Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Atom-Economical, Catalyst-Free Hydrosulfonation of Densely Functionalized Alkenes: Access to Oxindole Containing Sulfones

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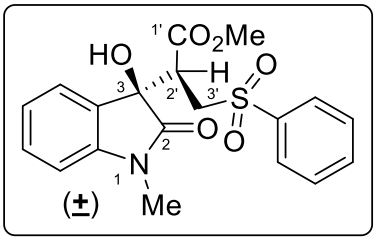
General information:

General remarks

All chemicals were purchased from commercial suppliers and used without further purification. NMR spectra were recorded on a JEOL Ressonanc-400 instrument using $CDCl_3$ or DMSO as solvent. Chemical shifts are reported in parts per million (ppm) and referenced to the residual solvent resonance. Coupling constant (*J*) are reported in hertz (Hz). Standard abbreviations indicating multiplicity were used as follows: s = singlet, d = doublet, t = triplet, dd = double doublet, dt = double triplet, q = quartet, ABq = AB quartet, m = multiplet. HRMS data were collected on Waters - Xevo G2S QTof with UPLC H-Class Ultra Performance Liquid chromatography - mass spectrometry (LC-MS) facility. The X-ray diffraction measurements were carried out at 298 K on a Bruker SMART APEX CCD area detector system equipped with a graphite monochromator and a Mo-Kα fine-focus sealed tube ($\lambda = 0.71073$ Å). The Baylis-Hillman alcohols **1** were prepared *via* the reaction between methyl or ethyl acrylate with isatin derivatives under the influence of DABCO following the known procedure.[1]

General procedure for Table 1: To a stirred solution of allylic alcohol **1a** *i.e.* 3-(methyl propenoate-2'-yl)-3-hydroxy-1-methylindolin-2-one (1.0 mmol, 0.247 g) in solvent, or benzenesulfinic acid sodium salt **2a'**(3.0 mmol, 0.492 g) **or** benzenesulfinic acid **2a** (3.0 mmol, 0.426 g) was added. The reaction mixture was then stirred at different temperatures. After complete conversion, the reaction mixture was diluted with water and extracted with ethyl acetate. The combined organic layer was washed with saturated $NaHCO_3$ solution and dried over Na_2SO_4.The solvent was evaporated and the residue thus obtained was purified *via* crystallization (EtOAc in hexanes) to afford the corresponding products **3aa** as white solid.

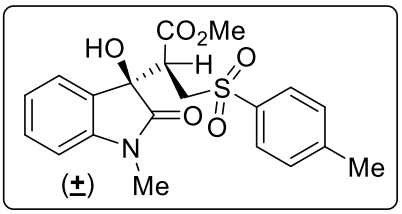
Representative example of Table 1, entry-1: 3-(Methyl-3'-(phenylsulfonyl)-propanoate-2'-yl)-3-hydroxy-1-methylindolin-2-one (3aa)



Yield: 0.318 g, 82%; M.P.: 126 ^{o}C; ^{1}H NMR (400 MHz, DMSO-d_6): δ 3.05 (s, 3 H), 3.16 (s, 3 H), 3.24 & 4.07 (dABq, J = 1.6 Hz & 14.4 Hz, 2 H), 3.84-3.91 (m, 1 H), 6.74 (s, 1 H), 6.95-7.01 (m, 2 H), 7.23 (d, J = 6.8 Hz, 1 H), 7.31 (td, J = 1.6 Hz & 8 Hz, 1 H), 7.65-7.69 (m, 2 H), 7.75-7.79 (m, 1 H), 7.83-7.86 (m, 2 H), ^{13}C NMR (100 MHz, DMSO-d_6): δ 25.9, 47.2, 51.7, 51.8, 74.2, 108.6, 122.3, 124.5, 127.6, 127.8, 129.5, 129.9, 134.1, 138.6, 142.8, 168.4, 175.2; HRMS (ESI) exact mass calcd for $C_{19}H_{20}NO_6S$ + H (M + H), 390.1011; found: 390.1006.

General procedure for Table 2: To a stirred solution of allylic alcohol in ethanol/water (1/1) (4.0 ml), aryl sulfinic acid **2** was added. The reaction mixture was then stirred at 35 ^{o}C for 48 h. The reaction mixture was then diluted with water and extracted with ethyl acetate. The combined organic layer was washed with saturated $NaHCO_3$ solution and dried over Na_2SO_4.The solvent was evaporated and the residue thus obtained was purified *via* crystallization (EtOAc in hexanes) to afford the corresponding products **3**.

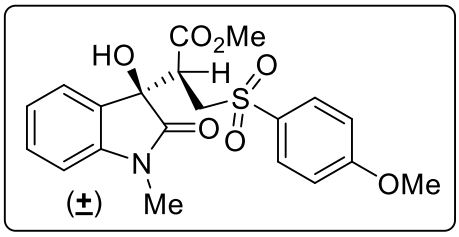
3-(Methyl-3'-(4-methylphenylsulfonyl)-propanoate-2'-yl)-3-hydroxy-1-methylindolin-2-one (3ab)



The title compound **3ab** was prepared following the general procedure for Table 2, using allylic alcohol **1a** *i.e.* 3-(methyl propenoate-2'-yl)-3-hydroxy-1-methylindolin-2-one (1.0 mmol, 0.247 g), and *p*-toluenesulfinic acid **2b** (3.0 mmol, 0.468 g). Yield: 0.330 g, 82%; White solid; M.P.: 142 ^{o}C; ^{1}H NMR

(400 MHz, $CDCl_3$): δ 2.38 (s, 3 H), 3.08 (s, 3 H), 3.38 & 3.67 (dABq, J = 1.6 Hz & 14.4 Hz, 2 H), 3.41 (s, 1 H) 3.78-3.84 (m, 1 H), 3.97 (s, 1 H), 6.74 (d, J = 7.6 Hz, 1 H), 6.94-7.06 (m, 2 H), 7.25-7.28 (m, 3 H), 7.68 (d, J = 8.0 Hz, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.7, 26.4, 46.5, 52.1, 52.7, 75.3, 108.8, 123.4, 124.1, 126.7, 128.4, 130.0, 130.8, 135.7, 143.3, 145.1, 169.8, 175.2; HRMS (ESI) exact mass calcd for $C_{20}H_{21}NO_6S$ + Na (M + Na), 426.0987; found: 426.0983.

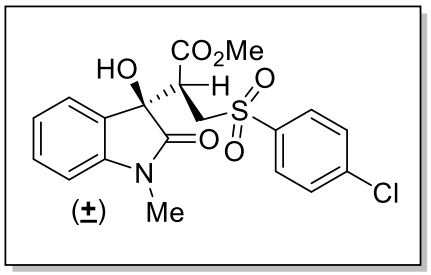
3-(Methyl-3'-(4-methoxyphenylsulfonyl)-propanoate-2'-yl)-3-hydroxy-1-methylindolin-2-one (3ac)



The title compound **3ac** was prepared following the general procedure for Table 2, using allylic alcohol **1a** *i.e.* 3-(methyl propenoate-2'-yl)-3-hydroxy-1-methylindolin-2-one (1.0 mmol, 0.247 g) and *p*-methoxybenzenesulfinic acid **2c** (3.0 mmol, 0.516 g). Yield: 0.347 g, 83%; White solid; M.P.: 160 ^{o}C; ^{1}H NMR (400 MHz, DMSO-d_6): δ 3.05 (s, 3 H), 3.19 (s, 3 H), 3.20 & 4.02 (dABq, J = 1.6 Hz & 14.4 Hz, 2 H), 3.78-3.86 (m*, 4 H), 6.71 (s, 1 H), 6.94-7.01 (m, 2 H), 7.17 (d, J = 7.2 Hz, 2 H), 7.22 (d, J = 7.2 Hz, 1 H), 7.31 (td, J = 1.6 Hz & 8.0 Hz, 1 H), 7.76 (d, J = 7.2Hz, 2 H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 25.9, 47.3, 51.8, 52.0, 55.8, 74.3, 108.6, 114.7, 122.3, 124.5, 127.6, 129.9, 130.12, 130.17, 142.8, 163.4, 168.5, 175.3; HRMS (ESI) exact mass calcd for $C_{20}H_{21}NO_7S$ + H (M + H), 420.1117; found: 420.1113.

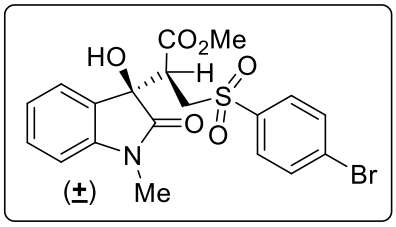
*This multiplet contains one singlet for 3 protons and one multiplet for 1 proton

3-(Methyl-3'-(4-chlorophenylsulfonyl)-propanoate-2'-yl)-3-hydroxy-1-methylindolin-2-one (3ad)



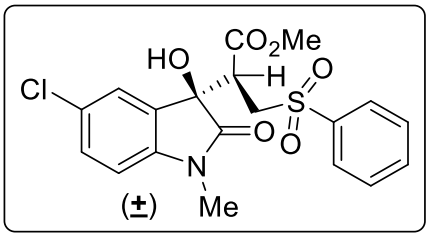
The title compound **3ad** was prepared following the general procedure for Table 2, using allylic alcohol **1a** *i.e.* 3-(methyl propenoate-2'-yl)-3-hydroxy-1-methylindolin-2-one (1.0 mmol, 0.247 g), and *p*-chlorobenzenesulfinic acid **2d** (3.0 mmol, 0.529 g). Yield: 0.359 g, 85%; White solid; M.P.: 182 ^{o}C; ^{1}H NMR (400 MHz, DMSO-d_6): δ 3.05 (s, 3 H), 3.19 (s, 3 H), 3.24 & 4.10 (dABq, *J* = 1.6 Hz & 14.4, 2 H), 3.88-3.95 (m, 1 H), 6.76 (s, 1 H), 6.95-7.01 (m, 2 H), 7.24 (d, *J* = 7.6 Hz, 1 H), 7.31 (td, *J* = 1.6 Hz & 8.0 Hz, 1 H), 7.75 (d, *J* = 8.4 Hz, 2 H), 7.87 (d, *J* = 8.4 Hz, 2 H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 25.9, 47.1, 51.7, 51.9, 74.2, 108.7, 122.3, 124.6, 127.5, 129.7, 129.9, 137.5, 139.2, 142.9, 168.4, 175.2; HRMS (ESI) exact mass calcd for $C_{19}H_{18}ClNO_6S$ + H (M + H), 424.0622; found: 424.0618.

3-(Methyl-3'-(4-bromophenylsulfonyl)-propanoate-2'-yl)-3-hydroxy-1-methylindolin-2-one (3ae)



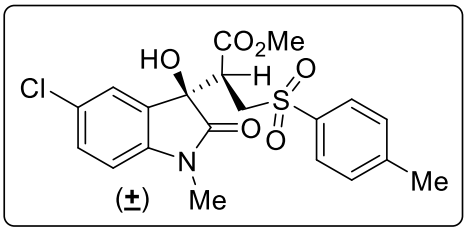
The title compound **3ae** was prepared following the general procedure for Table 2, using allylic alcohol **1a** *i.e.* 3-(methyl propenoate-2'-yl)-3-hydroxy-1-methylindolin-2-one (1.0 mmol, 0.247 g), and *p*-bromobenzenesulfinic acid **2e** (3.0 mmol, 0.663 g). Yield: 0.397 g, 85%; White solid; M.P.: 198 ^{o}C; ^{1}H NMR (400 MHz, DMSO-d_6): δ 3.05 (s, 3 H), 3.19 (s, 3 H), 3.23 & 4.09 (dABq, *J* = 1.6 Hz & 14.4 Hz, 2 H), 3.88-3.94 (m, 1 H), 6.76 (s, 1 H), 6.95-7.01 (m, 2 H), 7.24 (d, *J* = 7.2 Hz, 1 H), 7.31 (td, *J* = 1.6 Hz & 8.0 Hz, 1 H), 7.77-7.80 (m, 2 H), 7.88-7.91 (m, 2 H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 25.9, 47.1, 51.7, 51.9, 74.2, 108.7, 122.3, 124.6, 127.5, 128.4, 129.94, 129.99, 132.6, 137.9, 142.9, 168.4, 175.2; HRMS (ESI) exact mass calcd for $C_{19}H_{18}BrNO_6S$ + H (M + H), 468.0116; found: 468.0121

3-(Methyl-3'-(phenylsulfonyl)-propanoate-2'-yl)-5-chloro-3-hydroxy-1-methylindolin-2-one (3ba)



The title compound **3ba** was prepared following the general procedure for Table 2, using allylic alcohol **1b** *i.e.* 3-(methyl propenoate-2'-yl)-5-chloro-3-hydroxy-1-methylindolin-2-one (1.0 mmol, 0.281 g) and benzenesulfinic acid **2a** (3.0 mmol, 0.426 g). Yield: 0.346 g, 82%; White solid; M.P.: 152 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.08 (s, 3 H), 3.36 & 3.67 (dABq, *J* = 1.6 Hz & 12.4 Hz, 2 H), 3.47 (s, 3 H), 3.78-3.84 (m, 1 H), 3.96-3.97 (m, 1 H), 6.68 (d, *J* = 8.0 Hz, 1 H), 6.98 (d, *J* = 2.0 Hz , 1 H), 7.25 (dd *J* = 2.0 Hz & 8.4 Hz, 1 H), 7.50-7.54 (m, 2 H), 7.60-7.64 (m, 1 H), 7.82 (dd, *J* = 1.2 Hz & 8.4 Hz, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 26.6, 46.2, 52.0, 52.9, 75.2, 109.8, 124.6, 128.3, 128.9, 129.5, 130.7, 134.3, 138.5, 141.9, 169.8, 174.6; HRMS (ESI) exact mass calcd for $C_{19}H_{18}ClNO_6S$ + H (M + H), 424.0622; found: 424.0618.

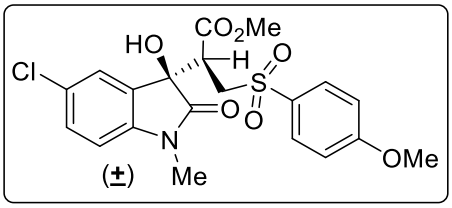
3-(Methyl-3'-(4-methylphenylsulfonyl)-propanoate-2'-yl)-5-chloro-3-hydroxy-1-methylindolin-2-one (3bb)



The title compound **3bb** was prepared following the general procedure for Table 2, using allylic alcohol **1b** *i.e.* 3-(methyl propenoate-2'-yl)-5-chloro-3-hydroxy-1-methylindolin-2-one (1.0 mmol, 0.281 g) and *p*-toluenesulfinic acid **2b** (3.0 mmol, 0.468 g). Yield: 0.358 g, White solid; 82%; M.P.: 189 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): *δ* 2.46 (s, 3 H), 3.15 (s, 3 H), 3.40 & 3.64 (dABq, *J* = 1.6 Hz & 14.4 Hz, 2 H), 3.56 (s, 3 H), 3.82-3.88 (m, 1 H), 4.11 (d, *J* = 2.0 Hz, 1 H), 6.75 (d, *J* = 8.4 Hz, 1 H), 7.00 (d, *J* = 1.6 Hz, 1 H), 7.31 (dd, *J* = 1.6 Hz & 8.4 Hz, 1 H), 7.37 (d, *J* = 7.6 Hz, 2 H), 7.75 (d, *J* = 8.4 Hz, 2 H); ^{13}C NMR (100

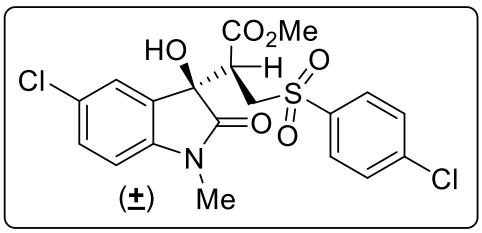
MHz, $CDCl_3$): δ 21.8, 26.8, 46.3, 52.0, 53.0, 75.2, 109.8, 124.7, 128.3, 128.4, 128.9, 130.2, 130.6, 135.4, 141.9, 145.4, 169.8, 174.6; HRMS (ESI) exact mass calcd for $C_{20}H_{20}ClNO_6S$ + H (M + H), 438.0778; found: 438.0786.

3-(Methyl-3'-(4-methoxyphenylsulfonyl)-propanoate-2'-yl)-5-chloro-3-hydroxy-1-methylindolin-2-one (3bc)



The title compound **3bc** was prepared following the general procedure for Table 2, using allylic alcohol **1b** *i.e.* 3-(methyl propenoate-2'-yl)-5-chloro-3-hydroxy-1-methylindolin-2-one (1.0 mmol, 0.281 g) and *p*-methoxybenzenesulfinic acid **2c** (3.0 mmol, 0.516 g). Yield: 0.344 g, 76%; White solid; M.P.: 168 ^oC; ^1H NMR (400 MHz, DMSO-d_6): δ 3.05 (s, 3 H), 3.25 & 3.99 (dABq, *J* = 1.6 Hz & 14.4 Hz, 2 H), 3.35 (s, 3 H), 3.78-3.86 (m*, 4 H), 6.87 (s, 1 H), 6.99 (d, *J* = 8.4 Hz, 1 H), 7.17 (dd, *J* = 2.0 Hz & 6.8 Hz, 2 H), 7.35-7.39 (m, 2 H), 7.76 (dd, *J* = 2.0 Hz & 6.8 Hz, 2 H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 26.1, 47.3, 51.9, 52.0, 55.8, 74.4, 110.2, 114.7, 124.7, 126.6, 129.61, 129.63, 129.7, 130.1, 130.2, 141.8, 163.5, 168.5, 175.0; HRMS (ESI) exact mass calcd for $C_{20}H_{20}ClNO_7S$ + H (M + H), 454.0727; found: 454.0722. *This multiplet contains one singlet for 3 protons and one multiplet for 1 proton.

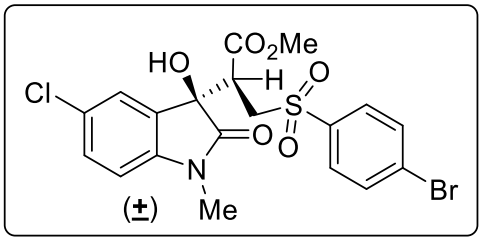
3-(Methyl-3'-(4-chlorophenylsulfonyl)-propanoate-2'-yl)-5-chloro-3-hydroxy-1-methylindolin-2-one (3bd)



The title compound **3bd** was prepared following the general procedure for Table 2, using allylic alcohol

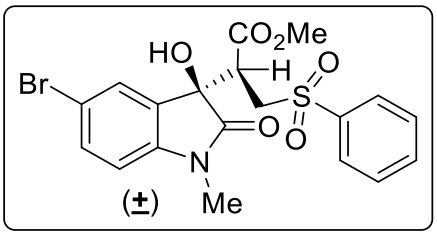
1b *i.e.* 3-(methyl propenoate-2'-yl)-5-chloro-3-hydroxy-1-methylindolin-2-one (1.0 mmol, 0.281 g) and *p*-chlorobenzenesulfinic acid **2d** (3.0 mmol, 0.529 g). Yield: 0.380 g, 83%; White solid; M.P.: 185 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.16 (s, 3 H), 3.39 & 3.78 (dABq, *J* = 2.0 Hz & 14.4 Hz, 2 H), 3.56 (s, 3 H), 3.85-3.91 (m, 1 H), 3.95 (s, 1 H), 6.76 (d, *J* = 8.4 Hz, 1 H), 7.06 (d, *J* = 2.0 Hz, 1 H), 7.33 (dd, *J* = 2.0 Hz & 8.4 Hz, 1 H), 7.54-7.56 (m, 2 H), 7.81-7.84 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 29.7, 46.2, 52.1, 53.0, 75.1, 109.9, 124.6, 128.3, 129.0, 129.8, 130.8, 137.0, 141.1, 141.9, 169.8, 174.5; HRMS (ESI) exact mass calcd for $C_{19}H_{17}Cl_2NO_6S$ + H (M + H), 458.0232; found: 458.0238.

3-(Methyl-3'-(4-bromophenylsulfonyl)-propanoate-2'-yl)-5-chloro-3-hydroxy-1-methylindolin-2-one (3be)



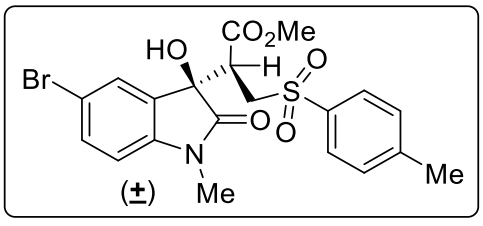
The title compound **3be** was prepared following the general procedure for Table 2, using allylic alcohol **1b** *i.e.* 3-(methyl propenoate-2'-yl)-5-chloro-3-hydroxy-1-methylindolin-2-one (1.0 mmol, 0.281 g) and *p*-bromobenzenesulfinic acid **2e** (3.0 mmol, 0.663 g). Yield: 0.426 g, 85%; White solid; M.P.: 180 ^{o}C; ^{1}H NMR (400 MHz, DMSO-d_6): δ 3.05 (s, 3 H), 3.22-3.29 (m*, 4 H), 3.90-3.96 (m, 1 H), 4.06-4.09 (m, 1 H), 6.91 (s, 1 H), 7.00 (d, *J* = 8.4 Hz, 1 H), 7.38 (s, 2 H), 7.79 (d, *J* = 8.4 Hz, 2 H), 7.90 (d, *J* = 8.0 Hz, 2 H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 26.1, 47.0, 51.6, 52.1, 74.3, 110.2, 124.7, 126.6, 128.4, 129.4, 129.8, 129.9, 132.6, 137.9, 141.8, 168.4, 174.9; HRMS (ESI) exact mass calcd for $C_{19}H_{17}BrClNO_6S$ + H (M + H), 501.9727; found: 501.9735. *This multiplet contains one singlet for 3 protons and one multiplet for 1 proton.

3-(Methyl-3'-(phenylsulfonyl)-propanoate-2'-yl)-5-bromo-3-hydroxy-1-methylindolin-2-one (3ca)



The title compound **3ca** was prepared following the general procedure for Table 2, using allylic alcohol **1c** *i.e.* 3-(methyl propenoate-2'-yl)-5-bromo-3-hydroxy-1-methylindolin-2-one (1.0 mmol, 0.326 g) and benzenesulfinic acid **2a** (3.0 mmol, 0.426 g). Yield: 0.388 g, 83%; White solid; M.P.: 173 ^{o}C; ^{1}H NMR (400 MHz, DMSO-d_6): δ 3.04 (s, 3 H), 3.19 (s, 3 H), 3.26 & 4.07 (dABq, *J* = 1.6 Hz & 14.8 Hz, 2 H), 3.85-3.92 (m, 1 H), 6.88 (s, 1 H), 6.95 (d, *J* = 8.4 Hz, 1 H), 7.47 (d, *J* = 2.0 Hz, 1 H), 7.51 (dd, *J* = 2.0 Hz & 8.4 Hz, 1 H), 7.65-7.69 (m, 2 H), 7.75-7.82 (m, 1 H), 7.84-7.87 (m, 2 H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 26.0, 47.1, 51.5, 74.3, 110.7, 114.3, 127.4, 127.8, 129.5, 129.9, 132.6, 134.2, 138.6, 142.2, 168.4, 174.9; HRMS (ESI) exact mass calcd for $C_{19}H_{18}BrNO_6S$ + H (M + H), 468.0116; found: 468.0109.

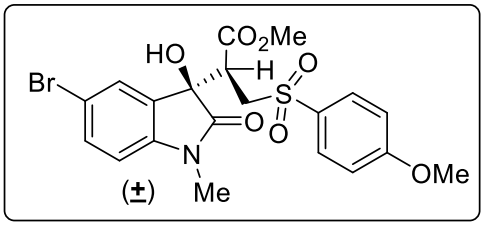
3-(Methyl-3'-(4-methylphenylsulfonyl)-propanoate-2'-yl)-5-bromo-3-hydroxy-1-methylindolin-2-one (3cb)



The title compound **3cb** was prepared following the general procedure for Table 2, using allylic alcohol **1c** *i.e.* 3-(methyl propenoate-2'-yl)-5-bromo-3-hydroxy-1-methylindolin-2-one (1.0 mmol, 0.326 g) and *p*-toluenesulfinic acid **2b** (3.0 mmol, 0.468 g). Yield: 0.390 g, 81%; White solid; M.P.: 180 ^{o}C; ^{1}H NMR (400 MHz, DMSO-d_6): δ 2.41 (s, 3 H), 3.04 (s, 3 H), 3.21 (s, 3 H), 3.22 & 4.02 (dABq, *J* = 1.6 Hz & 14.4 Hz, 2 H), 3.79-3.86 (m, 1 H), 6.86 (s, 1 H), 6.94 (d, *J* = 8.4 Hz, 1 H), 7.45 (d, *J* = 2.0 Hz, 1 H), 7.47 (d, *J*

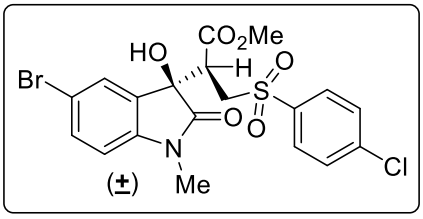
= 8.0 Hz, 2 H), 7.51 (dd, *J* = 2.0 Hz & 8.4 Hz, 1 H), 7.72 (d, *J* = 8.0 Hz, 2 H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 21.1, 26.1, 47.2, 51.7, 52.0, 74.4, 110.8, 114.3, 127.3, 127.9, 129.9, 130.0, 132.6, 135.8, 142.2, 144.8, 168.5, 174.9; HRMS (ESI) exact mass calcd for $C_{20}H_{20}BrNO_6S$ + H (M + H), 482.0273; found: 482.0278.

3-(Methyl-3'-(4-methoxyphenylsulfonyl)-propanoate-2'-yl)-5-bromo-3-hydroxy-1-methylindolin-2-one (3cc)



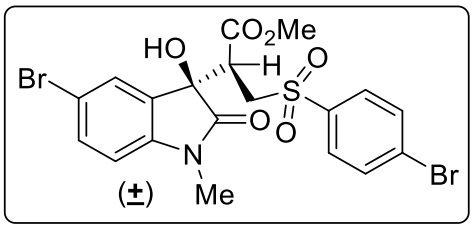
The title compound **3cc** was prepared following the general procedure for Table 2, using allylic alcohol **1c** *i.e.* 3-(methyl propenoate-2'-yl)-5-bromo-3-hydroxy-1-methylindolin-2-one (1.0 mmol, 0.326 g) and *p*-methoxybenzenesulfinic acid **2c** (3.0 mmol, 0.516 g). Yield: 0.413 g, 83%; White solid; M.P.: 158 ^{o}C; ^{1}H NMR (400 MHz, DMSO-d_6): δ 3.04 (s, 3 H), 3.19 (s, 3H), 3.20 & 4.00 (ABq, *J* = 14.0 Hz, 2 H), 3.77-3.86 (m*, 4 H), 6.85 (s, 1 H), 6.94 (d, *J* = 8.4 Hz, 1 H), 7.17 (d, *J* = 8.8 Hz, 2 H), 7.45 (s, 1 H), 7.51 (d, *J* = 8.4 Hz, 1 H), 7.76 (d, *J* = 8.8 Hz, 2 H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 26.0, 47.3, 51.9, 52.0, 55.8, 74.4, 110.8, 114.3, 114.7, 127.3, 129.9, 130.1, 130.2, 132.6, 142.2, 163.5, 168.5, 174.9; HRMS (ESI) exact mass calcd for $C_{20}H_{20}BrNO_7S$ + H (M + H), 498.0222; found: 498.0216. *This multiplet contains one singlet for 3 protons and one multiplet for one proton.

3-(Methyl-3'-(4-chlorophenylsulfonyl)-propanoate-2'-yl)-5-bromo-3-hydroxy-1-methylindolin-2-one (3cd)



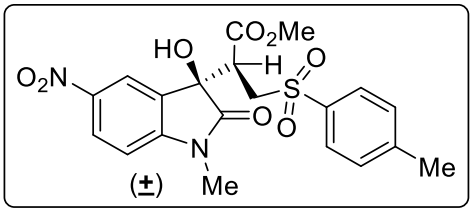
The title compound **3cd** was prepared following the general procedure for Table 2, using allylic alcohol **1c** *i.e.* 3-(methyl propenoate-2'-yl)-5-bromo-3-hydroxy-1-methylindolin-2-one (1.0 mmol, 0.326 g) and *p*-chlorobenzenesulfinic acid **2d** (3.0 mmol, 0.529 g). Yield: 0.431 g, 86%; White solid; M.P.: 170 ^{o}C; ^{1}H NMR (400 MHz, DMSO-d_6): δ 3.05 (s, 3 H), 3.22 (s, 3 H), 3.26 & 4.09 (dABq, *J* = 1.6 Hz & 14.8 Hz, 2 H), 3.89-3.96 (m, 1 H), 6.90 (s, 1 H), 6.95 (d, *J* = 8.4 Hz, 1 H), 7.47 (d, *J* = 2.0 Hz, 1 H), 7.51 (dd, *J* = 2.0 Hz & 8.4 Hz, 1 H), 7.74-7.77 (m, 2 H), 7.86-7.89 (m, 2 H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 26.1, 47.0, 51.6, 52.0, 74.3, 110.8, 114.3, 127.3, 129.7, 129.8, 129.9, 130.0, 132.7, 137.5, 139.3, 142.3, 168.4, 174.9; HRMS (ESI) exact mass calcd for $C_{19}H_{17}BrClNO_6S$ + H (M + H), 501.9727; found: 501.9732.

3-(Methyl-3'-(4-bromophenylsulfonyl)-propanoate-2'-yl)-5-bromo-3-hydroxy-1-methylindolin-2-one (3ce)



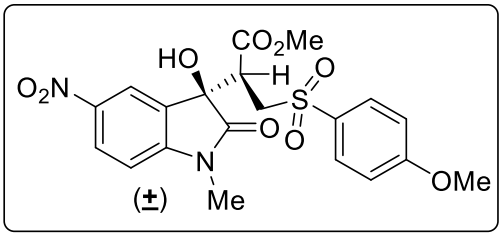
The title compound **3ce** was prepared following the general procedure for Table 2, using allylic alcohol **1c** *i.e.* 3-(methyl propenoate-2'-yl)-5-bromo-3-hydroxy-1-methylindolin-2-one (1.0 mmol, 0.326 g) and *p*-bromobenzenesulfinic acid **2e** (3.0 mmol, 0.663 g). Yield: 0.464 g, 85%; White solid; M.P.: 170 ^{o}C; ^{1}H NMR (400 MHz, DMSO-d_6): δ 3.05 (s, 3 H), 3.23 (s, 3 H), 3.26, 4.08 (dABq, *J* = 1.6 Hz & 14.4 Hz, 2 H), 3.89-3.95 (m, 1 H), 6.89 (s, 1 H), 6.95 (d, *J* = 8.4 Hz, 1 H), 7.47 (d, *J* = 2.0 Hz, 1 H), 7.52 (dd, *J* = 2.0 Hz & 8.4 Hz, 1 H), 7.77-7.81 (m, 2 H), 7.88-7.92 (m, 2 H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 26.0, 47.0, 51.6, 52.0, 74.3, 110.7, 114.3, 127.3, 128.4, 129.8, 129.9, 132.65, 132.68, 137.9, 142.3, 168.4, 174.8; HRMS (ESI) exact mass calcd for $C_{19}H_{17}Br_2NO_6S$ + H (M + H), 545.9222; found: 545.9228.

3-(Methyl-3'-(4-methylphenylsulfonyl)-propanoate-2'-yl)-5-nitro-3-hydroxy-1-methylindolin-2-one (3db)



The title compound **3db** was prepared following the general procedure for Table 2, using allylic alcohol **1d** *i.e.* 3-(methyl propenoate-2'-yl)-5-nitro-3-hydroxy-1-methylindolin-2-one (1.0 mmol, 0.292 g) and *p*-toluenesulfinic acid **2b** (3.0 mmol, 0.468 g). Yield: 0.376 g, 84%; off-white solid; M.P.: 172 ^{o}C; ^{1}H NMR (400 MHz, DMSO-d_6): δ 2.41 (s, 3 H), 3.14 (s, 3 H), 3.24 (s, 3 H), 3.25 & 4.10 (dABq, *J* = 1.6 Hz & 14.4 Hz, 2 H), 3.82-3.89 (m, 1 H), 7.06 (s, 1 H), 7.22 (d, *J* = 8.8 Hz, 1H), 7.46 (d, *J* = 8.0 Hz, 2 H), 7.74 (d, *J* = 8.0 Hz, 2 H), 8.05 (d, *J* = 2.4 Hz, 1 H), 8.30 (dd, *J* = 2.4 Hz & 8.8 Hz, 1 H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 21.1, 26.4, 47.2, 51.6, 52.1, 74.0, 109.2, 119.9, 127.1, 127.9, 128.6, 129.9, 135.6, 142.6, 144.8, 148.9, 168.5, 175.7; HRMS (ESI) exact mass calcd for $C_{20}H_{20}N_2O_8S$ + H (M + H), 449.1019; found: 449.1014.

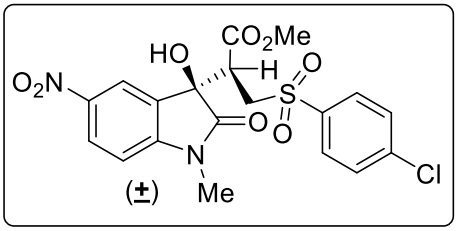
3-(Methyl-3'-(4-methoxyphenylsulfonyl)-propanoate-2'-yl)-5-nitro-3-hydroxy-1-methylindolin-2-one (3dc)



The title compound **3dc** was prepared following the general procedure for Table 2, using allylic alcohol **1d** *i.e.* 3-(methyl propenoate-2'-yl)-5-nitro-3-hydroxy-1-methylindolin-2-one (1.0 mmol, 0.292 g) and *p*-methoxybenzenesulfinic acid **2c** (3.0 mmol, 0.516 g). Yield: 0.366 g, 79%; off-white solid; M.P.: 184 ^{o}C; ^{1}H NMR (400 MHz, DMSO-d_6): δ 3.14 (s, 3 H), 3.22 & 4.07 (ABq, *J* = 14.4 Hz, 2 H), 3.23 (s, 3 H), 3.80-3.86 (m*, 4 H), 7.05 (s, 1 H), 7.16 (d, *J* = 8.8 Hz, 2 H), 7.22 (d, *J* = 8.4 Hz, 1 H), 7.77 (d, *J* = 8.8 Hz, 2 H), 8.04 (s, 1 H), 8.30 (d, *J* = 8.4 Hz, 1 H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 26.4, 47.3, 51.8,

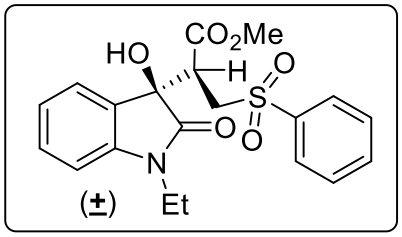
52.2, 55.8, 74.0, 109.3, 114.7, 119.9, 127.1, 128.6, 129.9, 130.2, 142.6, 148.9, 163.5, 168.5, 175.7; HRMS (ESI) exact mass calcd for $C_{20}H_{20}N_2O_9S$ + H (M + H), 465.0968; found: 465.0963. *This multiplet contains one singlet for 3 protons and one multiplet for 1 proton.

3-(Methyl-3'-(4-chlorophenylsulfonyl)-propanoate-2'-yl)-5-nitro-3-hydroxy-1-methylindolin-2-one (3dd)



The title compound **3dd** was prepared following the general procedure for Table 2, using allylic alcohol **1d** *i.e.* 3-(methyl propenoate-2'-yl)-5-nitro-3-hydroxy-1-methylindolin-2-one (1.0 mmol, 0.292 g) and *p*-chlorobenzenesulfinic acid **2d** (3.0 mmol, 0.529 g). Yield: 0.402 g, 86%; off-white solid; M.P.: 130 ^{o}C; ^{1}H NMR (400 MHz, DMSO-d_6): δ 3.15 (s, 3 H), 3.25 (s, 3 H), 3.29 & 4.20 (ABq, *J* = 14.4 Hz, 2 H), 3.93-4.00 (m, 1 H), 7.10 (s, 1 H), 7.23 (d, *J* = 8.8 Hz, 1 H), 7.75 (d, *J* = 8.4 Hz, 2 H), 7.89 (d, *J* = 8.4 Hz, 2 H), 8.09 (d, *J* = 2.4 Hz, 1 H), 8.30 (dd, *J* = 2.4 Hz & 8.8 Hz, 1 H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 26.5, 47.1, 51.5, 52.2, 73.9, 109.3, 120.0, 127.2, 128.5, 129.7, 130.0, 137.3, 139.3, 142.7, 148.9, 168.4, 175.8; HRMS (ESI) exact mass calcd for $C_{19}H_{17}ClN_2O_8S$ + H (M + H), 469.0472; found: 469.0478.

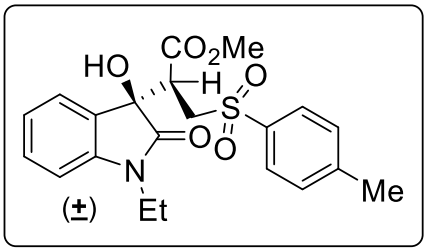
3-(Methyl-3-(phenylsulfonyl)-propanoate-2-yl)-3-hydroxy-1-ethylindolin-2-one (3ea)



The title compound **3ea** was prepared following the general procedure for Table 2, using allylic alcohol **1e** *i.e.* 3-(methyl propenoate-2'-yl)-3-hydroxy-1-ethylindolin-2-one (1.0 mmol, 0.261 g) and benzenesulfinic acid **2a** (3.0 mmol, 0.426 g). Yield: 0.302 g, 75%; White solid; M.P.: 136 ^{o}C; ^{1}H NMR

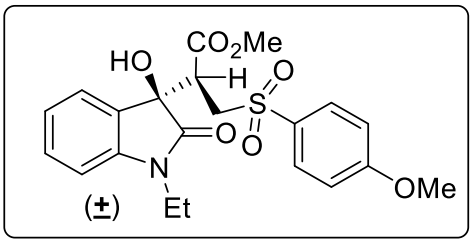
(400 MHz, $CDCl_3$): δ 1.15 (t, J = 7.6 Hz, 3 H), 3.38 (s, 3 H), 3.39, 3.74 (dABq, *J* = 2.0 & 14.4 Hz, 2 H), 3.50-3.59 (m, 1 H), 3.65-3.72 (m, 1 H), 3.82-3.88 (m, 2 H), 6.76 (d, *J* = 7.6 Hz, 1 H), 6.95 (t, *J* = 7.6 Hz, 1 H), 7.05 (d, *J* = 7.2 Hz, 1 H), 7.25 (td, *J* = 1.6 Hz & 8.0 Hz, 1 H), 7.47-7.51 (m, 2 H), 7.60 (t, *J* = 7.6 Hz, 1 H), 7.83 (d, *J* = 7.6 Hz, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 12.4, 35.0, 46.6, 52.1, 52.7, 75.1, 109.0, 123.3, 124.3, 126.8, 128.4, 129.4, 130.7, 134.1, 138.6, 142.5, 169.7, 174.8; HRMS (ESI) exact mass calcd for $C_{20}H_{21}NO_6S$ + H (M + H), 404.1168; found: 404.1172.

3-(Methyl-3'-(4-methylphenylsulfonyl)-propanoate-2'-yl)-3-hydroxy-1-ethylindolin-2-one (3eb)



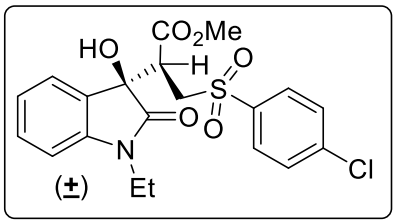
The title compound **3eb** was prepared following the general procedure for Table 2, using allylic alcohol **1e** *i.e.* 3-(methyl propenoate-2'-yl)-3-hydroxy-1-ethylindolin-2-one (1.0 mmol, 0.261 g) and *p*-toluenesulfinic acid **2b** (3.0 mmol, 0.468 g). Yield: 0.321 g, 77%; White solid; M.P.: 158 ^oC; ^1H NMR (400 MHz, $CDCl_3$): δ 1.22 (t, *J* = 7.2 Hz, 3 H), 2.44 (s, 3 H), 3.43-3.46 (m*, 4 H), 3.57-3.66 (m, 1 H), 3.72-3.82 (m, 2 H), 3.87-3.97 (m, 2 H), 6.82 (d, *J* = 8.0 Hz, 1 H), 7.01 (t, *J* = 7.6 Hz, 1 H), 7.12 (d, *J* = 7.6 Hz, 1 H), 7.31 (dd, *J* = 1.2 & 8.0 Hz, 1 H), 7.34 (d, *J* = 8.4 Hz, 2 H), 7.76 (d, J = 8.4 Hz, 2 H); ^{13}C NMR (100 MHz, CDCl3): δ 12.4, 21.7, 35.0, 46.7, 52.1, 52.6, 75.1, 108.9, 123.1, 124.4, 126.8, 128.4, 130.0, 130.7, 135.6, 142.4, 145.1, 169.7, 174.8; HRMS (ESI) exact mass calcd for $C_{21}H_{23}NO_6S$ + H (M + H), 418.1324; found:418.1331. *This multiplet contains one singlet for 3 protons and one multiplet for 1 proton.

3-(Methyl-3'-(4-methoxyphenylsulfonyl)-propanoate-2'-yl)-3-hydroxy-1-ethylindolin-2-one (3ec)



The title compound was **3ec** prepared following the general procedure for Table 2, using allylic alcohol **1e** *i.e.* 3-(methyl propenoate-2'-yl)-3-hydroxy-1-ethylindolin-2-one (1.0 mmol, 0.261 g) and *p*-methoxybenzenesulfinic acid **2c** (3.0 mmol, 0.516 g). Yield: 0.355 g, 82%; off-white solid; M.P.: 138 ^{o}C; ^{1}H NMR (400 MHz, DMSO-d_6): δ 1.06 (t, J = 7.2 Hz, 3 H), 3.17 (s, 3 H), 3.18 & 4.03 (dABq, *J* = 1.2 Hz & 14.4 Hz, 2 H), 3.48-3.57 (m, 1 H), 3.63-3.72 (m, 1 H), 3.78-3.84 (m, 1 H), 3.85 (s, 3 H), 6.71 (s, 1 H), 6.99 (d, *J* = 8.0 Hz, 2 H), 7.17 (dd, *J* = 2.0 Hz & 6.8 Hz, 2 H), 7.23 (d, *J* = 6.8 Hz, 1 H), 7.29 (td, *J* = 1.2 & 7.6 Hz, 1 H), 7.75 (dd, *J* = 2.0 & 6.8 Hz, 2 H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 12.2, 34.0, 47.3, 51.8, 52.0, 55.8, 74.1, 108.6, 114.7, 122.1, 124.8, 127.8, 129.9, 130.0, 130.2, 141.8, 163.5, 168.5, 174.8; HRMS (ESI) exact mass calcd for $C_{21}H_{23}NO_7S$ + H (M + H), 434.1273; found: 434.1279.

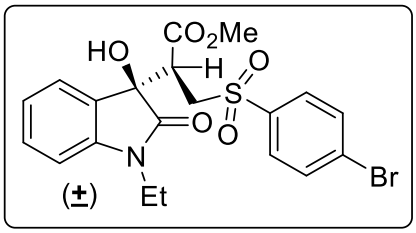
3-(Methyl-3'-(4-chlorophenylsulfonyl)-propanoate-2'-yl)-3-hydroxy-1-ethylindolin-2-one (3ed)



The title compound **3ed** was prepared following the general procedure for Table 2, using allylic alcohol **1e** *i.e.* 3-(methyl propenoate-2'-yl)-3-hydroxy-1-ethylindolin-2-one (1.0 mmol, 0.261 g) and *p*-chlorobenzenesulfinic acid **2d** (3.0 mmol, 0.529 g). Yield: 0.345 g, 79%; White solid; M.P.: 150 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.22 (t, *J* = 7.2 Hz, 3 H), 3.42-3.46 (m*, 4 H), 3.57-3.66 (m, 1 H), 3.72-3.81 (m, 1 H), 3.87-3.94 (m, 2 H), 3.98 (s, 1 H), 6.84 (d, *J* = 8.0 Hz, 1 H), 7.03 (td, *J* = 1.2 Hz & 7.6 Hz, 1 H), 7.14 (dd, *J* = 0.8 Hz & 7.6 Hz, 1 H), 7.33 (td, *J* = 1.2 Hz & 7.6 Hz, 1 H), 7.51-7.54 (m, 2 H), 7.82-7.84

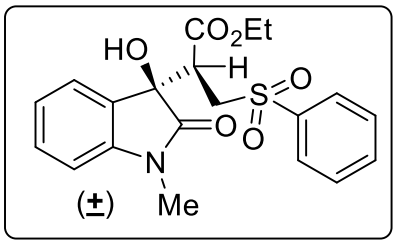
(m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 12.4, 35.0, 46.7, 52.2, 52.7, 75.1, 109.0, 123.2, 124.4, 126.8, 129.7, 129.9, 130.8, 137.1, 140.8, 142.4, 169.5, 174.8; HRMS (ESI) exact mass calcd for $C_{20}H_{20}ClNO_6S$ + Na (M + Na), 460.0598; found:460.0593. *This multiplet contains one singlet for 3 protons and one multiplet for 1 proton.

3-(Methyl-3'-(4-bromophenylsulfonyl)-propanoate-2'-yl)-3-hydroxy-1-ethylindolin-2-one (3ee)



The title compound **3ee** was prepared following the general procedure for Table 2, using allylic alcohol **1e** *i.e.* 3-(methyl propenoate-2'-yl)-3-hydroxy-1-ethylindolin-2-one (1.0 mmol, 0.261 g) and *p*-bromobenzenesulfinic acid **2e** (3.0 mmol, 0.663 g). Yield: 0.390 g, 81%; White solid; M.P.: 168 ^{o}C; ^{1}H NMR (400 MHz, DMSO-d_6): δ 1.07 (t, *J* = 7.2 Hz, 3 H), 3.18 (s, 3 H), 3.22 & 4.11 (dABq, *J* = 1.6 Hz & 14.4 Hz, 2 H), 3.51-3.56 (m, 1 H), 3.65-3.70 (m, 1 H), 3.88-3.95 (m, 1 H), 6.75 (s, 1 H), 6.96-7.01 (m, 2 H), 7.25-7.31 (m, 2 H), 7.78 (d, *J* = 8.0 Hz, 2 H), 7.90 (d, *J* = 8.0 Hz, 2 H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 12.2, 34.0, 47.1, 51.7, 51.9, 74.0, 108.6, 122.1, 124.8, 127.6, 128.4, 129.9, 132.6, 137.8, 141.9, 168.4, 174.8; HRMS (ESI) exact mass calcd for $C_{20}H_{20}BrNO_6S$ + H (M + H), 482.0273; found: 482.0277.

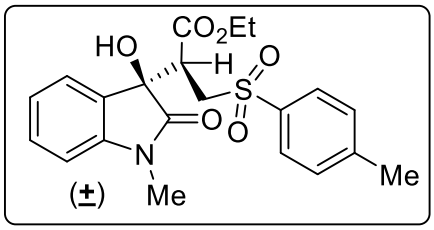
3-(ethyl-3'-(phenylsulfonyl)-propanoate-2'-yl)-3-hydroxy-1-methylindolin-2-one (3fa)



The title compound **3fa** was prepared following the general procedure for Table 2, using allylic alcohol **1f** *i.e.* 3-(ethyl propenoate-2'-yl)-3-hydroxy-1-methylindolin-2-one (1.0 mmol, 0.261 g) and

benzenesulfinic acid **2a** (3.0 mmol, 0.426 g). Yield: 0.322 g, 80%; White solid; M.P.: 178 ^{o}C; ^{1}H NMR (400 MHz, DMSO-d_6): δ 0.74 (t, *J* = 7.2 Hz, 3 H), 3.04 (s, 3 H), 3.27 & 4.07 (dABq, *J* = 1.6 Hz & 14.4 Hz, 2 H), 3.51-3.57 (m, 2 H), 3.89-3.95 (m, 1 H), 6.75 (s, 1 H), 6.94-6.97 (m, 1 H), 6.98-7.00 (m, 1 H), 7.26 (dd, *J* = 1.2 Hz & 7.6 Hz, 1 H), 7.30 (td, *J* = 1.2 Hz & 8.0 Hz, 1 H), 7.64-7.68 (m, 2 H), 7.74-7.78 (m, 1 H), 7.84-7.86 (m, 2 H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 13.3, 25.9, 47.1, 51.6, 60.6, 74.2, 108.6, 122.3, 124.7, 127.5, 127.8, 129.5, 129.9, 134.1, 138.8, 143.0, 167.7, 175.2; HRMS (ESI) exact mass calcd for $C_{20}H_{21}NO_6S$ + H (M + H), 404.1168; found: 404.1164.

3-(Ethyl-3'-(4-methylphenylsulfonyl)-propanoate-2'-yl)-3-hydroxy-1-methylindolin-2-one (3fb)



The title compound **3fb** was prepared following the general procedure for Table 2, using allylic alcohol **1f** *i.e.* 3-(ethyl propenoate-2'-yl)-3-hydroxy-1-methylindolin-2-one (1.0 mmol, 0.261 g) and p-toluenesulfinic acid **2b** (3.0 mmol, 0.468 g). Yield: 0.325 g, 78%; White solid; M.P.: 178 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.01 (t, J = 7.2 Hz , 3 H), 2.44 (s, 3 H), 3.16 (s, 3 H), 3.44-3.49 (m, 1 H), 3.76-3.96 (m, 5 H), 6.80 (d, *J* = 8.0 Hz, 1 H), 7.02 (t, *J* = 7.6 Hz, 1 H), 7.13 (d, J = 7.2 Hz, 1 H), 7.31-7.35 (m, 3 H), 7.77 (d, *J* = 6.8 Hz, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.7, 21.7, 26.4, 46.5, 52.1, 62.0, 75.2, 108.8, 123.3, 124.3, 126.7, 128.4, 130.0, 130.7, 135.8, 143.6, 145.1, 169.1, 175.3; HRMS (ESI) exact mass calcd for $C_{21}H_{23}NO_6S$ + H (M + H), 418.1324; found: 418.1329.

Crystal data for **3fb** Empirical formula, $C_{21}H_{23}NO_6S$; formula weight, 417.46; crystal color, habit: white, block; crystal dimensions, 0.24 X 0.19 X 0.13 mm^3; crystal system, monoclinic; lattice type, primitive; lattice parameters, *a* = 8.6303(7) Å, *b* = 10.9269(9) Å, *c* = 22.2548(18) Å; *α* = 90.00; *β* = 92.664(3); γ = 90.00; *V* = 2096.4(3) Å^3; space group, P 21/c; *Z* = 4; D_{calcd} = 1.323 g / cm^3; F_{000} = 880; λ(Mo-K_α) = 0.71073 Å; *R* (I≥2σ_1) = 0.0829, wR^2 = 0.1613. Detailed X-ray crystallographic data is

available from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK (**for compound 3fb CCDC # 2154710).**

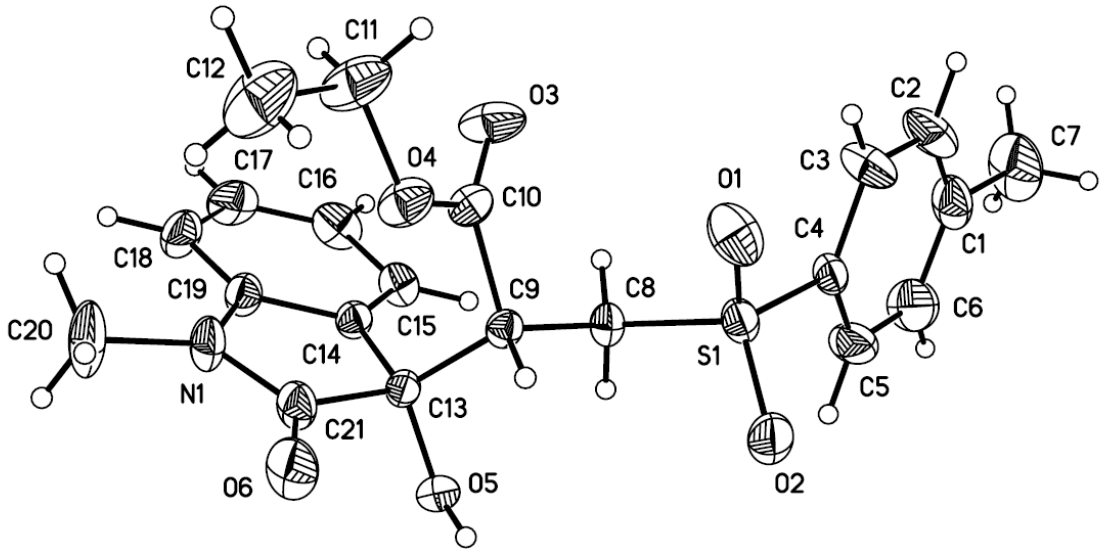
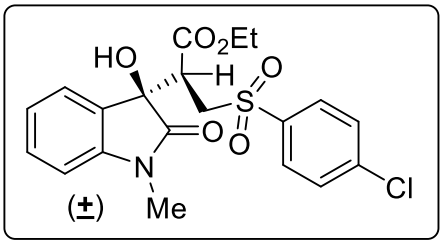


Figure 1. ORTEP diagram of compound **3fb**

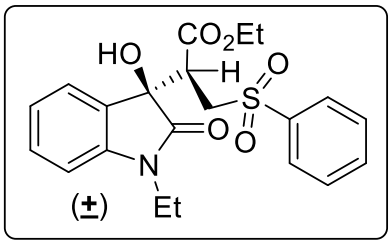
3-(Ethyl-3'-(4-chlorophenylsulfonyl)-propanoate-2'-yl)-3-hydroxy-1-methylindolin-2-one (3fd)



The title compound **3fd** was prepared following the general procedure for Table 2, using allylic alcohol **1f** *i.e.* 3-(ethyl propenoate-2'-yl)-3-hydroxy-1-methylindolin-2-one (1.0 mmol, 0.261 g) and p-chlorobenzenesulfinic acid **2d** (3.0 mmol, 0.529 g). Yield: 0.345 g, 79%; White solid; M.P.: 162 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.02 (t, *J* = 7.2 Hz, 3 H), 3.16 (s, 3 H), 3.45 (dd, *J* = 2.4 Hz & 9.2 Hz, 1 H), 3.85-3.99 (m, 5 H), 6.81 (d, *J* = 8.0 Hz, 1 H), 7.04 (t, *J* = 7.6 Hz, 1 H), 7.15 (dd, *J* = 0.8 Hz & 7.2 Hz, 1 H), 7.34 (td, *J* = 0.8 & 7.6 Hz, 1 H), 7.53 (dd, *J* = 0.8 Hz & 8.8 Hz, 2 H), 7.84 (dd, *J* = 0.8 Hz & 8.8 Hz,

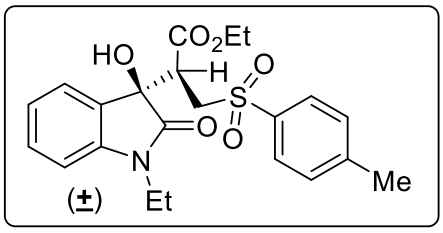
2 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.7, 26.4, 46.5, 52.2, 62.1, 75.1, 108.9, 123.3, 124.3, 126.6, 129.7, 129.9, 130.8, 137.2, 140.9, 143.5, 169.0, 175.2; HRMS (ESI) exact mass calcd for $C_{20}H_{20}ClNO_6S$ + Na (M + Na), 460.0598; found: 460.0591.

3-(Ethyl-3'-(phenylsulfonyl)-propanoate-2'-yl)-3-hydroxy-1-ethylindolin-2-one (3ga)



The title compound **3ga** was prepared following the general procedure for Table 2, using allylic alcohol **1g** *i.e.* 3-(ethyl propenoate-2'-yl)-3-hydroxy-1-ethylindolin-2-one (1.0 mmol, 0.275 g) and benzenesulfinic acid **2a** (3.0 mmol, 0.426 g). Yield: 0.308 g, 74%; White solid; M.P.: 158 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.93 (t, *J* = 7.2 Hz, 3 H), 1.16 (t, *J* = 7.2 Hz, 3 H), 3.34-3.38 (m, 1 H), 3.62 (q, *J* = 7.2 Hz, 1 H), 3.74-3.91 (m, 5 H), 6.75 (d, *J* = 8.0 Hz, 1 H), 6.94 (t, *J* = 7.6 Hz, 1 H), 7.06 (d, *J* = 7.6 Hz, 1 H), 7.25 (t, *J* = 8.0 Hz, 1 H), 7.49 (t, *J* = 8.0 Hz, 2 H), 7.59 (t, *J* = 7.6 Hz, 1 H), 7.83 (d, *J* = 8.0 Hz, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 12.4, 13.7, 35.0, 46.6, 52.1, 62.0, 75.1, 108.9, 123.1, 124.4, 126.9, 128.4, 129.4, 130.7, 134.0, 138.7, 142.6, 169.0, 174.9; HRMS (ESI) exact mass calcd for $C_{21}H_{23}ClNO_6S$ + H (M + H), 418.1324; found: 418.1320.

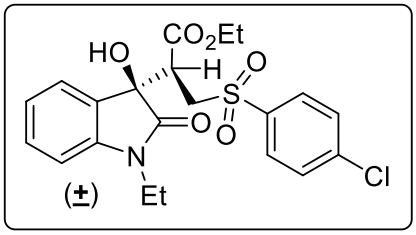
3-(Ethyl-3'-(4-methylphenylsulfonyl)-propanoate-2'-yl)-3-hydroxy-1-ethylindolin-2-one (3gb)



The title compound **3gb** was prepared following the general procedure for Table 2, using allylic alcohol **1g** *i.e.* 3-(ethyl propenoate-2'-yl)-3-hydroxy-1-ethylindolin-2-one (1.0 mmol, 0.275 g) and p-toluenesulfinic acid **2b** (3.0 mmol, 0.468 g). Yield: 0.310 g, 72%; White solid; M.P.: 167 ^{o}C; ^{1}H NMR

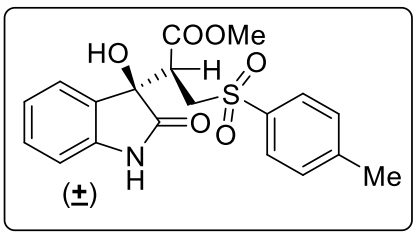
(400 MHz, $CDCl_3$): δ 0.94 (t, *J* = 7.2 Hz, 3 H), 1.16 (t, *J* = 7.2 Hz, 3 H), 2.38 (s, 3 H), 3.35 (dd, *J* = 2.4 & 9.2 Hz, 1 H), 3.62 (q, *J* = 7.2 Hz, 2 H), 3.69-3.75 (m, 2 H), 3.78-3.89 (m, 3 H), 6.75 (d, *J* = 8.0 Hz, 1 H), 6.94 (t, *J* = 8.0 Hz, 1 H), 7.06 (d, *J* = 7.2 Hz, 1 H), 7.23-7.29 (m, 3 H), 7.70 (d, *J* = 8.4 Hz, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 12.4, 13.7, 21.7, 35.0, 46.7, 52.1, 62.0, 75.1, 108.9, 123.1, 124.5, 126.9, 128.4, 130.0, 130.7, 135.7, 142.7, 145.1, 169.1, 174.9; HRMS (ESI) exact mass calcd for $C_{22}H_{25}NO_6S$ + H (M + H), 432.1481; found: 432.1476.

3-(Ethyl-3'-(4-chlorophenylsulfonyl)-propanoate-2'-yl)-3-hydroxy-1-ethylindolin-2-one (3gd)



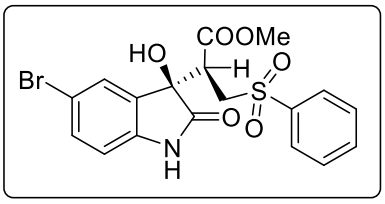
The title compound **3gd** was prepared following the general procedure for Table 2, using allylic alcohol **1g** *i.e.* 3-(ethyl propenoate-2'-yl)-3-hydroxy-1-ethylindolin-2-one (1.0 mmol, 0.275 g) and p-chlorobenzenesulfinic acid **2d** (3.0 mmol, 0.529 g). Yield: 0.351 g, 78%; White solid; M.P.: 156 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.01 (t, *J* = 7.2 Hz, 3 H), 1.23 (t, *J* = 7.2 Hz, 3 H), 3.41 (dd, *J* = 2.4 & 9.2 Hz, 1 H), 3.69 (q, *J* = 7.2 Hz, 2 H), 3.86-3.98 (m, 5 H), 6.83 (d, *J* = 8.0 Hz, 1 H), 7.03 (td, *J* = 0.8 & 7.6 Hz, 1 H), 7.15 (dd, *J* = 1.6 & 7.2 Hz, 1 H), 7.33 (td, *J* = 1.6 & 8.0 Hz, 1 H), 7.52-7.53 (m, 2 H), 7.82-7.84 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 12.4, 13.7, 35.1, 46.6, 52.2, 62.1, 75.0, 109.0, 124.5, 126.8, 129.7, 129.9, 130.8, 137.1, 140.9, 142.6, 168.9, 174.8; HRMS (ESI) exact mass calcd for $C_{21}H_{22}ClNO_6S$ + H (M + H), 452.0935; found: 452.0928.

3-(Methyl-3'-(4-methylphenylsulfonyl)-propanoate-2'-yl)-3-hydroxylindolin-2-one (3hb)



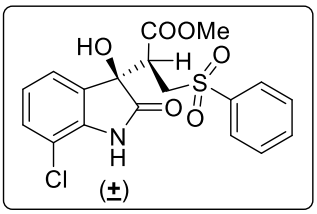
The title compound **3hb** was prepared following the general procedure for Table 2, using allylic alcohol **1h** *i.e.* 3-(methyl propenoate-2'-yl)-3-hydroxy indolin-2-one (1.0 mmol, 0.233 g) and p-chlorobenzenesulfinic acid **2b** (3.0 mmol, 0.468 g), providing **3hb**. Yield: 0.283 g, 73%; white solid; M.P.: 181 ^{o}C; ^{1}H NMR (400 MHz, DMSO-d_6): δ 2.42 (s, 3 H), 3.13 (s, 3 H), 3.27 (dd, *J* = 3.2 & 10.0 Hz, 1 H), 3.61-3.71 (m, 2 H), 6.65 (s, 1 H), 6.74 (d, *J* = 7.6 Hz, 1 H), 6.96 (td, *J* = 1.2 Hz & 7.6 Hz, 1 H), 7.21 (td, *J* = 1.6 Hz & 7.6 Hz, 1 H), 7.29 (d, *J* = 7.6 Hz, 1 H), 7.47 (d, *J* = 8.0 Hz, 2 H), 7.73 (d, *J* = 8.0 Hz, 2 H), 10.40 (s, 1 H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 21.1, 47.7, 51.6, 53.0, 74.0, 109.7, 121.6, 125.0, 127.9, 128.4, 129.9, 130.0, 135.3, 141.6, 144.9, 169.6, 175.8; HRMS (ESI) exact mass calcd for $C_{19}H_{19}NO_6S$ + H (M + H), 390.1011; found: 390.1017.

3-(Methyl-3'-(phenylsulfonyl) propanoate-2'-yl)-5-bromo-3-hydroxylindolin-2-one (3ia)



The title compound **3ia** was prepared following the general procedure for Table 2, using allylic alcohol **1i** *i.e.* 3-(methyl propenoate-2'-yl)-5-bromo-3-hydroxy indolin-2-one (1.0 mmol, 0.312 g) and benzenesulfinic acid **2a** (3.0 mmol, 0.426 g). Yield: 0.335 g, 74%; White solid; M.P.: 156 ^{o}C; ^{1}H NMR (400 MHz, DMSO-d_6): δ 3.20 (s, 3 H), 3.31-3.35 (m, 1 H), 3.59-3.72 (m, 2 H), 7.41 (dd, *J* = 2.0 Hz & 8.0 Hz, 1 H), 6.73 (d, *J* = 8.4 Hz, 1 H), 6.81 (s, 1 H), 7.51 (d, *J* = 2.0 Hz, 1 H), 7.65-7.70 (m, 2 H), 7.76-7.80 (m, 1 H), 7.86-7.88 (m, 2 H), 10.57 (s, 1 H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 47.4, 51.8, 51.9, 52.7, 74.2, 111.8, 113.3, 127.9, 129.6, 130.7, 132.8, 133.2, 134.3, 138.1, 141.0, 169.5, 175.4; HRMS (ESI) exact mass calcd for $C_{18}H_{16}BrNO_6S$ + H (M + H), 453.9960; found: 453.9953.

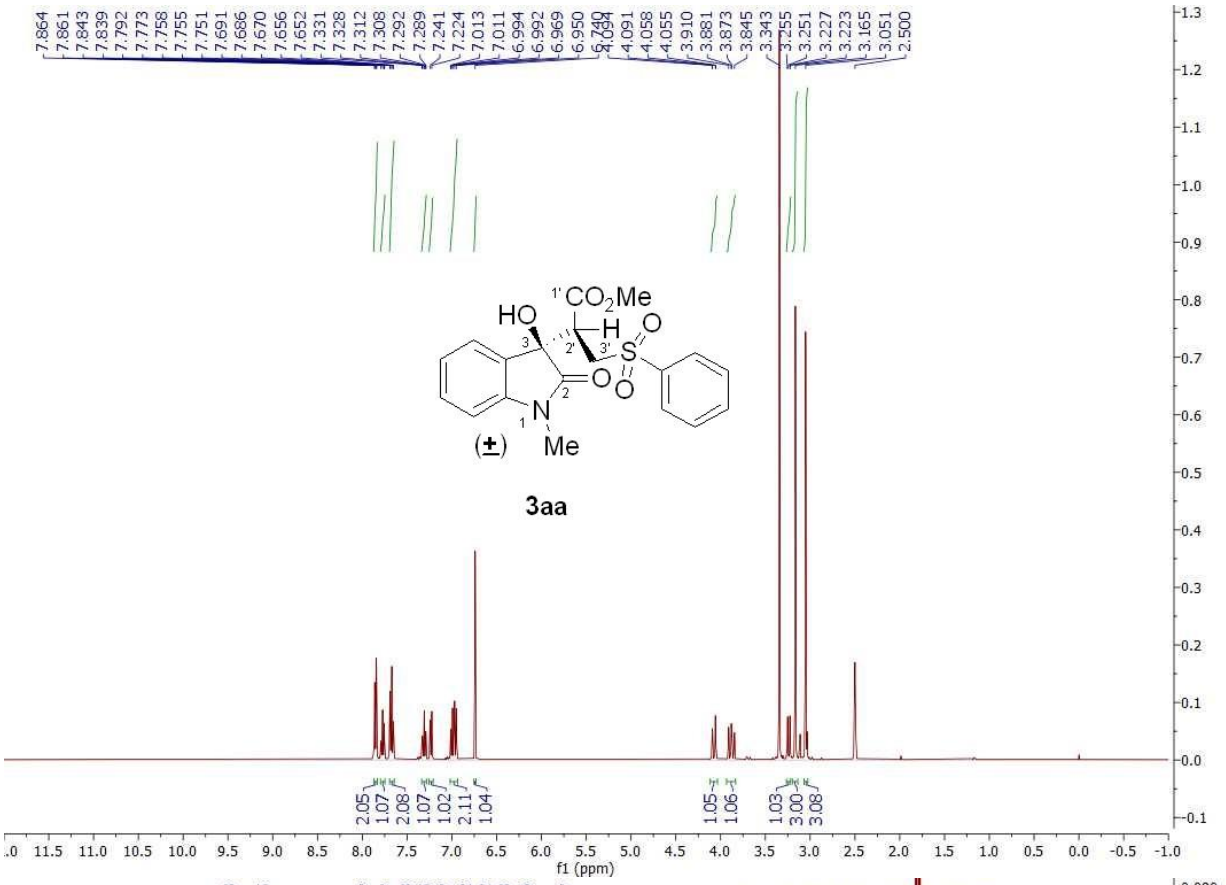
3-(Methyl-3'-(phenylsulfonyl) propanoate-2'-yl)-7-chloro-3-hydroxylindolin-2-one (3ja)



The title compound **3ja** was prepared following the general procedure for Table 2, using allylic alcohol **1j** *i.e.* 3-(methyl propenoate-2'-yl)-7-chloro-3-hydroxy indolin-2-one (1.0 mmol, 0.267 g) and benzenesulfinic acid **2a** (3.0 mmol, 0.426 g). Yield: 0.314 g, 77%; white semi solid; ^{1}H NMR (400 MHz, DMSO-d_6): δ 3.17-3.22 (m*, 4 H), 3.83-3.89 (m, 1 H), 4.01-4.08 (m, 1, H), 6.84 (s, 1 H), 6.94 (t, *J* = 8.0 Hz, 1 H), 7.18 (d, *J* = 7.2, Hz, 1 H), 7.28 (dd, *J* = 1.2 Hz & 8.0 Hz, 1 H), 7.65-7.69 (m, 2 H), 7.75-7.80 (m, 1 H), 7.84-7.87 (m, 2 H), 10.89 (s, 1 H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 47.2, 48.8, 51.7, 52.1, 75.1, 114.3, 123.3, 123.7, 128.0, 129.7, 129.9, 130.2, 134.4, 138.6, 139.3, 168.7, 177.1; HRMS (ESI) exact mass calcd for $C_{18}H_{16}ClNO_6S$ + H (M + H), 410.0465; found: 410.0471. *This multiplet contains one singlet for 3 protons and one multiplet for 1 proton.

Reference:

1. (a) D. Basavaiah, K. R. Reddy and N. Kumaragurubaran, *Nat. Protoc.* 2007, **2**, 2665; (b) D. Basavaiah, B. S. Reddy and S. S. Badsara, *Chem. Rev.* 2010, **110**, 5447; (c) S. J. Gardena and J. M. S. Skakle, *Tetrahedron Lett.*, 2002, **43**, 1969; (d) Y. M. Chung, Y. J. Im and J. N. Kim, *Bull. Korean Chem. Soc.* 2002, **23**, 1651.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H
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S
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O
N
Me
(±)
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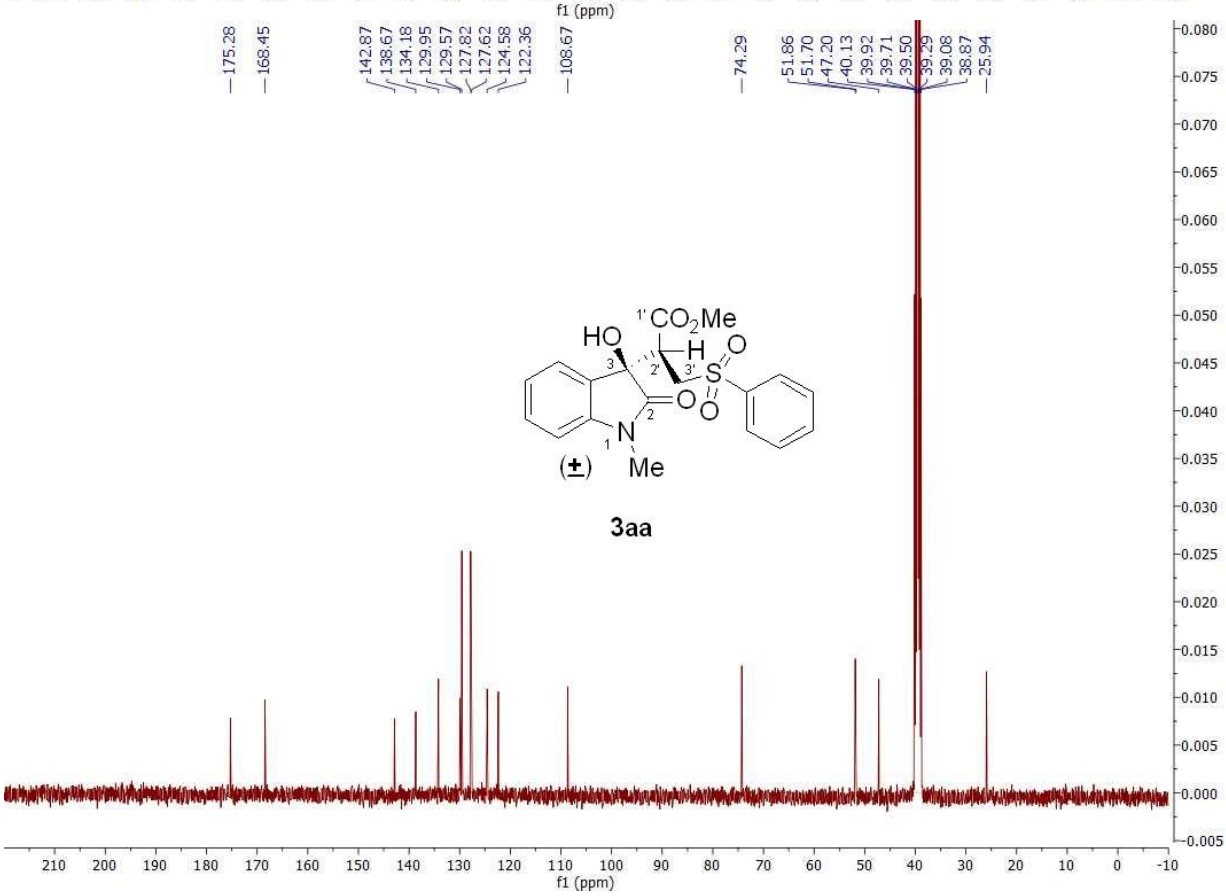
3.08
f1 (ppm)

3aa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39.50
39.29
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O
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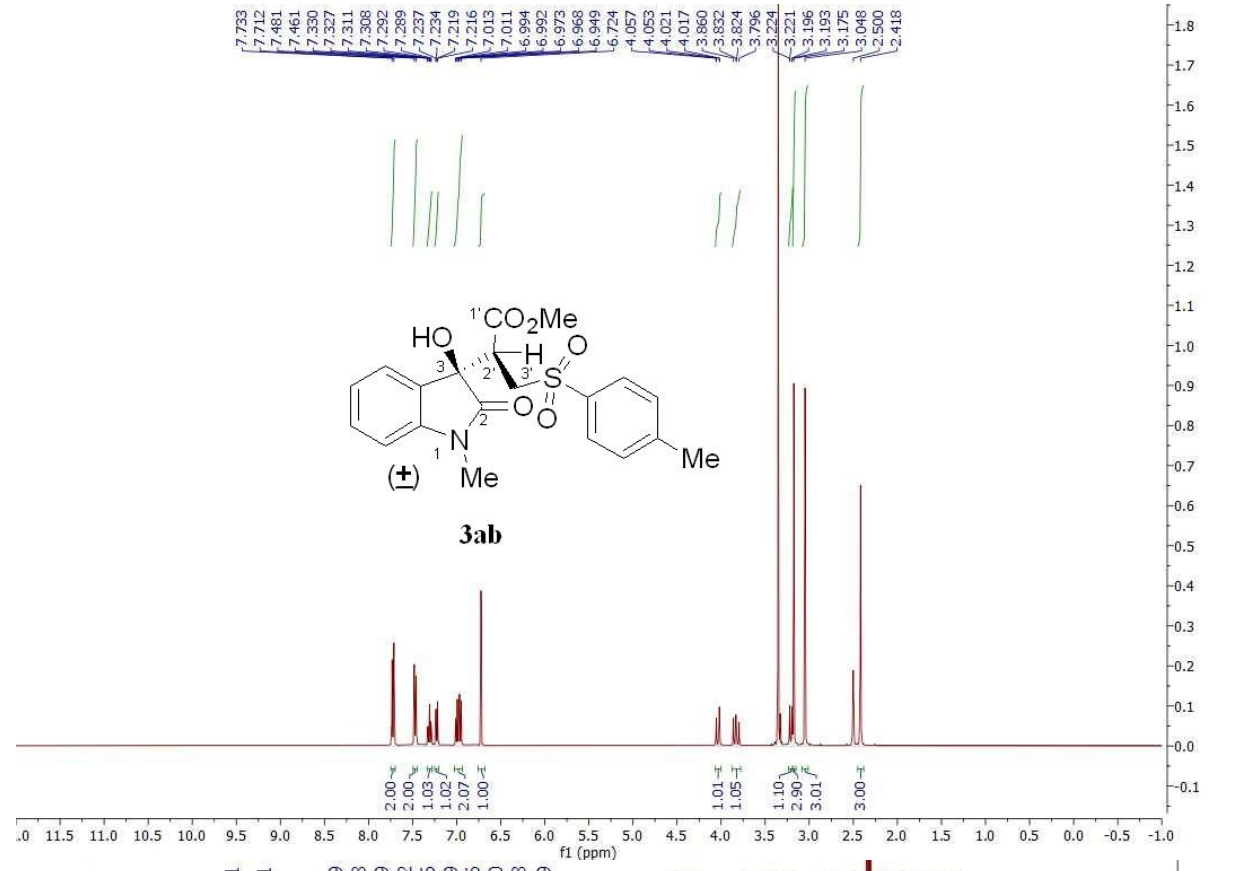
Me
(±)
f1 (ppm)

3aa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S
O
O
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N
1
Me
(±)
Me
2.00
2.00
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1.00
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1.05
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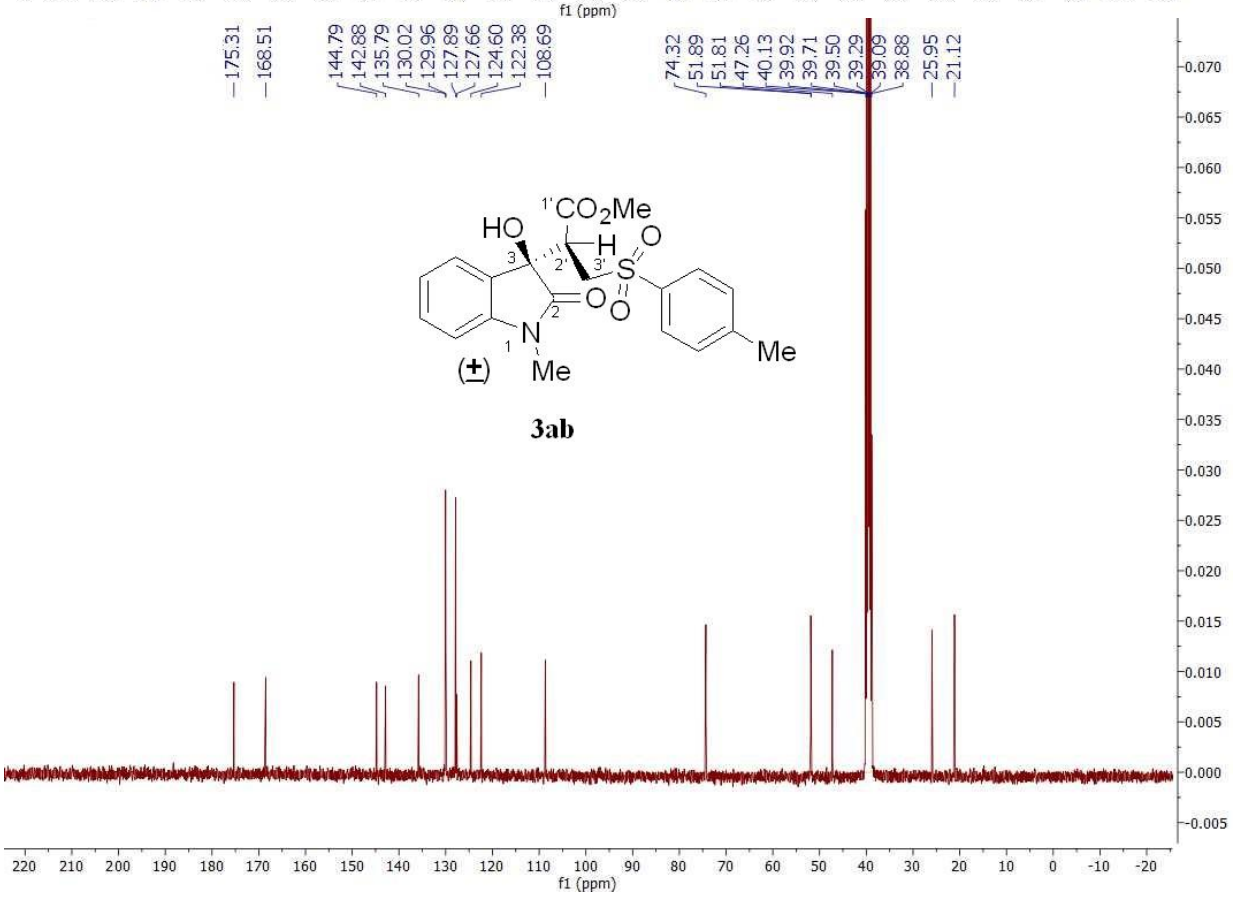
3.00
f1 (ppm)

3ab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25.95
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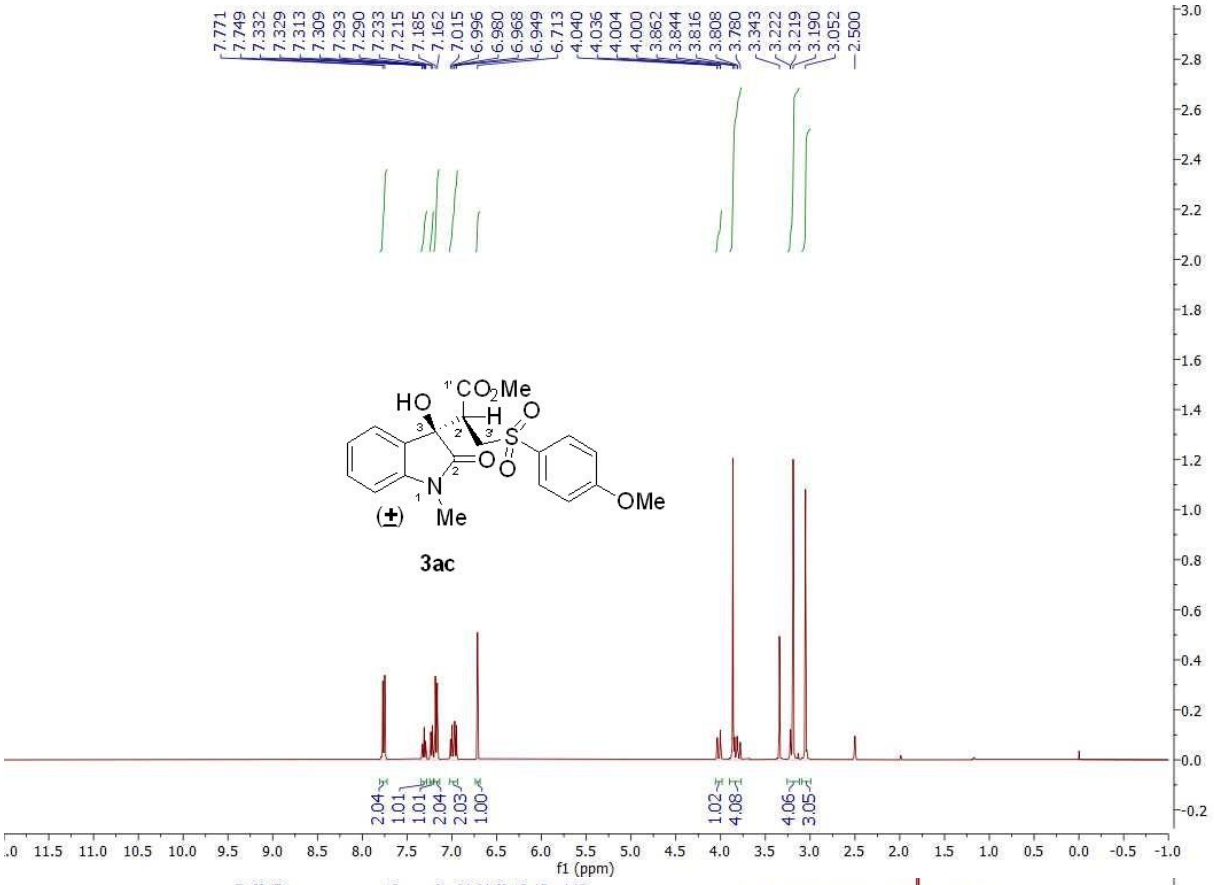
(±)
Me
f1 (ppm)

3ab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H
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(±)
OMe
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4.08
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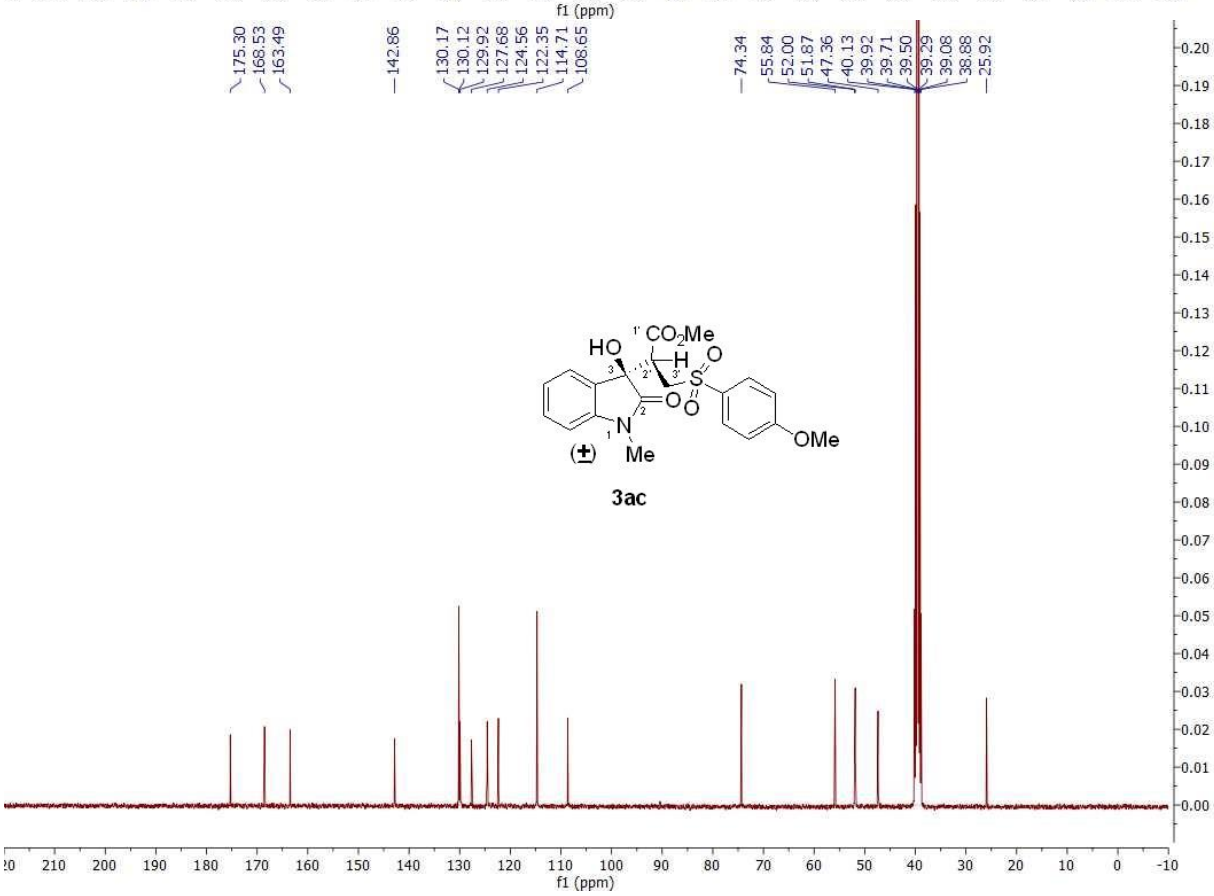
f1 (ppm)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OMe
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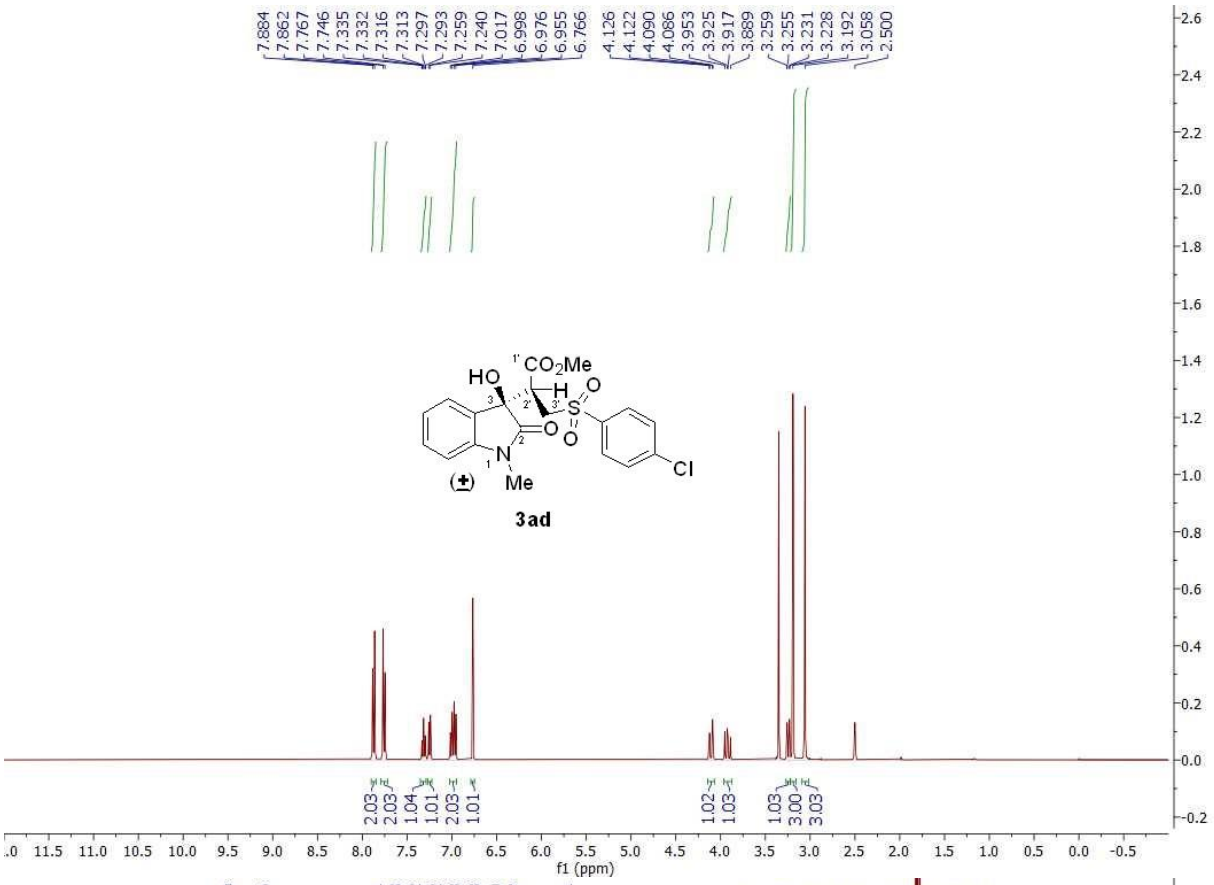
f1 (ppm)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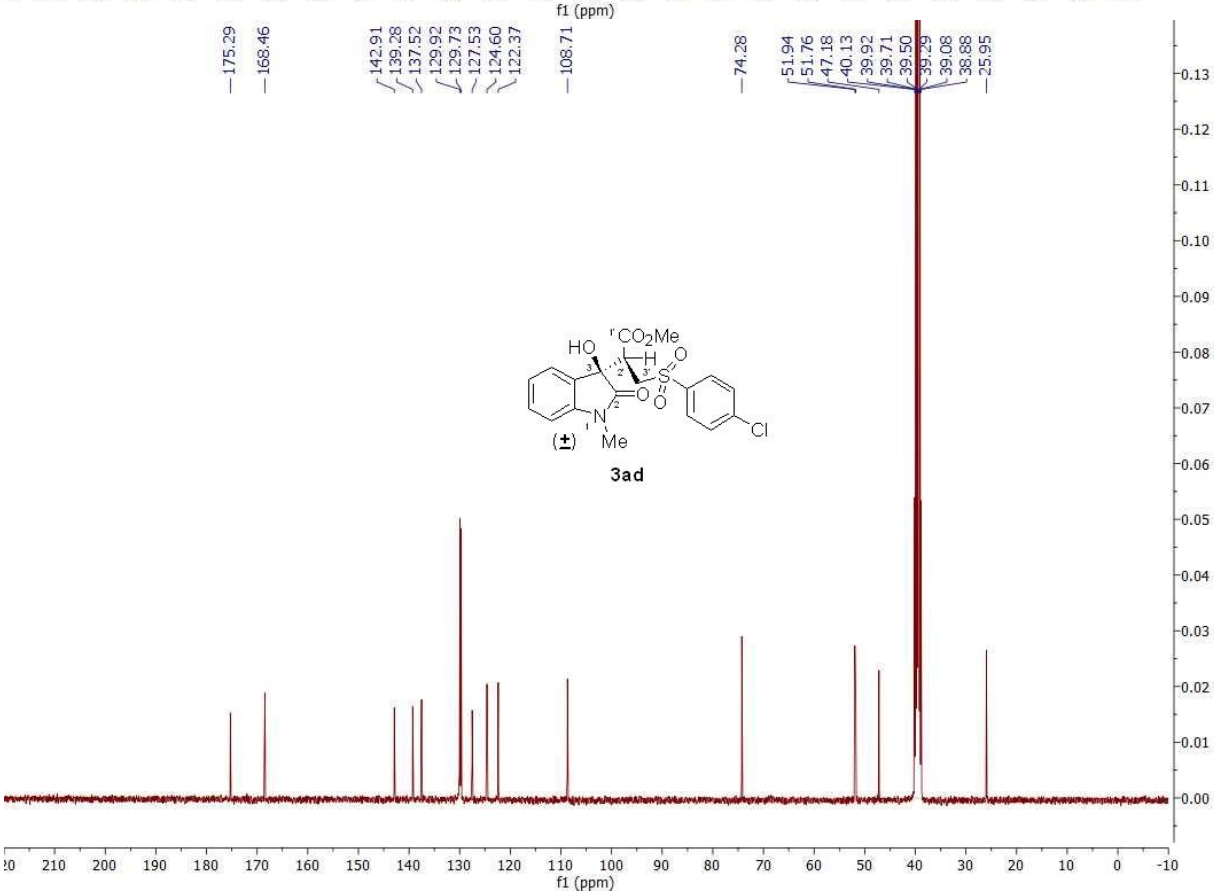
3.03
f1 (ppm)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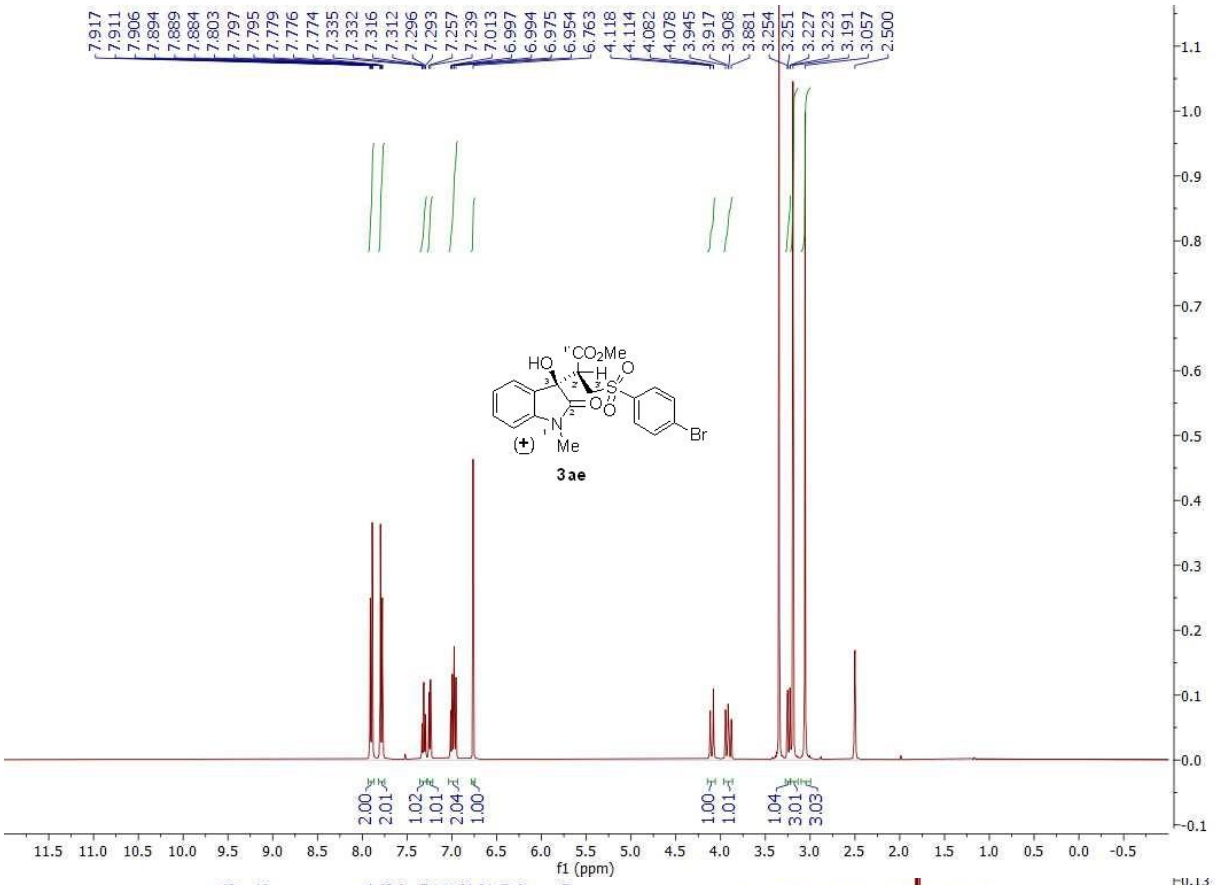
137.52
129.92
129.73
127.53
124.60
122.37
108.71
74.28
51.94
51.76
47.18
40.13
39.92
39.71
39.50
39.29
39.08
38.88
25.95
HO
1' CO2Me
H
O
S
O
O
N
Me
(±)
Cl
3ad
f1 (ppm)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7.906
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7.889
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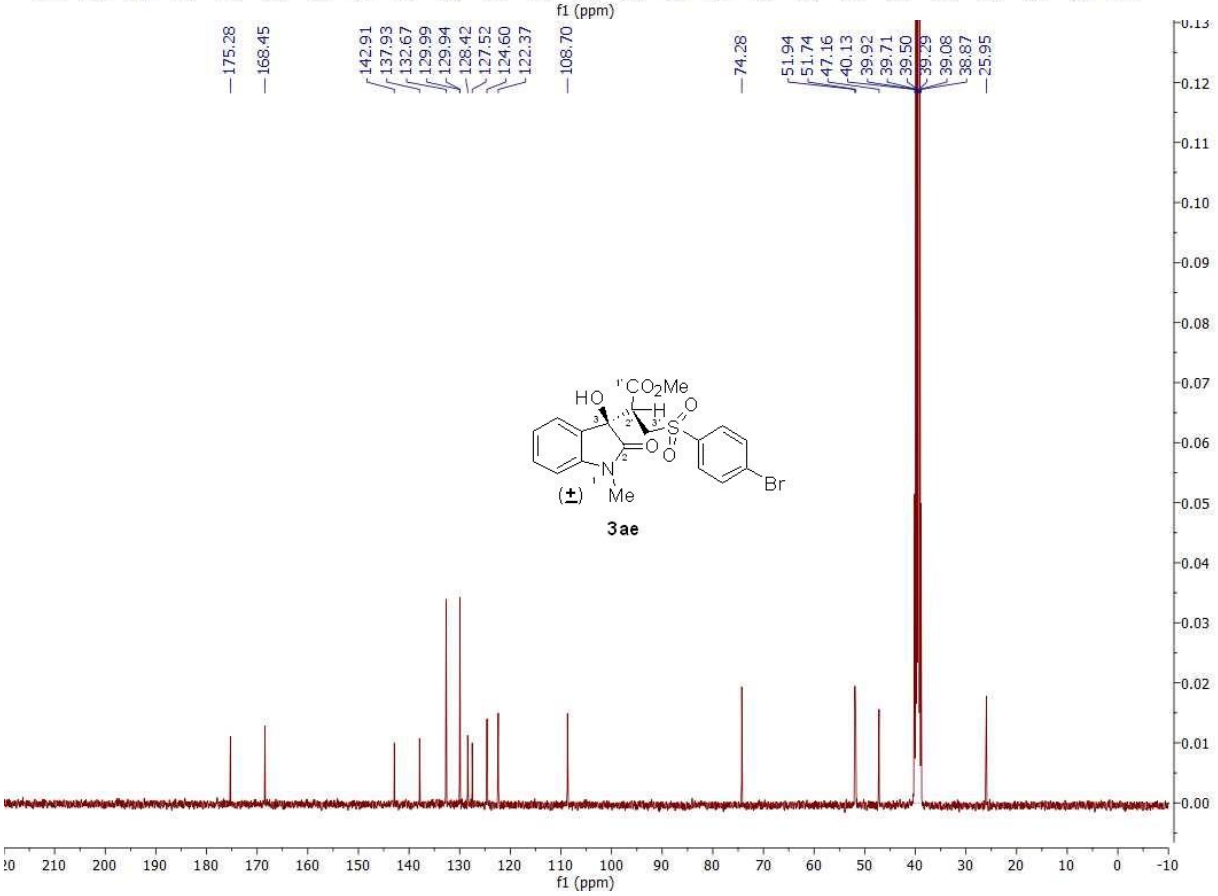
7.797
7.795
7.779
7.776
7.774
7.335
7.332
7.316
7.312
7.296
7.293
7.257
7.239
7.013
6.997
6.994
6.975
6.954
6.763
4.118
4.114
4.082
4.078
3.945
3.917
3.908
3.881
3.254
3.251
3.227
3.223
3.191
3.057
2.500
HO
CO2Me
O
S
O
O
N
Me
(±)
Br
3ae
2.00
2.01
1.02
1.01
2.04
1.00
1.00
1.01
1.04
3.01
3.03
f1 (ppm)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128.42
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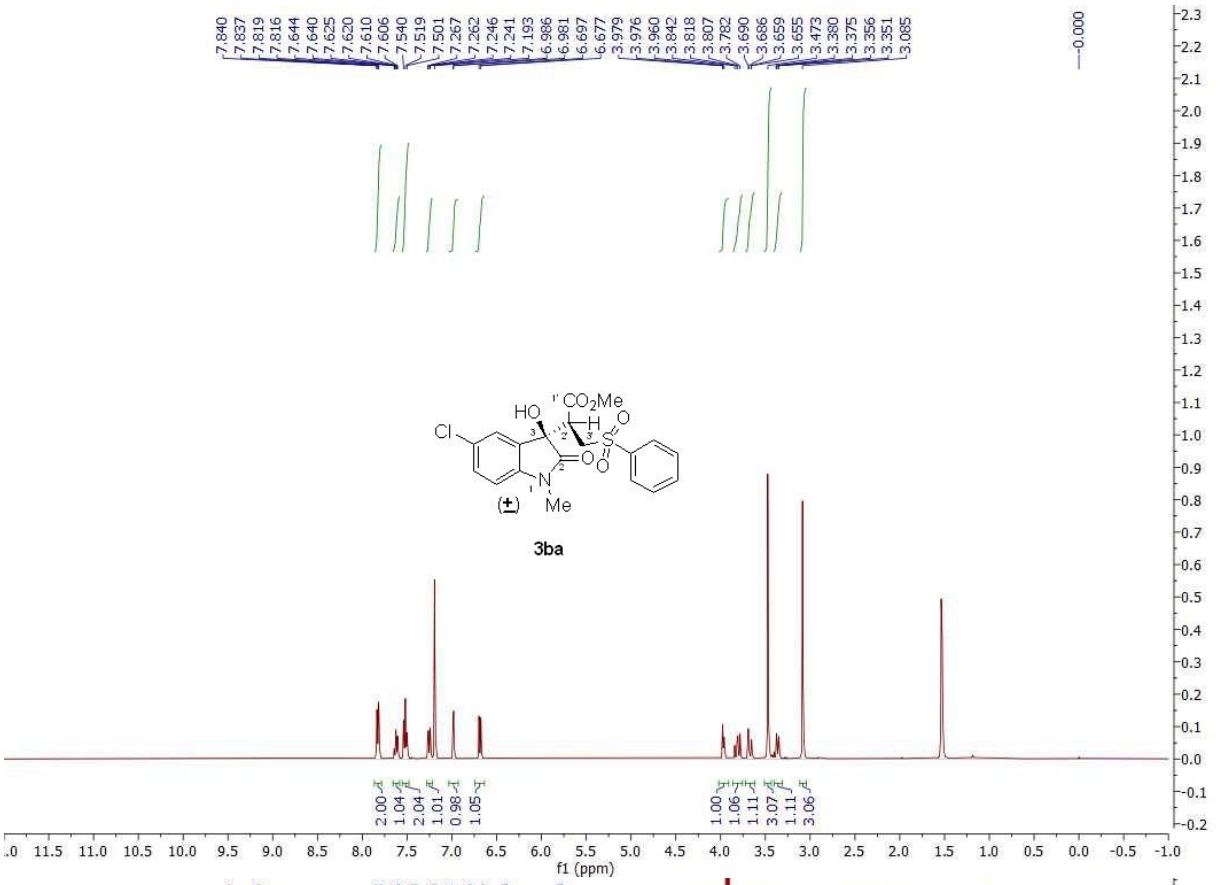
124.60
122.37
108.70
74.28
51.94
51.74
47.16
40.13
39.92
39.71
39.50
39.29
39.08
38.87
25.95
HO
CO2Me
O
S
O
O
N
Me
(±)
Br
3ae
f1 (ppm)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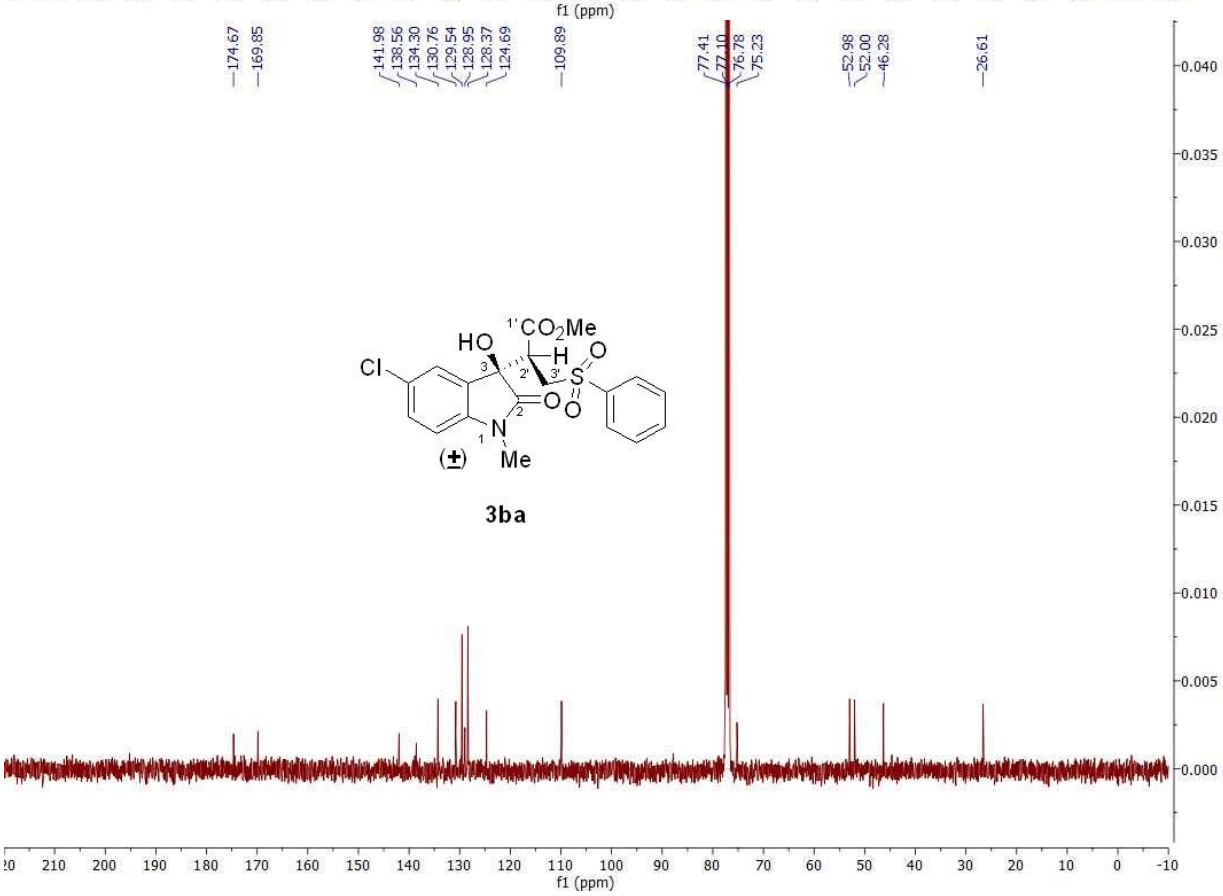
7.620
7.610
7.606
7.540
7.519
7.501
7.267
7.262
7.246
7.241
7.193
6.986
6.981
6.697
6.677
3.979
3.976
3.960
3.842
3.818
3.807
3.782
3.690
3.686
3.659
3.655
3.473
3.380
3.375
3.356
3.351
3.085
-0.000
HO
1' CO2Me
Cl
O
S
O
O
N
1
Me
(±)
3ba
2.00
1.04
2.04
1.01
0.98
1.05
1.00
1.06
1.11
3.07
1.11
3.06
f1 (ppm)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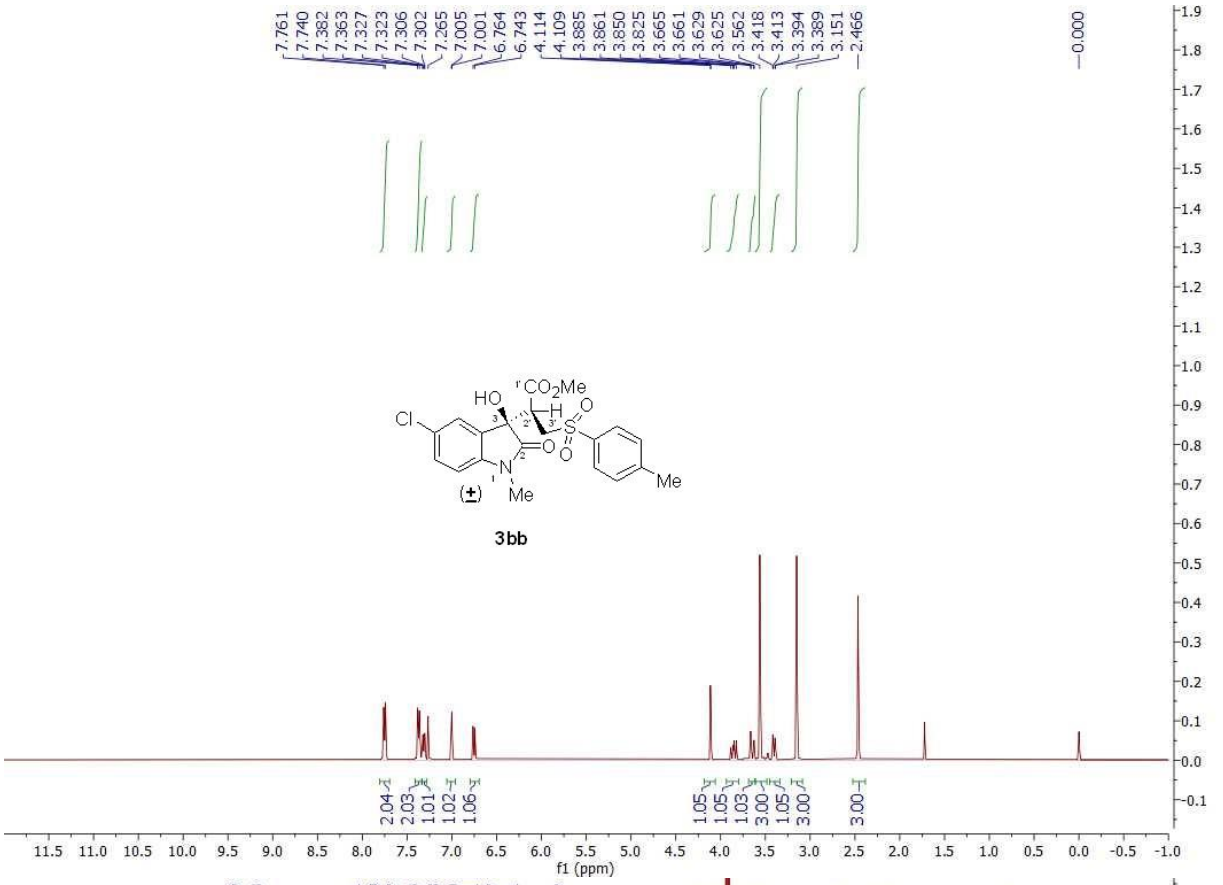
141.98
138.56
134.30
130.76
129.54
128.95
128.37
124.69
109.89
77.41
77.10
76.78
75.23
52.98
52.00
46.28
26.61
HO
1' CO2Me
Cl
O
S
O
O
N
1
Me
(±)
3ba
f1 (ppm)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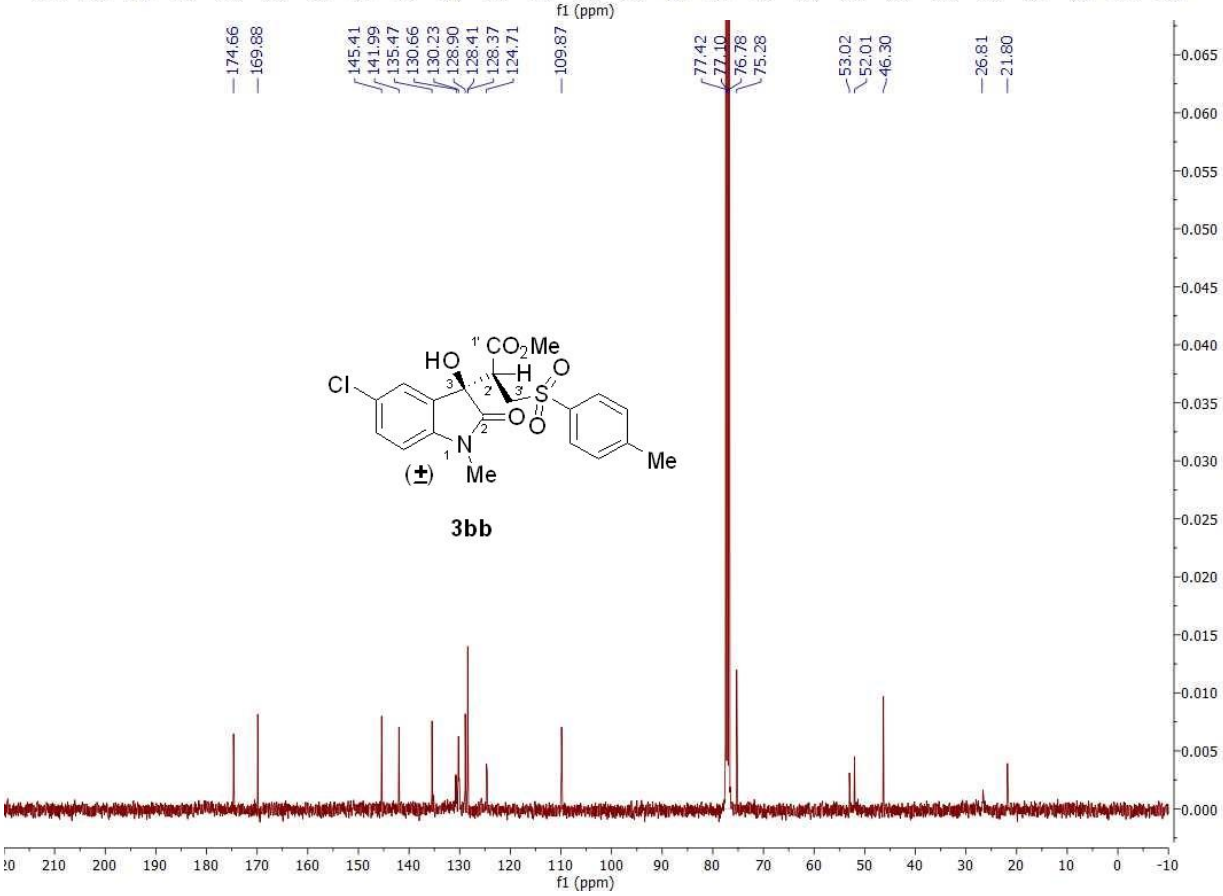
7.323
7.306
7.302
7.265
7.005
7.001
6.764
6.743
4.114
4.109
3.885
3.861
3.850
3.825
3.665
3.661
3.629
3.625
3.562
3.418
3.413
3.394
3.389
3.151
2.466
0.000
HO
1' CO2Me
Cl
Me
(±)
Me
2.04
2.03
1.01
1.02
1.06
1.05
1.05
1.03
3.00
1.05
3.00
3.00
f1 (ppm)

3bb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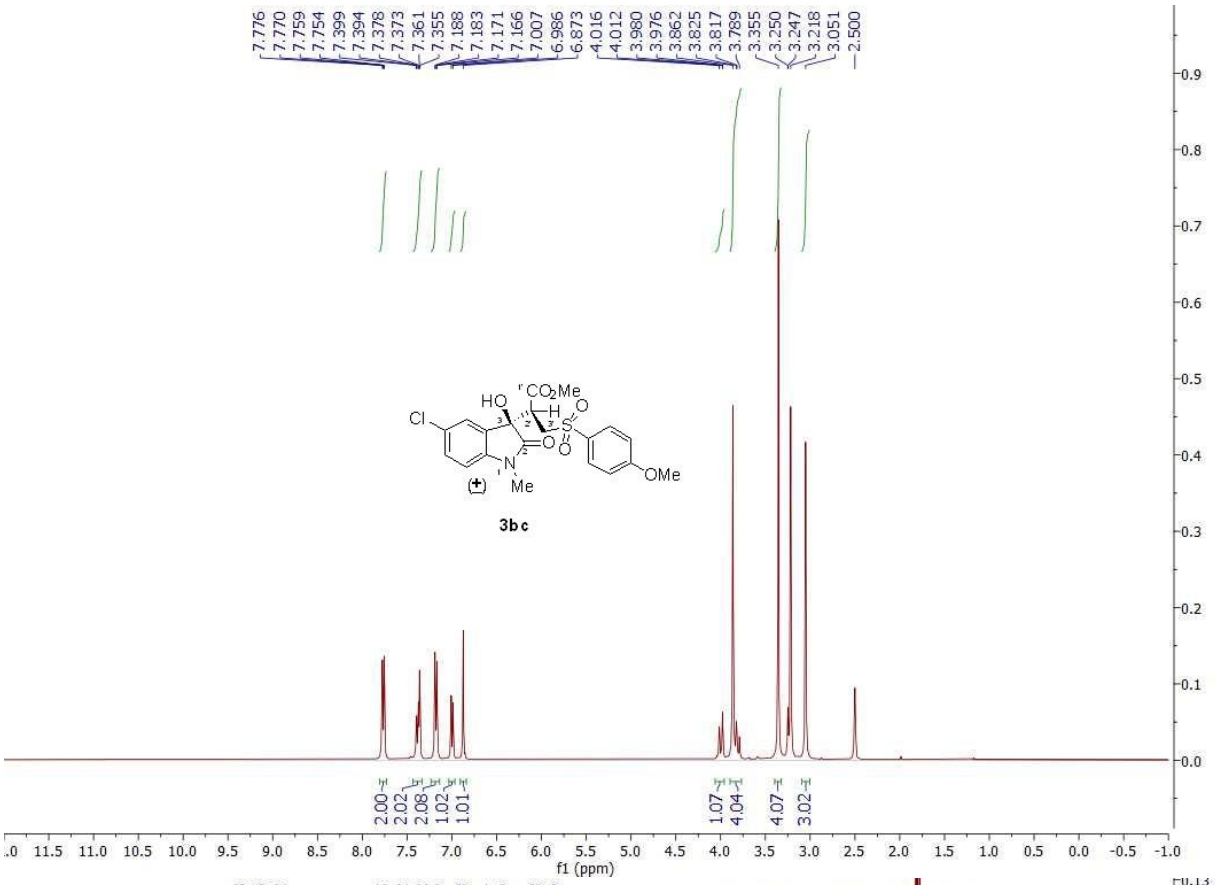
135.47
130.66
130.23
128.90
128.41
128.37
124.71
109.87
77.42
77.10
76.78
75.28
53.02
52.01
46.30
26.81
21.80
HO
1' CO2Me
Cl
Me
(±)
Me
f1 (ppm)

3bb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7.754
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7.394
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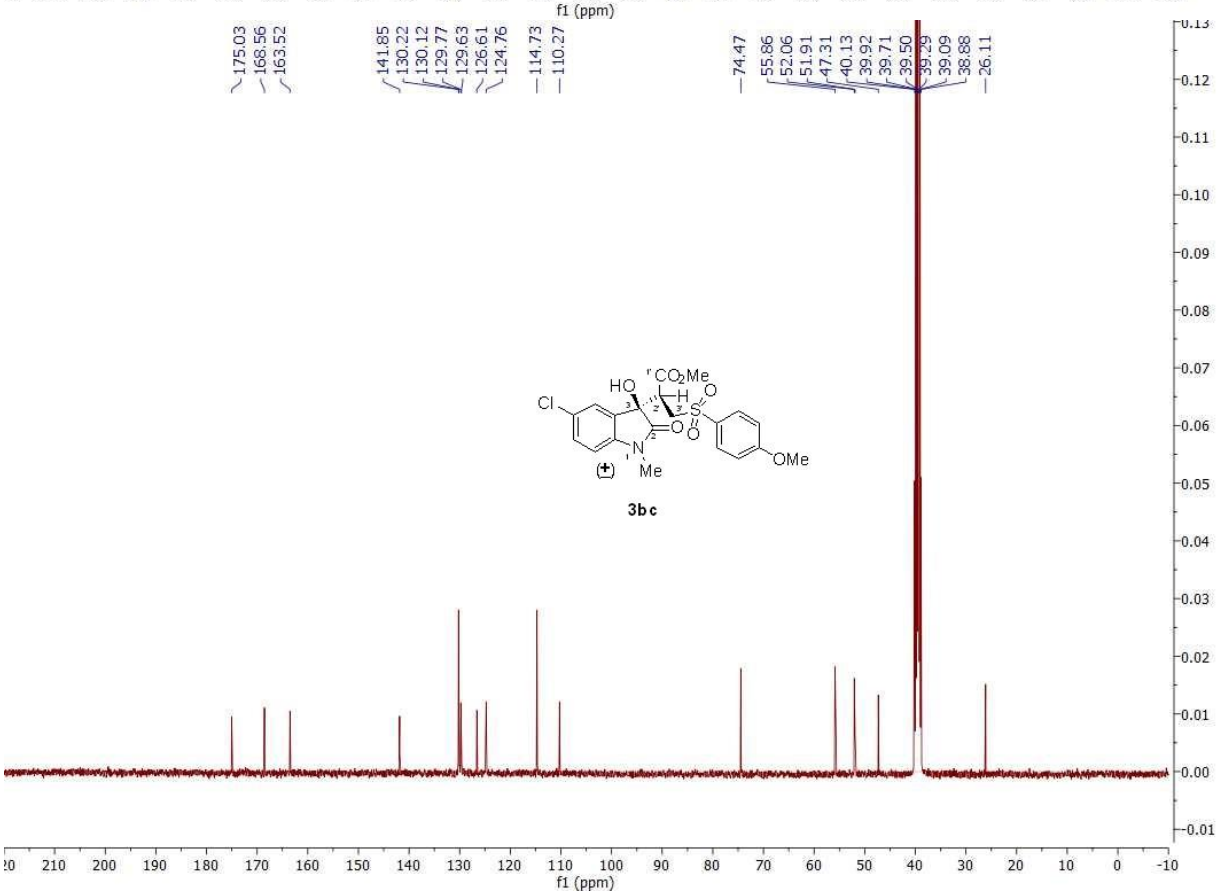
7.373
7.361
7.355
7.188
7.183
7.171
7.166
7.007
6.986
6.873
4.016
4.012
3.980
3.976
3.862
3.825
3.817
3.789
3.355
3.250
3.247
3.218
3.051
2.500
HO
CO2Me
Cl
O
S
O
O
N
Me
OMe
3bc
2.00
2.02
2.08
1.02
1.01
1.07
4.04
4.07
3.02
f1 (ppm)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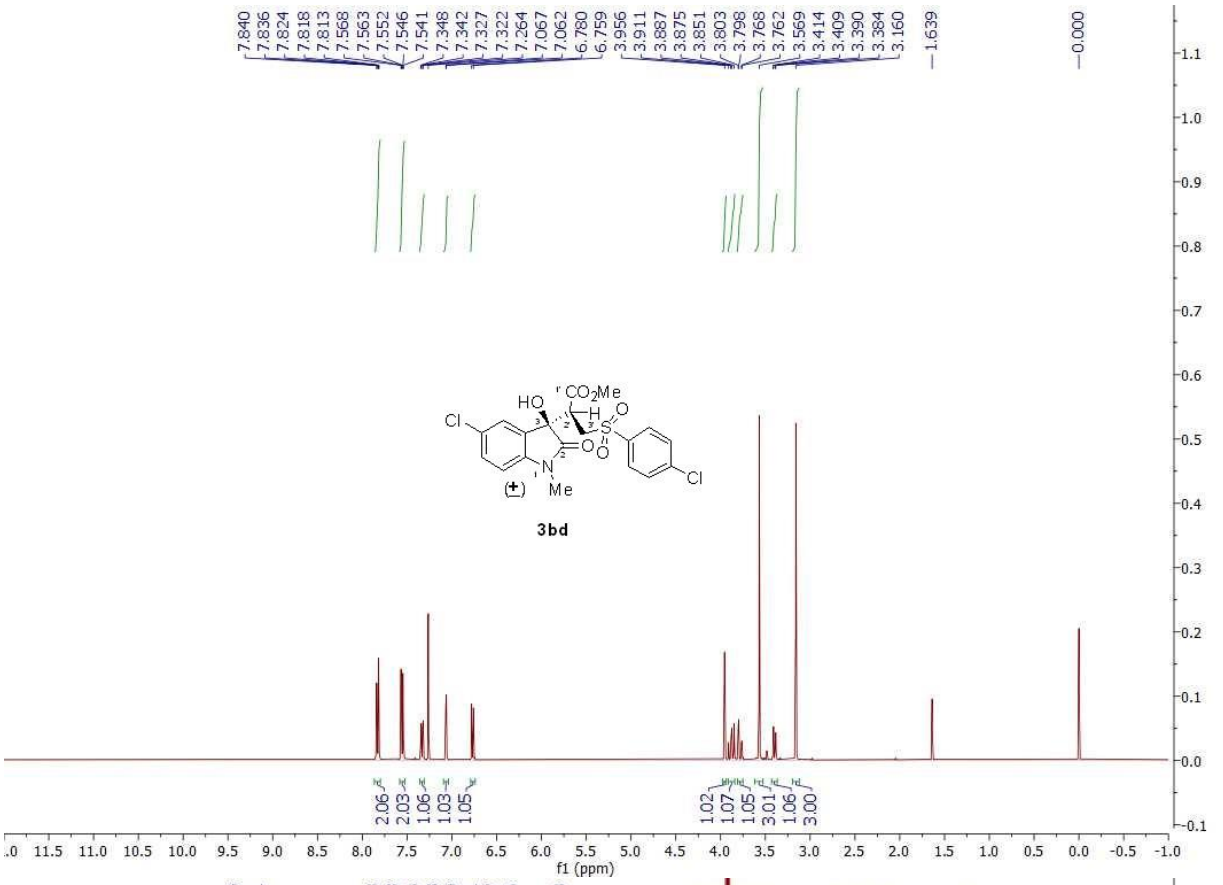
163.52
141.85
130.22
130.12
129.77
129.63
126.61
124.76
114.73
110.27
74.47
55.86
52.06
51.91
47.31
40.13
39.92
39.71
39.50
39.29
39.09
38.88
26.11
HO
CO2Me
Cl
O
S
O
O
N
Me
OMe
3bc
f1 (ppm)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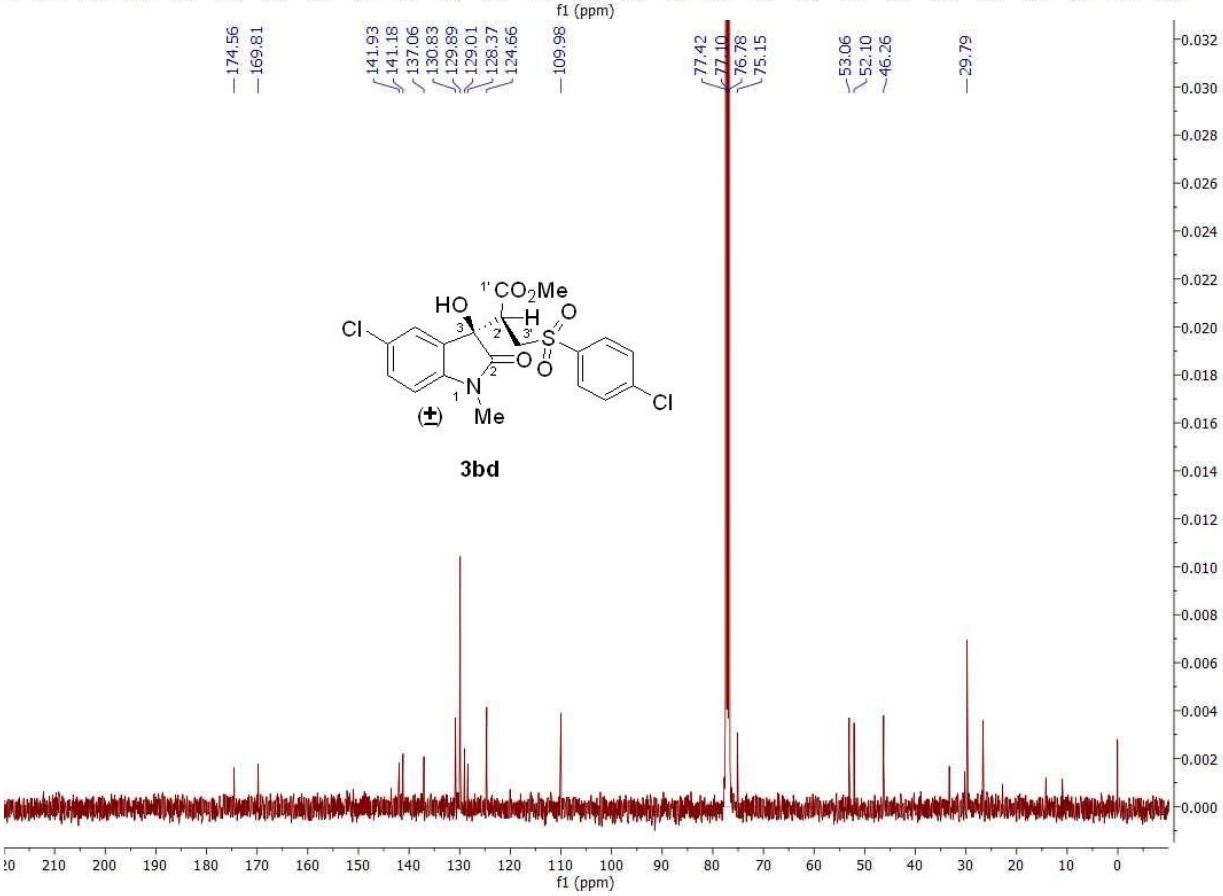
7.836
7.824
7.818
7.813
7.568
7.563
7.552
7.546
7.541
7.348
7.342
7.327
7.322
7.264
7.067
7.062
6.780
6.759
3.956
3.911
3.887
3.875
3.851
3.803
3.798
3.768
3.762
3.569
3.414
3.409
3.390
3.384
3.160
1.639
0.000
HO
1' CO2Me
Cl
O
O
O
Cl
N
Me
(±)
3bd
2.06
2.03
1.06
1.03
1.05
1.02
1.07
1.05
3.01
1.06
3.00
f1 (ppm)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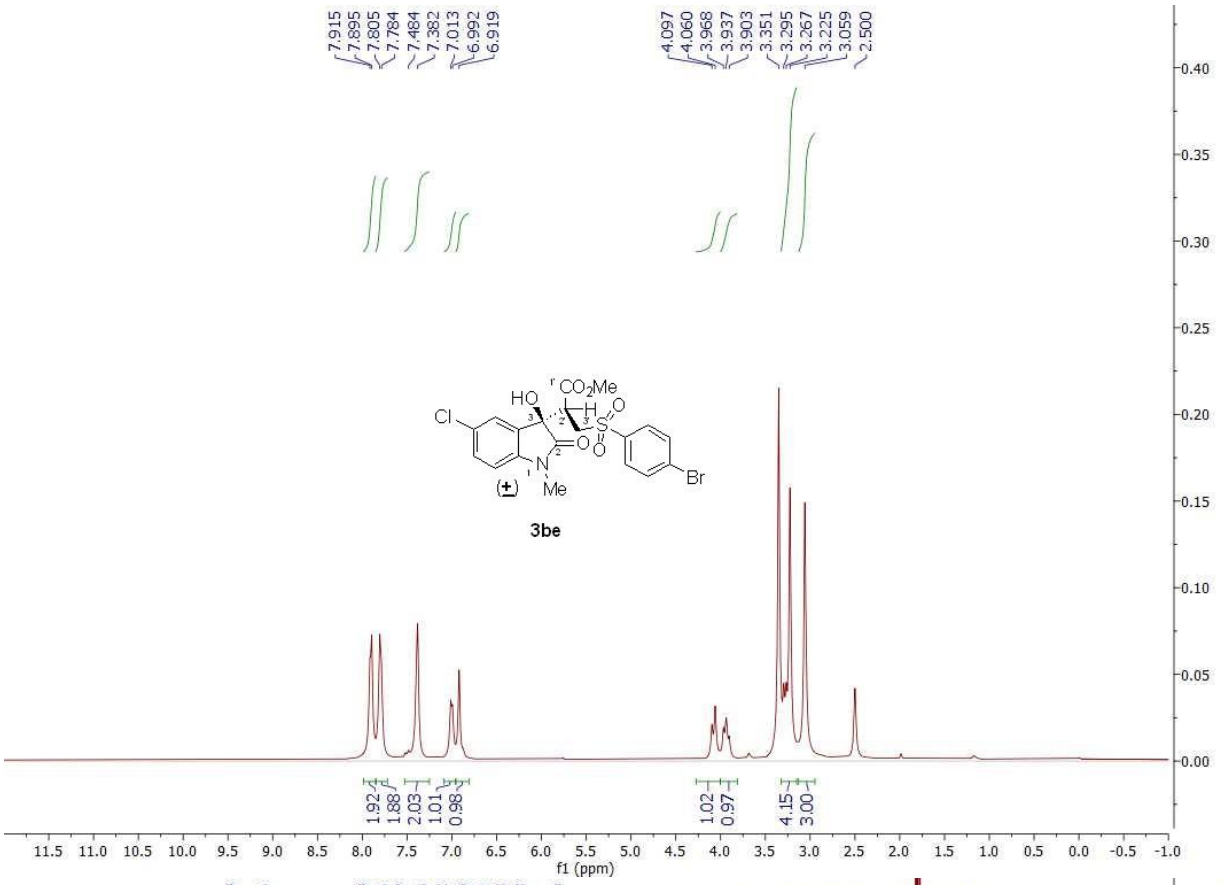
141.18
137.06
130.83
129.89
129.01
128.37
124.66
109.98
77.42
77.10
76.78
75.15
53.06
52.10
46.26
29.79
HO
1' CO2Me
Cl
O
O
O
Cl
N
Me
(±)
3bd
f1 (ppm)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7.784
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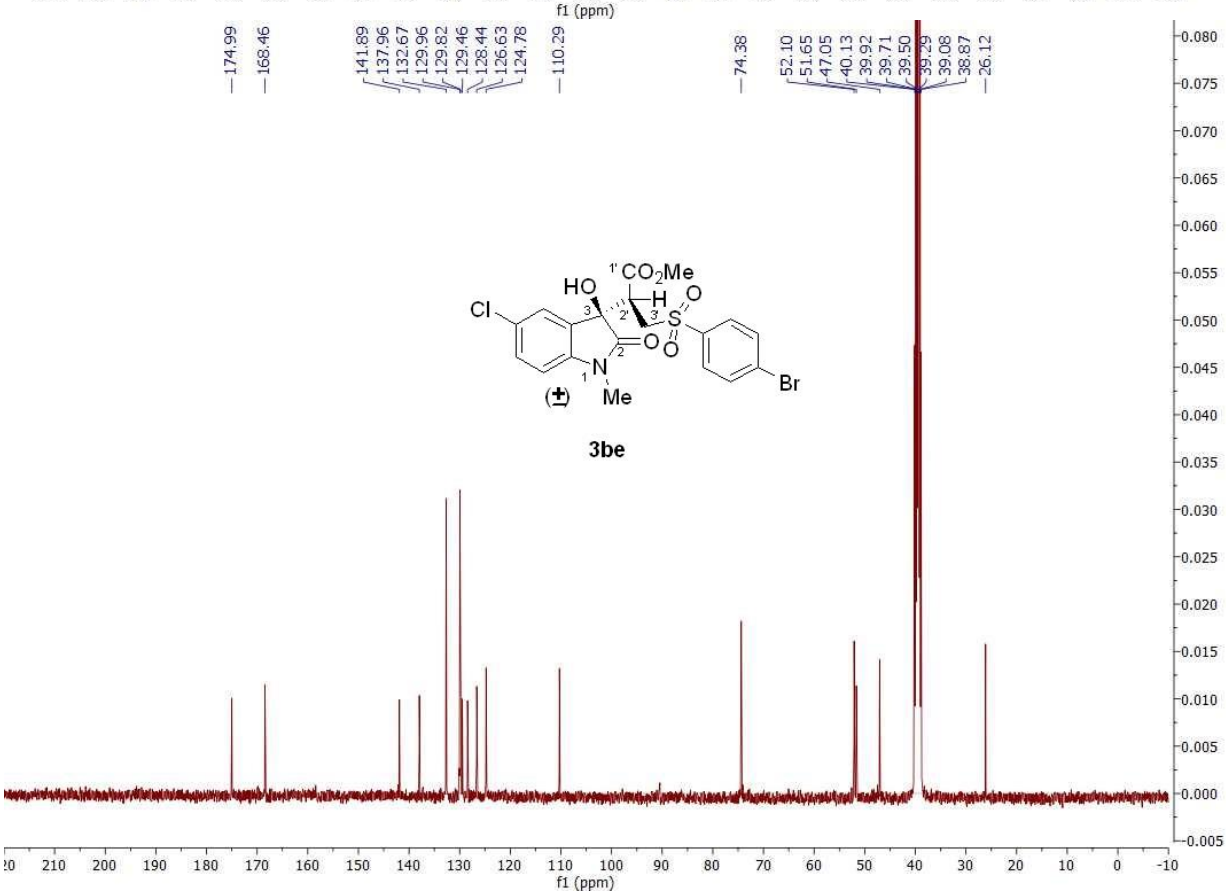
7.013
6.992
6.919
4.097
4.060
3.968
3.937
3.903
3.351
3.295
3.267
3.225
3.059
2.500
HO
CO2Me
Cl
O
O
O
N
Me
Br
(±)
3be
1.92
1.88
2.03
1.01
0.98
1.02
0.97
4.15
3.00
f1 (ppm)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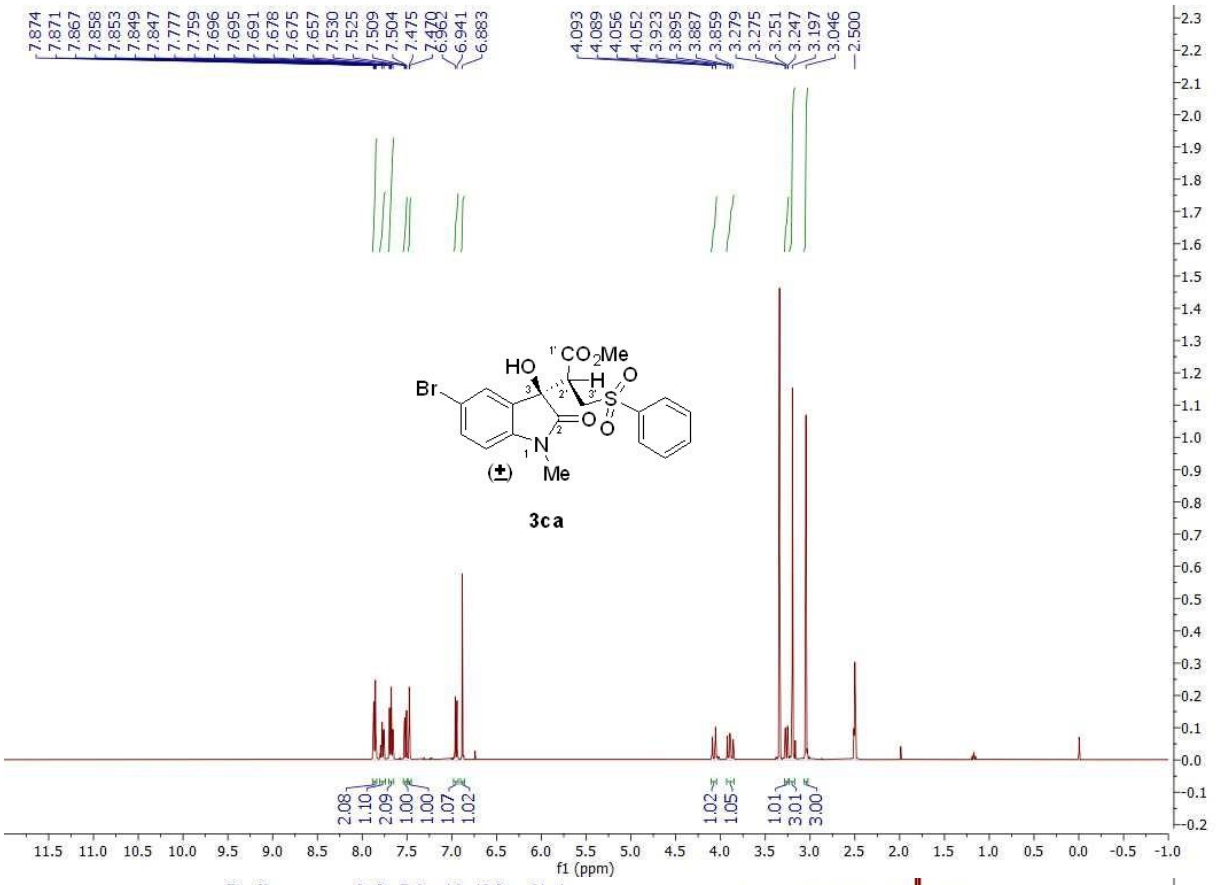
141.89
137.96
132.67
129.96
129.82
129.46
128.44
126.63
124.78
110.29
74.38
52.10
51.65
47.05
40.13
39.92
39.71
39.50
39.29
39.08
38.87
26.12
HO
CO2Me
Cl
O
O
O
N
Me
Br
(±)
3be
f1 (ppm)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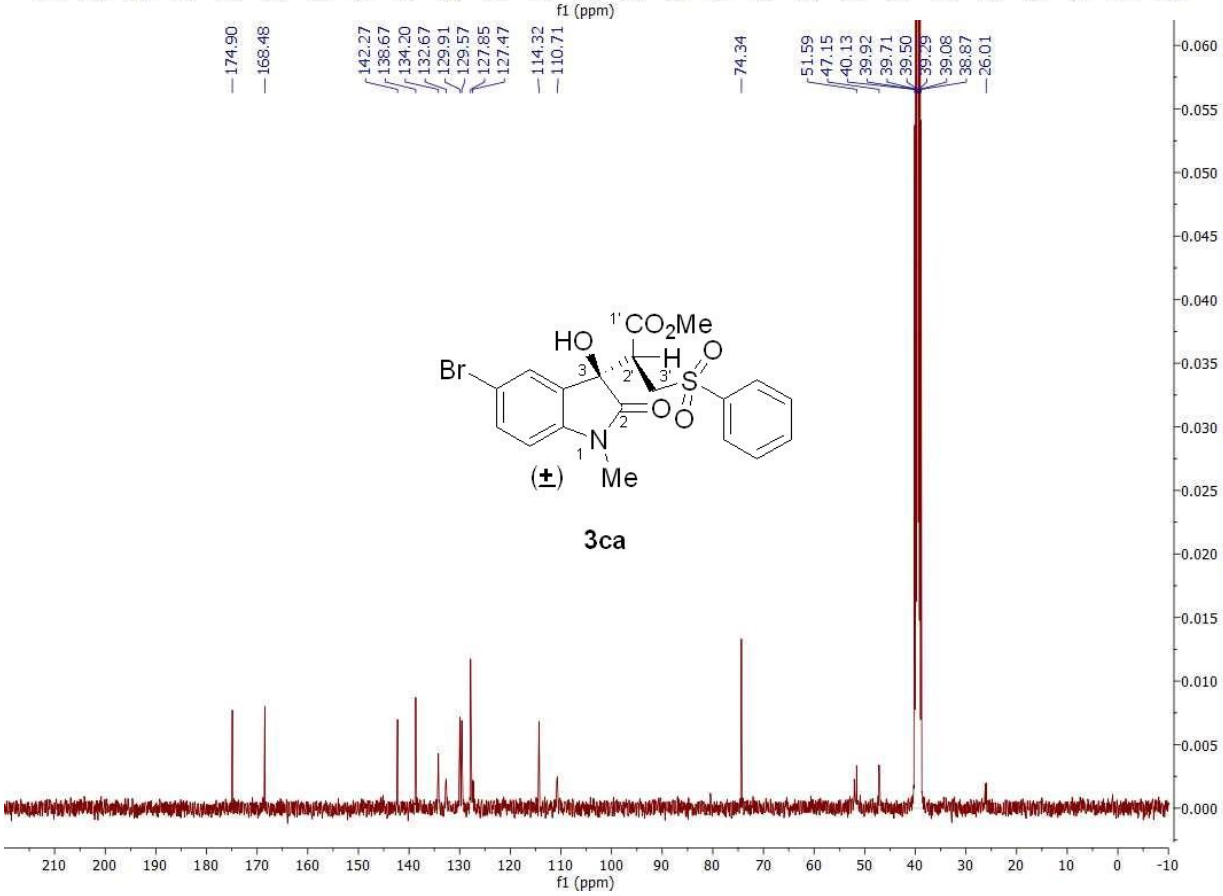
7.853
7.849
7.847
7.777
7.759
7.696
7.695
7.691
7.678
7.675
7.657
7.530
7.525
7.509
7.504
7.475
7.470
6.962
6.941
6.883
4.093
4.089
4.056
4.052
3.923
3.895
3.887
3.859
3.279
3.275
3.251
3.247
3.197
3.046
2.500
Br
HO
1' CO2Me
O
O
O
N
Me
(±)
2.08
1.10
2.09
1.00
1.00
1.07
1.02
1.02
1.05
1.01
3.01
3.00
f1 (ppm)

3ca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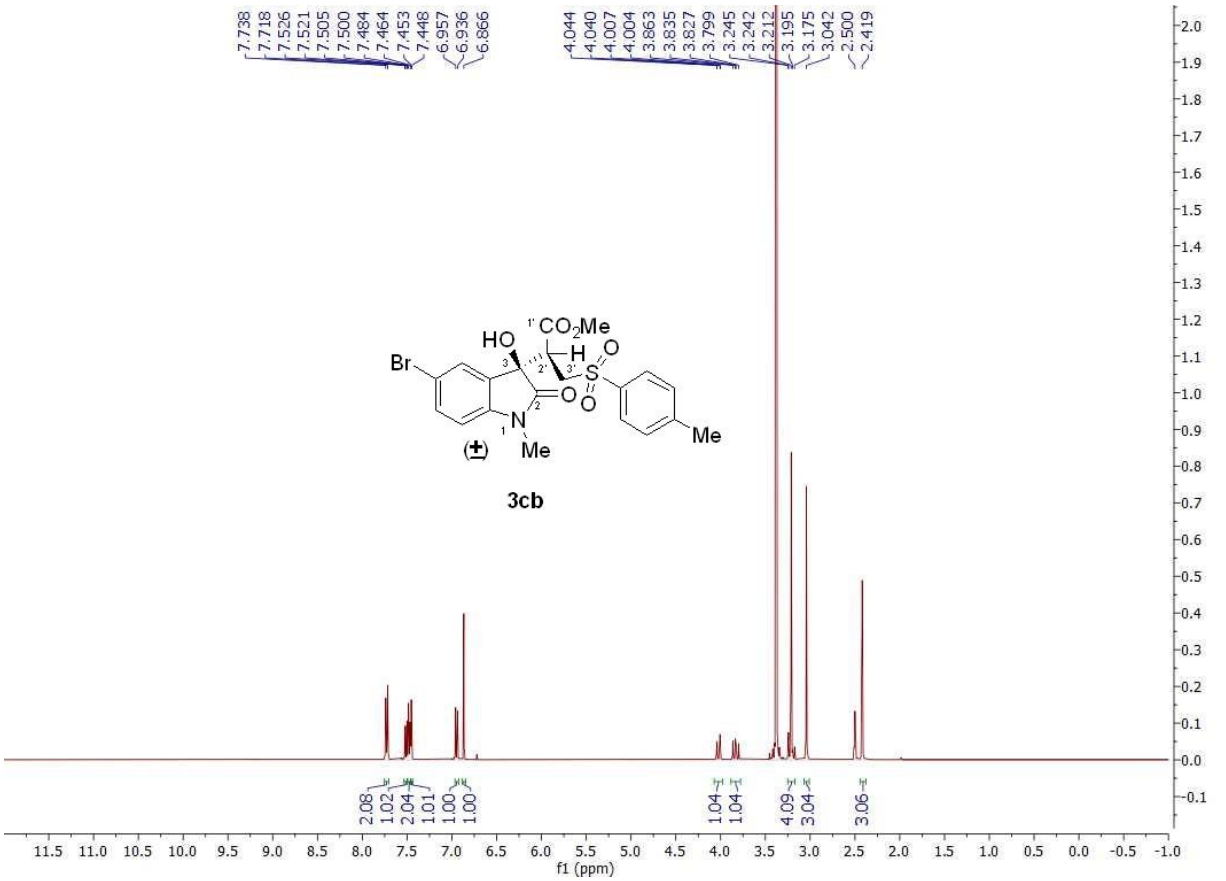
132.67
129.91
129.57
127.85
127.47
114.32
110.71
74.34
51.59
47.15
40.13
39.92
39.71
39.50
39.29
39.08
38.87
26.01
Br
HO
1' CO2Me
O
O
O
N
Me
(±)
f1 (ppm)

3ca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7.505
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7.464
7.453
7.448
6.957
6.936
6.866
4.044
4.040
4.007
4.004
3.863
3.835
3.827
3.799
3.245
3.242
3.212
3.195
3.175
3.042
2.500
2.419
HO
1' CO2Me
Br
Me
(±)
Me
2.08
1.02
2.04
1.01
1.00
1.00
1.04
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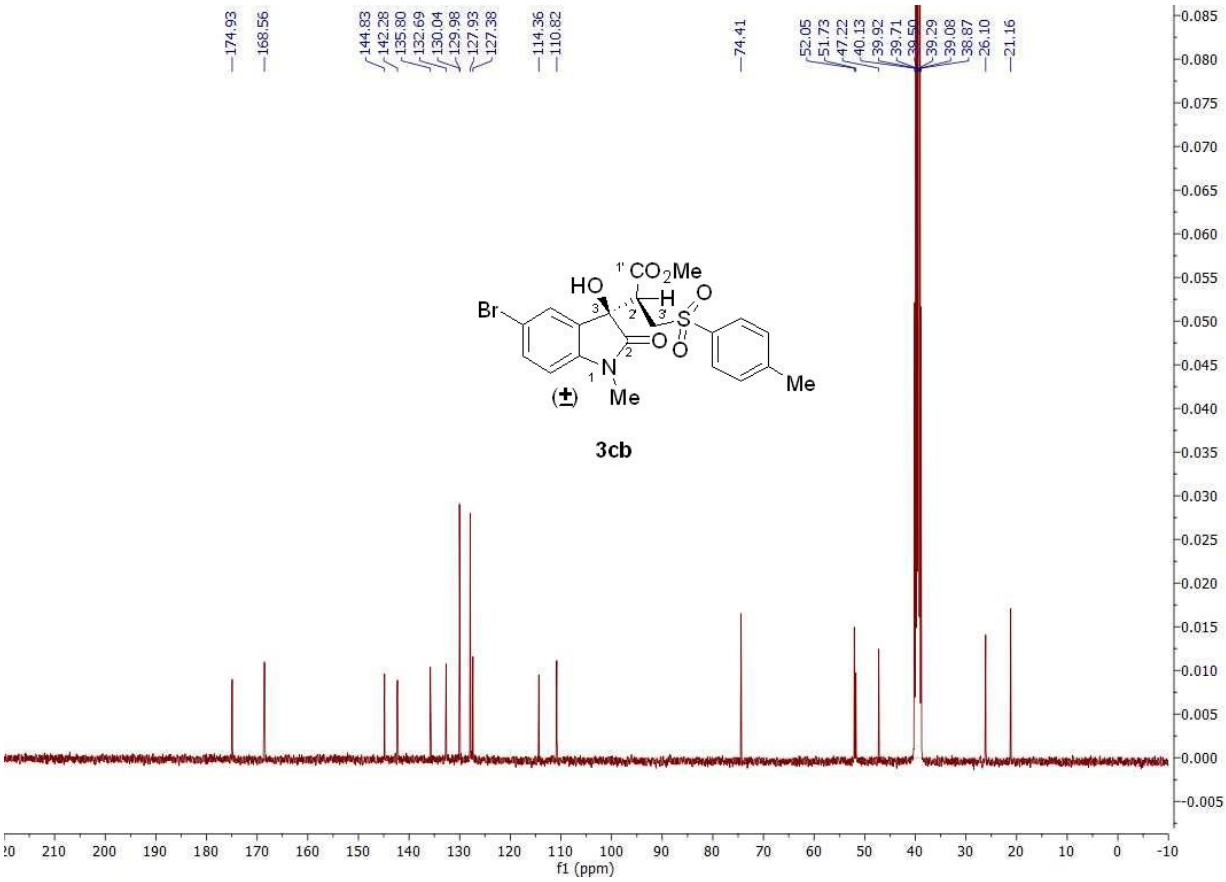
4.09
3.04
3.06
f1 (ppm)

3cb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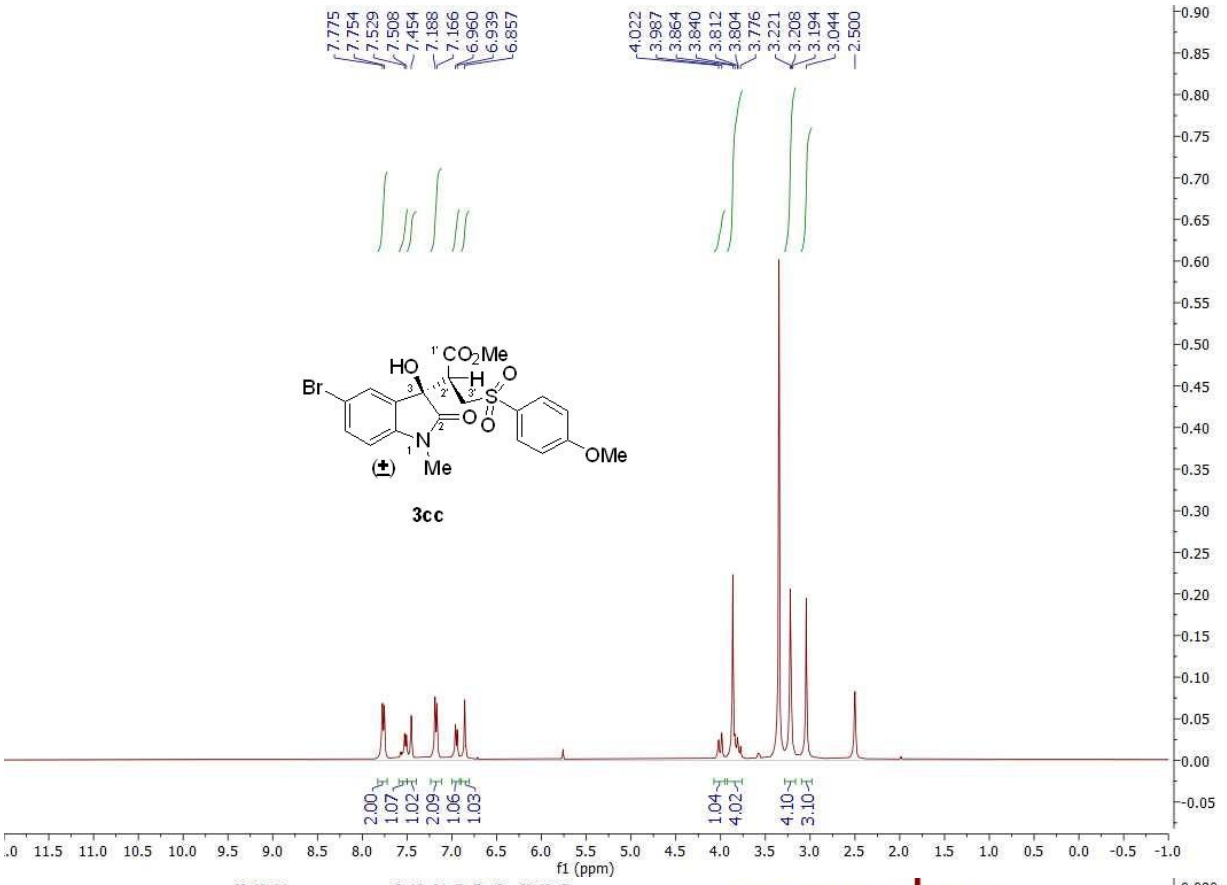
132.69
130.04
129.98
127.93
127.38
114.36
110.82
74.41
52.05
51.73
47.22
40.13
39.92
39.71
39.50
39.29
39.08
38.87
26.10
21.16
HO
1' CO2Me
Br
Me
(±)
Me
f1 (ppm)

3cb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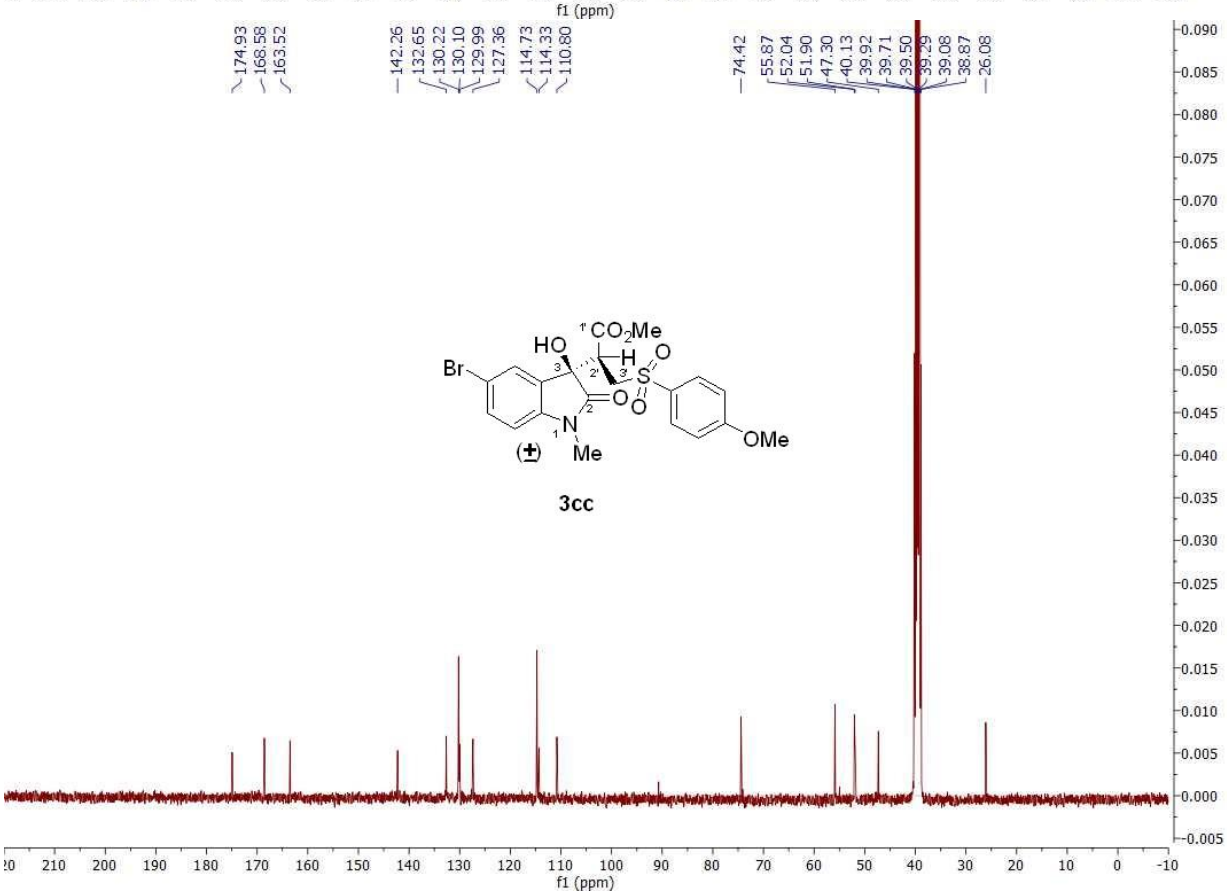
7.508
7.454
7.188
7.166
6.960
6.939
6.857
4.022
3.987
3.864
3.840
3.812
3.804
3.776
3.221
3.208
3.194
3.044
2.500
HO
1' CO2Me
Br
OMe
(±)
Me
3cc
2.00
1.07
1.02
2.09
1.06
1.03
1.04
4.02
4.10
3.10
f1 (ppm)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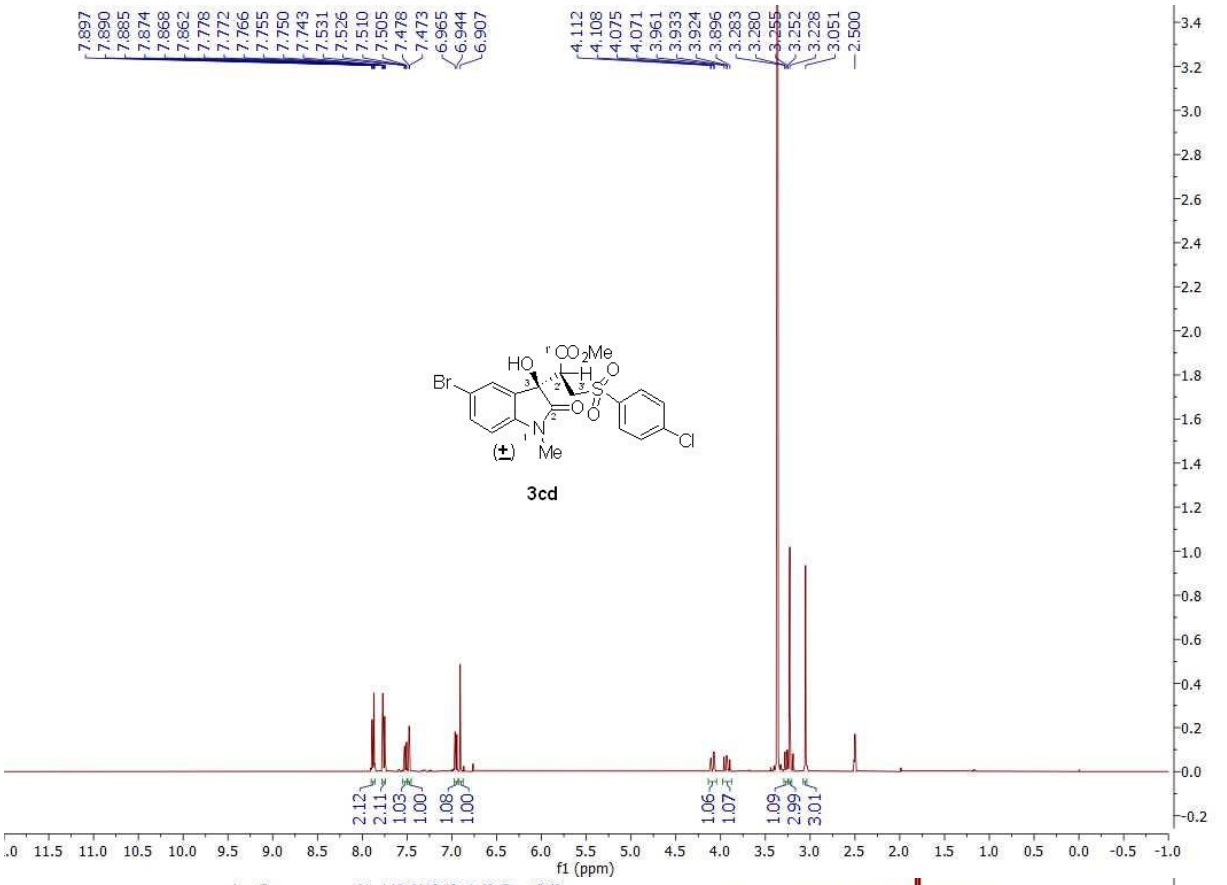
130.22
130.10
129.99
127.36
114.73
114.33
110.80
74.42
55.87
52.04
51.90
47.30
40.13
39.92
39.71
39.50
39.29
39.08
38.87
26.08
HO
1' CO2Me
Br
OMe
(±)
Me
3cc
f1 (ppm)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7.874
7.868
7.862
7.778
7.772
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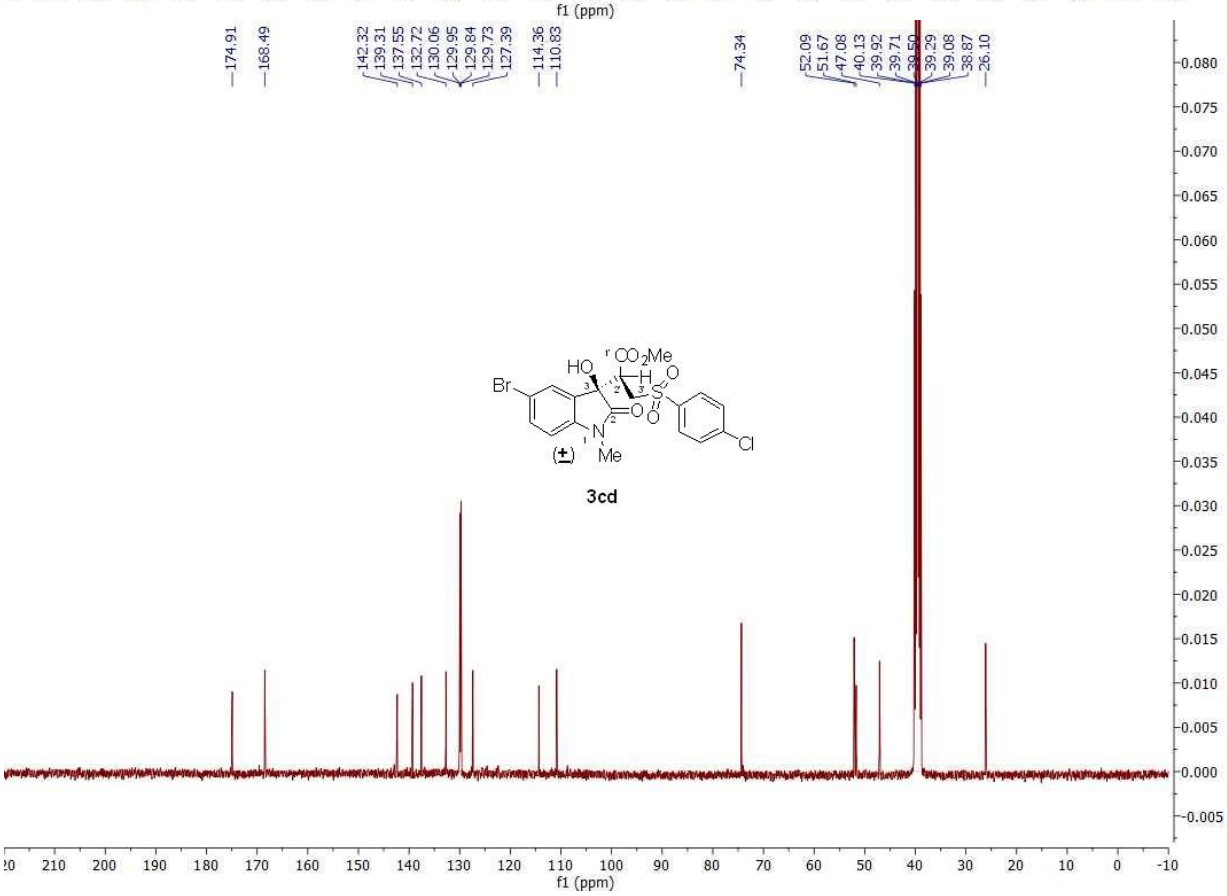
7.755
7.750
7.743
7.531
7.526
7.510
7.505
7.478
7.473
6.965
6.944
6.907
4.112
4.108
4.075
4.071
3.961
3.933
3.924
3.896
3.283
3.280
3.255
3.252
3.228
3.051
2.500
HO
CO2Me
Br
O
S
O
O
N
Me
Cl
(±)
3cd
2.12
2.11
1.03
1.00
1.08
1.00
1.06
1.07
1.09
2.99
3.01
f1 (ppm)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137.55
132.72
130.06
129.95
129.84
129.73
127.39
114.36
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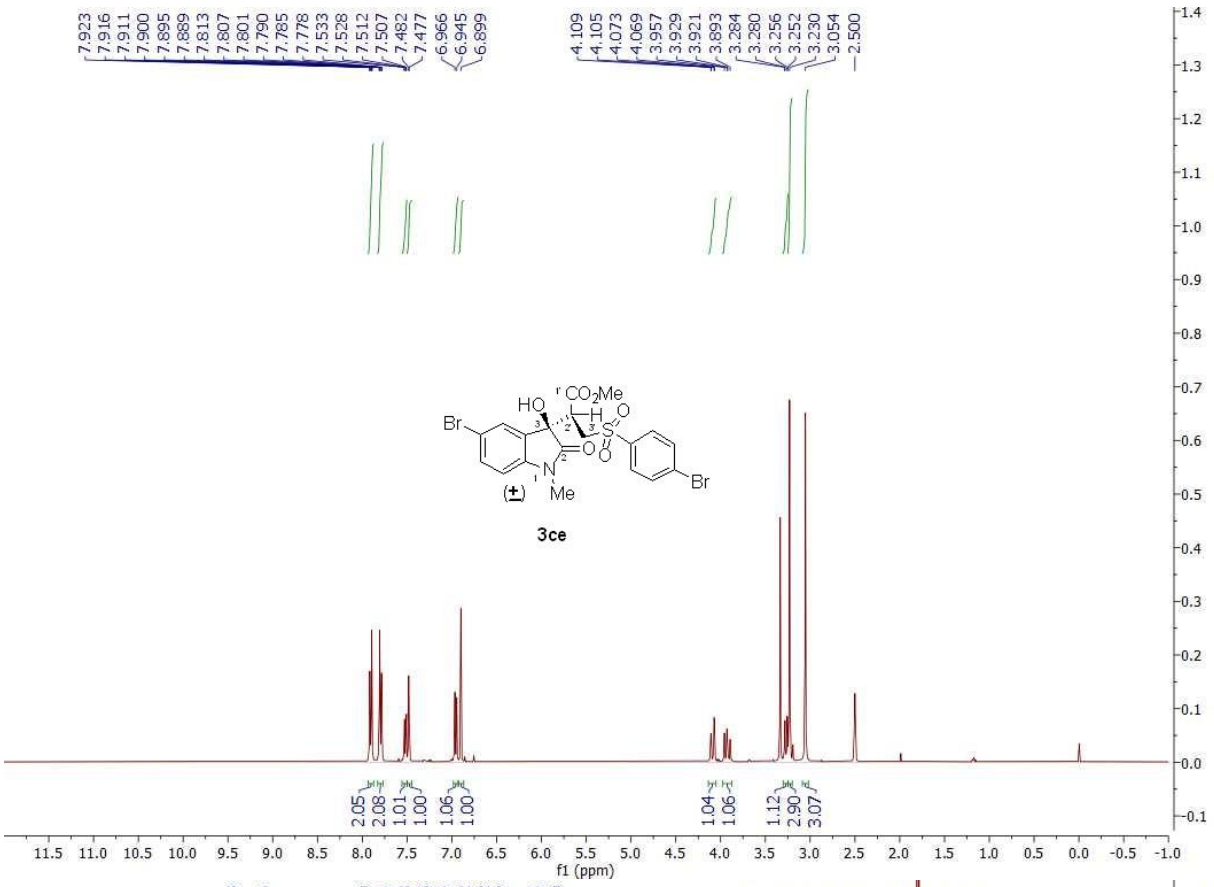
74.34
52.09
51.67
47.08
40.13
39.92
39.71
39.50
39.29
39.08
38.87
26.10
HO
CO2Me
Br
O
S
O
O
N
Me
Cl
(±)
3cd
f1 (ppm)


7.923
7.916
7.911
7.900
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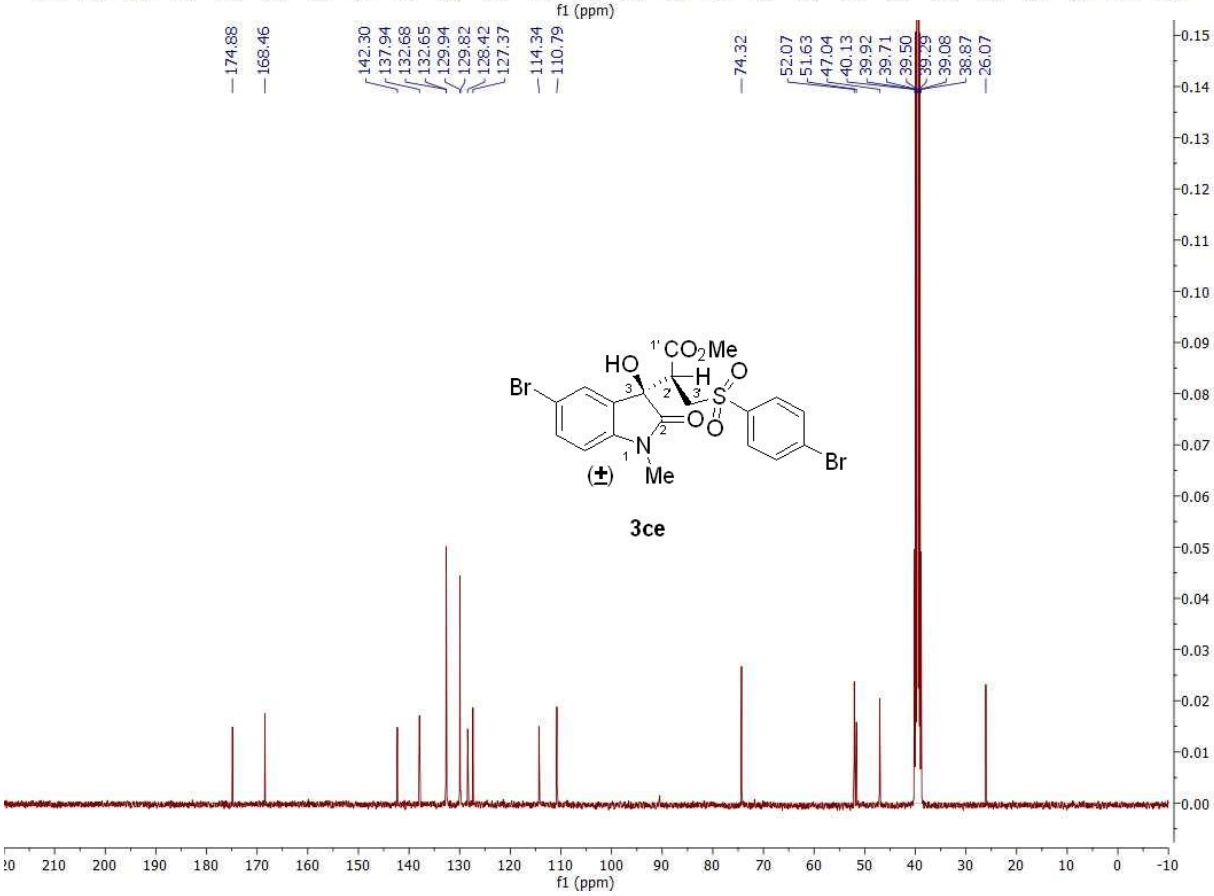
7.889
7.813
7.807
7.801
7.790
7.785
7.778
7.533
7.528
7.512
7.507
7.482
7.477
6.966
6.945
6.899
4.109
4.105
4.073
4.069
3.957
3.929
3.921
3.893
3.284
3.280
3.256
3.252
3.230
3.054
2.500
HO
1' CO2Me
Br
Br
N
Me
(±)
2.05
2.08
1.01
1.00
1.06
1.00
1.04
1.06
1.12
2.90
3.07
f1 (ppm)

3ce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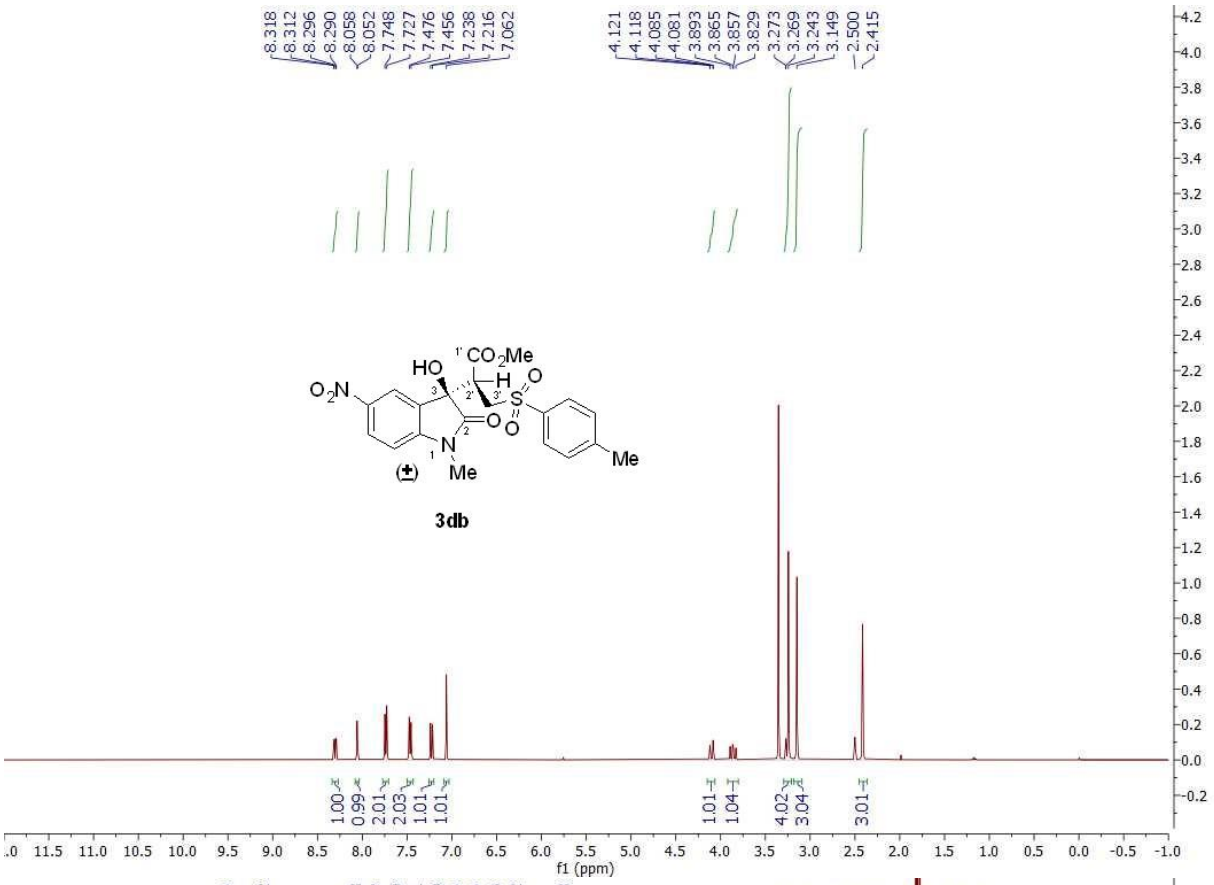
137.94
132.68
132.65
129.94
129.82
128.42
127.37
114.34
110.79
74.32
52.07
51.63
47.04
40.13
39.92
39.71
39.50
39.29
39.08
38.87
26.07
HO
1' CO2Me
Br
Br
N
Me
(±)
f1 (ppm)

3ce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8.290
8.058
8.052
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7.727
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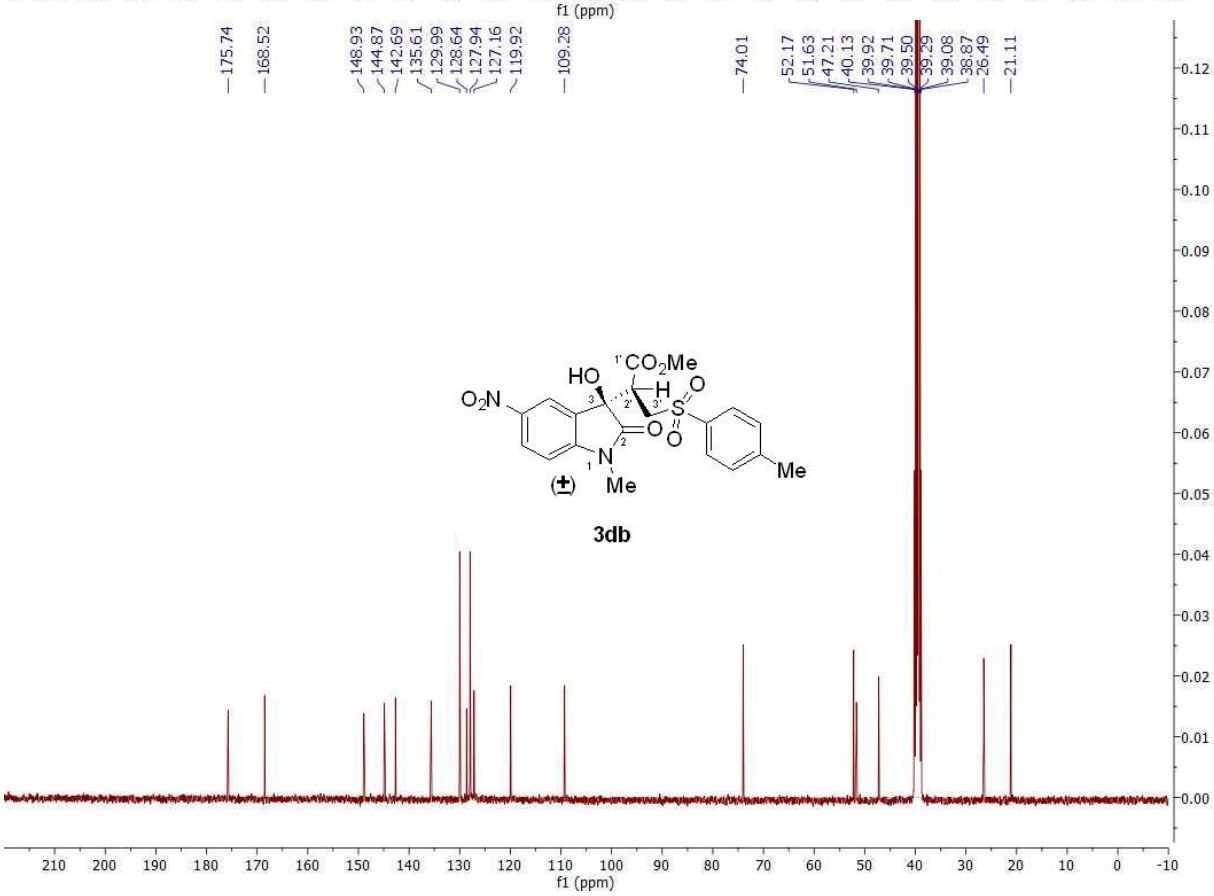
7.456
7.238
7.216
7.062
4.121
4.118
4.085
4.081
3.893
3.865
3.857
3.829
3.273
3.269
3.243
3.149
2.500
2.415
HO
1' CO2Me
O2N
Me
(±)
3db
1.00
0.99
2.01
2.03
1.01
1.01
1.01
1.04
4.02
3.04
3.01
f1 (ppm)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144.87
142.69
135.61
129.99
128.64
127.94
127.16
119.92
109.28
74.01
52.17
51.63
47.21
40.13
39.92
39.71
39.50
39.29
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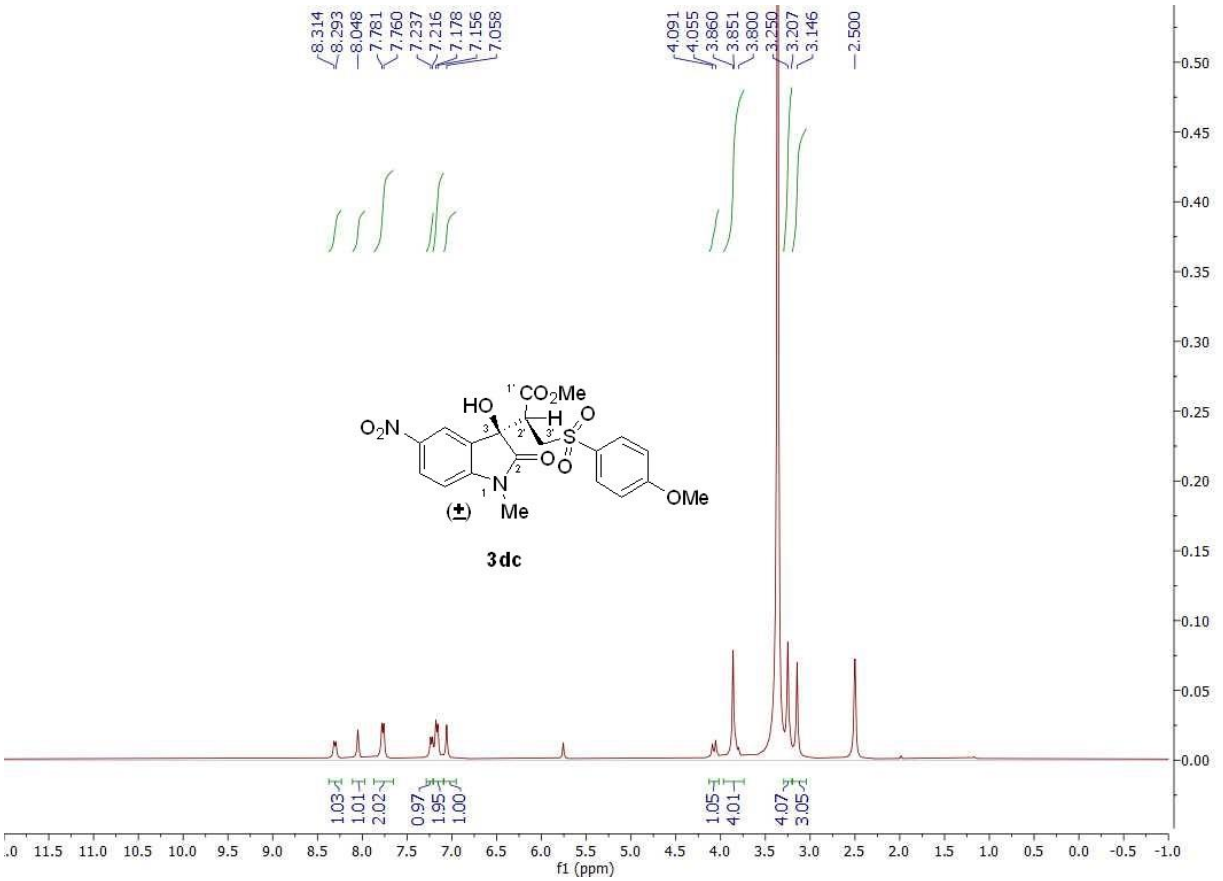
38.87
26.49
21.11
HO
1' CO2Me
O2N
Me
(±)
3db
f1 (ppm)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8.293
8.048
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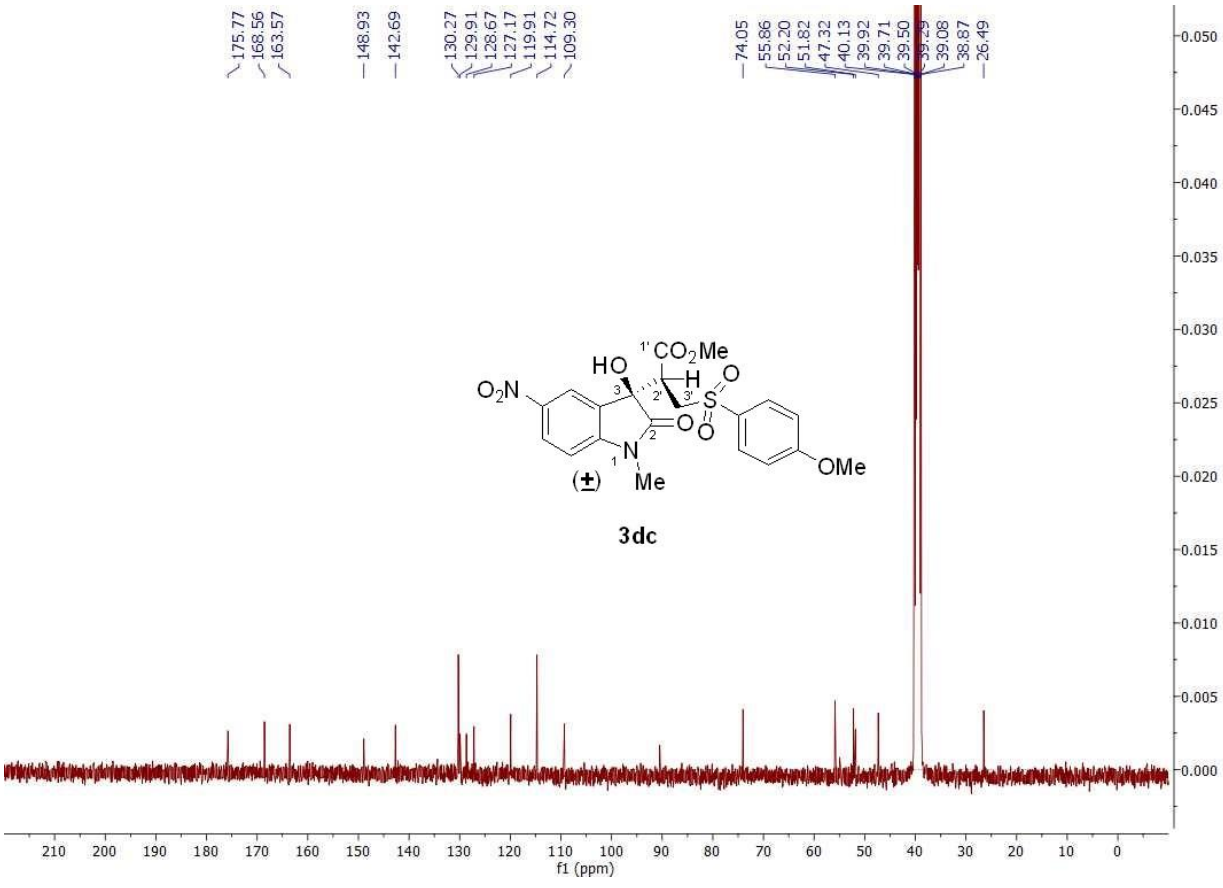
7.760
7.237
7.216
7.178
7.156
7.058
4.091
4.055
3.860
3.851
3.800
3.250
3.207
3.146
2.500
HO
1' CO2Me
H
O2N
OMe
Me
(±)
3dc
1.03
1.01
2.02
0.97
1.95
1.00
1.05
4.01
4.07
3.05
f1 (ppm)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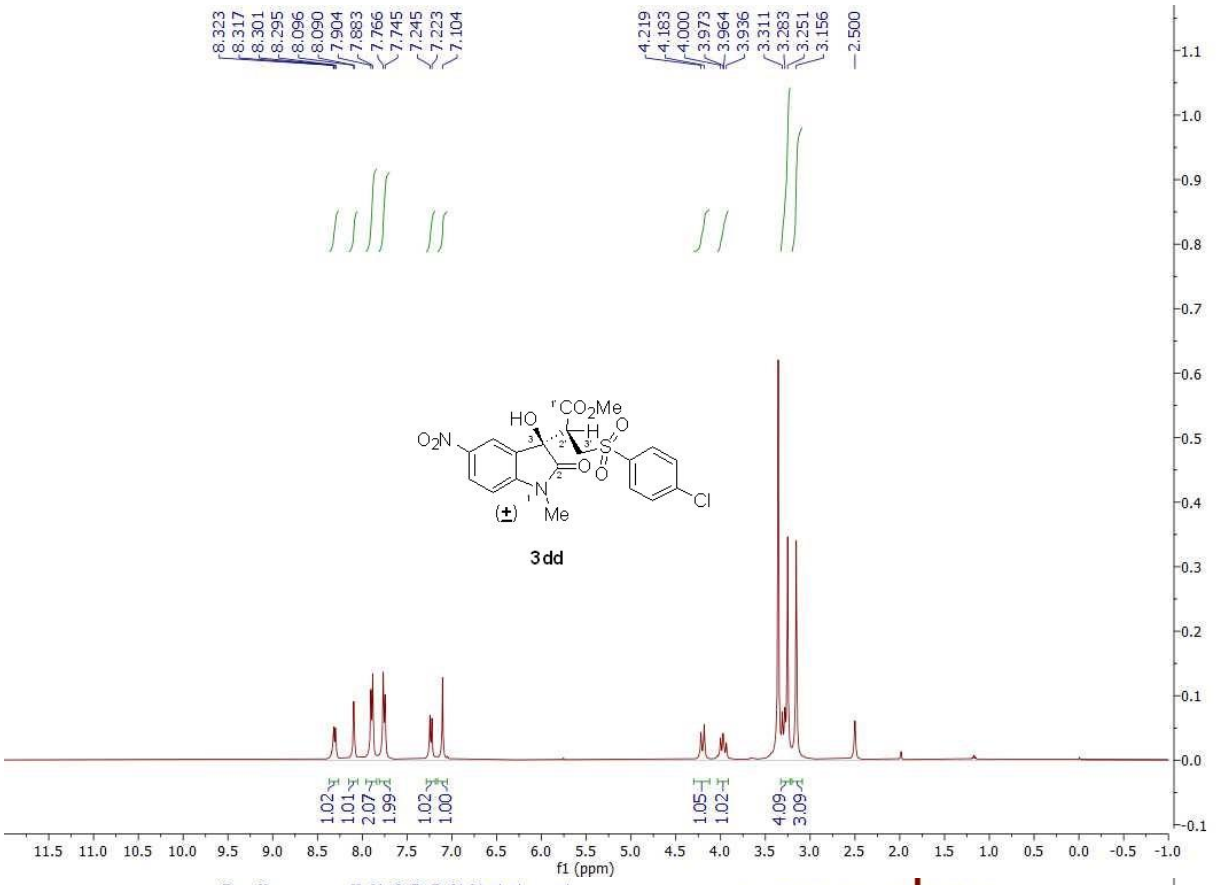
142.69
130.27
129.91
128.67
127.17
119.91
114.72
109.30
74.05
55.86
52.20
51.82
47.32
40.13
39.92
39.71
39.50
39.29
39.08
38.87
26.49
HO
1' CO2Me
H
O2N
OMe
Me
(±)
3dc
f1 (ppm)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8.301
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8.090
7.904
7.883
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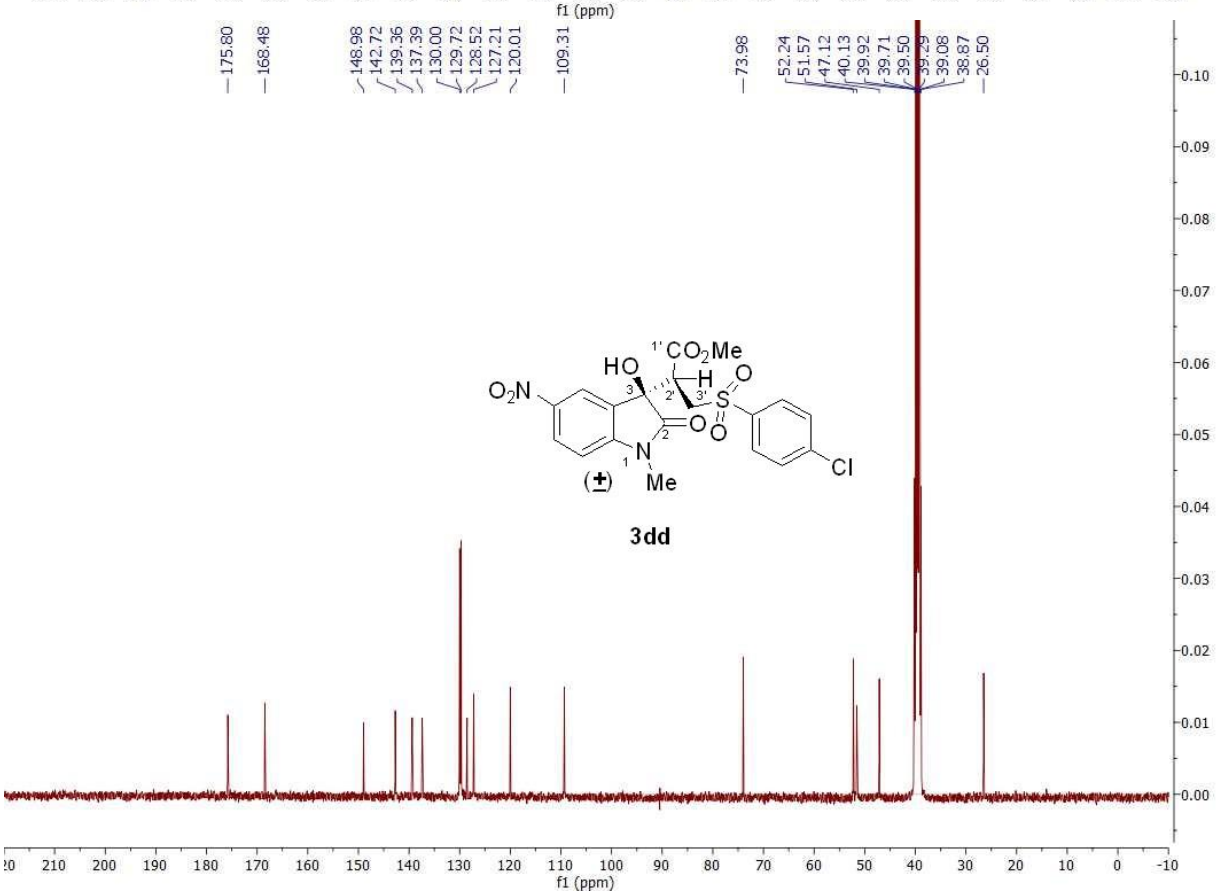
7.745
7.245
7.223
7.104
4.219
4.183
4.000
3.973
3.964
3.936
3.311
3.283
3.251
3.156
2.500
1.02
1.01
2.07
1.99
1.02
1.00
1.05
1.02
4.09
3.09
f1 (ppm)

3dd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129.72
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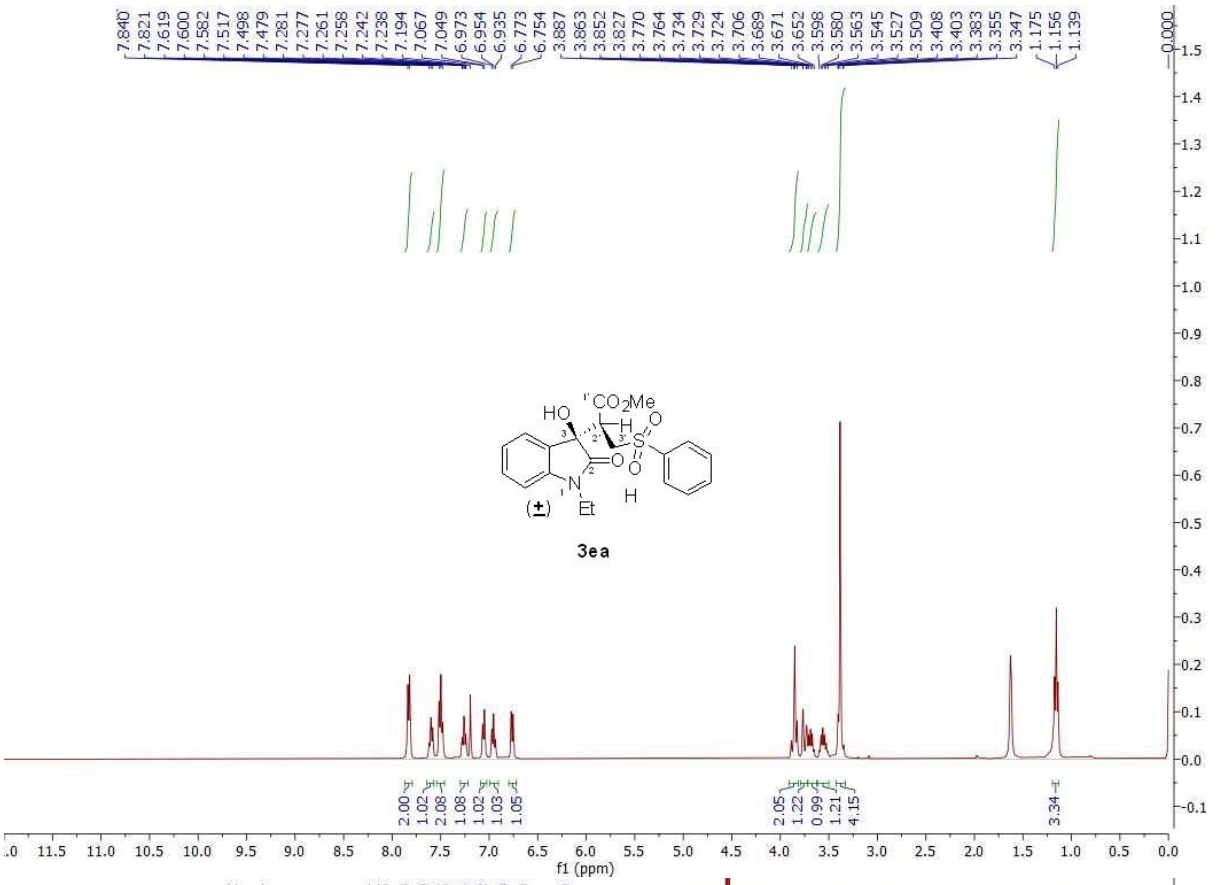
127.21
120.01
109.31
73.98
52.24
51.57
47.12
40.13
39.92
39.71
39.50
39.29
39.08
38.87
26.50
f1 (ppm)

3dd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7.619
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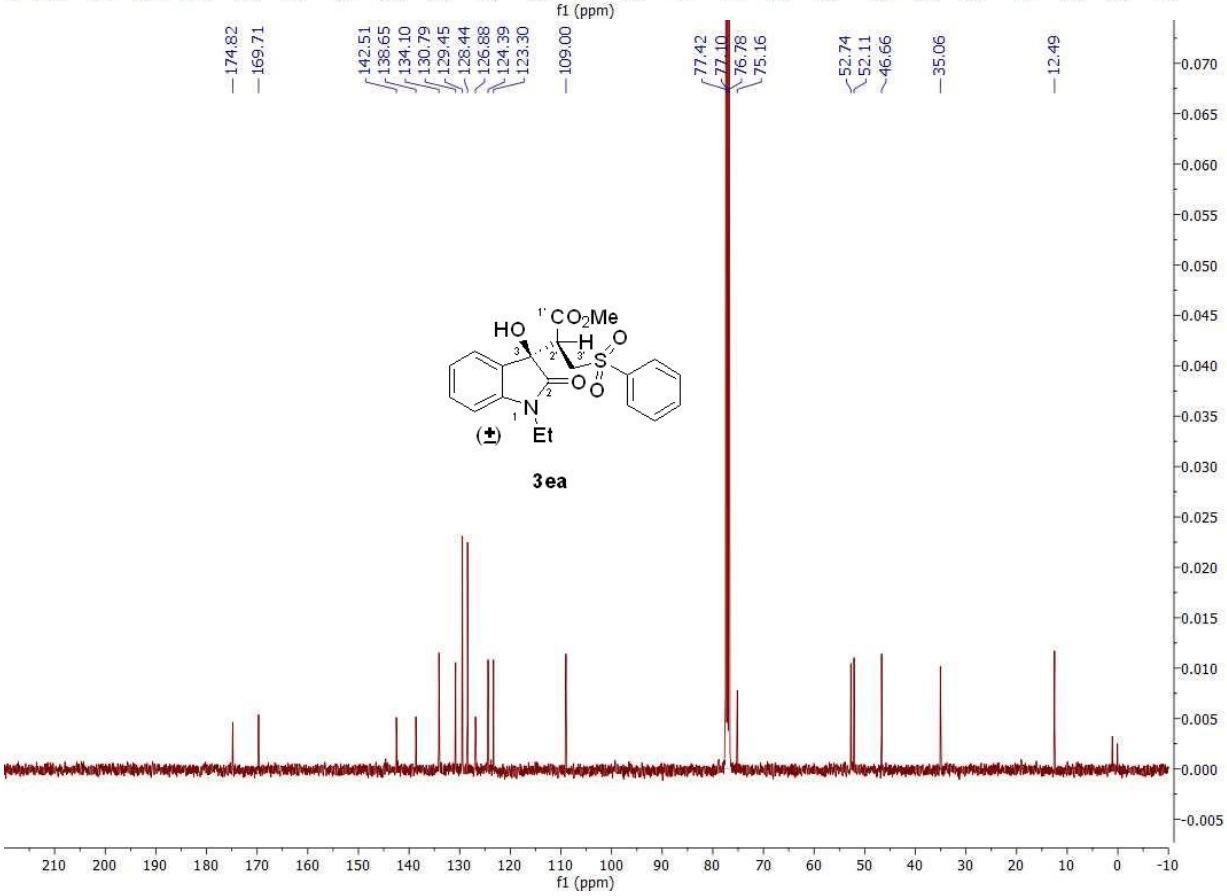
7.517
7.498
7.479
7.281
7.277
7.261
7.258
7.242
7.238
7.194
7.067
7.049
6.973
6.954
6.935
6.773
6.754
3.887
3.863
3.852
3.827
3.770
3.764
3.734
3.729
3.724
3.706
3.689
3.671
3.652
3.598
3.580
3.563
3.545
3.527
3.509
3.408
3.403
3.383
3.355
3.347
1.175
1.156
1.139
0.000
HO
1' CO2Me
N
Et
H
(±)
3ea
2.00
1.02
2.08
1.08
1.02
1.03
1.05
2.05
1.22
0.99
1.21
4.15
3.34
f1 (ppm)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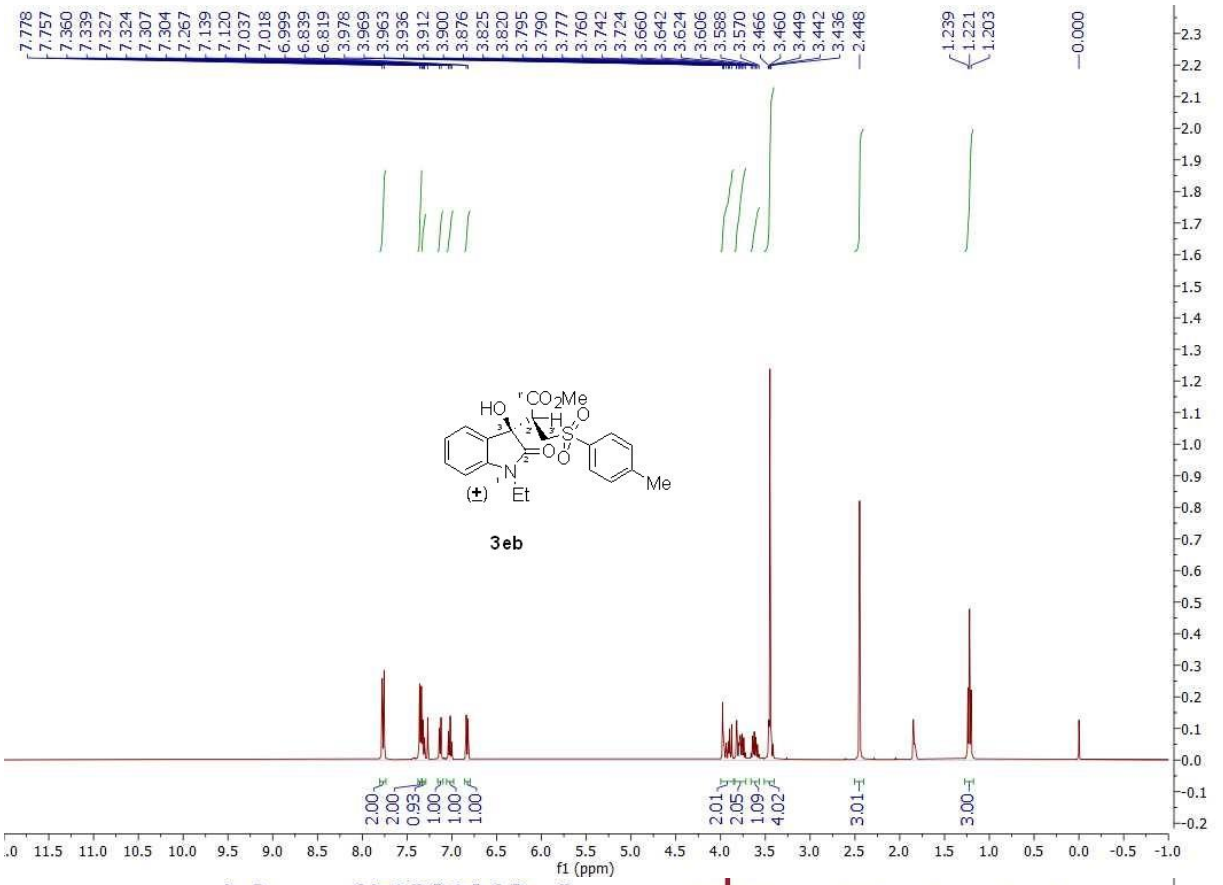
128.44
126.88
124.39
123.30
109.00
77.42
77.10
76.78
75.16
52.74
52.11
46.66
35.06
12.49
HO
1' CO2Me
N
Et
(±)
3ea
f1 (ppm)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7.324
7.307
7.304
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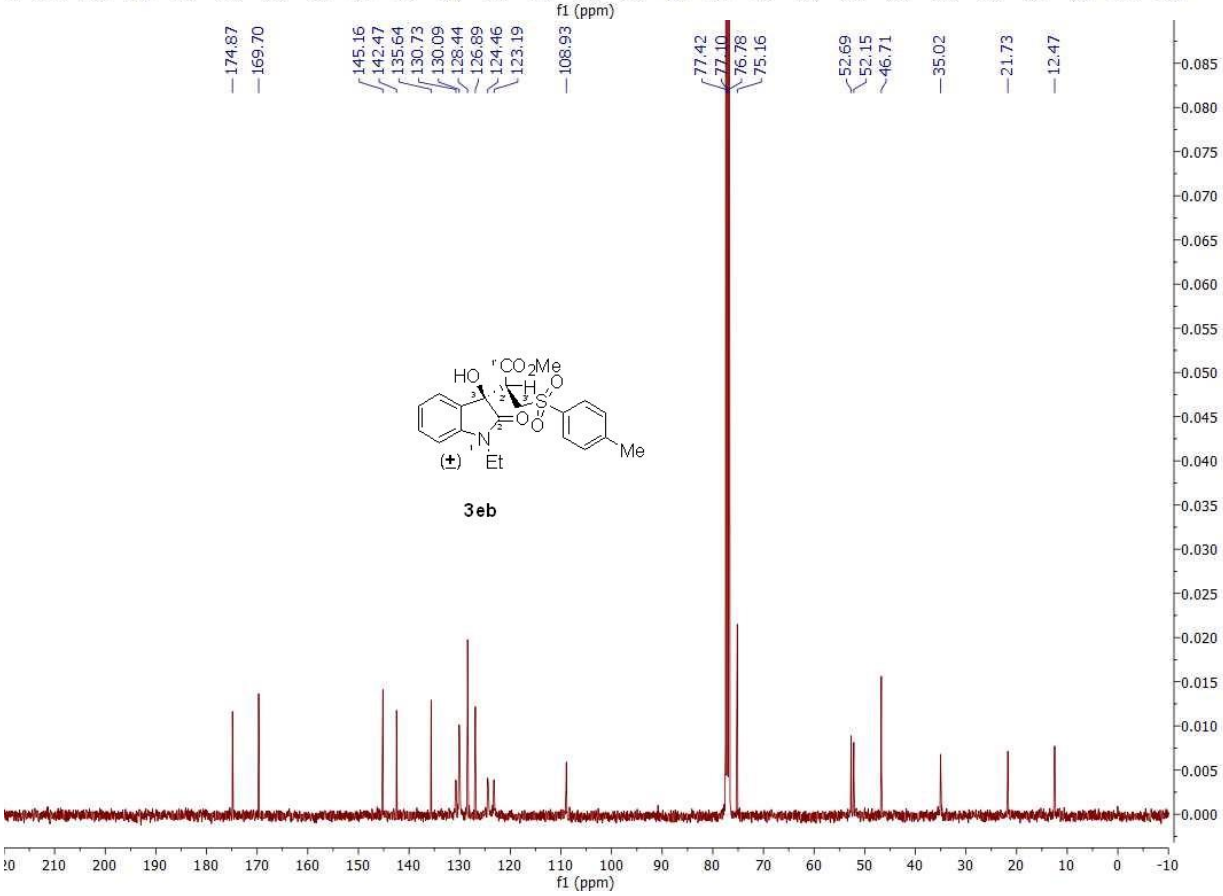
7.139
7.120
7.037
7.018
6.999
6.839
6.819
3.978
3.969
3.963
3.936
3.912
3.900
3.876
3.825
3.820
3.795
3.790
3.777
3.760
3.742
3.724
3.660
3.642
3.624
3.606
3.588
3.570
3.466
3.460
3.449
3.442
3.436
2.448
1.239
1.221
1.203
0.000
HO
CO2Me
O
S
O
O
N
Et
(±)
Me
3eb
2.00
2.00
0.93
1.00
1.00
1.00
2.01
2.05
1.09
4.02
3.01
3.00
f1 (ppm)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142.47
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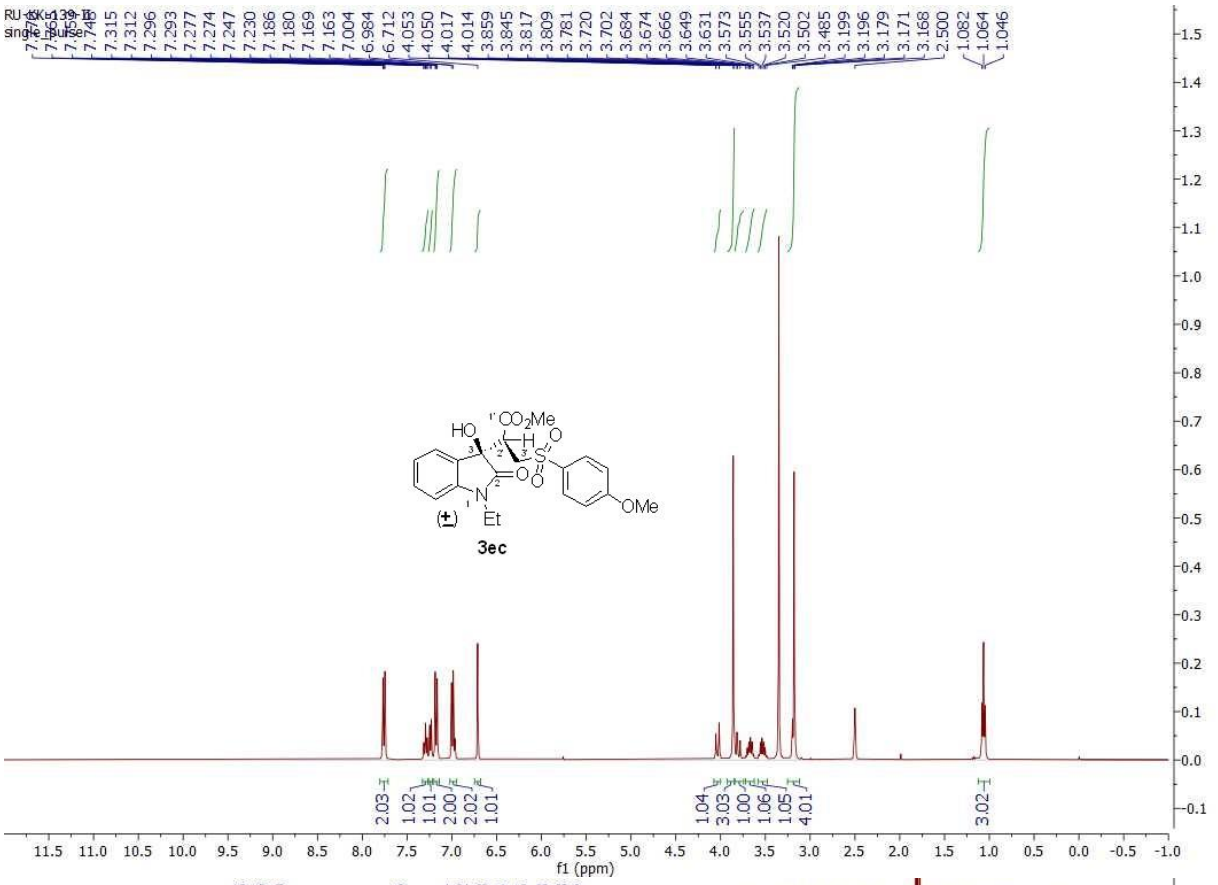
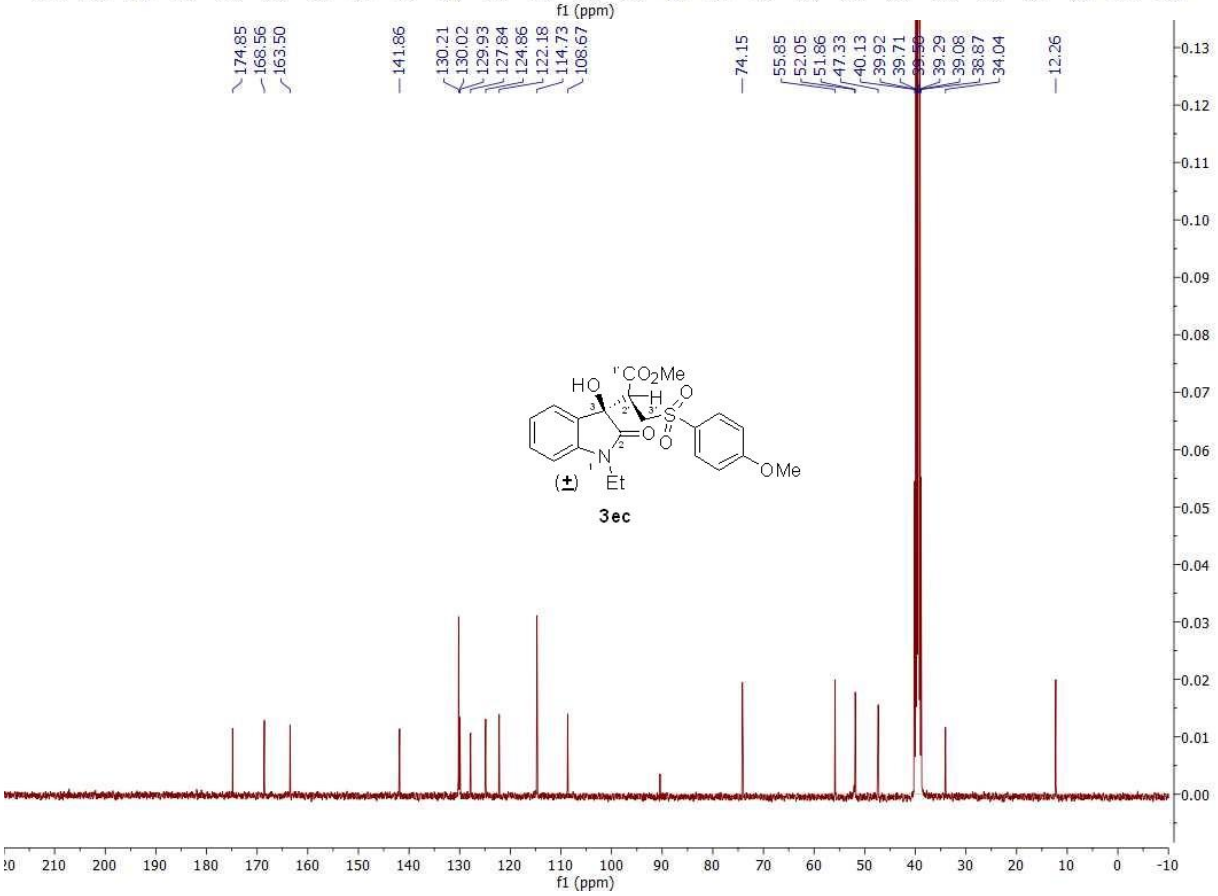
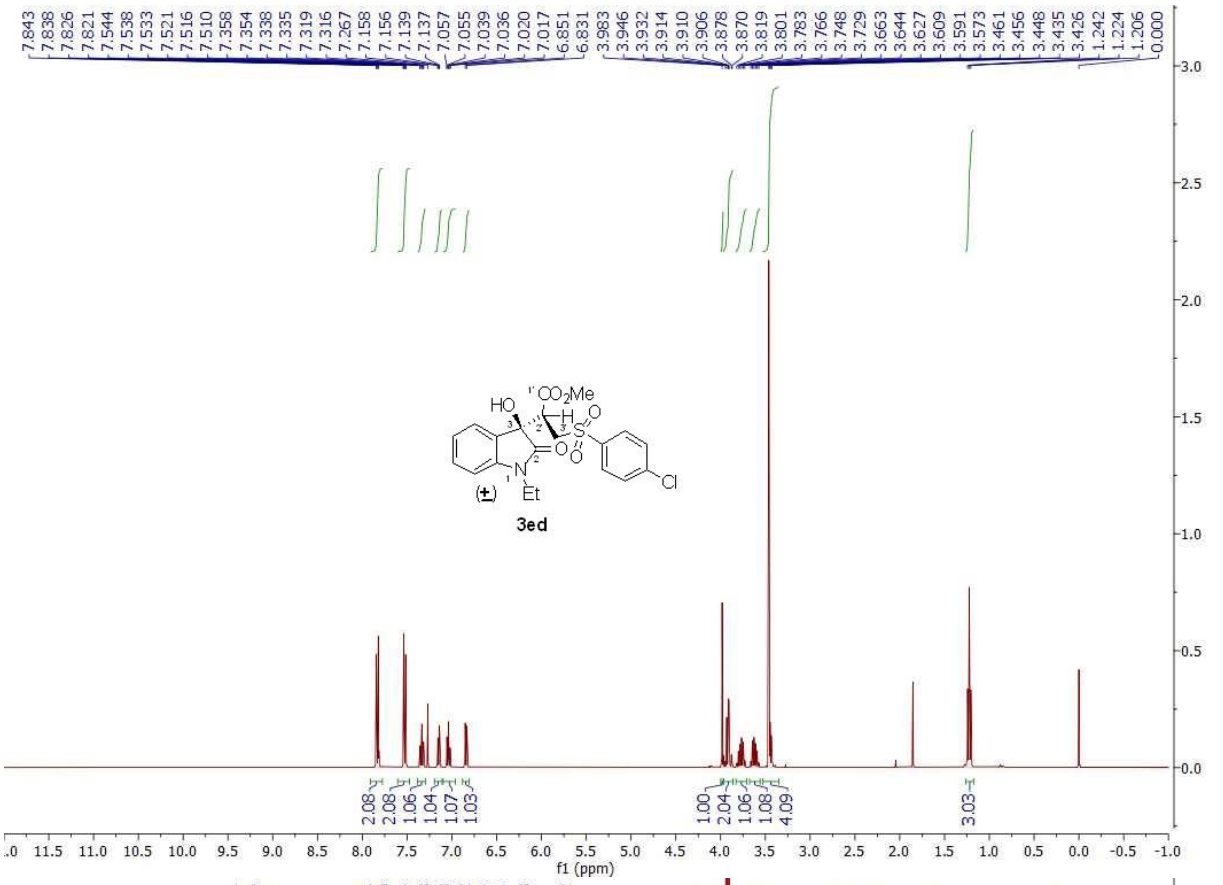
130.73
130.09
128.44
126.89
124.46
123.19
108.93
77.42
77.10
76.78
75.16
52.69
52.15
46.71
35.02
21.73
12.47
HO
CO2Me
O
S
O
O
N
Et
(±)
Me
3eb
f1 (ppm)


HO
CO2Me
O
S
O
O
N
Et
(±)
OMe
3ec
f1 (ppm)


HO
CO2Me
O
S
O
O
N
Et
(±)
OMe
3ec
f1 (ppm)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7.521
7.516
7.510
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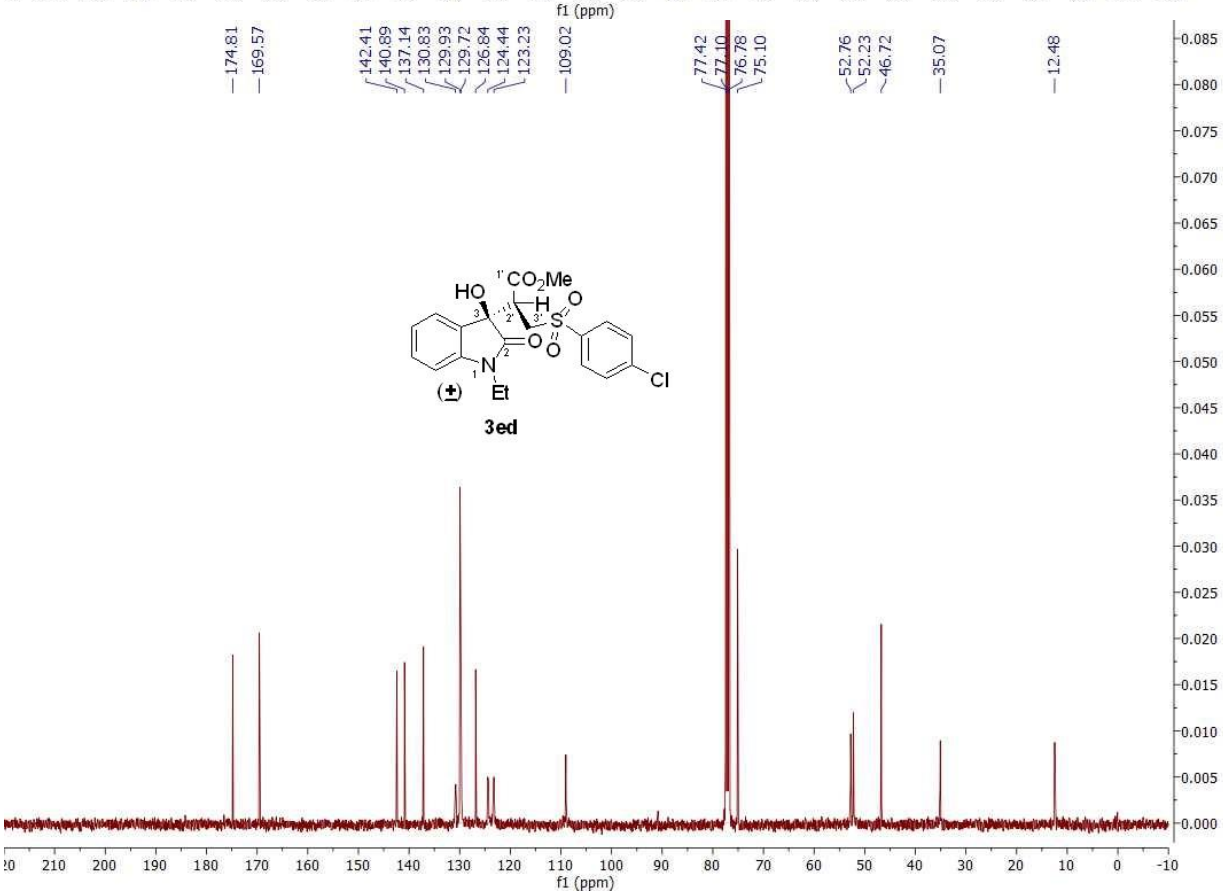
7.354
7.338
7.335
7.319
7.316
7.267
7.158
7.156
7.139
7.137
7.057
7.055
7.039
7.036
7.020
7.017
6.851
6.831
3.983
3.946
3.932
3.914
3.910
3.906
3.878
3.870
3.819
3.801
3.783
3.766
3.748
3.729
3.663
3.644
3.627
3.609
3.591
3.573
3.461
3.456
3.448
3.435
3.426
1.242
1.224
1.206
0.000
HO
1' CO2Me
Cl
(±)
Et
3ed
2.08
2.08
1.06
1.04
1.07
1.03
1.00
2.04
1.06
1.08
4.09
3.03
f1 (ppm)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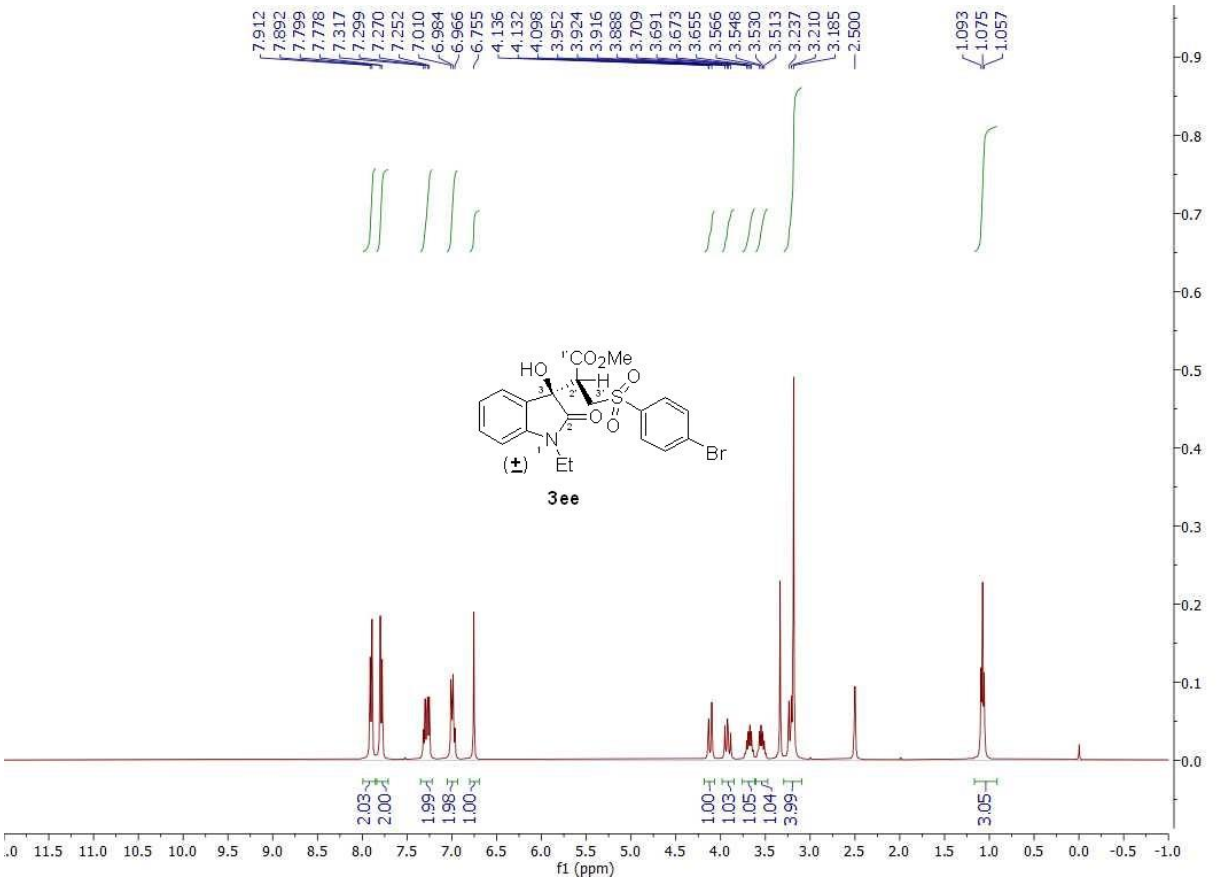
129.93
129.72
126.84
124.44
123.23
109.02
77.42
77.10
76.78
75.10
52.76
52.23
46.72
35.07
12.48
HO
1' CO2Me
Cl
(±)
Et
3ed
f1 (ppm)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7.270
7.252
7.010
6.984
6.966
6.755
4.136
4.132
4.098
3.952
3.924
3.916
3.888
3.709
3.691
3.673
3.655
3.566
3.548
3.530
3.513
3.237
3.210
3.185
2.500
1.093
1.075
1.057
HO
1'CO2Me
H
S
O
O
O
N
1'
Et
(±)
Br
3ee
2.03
2.00
1.99
1.98
1.00
1.00
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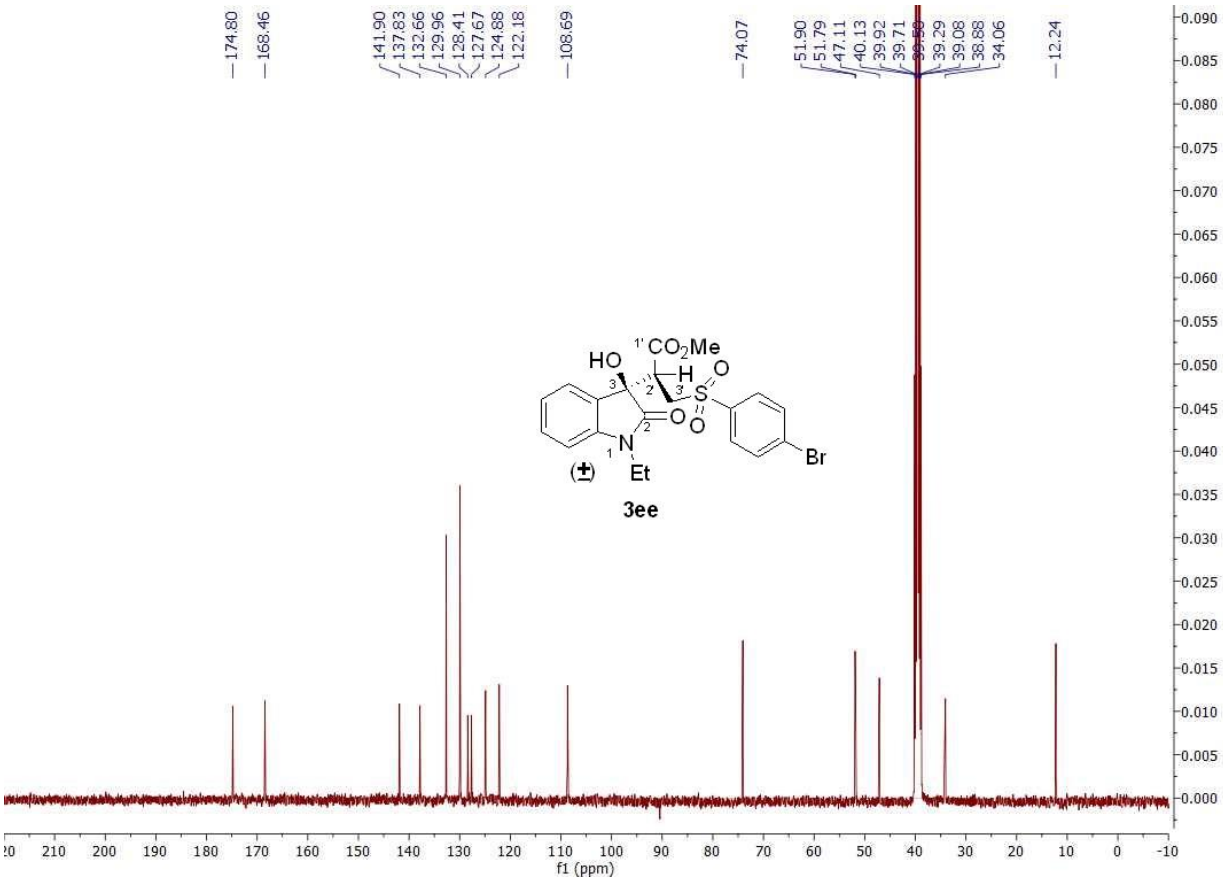
1.05
1.04
3.99
3.05
f1 (ppm)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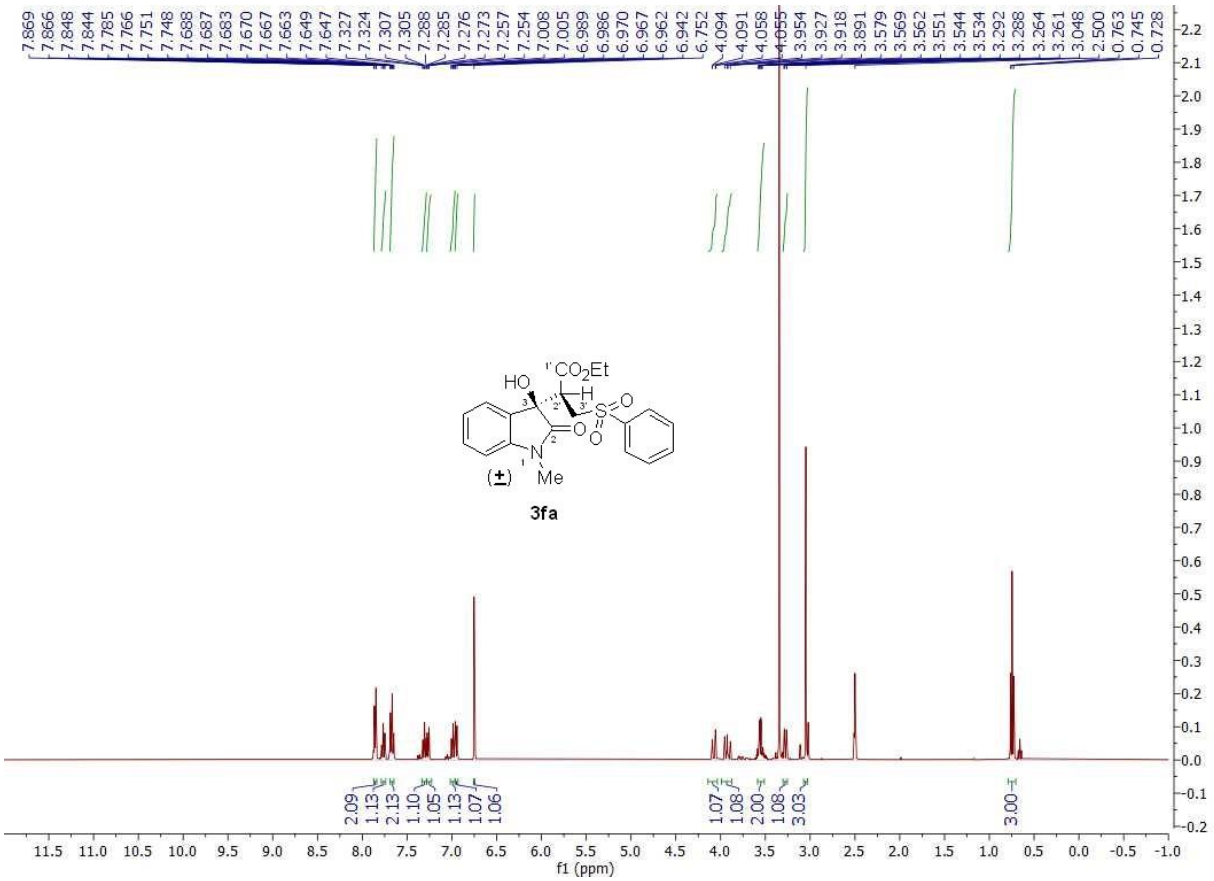
127.67
124.88
122.18
108.69
74.07
51.90
51.79
47.11
40.13
39.92
39.71
39.50
39.29
39.08
38.88
34.06
12.24
HO
1'CO2Me
H
S
O
O
O
N
1'
Et
(±)
Br
3ee
f1 (ppm)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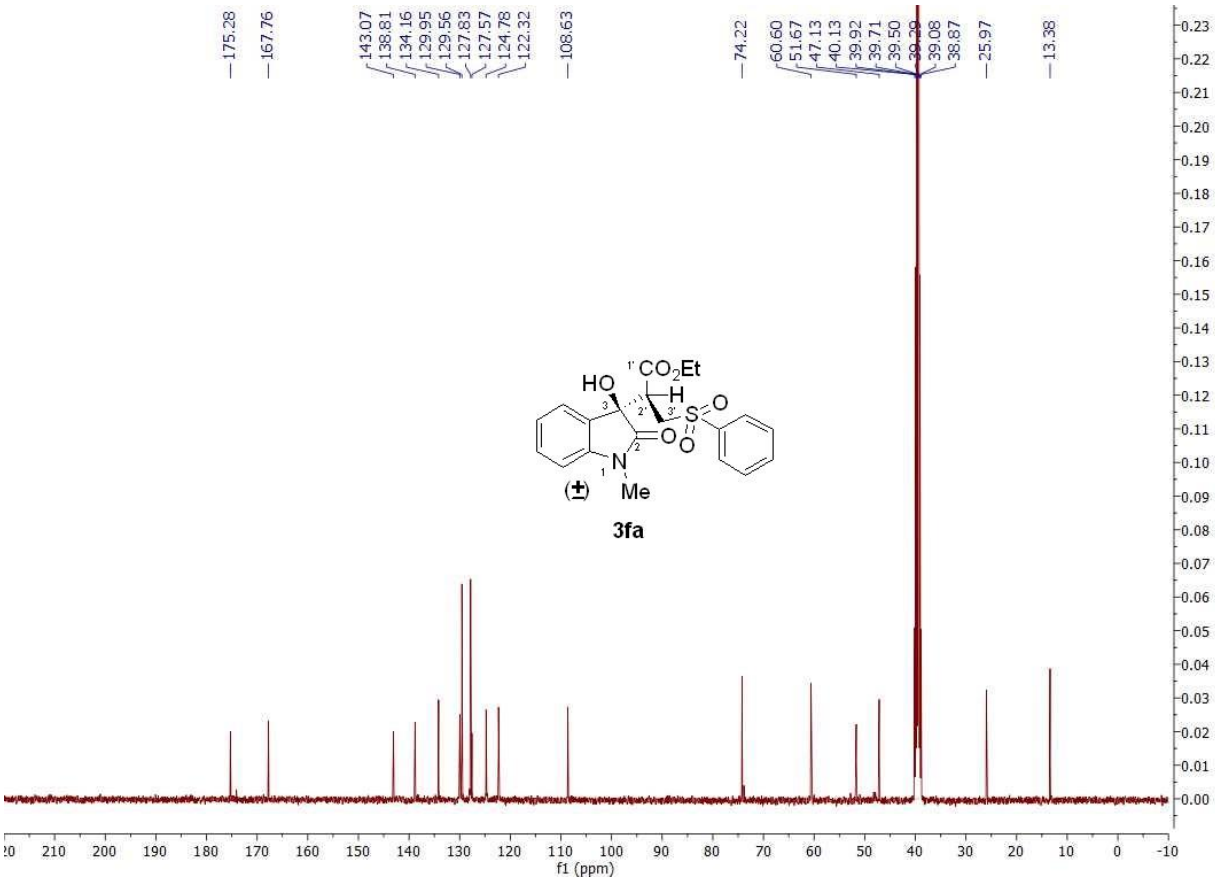
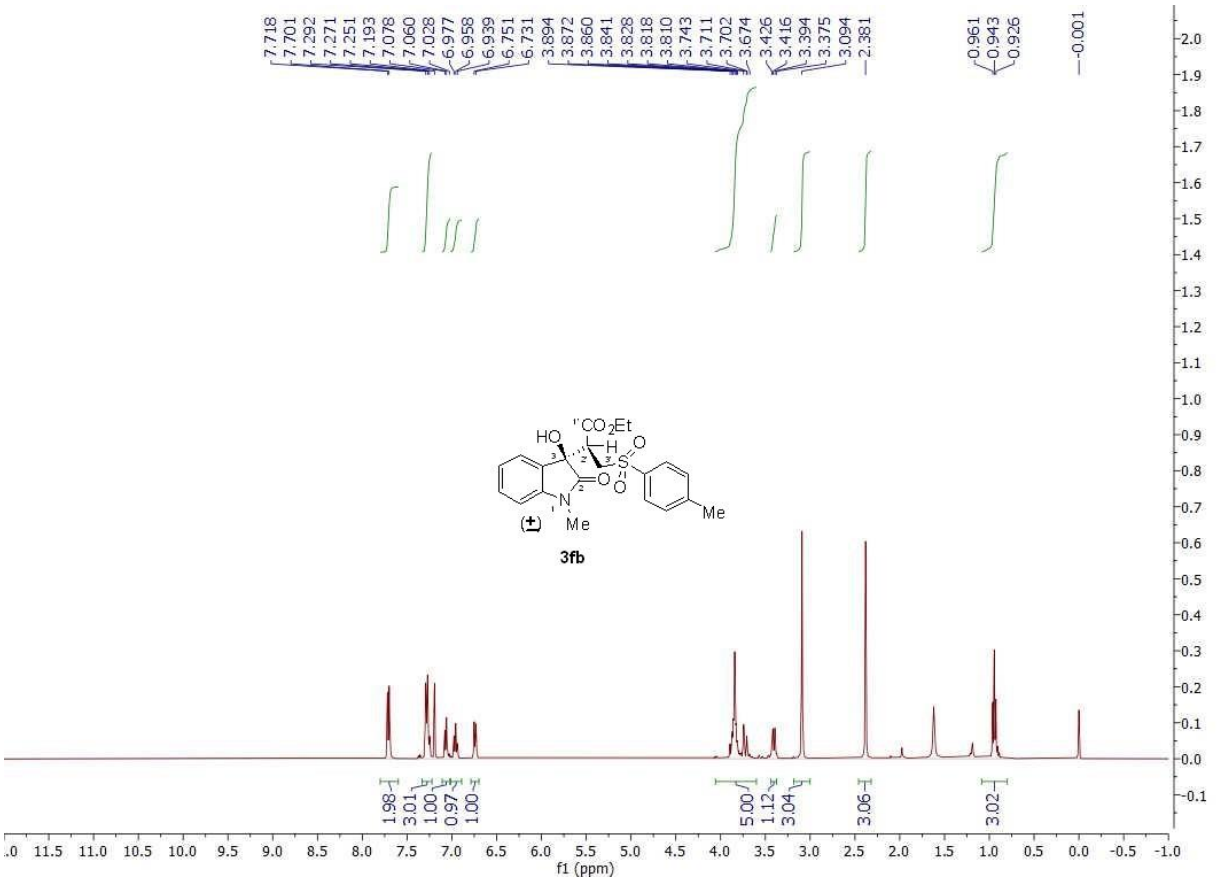
HO
1'CO2Et
H
S
O
O
O
N
Me
(±)
3fa
2.09 1.13 2.13 1.10 1.05 1.13 1.07 1.06 1.07 1.08 2.00 1.08 3.03 3.00
f1 (ppm)


175.28 167.76 143.07 138.81 134.16 129.95 129.56 127.83 127.57 124.78 122.32 108.63 74.22 60.60 51.67 47.13 40.13 39.92 39.71 39.50 39.29 39.08 38.87 25.97 13.38
HO
1'CO2Et
H
S
O
O
O
N
Me
(±)
3fa
f1 (ppm)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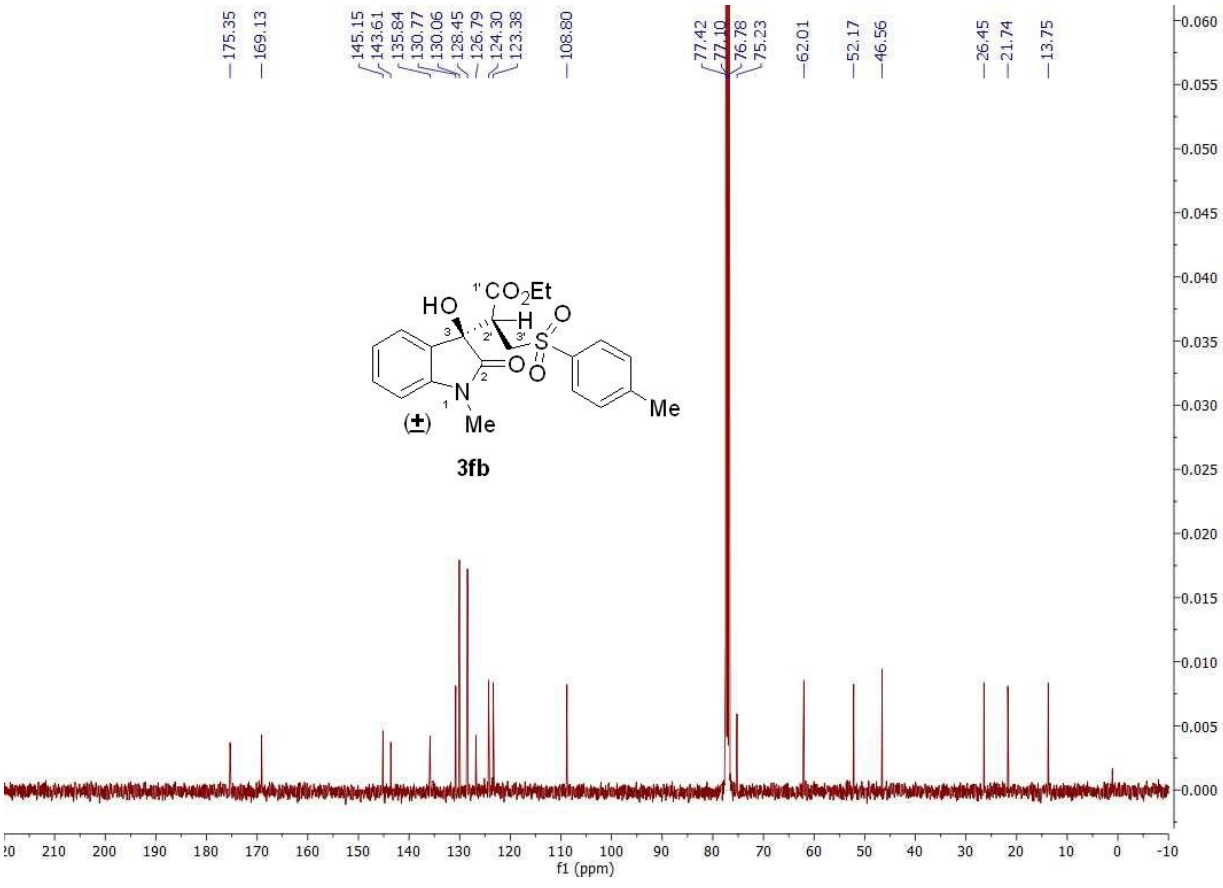
7.271
7.251
7.193
7.078
7.060
7.028
6.977
6.958
6.939
6.751
6.731
3.894
3.872
3.860
3.841
3.828
3.818
3.810
3.743
3.711
3.702
3.674
3.426
3.416
3.394
3.375
3.094
2.381
0.961
0.943
0.926
-0.001
1.98
3.01
1.00
0.97
1.00
5.00
1.12
3.04
3.06
3.02
f1 (ppm)

HO
1'CO2Et
H
O
S
O
O
N
Me
Me
(±)

3fb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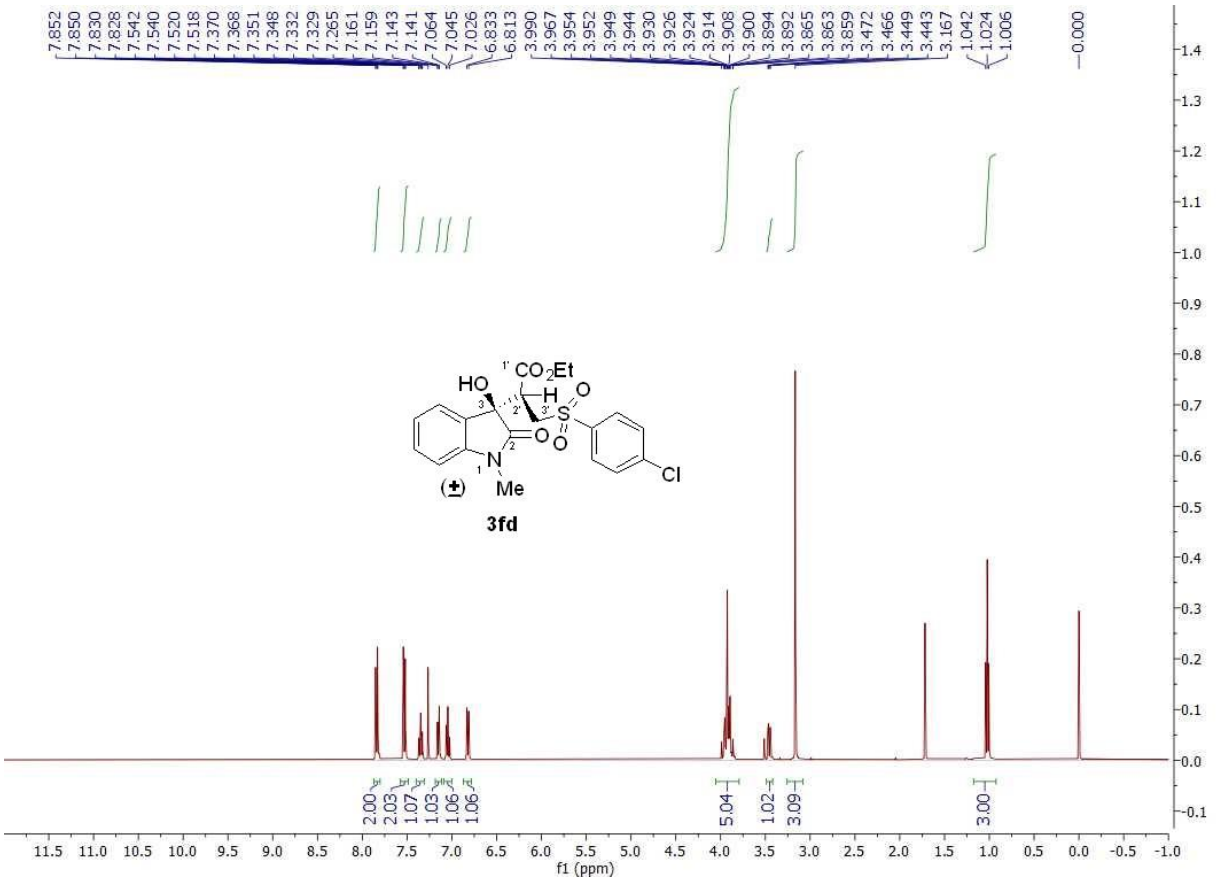
145.15
143.61
135.84
130.77
130.06
128.45
126.79
124.30
123.38
108.80
77.42
77.10
76.78
75.23
62.01
52.17
46.56
26.45
21.74
13.75
f1 (ppm)

HO
1'CO2Et
H
O
S
O
O
N
Me
Me
(±)

3fb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7.518
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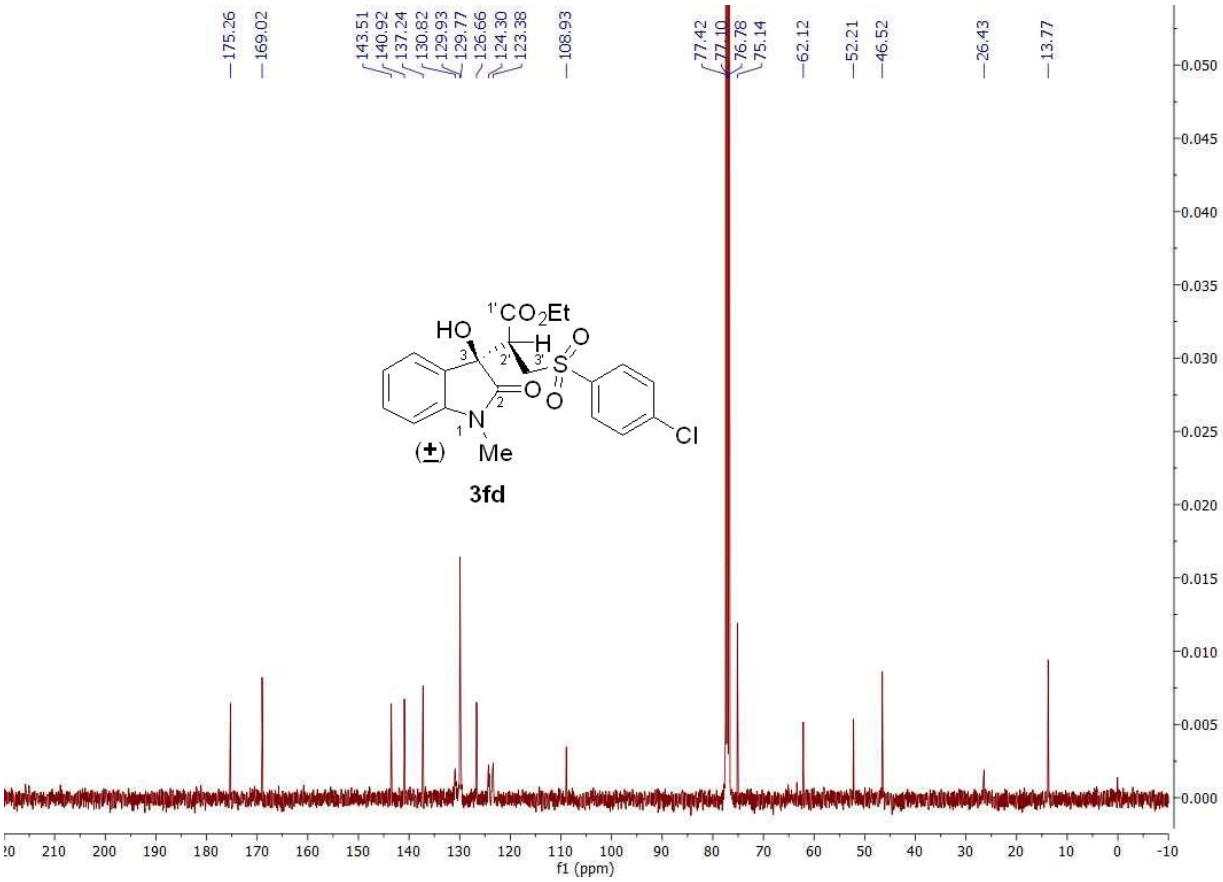
7.348
7.332
7.329
7.265
7.161
7.159
7.143
7.141
7.064
7.045
7.026
6.833
6.813
3.990
3.967
3.954
3.952
3.949
3.944
3.930
3.926
3.924
3.914
3.908
3.900
3.894
3.892
3.865
3.863
3.859
3.472
3.466
3.449
3.443
3.167
1.042
1.024
1.006
0.000
1' CO2Et
HO
3'
2'
3
2
1
O
S
O
O
N
Me
(±)
Cl
3fd
2.00
2.03
1.07
1.03
1.06
1.06
5.04
1.02
3.09
3.00
f1 (ppm)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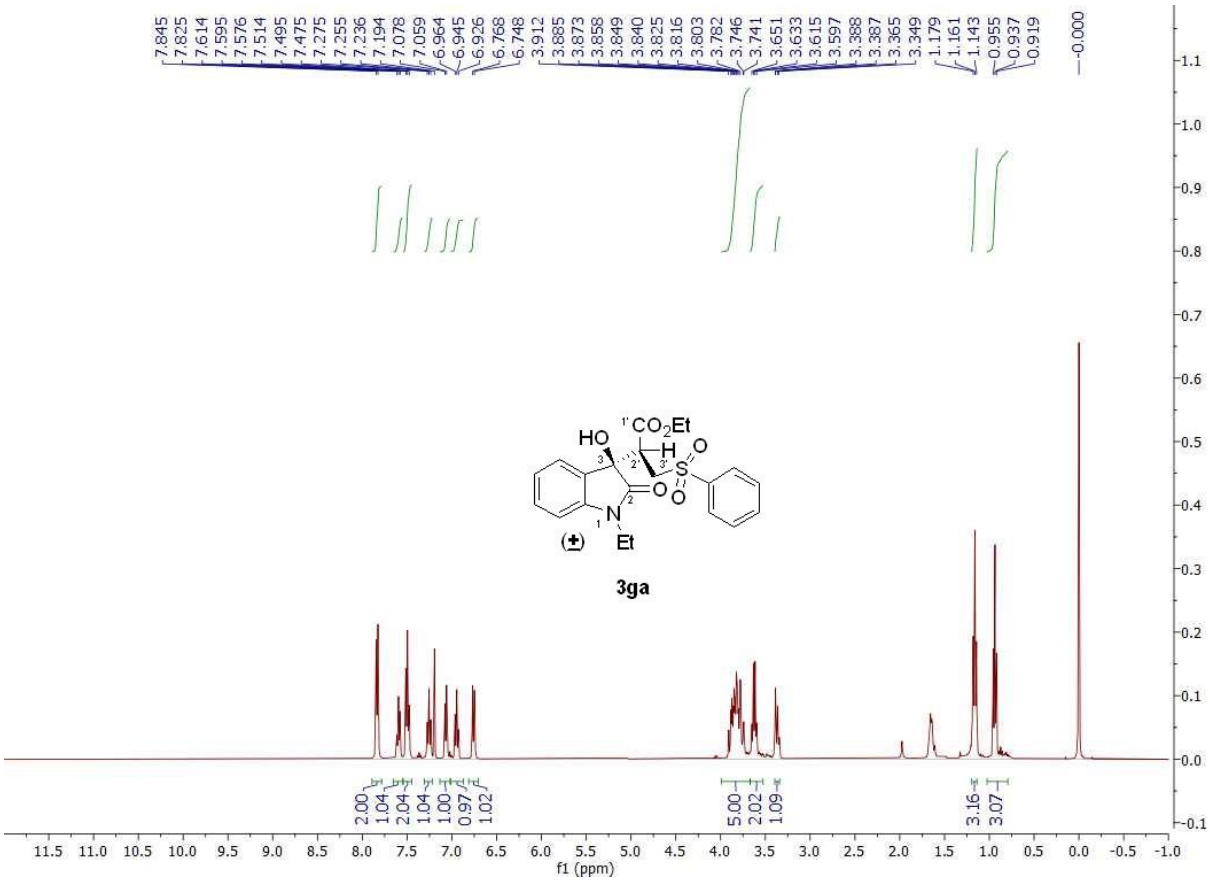
129.93
129.77
126.66
124.30
123.38
108.93
77.42
77.10
76.78
75.14
62.12
52.21
46.52
26.43
13.77
1' CO2Et
HO
3'
2'
3
2
1
O
S
O
O
N
Me
(±)
Cl
3fd
f1 (ppm)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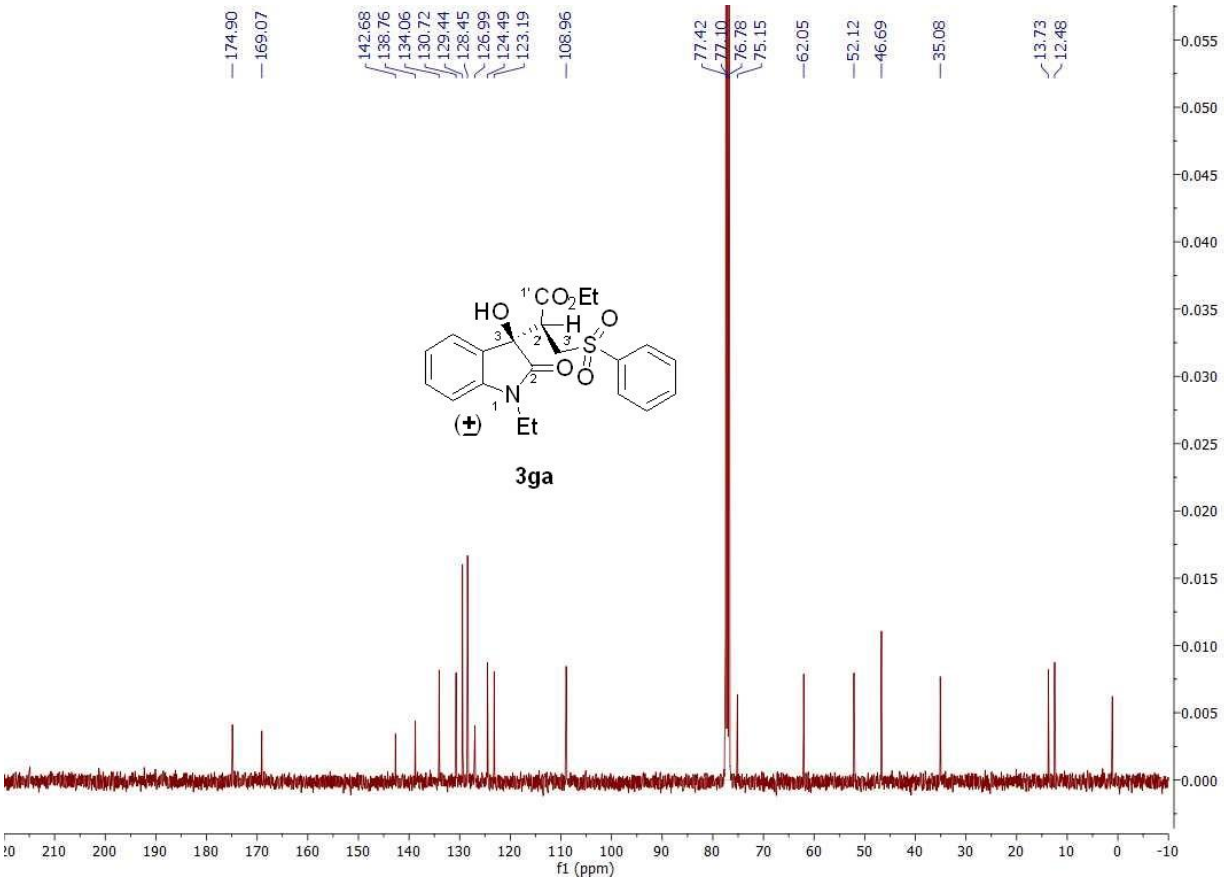
7.255
7.236
7.194
7.078
7.059
6.964
6.945
6.926
6.768
6.748
3.912
3.885
3.873
3.858
3.849
3.840
3.825
3.816
3.803
3.782
3.746
3.741
3.651
3.633
3.615
3.597
3.388
3.387
3.365
3.349
1.179
1.161
1.143
0.955
0.937
0.919
-0.000
HO
1' CO2Et
Et
3ga
2.00
1.04
2.04
1.04
1.00
0.97
1.02
5.00
2.02
1.09
3.16
3.07
f1 (ppm)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130.72
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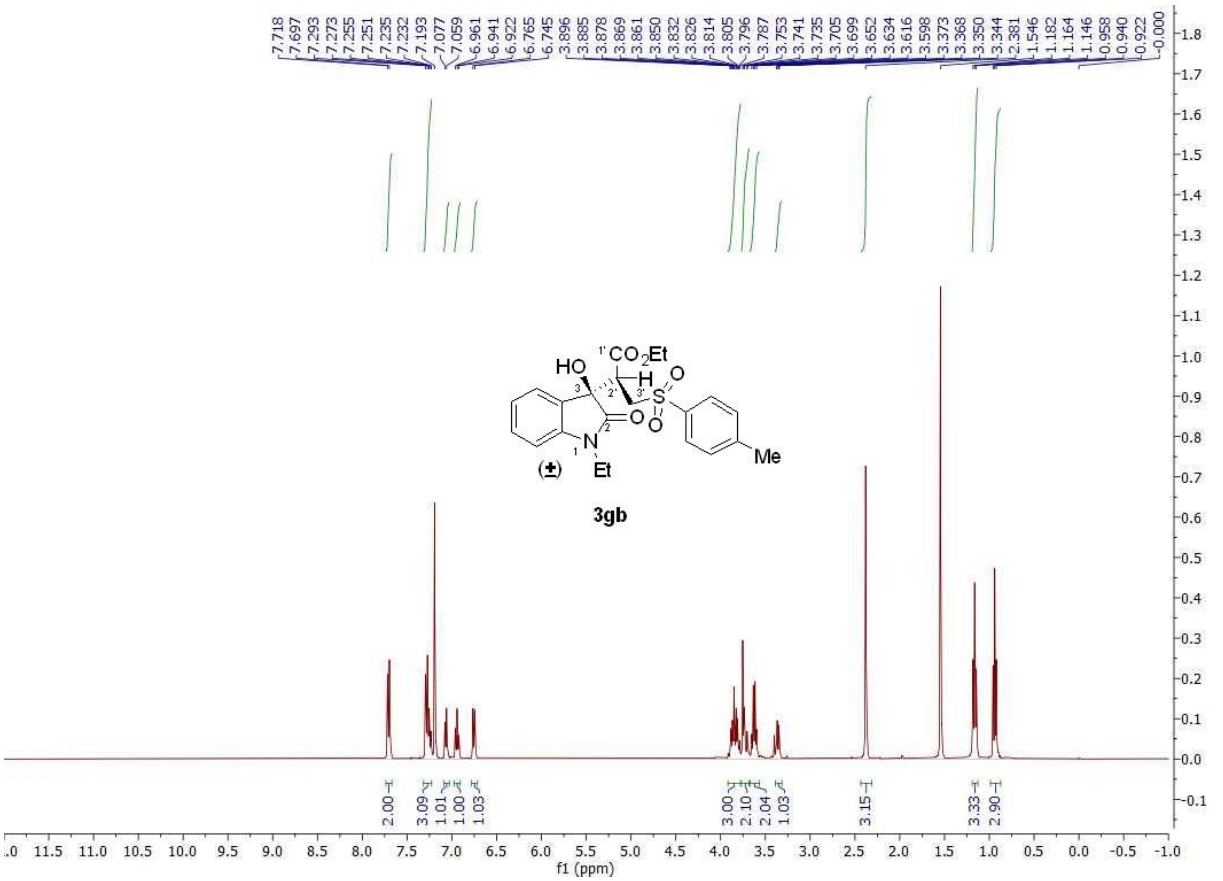
126.99
124.49
123.19
108.96
77.42
77.10
76.78
75.15
62.05
52.12
46.69
35.08
13.73
12.48
HO
1' CO2Et
Et
3ga
f1 (ppm)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7.232
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7.077
7.059
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6.941
6.922
6.765
6.745
3.896
3.885
3.878
3.869
3.861
3.850
3.832
3.826
3.814
3.805
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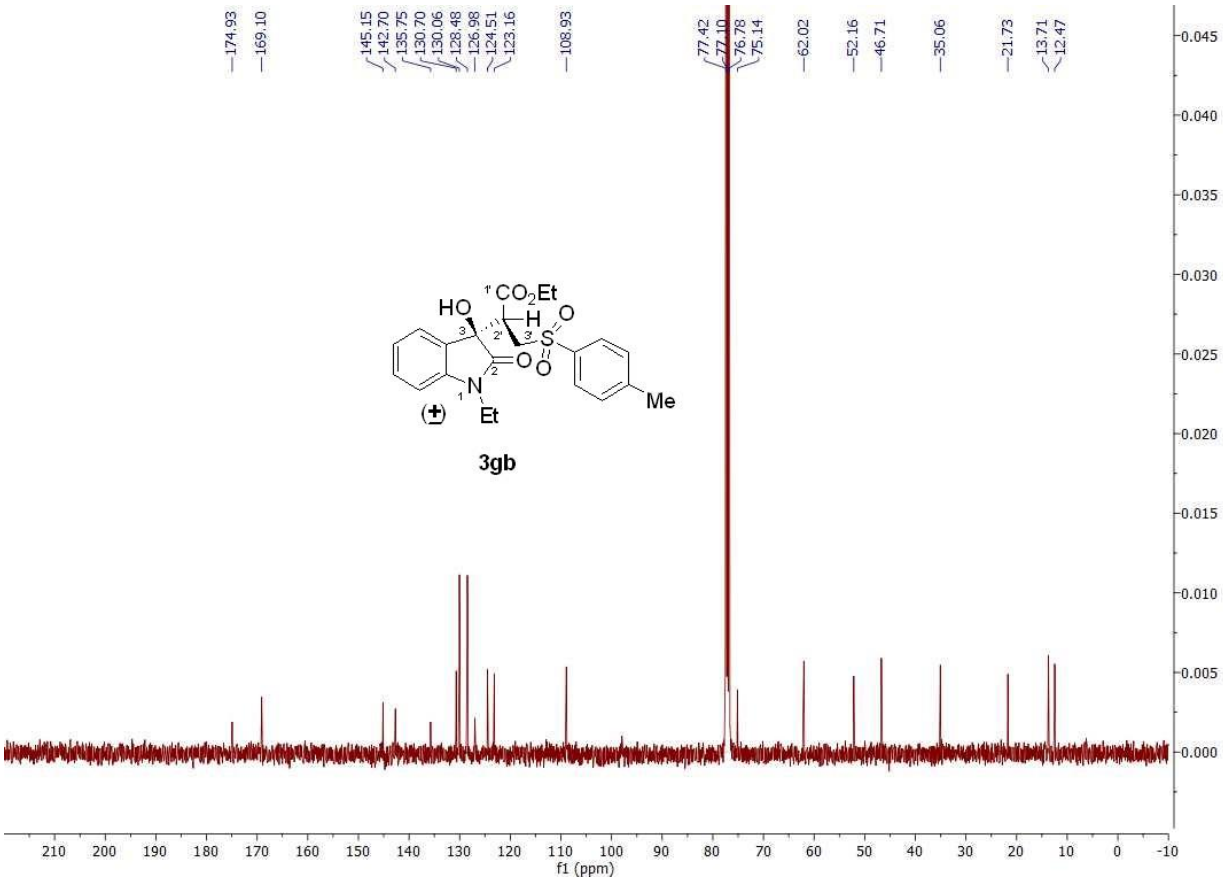
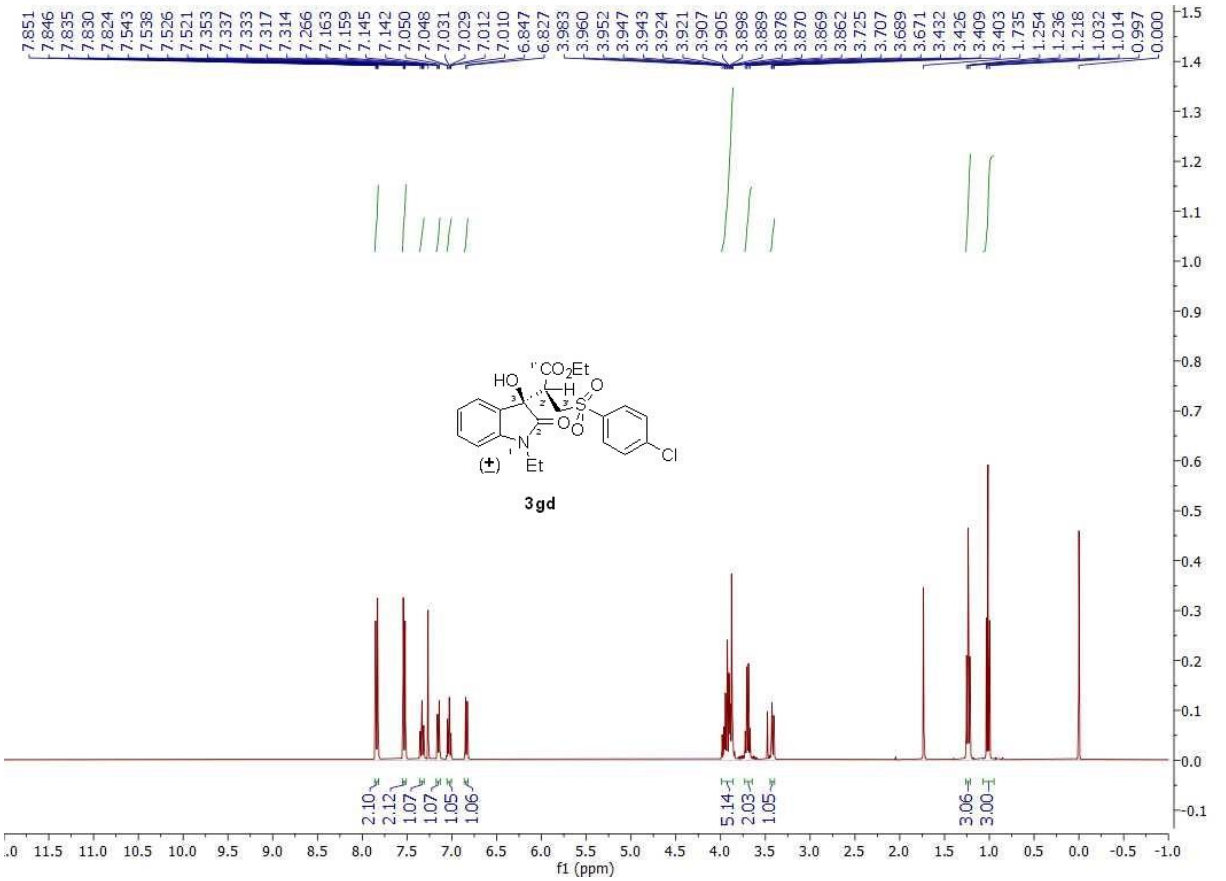
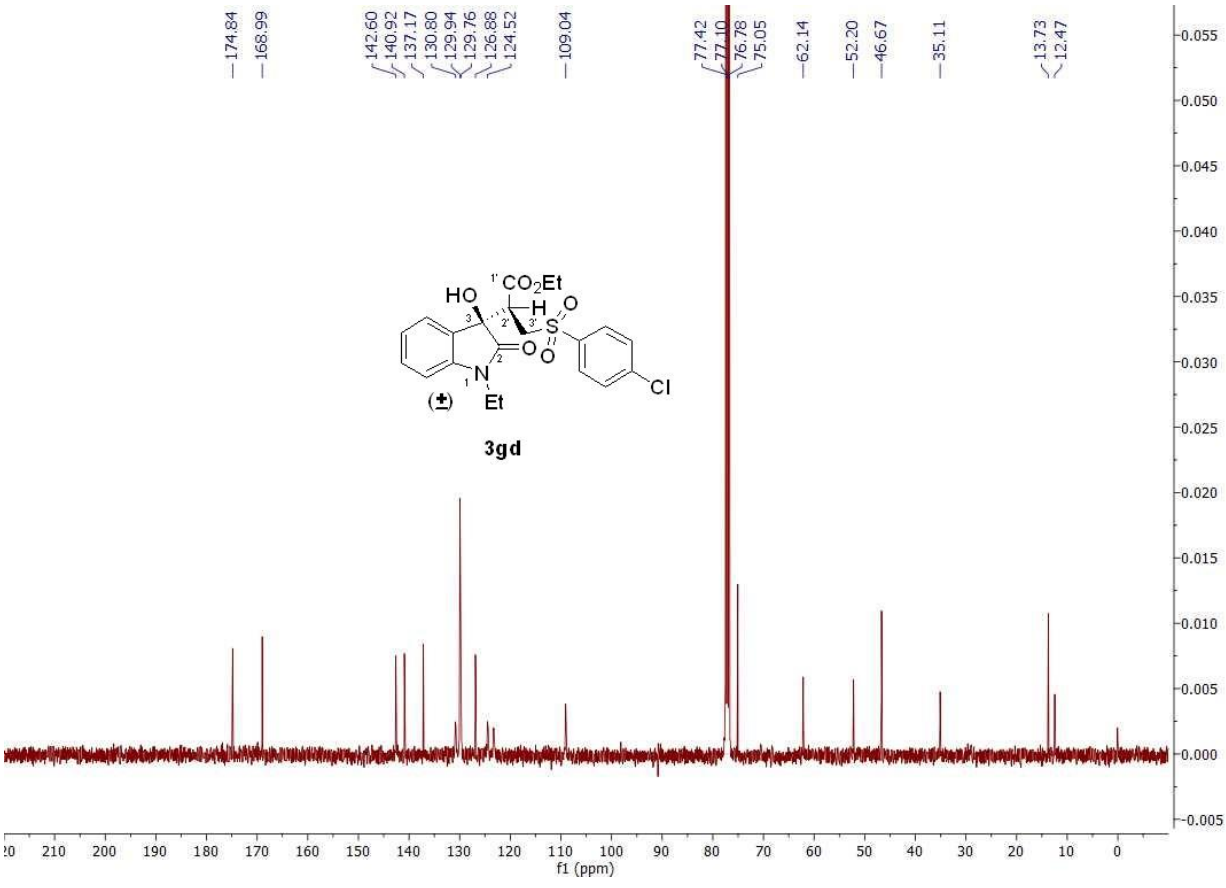
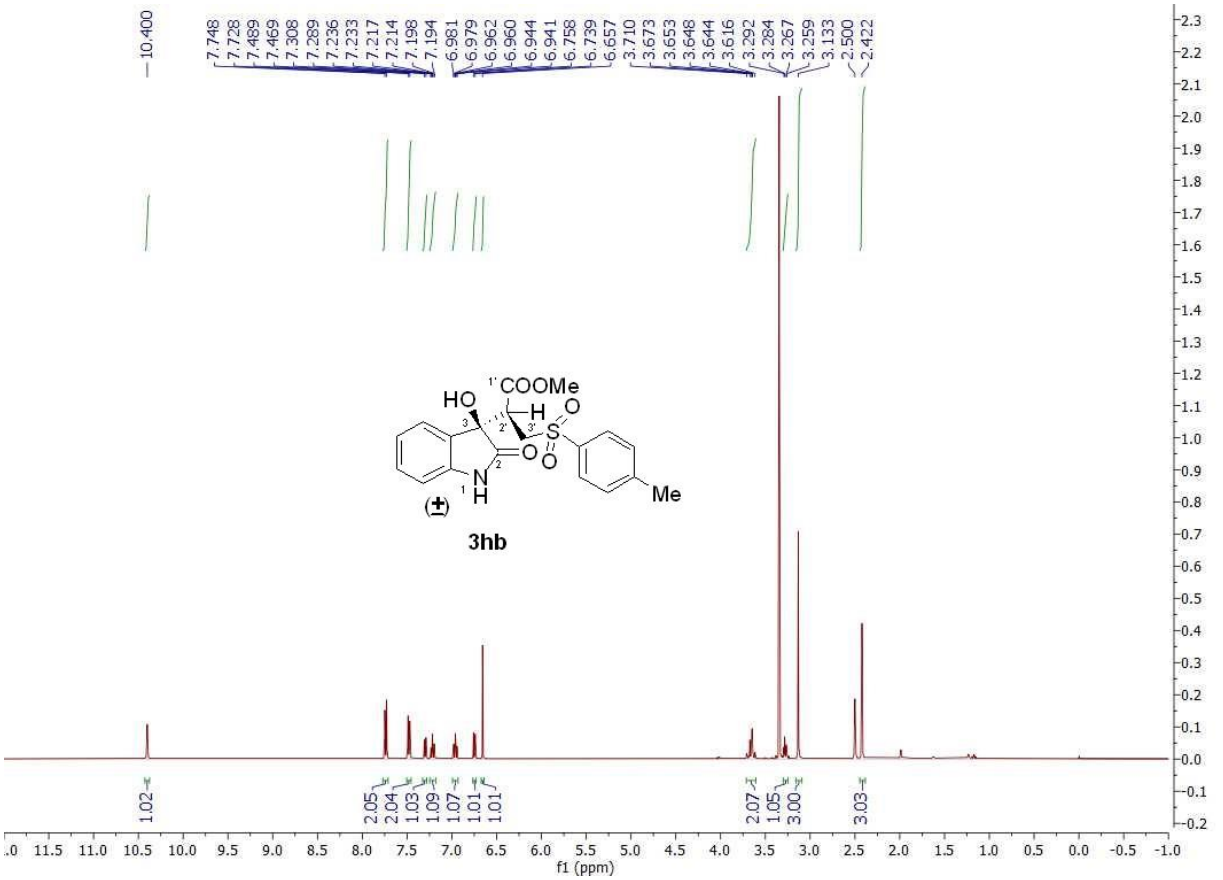
3.373
3.368
3.350
3.344
2.381
1.546
1.182
1.164
1.146
0.958
0.940
0.922
0.000
HO
1' CO2Et
O
O
O
N
Et
Me
(±)
3gb
2.00
3.09
1.01
1.00
1.03
3.00
2.10
2.04
1.03
3.15
3.33
2.90
f1 (ppm)


174.93
169.10
145.15
142.70
135.75
130.70
130.06
128.48
126.98
124.51
123.16
108.93
77.42
77.10
76.78
75.14
62.02
52.16
46.71
35.06
21.73
13.71
12.47
HO
1' CO2Et
O
O
O
N
Et
Me
(±)
3gb
f1 (ppm)

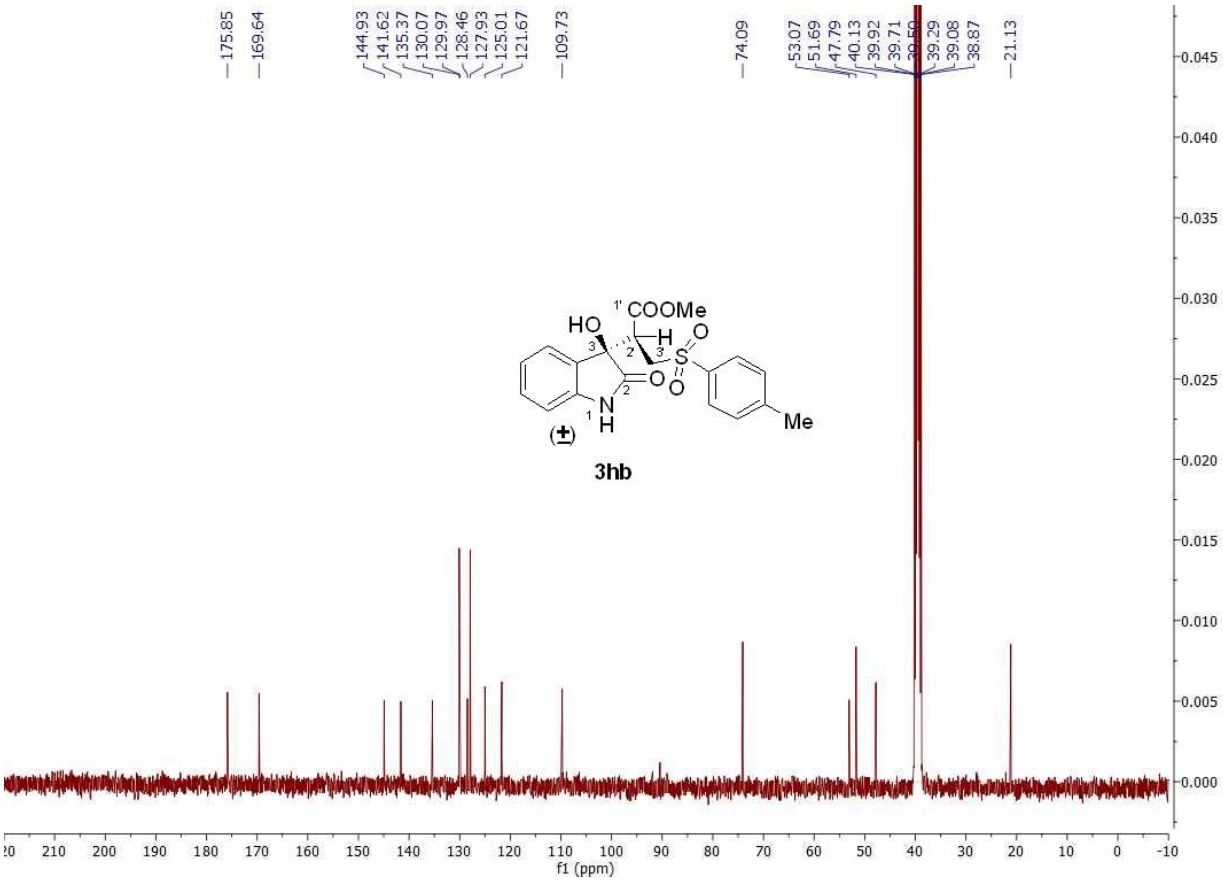

7.851
7.846
7.835
7.830
7.824
7.543
7.538
7.526
7.521
7.353
7.337
7.333
7.317
7.314
7.266
7.163
7.159
7.145
7.142
7.050
7.048
7.031
7.029
7.012
7.010
6.847
6.827
3.983
3.960
3.952
3.947
3.943
3.924
3.921
3.907
3.905
3.898
3.889
3.878
3.870
3.869
3.862
3.725
3.707
3.689
3.671
3.432
3.426
3.409
3.403
1.735
1.254
1.236
1.218
1.032
1.014
0.997
0.000
HO
CO2Et
H
O
S
O
O
N
Et
(±)
Cl
3gd
2.10
2.12
1.07
1.07
1.05
1.06
5.14
2.03
1.05
3.06
3.00
f1 (ppm)


174.84
168.99
142.60
140.92
137.17
130.80
129.94
129.76
126.88
124.52
109.04
77.42
77.10
76.78
75.05
62.14
52.20
46.67
35.11
13.73
12.47
HO
CO2Et
H
O
S
O
O
N
Et
(±)
Cl
3gd
f1 (ppm)


10.400
7.748
7.728
7.489
7.469
7.308
7.289
7.236
7.233
7.217
7.214
7.198
7.194
6.981
6.979
6.962
6.960
6.944
6.941
6.758
6.739
6.657
3.710
3.673
3.653
3.648
3.644
3.616
3.292
3.284
3.267
3.259
3.133
2.500
2.422
1.02
2.05
2.04
1.03
1.09
1.07
1.01
1.01
2.07
1.05
3.00
3.03
f1 (ppm)

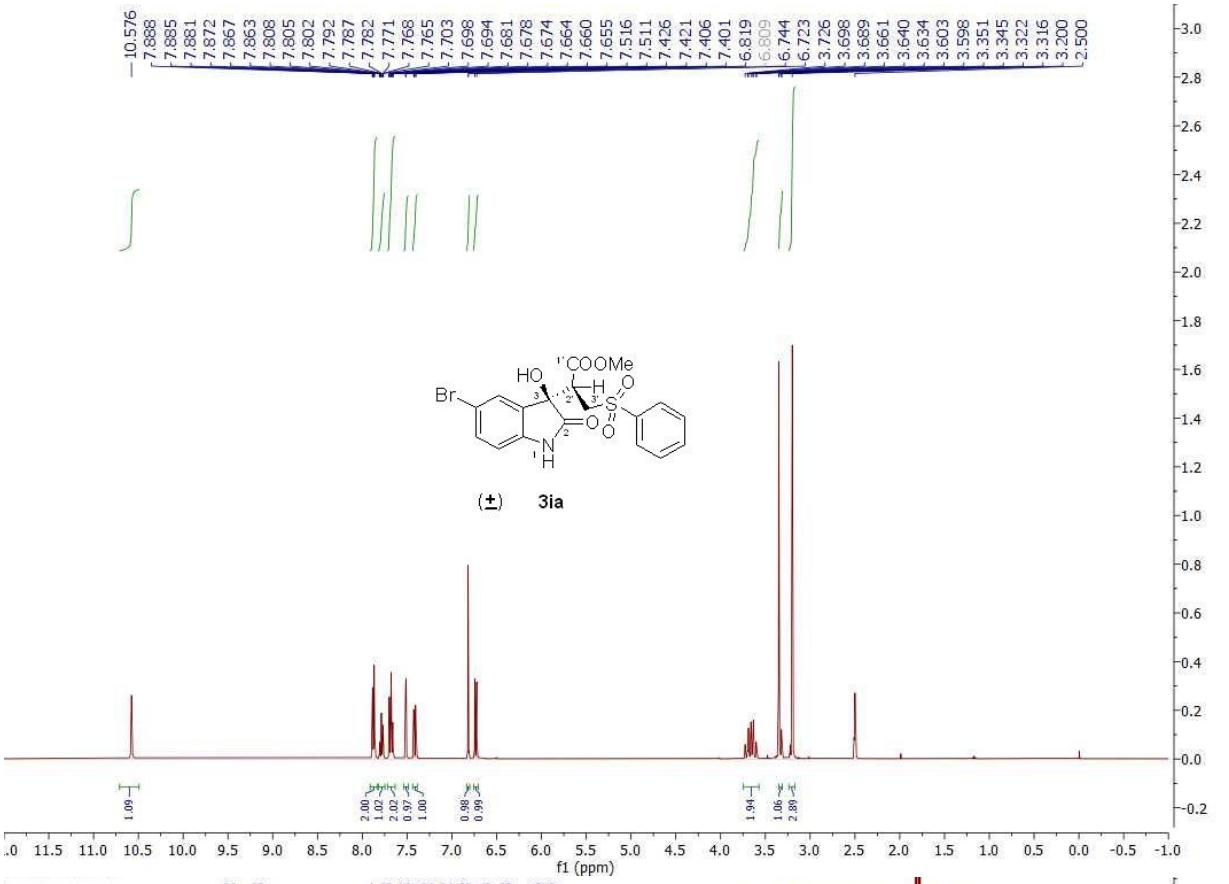
1'COOMe
HO
H
O
S
O
O
N
H
Me
(±)

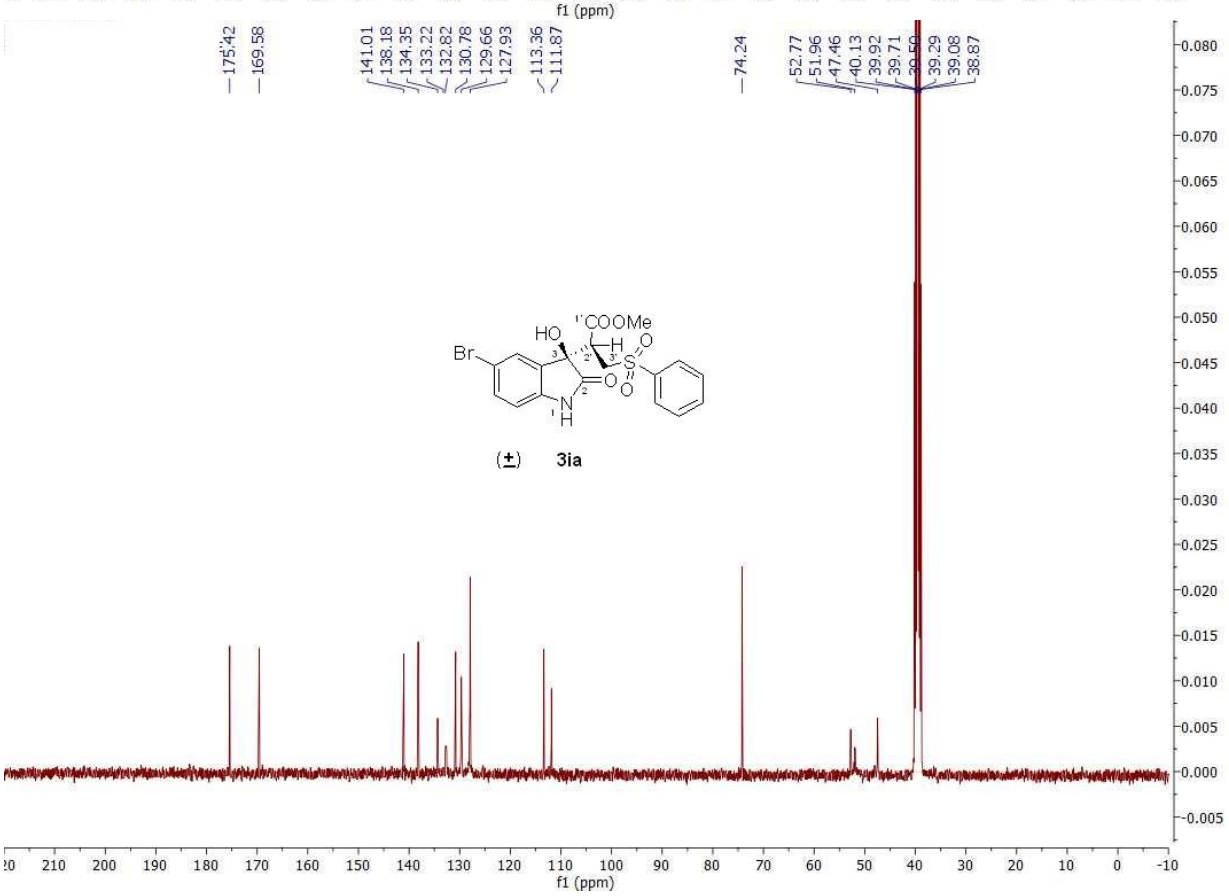
3hb

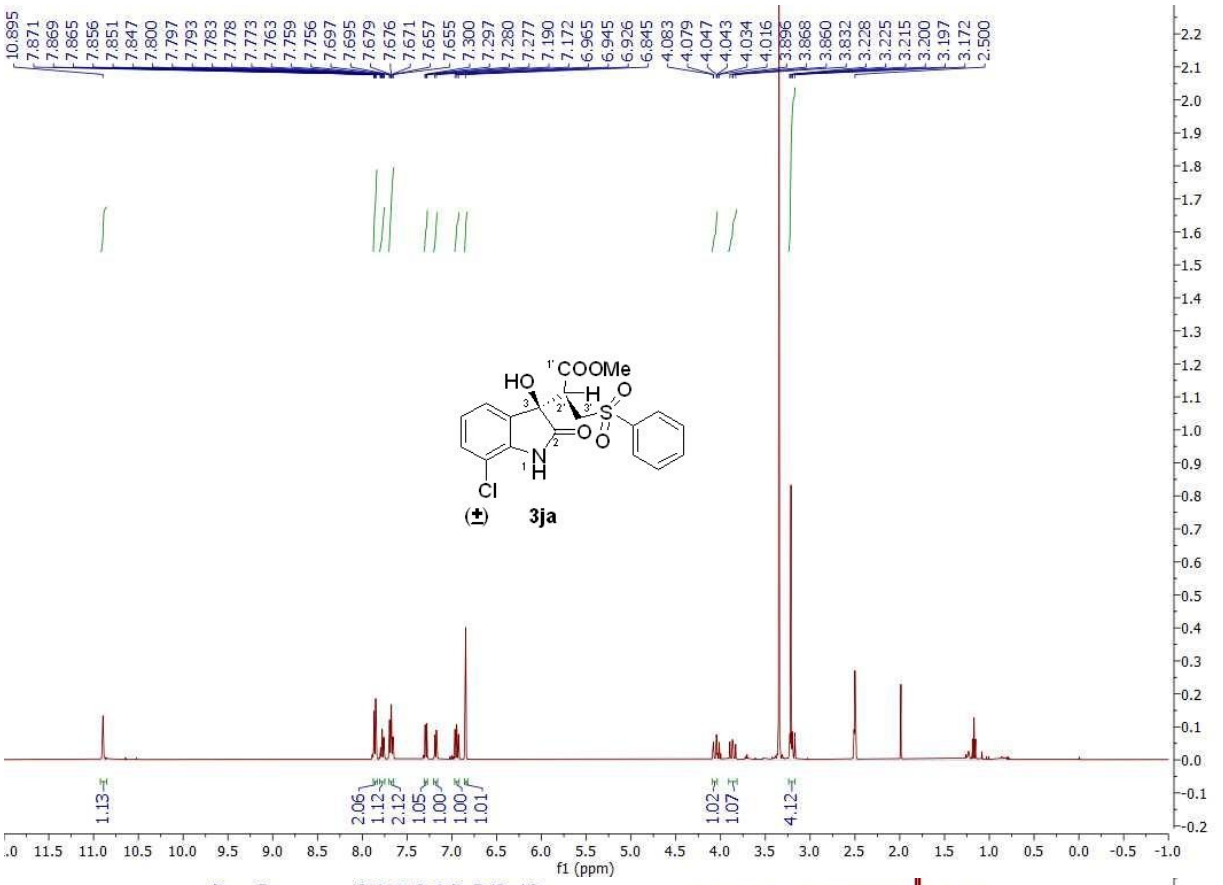

175.85
169.64
144.93
141.62
135.37
130.07
129.97
128.46
127.93
125.01
121.67
109.73
74.09
53.07
51.69
47.79
40.13
39.92
39.71
39.50
39.29
39.08
38.87
21.13
f1 (ppm)

1'COOMe
HO
H
O
S
O
O
N
H
Me
(±)

3hb

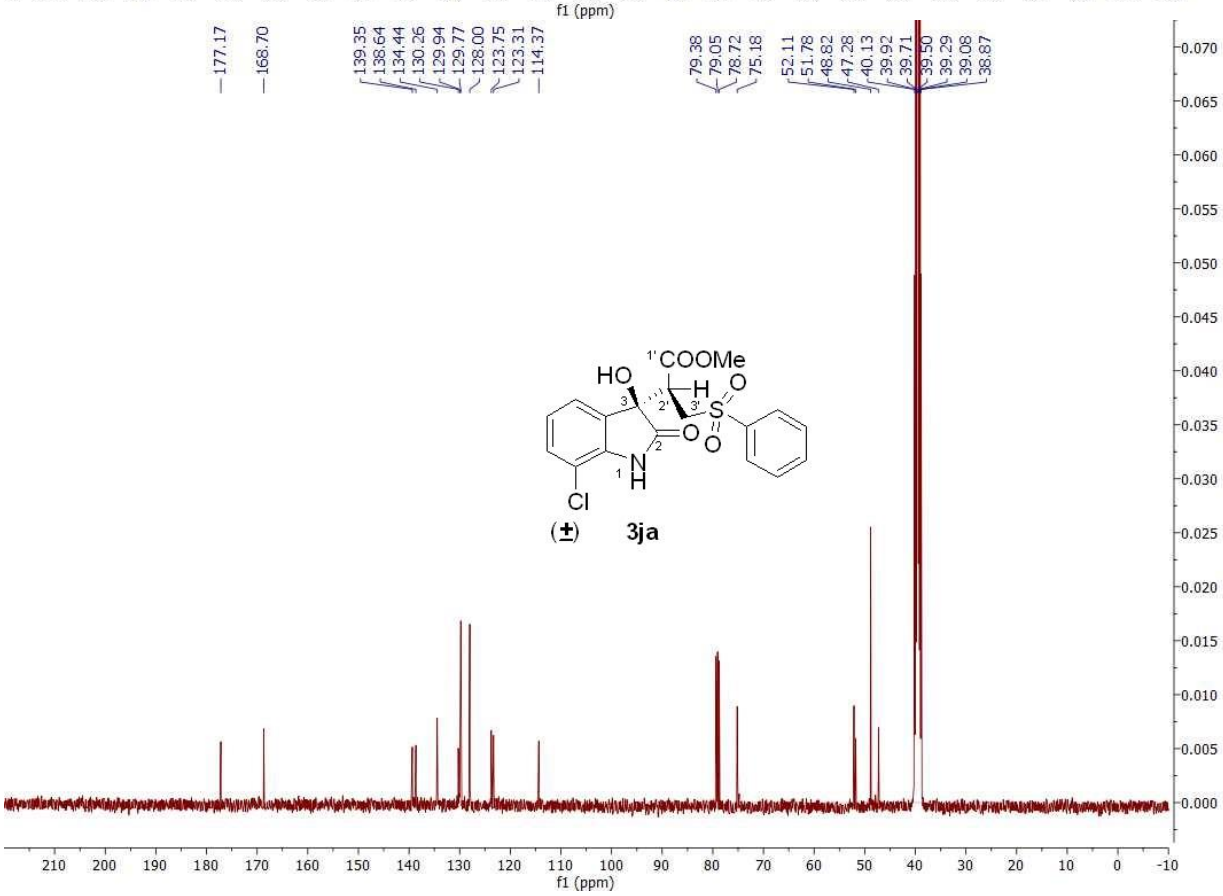

10.576
7.888
7.885
7.881
7.872
7.867
7.863
7.808
7.805
7.802
7.792
7.787
7.782
7.771
7.768
7.765
7.703
7.698
7.694
7.681
7.678
7.674
7.664
7.660
7.655
7.516
7.511
7.426
7.421
7.406
7.401
6.819
6.809
6.744
6.723
3.726
3.698
3.689
3.661
3.640
3.634
3.603
3.598
3.351
3.345
3.322
3.316
3.200
2.500
HO
COOMe
Br
O
S
N
H
(±) 3ia
f1 (ppm)


175.42
169.58
141.01
138.18
134.35
133.22
132.82
130.78
129.66
127.93
113.36
111.87
74.24
52.77
51.96
47.46
40.13
39.92
39.71
39.50
39.29
39.08
38.87
HO
COOMe
Br
O
S
N
H
(±) 3ia
f1 (ppm)


10.895
7.871
7.869
7.865
7.856
7.851
7.847
7.800
7.797
7.793
7.783
7.778
7.773
7.763
7.759
7.756
7.697
7.695
7.679
7.676
7.671
7.657
7.655
7.300
7.297
7.280
7.277
7.190
7.172
6.965
6.945
6.926
6.845
4.083
4.079
4.047
4.043
4.034
4.016
3.896
3.868
3.860
3.832
3.228
3.225
3.215
3.200
3.197
3.172
2.500
1.13
2.06
1.12
2.12
1.05
1.00
1.00
1.01
1.02
1.07
4.12
f1 (ppm)

HO
1'COOMe
H
O
S
O
O
N
H
Cl

(±) **3ja**

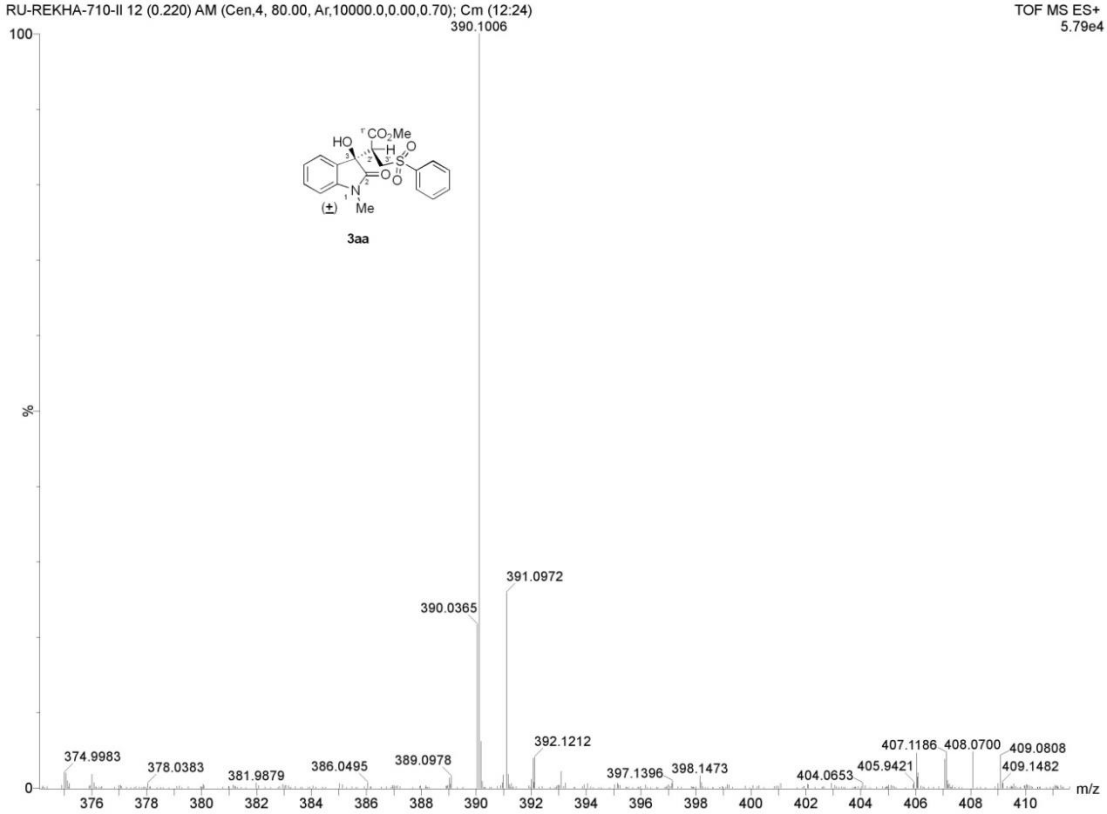

177.17
168.70
139.35
138.64
134.44
130.26
129.94
129.77
128.00
123.75
123.31
114.37
79.38
79.05
78.72
75.18
52.11
51.78
48.82
47.28
40.13
39.92
39.71
39.50
39.29
39.08
38.87
f1 (ppm)

HO
1'COOMe
H
O
S
O
O
N
H
Cl

(±) **3ja**

RU-REKHA-710-II 12 (0.220) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.70); Cm (12:24)

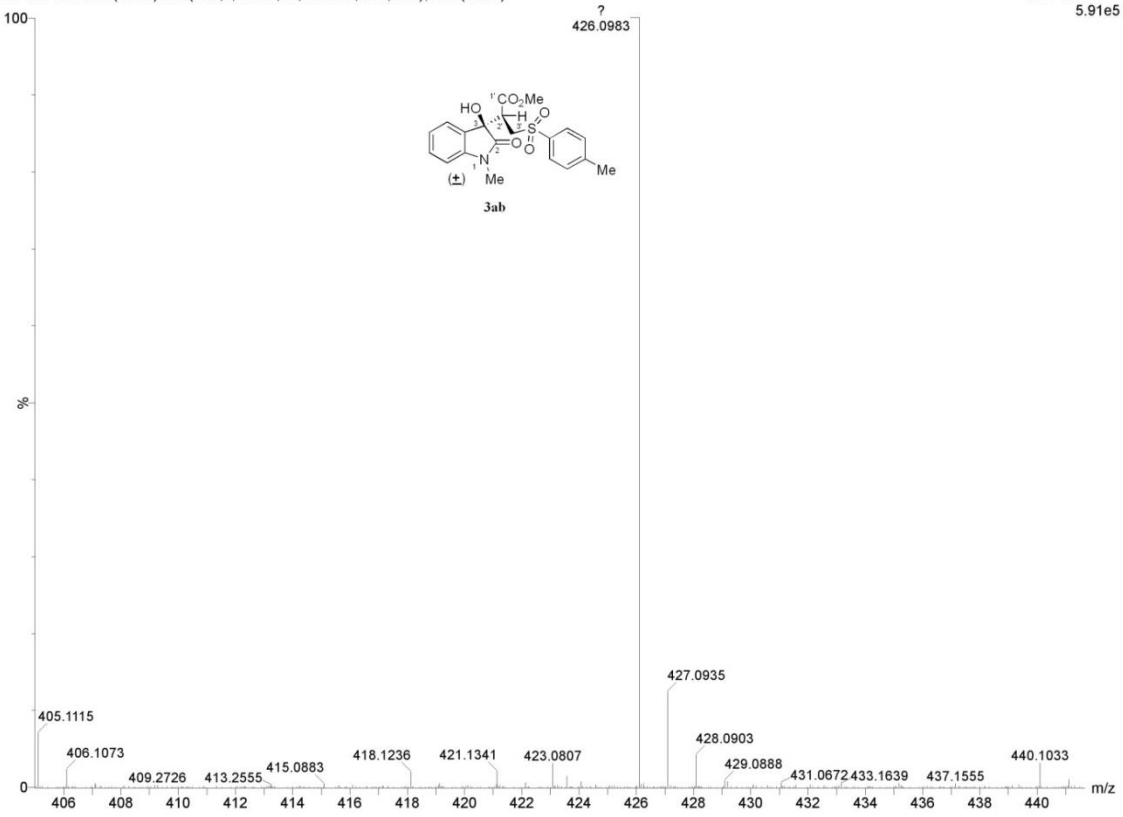
TOF MS ES+
5.79e4



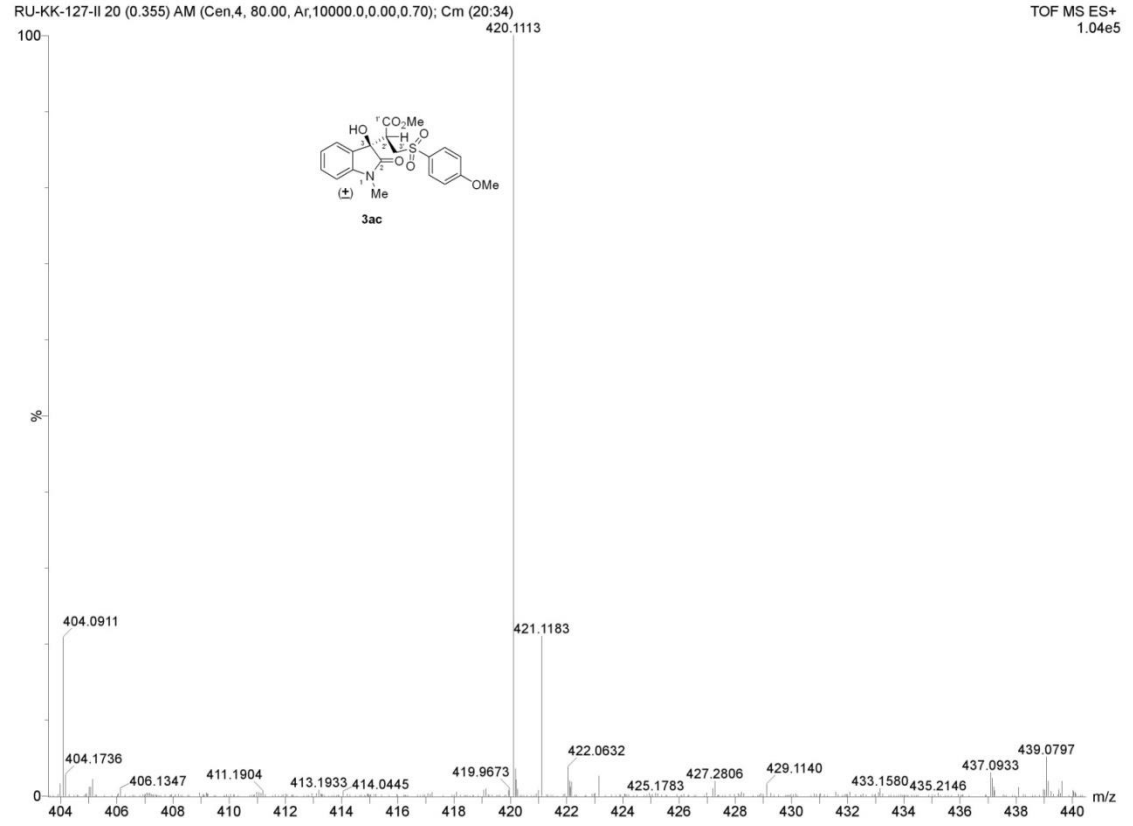
3aa

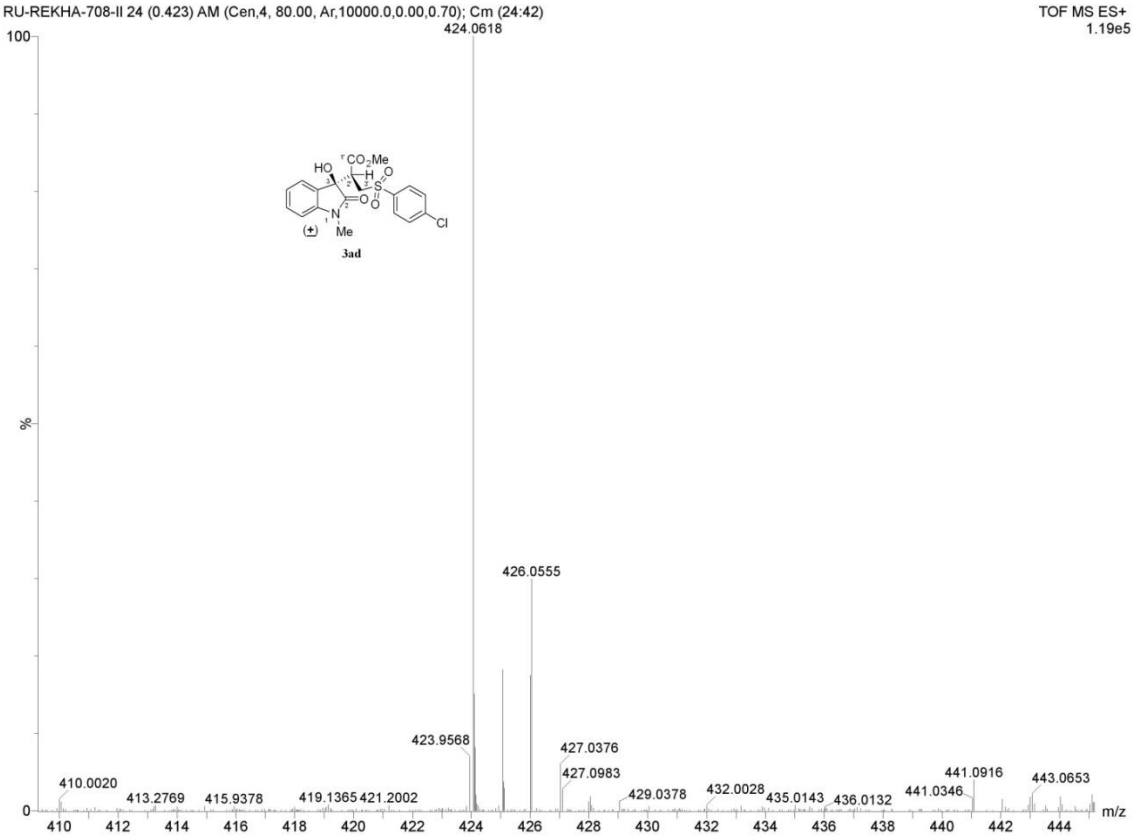
RU-KK-161-II 12 (0.220) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.70); Cm (12:27)

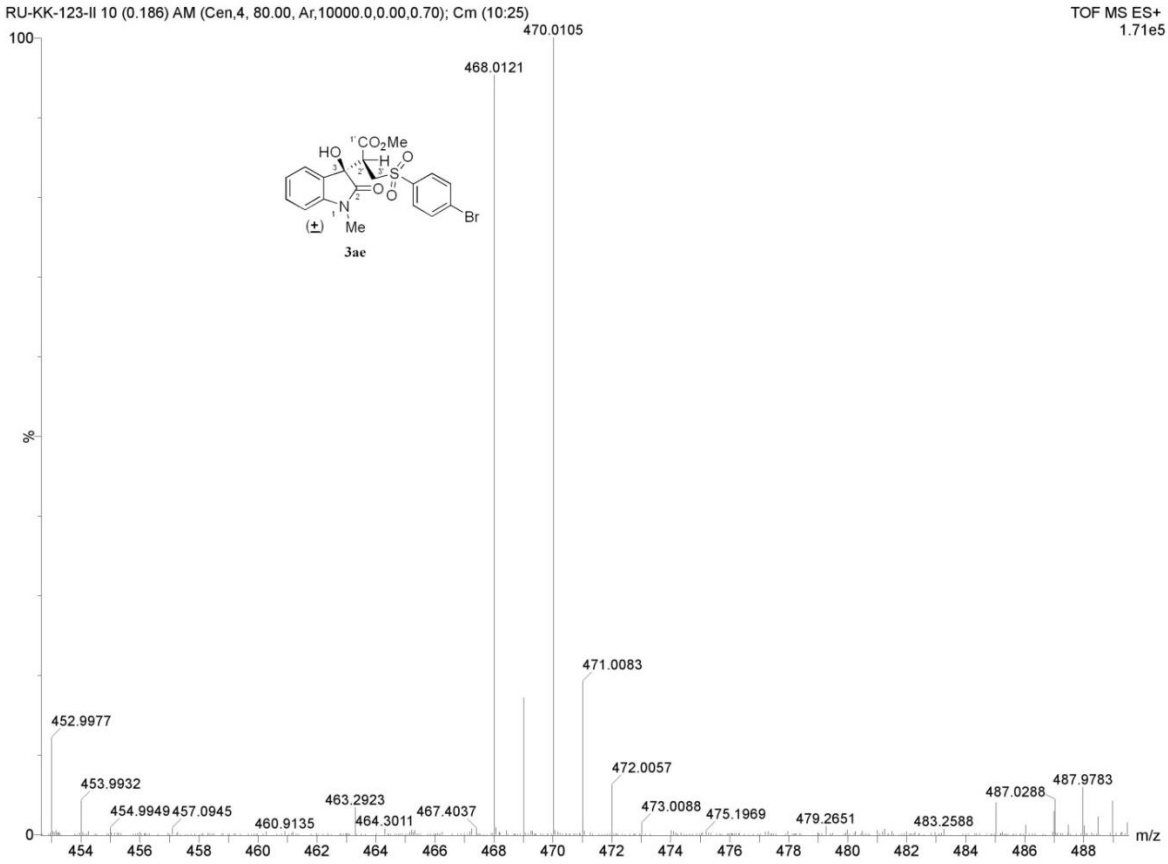
TOF MS ES+
5.91e5

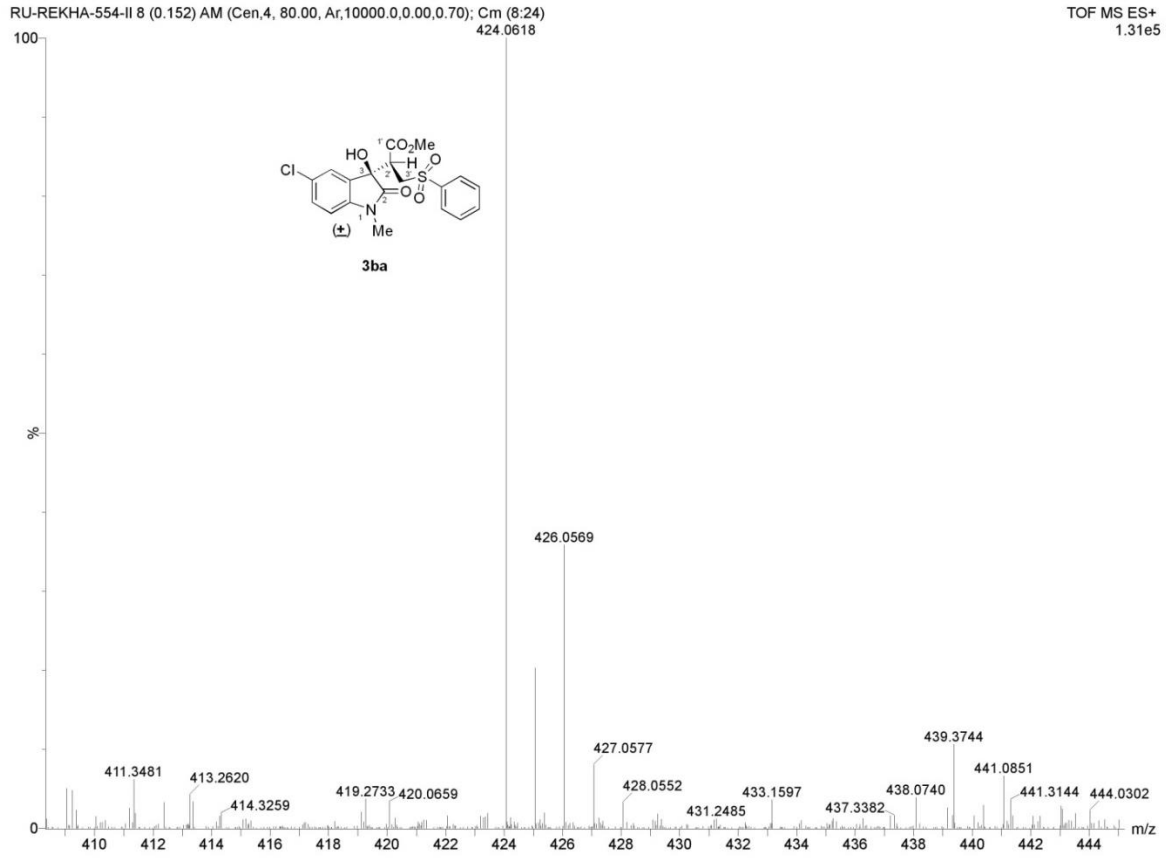


3ab


RU-KK-127-II 20 (0.355) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.70); Cm (20:34)
TOF MS ES+
1.04e5
100
%
0
420.1113
404.0911
421.1183
404.1736
406.1347
411.1904
413.1933
414.0445
419.9673
422.0632
425.1783
427.2806
429.1140
433.1580
435.2146
437.0933
439.0797
404
406
408
410
412
414
416
418
420
422
424
426
428
430
432
434
436
438
440
m/z
3ac

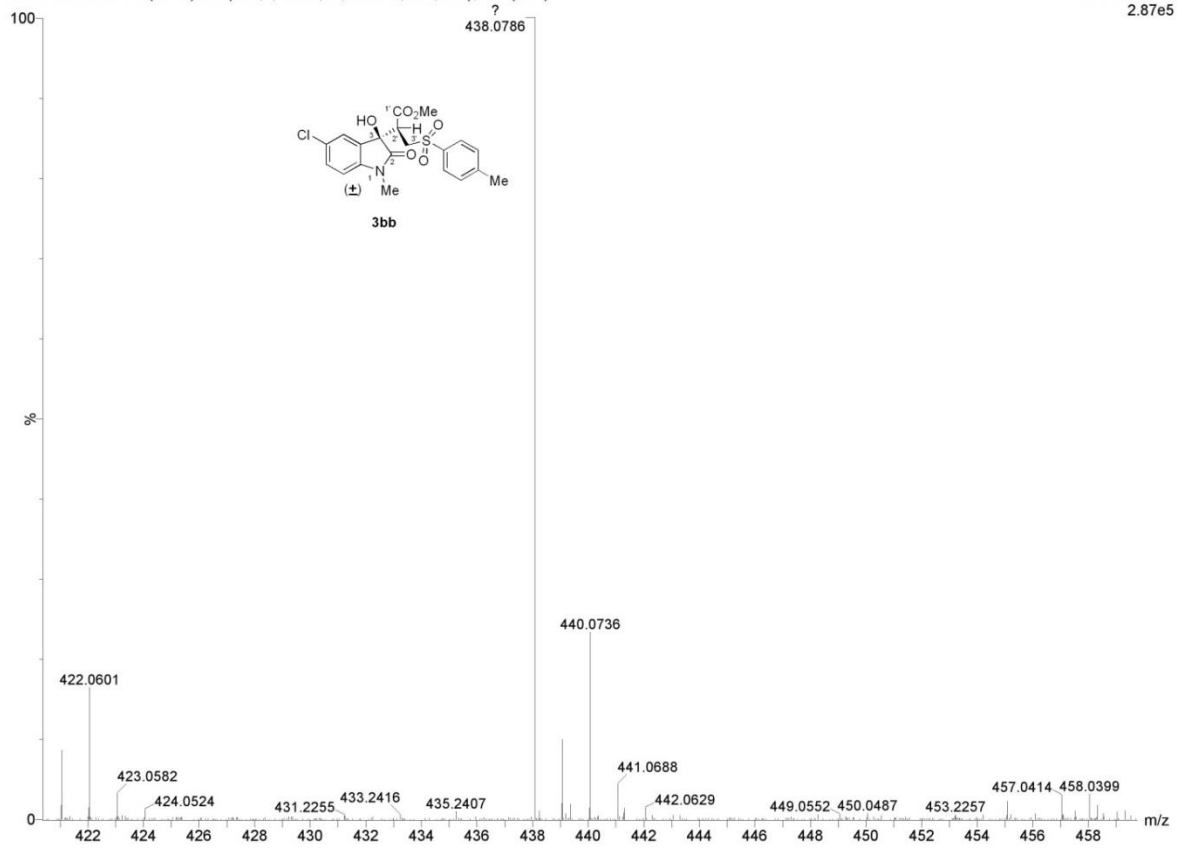

RU-REKHA-708-II 24 (0.423) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.70); Cm (24:42)
TOF MS ES+
1.19e5
100
%
0
424.0618
426.0555
423.9568
427.0376
427.0983
410.0020
413.2769
415.9378
419.1365
421.2002
429.0378
432.0028
435.0143
436.0132
441.0346
441.0916
443.0653
410
412
414
416
418
420
422
424
426
428
430
432
434
436
438
440
442
444
m/z
3ad


RU-KK-123-II 10 (0.186) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.70); Cm (10:25)
TOF MS ES+
1.71e5
100
%
0
470.0105
468.0121
471.0083
452.9977
472.0057
453.9932
487.9783
487.0288
454.9949
457.0945
463.2923
464.3011
467.4037
460.9135
473.0088
475.1969
479.2651
483.2588
454
456
458
460
462
464
466
468
470
472
474
476
478
480
482
484
486
488
m/z
HO
CO2Me
Br
Me
(±)
3ae


RU-REKHA-554-II 8 (0.152) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.70); Cm (8:24)
TOF MS ES+
1.31e5
100
%
0
424.0618
426.0569
427.0577
439.3744
411.3481
441.0851
413.2620
428.0552
438.0740
441.3144
444.0302
419.2733
420.0659
433.1597
414.3259
431.2485
437.3382
410
412
414
416
418
420
422
424
426
428
430
432
434
436
438
440
442
444
m/z
HO
CO2Me
Cl
Me
(±)
3ba

RU-REKHA-596-II 7 (0.135) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.70); Cm (7:12)

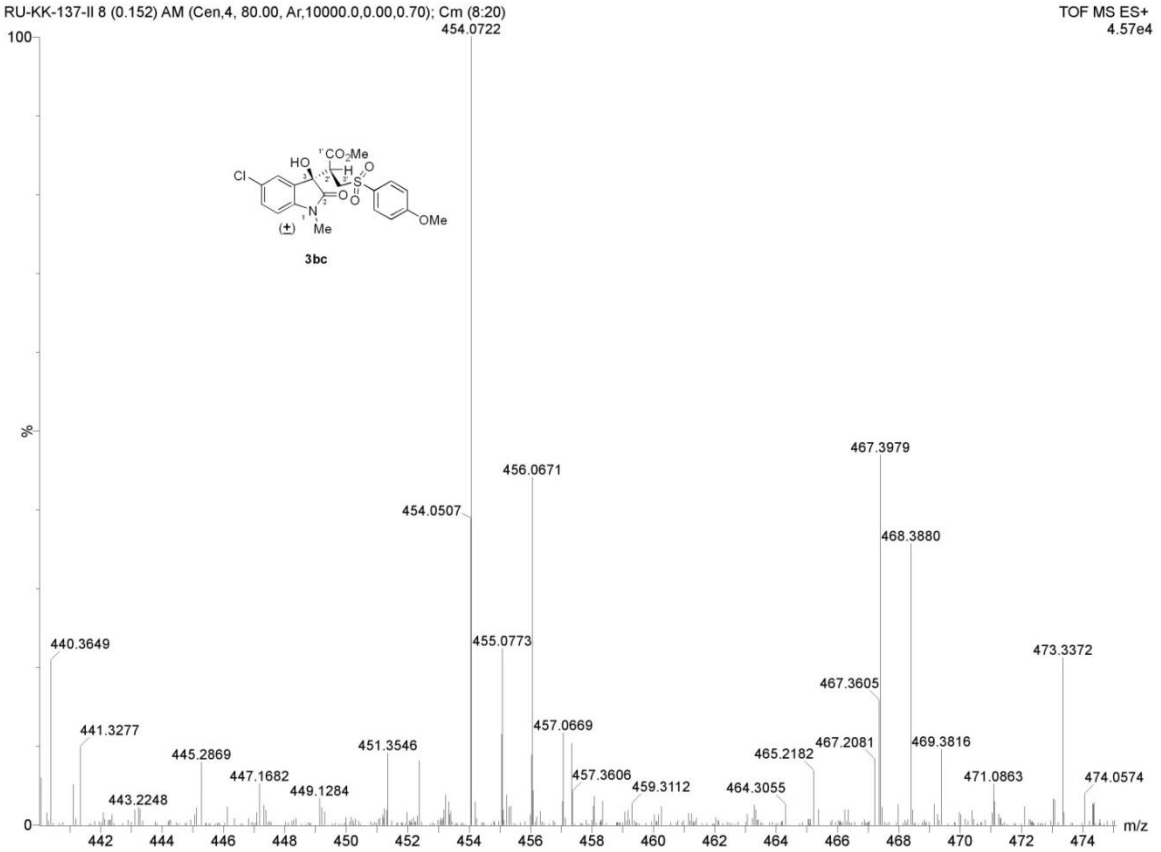
TOF MS ES+
2.87e5



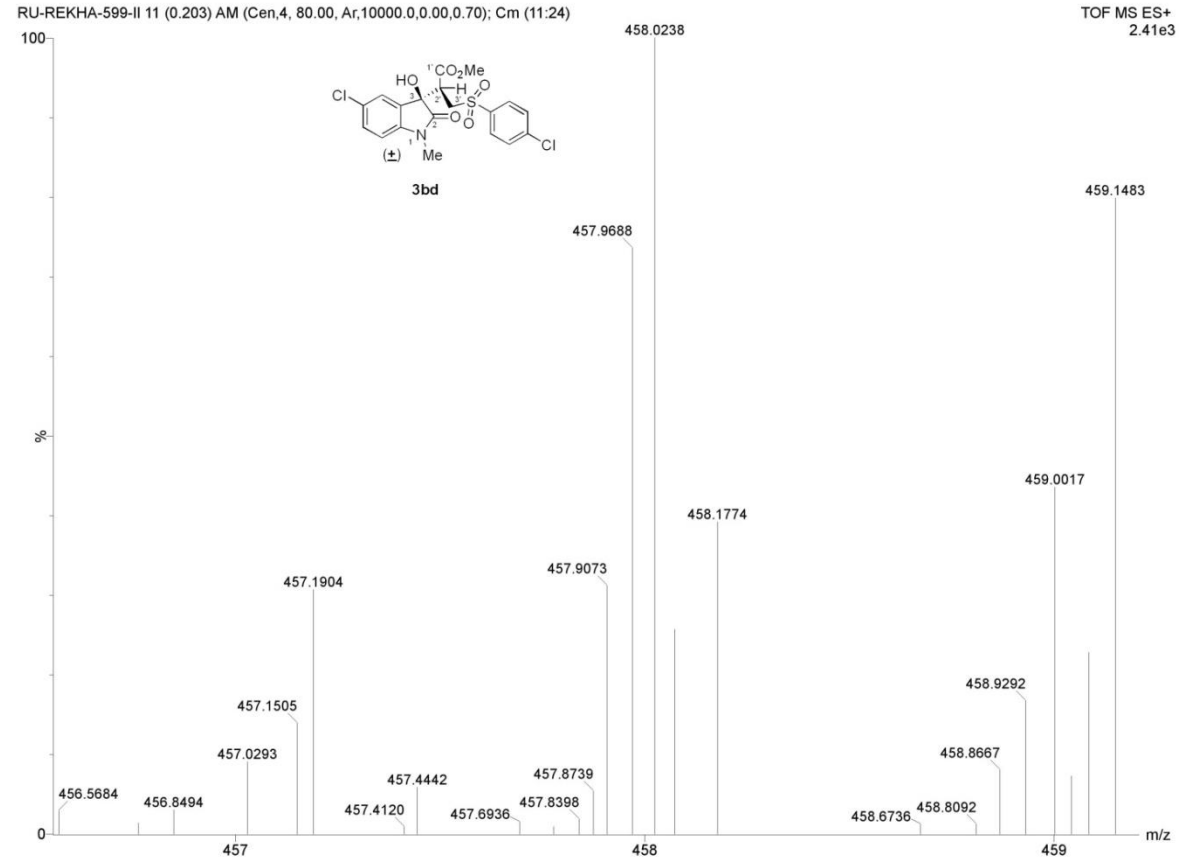
3bb

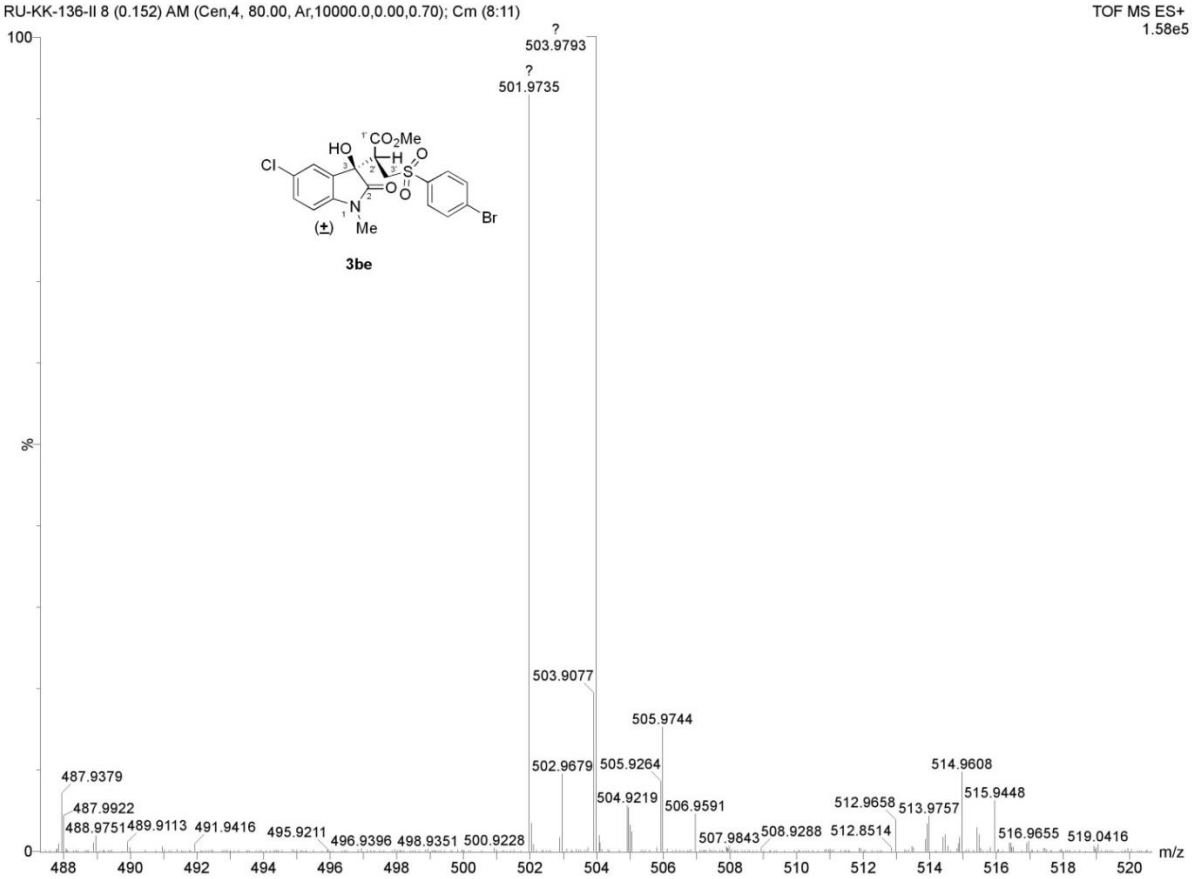
RU-KK-137-II 8 (0.152) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.70); Cm (8:20)

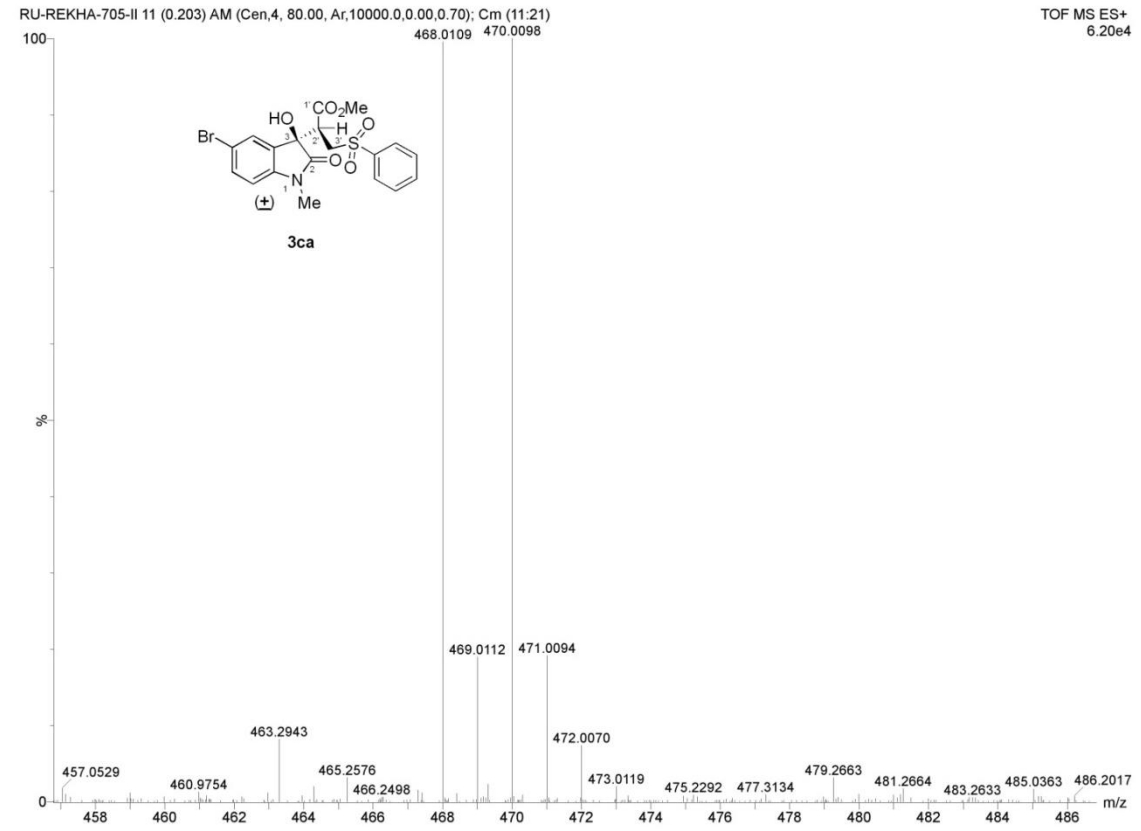
TOF MS ES+
4.57e4

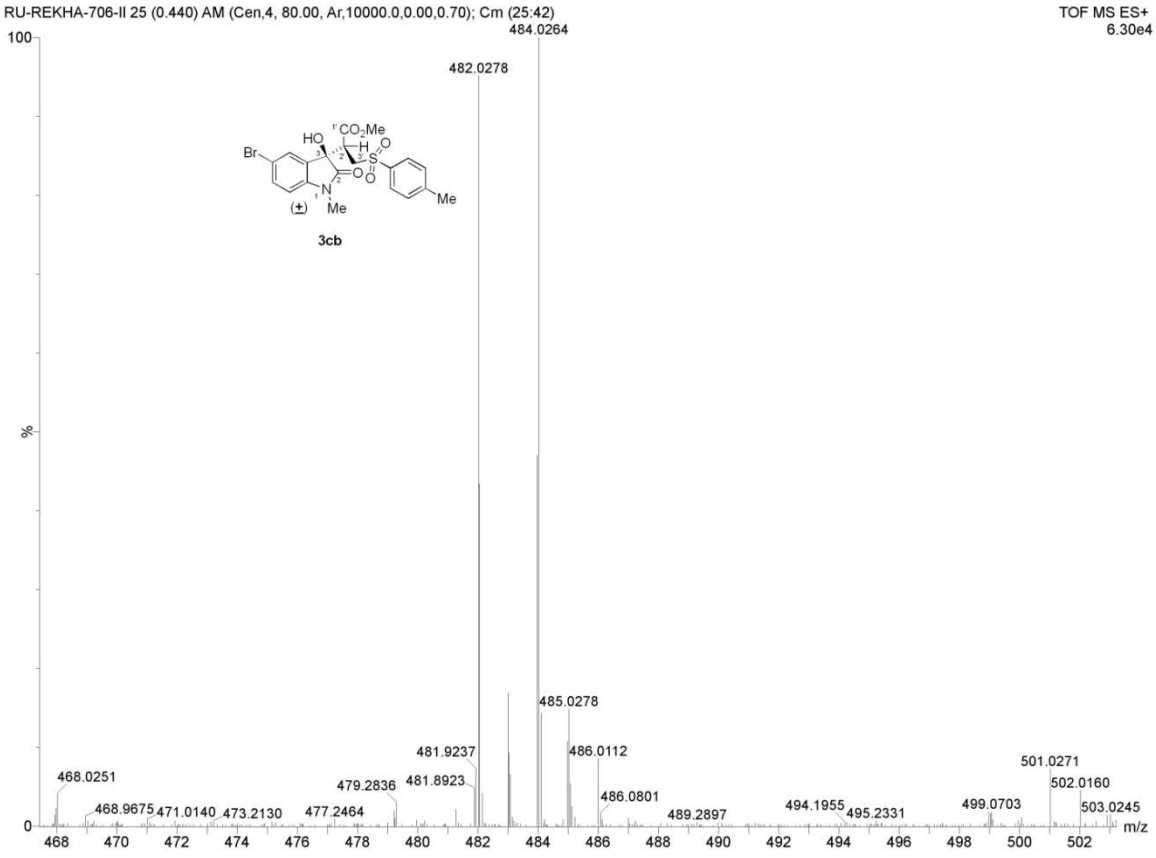


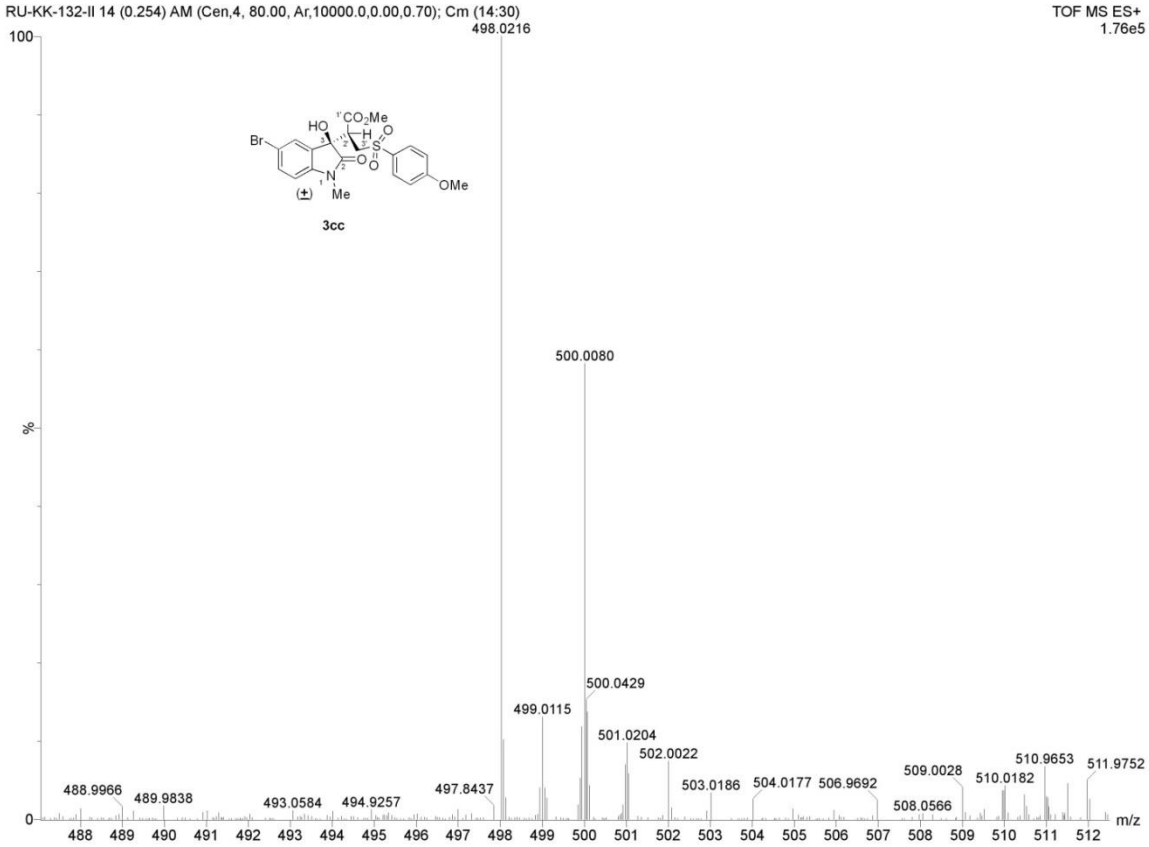
3bc

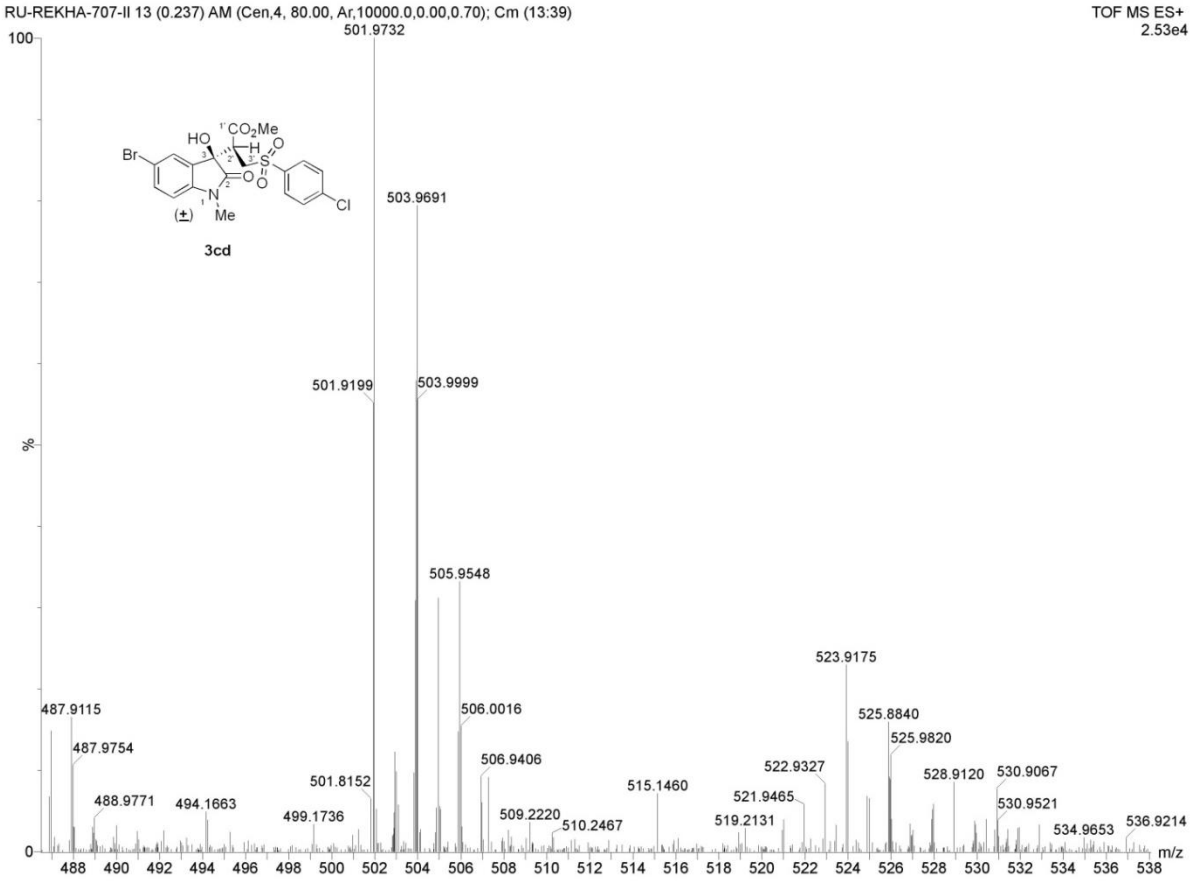

RU-REKHA-599-II 11 (0.203) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.70); Cm (11:24)
TOF MS ES+
2.41e3
100
%
0
458.0238
459.1483
457.9688
459.0017
458.1774
457.9073
457.1904
458.9292
457.1505
458.8667
457.0293
457.4442
457.8739
456.5684
456.8494
457.4120
457.6936
457.8398
458.6736
458.8092
457
458
459
m/z
3bd


RU-KK-136-II 8 (0.152) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.70); Cm (8:11)
TOF MS ES+
1.58e5
100
%
0
503.9793
501.9735
503.9077
505.9744
502.9679
505.9264
514.9608
487.9379
504.9219
506.9591
515.9448
487.9922
512.9658
513.9757
488.9751
489.9113
491.9416
495.9211
496.9396
498.9351
500.9228
507.9843
508.9288
512.8514
516.9655
519.0416
488
490
492
494
496
498
500
502
504
506
508
510
512
514
516
518
520
m/z
3be


RU-REKHA-705-II 11 (0.203) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.70); Cm (11:21)
TOF MS ES+
6.20e4
100
%
0
468.0109
470.0098
469.0112
471.0094
463.2943
472.0070
457.0529
460.9754
465.2576
466.2498
473.0119
475.2292
477.3134
479.2663
481.2664
483.2633
485.0363
486.2017
m/z
458
460
462
464
466
468
470
472
474
476
478
480
482
484
486
HO
CO2Me
H
Br
O
S
O
O
N
Me
(±)
3ca

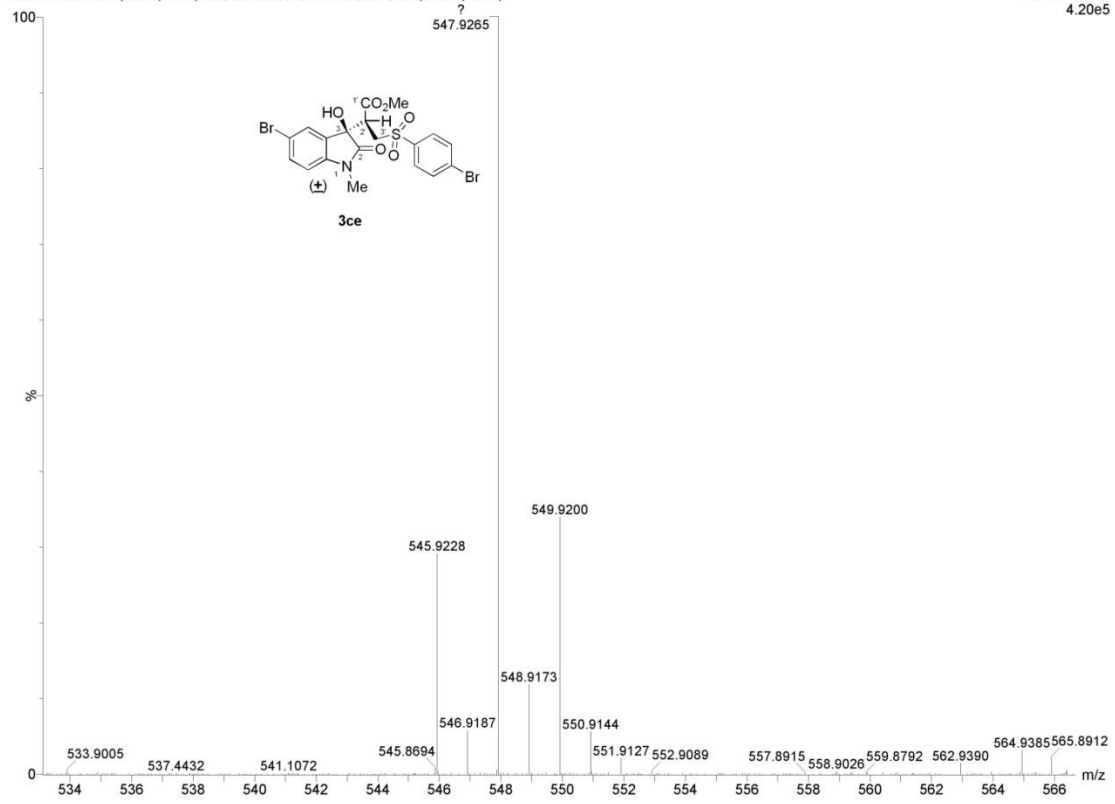

RU-REKHA-706-II 25 (0.440) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.70); Cm (25:42)
TOF MS ES+
6.30e4
100
%
0
484.0264
482.0278
485.0278
481.9237
486.0112
468.0251
481.8923
479.2836
501.0271
502.0160
486.0801
468.9675
471.0140
473.2130
477.2464
489.2897
494.1955
495.2331
499.0703
503.0245
m/z
468
470
472
474
476
478
480
482
484
486
488
490
492
494
496
498
500
502
HO
CO2Me
H
Br
O
S
O
O
N
Me
Me
(±)
3cb


RU-KK-132-II 14 (0.254) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.70); Cm (14:30)
TOF MS ES+
1.76e5
3cc
498.0216
500.0080
500.0429
499.0115
501.0204
502.0022
503.0186
504.0177
506.9692
509.0028
510.0182
510.9653
511.9752
488.9966
489.9838
493.0584
494.9257
497.8437
508.0566
m/z


RU-REKHA-707-II 13 (0.237) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.70); Cm (13:39)
TOF MS ES+
2.53e4
3cd
501.9732
503.9691
501.9199
503.9999
505.9548
523.9175
487.9115
506.0016
525.8840
525.9820
487.9754
506.9406
522.9327
528.9120
530.9067
501.8152
515.1460
521.9465
488.9771
494.1663
499.1736
509.2220
510.2467
519.2131
530.9521
534.9653
536.9214
m/z

RU-KK-124-II 11 (0.203) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.70); Cm (11:22)

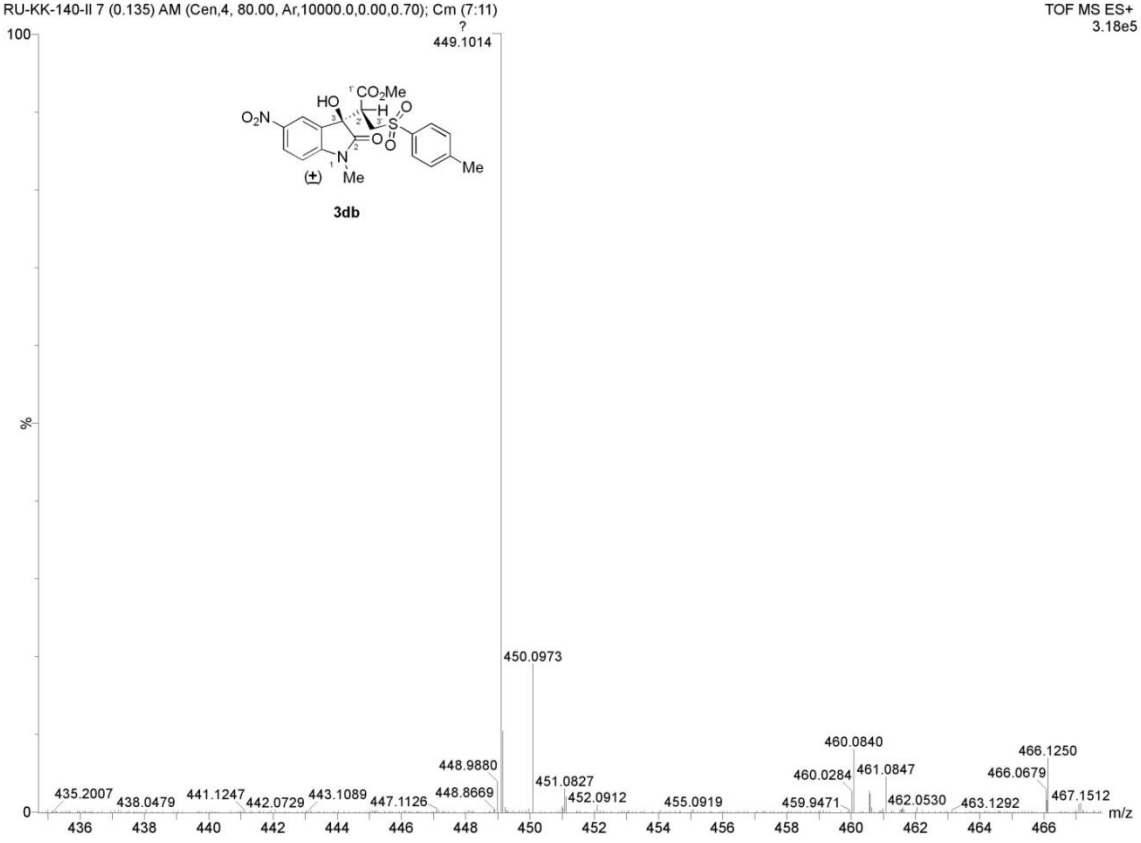
TOF MS ES+
4.20e5



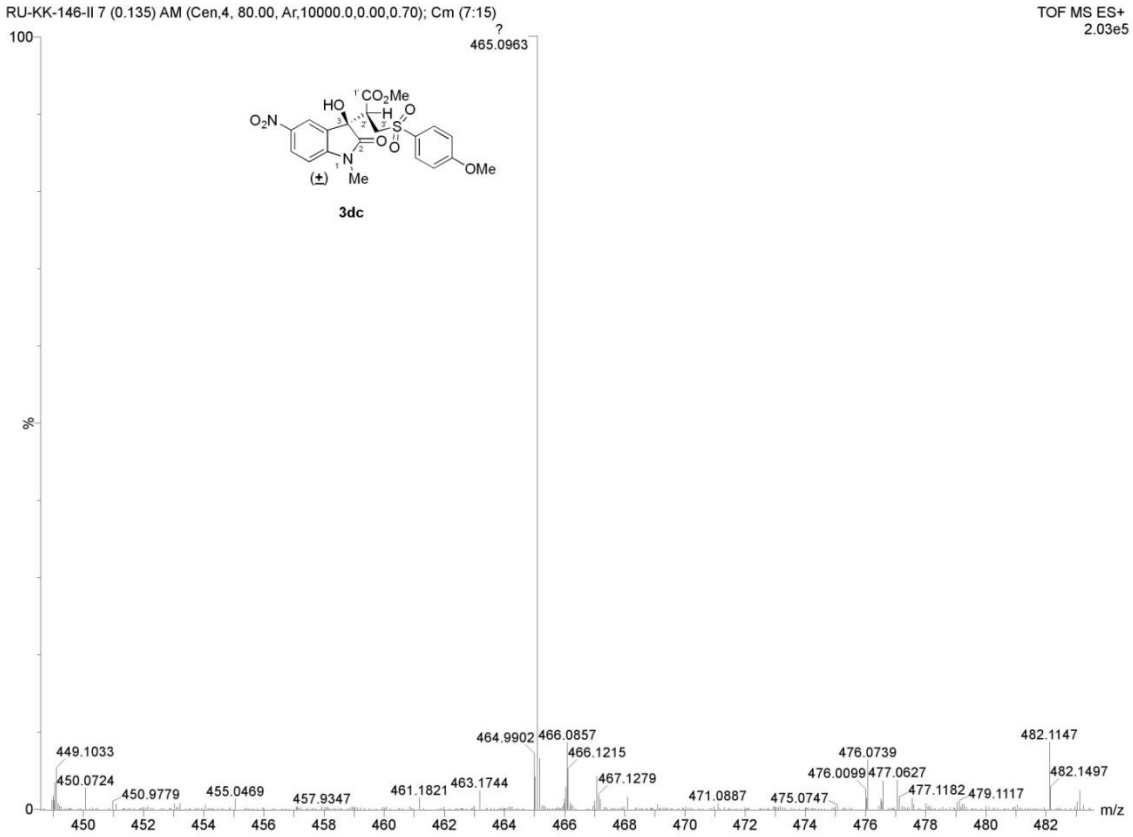
3ce

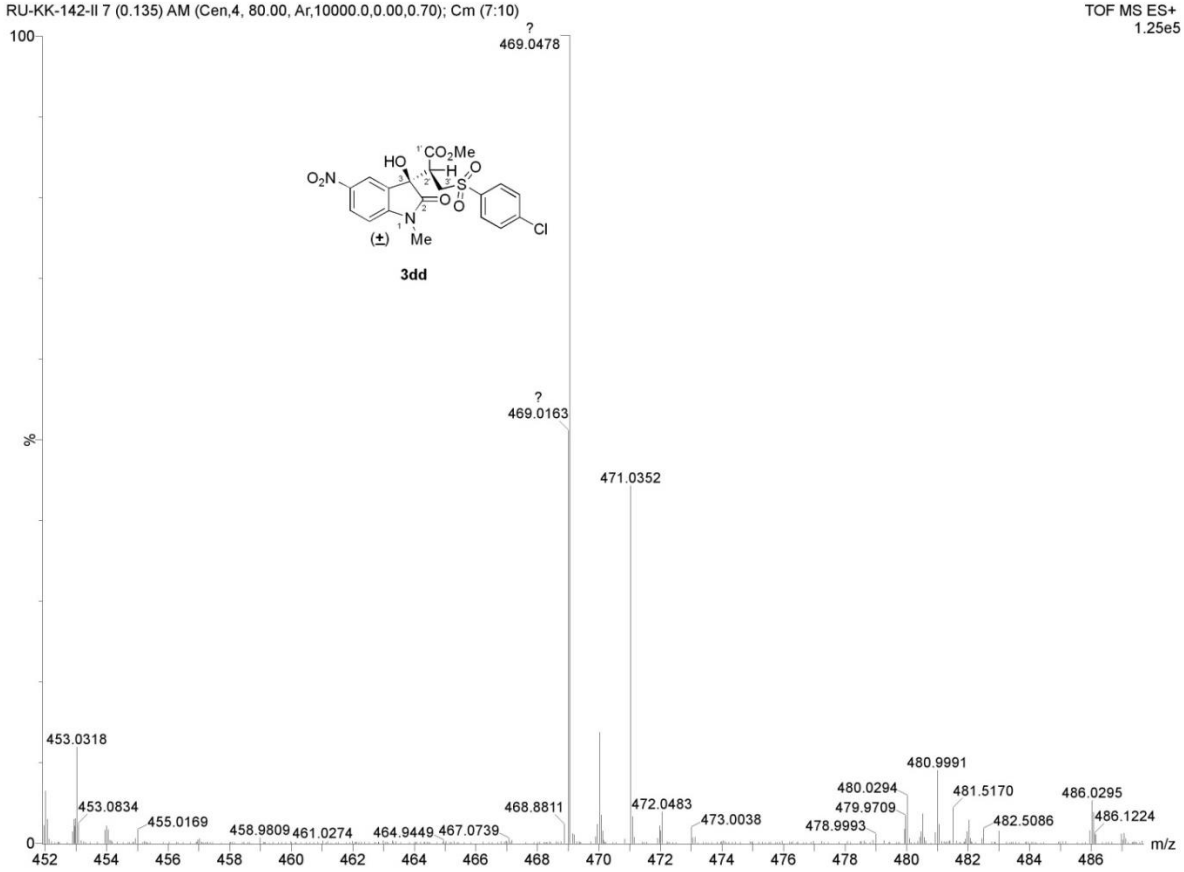
RU-KK-140-II 7 (0.135) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.70); Cm (7:11)

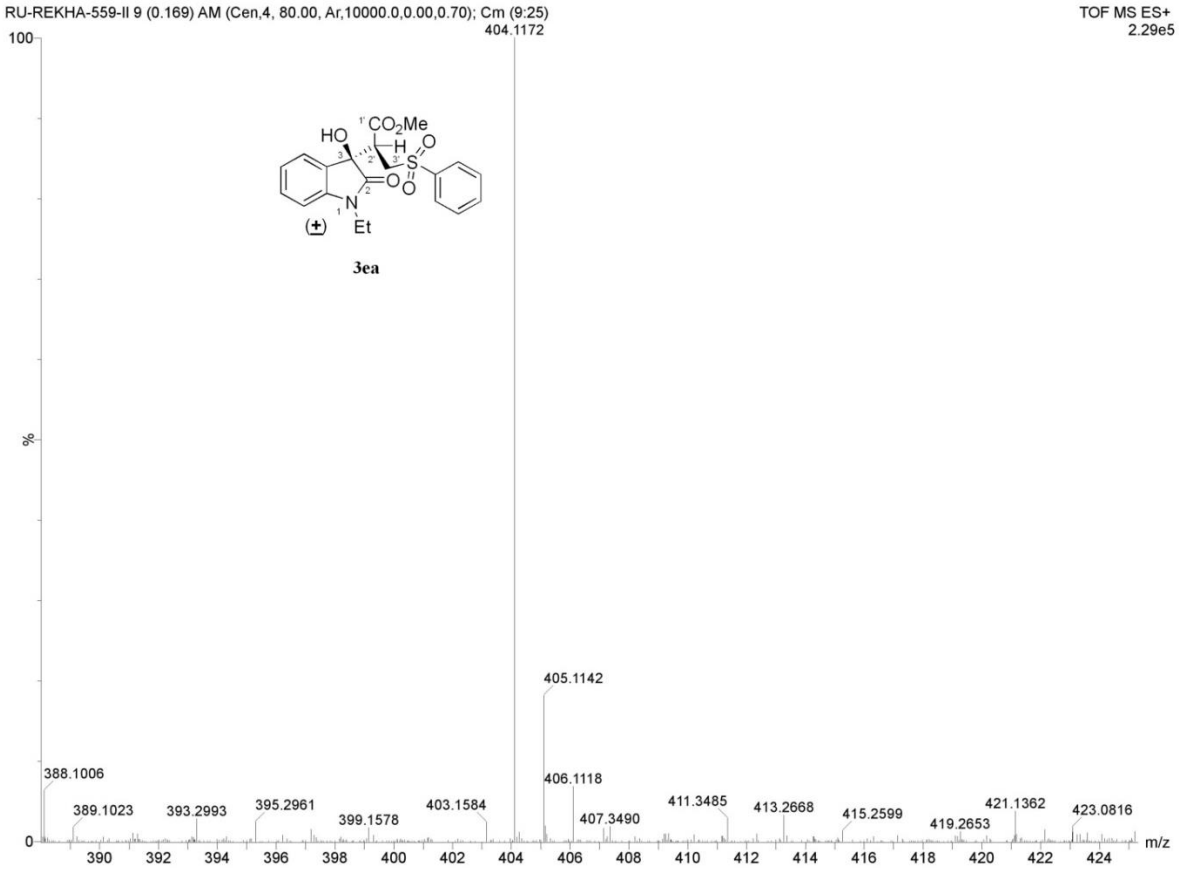
TOF MS ES+
3.18e5

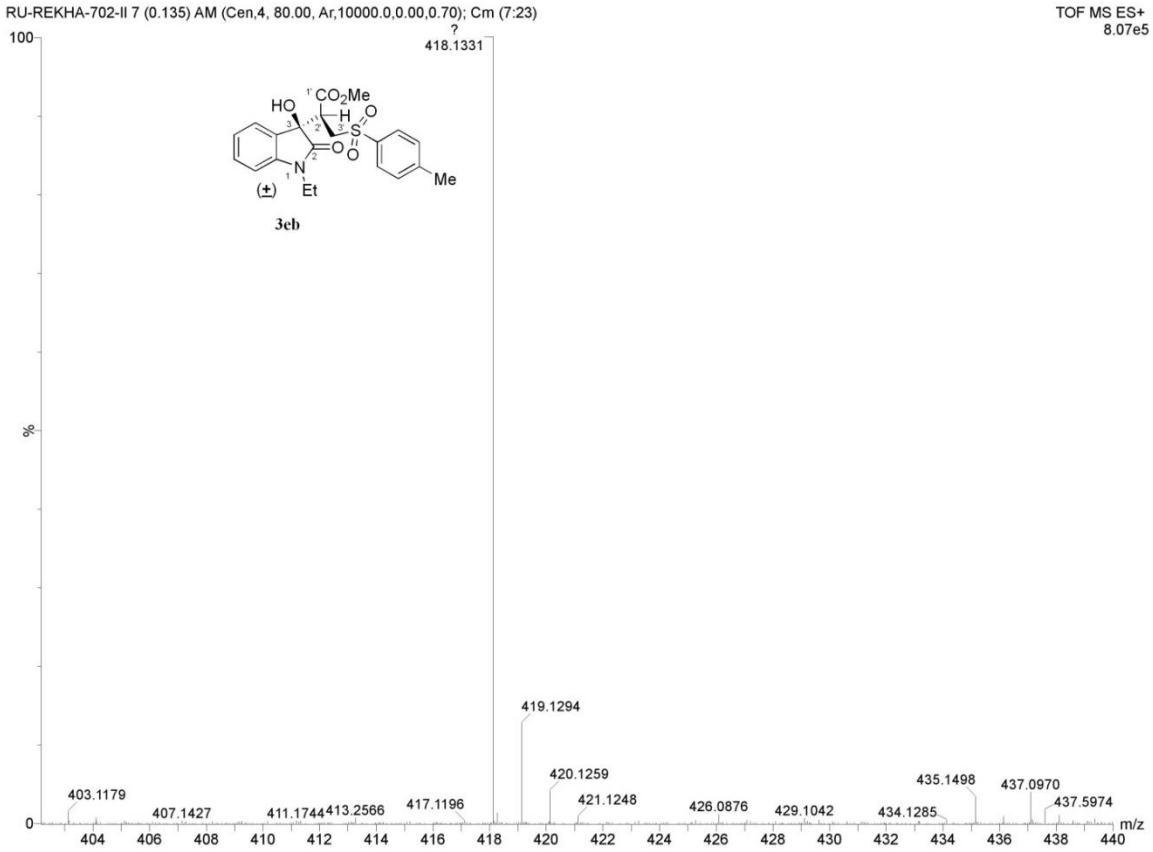


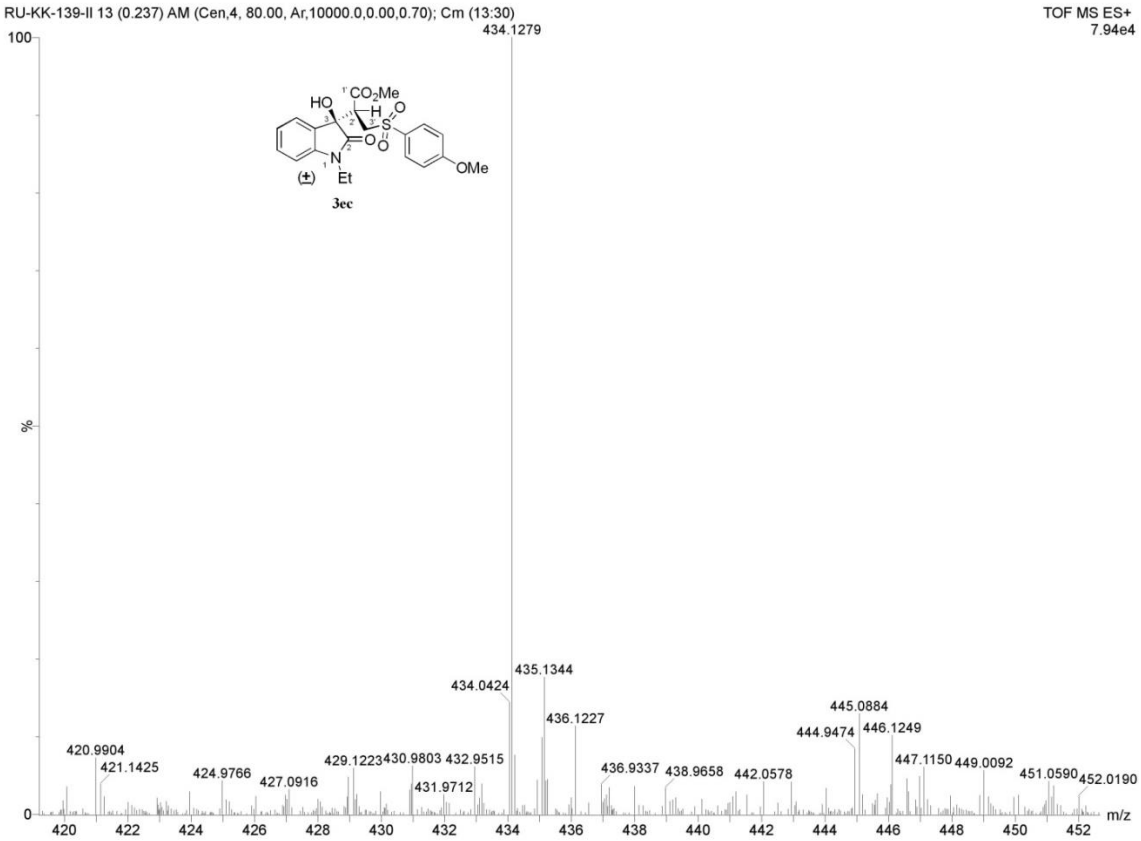
3db

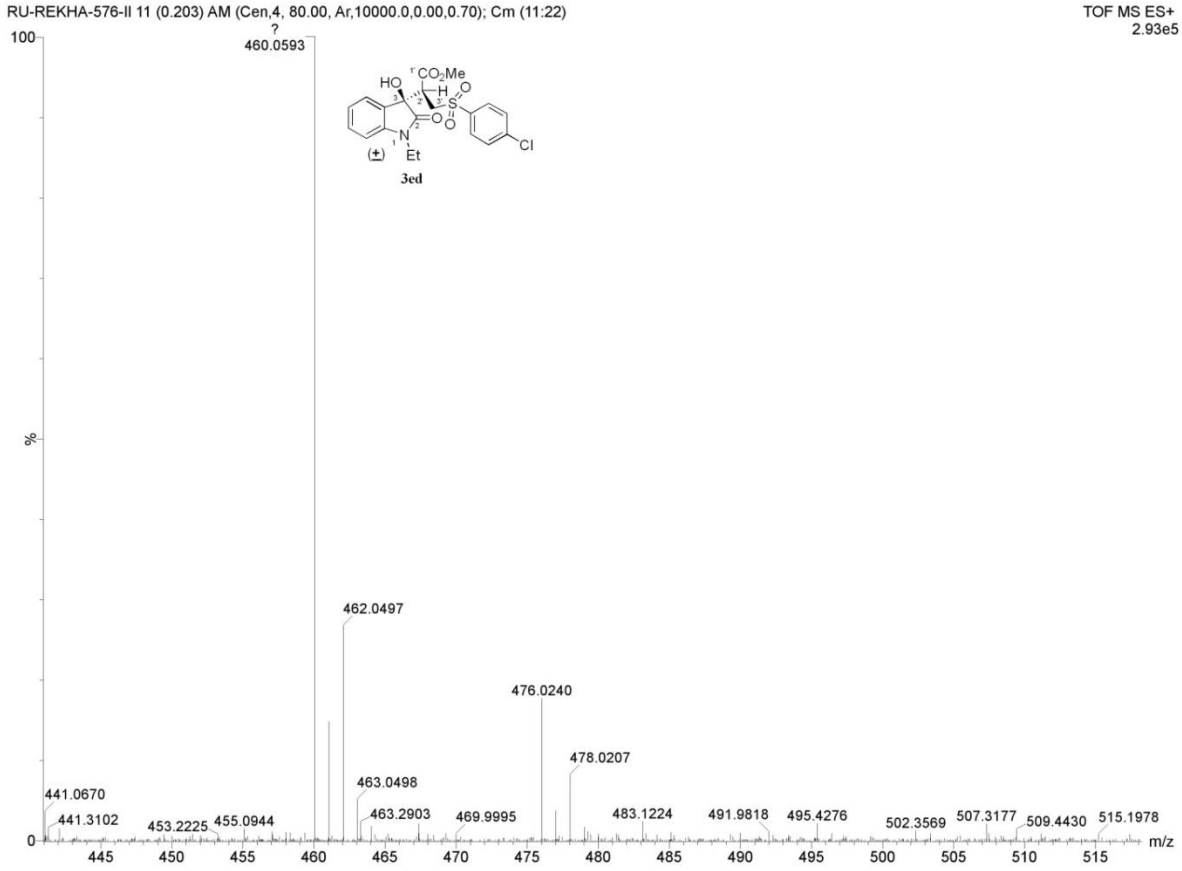

RU-KK-146-II 7 (0.135) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.70); Cm (7:15)
TOF MS ES+
2.03e5
100
%
0
465.0963
449.1033
450.0724
450.9779
455.0469
457.9347
461.1821
463.1744
464.9902
466.0857
466.1215
467.1279
471.0887
475.0747
476.0739
476.0099
477.0627
477.1182
479.1117
482.1147
482.1497
450
452
454
456
458
460
462
464
466
468
470
472
474
476
478
480
482
m/z
HO
CO2Me
O2N
N
Me
(±)
O
S
OMe
3dc

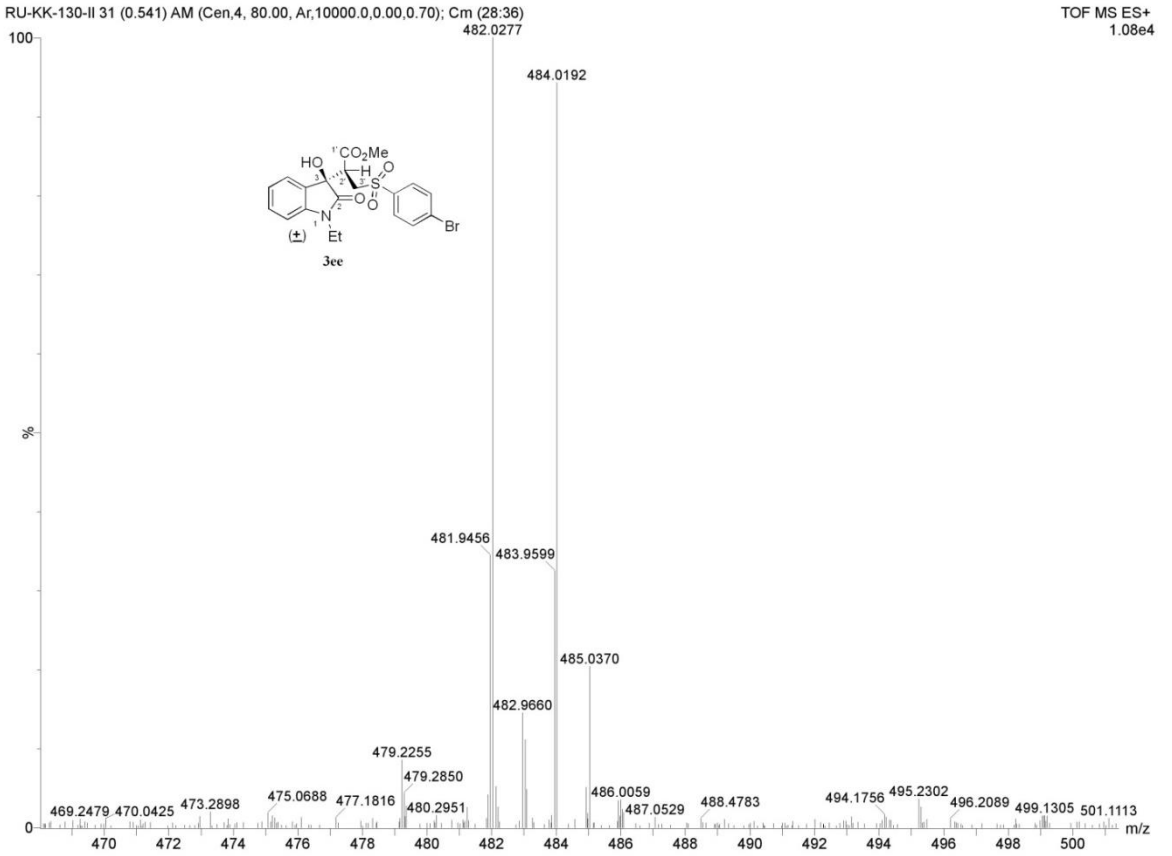

RU-KK-142-II 7 (0.135) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.70); Cm (7:10)
TOF MS ES+
1.25e5
100
%
0
469.0478
469.0163
471.0352
453.0318
453.0834
455.0169
458.9809
461.0274
464.9449
467.0739
468.8811
472.0483
473.0038
478.9993
479.9709
480.0294
480.9991
481.5170
482.5086
486.0295
486.1224
452
454
456
458
460
462
464
466
468
470
472
474
476
478
480
482
484
486
m/z
HO
CO2Me
O2N
N
Me
(±)
O
S
Cl
3dd

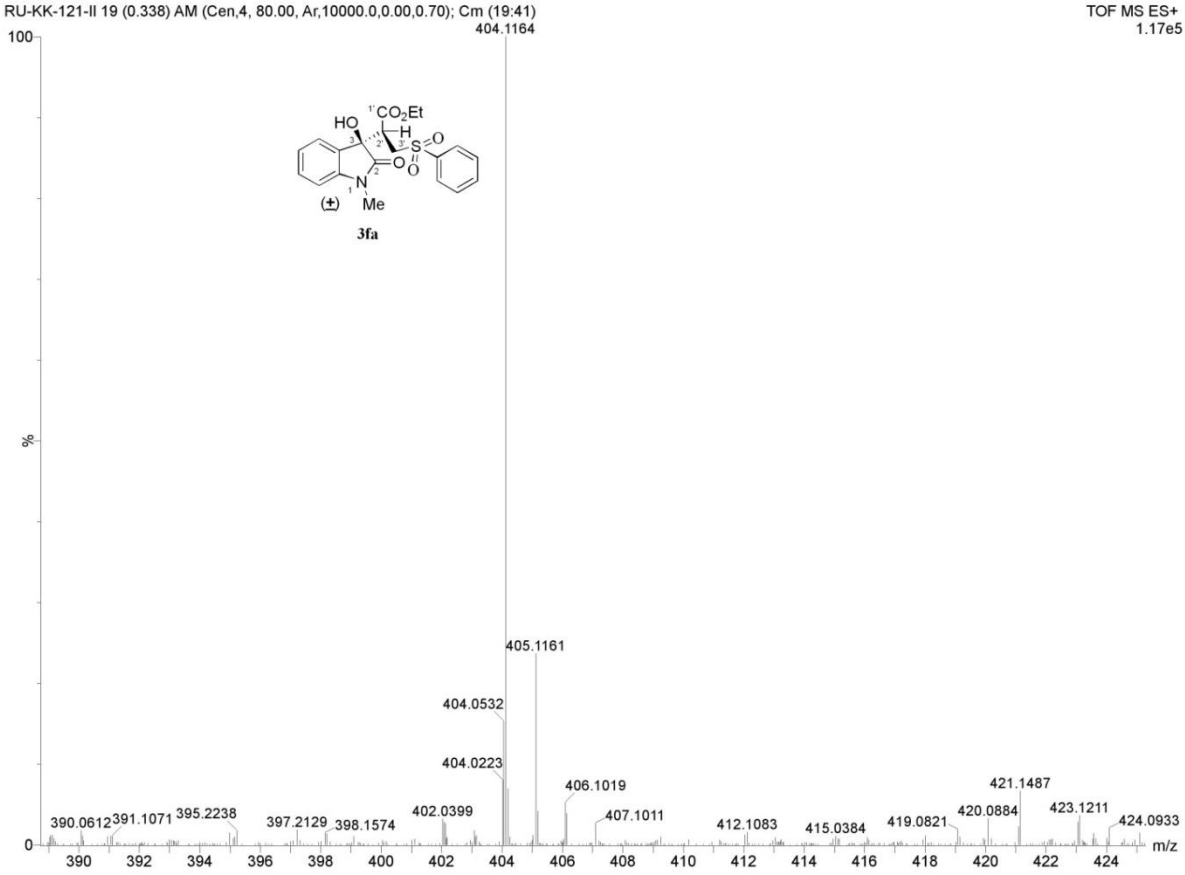

RU-REKHA-559-II 9 (0.169) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.70); Cm (9:25)
TOF MS ES+
2.29e5
404.1172
100
%
0
405.1142
388.1006
406.1118
389.1023
393.2993
395.2961
399.1578
403.1584
407.3490
411.3485
413.2668
415.2599
419.2653
421.1362
423.0816
390
392
394
396
398
400
402
404
406
408
410
412
414
416
418
420
422
424
m/z
HO
CO2Me
H
O
S
O
O
N
Et
(±)
3ea

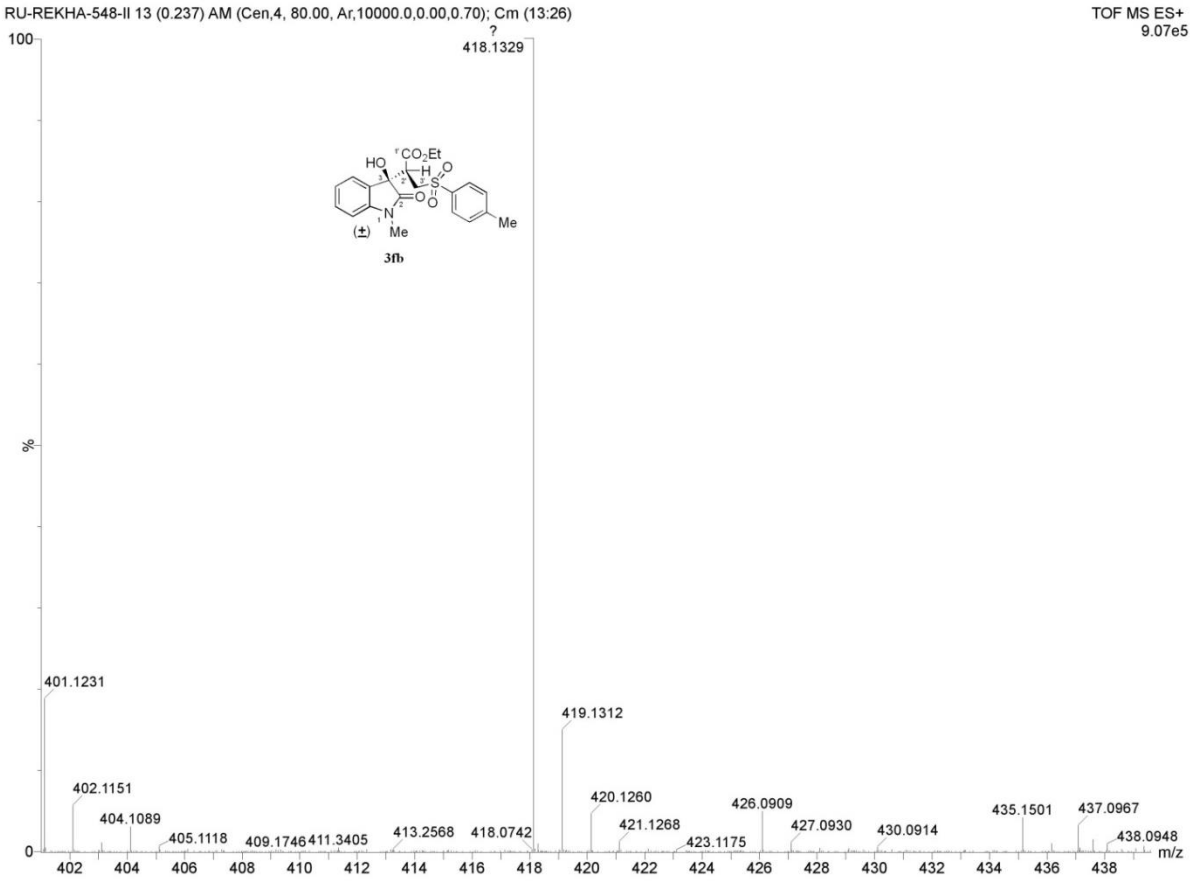

RU-REKHA-702-II 7 (0.135) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.70); Cm (7:23)
TOF MS ES+
8.07e5
?
418.1331
100
%
0
419.1294
403.1179
420.1259
421.1248
407.1427
411.1744
413.2566
417.1196
426.0876
429.1042
434.1285
435.1498
437.0970
437.5974
404
406
408
410
412
414
416
418
420
422
424
426
428
430
432
434
436
438
440
m/z
HO
CO2Me
H
O
S
O
O
N
Et
(±)
Me
3eb

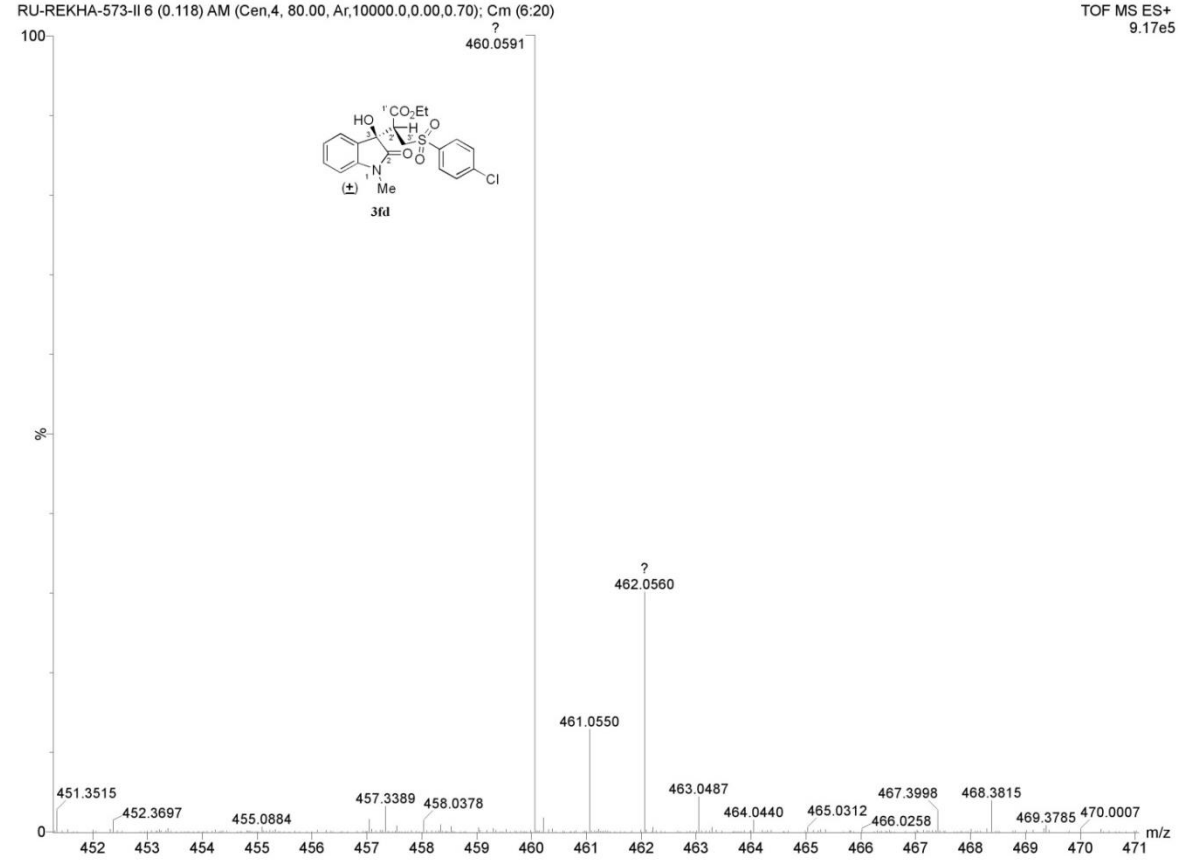

RU-KK-139-II 13 (0.237) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.70); Cm (13:30)
TOF MS ES+
7.94e4
100
%
0
434.1279
435.1344
434.0424
436.1227
445.0884
444.9474
446.1249
420.9904
421.1425
424.9766
427.0916
429.1223
430.9803
432.9515
431.9712
436.9337
438.9658
442.0578
447.1150
449.0092
451.0590
452.0190
m/z
420
422
424
426
428
430
432
434
436
438
440
442
444
446
448
450
452
HO
CO2Me
OMe
Et
3ec

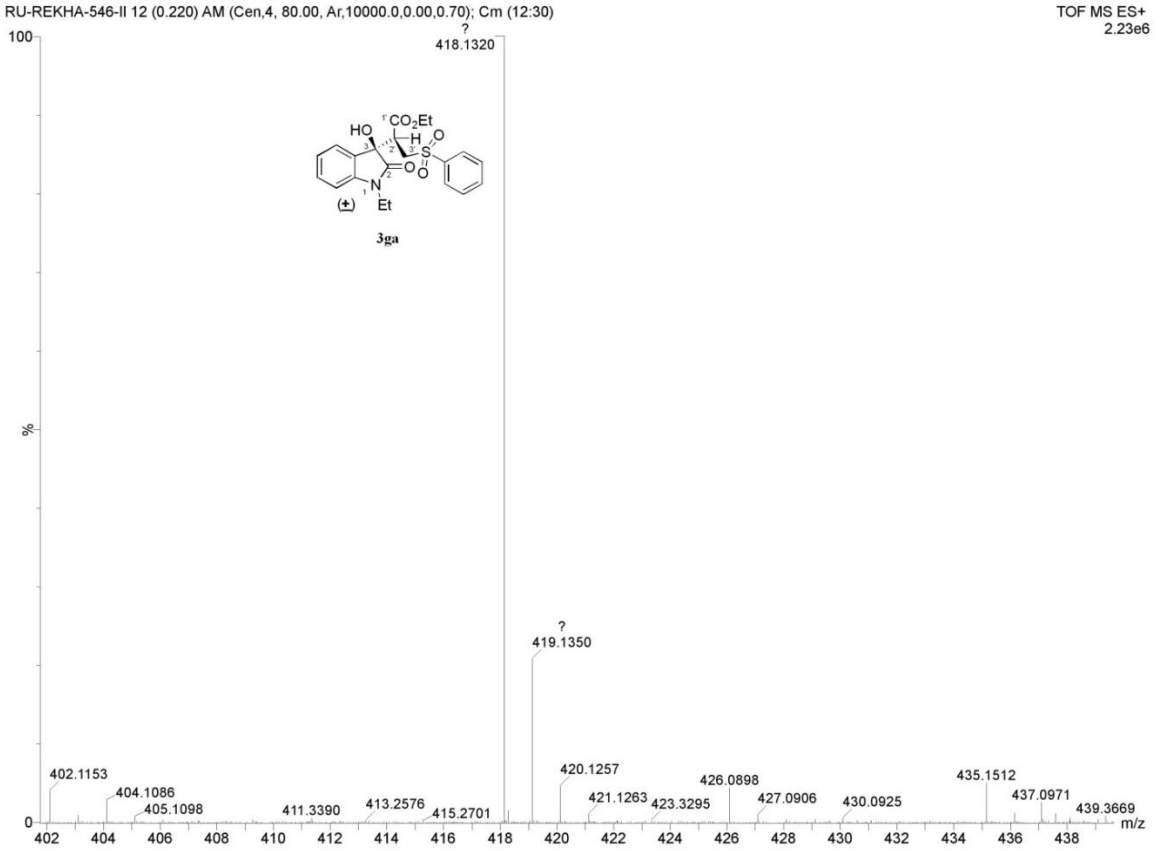

RU-REKHA-576-II 11 (0.203) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.70); Cm (11:22)
TOF MS ES+
2.93e5
100
%
0
460.0593
462.0497
476.0240
478.0207
463.0498
441.0670
441.3102
453.2225
455.0944
463.2903
469.9995
483.1224
491.9818
495.4276
502.3569
507.3177
509.4430
515.1978
m/z
445
450
455
460
465
470
475
480
485
490
495
500
505
510
515
HO
CO2Me
Cl
Et
3ed

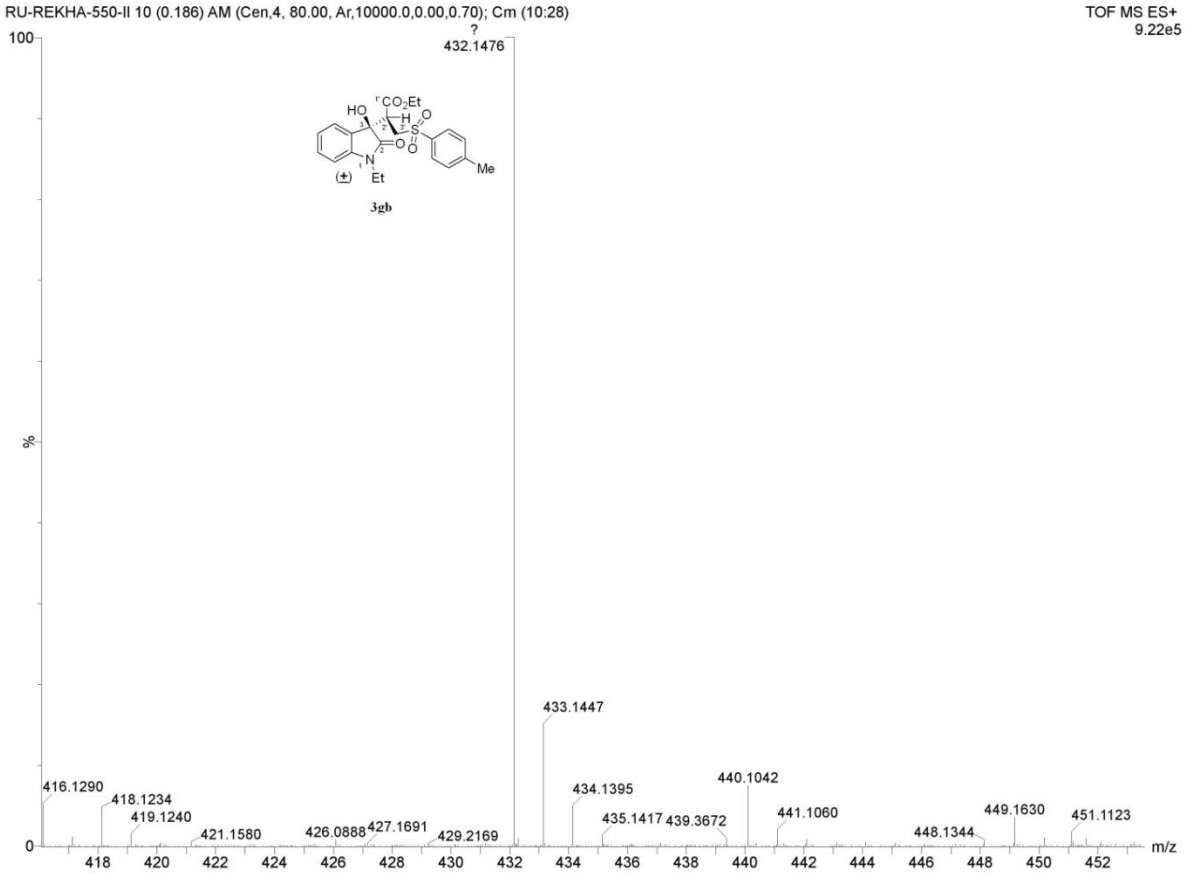

RU-KK-130-II 31 (0.541) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.70); Cm (28:36)
TOF MS ES+
1.08e4
482.0277
484.0192
481.9456
483.9599
485.0370
482.9660
479.2255
479.2850
486.0059
487.0529
488.4783
494.1756
495.2302
496.2089
499.1305
501.1113
469.2479
470.0425
473.2898
475.0688
477.1816
480.2951
%
m/z
3ee

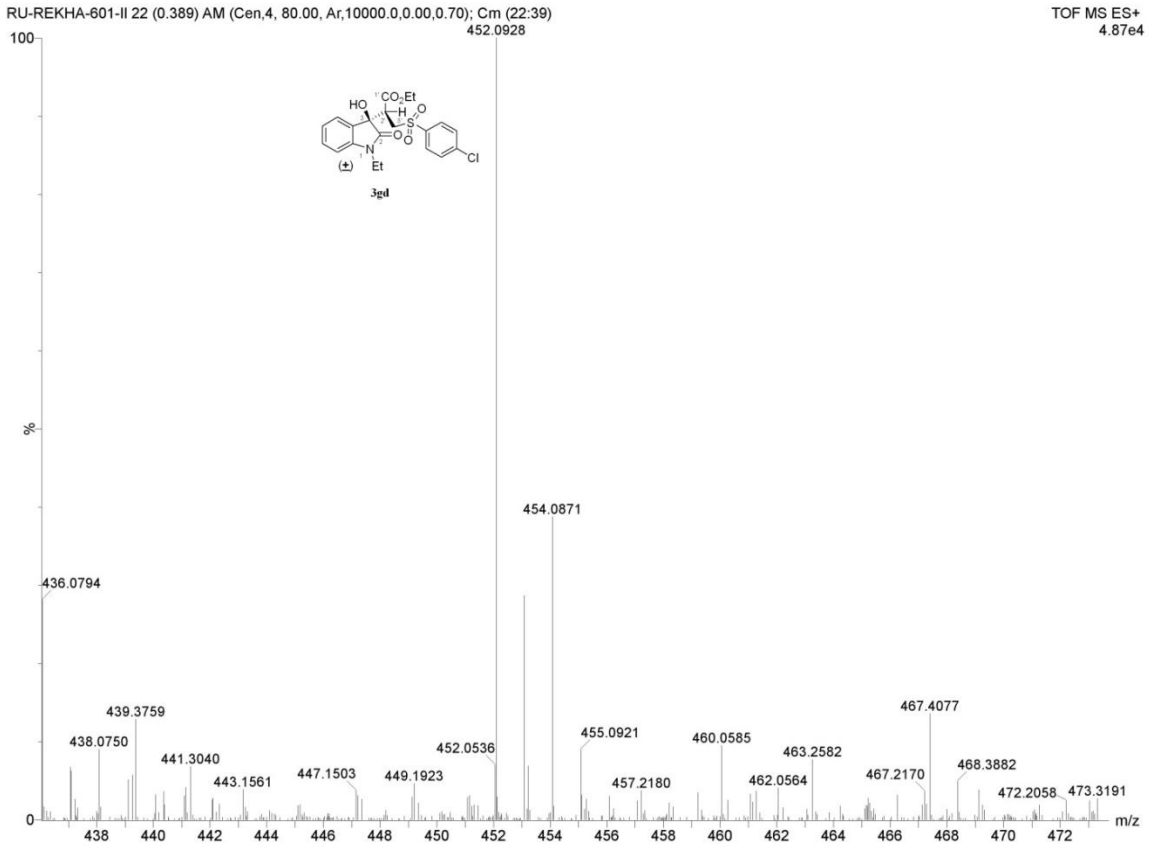

RU-KK-121-II 19 (0.338) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.70); Cm (19:41)
TOF MS ES+
1.17e5
404.1164
405.1161
404.0532
404.0223
406.1019
421.1487
407.1011
423.1211
424.0933
390.0612
391.1071
395.2238
397.2129
398.1574
402.0399
412.1083
415.0384
419.0821
420.0884
%
m/z
3fa

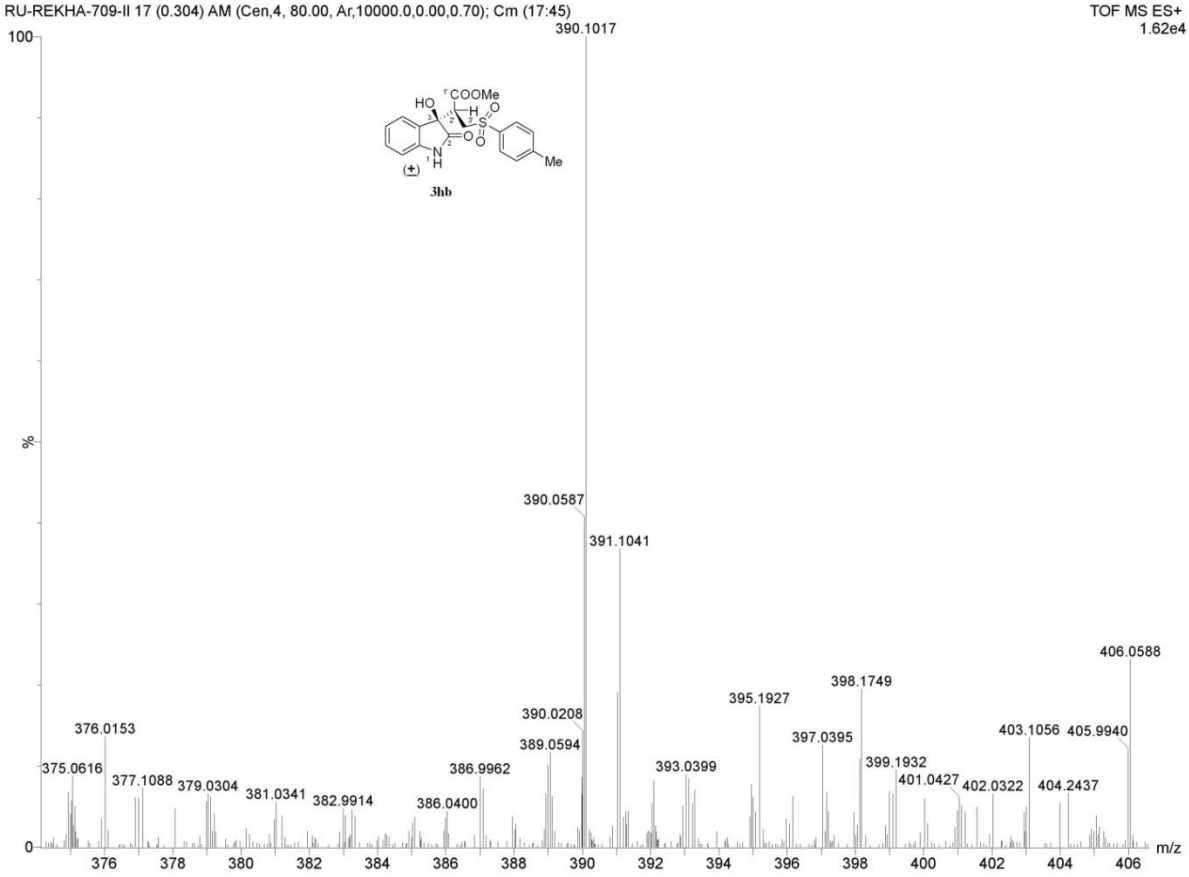

RU-REKHA-548-II 13 (0.237) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.70); Cm (13:26)
TOF MS ES+
9.07e5
100
%
0
418.1329
401.1231
419.1312
402.1151
420.1260
404.1089
426.0909
421.1268
435.1501
437.0967
427.0930
430.0914
405.1118
409.1746
411.3405
413.2568
418.0742
423.1175
438.0948
m/z
402
404
406
408
410
412
414
416
418
420
422
424
426
428
430
432
434
436
438
3fb

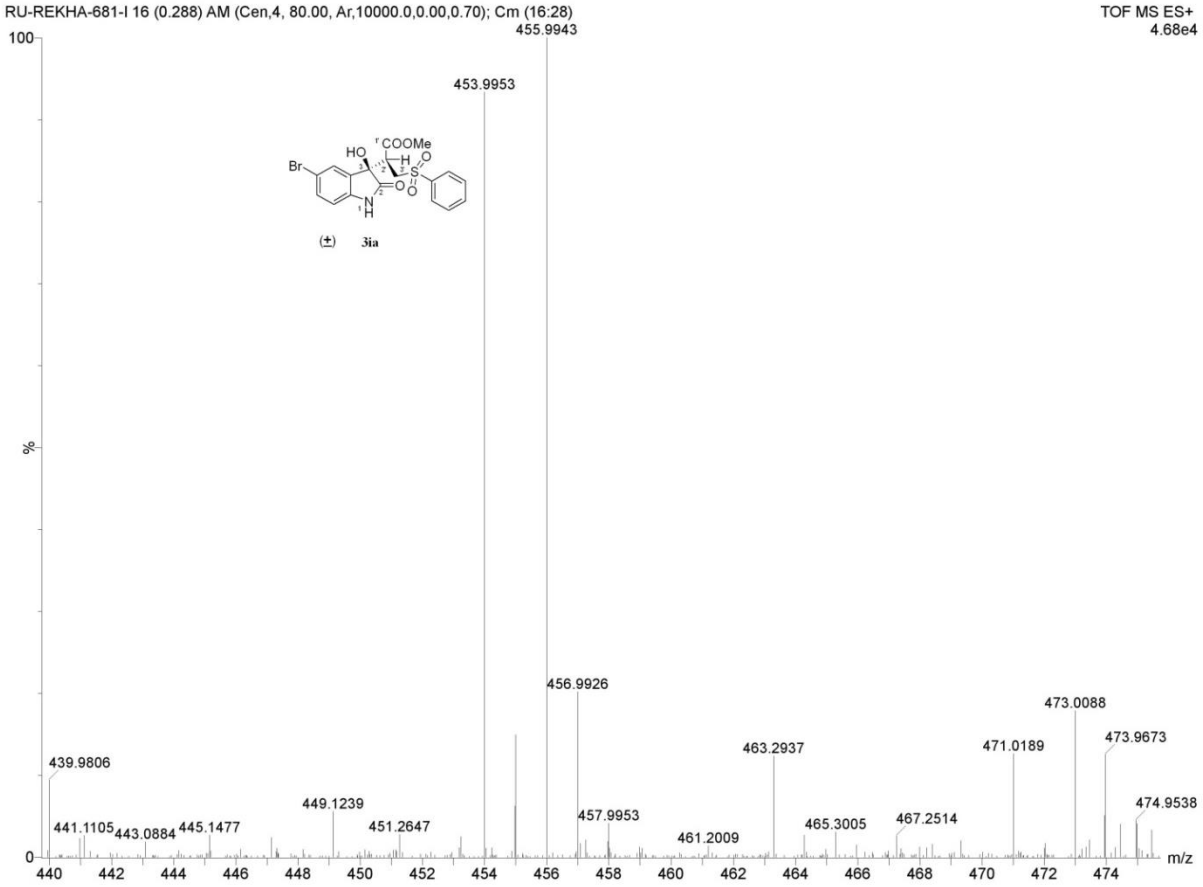

RU-REKHA-573-II 6 (0.118) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.70); Cm (6:20)
TOF MS ES+
9.17e5
100
%
0
460.0591
462.0560
461.0550
451.3515
463.0487
452.3697
457.3389
458.0378
455.0884
464.0440
465.0312
467.3998
468.3815
466.0258
469.3785
470.0007
m/z
452
453
454
455
456
457
458
459
460
461
462
463
464
465
466
467
468
469
470
471
3fd

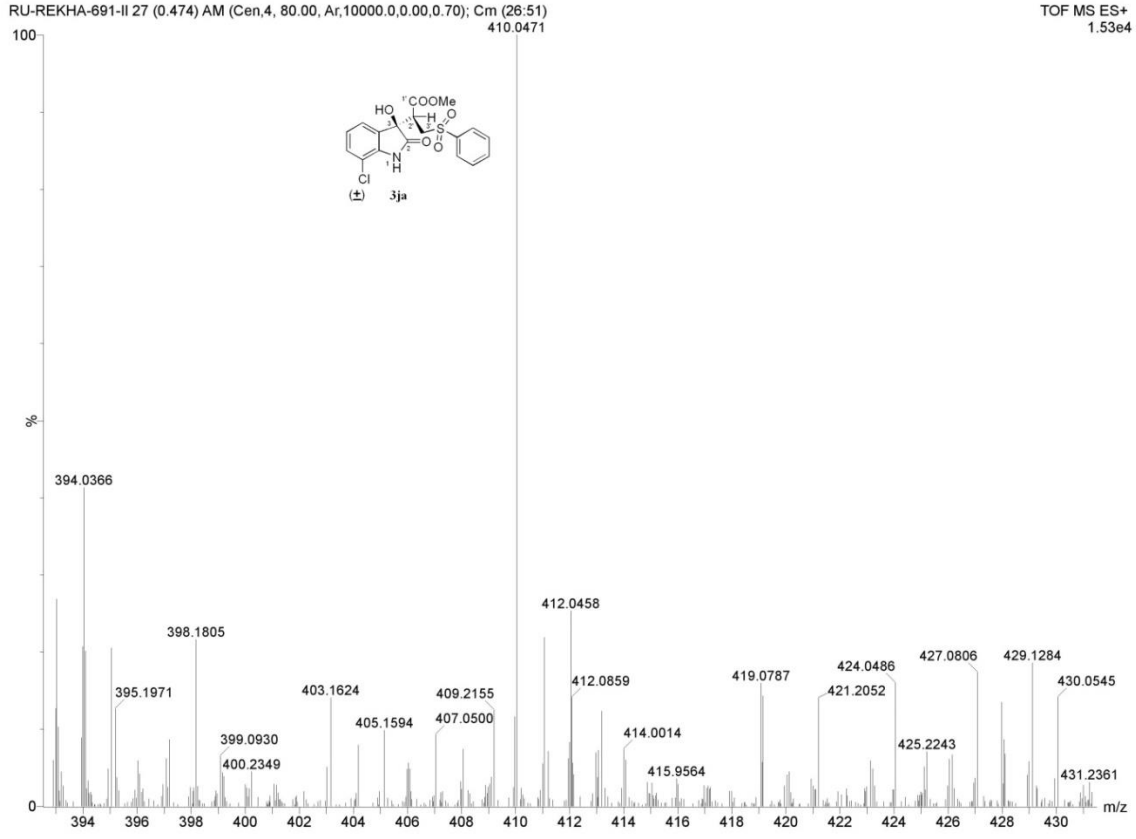

RU-REKHA-546-II 12 (0.220) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.70); Cm (12:30)
TOF MS ES+
2.23e6
100
%
0
418.1320
419.1350
402.1153
404.1086
405.1098
411.3390
413.2576
415.2701
420.1257
421.1263
423.3295
426.0898
427.0906
430.0925
435.1512
437.0971
439.3669
m/z
402
404
406
408
410
412
414
416
418
420
422
424
426
428
430
432
434
436
438
3ga


RU-REKHA-550-II 10 (0.186) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.70); Cm (10:28)
TOF MS ES+
9.22e5
100
%
0
432.1476
433.1447
416.1290
418.1234
419.1240
421.1580
426.0888
427.1691
429.2169
434.1395
435.1417
439.3672
440.1042
441.1060
448.1344
449.1630
451.1123
m/z
418
420
422
424
426
428
430
432
434
436
438
440
442
444
446
448
450
452
3gb


RU-REKHA-601-II 22 (0.389) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.70); Cm (22:39)
TOF MS ES+
4.87e4
100
%
0
452.0928
454.0871
436.0794
439.3759
438.0750
441.3040
443.1561
447.1503
449.1923
452.0536
455.0921
457.2180
460.0585
462.0564
463.2582
467.4077
467.2170
468.3882
472.2058
473.3191
438
440
442
444
446
448
450
452
454
456
458
460
462
464
466
468
470
472
m/z
3gd


RU-REKHA-709-II 17 (0.304) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.70); Cm (17:45)
TOF MS ES+
1.62e4
100
%
0
390.1017
390.0587
391.1041
406.0588
398.1749
395.1927
390.0208
376.0153
389.0594
397.0395
403.1056
405.9940
375.0616
386.9962
393.0399
399.1932
401.0427
377.1088
379.0304
381.0341
382.9914
386.0400
402.0322
404.2437
376
378
380
382
384
386
388
390
392
394
396
398
400
402
404
406
m/z
3hb


RU-REKHA-681-I 16 (0.288) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.70); Cm (16:28)
TOF MS ES+
4.68e4
455.9943
453.9953
456.9926
473.0088
473.9673
463.2937
471.0189
439.9806
474.9538
449.1239
457.9953
441.1105
443.0884
445.1477
451.2647
461.2009
465.3005
467.2514
(±) 3ia
%
m/z


RU-REKHA-691-II 27 (0.474) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.70); Cm (26:51)
TOF MS ES+
1.53e4
410.0471
394.0366
412.0458
398.1805
412.0859
427.0806
429.1284
424.0486
419.0787
430.0545
395.1971
403.1624
409.2155
421.2052
405.1594
407.0500
414.0014
399.0930
425.2243
400.2349
415.9564
431.2361
(±) 3ja
%
m/z