A facile access to novel heterocyclic analogues of chalcone from newly synthesized ketone containing isoxazole and benzoxazinone ring

Nishant Verma,* Sumit Kumar, Naseem Ahmed*

[a]*Department of Chemistry, Indian Institute of Technology Roorkee, Roorkee 247667, Uttarakhand, India.*

**Corresponding author. Fax and Tel.: +91 1332 285745.*

E-mail address: nasemfcy@iitr.ac.in

SUPPORTING INFORMATION

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General Information

Unless otherwise noted, chemicals were purchased from commercial suppliers at the highest purity grade available and were used without further purification. Solvents were distilled by standard methods. Thin layer chromatography was performed on Merck precoated 0.25 mm silica gel plates (60F-254) using UV light as visualizing agent and/or iodine as developing agent. Silica gel (100-200 mesh) was used for column chromatography. IR spectra were recorded on FT-IR spectrometer and expressed as wave numbers (cm^{-1}). ^{1}H and ^{13}C NMR spectra were recorded on a Brüker (500 MHz & 125 MHz) & Jeol (400 MHz & 100 MHz) spectrometer. Spectra were referenced internally to the residual proton resonance in $CDCl_3$ (δ 7.26 ppm) or with tetramethylsilane (TMS, δ 0.00 ppm) as the internal standard. Chemical shifts (δ) were reported as part per million (ppm) in δ scale downfield from TMS. ^{13}C NMR spectra were referenced to $CDCl_3$ (δ 77.23 ppm, the middle peak). Coupling constants are expressed in Hz. The following abbreviations are used to explain the multiplicities: s = singlet, d = doublet, t = triplet, dd = doublet of doublets, m = multiplet, br = broad. High-resolution mass spectra (HRMS) were obtained on a Brüker micrOTOF™-Q II mass spectrometer (ESIMS).

General procedure for synthesis of compounds

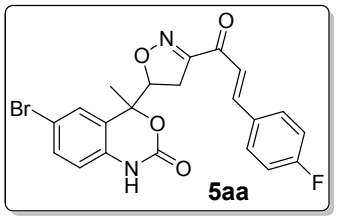
Preparation of compound 5a and 5b: A mixture of 6-bromo-4-methyl-4-vinyl-1H-benzo[d][1,3]oxazin-2(4H)-one (4a) or 4-allyl-6-bromo-4-methyl-1H-benzo[d][1,3]oxazin-2(4H)-one (4b) (5 mmol) and ammonium cerium(IV) nitrate (2.74 g, 5 mmol) in acetone (20 ml) was stirred under reflux for 12 h. The reaction mixture was extracted with EtOAc (50 ml) and washed with aq. $NaHCO_3$ solution (2 ×30 ml), saturated aq. NaCl (2 ×30 ml), and water (2 ×30 ml). The ethereal solution was dried over Na_2SO_4 and concentrated in a vacuum. The resulting

solid was chromatographed on silica gel. Elution with hexane– EtOAc (8:2) gave 4-(3-acetyl-4,5-dihydroisoxazol-5-yl)-6-bromo-4-methyl-1H-benzo[d][1,3]oxazin-2(4H)-one (5a) and 4-((3-acetyl-4,5-dihydroisoxazol-5-yl)methyl)-6-bromo-4-methyl-1H-benzo[d][1,3]oxazin-2(4H)-one (5b) as white solid (70%).

Preparation of Chalcones 5aa-ak and 5ba-bj: Dissolve 1 mmol of the substituted aldehyde and 1 mmol of the 5a or 5b in 10 mL of ethanol in a G-10 process vial capped with Teflon septum. 2 mmol of piperidine then added to the reaction vial using a micropipette. After a pre-stirring for one minute, the vial was subjected to microwave irradiation with the initial ramp time of 1 minute at 70 °C. The temperature was then raised to 80 ^{0}C with the holding time of 10-16 min. After completion of the reaction, cool the mixture in an ice-water bath until crystal formation is complete. Add 10 mL of ice-cold water to the flask and vacuum filter. Wash the crystals with water followed by ice-cold ethanol. Allow to air-dry. Recrystallize from 95% ethanol if necessary to afford the pure chalcones 5aa-ak and 5ba-bj in 81–93% yield.

Characterization Data:-

(*E*)-6-bromo-4-(3-(3-(4-fluorophenyl)acryloyl)-4,5-dihydroisoxazol-5-yl)-4-methyl-1H-benzo[d][1,3]oxazin-2(4H)-one (5aa)



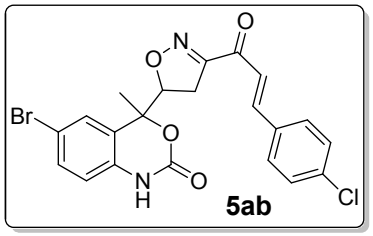
5aa

Yield: 0.42g (92%) as yellow solid; MP 212-214 °C; ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 1.78 (s, 3H), 2.87 – 2.94 (m, 1H), 3.0 – 3.06 (m, 1H), 3.89 – 3.97 (m, 1H), 6.78 (d, *J* = 14.0 Hz, 1H), 7.24 (s, 1H), 7.34 (d, *J* = 9.5 Hz, 1H), 7.40 (d, *J* = 9.5 Hz, 2H), 7.48 (d, *J* = 6.5 Hz, 2H), 7.56 (d, *J* = 8.5 Hz, 1H), 7.94 (d, *J* = 14.0 Hz, 1H), 9.67 (s, br, D_2O exchangeable, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 22.1, 26.7, 84.9, 86.1, 117.0, 120.9, 126.9, 127.5,

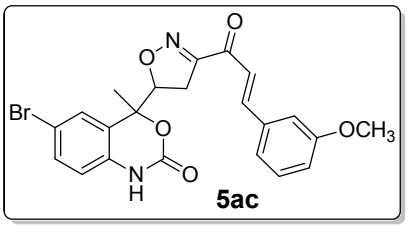
129.1, 130.3, 130.9, 131.5, 132.4, 134.0, 138.0, 138.3, 138.8, 153.3, 189.3; FTIR (KBr, ν = cm^{-1}): 1638, 1716, 3331; HRMS (ESI+): m/z calcd. for $C_{21}H_{16}BrFN_2NaO_4$ $[M+Na]^+$: 481.0175 found : 481.0171.

(*E*)-6-bromo-4-(3-(3-(4-chlorophenyl)acryloyl)-4,5-dihydroisoxazol-5-yl)-4-methyl-1H-benzo[d][1,3]oxazin-2(4H)-one (5ab)

Yield: 0.42g (89%) as yellow solid; MP 208-210 °C; ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 1.77 (s, 3H), 2.90 – 2.96 (m, 1H), 3.03 – 3.08 (m, 1H), 3.91 – 4.00 (m, 1H), 6.77 (d, *J* = 13.5 Hz, 1H), 7.23 (s, 1H), 7.33(d, *J* = 15.5 Hz, 1H), 7.40 (d, *J* = 8.5 Hz, 2H), 7.47 (d, *J* = 6.5 Hz, 2H), 7.55 (d, *J* = 8.5 Hz, 1H), 7.94 (d, *J* = 13.5 Hz, 1H), 9.66 (s, br, D_2O exchangeable, 1H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 21.2, 25.9, 84.1, 87.2, 116.2, 120.2, 126.1, 126.7, 128.3, 129.5, 130.1, 130.7, 131.6, 133.2, 137.2, 137.5, 138.0, 152.5, 189.3; FTIR (KBr, ν = cm^{-1}): 1637, 1715, 3329; HRMS (ESI+): m/z calcd. for $C_{21}H_{16}BrClN_2NaO_4$ $[M+Na]^+$: 496.9880 found : 496.9878



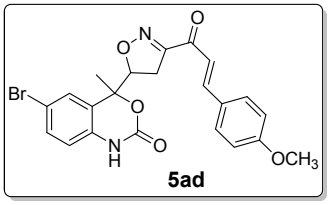
(*E*)-6-bromo-4-(3-(3-(3-methoxyphenyl)acryloyl)-4,5-dihydroisoxazol-5-yl)-4-methyl-1H-benzo[d][1,3]oxazin-2(4H)-one (5ac)



Yield: 0.4g (87%) as yellow solid; MP 203-205 °C; ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 1.67 (s, 3H), 2.92 – 2.93 (m, 1H), 3.01 – 3.04 (m, 1H), 3.72 – 3.76 (m, 1H), 3.81 (s, 3H), 6.77 (d, *J* = 13.5 Hz, 1H), 7.01 (d, *J* = 6.0 Hz, 2H), 7.11 (d, *J* = 7.5 Hz, 1H), 7.17 (d, *J* = 1.5 Hz, 1H), 7.30-7.34 (m, 2H), 7.55 (d, *J* = 8.5 Hz, 2H), 7.94 (d, *J* = 14.0 Hz, 1H), 9.85 (s, br, D_2O exchangeable, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 22.1, 26.3, 55.3, 84.6, 86.5, 116.6,

117.1, 117.3, 124.4, 126.5, 127.1, 128.2, 131.5, 132.7, 133.0, 134.6, 135.4, 137.2, 139.4, 140.2, 153.6, 188.8; FTIR (KBr, v = cm^{-1}): 1640, 1719, 3333; HRMS (ESI+): m/z calcd. for $C_{22}H_{19}BrN_2NaO_5$ $[M+Na]^+$: 493.0375 found : 493.0379.

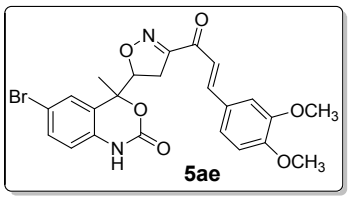
(*E*)-6-bromo-4-(3-(3-(4-methoxyphenyl)acryloyl)-4,5-dihydroisoxazol-5-yl)-4-methyl-1H-benzo[d][1,3]oxazin-2(4H)-one (5ad)



5ad

Yield: 0.39g (85%) as yellow solid; MP 206-208 °C; ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 1.66 (s, 3H), 2.88 – 2.94 (m, 1H), 2.99 – 3.05 (m, 1H), 3.69 – 3.75 (m, 1H), 3.83 (s, 3H), 6.76 (d, J = 14.0 Hz, 1H), 7.17 (s, 1H), 7.30 (d, J = 8.0 Hz, 1H), 7.38 (d, J =7.5.0 Hz, 2H), 7.47 (d, J = 8.0 Hz, 2H), 7.56 (d, J = 9.0 Hz, 1H), 7.92 (d, J = 13.5 Hz, 1H), 9.82 (s, br, D_2O exchangeable, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm): 21.9, 25.5, 55.7, 83.8, 85.3, 115.1, 115.9, 116.4, 122.7, 127.5, 128.1, 131.3, 132.3, 133.8, 135.1, 138.7, 139.2, 152.6, 163.1, 188.4; FTIR (KBr, v = cm^{-1}): 1641, 1722, 3335; HRMS (ESI+): m/z calcd. for $C_{22}H_{19}BrN_2NaO_5$ $[M+Na]^+$: 493.0375 found : 493.0371

(*E*)-6-bromo-4-(3-(3-(3,4-dimethoxyphenyl)acryloyl)-4,5-dihydroisoxazol-5-yl)-4-methyl-1H-benzo[d][1,3]oxazin-2(4H)-one (5ae)

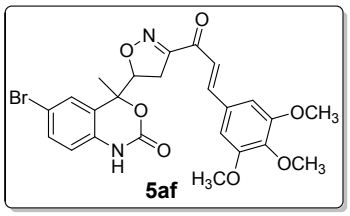


5ae

Yield: 0.42g (85%) as yellow solid; MP 197-199 °C; ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 1.78 (s, 3H), 2.89 – 2.97 (m, 1H), 3.05 – 3.12 (m, 1H), 3.74 – 3.80 (m, 1H), 3.88 - 3.89 (m, 6H), 6.75 (d, J = 14.0 Hz, 1H), 6.87 (d, J = 8.5 Hz, 1H), 6.98 (s, 1H), 7.13 (d, J = 8.5 Hz, 1H), 7.21 (s, 1H), 7.31 (d, J = 8.5 Hz, 1H), 7.51 (d, J = 8.5 Hz, 1H), 7.91 (d, J = 13.5 Hz, 1H), 9.50 (s, br, D_2O exchangeable, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ. 21.9, 26.2, 56.0, 56.1, 84.4, 86.5, 110.3, 111.3, 115.6, 116.5, 120.4, 122.4, 124.7, 126.3, 127.0, 131.0, 131.9, 133.4, 135.2, 139.4,

149.5, 152.9, 188.3; FTIR (KBr, v = cm^{-1}): 1638, 1719, 3332; HRMS (ESI+): m/z calcd. for $C_{23}H_{21}BrN_2NaO_6$ $[M+Na]^+$: 523.0481 found: 523.0486.

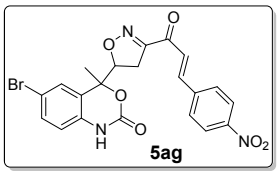
(*E*)-6-bromo-4-methyl-4-(3-(3-(3,4,5-trimethoxyphenyl)acryloyl)-4,5-dihydroisoxazol-5-yl)-1H-benzo[d][1,3]oxazin-2(4H)-one (5af)



5af

Yield: 0.44g (83%) as yellow solid; MP 193-195 °C; ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 1.78 (s, 3H), 2.90 – 2.97 (m, 1H), 3.04 – 3.11 (m, 1H), 3.76 – 3.82 (m, 1H), 3.86 (s, 6H), 3.87(s, 3H), 6.74-6.77 (m, 3H), 7.21 (s, 1H), 7.32 (dd, J = 1.5, 8.0 Hz, 1H), 7.53 (d, J = 8.5 Hz, 1H), 7.90 (d, J = 13.5 Hz, 1H), 9.65 (s, br, D_2O exchangeable, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 21.1, 25.9, 56.0, 60.7, 84.0, 86.3, 106.2, 115.3, 116.1, 120.1, 125.0, 126.0, 126.6, 130.6, 131.5, 133.1, 136.1, 139.0, 152.5, 153.3, 188.4; FTIR (KBr, v = cm^{-1}): 1644, 1728, 3341; HRMS (ESI+): m/z calcd. for $C_{24}H_{23}BrN_2NaO_7$ $[M+Na]^+$: 553.0586 found 553.0582.

(*E*)-6-bromo-4-methyl-4-(3-(3-(4-nitrophenyl)acryloyl)-4,5-dihydroisoxazol-5-yl)-1H-benzo[d][1,3]oxazin-2(4H)-one (5ag)

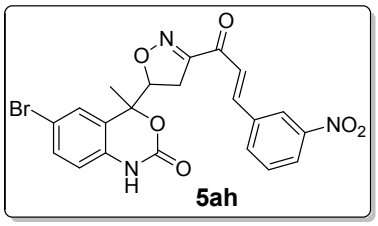


5ag

Yield: 0.45g (93%) as yellow solid; MP 198-200 °C; ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 1.77 (s, 3H), 2.89 – 2.94 (m, 1H), 3.03 – 3.08 (m, 1H), 3.85 – 3.90 (m, 1H), 6.77 (d, J = 13.5 Hz, 1H), 7.23 (s, 1H), 7.33 (d, J = 15.5Hz, 1H), 7.40 (d, J = 8.0 Hz, 2H), 7.47 (d, J = 8.5 Hz, 2H), 7.55 (d, J = 8.0 Hz, 1H), 7.93 (d, J = 13.5 Hz, 1H), 9.39 (s, br, D_2O exchangeable, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 23.9, 26.0, 85.1, 87.1, 116.4, 117.2, 121.2, 123.3, 127.2, 127.8, 131.8, 132.0, 132.7, 134.2, 135.8, 139.9, 153.6, 163.8, 190.2; FTIR (KBr, v = cm^{-1}): 1636, 1720, 3334; HRMS (ESI+): m/z calcd. for $C_{21}H_{16}BrN_3NaO_6$ $[M+Na]^+$: 508.0120 found : 508.0125.

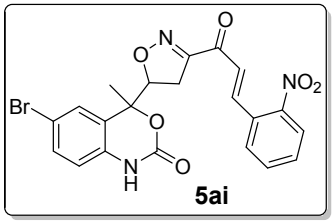
(*E*)-6-bromo-4-methyl-4-(3-(3-(3-nitrophenyl)acryloyl)-4,5-dihydroisoxazol-5-yl)-1H-benzo[d][1,3]oxazin-2(4H)-one (5ah)

Yield: 0.42g (88%) as yellow solid; MP 191-193 °C; ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 1.78 (s, 3H), 2.88 – 2.92 (m, 1H), 3.00 – 3.02 (m, 1H), 3.92 – 3.96 (m, 1H), 6.78 (d, *J* = 13.5 Hz, 1H), 7.33 - 7.35 (m, 2H), 7.66 - 7.69 (m, 2H), 7.86 (d, *J* = 7.5 Hz, 1H), 8.02 (d, *J* = 13.5 Hz, 1H), 8.16 (s, 1H), 8.31-8.40 (m, 1H), 9.78 (s, br, D_2O exchangeable, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 22.1, 26.2, 84.4, 86.8, 114.9, 115.7, 116.5, 120.4, 122.6, 126.4, 127.0, 131.0, 131.2, 131.9, 132.4, 133.5, 135.0, 139.1, 152.9, 163.0, 189.7; FTIR (KBr, *v* = cm^{-1}): 1639, 1728, 3331; HRMS (ESI+): m/z calcd. for $C_{21}H_{16}BrN_3NaO_6$ $[M+Na]^+$: 508.0120 found : 508.125.



5ah

(*E*)-6-bromo-4-methyl-4-(3-(3-(2-nitrophenyl)acryloyl)-4,5-dihydroisoxazol-5-yl)-1H-benzo[d] [1,3]oxazin-2(4H)-one (5ai)

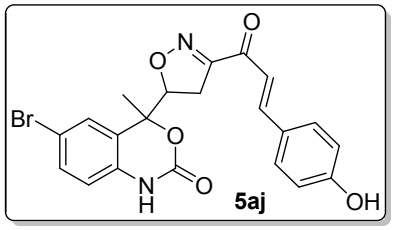


5ai

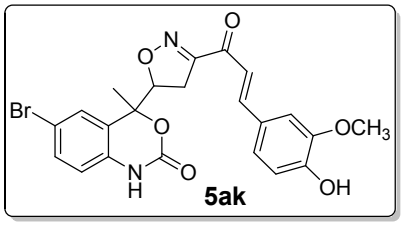
Yield: 0.4g (84%) as yellow solid; MP 188-190 °C; ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 1.77 (s, 3H), 2.89 – 2.96 (m, 1H), 3.03 – 3.11 (m, 1H), 3.83 – 3.90 (m, 1H), 6.77 (d, *J* = 13.5 Hz, 1H), 7.23 (s, 1H), 7.34 (d, *J* = 8.5 Hz, 1H), 7.42 (d, *J* = 8.5 Hz, 1H), 7.59 (d, *J* = 7.5 Hz, 1H), 7.65 (d, *J* = 7.5 Hz, 1H), 7.68-7.74 (m, 1H), 8.17 (d, *J* = 8.0 Hz, 1H), 8.49 (d, *J* = 13.5 Hz, 1H), 9.62 (s, br, D_2O exchangeable, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 21.9, 26.3, 84.5, 85.9, 115.7, 116.5, 120.5, 125.8, 126.3, 126.4, 127.1, 129.7, 131.0, 132.0,132.08, 133.5, 134.3, 135.5, 140.0, 152.9, 189.1; FTIR (KBr, *v* = cm^{-1}): 1638, 1716, 3331; HRMS (ESI+): m/z calcd. For for $C_{21}H_{16}BrN_3NaO_6$ $[M+Na]^+$: 508.0120 found : 508.0126.

