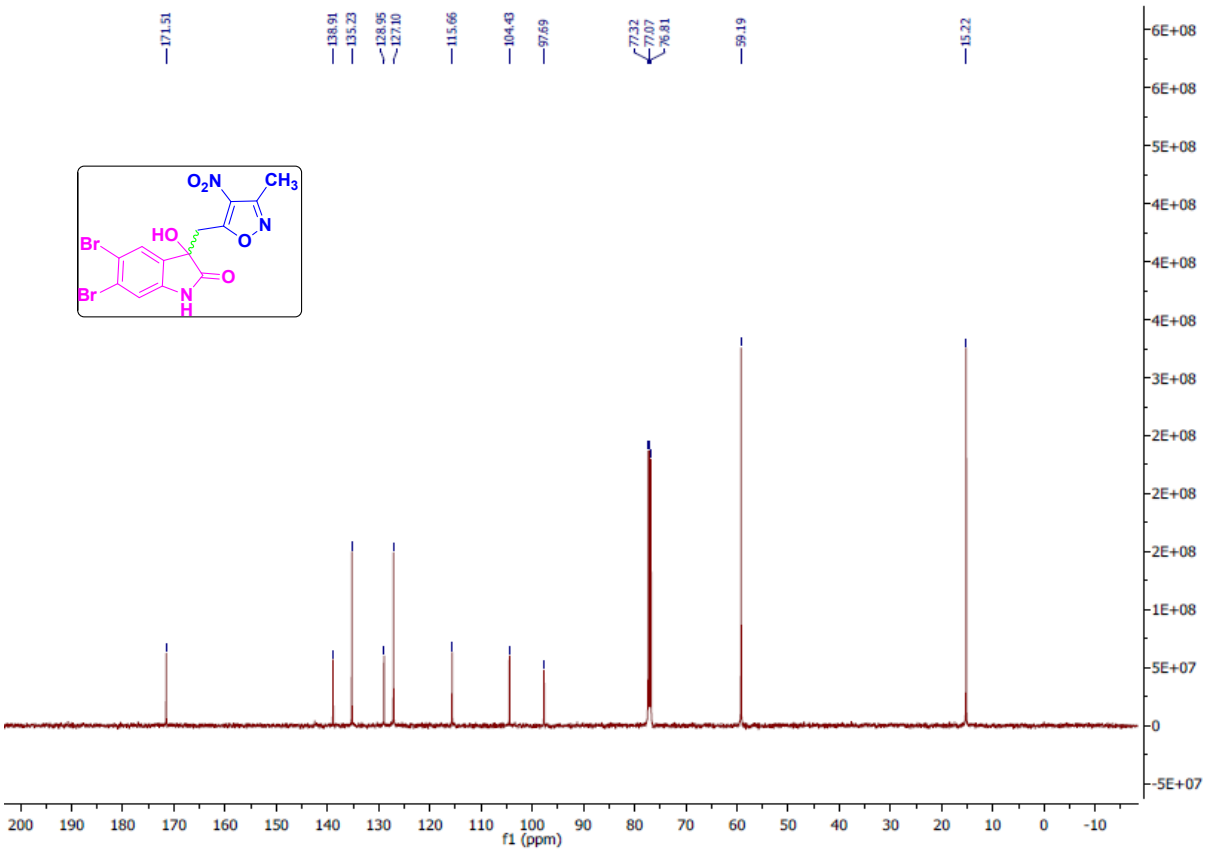


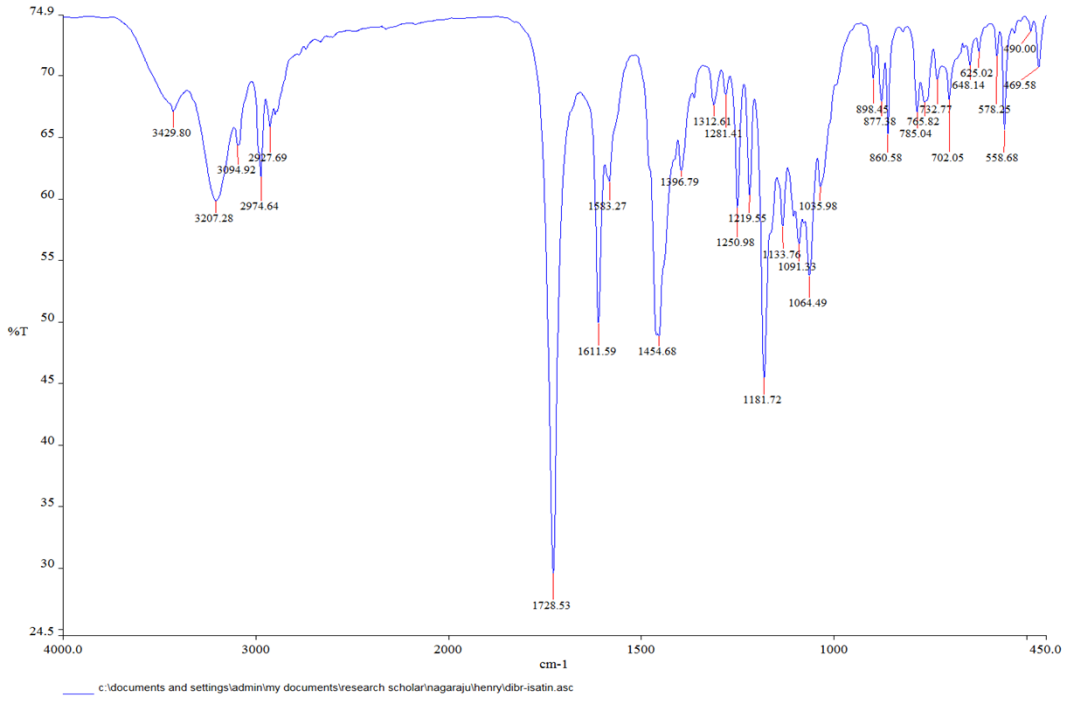
1-benzyl-5-bromo-3-hydroxy-3-((3-methyl-4-nitroisoxazol-5-yl)methyl)indolin-2-one:



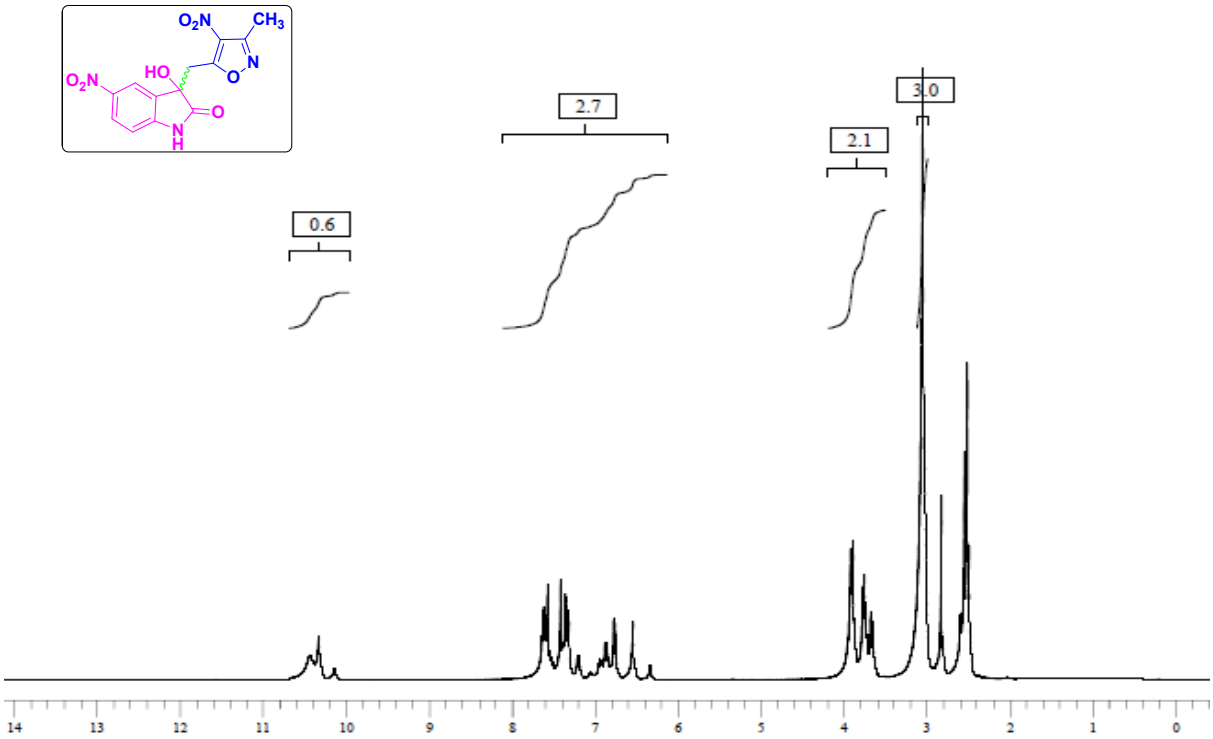
5,6-dibromo-3-hydroxy-3-((3-methyl-4-nitroisoxazol-5-yl)methyl)indolin-2-one:

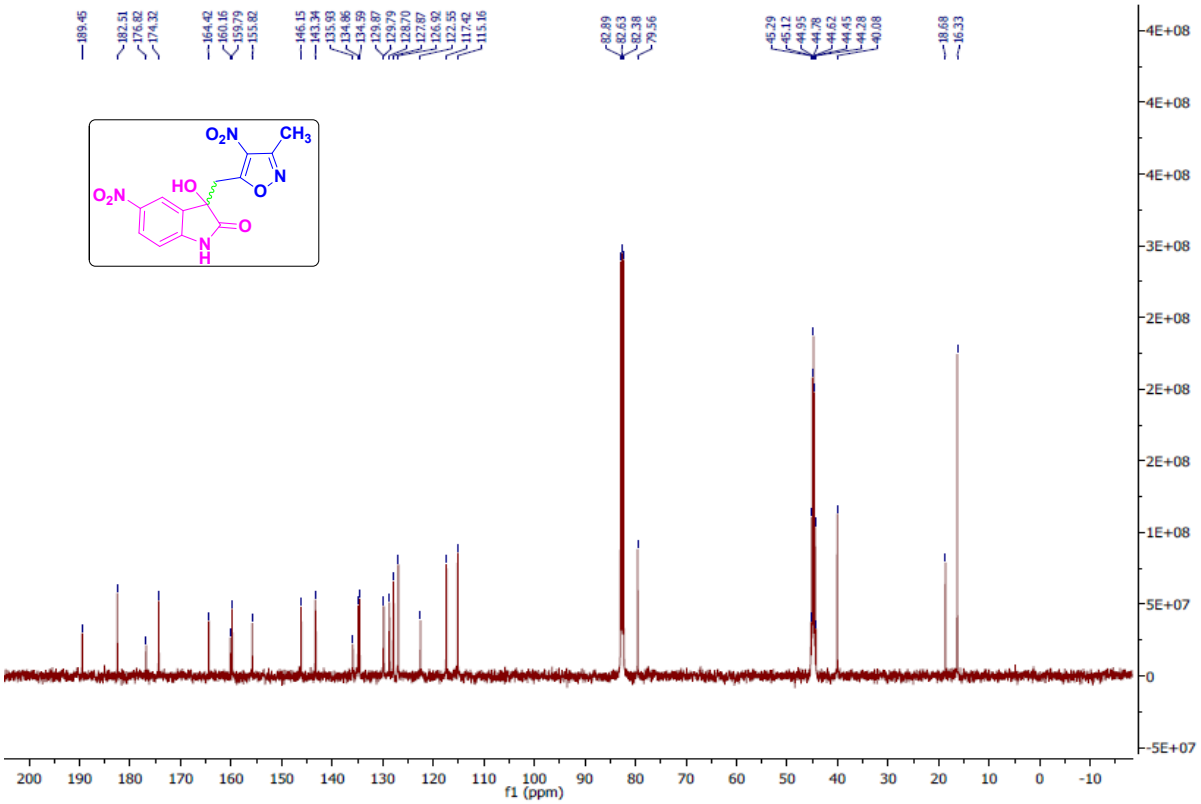






3-hydroxy-3-((3-methyl-4-nitroisoxazol-5-yl)methyl)-5-nitroindolin-2-one:

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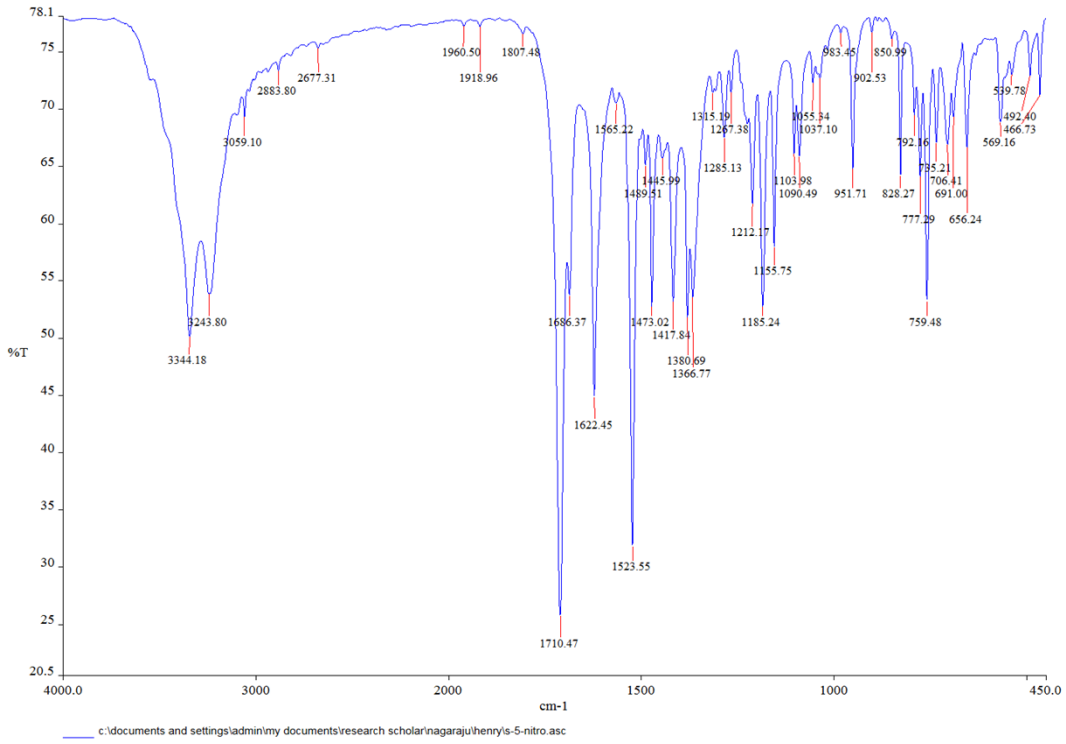
176.82
174.32
164.42
160.16
159.79
155.82
146.15
143.34
135.93
134.86
134.59
129.87
129.79
128.70
127.87
126.92
122.55
117.42
115.16
82.89
82.63
82.38
79.56
45.29
45.12
44.95
44.78
44.62
44.45
44.28
40.08
18.68
16.33
O2N
CH3
HO
O2N
N
O
O
N
H
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


78.1
75
70
65
60
55
50
45
40
35
30
25
20.5
%T
4000.0
3000
2000
1500
1000
450.0
cm-1
3344.18
3243.80
3059.10
2883.80
2677.31
1960.50
1918.96
1807.48
1710.47
1686.37
1622.45
1565.22
1523.55
1489.51
1473.02
1445.99
1417.84
1380.69
1366.77
1315.19
1285.13
1267.38
1212.17
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1037.10
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828.27
792.16
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759.48
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706.41
691.00
656.24
569.16
539.78
492.40
466.73
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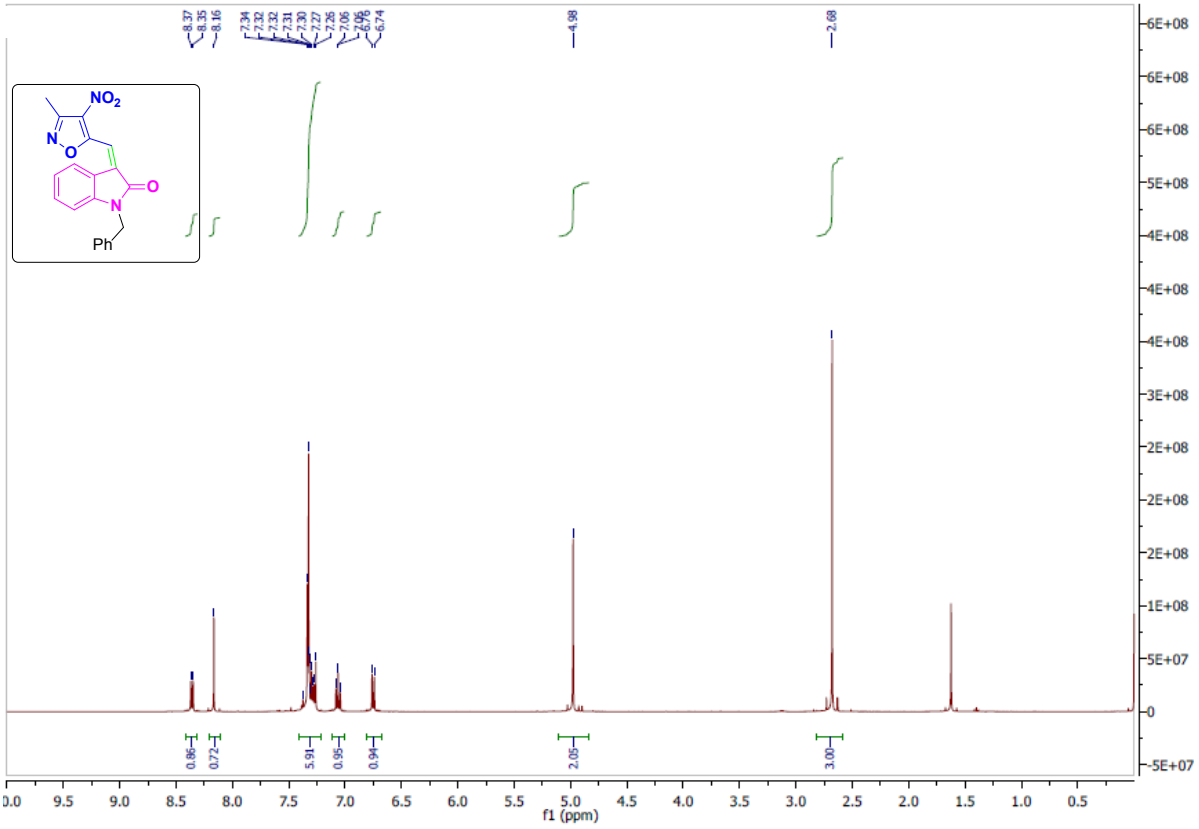
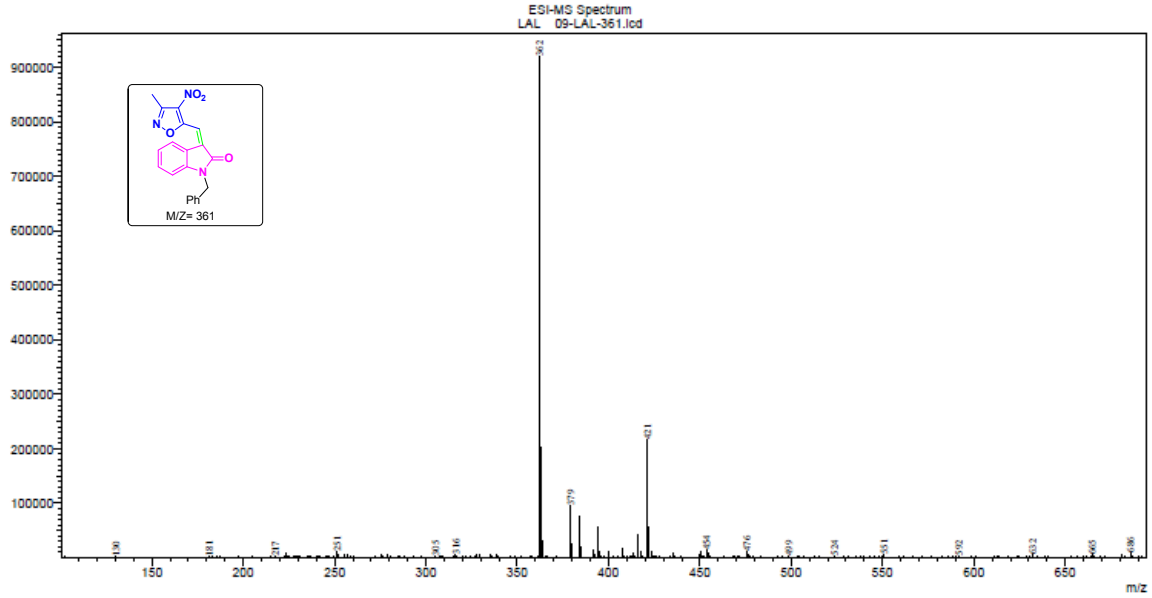
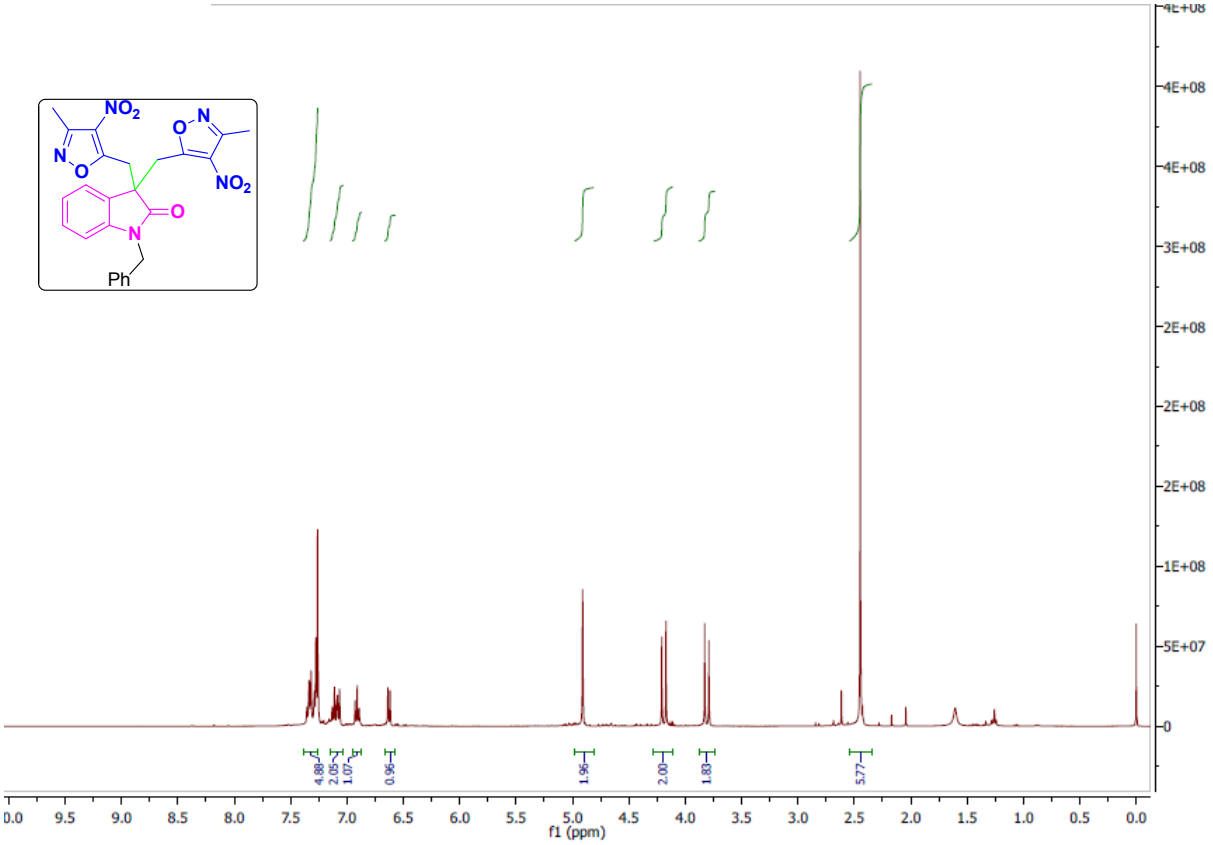
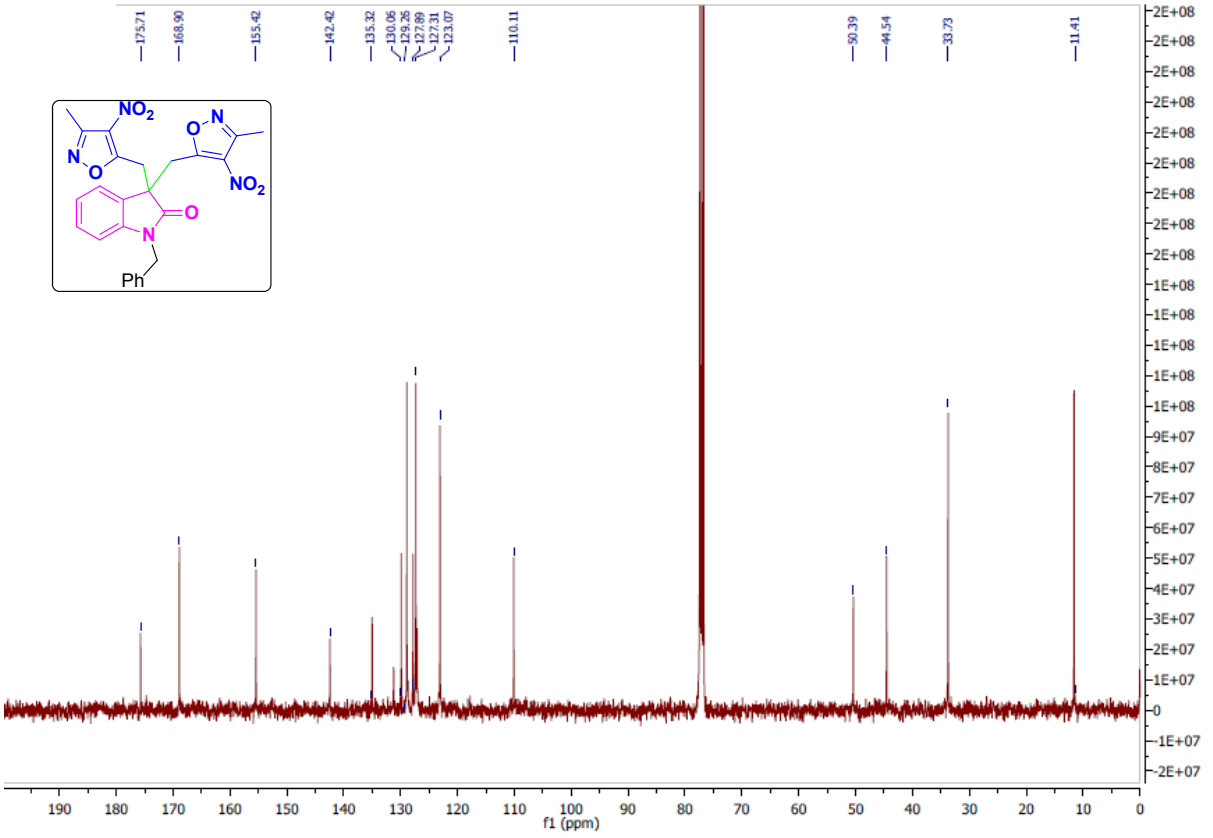
(E)-1-benzyl-3-((3-methyl-4-nitroisoxazol-5-yl)methylene)indolin-2-one

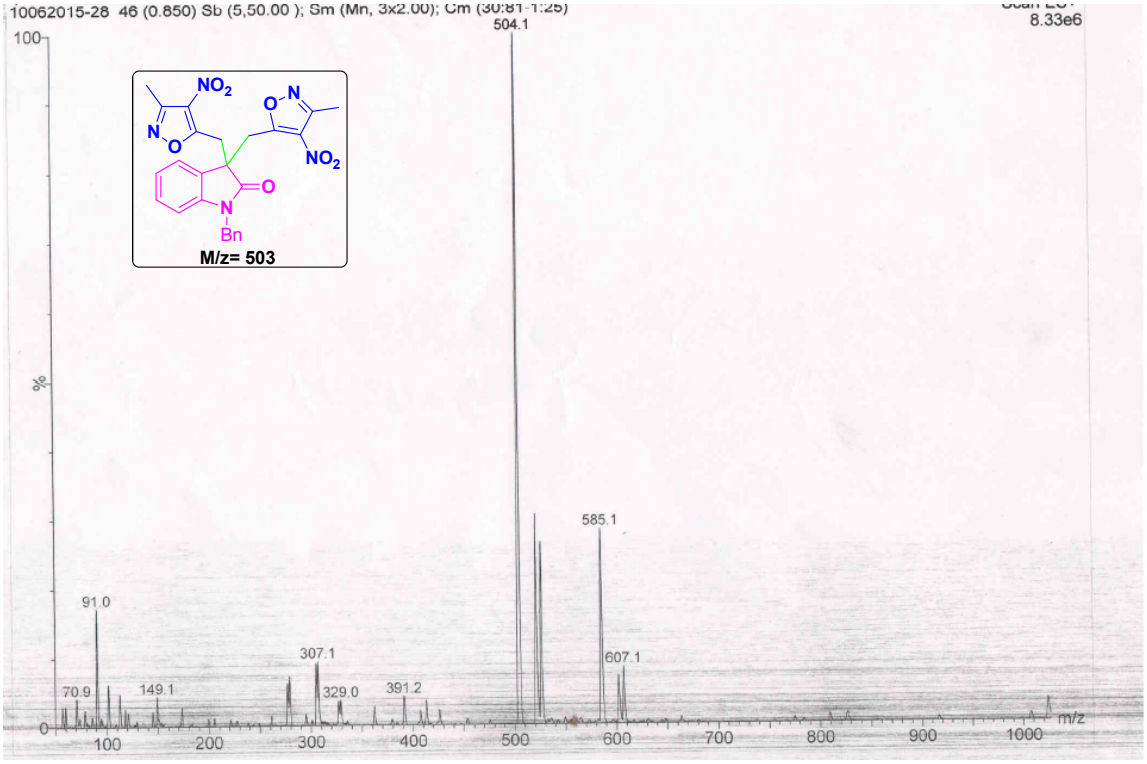




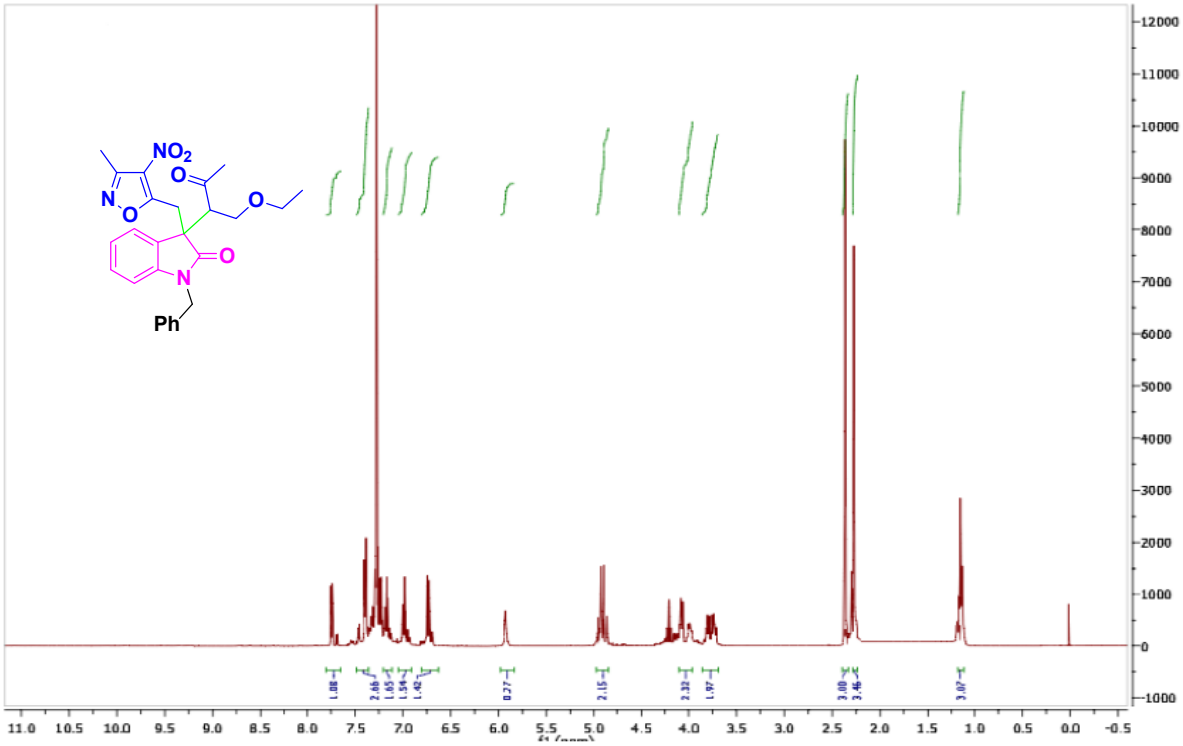
1-benzyl-3,3-bis((3-methyl-4-nitroisoxazol-5-yl)methyl)indolin-2-one:

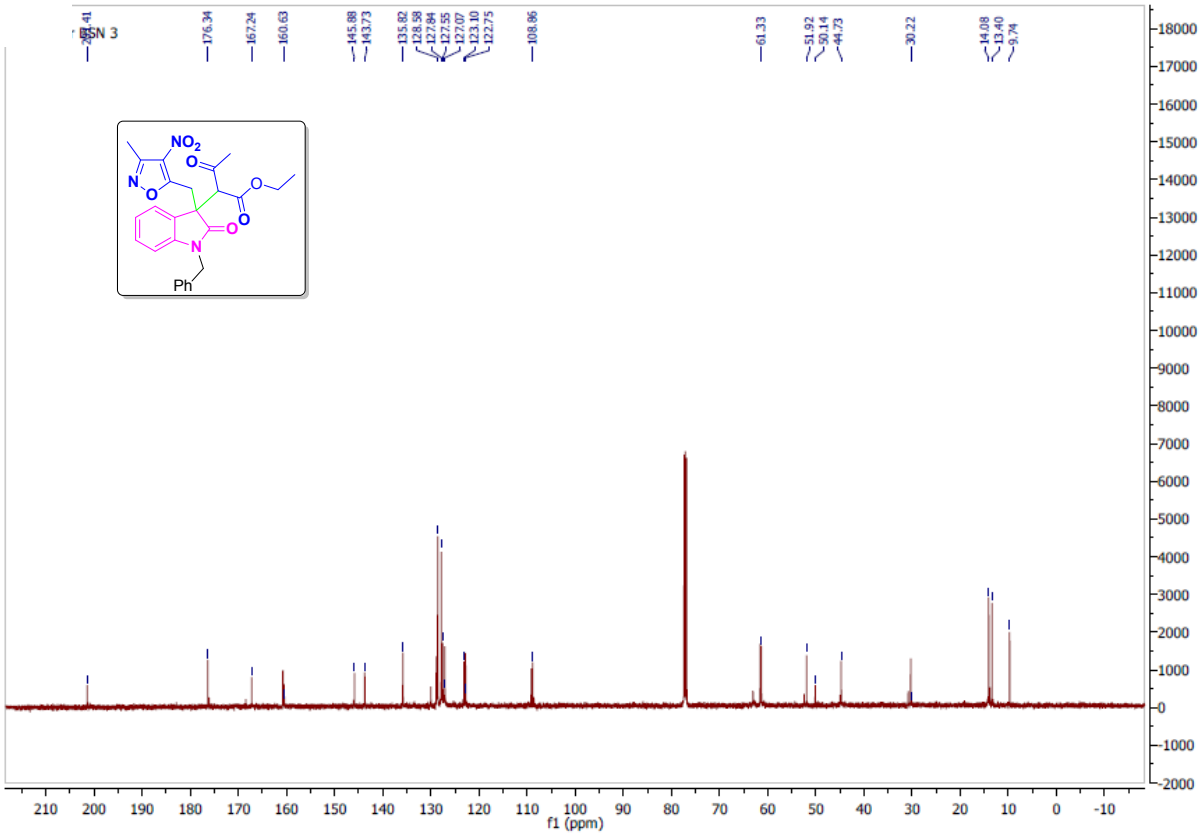




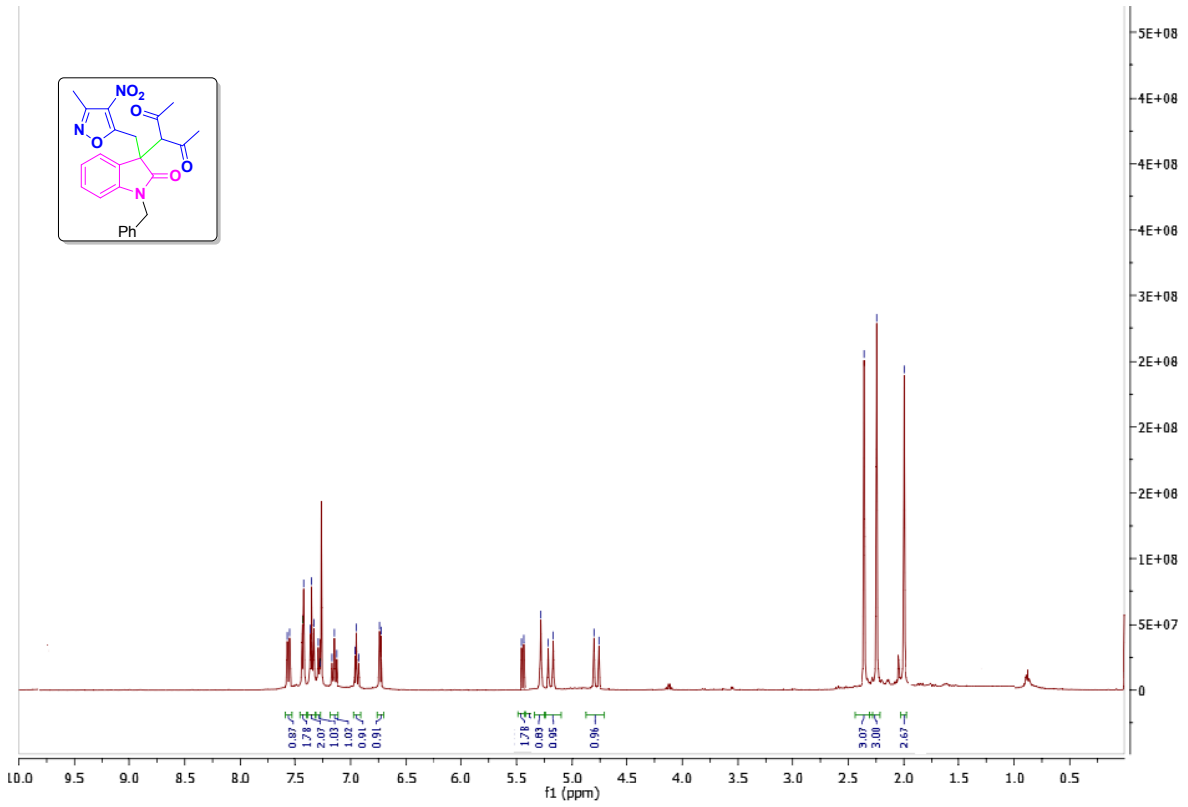


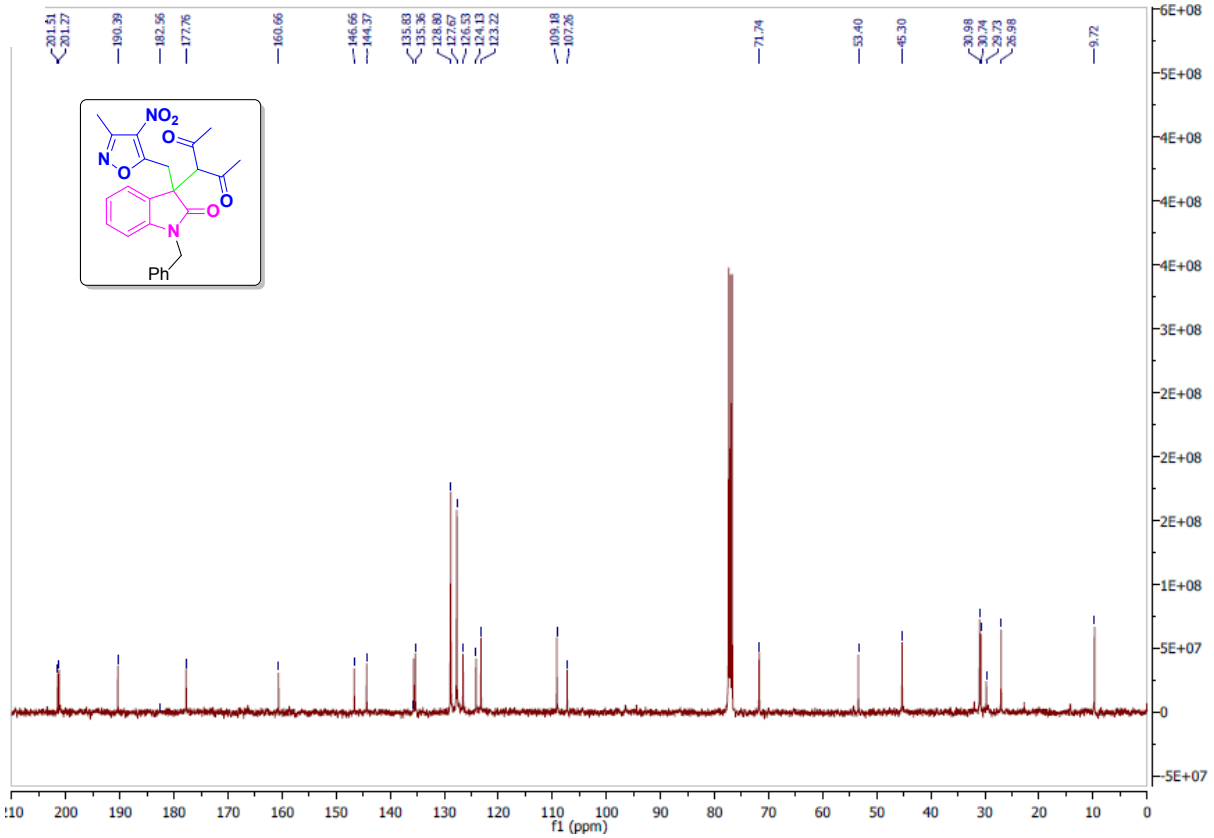
ethyl 2-(1-benzyl-3-((3-methyl-4-nitroisoxazol-5-yl)methyl)-2-oxoindolin-3-yl)-3-oxobutanoate

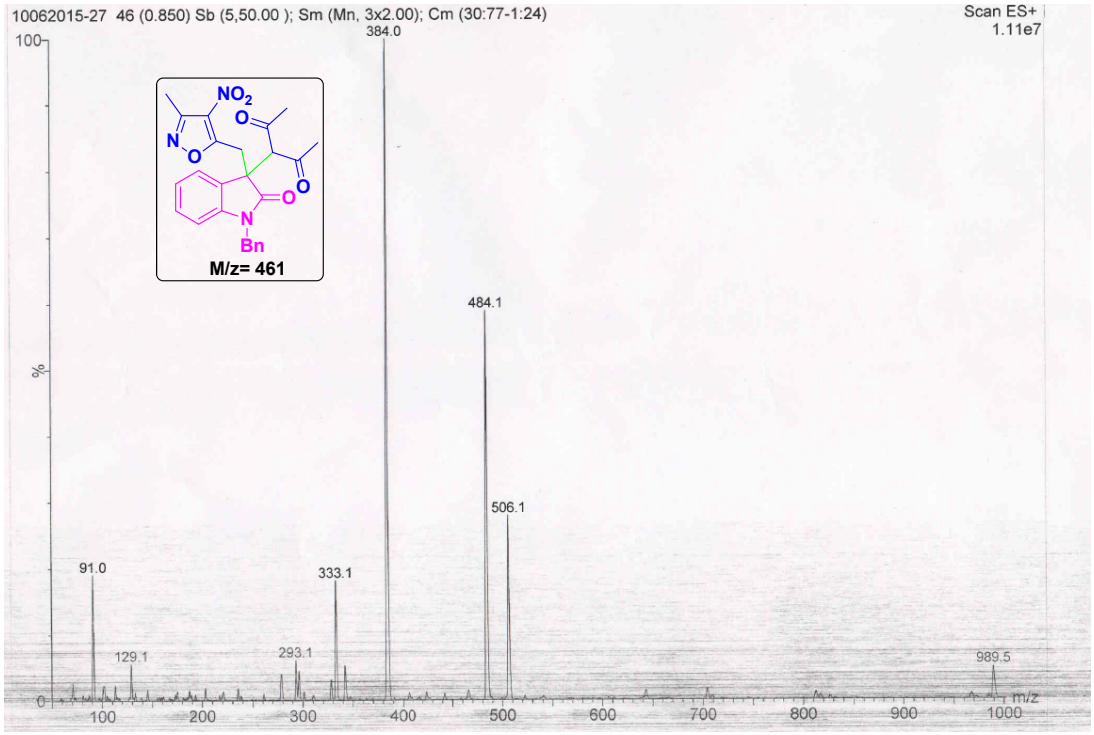




3-(1-benzyl-3-((3-methyl-4-nitroisoxazol-5-yl)methyl)-2-oxoindolin-3-yl)pentane-2,4-dione:




201.51
201.27
190.39
182.56
177.76
160.66
146.66
144.37
135.83
135.36
128.80
127.67
126.53
124.13
123.22
109.18
107.26
71.74
53.40
45.30
30.98
30.74
29.73
26.98
9.72
NO2
O
N
O
O
O
N
Ph
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
f1 (ppm)


10062015-27 46 (0.850) Sb (5,50.00); Sm (Mn, 3x2.00); Cm (30:77-1:24)
Scan ES+
1.11e7
100
%
384.0
484.1
506.1
91.0
333.1
129.1
293.1
989.5
NO2
O
N
O
O
O
N
Bn
M/z= 461
m/z

2-(3-((3-methyl-4-nitroisoxazol-5-yl)methyl)-2-oxoindolin-3-yl)malononitrile: