Electrophile Promoted Cyclization of *ortho*-Aryl Substituted Ynamides: Construction of 3-Amino-4-Halo- or 4-Seleno-Isocoumarin Derivatives

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1. General Considerations

Unless otherwise noted, all reagents and solvents were purchased from commercial sources and used as received. o-Ynamidyl benzoate esters **2** were prepared following reported procedures.[1] All manipulations were conducted under argon (1atm). The reactions were monitored by thin-layer chromatography (TLC) using silica gel gel (60 F254) plates. Compounds were visualized using a UV lamp (254 nm) and/or by potassium permanganate stain. Flash column chromatography was carried out on silica gel 60 (230-400 mesh, 0.040-0.063 mm). Melting points (mp [°C]) were taken on samples in open capillary tubes and are uncorrected. NMR spectra were recorded at 298 K with a Bruker Avance III HD nanobay (400 and 250 MHz) spectrometer equipped with a BBO probe. ^{1}H and ^{13}C spectra were recorded at 250 MHz (^{13}C, 62.9 MHz) or at 400 MHz (^{13}C, 100 MHz). Chemical shifts are given in parts per million from tetramethylsilane (TMS) as internal standard. The following abbreviations are used for the proton spectra multiplicities: s: singulet, d: doublet, t: triplet, q: quartet, qt: quintuplet, m: multiplet, br.: broad, dd: double doublet, dt: double triplet. High-resolution mass spectra were recorded with a Brucker maXis ESI qTOF ultrahigh-resolution mass spectrometer coupled to a Dionex Ultimate 3000 RSLC system (FR2708, Orléans). MS data were acquired in positive mode and were processed using Data Analysis 4.4 software (Bruker). Infrared spectra were recorded with a Thermo Scientific Nicolet IS10 FTIR spectrometer using diamond ATR golden gate sampling and are reported in wave numbers (cm^{-1}).

1. L. Habert, P. Retailleau, I. Gillaizeau, *Org. Biomol. Chem.* 2018, **16**, 7351.

2. General procedure

***2.1) Synthesis of 3-amino-4-halo or 4-seleno-isocoumarins (3a,d,t) from ynamides (2a,d) using NIS or PhSeCl (GP1)*:** To a solution of ynamide **2a** or **2d** (0.2 mmol), prepared as reported in the literature,[1] in DCM (2 mL) was added NIS (1 equiv) or PhSeCl (1.5 equiv) at room temperature. The reaction was completed within 1 minute. The crude compound **3a** or **3d** was purified by flash-column chromatography on silica gel with a petroleum ether/EtOAc elution system.

***2.2) Synthesis of 3-amino-4-iodo or 4-bromo isocoumarins (3) via a one-pot procedure from (1) using NIS or NBS (GP2)*:** In a sealed tube flushed with argon and equipped with a stirring bar were added the appropriate bromoalkyne **1**[1] (1.1 equiv.), the protected amine (1.0 equiv.), $CuSO_4$•$5H_2O$ (10 mol%), 1,10-phenantroline (20 mol%), K_3PO_4 (2.0 equiv.) and toluene (0.33 M). The reaction mixture was heated at 80 °C until completion to **2** (24-48h) (TLC monitoring). The reaction mixture was then allowed to cool down to room temperature, filtrated through a pad of Celite and rinsed with DCM (10 mL). After addition of NIS (1 equiv) or NBS (1.5 equiv), the reaction was completed in 1 minute. The crude compounds **3** were purified by flash-column chromatography on silica gel with a petroleum ether/EtOAc elution system.

***2.3) Synthesis of (8,9) via Heck cross-coupling (GP3)*:** To a mixture of **3f** or **3g** (0.125 mmol, 1 equiv) and 4-methoxystyrene (0.25 mmol, 2 equiv) in DMF (1.0 mL) were added TBAC (0.138 mmol, 1.1 equiv) and Na_2CO_3 (0.313 mmol, 2.5 equiv). The reaction mixture was degassed under argon (3 times), $Pd(OAc)_2$ (15 mol%) was added and it was heated at 80°C for 20 h. After cooling down to room temperature, water (25 mL) was added. The reaction mixture was extracted with ethyl acetate (3 x 30 mL). The organic extracts were combined, washed with water (2 x 25 mL) and brine (50 mL), and dried over $MgSO_4$. After filtration, the solvent was evaporated under reduced pressure and the residue was purified by flash-column chromatography on silica gel with a petroleum ether/EtOAc elution system.

***2.4) Synthesis of (11,12) via Sonogashira cross-coupling (GP4)*:** To a mixture of **3f** or **3g** (0.125 mmol, 1 equiv), $PdCl_2(PPh_3)_2$ (3 mg, 0.003 mmol, 3 mol %), CuI (1 mg, 0.002 mmol, 2 mol %) in DMF (0.7 mL) was added a solution of alkyne (0.188 mmol, 1.5 equiv) in DMF (0.3 mL) followed by triethylamine (0.5 mL). The reaction mixture was degassed under argon (3 times) and heated at 55°C for 16 h. After cooling down to room temperature, water (25 mL) was added and the reaction mixture was extracted with ethyl acetate (3 x 30 mL). The organic extracts were combined, washed with water (2 x 25 mL) and brine (50 mL), and dried over $MgSO_4$. After filtration, the solvent was evaporated under reduced pressure and the residue was purified by flash-column chromatography on silica gel with petroleum ether/ethyl acetate as eluent.

***2.5) Synthesis of ynamide (6a-6b) (GP5)*:** To a mixture of amine (1.0 mmol) K_3PO_4 (2.0 equiv.), $CuSO_4.5H_2O$ (0.10 equiv.), and 1,10-phenanthroline (0.20 equiv.) in a reaction vial was added a solution of bromoalkyne (**5a-5b**) (0.9 mmol, 1.0 M) in toluene. The reaction mixture was capped and heated in an oil bath at 80°C for 48 h while being monitored with TLC analysis. Upon completion, the reaction mixture was cooled to room temperature and diluted with EtOAc, filtered through Celite™, and the filtrate was concentrated in vacuo. The crude products were purified by silica gel flash column chromatography [gradient eluent: EtOAc in hexane].

3. Compounds characterization

***(R)*-4-benzyl-3-(4-iodo-1-oxo-1*H*-isochromen-3-yl)oxazolidin-2-one** (**3a**). Flash-column chromatography on silica gel with petroleum ether/ethyl acetate (80:20) as eluent gave **3a** as a white solid (67 mg, 75 % according to **GP1**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.18 (d, *J* = 7.8 Hz, 1H), 7.81-7.74 (m, 2H), 7.59-7.55 (m, 1H), 7.19-7.14 (m, 4H), 7.10-7.07 (m, 1H), 4.84 (s, 1H), 4.53 (t, *J* = 8.5 Hz, 1H), 4.25 (t, *J* = 8.4 Hz, 1H), 3.17-2.99 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.4, 153.6, 143.4, 137.3, 135.8, 134.6, 131.3, 129.8, 128.7, 128.7, 127.2, 120.2, 78.8, 68.5, 57.6, 39.5. HRMS (ESI+): calcd for $C_{19}H_{15}O_4NI$ [M+H]+ : 448.0040 found 448.0033. Mp : 171-172°C.

3-(4-iodo-1-oxo-1*H*-isochromen-3-yl)-1,3-oxazolidin-2-one (**3b**). Flash-column chromatography on silica gel with petroleum ether/ethyl acetate (60:40) as eluent afforded **3b** as a white solid (315 mg, 52 % according to **GP2**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.26 (d, *J* = 7.8 Hz, 1H), 7.83-7.79 (m, 2H), 7.63-7.58 (m, 1H), 4.59 (t, *J* = 7.8 Hz, 2H), 4.10 (t, *J* = 7.8 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.7, 153.8, 144.0, 137.4, 135.9, 131.4, 130.1, 129.9, 120.4, 77.2, 63.1, 44.7. HRMS (ESI^+): calcd for $C_{12}H_9O_4NI$ [M+H]+ : 357.9570 found 357.9571. Mp : 189-190°C.

***tert*-butyl (4-iodo-1-oxo-1*H*-isochromen-3-yl)(phenyl)carbamate** (**3c**). Flash-column chromatography on silica gel with petroleum ether/ethyl acetate (80:20) as eluent afforded **3c** as a white gum (574 mg, 80 % according to **GP2**). ^{1}H NMR (400 MHz, $CDCl_3$): 8.27 (d, *J* = 7.8 Hz, 1H), 7.82-7.77 (m, 2H), 7.60-7.56 (m, 1H), 7.51-7.49 (m, 2H), 7.38-7.35 (m, 2H), 7.28-7.25 (m, 1H), 1.49 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.5, 151.5, 148.1, 138.6, 137.9, 135.8, 131.3, 130.0, 129.6, 128.9, 127.1, 125.9, 120.2, 83.1, 78.6, 28.1. HRMS (ESI^+): calcd for $C_{20}H_{19}O_4NI$ $[M+H]^+$: 464.0353 found 464.0349.

2-(4-iodo-1-oxo-1*H*-isochromen-3-yl)-2,3-dihydro-1*H*-1,2-benzothiazole-1,1-dione (**3d**). Flash-column chromatography on silica gel with petroleum ether/ethyl acetate (60:40) as eluent afforded **3d** as a white solid (65 mg, 74 % according to **GP1**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.20-8.18 (m, 1H), 8.05-8.01 (m, 2H), 7.89 (d, *J* = 7.5 Hz, 1H), 7.87-7.83 (m, 1H), 7.78-7.69 (m, 3H), 5.07 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.8, 149.0, 142.6, 141.7, 139.6, 139.4, 139.0, 137.1, 135.6, 134.9, 130.8, 126.4, 125.3, 87.0, 55.3. HRMS (ESI^+): calcd for $C_{16}H_{11}O_4SIN$ [M+H]+ : 439.9448 found 439.9446. Mp : 231-232°C.

***N*-(3-((tert-butyl(dimethyl)silyl)oxy)propyl)-*N*-(4-iodo-1-oxo-1*H*-isochromen-3-yl)-4-methylbenzenesulfonamide** (**3e**). Flash-column chromatography on silica gel with petroleum ether/ethyl acetate (80:20) as eluent afforded **3e** as a white solid (746 mg, 84% according to **GP2**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.25 (d, *J* = 7.6 Hz, 1H), 7.90 (dd, *J* = 8.1, 1.2 Hz, 1H), 7.85-7.80 (m, 3H), 7.63-7.59 (m, 1H), 7.36 (d, *J* = 8.1 Hz, 2H), 3.62-3.42 (m, 4H), 2.46 (s, 3H), 1.79 (s, 2H), 0.83 (s, 9H), -0.01 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.0, 146.1, 144.5, 137.9, 135.9, 135.4, 132.4, 129.9, 129.9, 129.8, 128.4, 120.4, 83.1, 60.1, 46.7, 30.9, 25.8, 21.6, 18.2, -5.4. HRMS (ESI^+): calcd for $C_{25}H_{33}O_5SNISi$ $[M+H]^+$: 614.0887 found 614.0882. Mp : 115-116°C.

***N*-(2-(3,4-dimethoxyphenyl)ethyl)-*N*-(4-iodo-1-oxo-1H-isochromen-3-yl)-4-methylbenzenesulfonamide** (**3f**). Flash-column chromatography on silica gel with petroleum ether/ethyl acetate (80:20) as eluent afforded **3f** as a white solid (801 mg, 74% according to **GP2**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.23 (d, *J* = 8.5 Hz, 1H), 7.89-7.78 (m, 4H), 7.63-7.59 (m, 1H), 7.35 (d, *J* = 8.0 Hz, 2H), 6.67-6.60 (m, 3H), 3.79 (s, 3H), 3.76 (s, 3H), 3.58 (brs, 2H), 2.88 (brs, 2H), 2.45 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.0, 148.8, 147.7, 145.7, 144.7, 137.9, 135.8, 135.3, 132.4, 130.0, 129.9, 129.8, 129.8, 128.3, 120.5, 120.4, 111.8, 111.1, 83.7, 55.8, 55.8, 50.3, 34.0, 21.6. HRMS (ESI^+): calcd for $C_{26}H_{25}O_6SNI$ $[M+H]^+$: 606.0441 found 606.0432. Mp : 171-172°C.

***N*-(2-(3,4-dimethoxyphenyl)ethyl)-*N*-(4-iodo-1-oxo-1*H*-isochromen-3-yl)-4-nitrobenzenesulfonamide** (**3g**). Flash-column chromatography on silica gel with petroleum ether/ethyl acetate (70:30) as eluent afforded **3g** as a white solid (640 mg, 76% according to **GP2**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.37 (d, *J* = 8.9 Hz, 2H), 8.25 (d, *J* = 7.9 Hz, 1H), 8.06 (d, *J* = 8.8 Hz, 2H), 7.90-7.83 (m, 2H), 7.67-7.63 (m, 1H), 6.63-6.58 (m, 3H), 3.96-3.57 (m, 8H), 2.77 (m, 2H).^{13}C NMR (100 MHz, $CDCl_3$): δ 160.6, 150.5, 148.8, 147.9, 144.9, 144.1, 137.5, 136.1, 132.4, 130.4, 130.0, 129.4, 129.3, 124.4, 120.5, 120.3, 111.8, 111.1, 83.9, 55.8, 51.1, 34. HRMS (ESI^+): calcd for $C_{25}H_{22}O_8SN_2I$ $[M+H]^+$: 637.0136 found 637.0130. Mp : 139-140°C.

***N*-(4-iodo-1-oxo-1*H*-isochromen-3-yl)-4-methyl-*N*-(prop-2-en-1-yl)benzenesulfonamide** (**3h**). Flash-column chromatography on silica gel with petroleum ether/ethyl acetate (80:20) as eluent afforded **3h** as a white solid (549 mg, 60% according to **GP2**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.26 (d, *J* = 8.3 Hz, 1H), 7.91 (d, *J* = 6.9 Hz, 1H), 7.86-7.83 (m, 3H), 7.64-7.60 (m, 1H), 7.41-7.39 (m, 2H), 5.93-5.82 (m, 1H), 5.19-5.09 (m, 2H), 4.12 (brs, 2H), 2.49 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.0, 145.8, 144.7, 137.8, 135.8, 135.3, 132.4, 130.5, 129.9, 129.9, 129.9, 128.4, 121.0, 120.4, 83.6, 52.3, 21.6. HRMS (ESI^+): calcd for $C_{19}H_{17}O_4SIN$ $[M+H]^+$: 481.0183 found 481.9915. Mp : 169-170°C. The current reaction is also amenable to gram-scale synthesis starting from **1h** (6 mmol) with a good 57% isolated yield (**3h**).

***N*-allyl-*N*-(4-iodo-1-oxo-1*H*-isochromen-3-yl)-4-nitrobenzenesulfonamide** (**3i**). Flash-column chromatography on silica gel with petroleum ether/ethyl acetate (80:20) as eluent afforded **3i** as a white solid (354 mg, 63 % according to **GP2**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (d, *J* = 8.8 Hz, 2H), 8.27 (d, *J* = 7.7 Hz, 1H), 8.17 (d, *J* = 8.9 Hz, 2H), 7.94-7.81 (m, 2H), 7.64 – 7.68 (m, 1H), 5.99-5.59 (m, 1H), 5.23-5.01 (m, 2H), 4.23 (d, *J* = 6.5 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.6, 150.7, 145.1, 144.2, 137.2, 136.1, 132.5, 130.4, 130.1, 129.8, 129.7 (2 x C), 124.5 (2 x C), 121.9, 120.4, 83.8, 52.9. HRMS (ESI^+): calcd for $C_{18}H_{14}O_6SN_2$ $[M+H]^+$: 512.9612 found 512.9609. Mp : 124-127°C.

N-(4-iodo-7-methoxy-1-oxo-1H-isochromen-3-yl)-4-methyl-N-(prop-2-en-1-yl)benzenesulfonamide (**3j**). Flash-column chromatography on silica gel with petroleum ether/ethyl acetate (80:20) as eluent afforded **3j** as a white solid (367 mg, 62% according to **GP2**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.83-7.78 (m, 3H), 7.64 (d, *J* = 2.8 Hz, 1H), 7.38-7.33 (m, 3H), 5.90-5.80 (m, 1H), 5.17-5.05 (m, 2H), 4.30-4.10 (m, 2H), 3.92 (s, 3H), 2.46 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.1, 160.9, 144.6, 143.9, 135.4, 134.0, 131.2, 130.6, 129.9, 128.4, 124.6, 121.4, 120.9, 110.7, 83.2, 56.0, 52.3, 21.7. HRMS (ESI^+): calcd for $C_{20}H_{19}O_5SNI$ $[M+H]^+$: 512.0023 found 512.0016. Mp : 155-156°C.

N-(7-fluoro-4-iodo-1-oxo-1H-isochromen-3-yl)-4-methyl-N-(prop-2-en-1-yl)benzenesulfonamide (**3k**). Flash-column chromatography on silica gel with petroleum ether/ethyl acetate (80:20) as eluent afforded **3k** as a white solid (205 mg, 62 % according to **GP2**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.96-7.93 (m, 2H), 7.84-7.81 (m, 2H), 7.56-7.51 (m, 1H), 7.40 (d, *J* = 8.2 Hz, 2H), 5.91-5.81 (m, 1H), 5.19-5.09 (m, 2H), 4.03 (brs, 2H), 2.49 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.0, 160.1, 145.3, 144.8, 135.2, 135.1, 134.3 (C_{ar}), 130.4, 129.9, 128.3, 123.8, 121.9, 121.2, 115.4, 82.3, 52.3, 21.7. ^{19}F NMR (376 MHz, $CDCl_3$) δ -108.7. HRMS (ESI^+): calcd for $C_{19}H_{16}O_4SNIF$ $[M+H]^+$: 499.9823 found 499.9818. Mp : 170-171°C.

N-(7-chloro-4-iodo-1-oxo-1H-isochromen-3-yl)-4-methyl-N-(prop-2-en-1-yl)benzenesulfonamide (**3l**). Flash-column chromatography on silica gel with petroleum ether/ethyl acetate (80:20) as eluent afforded **3l** as a white solid (207 mg, 60% according to **GP2**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.21 (d, *J* = 2.2 Hz, 1H), 7.85-7.79 (m, 3H), 7.75 (dd, *J* = 8.6, 2.2 Hz, 1H), 7.39-7.37 (m, 2H), 5.88-5.78 (m, 1H), 5.17-5.07 (m, 2H), 4.15-4.05 (m, 2H), 2.47 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.9, 146.0, 144.9, 136.4, 136.3, 135.9, 135.2, 134.0, 130.3, 129.9, 129.2, 128.3, 121.4, 121.2, 82.4, 52.3, 21.7. HRMS (ESI^+): calcd for $C_{19}H_{16}O_4SNClI$ $[M+H]^+$: 515.9527 found 515.9523. Mp : 164-165°C.

N-(7-bromo-4-iodo-1-oxo-1H-isochromen-3-yl)-4-methyl-N-(prop-2-en-1-yl)benzenesulfonamide (**3m**). Flash-column chromatography on silica gel with petroleum ether/ethyl acetate (80:20) as eluent afforded **3m** as a white solid (253 mg, 57 % according to **GP2**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.35 (d, *J* = 2.1 Hz, 1H), 7.88 (dd, *J* = 8.6, 2.1 Hz, 1H), 7.77 (dd, *J* = 18.3, 8.5 Hz, 3H), 7.37 (d, *J* = 8.1 Hz, 2H), 5.87-5.77 (m, 1H), 5.16-5.06 (m, 2H), 4.04 (brs, 2H), 2.46 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.7, 146.1, 144.9, 138.8, 136.8, 135.2, 134.1, 132.2, 130.4, 129.9, 128.3, 124.1, 121.5, 121.2, 82.5, 52.3, 21.7. HRMS (ESI^+): calcd for $C_{19}H_{16}O_4SNIBr$ $[M+H]^+$: 559.9022 found 559.9014. Mp : 148-149°C.

N-(2-(3,4-dimethoxyphenyl)ethyl)-N-(4-iodo-1-oxo-1H-isochromen-3-yl)-4-methoxybenzenesulfonamide (**3n**). Flash-column chromatography on silica gel with petroleum ether/ethyl acetate (70:30) as eluent afforded **3n** as a white solid (545 mg, 90 % according to **GP2**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.23 (d, *J* = 9.2 Hz, 1H), 7.89-7.80 (m, 4H), 7.63-7.59 (m, 1H), 7.01 (d, *J* = 9.0 Hz, 2H), 6.67-6.60 (m, 3H), 3.89 (s, 3H), 3.79 (s, 3H), 3.75 (s, 3H), 3.75-3.57 (m, 2H), 2.89-2.73 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): 163.7, 161.0, 148.8, 147.7, 145.8, 137.9, 135.9, 132.4, 130.5, 129.9, 129.8, 129.8, 129.8, 120.5, 120.4, 114.4, 111.8, 111.2, 83.6, 55.8, 55.7, 50.3, 34.0. HRMS (ESI^+): calcd for $C_{26}H_{25}O_7SNI$ $[M+H]^+$: 622.0390 found 622.0391. Mp : 135-136°C.

Methyl 1-(4-iodo-1-oxo-1H-isochromen-3-yl)-1H-indole-3-carboxylate (**3o**). Flash-column chromatography on silica gel with petroleum ether/ethyl acetate (70:30) as eluent afforded **3o** as a white solid (244 mg, 55 % according to **GP2**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.35 (d, *J* = 7.8 Hz, 1H), 8.26-8.24 (m, 1H), 8.05 (s, 1H), 7.89-7.88 (m, 2H), 7.70-7.65 (m, 1H), 7.39-7.35 (m, 3H), 3.96 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.6, 160.2, 144.8, 137.4, 136.3, 136.1, 133.7, 131.9, 130.3, 126.1, 124.4, 123.4, 122.1, 120.5, 111.8, 111.4, 74.8, 51.4. HRMS (ESI^+): calcd for $C_{19}H_{13}O_4NI$ [M+H]+ : 445.9883 found 445.9886. Mp : 204-205°C.

N-(4-bromo-1-oxo-1H-isochromen-3-yl)-N-(2-(3,4-dimethoxyphenyl)ethyl)-4-nitrobenzenesulfonamide (**3q**). Flash-column chromatography on silica gel with petroleum ether/ethyl acetate (70:30) as eluent afforded **3q** as a white solid (616 mg, 77 % according to **GP2**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.35 (d, *J* = 8.9 Hz, 2H), 8.29 (d, *J* = 8.0 Hz, 1H), 8.05 (d, *J* = 8.8 Hz, 2H), 7.95-7.86 (m, 2H), 7.69-7.65 (m, 1H), 6.63-6.56 (m, 3H), 3.96 (brs, 2H), 3.78 (s, 2H), 3.74 (s, 2H), 2.82 (t, *J* = 7.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.1, 150.4, 148.7, 147.9, 144.3, 142.3, 135.8, 135.6, 130.4, 130.1, 129.3, 129.2, 127.5, 124.3, 120.9, 120.4, 111.7, 111.1, 107.2, 55.8, 50.8, 34.3. HRMS (ESI^+): calcd for $C_{25}H_{22}O_8SN_2Br$ $[M+H]^+$: 589.0274 found 589.0266. Mp : 156-157°C.

N-(4-bromo-1-oxo-1H-isochromen-3-yl)-N-(2-(3,4-dimethoxyphenyl)ethyl)-4-methoxybenzenesulfonamide (**3r**). Flash-column chromatography on silica gel with petroleum ether/ethyl acetate (70:30) as eluent afforded **3r** as a white solid (410 mg, 74 % according to **GP2**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.28 (d, *J* = 9.2 Hz, 1H), 7.94 (d, *J* = 9.3 Hz, 1H), 7.87-7.83 (m, 3H), 7.65-7.61 (m, 1H), 7.00 (d, *J* = 9.0 Hz, 2H), 6.65-6.59 (m, 3H), 3.89 (s, 3H), 3.79 (s, 3H), 3.74 (s, 3H), 3.70 (t, *J* = 7.7 Hz, 2H), 2.81 (t, *J* = 7.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.6, 160.5, 148.8, 147.7, 143.3, 136.0, 135.6, 130.4, 130.0, 129.8, 127.4, 120.9, 120.5, 114.4, 111.8, 111.2, 106.9, 55.8, 55.7, 50.0, 34.2. HRMS (ESI^+): calcd for $C_{26}H_{25}O_7SNBr$ $[M+H]^+$: 574.0795 found 574.0531. Mp : 129-130°C.

N-(4-bromo-1-oxo-1H-isochromen-3-yl)-4-methyl-N-(prop-2-en-1-yl)benzenesulfonamide (**3s**). Flash-column chromatography on silica gel with petroleum ether/ethyl acetate (80:20) as eluent afforded **3s** as a white solid (411 mg, 50 % according to **GP2**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.28 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.95 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.87-7.82 (m, 3H), 7.65-7.60 (m, 1H), 7.37 (d, *J* = 8.0 Hz, 2H), 5.85-5.75 (m, 1H), 5.18-5.06 (m, 2H), 4.07 (d, *J* = 6.8 Hz, 2H), 2.47 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.5, 144.7, 143.2, 136.0, 135.6, 135.5, 130.7, 130.0, 129.9, 129.9, 128.3, 127.5, 120.9, 120.8, 106.9, 52.0, 21.7. HRMS (ESI^+): calcd for $C_{19}H_{17}O_4SNBr$ [M+H]+ : 434.0056 found 434.0054. Mp : 161-162°C.

2-(1-oxo-4-(phenylselanyl)-1H-isochromen-3-yl)-2,3-dihydro-1H-1,2-benzothiazole-1,1-dione (**3t**). Flash-column chromatography on silica gel with petroleum ether/ethyl acetate (80:20) as eluent afforded **3t** as a white gum (43 mg, 47 % according to **GP1**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.29 (d, *J* = 7.8 Hz, 1H), 8.00 (d, *J* = 8.0 Hz, 1H), 7.84 (d, *J* = 7.8 Hz, 1H), 7.71-7.66 (m, 2H), 7.60-7.51 (m, 2H), 7.46 (d, *J* = 7.6 Hz, 1H), 7.34-7.32 (m, 2H), 7.20-7.18 (m, 3H), 4.98 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.0, 145.3, 137.6, 135.5, 134.3, 133.4, 131.0, 130.2, 130, 129.5, 129.4, 129.3, 129.1, 126.9, 124.7, 121.7, 121.1, 109.3, 50.0. HRMS (ESI$^+$): calcd for $C_{22}H_{16}O_4SSeN_2$ $[M+H]^+$: 469.9959 found 469.9955.

***N*-(2-(3,4-dimethoxyphenyl)ethyl)-*N*-(4-((E)-2-(4-methoxyphenyl)ethenyl)-1-oxo-1*H*-isochromen-3-yl)-4-methylbenzenesulfonamide** (**8**). Flash-column chromatography on silica gel with petroleum ether/ethyl acetate (70:30) as eluent afforded **8** as a colorless oil (42 mg, 55 % according to **GP3**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.36 (d, *J* = 7.8 Hz, 1H), 7.88 (d, *J* = 7.8 Hz, 1H), 7.78 (d, *J* = 8.2 Hz, 3H), 7.62-7.58 (m, 1H), 7.44 (d, *J* = 8.7 Hz, 2H), 7.31 (d, *J* = 8.2 Hz, 2H), 6.98-6.81 (m, 4H), 6.64-6.55 (m, 3H), 3.86 (s, 3H), 3.86 (s, 3H), 3.76 (s, 6H), 3.66 (t, *J* = 7.6 Hz, 2H), 2.73 (t, *J* = 7.6 Hz, 2H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.4, 159.9, 148.8, 147.6, 144.4, 141.4, 137.1, 136.3, 135.6, 134.8, 130.1, 130.0, 129.8, 129.4, 128.9, 128.2, 128.0, 125.6, 121.3, 120.5, 117.3, 116.4, 114.2, 111.7, 111.1, 55.8, 55.4, 49.9, 33.9, 21.6. HRMS (ESI$^+$): calcd for $C_{35}H_{34}O_7NS$ $[M+H]^+$: 612.2050 found 612.2043

***N*-(2-(3,4-dimethoxyphenyl)ethyl)-*N*-(4-((E)-2-(4-methoxyphenyl)ethenyl)-1-oxo-1*H*-isochromen-3-yl)-4-nitrobenzenesulfonamide** (**9**). Flash-column chromatography on silica gel with petroleum ether/ethyl acetate (70:30) as eluent afforded **9** as a yellow oil (43 mg, 53 % according to **GP3**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.37 (d, *J* = 7.9 Hz, 1H), 8.28 (d, *J* = 8.9 Hz, 2H), 8.02 (d, *J* = 8.8 Hz, 2H), 7.91 (d, *J* = 8.0 Hz, 1H), 7.83-7.79 (m, 1H), 7.66-7.61 (m, 1H), 7.43 (d, *J* = 8.7 Hz, 2H), 7.00-6.93 (m, 3H), 6.75 (d, *J* = 16.6 Hz, 1H), 6.63-6.54 (m, 3H), 3.86 (s, 3H), 3.82-3.76 (m, 8H), 2.74 (t, *J* = 7.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.0, 160.1, 150.2, 148.8, 147.9, 144.4, 140.7, 136.9, 136.9, 135.1, 130.2, 129.5, 129.3, 129.3, 129.0, 128.0, 125.6, 124.2, 121.3, 120.5, 117.4, 115.4, 114.3, 111.8, 111.1, 55.8, 55.7, 55.4, 50.8, 33.9. HRMS (ESI$^+$): calcd for $C_{34}H_{31}O_9SN_2$ $[M+H]^+$: 643.1744 found 643.1736.

***N*-(2-(3,4-dimethoxyphenyl)ethyl)-4-methyl-*N*-(1-oxo-4-(trifluoromethyl)-1*H*-isochromen-3-yl)benzenesulfonamide** (**10**). To a mixture of **3f** (60 mg, 0.1 mmol, 1 equiv), CuI (19 mg, 0.1 mmol, 1 equiv) in DMF (1 mL) was added $FSO_2CF_2CO_2Me$ (64 µl, 0.5 mmol, 5 equiv). The reaction mixture was degassed under argon and heated at 70°C for 10 h. After cooling down to room temperature, water (25 mL) was added and the reaction mixture was extracted with ethyl acetate (3 x 30 mL). The organic extracts were combined, washed with water (2 x 25 mL) and brine (50 mL), and dried over $MgSO_4$. The solvent was evaporated under reduced pressure and the residue was purified by flash-column chromatography on silica gel with petroleum ether/ethyl acetate (70:30) as eluent to give **10** as a yellow oil (42 mg, 77 %). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.31 (d, *J* = 7.8 Hz, 1H), 7.88-7.83 (m, 2H), 7.71 (d, *J* = 8.3 Hz, 2H), 7.67-7.63 (m, 1H), 7.33 (d, *J* = 8.1 Hz, 2H), 6.67-6.59 (m, 3H), 3.84-3.74 (m, 7H), 3.64-3.57 (m, 1H), 2.95-2.88 (m, 1H), 2.77-2.70 (m, 1H), 2.45 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.7, 148.9, 147.8, 144.9, 135.5, 134.9, 132.7, 130.1, 130.0, 129.8, 129.4, 128.1, 125.4, 120.7, 120.5, 111.8, 111.3, 55.8, 55.7, 49.8, 34.3, 21.7. ^{19}F NMR (376 MHz, $CDCl_3$) δ -56.1. HRMS (ESI$^+$): calcd for $C_{27}H_{25}O_6SNF_3$ [M+H]+ : 548.1349 found 548.1344.

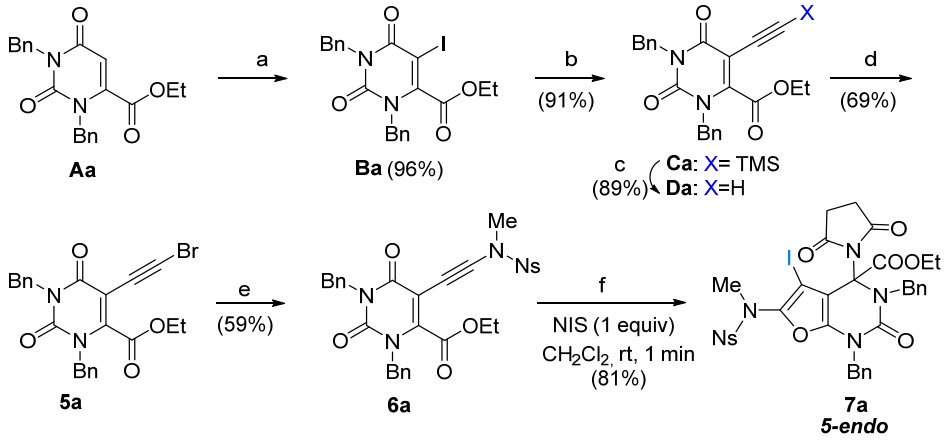
***N*-(2-(3,4-dimethoxyphenyl)ethyl)-*N*-(4-((4-methoxyphenyl)ethynyl)-1-oxo-1*H*-isochromen-3-yl)-4-methylbenzenesulfonamide** (**11**). Flash-column chromatography on silica gel with petroleum ether/ethyl acetate (70:30) as eluent afforded **11** as a pale-yellow oil (45 mg, 60 % according to **GP4**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.31 (d, *J* = 9.3 Hz, 1H), 8.03 (d, *J* = 8.5 Hz, 1H), 7.88-7.84 (m, 3H), 7.65-7.61 (m, 1H), 7.51 (d, *J* = 8.7 Hz, 2H), 7.29 (d, *J* = 9.5 Hz, 2H), 6.93 (d, *J* = 8.8 Hz, 2H), 6.64-6.60 (m, 3H), 3.87 (s, 3H), 3.87-3.83 (m, 2H), 3.76 (s, 3H), 3.73 (s, 3H), 2.88 (t, *J* = 7.5 Hz, 2H) 2.41 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.6, 160.2, 148.7, 147.6, 147.3, 144.3, 136.2, 136.1, 135.2, 133.2, 130.0, 129.8, 129.7, 129.3, 128.1, 125.8, 120.7, 120.2, 114.5, 114.1, 111.8, 111.1, 105.0, 98.9, 78.8,

55.7, 55.7, 55.4, 50.3, 34.7, 21.6. HRMS (ESI$^+$): calcd for $C_{35}H_{32}O_7SN$ $[M+H]^+$: 610.1894 found 610.1887.

***N*-(3,4-dimethoxyphenethyl)-4-nitro-*N*-(1-oxo-4-((trimethylsilyl)ethynyl)-1*H*-isochromen-3-yl)benzenesulfonamide** (**12**). Flash-column chromatography on silica gel with petroleum ether/ethyl acetate (80:20) as eluent afforded **12** as a pale yellow oil (44 mg, 58 % according to **GP4**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (d, *J* = 8.9 Hz, 2H), 8.29 (d, *J* = 7.0 Hz, 1H), 8.07 (d, *J* = 8.9 Hz, 2H), 7.94 (d, *J* = 7.3 Hz, 1H), 7.88 (t, *J* = 8.2 Hz, 1H), 7.65 (t, *J* = 8.1 Hz, 1H), 6.62 (s, 1H), 6.61 (d, *J* = 1.9 Hz, 1H), 6.55 (d, *J* = 1.7 Hz, 1H), 3.93 (t, *J* = 7.2 Hz, 2H), 3.79 (s, 3H), 3.76 (s, 3H), 2.83 (t, *J* = 7.2 Hz, 2H), 0.35 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.8, 152.0, 150.5, 149.7, 149.6, 146.7, 137.5, 137.2, 131.5 (2 x C), 131.3, 130.9 (2 x C), 127.7, 126.0 (2 x C), 122.3, 121.7, 113.5, 112.8, 108.2, 106.4, 96.2, 57.5, 57.42, 5.86, 36.5, 1.5 (3 x C). HRMS (ESI$^+$): calcd for $C_{30}H_{31}O_8SN_2Si$ $[M+H]^+$: 607.1565 found 607.1556.

4-azido-3-((3,4-dimethoxyphenethyl)(4-nitrophenyl)amino)-1*H*-isochromen-1-one (**13**). Under an argon atmosphere, 1N NaOH solution (40 µl, 0.04 mmol, 0.2 equiv), L-proline (4.6 mg, 0.04 mmol, 0.2 equiv), CuI (3.8 mg, 0.02 mmol, 0.1 equiv) and NaN_3 (15.6 mg, 0.24 mmol, 1.2 equiv) were added to a solution of **3g** (127 mg, 0.2 mmol, 1 equiv) in 2 mL of DMSO. The mixture was heated to 60°C for 18 h. NaN_3, NaOH and L-proline were added again in the same amounts and the reaction was heated at 60°C for 5 h. After cooling to room temperature, water was then added. The precipitate was filtered, washed with water and concentrated *in vacuo*. Flash-column chromatography on silica gel with petroleum ether/ethyl acetate (70:30) as eluent afforded **13** as a yellow oil (25 mg, 23 %). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.33 (d, *J* = 7.7 Hz, 1H), 8.15 (d, *J* = 8.6 Hz, 2H), 7.83 – 7.71 (m, 1H), 7.65 (t, *J* = 7.6 Hz, 1H), 7.45 (d, *J* = 7.7 Hz, 1H), 7.31 (d, *J* = 8.6 Hz, 2H), 6.74 (s, 1H), 6.71 (s, 2H), 4.45 – 4.30 (m, 1H), 4.28 – 4.16 (m, 1H), 3.85 (s, 3H), 3.82 (s, 3H), 2.92 (t, *J* = 7.5 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 169.5, 162.8, 148.8, 148.0, 147.8, 145.2, 136.7, 135.0, 134.3, 130.1, 129.9, 129.3, 127.7, 127.5 (2 x C), 125.0, 124.0 (2 x C), 121.0, 111.9, 111.1, 69.8, 55.8, 42.2, 33.3. HRMS (ESI$^+$): calcd for $C_{25}H_{22}O_8SN_5$ $[M+H]^+$: 552.1384 found 552.1378. Mp : 170-171°C.

4. Synthesis of substituted furanopyrimidinone 7a *via* iodocyclization.



Reaction conditions: a) **Aa**[2] (3 mmol), TFA (5ml), TFAA (1 ml), NIS (5.7 mmol), reflux 8h. b) **Ba** (1 mmol, 1 equiv), Et_3N (1.5 mL/mmol), TMSC≡CH (1.1 equiv), CuI (5 mol%), dichlorobis(triphenylphosphine)palladium (2.5 mol%), rt, 18h. c) **Ca** in THF (2 mL/mmol), TBAF (1.1 equiv, 1M in THF) at 0 °C 5 min. d) **Da** (1.0 mmol) in MeCN (2.0 mL), NBS (1.5 equiv), DBU (1.0 equiv), 1 min. e) Amine[1] (1.0 mmol) K_3PO_4 (2.0 equiv.), $CuSO_4.5H_2O$ (0.10 equiv.), 1,10-phenanthroline (0.20 equiv.), bromoalkyne (**5a**) (0.9 mmol, 1.0 M) in toluene, 80°C for 48 h then diluted with EtOAc and filtered through Celite™. f) **6a** (0.2 mmol), NIS (1 equiv), DCM (2 mL) rt, 1 min.

2. a) N. G Kundu ; S. Sikdar ; R. P. Hertzberg ; S. A. Schmitz ; S. G. Khatri, *J. Chem. Soc., Perkin Trans. 1*, **1985**, 1295. b) S. J. Hannon, N. G. Kundu, R. P. Hertzberg, R. S. Bhatt, C. Heidelberger, *Tetrahedron Lett.*, **1980**, 21, 1105.

a) Ethyl 1,3-dibenzyl-5-iodo-2,6-dioxo-1,2,3,6-tetrahydropyrimidine-4-carboxylate (Ba).[3] Ethyl 1,3-dibenzylorotate, respectively **Aa** (3 mmol), was refluxed with trifluoroacetic acid (5 ml) and trifluoroacetic anhydride (1 ml). *N*-Iodosuccinimide (1.3 g, 1.9 equiv., 5.7 mmol) was added to the reaction mixture which was further refluxed for 8 h. The solvent was removed under vacuum and the residue was taken up in chloroform (10 ml). The chloroform solution was washed with aqueous saturated sodium bicarbonate solution, sodium thiosulphate solution (10%) and dried (over anhydrous sodium sulphate). The solvent was removed under reduced pressure leading to the crude desired product **Ba** which was directly engaged in the next step. Pale pink solid (1.41 g, 96 %). ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.57 – 7.41 (m, 2H), 7.35 – 7.13 (m, 8H), 5.17 (s, 2H), 5.03 (s, 2H), 4.30 – 4.06 (m, 2H), 1.26 – 0.81 (m, 3H). HRMS (ESI$^+$): calcd for $C_{21}H_{19}O_4N_2I$ [M+H]+ : 492.0494 found 492.0459. Mp : 111-113°C. *Sample degradation was observed preventing to obtain a good quality spectrum.*

b) Ethyl 1,3-dibenzyl-2,6-dioxo-5-((trimethylsilyl)ethynyl)-1,2,3,6-tetrahydropyrimidine-4-carboxylate (**Ca**). To a solution of crude ethyl-1,3-dibenzyl-5-iodo-2,6-dioxo-1,2,3,6-tetrahydropyrimidine-4-carboxylate **Ba** (1mmol, 1 equiv), in anhydrous triethylamine (1.5 mL/mmol) was added trimethylsilylacetylene (1.1 equiv). The solution was degassed under argon then copper iodide (5 mol%) and dichlorobis(triphenylphosphine)palladium (2.5 mol%) were added at room temperature. The reaction mixture was stirred at room temperature overnight then filtered through a pad of celite. The residue was washed with diethyl ether. Solvents were removed under vacuum and the expected product was purified by flash column chromatography on silica gel with petroleum ether/ethyl acetate (80:20) as eluent afforded **Ca** as a colorless oil (418 mg, 91 %). ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.53 – 7.39 (m, 2H), 7.38 – 7.24 (m, 6H), 7.23 – 7.07 (m, 2H), 5.15 (s, 2H), 5.08 (s, 2H), 4.24 – 4.05 (m, 2H), 1.15 (t, J = 7.2 Hz, 3H), 0.19 (s, 9H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 162.9, 162.1, 152.2, 149.8, 137.8, 136.7, 130.9 (2 x C), 130.5 (2 x C), 130.2 (2 x C), 129.9, 129.6, 129.2 (2 x C), 104.7, 100.3, 95.7, 64.8, 51.5, 47.2, 15.1, 1.5 (3 x C).

c) Ethyl 1,3-dibenzyl-5-ethynyl-2,6-dioxo-1,2,3,6-tetrahydropyrimidine-4-carboxylate Da. To a solution of silylated compound **Ca** in THF (2 mL/mmol) was added TBAF (1.1 equiv, 1M in THF) at 0 °C. The solution was stirred at this temperature for 5 minutes then diluted with water. The mixture was extracted with diethyl ether, the combined organic phases were dried over anhydrous $MgSO_4$ and concentrated under vacuum. The expected product was purified by flash column chromatography on silica gel with petroleum ether/ethyl acetate (80:20) as eluent afforded **Da** as a colorless oil (345 mg, 89 %). ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.53 – 7.39 (m, 2H), 7.38 – 7.17 (m, 6H), 7.14 – 7.19 (m, 2H), 5.15 (s, 2H), 5.07 (s, 2H), 4.16 (q, J = 7.2 Hz, 2H), 3.24 (s, 1H), 1.12 (t, J = 7.1 Hz, 3H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 161.0, 160.6, 150.4, 148.5, 136.0, 134.9, 129.4 (2 x C), 128.8 (2 x C), 128.5 (2 x C), 128.3, 128.0, 127.5 (2 x C), 97.6, 85.0, 73.5, 63.3, 49.9, 45.5, 13.4.

d) Ethyl 1,3-dibenzyl-5-(bromoethynyl)-2,6-dioxo-1,2,3,6-tetrahydropyrimidine-4-carboxylate (**5a**). To a solution of aryl alkyne **Da** (1.0 mmol) in MeCN (2.0 mL) was added NBS (1.5 equiv) and DBU (1.0 equiv). The mixture was stirred at room temperature for 1 min. The reaction mixture was then poured into water and extracted with CH_2Cl_2 (3×10 mL). The combined organic phases were washed with water (3×10 mL), filtered and concentrated under reduced pressure. The crude product was purified by flash-column chromatography on silica gel with petroleum ether/ethyl acetate (80:20) as eluent afforded **5a** as a pale yellow oil (322 mg, 69 %). ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.52 – 7.40 (m, 2H), 7.34 – 7.22 (m, 6H), 7.20 – 7.09 (m, 2H), 5.13 (s, 2H), 5.08 (s, 2H), 4.15 (q, J = 7.2 Hz, 2H), 1.15 (t, J = 7.1 Hz, 3H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 161.0, 160.5, 150.4, 148.2, 135.9, 134.9, 129.3 (2 x C), 128.8 (2 x C), 128.5 (2 x C), 128.3, 128.0, 127.6 (2 x C), 98.5, 77.1, 70.3, 63.3, 57.7, 49.8, 45.6, 13.7.

3. B. Das, N. G. Kundu, *Synth. Commun.,* 2006, 855.

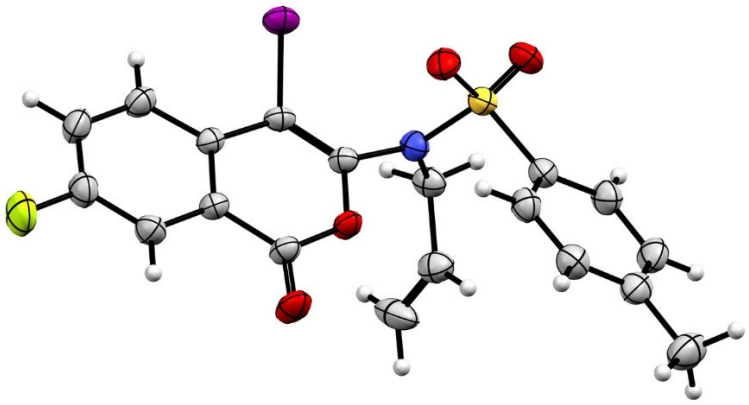
e) Ethyl 1,3-dibenzyl-5-((*N*-methyl-4-nitrophenylsulfonamido)ethynyl)-2,6-dioxo-1,2,3,6-tetrahydro-pyrimidine-4-carboxylate (**6a**). Flash-column chromatography on silica gel with petroleum ether/ethyl acetate (80:20) as eluent afforded **6a** as a pale yellow solid (36 mg, 59 % according to **GP5**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (d, *J* = 8.8 Hz, 2H), 8.17 (d, *J* = 8.8 Hz, 2H), 7.54 – 7.47 (m, 2H), 7.40 – 7.29 (m, 6H), 7.28 – 7.13 (m, 2H), 5.18 (s, 2H), 5.13 (s, 2H), 4.25 (q, *J* = 7.1 Hz, 2H), 3.16 (s, 3H), 1.16 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.2, 160.6, 150.8, 150.5, 147.5, 141.4, 136.0, 134.9, 129.3 (2 x C), 129.2 (2 x C), 128.8 (2 x C), 128.5 (2 x C), 128.3, 128.1, 127.5 (2 x C), 124.6 (2 x C), 97.5, 89.3, 63.6, 60.5, 50.0, 45.6, 39.4, 13.5. HRMS (ESI^+): calcd for $C_{30}H_{26}O_8SN_4$ $[M+H]^+$: 603.1544 found 603.1536. IR (ν cm^{-1}): 2915, 1660, 1594, 1515, 1498, 1454, 1347, 1259, 1086, 1025, 803, 734, 696, 560, 542, 531.

f) Ethyl 1,3-dibenzyl-4-(2,5-dioxopyrrolidin-1-yl)-5-iodo-6-(N-methyl-4-nitrophenylsulfonamido)-2-oxo-1,2,3,4-tetrahydrofuro[2,3-d]pyrimidine-4-carboxylate (7a). Flash-column chromatography on silica gel with petroleum ether/ethyl acetate (80:20) as eluent afforded **7a** as a yellow solid (67 mg, 81 % according to **GP1**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, *J* = 8.5 Hz, 2H), 7.83 (d, *J* = 8.5 Hz, 2H), 7.44 (t, *J* = 7.4 Hz, 2H), 7.41 – 7.30 (m, 3H), 7.30 – 7.23 (m, 3H), 7.09 (d, *J* = 7.1 Hz, 2H), 5.73 (d, *J* = 17.1 Hz, 1H), 5.19 (d, *J* = 16.0 Hz, 1H), 4.94 (d, *J* = 16.0 Hz, 1H), 4.42 – 4.27 (m, 2H), 4.25 (d, *J* = 16.9 Hz, 1H), 3.17 (s, 3H), 2.14 (s, 4H), 1.33 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.2, 165.2, 151.1, 150.5, 145.3, 143.3, 141.4, 137.5, 136.3, 129.3 (2 x C), 128.9 (2 x C), 128.3 (2 x C), 127.7, 127.3, 126.6 (2 x C), 126.5 (2 x C), 124.4 (2 x C), 91.2, 73.0, 63.3, 48.6, 45.5, 38.1, 27.5, 14.0. HRMS (ESI^+): calcd for $C_{34}H_{30}O_{10}SN_5I$ $[M+H]^+$: 828.0831 found 828.0814. IR (ν cm^{-1}): 2983, 1788, 1750, 1724, 1674, 1531, 1477, 1454, 1348, 1332, 1241, 1180, 1030, 969, 855, 738, 700, 637. Mp : 279-282°C.

5. Crystal structure determination of 3k[4]

Crystal Data for $C_{19}H_{15}FINO_4S$ (M = 499.28 g/mol): monoclinic, space group $P2_1/n$ (no. 14), a = 8.4116(4) Å, b = 18.7873(10) Å, c = 12.5260(6) Å, β = 98.829(5)°, V = 1956.04(17) $Å^3$, Z = 4, T = 293 (2) K, μ(MoKα) =1.777 mm^{-1}, Dcalc = 1.695 g/cm^3, 24947 reflections measured (3.629° ≤ θ ≤ 29.645°), 5266 unique (Rint=0.054) which were used in all calculations. The final R1 was 0.0354 (for 3919 $I > 2\sigma(I)$) and wR2 was 0.091 (all data). The final difference Fourier map showed minimum and maximum values of 1.057 and -0.714 e $Å^{-3}$, respectively. The single crystal X-ray diffraction experiment was carried out using a RIGAKU XtaLabPro diffractometer equipped with a Mo microfocus sealed tube generator coupled to a double-bounce confocal Max-Flux® multilayer optic and a HPAD PILATUS3 R 200K detector, on a colorless crystalline parallelepipedic stick. was the data collection and reduction were performed by the CrysalisPro [1] software. The structure was solved by Iterative dual-space direct methods (SHELXD program) [2] in the centrosymmetric triclinic space group. Structure refinement was performed by full-matrix least-squares methods (SHELXL-2018/1 program)[3] on 274 parameters, weighted refinement: $w = 1/[\sigma^2(F_o^2) + (0.0321P)^2 + 1.0040P]$ with $P = [\max(F_o^2,0) + 2F_o^2]/3$ and hydrogen atoms located from difference Fourier synthesis and refined isotropically assuming a riding motion model and their isotropic U's were set to -1.2 (-1.5 for methyl) times the equivalent isotropic displacement parameter of the parent atom. Butene group appeared as disordered over two atomic sites in a 0.833(8)/0.167(8) ratio. Both sites were subjected to RIGU rigid bond and SADI distance restraints. All non-hydrogen atoms were refined with anisotropic displacement parameters.

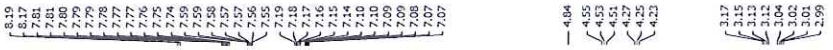
CCDC 2082041 (compound **3k**) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.



Ortep view of compound **3k**. Minor site for the butene group is not shown for clarity. Ellipsoids are drawn at 30% of probability.

4. (a) Rigaku OD (2015). *CrysAlis PRO*. Rigaku Oxford Diffraction, Yarnton, Oxfordshire, England. (b) Schneider, T.R., Sheldrick, G. M. (2002). *Acta Crystallogr.,* **D**58, 1772-1779. (c) Sheldrick, G. M. (2015). *Acta Crystallogr.,* **C**71, 3-8.

6. Spectra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7.57
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7.56
7.55
7.19
7.18
7.17
7.16
7.15
7.14
7.10
7.10
7.09
7.09
7.08
7.07
7.07
4.84
4.55
4.53
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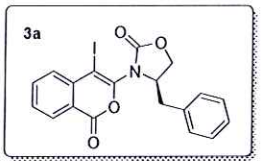
3.04
3.02
3.01
2.99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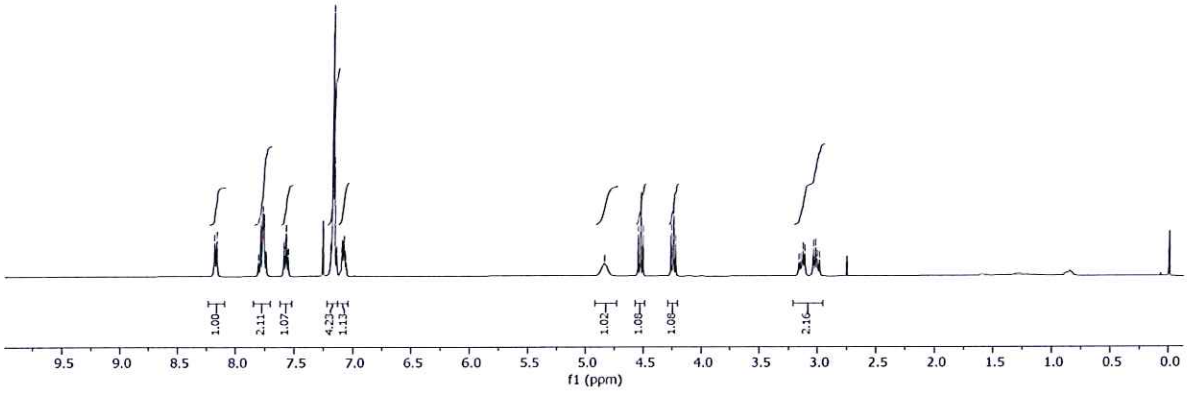
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8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


160.41
153.58
143.41
137.35
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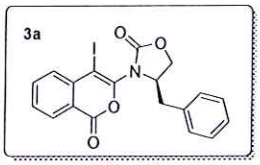
57.58
39.49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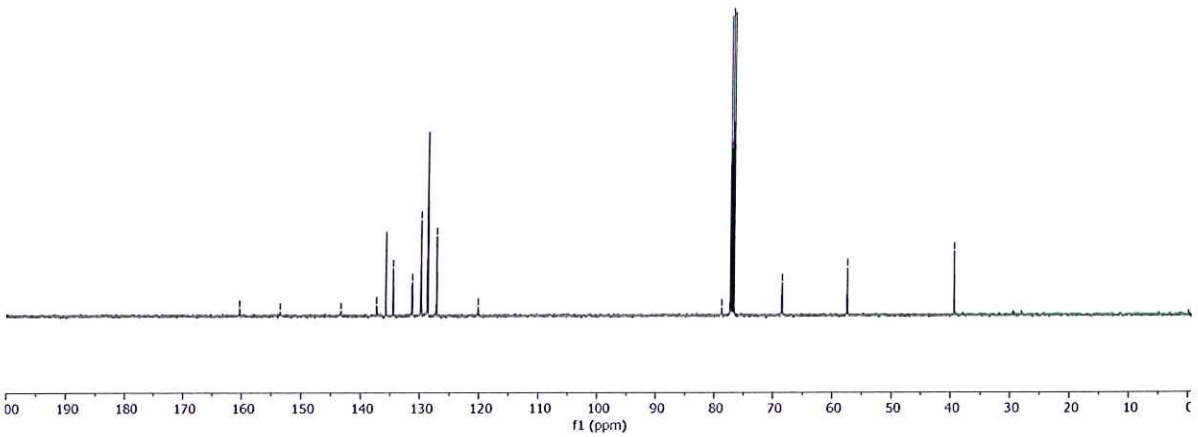
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160
150
140
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120
110
100
90
80
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40
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20
10
f1 (ppm)


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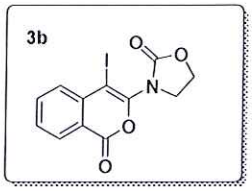
4.10
4.08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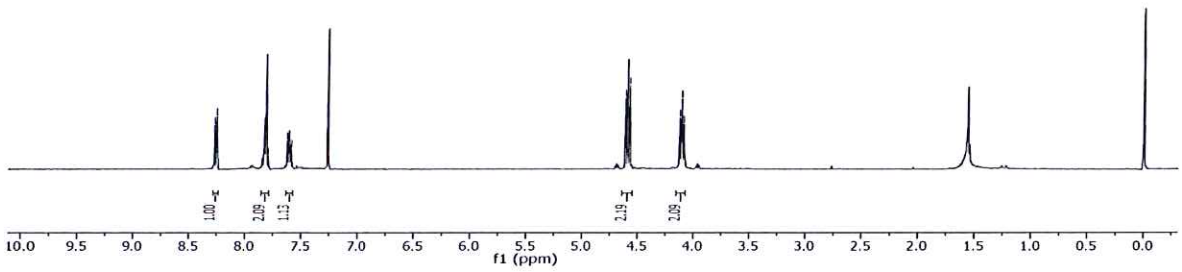
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9.0
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6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


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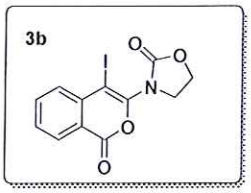
44.69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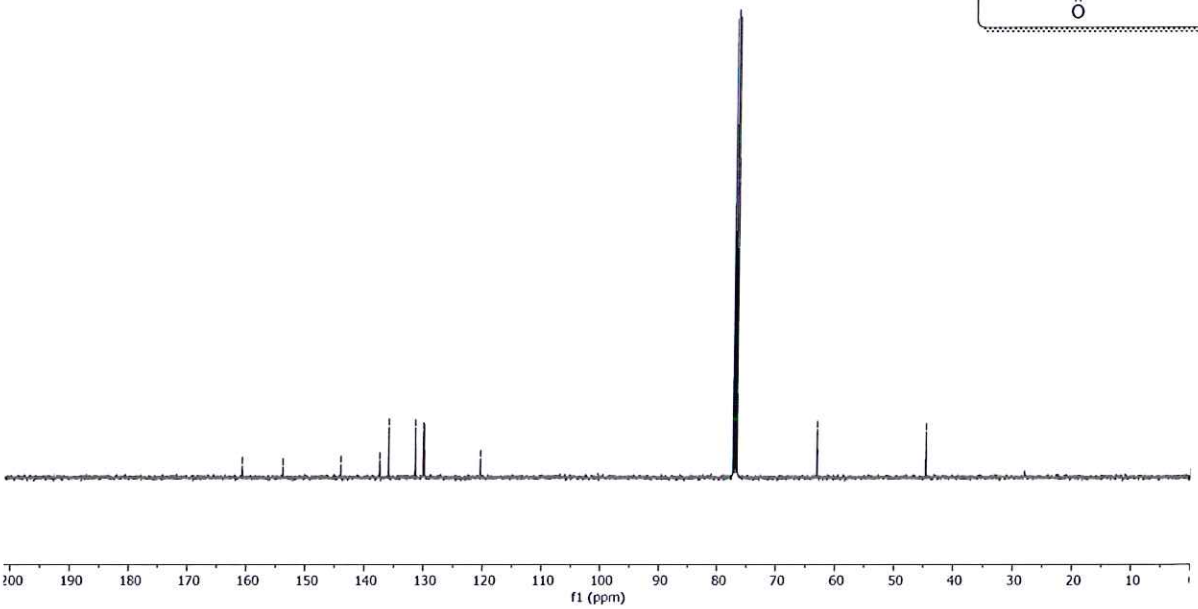
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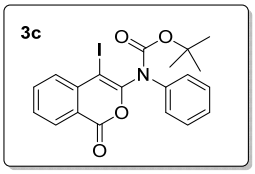
20
10
f1 (ppm)


3c

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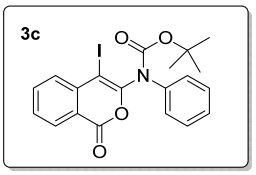
f1 (ppm)


3c

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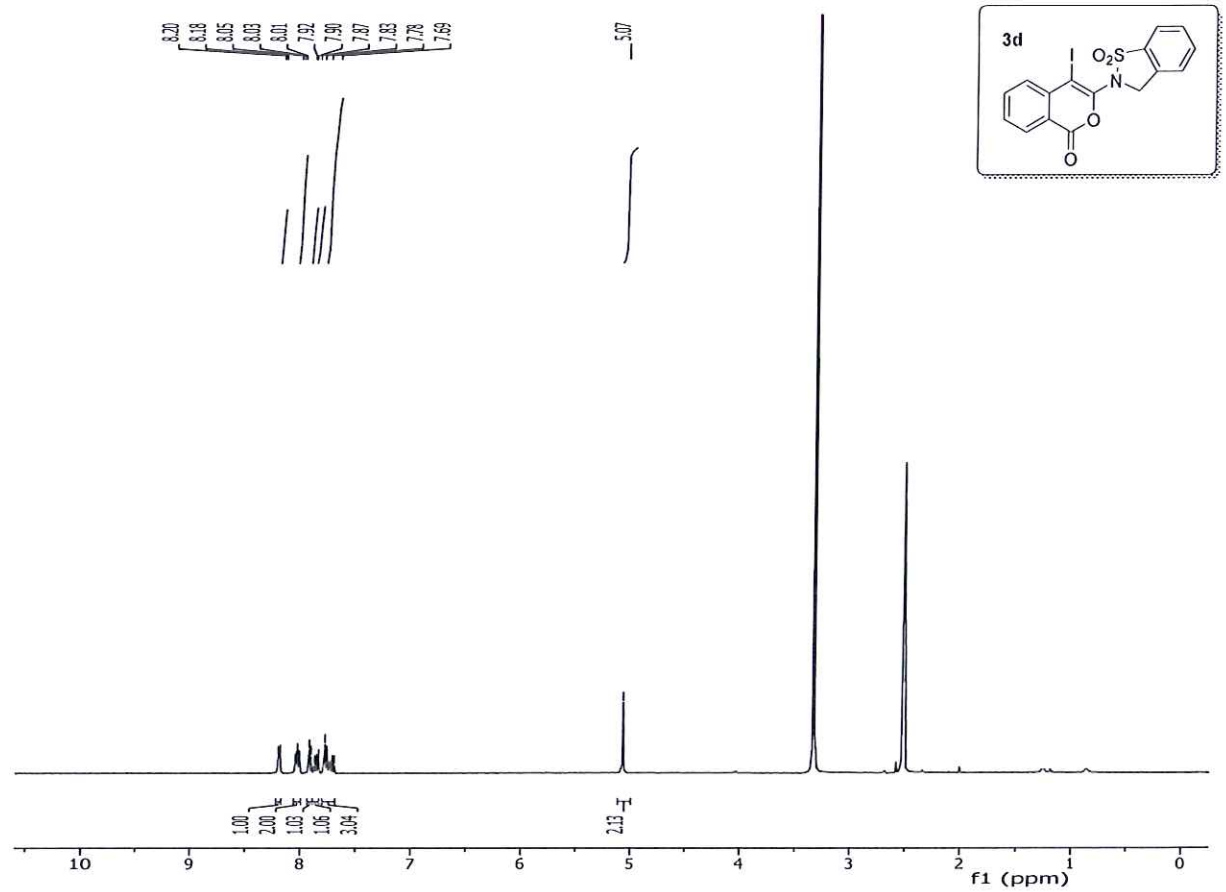
f1 (ppm)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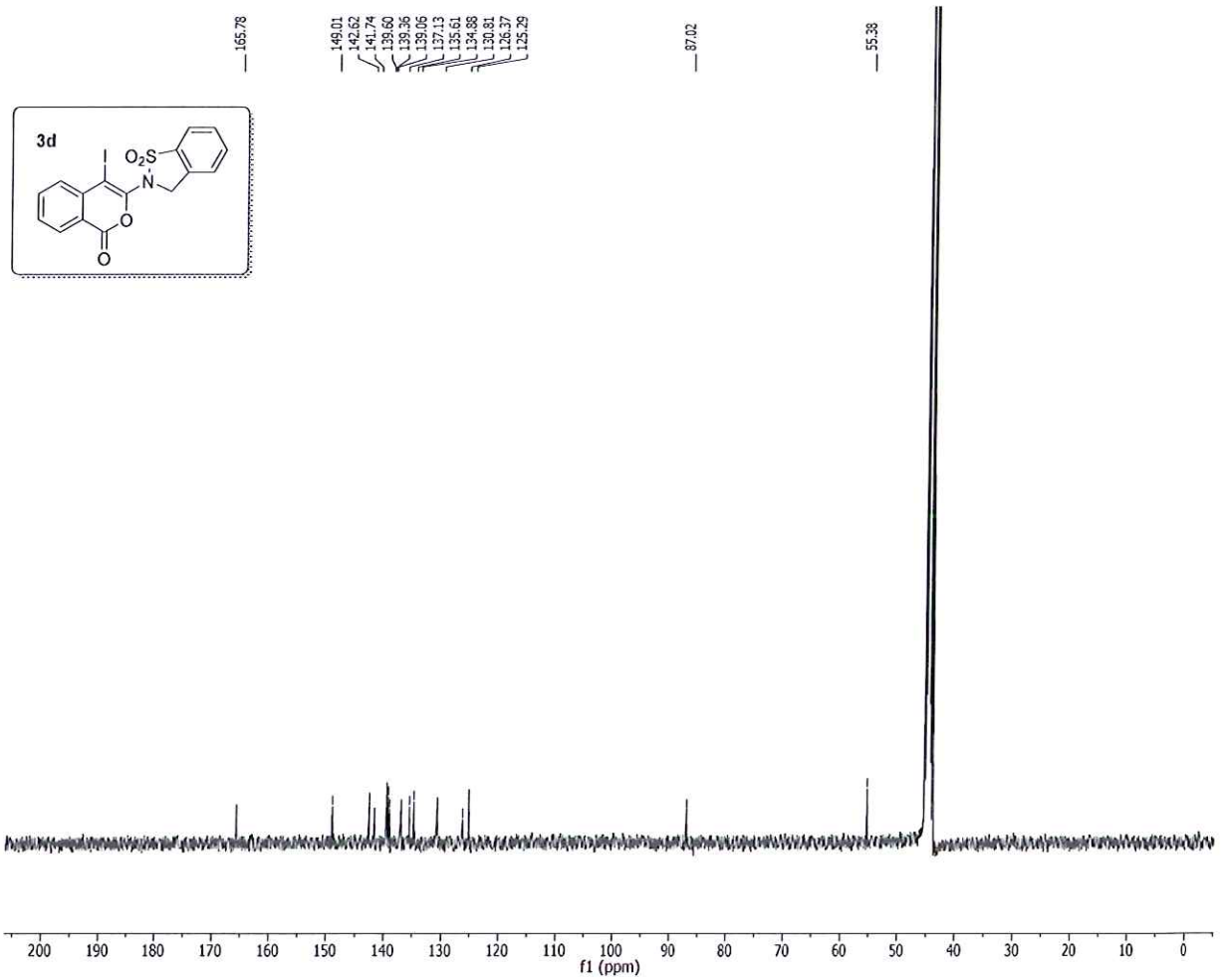
1.03
1.06
3.04
2.13
f1 (ppm)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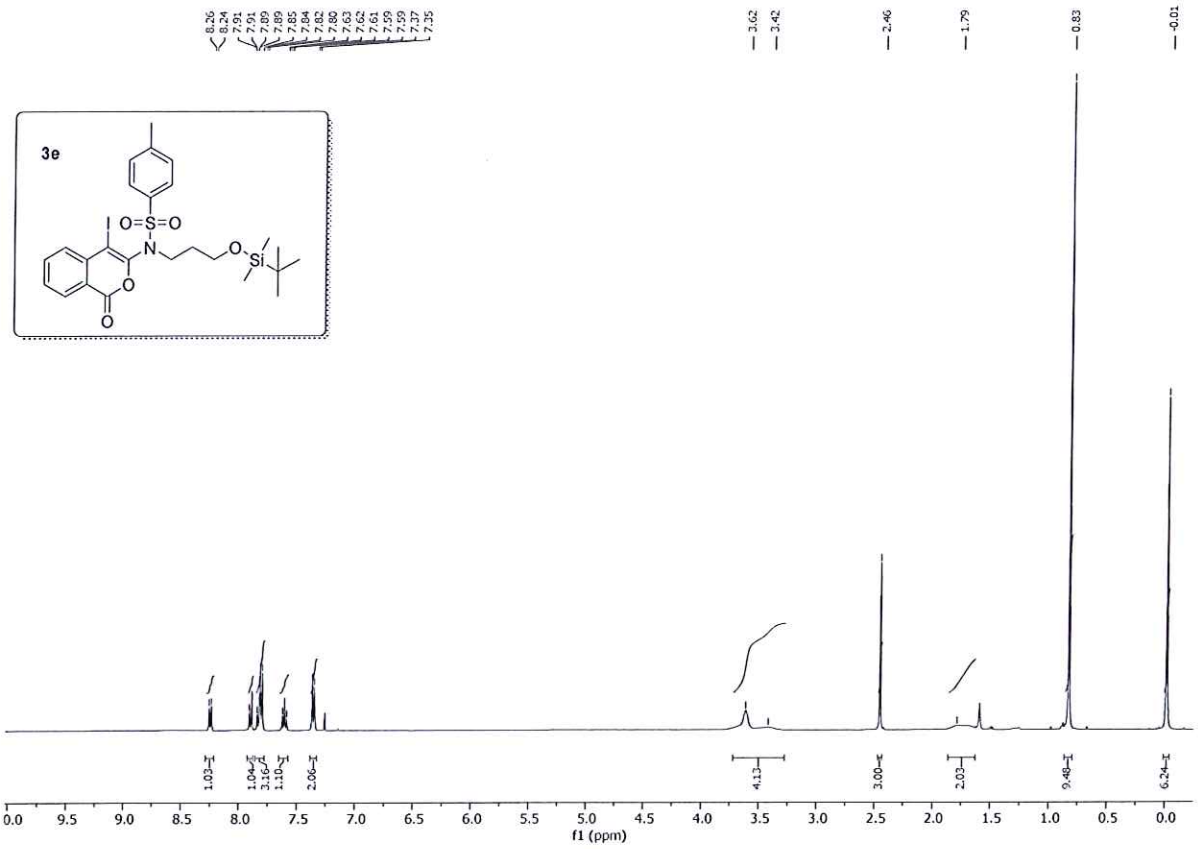
3d
f1 (ppm)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7.62
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7.37
7.35
3.62
3.42
2.46
1.79
0.83
-0.01
3e
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2.06
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2.03
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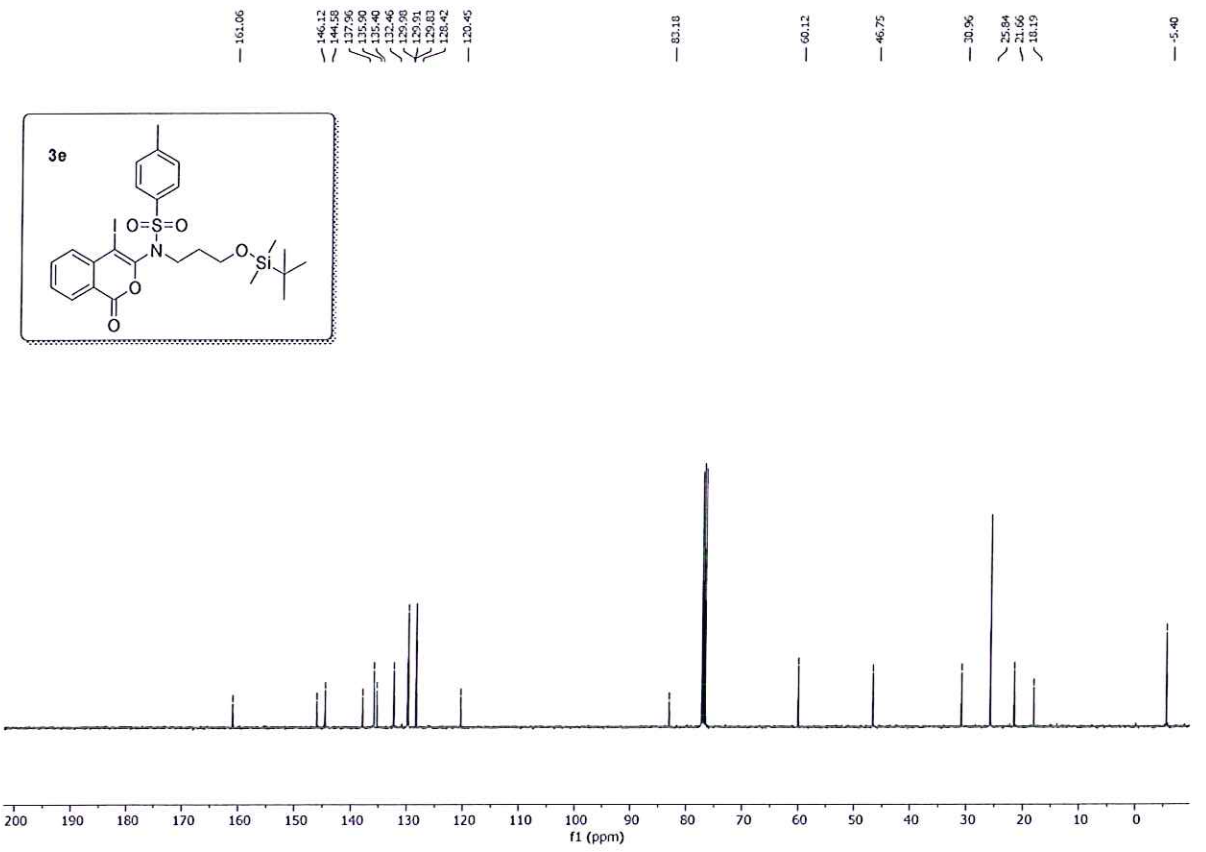
6.24
f1 (ppm)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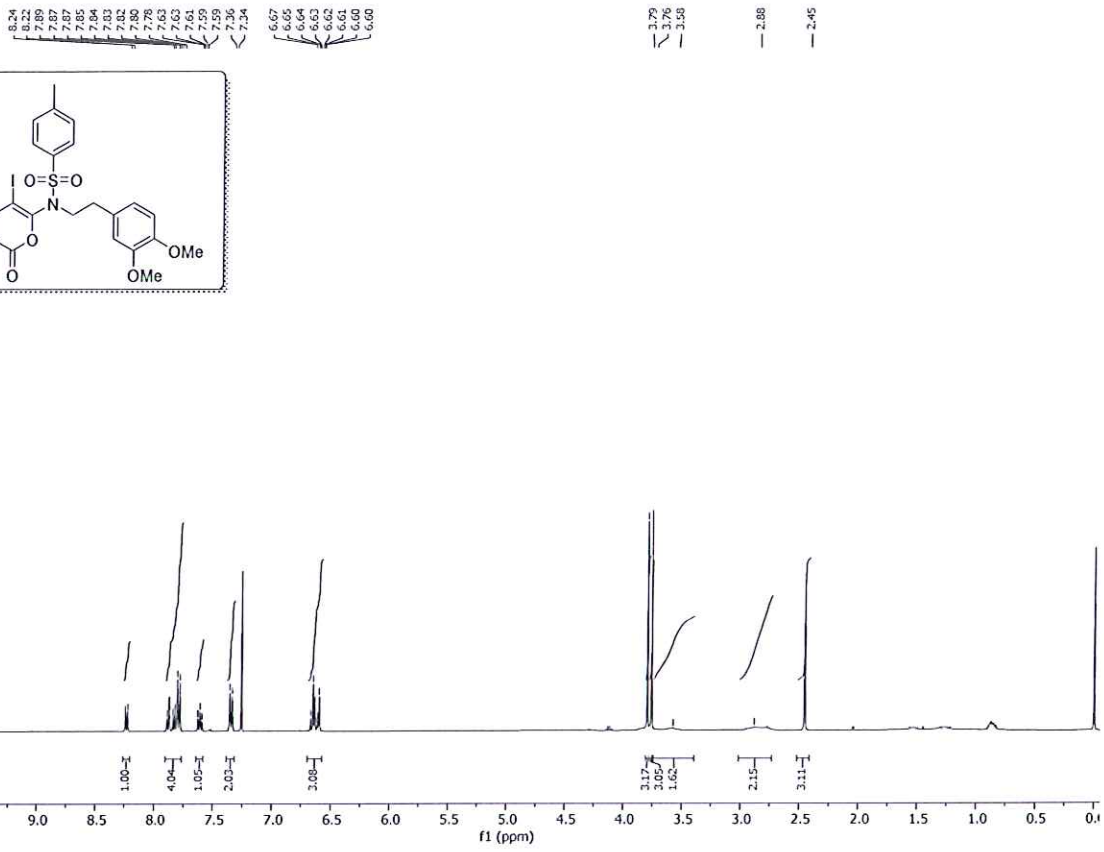
18.19
-5.40
3e
f1 (ppm)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6.63
6.62
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3.76
3.58
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2.45
3f
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N
O
OMe
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3.17
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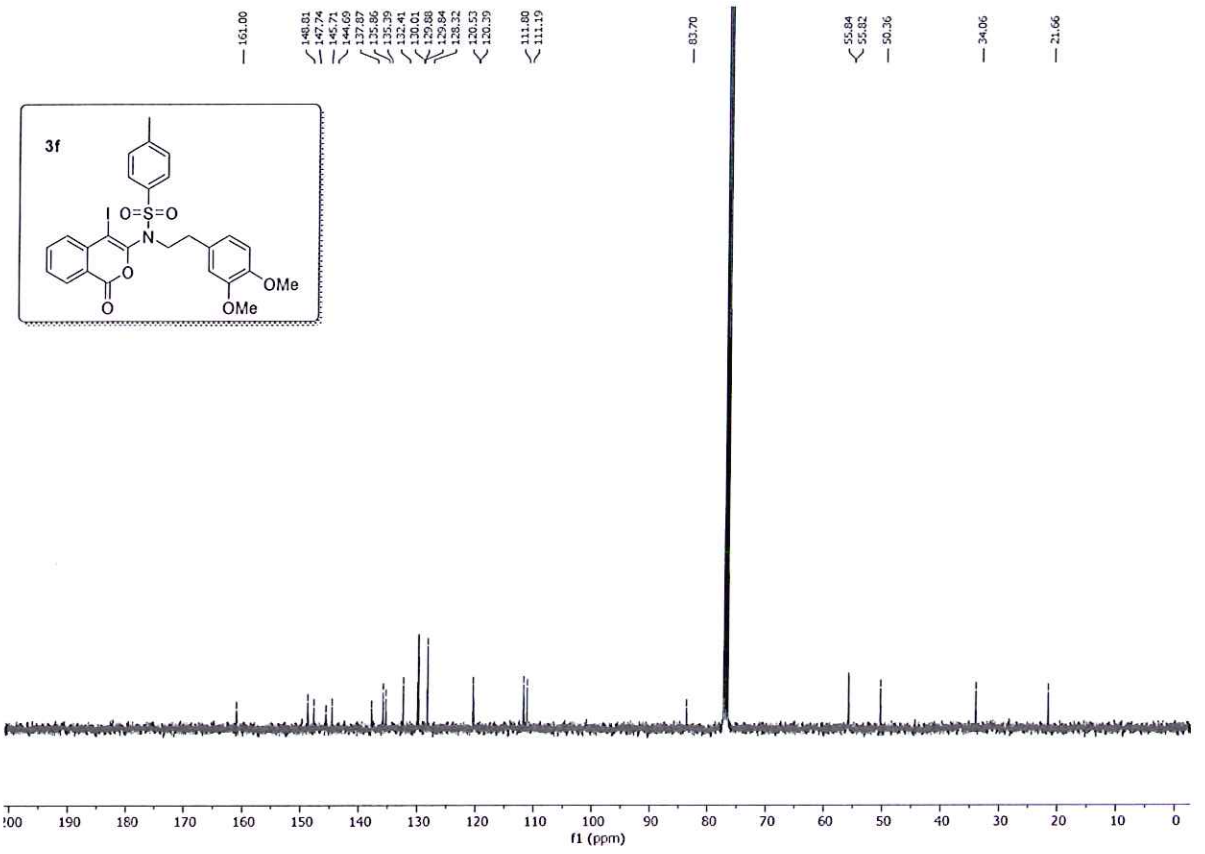
f1 (ppm)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55.84
55.82
50.36
34.06
21.66
3f
O=S=O
N
O
OMe
OMe
f1 (ppm)


8.38
8.36
8.26
8.24
8.07
8.05
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7.88
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7.86
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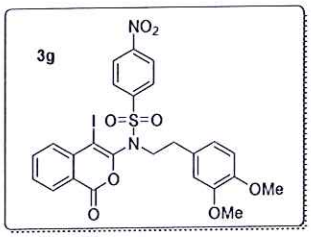
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O
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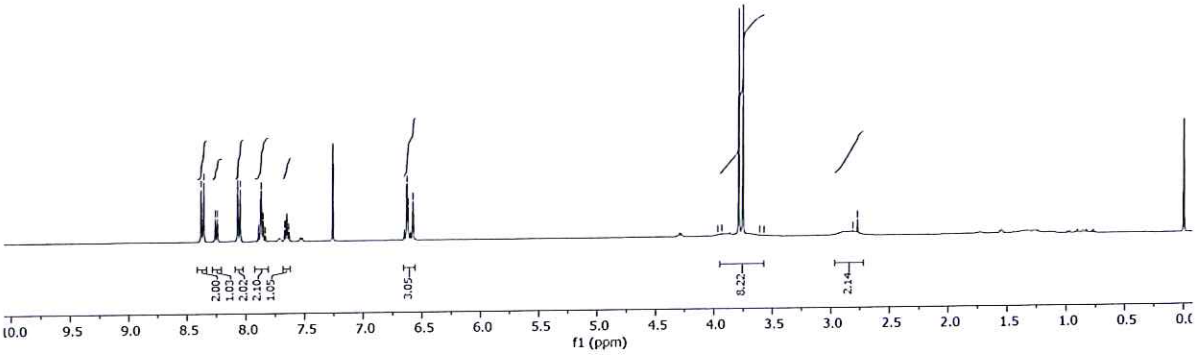
OMe
O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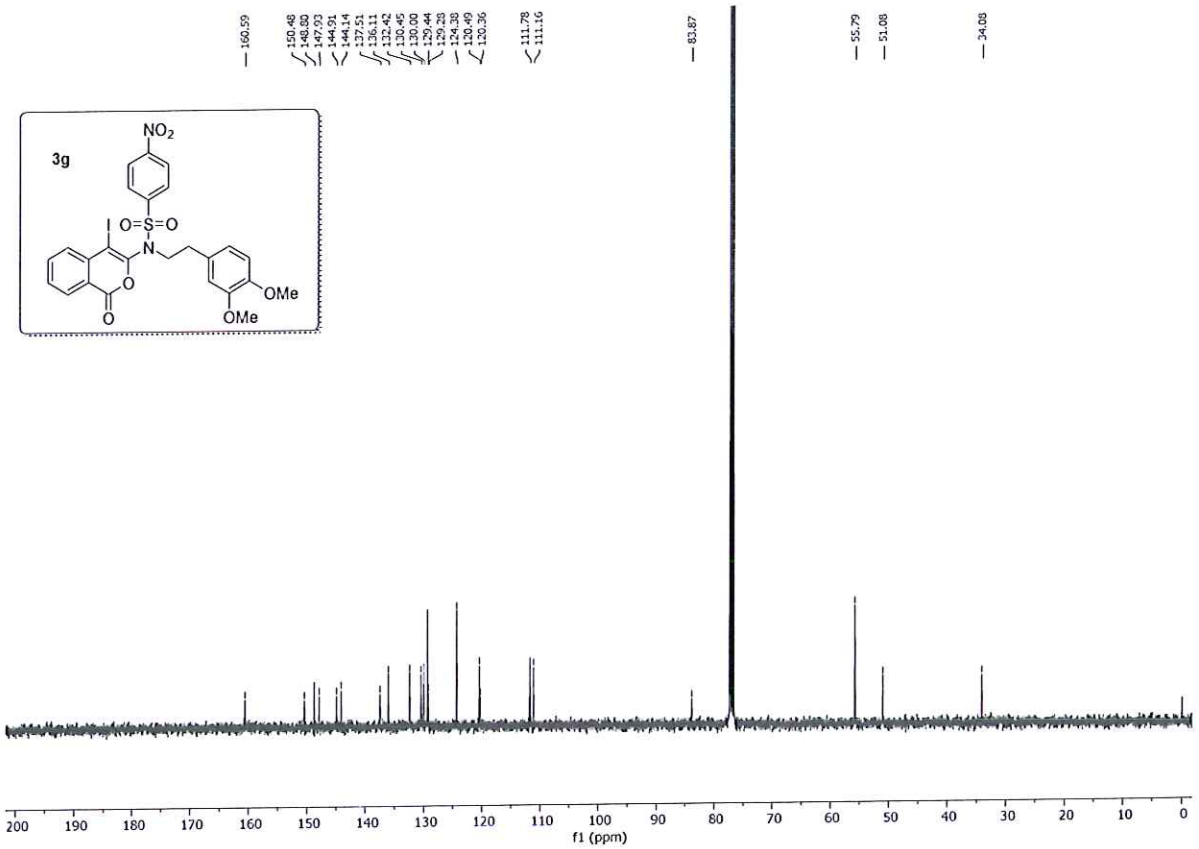
0.0
f1 (ppm)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120.49
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111.16
83.87
55.79
51.08
34.08
200
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180
170
160
150
140
130
120
110
100
90
80
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10
0
f1 (ppm)

3g
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O=S=O
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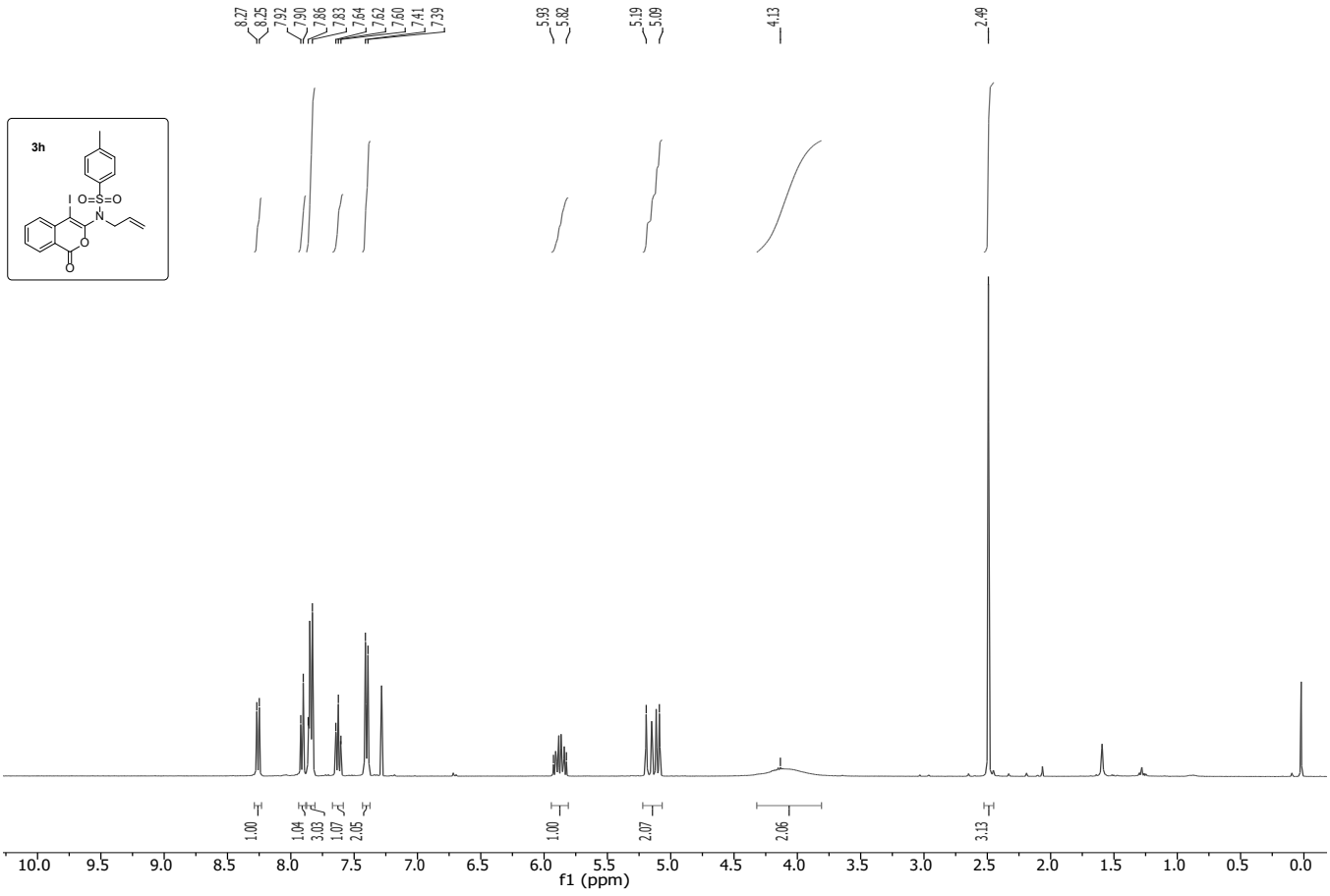
O
OMe
OMe
O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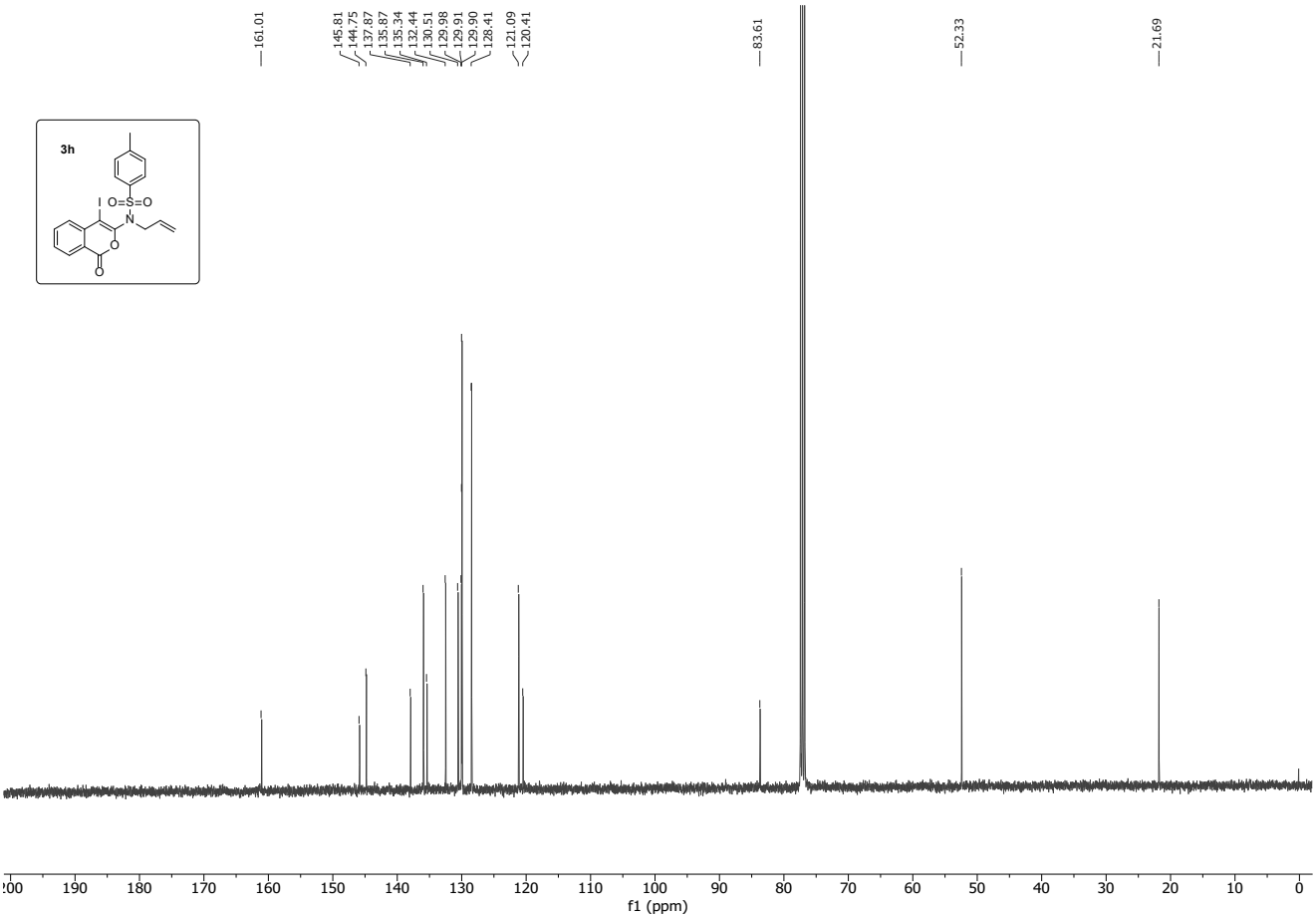
1.00
2.07
2.06
3.13
f1 (ppm)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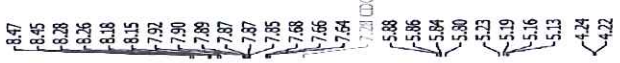
52.33
21.69
3h
f1 (ppm)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5.19
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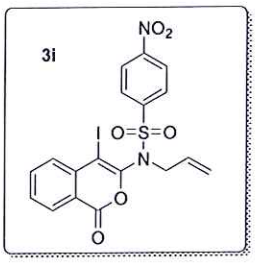
5.13
4.24
4.22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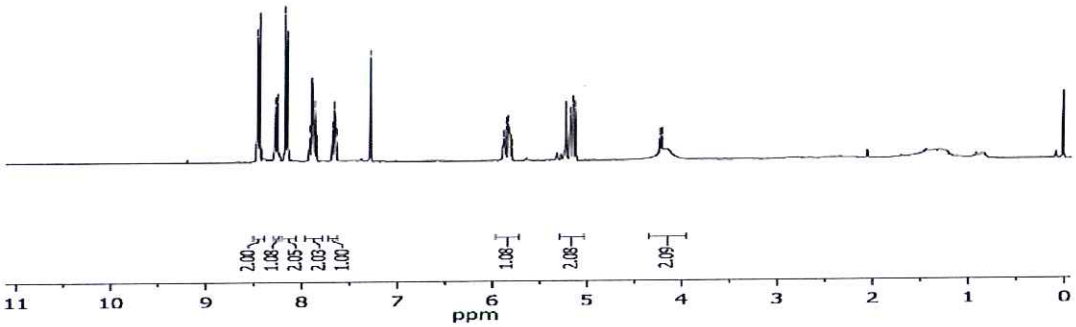
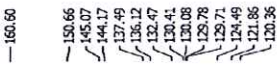
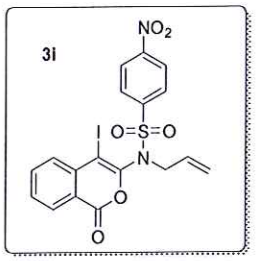
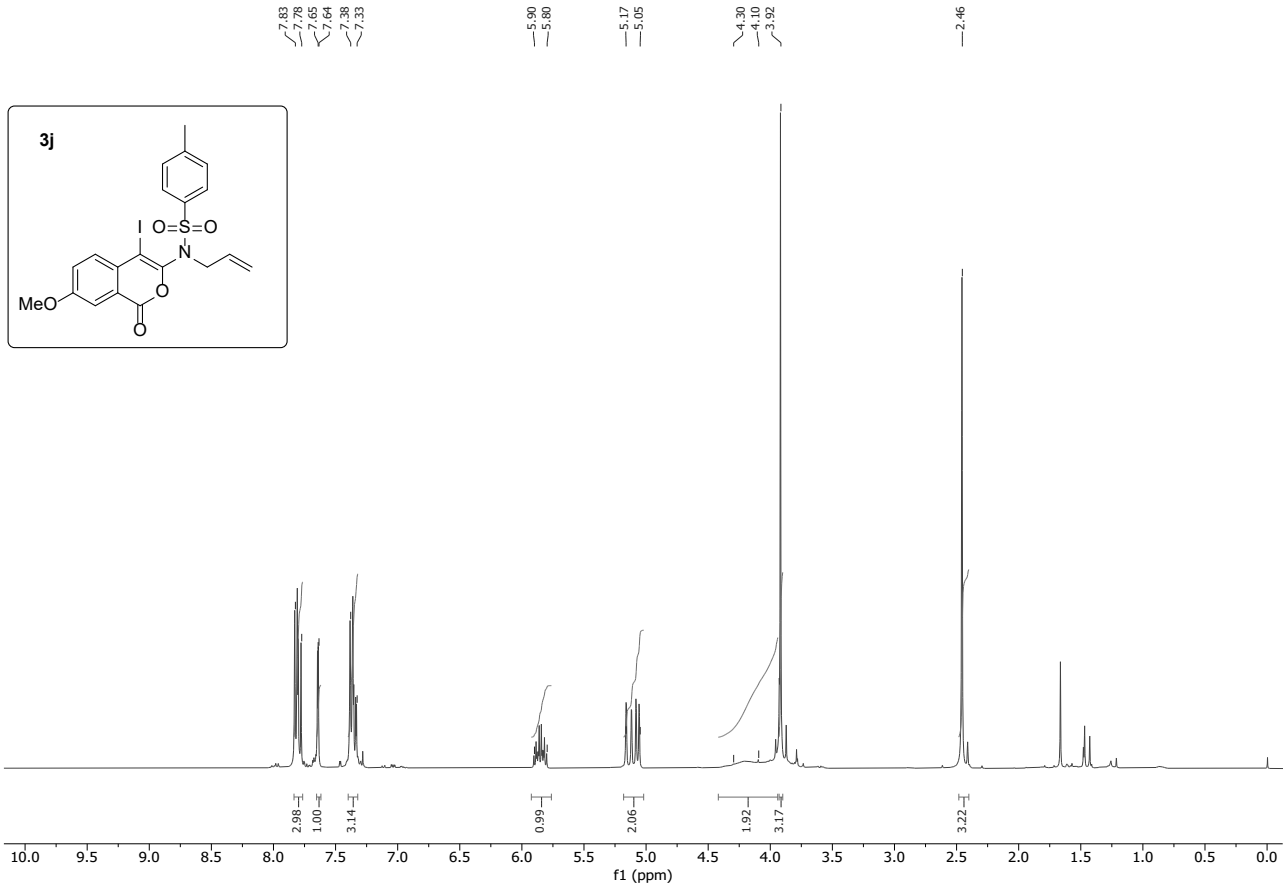
NO2
O=S=O
N
I
O
O

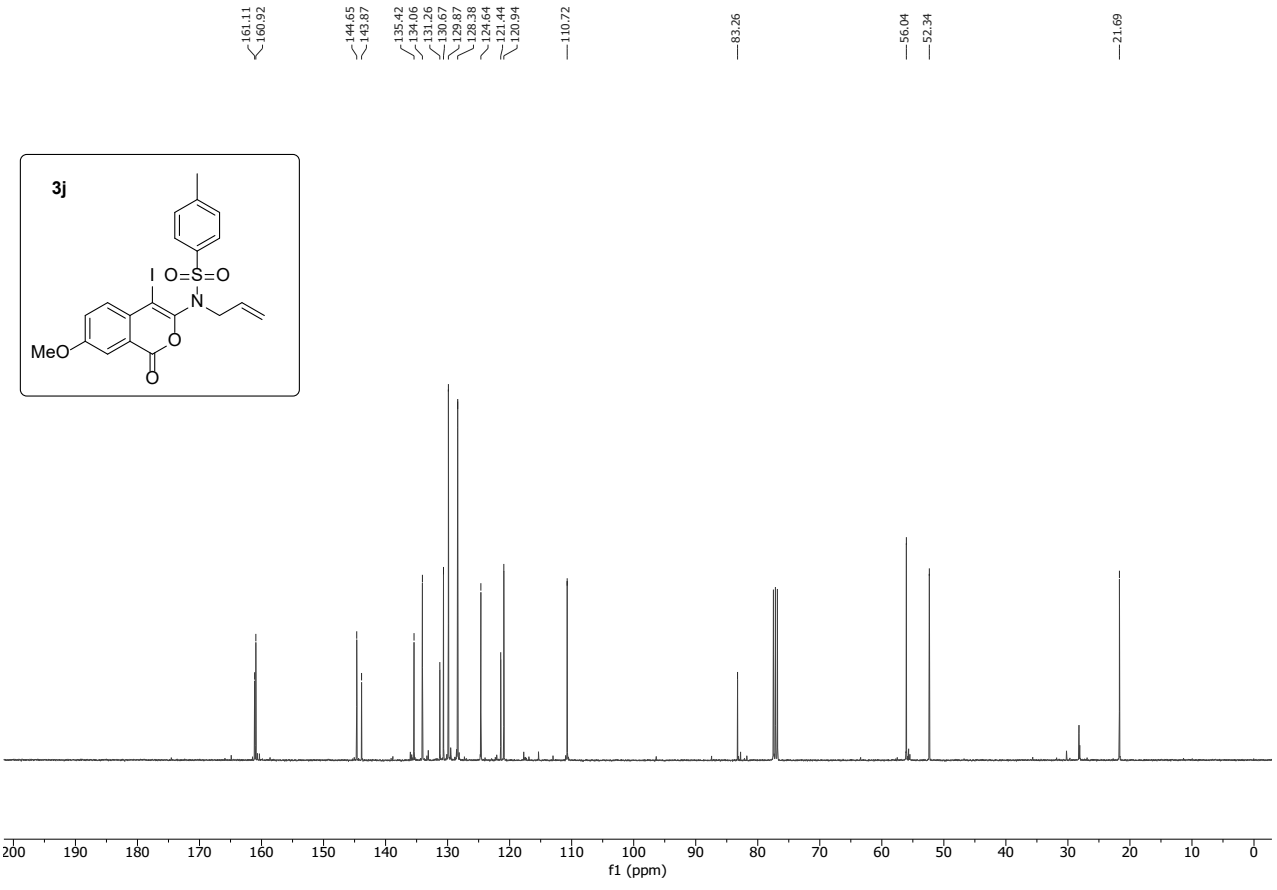

2.00
1.08
2.05
2.03
1.00
1.08
2.08
2.09
11
10
9
8
7
6
5
4
3
2
1
0
ppm

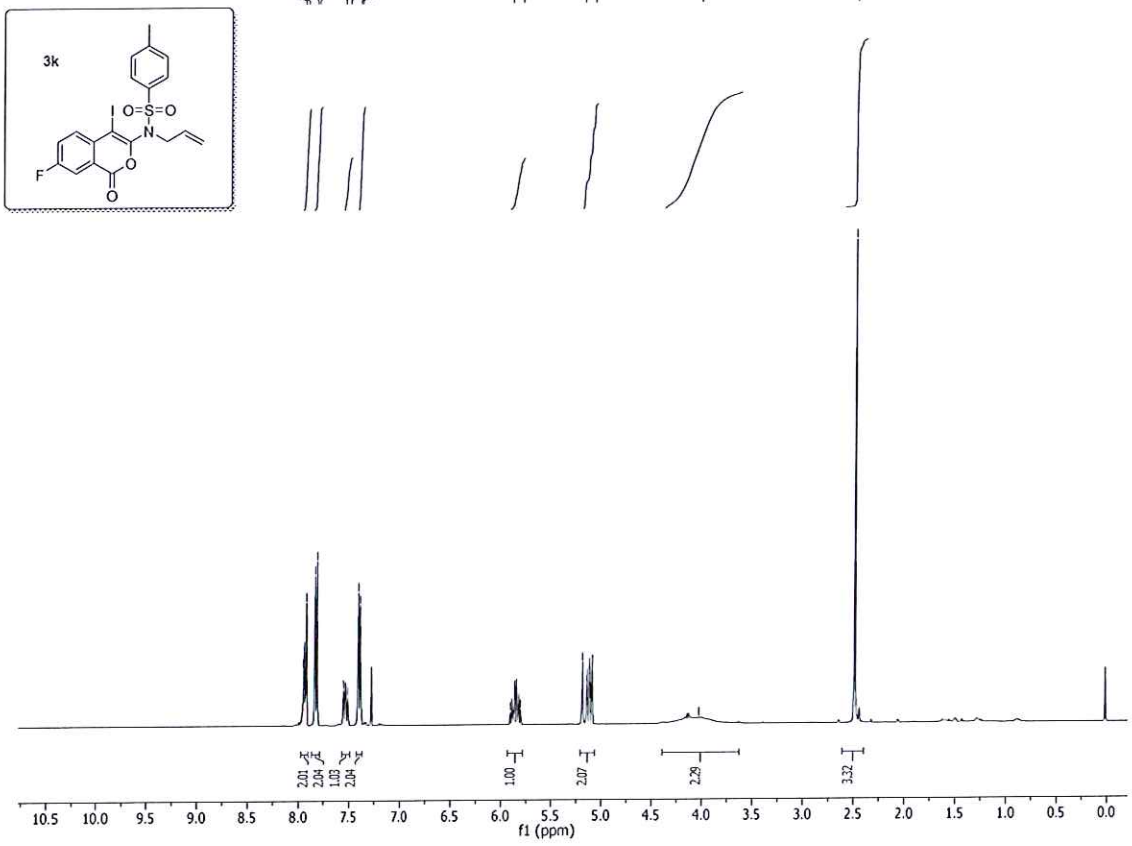

160.60
150.66
145.07
144.17
137.49
136.12
132.47
130.41
130.08
129.78
129.71
124.49
121.86
120.36
83.76
52.93
29.63

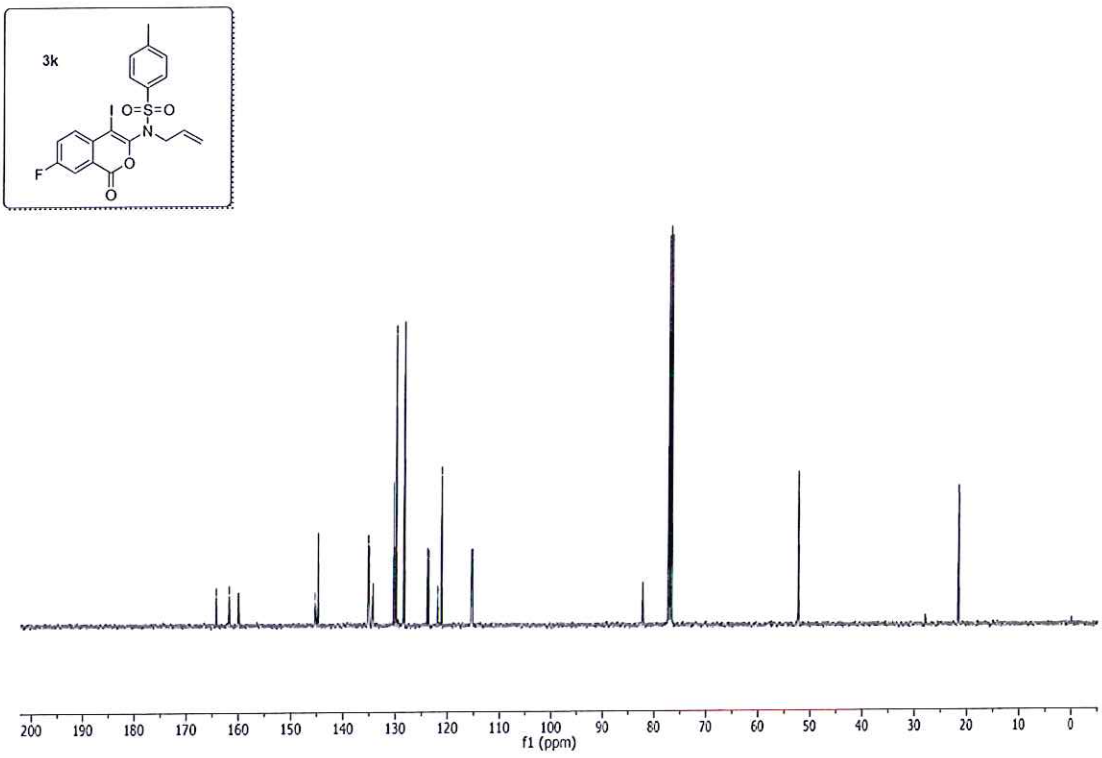

3i
NO2
O=S=O
N
I
O
O

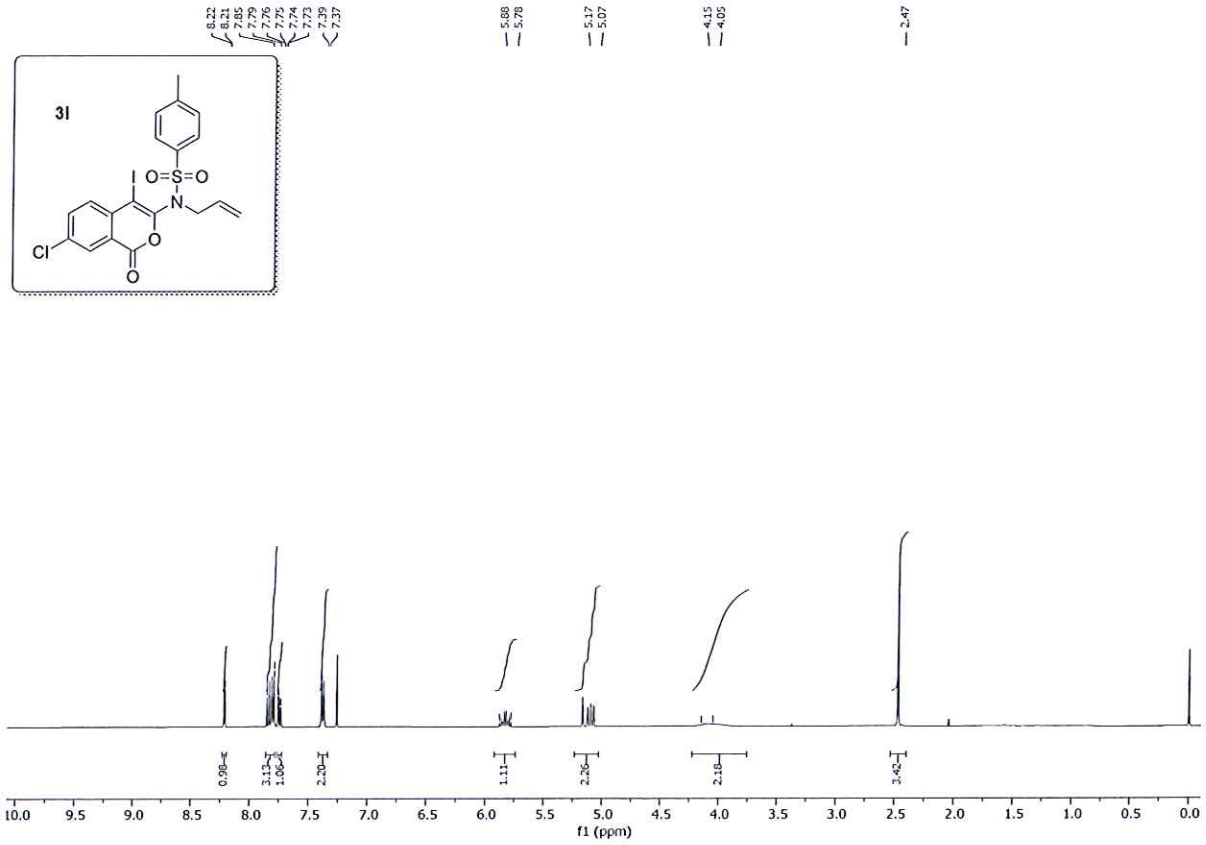
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

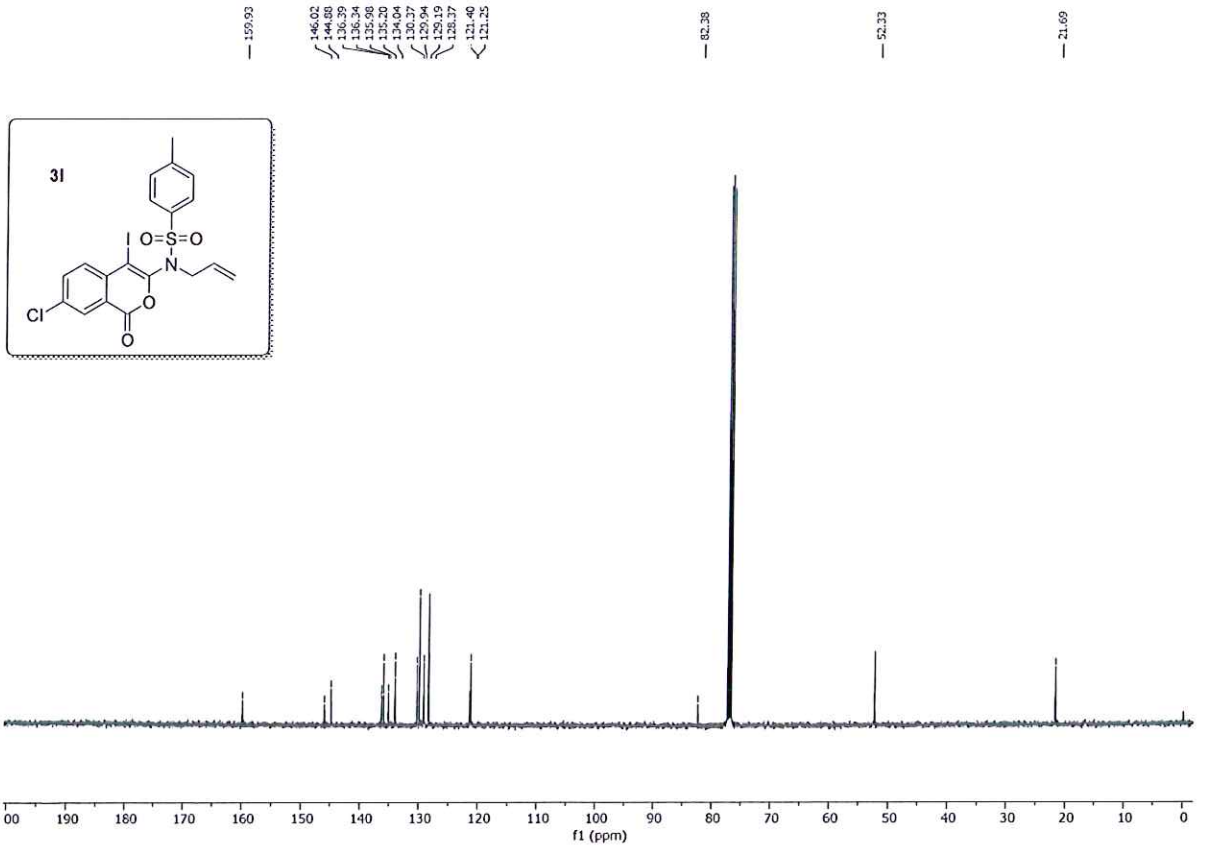

7.83
7.78
7.65
7.64
7.38
7.33
5.90
5.80
5.17
5.05
4.30
4.10
3.92
2.46
3j
I
O=S=O
N
O
MeO
O
2.98
1.00
3.14
0.99
2.06
1.92
3.17
3.22
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


161.11
160.92
144.65
143.87
135.42
134.06
131.26
130.67
129.87
128.38
124.64
121.44
120.94
110.72
83.26
56.04
52.34
21.69
3j
I
O=S=O
N
O
MeO
O
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

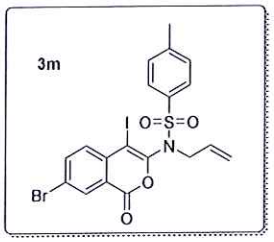

3k
7.96
7.93
7.84
7.82
7.56
7.51
7.41
7.39
5.91
5.81
5.19
5.09
4.03
2.49
2.01
2.04
1.03
2.04
1.00
2.07
2.29
3.32
f1 (ppm)

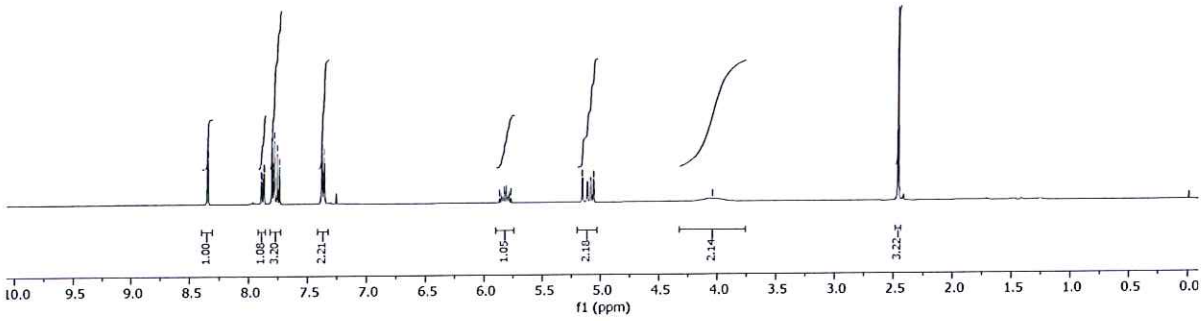

3k
164.25
161.83
160.14
160.11
145.39
144.83
135.23
135.16
135.08
134.29
134.36
129.92
128.36
123.93
123.71
121.94
121.85
121.18
115.52
115.29
82.34
82.33
52.33
21.68
f1 (ppm)


8.22
8.21
7.85
7.79
7.76
7.75
7.74
7.73
7.39
7.37
5.88
5.78
5.17
5.07
4.15
4.05
2.47
3l
I
O=S=O
N
Cl
O
O
0.98
3.13
1.06
2.20
1.11
2.26
2.16
3.42
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

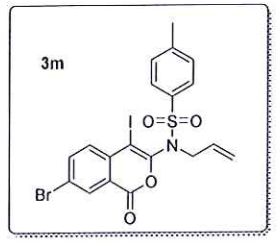

159.93
146.02
144.88
136.39
136.24
135.98
135.20
134.64
130.37
129.94
129.19
128.37
121.40
121.25
82.38
52.33
21.69
3l
I
O=S=O
N
Cl
O
O
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

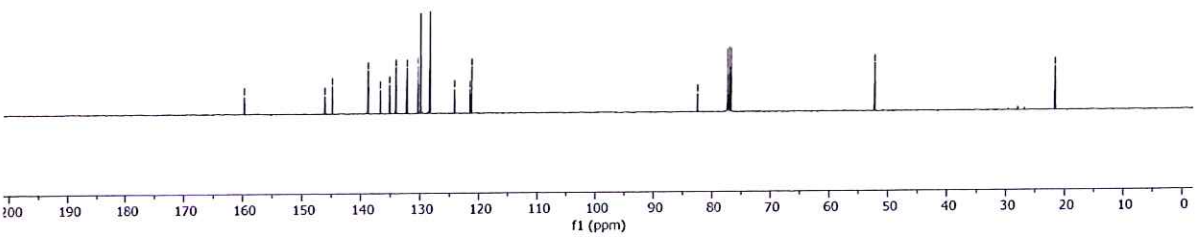
8.35
8.35
7.90
7.89
7.88
7.87
7.81
7.79
7.76
7.74
7.38
7.36
5.87
5.77
5.16
5.06
4.04
2.46

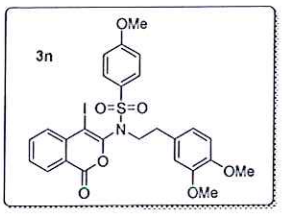




159.77
146.12
144.88
138.84
136.78
135.19
134.13
132.25
130.38
129.95
128.37
124.16
121.55
121.26
82.49
52.32
21.71

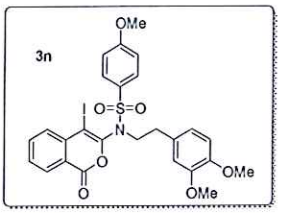


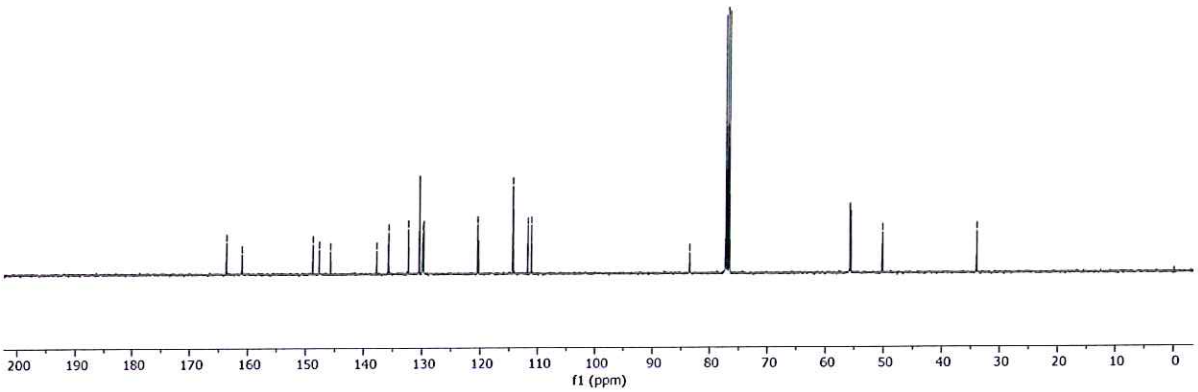



3n
OMe
O=S=O
I
N
O
O
OMe
OMe

8.24
8.22
7.89
7.80
7.63
7.59
7.02
7.00
6.67
6.60
3.89
3.79
3.75
3.75
3.57
2.89
2.73
1.00
4.06
1.10
2.10
3.01
3.10
3.21
3.00
1.40
1.95
f1 (ppm)

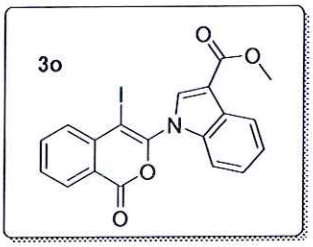

163.68
161.05
148.81
147.72
145.83
137.88
135.86
132.38
130.52
129.99
129.88
129.86
129.83
120.53
120.38
114.43
111.81
111.21
83.63
55.84
55.83
55.69
50.32
34.05

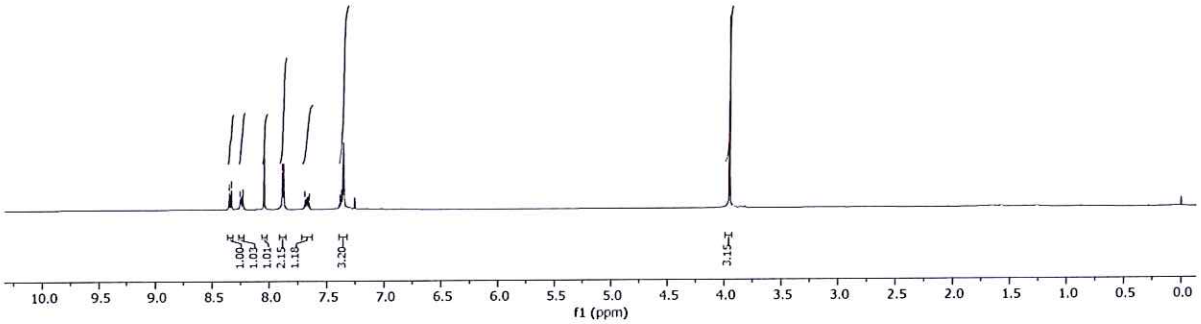

3n
OMe
O=S=O
I
N
O
O
OMe
OMe


200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

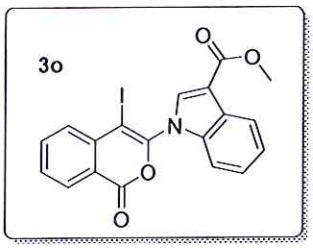
8.36
8.34
8.26
8.24
8.05
7.89
7.88
7.70
7.65
7.39
7.35

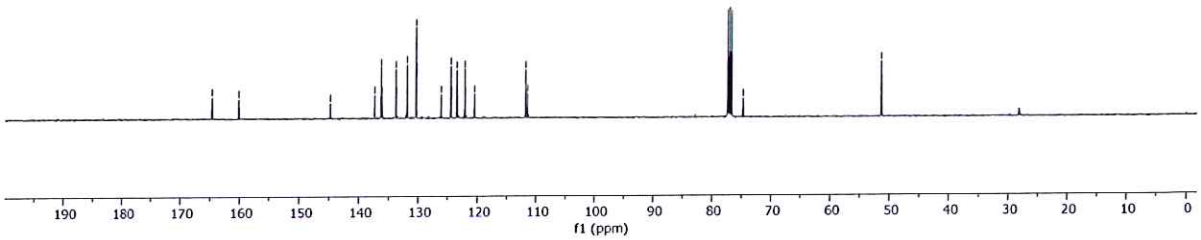
3.96



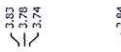


164.67
160.20
144.80
137.37
136.28
136.14
133.72
131.85
130.34
126.13
124.46
123.46
122.14
120.52
111.83
111.46
74.79
51.45

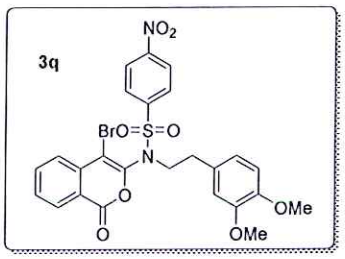


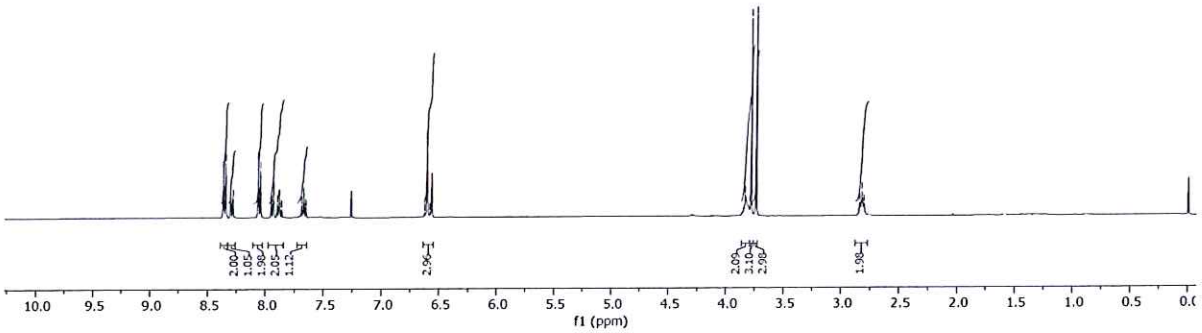



8.36
8.34
8.30
8.28
8.07
8.04
7.95
7.95
7.93
7.93
7.90
7.90
7.88
7.88
7.86
7.86
7.69
7.69
7.67
7.67
7.67
7.67
7.65
7.65
6.63
6.61
6.60
6.58
6.57
6.56

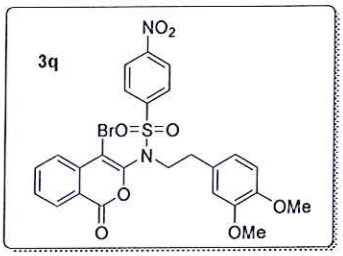

3.83
3.78
3.74

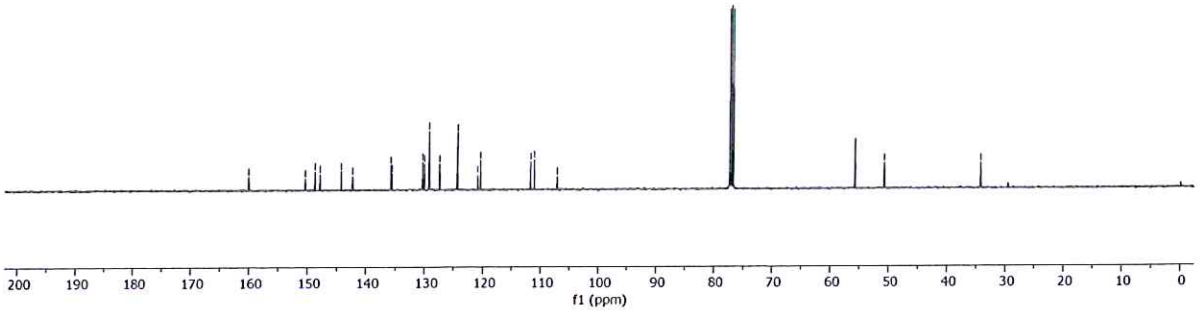

2.84
2.82
2.80

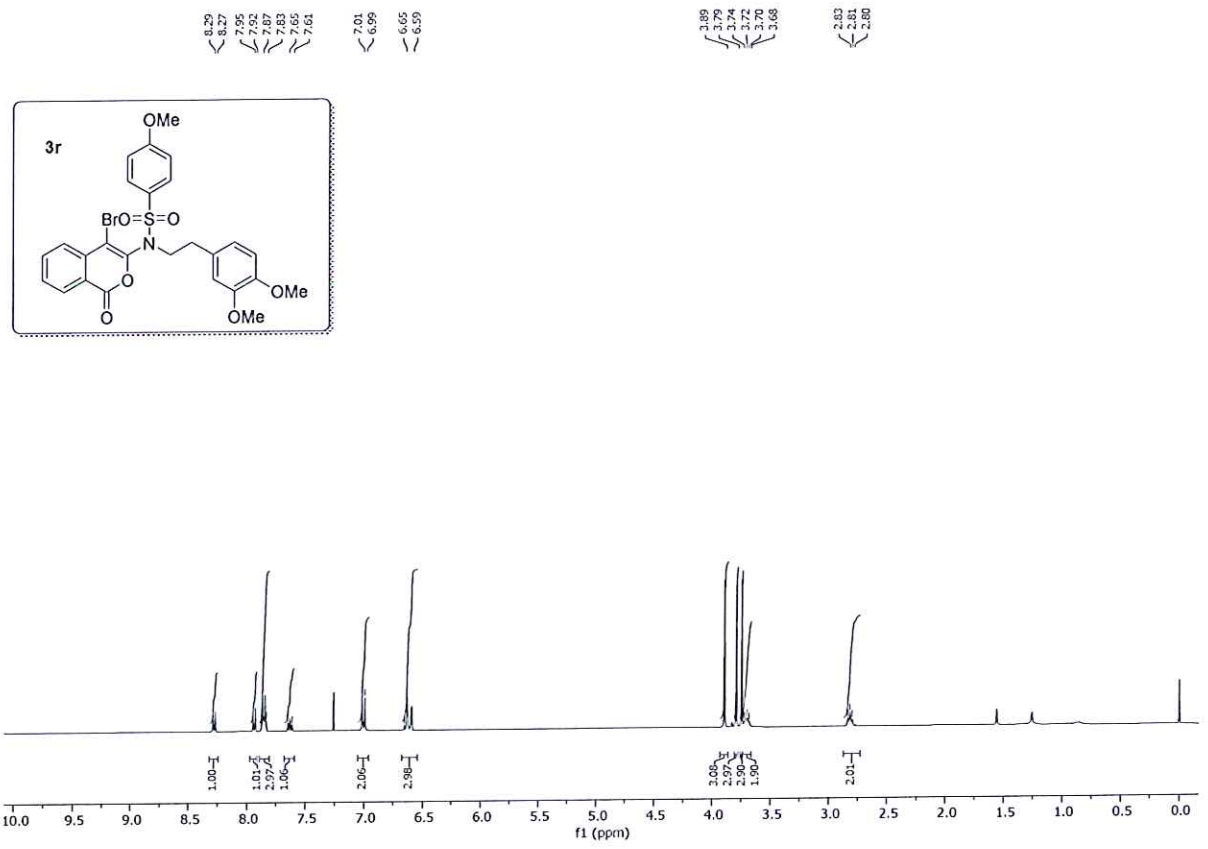

3q
NO2
BrO=S=O
N
O
O
OMe
OMe

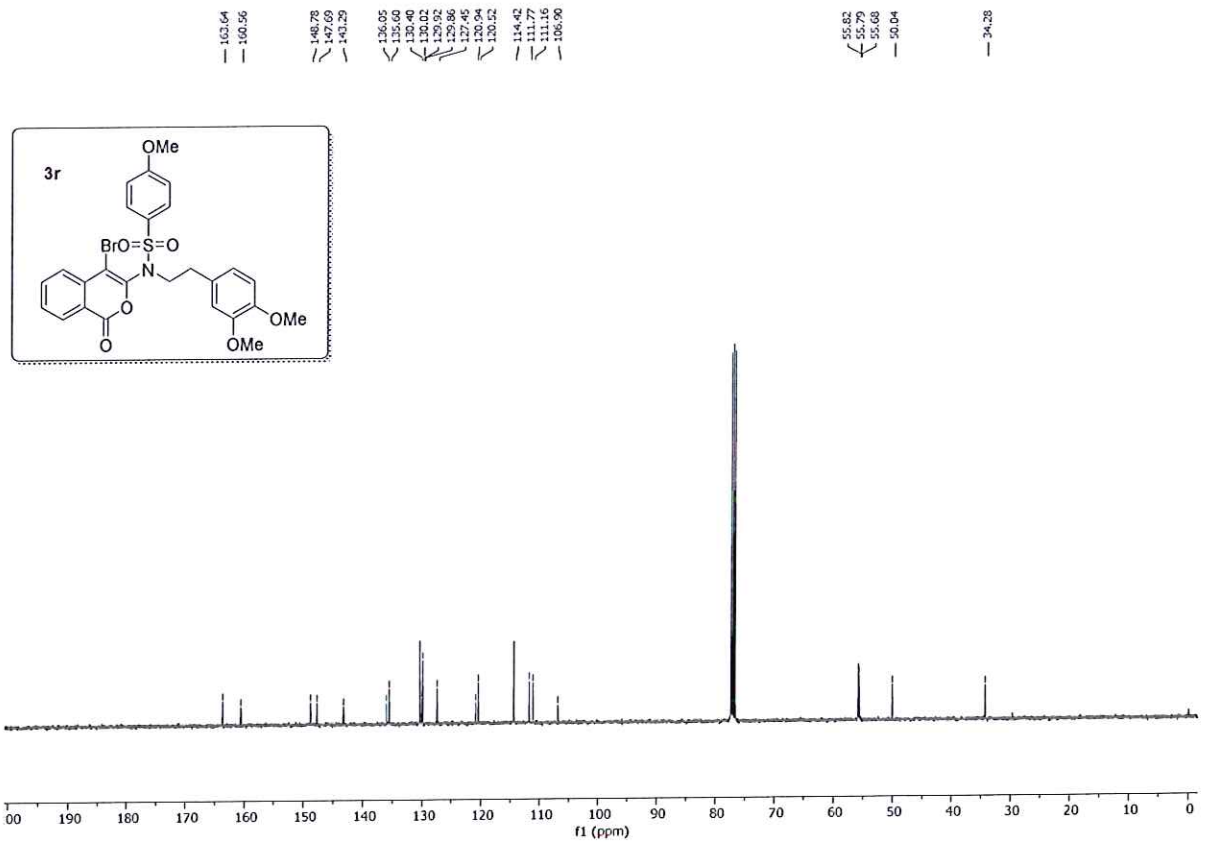

2.00
1.05
1.96
2.05
1.12
2.96
2.09
3.10
2.98
1.98
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


160.10
150.43
148.76
147.90
144.32
142.36
135.85
135.66
130.40
130.09
129.30
129.29
127.51
124.37
120.93
120.48
111.75
111.11
107.20
55.76
50.83
34.38

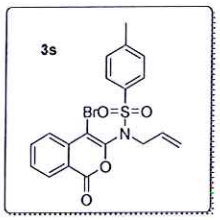

3q
NO2
BrO=S=O
N
O
O
OMe
OMe

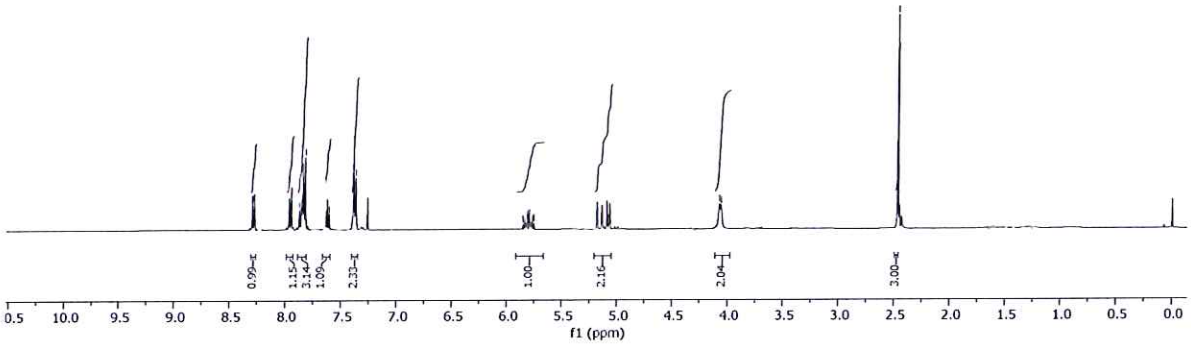

200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.29
8.27
7.95
7.92
7.87
7.83
7.65
7.61
7.01
6.99
6.65
6.59
3.89
3.79
3.74
3.72
3.70
3.68
2.83
2.81
2.80
3r
OMe
BrO=S=O
N
O
O
OMe
OMe
1.00
1.01
2.07
1.06
2.06
2.98
3.08
2.97
2.90
1.90
2.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

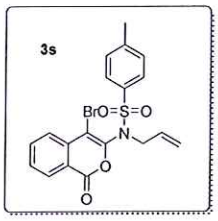

163.64
160.56
148.78
147.69
143.29
136.05
135.60
130.40
130.02
129.92
129.86
127.45
120.94
120.52
114.42
111.77
111.16
106.90
55.82
55.79
55.68
50.04
34.28
3r
OMe
BrO=S=O
N
O
O
OMe
OMe
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

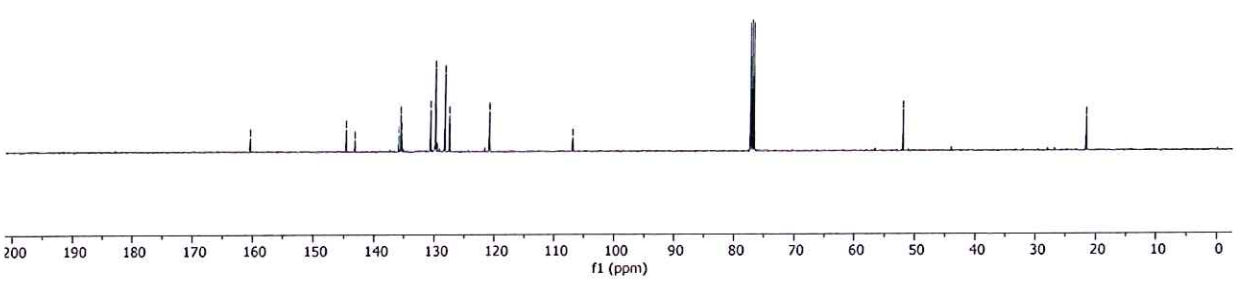

8.29
8.29
8.27
8.27
7.96
7.96
7.94
7.94
7.87
7.82
7.65
7.60
7.38
7.36
5.85
5.75
5.18
5.06
4.07
4.06
2.47

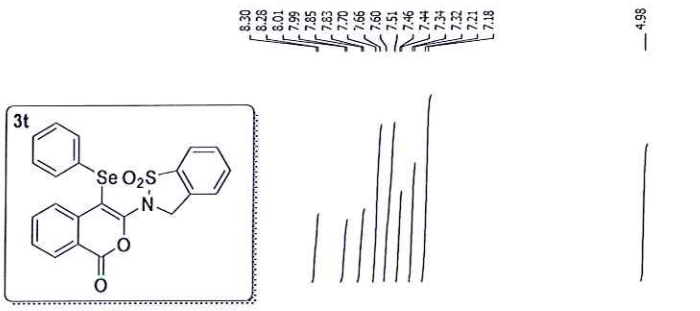

3s
Br
O
S
O
N
O
O

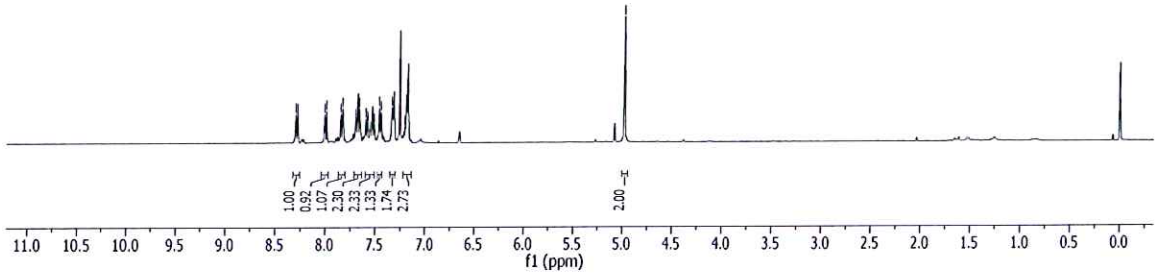

0.99
1.15
3.14
1.09
2.33
1.00
2.16
2.04
3.00
0.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

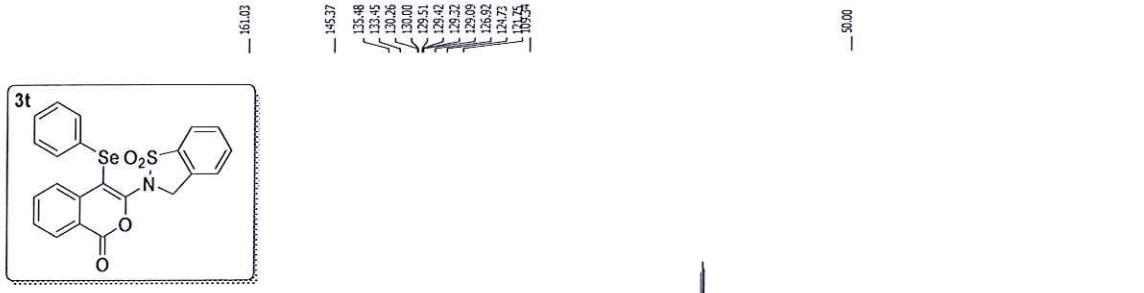

160.52
144.72
143.25
136.04
135.64
135.51
130.70
130.01
129.94
129.92
128.29
127.56
120.96
120.88
106.98
52.00
21.68

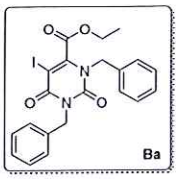

3s
Br
O
S
O
N
O
O


200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

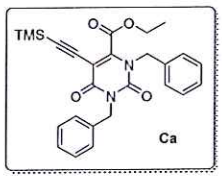

8.30
8.28
8.01
7.99
7.85
7.83
7.70
7.66
7.60
7.51
7.46
7.44
7.34
7.32
7.21
7.18
4.98
3t
Se
O2S
N
O
O


1.00
0.92
1.07
2.30
2.33
1.33
1.74
2.73
2.00
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

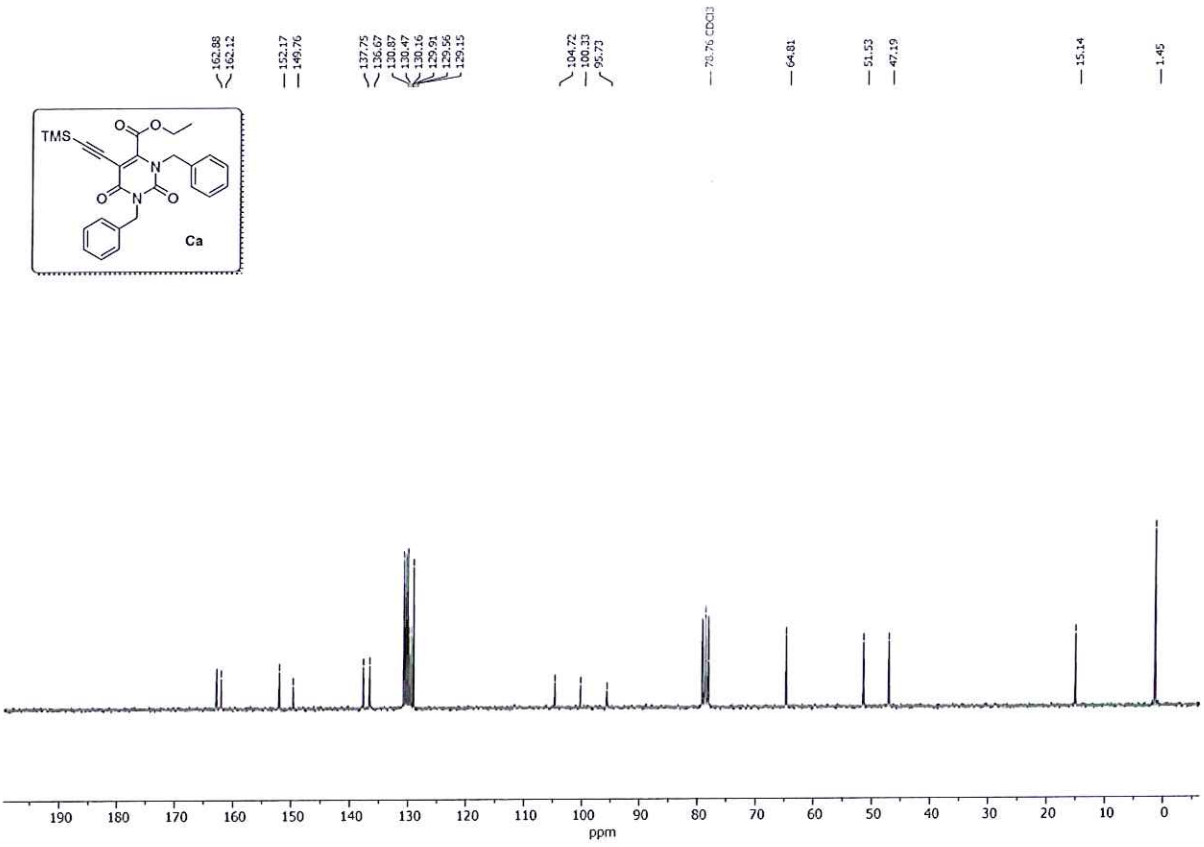

161.03
145.37
135.48
133.45
130.26
130.00
129.51
129.42
129.32
129.09
126.92
124.73
121.75
109.54
50.00
3t
Se
O2S
N
O
O
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

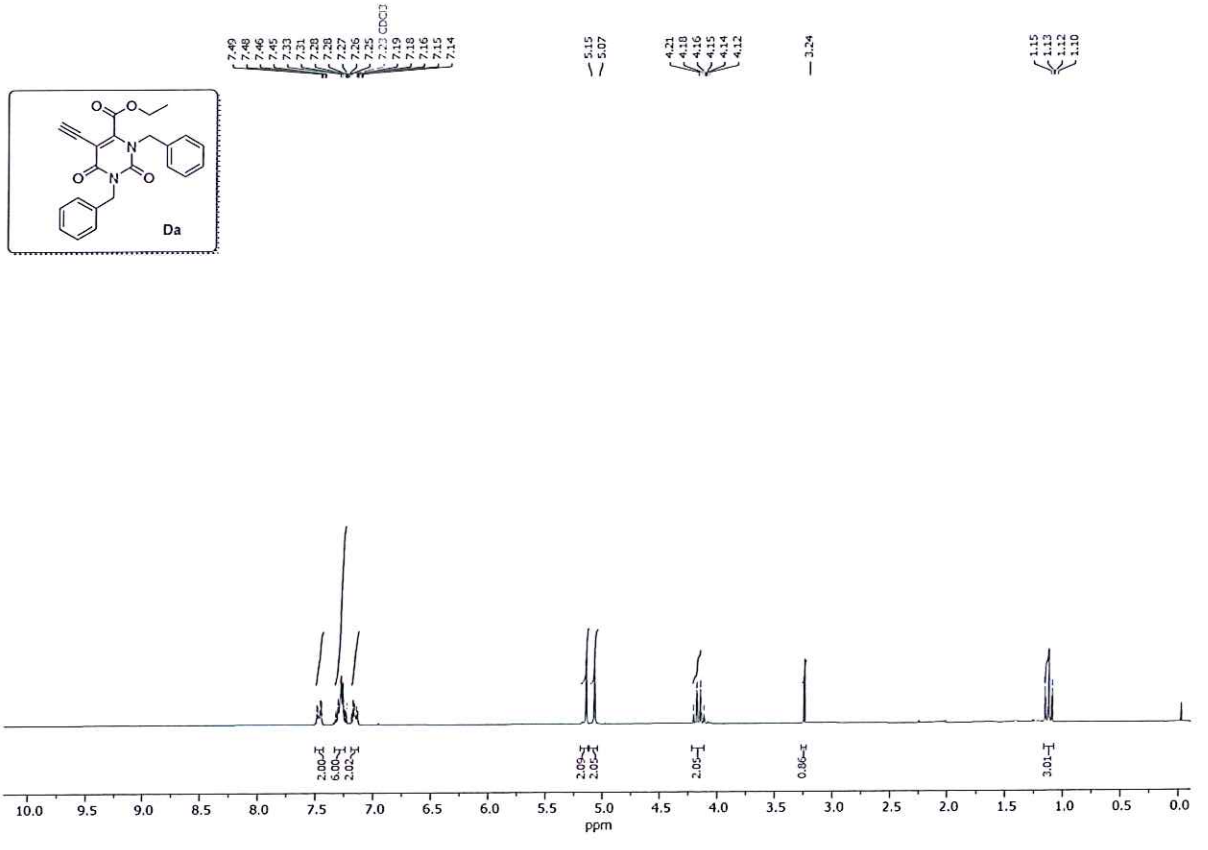

Ba

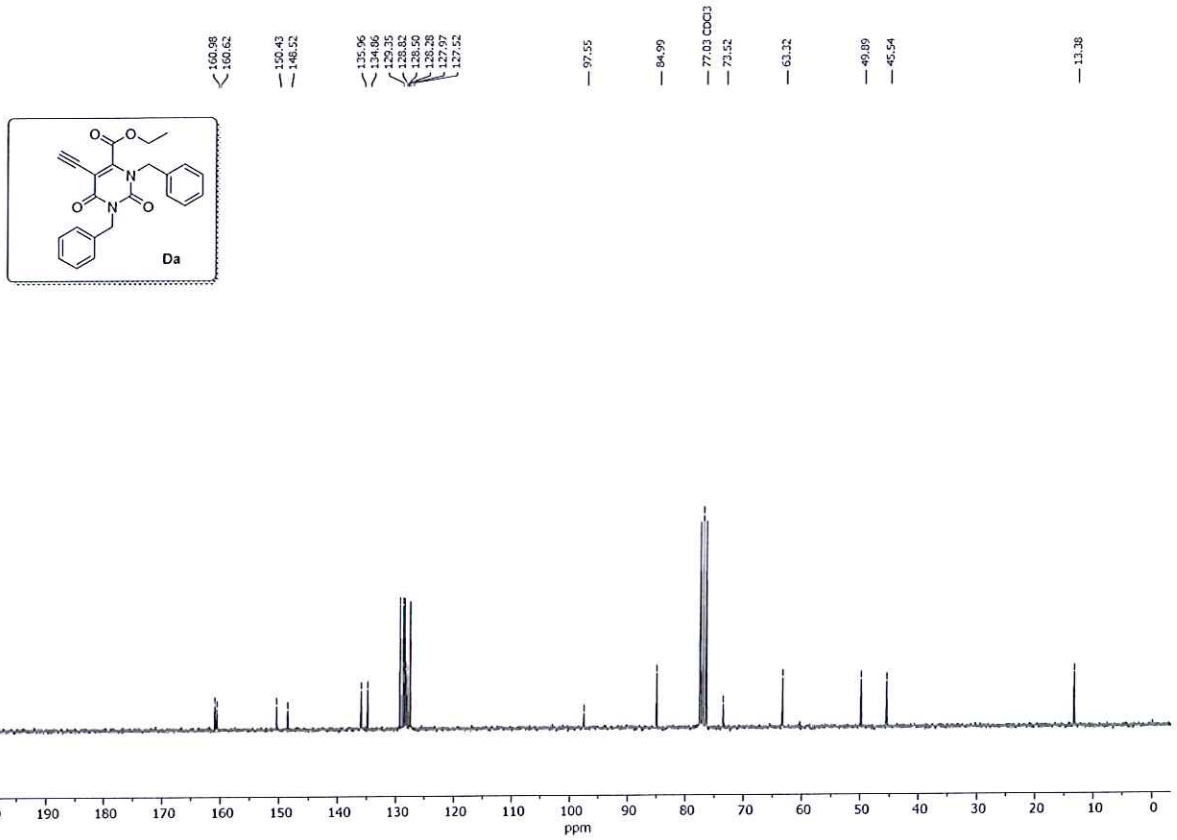
7.49
7.47
7.46
7.31
7.28
7.26
7.26
7.24
7.20
7.17
5.17
5.03
4.18
4.15
4.13
1.15
1.13
1.10
1.07
1.83
7.71
1.90
1.69
2.00
2.62
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm

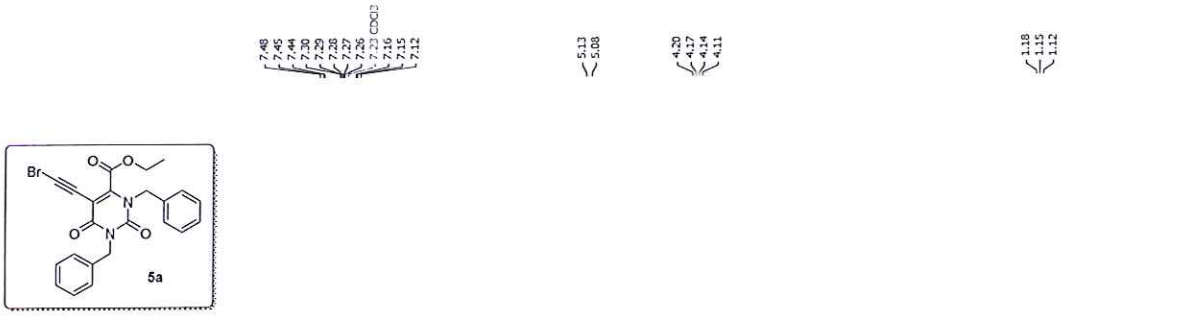

TMS
Ca

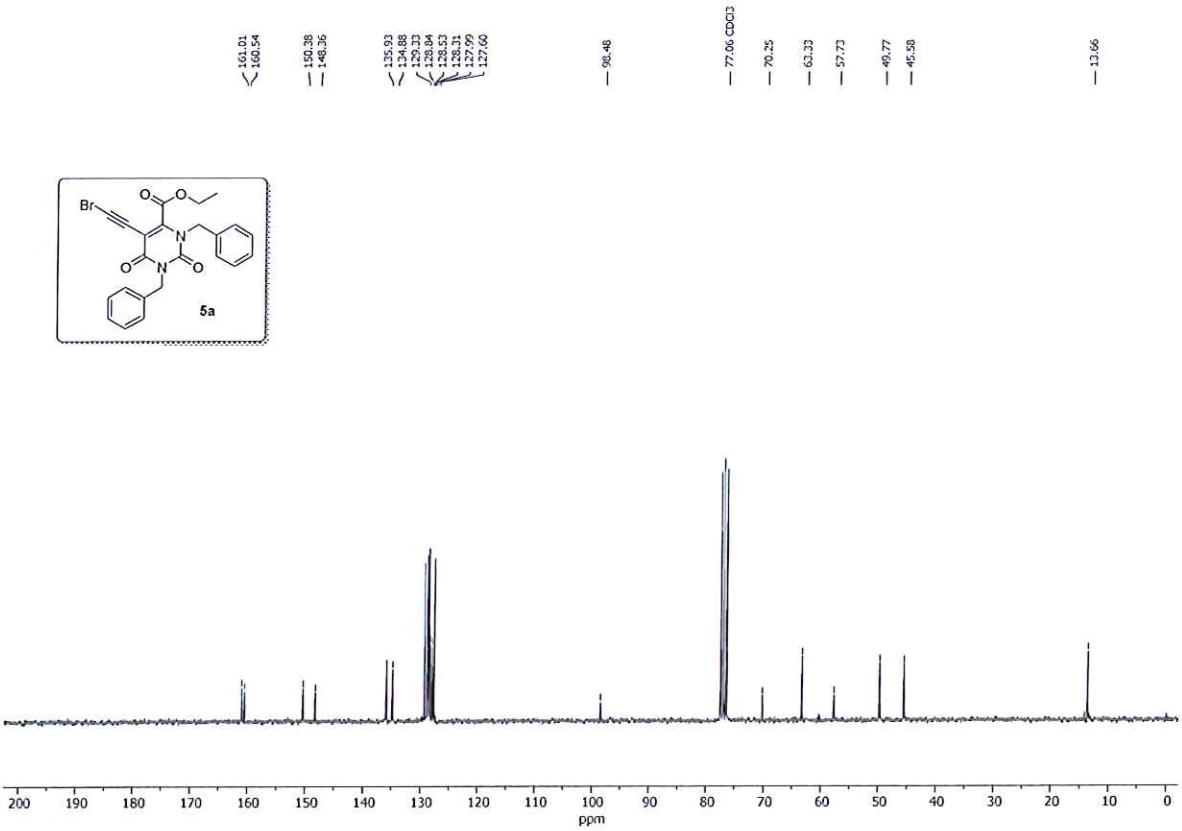
7.49
7.47
7.46
7.45
7.29
7.29
7.28
7.26 CDCl3
7.20
7.17
7.16
7.15
7.14
5.15
5.08
4.20
4.19
4.17
4.16
4.15
4.14
4.13
4.12
4.12
4.11
4.10
4.09
4.08
1.18
1.15
1.12
0.21
0.19
2.00
6.06
2.02
2.02
2.09
2.00
3.05
9.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm


162.88
162.12
152.17
149.76
137.75
136.67
130.87
130.47
130.16
129.91
129.56
129.15
104.72
100.33
95.73
78.76 CDCl3
64.81
51.53
47.19
15.14
1.45
TMS
Ca
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

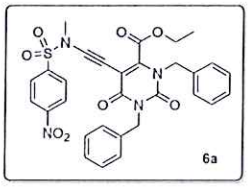

7.49
7.48
7.46
7.45
7.33
7.31
7.28
7.28
7.27
7.26
7.25
7.23 CDCl3
7.19
7.18
7.16
7.15
7.14
5.15
5.07
4.21
4.18
4.16
4.15
4.14
4.12
3.24
1.15
1.13
1.12
1.10
Da
2.00
6.00
2.02
2.09
2.05
2.05
0.86
3.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm

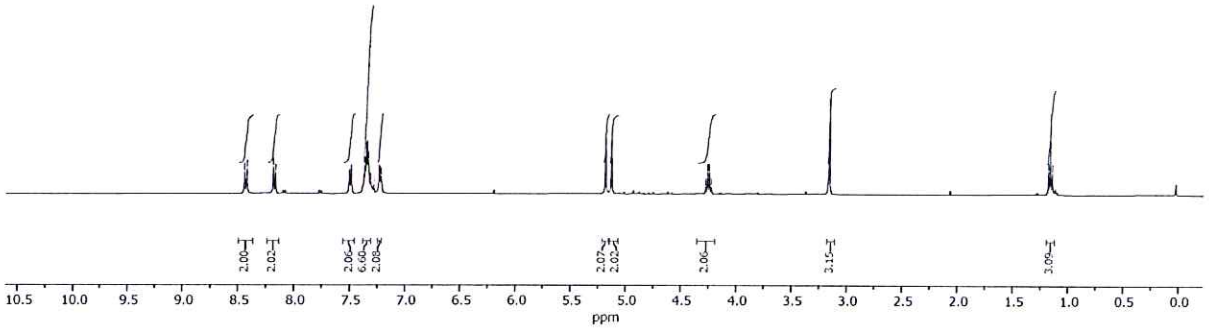

160.98
160.62
150.43
146.52
135.96
134.86
129.35
128.82
128.50
128.28
127.97
127.52
97.55
84.99
77.03 CDCl3
73.52
63.32
49.89
45.54
13.38
Da
ppm


7.48
7.45
7.44
7.30
7.29
7.28
7.27
7.26
7.16
7.15
7.12
5.13
5.08
4.20
4.17
4.14
4.11
1.18
1.15
1.12
5a
2.07
6.10
2.07
2.07
2.00
2.09
3.08
ppm

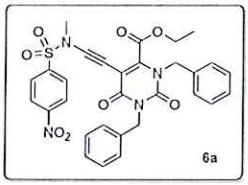

161.01
160.54
150.38
148.36
135.93
134.88
129.33
128.94
128.53
128.31
127.99
127.60
98.48
77.06 CDCl3
70.25
63.33
57.73
49.77
45.58
13.66
Br
O
O
N
N
O
O
5a
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

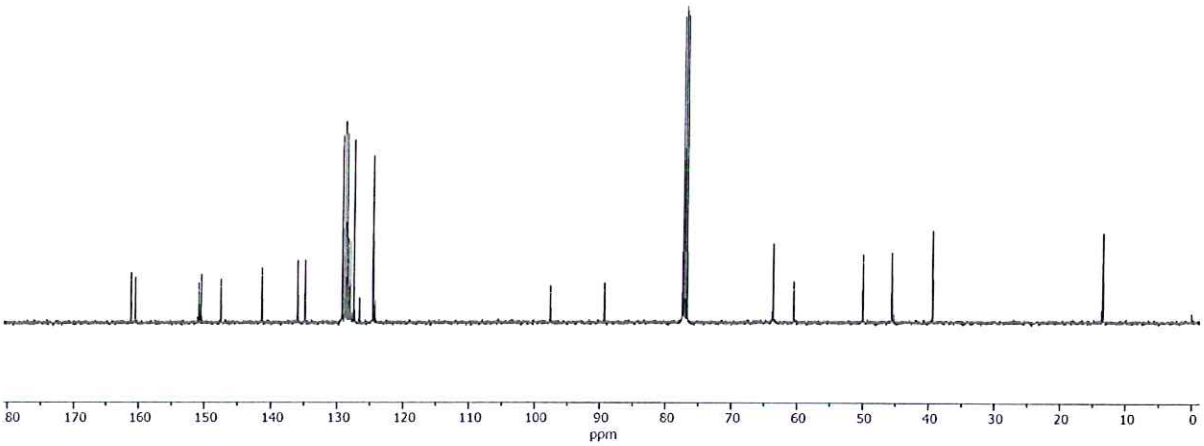

8.44
8.42
8.19
8.16
7.51
7.50
7.49
7.48
7.36
7.35
7.34
7.33
7.31
7.24
7.23
7.22
5.18
5.13
4.28
4.26
4.24
4.22
3.16
1.18
1.16
1.15

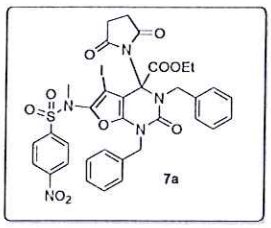

6a

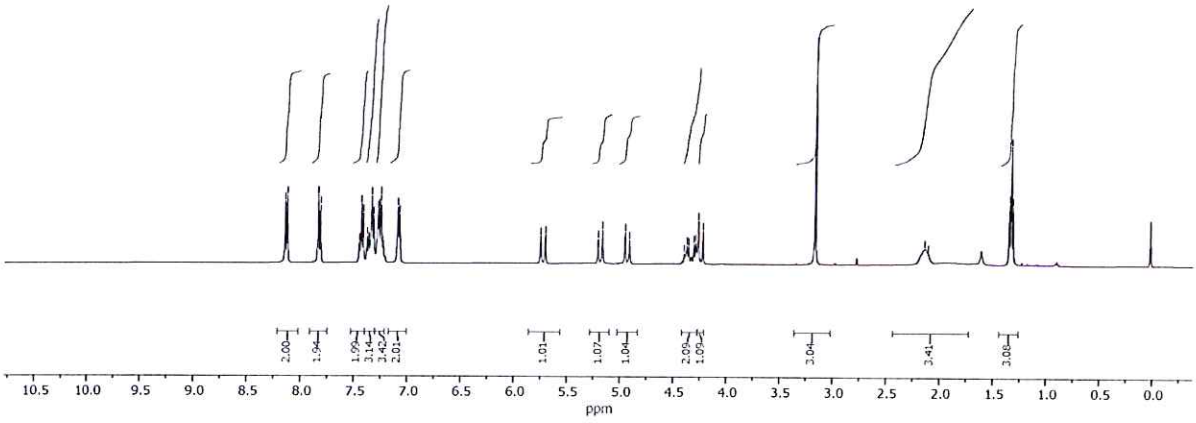

2.00
2.02
2.06
6.60
2.08
2.07
2.02
2.06
3.15
3.09
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm

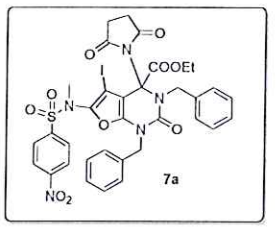

161.22
160.58
150.84
150.47
147.54
141.38
135.97
134.87
129.26
129.22
128.84
128.54
128.33
128.01
127.52
124.59
97.54
89.34
63.60
60.51
50.01
45.59
39.41
13.51


6a

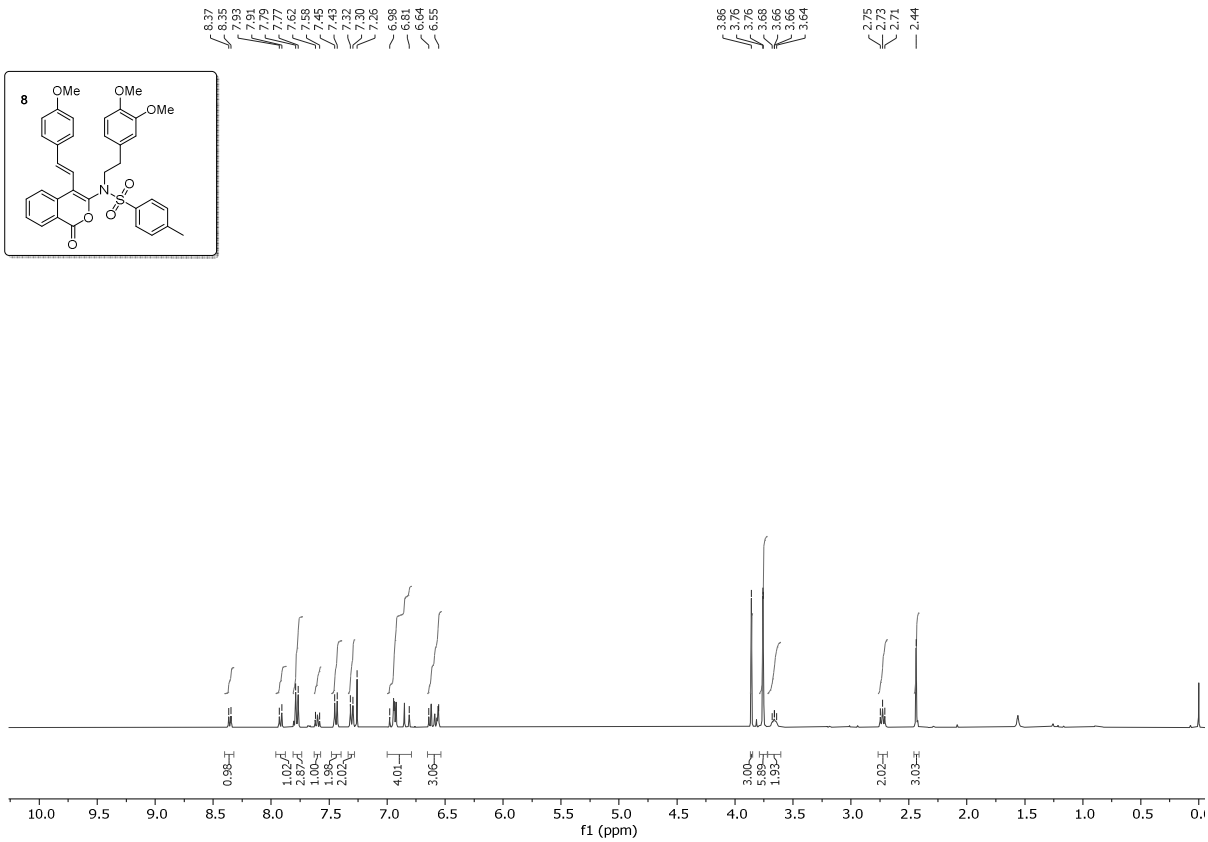

80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

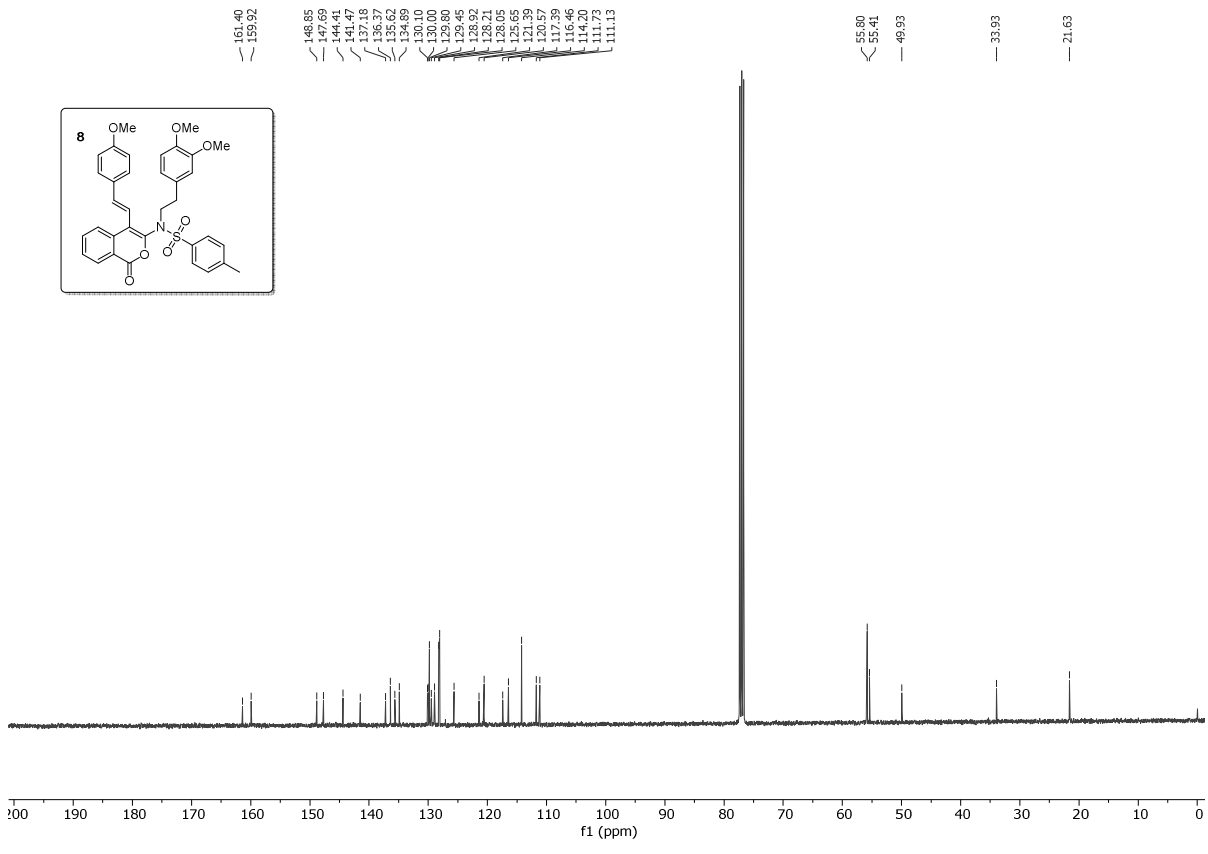

COOEt
7a


ppm


COOEt
7a

ppm

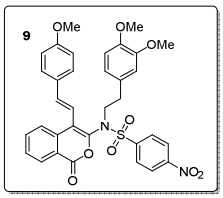

8.37
8.35
7.93
7.91
7.79
7.77
7.62
7.58
7.45
7.43
7.32
7.30
7.26
6.98
6.81
6.64
6.55
3.86
3.76
3.76
3.68
3.66
3.66
3.64
2.75
2.73
2.71
2.44
8
OMe
OMe
OMe
0.98
1.02
2.87
1.00
1.98
2.02
4.01
3.06
3.00
5.89
1.93
2.02
3.03
f1 (ppm)

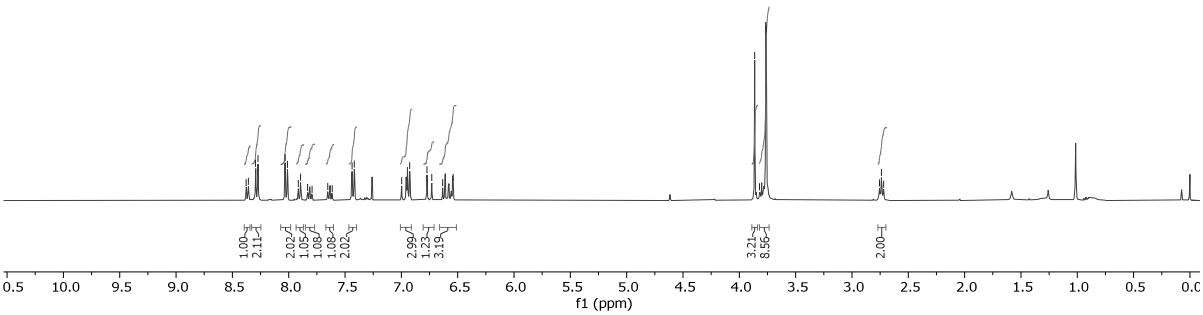

161.40
159.92
148.85
147.69
144.41
141.47
137.18
136.37
135.62
134.89
130.10
130.00
129.80
129.45
128.92
128.21
128.05
125.65
121.39
120.57
117.39
116.46
114.20
111.73
111.13
55.80
55.41
49.93
33.93
21.63
8
OMe
OMe
OMe
f1 (ppm)

8.38
8.36
8.29
8.27
8.03
8.01
7.92
7.90
7.83
7.79
7.66
7.61
7.44
7.42
7.00
6.93
6.77
6.73
6.63
6.54

3.86
3.82
3.76

2.76
2.74
2.72



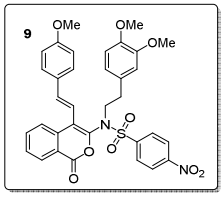


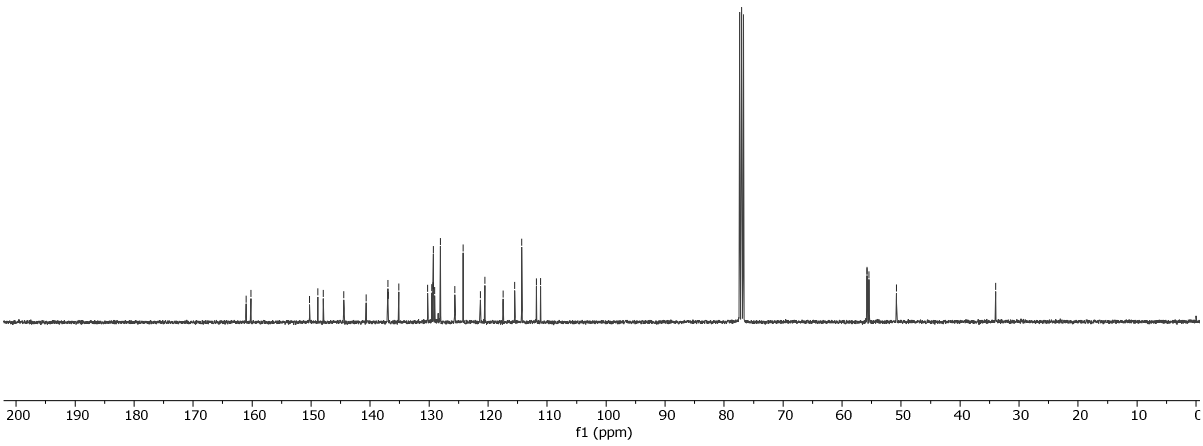
161.00
160.17

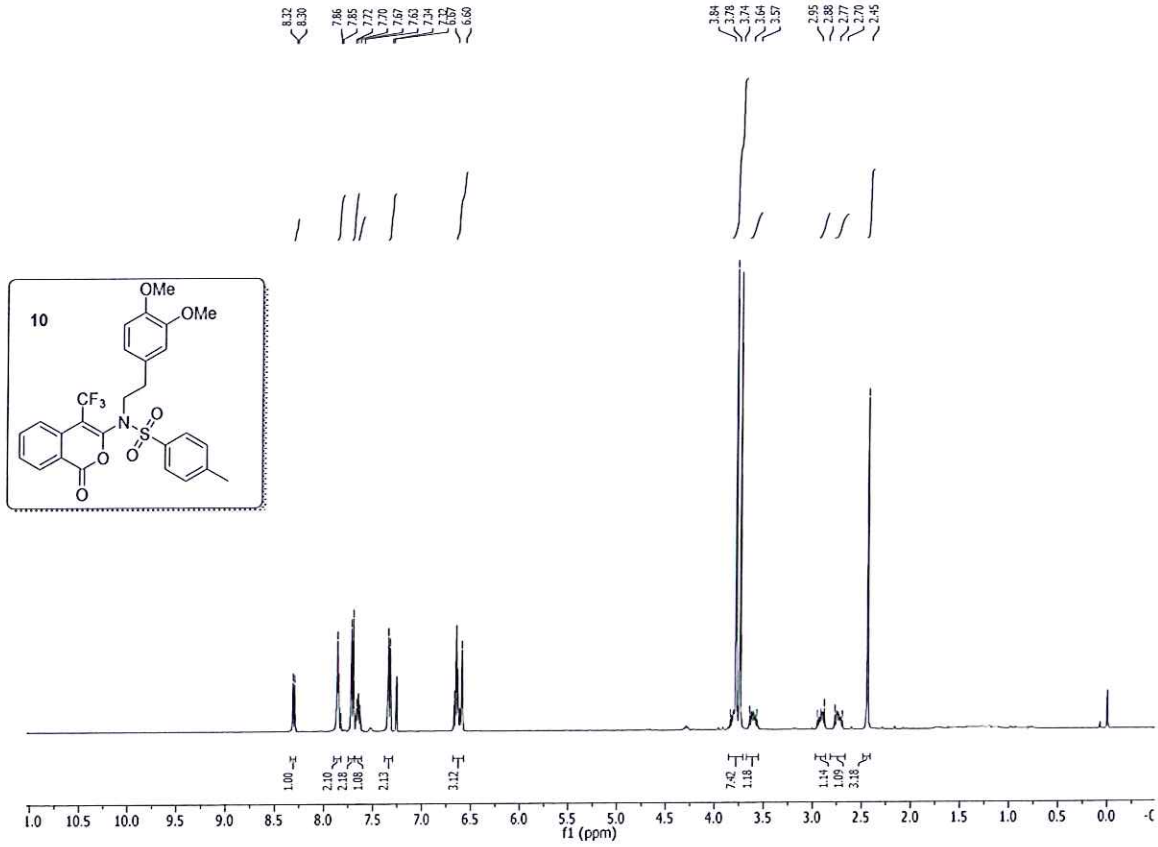
150.24
148.85
147.91
144.44
140.68
136.99
136.91
135.14
130.25
129.53
129.34
129.28
129.04
128.06
125.64
124.23
121.32
120.53
117.45
115.49
114.30
111.81
111.12

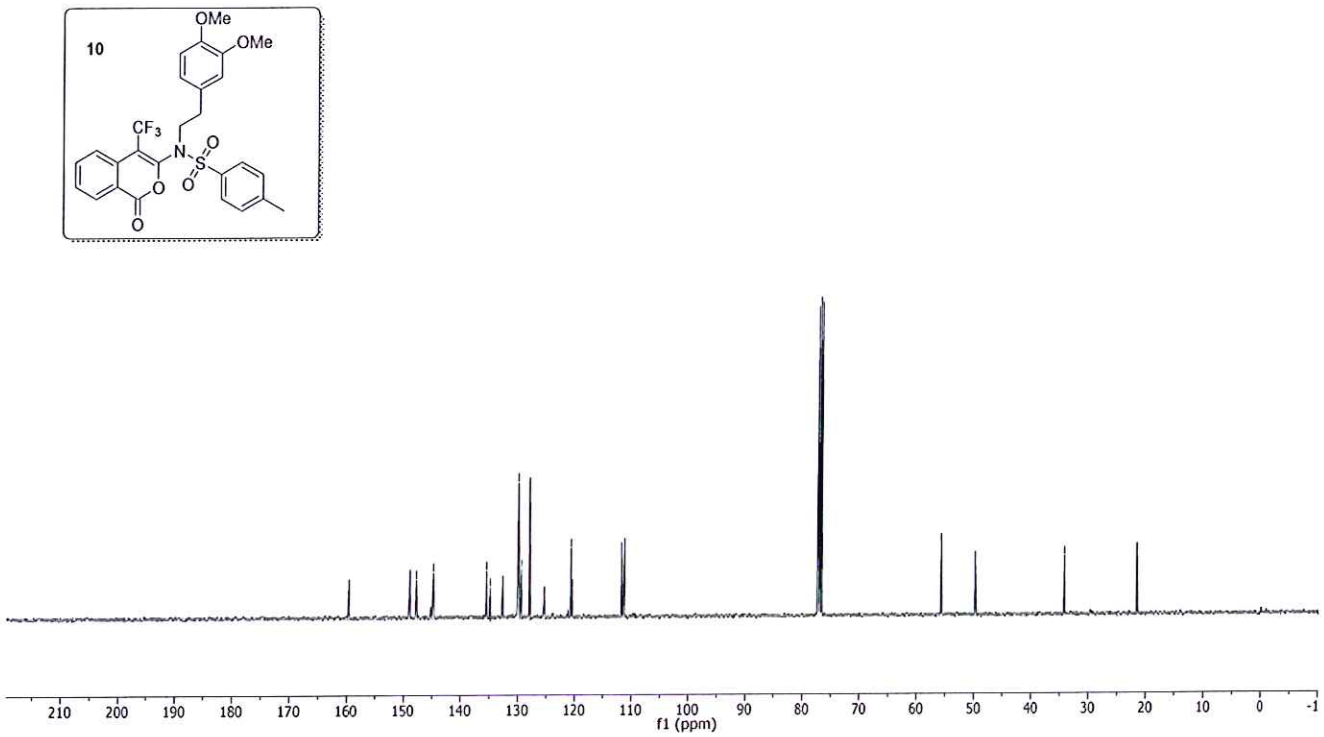
55.80
55.77
55.43
50.80

33.99



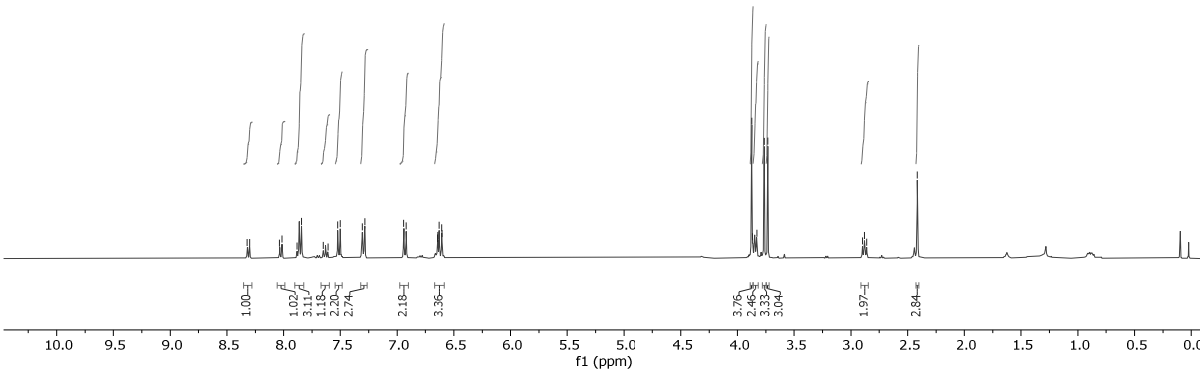


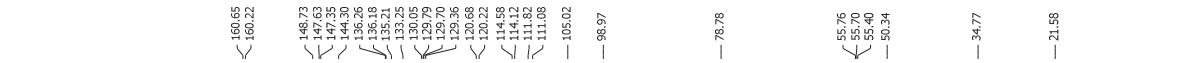

10
OMe
OMe
CF3
N
S
O
O
O
f1 (ppm)


10
OMe
OMe
CF3
N
S
O
O
O
f1 (ppm)


8.32
8.30
8.04
8.01
7.88
7.84
7.65
7.61
7.52
7.50
7.31
7.28
6.94
6.92
6.64
6.64
6.64
6.63
6.61
6.60
3.87
3.87
3.83
3.76
3.73
2.90
2.88
2.86
2.41

11
OMe
OMe
OMe
N
S
O
O
O
O


1.00
1.02
3.11
1.18
2.20
2.74
2.18
3.36
3.76
2.46
3.33
3.04
1.97
2.84
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


160.65
160.22
148.73
147.63
147.35
144.30
136.26
136.18
135.21
133.25
130.05
129.79
129.70
129.36
120.68
120.22
114.58
114.12
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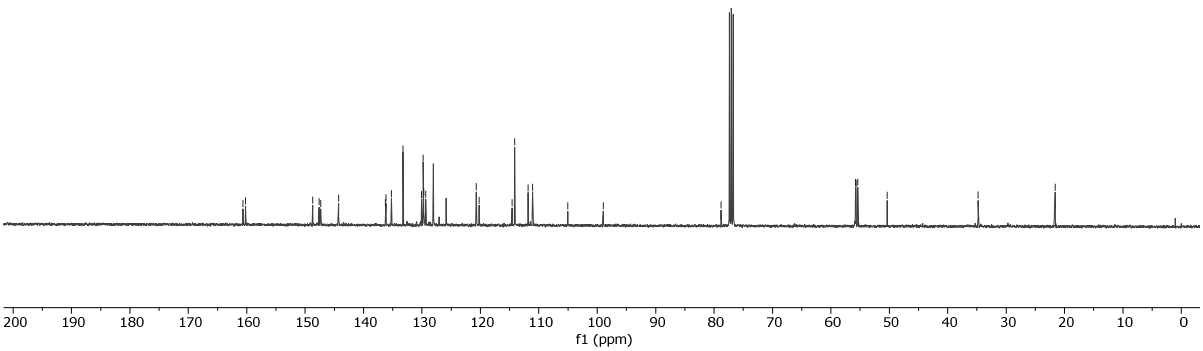
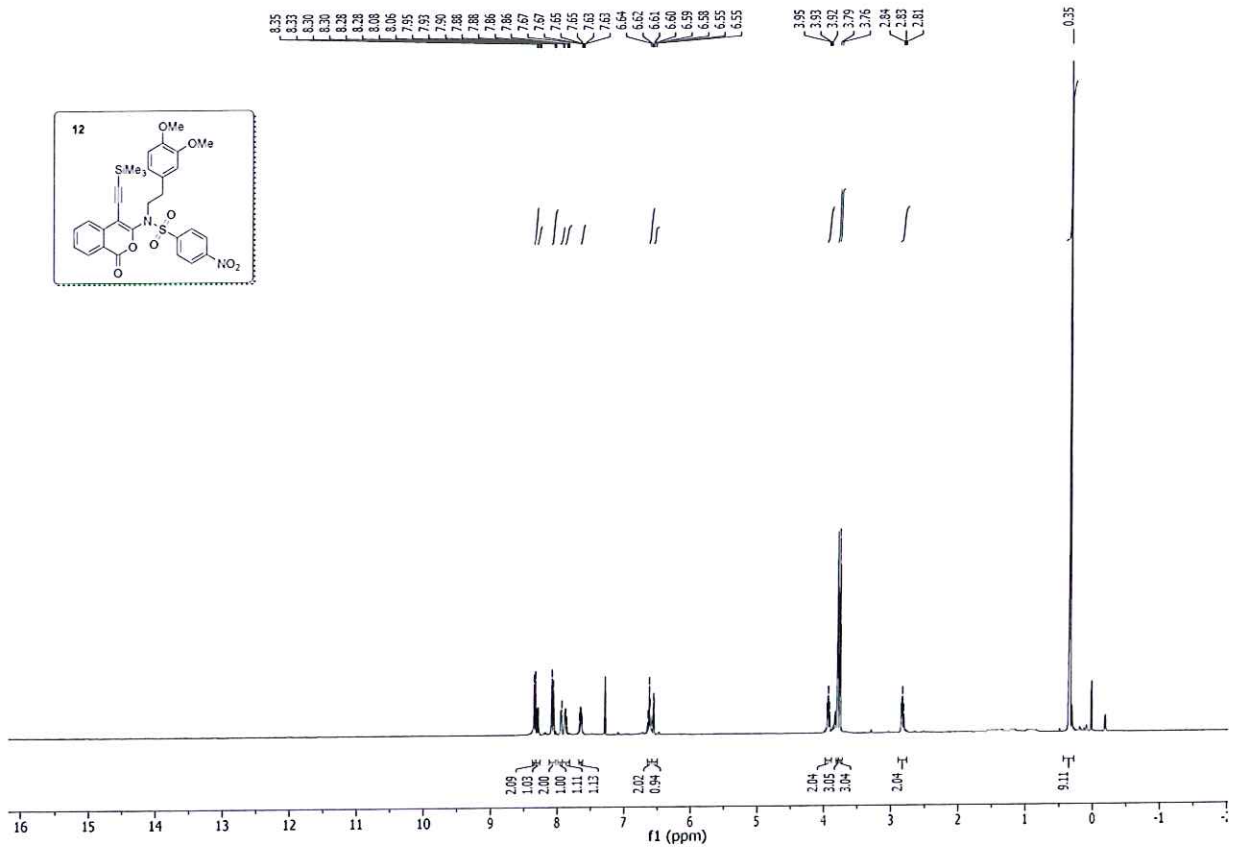
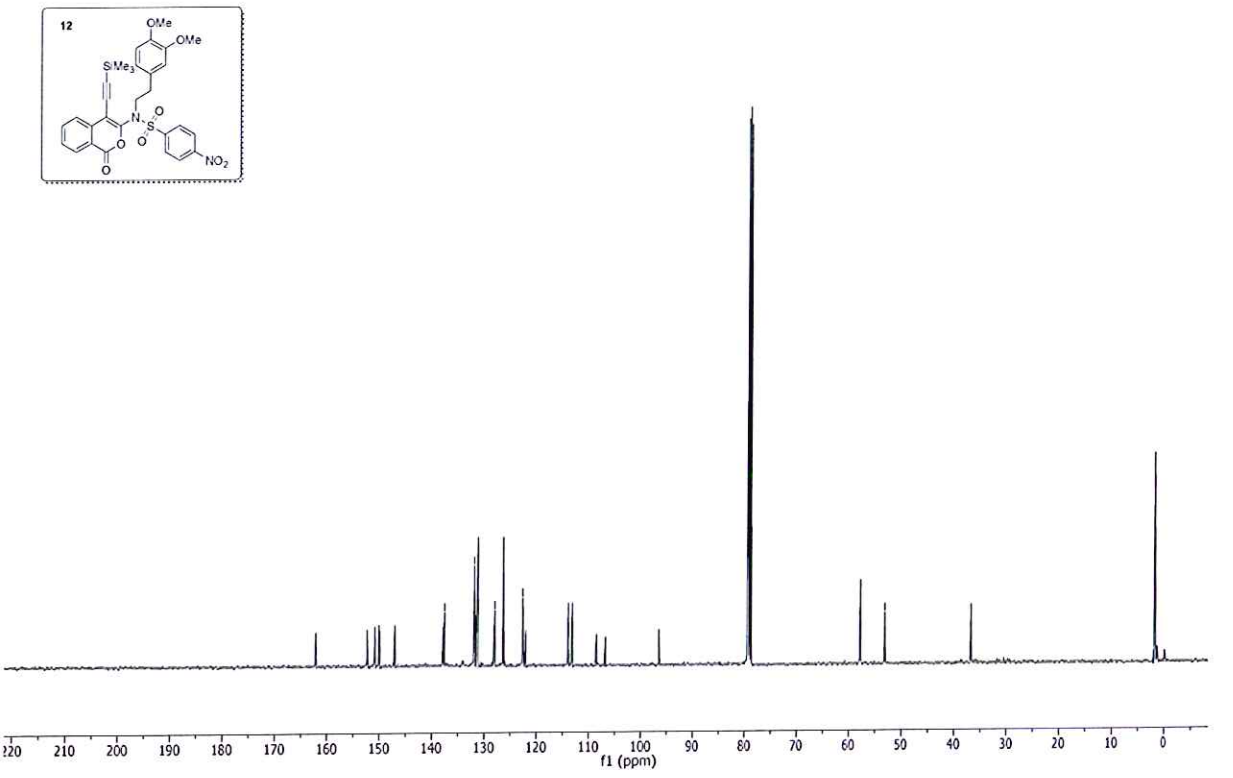
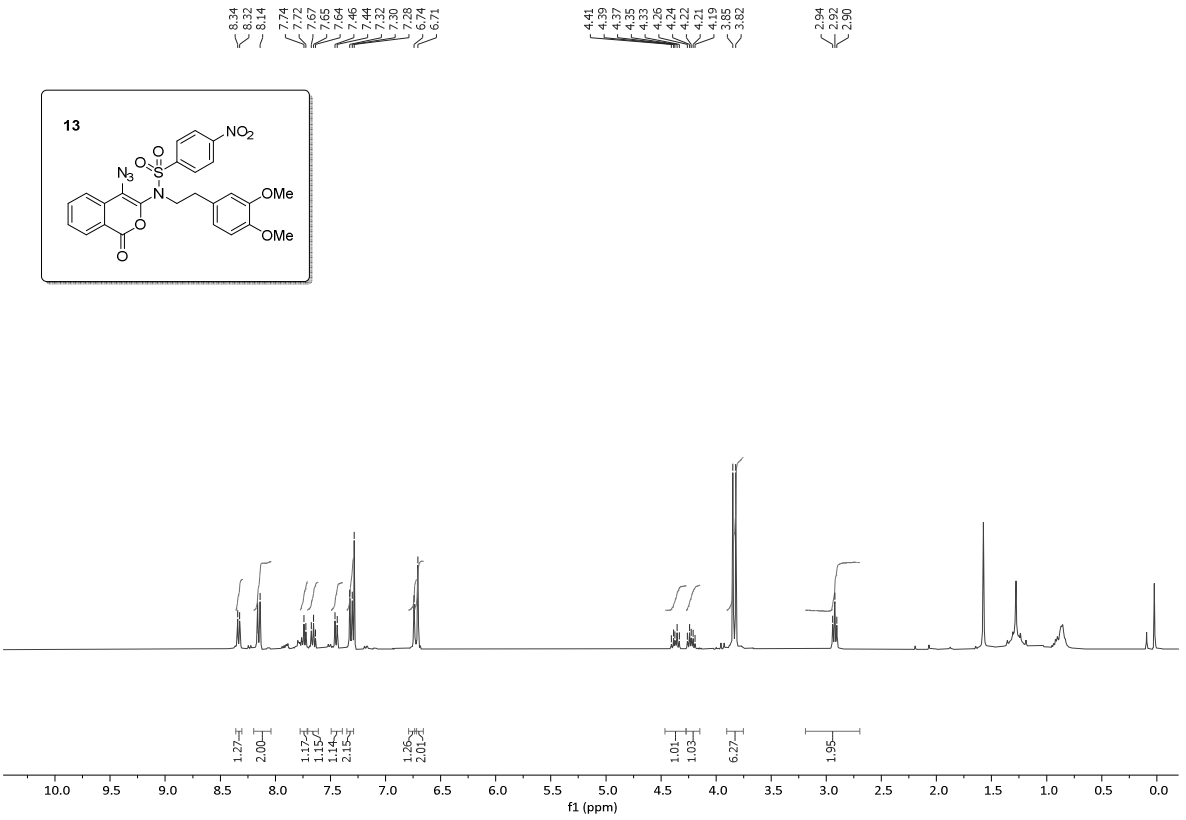
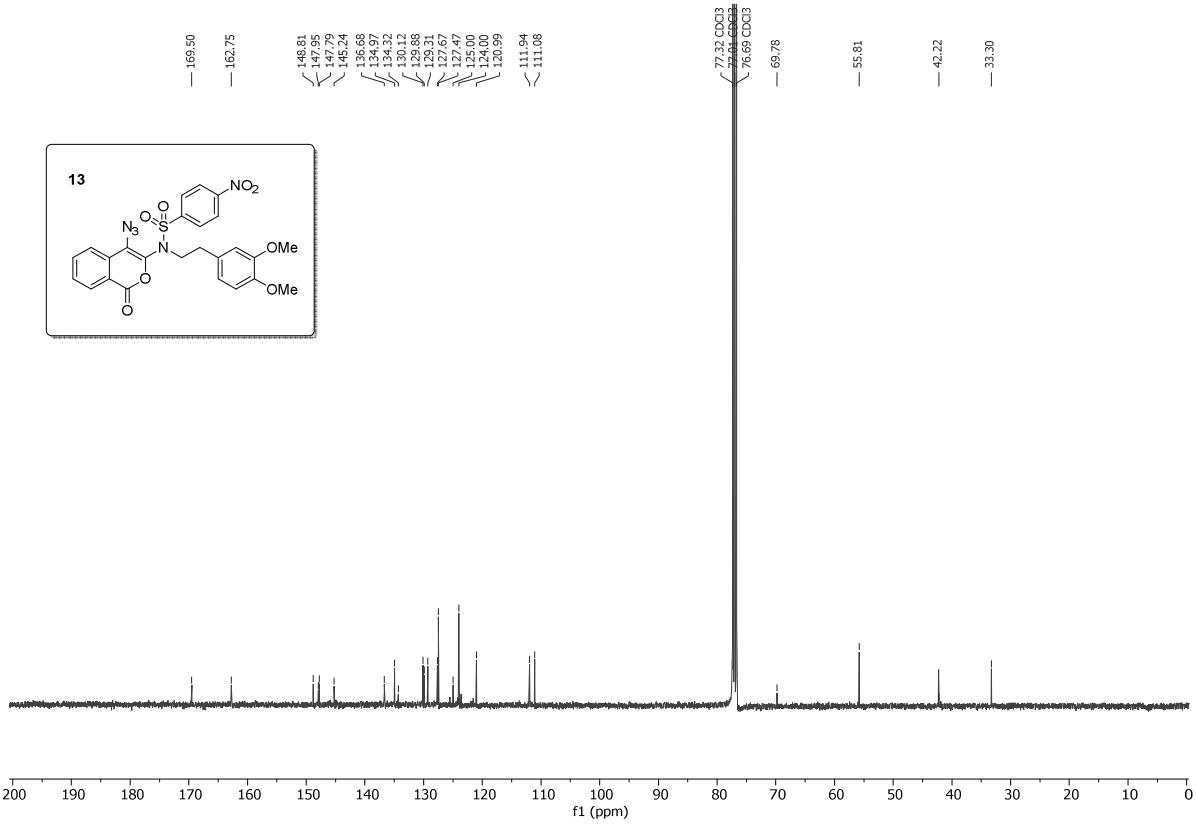
55.76
55.70
55.40
50.34
34.77
21.58


200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


12
OMe
OMe
SiMe3
NO2
f1 (ppm)


12
OMe
OMe
SiMe3
NO2
f1 (ppm)


8.34
8.32
8.14
7.74
7.72
7.67
7.65
7.64
7.46
7.44
7.32
7.30
7.28
6.74
6.71
4.41
4.39
4.37
4.35
4.33
4.26
4.24
4.22
4.21
4.19
3.85
3.82
2.94
2.92
2.90
13
NO2
N3
O
S
N
OMe
OMe
O
1.27
2.00
1.17
1.15
1.14
2.15
1.26
2.01
1.01
1.03
6.27
1.95
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


169.50
162.75
148.81
147.95
147.79
145.24
136.68
134.97
134.32
130.12
129.88
129.31
127.67
127.47
125.00
124.00
120.99
111.94
111.08
77.32 CDCl3
77.01 CDCl3
76.69 CDCl3
69.78
55.81
42.22
33.30
13
NO2
N3
O
S
N
OMe
OMe
O
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)