(*E*)-4-(3-(3-(4-aminophenyl)acryloyl)-4,5-dihydroisoxazol-5-yl)-6-bromo-4-methyl-1H-benzo[d][1,3]oxazin-2(4H)-one (5aj)

Yield: 0.38g (85%) as yellow solid; MP 209-211 °C; ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 1.79 (s, 3H), 2.88 – 2.92 (m, 1H), 2.99 – 3.02 (m, 1H), 3.93 – 3.97 (m, 1H), 6.78 (d, *J* = 8.5 Hz, 1H), 6.98 - 7.04 (m, 3H), 7.23-7.24 (m, 2H), 7.34 - 7.36 (m, 1H), 7.51 (d, *J* = 8.5 Hz, 1H), 7.88 (d, *J* = 13.5 Hz, 1H), 9.44 (s, br, D_2O exchangeable, 1H), 9.69 (s, br, D_2O exchangeable, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 22.5, 25.6, 84.1, 87.2, 116.6, 120.0, 121.6, 125.7, 127.6, 130.7, 131.4, 132.4, 133.6, 137.2, 138.6, 139.5, 153.1, 157.5, 189.7; FTIR (KBr, *v* = cm^{-1}): 1642, 1716, 3458; HRMS (ESI+): m/z calcd. for $C_{21}H_{17}BrN_2NaO_5$ $[M+Na]^+$: 479.0219 found: 479.0212**.**

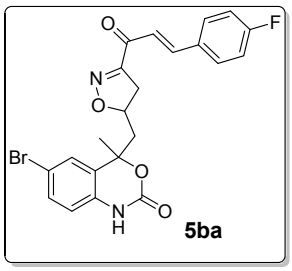


(*E*)-6-bromo-4-(3-(3-(4-hydroxyphenyl)acryloyl)-4,5-dihydroisoxazol-5-yl)-4-methyl-1H-benzo[d][1,3]oxazin-2(4H)-one (5ak)



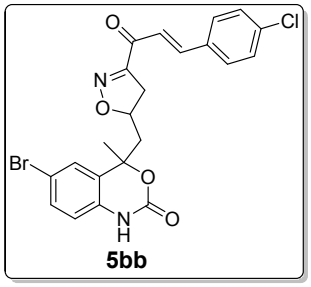
Yield: 0.42g (87%) as yellow solid; MP 207-209 °C; ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 1.75 (s, 3H), 2.89 – 2.94 (m, 1H), 3.02 – 3.07 (m, 1H), 3.71 – 3.78 (m, 1H), 3.89 (s, 3H), 6.77 (d, *J* = 14.0 Hz, 1H), 6.99 (d, *J* = 8.0 Hz, 1H), 7.21 (s, 1H), 7.32 (d, *J* = 8.0 Hz, 1H), 7.37 (m, 2H), 7.49 (d, *J* = 8.5 Hz, 1H), 7.73 (d, *J* = 13.5 Hz, 1H), 9.41 (s, br, D_2O exchangeable, 1H), 9.76 (s, br, D_2O exchangeable, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 21.4, 25.9, 58.0, 84.2, 86.8, 116.2, 116.7, 116.9, 123.9, 126.1, 126.6, 127.8, 131.1, 132.6, 134.2, 134.9, 136.7, 139.7, 139.0, 149.2, 153.2, 189.9; FTIR (KBr, *v* = cm^{-1}): 1646, 1726, 3422; HRMS (ESI+): m/z calcd. for $C_{22}H_{19}BrN_2NaO_6$ $[M+Na]^+$: 509.0324 found : 509.0319.

(*E*)-6-bromo-4-((3-(3-(4-fluorophenyl)acryloyl)-4,5-dihydroisoxazol-5-yl)methyl)-4-methyl-1H-benzo[d][1,3]oxazin-2(4H)-one (5ba)



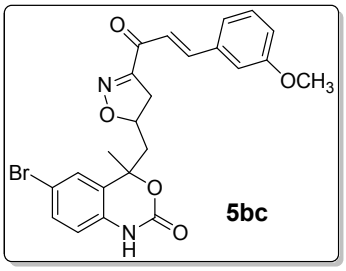
Yield: 0.4g (86%) as yellow solid; MP 196-198 °C; ^{1}H NMR (500 MHz, $CDCl_3$, ppm): 1.68 (s, 3H), 1.98 (d, *J* = 8.0 Hz, 2H), 2.88 – 2.93 (m, 1H), 3.01 – 3.04 (m, 1H), 3.25 – 3.30 (m, 1H), 6.78 (d, *J* = 14.0 Hz, 1H), 7.18 (s, 1H), 7.31 (d, *J* = 8.5 Hz, 1H), 7.40 (d, *J* = 8.0 Hz, 2H), 7.48 (d, *J* = 8.0 Hz, 2H), 7.58 (d, *J* = 8.5 Hz, 1H), 7.94 (d, *J* = 14.0 Hz, 1H), 9.84 (s, br, D_2O exchangeable, 1H); δ ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 28.6, 31.4, 45.5, 57.7, 71.9, 117.2, 121.2, 127.1, 127.7, 129.3, 130.5, 131.1, 131.7, 132.6, 134.2, 138.2, 138.5, 139.0, 153.5, 188.3; FTIR (KBr, *v* = cm^{-1}): 1636, 1720, 3338; HRMS (ESI+): m/z calcd. for $C_{22}H_{18}BrFN_2NaO_4$ $[M+Na]^+$: 495.0332 found : 495.3328**.**

(*E*)-6-bromo-4-((3-(3-(4-chlorophenyl)acryloyl)-4,5-dihydroisoxazol-5-yl)methyl)-4-methyl-1H-benzo[d][1,3]oxazin-2(4H)-one (5bb)



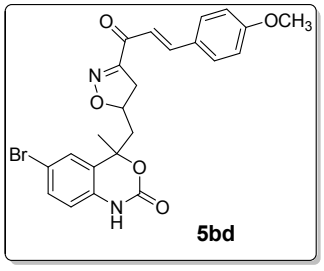
Yield: 0.4g (84%) as yellow solid; MP 192-194 °C; ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 1.65 (s, 3H), 1.95 (d, *J* = 8.0 Hz, 2H), 2.85 – 2.90 (m, 1H), 2.96 – 3.01 (m, 1H), 3.22 – 3.27 (m, 1H), 6.77(d, *J* = 13.5 Hz, 1H), 7.16 (s, 1H), 7.29 (d, *J* = 8.0 Hz, 1H), 7.38 (d, *J* = 7.5 Hz, 2H), 7.46 (d, *J* = 8.0 Hz, 2H), 7.55 (d, *J* = 8.0 Hz, 1H), 7.91 (d, *J* = 13.5 Hz, 1H), 9.81 (s, br, D_2O exchangeable, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 28.4, 31.2, 45.4, 57.6, 71.3, 115.6, 116.4, 120.4, 126.4, 127.0, 128.6, 129.7, 130.4, 131.0, 131.9, 133.4, 137.5, 138.3, 152.8, 188.8; FTIR (KBr, *v* = cm^{-1}): 1639, 1729, 3339; HRMS (ESI+): m/z calcd. for $C_{22}H_{18}BrClN_2NaO_4$ $[M+Na]^+$: 511.0036 found : 511.0031.

(*E*)-6-bromo-4-((3-(3-(3-methoxyphenyl)acryloyl)-4,5-dihydroisoxazol-5-yl)methyl)-4-methyl-1H-benzo[d][1,3]oxazin-2(4H)-one (5bc)



Yield: 0..41g (86%) as yellow solid; MP 188-190 °C; ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 1.70 (s, 3H), 1.91 (d, *J* = 8 Hz, 2H), 2.92 – 2.94 (m, 1H), 3.02 – 3.07 (m, 1H), 3.20 – 3.22 (m, 1H), 3.82 (s, 3H), 6.78 (d, *J* = 13.5 Hz, 1H), 7.01 (d, *J* = 6.5 Hz, 2H), 7.12 (d, *J* = 8.0 Hz, 1H), 7.30-7.35 (s, 2H), 7.56 (d, *J* = 13.5 Hz, 1H), 7.55 (d, *J* = 8.5 Hz, 1H), 7.94 (d, *J* = 13.5 Hz, 1H), 9.86 (s, br, D_2O exchangeable, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 28.5, 31.6, 46.2, 57.5, 69.5, 115.8, 116.3, 116.5, 123.6, 125.7, 126.3, 127.5, 130.7, 131.9, 132.2, 133.9, 134.6, 136.4, 138.7, 139.4, 148.9, 152.9, 188.8; FTIR (KBr, *v* = cm^{-1}): 1638, 1716, 3340; HRMS (ESI+): m/z calcd. for $C_{23}H_{21}BrClN_2NaO_5$ $[M+Na]^+$: 507.0532 found: 507.0538.

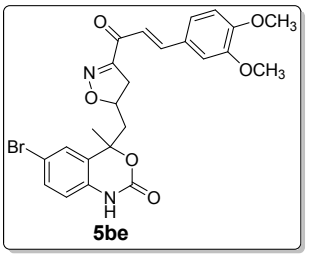
(*E*)-6-bromo-4-((3-(3-(4-methoxyphenyl)acryloyl)-4,5-dihydroisoxazol-5-yl)methyl)-4-methyl-1H-benzo[d][1,3]oxazin-2(4H)-one (5bd)



Yield: 0.39g (82%) as yellow solid; MP 191-193 °C; ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 1.69 (s, 3H), 1.91 (d, *J* = 7.5 Hz, 2H), 2.88-2.93 (m, 1H), 3.01 - 3.06 (m, 1H), 3.20-3.25 (m, 1H), 3.82 (s, 3H), 6.78 (d, *J* = 13.5 Hz, 1H), 6.91 (d, *J* = 8.0 Hz, 2H), 7.16 (s, 1H), 7.30 (d, *J* = 8.0 Hz, 1H), 7.45 - 7.91 (m, 3H), 7.92 (d, *J* = 13.5 Hz, 1H), 9.88 (s, br, D_2O exchangeable, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 29.0, 31.6, 45.5, 57.5, 70.6, 115.7, 116.5, 118.0, 120.5, 121.9, 126.4, 127.1, 130.5, 131.0, 132.0, 133.5, 137.4, 139.2, 152.9,

160.2, 188.8; FTIR (KBr, v = cm^{-1}): 1645, 1718, 3335; HRMS (ESI+): m/z calcd. for $C_{23}H_{21}BrClN_2NaO_5$ $[M+Na]^+$: 507.0532 found 507.0527.

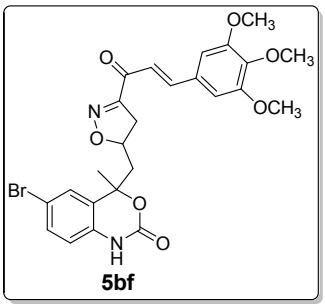
(*E*)-6-bromo-4-((3-(3-(3,4-dimethoxyphenyl)acryloyl)-4,5-dihydroisoxazol-5-yl)methyl)-4-methyl-1H-benzo[d][1,3]oxazin-2(4H)-one (5be)



5be

Yield: 0.41g (80%) as yellow solid; MP 184-186 °C; ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 1.67 (s, 3H), 1.93 (d, J = 7.5 Hz, 2H), 2.91 - 2.95(m, 1H), 3.01 - 3.04 (m, 1H), 3.14 - 3.18 (m, 1H), 3.87 (s, 6H), 6.77 (d, J = 13.5 Hz, 1H), 6.87 (d, J = 8.0 Hz, 1H), 6.98 (s, 1H), 7.14 (d, J = 8.5 Hz, 1H), 7.27 - 7.29 (m, 2H), 7.52 (d, J = 7.5 Hz, 1H), 7.91 (d, J = 13.5 Hz, 1H), 9.92 (s, br, D_2O exchangeable, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 28.1, 30.7, 45.4, 56.0, 56.1, 61.5, 71.9, 110.3, 111.3, 115.6, 116.5, 120.4, 122.8, 124.7, 126.3, 127.0, 131.0, 131.9, 133.4, 135.2, 139.4, 149.5, 152.9, 188.8; FTIR (KBr, v = cm^{-1}): 1640, 1721, 3336; HRMS (ESI+): m/z calcd. for $C_{24}H_{23}BrN_2NaO_6$ $[M+Na]^+$: 537.0637 found :537.0632.

(*E*)-6-bromo-4-methyl-4-((3-(3-(3,4,5-trimethoxyphenyl)acryloyl)-4,5-dihydroisoxazol-5-yl)methyl)-1H-benzo[d][1,3]oxazin-2(4H)-one (5bf)

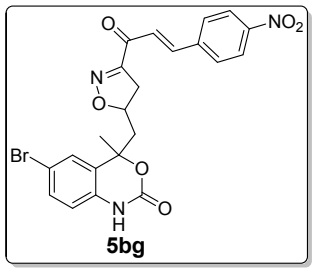


5bf

Yield: 0.4g (75%) as yellow solid; MP 191-193 °C; ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 1.66 (s, 3H), 1.92 (d, J = 7.5 Hz, 2H), 2.90 - 2.94 (m, 1H), 3.03 - 3.06 (m, 1H), 3.12 - 3.15 (m, 1H), 3.86 (s, 6H), 3.87 (s, 3H), 6.73 - 6.78 (m, 2H), 7.15 (s, 1H), 7.28 - 7.30 (m, 2H), 7.54 (d, J = 8.5 Hz, 1H), 7.90 (d, J = 13.5 Hz, 1H), 9.95 (s, br, D_2O exchangeable, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 28.3, 31.4, 45.4, 56.3, 59.3, 61.1, 70.6, 115.7, 116.5, 120.4, 125.4, 126.4, 127.0, 131.0, 131.9, 133.5, 136.5, 139.4, 141.8, 152.9,

153.7, 188.8; FTIR (KBr, v = cm^{-1}): 1639, 1719, 3343; HRMS (ESI+): m/z calcd. for $C_{25}H_{25}BrN_2NaO_7$ $[M+Na]^+$: 567.0743 found :567.0742.

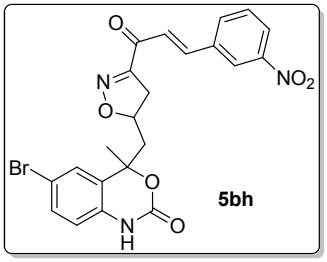
(*E*)-6-bromo-4-methyl-4-((3-(3-(4-nitrophenyl)acryloyl)-4,5-dihydroisoxazol-5-yl)methyl)-1H-benzo[d][1,3]oxazin-2(4H)-one (5bg)



5bg

Yield: 0.43g (87%) as yellow solid; MP 185-187 °C; ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 1.69 (s, 3H), 1.92 (d, J = 8.5Hz, 2H), 2.90 - 2.93 (m, 1H), 3.02 - 3.05 (m, 1H), 3.11 - 3.15 (m, 1H), 6.78 (d, J = 13.5Hz, 1H), 7.17 (s, 1H), 7.30-7.32 (m, 3H), 7.62 - 7.73 (m, 2H), 8.02 (d, J = 14.0 Hz, 1H), 8.28 (d, J = 8.5 Hz, 1H), 9.81 (s, br, D_2O exchangeable, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 28.7, 31.0, 45.5, 57.5, 70.6, 115.8, 116.5, 120.5, 124.6, 126.4, 127.1, 128.3, 129.9, 131.0, 132.0, 133.5, 136.2, 140.0, 152.9, 189.7; FTIR (KBr, v = cm^{-1}): 1648, 1719, 3333; HRMS (ESI+): m/z calcd. for $C_{22}H_{18}BrN_3NaO_6$ $[M+Na]^+$: 522.0277 found : 522.0275.

(*E*)-6-bromo-4-methyl-4-((3-(3-(3-nitrophenyl)acryloyl)-4,5-dihydroisoxazol-5-yl)methyl)-1H-benzo[d][1,3]oxazin-2(4H)-one (5bh)

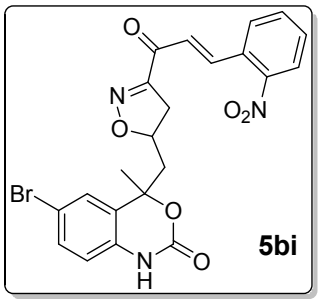


5bh

Yield: 0.44g (89%) as yellow solid; MP 181-183 °C; ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 1.68 (s, 3H), 1.91 (d, J = 7.5 Hz, 2H), 2.91 - 2.94 (m, 1H), 3.03 - 3.07 (m, 1H), 3.14 - 3.18 (m, 1H), 6.78 (d, J = 8.5 Hz, 1H), 7.16 (s, 1H), 7.30 (d, J = 8.0 Hz, 2H), 7.63 - 7.68 (m, 2H), 7.86 (d, J = 7.5 Hz, 1H), 8.02 (d, J = 14.0 Hz, 1H), 8.31 (d, J = 7.5 Hz, 1H), 9.93 (s, br, D_2O exchangeable, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 28.3, 30.5, 45.5, 59.5, 70.4, 115.7, 116.5, 120.5, 123.6, 126.2, 126.4, 127.0, 130.7, 131.0,

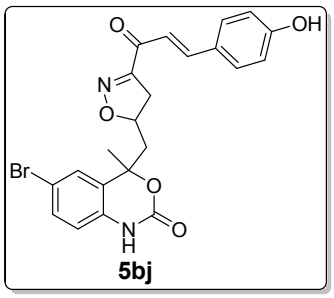
132.0, 133.5, 134.5, 136.3, 139.4, 148.8, 153.0, 189.0; FTIR (KBr, ν = cm^{-1}): 1648, 1719, 3336; HRMS (ESI+): m/z calcd. for $C_{22}H_{18}BrN_3NaO_6$ $[M+Na]^+$: 522.0277 found : 522.0279.

(*E*)-6-bromo-4-methyl-4-((3-(3-(2-nitrophenyl)acryloyl)-4,5-dihydroisoxazol-5-yl)methyl)-1H-benzo[d][1,3]oxazin-2(4H)-one (5bi)



Yield: 0.44g (88%) as yellow solid; MP 178-180 °C; ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 1.69(s, 3H), 1.89 (d, *J* = 8.0 Hz, 2H), 2.94 - 2.99 (m, 1H), 3.01 - 3.05 (m, 1H), 3.11 - 3.14 (m, 1H), 6.78 (d, *J* = 13.5 Hz, 1H), 7.17 (s, 1H), 7.29 - 7.31 (m, 1H), 7.42 (d, *J* = 13.5 Hz, 1H), 7.58 - 7.73 (m, 3H), 8.17 (d, *J* = 14.0 Hz, 1H), 8.49 (d, *J* = 8.5 Hz, 1H), 9.85 (s, br, D_2O exchangeable, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 28.7, 31.2, 45.5, 57.1, 70.4, 115.7, 116.5, 120.5, 125.8, 126.4, 127.1, 129.7, 131.0, 132.0, 132.08, 133.5, 134.3, 135.5, 140.0, 148.3, 152.9, 189.3; FTIR (KBr, ν = cm^{-1}): 1649, 1722, 3334; HRMS (ESI+): m/z calcd. for $C_{22}H_{18}BrN_3NaO_6$ $[M+Na]^+$: 522.0277 found : 522.0271.

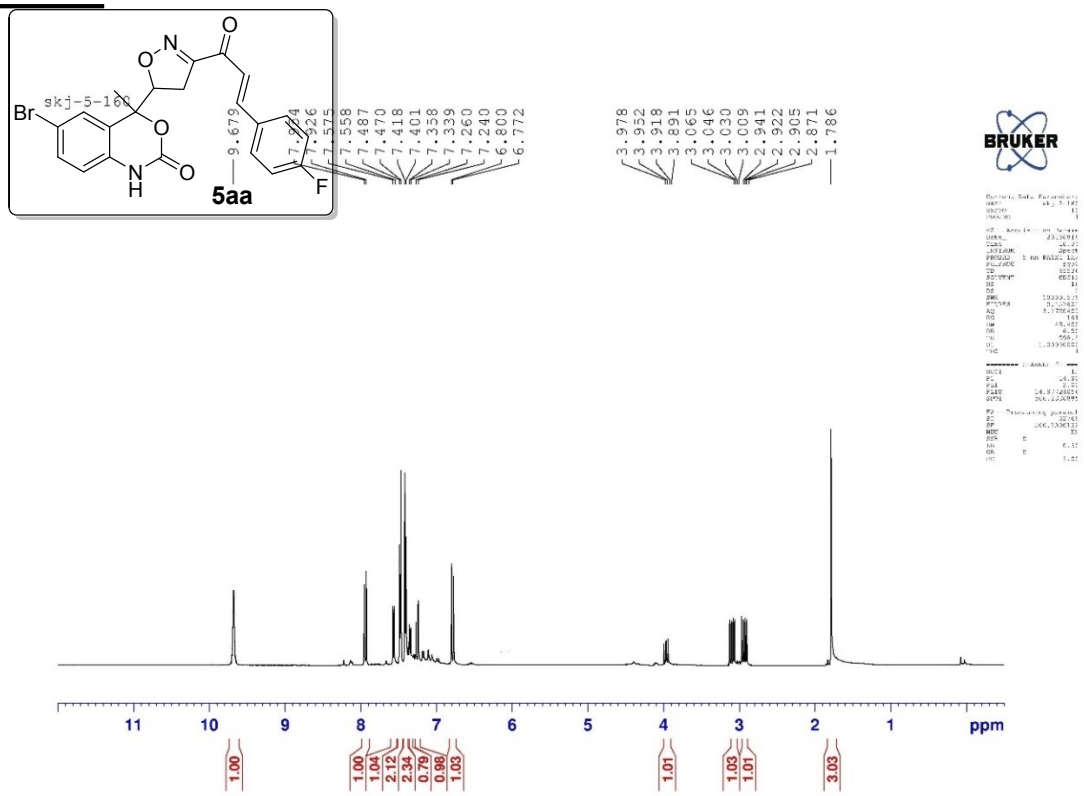
(*E*)-6-bromo-4-((3-(3-(4-hydroxyphenyl)acryloyl)-4,5-dihydroisoxazol-5-yl)methyl)-4-methyl-1H-benzo[d][1,3]oxazin-2(4H)-one (5bj)

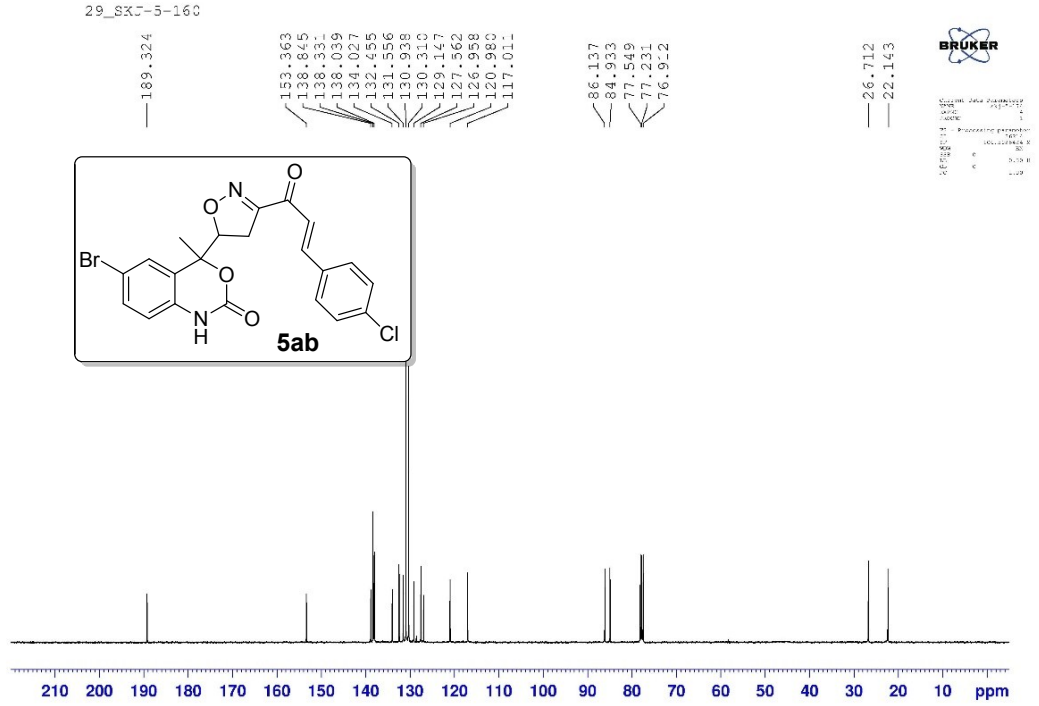


Yield: 0.4g (86%) as yellow solid; MP 194-196 °C; ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 1.70 (s, 3H), 1.91 (d, *J* = 8.0Hz, 2H), 2.93 - 2.96 (m, 1H), 3.01 - 3.04 (m, 1H), 3.19 - 3.24 (m, 1H), 6.78 (d, *J* = 13.5 Hz, 1H), 7.01 - 7.05 (m, 2H), 7.18 (d, *J* = 2.0 Hz, 1H), 7.24 (s, 1H), 7.27 (d, *J* = 8.0 Hz, 2H), 7.32 (dd, *J* = 2, 8.5 Hz, 1H), 7.54 (d, *J* = 8.5 Hz, 1H), 7.89 (d, *J*= 14.0 Hz, 1H), 9.47 (s, br, D_2O exchangeable, 1H), 9.71 (s, br, D_2O exchangeable, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ. 28.3, 30.5, 45.6, 58.2, 69.5,

116.5, 119.9, 120.7, 121.6, 126.4, 127.1, 130.6, 130.9, 132.1, 133.2, 137.3, 139.4, 153.1, 157.2, 188.6; FTIR (KBr, ν = cm^{-1}): 1643, 1724, 3432; HRMS (ESI+): m/z calcd. for $C_{22}H_{19}BrN_2NaO_5$ $[M+Na]^+$: 493.0375 found : 493.0377.

Spectra:-

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127.362
126.958
120.980
117.011
86.137
84.933
77.549
77.231
76.912
26.712
22.143
BRUKER
Br
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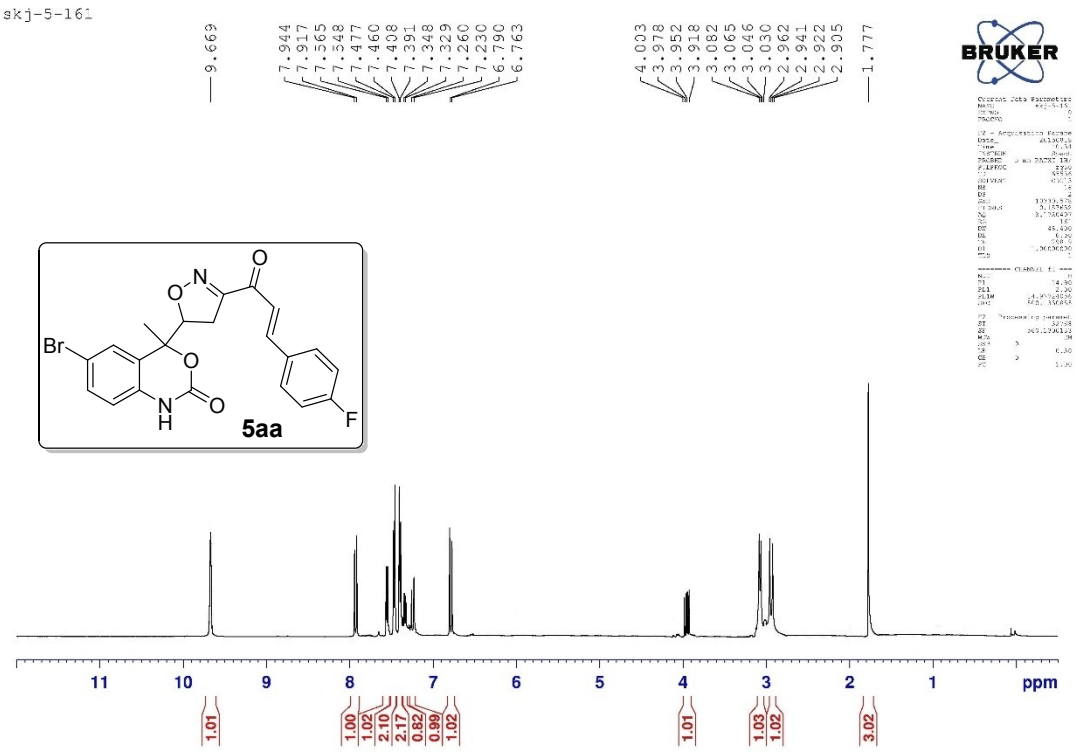
N
O
O
N
H
O
Cl
5ab
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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7.917
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7.548
7.477
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7.391
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7.329
7.260
7.230
6.790
6.763
4.003
3.978
3.952
3.918
3.082
3.065
3.046
3.030
2.962
2.941
2.922
2.905
1.777
BRUKER
Br
O
N
O
O
N
H
O
F
5aa
11 10 9 8 7 6 5 4 3 2 1 ppm
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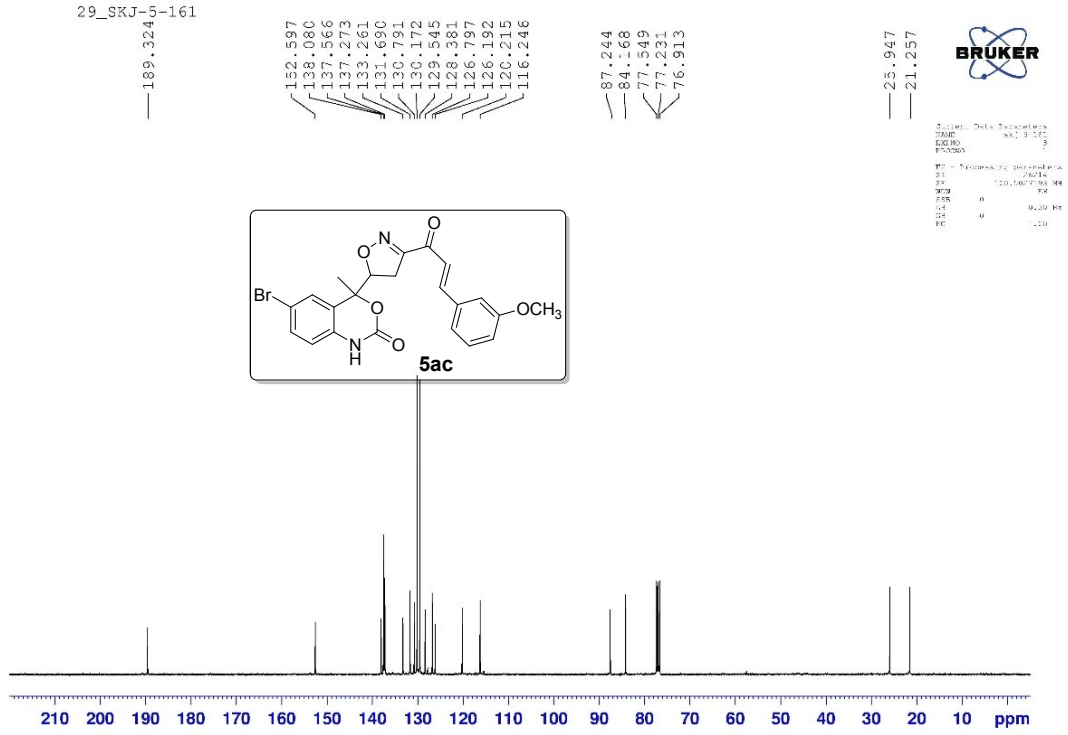
1.00
1.02
2.10
2.17
0.82
0.99
1.02
1.01
1.03
1.02
3.02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126.192
120.215
116.246
87.244
84.168
77.549
77.231
76.913
25.947
21.257
BRUKER
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H
O
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5ac
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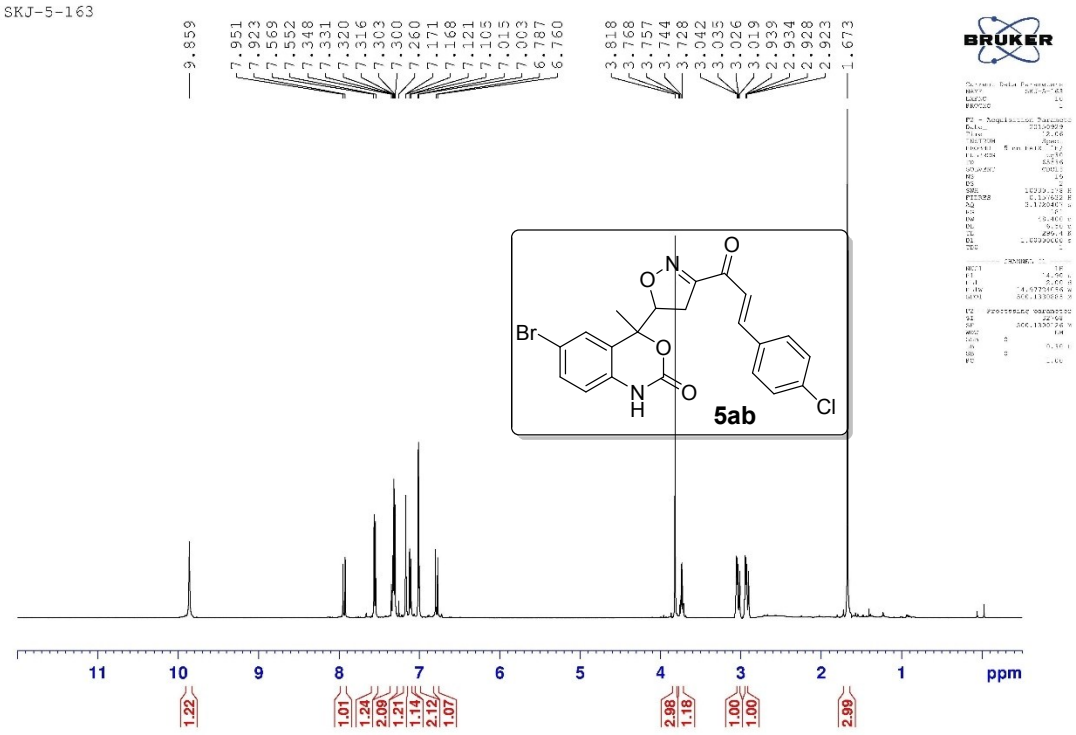
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7.003
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3.757
3.744
3.728
3.042
3.035
3.026
3.019
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2.934
2.928
2.923
1.673
BRUKER
Br
O
N
O
O
O
N
H
Cl
5ab
11 10 9 8 7 6 5 4 3 2 1 ppm
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2.98
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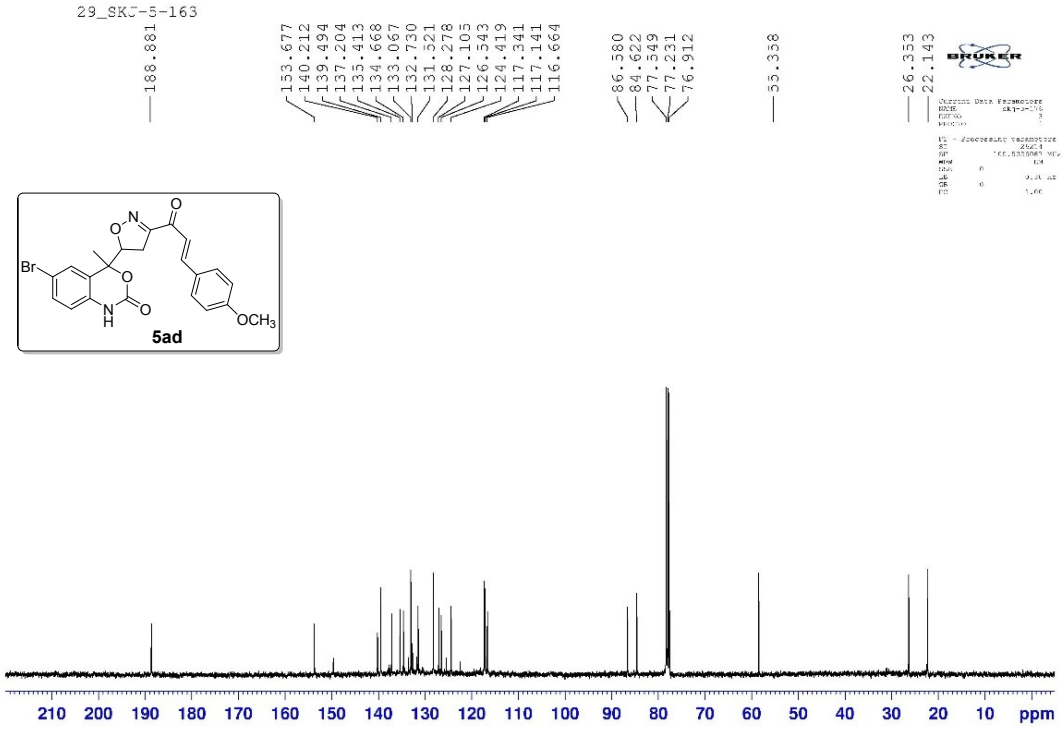
1.00
1.00
2.99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117.141
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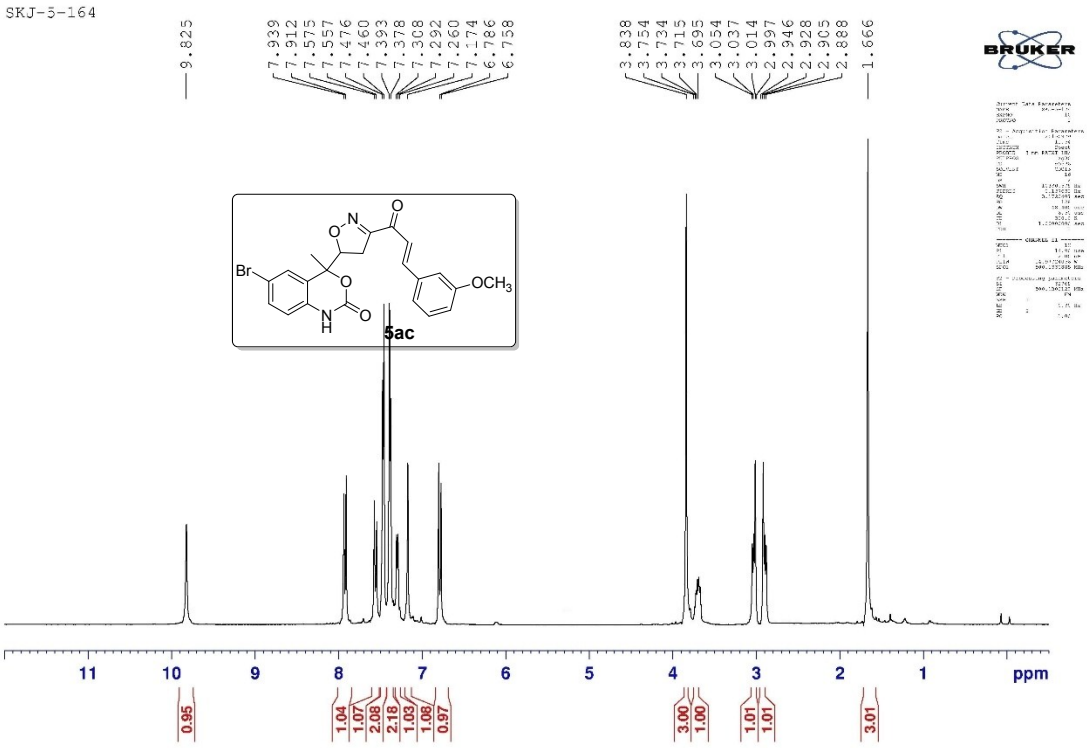
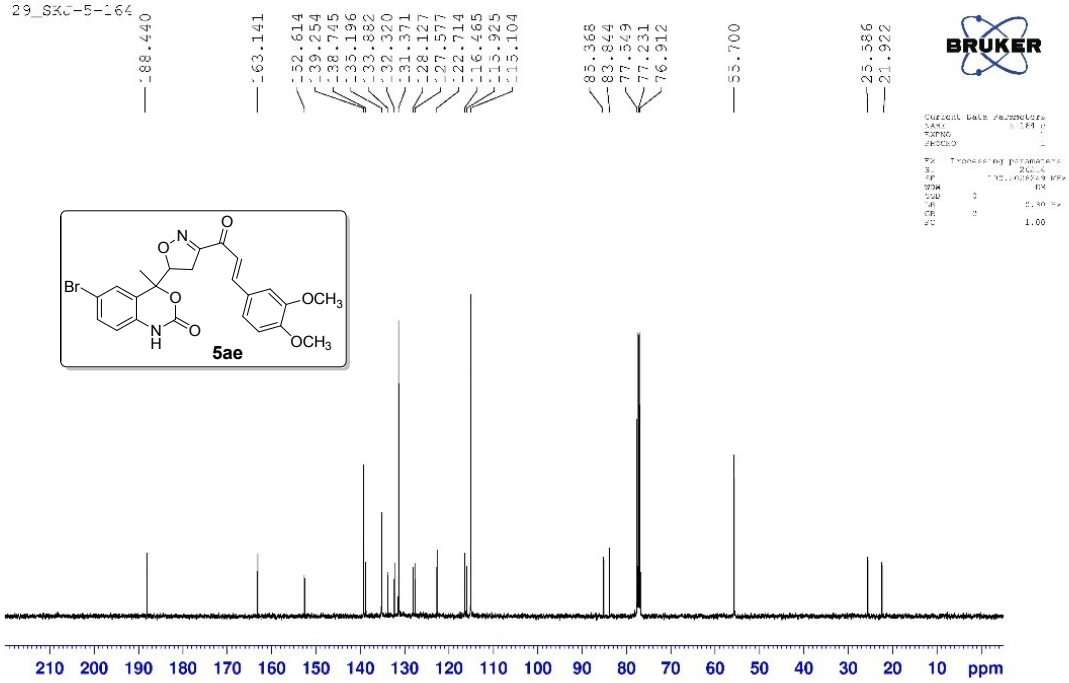
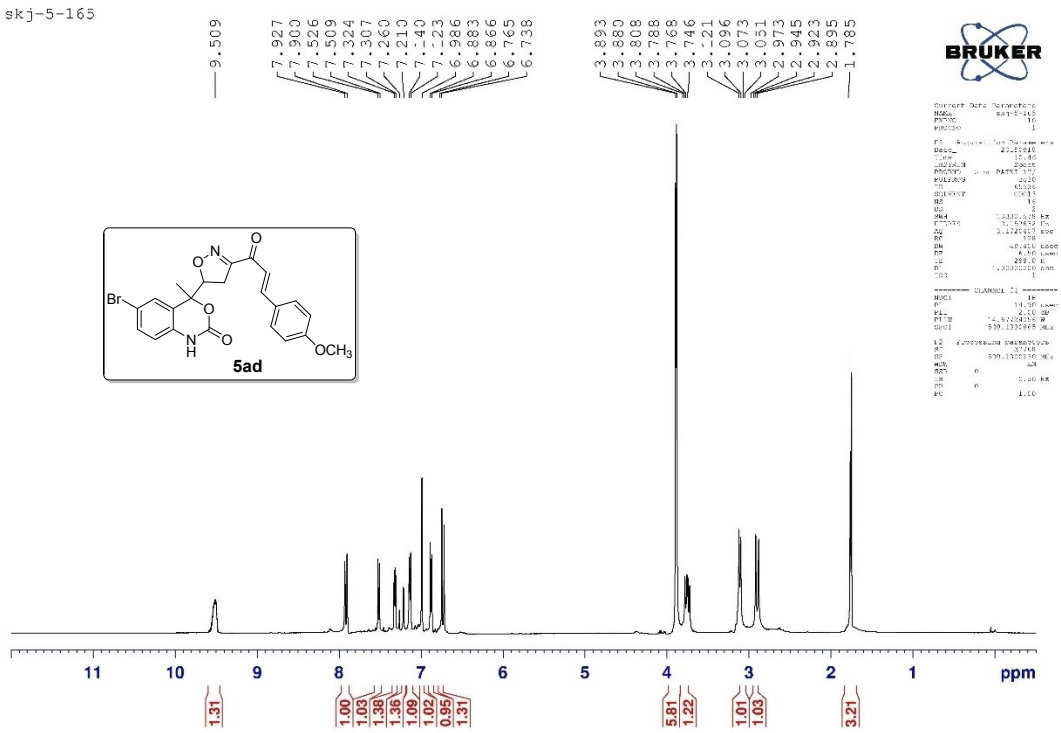
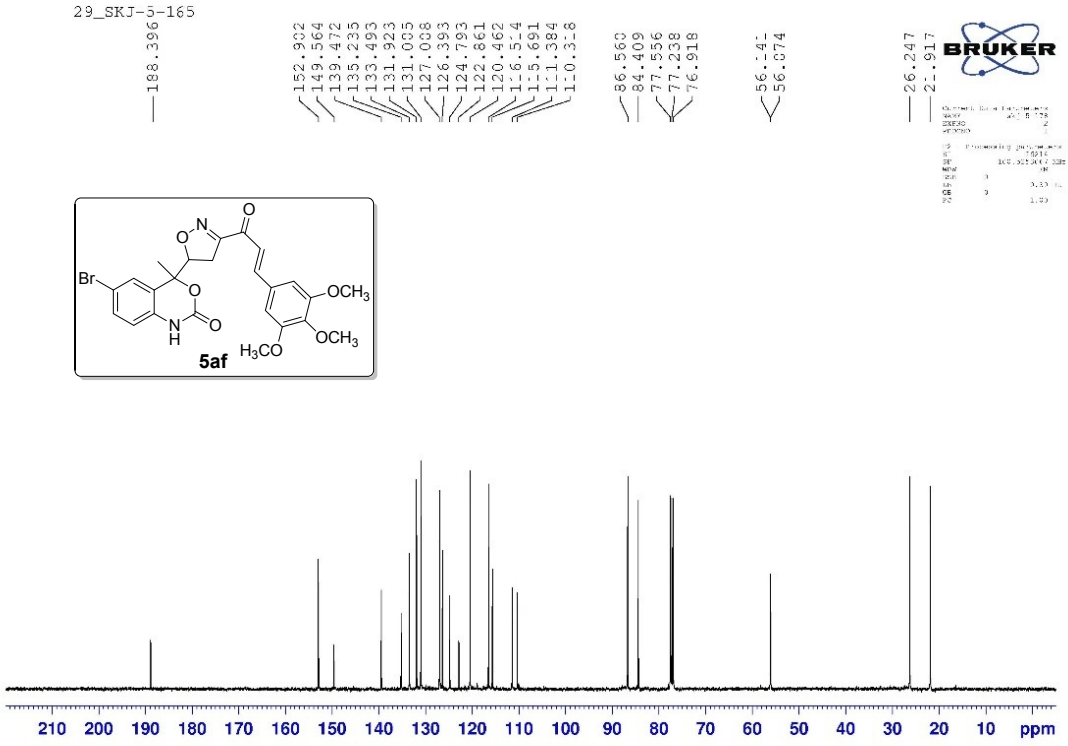
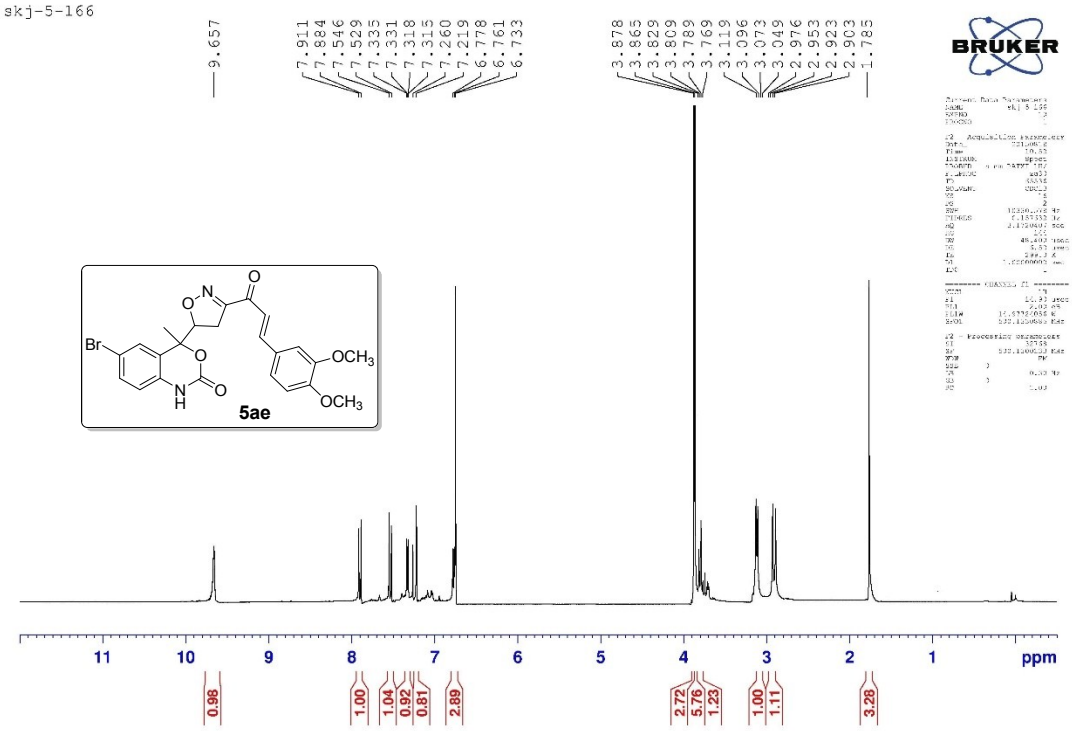
77.549
77.231
76.912
55.358
26.353
22.143
BRUKER
Br
O
N
O
O
N
H
O
OCH3
5ad
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

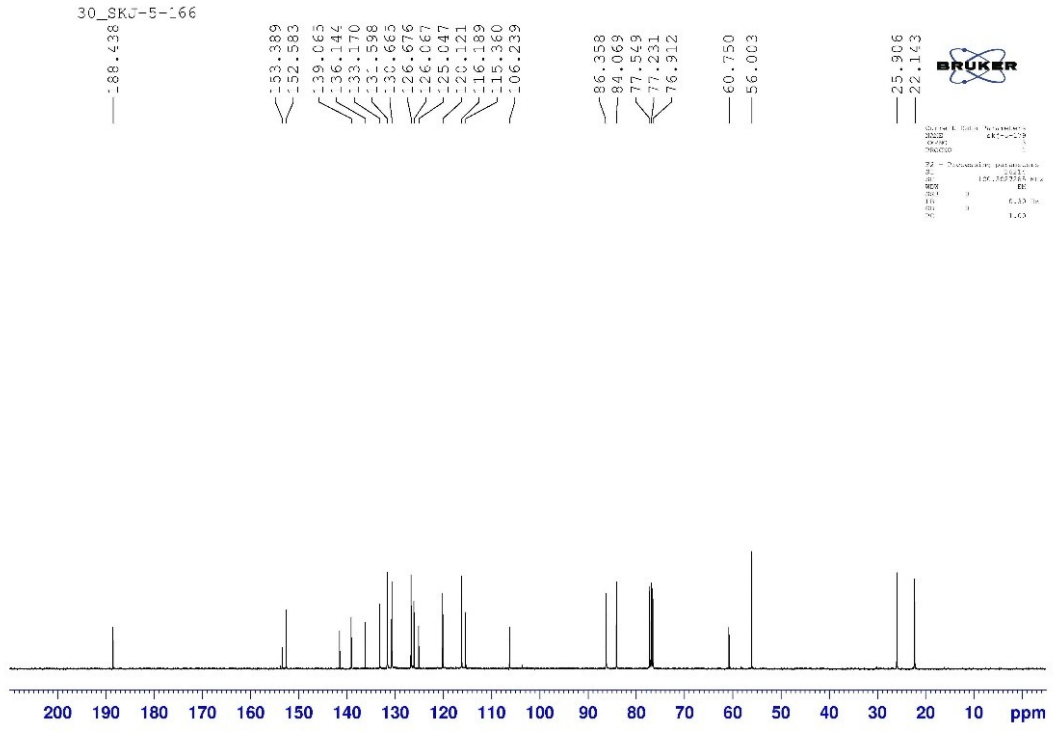

SKJ-5-164
9.825
7.939
7.912
7.575
7.557
7.476
7.460
7.393
7.378
7.308
7.292
7.260
7.174
6.786
6.758
3.838
3.754
3.734
3.715
3.695
3.054
3.037
3.014
2.997
2.946
2.928
2.905
2.888
1.666
BRUKER
Br
O
N
O
O
N
H
O
OCH3
5ac
11 10 9 8 7 6 5 4 3 2 1 ppm
0.95
1.04
1.07
2.08
2.18
1.03
1.08
0.97
3.00
1.00
1.01
1.01
3.01

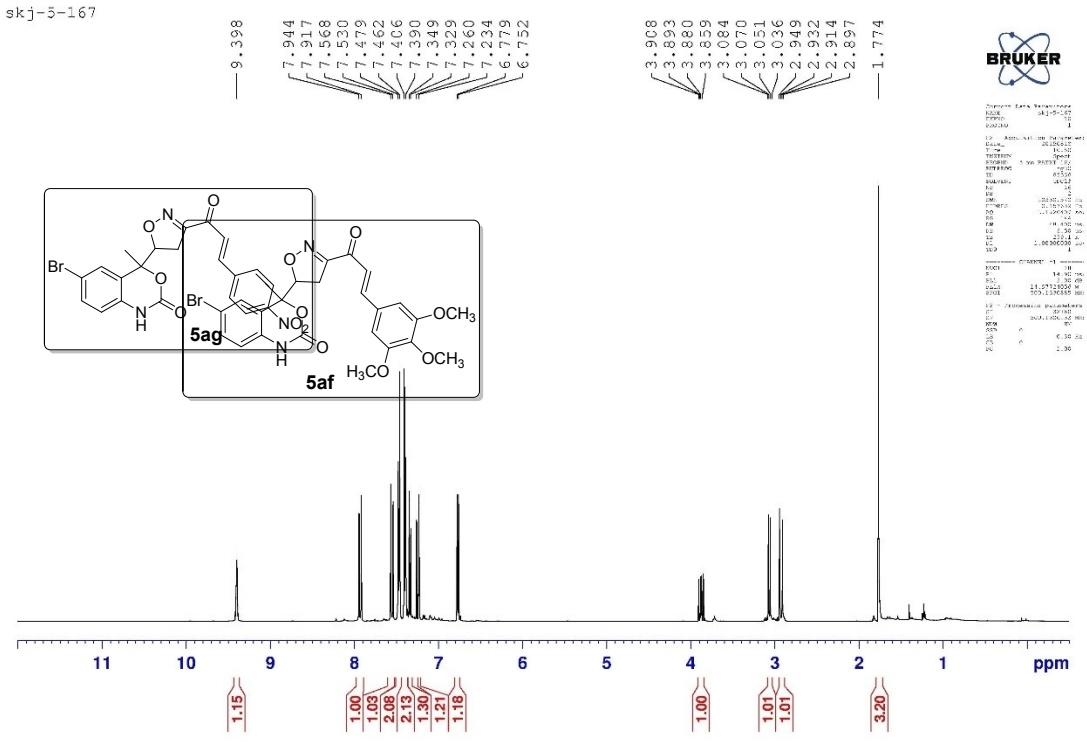

29_SKJ-5-164
188.440
163.141
152.614
139.254
138.745
135.196
133.882
132.320
131.371
128.127
127.577
122.714
116.465
115.925
115.104
85.368
83.844
77.549
77.231
76.912
55.700
25.386
21.922
BRUKER
Br
O
N
O
O
N
H
O
OCH3
OCH3
5ae
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

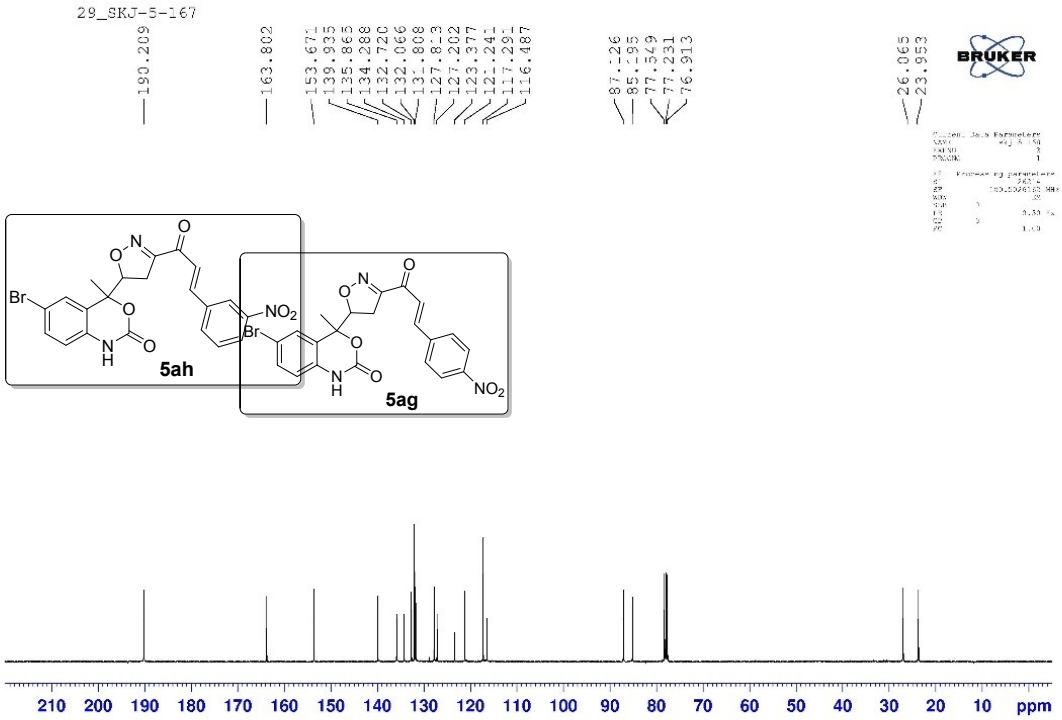

skj-5-165
9.509
7.927
7.900
7.526
7.509
7.324
7.307
7.260
7.210
7.140
7.123
6.986
6.883
6.866
6.765
6.738
3.893
3.880
3.808
3.788
3.768
3.746
3.121
3.096
3.073
3.051
2.973
2.945
2.923
2.895
1.785
BRUKER
Br
O
N
O
O
N
H
O
OCH3
5ad
11 10 9 8 7 6 5 4 3 2 1 ppm
1.31
1.00
1.03
1.38
1.36
1.09
1.02
0.95
1.31
5.81
1.22
1.01
1.03
3.21

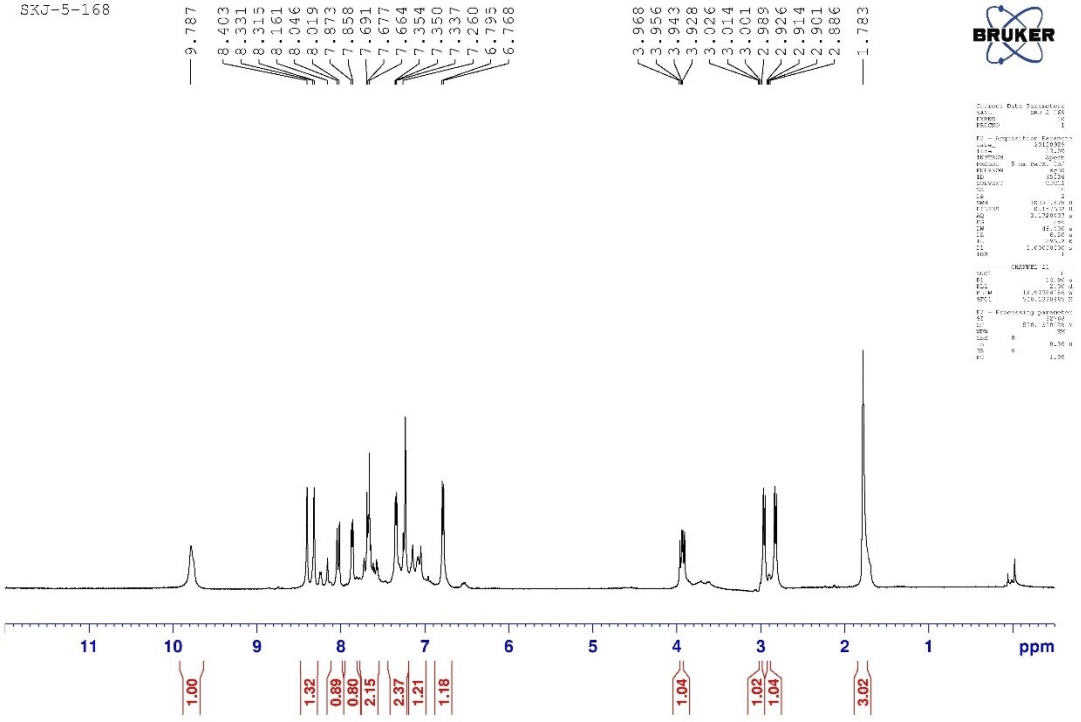

29_SKJ-5-165
188.396
152.932
149.564
139.472
135.235
133.493
131.923
131.005
127.038
126.393
124.793
122.861
120.462
116.5.4
115.691
111.384
110.318
86.560
84.409
77.556
77.238
76.918
56.141
56.074
26.247
21.917
BRUKER
Br
O
N
O
O
N
H
O
OCH3
H3CO
OCH3
5af
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

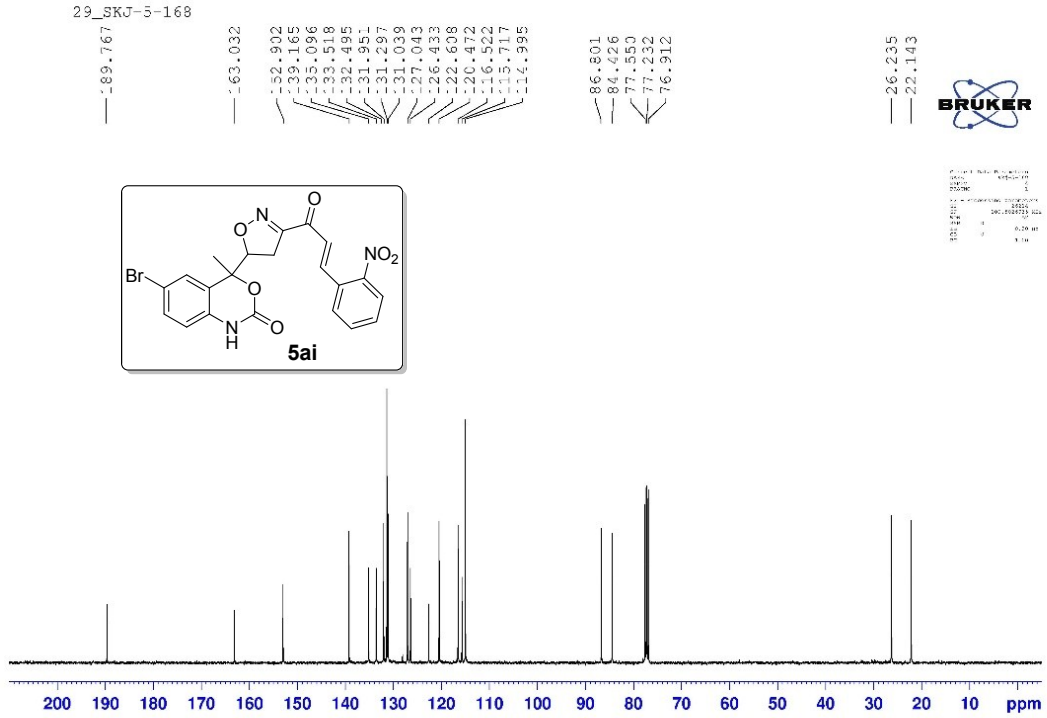

skj-5-166
9.657
7.911
7.884
7.546
7.529
7.335
7.331
7.318
7.315
7.260
7.219
6.778
6.761
6.733
3.878
3.865
3.829
3.809
3.789
3.769
3.119
3.096
3.073
3.049
2.976
2.953
2.923
2.903
1.785
BRUKER
Br
O
N
O
O
N
H
O
OCH3
OCH3
5ae
11 10 9 8 7 6 5 4 3 2 1 ppm
0.98
1.00
1.04
0.92
0.81
2.89
2.72
5.76
1.23
1.00
1.11
3.28

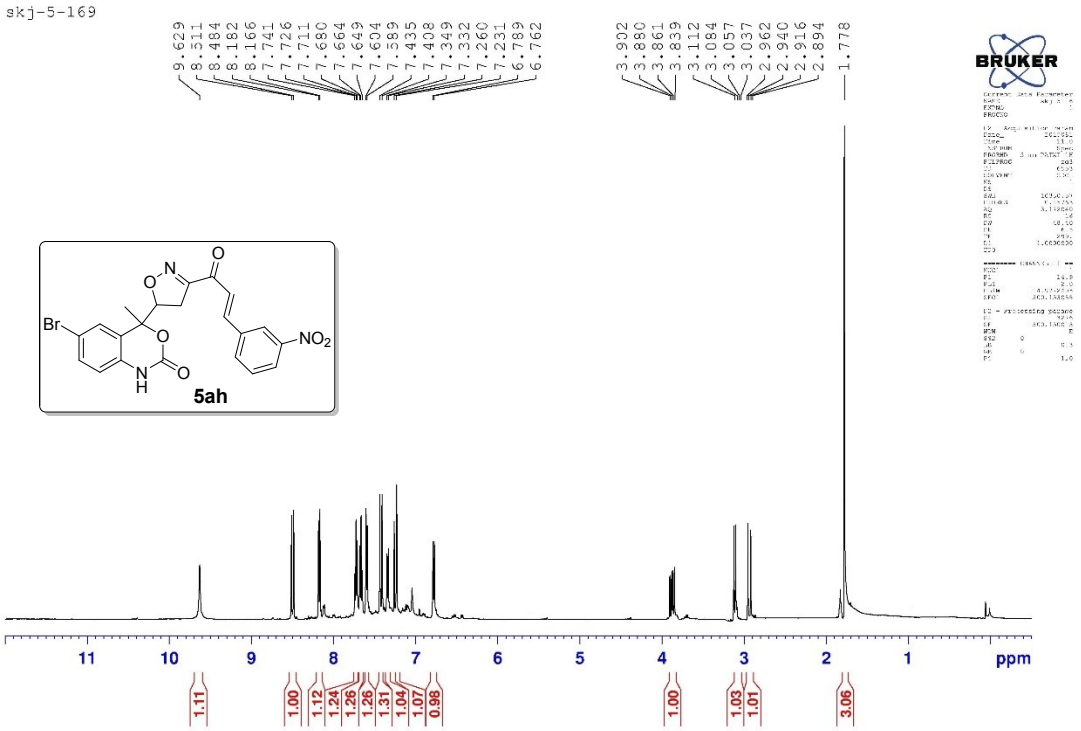

30_SKJ-5-166
188.438
153.389
152.583
139.065
136.144
133.170
131.598
130.665
126.676
126.067
125.047
120.121
116.189
115.360
106.239
86.358
84.069
77.549
77.231
76.912
60.750
56.003
25.906
22.143
BRUKER
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

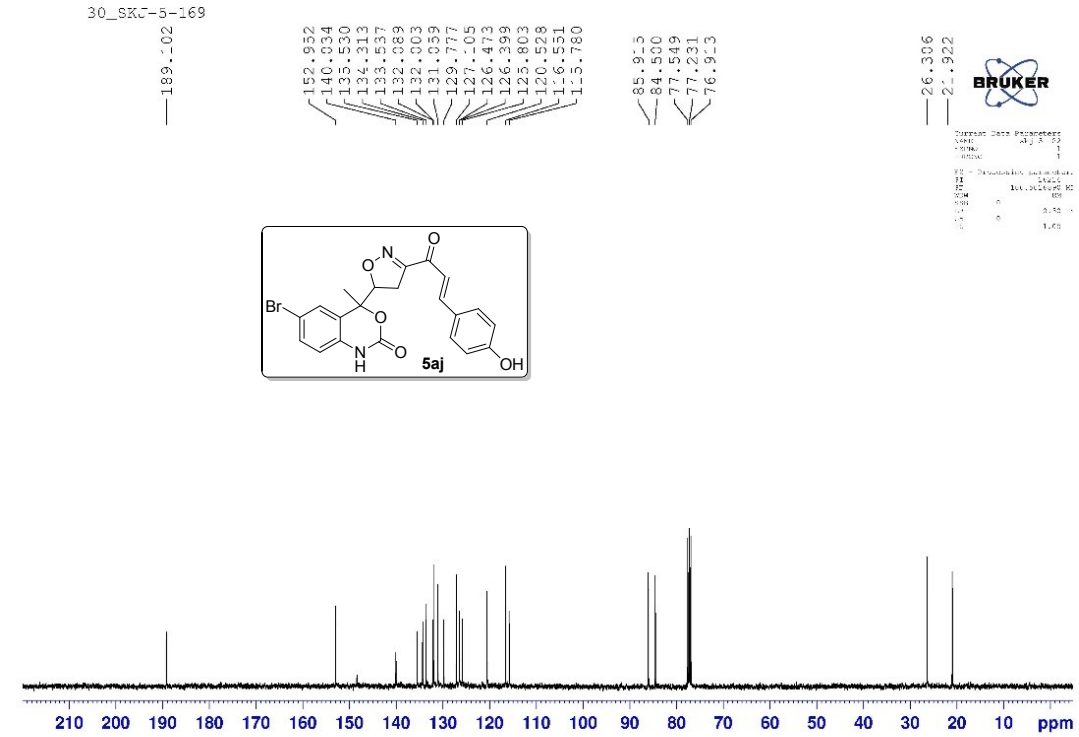

skj-5-167
9.398
7.944
7.917
7.568
7.530
7.479
7.462
7.406
7.390
7.349
7.329
7.260
7.234
6.779
6.752
3.908
3.893
3.880
3.859
3.084
3.070
3.051
3.036
2.949
2.932
2.914
2.897
1.774
BRUKER
5ag
5af
11 10 9 8 7 6 5 4 3 2 1 ppm
1.15
1.00
1.03
2.08
2.13
1.30
1.21
1.18
1.00
1.01
1.01
3.20

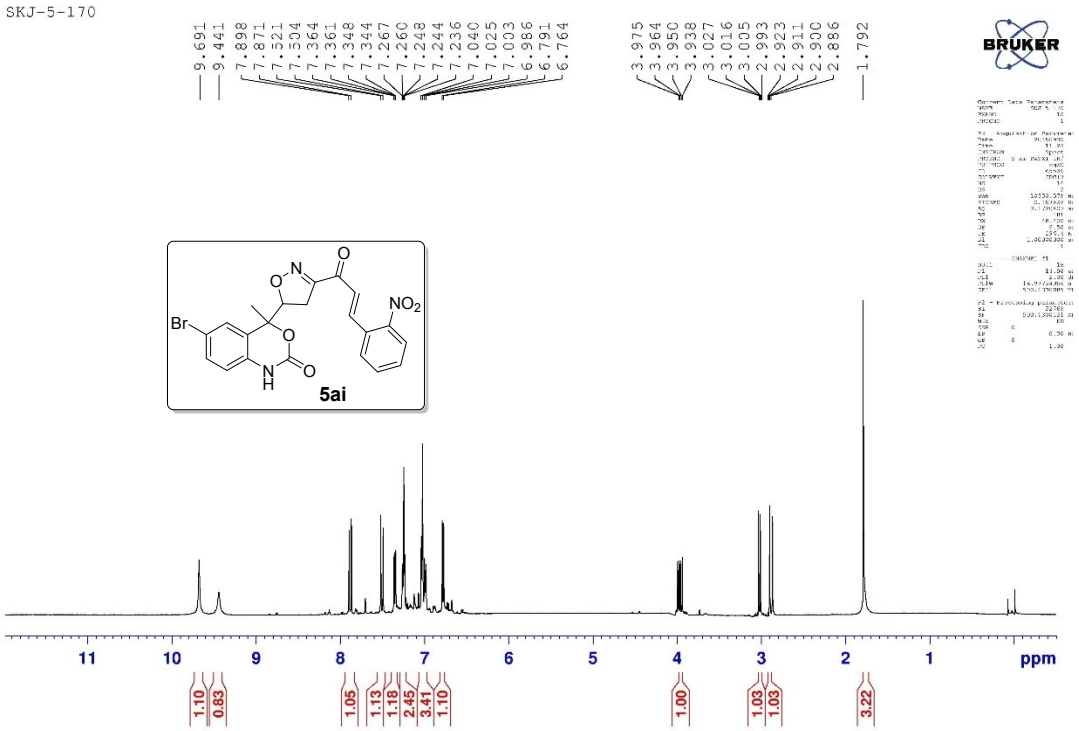

29_SKJ-5-167
190.209
163.802
153.671
139.935
135.865
134.288
132.720
132.066
131.808
127.813
127.202
123.377
122.241
117.291
116.487
87.126
85.195
77.349
77.231
76.913
26.065
23.953
BRUKER
Br
NO2
Br
NO2
5ah
5ag
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

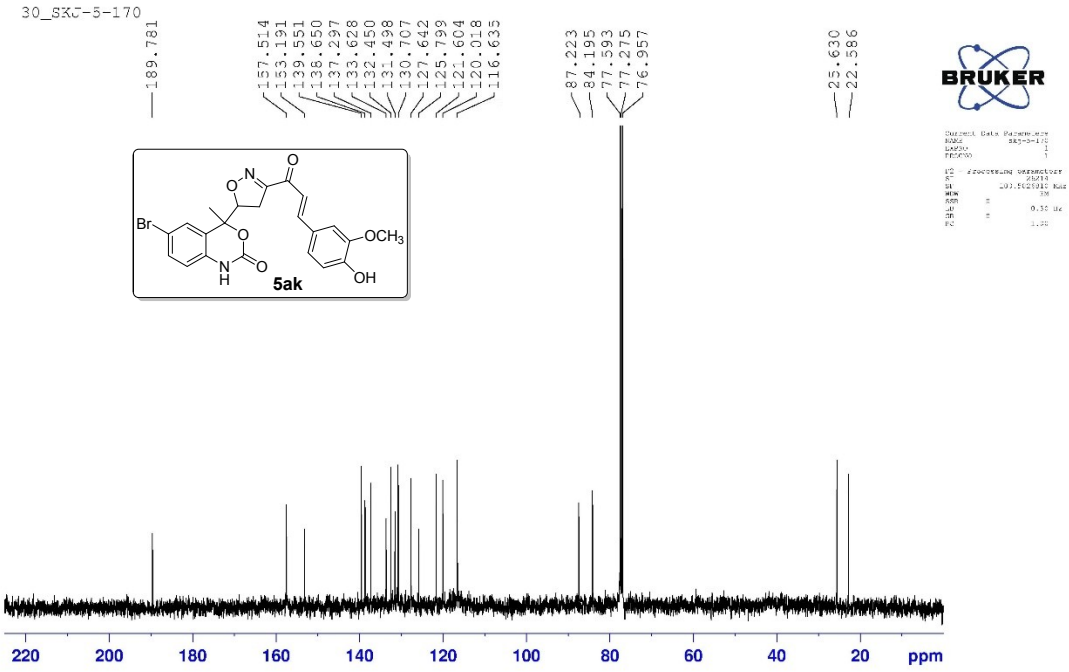

SKJ-5-168
9.787
8.403
8.331
8.315
8.161
8.046
8.019
7.873
7.858
7.691
7.677
7.664
7.354
7.350
7.337
7.260
6.795
6.768
3.968
3.956
3.943
3.928
3.026
3.014
3.001
2.989
2.926
2.914
2.901
2.886
1.783
BRUKER
11 10 9 8 7 6 5 4 3 2 1 ppm
1.00
1.32
0.89
0.80
2.15
2.37
1.21
1.18
1.04
1.02
1.04
3.02

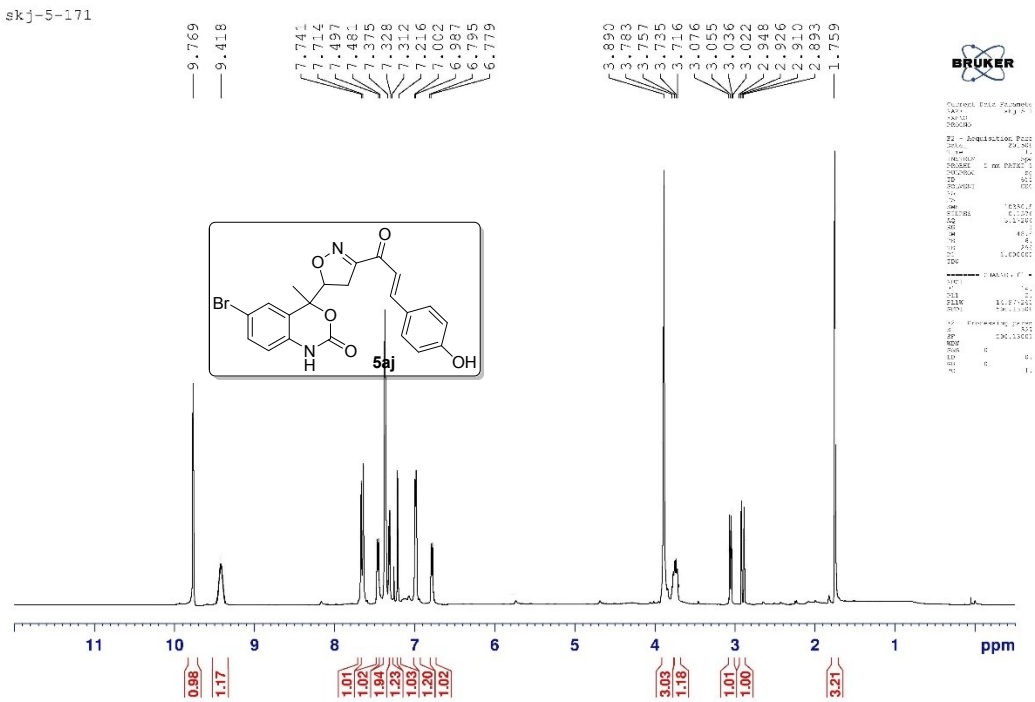

29_SKJ-5-168
189.767
163.032
152.902
139.165
135.096
133.518
132.495
131.951
131.297
131.039
127.043
126.433
122.608
120.472
116.522
113.717
114.995
86.801
84.426
77.550
77.232
76.912
26.235
22.143
BRUKER
Br
O
N
O
NO2
O
N
H
O
5ai
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

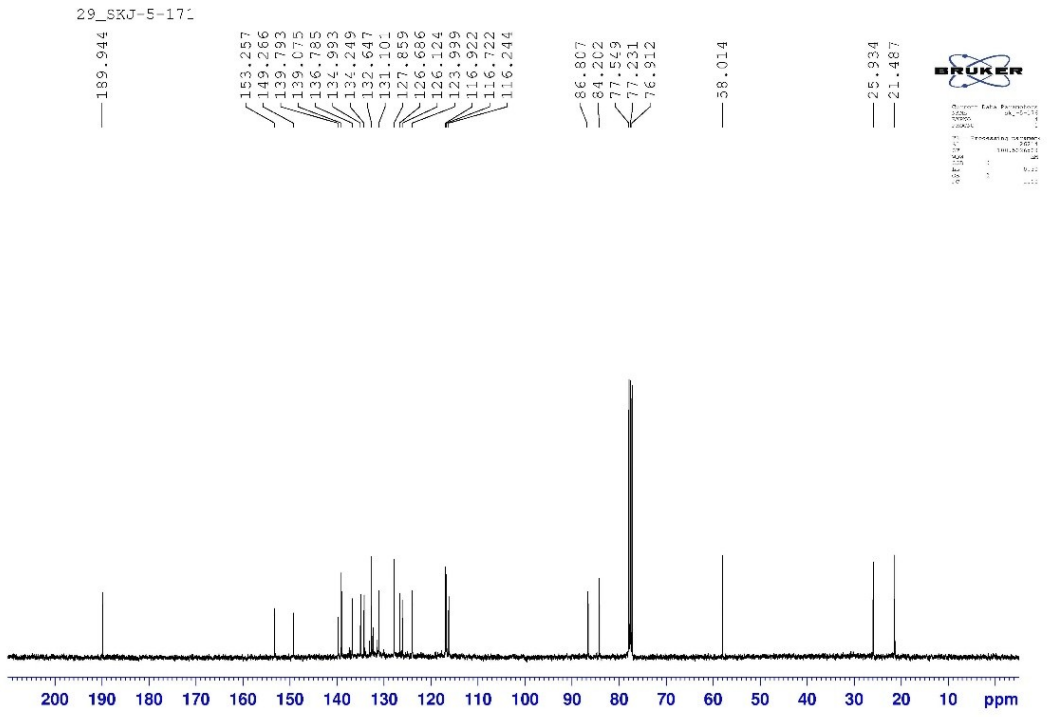

skj-5-169
9.629
8.511
8.484
8.182
8.166
7.741
7.726
7.711
7.680
7.664
7.649
7.604
7.589
7.435
7.408
7.349
7.332
7.260
7.231
6.789
6.762
3.902
3.880
3.861
3.839
3.112
3.084
3.057
3.037
2.962
2.940
2.916
2.894
1.778
BRUKER
Br
O
N
O
NO2
O
N
H
O
5ah
11 10 9 8 7 6 5 4 3 2 1 ppm
1.11
1.00
1.12
1.24
1.26
1.26
1.31
1.04
1.07
0.98
1.00
1.03
1.01
3.06

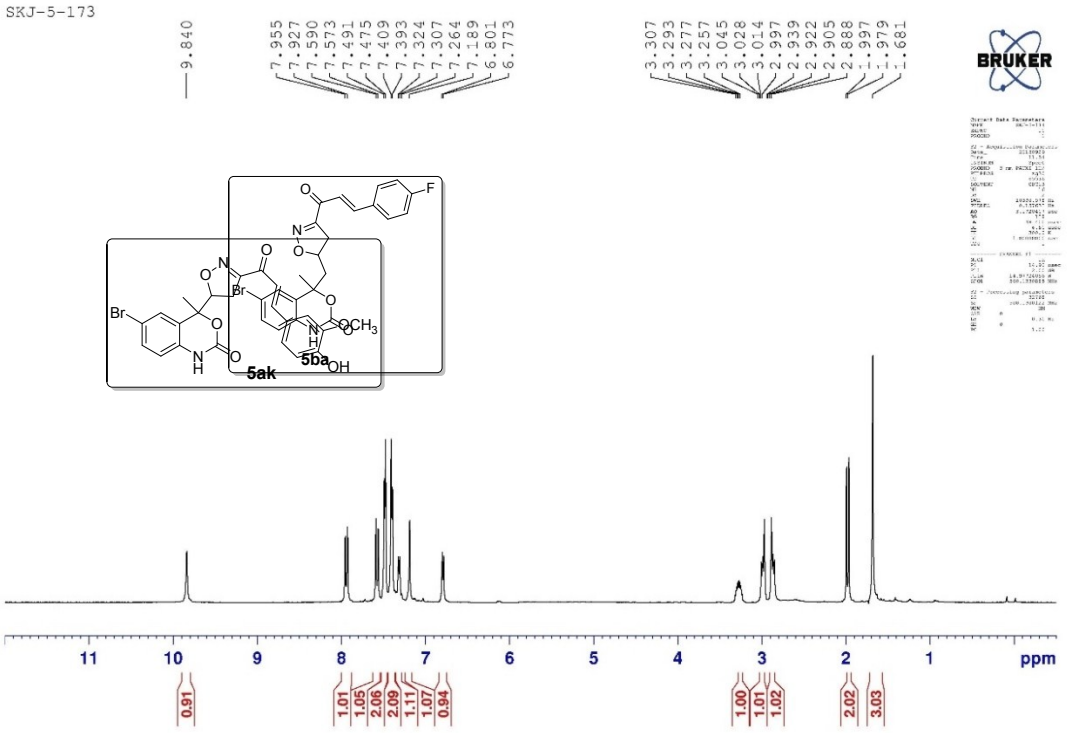

30_SKJ-5-169
189.102
152.932
140.034
135.530
134.313
133.537
132.089
132.003
131.059
129.777
127.005
126.473
126.399
125.803
120.528
116.551
115.780
85.915
84.500
77.549
77.231
76.913
26.306
22.922
BRUKER
Br
O
N
O
O
N
H
O
OH
5aj
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

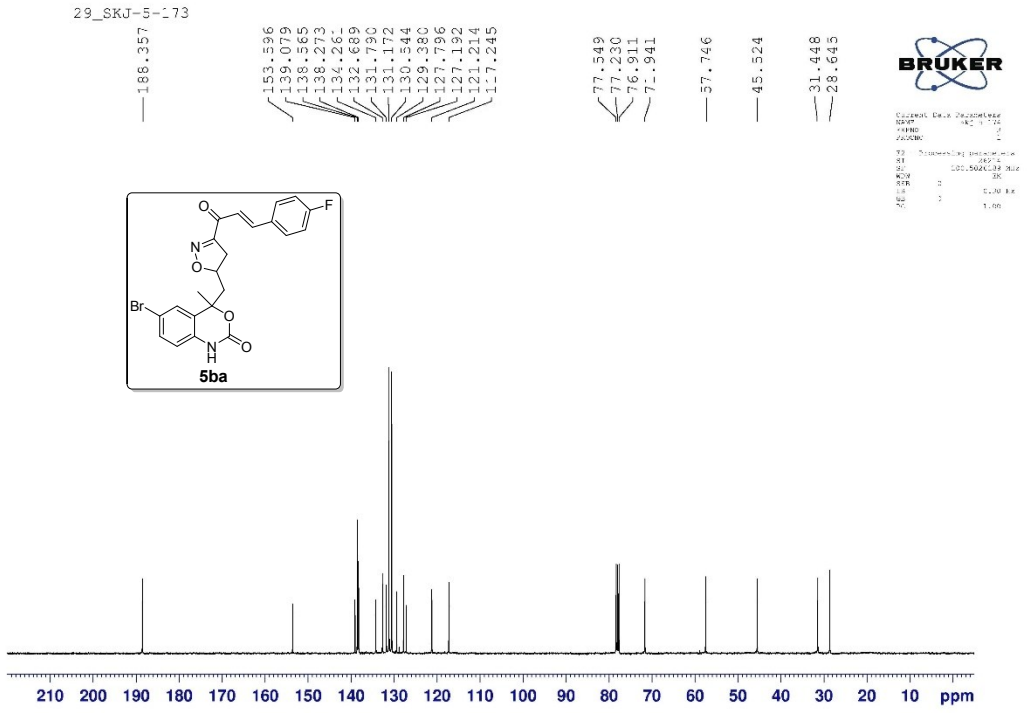

SKJ-5-170
9.691
9.441
7.898
7.871
7.521
7.504
7.364
7.361
7.348
7.344
7.267
7.260
7.248
7.244
7.236
7.040
7.025
7.003
6.986
6.791
6.764
3.975
3.964
3.950
3.938
3.027
3.016
3.005
2.993
2.923
2.911
2.900
2.886
1.792
BRUKER
Br
O
N
O
O
N
H
O
NO2
5ai
11 10 9 8 7 6 5 4 3 2 1 ppm
1.10
0.83
1.05
1.13
1.18
2.45
3.41
1.10
1.00
1.03
1.03
3.22

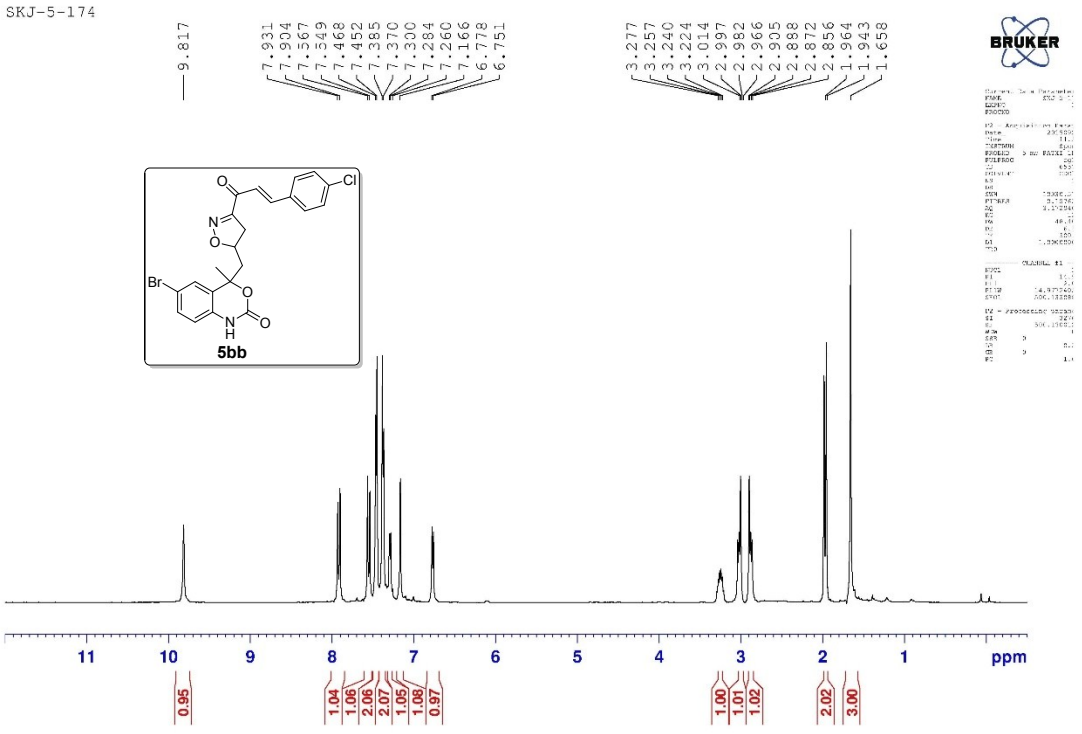

30_SKJ-5-170
189.781
157.514
153.191
139.551
138.650
137.297
133.628
132.450
131.498
130.707
127.642
125.799
121.604
120.018
116.635
87.223
84.195
77.593
77.275
76.957
25.630
22.586
BRUKER
Br
O
N
O
O
N
H
O
OCH3
OH
5ak
220
200
180
160
140
120
100
80
60
40
20
ppm

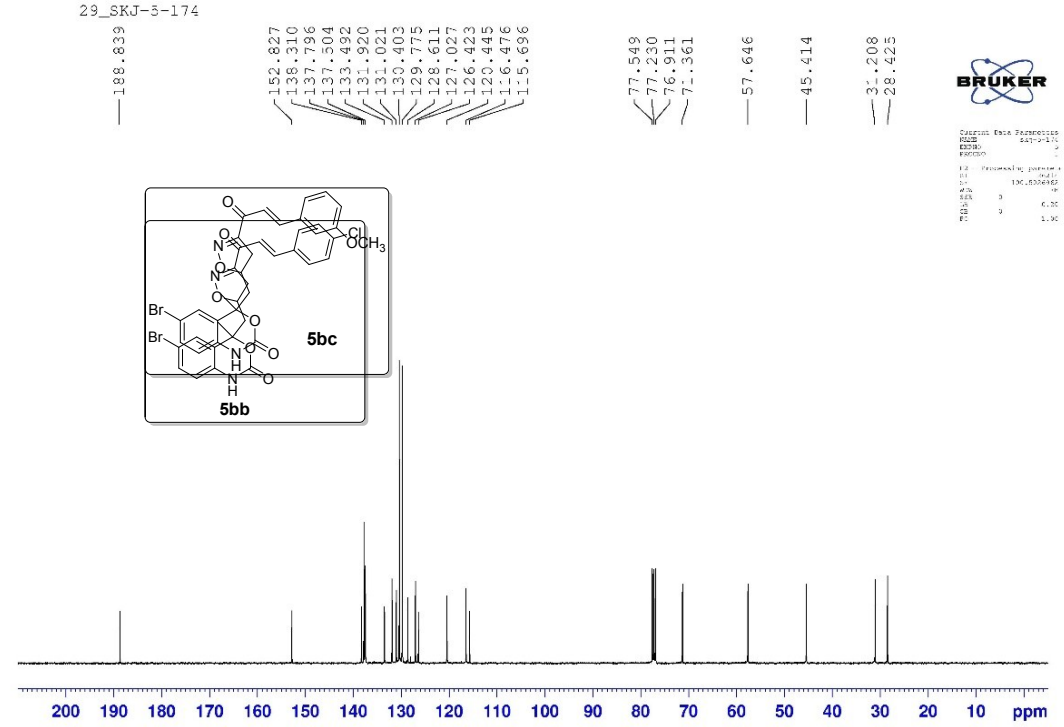

skj-5-171
9.769
9.418
7.744
7.714
7.497
7.481
7.375
7.328
7.312
7.216
7.002
6.987
6.795
6.779
3.890
3.783
3.757
3.735
3.716
3.076
3.055
3.036
3.022
2.948
2.926
2.910
2.893
1.759
BRUKER
Br
O
N
O
O
N
H
O
OH
5aj
11
10
9
8
7
6
5
4
3
2
1
ppm
0.98
1.17
1.01
1.02
1.94
1.23
1.03
1.20
1.02
3.03
1.18
1.01
1.00
3.21

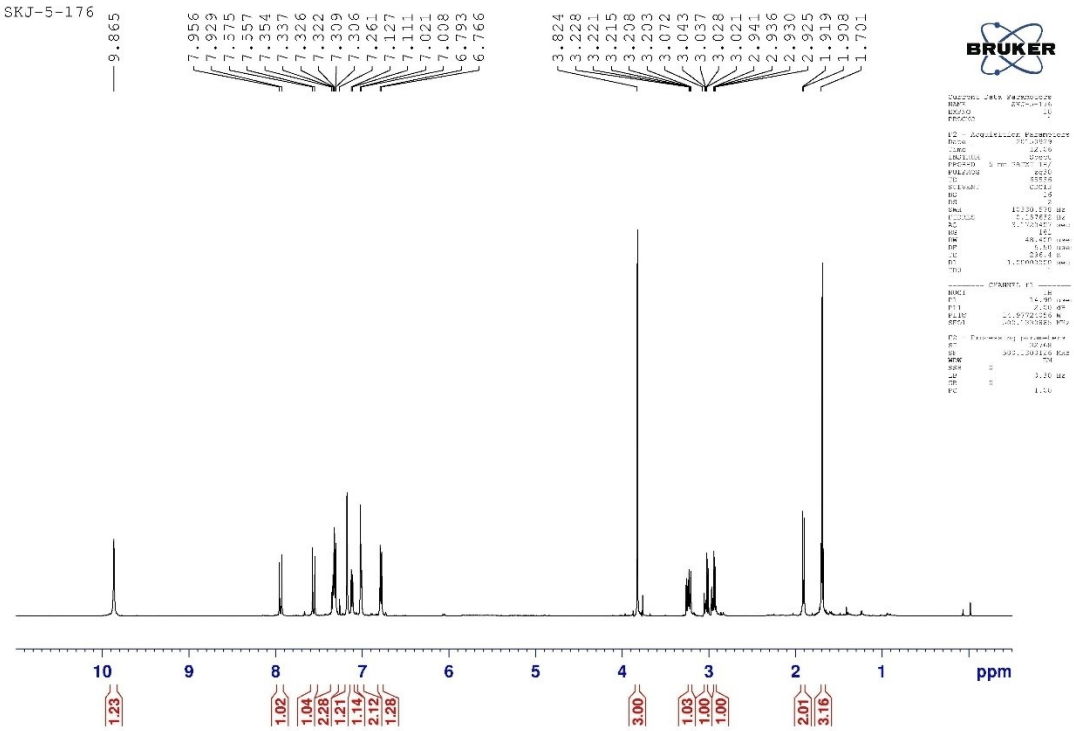

29_SKJ-5-171
189.944
153.257
149.266
139.793
139.075
136.785
134.993
134.249
132.647
131.101
127.859
126.686
126.124
123.999
116.922
116.722
116.244
86.807
84.202
77.549
77.231
76.912
38.014
25.934
21.487
BRUKER
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

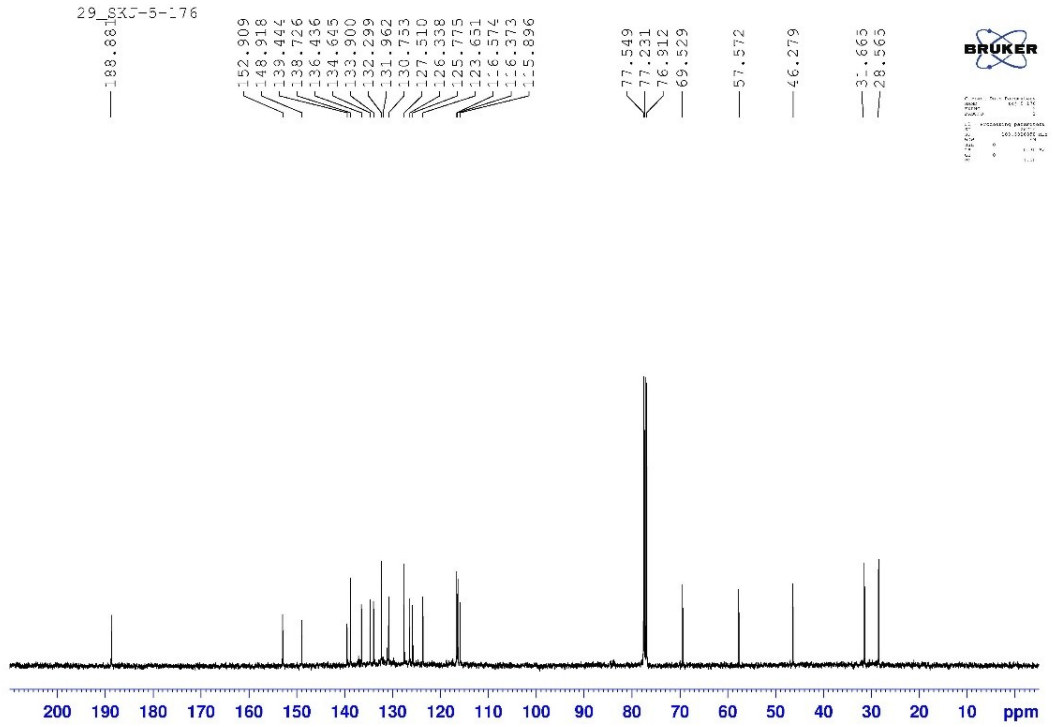

SKJ-5-173
9.840
7.955
7.927
7.590
7.573
7.491
7.475
7.409
7.393
7.324
7.307
7.264
7.189
6.801
6.773
3.307
3.293
3.277
3.257
3.045
3.028
3.014
2.997
2.939
2.922
2.905
2.888
1.997
1.979
1.681
BRUKER
5ak
5ba
11 10 9 8 7 6 5 4 3 2 1 ppm
0.91
1.01
1.05
2.06
2.09
1.11
1.07
0.94
1.00
1.01
1.02
2.02
3.03

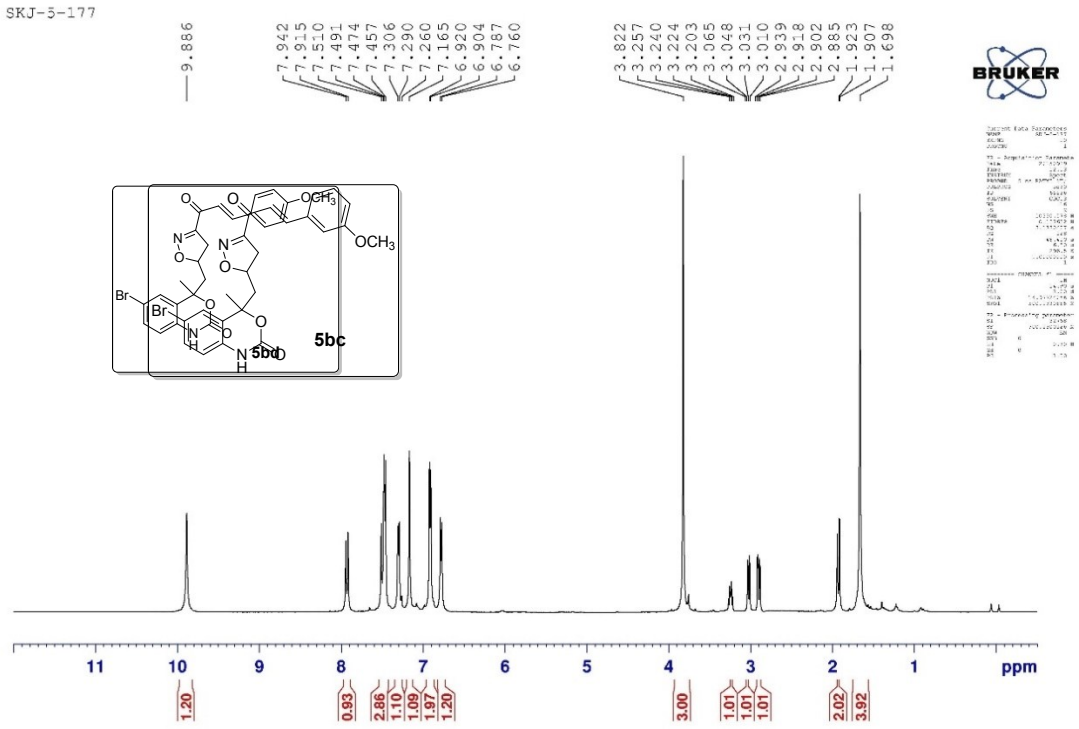

29_SKJ-5-173
188.357
153.596
139.079
138.565
138.273
134.261
132.689
131.790
131.172
130.544
129.380
127.796
127.192
121.214
117.245
77.549
77.230
76.911
57.746
45.524
31.448
28.645
BRUKER
5ba
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


SKJ-5-174
9.817
7.931
7.904
7.567
7.549
7.468
7.452
7.385
7.370
7.300
7.284
7.260
7.166
6.778
6.751
3.277
3.257
3.240
3.224
3.014
2.997
2.982
2.966
2.905
2.888
2.872
2.856
1.964
1.943
1.658
BRUKER
5bb
11 10 9 8 7 6 5 4 3 2 1 ppm
0.95
1.04
1.06
2.06
2.07
1.05
1.08
0.97
1.00
1.01
1.02
2.02
3.00


29_SKJ-5-174
188.839
152.827
138.310
137.796
137.504
133.492
131.920
131.021
130.403
129.775
128.611
127.027
126.423
120.445
116.476
115.696
77.549
77.230
76.911
57.646
45.414
31.208
28.425
BRUKER
5bc
5bb
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

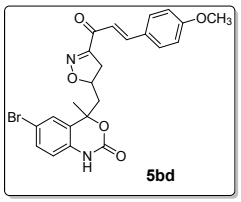

SKJ-5-176
9.865
7.956
7.929
7.575
7.557
7.354
7.337
7.326
7.322
7.309
7.306
7.261
7.127
7.111
7.021
7.008
6.793
6.766
3.824
3.228
3.221
3.215
3.208
3.203
3.072
3.043
3.037
3.028
3.021
2.941
2.936
2.930
2.925
1.919
1.908
1.701
BRUKER
10 9 8 7 6 5 4 3 2 1 ppm
1.23
1.02
1.04
2.26
1.21
1.14
2.12
1.28
3.00
1.03
1.00
1.00
2.01
3.16


29_SKJ-5-176
188.881
152.909
148.918
139.444
138.726
136.436
134.665
133.900
132.299
131.962
130.753
127.510
126.338
125.775
123.651
116.574
116.373
115.896
77.549
77.231
76.912
69.529
57.572
46.279
31.665
29.563
BRUKER
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

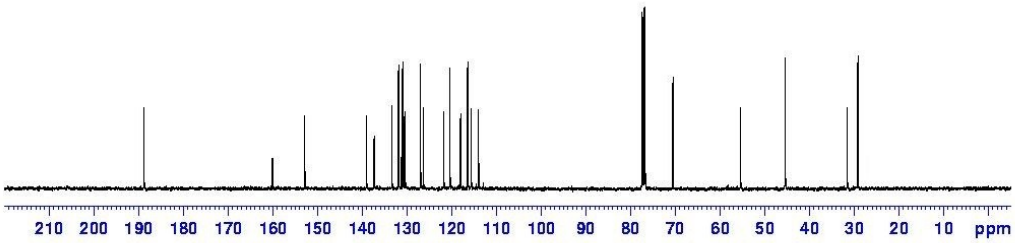

SKJ-5-177
9.886
7.942
7.915
7.510
7.491
7.474
7.457
7.306
7.290
7.260
7.165
6.920
6.904
6.787
6.760
3.822
3.257
3.240
3.224
3.203
3.065
3.048
3.031
3.010
2.939
2.918
2.902
2.885
1.923
1.907
1.698
BRUKER
OCH3
OCH3
Br
Br
5bc
11 10 9 8 7 6 5 4 3 2 1 ppm
1.20
0.93
2.86
1.10
1.09
1.97
1.20
3.00
1.01
1.01
1.01
2.02
3.92

29_SKJ-5-177

188.881
160.231
152.984
139.213
137.469
133.543
132.021
131.072
130.551
127.109
126.473
121.904
120.551
118.098
116.569
115.794
77.549
77.230
76.912
70.636
57.572
45.536
31.665
29.008

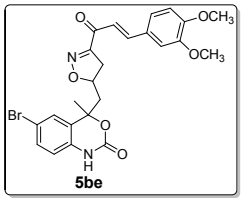


5bd

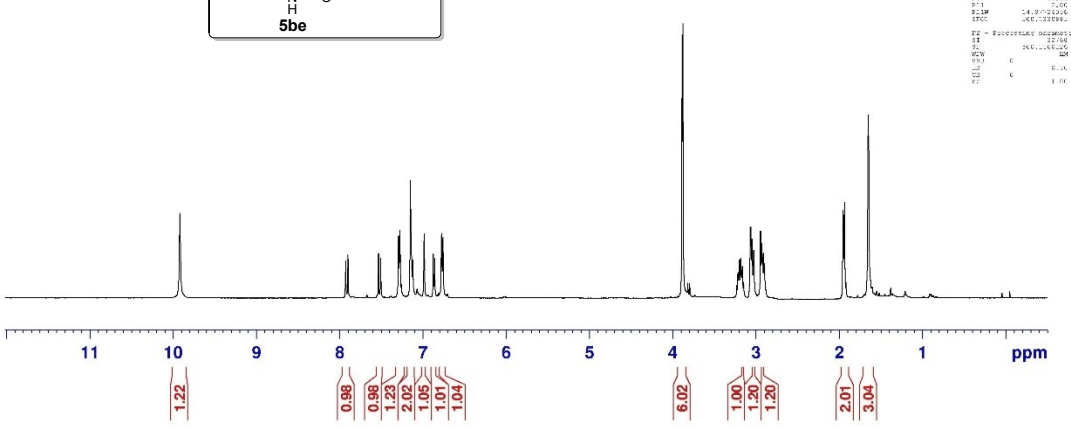


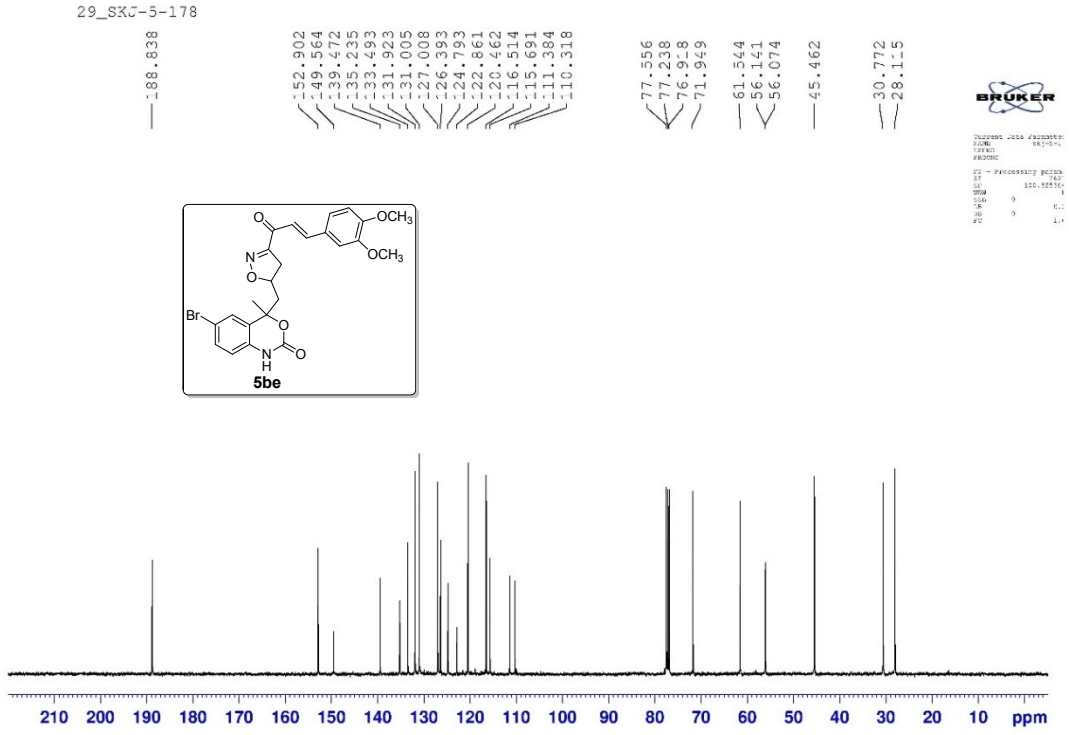
SKJ-5-178

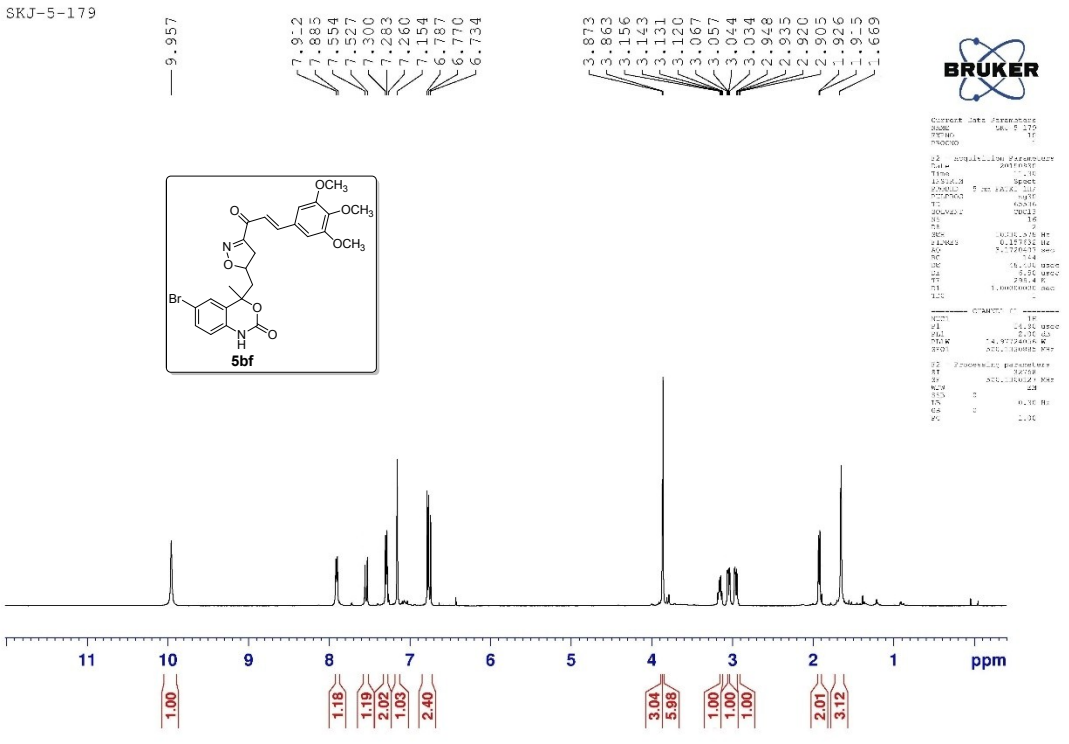
9.920
7.929
7.902
7.535
7.508
7.294
7.277
7.260
7.152
7.124
6.987
6.877
6.861
6.788
6.761
3.888
3.879
3.182
3.170
3.158
3.148
3.046
3.034
3.022
3.012
2.950
2.936
2.924
2.910
1.938
1.929
1.676

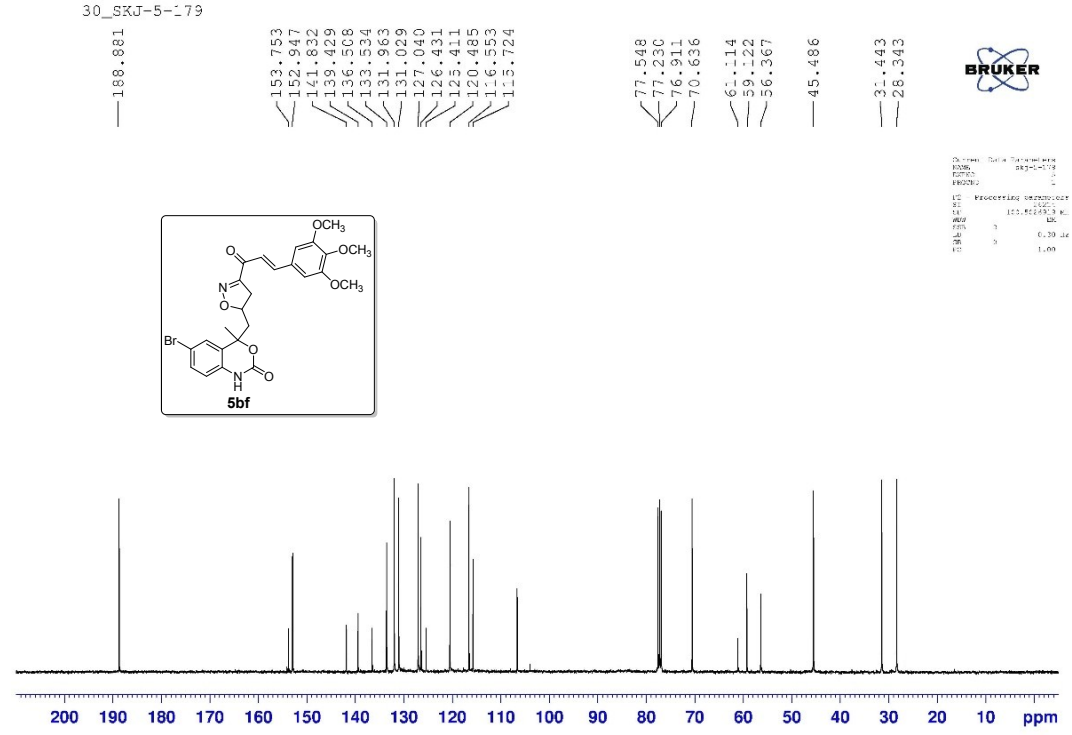


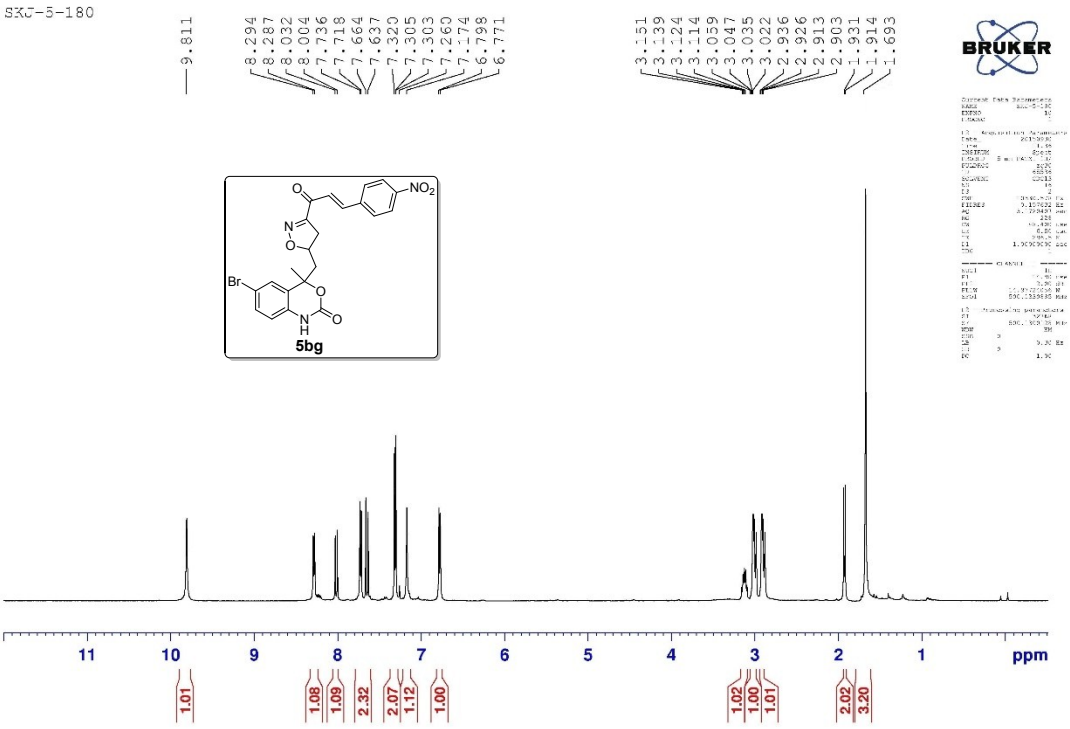
5be

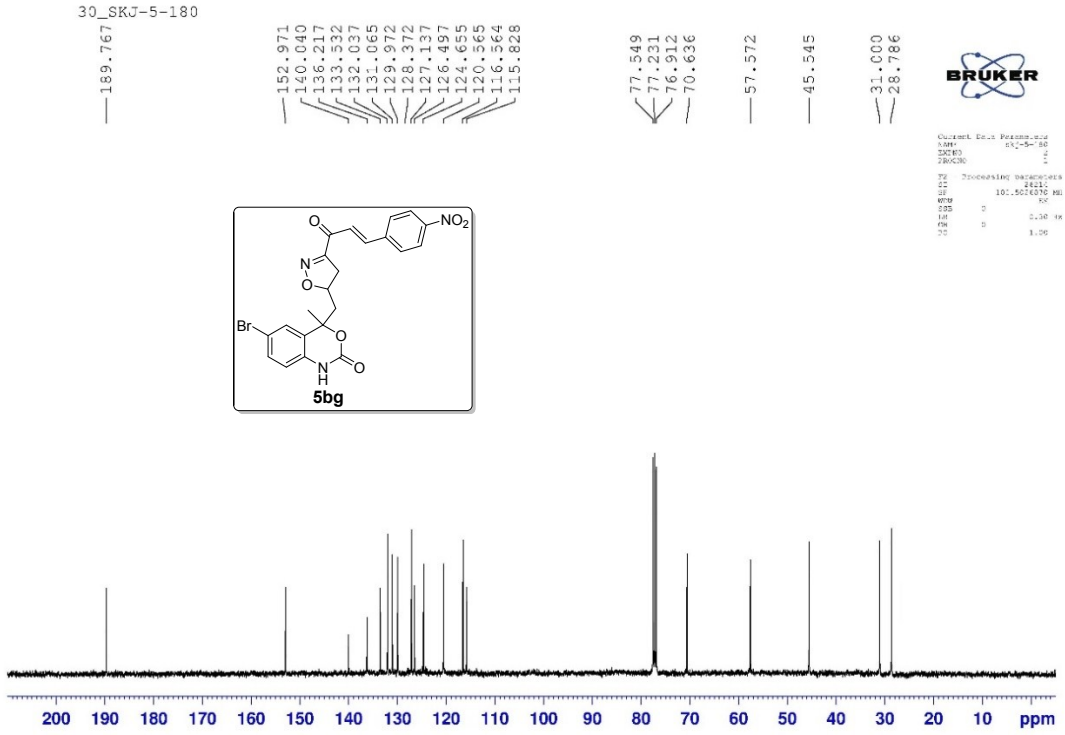


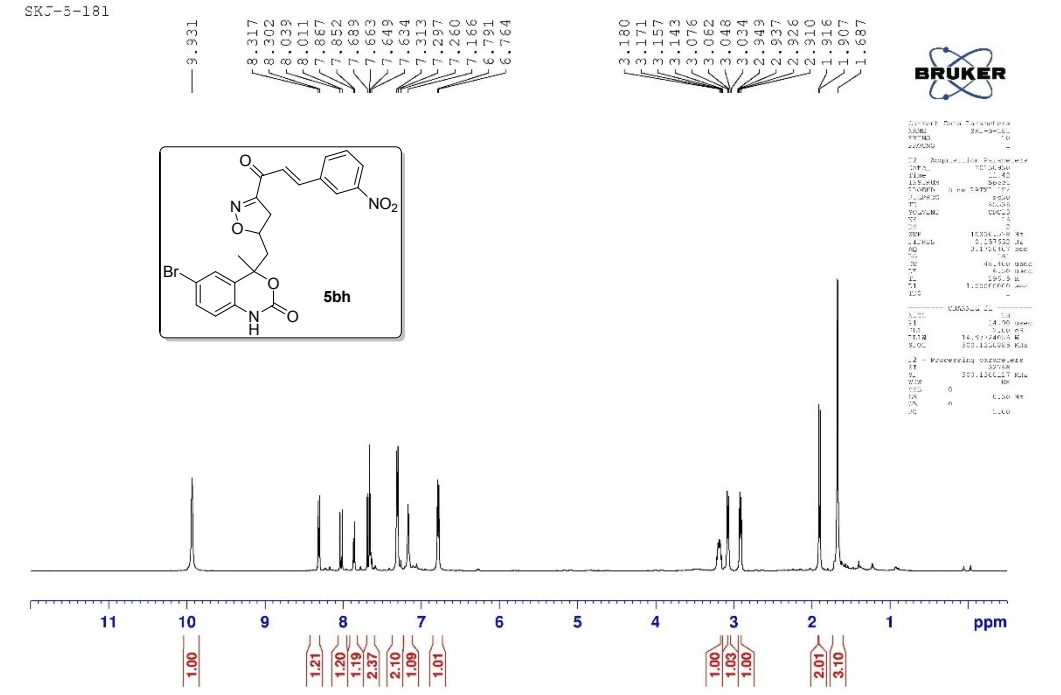

29_SKJ-5-178
188.838
152.902
149.564
139.472
135.235
133.693
131.923
131.005
127.008
126.393
124.793
122.861
120.462
116.514
115.691
111.384
110.318
77.556
77.238
76.958
71.949
61.544
56.141
56.074
45.462
30.772
28.115
BRUKER
OCH3
OCH3
Br
5be
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

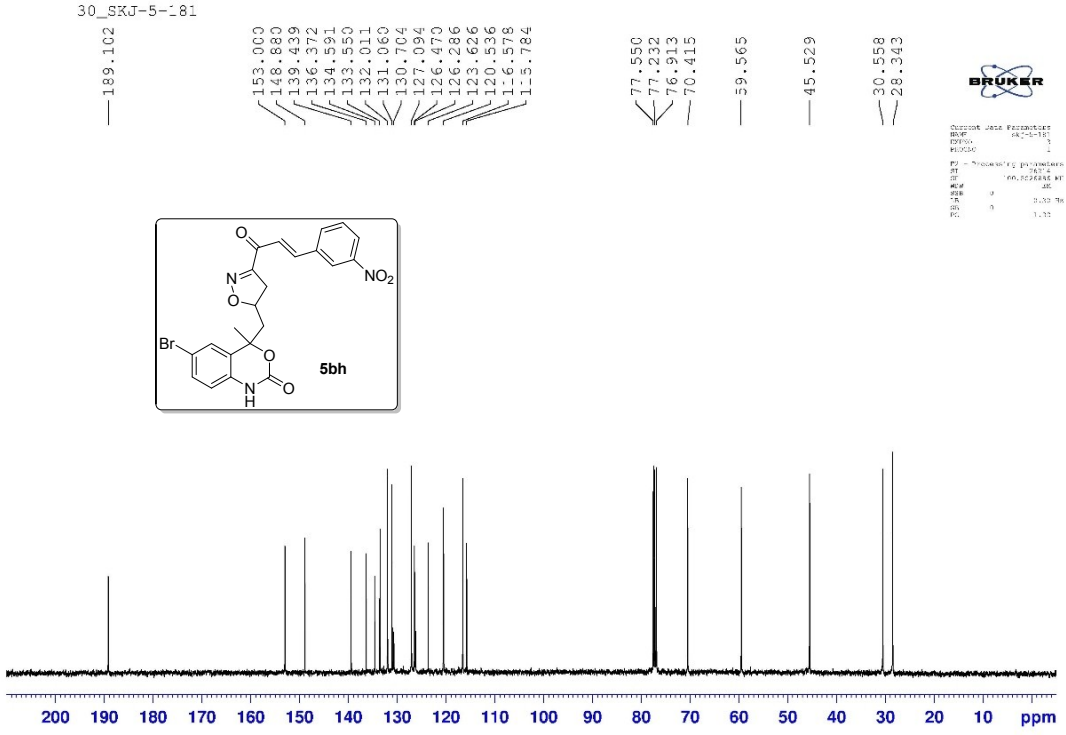

SKJ-5-179
9.957
7.902
7.885
7.554
7.527
7.300
7.283
7.260
7.154
6.787
6.770
6.734
3.873
3.863
3.156
3.143
3.131
3.120
3.067
3.057
3.044
3.034
2.948
2.935
2.920
2.905
2.926
1.915
1.669
BRUKER
OCH3
OCH3
OCH3
Br
5bf
11 10 9 8 7 6 5 4 3 2 1 ppm
1.00
1.18
1.19
2.02
1.03
2.40
3.04
5.98
1.00
1.00
1.00
2.01
3.12

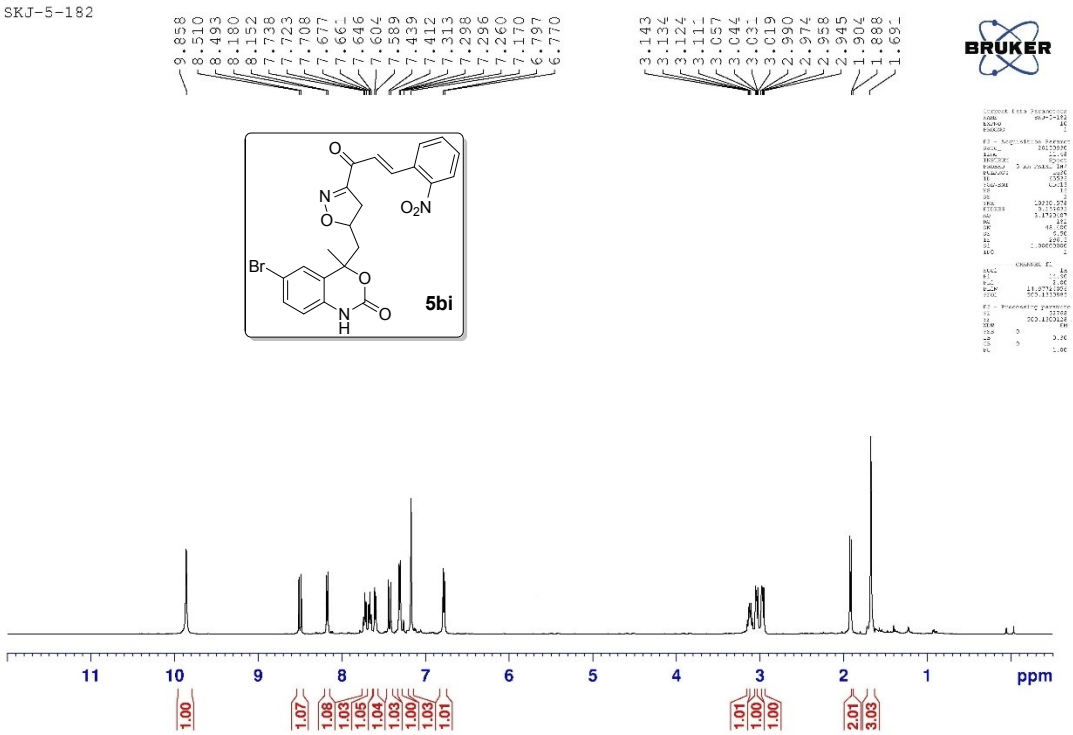

30_SKJ-5-179
188.881
153.753
152.947
141.832
139.429
136.568
133.534
131.963
131.029
127.040
126.431
125.411
120.485
116.553
113.724
77.548
77.230
76.911
70.636
61.114
59.122
56.367
45.486
31.443
28.343
BRUKER
OCH3
OCH3
OCH3
Br
5bf
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


SKJ-5-180
9.811
8.294
8.287
8.032
8.004
7.736
7.718
7.664
7.637
7.320
7.305
7.303
7.260
7.174
6.798
6.771
3.151
3.139
3.124
3.114
3.059
3.047
3.035
3.022
2.936
2.926
2.913
2.903
1.931
1.914
1.693
BRUKER
NO2
Br
5bg
11 10 9 8 7 6 5 4 3 2 1 ppm
1.01
1.08
1.09
2.32
2.07
1.12
1.00
1.02
1.00
1.01
2.02
3.20

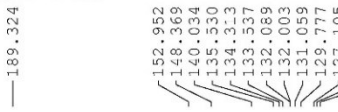

30_SKJ-5-180
189.767
152.971
140.040
136.217
133.532
132.037
131.065
129.972
128.372
127.137
126.497
124.655
120.565
116.564
115.828
77.549
77.231
76.912
70.636
57.572
45.545
31.000
28.786
BRUKER
5bg
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

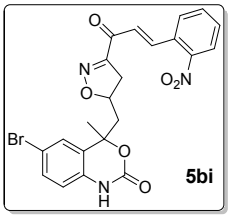

SKJ-5-181
9.931
8.317
8.302
8.039
8.011
7.867
7.852
7.689
7.663
7.649
7.634
7.313
7.297
7.260
7.166
6.791
6.764
3.180
3.171
3.157
3.143
3.076
3.062
3.048
3.034
2.949
2.937
2.926
2.910
1.916
1.907
1.687
BRUKER
5bh
11 10 9 8 7 6 5 4 3 2 1 ppm
1.00
1.21
1.20
1.19
2.37
2.10
1.09
1.01
1.00
1.03
1.00
2.01
3.10

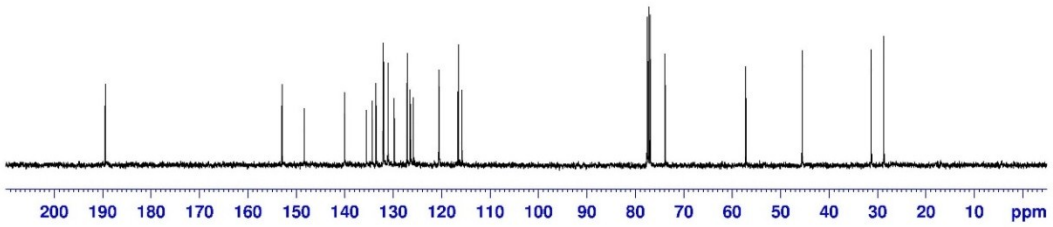

30_SKJ-5-181
189.102
153.000
148.880
139.439
136.372
134.591
133.550
132.011
131.060
130.704
127.094
126.470
126.286
123.626
120.536
77.550
77.232
76.913
70.415
59.565
45.529
30.558
28.343
BRUKER
5bh
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


SKJ-5-182
9.858
8.510
8.493
8.180
8.152
7.738
7.723
7.708
7.677
7.646
7.604
7.589
7.439
7.412
7.313
7.298
7.296
7.260
7.170
6.797
6.770
3.143
3.134
3.124
3.057
3.044
3.019
2.990
2.974
2.958
2.945
1.904
1.888
BRUKER
5bi
11 10 9 8 7 6 5 4 3 2 1 ppm
1.00
1.07
1.08
1.03
1.05
1.04
1.03
1.00
1.03
1.01
1.01
1.00
1.00
2.01
3.03

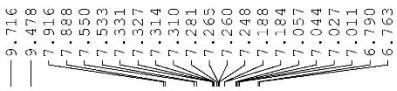
30_SKJ-5-182

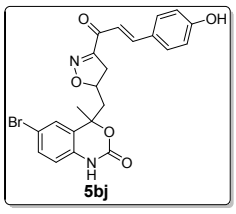


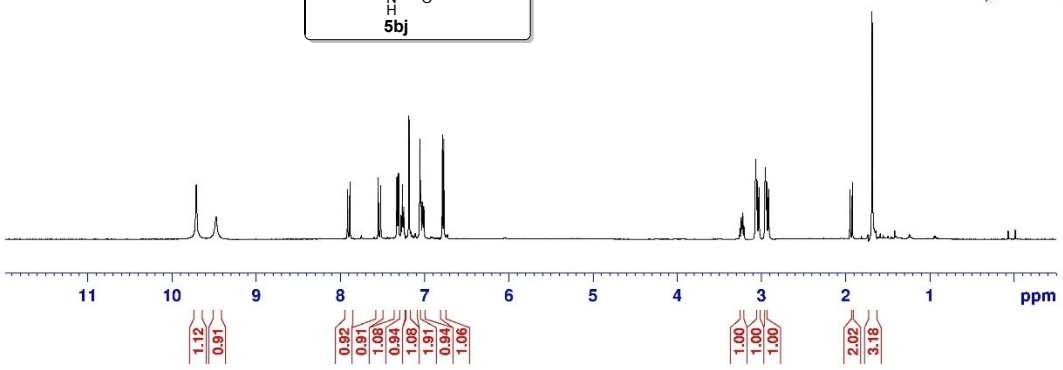


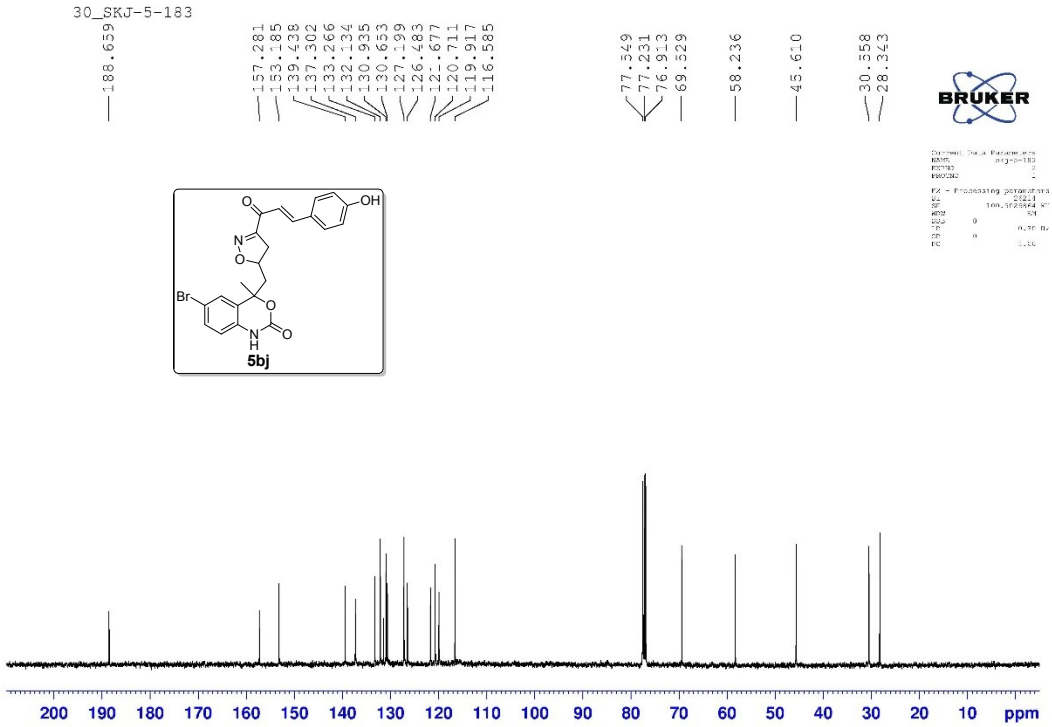


SKJ-5-183








30_SKJ-5-183
188.659
157.281
153.185
139.438
137.302
133.266
132.134
130.935
130.653
127.199
126.483
122.677
120.711
119.917
116.585
77.549
77.231
76.913
69.529
58.236
45.610
30.558
28.343
BRUKER
OH
O
N
O
Br
O
N
H
O
5bj
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm