Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Rongalite-Induced Transition-Metal and Hydride-Free Reductive Aldol Reaction: A Rapid access to 3,3´-Disubstituted Oxindoles and Its Mechanistic Studies

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1. General procedures

General procedure for synthesis of *N*-alkyl isatins (1k-s, 1w).[1] An oven dried 50 mL reaction flask equipped with a magnetic stirring bar was charged with appropriate isatin (10 mmol) and *N*, *N*-Dimethyl formamide (DMF) solvent (15 mL), the mixture was cooled to 0-5 ^{o}C. After 5 minutes NaH (12 mmol) was added in portion wise to above mixture with the duration of 15 minutes, then the corresponding alkyl bromide (10 mmol) (for methylation, methyl iodide is used) was added in dropwise. The reaction mixture was continued to stir under cooling condition until the completion of starting material, monitored by TLC. After completion of reaction, ice cold water is added and the resulted solid is filtered under vacuum, washed with water and dried.

General procedure for synthesis of *N*-benzyl isatins (1t-u).[2] An oven dried 50 mL reaction flask equipped with a magnetic stirring bar was charged with appropriate isatin (10 mmol), K_2CO_3 (12 mmol) and *N*, *N*-Dimethyl formamide (DMF) solvent (15 mL), then benzyl bromide (10 mmol) was added dropwise at ambient temperature. The reaction mixture was allowed to stir at room temperature to complete the reaction. After completion of reaction (monitored by TLC), cold water is added and stirring was continued to form the precipitation of product. Finally, the precipitate was filtered under vacuum, washed with water and dried.

General procedure for synthesis of *N*-aryl isatins (1v).[3] An oven dried 50 mL reaction flask equipped with a magnetic stirring bar was charged with appropriate isatin (10 mmol), appropriate phenylboronic acid (20 mmol), cupric acetate (10 mmol), pyridine (20 mmol) and dichloromethane (DCM) solvent (15 mL). The reaction mixture was stirred at room temperature and progress of the reaction was monitored by TLC using hexanes and ethyl acetate as an eluent. After completion of reaction, mixture is extracted with DCM and the organic layers were

separated, dried (Na_2SO_4) and evaporated to give a residue that was purified on silica gel column chromatography using hexanes and ethyl acetate as an eluent.

General procedure for synthesis of bis-isatins (1x-y).[4] An oven dried 50 mL reaction flask equipped with a magnetic stirring bar was charged with appropriate isatin (10 mmol), K_2CO_3 (12 mmol) and dimethyl sulfoxide (DMSO) solvent (15 mL), then the corresponding dibromo alkane (5 mmol) was added in dropwise. After completion of the reaction (monitored by TLC), ice cold water was added and continued to stir for precipitation of product. The solid product was then filtered under vacuum, washed with water and cold methanol.

General procedure for synthesis of isatin Schiff bases (4a-r).[5] An oven dried 50 mL reaction flask equipped with a magnetic stirring bar was charged with appropriate isatin (10 mmol), aniline (10 mmol) and EtOH (15 mL). The mixture was stirred at 60 °C, then the catalytic amount of glacial CH_3COOH is added. After the completion of reaction (monitored by TLC) ice cold water was added and the resulted solid was filtered under vacuum, washed with cold methanol and dried.

General procedure for synthesis of isatin-derived ketimines (6a-e).[6] An oven dried 25 mL reaction flask equipped with a magnetic stirring bar was charged with appropriate isatin (1 mmol), *N*-Boc-triphenyliminophosphorane (2 mmol) and anhydrous 1,4-dioxane (2 mL). The mixture is refluxed for 4-5 h under nitrogen atmosphere. Progress of the reaction is monitored by TLC. Later, crude is purified by silica gel column chromatography using hexanes/ethyl acetate as mobile phase.

General procedure (A) for synthesis of 3-hydroxy-3-(hydroxymethyl)indolin-2-one derivatives (3a-y). An oven dried 10 mL reaction flask equipped with a magnetic stirring bar was charged with appropriate isatin-derivative (1 mmol), rongalite (2 mmol), K_2CO_3 (2 mmol)

and EtOH+H_2O (2 mL, 8:2 v/v). The mixture was stirred at 70 °C for the appropriate time (10-20 min). The progress of the reaction was monitored by TLC using hexanes and ethyl acetate as an eluent. After completion of reaction, EtOH is evaporated under vacuum and extracted with ethyl acetate (3 x 10 mL). The organic layers were separated, dried (Na_2SO_4) and evaporated to give a residue that was purified on a short pad of silica gel column chromatography using hexanes and ethyl acetate as an eluent.

General experimental procedure (B) for synthesis of 3-(hydroxymethyl)-3-(phenylamino)indolin-2-one derivatives (5a-r). An oven dried 10 mL reaction flask equipped with a magnetic stirring bar was charged with appropriate isatin Schiff base/*N*-protected isatin Schiff base (1 mmol), rongalite (2 mmol), K_2CO_3 (2 mmol) and EtOH+H_2O (2 mL, 8:2 v/v). The mixture was stirred at 70 °C for the appropriate time (20-50 min). The progress of the reaction was monitored by TLC using hexanes and ethyl acetate as an eluent. After completion of reaction, EtOH is evaporated under vacuum and extracted with ethyl acetate (3 x 10 mL). The organic layers were separated, dried (Na_2SO_4) and evaporated to give a residue that was purified on a short pad of silica gel column chromatography using hexanes and ethyl acetate as an eluent.

General experimental procedure (C) for synthesis of *tert*-butyl (3-(hydroxymethyl)-2-oxoindolin-3-yl)carbamate derivatives (7a-e). An oven dried 10 mL reaction flask equipped with a magnetic stirring bar was charged with appropriate isatin-derived ketimine (0.5 mmol), rongalite (1 mmol), K_2CO_3 (1 mmol) and EtOH+H_2O (2 mL, 8:2 v/v). The mixture was stirred at 70 °C for the appropriate time (20-60 min). The progress of the reaction was monitored by TLC using hexanes and ethyl acetate as an eluent. After completion of reaction, EtOH is evaporated under vacuum and extracted with ethyl acetate (3 x 10 mL). The organic layers were separated,

dried (Na_2SO_4) and evaporated to give a residue that was purified on a short pad of silica gel column chromatography using hexanes and ethyl acetate as an eluent.

Experimental procedure (D) for synthesis of 3-hydroxyindolin-2-one (8). An oven dried 10 mL reaction flask equipped with a magnetic stirring bar was charged with isatin **1a** (1 mmol), rongalite **2** (1 mmol) and EtOH+H_2O (2 mL, 8:2 v/v). The mixture was stirred at 70 °C for 10 min. The progress of the reaction was monitored by TLC using hexanes and ethyl acetate as an eluent. After completion, EtOH is evaporated under vacuum and extracted with ethyl acetate (3 x 10 mL). The organic layers were separated, dried (Na_2SO_4) and evaporated to give a residue that was purified on a short pad of silica gel column chromatography using hexanes and ethyl acetate as an eluent.

2. ^{1}H NMR Experiment on isatin Schiff base 4j

Mechanistic Study of Reductive Aldol reactions through ^{1}H NMR Spectroscopy

We have conducted similar ^{1}H NMR experiment on isatin Schiff base to check whether isatin Schiff bases follow the same pathway like isatins or not. Isatin Schiff base **4j** (50 mg, 0.15 mmol) was treated with rongalite **2** (2 equiv.) and K_2CO_3 (2 equiv.) in 1 mL of DMSO-d_6 at 70 °C. A 10 μL aliquot of the reaction mixture was transferred to a NMR tube, diluted with DMSO-d_6 (0.5 mL), and recorded ^{1}H NMR spectra at noted times. The ^{1}H NMR spectra are shown in Figure S1. Characterization data of the identified compounds are as follows. When the reaction mixture is recorded at 25 min, peaks at δ 10.63, 6.31, 5.10 and 2.13 ppm are observed, which are correspond to the intermediate i.e., 5-bromo-3-(*p*-tolylamino)indolin-2-one. The peaks at 10.63 ppm represents the NH proton of oxindole moiety, 6.31 ppm represents the NH proton of aniline,

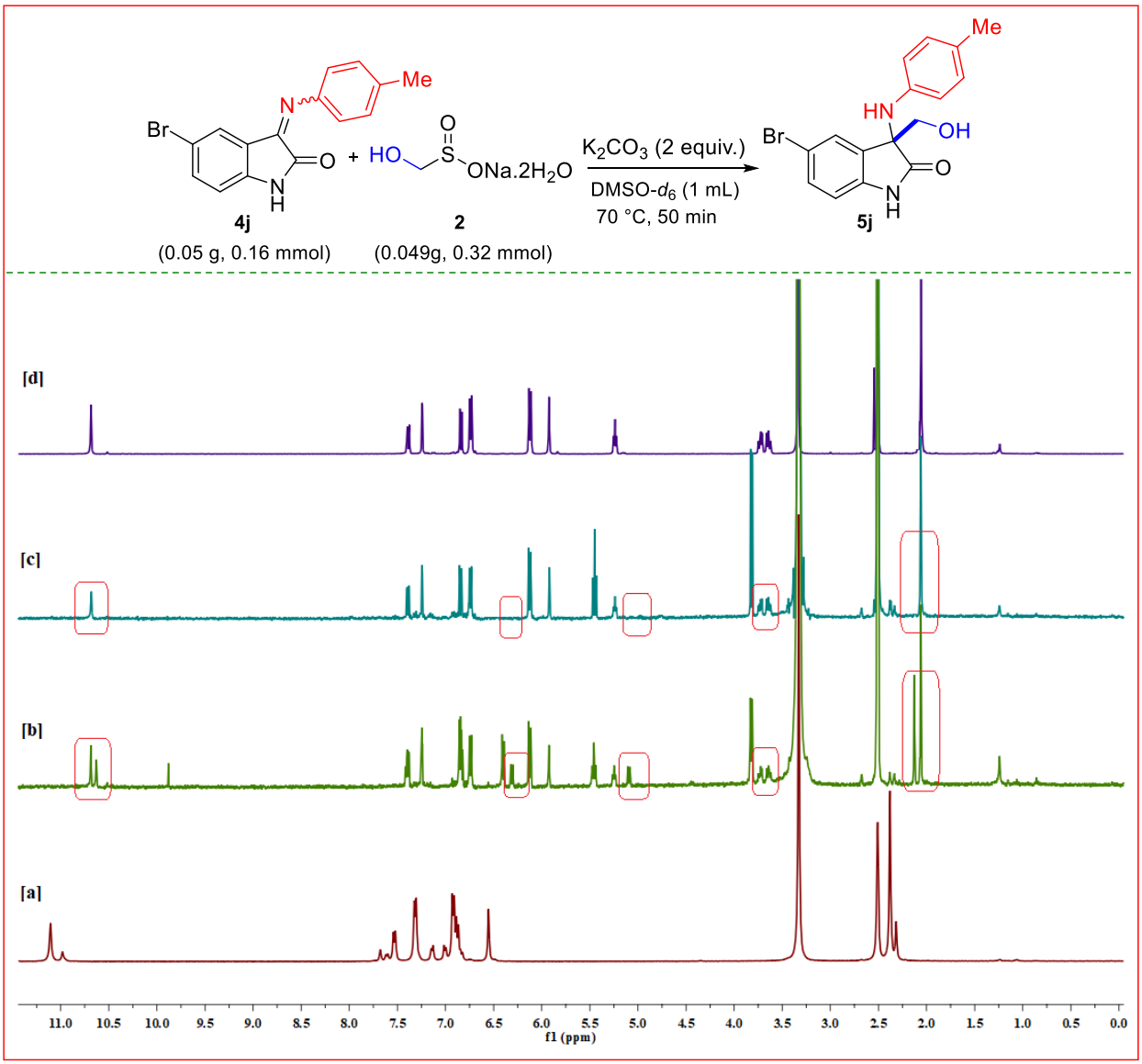


Figure S1. 400 MHz ^{1}H NMR spectra of aliquots taken at noted times. All spectra were recorded by diluting an aliquot of the reaction mixture in DMSO-d_6. Panel a: isatin Schiff base **4j**; panel b: isatin Schiff base, rongalite and K_2CO_3, after 25 min; panel c: after 50 min; panel d: purified compound **5j**.

5.10 ppm represents the CH proton and 2.13 ppm represents the CH_3 protons of aniline. Notably, at 25 min observed the formation of final product also i.e., 5-bromo-3-(hydroxymethyl)-3-(*p*-tolylamino)indolin-2-one and the corresponding peaks are observed at 10.68 ppm (NH proton of

oxindoles, 5.92 ppm (NH proton of aniline), 5.24 ppm (OH proton) and 2.06 ppm (CH_3 protons). From ^{1}H NMR spectrum at 25 min, it is clear that no Schiff base is remained and mixture of intermediate and product is observed. When reaction mixture is recorded at 50 min, the peaks correspond to intermediate are completely diminished and observed only the peaks respective to final product which was compared with ^{1}H NMR spectrum of purified product **5j**.

3. Deuterium labeling studies

3.1 Preparation of deuterated rongalite

An oven dried 10 mL reaction flask equipped with a magnetic stirring bar was charged with anhydrous rongalite (0.3 g) and mehanol-d_4 (3 mL), the resulting mixture was stirred for 1h. Then the mehanol-d_4 was evaporated, dried under vacuum and recorded ^{1}H NMR. The Proton NMR spectra of both anhydrus rongalite **2** and deuterated rongalite **2-D** were shown in Figure S2. The O-H peak in rongalite at δ 5.41 ppm (Figure S2a) was completely disappeared in deuterated rongalite **2-D** (Figure S2b), which indicate the complete deuteration of the O-H group of rogalite.

3.2 ^{1}H NMR (400 MHz, DMSO-d_6) spectra of rongalite and deuterated rongalite

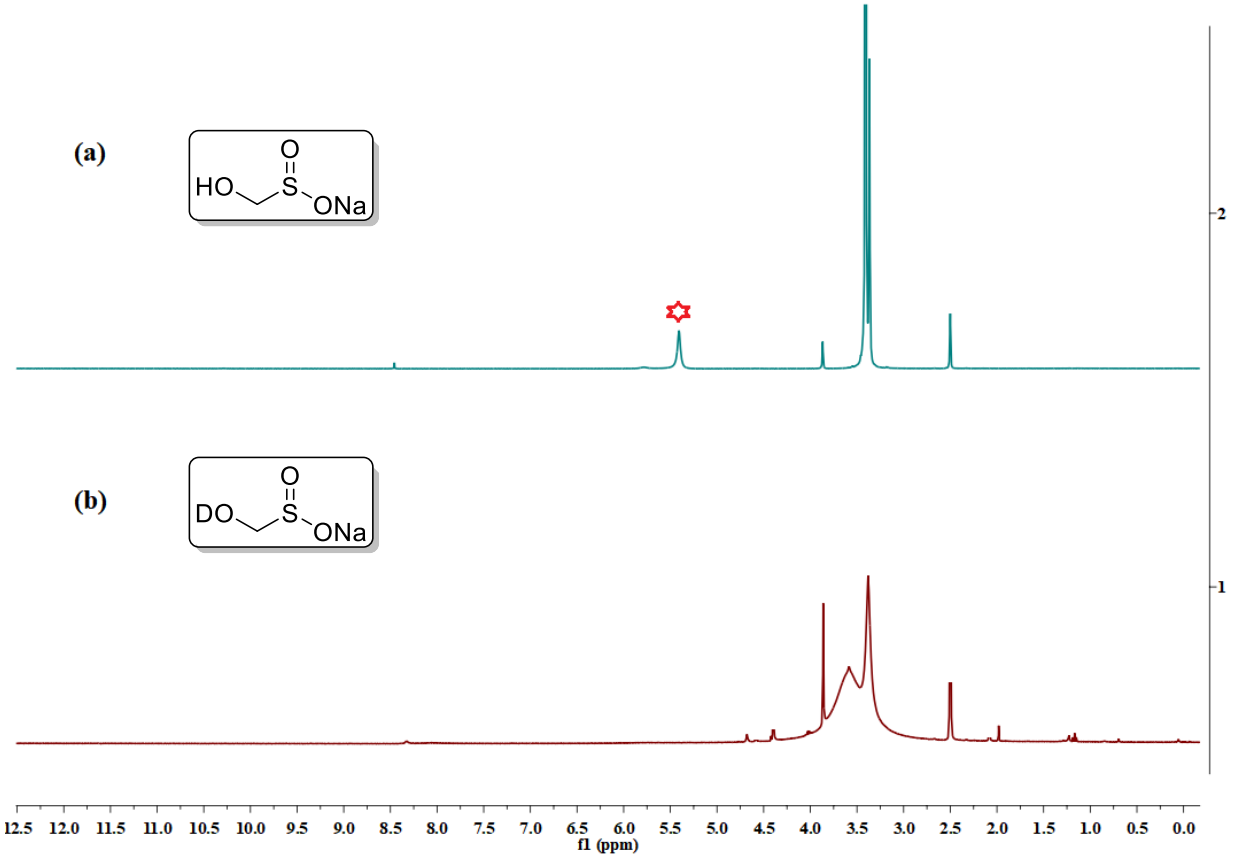
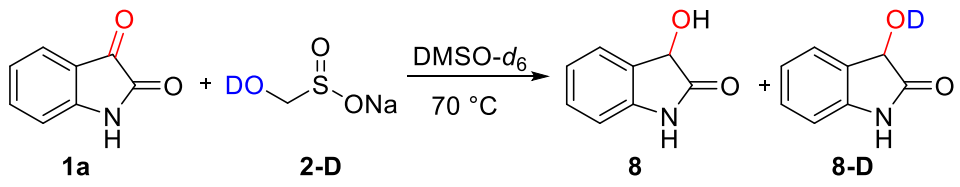


Figure S2. ^{1}H NMR spectra of (a) Rongalite; (b) Deuterated rongalite.

3.3 Deuterium labeling experiment



An oven dried 10 mL reaction flask equipped with a magnetic stirring bar was charged with isatin **1a** (0.05 mmol) and deuterated rongalite **2-D** (0.05 mmol) in DMSO-d_6 (1 mL) and the

mixture was stirred at 70 °C for 5 min under N_2 atmosphere . The crude mixture was recorded for ^{1}H NMR and results are shown in Figure S3b. Based on ^{1}H NMR, we have found that 35% of deuterium was incorporated in the product **8-D**. This result suggested that the proton from the rongalite got itself incorporated into the final product.

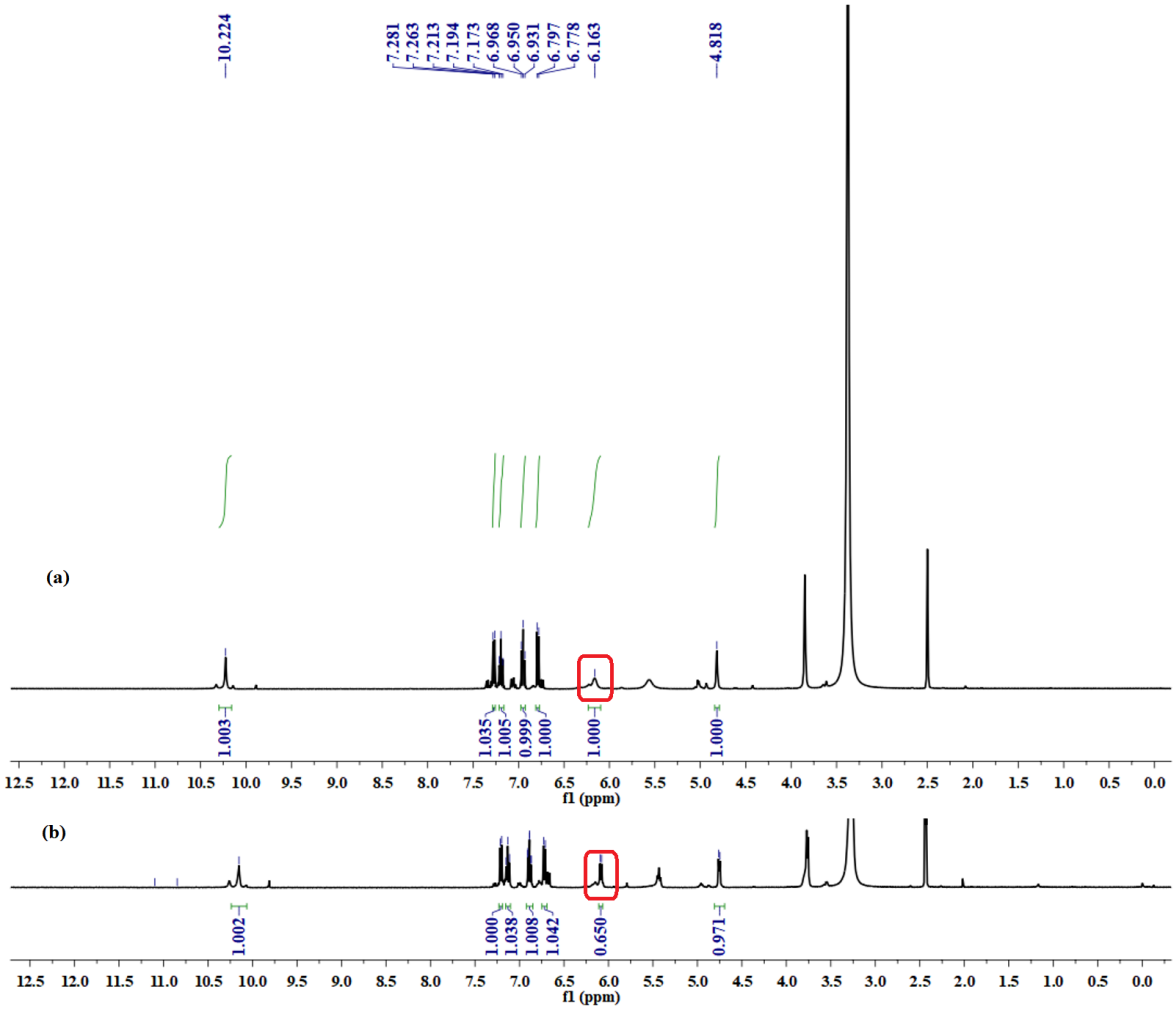
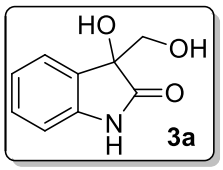


Figure S3. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of reaction mixture of (a) Isatin **1a** (0.05 mmol) and rongalite **2** (0.05 mmol) in DMSO-d_6 at 70 °C; (b) Isatin **1a** (0.05 mmol) and deuterated rongalite **2-D** (0.05 mmol) in DMSO-d_6 at 70 °C.

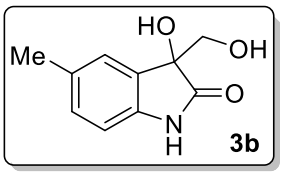
4.0 Characterization data

3-hydroxy-3-(hydroxymethyl)indolin-2-one (3a). White solid; Yield (165 mg, 92%); mp 146-



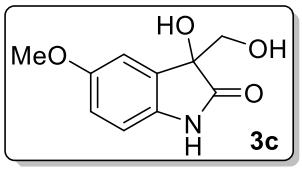
147 °C; The title compound is prepared according to the general procedure (A) described as above; FT-IR (KBr, cm^{-1}) 3425, 3370, 3062, 1723, 1681, 1265; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 10.14 (s, 1H), 7.28 (d, J = 7.2 Hz, 1H), 7.20 (t, J = 7.6 Hz, 1H), 6.96 (t, J = 7.6 Hz, 1H), 6.78 (d, J = 7.6 Hz, 1H), 5.87 (s, 1H), 4.80 (t, J = 5.6 Hz, 1H), 3.66 – 3.60 (m, 2H); $^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO-d_6) δ (ppm): 179.2, 143.2, 131.8, 129.2, 124.9, 121.7, 109.7, 76.6, 65.8; HRMS (ESI) *m/z*: $[M+Na]^+$ calcd for $C_9H_9NNaO_3$ 202.0480; found 202.0475.

3-hydroxy-3-(hydroxymethyl)-5-methylindolin-2-one (3b). White solid; Yield (155 mg, 80%);



mp 187-188 °C; The title compound is prepared according to the general procedure (A) described as above; FT-IR (KBr, cm^{-1}) 3425, 3306, 3191, 3059, 1710, 1623; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 10.04 (s, 1H), 7.09 (s, 1H), 6.99 (d, J = 7.6 Hz, 1H), 6.66 (d, J = 7.6 Hz, 1H), 5.81 (s, 1H), 4.78 (t, J = 5.6 Hz, 1H), 3.60 (d, J = 5.6 Hz, 2H), 2.26 (s, 3H); $^{13}C\{^{1}H\}$ NMR (125 MHz, DMSO-d_6) δ (ppm): 179.2, 140.7, 131.8, 130.5, 129.4, 125.6, 109.4, 76.7, 65.8, 21.2; HRMS (ESI) *m/z*: $[M+Na]^+$ calcd for $C_{10}H_{11}NNaO_3$ 216.0637; found 216.0360.

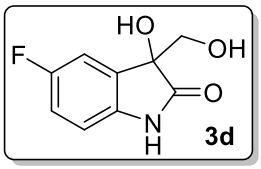
3-hydroxy-3-(hydroxymethyl)-5-methoxyindolin-2-one (3c). Off white solid; Yield (165 mg,



79%); mp 182-183 °C; The title compound is prepared according to the general procedure (A) described as above; FT-IR (KBr, cm^{-1}) 3476, 3322, 3061, 1702, 1613; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 9.98 (s, 1H), 6.91 (d, J = 2.4 Hz, 1H), 6.76 (dd, J = 8.4, 2.4 Hz, 1H), 6.68 (d, J = 8.4 Hz, 1H), 5.87 (s, 1H), 4.79 (t, J = 5.6 Hz,

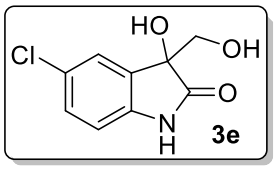
1H), 3.71 (s, 3H), 3.64 – 3.57 (m, 2H); $^{13}C\{^{1}H\}$ NMR (75 MHz, DMSO-d_6) δ (ppm): 178.5, 154.8, 135.8, 132.4, 113.5, 111.6, 109.5, 76.5, 65.4, 55.5; HRMS (ESI) *m/z*: $[M+Na]^+$ calcd for $C_{10}H_{11}NNaO_4$ 232.0586; found 232.0590.

5-fluoro-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3d). White solid; Yield (162 mg, 82%);



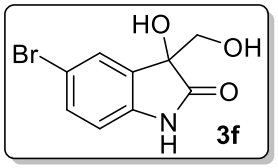
mp 174-175 °C; The title compound is prepared according to the general procedure (A) described as above; FT-IR (KBr, cm^{-1}) 3425, 3366, 3176, 3082, 1727, 1682; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 10.18 (s, 1H), 7.14 – 7.12 (m, 1H), 7.05 – 6.99 (m, 1H), 6.76 (dd, J = 8.4, 4.4 Hz, 1H), 6.01 (s, 1H), 4.87 (t, J = 5.6 Hz, 1H), 3.62 (m, 2H); $^{13}C\{^{1}H\}$ NMR (75 MHz, DMSO-d_6) δ (ppm): 178.5, 157.9 (d, $^{1}J_{C\text{-}F}$ = 234.8 Hz), 138.7, 133.0 (d, $^{3}J_{C\text{-}F}$ = 7.5 Hz), 114.8 (d, $^{2}J_{C\text{-}F}$ = 23.3 Hz), 112.1 (d, $^{2}J_{C\text{-}F}$ = 24 Hz), 109.9 (d, $^{3}J_{C\text{-}F}$ = 7.5 Hz), 76.5, 65.3; HRMS (ESI) *m/z*: $[M+Na]^+$ calcd for $C_9H_8FNNaO_3$ 220.0386; found 220.0387.

5-chloro-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3e). White solid; Yield (181 mg, 85%);



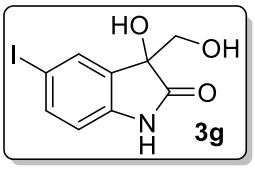
mp 192-193 °C; The title compound is prepared according to the general procedure (A) described as above; FT-IR (KBr, cm^{-1}) 3424, 3277, 3072, 1711, 1616; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 10.30 (s, 1H), 7.30 (d, J = 2.0 Hz, 1H), 7.25 (dd, J = 8.0, 2.0 Hz, 1H), 6.79 (d, J = 8.0 Hz, 1H), 6.04 (s, 1H), 4.90 (t, J = 5.6 Hz, 1H), 3.62 (m, 2H); $^{13}C\{^{1}H\}$ NMR (75 MHz, DMSO-d_6) δ (ppm): 178.2, 141.5, 133.3, 128.5, 125.4, 124.6, 110.6, 76.3, 65.2; HRMS (ESI) *m/z*: $[M+Na]^+$ calcd for $C_9H_8ClNNaO_3$ 236.0090; found 236.0089.

5-bromo-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3f). White solid; Yield (230 mg, 89%);



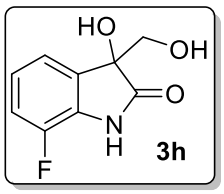
mp 194-195 °C; The title compound is prepared according to the general procedure (A) described as above; FT-IR (KBr, cm^{-1}) 3400, 3251, 3082, 1710, 1632; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 10.31 (s, 1H), 7.42 (d, J = 2.0 Hz, 1H), 7.39 – 7.36 (m, 1H), 6.75 (d, J = 8.4 Hz, 1H), 6.04 (s, 1H), 4.92 (t, J = 5.6 Hz, 1H), 3.63 (m, 2H); $^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO-d_6) δ (ppm): 178.7, 142.5, 134.3, 131.9, 127.8, 113.6, 111.7, 76.8, 65.7; HRMS (ESI) *m/z*: $[M+Na]^+$ calcd for $C_9H_8BrNNaO_3$ 279.9585; found 279.9571.

3-hydroxy-3-(hydroxymethyl)-5-iodoindolin-2-one (3g). White crystalline solid; Yield (262



mg, 86%); mp 188-189 °C; The title compound is prepared according to the general procedure (A) described as above; FT-IR (KBr, cm^{-1}) 3421, 3368, 3167, 3080, 1725, 1679; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 10.28 (s, 1H), 7.56 – 7.53 (m, 2H), 6.64 (d, J = 8.0 Hz, 1H), 6.01 (s, 1H), 4.90 (t, J = 5.6 Hz, 1H), 3.66 – 3.57 (m, 2H); $^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO-d_6) δ (ppm): 178.5, 143.0, 137.7, 134.6, 133.3, 112.2, 84.7, 76.7, 65.6; HRMS (ESI) *m/z*: $[M+Na]^+$ calcd for $C_9H_8INNaO_3$ 327.9447; found 327.9444.

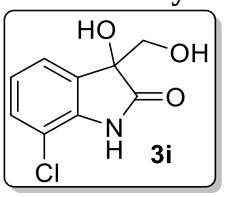
7-fluoro-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3h). White solid; Yield (170 mg, 86%);



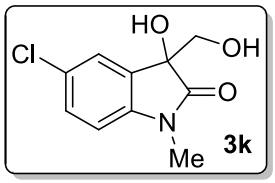
mp 177-178 °C; The title compound is prepared according to the general procedure (A) described as above; FT-IR (KBr, cm^{-1}) 3420, 3366, 3176, 3082, 1727, 1682; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 10.66 (s, 1H), 7.16 – 7.09 (m, 2H), 7.00 – 6.99 (m, 1H), 6.04 (s, 1H), 4.88 (t, J = 5.6 Hz, 1H), 3.65 (d, J = 5.6 Hz, 2H); $^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO-d_6) δ (ppm): 179.1, 146.7 (d, $^{1}J_{C\text{-}F}$ = 240.2 Hz), 134.9 (d, $^{3}J_{C\text{-}F}$ = 3.5 Hz), 130.0 (d, $^{2}J_{C\text{-}F}$ = 11.8 Hz), 122.7 (d, $^{3}J_{C\text{-}F}$ = 5.6 Hz), 120.9 (d, $^{4}J_{C\text{-}F}$ = 2.9 Hz),

116.3 (d, $^{2}J_{C\text{-}F}$ = 17.2 Hz), 76.8 (d, $^{4}J_{C\text{-}F}$ = 2.7 Hz), 65.8; HRMS (ESI) *m/z*: $[M+Na]^+$ calcd for $C_9H_8FNNaO_3$ 220.0386; found 220.0389.

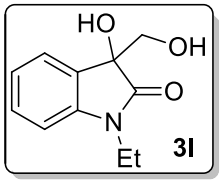
7-chloro-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3i). White crystalline solid; Yield (183 mg, 86%); mp 168-169 °C; The title compound is prepared according to the general procedure (A) described as above; FT-IR (KBr, cm^{-1}) 3424, 3277, 3081, 1711, 1616; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 10.59 (s, 1H), 7.297 – 7.230 (m, 2H), 6.99 (t, *J* = 7.6 Hz, 1H), 6.06 (s, 1H), 4.90 (t, *J* = 5.6 Hz, 1H), 3.65 (d, *J* = 5.6 Hz, 2H); ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ (ppm): 179.2, 140.8, 133.9, 129.2, 123.4, 123.2, 114.0, 77.3, 65.8; HRMS (ESI) *m/z*: $[M+Na]^+$ calcd for $C_9H_8ClNNaO_3$ 236.0090; found 236.0088.



5-chloro-3-hydroxy-3-(hydroxymethyl)-1-methylindolin-2-one (3k). White solid; Yield (204 mg, 90%); mp 174-175; The title compound is prepared according to the general procedure (A) described as above; FT-IR (KBr, cm^{-1}) 3422, 3223, 3061, 1689, 1612, 1492; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 7.39 – 7.34 (m, 2H), 6.99 (d, *J* = 8.8 Hz, 1H), 6.12 (s, 1H), 4.93 (t, *J* = 5.6 Hz, 1H), 3.71 – 3.61 (m, 2H), 3.09 (s, 3H); ^{13}C{^{1}H} NMR (75 MHz, DMSO-d_6) δ (ppm): 176.4, 142.9, 132.6, 128.6, 126.1, 124.2, 109.4, 76.1, 65.1, 25.8; HRMS (ESI) *m/z*: $[M+Na]^+$ calcd for $C_{10}H_{10}ClNNaO_3$ 250.0247; found 250.0241.

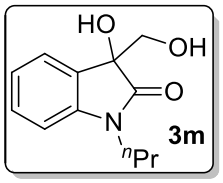


1-ethyl-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3l). White solid; Yield (197 mg, 95%); mp 118-119 °C; The title compound is prepared according to the general procedure (A) described as above; FT-IR (KBr, cm^{-1}) 3354, 3305, 3092,



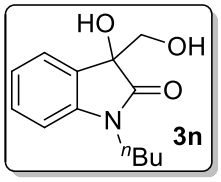
3059, 2925, 1698, 1614, 1493; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 7.39 (d, J = 7.2 Hz, 1H), 7.37 – 7.33 (m, 1H), 7.11 – 7.04 (m, 2H), 6.01 (s, 1H), 4.88 (t, J = 5.6 Hz, 1H), 3.75 – 3.67 (m, 4H), 1.19 (t, J = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (125 MHz, DMSO-d_6) δ (ppm): 177.0, 143.7, 131.3, 129.4, 124.6, 122.3, 108.6, 76.4, 65.8, 34.3, 13.0; HRMS (ESI) *m/z*: $[M+Na]^+$ calcd for $C_{11}H_{13}NNaO_3$ 230.0793; found 230.0789.

3-hydroxy-3-(hydroxymethyl)-1-propylindolin-2-one (3m). White crystalline solid; Yield



(208 mg, 94%); mp 104-105 °C; The title compound is prepared according to the general procedure (A) described as above; FT-IR (KBr, cm^{-1}) 3394, 3063, 2966, 2934, 1702, 1614, 1489; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 7.33 (d, J = 7.2 Hz, 1H), 7.30 – 7.26 (m, 1H), 7.02 (t, J = 7.6 Hz, 1H), 6.99 (d, J = 7.6 Hz, 1H), 5.95 (s, 1H), 4.82 (t, J = 5.6 Hz, 1H), 3.67 – 3.65 (m, 2H), 3.64 – 3.52 (m, 2H), 1.64 – 1.54 (m, 2H), 0.88 (t, J = 7.6 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ (ppm): 177.5, 144.1, 131.2, 129.4, 124.6, 122.2, 108.7, 76.4, 65.8, 41.0, 20.8, 11.6; HRMS (ESI) *m/z*: $[M+Na]^+$ calcd for $C_{12}H_{15}NNaO_3$ 244.0950; found 244.0947.

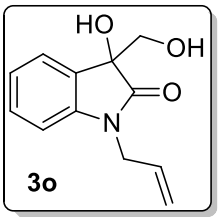
1-butyl-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3n). Colorless liquid; Yield (221 mg,



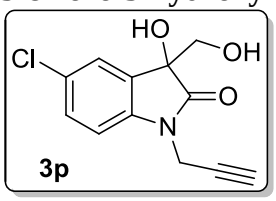
94%); The title compound is prepared according to the general procedure (A) described as above; FT-IR (KBr, cm^{-1}) 3402, 3058, 2959, 2934, 1703, 1614; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 7.33 (d, J = 7.2 Hz, 1H), 7.30 – 7.26 (m, 1H), 7.02 (t, J = 7.6 Hz, 1H), 6.97 (d, J = 7.6 Hz, 1H), 5.95 (s, 1H), 4.82 (t, J = 5.6 Hz, 1H), 3.69 – 3.54 (m, 4H), 1.59 – 1.50 (m, 2H), 1.36 – 1.27 (m, 2H), 0.89 (t, J = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (100

MHz, DMSO-d_6) δ (ppm): 177.4, 144.1, 131.3, 129.4, 124.6, 122.2, 108.7, 76.4, 65.8, 39.2, 29.6, 19.8, 14.2; HRMS (ESI) *m/z*: $[M+Na]^+$ calcd for $C_{13}H_{17}NNaO_3$ 258.1106; found 258.1108.

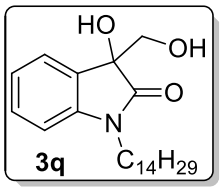
1-allyl-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3o). White crystalline solid; Yield (208 mg, 95%); mp 100-101 °C; The title compound is prepared according to the general procedure (A) described as above; FT-IR (KBr, cm^{-1}) 3322, 3061, 2920, 1694, 1614, 1468; ^1H NMR (400 MHz, DMSO-d_6) δ (ppm): 7.35 (d, *J* = 7.2 Hz, 1H), 7.26 (t, *J* = 7.6 Hz, 1H), 7.04 (t, *J* = 7.2 Hz, 1H), 6.86 (d, *J* = 7.6 Hz, 1H), 6.03 (s, 1H), 5.87 – 5.76 (m, 1H), 5.21 (d, *J* = 17.2 Hz, 1H), 5.12 (d, *J* = 10.4 Hz, 1H), 4.88 (s, 1H), 4.26 (dd, *J* = 45.2, 16.8 Hz, 2H), 3.69 (m, 2H); $^{13}C\{^1H\}$ NMR (125 MHz, DMSO-d_6) δ (ppm): 177.3, 143.8, 132.2, 131.2, 129.3, 124.5, 122.4, 116.9, 109.1, 76.5, 65.8, 41.7; HRMS (ESI) *m/z*: $[M+Na]^+$ calcd for $C_{12}H_{13}NNaO_3$ 242.0793; found 242.0784.



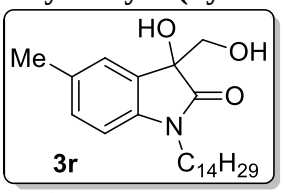
5-chloro-3-hydroxy-3-(hydroxymethyl)-1-(prop-2-yn-1-yl)indolin-2-one (3p). White solid; Yield (228 mg, 91%); mp 120-121 °C; The title compound is prepared according to the general procedure (A) described as above; FT-IR (KBr, cm^{-1}) 3287, 3229, 3063, 2921, 2120, 1716, 1612, 1487; ^1H NMR (400 MHz, DMSO-d_6) δ (ppm): 7.43 – 7.39 (m, 2H), 7.07 (d, *J* = 8.4 Hz, 1H), 6.26 (s, 1H), 4.97 (t, *J* = 5.6 Hz, 1H), 4.55 – 4.43 (m, 2H), 3.72 – 3.62 (m, 2H), 3.27 (s, 1H); $^{13}C\{^1H\}$ NMR (75 MHz, DMSO-d_6) δ (ppm): 175.7, 141.0, 132.5, 128.6, 126.6, 124.4, 110.2, 77.7, 76.1, 74.3, 65.2, 28.7; HRMS (ESI) *m/z*: $[M+Na]^+$ calcd for $C_{12}H_{10}ClNNaO_3$ 274.0247; found 274.0254.



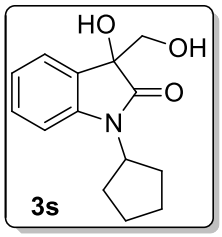
3-hydroxy-3-(hydroxymethyl)-1-tetradecylindolin-2-one (3q). White solid; Yield (353 mg, 94%); mp 85-86 °C; The title compound is prepared according to the general procedure (A) described as above; FT-IR (KBr, cm^{-1}) 3294, 2955, 2915, 2848, 1713, 1615, 1470; ^1H NMR (400 MHz, DMSO-d_6) δ (ppm): 7.33 (d, J = 7.2 Hz, 1H), 7.30 – 7.25 (m, 1H), 7.02 (t, J = 7.4 Hz, 1H), 6.96 (d, J = 7.6 Hz, 1H), 5.94 (s, 1H), 4.80 (t, J = 5.6 Hz, 1H), 3.69 – 3.53 (m, 4H), 1.60 – 1.50 (m, 2H), 1.31 – 1.21 (m, 22H), 0.86 (t, J = 6.8 Hz, 3H); $^{13}C\{^1H\}$ NMR (100 MHz, DMSO-d_6) δ (ppm): 177.3, 144.0, 131.3, 129.3, 124.6, 122.2, 108.6, 76.3, 65.8, 39.4, 31.8, 29.5, 29.5, 29.5, 29.2, 29.2, 27.4, 26.6, 22.6, 14.4; HRMS (ESI) *m/z*: $[M+Na]^+$ calcd for $C_{12}H_{10}ClNNaO_3$ 274.0247; found 274.0254.



3-hydroxy-3-(hydroxymethyl)-5-methyl-1-tetradecylindolin-2-one (3r). White solid; Yield (346 mg, 89%); mp 99-100 °C; The title compound is prepared according to the general procedure (A) described as above; FT-IR (KBr, cm^{-1}) 3437, 3388, 3023, 2954, 2840, 1710, 1614, 1465; ^1H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.15 (s, 1H), 7.07 (d, J = 8.0 Hz, 1H), 6.69 (d, J = 8.0 Hz, 1H), 3.78 – 3.68 (m, 2H), 3.64 – 3.51 (m, 2H), 2.27 (s, 3H), 1.62 – 1.56 (m, 2H), 1.23 – 1.17 (m, 22H), 0.82 (d, J = 6.8 Hz, 3H); $^{13}C\{^1H\}$ NMR (75 MHz, DMSO-d_6) δ (ppm): 176.6, 141.1, 130.7, 130.5, 128.8, 124.9, 107.8, 75.9, 65.4, 31.1, 28.9, 28.6, 28.5, 26.8, 26.0, 21.9, 20.5, 13.7; HRMS (ESI) *m/z*: $[M+Na]^+$ calcd for $C_{24}H_{39}NNaO_3$ 412.2828; found 412.2832.

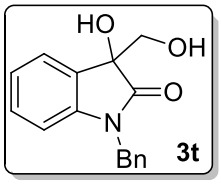


1-cyclopentyl-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3s). Colorless liquid; Yield (235 mg, 95%); The title compound is prepared according to the general procedure (A) described as above; FT-IR (KBr, cm^{-1}) 3302, 3058, 2921, 2873, 1703, 1614; ^1H NMR (400 MHz, DMSO-d_6) δ (ppm): 7.34 (d, J = 7.6 Hz, 1H), 7.30

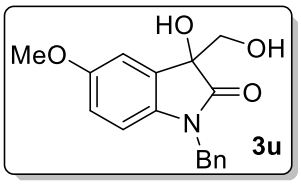


– 7.25 (m, 1H), 7.04 – 6.99 (m, 2H), 5.91 (s, 1H), 4.80 (t, *J* = 5.6 Hz, 1H), 4.63 (quint, *J* = 8.4 Hz, 1H), 3.63 (d, *J* = 5.6 Hz, 2H), 2.03 – 1.78 (m, 6H), 1.69 – 1.60 (m, 2H); $^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO-d_6) δ (ppm): 177.4, 143.3, 131.5, 129.3, 124.8, 122.0, 109.6, 76.1, 66.0, 52.1, 28.0, 27.7, 25.2, 25.2; HRMS (ESI) *m/z*: $[M+Na]^+$ calcd for $C_{14}H_{17}NNaO_3$ 270.1106; found 270.1107.

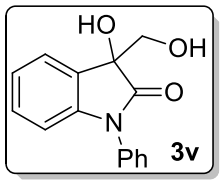
1-benzyl-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3t). White solid; Yield (256 mg, 95%); mp 123-124 °C; The title compound is prepared according to the general procedure (A) described as above; FT-IR (KBr, cm^{-1}) 3305, 3256, 3061, 2965, 1690, 1618; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 7.39 – 7.29 (m, 5H), 7.25 (t, *J* = 7.2 Hz, 1H), 7.19 (t, *J* = 7.6 Hz, 1H), 7.02 (t, *J* = 7.6 Hz, 1H), 6.76 (d, *J* = 7.6 Hz, 1H), 6.11 (s, 1H), 4.98 – 4.94 (m, 2H), 4.80 (d, *J* = 16.0 Hz, 1H), 3.80 – 3.72 (m, 2H); $^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO-d_6) δ (ppm): 177.7, 143.7, 136.7, 131.3, 129.3, 128.9, 127.7, 127.6, 124.6, 122.6, 109.2, 76.6, 65.9, 42.9; HRMS (ESI) *m/z*: $[M+Na]^+$ calcd for $C_{16}H_{15}NNaO_3$ 292.0950; found 292.0958.



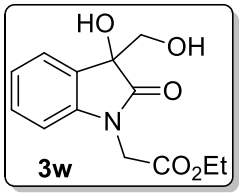
1-benzyl-3-hydroxy-3-(hydroxymethyl)-5-methoxyindolin-2-one (3u). White solid; Yield (257 mg, 86%); mp 158-159 °C; The title compound is prepared according to the general procedure (A) described as above; FT-IR (KBr, cm^{-1}) 3406, 3051, 2928, 1703, 1602, 1490; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 7.35 – 7.22 (m, 5H), 7.00 (d, *J* = 2.4 Hz, 1H), 6.75 (dd, *J* = 8.4, 2.4 Hz, 1H), 6.64 (d, *J* = 8.4 Hz, 1H), 6.11 (s, 1H), 4.96 – 4.89 (m, 2H), 4.76 (d, *J* = 16.0 Hz, 1H), 3.73 (d, *J* = 5.6 Hz, 2H), 3.70 (s, 3H); $^{13}C\{^{1}H\}$ NMR (75 MHz, DMSO-d_6) δ (ppm): 176.8, 155.4, 136.4, 136.2, 132.0, 128.3, 127.1, 127.0, 113.2, 111.6, 109.0, 76.4, 65.5, 55.5, 42.5; HRMS (ESI) *m/z*: $[M+Na]^+$ calcd for $C_{17}H_{17}NNaO_4$ 322.1055; found 322.1052.



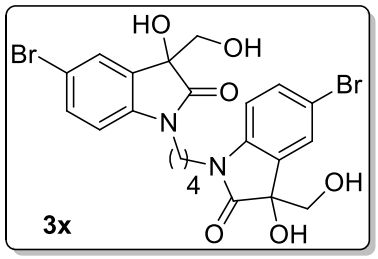
3-hydroxy-3-(hydroxymethyl)-1-phenylindolin-2-one (3v). Colorless semisolid; Yield (243 mg, 95%); The title compound is prepared according to the general procedure (A) described as above; FT-IR (KBr, cm^{-1}) 3390, 3260, 3065, 1712, 1265; ^1H NMR (400 MHz, DMSO-d_6) δ (ppm): 7.58 (t, J = 7.6 Hz, 2H), 7.46 (t, J = 7.2 Hz, 2H), 7.40 (d, J = 7.2 Hz, 2H), 7.26 (t, J = 7.6 Hz, 1H), 7.11 (t, J = 7.6 Hz, 1H), 6.73 (d, J = 8.0 Hz, 1H), 6.20 (s, 1H), 5.00 (t, J = 5.6 Hz, 1H), 3.82 – 3.74 (m, 2H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ (ppm): 177.2, 143.4, 133.8, 129.7, 129.7, 128.3, 128.3, 126.6, 124.9, 123.8, 109.8, 76.4, 66.8; HRMS (ESI) *m/z:* $[M+Na]^+$ calcd for $C_{15}H_{13}NNaO_3$ 278.0793; found 278.0789.



ethyl 2-(3-hydroxy-3-(hydroxymethyl)-2-oxoindolin-1-yl)acetate (3w). Colorless liquid; Yield (244 mg, 92%); The title compound is prepared according to the general procedure (A) described as above; FT-IR (KBr, cm^{-1}) 3432, 3059, 2951, 2257, 1735, 1645, 1492; ^1H NMR (400 MHz, DMSO-d_6) δ (ppm): 7.37 (d, J = 6.8 Hz, 1H), 7.28 (t, J = 7.6 Hz, 1H), 7.05 (t, J = 7.6 Hz, 1H), 6.93 (d, J = 7.6 Hz, 1H), 6.09 (s, 1H), 4.90 (t, J = 5.6 Hz, 1H), 4.49 (s, 2H), 4.14 (q, J = 7.2 Hz, 2H), 3.70 – 3.57 (m, 2H), 1.21 (t, J = 7.2 Hz, 3H); $^{13}C\{^1H\}$ NMR (100 MHz, DMSO-d_6) δ (ppm): 177.5, 168.3, 143.4, 130.7, 129.3, 124.9, 122.7, 108.9, 76.5, 66.0, 61.5, 41.3, 14.5; HRMS (ESI) *m/z:* $[M+Na]^+$ calcd for $C_{13}H_{15}NNaO_5$ 288.0848; found 288.0837.

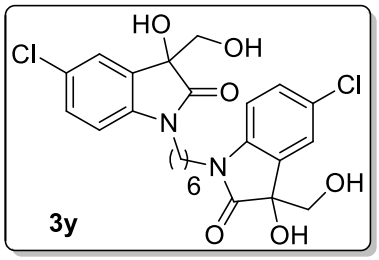


1,1'-(butane-1,4-diyl)bis(5-bromo-3-hydroxy-3-(hydroxymethyl)indolin-2-one) (3x). White solid; Yield (485 mg, 85%); mp 203-204 °C; The title compound is prepared according to the general procedure (A) described as above; FT-IR (KBr, cm^{-1}) 3401, 3249, 3081, 2954, 1712, 1623; ^1H NMR (400 MHz, DMSO-d_6) δ (ppm): 7.50 – 7.44 (m, 4H),



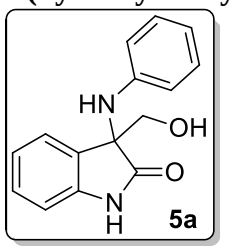
6.98 (dd, *J* = 8.0, 2.4 Hz, 2H), 6.13 (s, 2H), 4.92 (t, *J* = 5.6 Hz, 2H), 3.72 – 3.59 (m, 8H); $^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO-d_6) δ (ppm): 177.0, 143.2, 133.7, 132.0, 127.5, 114.3, 110.9, 76.5, 65.6, 39.1, 24.3; HRMS (ESI) *m/z:* $[M+H]^+$ calcd for $C_{22}H_{23}Br_2N_2O_6$ 568.9923; found 568.9913.

1,1'-(hexane-1,6-diyl)bis(5-chloro-3-hydroxy-3-(hydroxymethyl)indolin-2-one) (3y). White

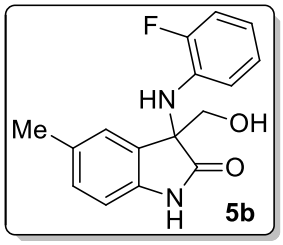


solid; Yield (438 mg, 86%); mp 168-169 °C; The title compound is prepared according to the general procedure (A) described as above; FT-IR (KBr, cm^{-1}) 3421, 3228, 3056, 2962, 1690, 1610, 1493; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 7.35 (d, *J* = 2.4 Hz, 2H), 7.31 (d, *J* = 8.4 Hz, 2H), 6.98 (d, *J* = 8.4 Hz, 2H), 6.10 (s, 2H), 4.90 (t, *J* = 5.6 Hz, 2H), 3.69 – 3.51 (m, 8H), 1.50 (s, 4H), 1.29 (s, 4H); $^{13}C\{^{1}H\}$ NMR (100 MHz, MeOD) δ (ppm): 177.6, 142.1, 131.9, 129.1, 127.8, 124.5, 109.9, 76.3, 65.4, 39.4, 26.7, 25.8; HRMS (ESI) *m/z:* $[M+Na]^+$ calcd for $C_{24}H_{26}Cl_2N_2NaO_6$ 531.1066; found 531.1045.

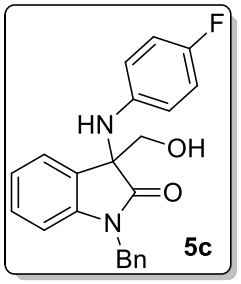
3-(hydroxymethyl)-3-(phenylamino)indolin-2-one (5a). White crystalline solid; Yield (241



mg, 95%); mp 171-172 °C; The title compound is prepared according to the general procedure (B) described as above; FT-IR (KBr, cm^{-1}) 3421, 3321, 3280, 3068, 2911, 1710, 1680; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 10.56 (s, 1H), 7.21 (td, *J* = 7.6, 1.2 Hz, 1H), 7.14 (d, *J* = 7.6 Hz, 1H), 6.95 – 6.86 (m, 4H), 6.46 (t, *J* = 7.6 Hz, 1H), 6.20 (d, *J* = 8.8 Hz, 2H), 6.06 (s, 1H), 5.17 (t, *J* = 6.0 Hz, 1H), 3.73 – 3.62 (m, 2H); $^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO-d_6) δ (ppm): 178.4, 146.8, 142.4, 130.1, 129.1, 129.0, 124.4, 122.0, 117.1, 113.6, 110.1, 67.8, 66.1; HRMS (ESI) *m/z:* $[M+Na]^+$ calcd for $C_{15}H_{14}N_2NaO_2$ 277.0953; found 277.0952.

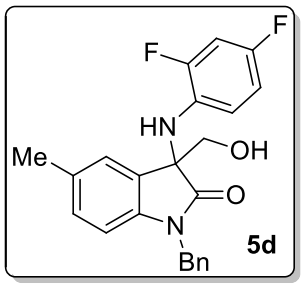
3-((2-fluorophenyl)amino)-3-(hydroxymethyl)-5-methylindolin-2-one (5b). Off white solid; 

Yield (249 mg, 87%); mp 181-182 °C; The title compound is prepared according to the general procedure (B) described as above; FT-IR (KBr, cm^{-1}) 3392, 3354, 3250, 3080, 1706, 1673; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 10.58 (s, 1H), 7.06 – 7.01 (m, 3H), 6.81 (d, J = 7.6 Hz, 1H), 6.68 (t, J = 7.6 Hz, 1H), 6.53 (dd, J = 12.4, 6.8 Hz, 1H), 5.82 (t, J = 8.0 Hz, 1H), 5.66 (s, 1H), 5.46 (t, J = 6.0 Hz, 1H), 3.75 – 3.58 (m, 2H), 2.21 (s, 3H); $^{13}C\{^{1}H\}$ NMR (125 MHz, DMSO-d_6) δ (ppm): 177.6, 151.6 (d, $^{1}J_{C\text{-}F}$ = 238 Hz), 150.6, 139.5, 134.6 (d, $^{3}J_{C\text{-}F}$ = 11.2 Hz), 131.0, 129.5 (d, $^{2}J_{C\text{-}F}$ = 28.2 Hz), 125.1, 124.9 (d, $^{4}J_{C\text{-}F}$ = 1.25 Hz), 117.4 (d, $^{3}J_{C\text{-}F}$ = 7.5 Hz), 114.9 (d, $^{2}J_{C\text{-}F}$ = 18.8 Hz), 113.3, 110.2, 67.7, 65.7, 21.1; HRMS (ESI) *m/z:* $[M+Na]^{+}$ calcd for $C_{16}H_{15}FN_2NaO_2$ 309.1015; found 309.1006.

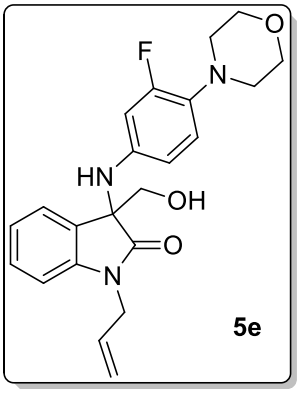
1-benzyl-3-((4-fluorophenyl)amino)-3-(hydroxymethyl)indolin-2-one (5c). Colorless 

semisolid; Yield (340 mg, 94%); The title compound is prepared according to the general procedure (B) described as above; FT-IR (KBr, cm^{-1}) 3371, 3356, 3091, 1701, 1612; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 7.40 – 7.27 (m, 5H), 7.25 – 7.21 (m, 2H), 7.00 (t, J = 7.6 Hz, 1H), 6.95 (d, J = 7.6 Hz, 1H), 6.67 (t, J = 8.8 Hz, 2H), 6.17 (s, 1H), 6.15 – 6.12 (m, 2H), 5.30 (t, J = 5.6 Hz, 1H), 5.00 – 4.91 (m, 2H), 3.85 – 3.75 (m, 2H); $^{13}C\{^{1}H\}$ NMR (125 MHz, DMSO-d_6) δ (ppm): 177.0, 155.4 (d, $^{1}J_{C\text{-}F}$ = 231.2 Hz), 143.1, 143.0, 136.7, 129.3, 129.2, 129.1, 128.0, 127.9, 124.1, 123.0, 115.4 (d, $^{2}J_{C\text{-}F}$ = 22.4 Hz), 115.3 (d, $^{3}J_{C\text{-}F}$ = 7.8 Hz), 109.7, 67.7, 66.4, 43.5; HRMS (ESI) *m/z:* $[M+H]^{+}$ calcd for $C_{22}H_{20}FN_2O_2$ 363.1509; found 363.1507.

1-benzyl-3-((2,4-difluorophenyl)amino)-3-(hydroxymethyl)-5-methylindolin-2-one (5d). Off white solid; Yield (355 mg, 90%); mp 120-121 °C; The title compound is prepared according to the general procedure (B) described as above; FT-IR (KBr, cm^{-1}) 3421, 3381, 3341, 3068, 2910, 1686, 1619; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.22 – 7.18 (m, 3H), 7.17 – 7.11 (m, 2H), 7.09 – 7.06 (m, 1H), 7.01 – 6.97 (m, 1H), 6.72 – 6.63 (m, 2H), 6.23 – 6.16 (m, 1H), 5.67 – 5.61 (m, 1H), 5.01 (d, J = 15.6 Hz, 1H), 4.64 (d, J = 15.6 Hz, 1H), 3.86 (d, J = 11.6 Hz, 1H), 3.65 (d, J = 11.6 Hz, 1H), 2.20 (s, 3H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ (ppm): 177.4, 155.5 (dd, $^{1}J_{C\text{-}F}$ = 238 Hz, $^{3}J_{C\text{-}F}$ = 11.1 Hz), 152.1 (dd, $^{1}J_{C\text{-}F}$ = 242 Hz, $^{3}J_{C\text{-}F}$ = 11.1 Hz), 139.5, 135.4, 133.5, 130.5 (dd, $^{2}J_{C\text{-}F}$ = 11.4 Hz, $^{4}J_{C\text{-}F}$ = 3.1 Hz), 130.2, 128.8, 128.0, 127.7, 127.2, 124.8, 115.1 (dd, $^{3}J_{C\text{-}F}$ = 8.8 Hz, $^{3}J_{C\text{-}F}$ = 3.5 Hz), 110.4 (dd, $^{2}J_{C\text{-}F}$ = 21.5 Hz, $^{4}J_{C\text{-}F}$ = 3.8 Hz), 110.0, 103.7 (dd, $^{2}J_{C\text{-}F}$ = 23.2 Hz, $^{2}J_{C\text{-}F}$ = 26.4 Hz), 67.9, 64.9, 44.2, 21.1; HRMS (ESI) *m/z:* $[M+Na]^{+}$ calcd for $C_{23}H_{20}F_2N_2NaO_2$ 417.1391; found 417.1387.

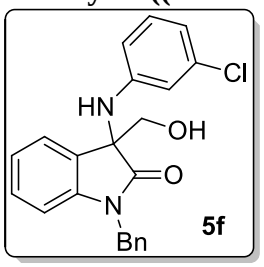


1-allyl-3-((3-fluoro-4-morpholinophenyl)amino)-3-(hydroxymethyl)indolin-2-one (5e). Off white solid; Yield (373 mg, 94%); mp 105-106 °C; The title compound is prepared according to the general procedure (B) described as above; FT-IR (KBr, cm^{-1}) 3336, 3312, 3091, 2833, 1707, 1703, 1507; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 7.30 (td, J = 7.6, 1.2 Hz, 1H), 7.23 (d, J = 7.6 Hz, 1H), 7.05 – 6.99 (m, 2H), 6.66 – 6.58 (m, 1H), 6.19 (s, 1H), 5.98 (dd, J = 15.2, 2.4 Hz, 1H), 5.89 (dd, J = 8.4, 2.4 Hz, 1H), 5.87 – 5.77 (m, 1H), 5.30 (dd, J = 17.2, 1.6 Hz, 1H), 5.21 (t, J = 5.6 Hz, 1H), 5.18 (dd, J = 10.4, 1.6 Hz, 1H), 4.42 – 4.29 (m, 2H), 3.76 – 3.68 (m, 2H), 3.63 (t, J = 4.4 Hz, 4H), 2.73 (t, J = 4.4 Hz, 4H); $^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO-d_6) δ (ppm): 176.4, 156.2 (d, $^{1}J_{C\text{-}F}$ = 240.0 Hz), 143.2, 143.1 (d, $^{3}J_{C\text{-}F}$ = 4.2 Hz), 132.2,

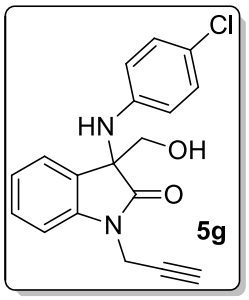


130.6 (d, $^{2}J_{C\text{-}F}$ = 9.5 Hz), 129.3 (d, $^{2}J_{C\text{-}F}$ = 11.6 Hz), 124.1, 122.8, 120.6 (d, $^{3}J_{C\text{-}F}$ = 4.2 Hz), 117.7, 109.7, 109.6 (d, $^{4}J_{C\text{-}F}$ = 1.8 Hz), 102.5, 102.2, 67.6, 66.8, 66.2, 51.8, 42.2; HRMS (ESI) *m/z:* $[M+H]^+$ calcd for $C_{22}H_{25}FN_3O_3$ 398.1880; found 398.1880.

1-benzyl-3-((3-chlorophenyl)amino)-3-(hydroxymethyl)indolin-2-one (5f). Pale yellow liquid; Yield (355 mg, 94%); The title compound is prepared according to the general procedure (B) described as above; FT-IR (KBr, cm^{-1}) 3376, 3345, 3068, 2910, 1708, 1613, 1596; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 7.41 (d, J = 7.2 Hz, 2H), 7.35 –7.23 (m, 5H), 7.01 (t, J = 7.2 Hz, 1H), 6.95 (d, J = 8.0 Hz, 1H), 6.82 (t, J = 8.0 Hz, 1H), 6.60 (s, 1H), 6.50 (dd, J = 8.0, 1.2 Hz, 1H), 6.23 (s, 1H), 6.06 (dd, J = 8.0, 1.6 Hz, 1H), 5.34 (t, J = 5.6 Hz, 1H), 5.02 – 4.93 (m, 2H), 3.85 – 3.76 (m, 2H); ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ (ppm): 176.5, 148.1, 143.1, 136.7, 133.8, 130.6, 129.3, 129.1, 128.9, 127.9, 124.1, 123.1, 116.9, 113.3, 112.4, 109.8, 67.7, 66.0, 43.6; HRMS (ESI) *m/z:* $[M+H]^+$ calcd for $C_{22}H_{20}ClN_2O_2$ 379.1213; found 379.1200.

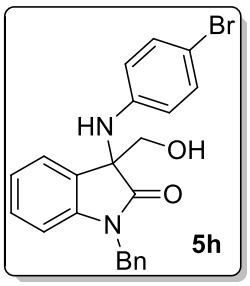


3-((4-chlorophenyl)amino)-3-(hydroxymethyl)-1-(prop-2-yn-1-yl)indolin-2-one (5g). Pale yellow liquid; Yield (310 mg, 95%); The title compound is prepared according to the general procedure (B) described as above; FT-IR (KBr, cm^{-1}) 3394, 3341, 3065, 2965, 2934, 2135, 1706, 1610; ^{1}H NMR (400 MHz, $CDCL_3$+DMSO-d_6) δ (ppm): 7.34 (t, J = 7.6 Hz, 1H), 7.25 (d, J = 7.2 Hz, 1H), 7.14 (d, J = 7.6 Hz, 1H), 7.05 (t, J = 7.6 Hz, 1H), 6.84 (d, J = 8.8 Hz, 2H), 6.21 (s, 1H), 6.14 (d, J = 8.8 Hz, 2H), 5.23 (t, J = 6.0 Hz, 1H), 4.69 (dd, J = 17.6, 2.4 Hz, 1H), 4.47 (dd, J = 17.6, 2.4 Hz, 1H), 3.79 – 3.67 (m, 2H), 2.99 (s, 1H); ^{13}C{^{1}H} NMR (125 MHz, DMSO-d_6) δ (ppm): 175.9, 145.0, 141.7, 129.1, 128.8, 128.6, 124.2, 123.2, 121.3, 115.3, 109.8, 77.6, 73.9,

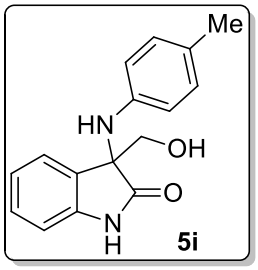


67.4, 65.9, 29.4; HRMS (ESI) *m/z:* $[M+Na]^+$ calcd for $C_{18}H_{15}ClN_2NaO_2$ 349.0720; found 349.0728.

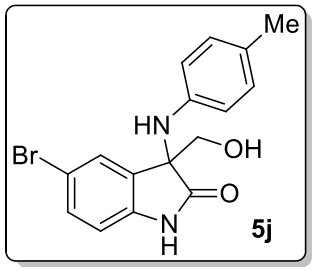
1-benzyl-3-((4-bromophenyl)amino)-3-(hydroxymethyl)indolin-2-one (5h). Brown crystalline solid; Yield (394 mg, 93%); mp 140-141 °C; The title compound is prepared according to the general procedure (B) described as above; FT-IR (KBr, cm^{-1}) 3374, 3560, 3392, 2916, 1702, 1614; ^1H NMR (400 MHz, DMSO-d_6) δ (ppm): 7.41 (d, J = 8.4 Hz, 2H), 7.37 – 7.32 (m, 2H), 7.32 – 7.27 (m, 1H), 7.26 – 7.21 (m, 2H), 7.03 – 6.94 (m, 4H), 6.46 (s, 1H), 6.08 (d, J = 9.2 Hz, 2H), 5.31 (t, J = 5.6 Hz, 1H), 5.01 – 4.91 (m, 2H), 3.84 – 3.75 (m, 2H); $^{13}C\{^1H\}$ NMR (100 MHz, DMSO-d_6) δ (ppm): 176.6, 145.9, 143.1, 136.8, 131.6, 129.2, 129.0, 128.1, 127.9, 124.1, 122.9, 115.9, 109.8, 108.3, 67.7, 66.0, 43.6; HRMS (ESI) *m/z:* $[M+H]^+$ calcd for $C_{22}H_{20}BrN_2O_2$ 423.0708; found 423.0706.



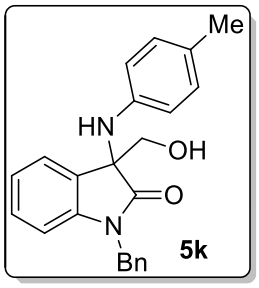
3-(hydroxymethyl)-3-(*p*-tolylamino)indolin-2-one (5i). colorless semi solid; Yield (242 mg, 90%); The title compound is prepared according to the general procedure (B) described as above; FT-IR (KBr, cm^{-1}) 3415, 3335, 3291, 2930, 1720, 1699, 1616; ^1H NMR (400 MHz, DMSO-d_6) δ (ppm): 10.52 (s, 1H), 7.20 (t, J = 7.6 Hz, 1H), 7.13 (d, J = 7.2 Hz, 1H), 6.92 (t, J = 7.2 Hz, 1H), 6.87 (d, J = 7.6 Hz, 1H), 6.70 (d, J = 8.0 Hz, 2H), 6.12 (d, J = 8.0 Hz, 2H), 5.83 (s, 1H), 5.15 (t, J = 6.0 Hz, 1H), 3.71 – 3.61 (m, 2H), 2.04 (s, 3H); $^{13}C\{^1H\}$ NMR (100 MHz, DMSO-d_6) δ (ppm): 178.6, 144.4, 142.4, 130.3, 129.5, 128.9, 125.6, 124.4, 122.0, 114.0, 110.0, 67.8, 66.3, 20.4; HRMS (ESI) *m/z:* $[M+H]^+$ calcd for $C_{16}H_{17}N_2O_2$ 269.1290; found 269.1292.

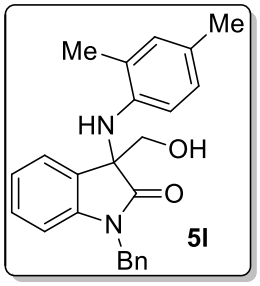


5-bromo-3-(hydroxymethyl)-3-(*p*-tolylamino)indolin-2-one (5j). Off white solid; Yield (305 mg, 88%); mp 172-173 °C; The title compound is prepared according to the general procedure (B) described as above; FT-IR (KBr, cm^{-1}) 3391, 3315, 3286, 3081, 2925, 1720, 1698, 1612; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 10.68 (s, 1H), 7.39 (dd, J = 8.0, 2.4 Hz, 1H), 7.24 (d, J = 1.6 Hz, 1H), 6.84 (d, J = 8.0 Hz, 1H), 6.74 (d, J = 8.0 Hz, 2H), 6.12 (d, J = 8.4 Hz, 2H), 5.92 (s, 1H), 5.24 (t, J = 6.0 Hz, 1H), 3.75 – 3.62 (m, 2H), 2.06 (s, 3H); $^{13}C\{^{1}H\}$ NMR (125 MHz, DMSO-d_6) δ (ppm): 178.1, 144.1, 141.9, 133.0, 131.7, 129.7, 127.0, 125.9, 113.9, 113.9, 112.0, 67.6, 66.5, 20.4; HRMS (ESI) *m/z:* $[M+H]^+$ calcd for $C_{16}H_{16}BrN_2O_2$ 347.0395; found 347.0382.

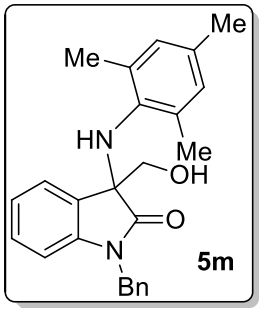


1-benzyl-3-(hydroxymethyl)-3-(*p*-tolylamino)indolin-2-one (5k). White crystalline solid; Yield (341 mg, 95%); mp 141-142 °C; The title compound is prepared according to the general procedure (B) described as above; FT-IR (KBr, cm^{-1}) 3391, 3311, 3092, 2920, 1703, 1614; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 7.39 (d, J = 7.2 Hz, 2H), 7.36 – 7.27 (m, 3H), 7.22 – 7.19 (m, 2H), 6.98 (t, J = 7.6 Hz, 1H), 6.92 (d, J = 7.6 Hz, 1H), 6.64 (d, J = 8.0 Hz, 2H), 6.06 (d, J = 8.0 Hz, 2H), 5.97 (s, 1H), 5.26 (t, J = 5.6 Hz, 1H), 5.00 – 4.89 (m, 2H), 3.81 – 3.73 (m, 2H), 2.05 (s, 3H); $^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO-d_6) δ (ppm): 177.1, 144.2, 143.2, 136.9, 129.8, 129.5, 128.9, 128.0, 127.9, 126.0, 124.1, 122.8, 114.4, 109.6, 67.8, 66.3, 43.5, 20.4; HRMS (ESI) *m/z:* $[M+H]^+$ calcd for $C_{23}H_{23}N_2O_2$ 359.1760; found 359.1760.



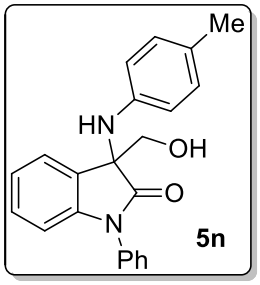
1-benzyl-3-((2,4-dimethylphenyl)amino)-3-(hydroxymethyl)indolin-2-one (5l). White solid; 

Yield (357 mg, 96%); mp 160-161 °C; The title compound is prepared according to the general procedure (B) described as above; FT-IR (KBr, cm^{-1}) 3375, 3325, 3067, 2916, 1691, 1614; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 7.40 – 7.29 (m, 5H), 7.24 – 7.17 (m, 2H), 6.99 – 6.94 (m, 2H), 6.79 (s, 1H), 6.31 (d, J = 8.0 Hz, 1H), 5.55 (t, J = 6.0 Hz, 1H), 5.44 (d, J = 8.4 Hz, 1H), 5.03 – 4.89 (m, 3H), 3.82 – 3.68 (m, 2H), 2.19 (s, 3H), 2.04 (s, 3H); $^{13}C\{^{1}H\}$ NMR (125 MHz, DMSO-d_6) δ (ppm): 176.8, 142.7, 141.7, 136.8, 131.3, 129.5, 129.0, 129.0, 128.1, 127.9, 126.9, 126.4, 124.2, 123.7, 122.8, 112.3, 109.7, 68.0, 66.1, 43.5, 20.4, 18.1; HRMS (ESI) *m/z:* $[M+H]^+$ calcd for $C_{24}H_{25}N_2O_2$ 373.1916; found 373.1907.

1-benzyl-3-(hydroxymethyl)-3-(mesitylamino)indolin-2-one (5m). Pale yellow solid; Yield 

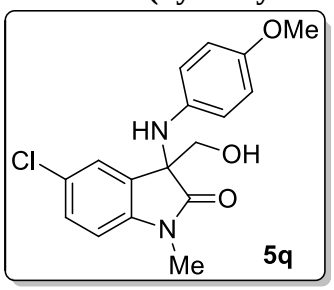
(371 mg, 96%); mp 122-123 °C; The title compound is prepared according to the general procedure (B) described as above; FT-IR (KBr, cm^{-1}) 3362, 3311, 3061, 2912, 1701, 1614, 1484; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 7.30 – 7.22 (m, 5H), 7.09 (td, J = 7.6, 1.2 Hz, 1H), 6.83 – 6.73 (m, 3H), 6.61 (s, 2H), 5.41 (t, J = 5.6 Hz, 1H), 4.89 (d, J = 15.6 Hz, 1H), 4.79 (d, J = 15.6 Hz, 1H), 4.20 (s, 1H), 3.87 – 3.78 (m, 2H), 2.09 (s, 3H), 1.94 (s, 6H); $^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO-d_6) δ (ppm): 176.4, 155.9, 141.7, 136.8, 135.9, 131.3, 131.0, 129.0, 128.1, 127.9, 126.9, 126.5, 123.7, 112.3, 110.2, 68.0, 66.3, 43.5, 20.4, 18.0; HRMS (ESI) *m/z:* $[M+H]^+$ calcd for $C_{25}H_{27}N_2O_2$ 387.2073; found 387.2066.

3-(hydroxymethyl)-1-phenyl-3-(*p*-tolylamino)indolin-2-one (5n). colorless semisolid, Yield



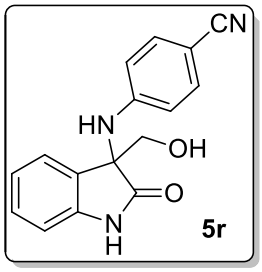
(327 mg); The title compound is prepared according to the general procedure (B) described as above; FT-IR (KBr, cm^{-1}) 3392, 3316, 3069, 2918, 1713, 1604; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.43 (t, J = 7.6 Hz, 2H), 7.36 – 7.31 (m, 2H), 7.28 – 7.20 (m, 3H), 7.06 (t, J = 7.6 Hz, 1H), 6.82 (d, J = 7.6 Hz, 1H), 6.75 (d, J = 8.4 Hz, 2H), 6.24 (d, J = 8.8 Hz, 2H), 3.90 (d, J = 11.6 Hz, 1H), 3.74 (d, J = 11.6 Hz, 1H), 3.09 (s, 1H), 2.08 (s, 3H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ (ppm): 177.8, 143.3, 142.9, 134.1, 129.8, 129.7, 129.5, 128.8, 128.5, 127.9, 126.5, 124.5, 123.9, 115.6, 110.1, 67.9, 65.5, 20.5; HRMS (ESI) *m/z:* $[M+Na]^+$ calcd for $C_{22}H_{20}N_2NaO_2$ 367.1422; found 367.1419.

5-chloro-3-(hydroxymethyl)-3-((4-methoxyphenyl)amino)-1-methylindolin-2-one (5q).

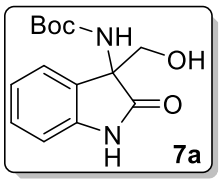


White solid; Yield (305 mg, 92%); mp 119-120 °C; The title compound is prepared according to the general procedure (B) described as above; FT-IR (KBr, cm^{-1}) 3350, 3319, 3012, 1725, 1689, 1609; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 7.37 (dd, J = 8.0, 2.4 Hz, 1H), 7.21 (d, J = 2.4 Hz, 1H), 7.09 (d, J = 8.4 Hz, 1H), 6.54 (d, J = 8.8 Hz, 2H), 6.11 (d, J = 9.2 Hz, 2H), 5.79 (s, 1H), 5.22 (t, J = 5.6 Hz, 1H), 3.77 – 3.66 (m, 2H), 3.55 (s, 3H), 3.18 (s, 3H); $^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO-d_6) δ (ppm): 176.7, 152.0, 143.2, 140.2, 132.1, 128.9, 126.9, 124.1, 115.3, 114.8, 110.4, 67.5, 66.7, 55.5, 26.8; HRMS (ESI) *m/z:* $[M+H]^+$ calcd for $C_{17}H_{18}ClN_2O_3$ 333.1006; found 333.1009.

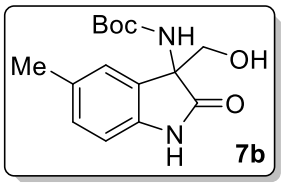
4-((3-(hydroxymethyl)-2-oxoindolin-3-yl)amino)benzonitrile (5r). White solid; Yield (251 mg, 90%); mp 121-122 °C; The title compound is prepared according to the general procedure (B) described as above; FT-IR (KBr, cm^{-1}) 3382, 3319, 3053, 2923, 2242, 1710, 1689, 1602; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 10.76 (s, 1H), 7.38 (d, J = 8.8 Hz, 2H), 7.29 (t, J = 7.6 Hz, 1H), 7.20 (d, J = 7.2 Hz, 1H), 7.17 (s, 1H), 7.02 – 6.95 (m, 2H), 6.31 (d, J = 8.8 Hz, 2H), 5.32 (t, J = 6.0 Hz, 1H), 3.83 – 3.70 (m, 2H); $^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO-d_6) δ (ppm): 178.5, 144.4, 142.4, 130.3, 129.5, 128.9, 125.6, 124.4, 121.9, 113.9, 110.0, 67.8, 66.3, 20.4; HRMS (ESI) *m/z:* $[M+Na]^+$ calcd for $C_{16}H_{13}N_3NaO_2$ 302.0905; found 302.0903.



***tert*-butyl (3-(hydroxymethyl)-2-oxoindolin-3-yl)carbamate (7a).** Colorless solid; Yield (120 mg, 86%); mp 185-186 °C; The title compound is prepared according to the general procedure (C) described as above; FT-IR (KBr, cm^{-1}) 3645, 3418, 2979, 1712, 1623, 1255, 1166, 1077; ^{1}H NMR (400 MHz, MeOD) δ (ppm): 10.06 (s, 1H), 7.17 – 7.11 (m, 2H), 6.93 (t, J = 7.6 Hz, 1H), 6.79 (d, J = 7.6 Hz, 1H), 5.42 (s, 1H), 3.67 – 3.53 (m, 2H), 1.13 (s, 9H).; $^{13}C\{^{1}H\}$ NMR (100 MHz, MeOD) δ (ppm): 178.8, 155.0, 141.8, 130.3, 128.5, 122.9, 122.1, 109.7, 80.3, 65.3, 63.9, 27.0.

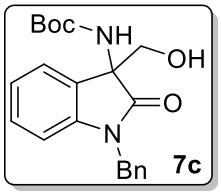


***tert*-butyl (3-(hydroxymethyl)-5-methyl-2-oxoindolin-3-yl)carbamate (7b).** Colorless semisolid; Yield (127 mg, 87%); The title compound is prepared according to the general procedure (C) described as above; FT-IR (KBr, cm^{-1}) 3644, 3402, 2981, 1711, 1613, 1251, 1156, 1076; ^{1}H NMR (400 MHz, MeOD) δ (ppm): 10.08 (s, 1H), 7.11 (s, 1H), 7.07 (d, J = 7.6 Hz, 1H), 6.80 (d, J = 7.6 Hz, 1H), 5.51 (s, 1H), 3.82 – 3.64 (m, 2H), 2.32 (s, 3H), 1.27 (s, 9H).; $^{13}C\{^{1}H\}$ NMR (100 MHz,



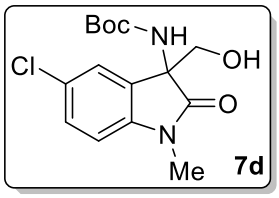
MeOD) δ (ppm): 178.7, 155.0, 139.3, 131.7, 130.4, 128.8, 123.7, 109.5, 80.1, 65.4, 63.9, 27.1, 19.9.

***tert*-butyl (1-benzyl-3-(hydroxymethyl)-2-oxoindolin-3-yl)carbamate (7c).**[7] Colorless



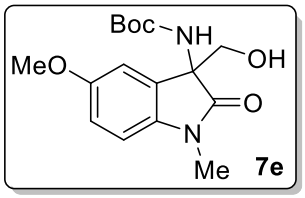
semisolid; Yield (175 mg, 95%); The title compound is prepared according to the general procedure (C) described as above; FT-IR (KBr, cm^{-1}) 3433, 2256, 1654, 1648, 1166, 1048, 1025; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 7.51 (s, 1H), 7.43 (d, J = 7.2 Hz, 2H), 7.31 – 7.20 (m, 4H), 7.15 (s, 1H), 6.99 (s, 1H), 6.69 (s, 1H), 5.29 – 4.45 (m, 3H), 3.76 – 3.61 (m, 2H), 1.31 (s, 6H), 0.95 (s, 3H); $^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO-d_6) δ (ppm): 176.0, 154.2, 143.7, 136.9, 130.7, 128.8, 128.5, 127.6, 127.5, 123.0, 122.3, 108.8, 79.1, 65.8, 63.5, 43.3, 28.5.

***tert*-butyl (5-chloro-3-(hydroxymethyl)-1-methyl-2-oxoindolin-3-yl)carbamate (7d).**[7]



Colorless semisolid; Yield (152 mg, 93%); The title compound is prepared according to the general procedure (C) described as above; FT-IR (KBr, cm^{-1}) 3432, 2256, 1654, 1647, 1165, 1047, 1025; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 7.54 (s, 1H), 7.37 (d, J = 7.6 Hz, 1H), 7.25 (s, 1H), 7.02 (d, J = 8.4 Hz, 1H), 5.12 (s, 1H), 3.75 – 3.54 (m, 2H), 3.15 (s, 3H), 1.32 (s, 6H), 1.04 (s, 3H); $^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO-d_6) δ (ppm): 175.5, 154.1, 143.6, 132.8, 128.4, 126.3, 123.1, 109.7, 79.2, 65.4, 63.6, 28.4, 26.7.

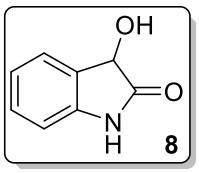
***tert*-butyl (3-(hydroxymethyl)-5-methoxy-1-methyl-2-oxoindolin-3-yl)carbamate (7e).**[7]



White solid; mp 174 – 175 °C; Yield (146 mg, 91%); The title compound is prepared according to the general procedure (C) described

as above; FT-IR (KBr, cm^{-1}) 3434, 2256, 1647, 1654, 1165, 1047, 1025; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 7.39 (s, 1H), 6.92 – 6.82 (m, 3H), 5.03 (s, 1H), 3.77 (s, 3H), 3.70 – 3.50 (m, 2H), 3.12 (s, 3H), 1.32 (s, 6H), 1.03 (s, 3H); $^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO-d_6) δ (ppm): 175.4, 155.6, 154.1, 138.1, 131.9, 112.5, 110.7, 108.5, 78.9, 65.6, 63.8, 55.9, 28.4, 26.6.

3-hydroxyindolin-2-one (**8**).[8] White solid; Yield (144 mg, 97%); mp 165-166 °C; The title compound is prepared according to the procedure (C) described as above; FT-IR (KBr, cm^{-1}) 3440, 3350, 3051, 2923, 1710, 1635, 1480; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 10.27 (s, 1H), 7.33 (d, J = 7.2 Hz, 1H), 7.26 (t, J = 7.6 Hz, 1H), 7.01 (t, J = 7.6 Hz, 1H), 6.84 (d, J = 7.6 Hz, 1H), 6.21 (d, J = 7.6 Hz, 1H), 4.88 (d, J = 7.6 Hz, 1H); $^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO-d_6) δ (ppm): 178.6, 142.3, 129.6, 129.5, 125.3, 122.3, 110.2, 69.6.



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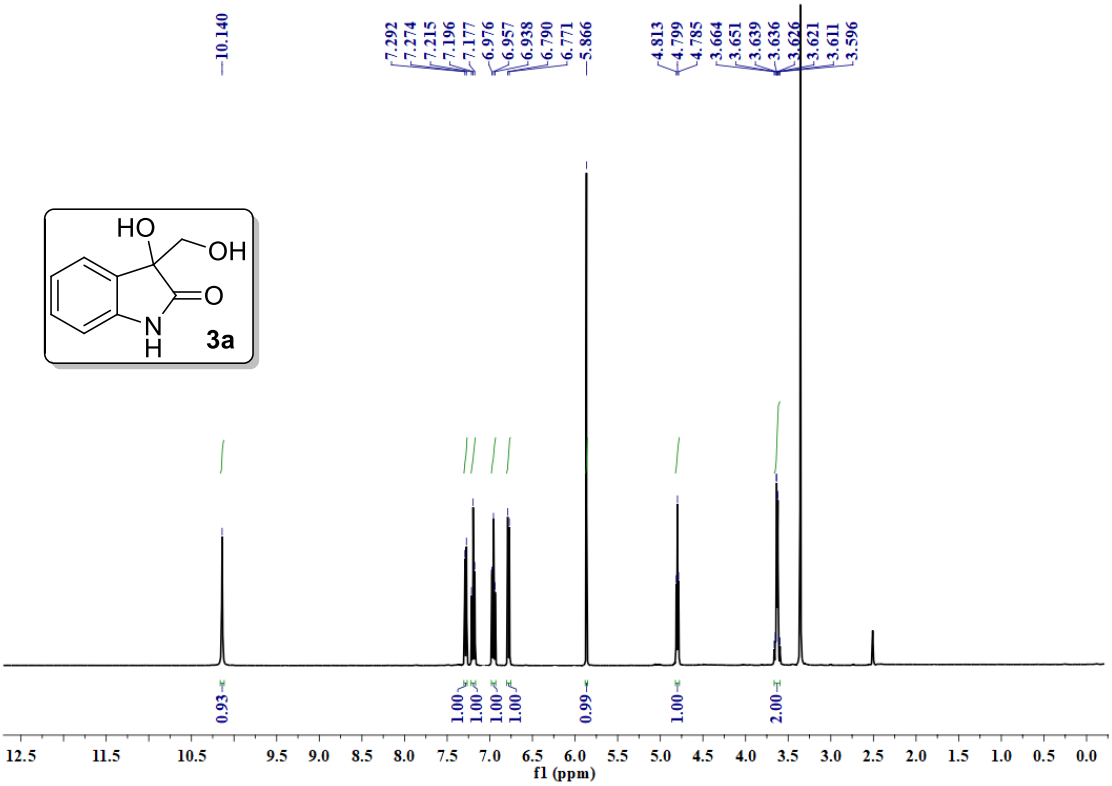
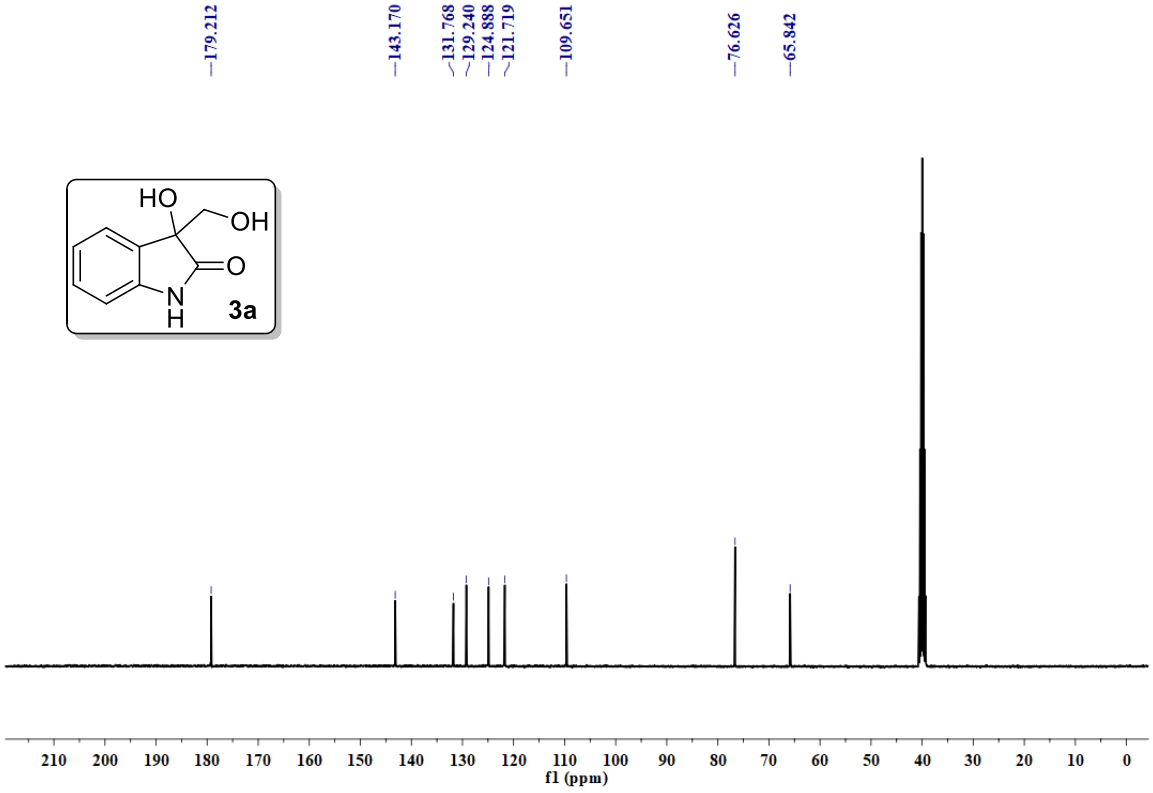
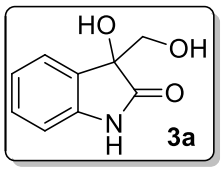
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 3-hydroxy-3-(hydroxymethyl)indolin-2-one (3a)

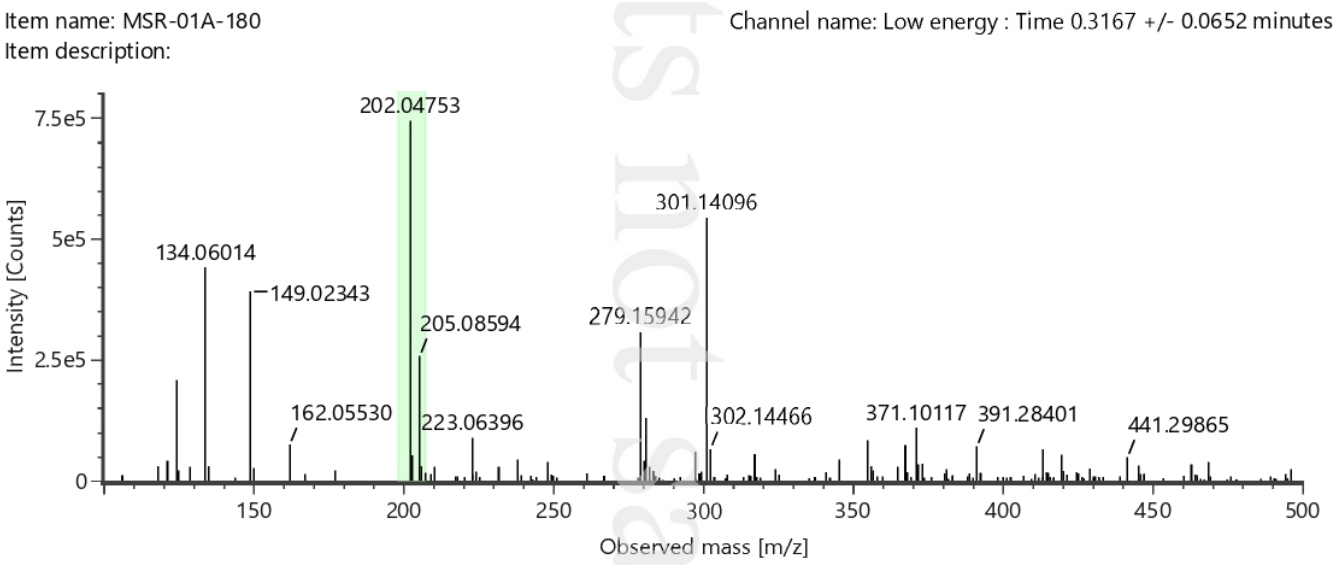


^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of 3-hydroxy-3-(hydroxymethyl)indolin-2-one (3a)

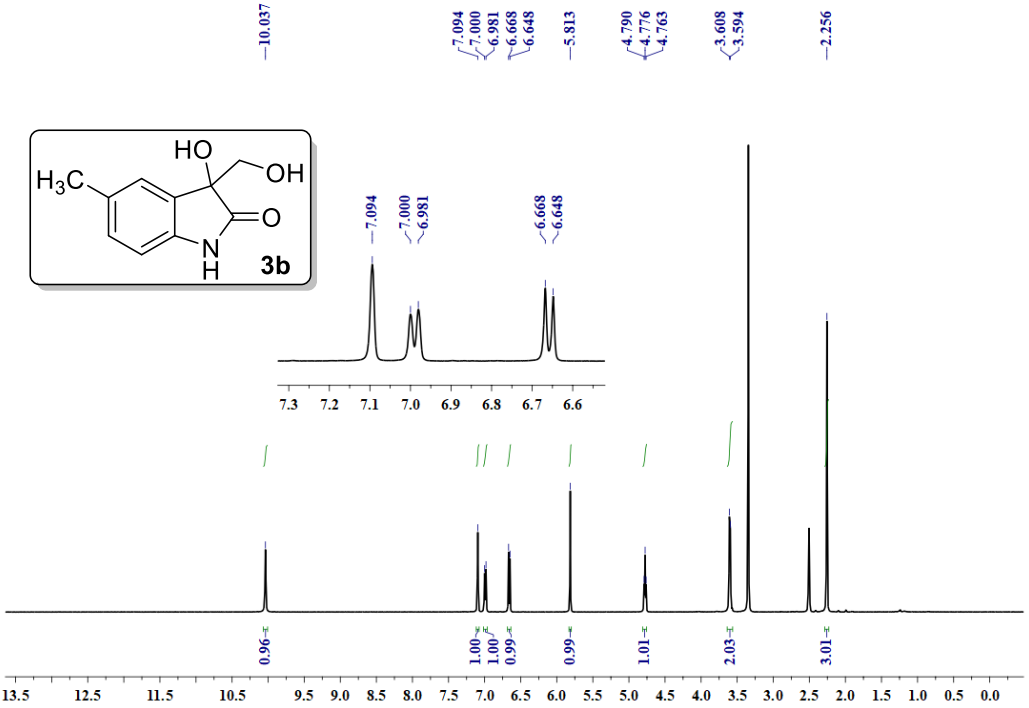


HRMS of 3-hydroxy-3-(hydroxymethyl)indolin-2-one (3a)

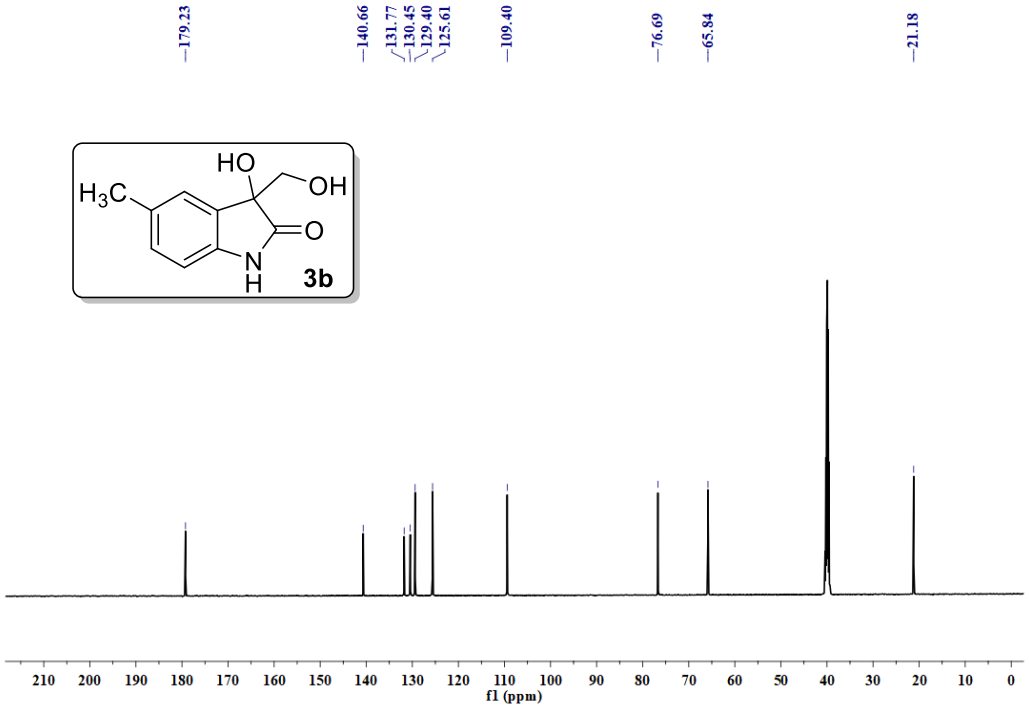




^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 3-hydroxy-3-(hydroxymethyl)-5-methylindolin-2-one (3b)

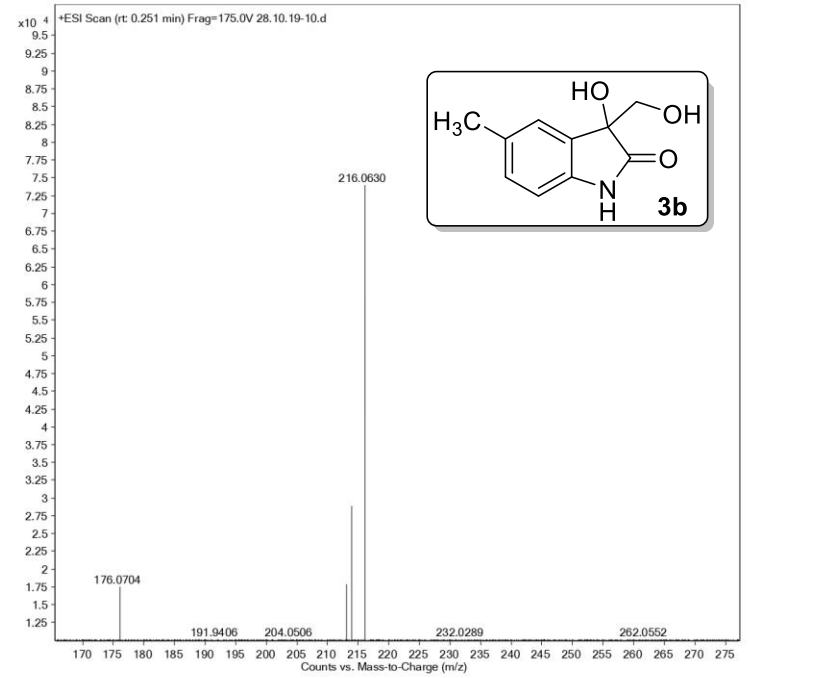


^{13}C{^{1}H} NMR (125 MHz, DMSO-d_6) spectrum of 3-hydroxy-3-(hydroxymethyl)-5-methylindolin-2-one (3b)

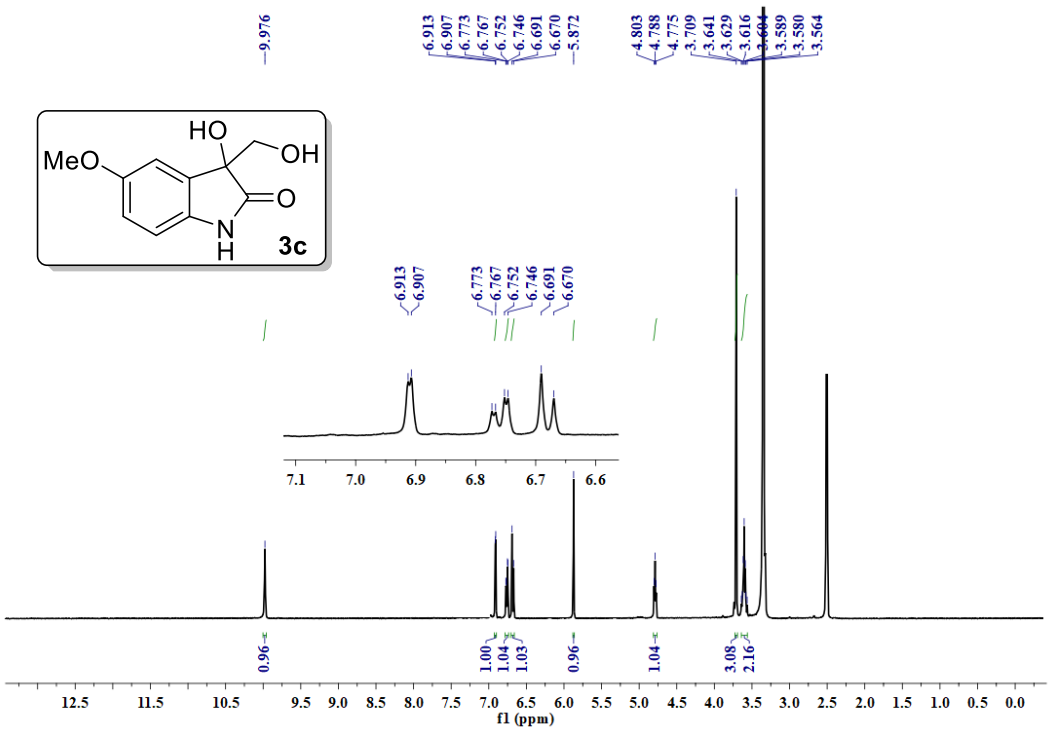


HRMS of 3-hydroxy-3-(hydroxymethyl)-5-methylindolin-2-one (3b)

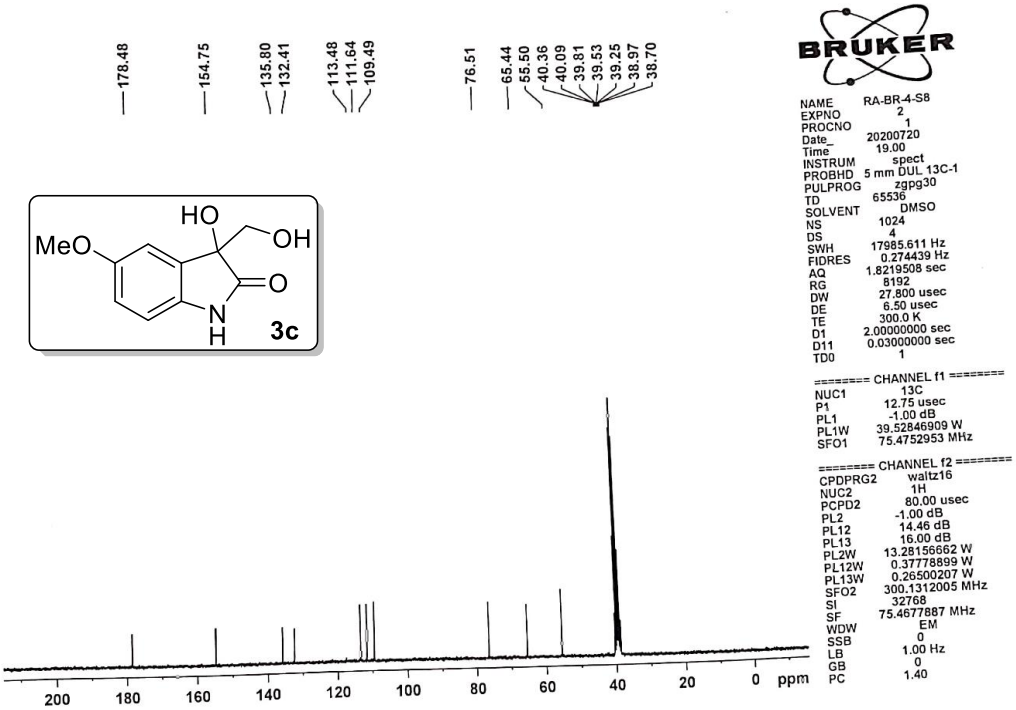
Sample Name	gsp 9	**Position**	P1-B1	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	2	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	28.10.19-10.d
ACQ Method	srinu.m	**Comment**		**Acquired Time**	28-Oct-19 3:03:36 PM



^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 3-hydroxy-3-(hydroxymethyl)-5-methoxyindolin-2-one (3c)

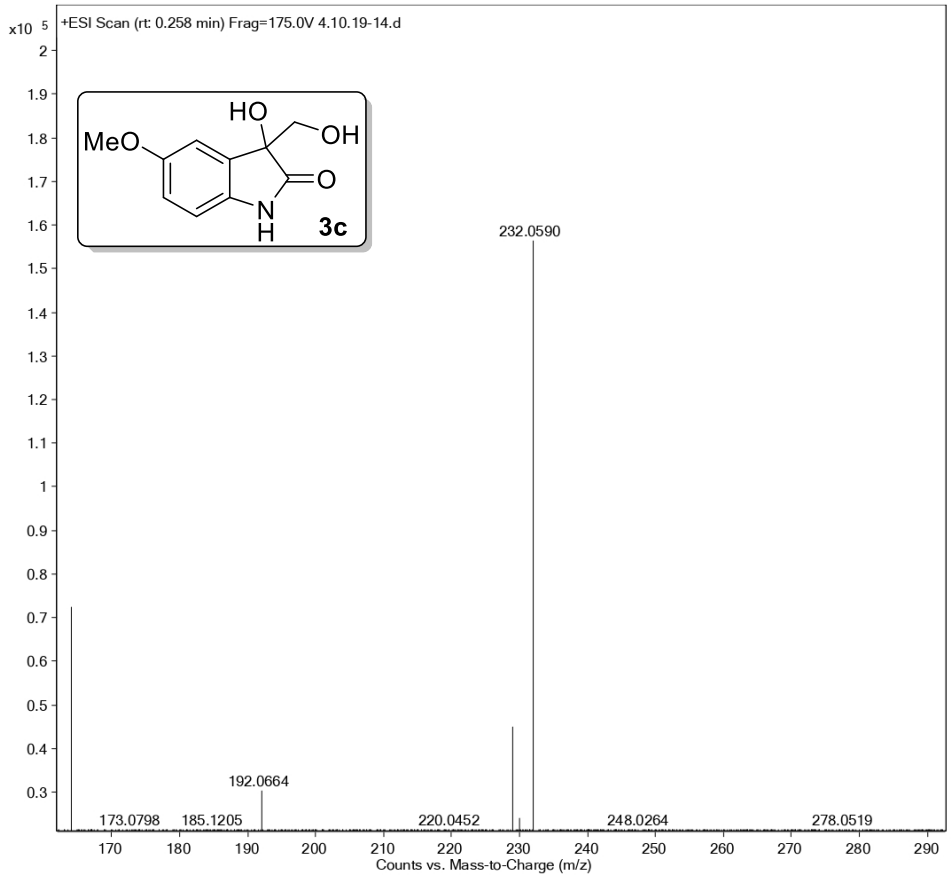


^{13}C{^{1}H} NMR (75 MHz, DMSO-d_6) spectrum of 3-hydroxy-3-(hydroxymethyl)-5-methoxyindolin-2-one (3c)

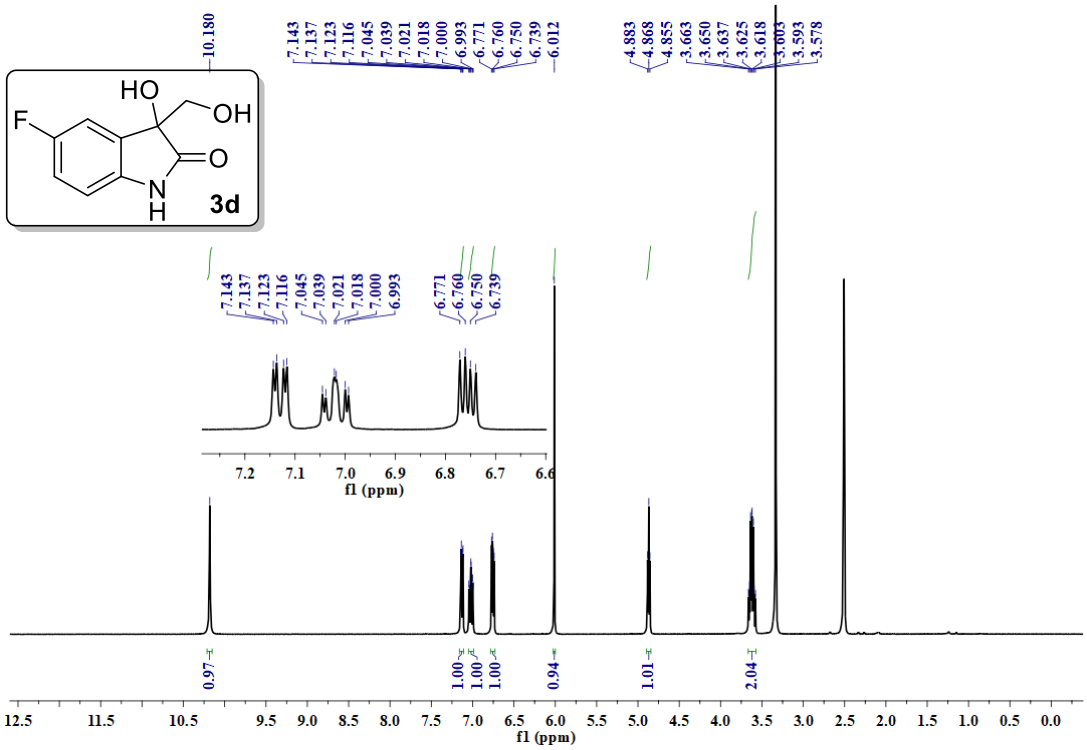


HRMS of 3-hydroxy-3-(hydroxymethyl)-5-methoxyindolin-2-one (3c)

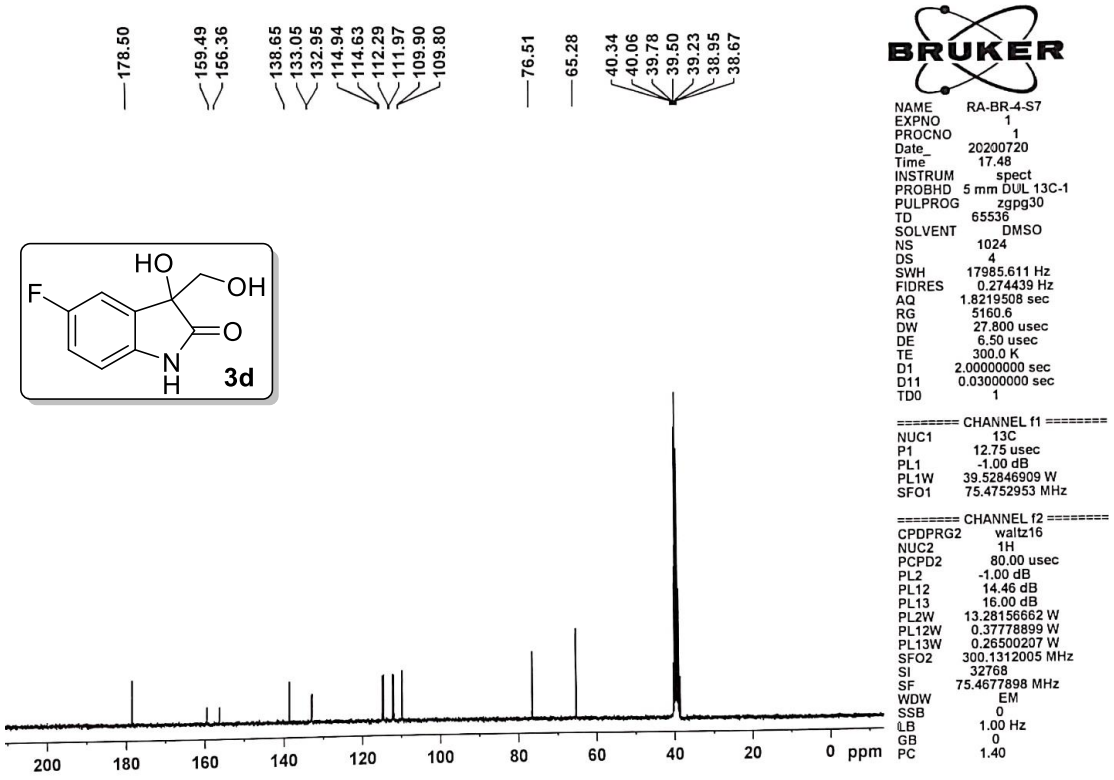
Sample Name	OMEISRG	**Position**	P1-B5	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	2	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	4.10.19-14.d
ACQ Method	srinu.m	**Comment**		**Acquired Time**	04-Oct-19 5:10:07 PM



^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 5-fluoro-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3d)

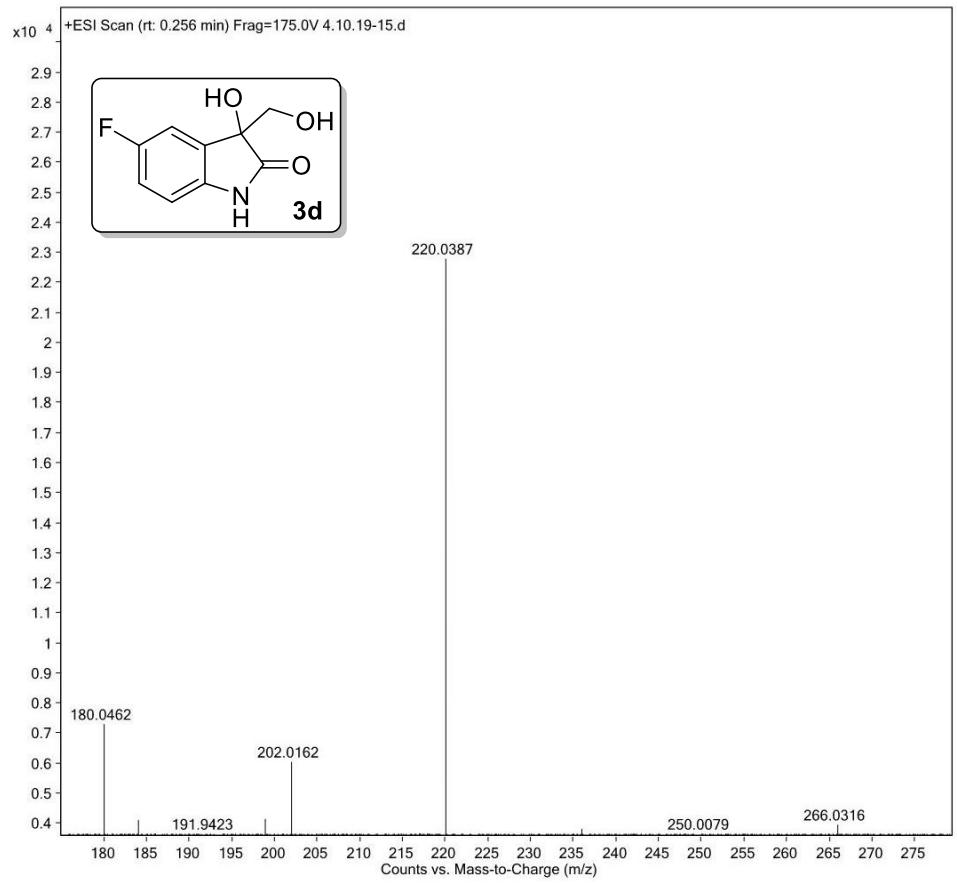


^{13}C{^{1}H} NMR (75 MHz, DMSO-d_6) spectrum of 5-fluoro-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3d)

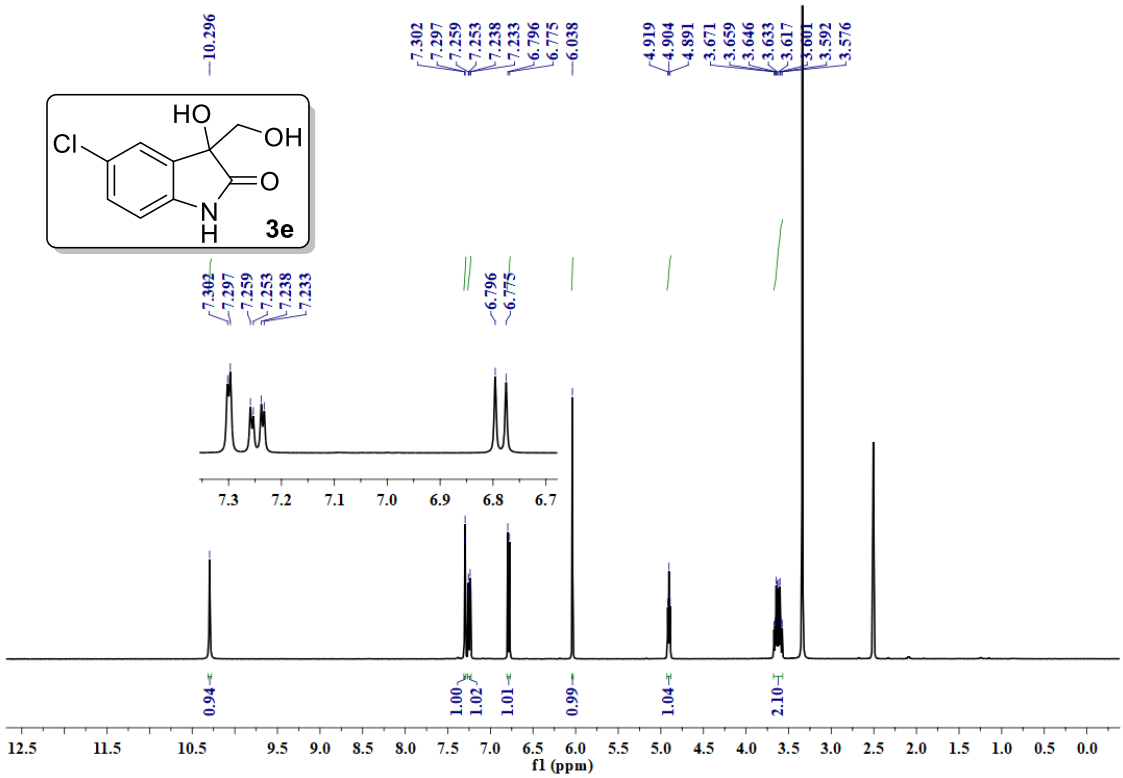


HRMS of 5-fluoro-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3d)

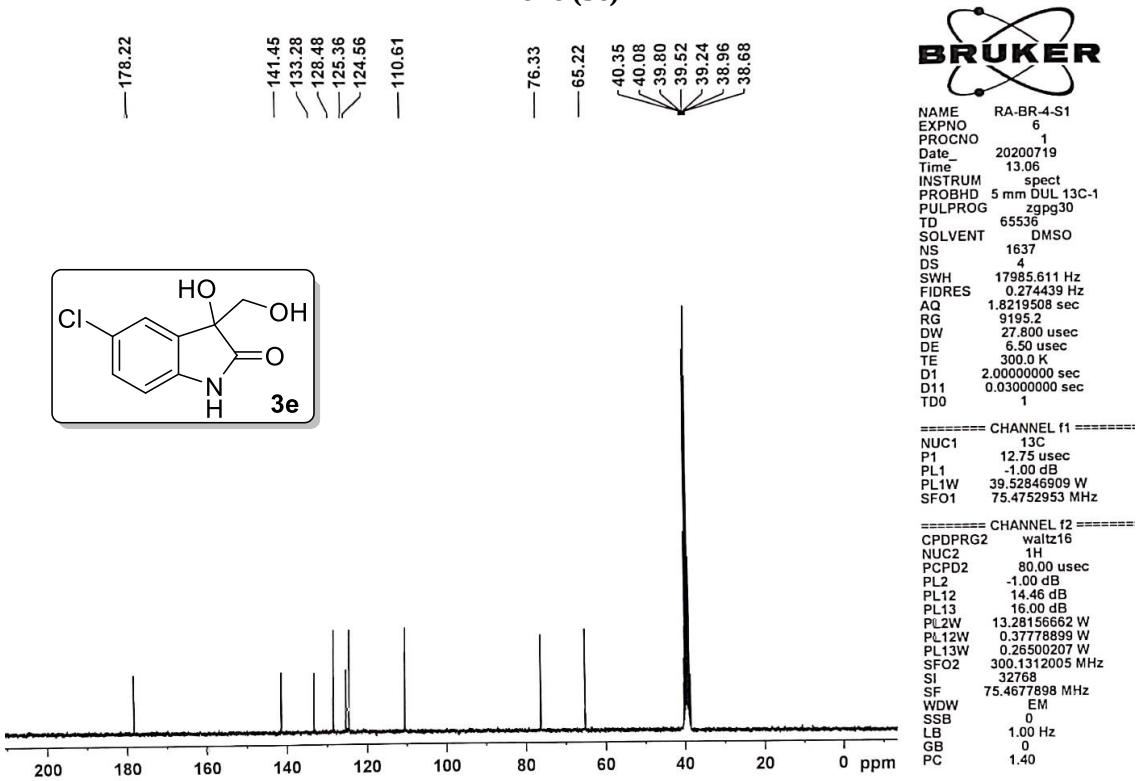
Sample Name	FISRG	**Position**	P1-B6	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	2	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	4.10.19-15.d
ACQ Method	srinu.m	**Comment**		**Acquired Time**	04-Oct-19 5:14:06 PM



^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 5-chloro-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3e)



^{13}C{^{1}H} NMR (75 MHz, DMSO-d_6) spectrum of 5-chloro-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3e)



BRUKER

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PL13 16.00 dB
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LB 1.00 Hz
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HRMS of 5-chloro-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3e)

Sample Name	CLISRG	**Position**	P1-A6	**Instrument Name**	Instrument 1
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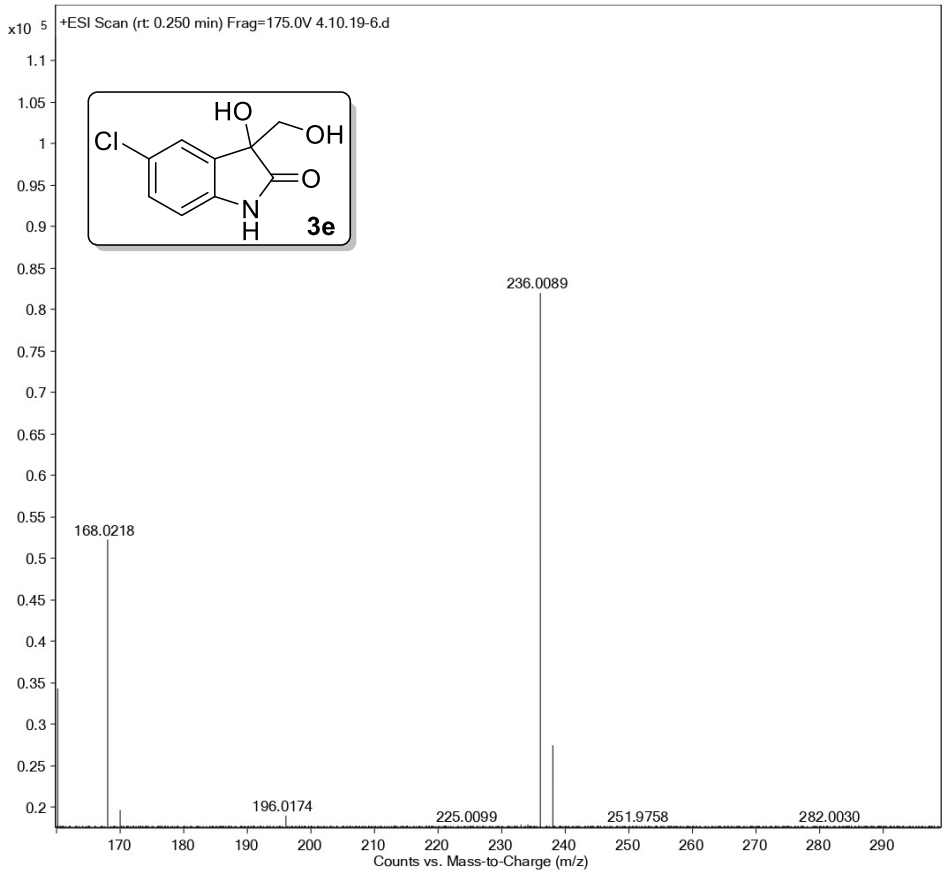
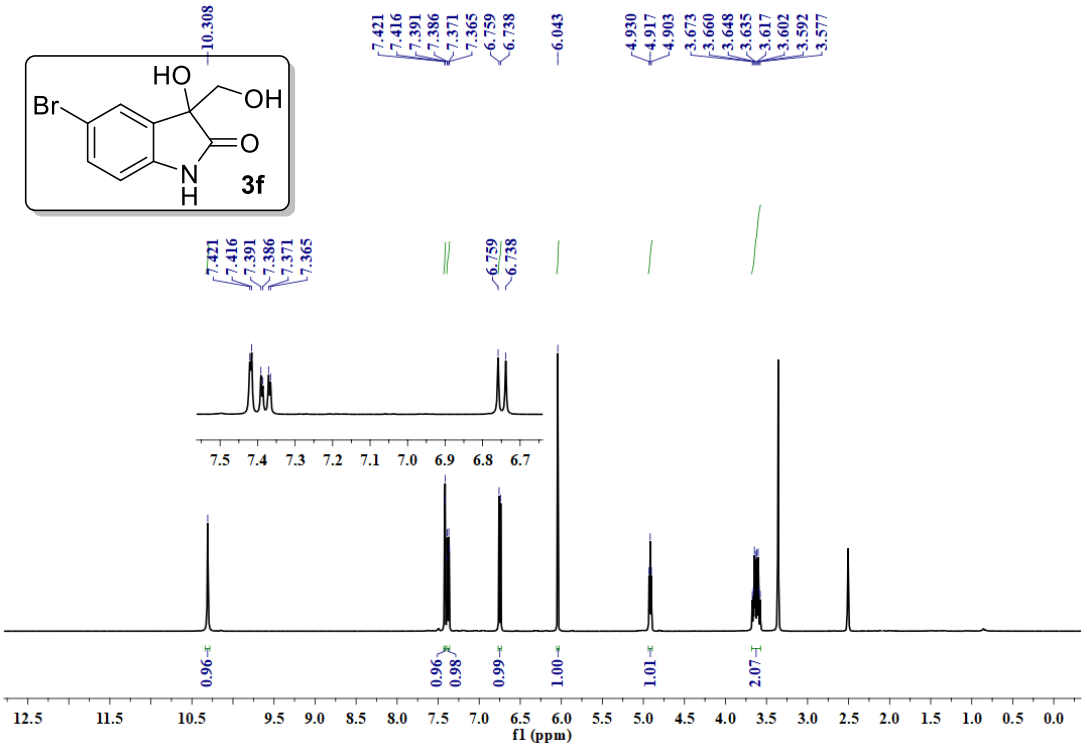
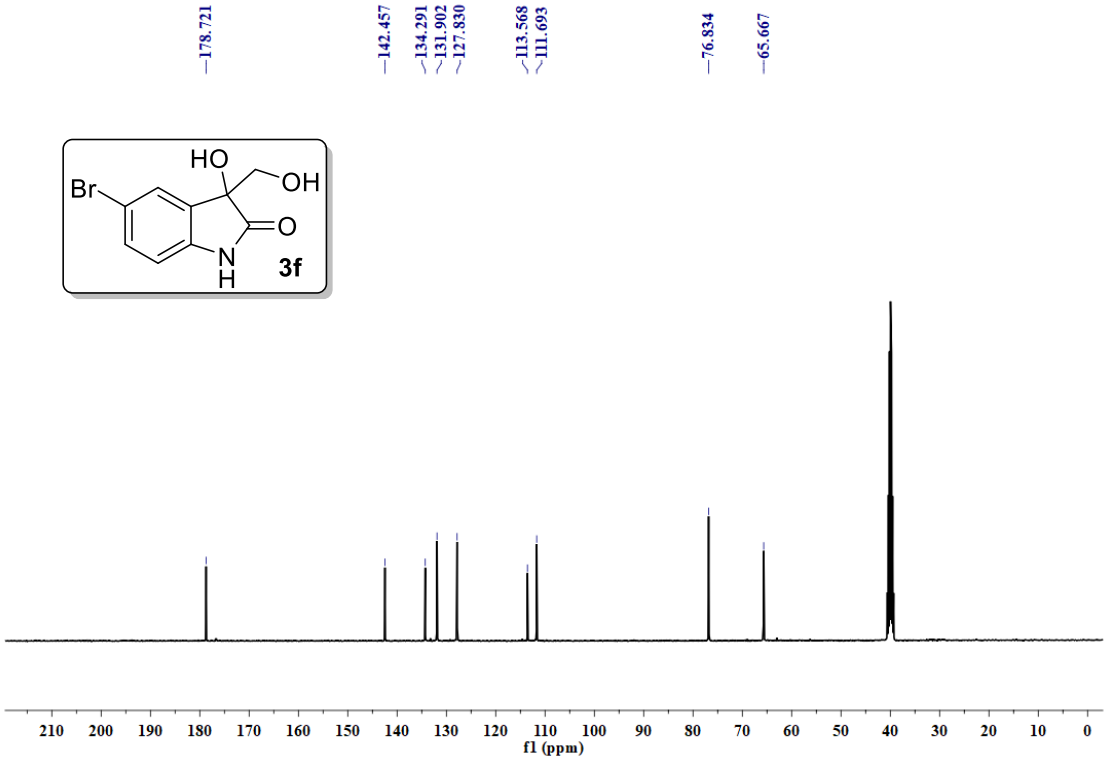


^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 5-bromo-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3f)

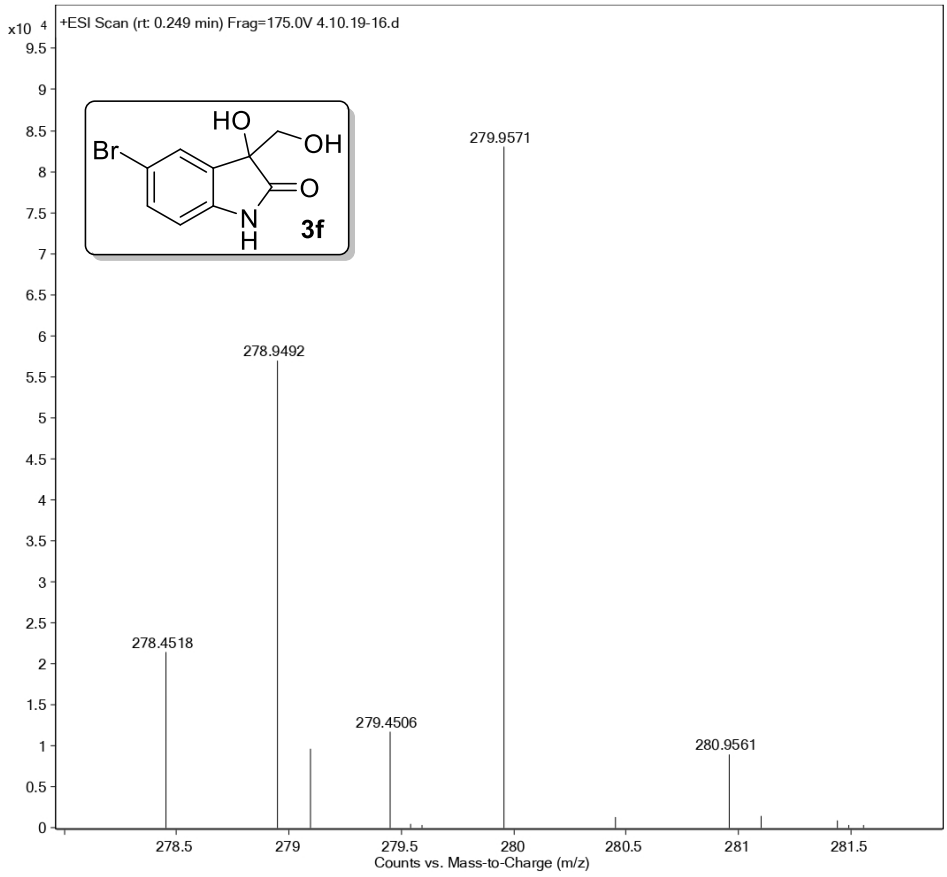


^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of 5-bromo-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3f)

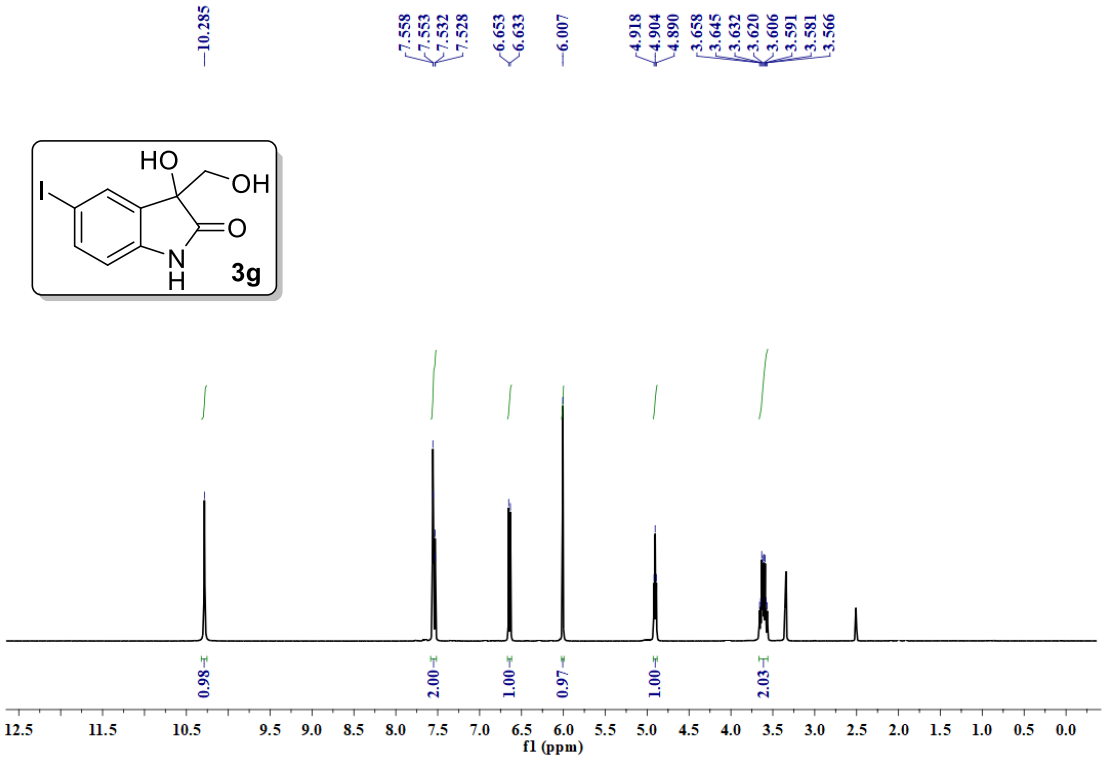


HRMS of 5-bromo-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3f)

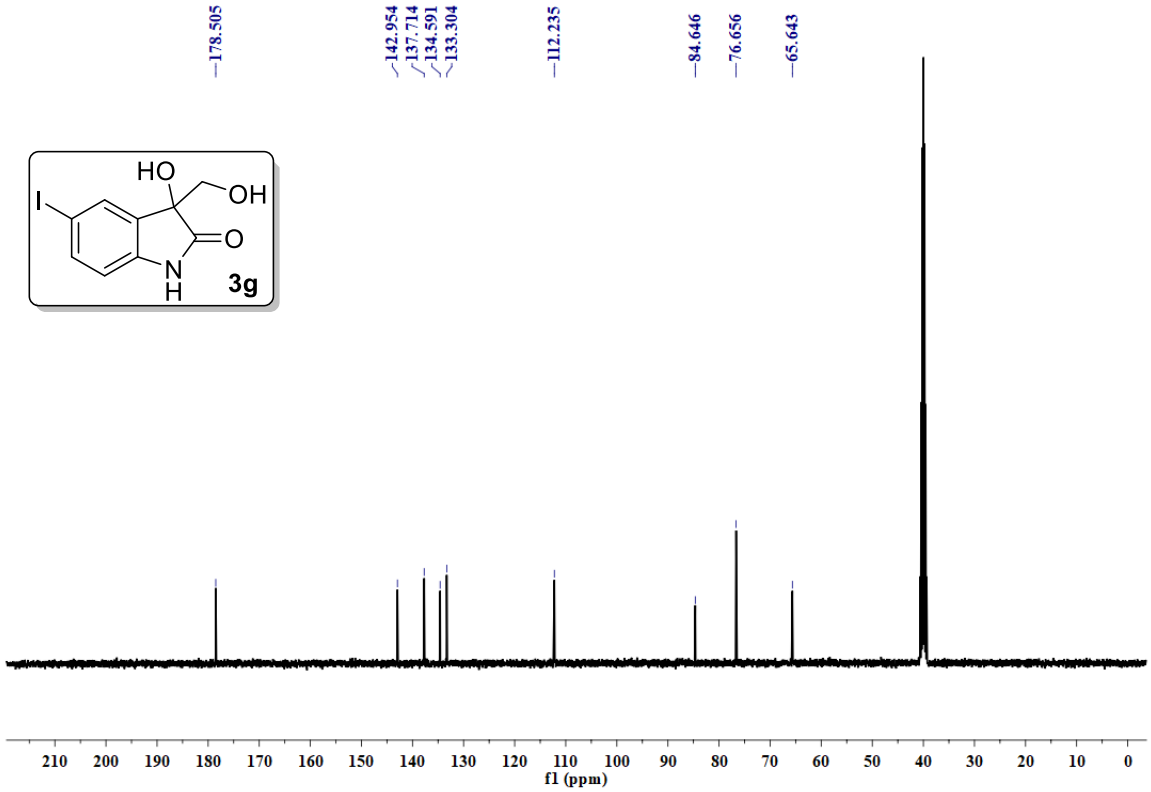
Sample Name	BRISRG	**Position**	P1-B7	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	2	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	4.10.19-16.d
ACQ Method	srinu.m	**Comment**		**Acquired Time**	04-Oct-19 5:18:05 PM



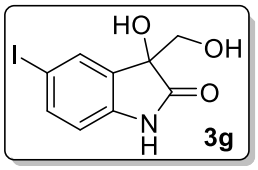
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 3-hydroxy-3-(hydroxymethyl)-5-iodoindolin-2-one (3g)

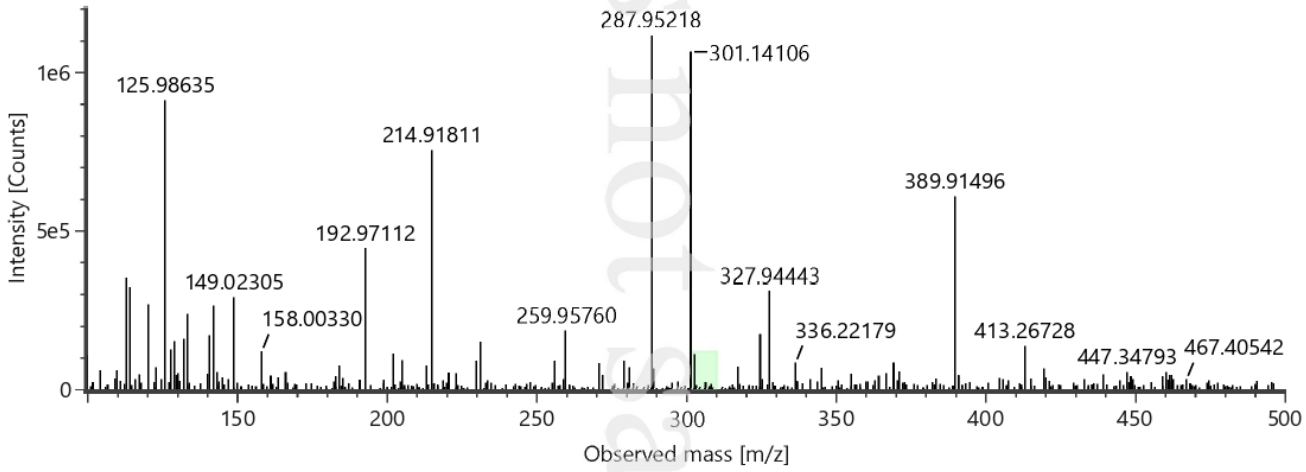


^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of 3-hydroxy-3-(hydroxymethyl)-5-iodoindolin-2-one (3g)

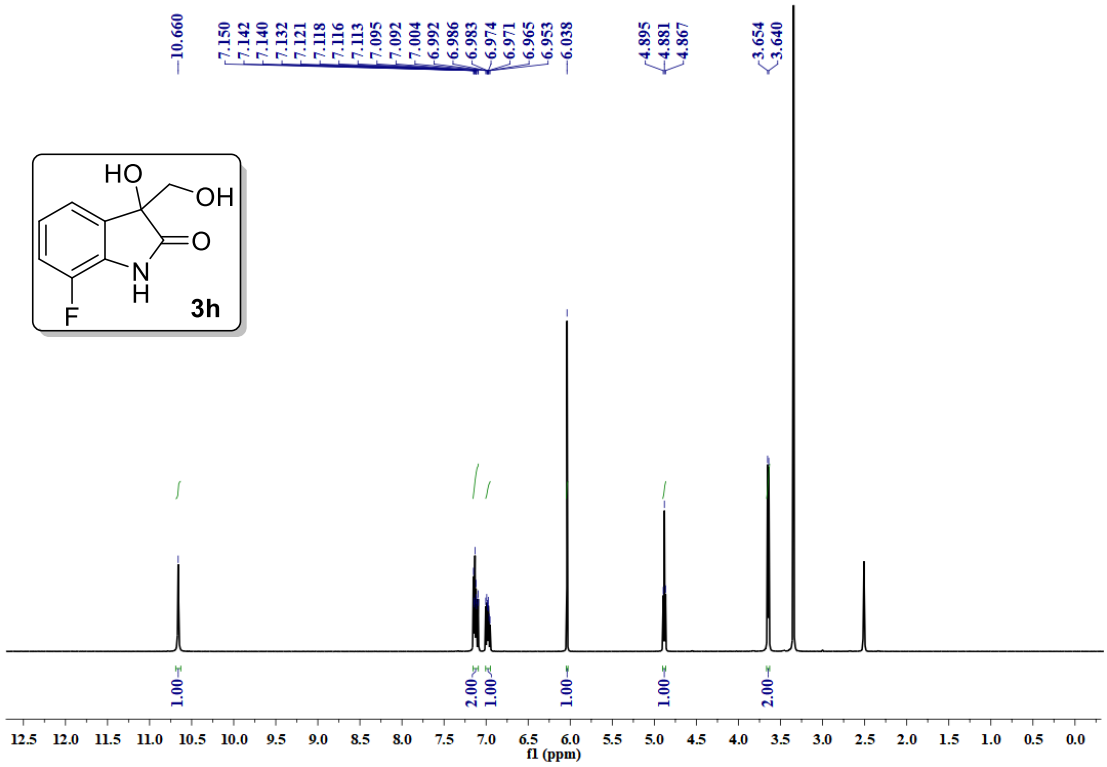


HRMS of 3-hydroxy-3-(hydroxymethyl)-5-iodoindolin-2-one (3g)

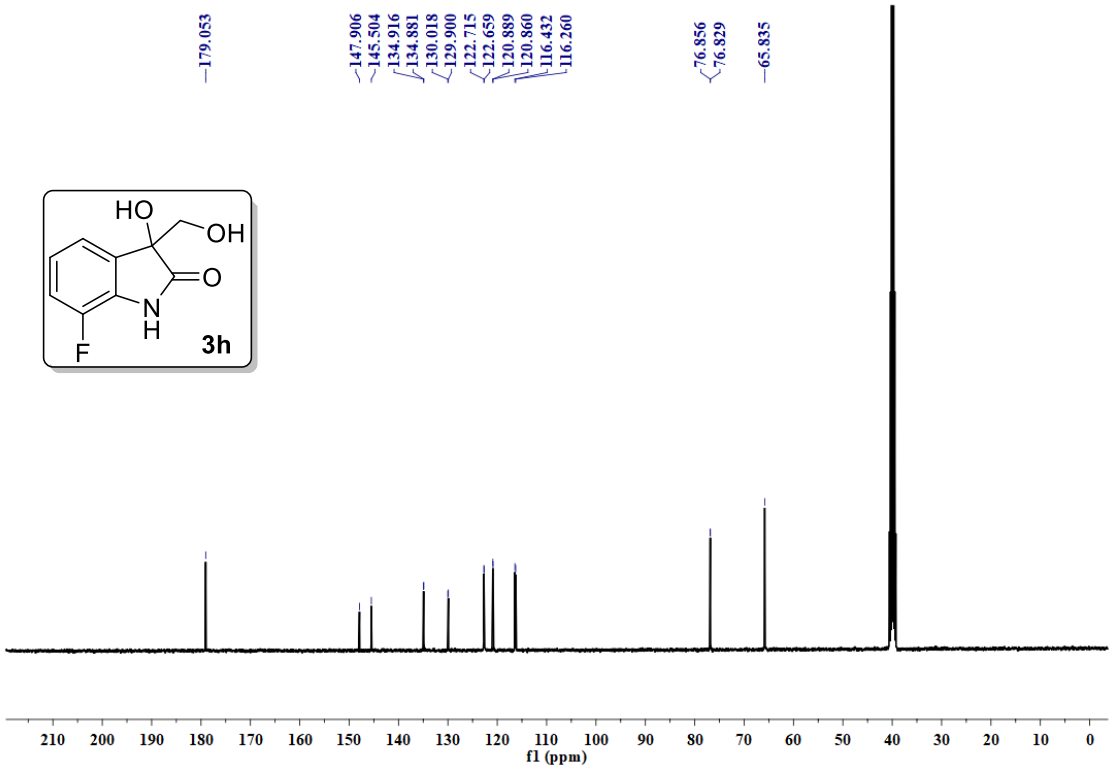




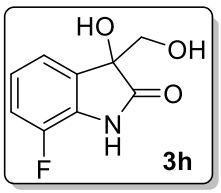
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 7-fluoro-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3h)

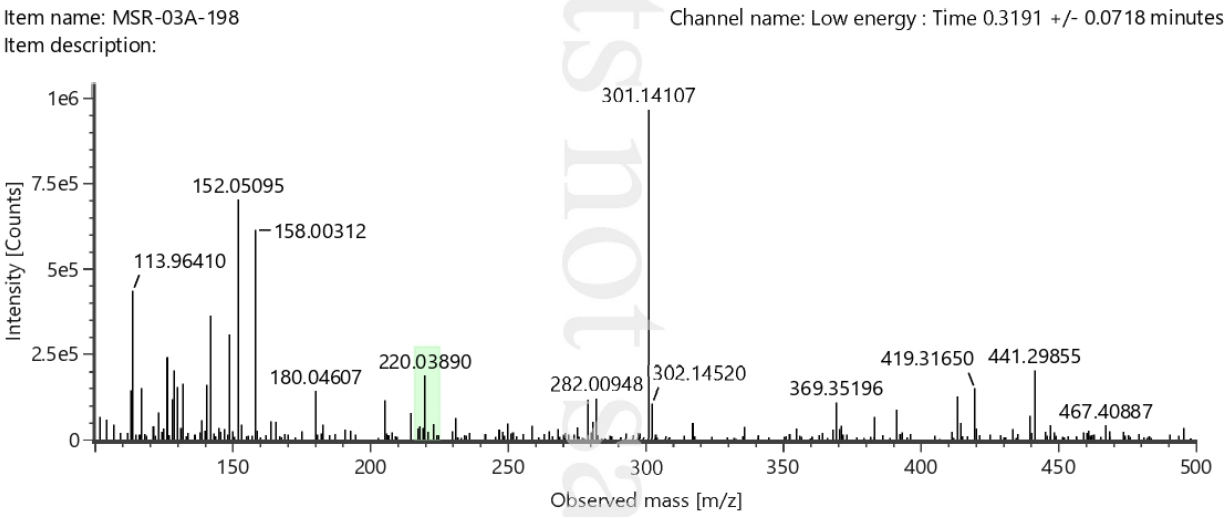


^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of 7-fluoro-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3h)

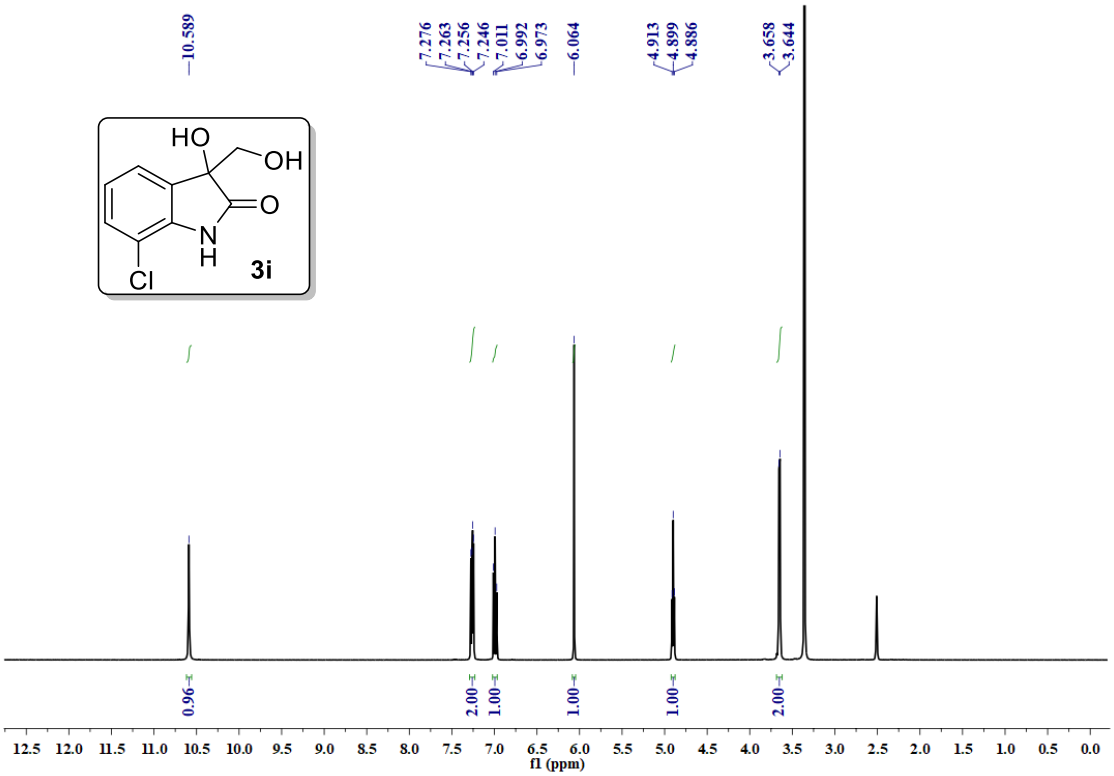


HRMS of 7-fluoro-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3h)

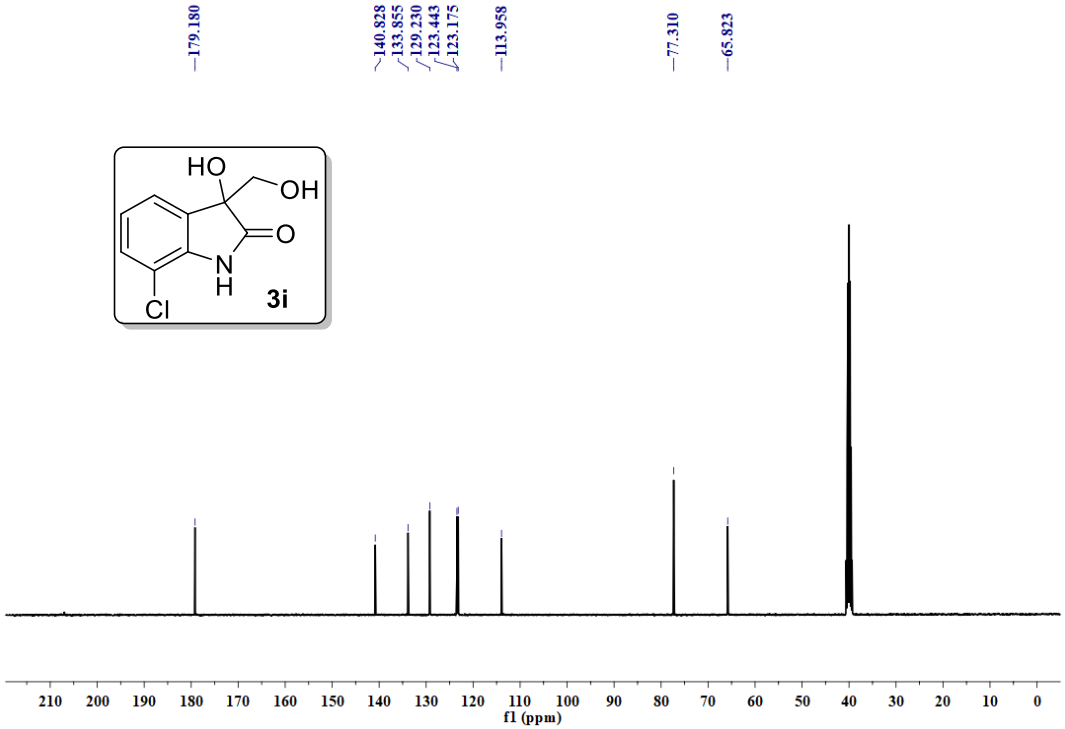




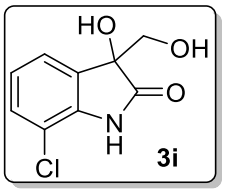
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 7-chloro-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3i)

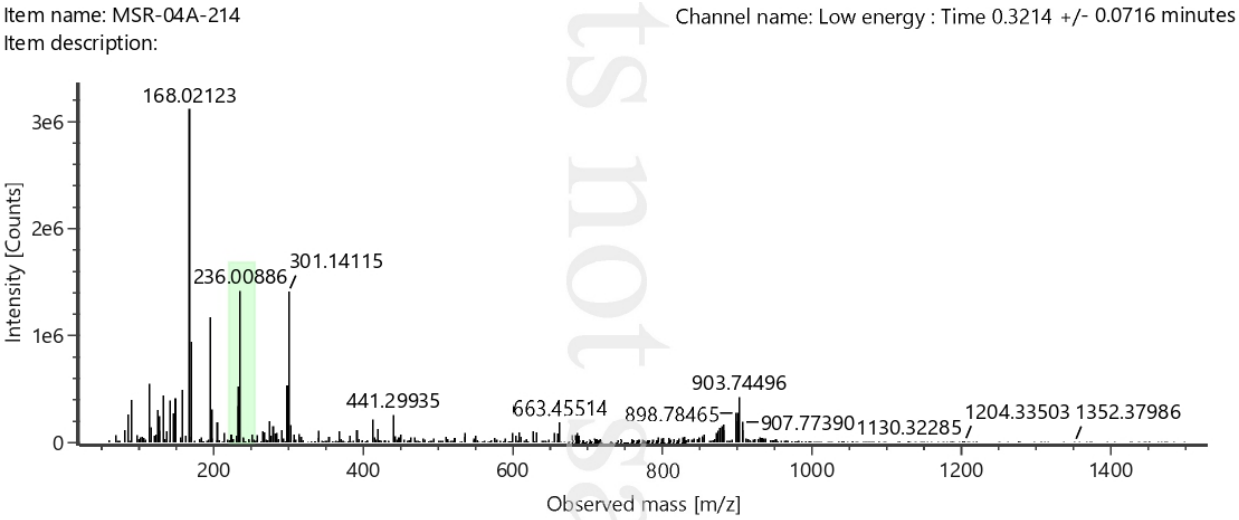


^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of 7-chloro-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3i)

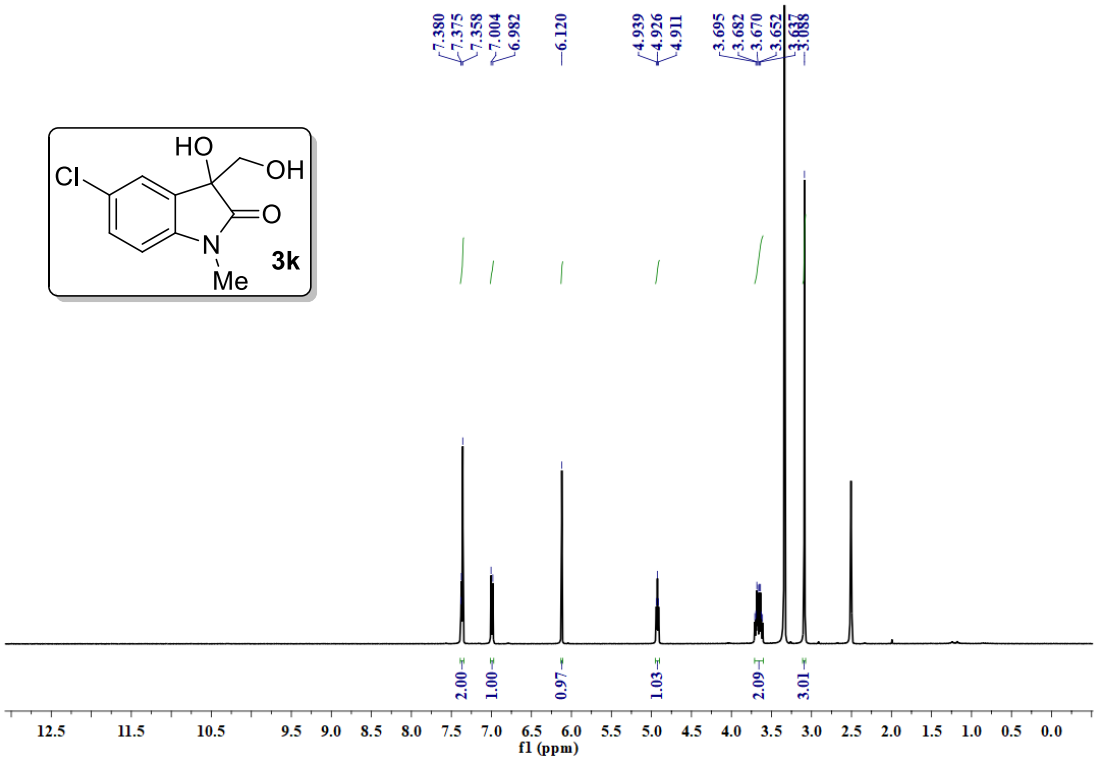


HRMS of 7-chloro-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3i)

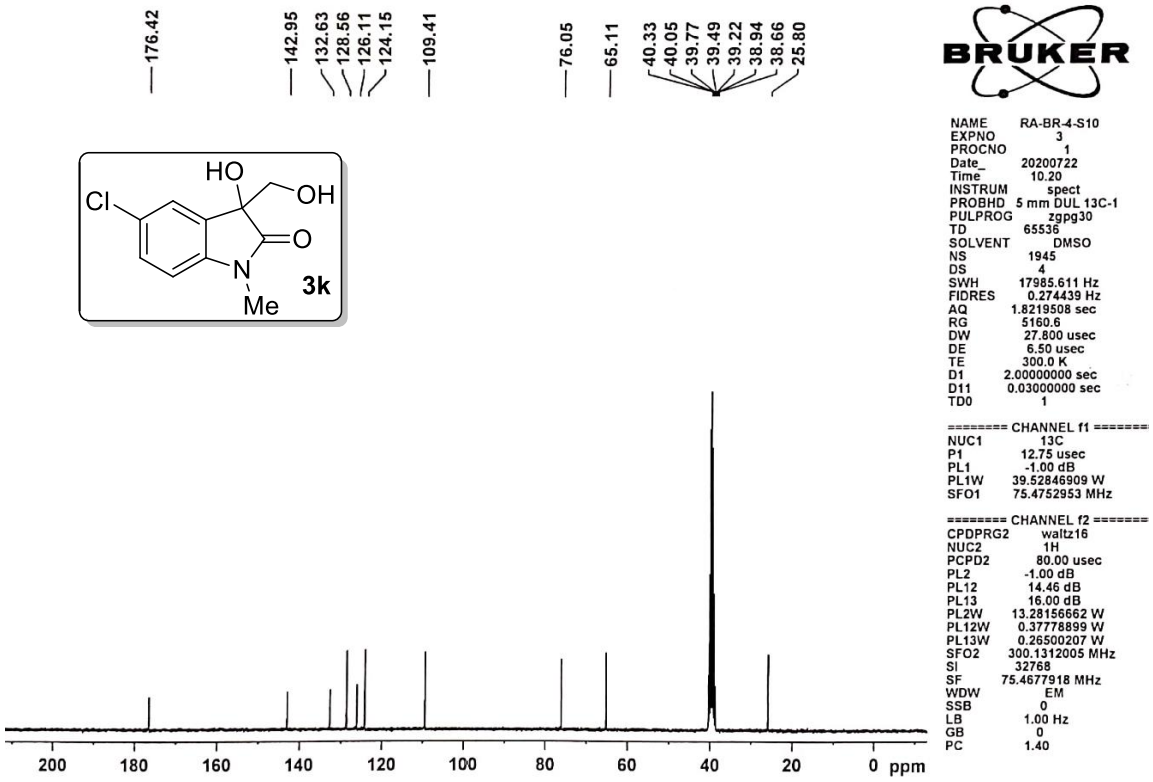




^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 5-chloro-3-hydroxy-3-(hydroxymethyl)-1-methylindolin-2-one (3k)



^{13}C{^{1}H} NMR (75 MHz, DMSO-d_6) spectrum of 5-chloro-3-hydroxy-3-(hydroxymethyl)-1-methylindolin-2-one (3k)

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PROCNO                  1
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Time                10.20
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NS                   1945
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SWH          17985.611 Hz
FIDRES        0.274439 Hz
AQ           1.8219508 sec
RG                5160.6
DW             27.800 usec
DE              6.50 usec
TE                300.0 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                     1

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P1             12.75 usec
PL1             -1.00 dB
PL1W       39.52846909 W
SFO1       75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2          80.00 usec
PL2             -1.00 dB
PL12            14.46 dB
PL13            16.00 dB
PL2W       13.28156662 W
PL12W       0.37778899 W
PL13W       0.26500207 W
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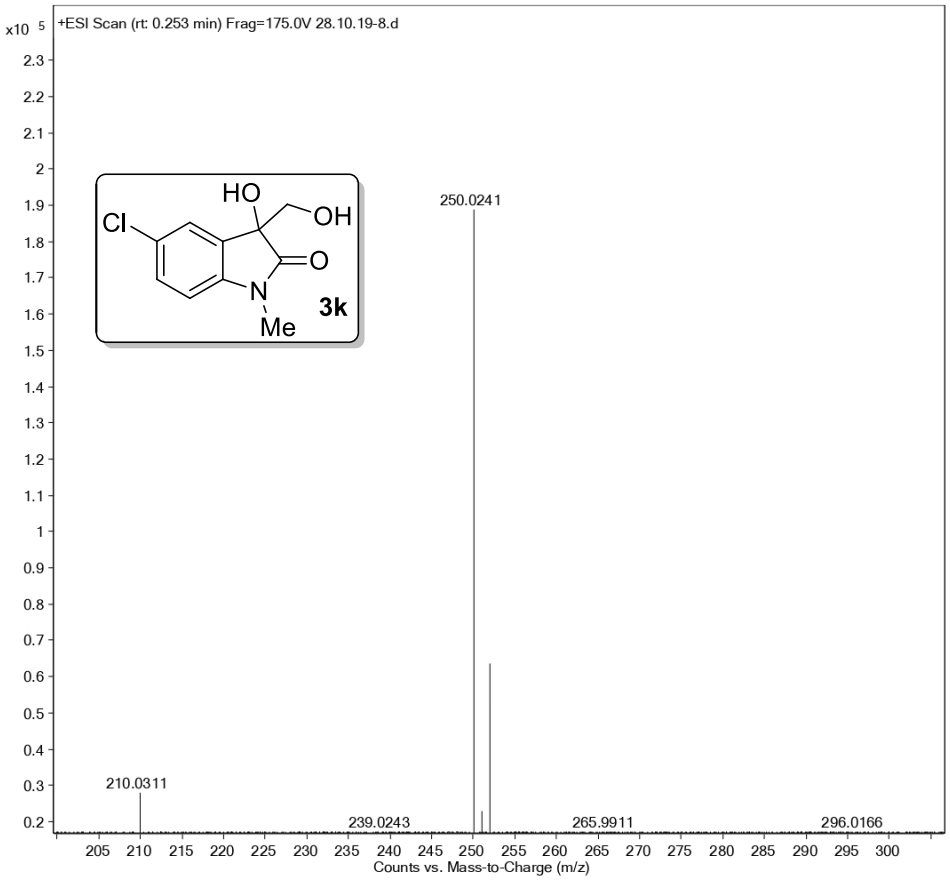
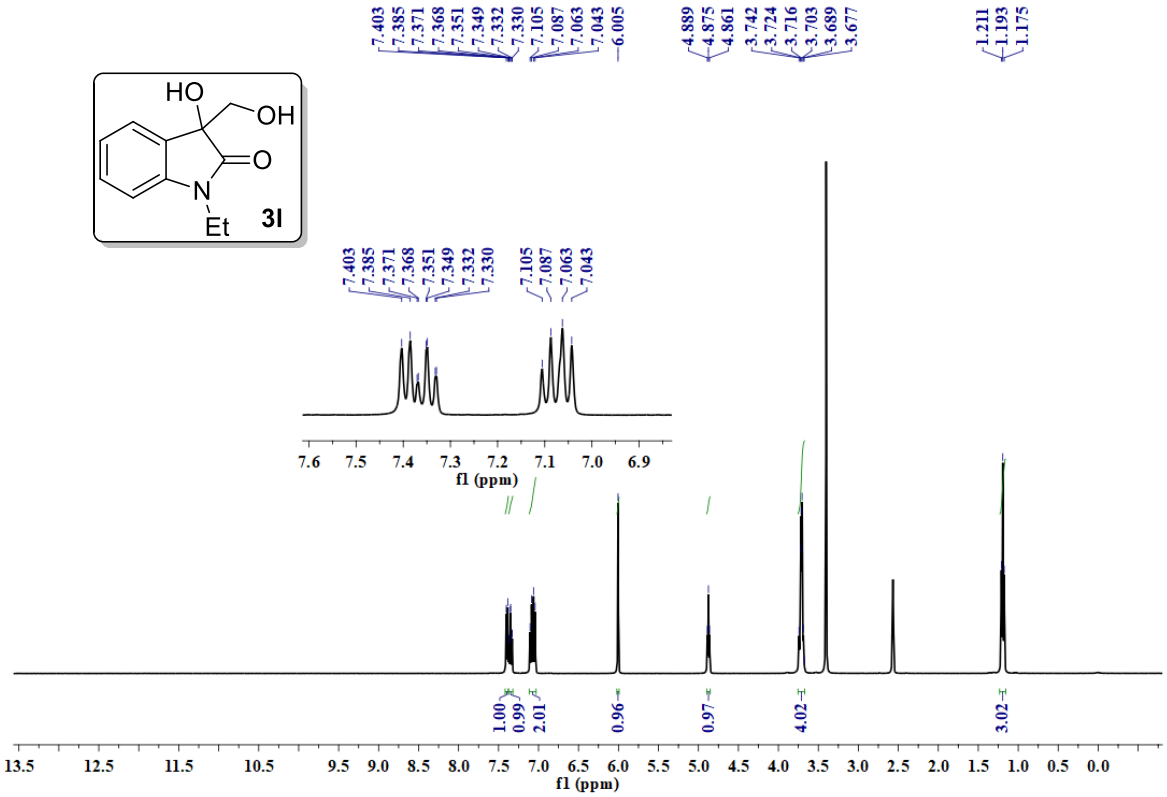
HRMS of 5-chloro-3-hydroxy-3-(hydroxymethyl)-1-methylindolin-2-one (3k)

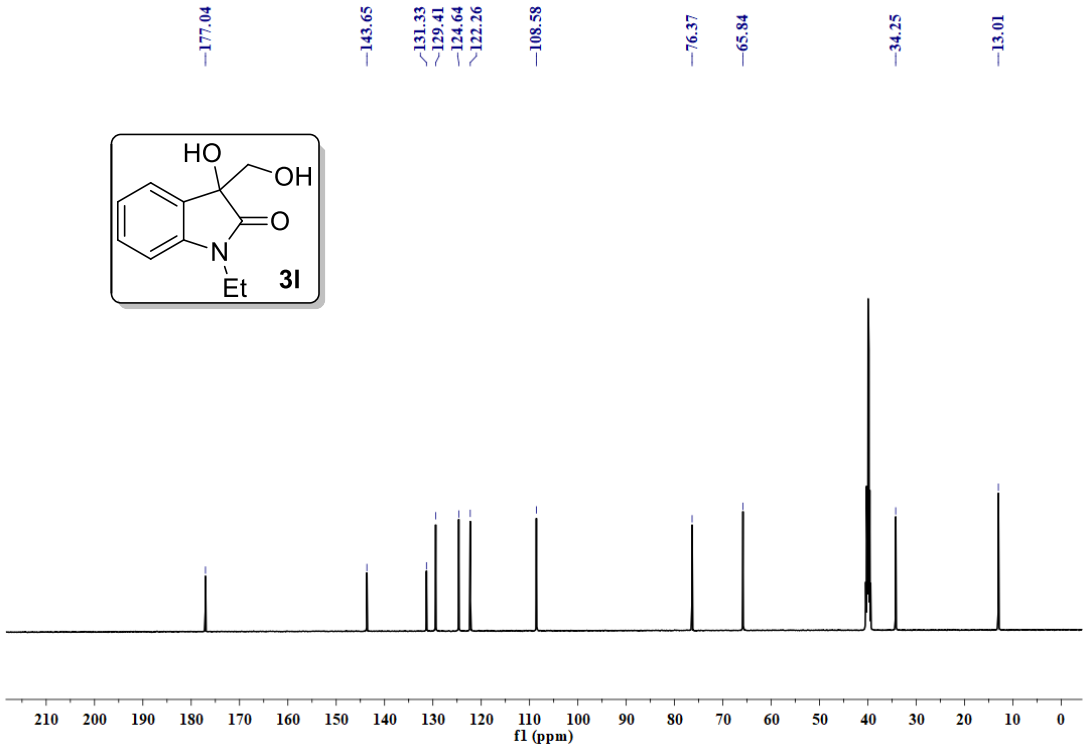
Sample Name	gsp 11	**Position**	P1-A8	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	2	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	28.10.19-8.d
ACQ Method	srinu.m	**Comment**		**Acquired Time**	28-Oct-19 2:55:39 PM



^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 1-ethyl-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3l)

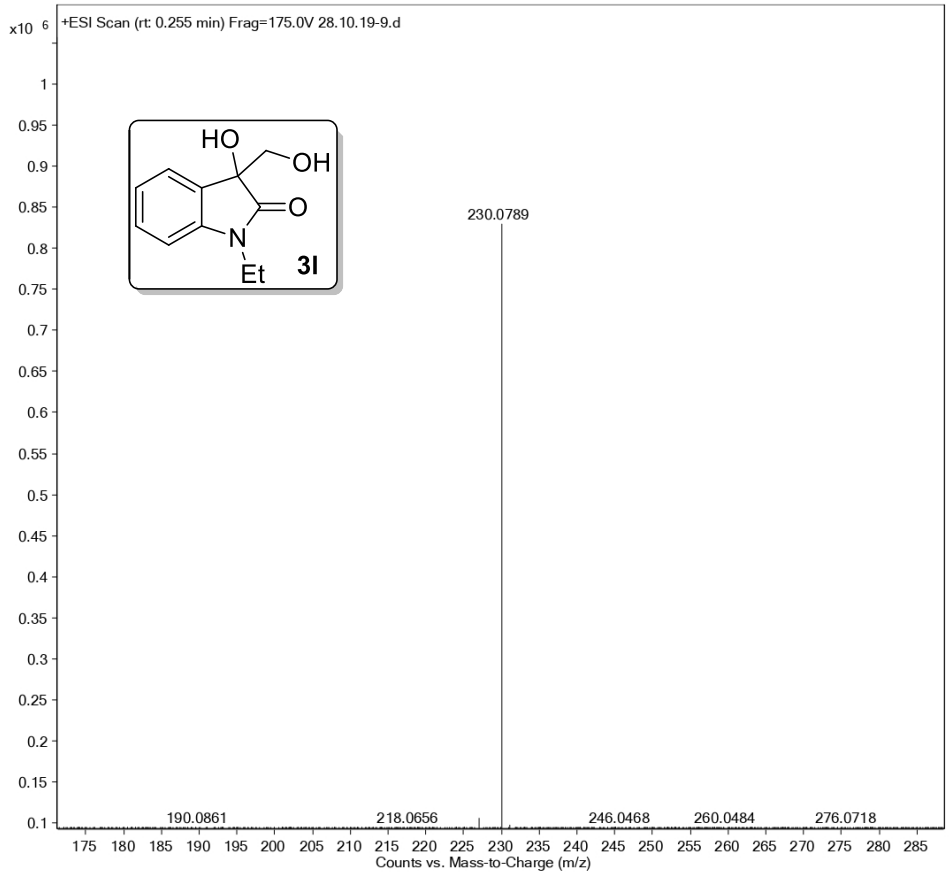


^{13}C{^{1}H} NMR (125 MHz, DMSO-d_6) spectrum of 1-ethyl-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3l)

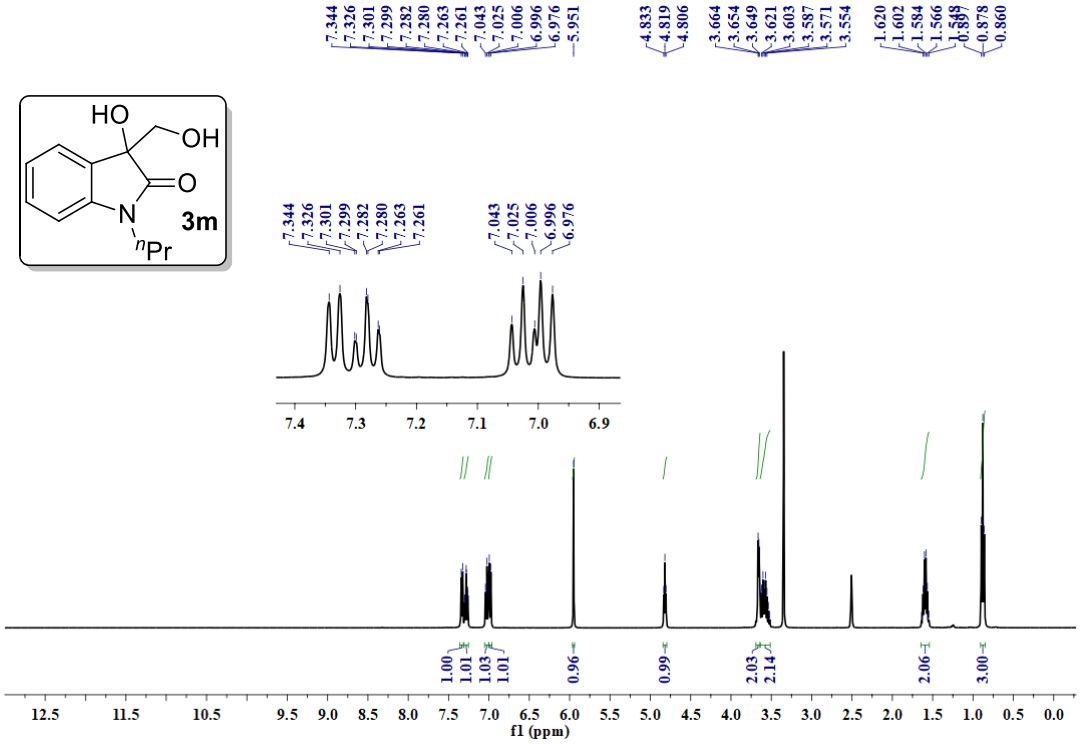


HRMS of 1-ethyl-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3l)

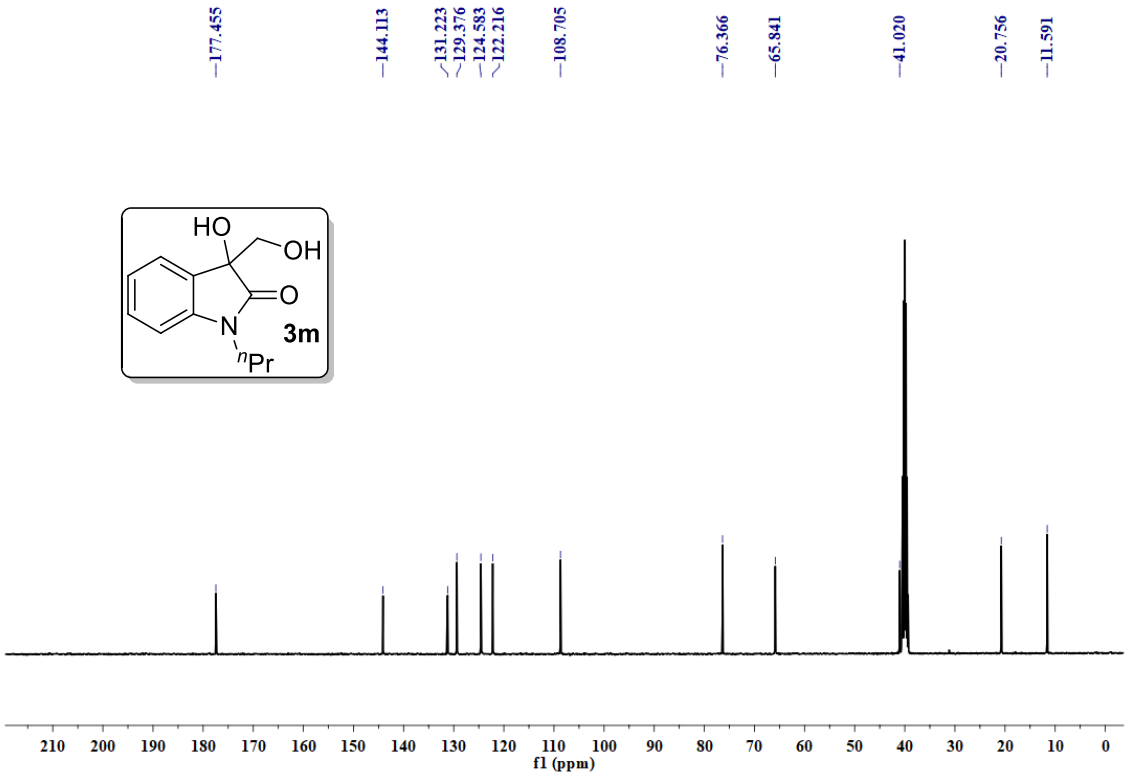
Sample Name	gsp 10	**Position**	P1-A9	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	2	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	28.10.19-9.d
ACQ Method	srinu.m	**Comment**		**Acquired Time**	28-Oct-19 2:59:37 PM



^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 3-hydroxy-3-(hydroxymethyl)-1-propylindolin-2-one (3m)

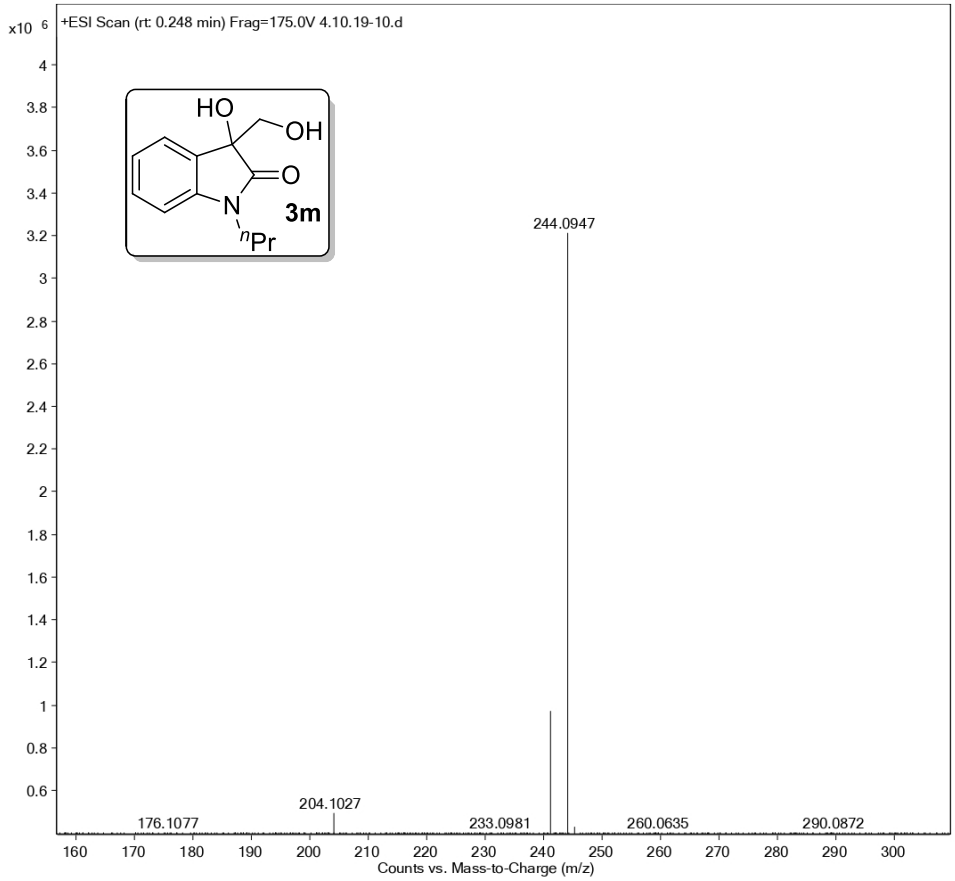


^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of 3-hydroxy-3-(hydroxymethyl)-1-propylindolin-2-one (3m)

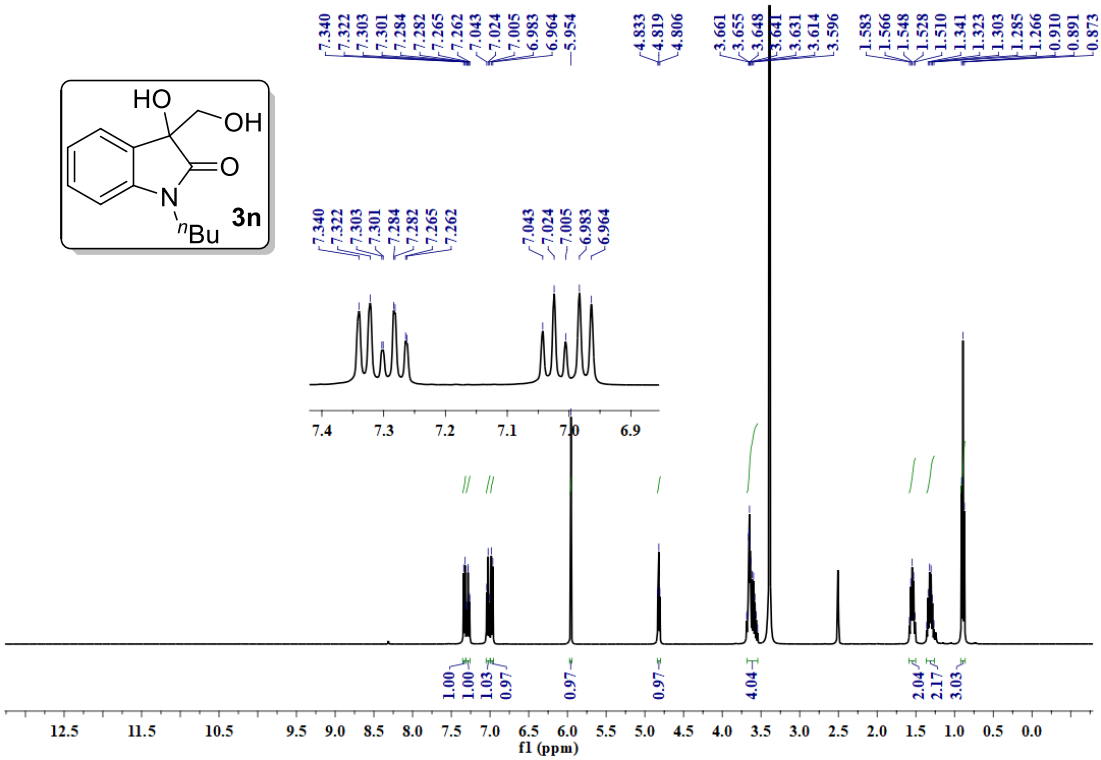


HRMS of 3-hydroxy-3-(hydroxymethyl)-1-propylindolin-2-one (3m)

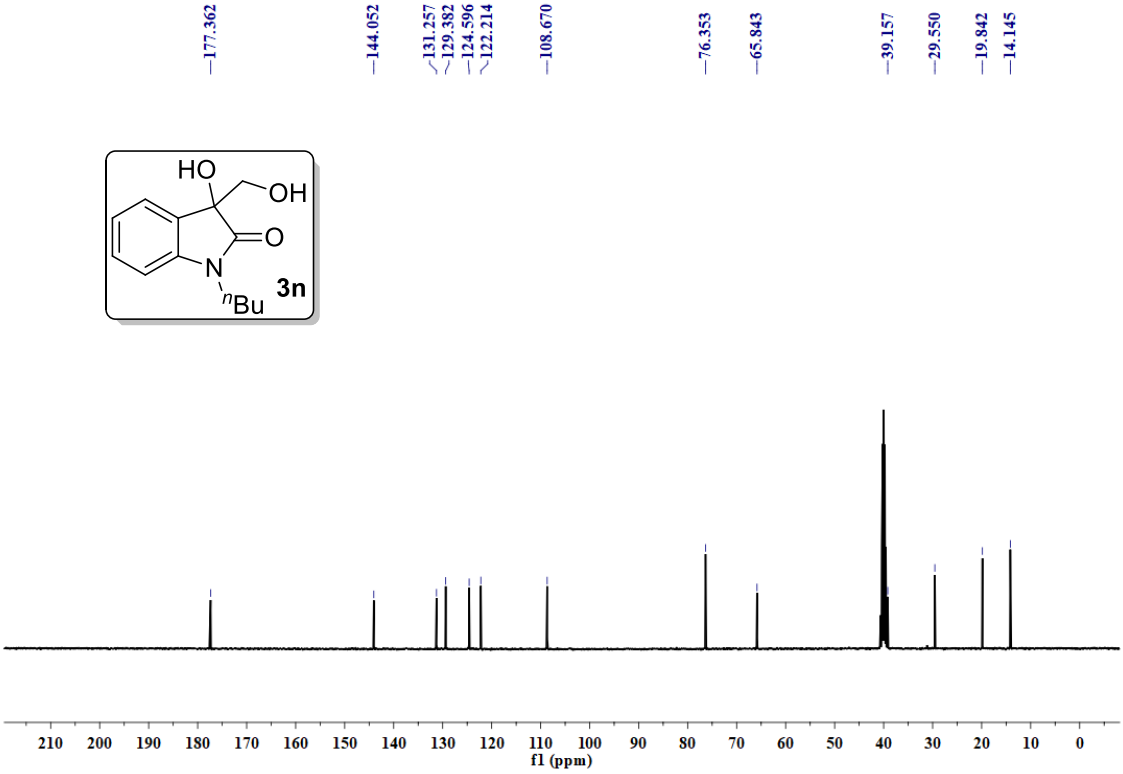
Sample Name	N-PYLISRG	**Position**	P1-B1	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	2	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	4.10.19-10.d
ACQ Method	srinu.m	**Comment**		**Acquired Time**	04-Oct-19 4:54:11 PM



^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 1-butyl-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3n)

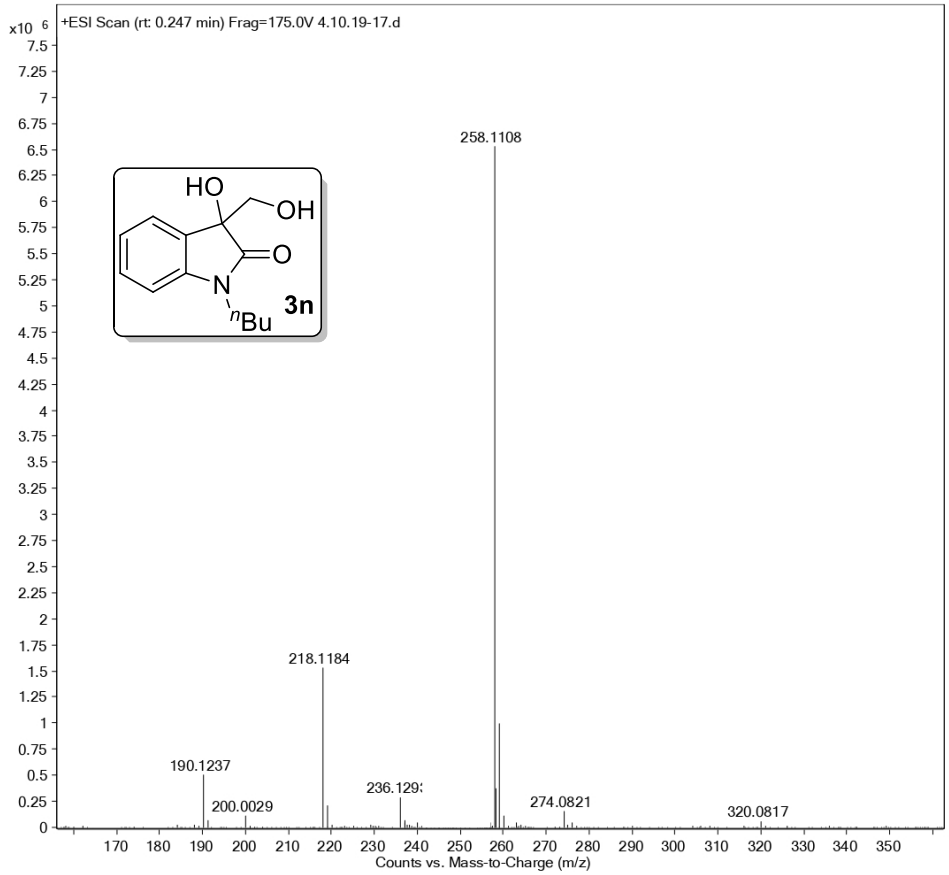


^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of 1-butyl-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3n)

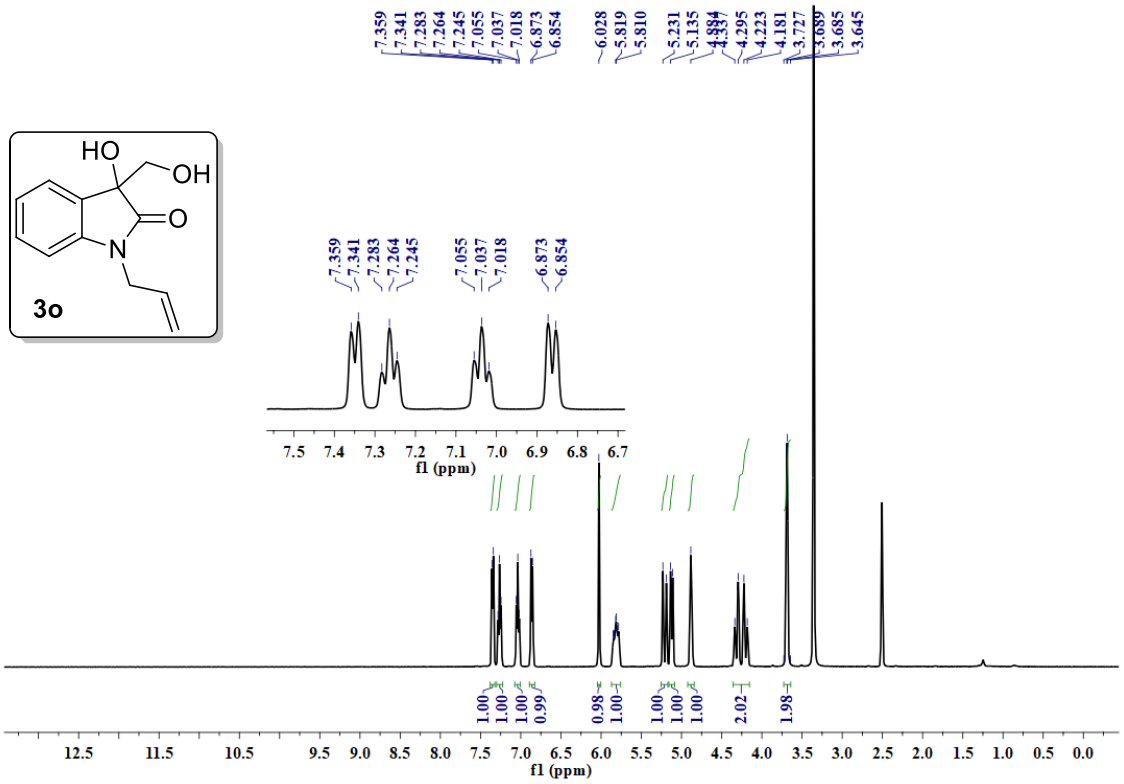


HRMS of 1-butyl-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3n)

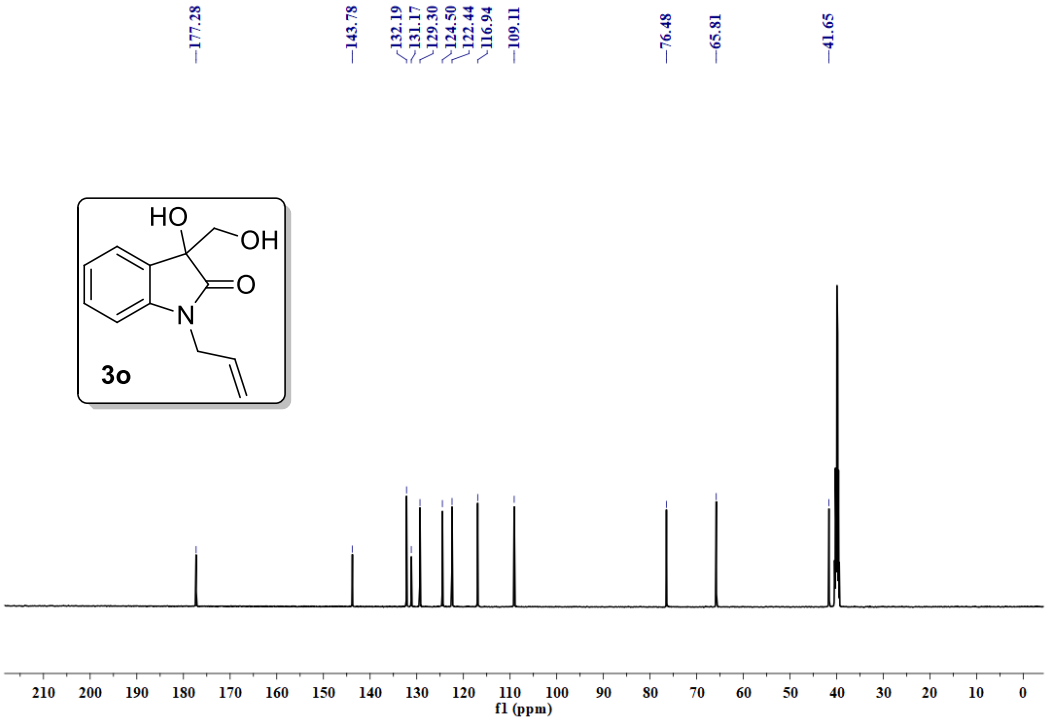
Sample Name	N-BUTYLISRG	**Position**	P1-B8	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	2	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	4.10.19-17.d
ACQ Method	srinu.m	**Comment**		**Acquired Time**	04-Oct-19 5:22:03 PM



^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 1-allyl-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3o)

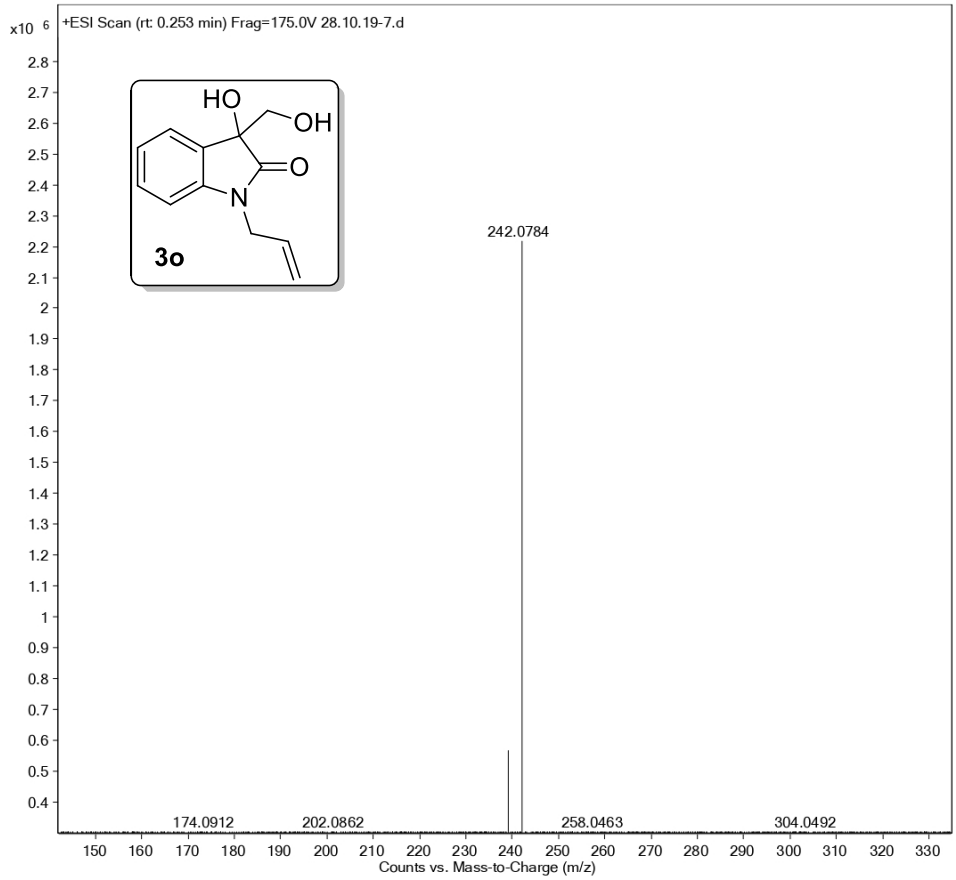


^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of 1-allyl-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3o)

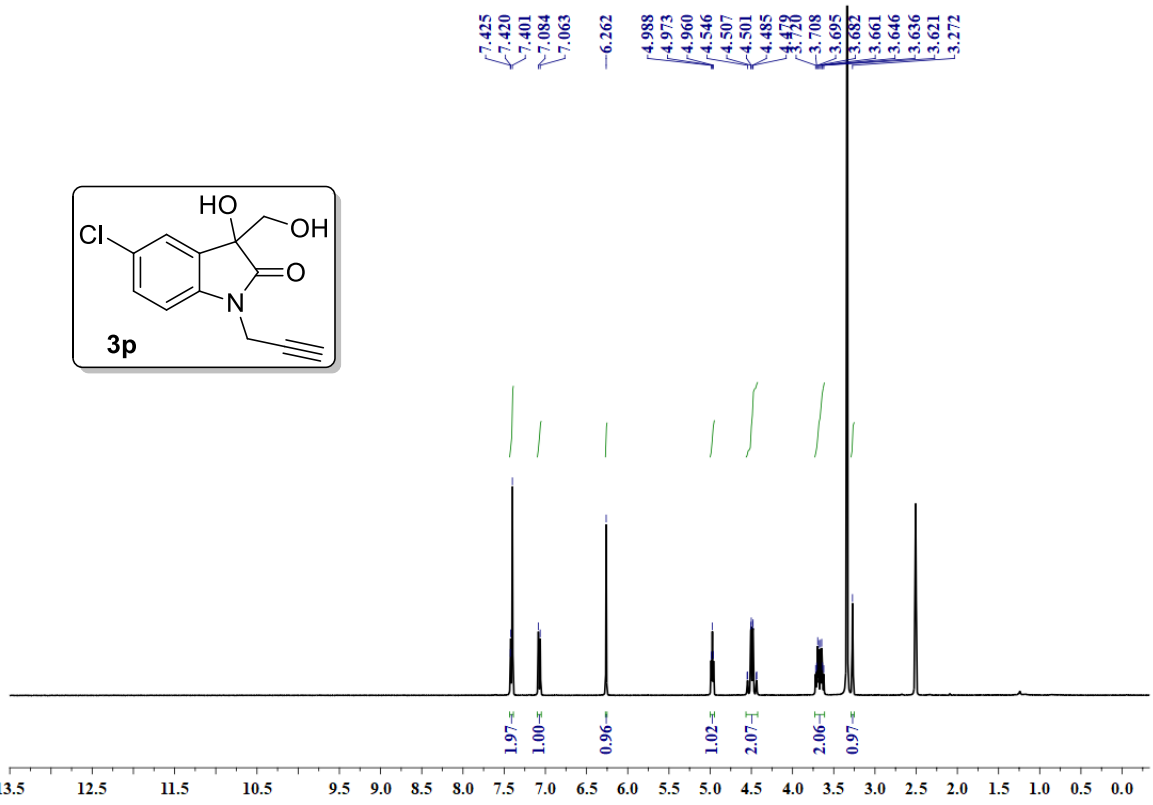


HRMS of 1-allyl-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3o)

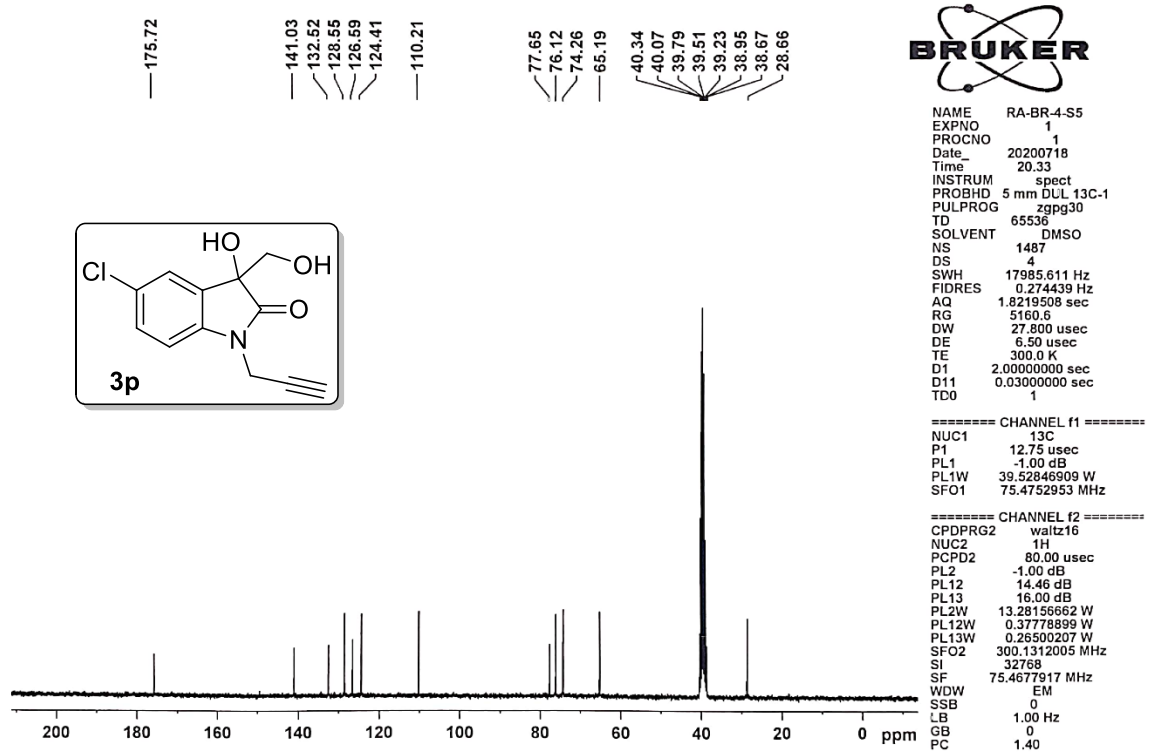
Sample Name	gsp 12	**Position**	P1-A7	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	2	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	28.10.19-7.d
ACQ Method	srinu.m	**Comment**		**Acquired Time**	28-Oct-19 2:51:41 PM



^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 5-chloro-3-hydroxy-3-(hydroxymethyl)-1-(prop-2-yn-1-yl)indolin-2-one (3p)

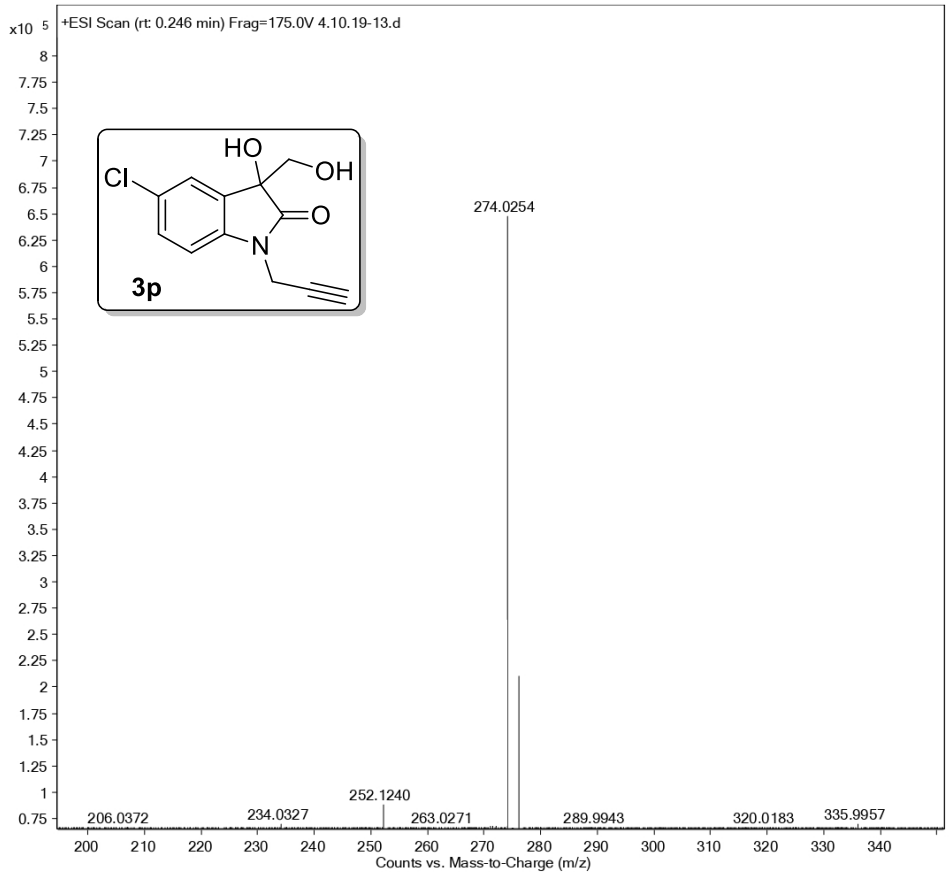


^{13}C{^{1}H} NMR (75 MHz, DMSO-d_6) spectrum of 5-chloro-3-hydroxy-3-(hydroxymethyl)-1-(prop-2-yn-1-yl)indolin-2-one (3p)

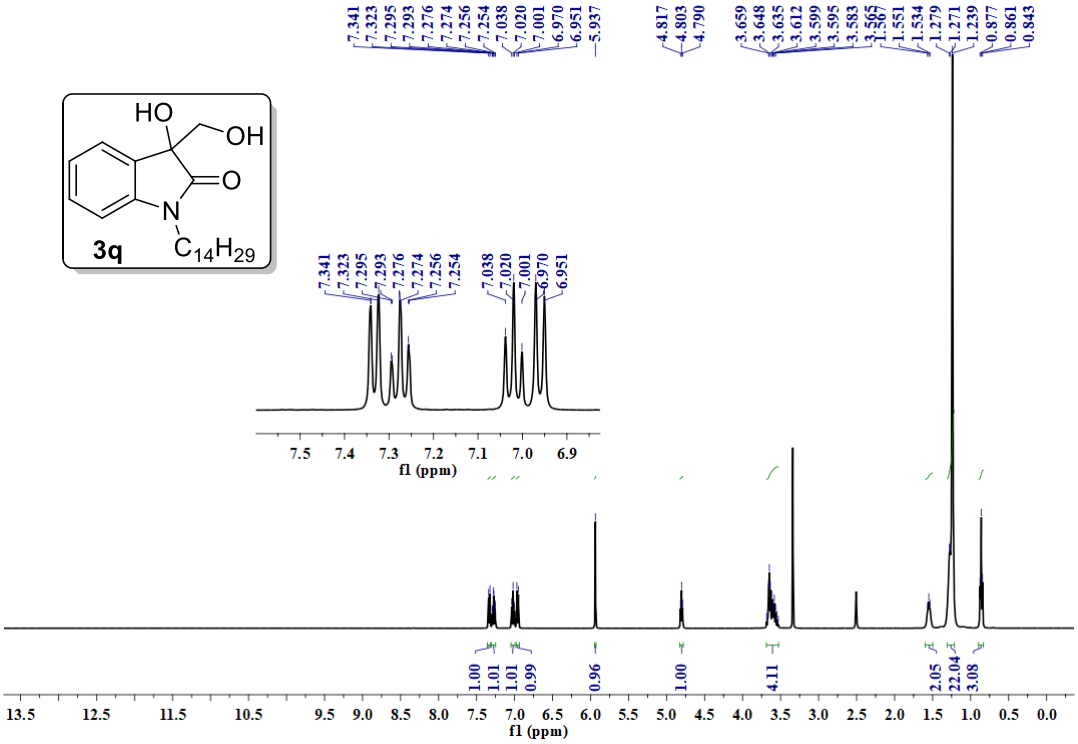


HRMS of 5-chloro-3-hydroxy-3-(hydroxymethyl)-1-(prop-2-yn-1-yl)indolin-2-one (3p)

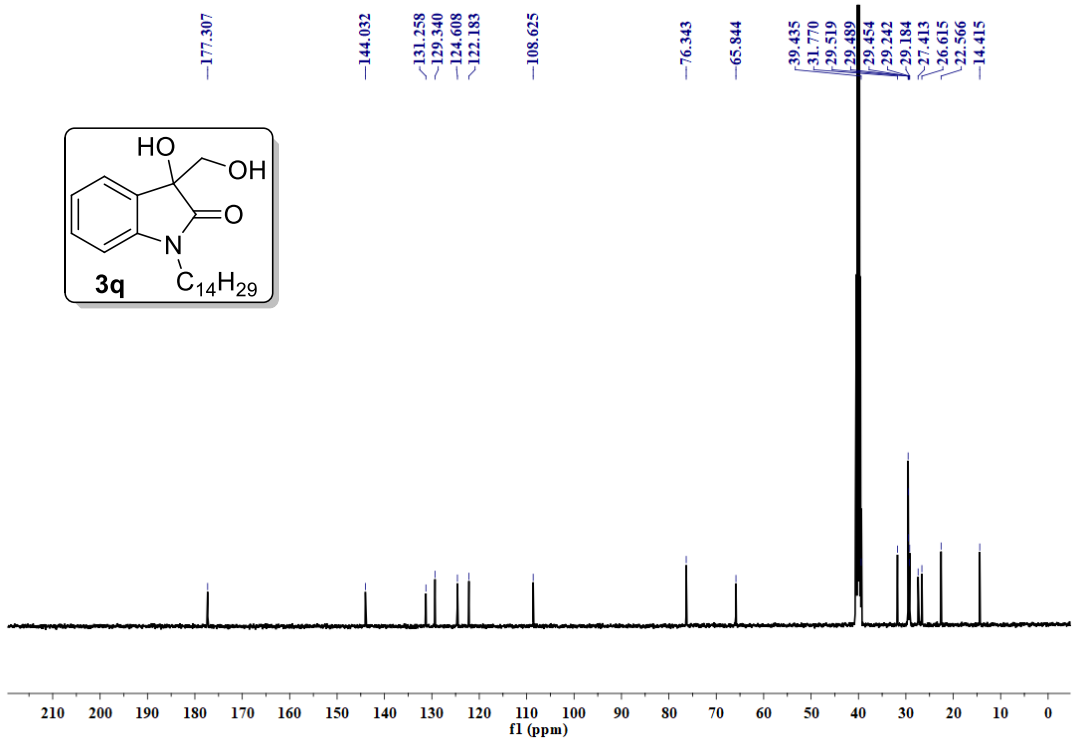
Sample Name	CLPGYLISRG	**Position**	P1-B4	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	2	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	4.10.19-13.d
ACQ Method	srinu.m	**Comment**		**Acquired Time**	04-Oct-19 5:06:08 PM



^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 3-hydroxy-3-(hydroxymethyl)-1-tetradecylindolin-2-one (3q)

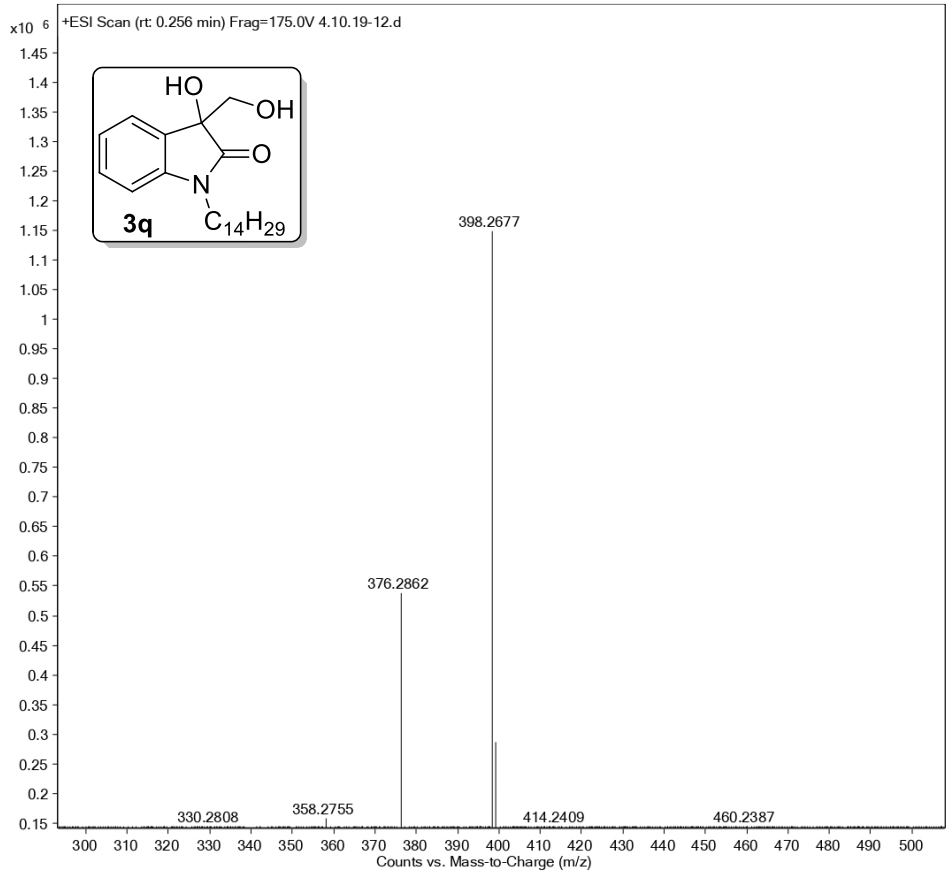


^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of 3-hydroxy-3-(hydroxymethyl)-1-tetradecylindolin-2-one (3q)

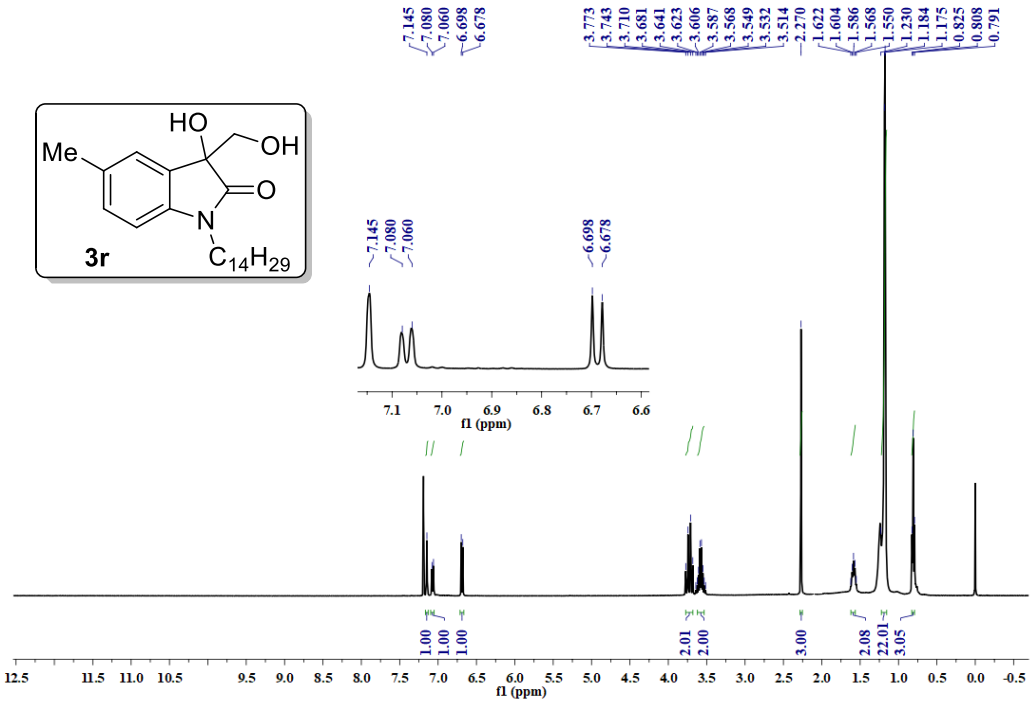


HRMS of 3-hydroxy-3-(hydroxymethyl)-1-tetradecylindolin-2-one (3q)

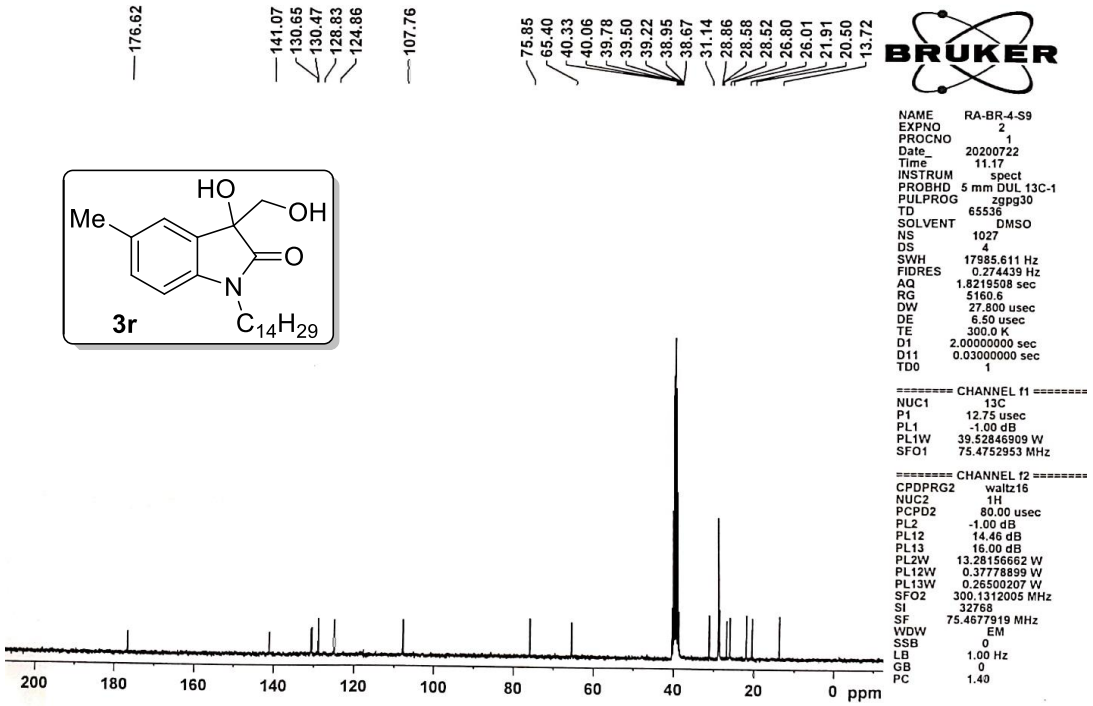
Sample Name	N-TDLISRG	**Position**	P1-B3	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	2	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	4.10.19-12.d
ACQ Method	srinu.m	**Comment**		**Acquired Time**	04-Oct-19 5:02:09 PM



^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3-hydroxy-3-(hydroxymethyl)-5-methyl-1-tetradecylindolin-2-one (3r)

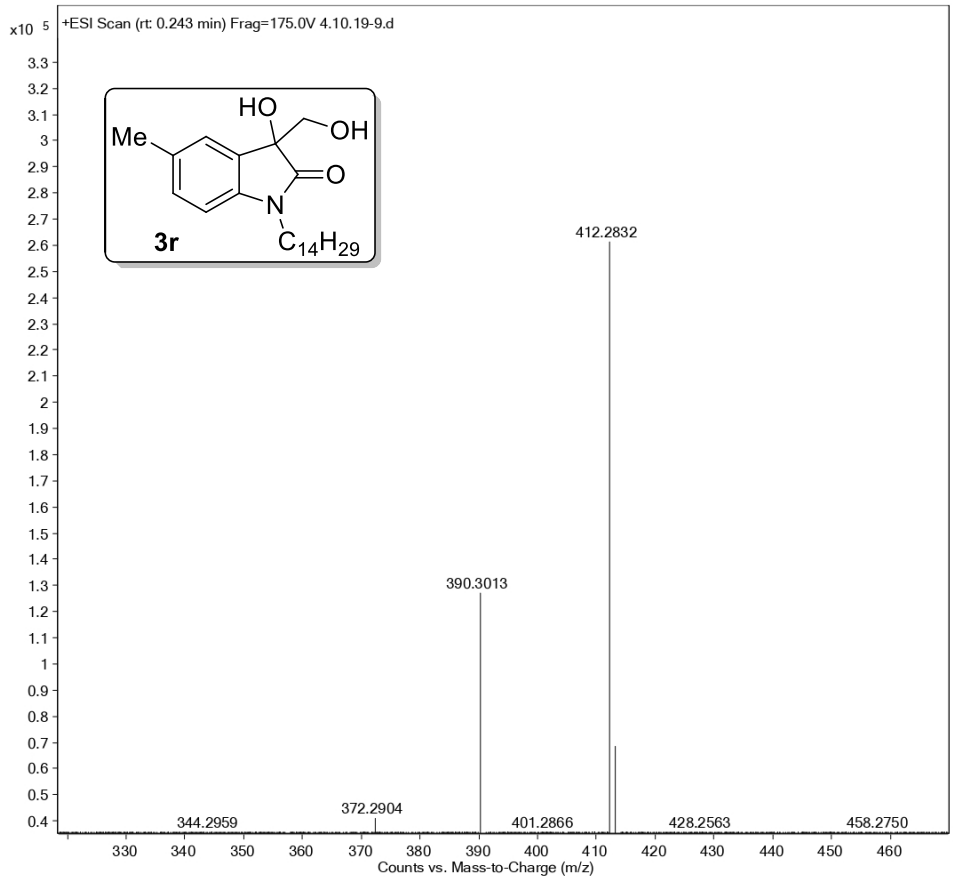


^{13}C{^{1}H} NMR (75 MHz, DMSO-d_6) spectrum of 3-hydroxy-3-(hydroxymethyl)-5-methyl-1-tetradecylindolin-2-one (3r)

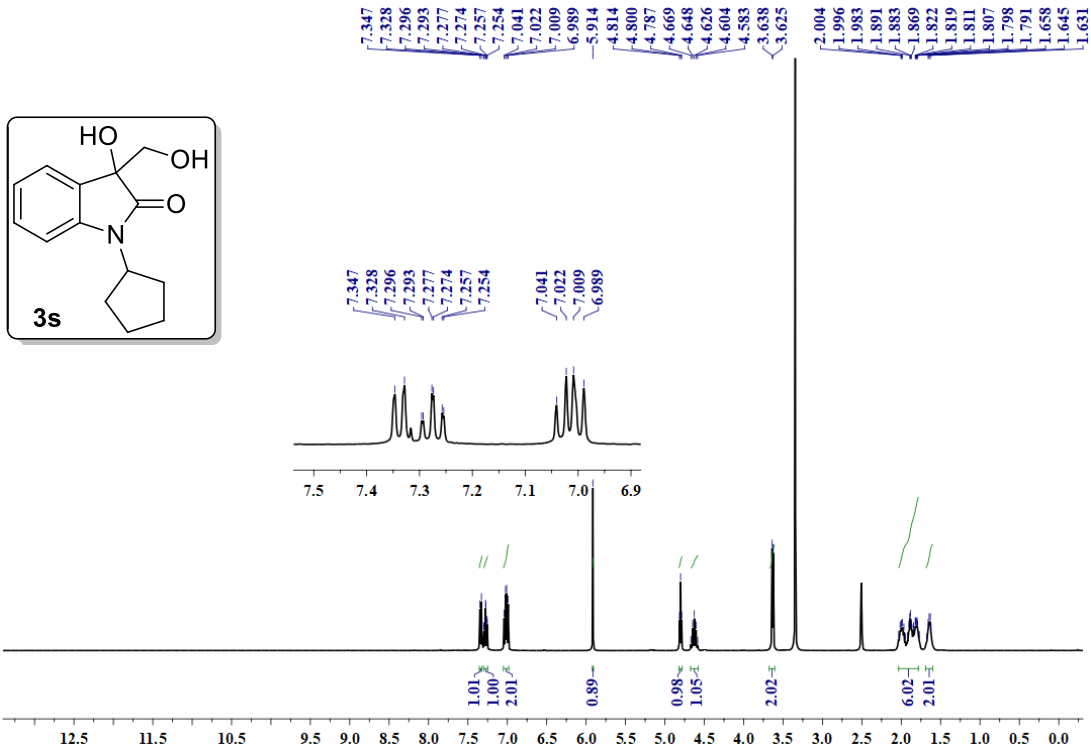


HRMS of 3-hydroxy-3-(hydroxymethyl)-5-methyl-1-tetradecylindolin-2-one (3r)

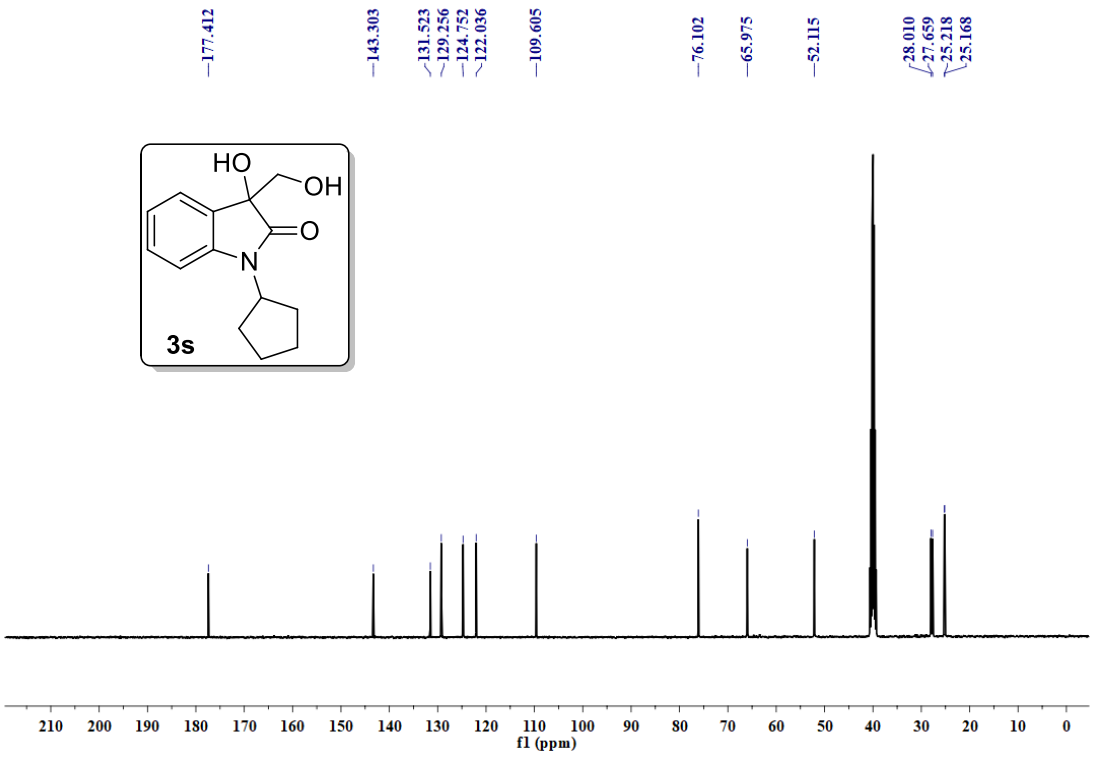
Sample Name	METDISRG	**Position**	P1-A9	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	2	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	4.10.19-9.d
ACQ Method	srinu.m	**Comment**		**Acquired Time**	04-Oct-19 4:50:12 PM



^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 1-cyclopentyl-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3s)

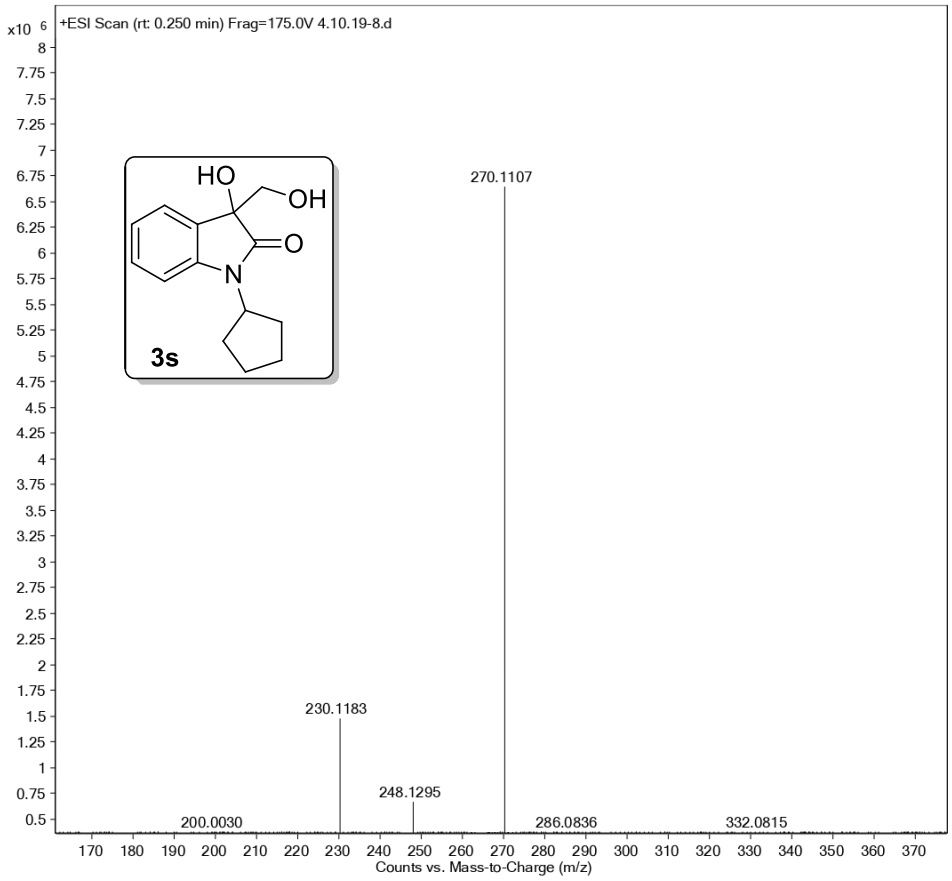


^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of 1-cyclopentyl-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3s)

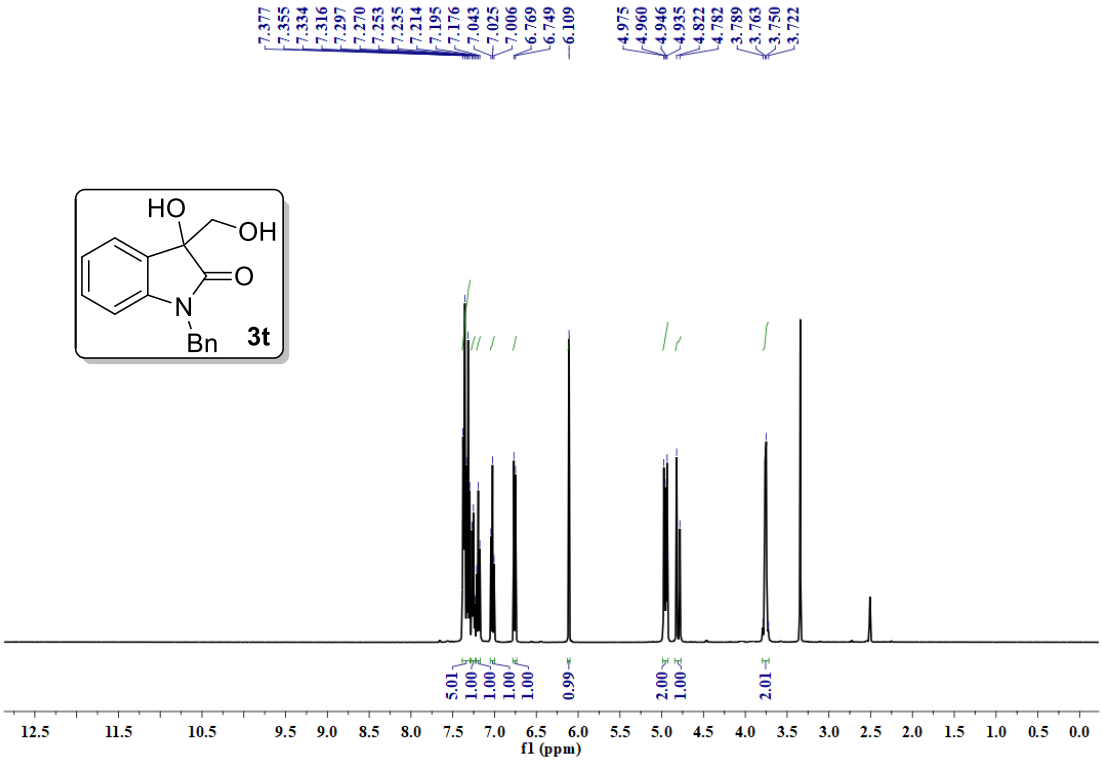


HRMS of 1-cyclopentyl-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3s)

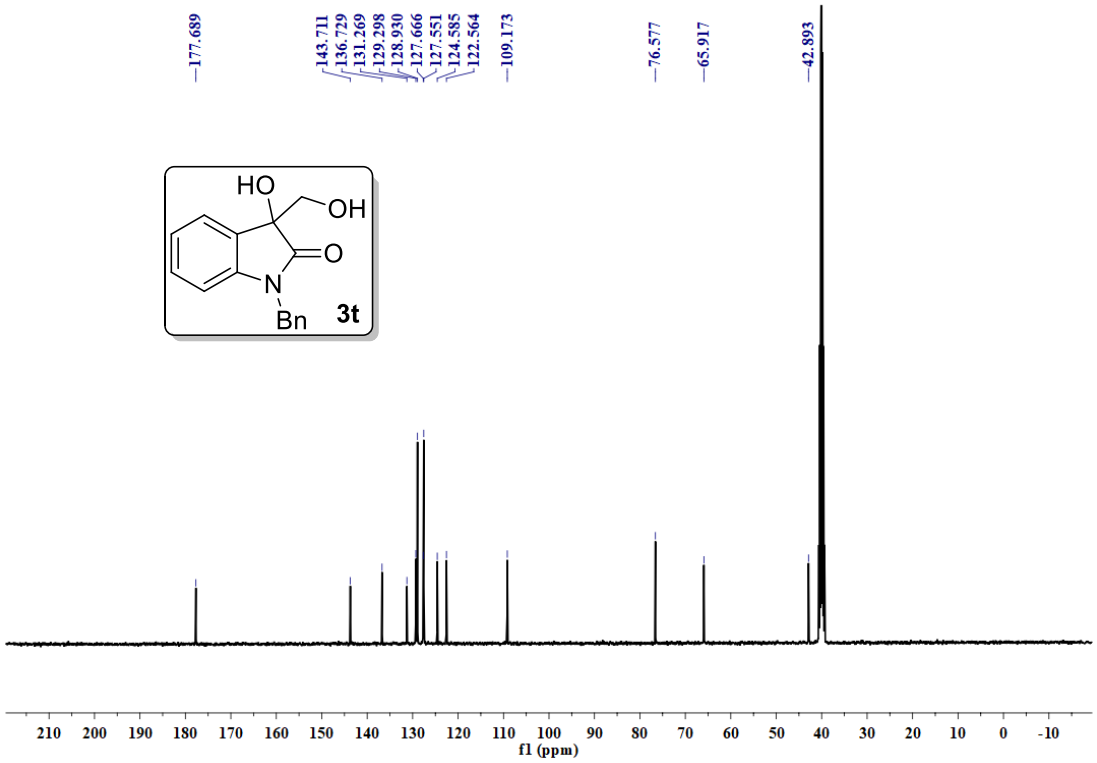
Sample Name	N-CYPLISRG	**Position**	P1-A8	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	2	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	4.10.19-8.d
ACQ Method	srinu.m	**Comment**		**Acquired Time**	04-Oct-19 4:46:15 PM



^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 1-benzyl-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3t)

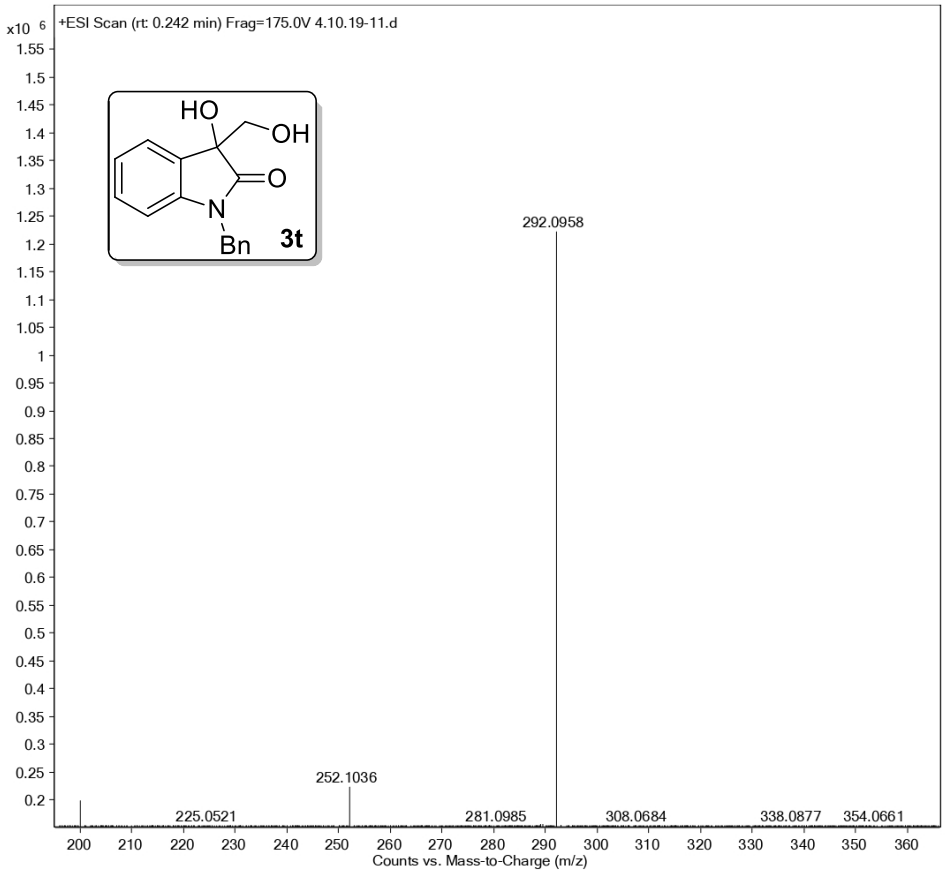


^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of 1-benzyl-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3t)

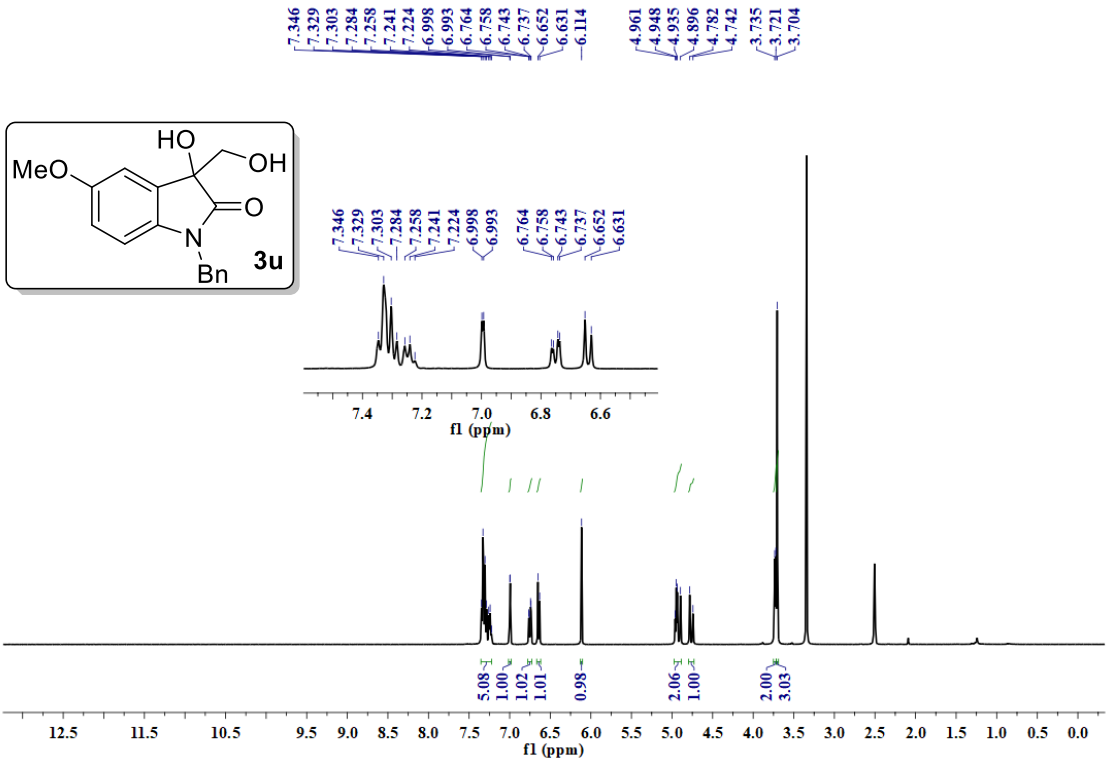


HRMS of 1-benzyl-3-hydroxy-3-(hydroxymethyl)indolin-2-one (3t)

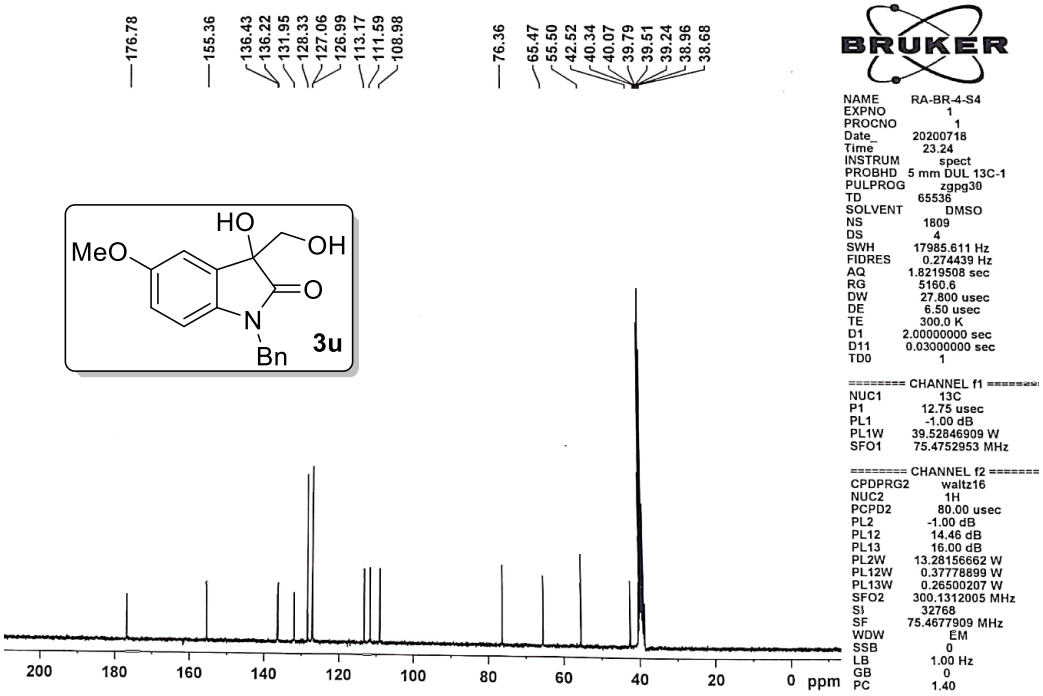
Sample Name	N-BNLISRG	**Position**	P1-B2	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	2	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	4.10.19-11.d
ACQ Method	srinu.m	**Comment**		**Acquired Time**	04-Oct-19 4:58:11 PM



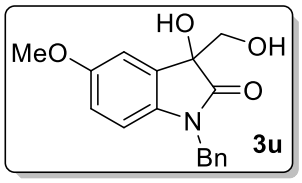
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 1-benzyl-3-hydroxy-3-(hydroxymethyl)-5-methoxyindolin-2-one (3u)

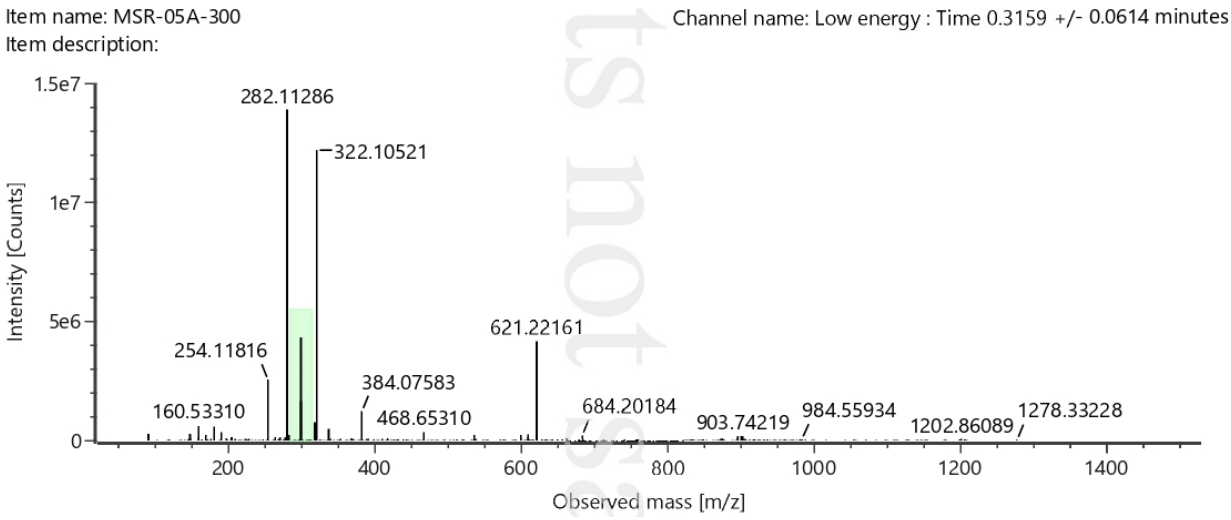


^{13}C{^{1}H} NMR (75 MHz, DMSO-d_6) spectrum of 1-benzyl-3-hydroxy-3-(hydroxymethyl)-5-methoxyindolin-2-one (3u)

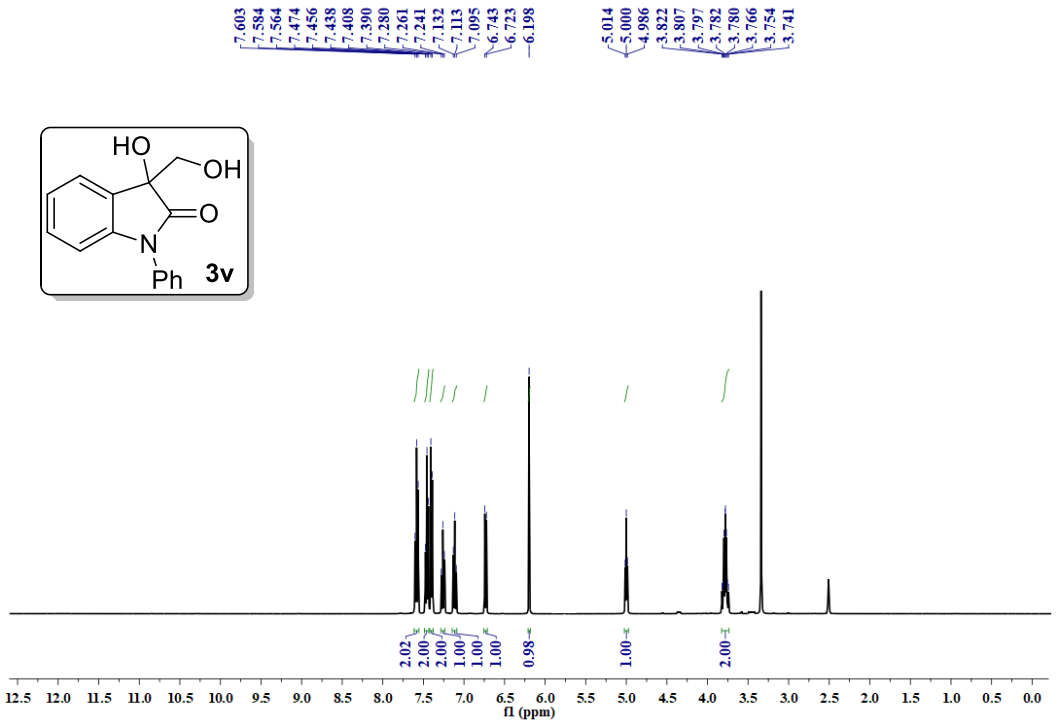


HRMS of 1-benzyl-3-hydroxy-3-(hydroxymethyl)-5-methoxyindolin-2-one (3u)

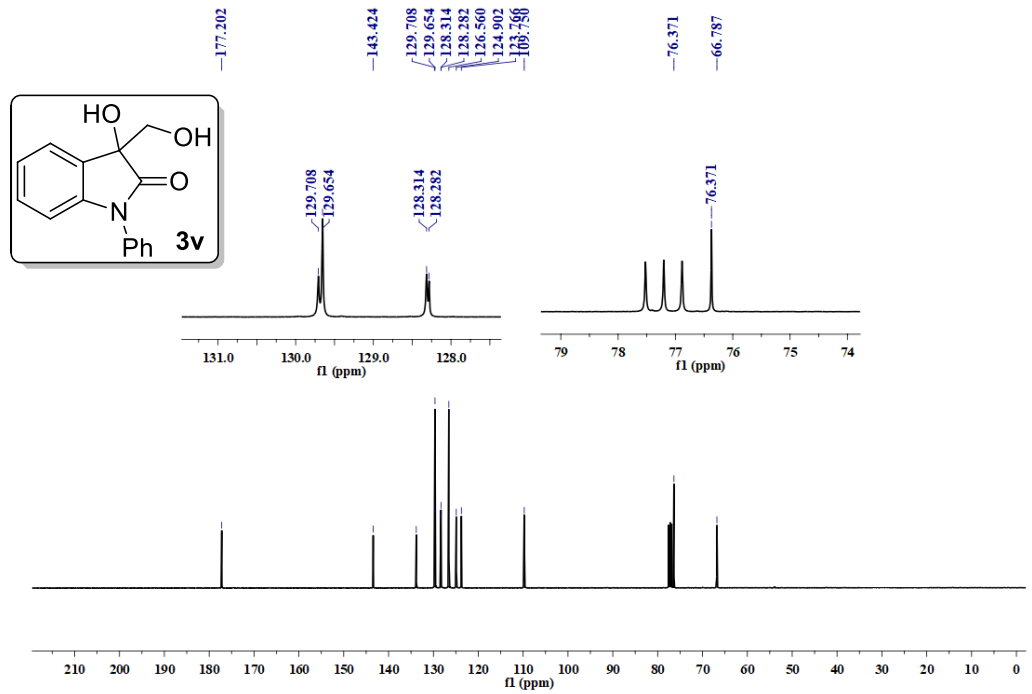




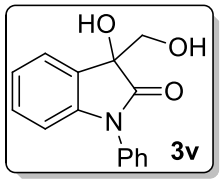
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 3-hydroxy-3-(hydroxymethyl)-1-phenylindolin-2-one (3v)

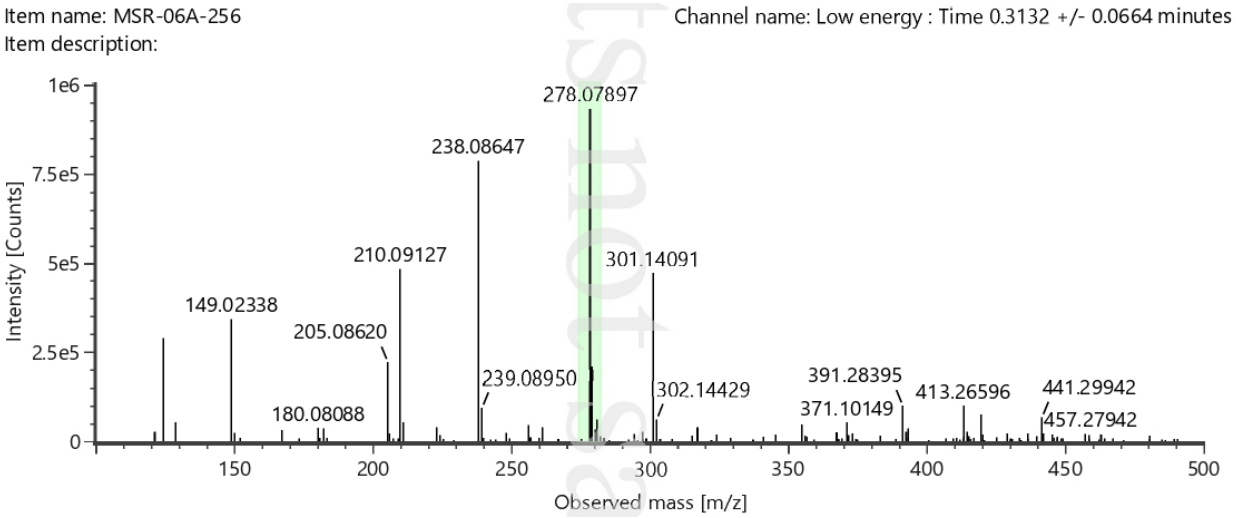


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of 3-hydroxy-3-(hydroxymethyl)-1-phenylindolin-2-one (3v)

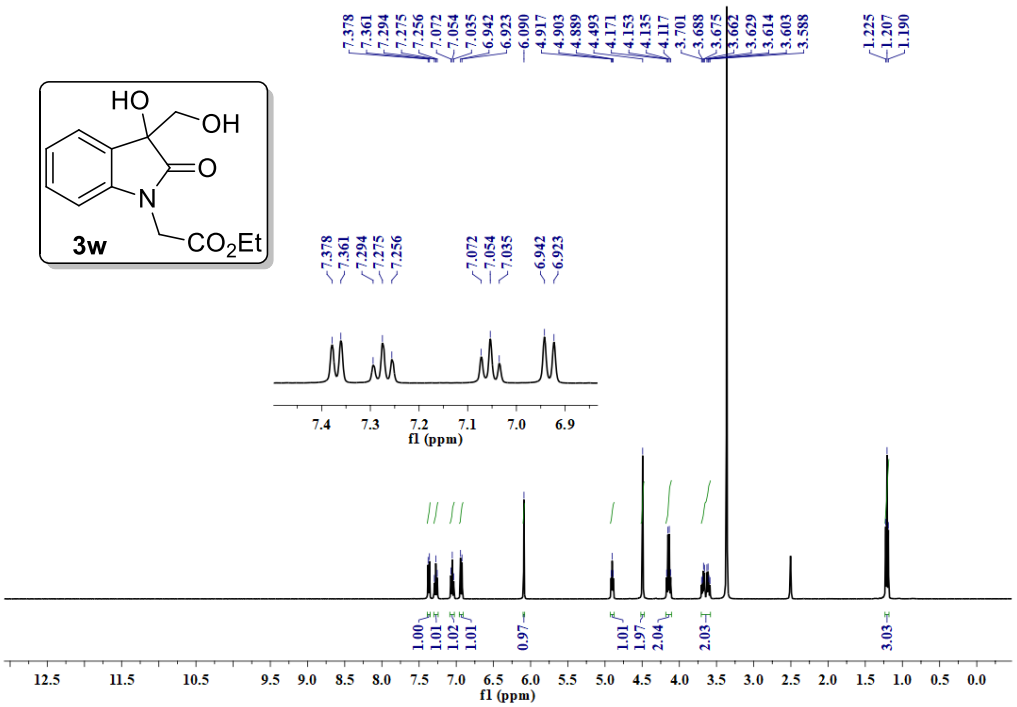


HRMS of 3-hydroxy-3-(hydroxymethyl)-1-phenylindolin-2-one (3v)

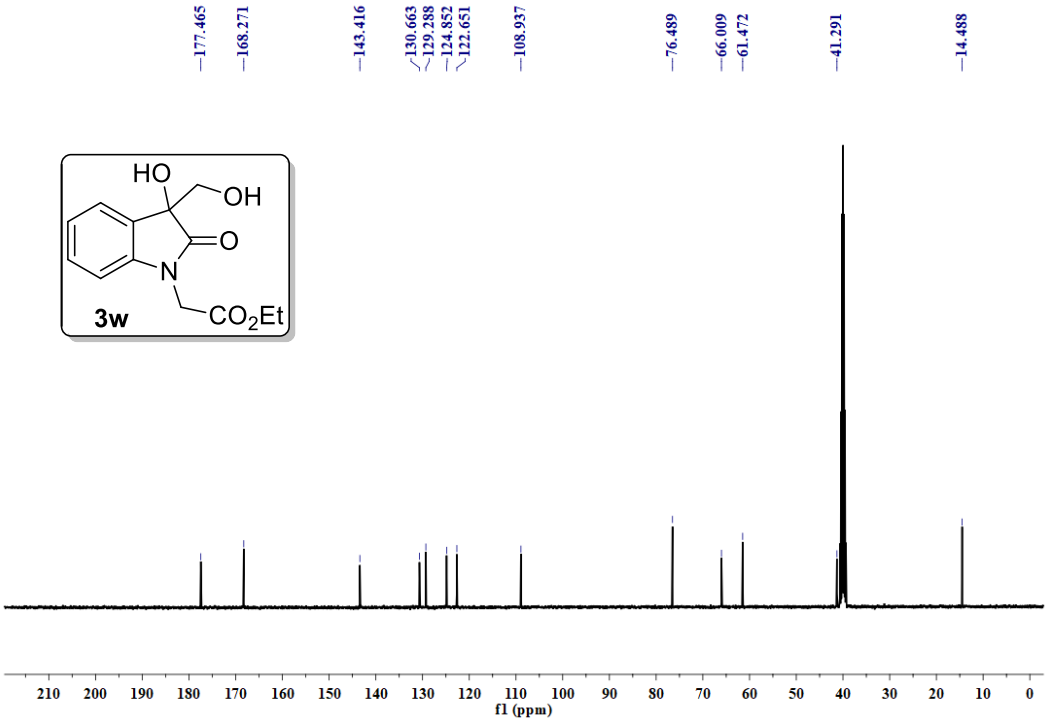




^{1}H NMR (400 MHz, DMSO-d_6) spectrum of ethyl 2-(3-hydroxy-3-(hydroxymethyl)-2-oxoindolin-1-yl)acetate (3w)

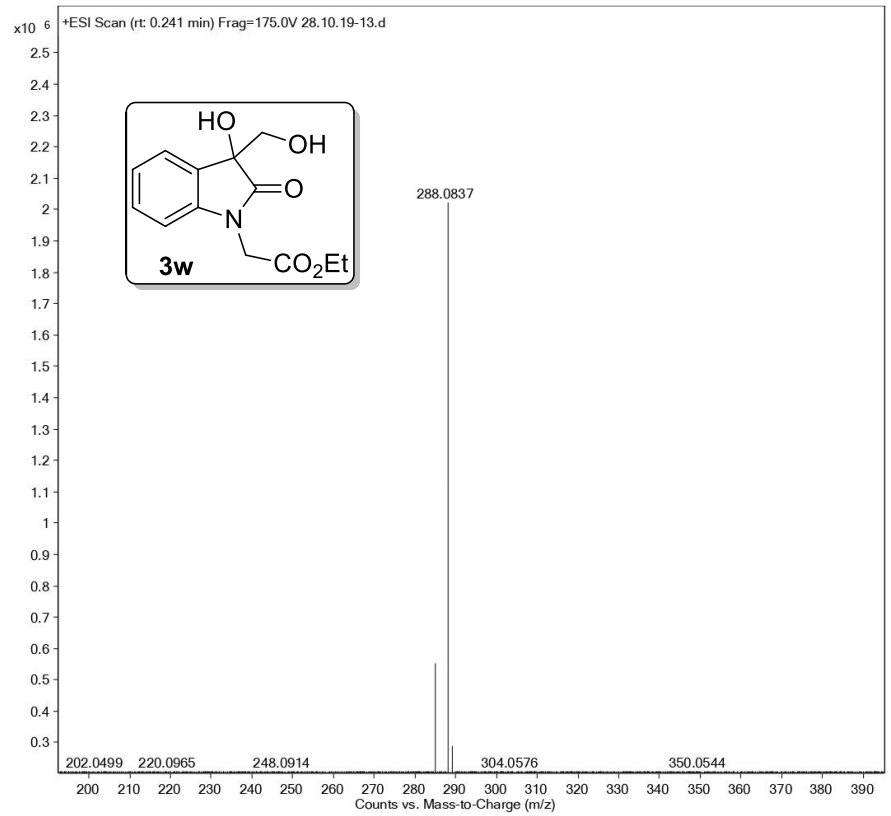


^{13}C{^{1}H} NMR (125 MHz, DMSO-d_6) spectrum of ethyl 2-(3-hydroxy-3-(hydroxymethyl)-2-oxoindolin-1-yl)acetate (3w)

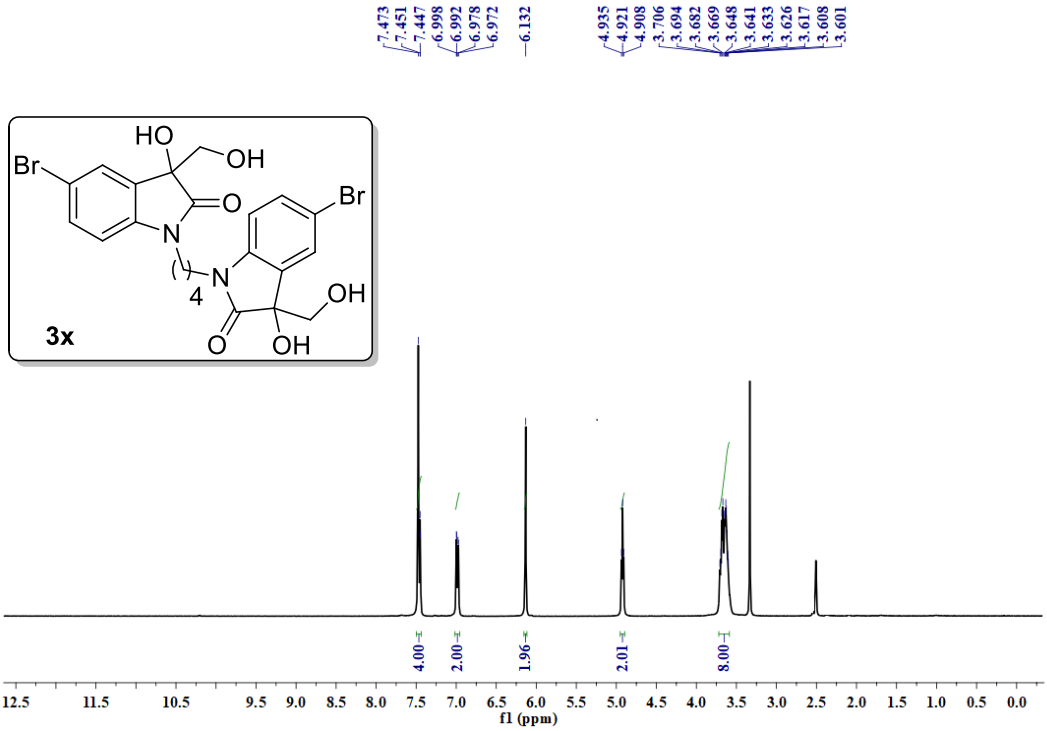


HRMS of ethyl 2-(3-hydroxy-3-(hydroxymethyl)-2-oxoindolin-1-yl)acetate (3w)

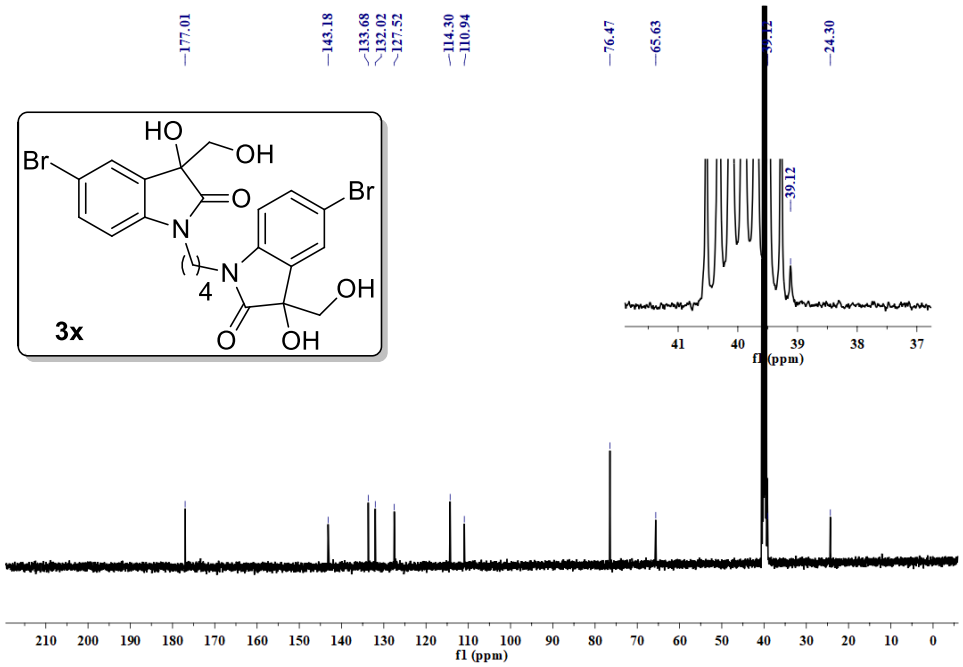
Sample Name	gsp 6	**Position**	P1-B4	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	2	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	28.10.19-13.d
ACQ Method	srinu.m	**Comment**		**Acquired Time**	28-Oct-19 3:15:32 PM



^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 1,1'-(butane-1,4-diyl)bis(5-bromo-3-hydroxy-3-(hydroxymethyl)indolin-2-one) (3x)

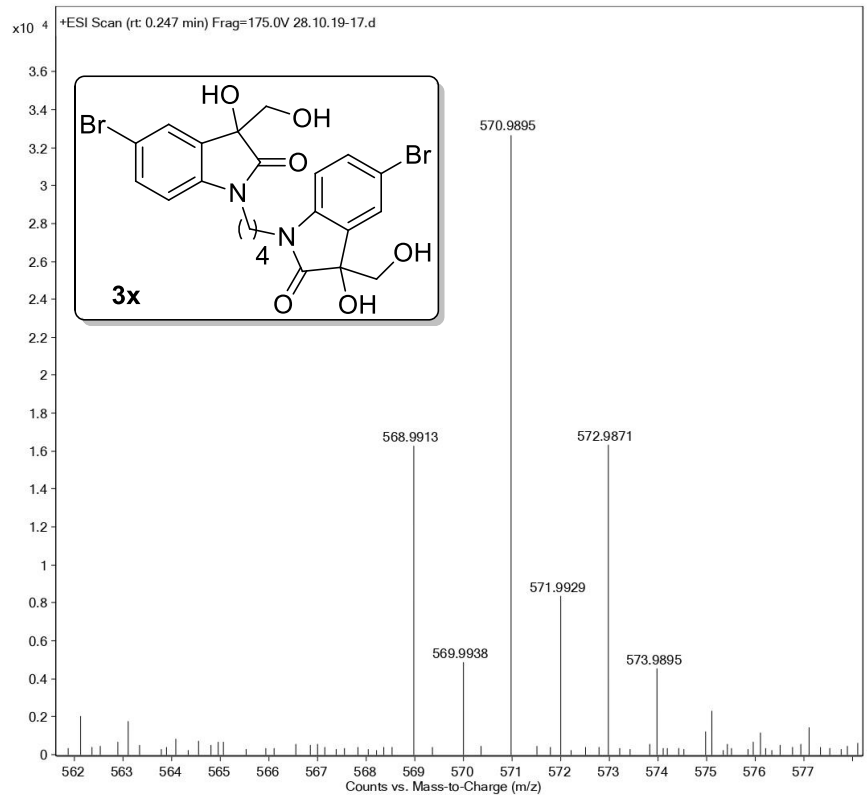


^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of 1,1'-(butane-1,4-diyl)bis(5-bromo-3-hydroxy-3-(hydroxymethyl)indolin-2-one) (3x)

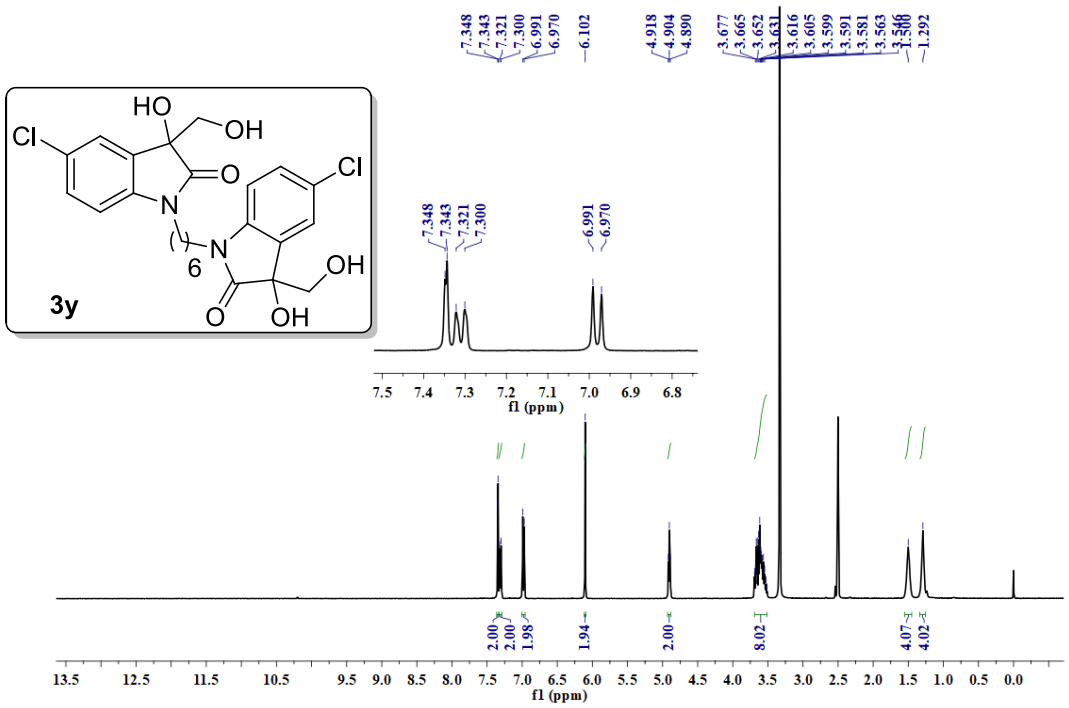


HRMS spectrum of 1,1'-(butane-1,4-diyl)bis(5-bromo-3-hydroxy-3-(hydroxymethyl)indolin-2-one) (3x)

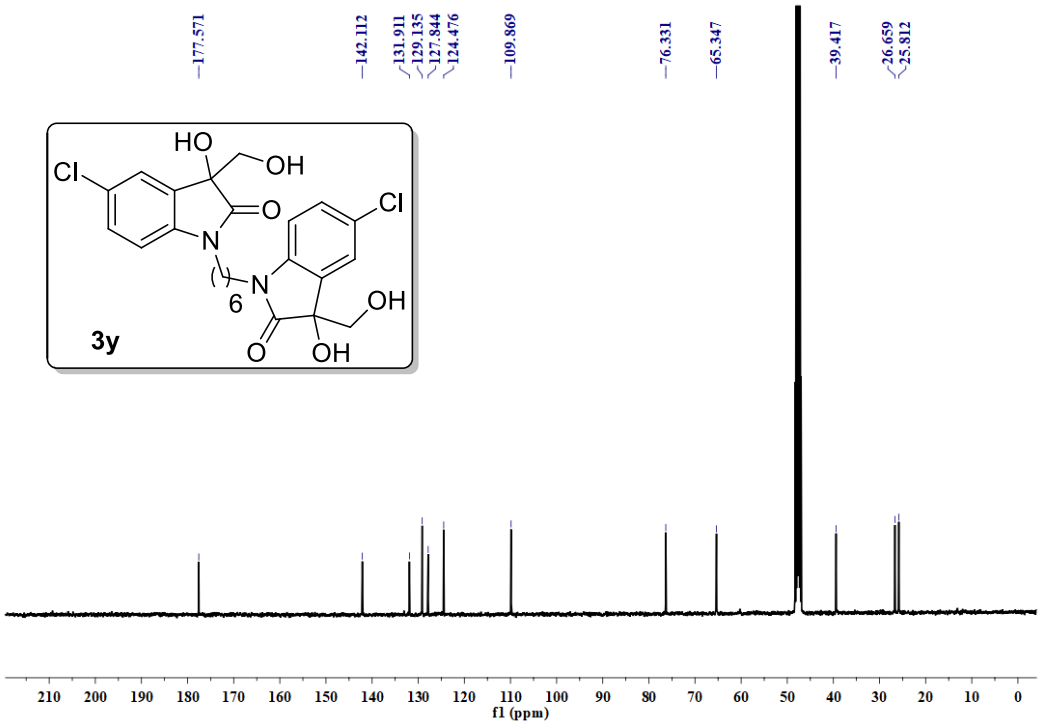
Sample Name	gsp 2	**Position**	P1-B8	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	2	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	28.10.19-17.d
ACQ Method	srinu.m	**Comment**		**Acquired Time**	28-Oct-19 3:31:27 PM



^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 1,1'-(hexane-1,6-diyl)bis(5-chloro-3-hydroxy-3-(hydroxymethyl)indolin-2-one) (3y)

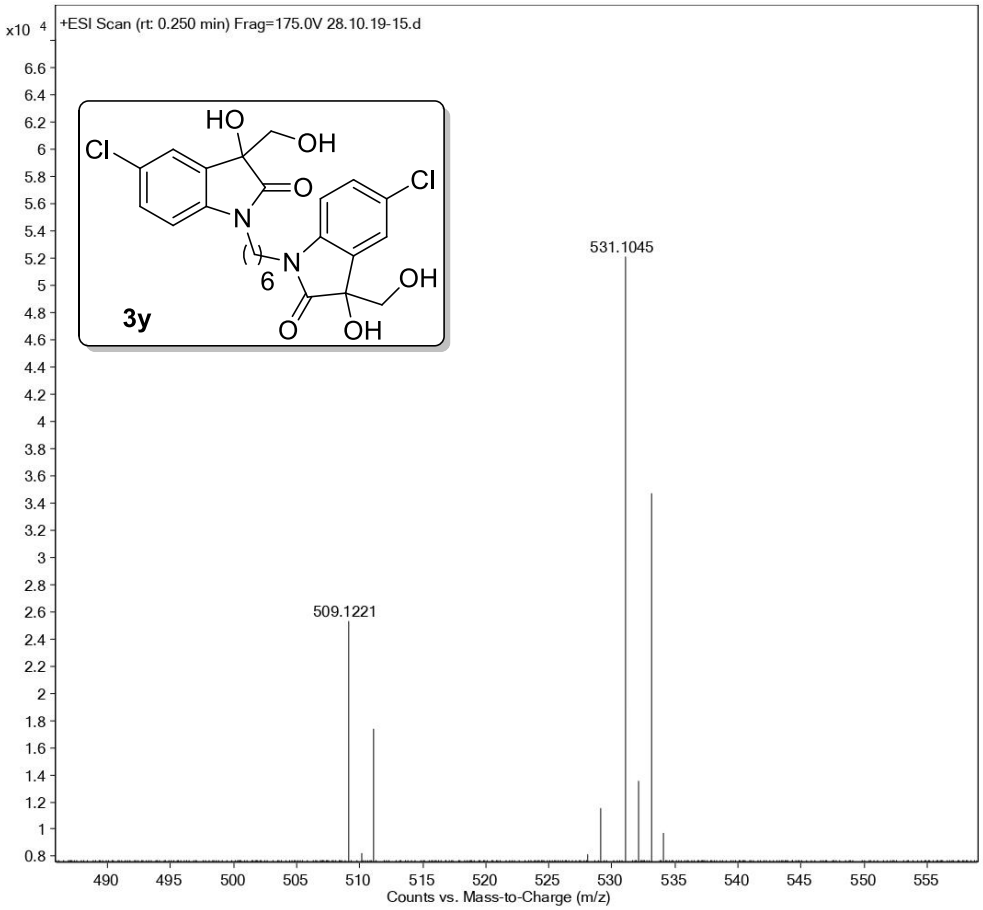


^{13}C{^{1}H} NMR (100 MHz, MeOD) spectrum of 1,1'-(hexane-1,6-diyl)bis(5-chloro-3-hydroxy-3-(hydroxymethyl)indolin-2-one) (3y)

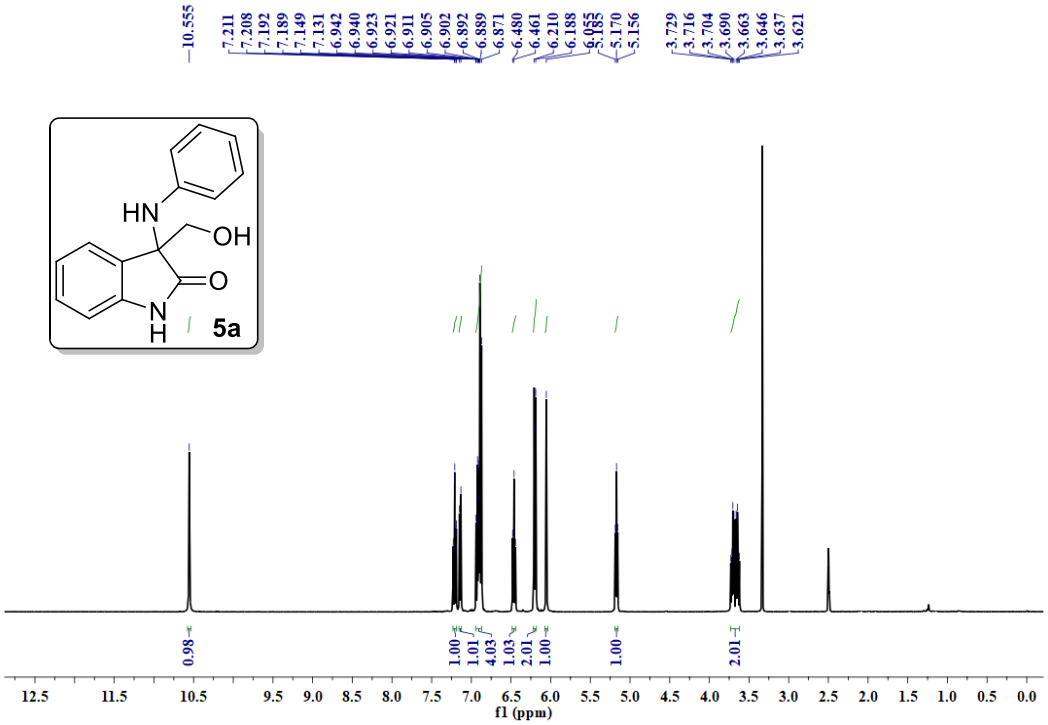


HRMS of 1,1'-(hexane-1,6-diyl)bis(5-chloro-3-hydroxy-3-(hydroxymethyl)indolin-2-one) (3y)

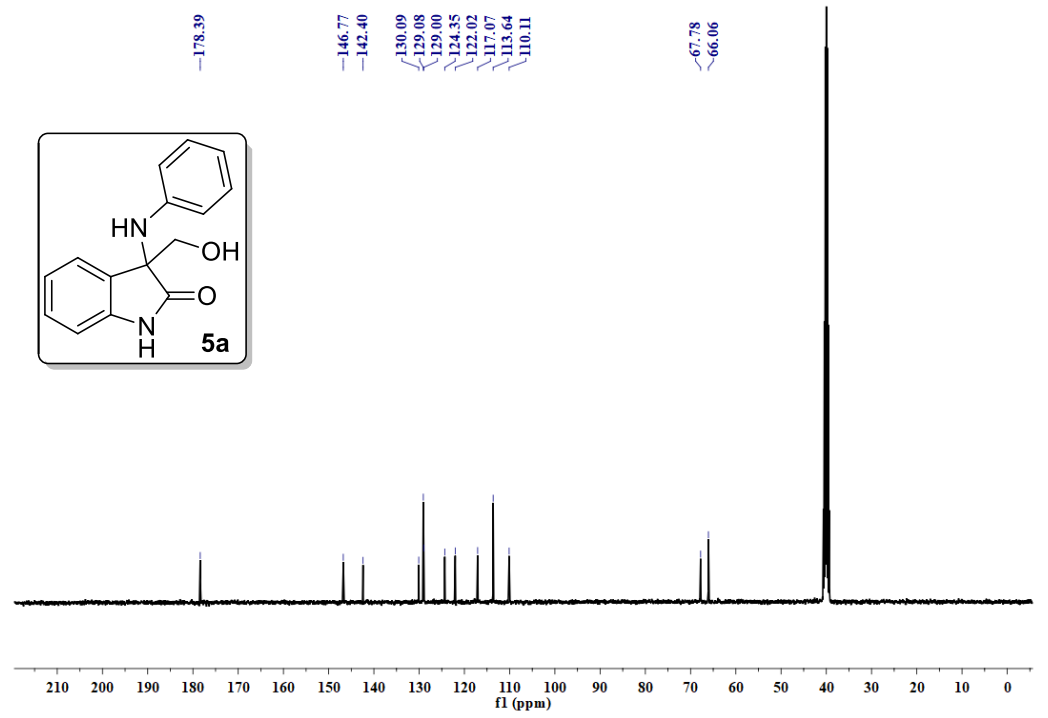
Sample Name	gsp 4	**Position**	P1-B6	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	2	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	28.10.19-15.d
ACQ Method	srinu.m	**Comment**		**Acquired Time**	28-Oct-19 3:23:30 PM



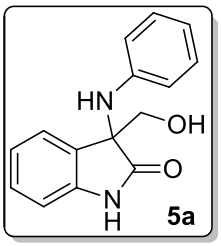
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 3-(hydroxymethyl)-3-(phenylamino)indolin-2-one (5a)



^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of 3-(hydroxymethyl)-3-(phenylamino)indolin-2-one (5a)

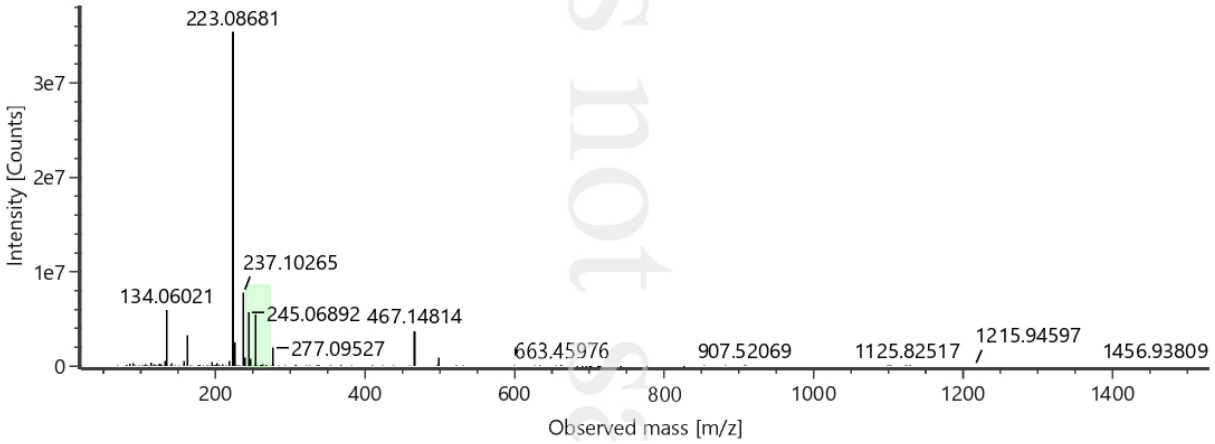


HRMS of 3-(hydroxymethyl)-3-(phenylamino)indolin-2-one (5a)

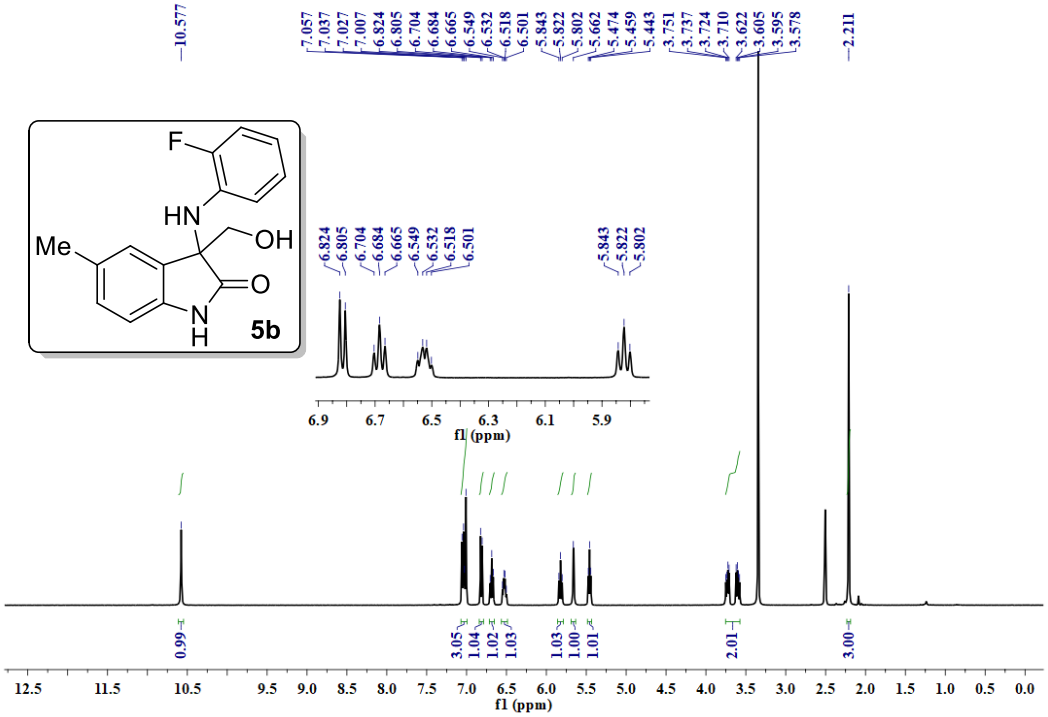


Item name: MSR-07A-255
Item description:

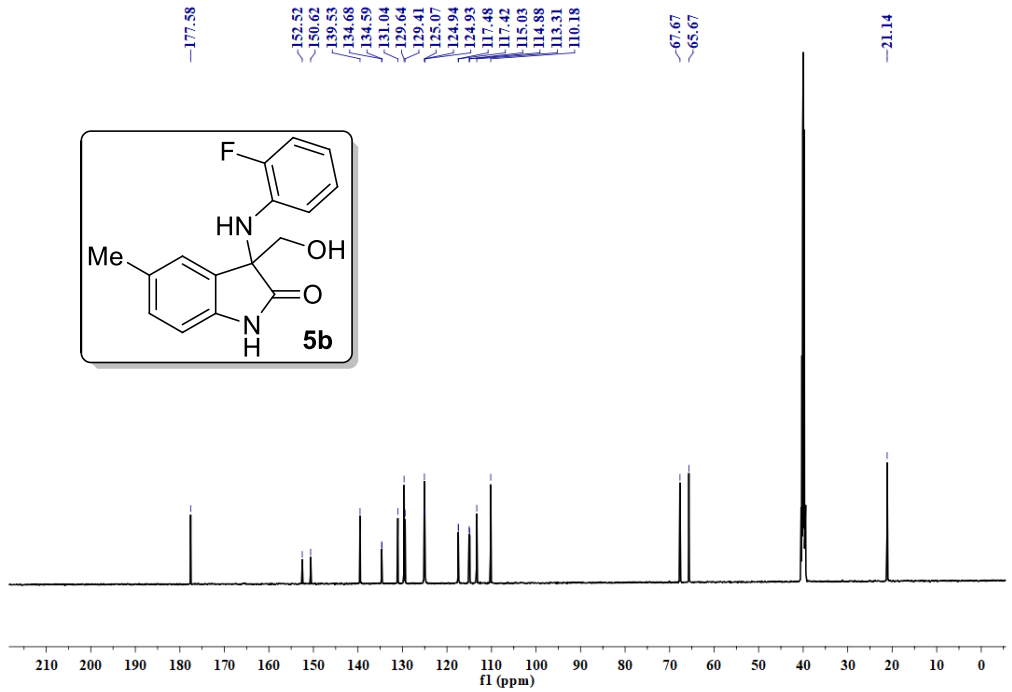
Channel name: Low energy : Time 0.3141 +/- 0.0655 minutes



^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 3-((2-fluorophenyl)amino)-3-(hydroxymethyl)-5-methylindolin-2-one (5b)

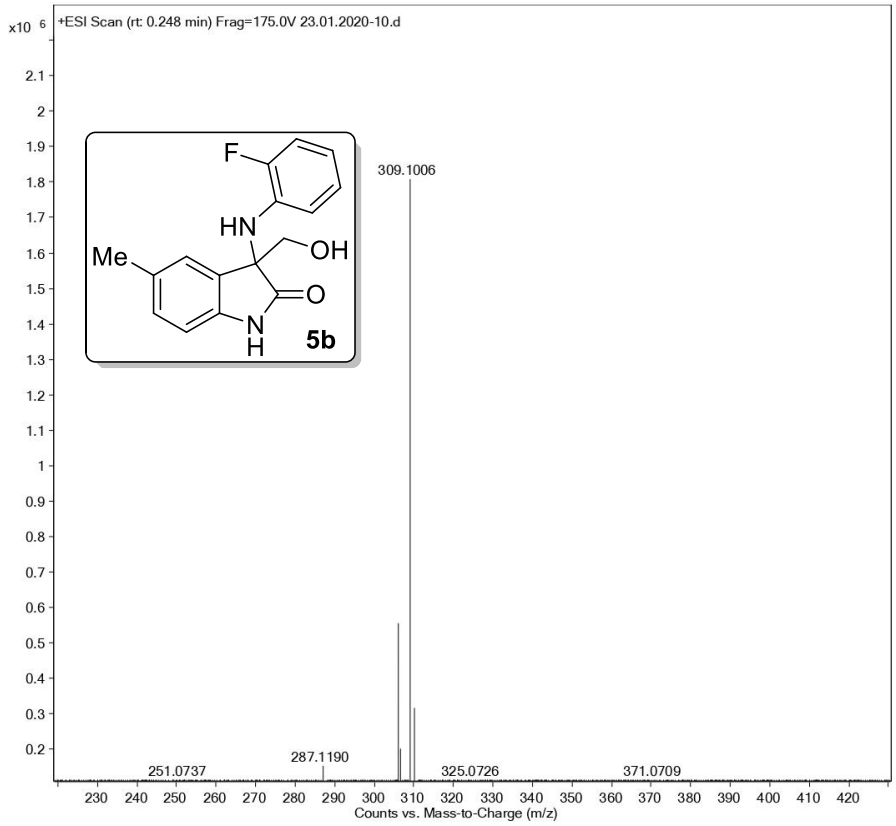


^{13}C{^{1}H} NMR (125 MHz, DMSO-d_6) spectrum of 3-((2-fluorophenyl)amino)-3-(hydroxymethyl)-5-methylindolin-2-one (5b)

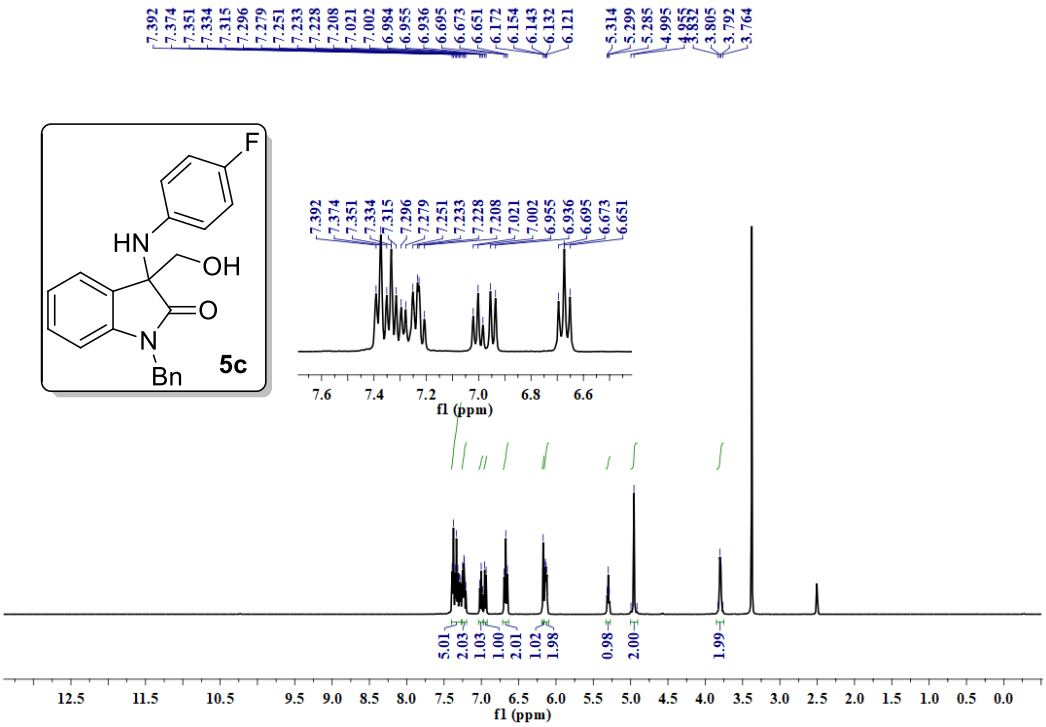


HRMS of 3-((2-fluorophenyl)amino)-3-(hydroxymethyl)-5-methylindolin-2-one (5b)

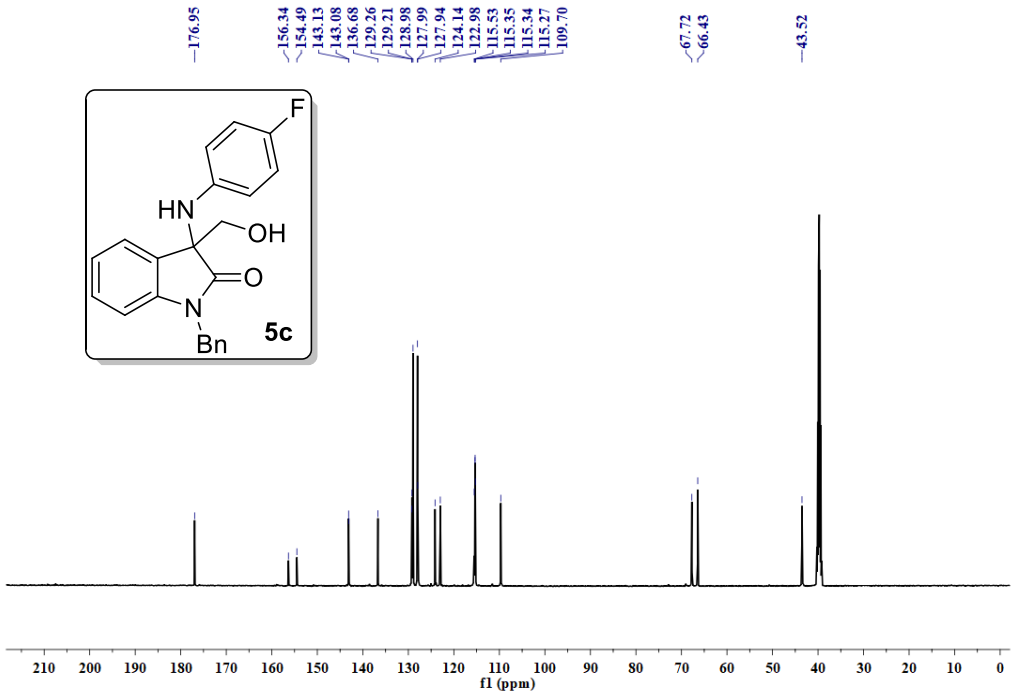
Sample Name	MEISFANI-2	**Position**	P1-B1	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	2	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	23.01.2020-10.d
ACQ Method	srinu.m	**Comment**		**Acquired Time**	23-Jan-20 4:54:09 PM



^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 1-benzyl-3-((4-fluorophenyl)amino)-3-(hydroxymethyl)indolin-2-one (5c)

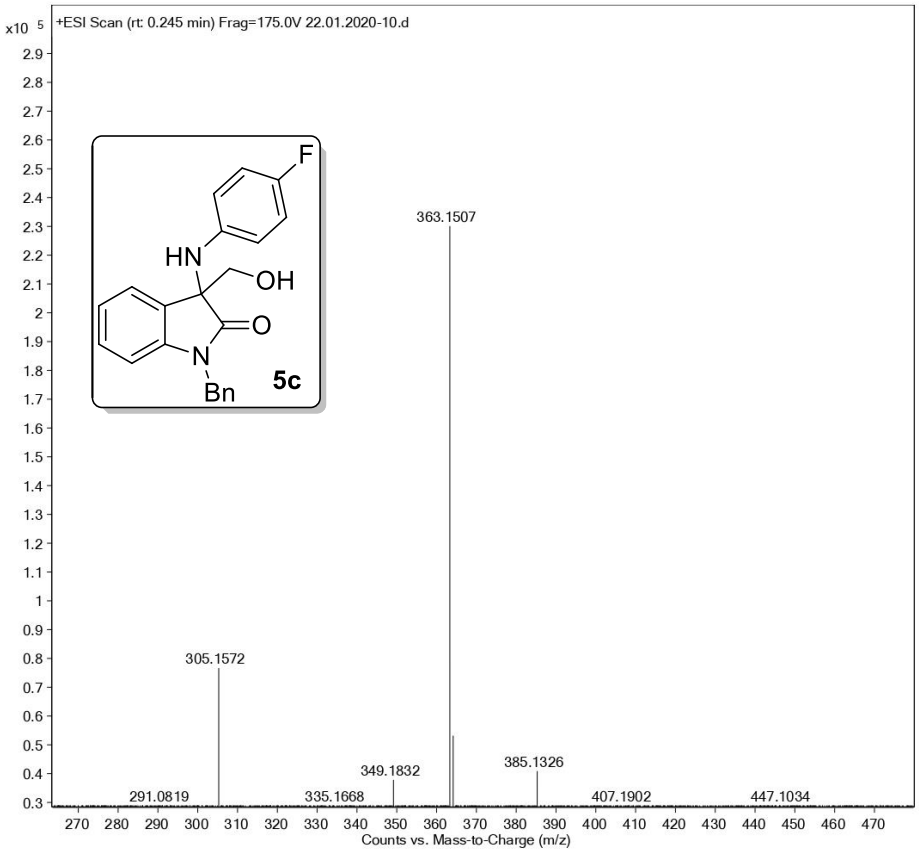


^{13}C{^{1}H} NMR (125 MHz, DMSO-d_6) spectrum of 1-benzyl-3-((4-fluorophenyl)amino)-3-(hydroxymethyl)indolin-2-one (5c)

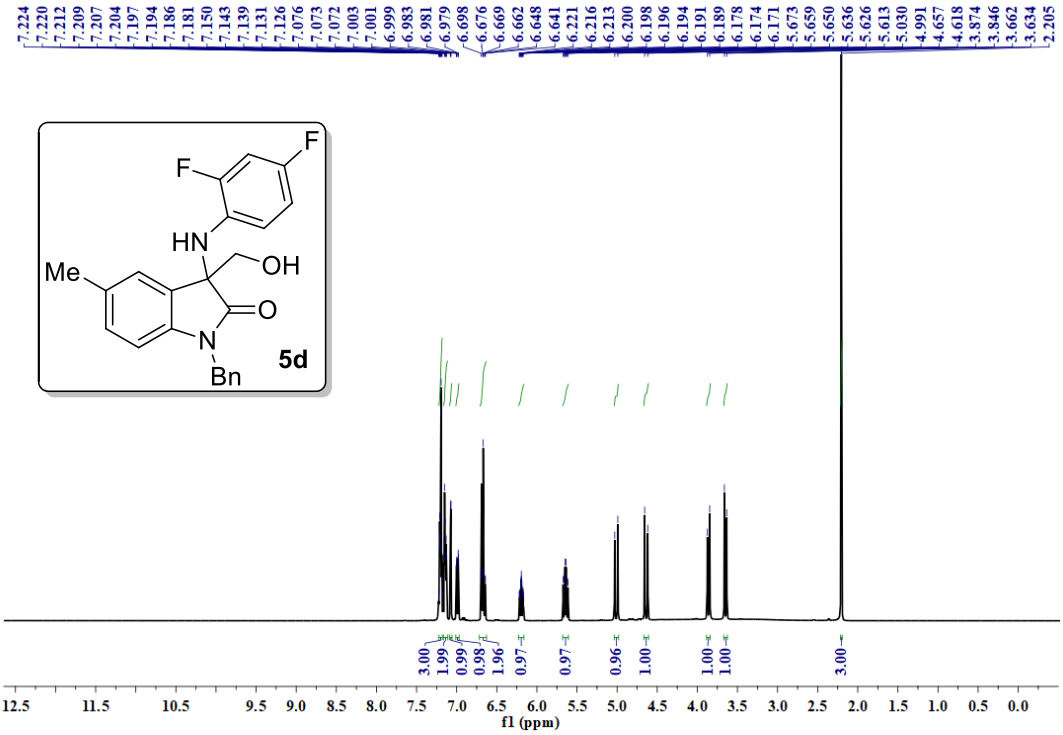


HRMS of 1-benzyl-3-((4-fluorophenyl)amino)-3-(hydroxymethyl)indolin-2-one (5c)

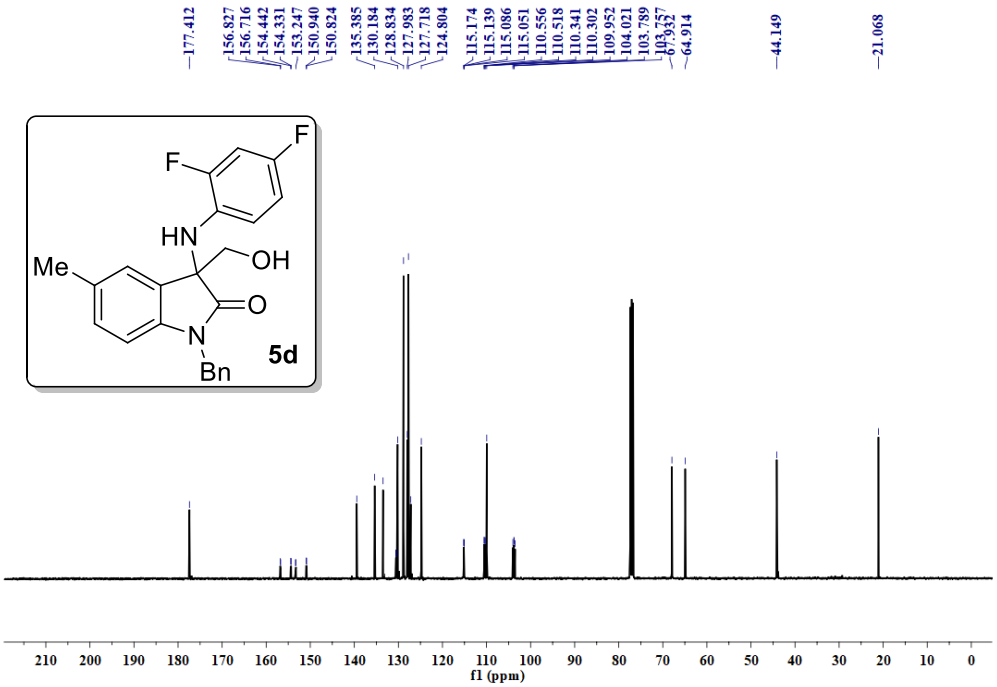
Sample Name	NBNISFANI-4	**Position**	P1-B1	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	2	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	22.01.2020-10.d
ACQ Method	srinu.m	**Comment**		**Acquired Time**	22-Jan-20 4:28:26 PM



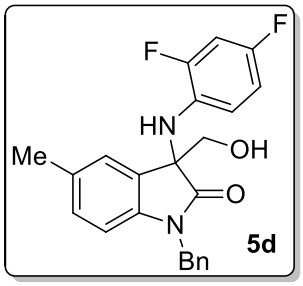
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 1-benzyl-3-((2,4-difluorophenyl)amino)-3-(hydroxymethyl)-5-methylindolin-2-one (5d)



^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spcetrum of 1-benzyl-3-((2,4-difluorophenyl)amino)-3-(hydroxymethyl)-5-methylindolin-2-one (5d)

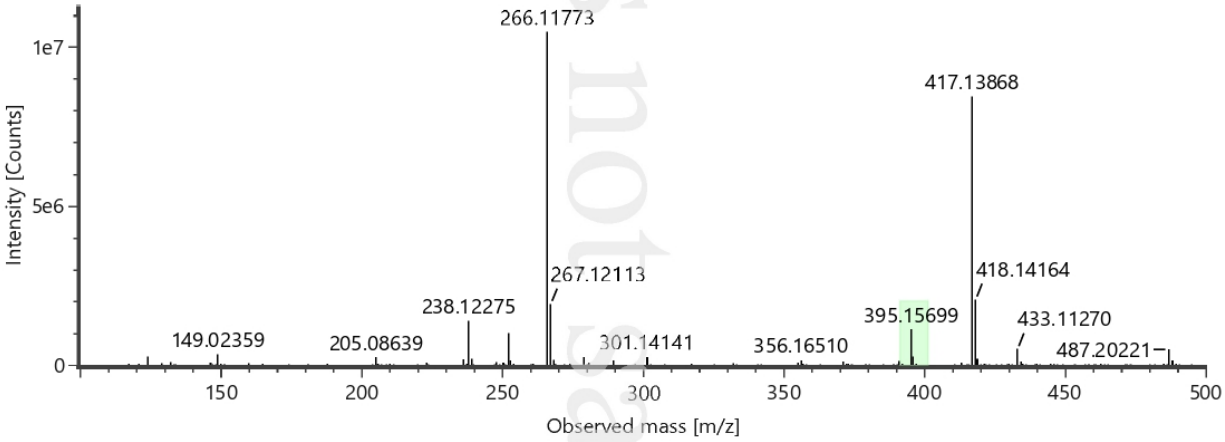


HRMS of 1-benzyl-3-((2,4-difluorophenyl)amino)-3-(hydroxymethyl)-5-methylindolin-2-one (5d)

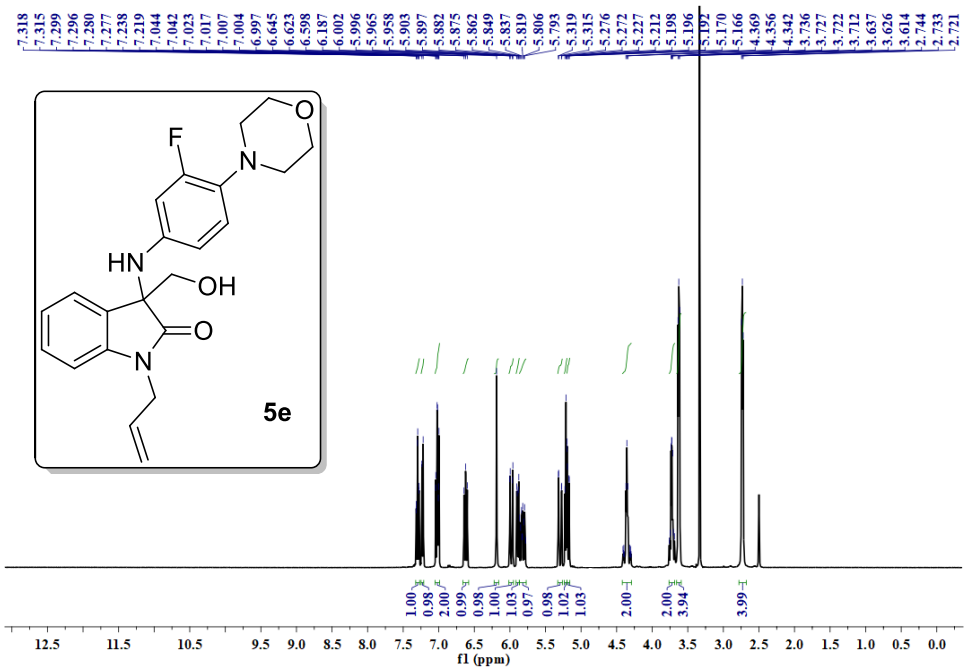


Item name: MSR-08A-395
Item description:

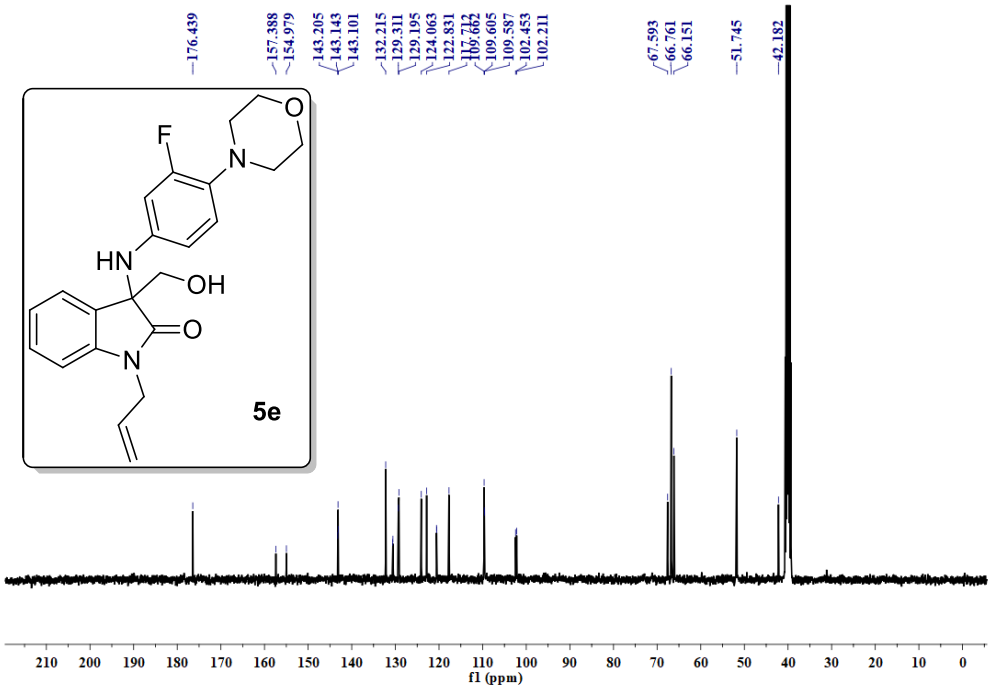
Channel name: Low energy : Time 0.3119 +/- 0.0681 minutes



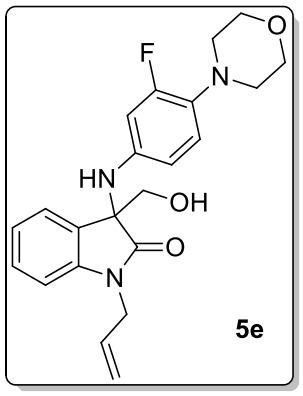
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 1-allyl-3-((3-fluoro-4-morpholinophenyl)amino)-3-(hydroxymethyl)indolin-2-one (5e)



^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of 1-allyl-3-((3-fluoro-4-morpholinophenyl)amino)-3-(hydroxymethyl)indolin-2-one (5e)

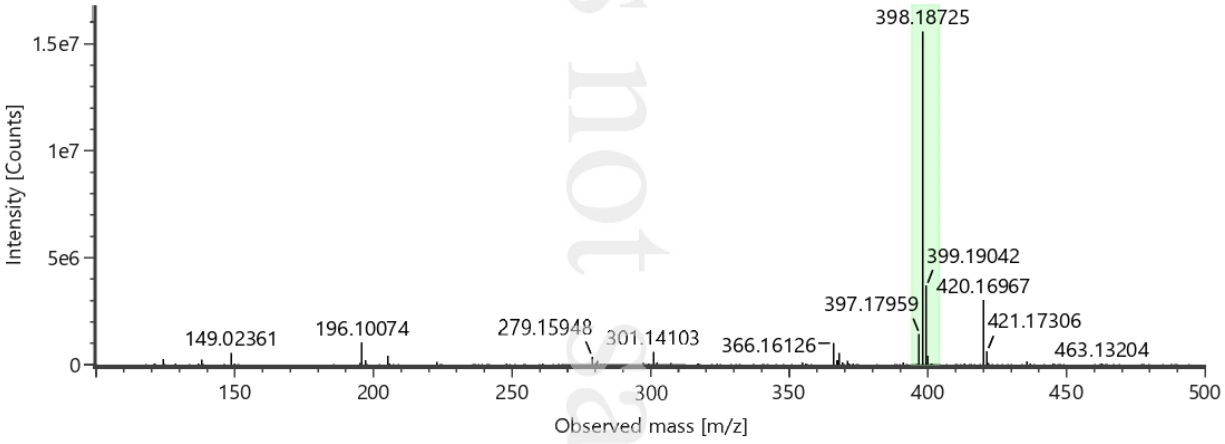


HRMS of 1-allyl-3-((3-fluoro-4-morpholinophenyl)amino)-3-(hydroxymethyl)indolin-2-one (5e)

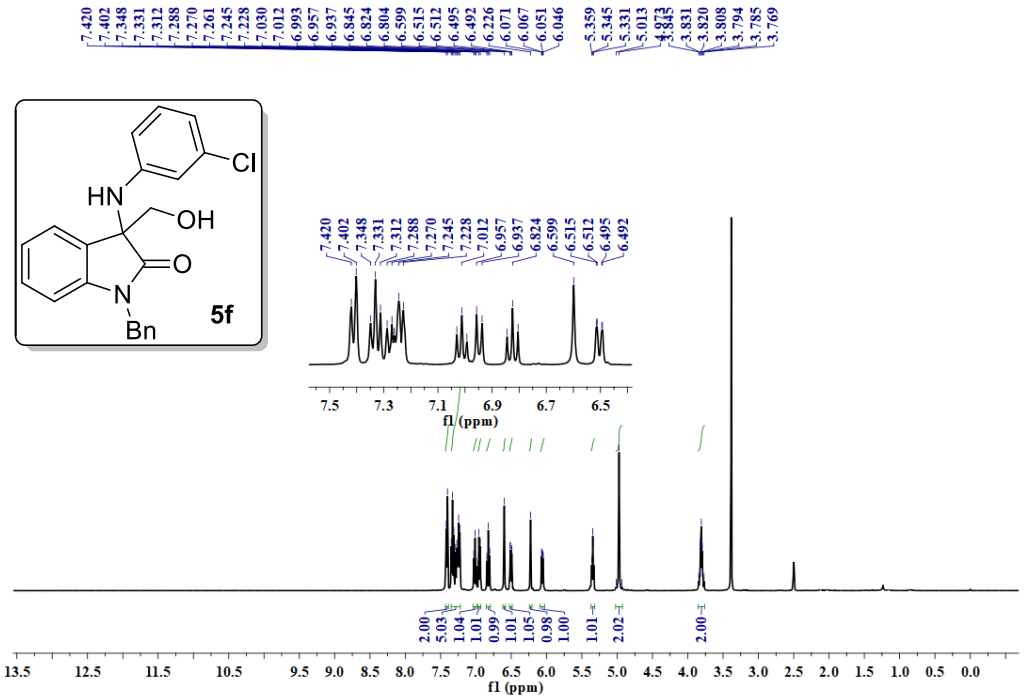


Item name: MSR-09A-398
Item description:

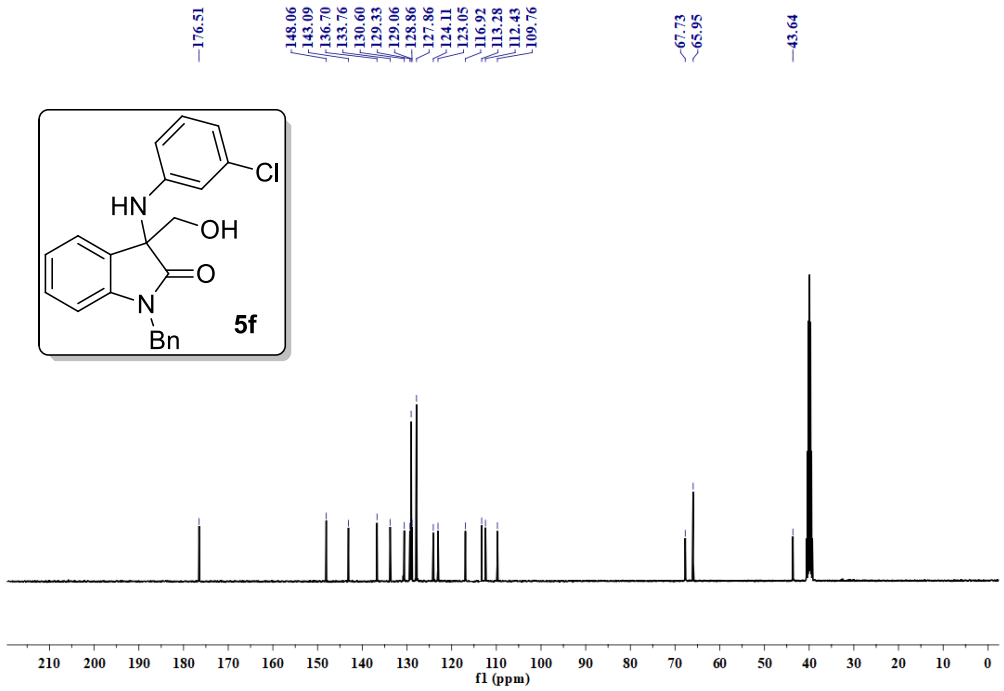
Channel name: Low energy : Time 0.3134 +/- 0.0646 minutes



^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 1-benzyl-3-((3-chlorophenyl)amino)-3-(hydroxymethyl)indolin-2-one (5f)

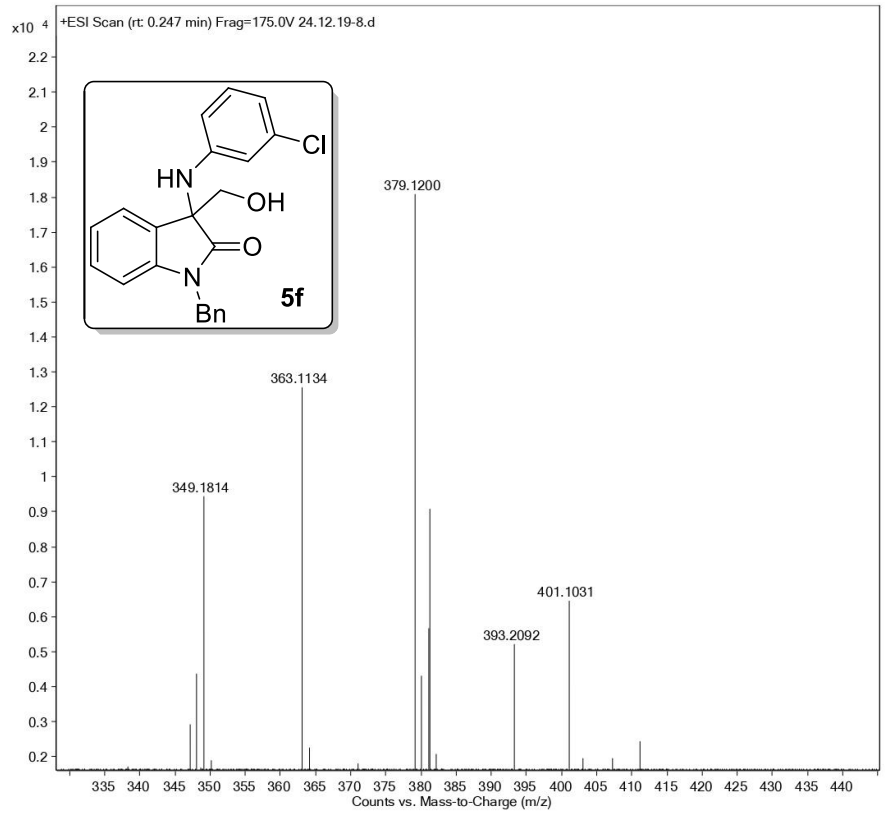


^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of 1-benzyl-3-((3-chlorophenyl)amino)-3-(hydroxymethyl)indolin-2-one (5f)

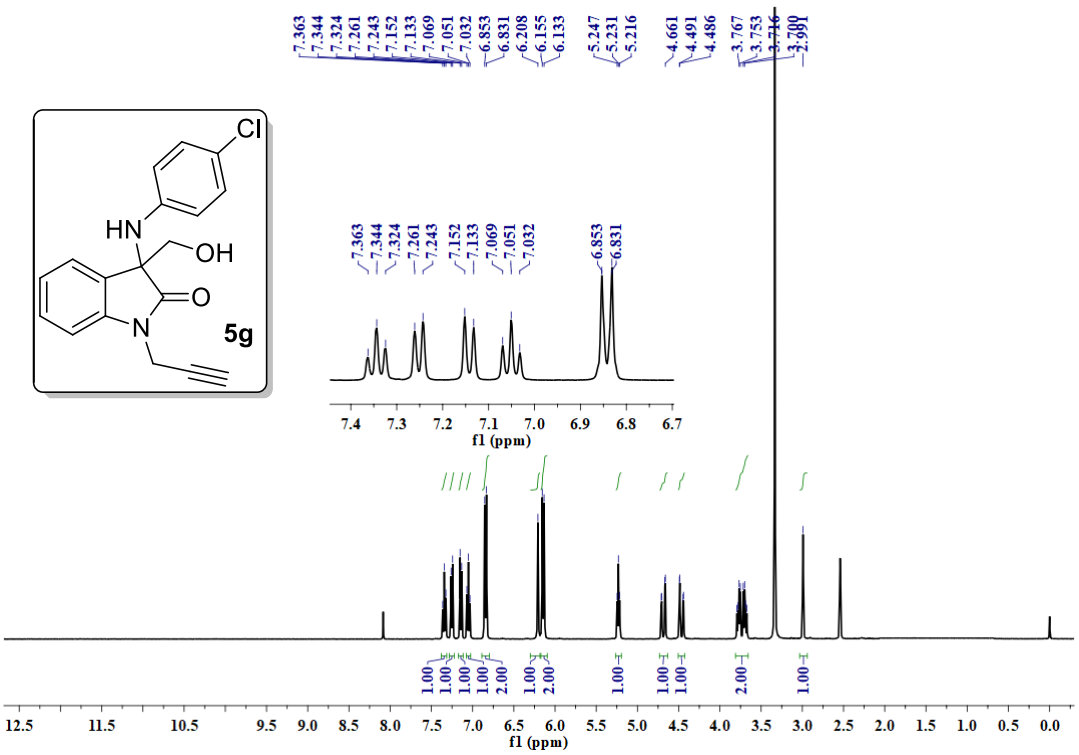


HRMS of 1-benzyl-3-((3-chlorophenyl)amino)-3-(hydroxymethyl)indolin-2-one (5f)

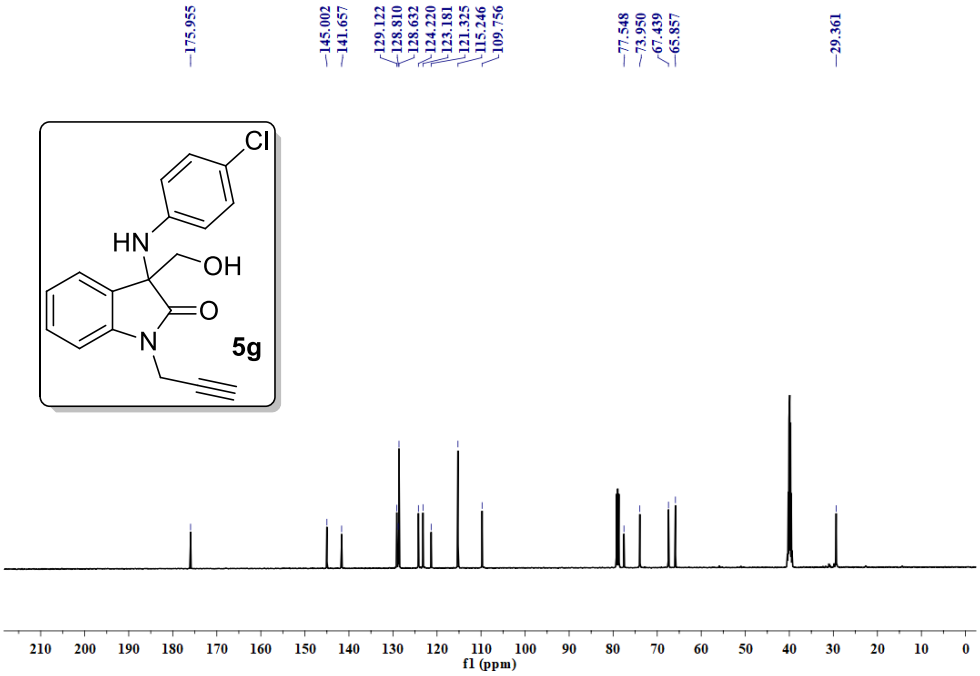
Sample Name	KHP-GSP-ISNBN-3CL	**Position**	P1-A8	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	2	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	24.12.19-8.d
ACQ Method	srinu.m	**Comment**		**Acquired Time**	24-Dec-19 4:47:38 PM



^{1}H NMR (400 MHz, $CDCl_3$+DMSO-d_6) spectrum of 3-((4-chlorophenyl)amino)-3-(hydroxymethyl)-1-(prop-2-yn-1-yl)indolin-2-one (5g)

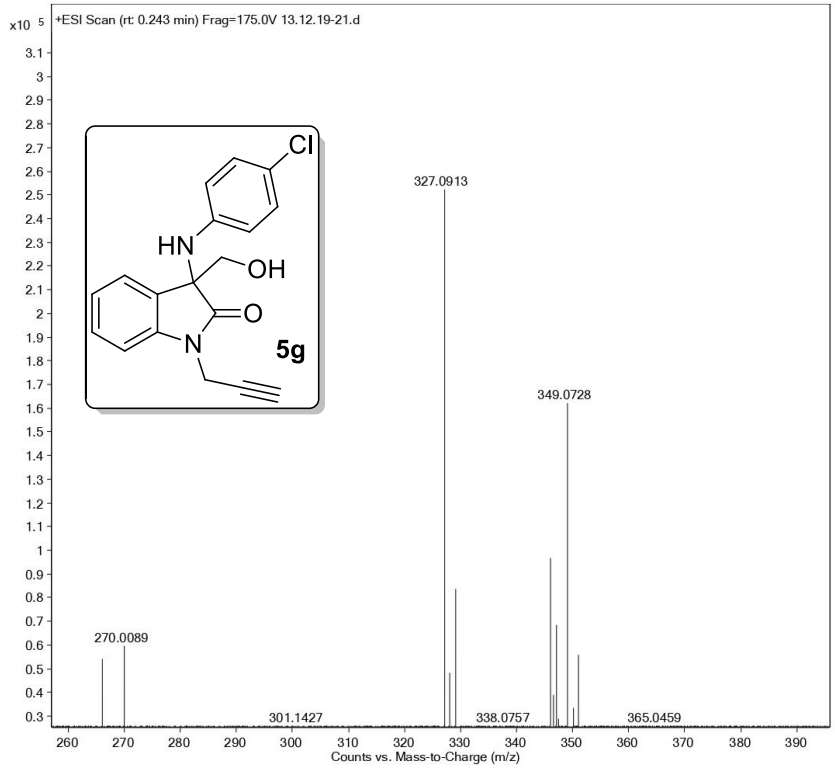


^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$+DMSO-d_6) spectrum of 3-((4-chlorophenyl)amino)-3-(hydroxymethyl)-1-(prop-2-yn-1-yl)indolin-2-one (5g)

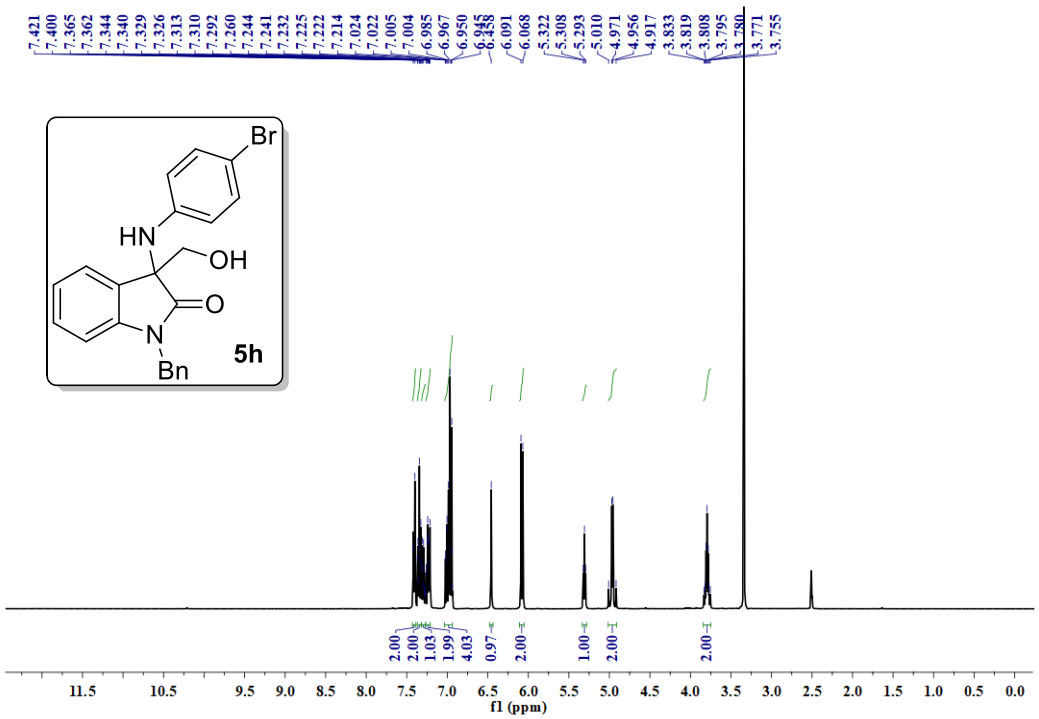


HRMS of 3-((4-chlorophenyl)amino)-3-(hydroxymethyl)-1-(prop-2-yn-1-yl)indolin-2-one (5g)

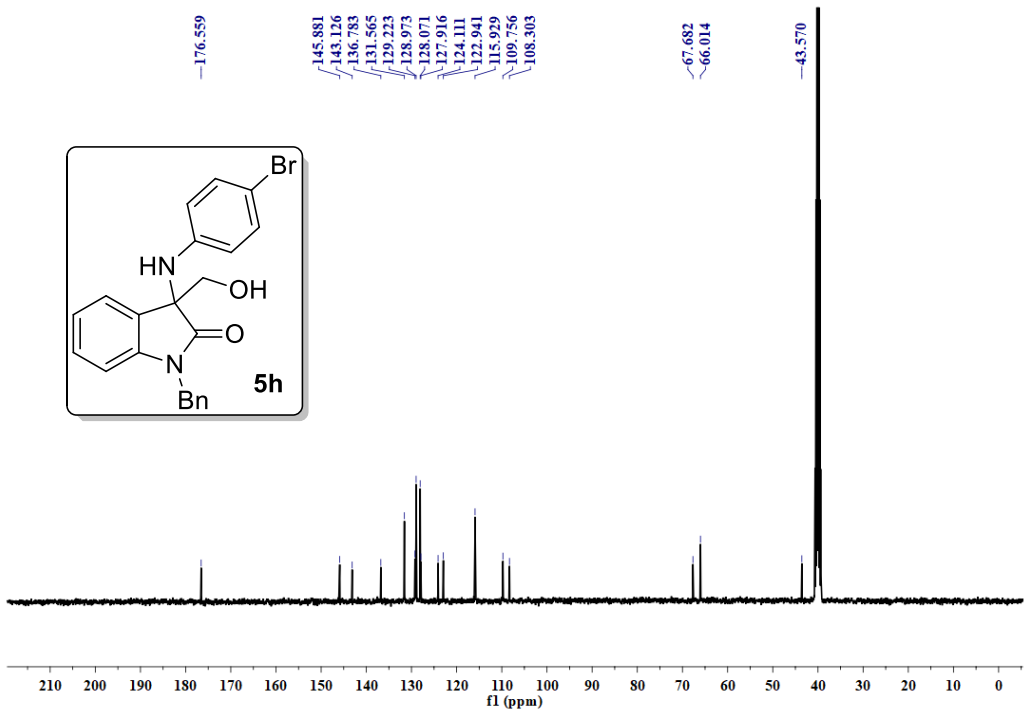
Sample Name	N-pgyl+4-d-aniline	**Position**	P1-A1	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	2	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	13.12.19-21.d
ACQ Method	srinu.m	**Comment**		**Acquired Time**	13-Dec-19 5:27:40 PM



^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 1-benzyl-3-((4-bromophenyl)amino)-3-(hydroxymethyl)indolin-2-one (5h)

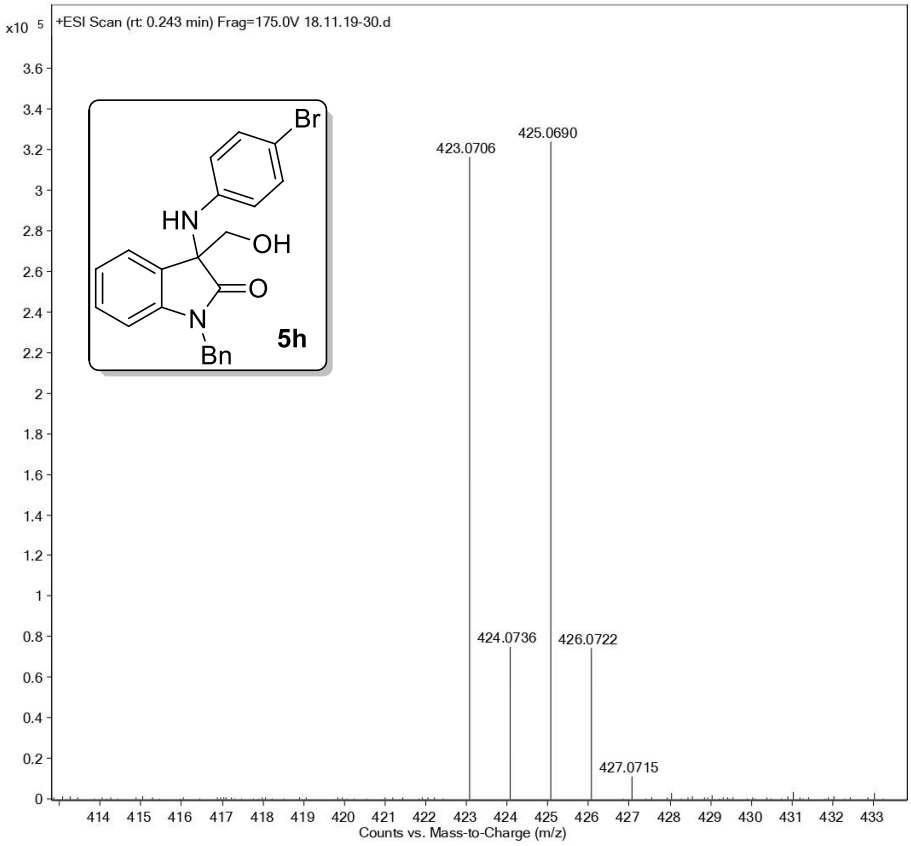


^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of 1-benzyl-3-((4-bromophenyl)amino)-3-(hydroxymethyl)indolin-2-one (5h)

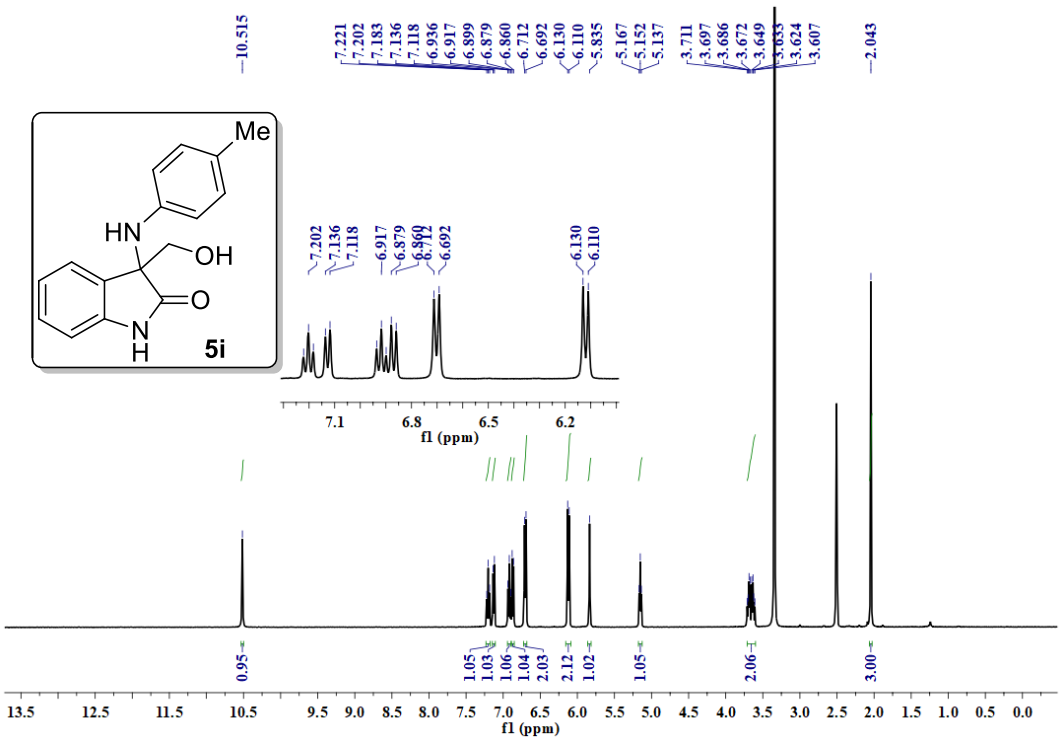


HRMS of 1-benzyl-3-((4-bromophenyl)amino)-3-(hydroxymethyl)indolin-2-one (5h)

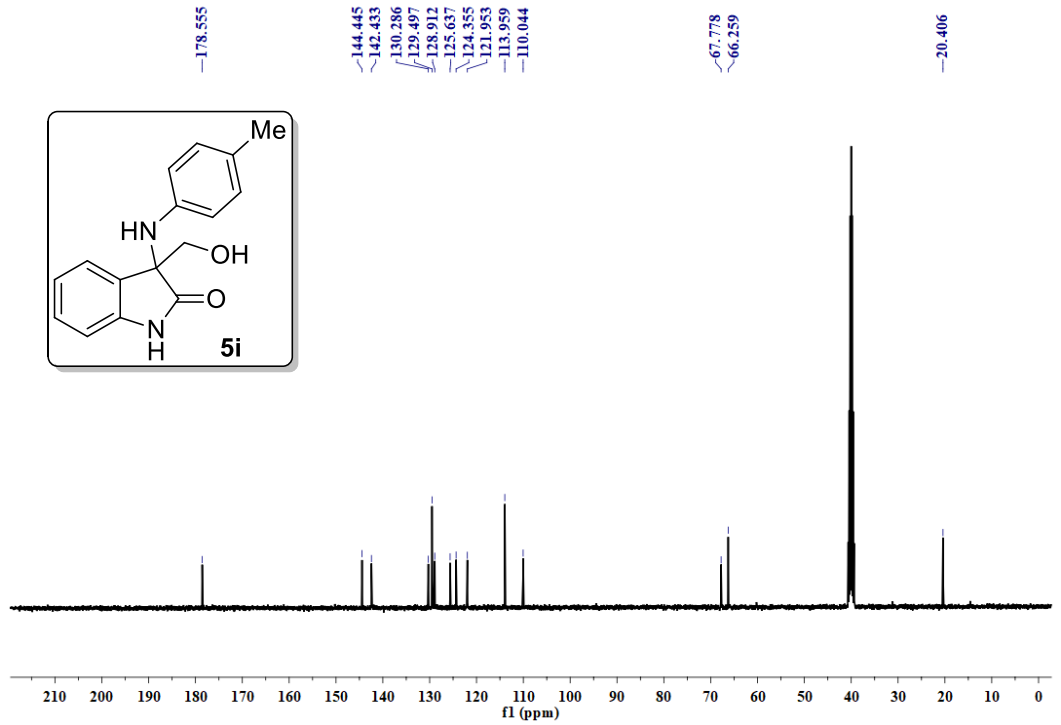
Sample Name	118 gsp5	**Position**	P1-D3	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	2	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	18.11.19-30.d
ACQ Method	srinu.m	**Comment**		**Acquired Time**	18-Nov-19 5:15:36 PM



^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 3-(hydroxymethyl)-3-(*p*-tolylamino)indolin-2-one (5i)

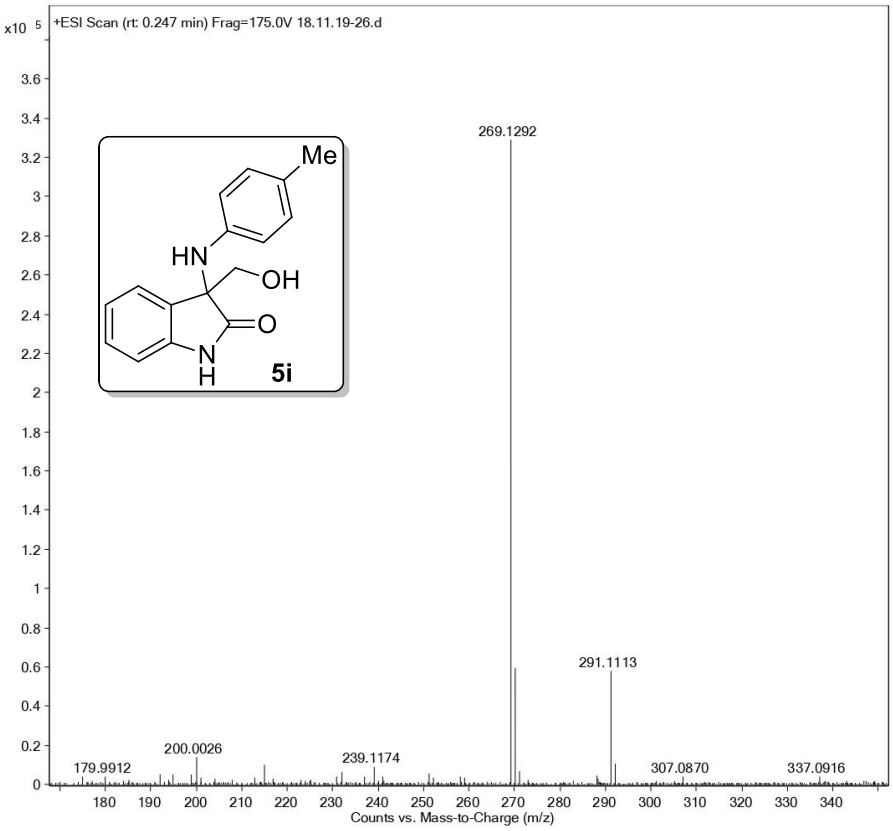


^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of 3-(hydroxymethyl)-3-(*p*-tolylamino)indolin-2-one (5i)

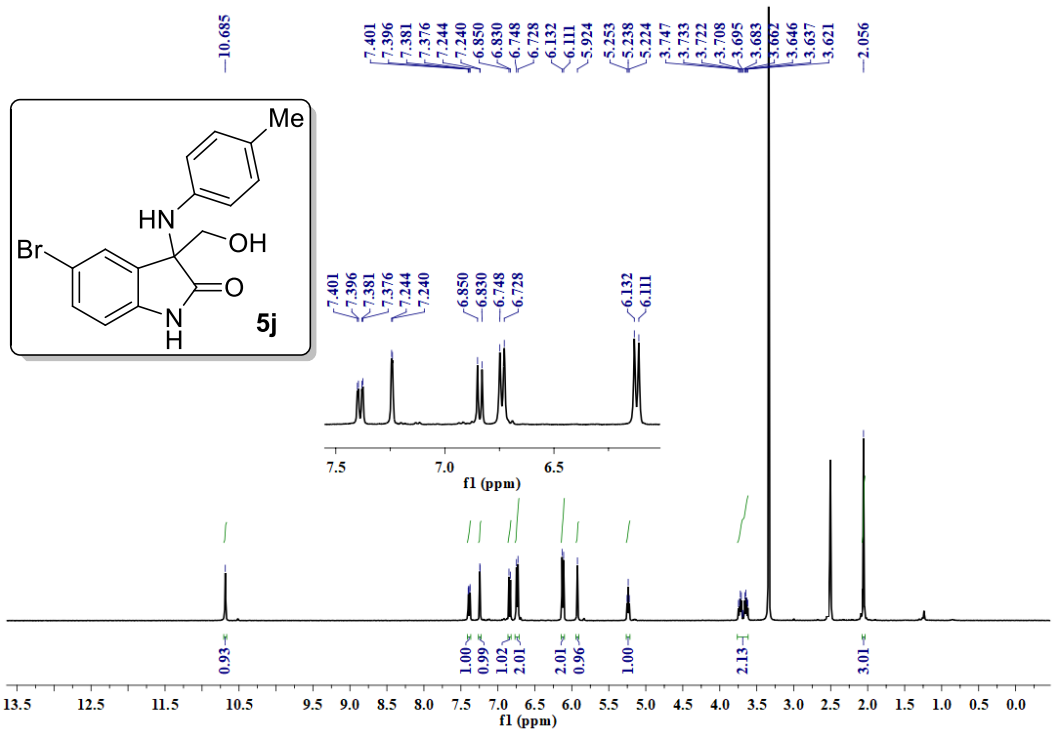


HRMS of 3-(hydroxymethyl)-3-(*p*-tolylamino)indolin-2-one (5i)

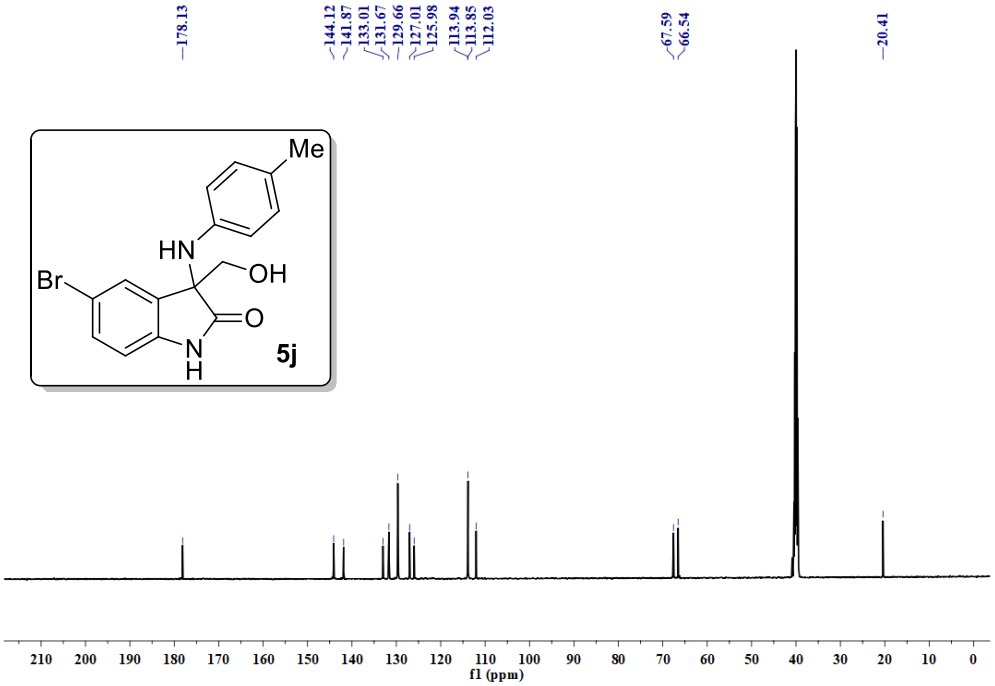
Sample Name	118 gsp1	**Position**	P1-C8	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	2	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	18.11.19-26.d
ACQ Method	srinu.m	**Comment**		**Acquired Time**	18-Nov-19 4:59:42 PM



^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 5-bromo-3-(hydroxymethyl)-3-(*p*-tolylamino)indolin-2-one (5j)

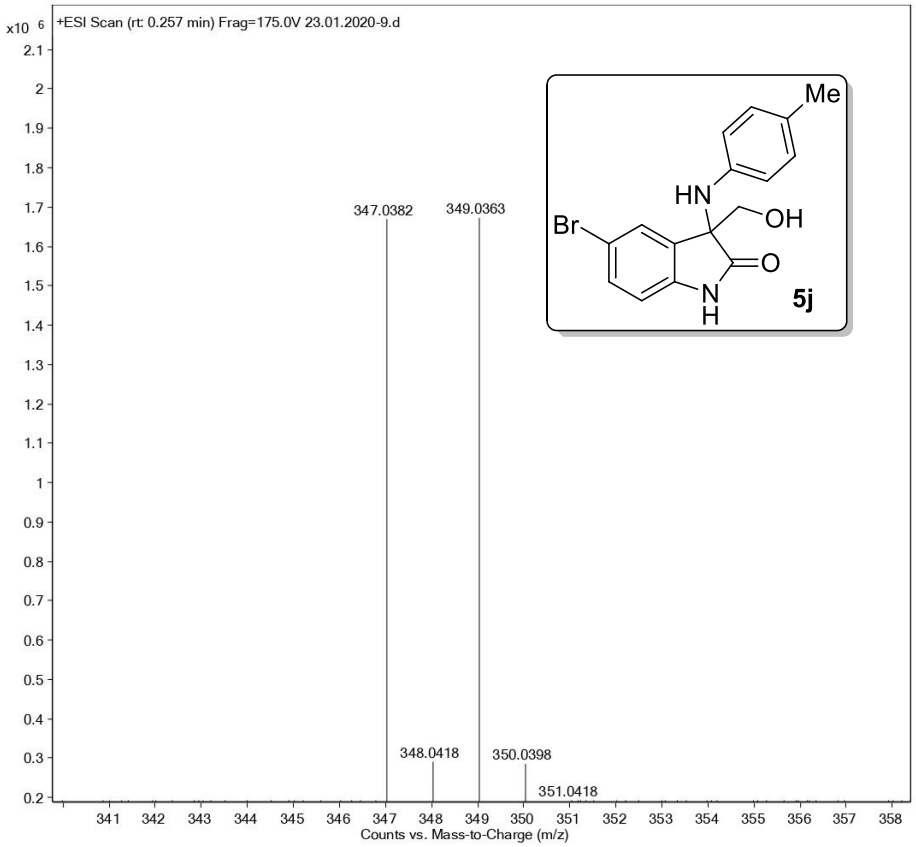


^{13}C{^{1}H} NMR (125 MHz, DMSO-d_6) spectrum of 5-bromo-3-(hydroxymethyl)-3-(*p*-tolylamino)indolin-2-one (5j)

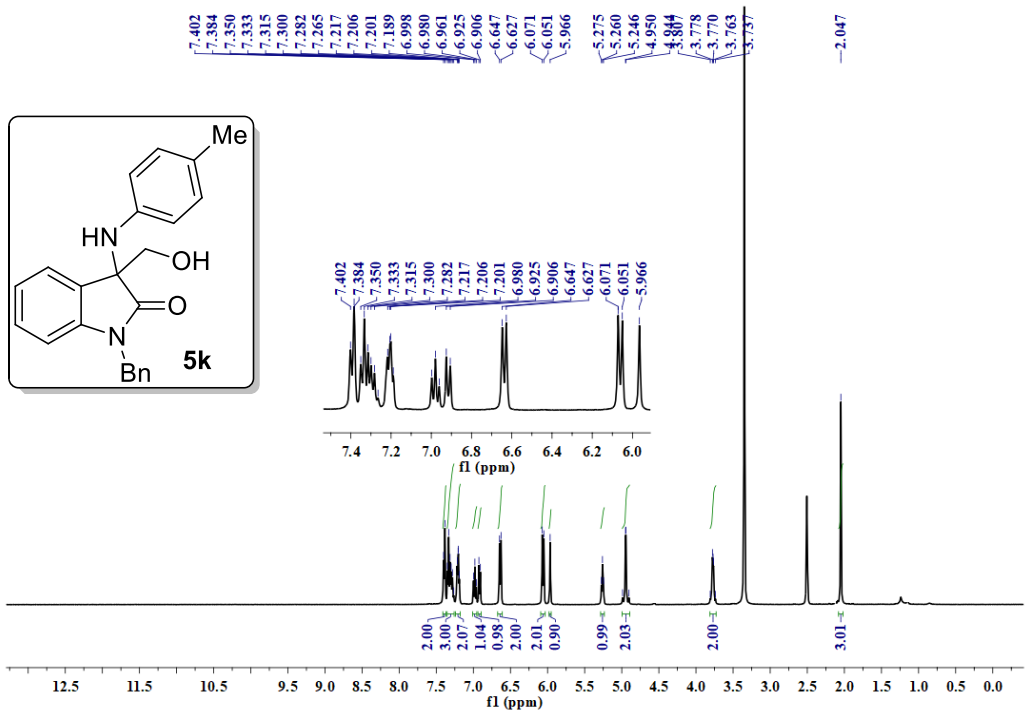


HRMS of 5-bromo-3-(hydroxymethyl)-3-(*p*-tolylamino)indolin-2-one (5j)

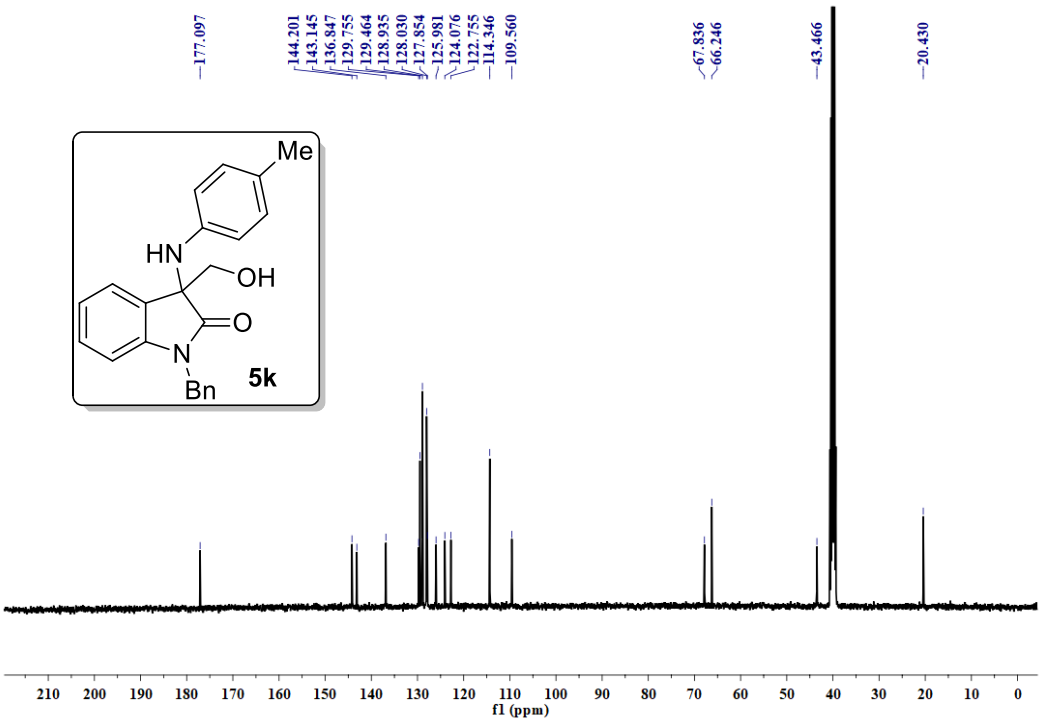
Sample Name	BRISCH3ANI	**Position**	P1-A9	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	2	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	23.01.2020-9.d
ACQ Method	srinu.m	**Comment**		**Acquired Time**	23-Jan-20 4:50:10 PM



^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 1-benzyl-3-(hydroxymethyl)-3-(*p*-tolylamino)indolin-2-one (5k)

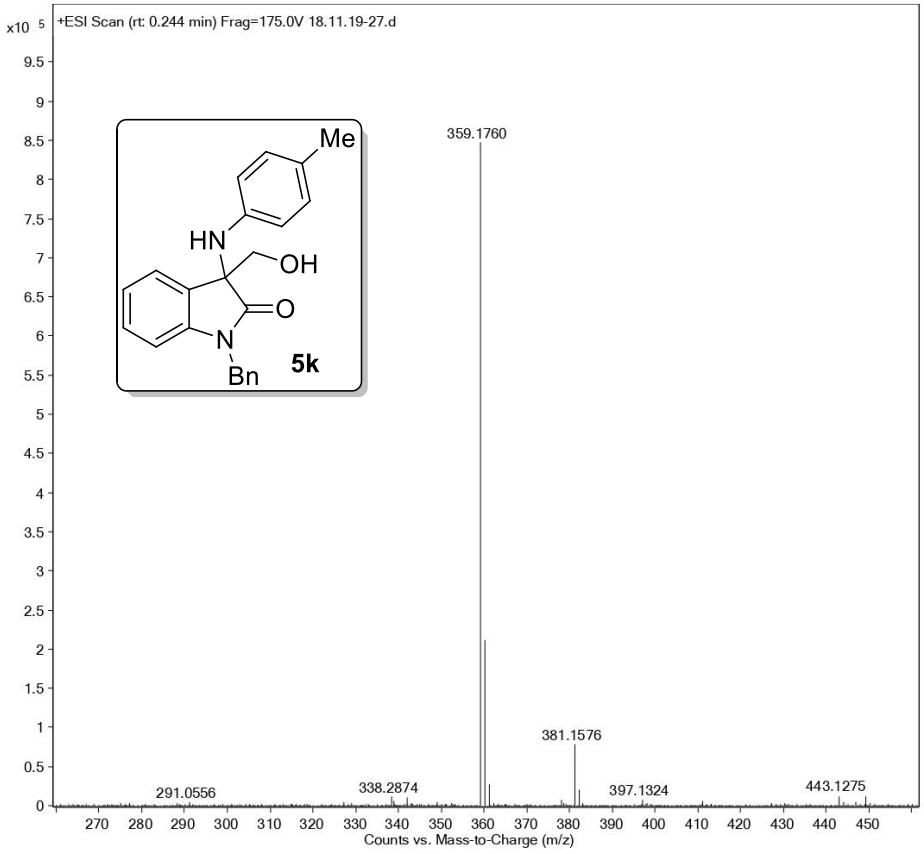


^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of 1-benzyl-3-(hydroxymethyl)-3-(*p*-tolylamino)indolin-2-one (5k)

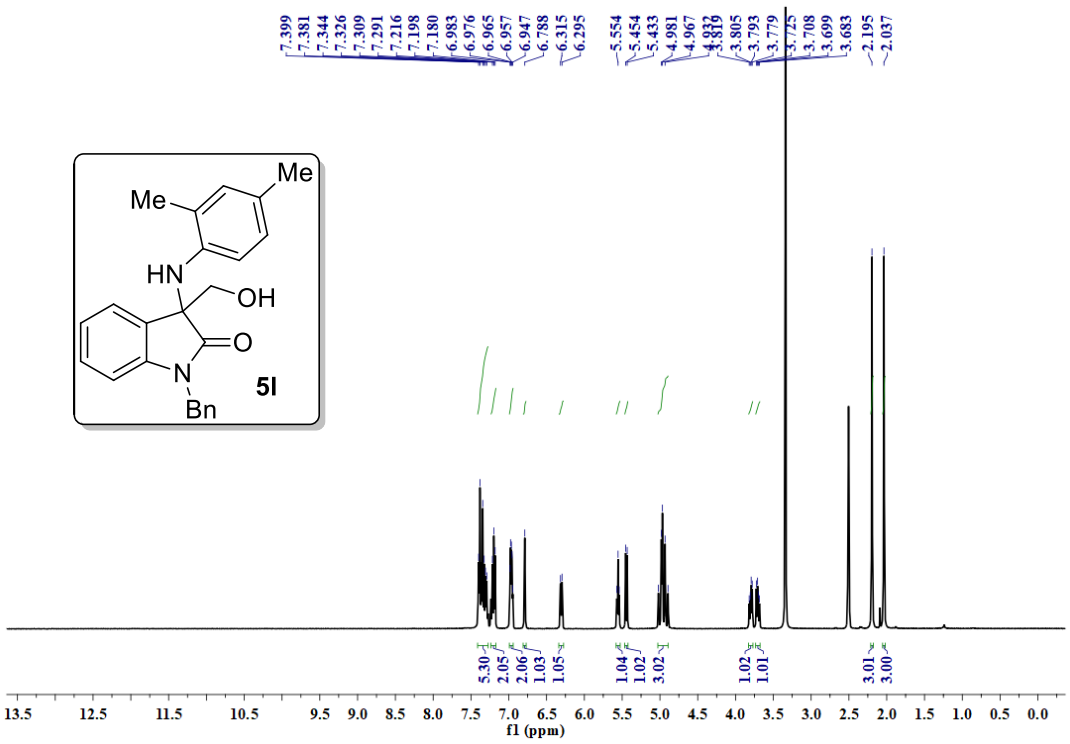


HRMS of 1-benzyl-3-(hydroxymethyl)-3-(*p*-tolylamino)indolin-2-one (5k)

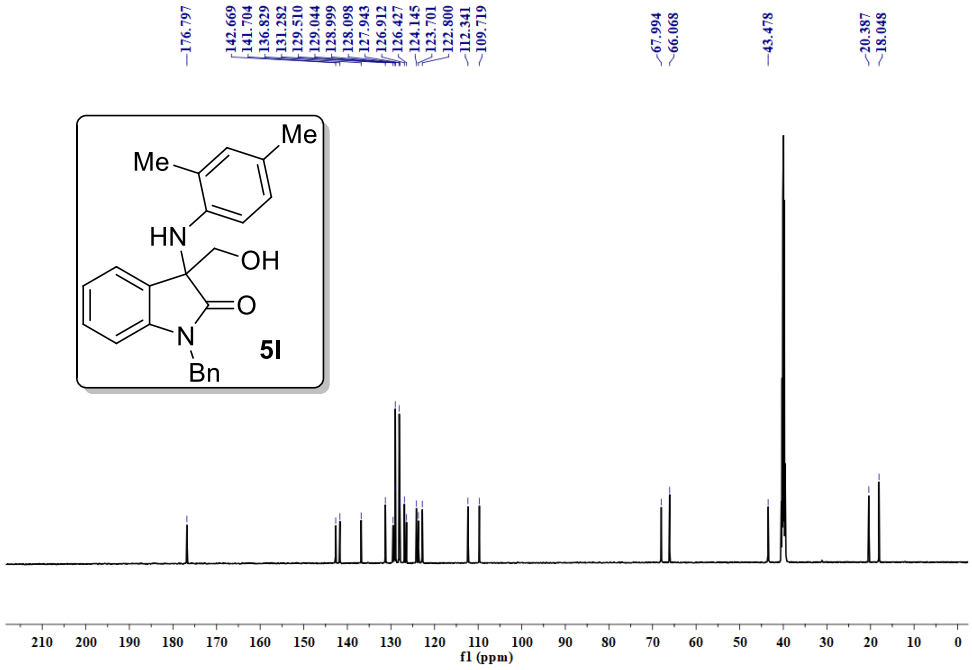
Sample Name	118 gsp2	**Position**	P1-C9	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	2	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	18.11.19-27.d
ACQ Method	srinu.m	**Comment**		**Acquired Time**	18-Nov-19 5:03:41 PM



^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 1-benzyl-3-((2,4-dimethylphenyl)amino)-3-(hydroxymethyl)indolin-2-one (5l)

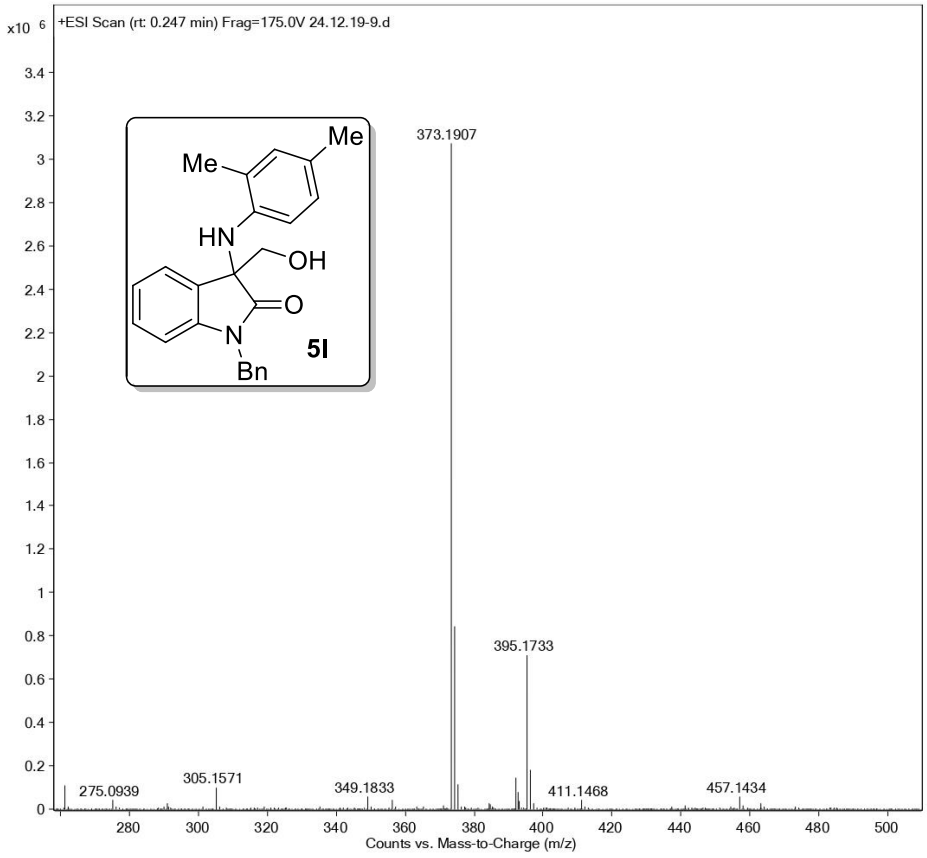


^{13}C{^{1}H} NMR (125 MHz, DMSO-d_6) spectrum of 1-benzyl-3-((2,4-dimethylphenyl)amino)-3-(hydroxymethyl)indolin-2-one (5l)

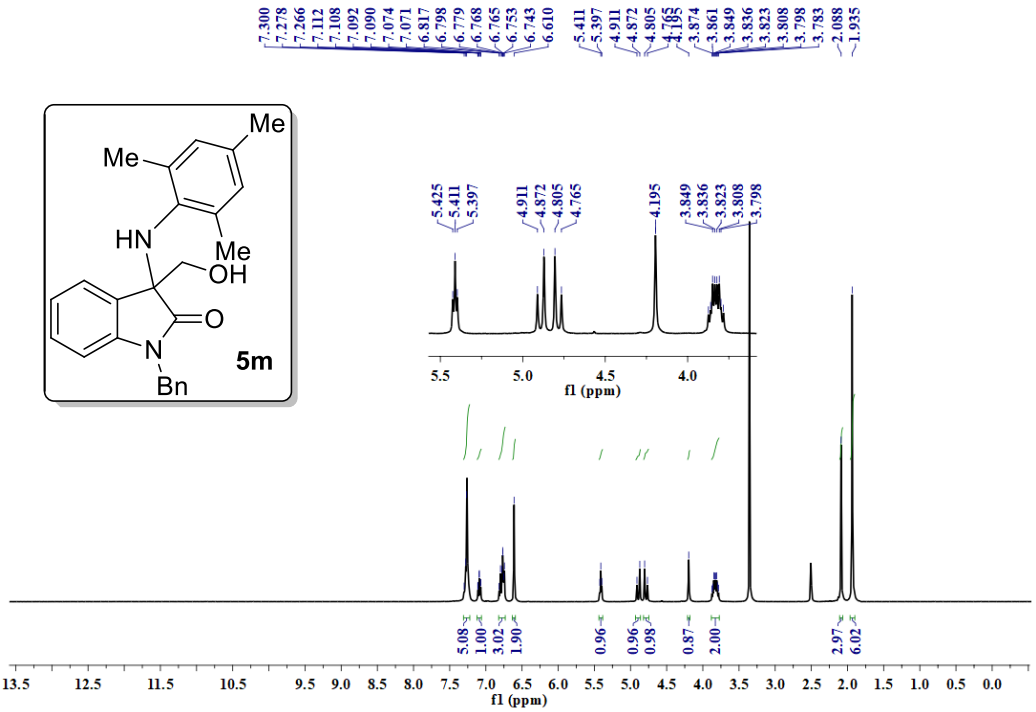


HRMS of 1-benzyl-3-((2,4-dimethylphenyl)amino)-3-(hydroxymethyl)indolin-2-one (5l)

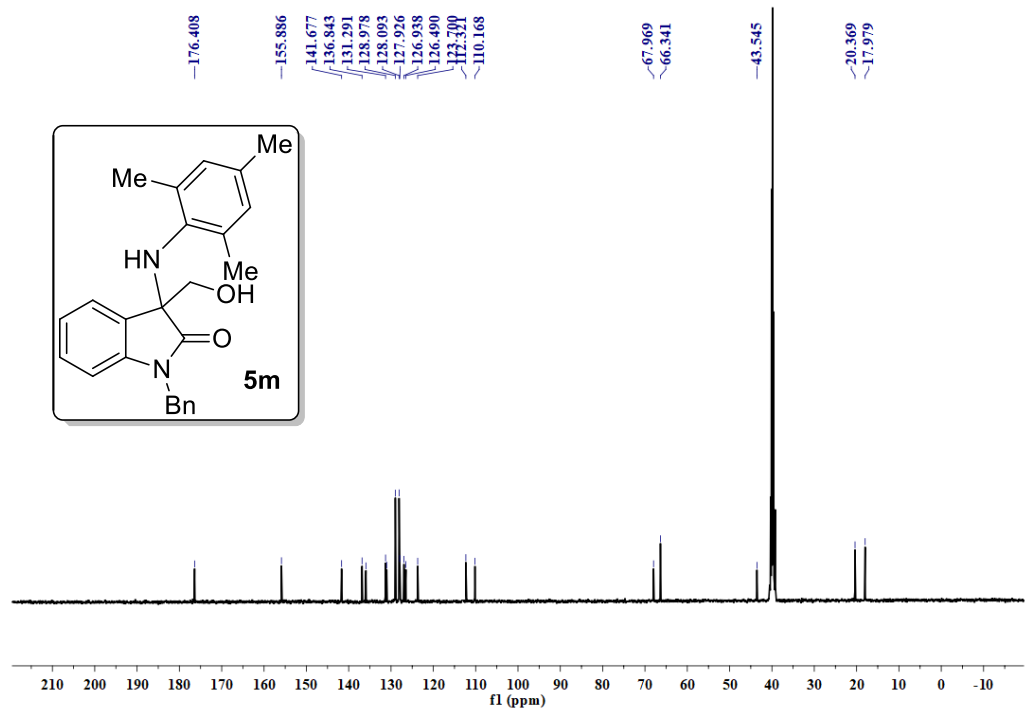
Sample Name	KHP-GSP-ISNBN-ME	**Position**	P1-A9	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	2	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	24.12.19-9.d
ACQ Method	srinu.m	**Comment**		**Acquired Time**	24-Dec-19 4:51:34 PM



^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 1-benzyl-3-(hydroxymethyl)-3-(mesitylamino)indolin-2-one (5m)

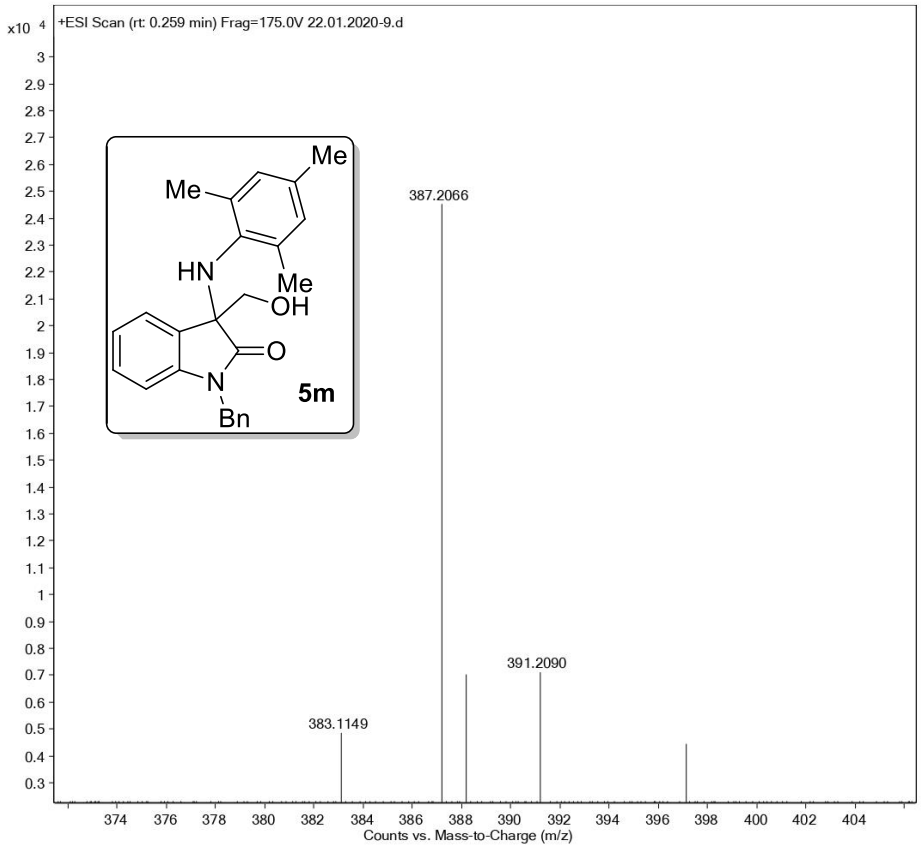


^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of 1-benzyl-3-(hydroxymethyl)-3-(mesitylamino)indolin-2-one (5m)

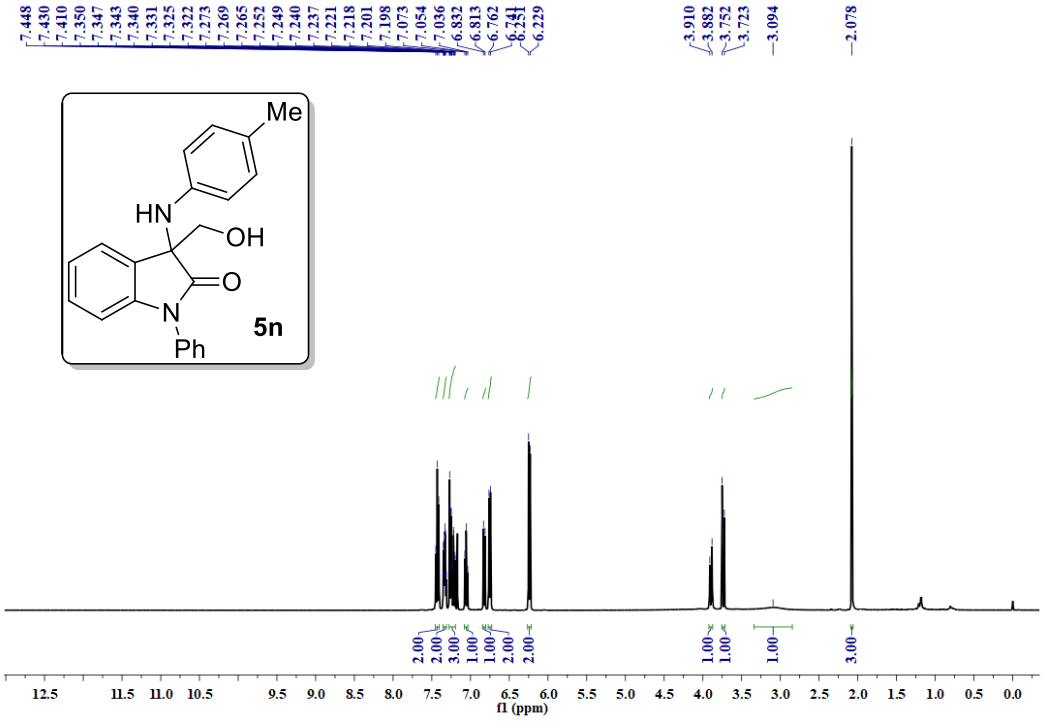


HRMS of 1-benzyl-3-(hydroxymethyl)-3-(mesitylamino)indolin-2-one (5m)

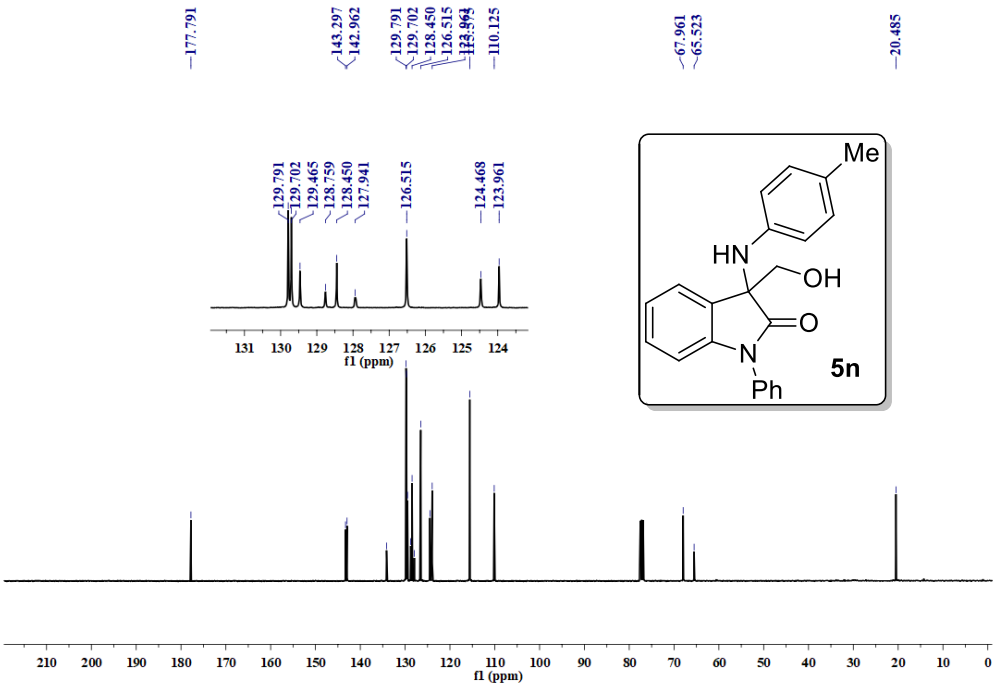
Sample Name	NBNIS2 4 6 ME ANI	**Position**	P1-A9	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	2	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	22.01.2020-9.d
ACQ Method	srinu.m	**Comment**		**Acquired Time**	22-Jan-20 4:24:27 PM



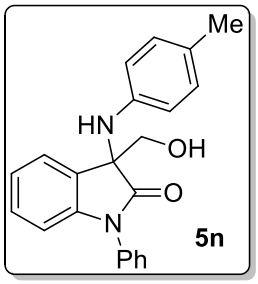
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3-(hydroxymethyl)-1-phenyl-3-(*p*-tolylamino)indolin-2-one (5n)

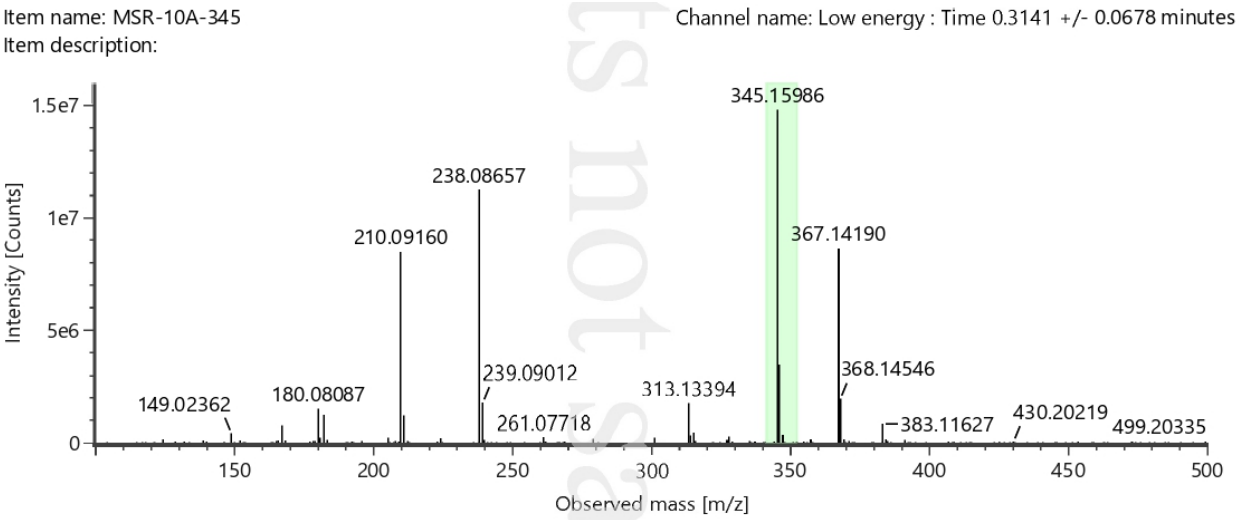


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of 3-(hydroxymethyl)-1-phenyl-3-(*p*-tolylamino)indolin-2-one (5n)

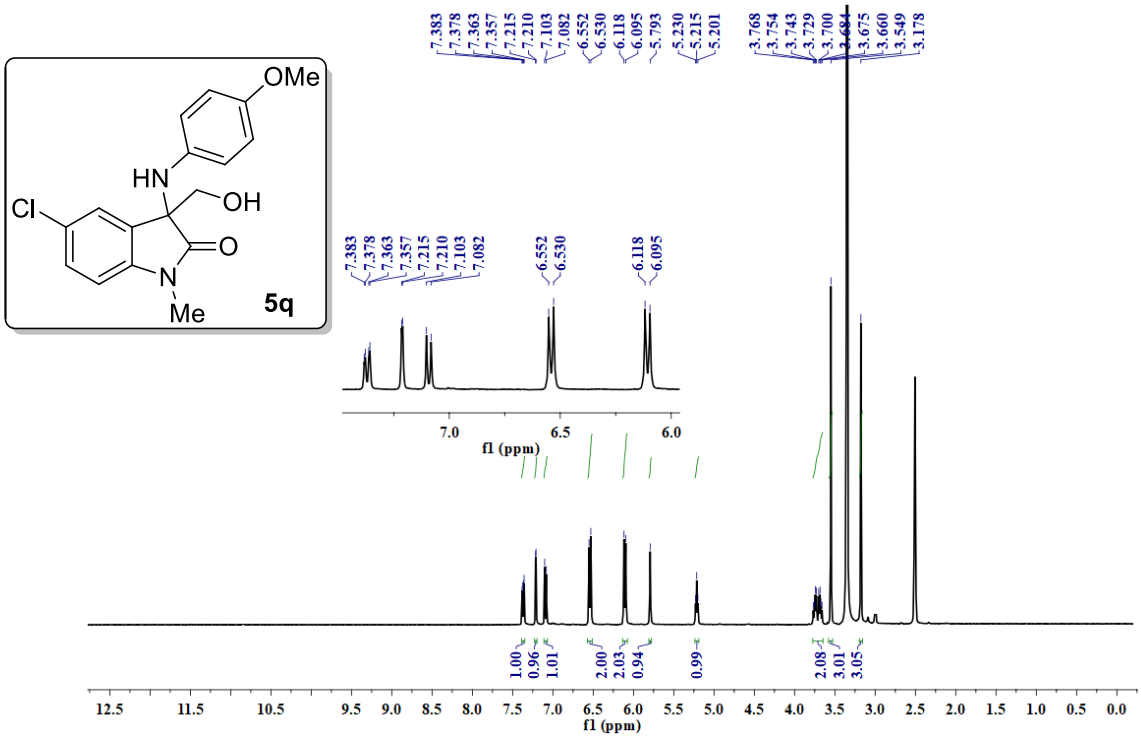


HRMS of 3-(hydroxymethyl)-1-phenyl-3-(*p*-tolylamino)indolin-2-one (5n)

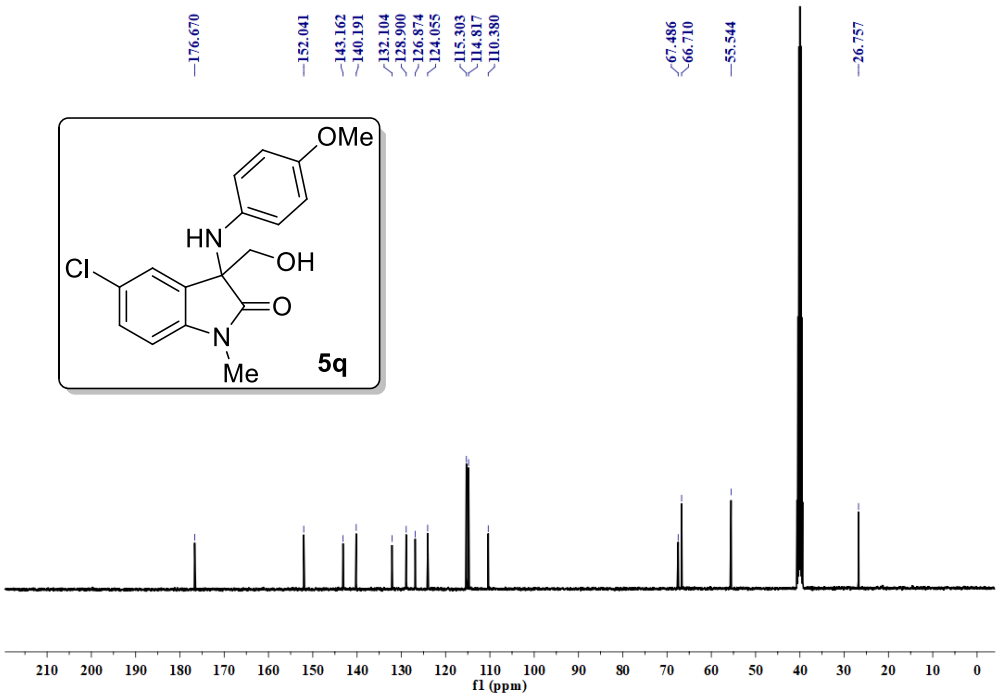




^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 5-chloro-3-(hydroxymethyl)-3-((4-methoxyphenyl)amino)-1-methylindolin-2-one (5q)

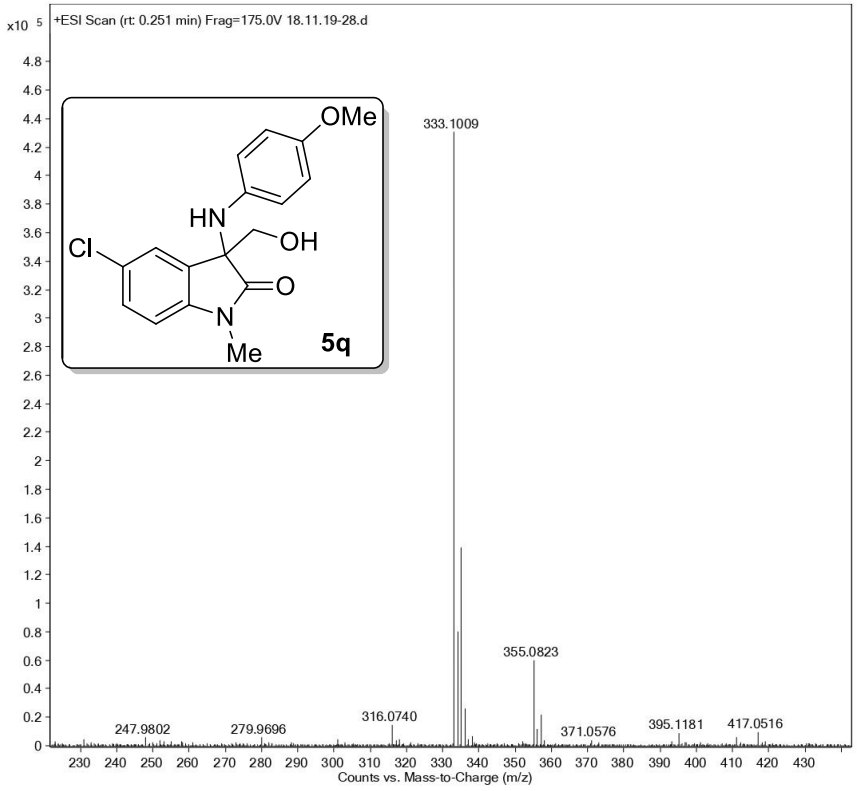


^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of 5-chloro-3-(hydroxymethyl)-3-((4-methoxyphenyl)amino)-1-methylindolin-2-one (5q)

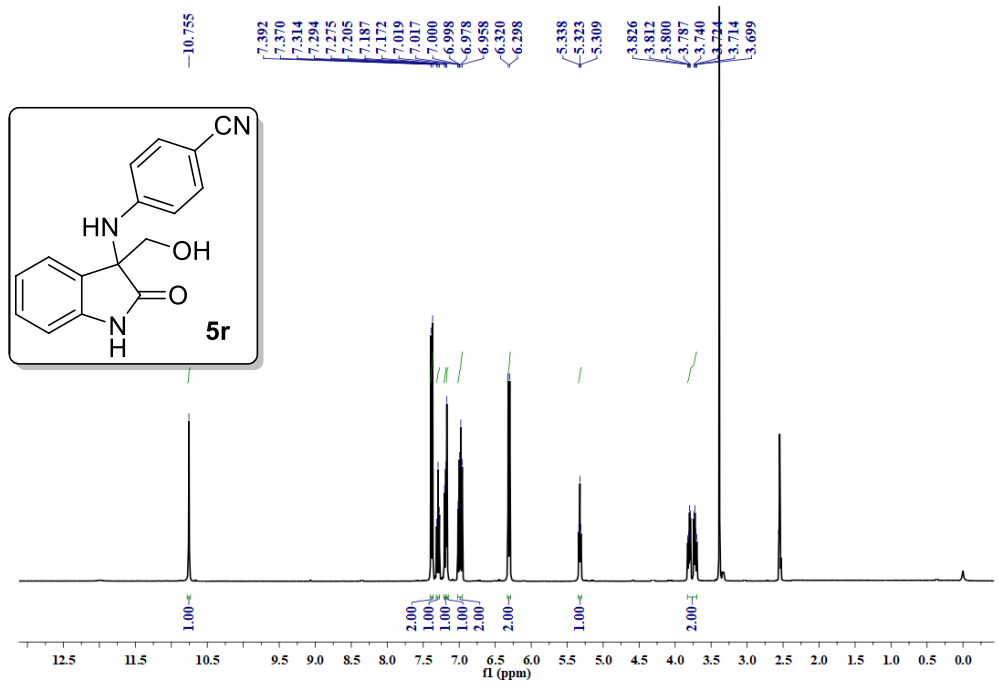


HRMS of 5-chloro-3-(hydroxymethyl)-3-((4-methoxyphenyl)amino)-1-methylindolin-2-one (5q)

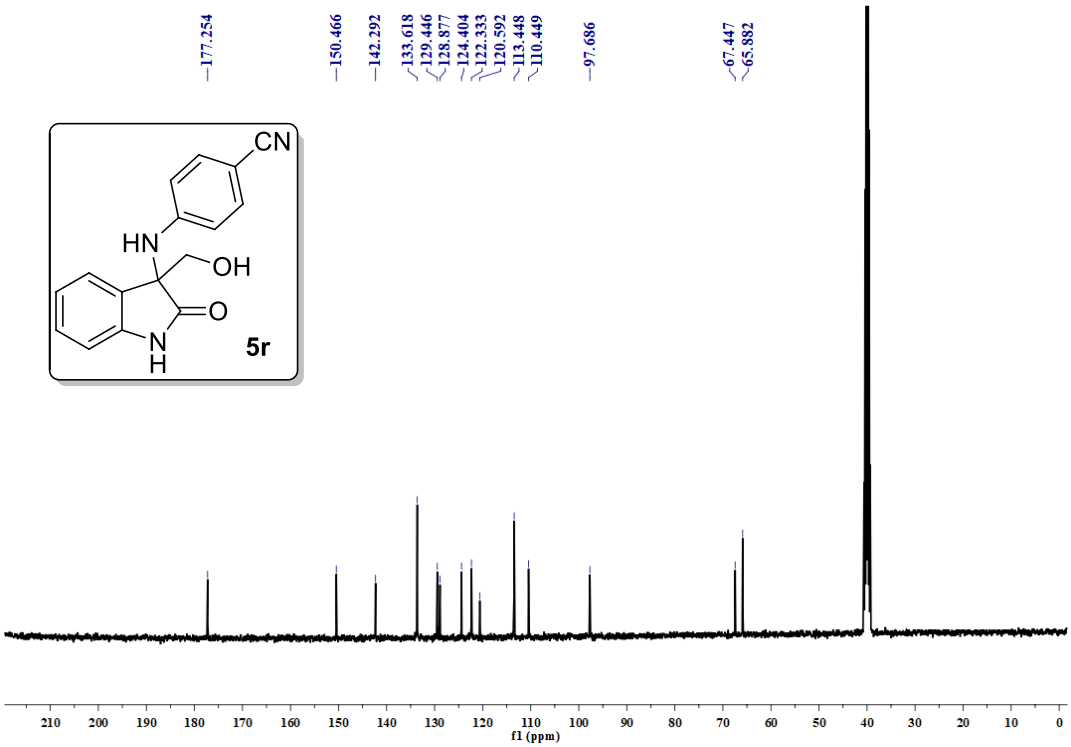
Sample Name	118 gsp3	**Position**	P1-D1	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	2	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	18.11.19-28.d
ACQ Method	srinu.m	**Comment**		**Acquired Time**	18-Nov-19 5:07:38 PM



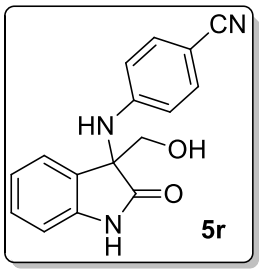
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of 4-((3-(hydroxymethyl)-2-oxoindolin-3-yl)amino)benzonitrile (5r)

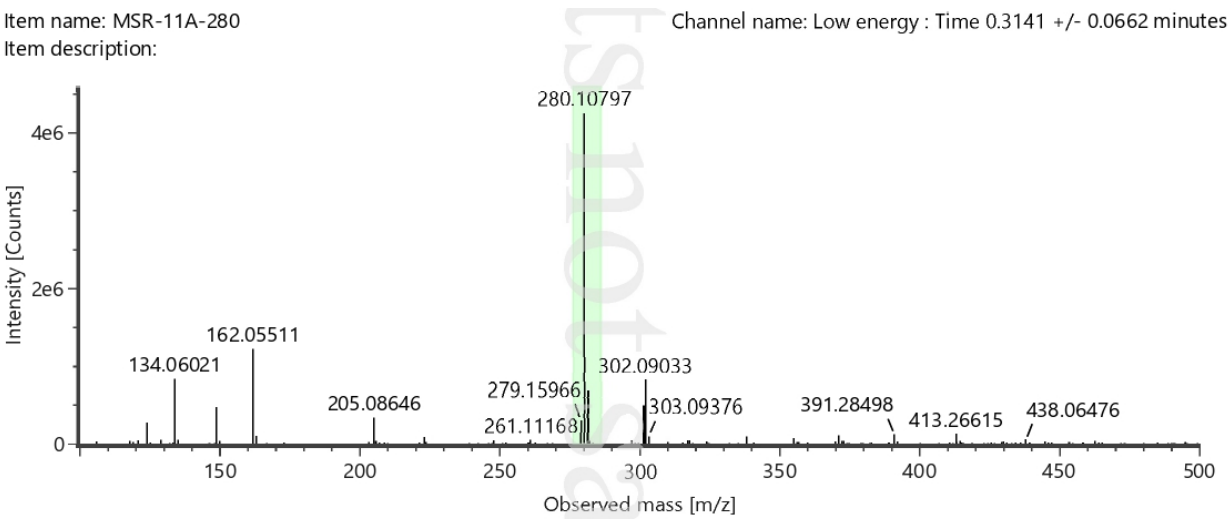


^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of 4-((3-(hydroxymethyl)-2-oxoindolin-3-yl)amino)benzonitrile (5r)

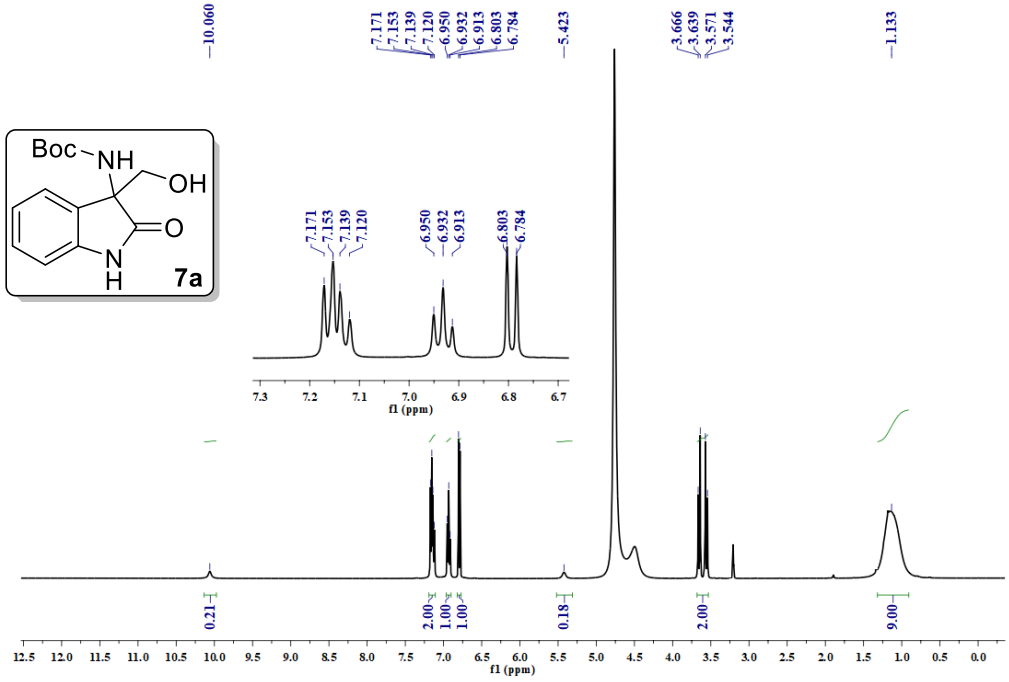


HRMS of 4-((3-(hydroxymethyl)-2-oxoindolin-3-yl)amino)benzonitrile (5r)

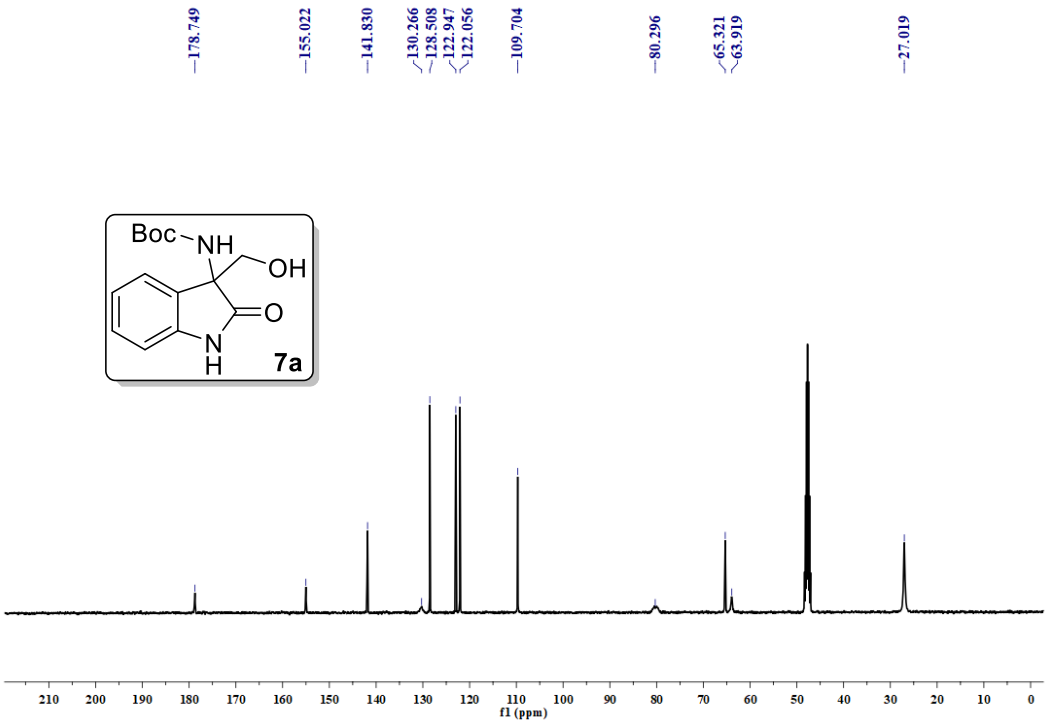




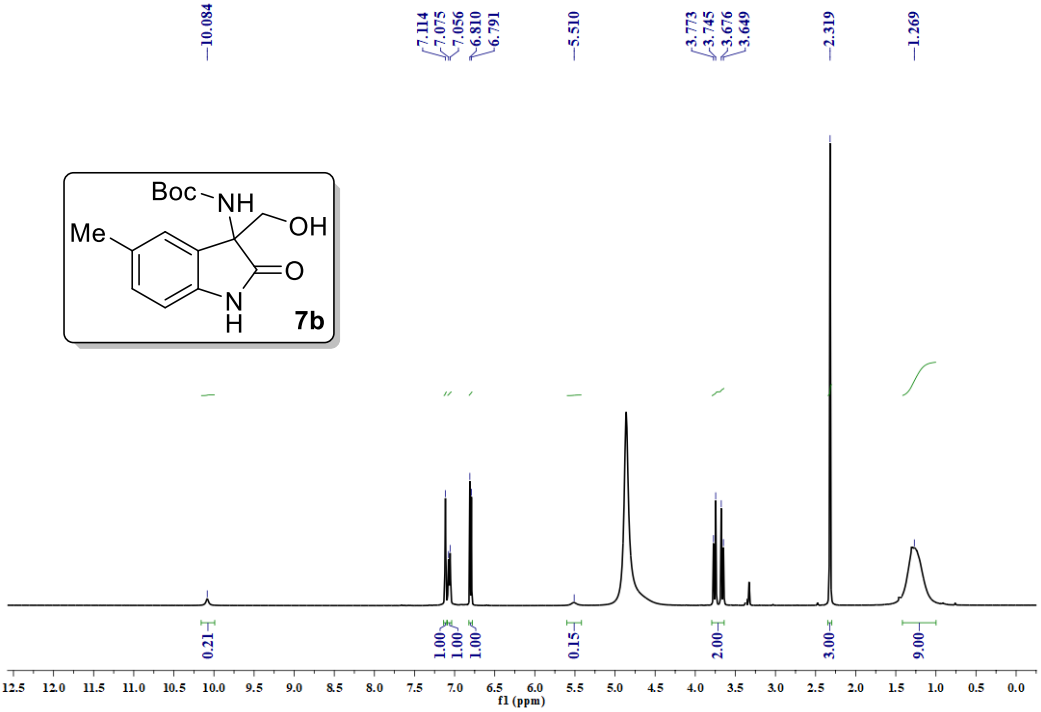
^{1}H NMR (400 MHz, MeOD) spectrum of *tert*-butyl (3-(hydroxymethyl)-2-oxoindolin-3-yl)carbamate (7a)



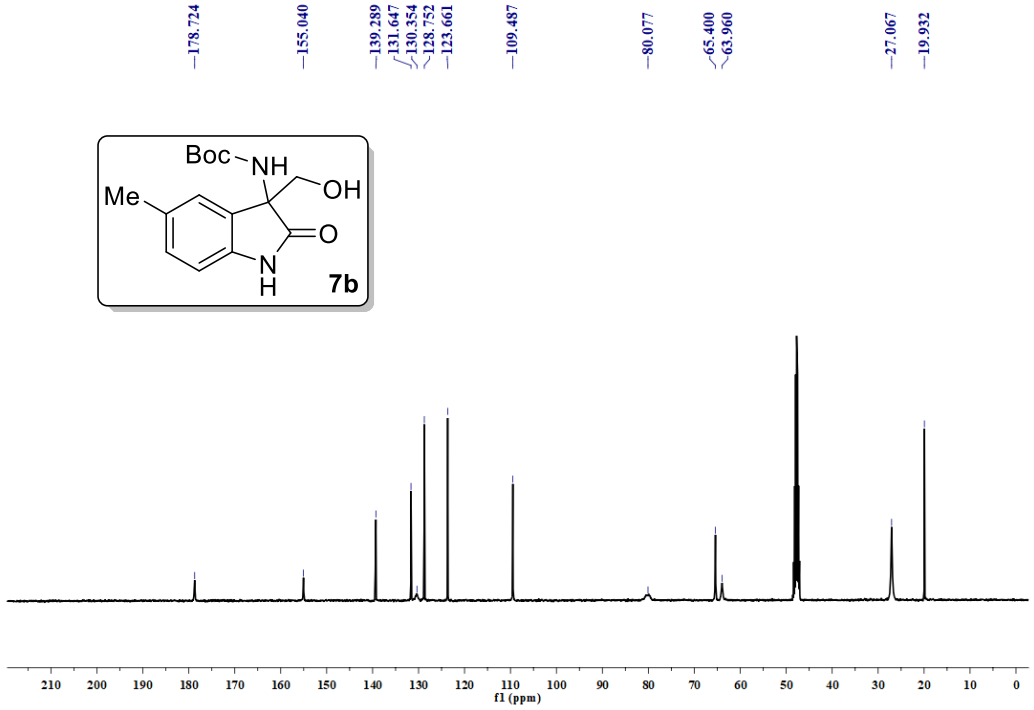
^{13}C{^{1}H} NMR (100 MHz, MeOD) spectrum of *tert*-butyl (3-(hydroxymethyl)-2-oxoindolin-3-yl)carbamate (7a)



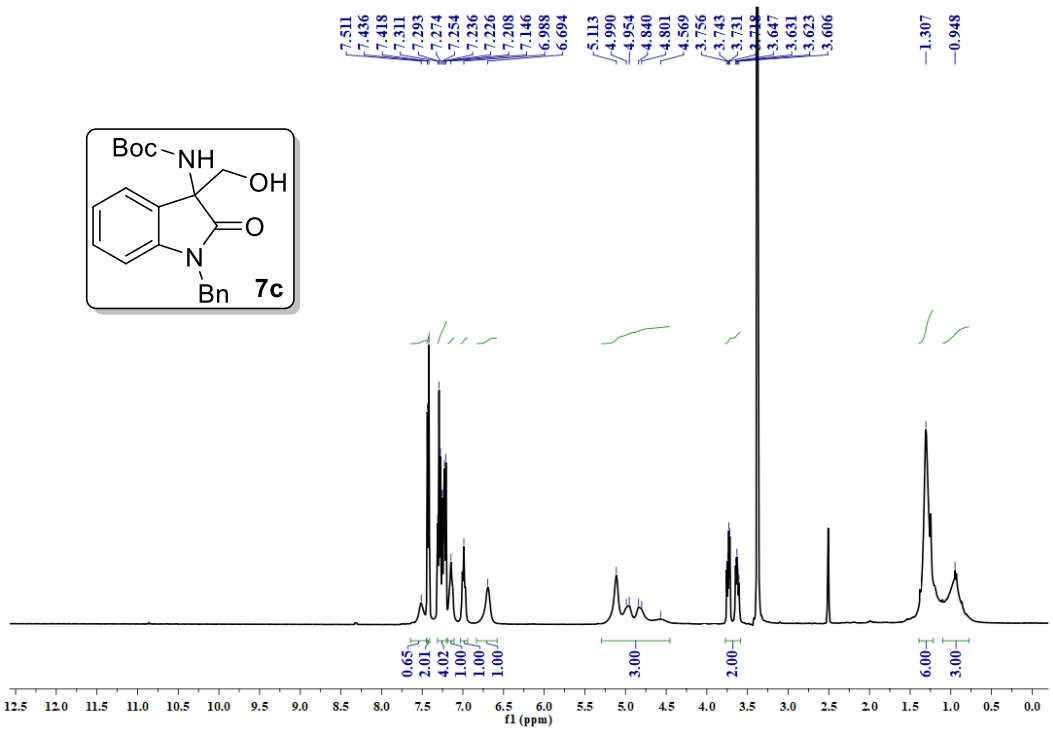
^{1}H NMR (400 MHz, MeOD) spectrum of *tert*-butyl (3-(hydroxymethyl)-5-methyl-2-oxoindolin-3-yl)carbamate (7b)



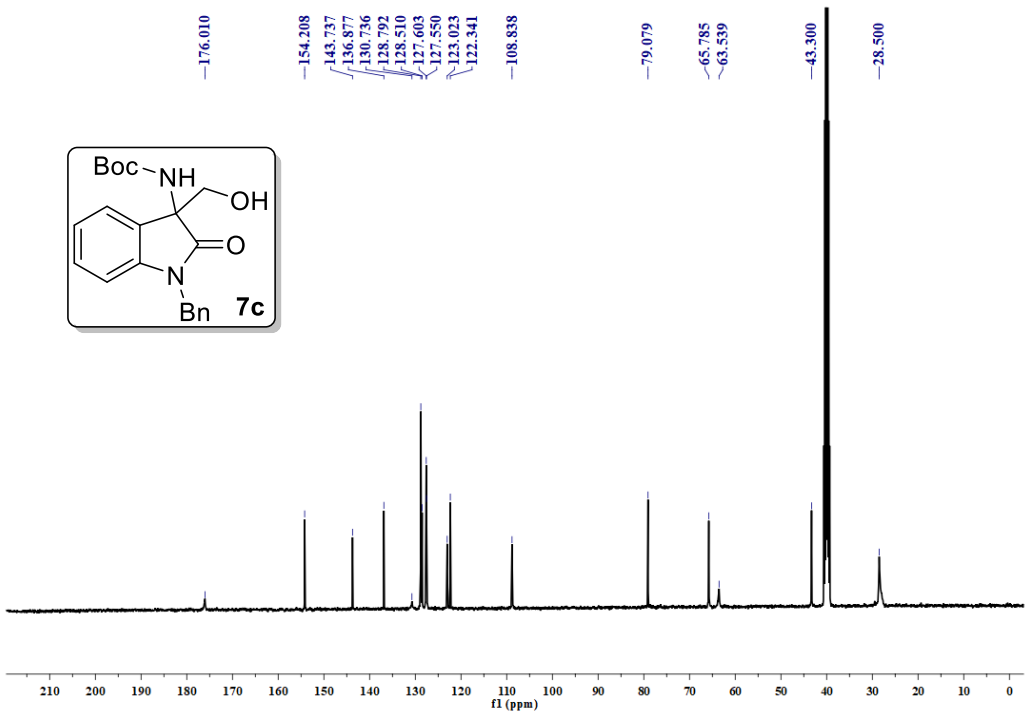
^{13}C{^{1}H} NMR (100 MHz, MeOD) spectrum of *tert*-butyl (3-(hydroxymethyl)-5-methyl-2-oxoindolin-3-yl)carbamate (7b)



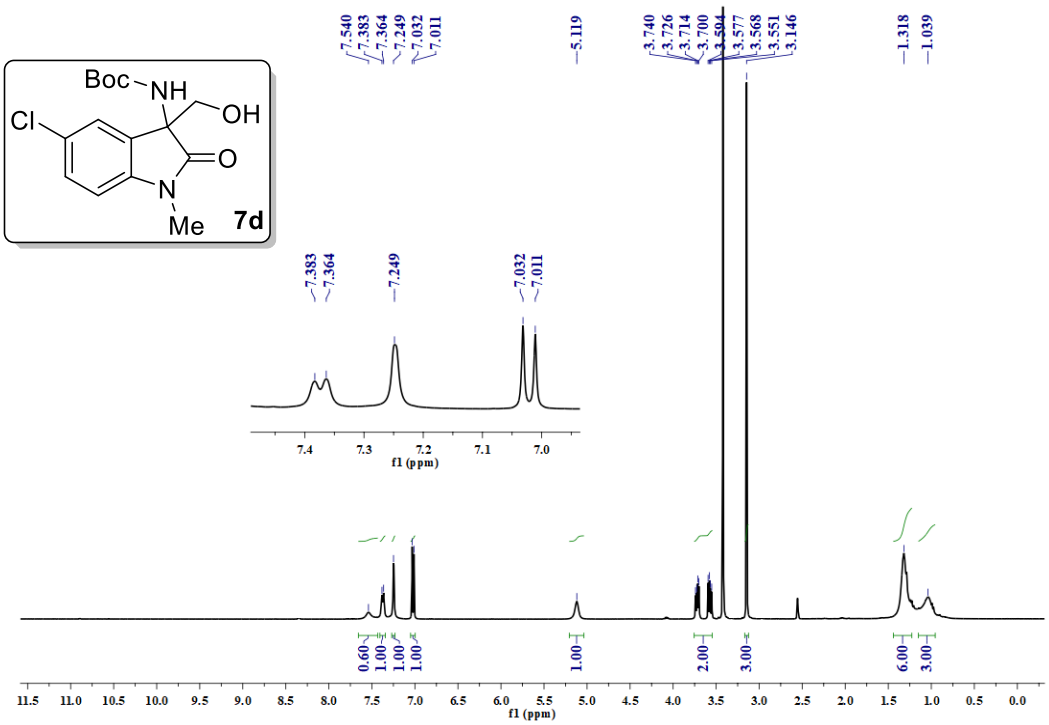
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of *tert*-butyl (1-benzyl-3-(hydroxymethyl)-2-oxoindolin-3-yl)carbamate (7c)



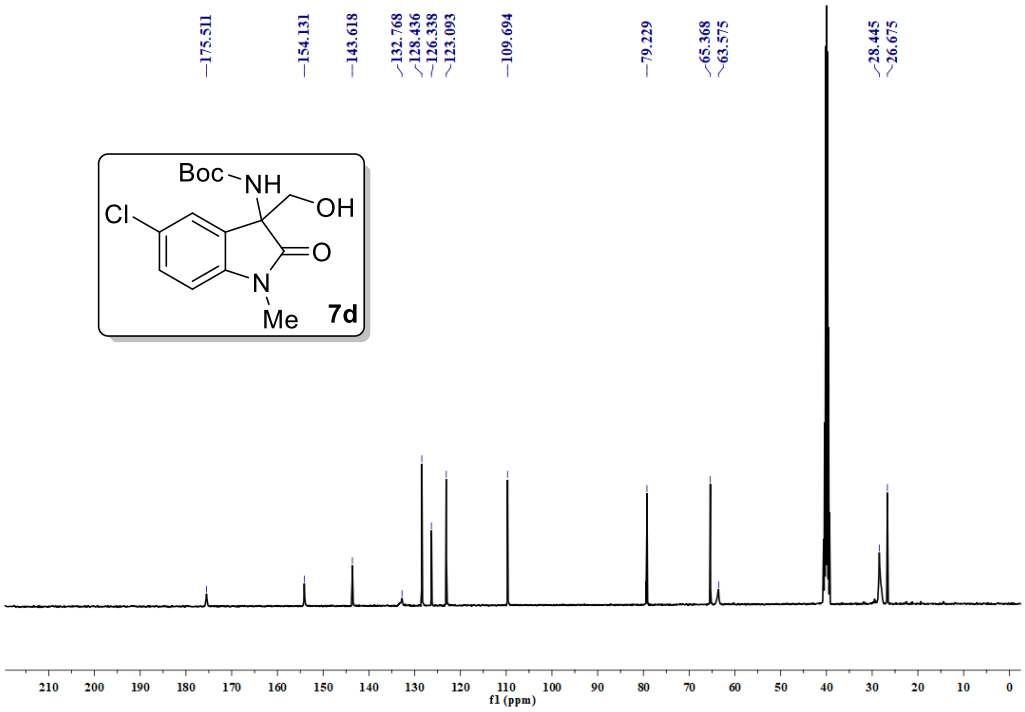
^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of *tert*-butyl (1-benzyl-3-(hydroxymethyl)-2-oxoindolin-3-yl)carbamate (7c)



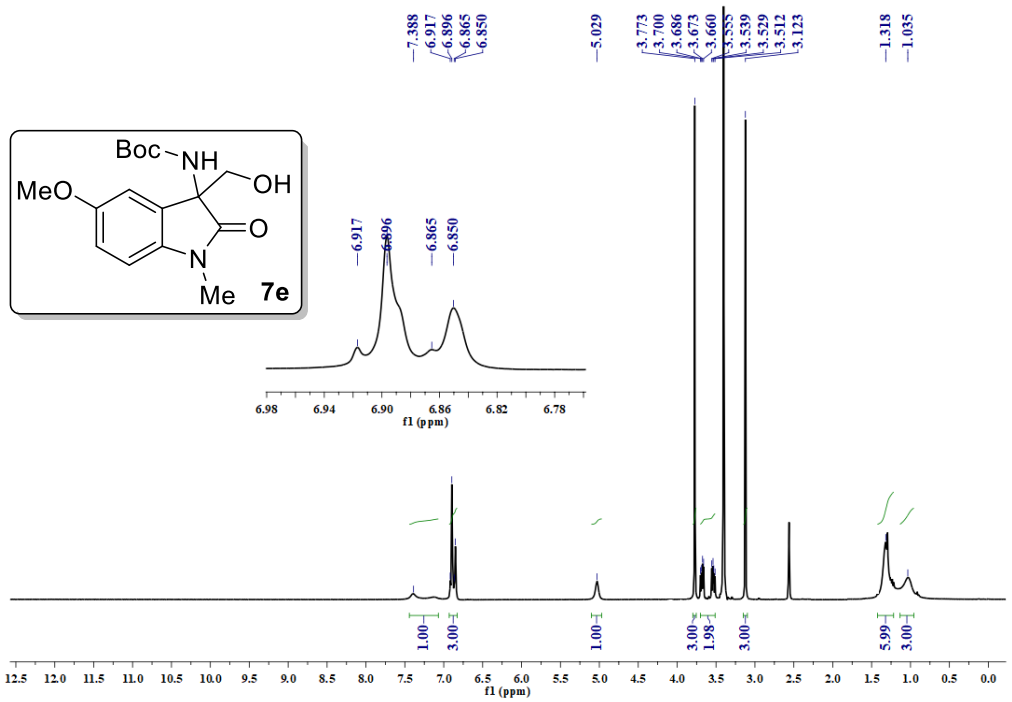
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of *tert*-butyl (5-chloro-3-(hydroxymethyl)-1-methyl-2-oxoindolin-3-yl)carbamate (7d)



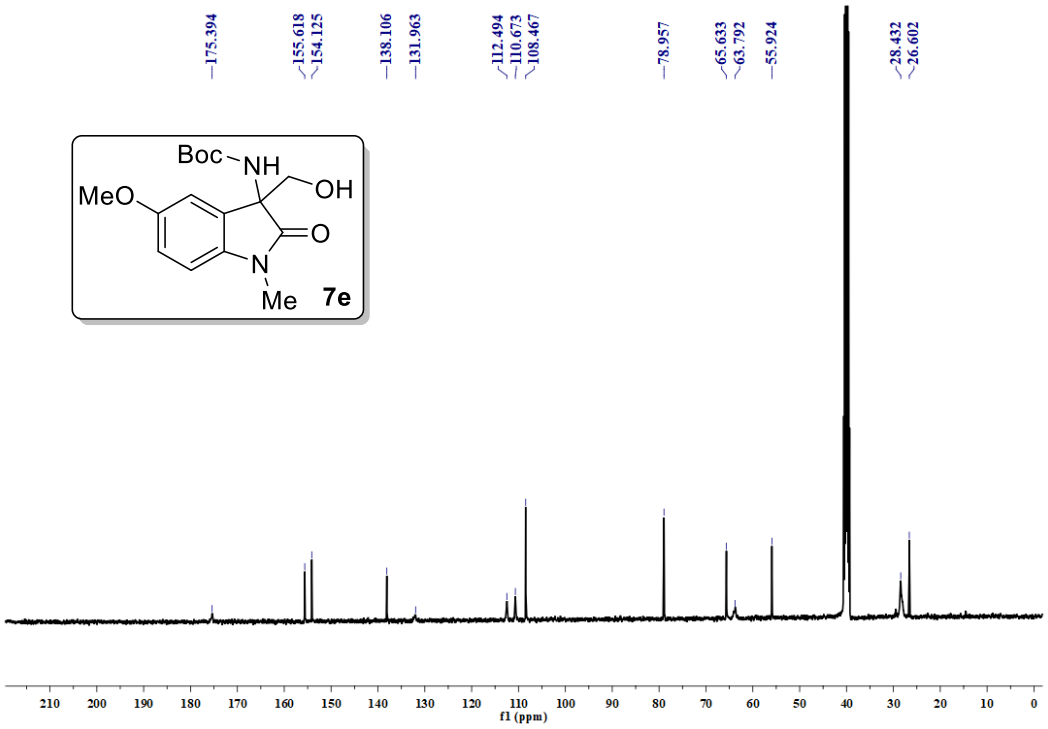
^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of *tert*-butyl (5-chloro-3-(hydroxymethyl)-1-methyl-2-oxoindolin-3-yl)carbamate (7d)



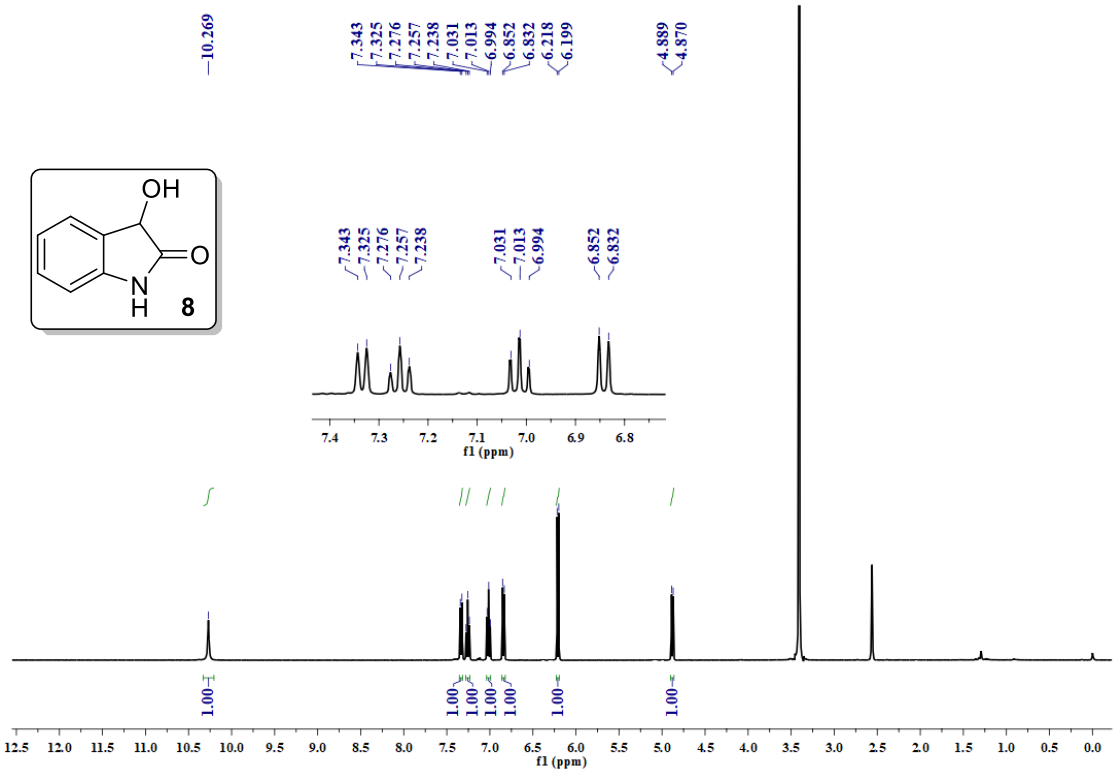
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of *tert*-butyl (3-(hydroxymethyl)-5-methoxy-1-methyl-2-oxoindolin-3-yl)carbamate (7e)



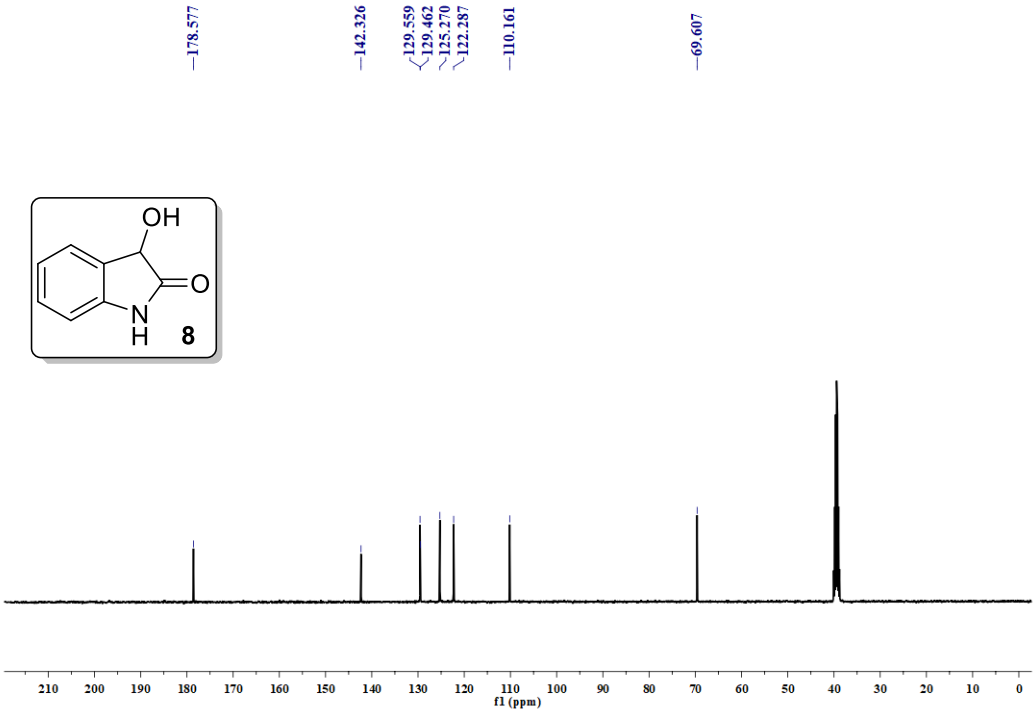
^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of *tert*-butyl (3-(hydroxymethyl)-5-methoxy-1-methyl-2-oxoindolin-3-yl)carbamate (7e)



^{1}H NMR (400 MHz, DMSO-d_6) of 3-hydroxyindolin-2-one (8)



^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) of 3-hydroxyindolin-2-one (8)



HRMS of **3-hydroxyindolin-2-one (8) and deuterated 3-hydroxyindolin-2-one (8-D)**

Sample Name	isrgod	**Position**	P1-A4	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	2	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	15.12.2021-4.d
ACQ Method	NITW-W.m	**Comment**		**Acquired Time**	15-Dec-21 5:02:23 PM