Supporting Information for

Oxidative Oxygen-Nucleophilic Bromo-Cyclization of Alkenyl Carbonyl Compounds Without Organic Wastes Using Alkali Metal Reagents in Green Solvent

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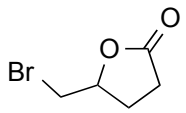
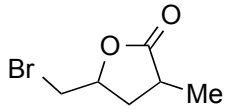
1. General Methods. ^{1}H NMR spectra were measured on a JEOL ECS-400 (400 MHz) spectrometer at ambient temperature. Data were recorded as follows: chemical shift in ppm from internal tetramethylsilane on the δ scale, multiplicity (s = singlet; d = doublet; t = triplet; q = quartet; sep = septet; m = multiplet; br = broad), coupling constant (Hz), integration, and assignment. ^{13}C NMR spectra were measured on a JEOL ECS-400 (100 MHz) spectrometer. Chemical shifts were recorded in ppm from the solvent resonance employed as the internal standard (deuterochloroform at 77.0 ppm). High-resolution mass spectra were recorded by Thermo Fisher Scientific Exactive Orbitrap mass spectrometers. Infrared (IR) spectra were recorded on a JASCO FT/IR 4100 spectrometer. Single crystal X-ray diffraction data were collected at 173K on a Bruker SMART APEX II CCD diffractometer with Mo Kα (λ = 0.71073) radiation and graphite monochromator. For thin-layer chromatography (TLC) analysis throughout this work, Merck precoated TLC plates (silica gel 60GF254 0.25 mm) were used. The products were purified by neutral column chromatography on silica gel (Kanto Chemical Co., Inc. silica gel 60N, Prod. No. 37560-84; Merck silica gel 60, Prod. No. 1.09385.9929). Visualization was accomplished by UV light (254 nm), anisaldehyde, $KMnO_4$, and phosphomolybdic acid. In experiments that required dry solvents were distilled in prior to use.

2. General Procedure for Oxidative Bromo-lactonization of Alkenyl Carboxylic Acids (1) (Table 1; Entry 15, Table 2; Entry 4, Table 3, and Scheme 1).

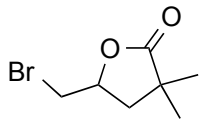
To a solution of **1a** (25.1 mg, 0.25 mmol) and KBr (44.7 mg, 0.375 mmol) in AcOEt (1.0 mL) was added Oxone® (184.4 mg, 0.30 mmol) at –10 ºC. After stirring at –10 ºC for 30 h, saturated Na_2SO_3 aqueous solution (10 mL) was added to the reaction mixture, and the product was extracted with AcOEt (15 mL×3). The combined extracts were washed with brine (10 mL) and dried over Na_2SO_4. The organic phase was concentrated under reduced pressure and the crude product was purified by silica gel column chromatography (eluent: hexane/AcOEt = 2/1) to give desired product **2a** (47.3 mg, 98%).



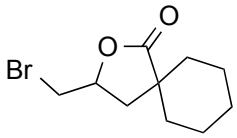
5-(Bromomethyl)dihydrofuran-2(3*H*)-one (2a): ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.13 (dddd, *J* = 13.0, 10.3, 8.0, 6.6 Hz, 1H), 2.45 (dddd, *J* = 13.0, 9.8, 7.3, 5.7 Hz, 1H), 2.57 (ddd, *J* = 18.1, 9.8, 8.0 Hz, 1H), 2.67 (ddd, *J* = 18.1, 10.3, 5.7 Hz, 1H), 3.54 (dd, *J* = 11.0, 6.0 Hz, 1H), 3.58 (dd, *J* = 11.0, 4.4 Hz, 1H), 4.69-4.75 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 26.2, 28.3, 34.0, 77.8, 176.1. IR (neat) 2927, 1768, 1420, 1337, 1160, 1020 cm^{-1}. MS (APCI) calcd for $C_5H_8BrO_2$ $[M+H]^+$ 178.9702, found 178.9701.



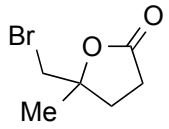
5-(Bromomethyl)-3-methyldihydrofuran-2(3*H*)-one (2b): (*cis*-isomer) ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.31 (d, *J* = 7.1 Hz, 3H), 1.65-1.78 (m, 1H), 2.64 (ddd, *J* = 12.8, 9.1, 6.1 Hz, 1H), 2.69-2.83 (m, 1H), 3.51 (dd, *J* = 11.0, 6.3 Hz, 1H), 3.59 (dd, *J* = 11.0, 4.8 Hz, 1H), 4.52-4.63 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 15.0, 33.3, 35.5, 35.6, 75.9, 178.4. IR (neat) 2973, 1766, 1454, 1344, 1154, 1014 cm^{-1}. MS (APCI) calcd for $C_6H_{10}BrO_2$ $[M+H]^+$ 192.9859, found 192.9861. (*trans*-isomer) ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.31 (d, *J* = 7.6 Hz, 3H), 2.10 (dt, *J* = 13.8, 8.5 Hz, 1H), 2.41 (ddd, *J* = 13.8, 9.7, 4.0 Hz, 1H), 2.77-2.90 (m, 1H), 3.50 (dd, *J* = 11.0, 6.2 Hz, 1H), 3.55 (dd, *J* = 11.0, 4.5 Hz, 1H), 4.71-4.80 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 16.1, 33.8 (2C), 33.9, 75.7, 179.1. IR (neat) 2973, 1766, 1455, 1343, 1158, 1012 cm^{-1}. MS (APCI) calcd for $C_6H_{10}BrO_2$ $[M+H]^+$ 192.9859, found 192.9868.



5-(Bromomethyl)-3,3-dimethyldihydrofuran-2(3*H*)-one (2c): ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.29 (s, 3H), 1.32 (s, 3H), 1.94 (dd, *J* = 13.3, 9.6 Hz, 1H), 2.28 (dd, *J* = 13.3, 6.4 Hz, 1H), 3.48 (dd, *J* = 10.8, 6.4 Hz, 1H), 3.58 (dd, *J* = 10.8, 4.8 Hz, 1H), 4.64 (dtd, *J* = 9.6, 6.4, 4.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 24.86, 24.89, 33.5, 40.5, 41.9, 74.6, 180.9. IR (neat) 2970, 1766, 1457, 1336, 1204, 1107, 1015 cm^{-1}. MS (APCI) calcd for $C_7H_{12}BrO_2$ $[M+H]^+$ 207.0015, found 207.0012.

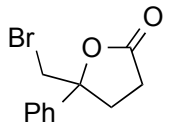


3-(Bromomethyl)-2-oxaspiro[4.5]decan-1-one (2d): ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.18-1.44 (m, 3H), 1.49-1.84 (m, 8H), 2.44 (dd, *J* = 13.3, 6.8 Hz, 1H), 3.47 (dd, *J* = 10.8, 6.6 Hz, 1H), 3.56 (dd, *J* = 10.8, 4.6 Hz, 1H), 4.55-4.64 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.97, 22.05, 25.1, 32.1, 33.9, 34.0, 38.0, 44.9, 74.9, 180.5. IR (neat) 2930, 1761, 1448, 1338, 1186, 1019 cm^{-1}. MS (APCI) calcd for $C_{10}H_{16}BrO_2$ $[M+H]^+$ 247.0328, found 247.0323.

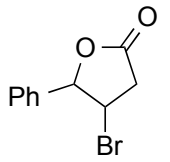


5-(Bromomethyl)-5-methyldihydrofuran-2(3*H*)-one (2e): ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.58 (s, 3H), 2.09 (ddd, *J* = 13.5, 10.3, 7.1 Hz, 1H), 2.39 (ddd, *J* = 13.5, 10.3, 7.1 Hz, 1H), 2.62 (ddd, *J* = 18.5, 10.3, 7.1 Hz, 1H), 2.73 (ddd, *J* = 18.5, 10.3, 7.1 Hz, 1H), 3.48 (d, *J* = 11.0 Hz, 1H), 3.54 (d, *J*

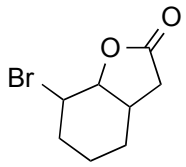
= 11.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 25.4, 29.2, 31.5, 39.4, 84.0, 175.8. IR (neat) 2923, 1767, 1420, 1276, 1164, 1072 cm^{-1}. MS (APCI) calcd for $C_6H_{10}BrO_2$ $[M+H]^+$ 192.9859, found 192.9857.



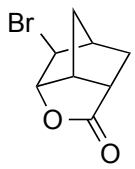
5-(Bromomethyl)-5-phenyldihydrofuran-2(3*H*)-one (2f): ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.48-2.62 (m, 2H), 2.74-2.88 (m, 2H), 3.70 (d, *J* = 11.4 Hz, 1H), 3.75 (d, *J* = 11.4 Hz, 1H), 7.32-7.45 (m, 5H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 29.0, 32.3, 41.0, 86.4, 124.9 (2C), 128.6, 128.8 (2C), 140.7, 175.5. IR (neat) 2926, 1777, 1447, 1257, 1184, 1038 cm^{-1}. MS (APCI) calcd for $C_{11}H_{12}BrO_2$ $[M+H]^+$ 255.0015, found 255.0010.



4-Bromo-5-phenyldihydrofuran-2(3*H*)-one (2g): ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.97 (dd, *J* = 18.6, 6.4 Hz, 1H), 3.23 (dd, *J* = 18.6, 7.6 Hz, 1H), 4.37 (ddd, *J* = 7.6, 6.4, 5.2 Hz, 1H), 5.66 (d, *J* = 5.2 Hz, 1H), 7.34-7.46 (m, 5H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 38.7, 45.5, 87.8, 125.3 (2C), 129.0 (2C), 129.3, 135.7, 172.9. IR (neat) 2935, 1789, 1406, 1323, 1210, 1139 cm^{-1}. MS (ESI) calcd for $C_{10}H_{10}BrO_2$ $[M+H]^+$ 240.9859, found 240.9858.

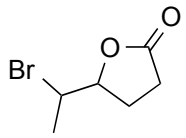


7-Bromohexahydrobenzofuran-2(3*H*)-one (2h): ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.23-1.39 (m, 1H), 1.48-1.61 (m, 1H), 1.73-1.87 (m, 2H), 1.91-2.00 (m, 1H), 2.01-2.11 (m, 1H), 2.29 (dd, *J* = 17.0, 3.4 Hz, 1H), 2.61 (dd, *J* = 17.0, 7.0 Hz, 1H), 2.72-2.83 (m, 1H), 4.47 (dt, *J* = 4.4, 4.1 Hz, 1H), 4.61 (t, *J* = 4.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 18.6, 26.2, 29.4, 32.6, 36.5, 48.4, 81.4, 175.9. IR (neat) 2929, 1778, 1450, 1321, 1172, 1017 cm^{-1}. MS (APCI) calcd for $C_8H_{12}BrO_2$ $[M+H]^+$ 219.0015, found 219.0013.

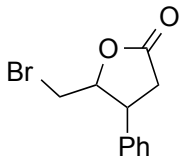


6-Bromohexahydro-2*H*-3,5-methanocyclopenta[*b*]furan-2-one (2i): ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.71-1.78 (m, 1H), 1.81 (dt, *J* = 14.0, 1.8 Hz, 1H), 2.15 (ddd, *J* = 14.0, 11.4, 4.1 Hz, 1H),

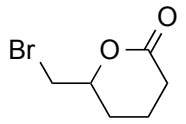
2.30-2.38 (m, 1H), 2.53-2.61 (m, 1H), 2.65-2.71 (m, 1H), 3.22-3.27 (m, 1H), 3.86 (d, J = 2.3 Hz, 1H), 4.94 (d, J = 5.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 34.0, 35.7, 37.5, 45.5, 45.9, 53.4, 87.7, 179.2. IR (neat) 2979, 1782, 1449, 1343, 1170, 1011 cm^{-1}. MS (APCI) calcd for $C_8H_{10}BrO_2$ $[M+H]^+$ 216.9859, found 216.9856.



5-(1-Bromoethyl)dihydrofuran-2(3*H*)-one (2j): ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.75 (d, J = 7.1 Hz, 3H), 2.16 (dddd, J = 13.3, 10.7, 8.0, 6.6 Hz, 1H), 2.39 (dddd, J = 13.3, 10.7, 8.0, 5.6 Hz, 1H), 2.56 (ddd, J = 18.6, 10.7, 8.0 Hz, 1H), 2.69 (dd, J = 18.6, 10.7, 5.6 Hz, 1H), 4.21 (qd, J = 7.1, 3.7 Hz, 1H), 4.59 (ddd, J = 8.0, 6.6, 3.7 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.2, 25.0, 28.3, 50.3, 81.8, 176.3. IR (neat) 2927, 1771, 1446, 1353, 1154, 1027 cm^{-1}. MS (APCI) calcd for $C_6H_{10}BrO_2$ $[M+H]^+$ 192.9859, found 192.9858.

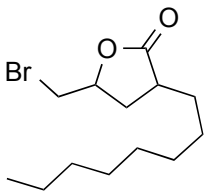


5-(Bromomethyl)-4-phenyldihydrofuran-2(3*H*)-one (2k): (*cis*-isomer) ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.87 (dd, J = 18.1, 3.9 Hz, 1H), 2.99 (dd, J = 11.0, 6.6 Hz, 1H), 3.07 (dd, J = 18.1, 9.0 Hz, 1H), 3.24 (dd, J = 11.0, 6.6 Hz, 1H), 3.90 (ddd, J = 9.0, 6.6, 3.9 Hz, 1H), 4.96 (q, J = 6.6 Hz, 1H), 7.18-7.24 (m, 2H), 7.31-7.42 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 29.6, 36.2, 43.7, 82.1, 127.9 (2C), 128.2, 129.0 (2C), 136.3, 175.6. IR (neat) 2925, 1775, 1419, 1326, 1142, 1029 cm^{-1}. MS (APCI) calcd for $C_{11}H_{12}BrO_2$ $[M+H]^+$ 255.0015, found 255.0018. (*trans*-isomer) ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.81 (dd, J = 18.3, 9.6 Hz, 1H), 3.08 (dd, J = 18.3, 9.6 Hz, 1H), 3.52 (dd, J = 11.7, 4.1 Hz, 1H), 3.67 (td, J = 9.6, 7.6 Hz, 1H), 3.69 (dd, J = 11.8, 4.1 Hz, 1H), 4.65 (dt, J = 7.6, 4.1 Hz, 1H), 7.24-7.29 (m, 2H), 7.30-7.36 (m, 1H), 7.36-7.43 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 32.6, 36.8, 45.1, 84.2, 127.1 (2C), 128.1, 129.4 (2C), 138.6, 174.6. IR (neat) 2925, 1779, 1419, 1329, 1165, 1031 cm^{-1}. MS (APCI) calcd for $C_{11}H_{12}BrO_2$ $[M+H]^+$ 255.0015, found 255.0018.

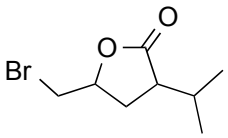


6-(Bromomethyl)tetrahydro-2*H*-pyran-2-one (2l): ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.73 (dtd, J = 13.8, 11.2, 5.2 Hz, 1H), 1.82-1.94 (m, 1H), 1.94-2.06 (m, 1H), 2.08-2.18 (m, 1H), 2.48 (ddd, J = 18.1, 9.8, 7.1 Hz, 1H), 2.57-2.68 (m, 1H), 3.50 (dd, J = 11.0, 6.1 Hz, 1H), 3.55 (dd, J = 11.0, 4.6

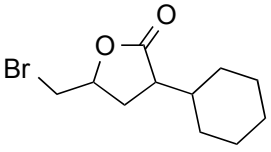
Hz, 1H), 4.47-4.57 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 18.1, 26.2, 29.3, 33.8, 78.5, 170.3. IR (neat) 2923, 1730, 1442, 1351, 1231, 1164, 1038 cm^{-1}. MS (APCI) calcd for $C_6H_{10}BrO_2$ $[M+H]^+$ 192.9859, found 192.9861.



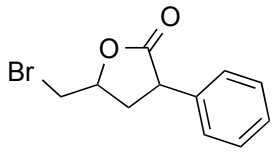
5-(Bromomethyl)-3-octyldihydrofuran-2(3*H*)-one (2m): (*cis*-isomer) ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.88 (t, *J* = 6.8 Hz, 3H), 1.16-1.53 (m, 13H), 1.65-1.78(m, 1H), 1.86-1.98 (m, 1H), 2.53-2.72 (m, 2H), 3.49 (dd, *J* = 10.8, 6.6 Hz, 1H), 3.59 (dd, *J* = 10.8, 4.7 Hz, 1H), 4.51-4.62 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.1, 22.6, 27.3, 29.2, 29.29, 29.34, 30.3, 31.8, 33.4, 33.6, 40.7, 76.1, 177.9. IR (neat) 2917, 1756, 1465, 1365, 1164, 1013 cm^{-1}. MS (APCI) calcd for $C_{13}H_{24}BrO_2$ $[M+H]^+$ 291.0954, found 291.0948. (*trans*-isomer) ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.88 (t, *J* = 7.0 Hz, 3H), 1.17-1.54 (m, 13H), 1.78-1.92 (m, 1H), 2.13 (dt, *J* = 13.5, 8.2 Hz, 1H), 2.33 (ddd, *J* = 13.5, 9.7, 4.6 Hz, 1H), 2.66-2.80 (m, 1H), 3.49 (dd, *J* = 11.0, 6.4 Hz, 1H), 3.54 (dd, *J* = 11.0, 4.4 Hz, 1H), 4.68-4.77 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.0, 22.6, 27.1, 29.1, 29.2, 29.3, 31.1, 31.8, 31.9, 34.1, 39.0, 76.0, 178.5. IR (neat) 2923, 1769, 1468, 1338, 1151, 1018 cm^{-1}. MS (APCI) calcd for $C_{13}H_{24}BrO_2$ $[M+H]^+$ 291.0954, found 291.0945.



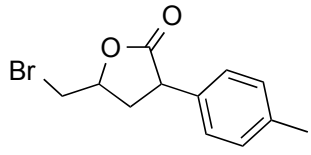
5-(Bromomethyl)-3-isopropyldihydrofuran-2(3*H*)-one (2n): (*cis*-isomer) ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.95 (d, *J* = 7.1 Hz, 3H), 1.06 (d, *J* = 7.1 Hz, 3H), 1.72-1.91 (m, 1H), 2.16-2.30 (m, 1H), 2.39 (ddd, *J* = 13.0, 9.3, 6.2 Hz, 1H), 2.65 (ddd, *J* = 12.4, 9.3, 5.2 Hz, 1H), 3.49 (dd, *J* = 10.9, 6.6 Hz, 1H), 3.60 (dd, *J* = 10.9, 4.8 Hz, 1H), 4.58-4.50 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 18.2, 20.5, 27.6, 29.1, 33.4, 46.8, 75.7, 176.9. IR (neat) 2961, 1766, 1467, 1335, 1152, 1011 cm^{-1}. MS (APCI) calcd for $C_8H_{14}BrO_2$ $[M+H]^+$ 221.0172, found 221.0167. (*trans*-isomer) ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.96 (d, *J* = 6.9 Hz, 3H), 1.04 (d, *J* = 6.9 Hz, 3H), 1.13-2.30 (m, 3H), 2.70 (ddd, *J* = 10.3, 7.8, 5.1 Hz, 1H), 3.49 (dd, *J* = 11.0, 6.3 Hz, 1H), 3.54 (dd, *J* = 11.0, 4.3 Hz, 1H), 4.64-4.73 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 18.3, 20.3, 27.9, 28.9, 34.5, 45.2, 76.1, 177.7. IR (neat) 2962, 1766, 1469, 1334, 1155, 1010 cm^{-1}. MS (APCI) calcd for $C_8H_{14}BrO_2$ $[M+H]^+$ 221.0172, found 221.0167.



5-(Bromomethyl)-3-cyclohexyldihydrofuran-2(3*H*)-one (2o): (*cis*-isomer) ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.00-1.21 (m, 3H), 1.22-1.38 (m, 2H), 1.52-1.93 (m, 7H), 2.39 (ddd, *J* = 13.0, 9.4, 6.2 Hz, 1H), 2.63 (ddd, *J* = 12.4, 9.3, 5.0 Hz, 1H), 3.48 (dd, *J* = 10.8, 6.6 Hz, 1H), 3.59 (dd, *J* = 10.8, 4.6 Hz, 1H), 4.48-4.58 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 26.0, 26.1, 26.2, 28.5, 29.7, 31.2, 33.4, 37.5, 46.1, 75.8, 176.9. IR (neat) 2924, 1768, 1448, 1339, 1164, 1021 cm^{-1}. MS (APCI) calcd for $C_{11}H_{18}BrO_2$ $[M+H]^+$ 261.0485, found 261.0179. (*trans*-isomer) ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.01-1.21 (m, 3H), 1.21-1.37 (m, 2H), 1.54-1.64 (m, 1H), 1.64-1.72 (m, 1H), 1.72-1.88 (m, 4H), 2.17 (ddd, *J* = 13.9, 10.6, 5.5 Hz, 1H), 2.27 (ddd, *J* = 13.9, 8.2, 7.3 Hz, 1H), 2.68 (ddd, *J* = 10.6, 7.3, 5.0 Hz, 1H), 3.48 (dd, *J* = 11.0, 6.4 Hz, 1H), 3.53 (dd, *J* = 11.0, 4.5 Hz, 1H), 4.62-4.72 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 26.0 (2C), 26.1, 28.6 (2C), 30.8, 34.4, 38.8, 44.9, 76.3, 177.8. IR (neat) 2924, 1764, 1449, 1340, 1156, 1018 cm^{-1}. MS (APCI) calcd for $C_{11}H_{18}BrO_2$ $[M+H]^+$ 261.0485, found 261.0478.

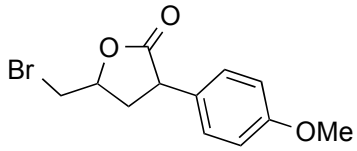


5-(Bromomethyl)-3-phenyldihydrofuran-2(3*H*)-one (2p): (*cis*-isomer) ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.22-2.36 (m, 1H), 2.88 (ddd, *J* = 13.1, 9.4, 6.0 Hz, 1H), 3.59 (dd, *J* = 11.0, 6.3 Hz, 1H), 3.66 (dd, *J* = 11.0, 4.6 Hz, 1H), 3.94 (dd, *J* = 12.6, 9.4 Hz, 1H), 4.66-4.75 (m, 1H), 7.28-7.35 (m, 3H), 7.35-7.42 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 33.1, 36.3, 46.9, 75.7, 127.8, 128.1 (2C), 128.9 (2C), 136.0, 175.7. IR (neat) 2951, 1767, 1450, 1352, 1146, 1015 cm^{-1}. MS (APPI) calcd for $C_{11}H_{11}BrO_2$ $[M]^+$ 253.9937, found 253.9936. (*trans*-isomer) ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.58 (dt, *J* = 13.9, 7.8 Hz, 1H), 2.67 (ddd, *J* = 13.9, 10.1, 5.3 Hz, 1H), 3.57-3.63 (m, 2H), 4.03 (dd, *J* = 10.1, 7.8 Hz, 1H), 4.83-4.92 (m, 1H), 7.24-7.34 (m, 3H), 7.34-7.41 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 33.9, 34.8, 45.4, 76.1, 127.5 (2C), 127.7, 129.0 (2C), 136.8, 176.3. IR (neat) 2958, 1768, 1452, 1334, 1149, 1011 cm^{-1}. MS (ESI) calcd for $C_{11}H_{12}BrO_2$ $[M+H]^+$ 255.0015, found 255.0019.

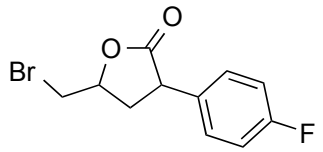


5-(Bromomethyl)-3-(*p*-tolyl)dihydrofuran-2(3*H*)-one (2q): (*cis*-isomer) ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.26 (td, *J* = 13.0, 10.1 Hz, 1H), 2.34 (s, 3H), 2.85 (ddd, *J* = 13.0, 9.4, 6.1 Hz, 1H), 3.58 (dd, *J* = 11.1, 6.1 Hz, 1H), 3.65 (dd, *J* = 11.1, 4.8 Hz, 1H), 3.90 (dd, *J* = 13.0, 9.4 Hz, 1H), 4.64-4.74 (m, 1H), 7.18 (s, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.1, 33.2, 36.3, 46.5, 75.7, 127.9 (2C), 129.6 (2C), 132.9, 137.6, 175.9. IR (neat) 2922, 1770, 1451, 1335, 1156, 1019 cm^{-1}. MS

(APCI) calcd for $C_{12}H_{14}BrO_2$ $[M+H]^+$ 269.0172, found 269.0168. (*trans*-isomer) ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.34 (s, 3H), 2.57 (dt, *J* = 13.7, 7.6 Hz, 1H), 2.66 (ddd, *J* = 13.7, 9.8, 5.0 Hz, 1H), 3.59 (dd, *J* = 11.0, 6.0 Hz, 1H), 3.62 (dd, *J* = 11.0, 4.6 Hz, 1H), 4.00 (dd, *J* = 9.8, 7.6 Hz, 1H), 4.82-4.92 (m, 1H), 7.13-7.21 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.0, 33.8, 34.9, 45.1, 76.1, 127.4 (2C), 129.7 (2C), 133.8, 137.5, 176.5. IR (neat) 2920, 1770, 1453, 1339, 1150, 1011 cm^{-1}. MS (APCI) calcd for $C_{12}H_{14}BrO_2$ $[M+H]^+$ 269.0172, found 269.0172.

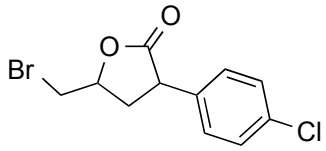


5-(Bromomethyl)-3-(4-methoxyphenyl)dihydrofuran-2(3*H*)-one (2r): (*cis*-isomer) ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.25 (dd, *J* = 13.0, 10.1 Hz, 1H), 2.86 (ddd, *J* = 13.0, 9.3, 6.0 Hz, 1H), 3.59 (dd, *J* = 11.0, 6.4 Hz, 1H), 3.66 (dd, *J* = 11.0, 4.6 Hz, 1H), 3.80 (s, 3H), 3.90 (dd, *J* = 13.0, 9.3 Hz, 1H), 4.65-4.74 (m, 1H), 6.88-6.94 (m, 2H), 7.19-7.25 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 33.2, 36.4, 46.2, 55.3, 75.7, 114.3 (2C), 127.9, 129.1 (2C), 159.1, 176.1. IR (neat) 2932, 1770, 1514, 1455, 1249, 1156, 1019 cm^{-1}. MS (APCI) calcd for $C_{12}H_{14}BrO_3$ $[M+H]^+$ 285.0121, found 285.0116. (*trans*-isomer) ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.55 (dt, *J* = 14.0, 8.0 Hz, 1H), 2.66 (ddd, *J* = 14.0, 10.0, 5.0 Hz, 1H), 3.58 (dd, *J* = 11.0, 6.0 Hz, 1H), 3.61 (dd, *J* = 11.0, 4.8 Hz, 1H), 3.80 (s, 3H), 3.99 (dd, *J* = 10.0, 8.0 Hz, 1H), 4.82-4.91 (m, 1H), 6.87-6.93 (m, 2H), 7.16-7.22 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 33.8, 34.9, 44.6, 55.3, 76.1, 114.4 (2C), 128.65 (2C), 128.69, 159.1, 176.7. IR (neat) 2931, 1768, 1513, 1459, 1249, 1150, 1031 cm^{-1}. MS (APCI) calcd for $C_{12}H_{14}BrO_3$ $[M+H]^+$ 285.0121, found 285.0121.

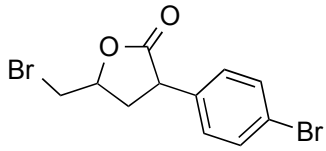


5-(Bromomethyl)-3-(4-fluorophenyl)dihydrofuran-2(3*H*)-one (2s): (*cis*-isomer) ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.26 (td, *J* = 12.7, 10.1 Hz, 1H), 2.89 (ddd, *J* = 13.0, 9.2, 6.0 Hz, 1H), 3.60 (dd, *J* = 11.0, 6.1 Hz, 1H), 3.67 (dd, *J* = 11.0, 4.6 Hz, 1H), 3.94 (dd, *J* = 12.7, 9.2 Hz, 1H), 4.67-4.76 (m, 1H), 7.03-7.12 (m, 2H), 7.24-7.33 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 33.1, 36.3, 46.1, 75.6, 115.9 (d, J_{C-F} = 21.1 Hz, 2C), 129.7 (d, J_{C-F} = 8.6 Hz, 2C), 131.7 (d, J_{C-F} = 2.9 Hz), 162.3 (d, J_{C-F} = 248.1 Hz), 175.5. IR (neat) 2925, 1770, 1551, 1338, 1225, 1156, 1018 cm^{-1}. MS (APCI) calcd for $C_{11}H_{11}BrFO_2$ $[M+H]^+$ 272.9921, found 272.9919. (*trans*-isomer) ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.52-2.60 (m, 1H), 2.66-2.74 (m, 1H), 3.61 (d, *J* = 5.3 Hz, 2H), 4.04 (t, *J* = 9.2 Hz, 1H), 4.84-4.93 (m, 1H), 7.02-7.10 (m, 2H), 7.22-7.30 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 33.9, 34.7, 44.6, 76.0, 116.0 (d, J_{C-F} = 21.9 Hz, 2C), 129.3 (d, J_{C-F} = 7.6 Hz, 2C), 132.5, 162.2 (d, J_{C-F} =

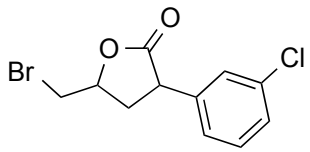
250.8 Hz), 176.3. IR (neat) 2958, 1769, 1510, 1339, 1226, 1152, 1012 cm^{-1}. MS (APPI) calcd for $C_{11}H_{10}BrFO_2$ $[M]^+$ 271.9843, found 271.9843.



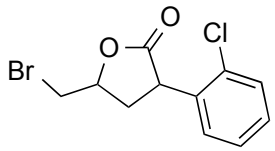
5-(Bromomethyl)-3-(4-chlorophenyl)dihydrofuran-2(3*H*)-one (2t): (*cis*-isomer) ^1H NMR (400 MHz, $CDCl_3$) δ 2.26 (td, *J* = 12.7, 10.1 Hz, 1H), 2.88 (ddd, *J* = 13.0, 9.1, 5.8 Hz, 1H), 3.60 (dd, *J* = 11.0, 6.2 Hz, 1H), 3.66 (dd, *J* = 11.0, 4.6 Hz, 1H), 3.93 (dd, *J* = 12.7, 9.1 Hz, 1H), 4.67-4.76 (m, 1H), 7.22-7.28 (m, 2H), 7.32-7.39 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 33.1, 36.1, 46.2, 75.7, 129.1 (2C), 129.4 (2C), 133.8, 134.4, 175.2. IR (neat) 2925, 1766, 1491, 1342, 1155, 1087, 1014 cm^{-1}. MS (APCI) calcd for $C_{11}H_{11}BrClO_2$ $[M+H]^+$ 288.9625, found 288.9627. (*trans*-isomer) ^1H NMR (400 MHz, $CDCl_3$) δ 2.49-2.61 (m, 1H), 2.64-2.75 (m, 1H), 3.57-3.65 (m, 2H), 4.03 (t, *J* = 9.1 Hz, 1H), 4.84-4.93 (m, 1H), 7.19-7.25 (m, 2H), 7.31-7.38 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 33.9, 34.5, 44.7, 76.0, 129.0 (2C), 129.2 (2C), 133.7, 135.2, 176.0. IR (neat) 2958, 1770, 1493, 1340, 1152, 1092, 1013 cm^{-1}. MS (APPI) calcd for $C_{11}H_{10}BrClO_2$ $[M]^+$ 287.9547, found 287.9548.



5-(Bromomethyl)-3-(4-bromophenyl)dihydrofuran-2(3*H*)-one (2u): (*cis*-isomer) ^1H NMR (400 MHz, $CDCl_3$) δ 2.25 (td, *J* = 12.6, 10.1 Hz, 1H), 2.88 (ddd, *J* = 13.0, 9.2, 6.0 Hz, 1H), 3.60 (dd, *J* = 11.0, 6.2 Hz, 1H), 3.66 (dd, *J* = 11.0, 4.6 Hz, 1H), 3.91 (dd, *J* = 12.6, 9.2 Hz, 1H), 4.66-4.76 (m, 1H), 7.15-7.22 (m, 2H), 7.47-7.55 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 33.0, 36.0, 46.3, 75.7, 121.9, 129.7 (2C), 132.1 (2C), 134.9, 175.1. IR (neat) 2920, 1766, 1488, 1341, 1153, 1010 cm^{-1}. MS (ESI) calcd for $C_{11}H_{10}Br_2O_2Na$ $[M+Na]^+$ 354.8940, found 354.8934. (*trans*-isomer) ^1H NMR (400 MHz, $CDCl_3$) δ 2.55 (dtd, *J* = 13.7, 8.2, 1.3 Hz, 1H), 2.64-2.75 (m, 1H), 3.58-3.65 (m, 2H), 4.02 (dd, *J* = 10.0, 8.2 Hz, 1H), 4.83-4.92 (m, 1H), 7.17 (d, *J* = 8.7 Hz, 2H), 7.50 (d, *J* = 8.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 33.8, 34.5, 44.8, 76.0, 121.9, 129.3 (2C), 132.2 (2C), 135.7, 175.8. IR (neat) 2962, 1771, 1489, 1339, 1151, 1010 cm^{-1}. MS (APCI) calcd for $C_{11}H_{10}Br_2O_2$ $[M]^+$ 331.9042, found 331.9046.



5-(Bromomethyl)-3-(3-chlorophenyl)dihydrofuran-2(3*H*)-one (2v): (*cis*-isomer) ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.27 (td, *J* = 13.0, 10.2 Hz, 1H), 2.89 (ddd, *J* = 13.0, 9.2, 6.0 Hz, 1H), 3.61 (dd, *J* = 11.0, 6.2 Hz, 1H), 3.67 (dd, *J* = 11.0, 4.3 Hz, 1H), 3.93 (dd, *J* = 12.6, 9.2 Hz, 1H), 4.72 (dtd, *J* = 10.2, 6.1, 4.3 Hz, 1H), 7.18-7.24 (m, 1H), 7.27-7.35 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 33.0, 36.0, 46.4, 75.7, 126.3, 128.1, 128.3, 130.2, 134.7, 137.8, 175.0. IR (neat) 2925, 1773, 1479, 1342, 1157, 1019 cm^{-1}. MS (APCI) calcd for $C_{11}H_{11}BrClO_2$ $[M+H]^+$ 288.9625, found 288.9617. (*trans*-isomer) ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.56 (dd, *J* = 13.7, 8.2 Hz, 1H), 2.69 (ddd, *J* = 13.7, 10.1, 4.6 Hz, 1H), 3.34 (d, *J* = 5.3 Hz, 2H), 4.03 (dd, *J* = 10.1, 8.2 Hz, 1H), 4.84-4.93 (m, 1H), 7.14-7.20 (m, 1H), 7.25-7.34 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 33.9, 34.4, 44.9, 76.0, 125.8, 127.8, 128.0, 130.3, 134.8, 138.6, 175.7. IR (neat) 2967, 1771, 1478, 1340, 1151, 1012 cm^{-1}. MS (APCI) calcd for $C_{11}H_{10}BrClO_2$ $[M]^+$ 287.9547, found 287.9553.

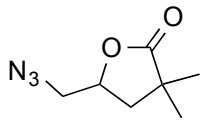


5-(Bromomethyl)-3-(2-chlorophenyl)dihydrofuran-2(3*H*)-one (2w): (*cis*-isomer) ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.19 (td, *J* = 13.0, 10.1 Hz, 1H), 2.95 (ddd, *J* = 13.0, 9.6, 6.2 Hz, 1H), 3.60 (dd, *J* = 11.0, 6.4 Hz, 1H), 3.68 (dd, *J* = 11.0, 4.6 Hz, 1H), 4.37 (dd, *J* = 13.0, 9.6 Hz, 1H), 4.71-4.82 (m, 1H), 7.24-7.34 (m, 3H), 7.39-7.45 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 33.0, 35.5, 45.1, 76.0, 127.5, 129.3, 129.8, 129.9, 134.0, 134.3, 174.9. IR (neat) 2922, 1762, 1421, 1347, 1177, 1025 cm^{-1}. MS (APCI) calcd for $C_{11}H_{11}BrClO_2$ $[M+H]^+$ 288.9625, found 288.9621. (*trans*-isomer) ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.52 (dt, *J* = 13.8, 8.7 Hz, 1H), 2.73 (ddd, *J* = 13.8, 10.7, 4.3 Hz, 1H), 3.61 (dd, *J* = 11.2, 4.1 Hz, 1H), 3.66 (dd, *J* = 11.2, 5.7 Hz, 1H), 4.38 (dd, *J* = 10.7, 8.7 Hz, 1H), 4.86-4.97 (m, 1H), 7.22-7.32 (m, 3H), 7.39-7.46 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 33.9, 34.3, 44.3, 76.0, 127.5, 129.3, 129.7, 130.1, 133.7, 135.1, 175.8. IR (neat) 2962, 1772, 1476, 1343, 1153, 1012 cm^{-1}. MS (APCI) calcd for $C_{11}H_{11}BrClO_2$ $[M+H]^+$ 288.9625, found 288.9624.

3. Transformation into γ-Azidomethyl Lactone (3c) from 1c without purification of 2c via Oxidative Bromo-lactonization Using KBr and Oxone® (Scheme 2).

To a solution of **1c** (32.1 mg, 0.25 mmol) and KBr (44.6 mg, 0.375 mmol) in AcOEt (1.0 mL) was added Oxone® (184.4 mg, 0.30 mmol) at –10 ºC. After stirring at –10 ºC for 12 h, the reaction mixture was filtered through Celite with AcOEt to remove the precipitate. The filtrate was concentrated under reduced pressure and the crude product was dissolved with MeCN (1.2 mL). 15-Crown-5-ether (10 μL, 0.05 mmol) and NaN_3 (32.5 mg, 0.50 mmol) were added to the solution at room temperature under argon atmosphere. After stirring at 90 ºC for 6 h, NaN_3 (8.2 mg, 0.125

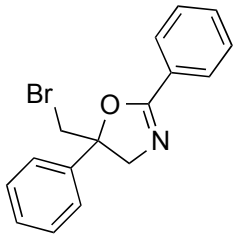
mmol) was again added to the reaction mixture. After stirring at 90 ºC for 18 h, the reaction mixture was cooled to room temperature, and the suspension was filtered through Celite with AcOEt. The filtrate was concentrated under reduced pressure and the crude product was purified by silica gel column chromatography (eluent: hexane/AcOEt = 3/1) to give desired product **3c** (37.6 mg, 89%).



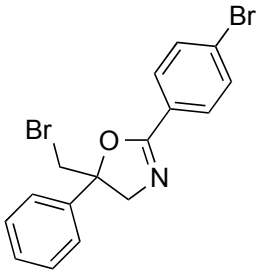
5-(Azidomethyl)-3,3-dimethyldihydrofuran-2(3*H*)-one (3c): ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.29 (s, 3H), 1.32 (s, 3H), 1.94 (dd, *J* = 12.9, 9.8 Hz, 1H), 2.13 (dd, *J* = 12.9, 6.5 Hz, 1H), 3.44 (dd, *J* = 13.5, 5.5 Hz, 1H), 3.58 (dd, *J* = 13.5, 3.9 Hz, 1H), 4.54-4.63 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 24.7, 24.9, 39.7, 40.1, 53.8, 74.7, 180.9. IR (neat) 2971, 2099, 1767, 1458, 1281, 1204, 1121, 1050 cm^{-1}. MS (APCI) calcd for $C_7H_{12}N_3O_2$ $[M+H]^+$ 170.0930, found 170.0922.

4. General Procedure for Oxidative Bromo-Cyclization of *N*-Allyl Amides (4) (Table 4; Entry 13, and Scheme 3).

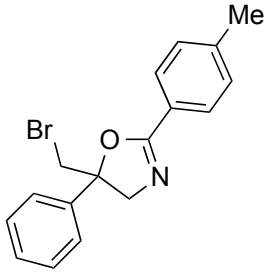
To a solution of **4a** (59.4 mg, 0.25 mmol) and KBr (35.7 mg, 0.30 mmol) in AcOEt (1.0 mL) was added Oxone® (153.7 mg, 0.25 mmol) at room temperature. After stirring at room temperature for 13 h, saturated Na_2SO_3 aqueous solution (10 mL) was added to the reaction mixture, and the product was extracted with AcOEt (15 mL×3). The combined extracts were washed with brine (10 mL) and dried over Na_2SO_4. The organic phase was concentrated under reduced pressure and the crude product was purified by silica gel column chromatography (eluent: hexane/AcOEt = 3/1) to give desired product **5a** (72.7 mg, 92%).



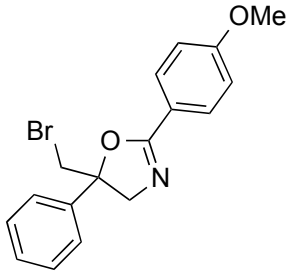
5-(Bromomethyl)-2,5-diphenyl-4,5-dihydrooxazole (5a): ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.77 (d, *J* = 11.4 Hz, 1H), 3.85 (d, *J* = 11.4 Hz, 1H), 4.28 (d, *J* = 15.1 Hz, 1H), 4.50 (d, *J* = 15.1 Hz, 1H), 7.30-7.57 (m, 8H), 8.03-8.09 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 40.1, 65.9, 87.0, 124.9 (2C), 127.4, 128.3 (3C), 128.4 (2C), 128.8 (2C), 131.6, 141.7, 162.9. IR (neat) 1656, 1446, 1345, 1270, 1065, 1021 cm^{-1}. MS (ESI) calcd for $C_{16}H_{15}BrNO$ $[M+H]^+$ 316.0332, found 316.0327.



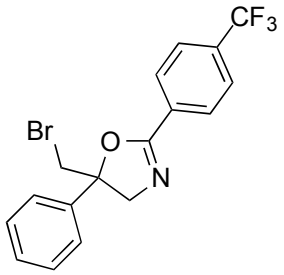
5-(Bromomethyl)-2-(4-bromophenyl)-5-phenyl-4,5-dihydrooxazole (5b): ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.75 (d, *J* = 11.2 Hz, 1H), 3.83 (d, *J* = 11.2 Hz, 1H), 4.27 (d, *J* = 15.1 Hz, 1H), 4.48 (d, *J* = 15.1 Hz, 1H), 7.31-7.39 (m, 1H), 7.39-7.44 (m, 4H), 7.56-7.62 (m, 2H), 7.88-7.95 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 40.1, 65.9, 87.2, 124.8 (2C), 126.3, 128.4 (2C), 128.8 (2C), 129.8 (2C), 131.7 (2C), 141.5, 162.1. IR (neat) 1655, 1486, 1345, 1268, 1079, 1010 cm^{-1}. MS (ESI) calcd for $C_{16}H_{14}Br_2NO$ $[M+H]^+$ 393.9437, found 393.9439.



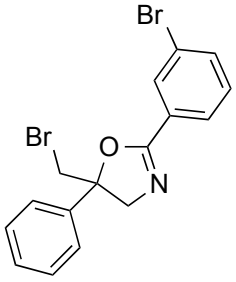
5-(Bromomethyl)-5-phenyl-2-(*p*-tolyl)-4,5-dihydrooxazole (5c): ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.41 (s, 3H), 3.76 (d, *J* = 8.9 Hz, 1H), 3.83 (d, *J* = 8.9 Hz, 1H), 4.26 (d, *J* = 11.9 Hz, 1H), 4.47 (d, *J* = 11.9 Hz, 1H), 7.26 (d, *J* = 6.4 Hz, 2H), 7.30-7.35 (m, 1H), 7.36-7.45 (m, 4H), 7.94 (d, *J* = 6.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.6, 40.1, 65.8, 86.8, 124.6, 124.9 (2C), 128.2 (3C), 128.7 (2C), 141.8, 142.0, 162.9. IR (neat) 1653, 1447, 1346, 1269, 1077, 1018 cm^{-1}. MS (ESI) calcd for $C_{17}H_{17}BrNO$ $[M+H]^+$ 330.0488, found 330.0487.



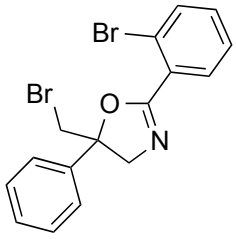
5-(Bromomethyl)-2-(4-methoxyphenyl)-5-phenyl-4,5-dihydrooxazole (5d): ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.76 (d, *J* = 11.2 Hz, 1H), 3.82 (d, *J* = 11.2 Hz, 1H), 3.85 (s, 3H), 4.24 (d, *J* = 14.9 Hz, 1H), 4.45 (d, *J* = 14.9 Hz, 1H), 6.91-6.98 (m, 2H), 7.28-7.45 (m, 5H), 7.95-8.02 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 40.1, 55.4, 65.8, 86.8, 113.8 (2C), 119.9, 124.9 (2C), 128.2, 128.7 (2C), 130.0 (2C), 141.8, 162.3, 162.7. IR (neat) 1647, 1606, 1510, 1444, 1348, 1254, 1167, 1020 cm^{-1}. MS (ESI) calcd for $C_{17}H_{17}BrNO_2$ $[M+H]^+$ 346.0437, found 346.0436.



5-(Bromomethyl)-5-phenyl-2-(4-(trifluoromethyl)phenyl)-4,5-dihydrooxazole (5e): ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.77 (d, J = 11.5 Hz, 1H), 3.85 (d, J = 11.5 Hz, 1H), 4.32 (d, J = 15.4 Hz, 1H), 4.54 (d, J = 15.4 Hz, 1H), 7.32-7.45 (m, 5H), 7.72 (d, J = 8.3 Hz, 2H), 8.17 (d, J = 8.3 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 40.0, 65.9, 87.5, 123.7 (q, $J_{C–F}$ = 274.0 Hz), 124.8 (2C), 125.4 (q, $J_{C–F}$ = 3.8 Hz, 2C), 128.5, 128.6 (2C), 128.9 (2C), 131.0, 133.2 (q, $J_{C–F}$ = 32.6 Hz), 141.4, 161.7. IR (neat) 1657, 1448, 1321, 1272, 1125, 1084, 1016 cm^{-1}. MS (ESI) calcd for $C_{17}H_{14}BrF_3NO$ $[M+H]^+$ 384.0205, found 384.0204.

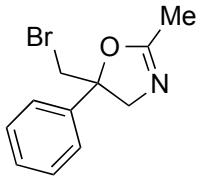


5-(Bromomethyl)-2-(3-bromophenyl)-5-phenyl-4,5-dihydrooxazole (5f): ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.74 (d, J = 11.3 Hz, 1H), 3.83 (d, J = 11.3 Hz, 1H), 4.28 (d, J = 15.2 Hz, 1H), 4.50 (d, J = 15.2 Hz, 1H), 7.29-7.44 (m, 6H), 7.61-7.66 (m, 1H), 7.97 (dt, J = 7.8, 1.8 Hz, 1H), 8.19 (t, J = 1.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 40.0, 65.8, 87.4, 122.5, 124.8 (2C), 126.8, 128.4, 128.8 (2C), 129.3, 130.0, 131.2, 134.5, 141.4, 161.6. IR (neat) 1653, 1561, 1478, 1346, 1257, 1064 cm^{-1}. MS (ESI) calcd for $C_{16}H_{14}Br_2NO$ $[M+H]^+$ 393.9437, found 393.9437.

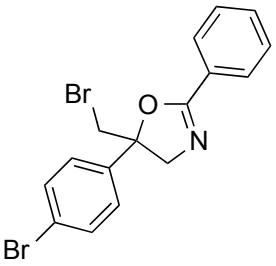


5-(Bromomethyl)-2-(2-bromophenyl)-5-phenyl-4,5-dihydrooxazole (5g): ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.76 (d, J = 11.2 Hz, 1H), 3.84 (d, J = 11.2 Hz, 1H), 4.34 (d, J = 15.1 Hz, 1H), 4.56 (d, J = 15.1 Hz, 1H), 7.29-7.49 (m, 7H), 7.68 (dd, J = 6.8, 1.4 Hz, 1H), 7.85 (dd, J = 7.8, 1.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 40.3, 65.9, 87.4, 121.8, 125.1 (2C), 127.2, 128.3, 128.8 (2C), 129.2, 131.6, 131.8, 134.0, 141.4, 162.1. IR (neat) 1658, 1434, 1343, 1249, 1095, 1020 cm^{-1}.

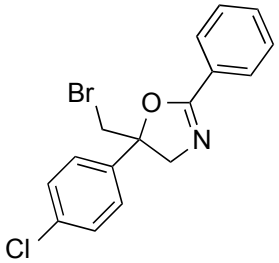
MS (ESI) calcd for $C_{16}H_{14}Br_2NO$ $[M+H]^+$ 393.9437, found 393.9438.



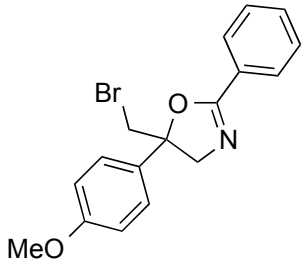
5-(Bromomethyl)-2-methyl-5-phenyl-4,5-dihydrooxazole (5h): ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.10 (t, *J* = 1.3 Hz, 3H), 3.65 (d, *J* = 11.3 Hz, 1H), 3.71 (d, *J* = 11.3 Hz, 1H), 4.04 (dd, *J* = 14.4, 1.3 Hz, 1H), 4.24 (dd, *J* = 14.4, 1.3 Hz, 1H), 7.30-7.43 (m, 5H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.0, 40.3, 65.4, 86.8, 124.9 (2C), 128.2, 128.7 (2C), 141.7, 163.9. IR (neat) 3286, 1641, 1539, 1446, 1285, 1110, 1046 cm^{-1}. MS (ESI) calcd for $C_{11}H_{13}BrNO$ $[M+H]^+$ 254.0175, found 254.0173.



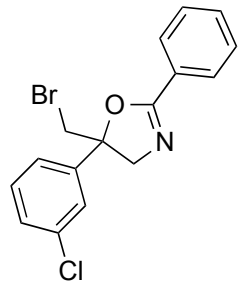
5-(Bromomethyl)-5-(4-bromophenyl)-2-phenyl-4,5-dihydrooxazole (5i): ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.74 (d, *J* = 11.4 Hz, 1H), 3.80 (d, *J* = 11.4 Hz, 1H), 4.23 (d, *J* = 15.2 Hz, 1H), 4.48 (d, *J* = 15.2 Hz, 1H), 7.28-7.36 (m, 2H), 7.42-7.50 (m, 2H), 7.50-7.58 (m, 3H), 8.00-8.08 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 39.5, 65.9, 86.6, 122.4, 126.7 (2C), 127.2, 128.3 (2C), 128.5 (2C), 131.7, 131.9 (2C), 140.7, 162.8. IR (neat) 1647, 1486, 1345, 1260, 1063, 1007 cm^{-1}. MS (ESI) calcd for $C_{16}H_{14}Br_2NO$ $[M+H]^+$ 393.9437, found 393.9432.



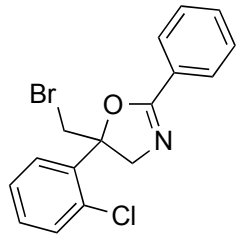
5-(Bromomethyl)-5-(4-chlorophenyl)-2-phenyl-4,5-dihydrooxazole (5j): ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.74 (d, *J* = 11.4 Hz, 1H), 3.80 (d, *J* = 11.4 Hz, 1H), 4.23 (d, *J* = 15.4 Hz, 1H), 4.48 (d, *J* = 15.4 Hz, 1H), 7.38 (s, 4H), 7.43-7.50 (m, 2H), 7.50-7.56 (m, 1H), 8.01-8.07 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 39.6, 65.9, 86.6, 126.4 (2C), 127.2, 128.2 (2C), 128.5 (2C), 128.9 (2C), 131.7, 134.2, 140.2, 162.8. IR (neat) 1649, 1490, 1345, 1261, 1065, 1011 cm^{-1}. MS (ESI) calcd for $C_{16}H_{14}BrClNO$ $[M+H]^+$ 349.9942, found 349.9936.



5-(Bromomethyl)-5-(4-methoxyphenyl)-2-phenyl-4,5-dihydrooxazole (5k): ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.74 (d, *J* = 11.5 Hz, 1H), 3.81 (s, 3H), 3.82 (d, *J* = 11.5 Hz, 1H), 4.26 (d, *J* = 15.1 Hz, 1H), 4.47 (d, *J* = 15.1 Hz, 1H), 6.88-6.96 (m, 2H), 7.32-7.39 (m, 2H), 7.42-7.48 (m, 2H), 7.48-7.55 (m, 1H), 8.01-8.08 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 40.2, 55.3, 65.8, 86.8, 114.1 (2C), 126.2 (2C), 127.5, 128.2 (2C), 128.4 (2C), 131.5, 133.6, 159.4, 162.8. IR (neat) 1644, 1611, 1510, 1346, 1250, 1184, 1021 cm^{-1}. MS (ESI) calcd for $C_{17}H_{17}BrNO_2$ $[M+H]^+$ 346.0437, found 346.0428.

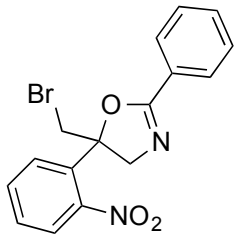


5-(Bromomethyl)-5-(3-chlorophenyl)-2-phenyl-4,5-dihydrooxazole (5l): ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.74 (d, *J* = 11.3 Hz, 1H), 3.80 (d, *J* = 11.3 Hz, 1H), 4.24 (d, *J* = 15.2 Hz, 1H), 4.47 (d, *J* = 15.2 Hz, 1H), 7.24-7.37 (m, 3H), 7.40-7.56 (m, 4H), 8.01-8.08 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 39.5, 65.9, 86.5, 123.1, 125.3, 127.1, 128.2 (2C), 128.5 (3C), 130.1, 131.7, 134.7, 143.7, 162.7. IR (neat) 1655, 1472, 1345, 1267, 1086, 1022 cm^{-1}. MS (ESI) calcd for $C_{16}H_{14}BrClNO$ $[M+H]^+$ 349.9942, found 349.9935.

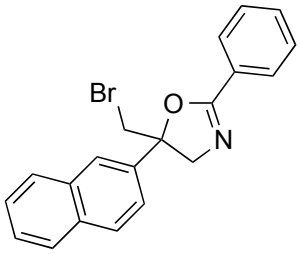


5-(Bromomethyl)-5-(2-chlorophenyl)-2-phenyl-4,5-dihydrooxazole (5m): ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.97 (d, *J* = 11.4 Hz, 1H), 4.11 (d, *J* = 11.4 Hz, 1H), 4.41 (d, *J* = 15.9 Hz, 1H), 4.62 (d, *J* = 15.9 Hz, 1H), 7.26-7.36 (m, 2H), 7.38-7.57 (m, 4H), 7.76-7.83 (m, 1H), 8.03-8.11 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 38.1, 65.3, 87.1, 127.16, 127.22, 127.8, 128.3 (2C), 128.5 (2C), 129.8, 129.9, 130.9, 131.6, 139.0, 162.0. IR (neat) 1659, 1450, 1345, 1267, 1088, 1022 cm^{-1}. MS

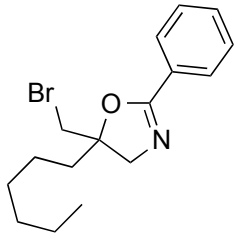
(ESI) calcd for $C_{16}H_{14}BrClNO$ $[M+H]^+$ 349.9942, found 349.9936.



5-(Bromomethyl)-5-(2-nitrophenyl)-2-phenyl-4,5-dihydrooxazole (5n): ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.80 (d, *J* = 11.2 Hz, 1H), 3.84 (d, *J* = 11.2 Hz, 1H), 4.29 (d, *J* = 15.2 Hz, 1H), 4.54 (d, *J* = 15.2 Hz, 1H), 7.44-7.52 (m, 2H), 7.52-7.58 (m, 1H), 7.62 (t, *J* = 8.1 Hz, 1H), 7.74-7.82 (m, 1H), 8.02-8.10 (m, 2H), 8.18-8.26 (m, 1H), 8.33 (t, *J* = 1.9 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 39.0, 66.0, 86.4, 120.4, 123.3, 126.8, 128.3 (2C), 128.6 (2C), 129.9, 131.3, 131.9, 143.8, 148.4, 162.8. IR (neat) 1732, 1656, 1528, 1347, 1268, 1064, 1022 cm^{-1}. MS (ESI) calcd for $C_{16}H_{14}BrN_2O_3$ $[M+H]^+$ 361.0182, found 361.0176.

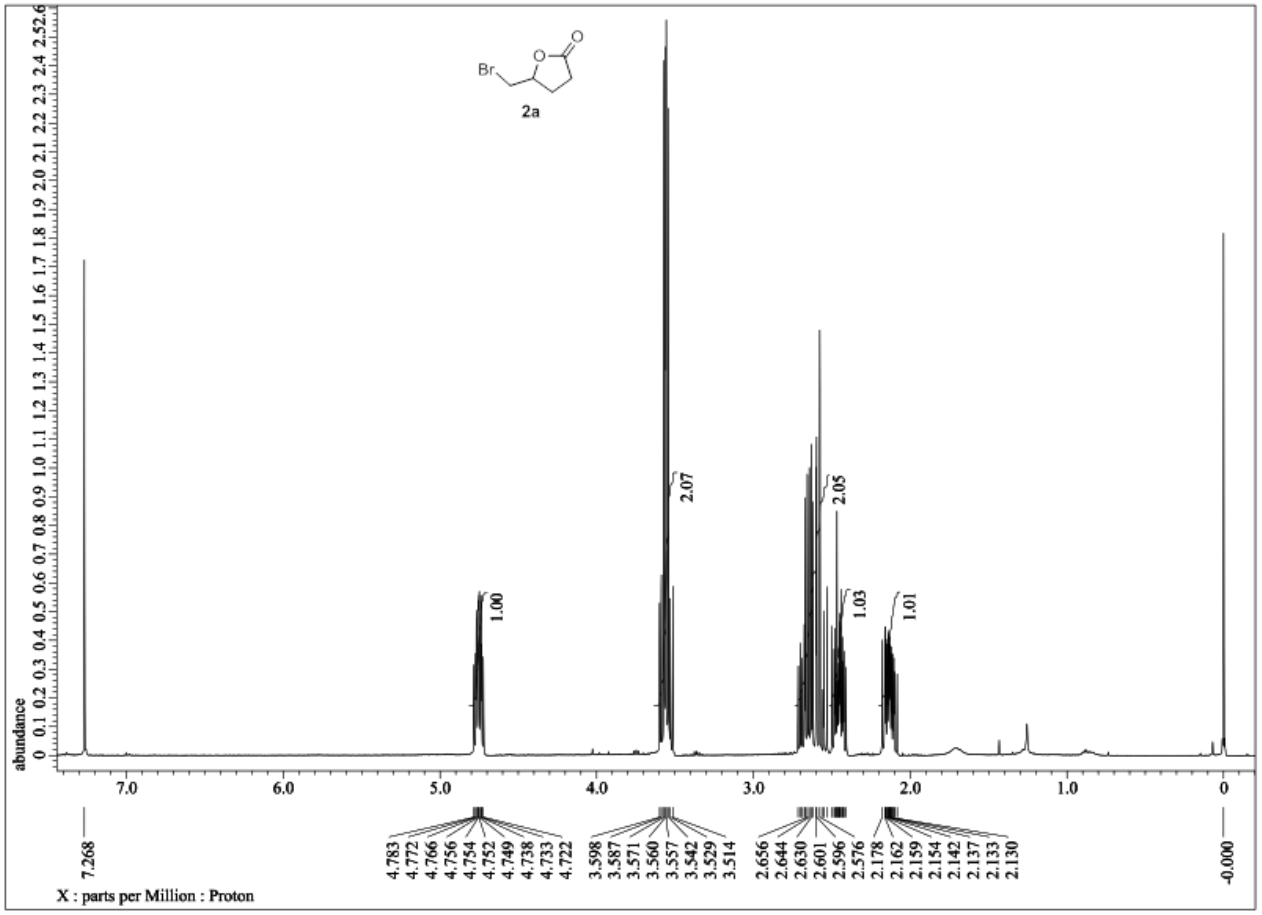


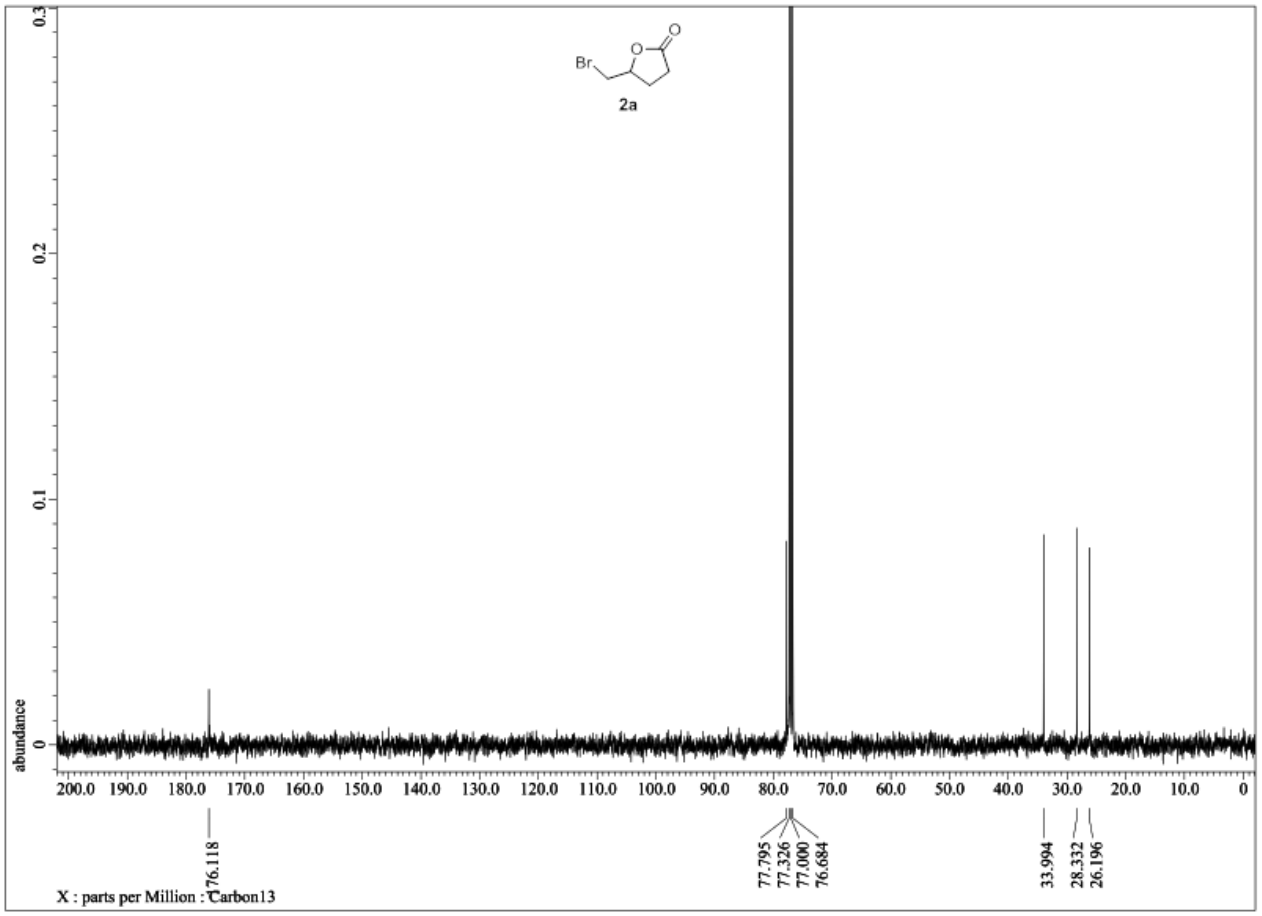
5-(Bromomethyl)-5-(naphthalen-2-yl)-2-phenyl-4,5-dihydrooxazole (5o): ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.88 (d, *J* = 11.4 Hz, 1H), 3.93 (d, *J* = 11.4 Hz, 1H), 4.38 (d, *J* = 15.1 Hz, 1H), 4.57 (d, *J* = 15.1 Hz, 1H), 7.44-7.58 (m, 6H), 7.81-7.95 (m, 4H), 8.07-8.14 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 40.0, 65.9, 87.2, 122.7, 124.0, 126.6, 126.7, 127.4, 127.7, 128.2, 128.3 (2C), 128.5 (2C), 128.9, 131.6, 132.9, 133.0, 138.8, 163.0. IR (neat) 1654, 1449, 1334, 1269, 1088, 1022 cm^{-1}. MS (ESI) calcd for $C_{20}H_{17}BrNO$ $[M+H]^+$ 366.0488, found 366.0486.

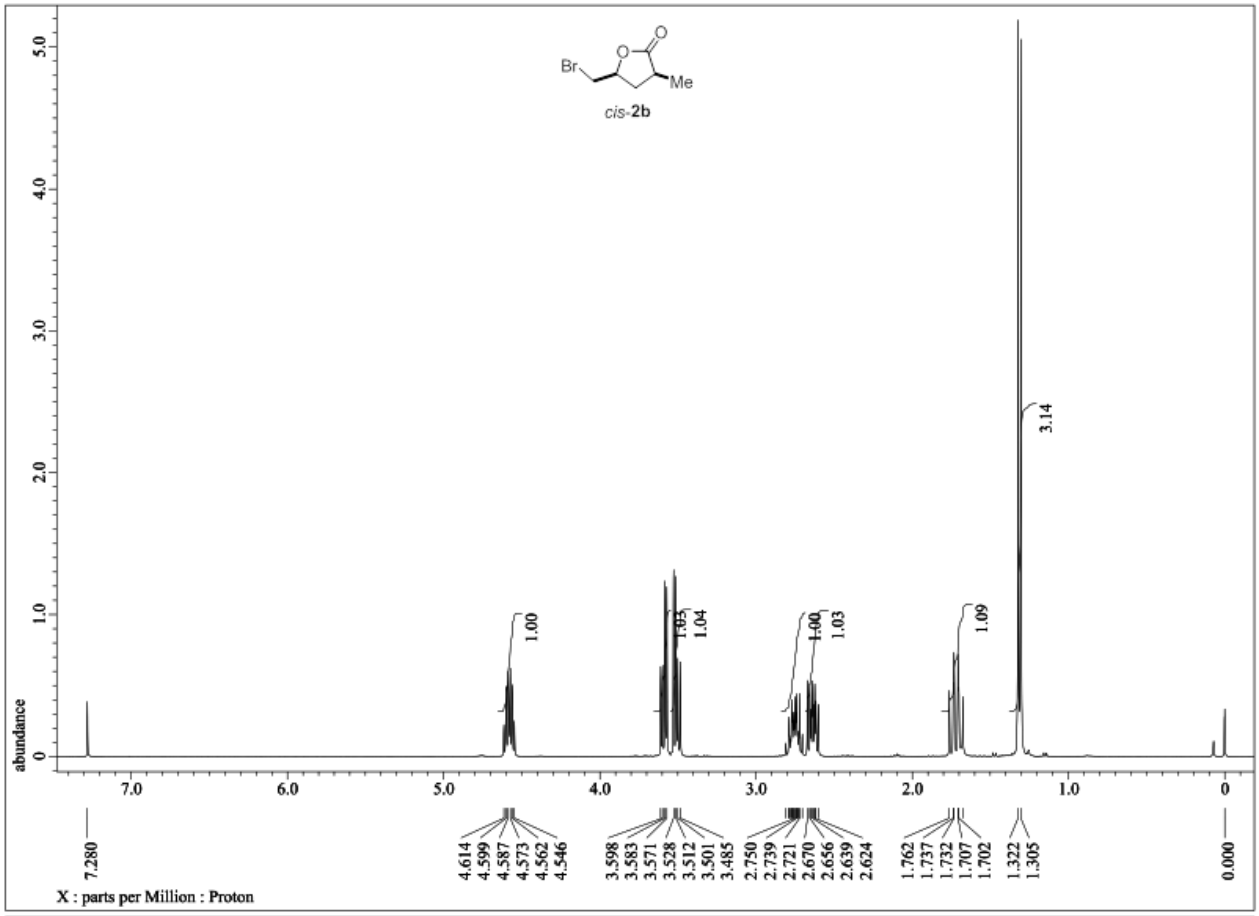


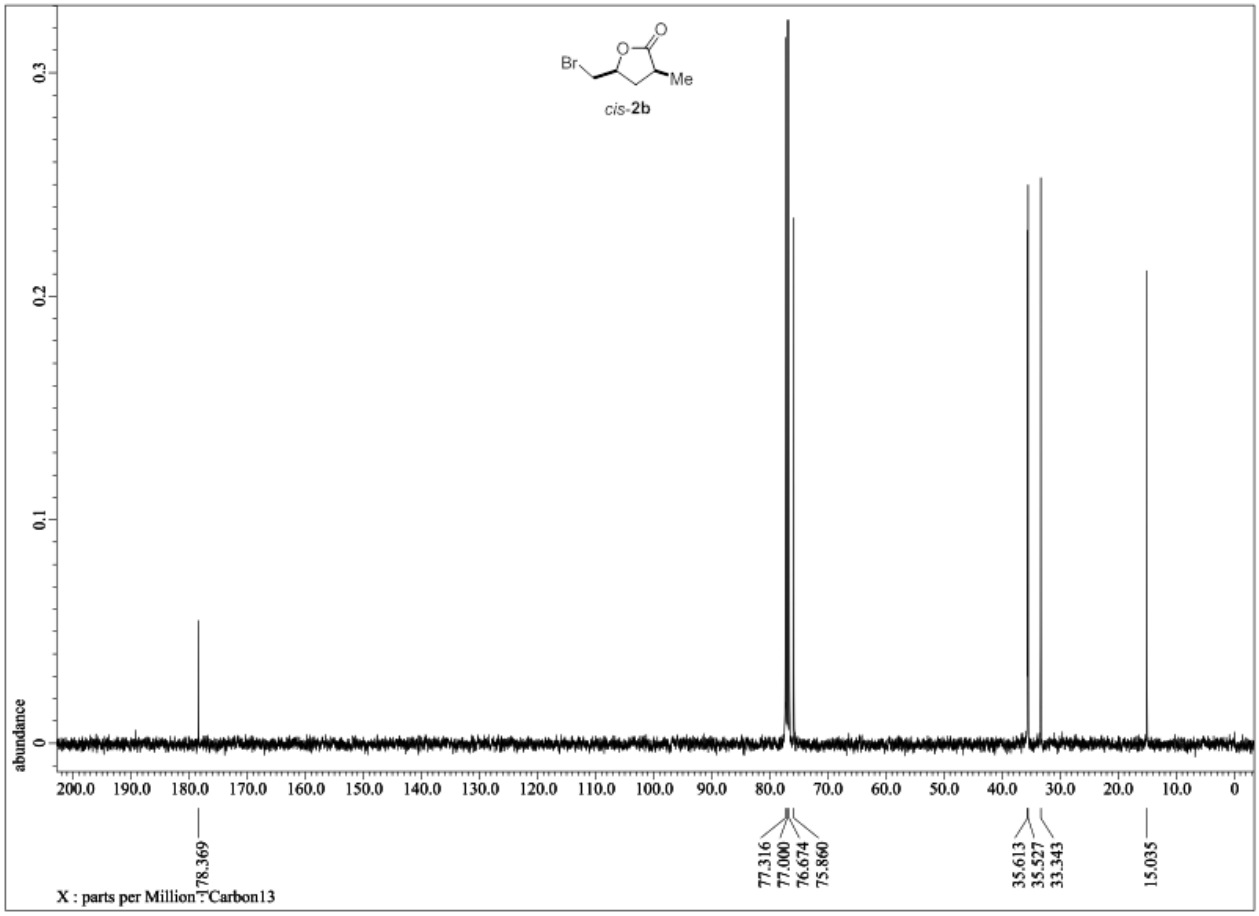
5-(Bromomethyl)-5-hexyl-2-phenyl-4,5-dihydrooxazole (5p): ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.88 (t, *J* = 6.9 Hz, 3H), 1.22-1.48 (m, 8H), 1.80-1.97 (m, 2H), 3.54 (d, *J* = 10.9 Hz, 1H), 3.58 (d, *J* = 10.9 Hz, 1H), 3.86 (d, *J* = 15.3 Hz, 1H), 4.03 (d, *J* = 15.3 Hz, 1H), 7.38-7.45 (m, 2H), 7.45-7.51 (m, 1H), 7.90-7.96 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.0, 22.5, 23.2, 29.4, 31.6, 37.0, 37.8, 63.0, 86.3, 127.6, 128.1 (2C), 128.3 (2C), 131.4, 168.2. IR (neat) 2928, 1651, 1450, 1348,

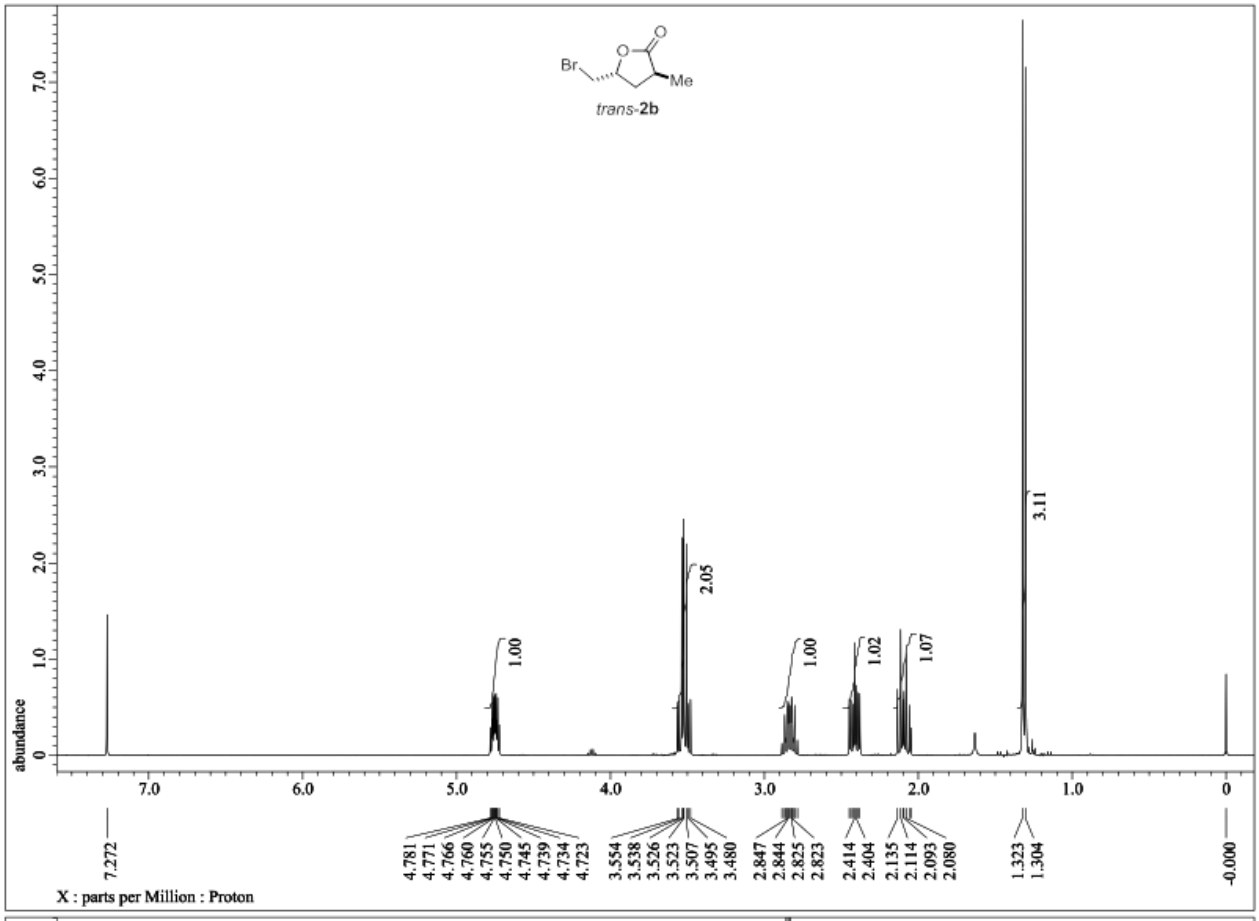
1265, 1086, 1024 cm^{-1}. MS (ESI) calcd for $C_{16}H_{23}BrNO$ $[M+H]^+$ 324.0958, found 324.0949.

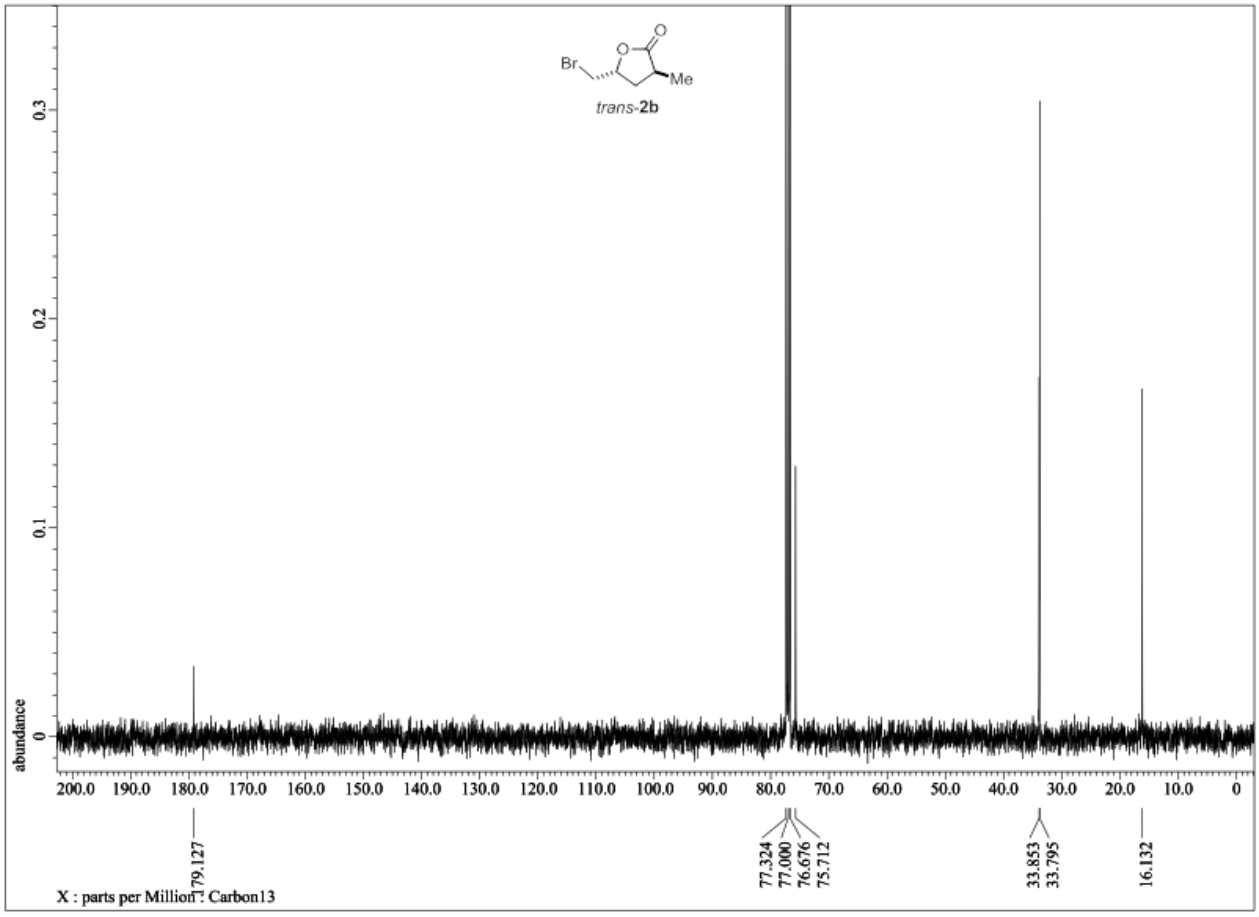

Br
O
O
2a
abundance
1.00
2.07
2.05
1.03
1.01
7.268
4.783
4.772
4.766
4.756
4.754
4.752
4.749
4.738
4.733
4.722
3.598
3.587
3.571
3.560
3.557
3.542
3.529
3.514
2.656
2.644
2.630
2.601
2.596
2.576
2.178
2.162
2.159
2.154
2.142
2.137
2.133
2.130
-0.000
X : parts per Million : Proton

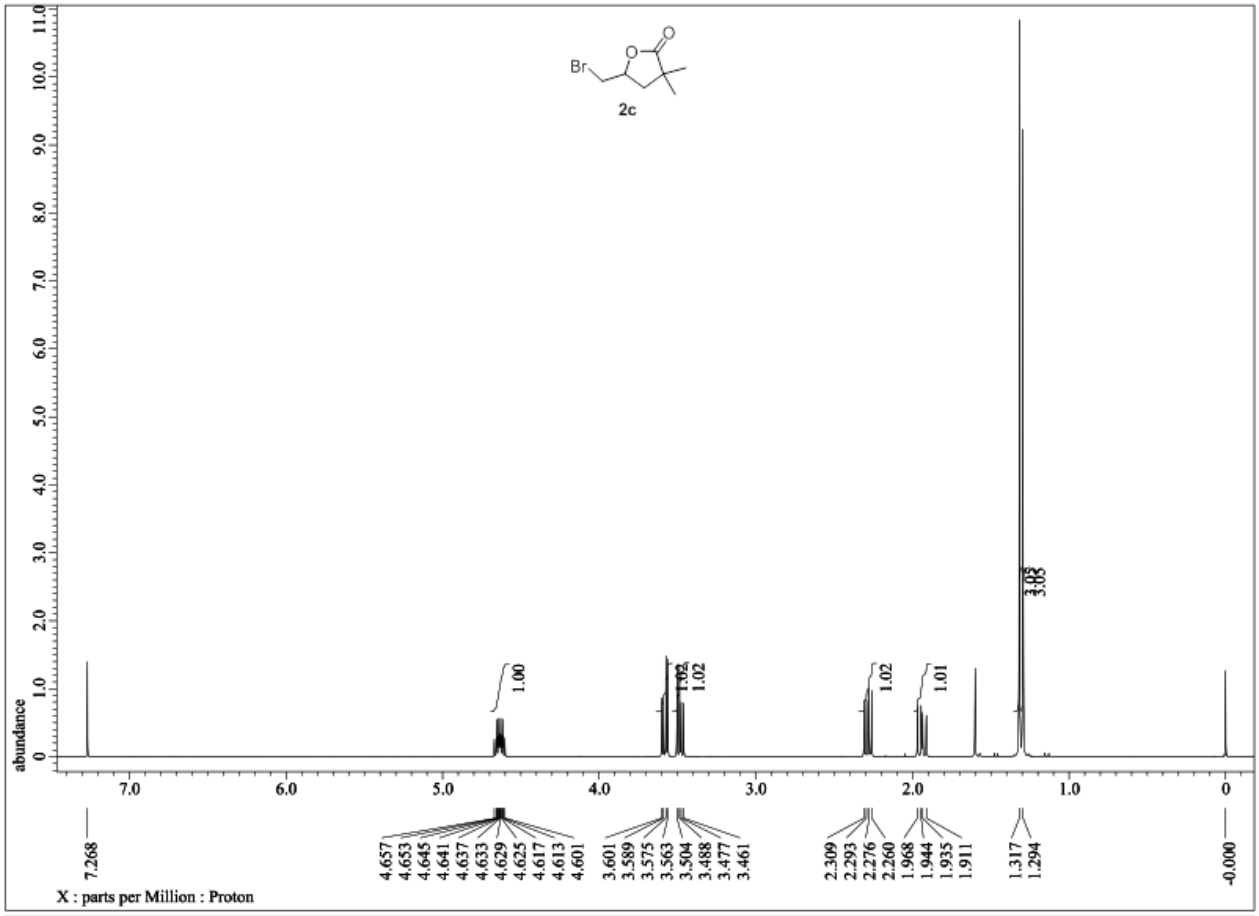

Br
O
O
2a
abundance
176.118
77.795
77.326
77.000
76.684
33.994
28.332
26.196
X : parts per Million : Carbon13

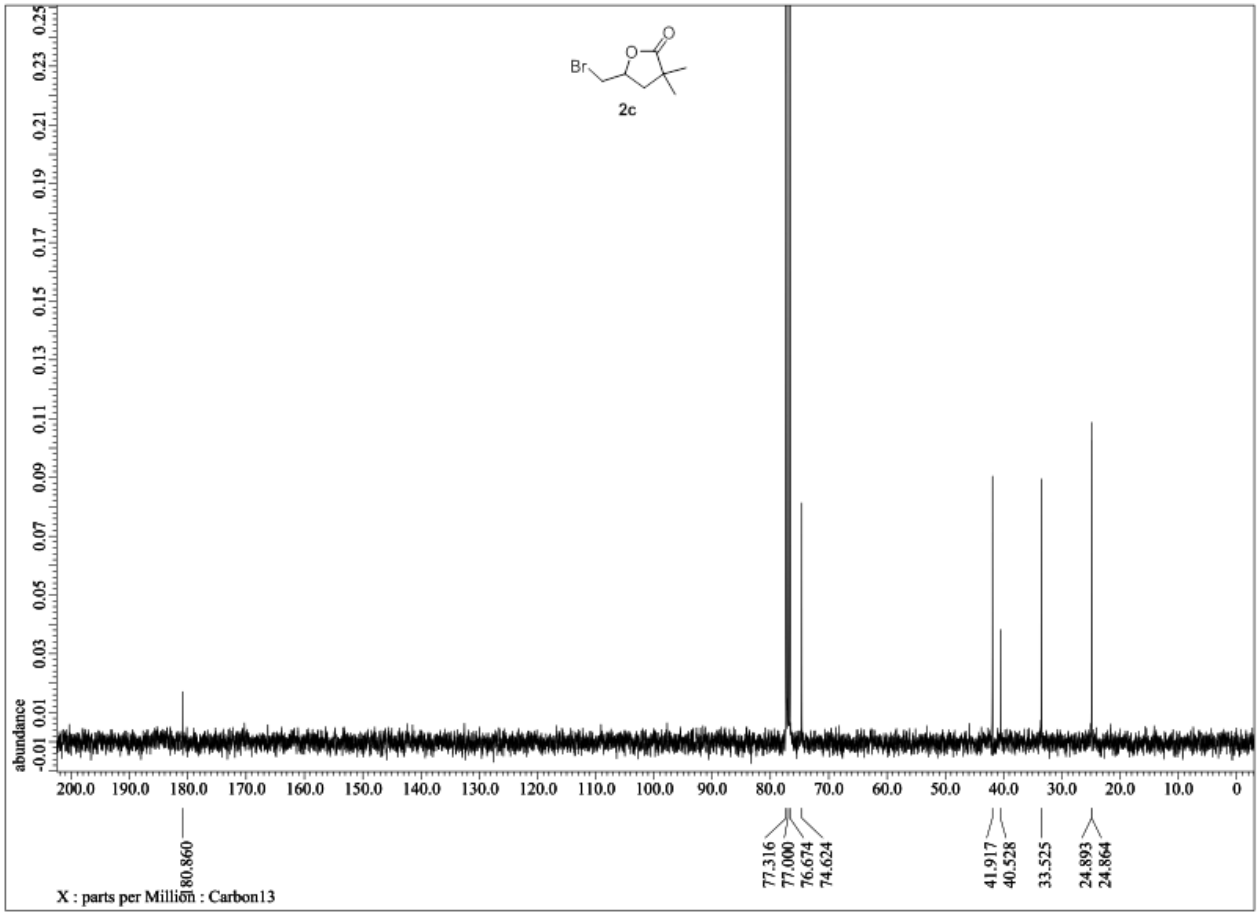

Br
O
O
Me
cis-2b
abundance
X : parts per Million : Proton
7.280
4.614
4.599
4.587
4.573
4.562
4.546
3.598
3.583
3.571
3.528
3.512
3.501
3.485
2.750
2.739
2.721
2.670
2.656
2.639
2.624
1.762
1.737
1.732
1.707
1.702
1.322
1.305
0.000
1.00
1.03
1.04
1.00
1.03
1.09
3.14

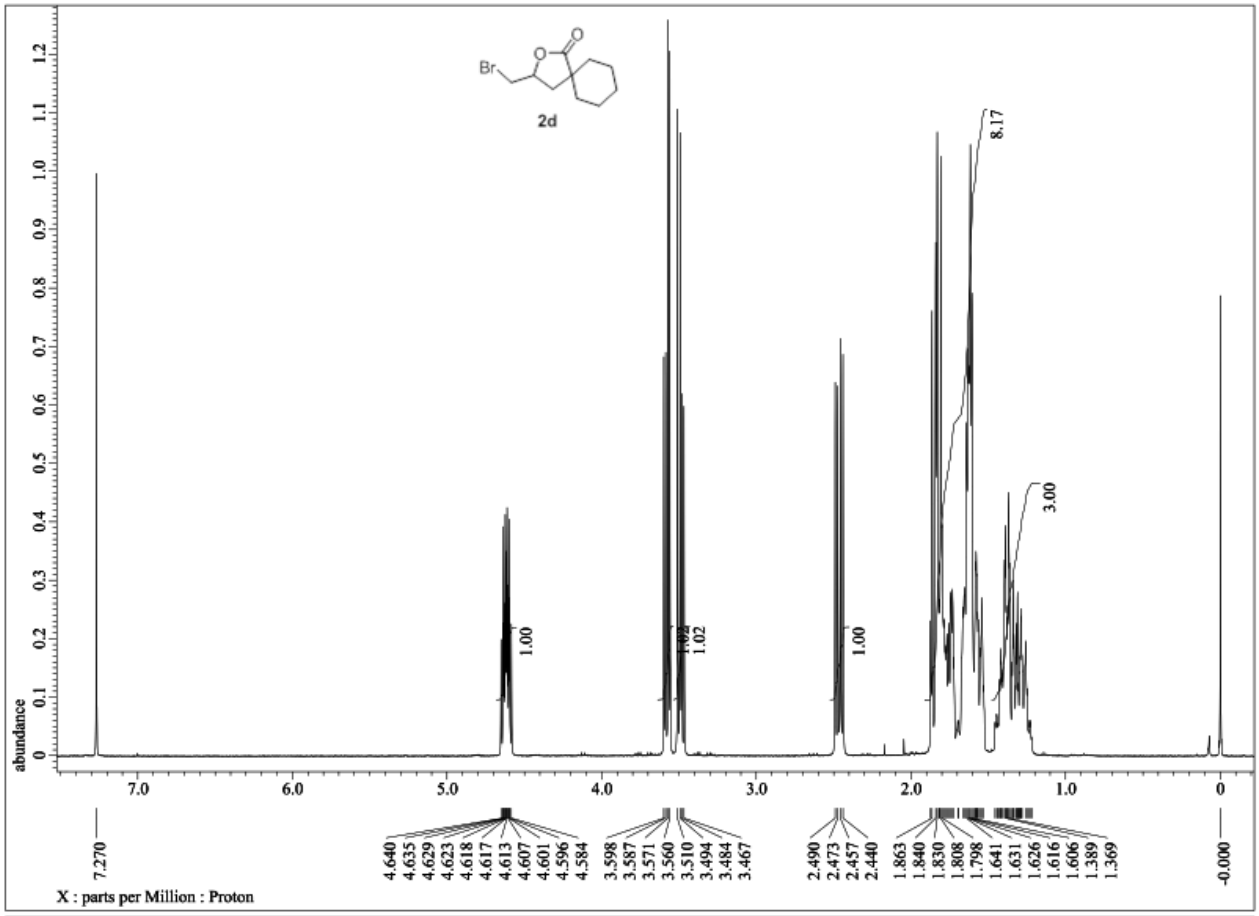

Br
O
O
Me
cis-2b
abundance
X : parts per Million : Carbon13
78.369
77.316
77.000
76.674
75.860
35.613
35.527
33.343
15.035

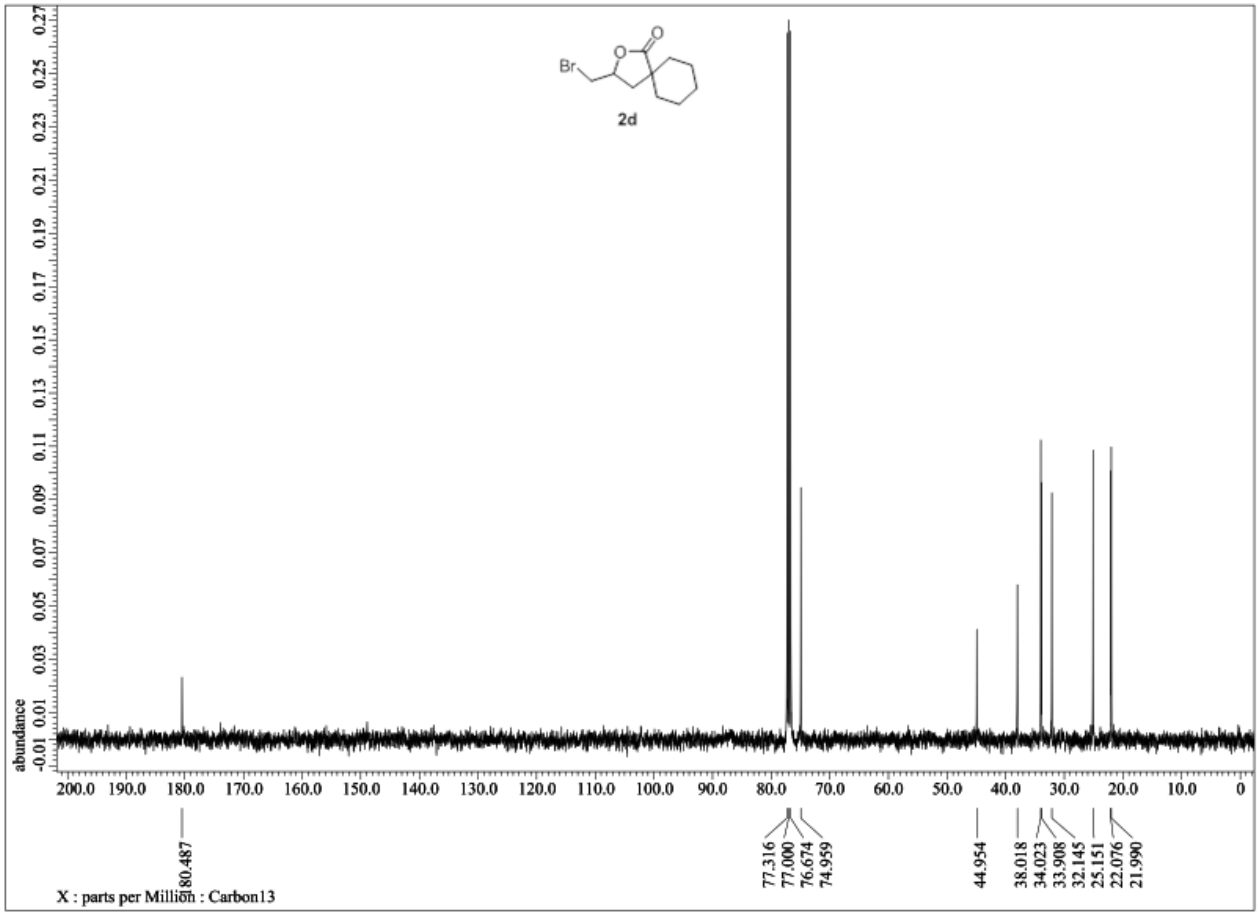

Br
O
O
Me
trans-2b
abundance
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
1.00
2.05
1.00
1.02
1.07
3.11
7.272
4.781
4.771
4.766
4.760
4.755
4.750
4.745
4.739
4.734
4.723
3.554
3.538
3.526
3.523
3.507
3.495
3.480
2.847
2.844
2.825
2.823
2.414
2.404
2.135
2.114
2.093
2.080
1.323
1.304
-0.000
X : parts per Million : Proton

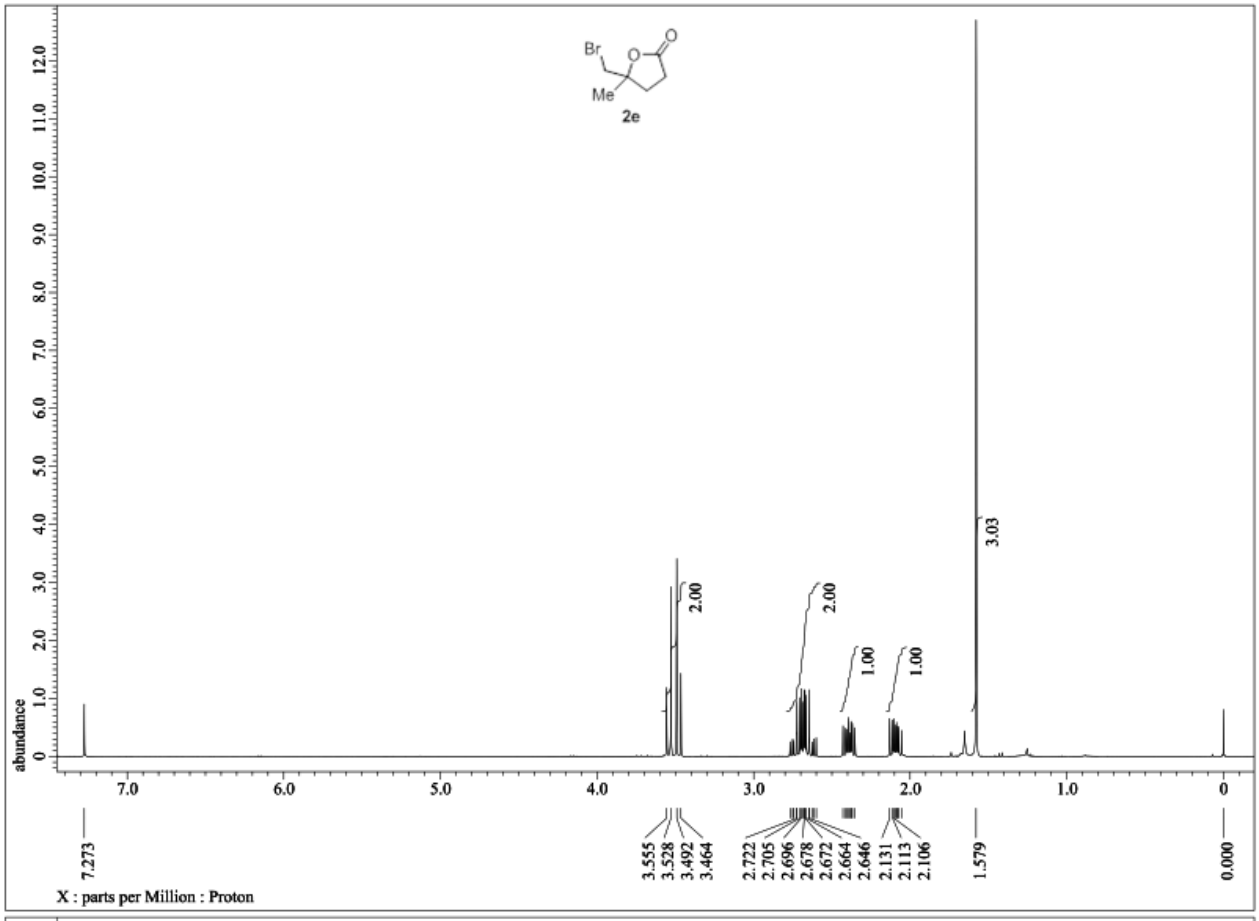

Br
O
O
Me
trans-2b
abundance
0.3
0.2
0.1
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
179.127
77.324
77.000
76.676
75.712
33.853
33.795
16.132
X : parts per Million : Carbon13

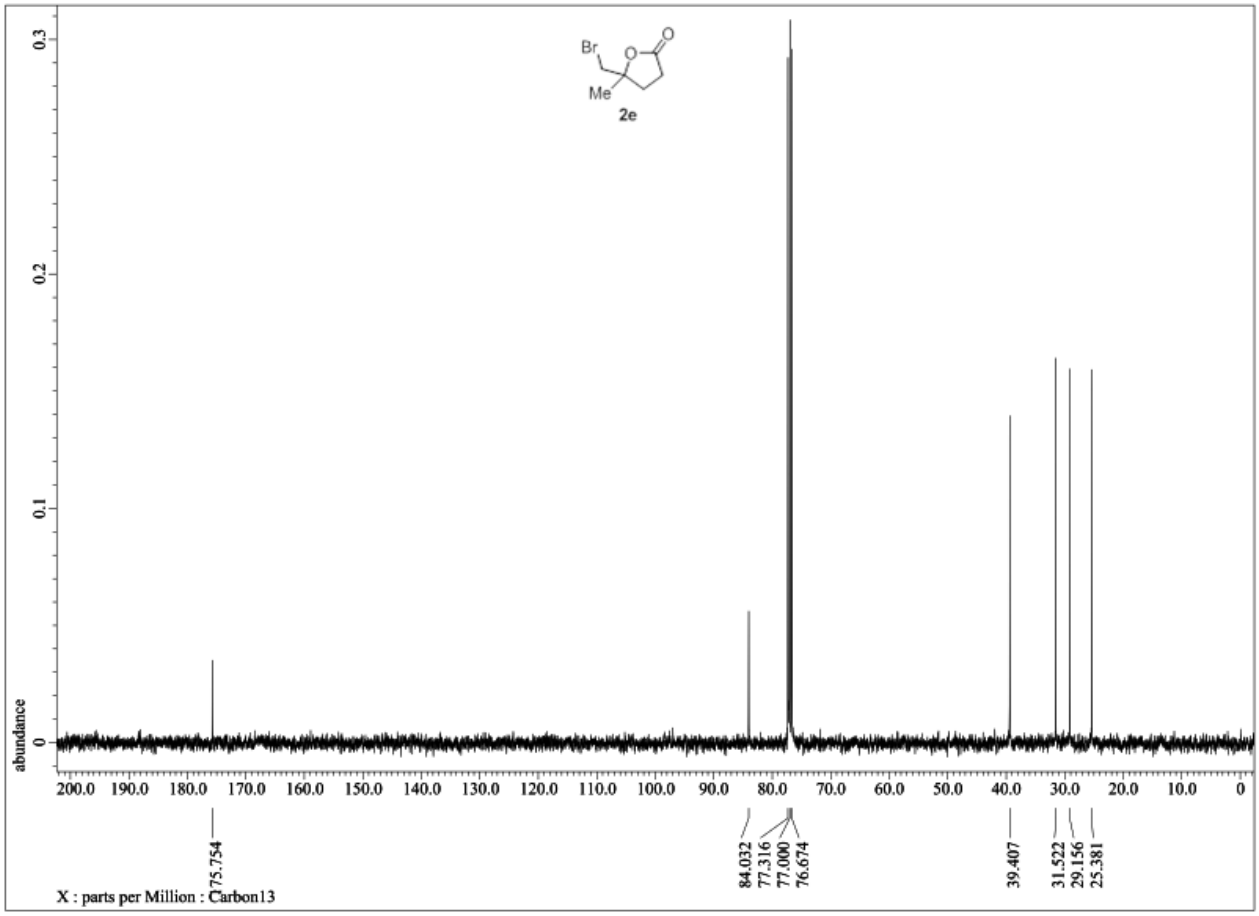

Br
O
O
2c
abundance
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
1.00
1.02
1.02
1.01
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.268
4.657
4.653
4.645
4.641
4.637
4.633
4.629
4.625
4.617
4.613
4.601
3.601
3.589
3.575
3.563
3.504
3.488
3.477
3.461
2.309
2.293
2.276
2.260
1.968
1.944
1.935
1.911
1.317
1.294
-0.000
X : parts per Million : Proton

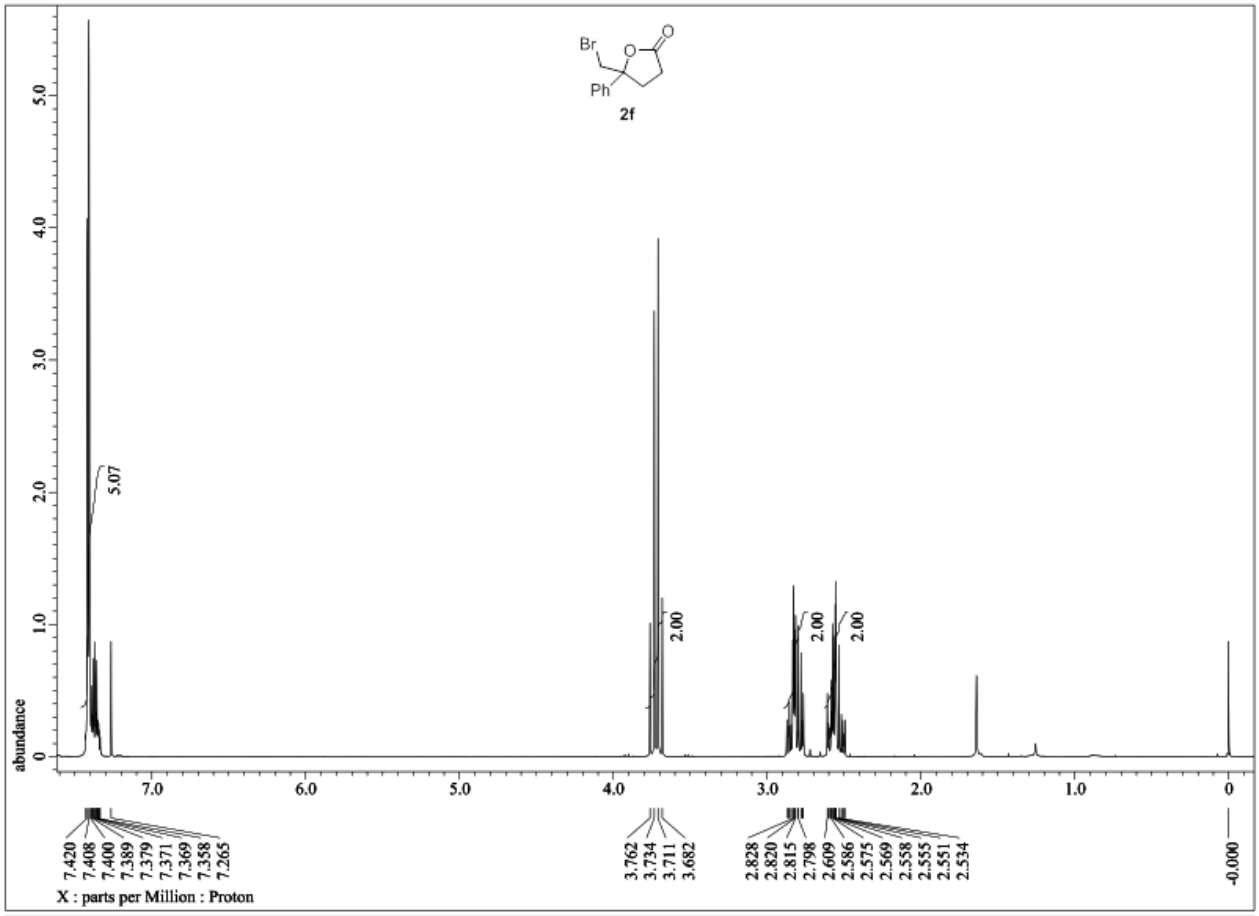

Br
O
O
2c
abundance
0.25
0.23
0.21
0.19
0.17
0.15
0.13
0.11
0.09
0.07
0.05
0.03
0.01
-0.01
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
180.860
77.316
77.000
76.674
74.624
41.917
40.528
33.525
24.893
24.864
X : parts per Million : Carbon13

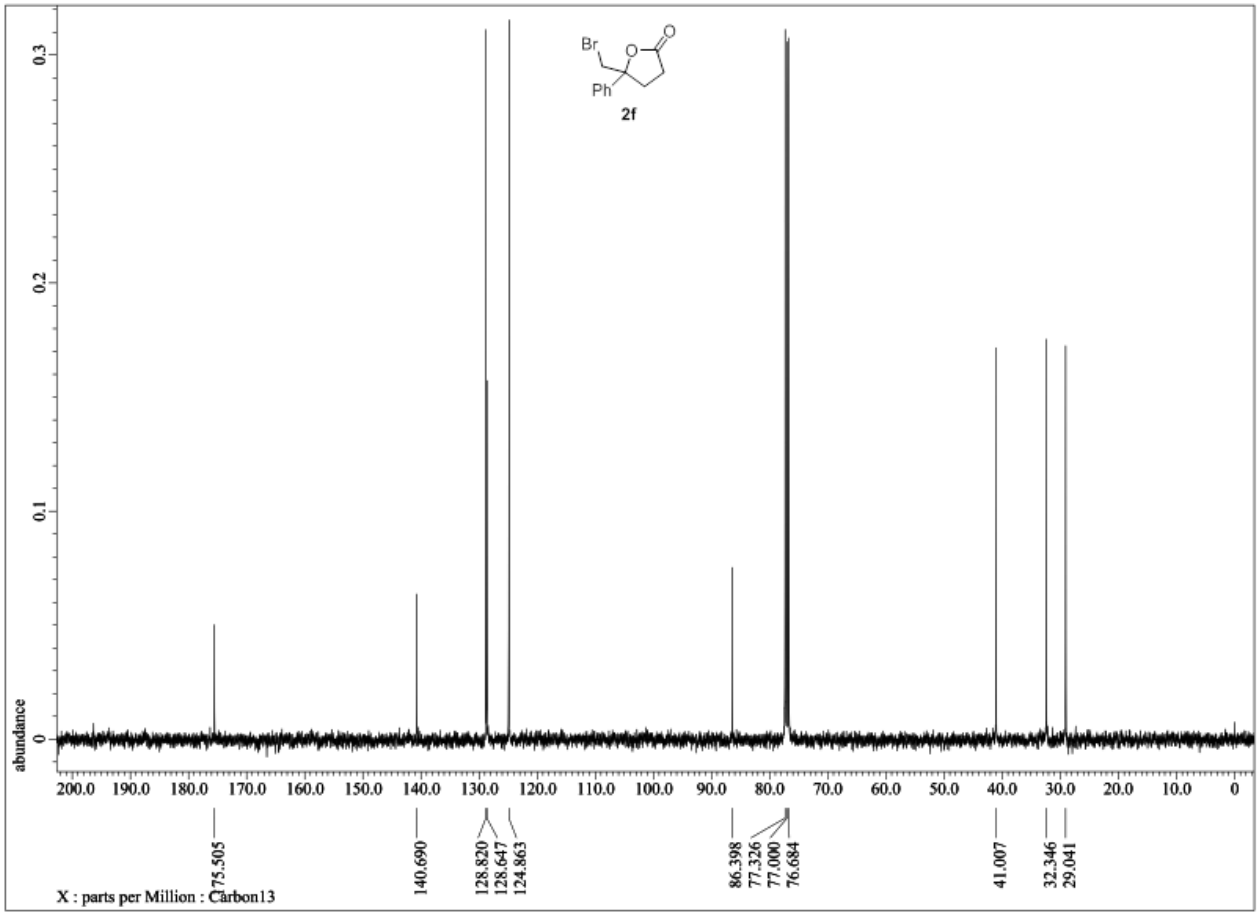

Br
O
O
2d
8.17
3.00
1.00
1.02
1.02
1.00
abundance
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.270
4.640
4.635
4.629
4.623
4.618
4.617
4.613
4.607
4.601
4.596
4.584
3.598
3.587
3.571
3.560
3.510
3.494
3.484
3.467
2.490
2.473
2.457
2.440
1.863
1.840
1.830
1.808
1.798
1.641
1.631
1.626
1.616
1.606
1.389
1.369
-0.000
X : parts per Million : Proton

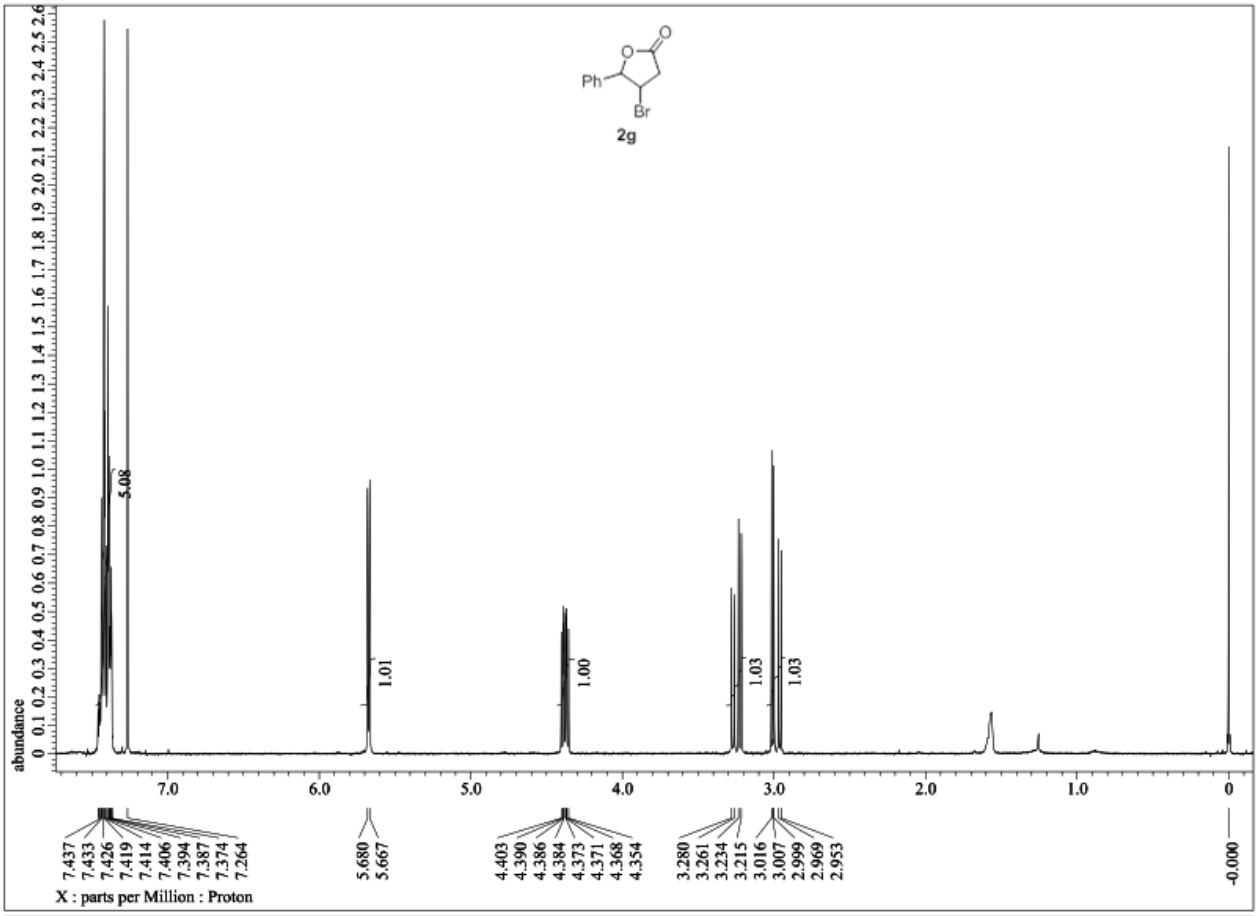

Br
O
O
2d
abundance
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
180.487
77.316
77.000
76.674
74.959
44.954
38.018
34.023
33.908
32.145
25.151
22.076
21.990
X : parts per Million : Carbon13

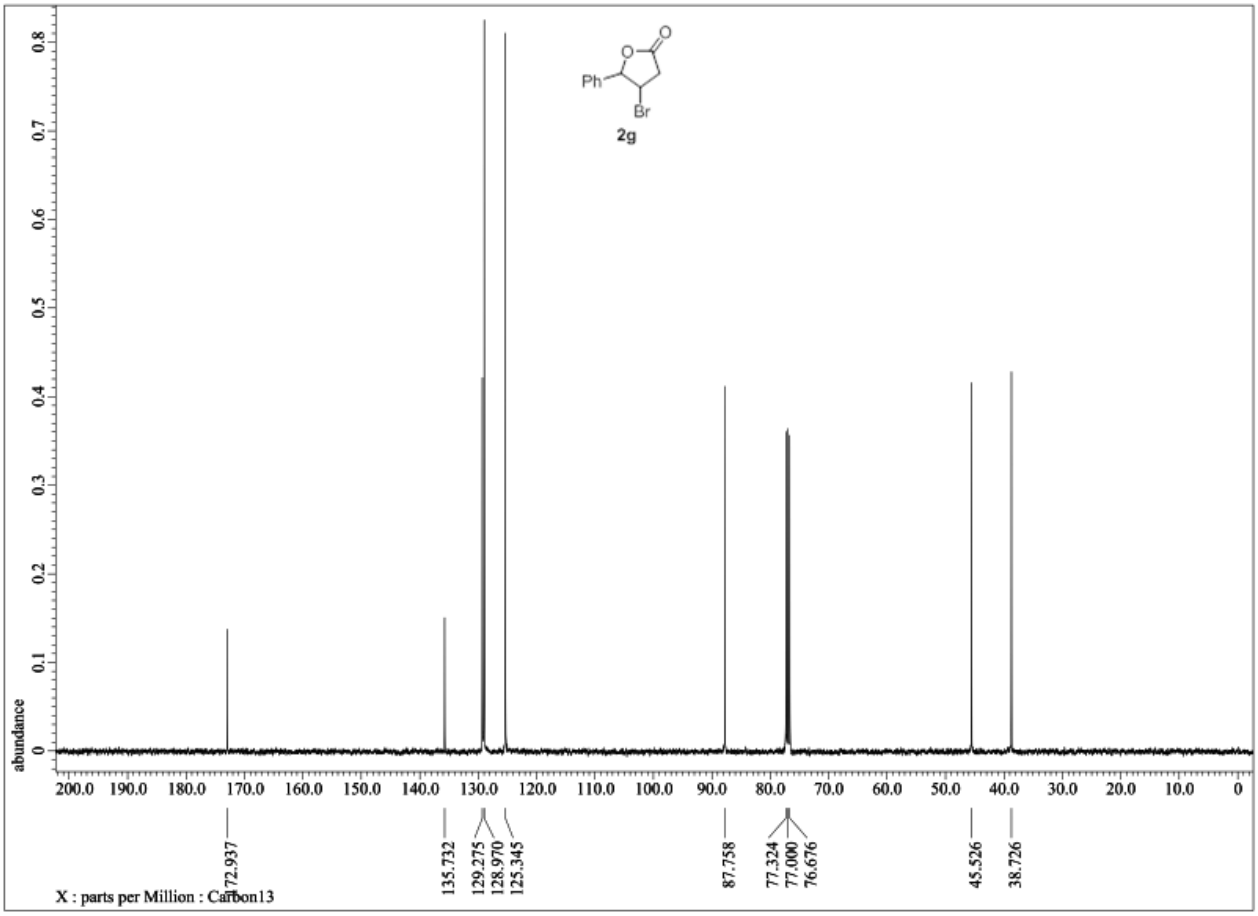

Br
O
O
Me
2e
abundance
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
2.00
2.00
1.00
1.00
3.03
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.273
3.555
3.528
3.492
3.464
2.722
2.705
2.696
2.678
2.672
2.664
2.646
2.131
2.113
2.106
1.579
0.000
X : parts per Million : Proton

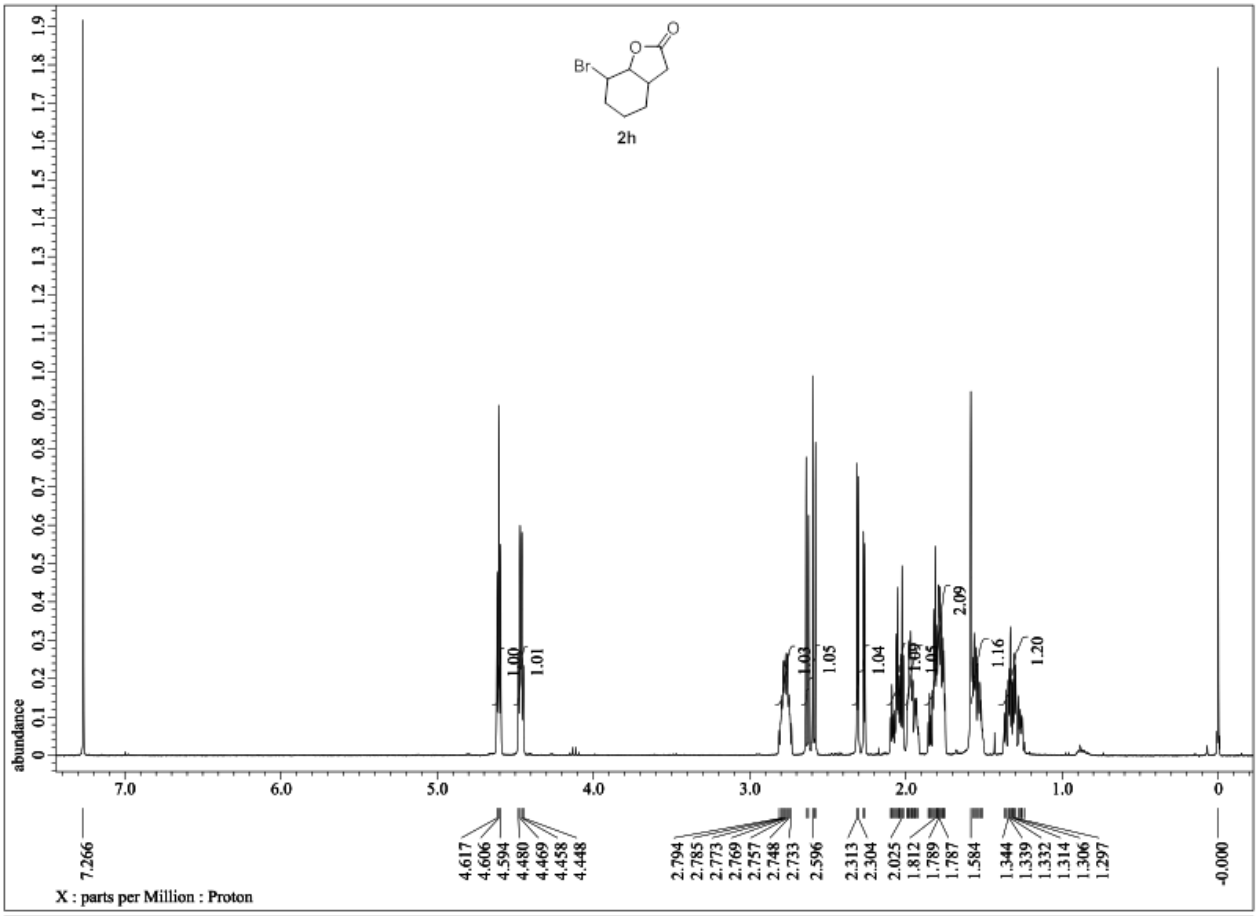

Br
O
O
Me
2e
abundance
0.3
0.2
0.1
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
75.754
84.032
77.316
77.000
76.674
39.407
31.522
29.156
25.381
X : parts per Million : Carbon13

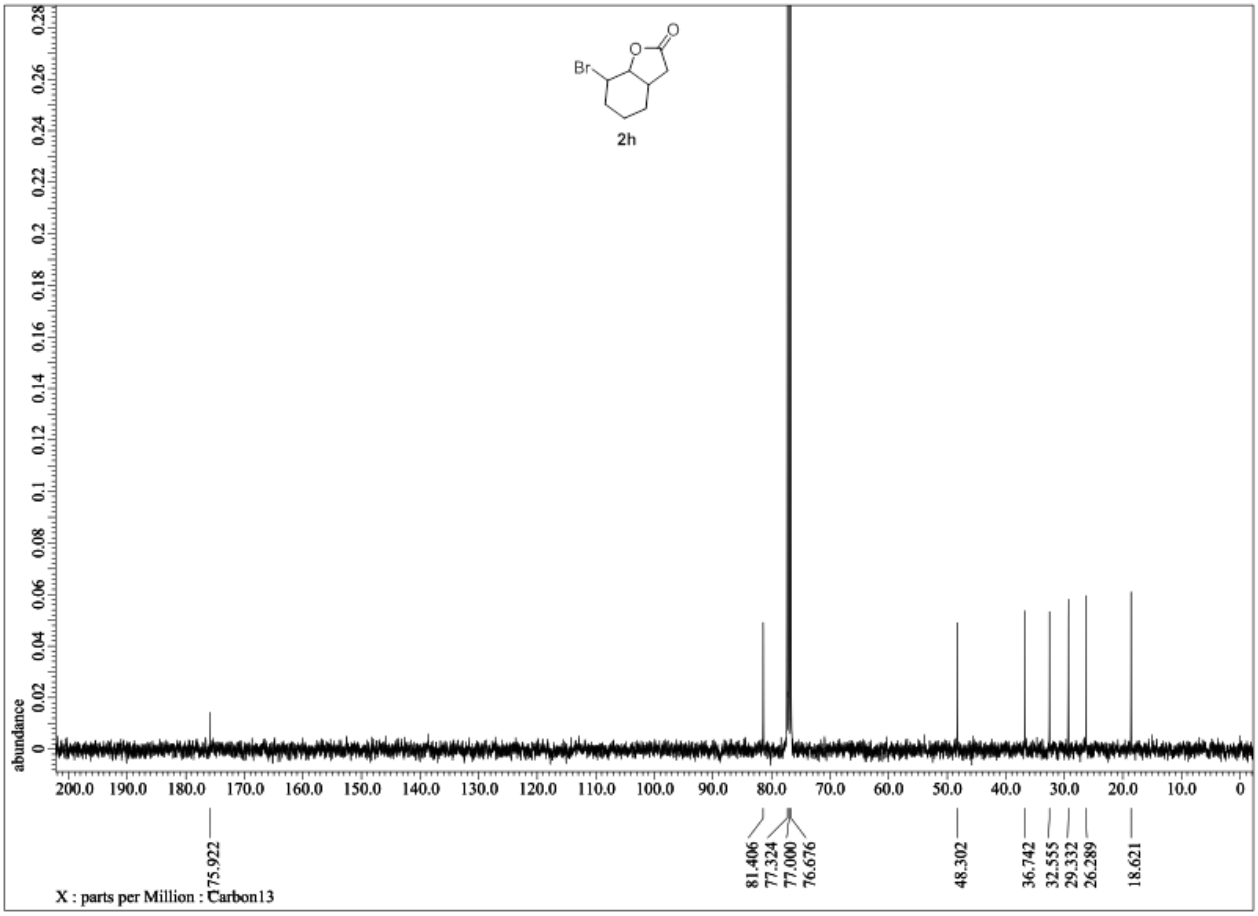

Br
O
O
Ph
2f
abundance
5.07
2.00
2.00
2.00
7.420
7.408
7.400
7.389
7.379
7.371
7.369
7.358
7.265
3.762
3.734
3.711
3.682
2.828
2.820
2.815
2.798
2.609
2.586
2.575
2.569
2.558
2.555
2.551
2.534
-0.000
X : parts per Million : Proton

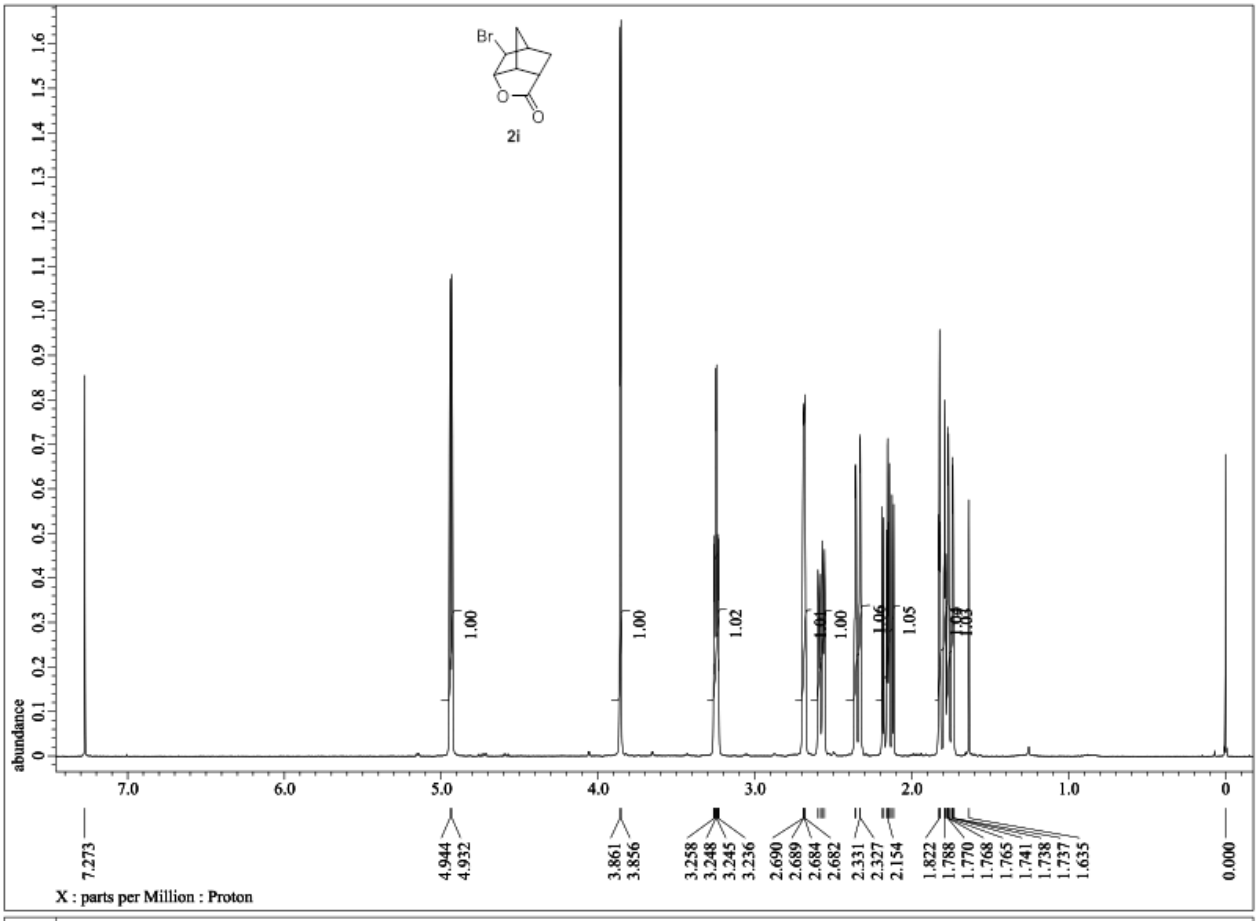

Br
O
O
Ph
2f
abundance
75.505
140.690
128.820
128.647
124.863
86.398
77.326
77.000
76.684
41.007
32.346
29.041
X : parts per Million : Carbon13

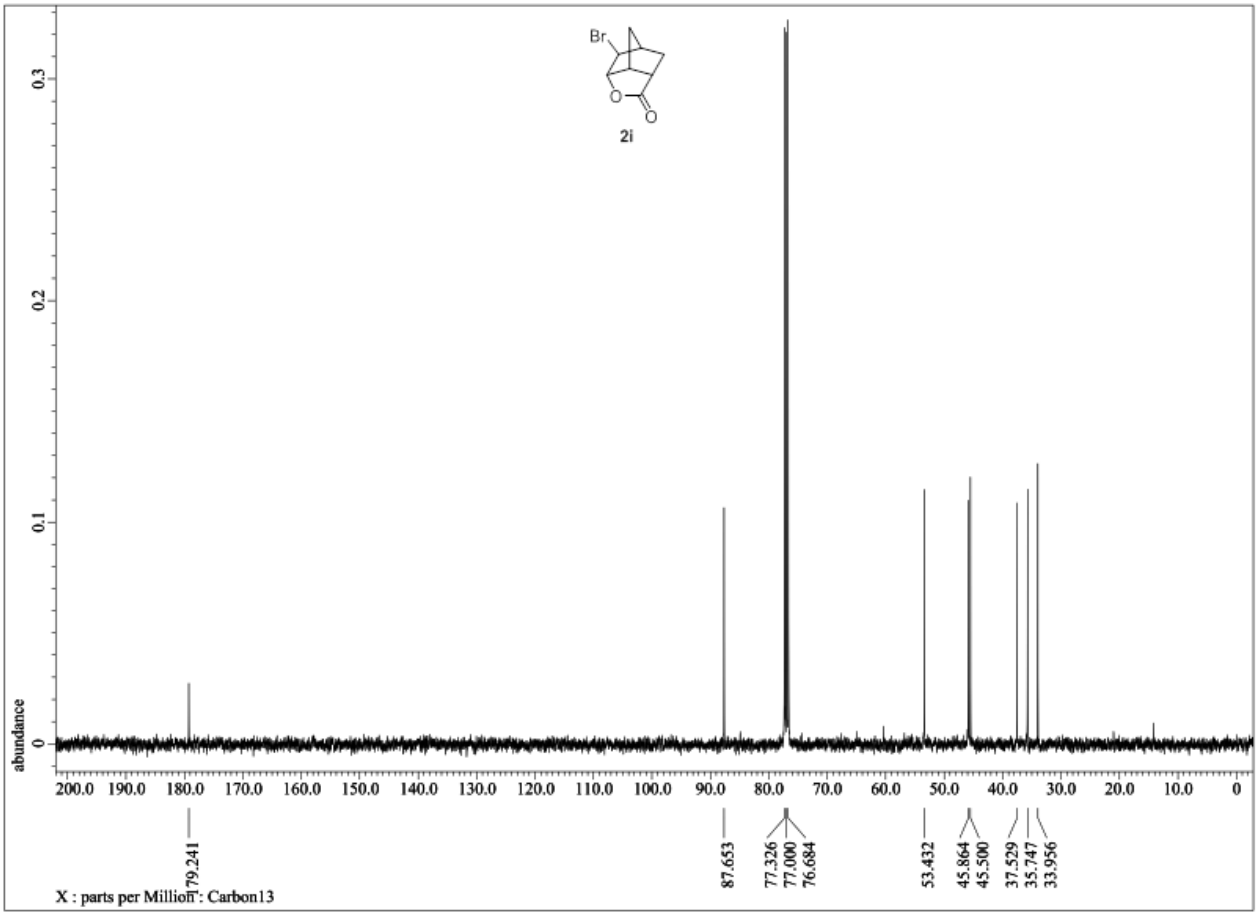

Ph
O
O
Br
2g
abundance
5.08
1.01
1.00
1.03
1.03
7.437
7.433
7.426
7.419
7.414
7.406
7.394
7.387
7.374
7.264
5.680
5.667
4.403
4.390
4.386
4.384
4.373
4.371
4.368
4.354
3.280
3.261
3.234
3.215
3.016
3.007
2.999
2.969
2.953
-0.000
X : parts per Million : Proton

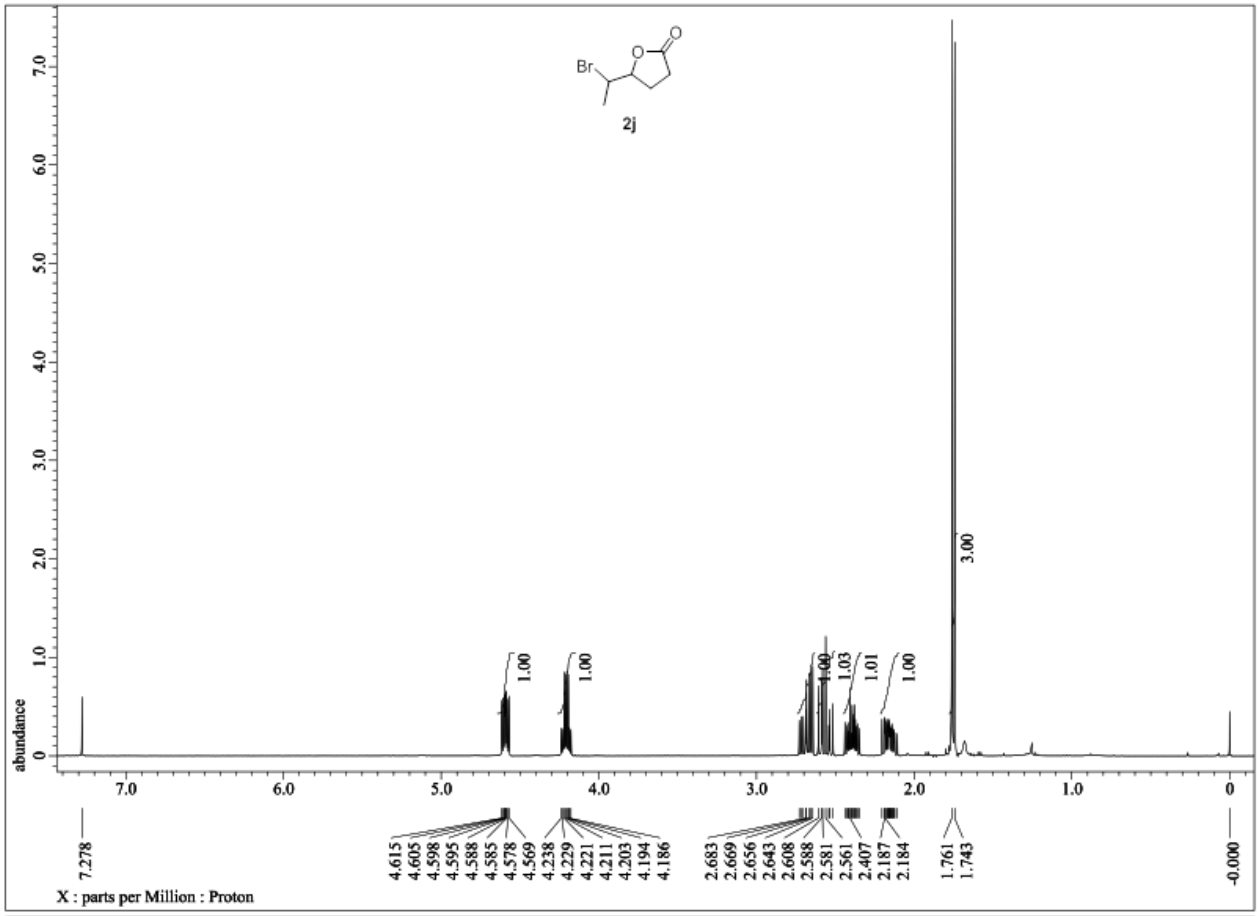

Ph
O
O
Br
2g
abundance
172.937
135.732
129.275
128.970
125.345
87.758
77.324
77.000
76.676
45.526
38.726
X : parts per Million : Carbon13

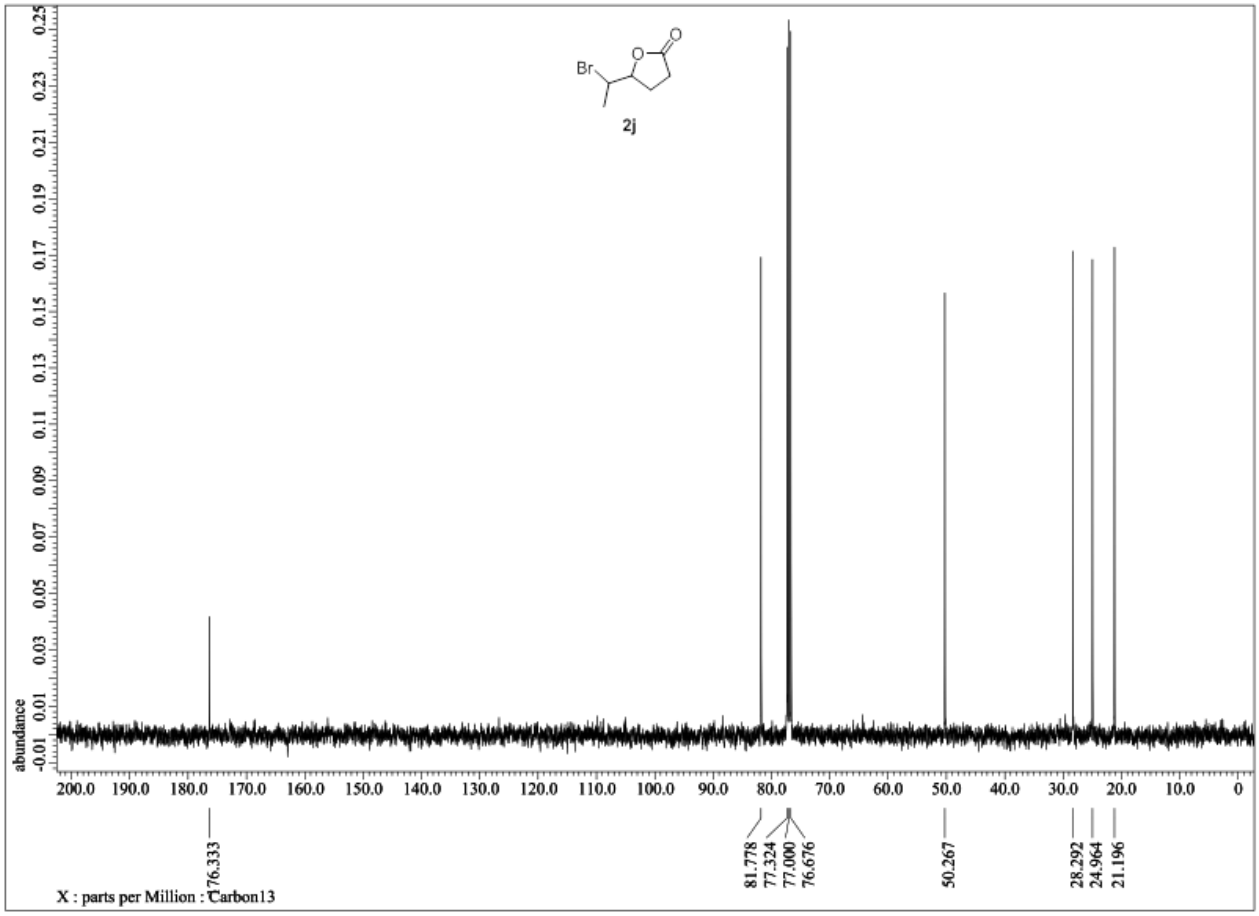

Br
O
O
2h
abundance
1.00
1.01
1.03
1.05
1.04
1.09
1.05
2.09
1.16
1.20
7.266
4.617
4.606
4.594
4.480
4.469
4.458
4.448
2.794
2.785
2.773
2.769
2.757
2.748
2.733
2.596
2.313
2.304
2.025
1.812
1.789
1.787
1.584
1.344
1.339
1.332
1.314
1.306
1.297
-0.000
X : parts per Million : Proton

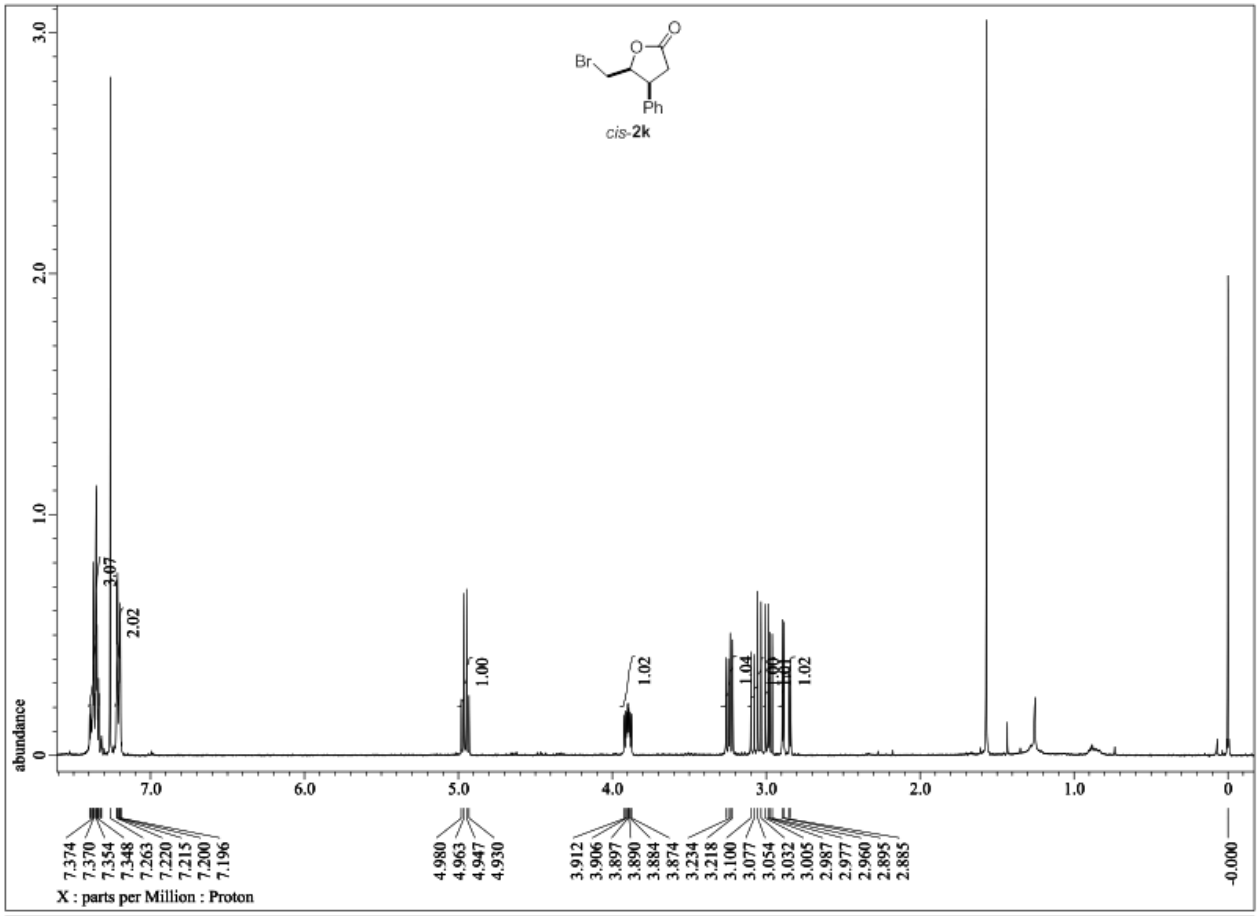

Br
O
O
2h
abundance
75.922
81.406
77.324
77.000
76.676
48.302
36.742
32.555
29.332
26.289
18.621
X : parts per Million : Carbon13

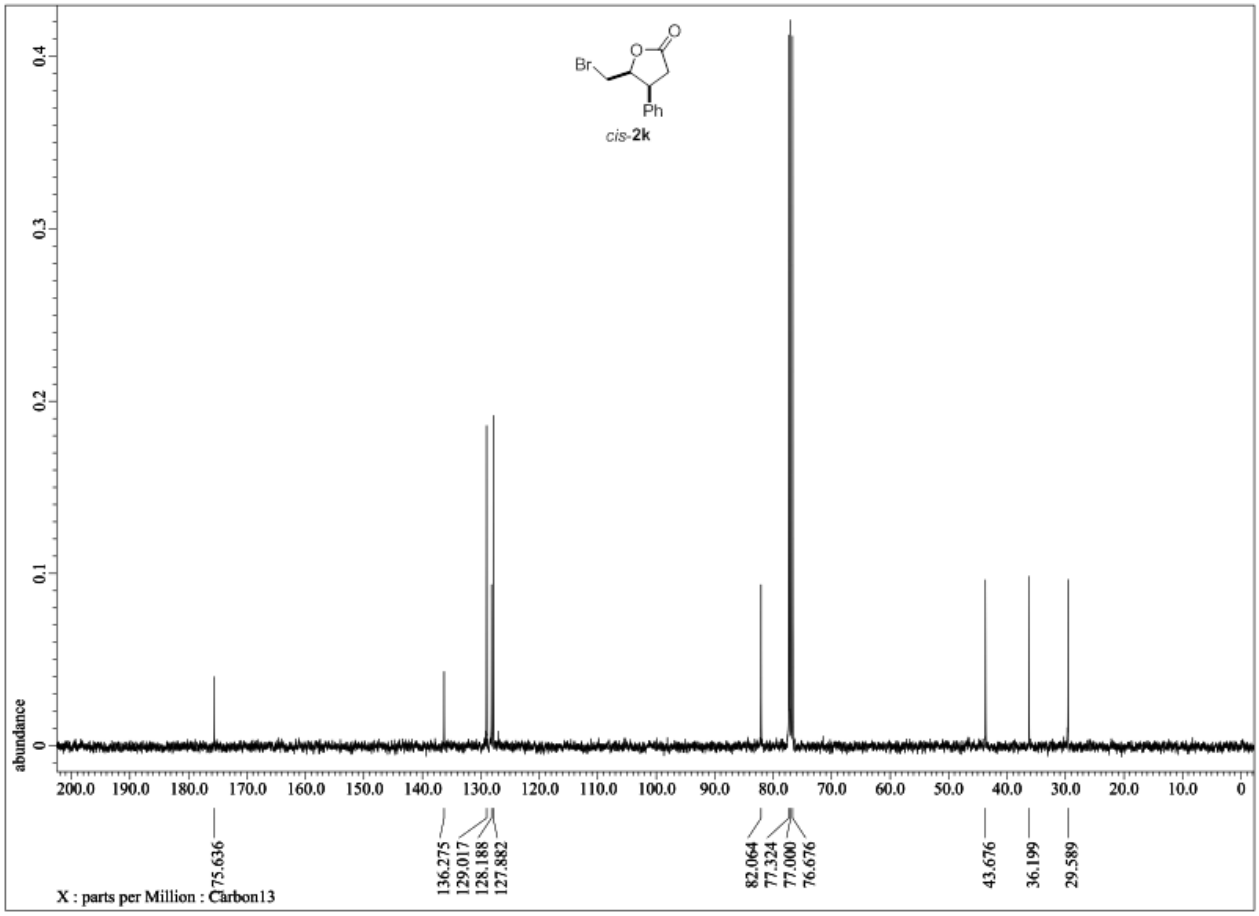

Br
O
O
2i
abundance
1.00
1.00
1.02
1.00
1.06
1.05
7.273
4.944
4.932
3.861
3.856
3.258
3.248
3.245
3.236
2.690
2.689
2.684
2.682
2.331
2.327
2.154
1.822
1.788
1.770
1.768
1.765
1.741
1.738
1.737
1.635
0.000
X : parts per Million : Proton

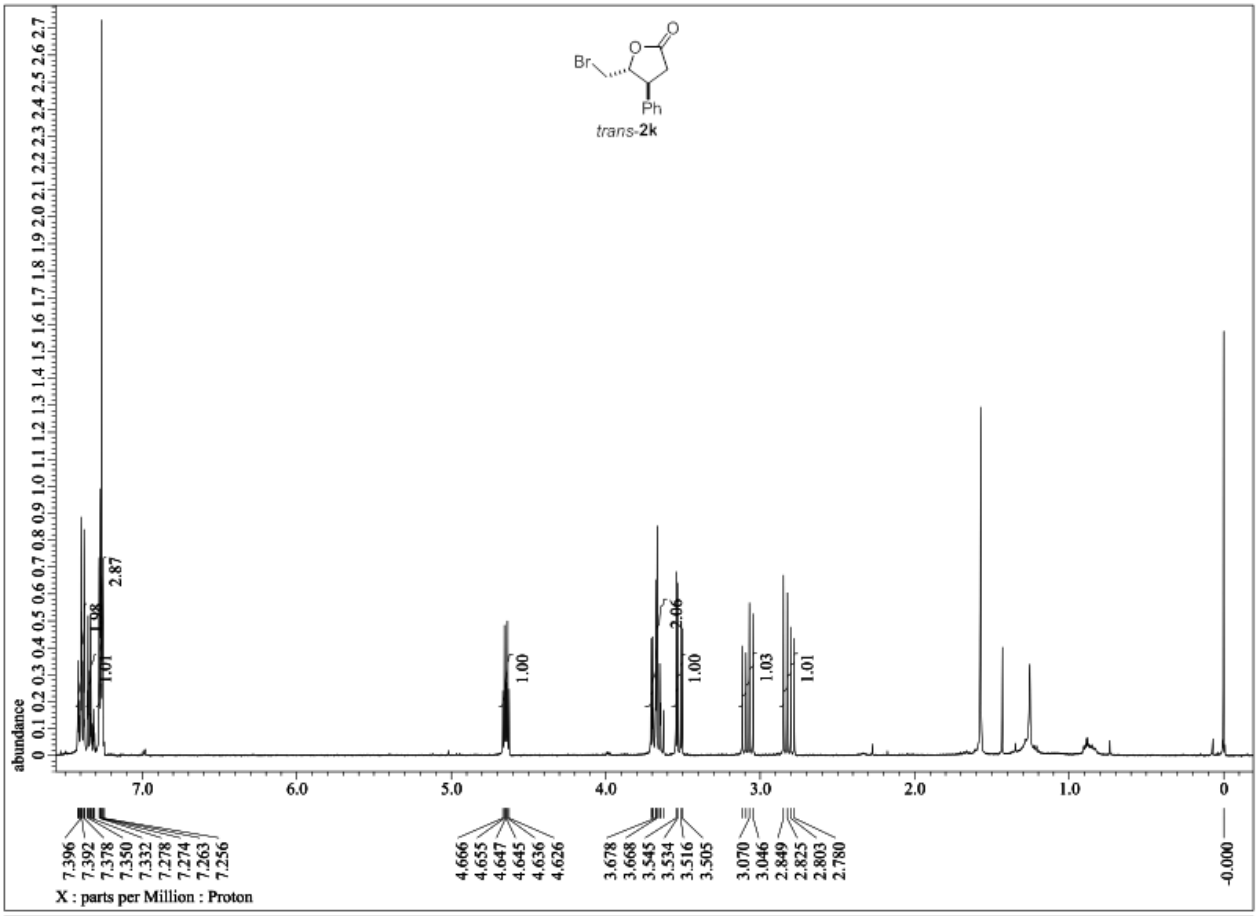

Br
O
O
2i
abundance
79.241
87.653
77.326
77.000
76.684
53.432
45.864
45.500
37.529
35.747
33.956
X : parts per Million : Carbon13

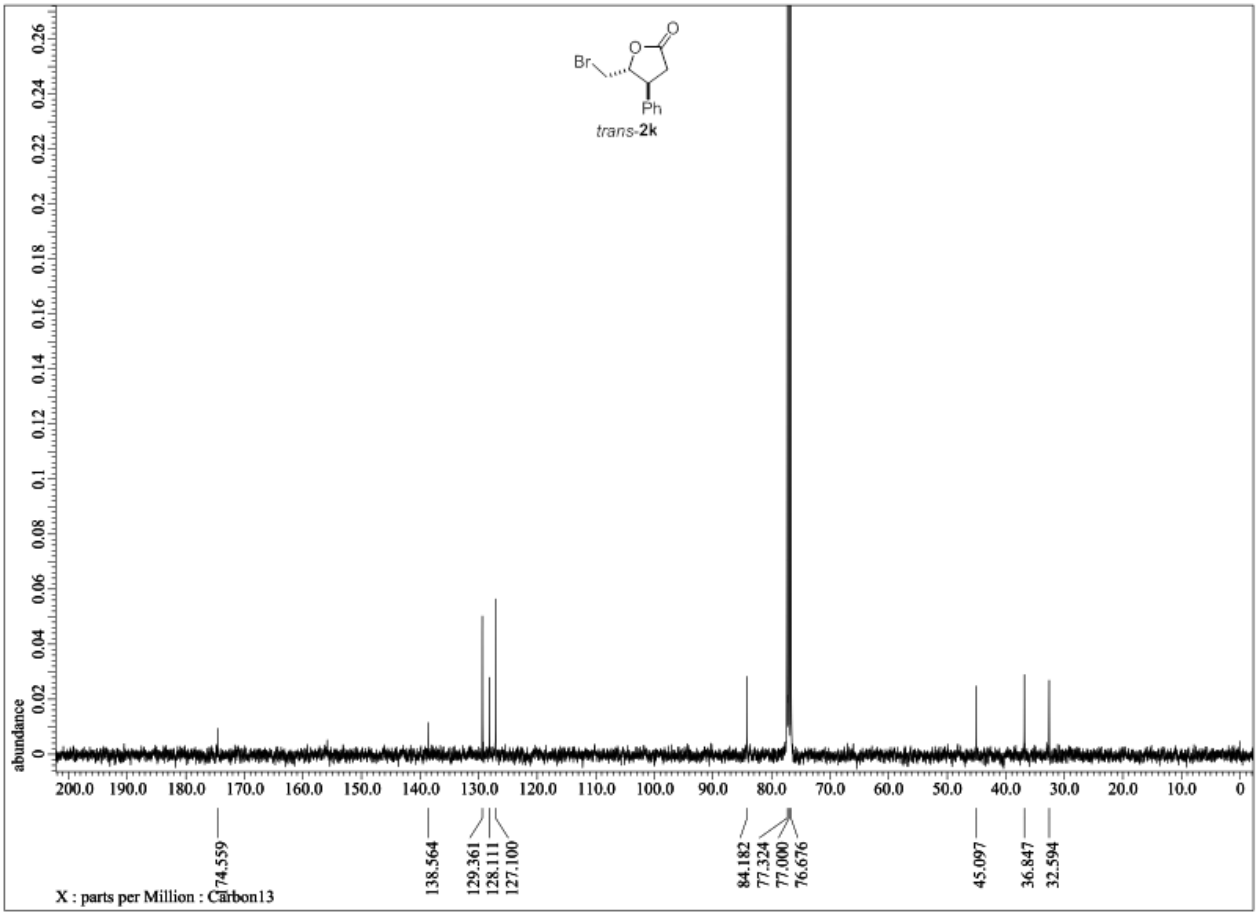

Br
O
O
2j
abundance
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
1.00
1.00
1.00
1.03
1.01
1.00
3.00
7.278
4.615
4.605
4.598
4.595
4.588
4.585
4.578
4.569
4.238
4.229
4.221
4.211
4.203
4.194
4.186
2.683
2.669
2.656
2.643
2.608
2.588
2.581
2.561
2.407
2.187
2.184
1.761
1.743
-0.000
X : parts per Million : Proton

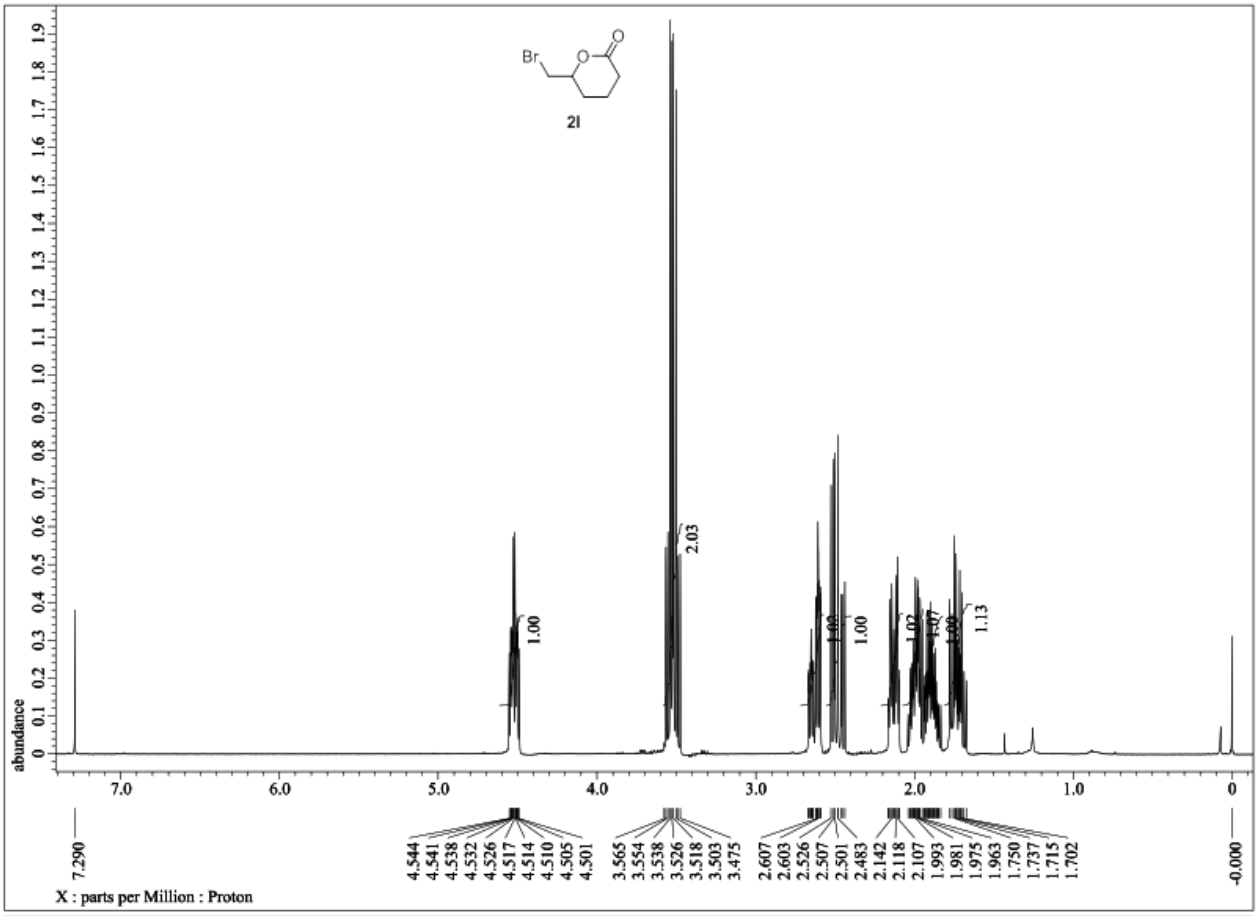

Br
O
O
2j
abundance
0.25
0.23
0.21
0.19
0.17
0.15
0.13
0.11
0.09
0.07
0.05
0.03
0.01
-0.01
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
176.333
81.778
77.324
77.000
76.676
50.267
28.292
24.964
21.196
X : parts per Million : Carbon13

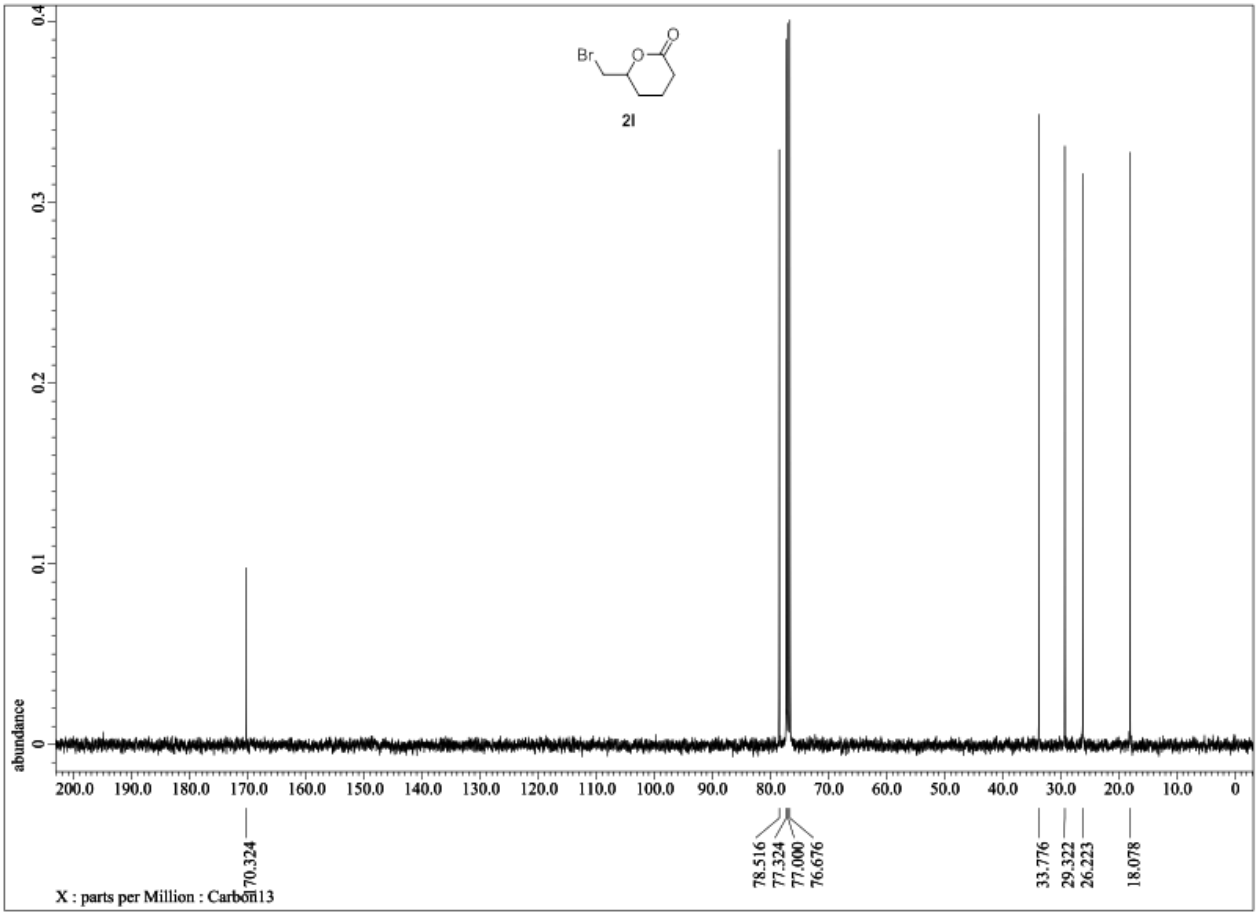

Br
O
O
Ph
cis-2k
abundance
3.0
2.0
1.0
0
3.07
2.02
1.00
1.02
1.04
1.02
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.374
7.370
7.354
7.348
7.263
7.220
7.215
7.200
7.196
4.980
4.963
4.947
4.930
3.912
3.906
3.897
3.890
3.884
3.874
3.234
3.218
3.100
3.077
3.054
3.032
3.005
2.987
2.977
2.960
2.895
2.885
-0.000
X : parts per Million : Proton

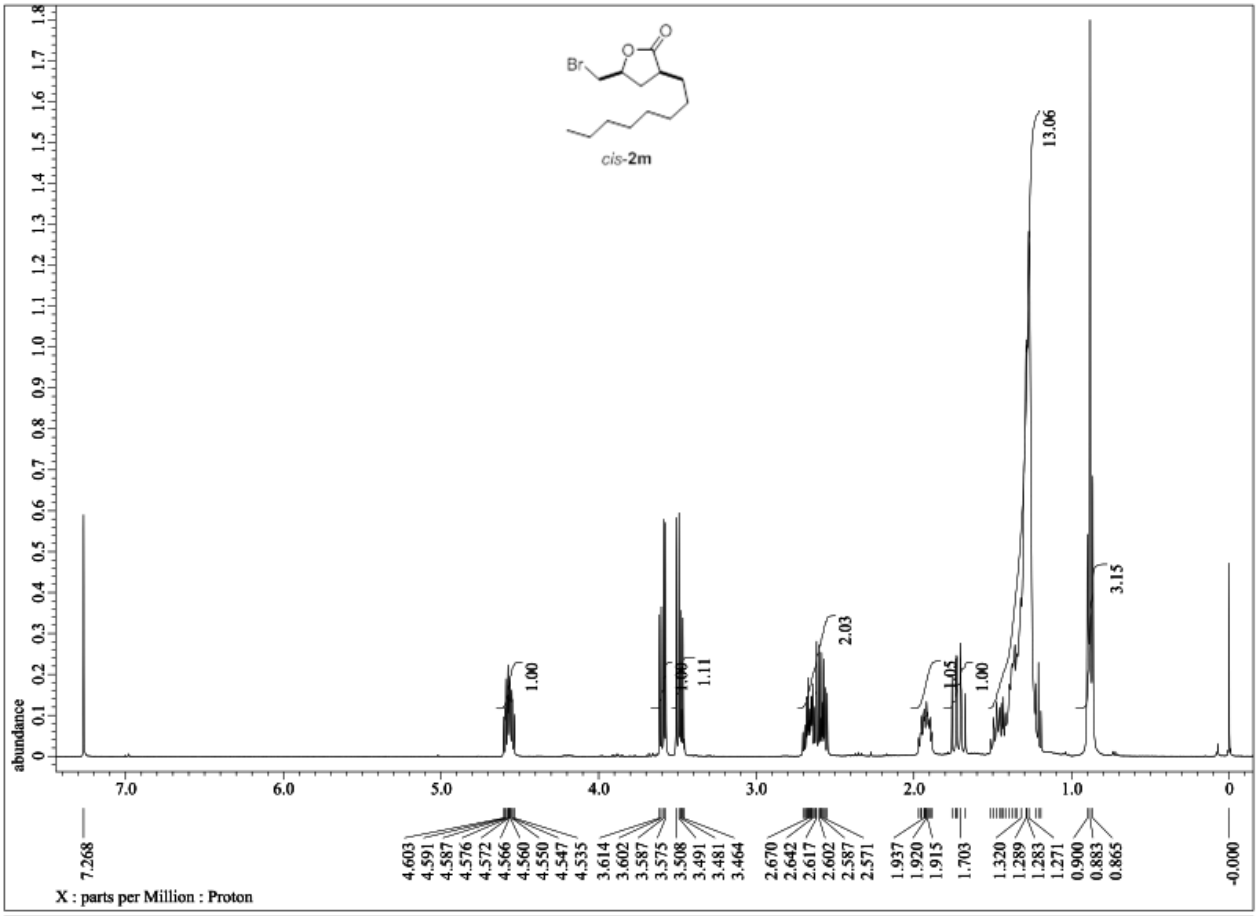

Br
O
O
Ph
cis-2k
abundance
0.4
0.3
0.2
0.1
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
175.636
136.275
129.017
128.188
127.882
82.064
77.324
77.000
76.676
43.676
36.199
29.589
X : parts per Million : Carbon13

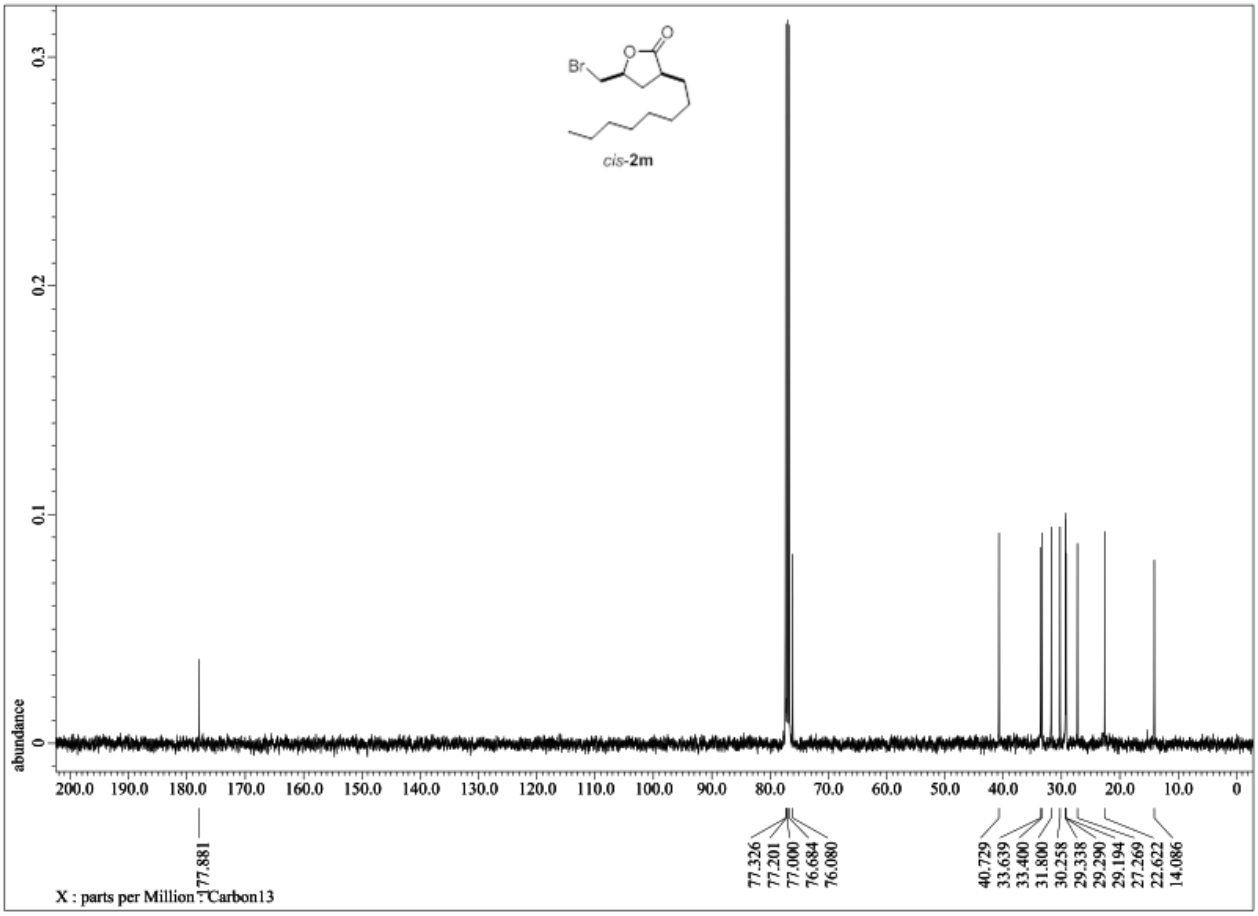

Br
O
O
Ph
trans-2k
abundance
X : parts per Million : Proton
7.396
7.392
7.378
7.350
7.332
7.278
7.274
7.263
7.256
4.666
4.655
4.647
4.645
4.636
4.626
3.678
3.668
3.545
3.534
3.516
3.505
3.070
3.046
2.849
2.825
2.803
2.780
-0.000
1.01
1.98
2.87
1.00
2.06
1.00
1.03
1.01

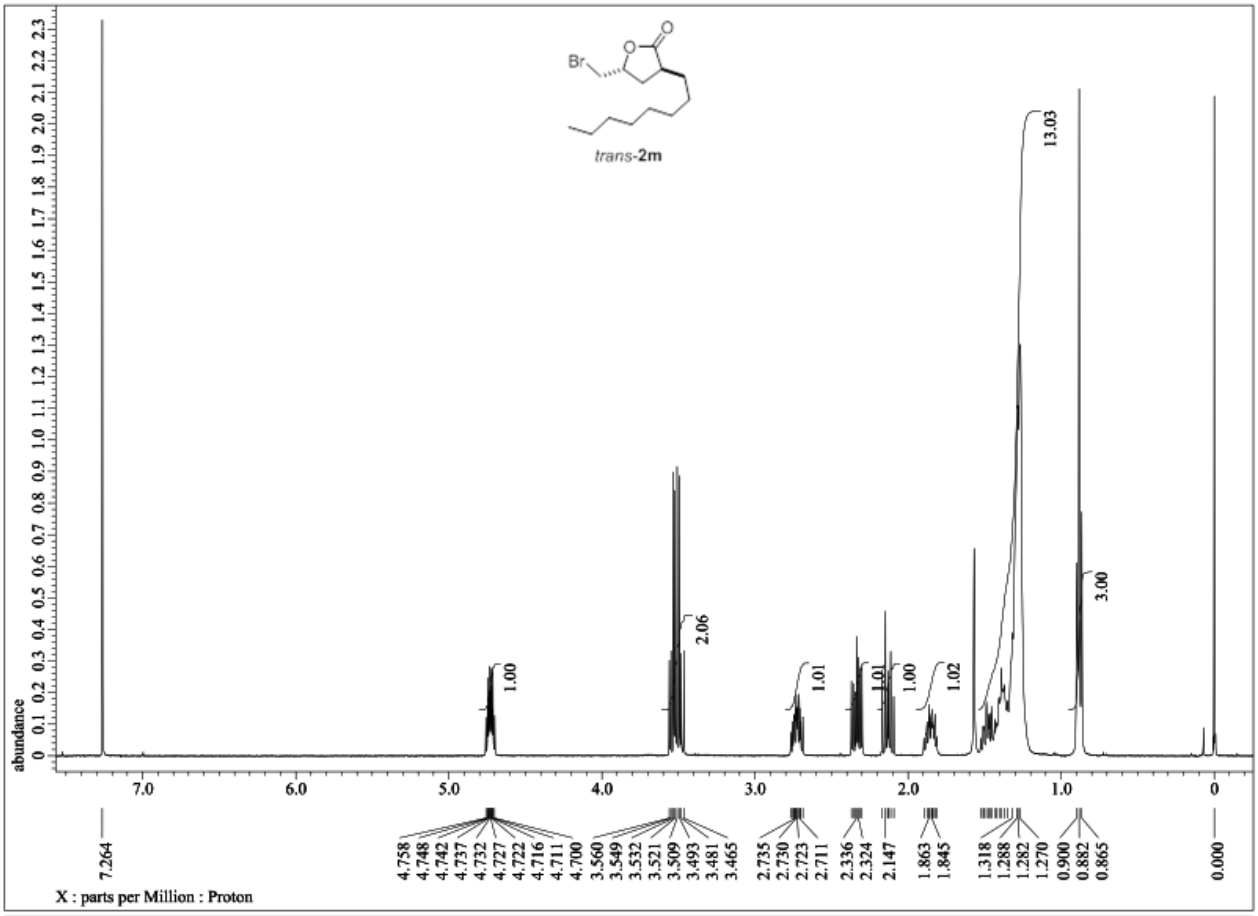

Br
O
O
Ph
trans-2k
abundance
X : parts per Million : Carbon13
174.559
138.564
129.361
128.111
127.100
84.182
77.324
77.000
76.676
45.097
36.847
32.594

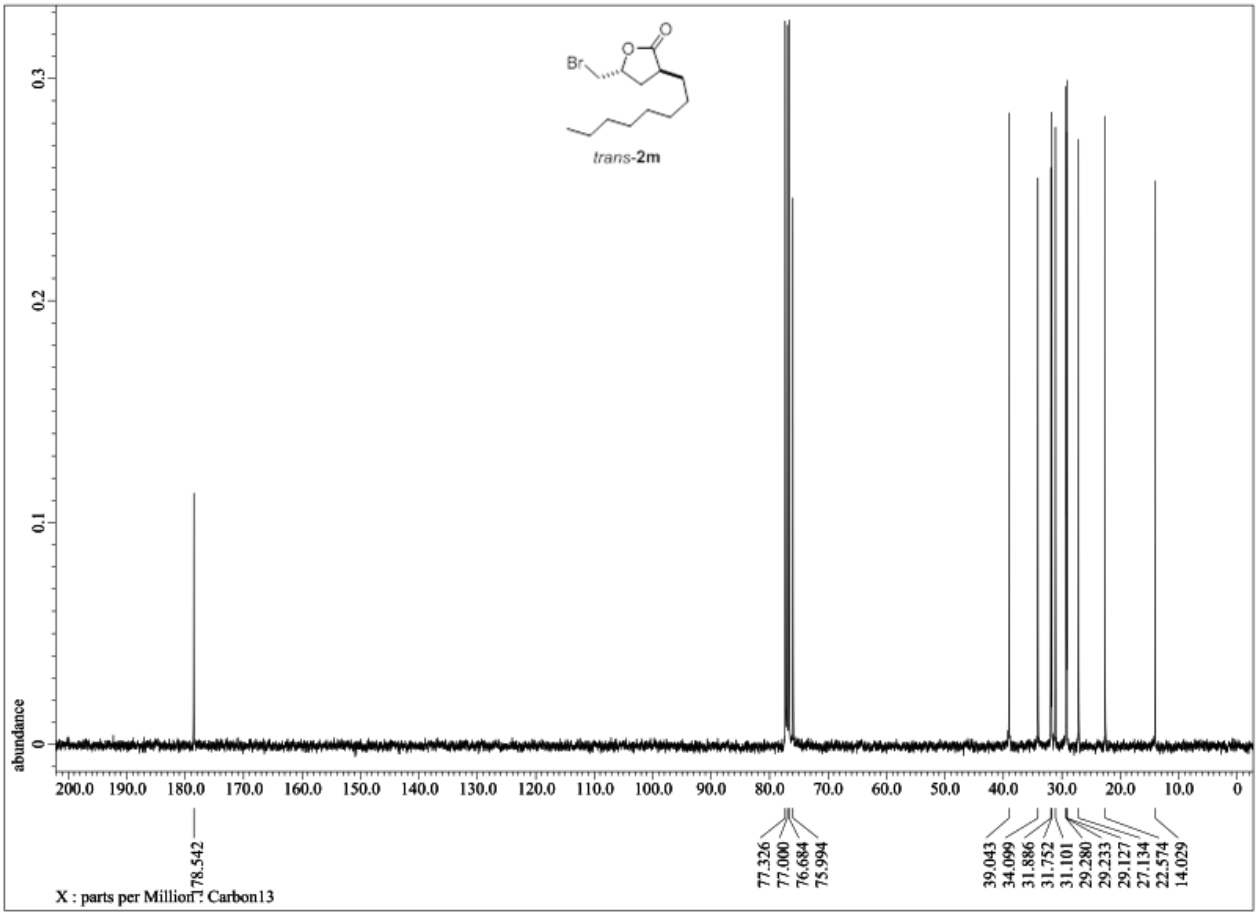

Br
O
O
2l
abundance
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
1.00
2.03
1.00
1.00
1.02
1.07
1.00
1.13
7.290
4.544
4.541
4.538
4.532
4.526
4.517
4.514
4.510
4.505
4.501
3.565
3.554
3.538
3.526
3.518
3.503
3.475
2.607
2.603
2.526
2.507
2.501
2.483
2.142
2.118
2.107
1.993
1.981
1.975
1.963
1.750
1.737
1.715
1.702
-0.000
X : parts per Million : Proton

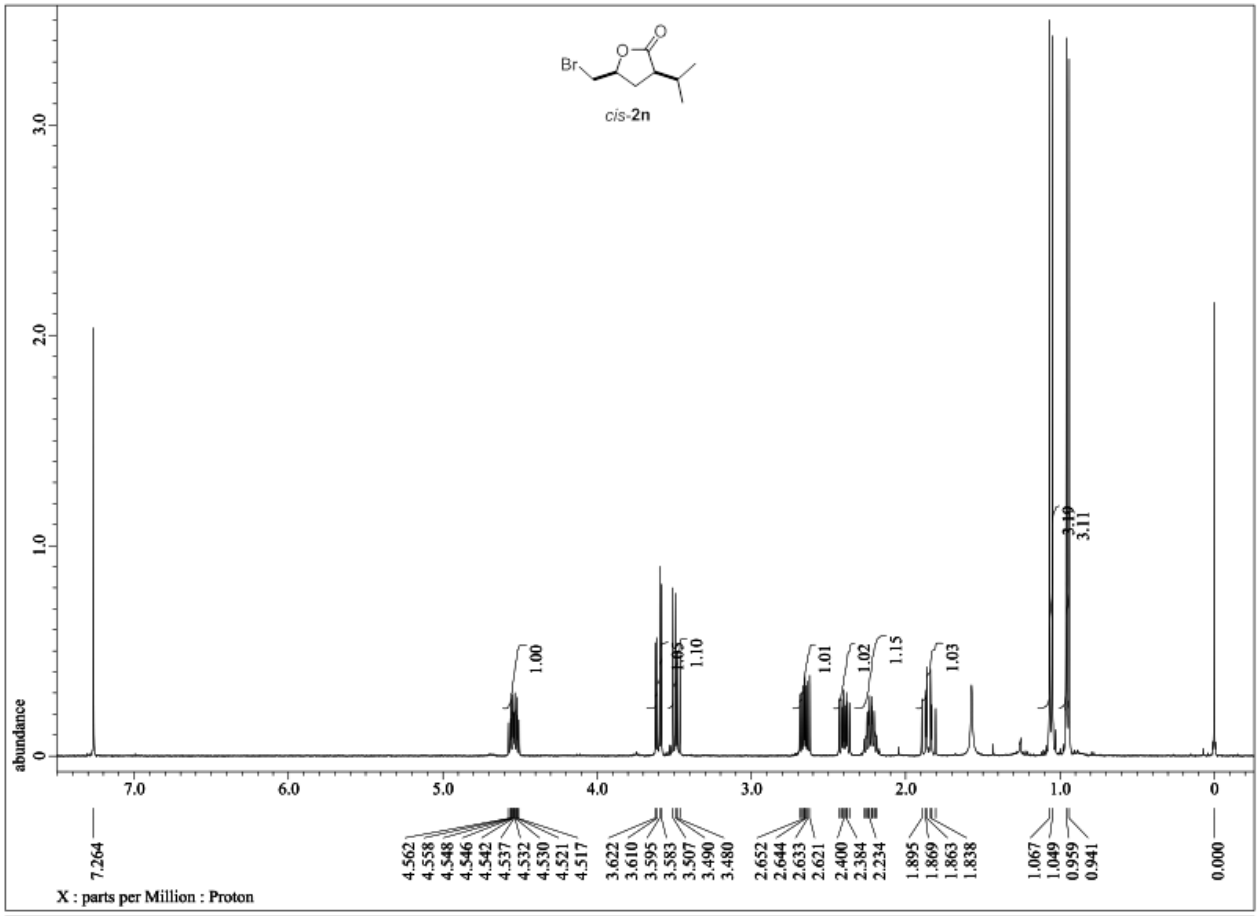

Br
O
O
2l
abundance
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
70.324
78.516
77.324
77.000
76.676
33.776
29.322
26.223
18.078
X : parts per Million : Carbon13

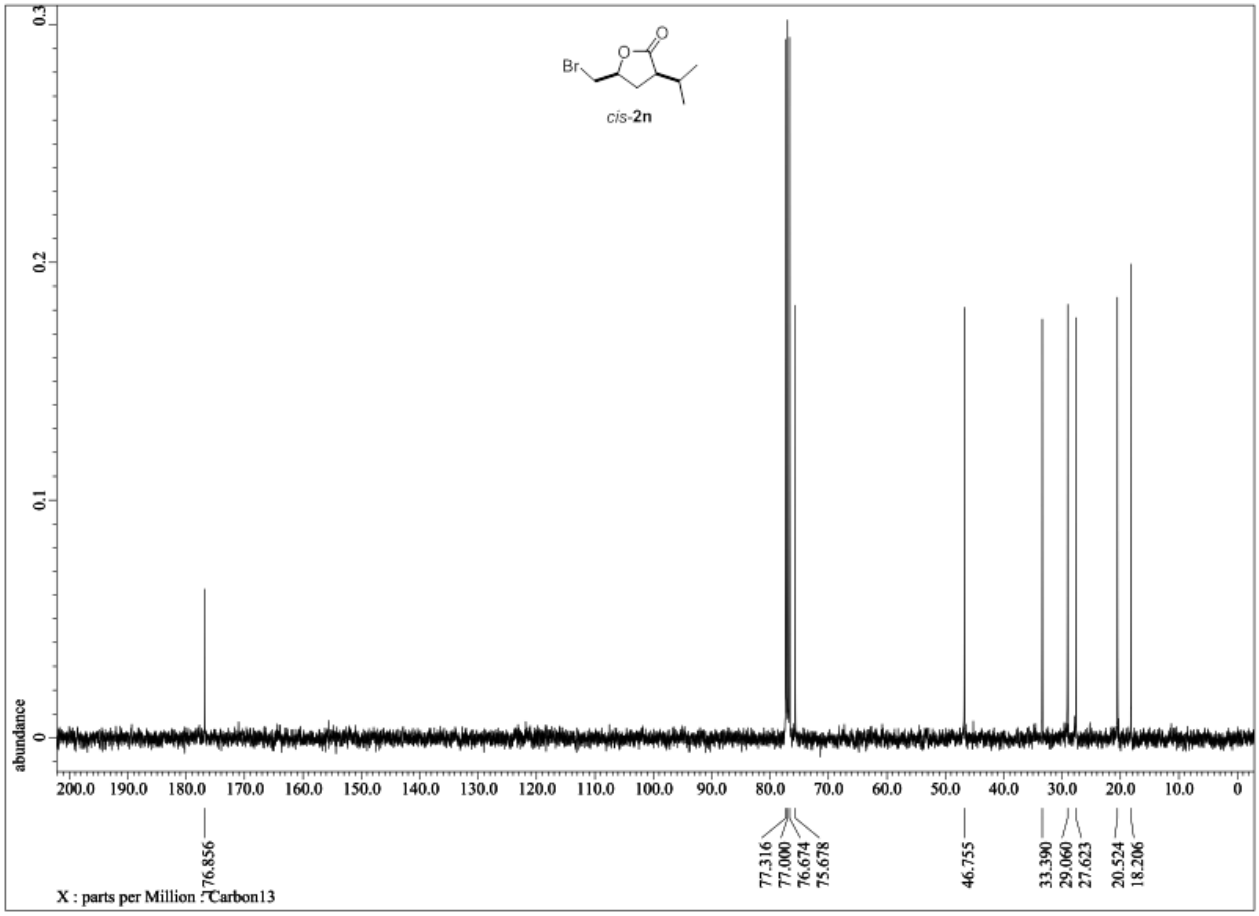

Br
O
O
cis-2m
abundance
X : parts per Million : Proton
7.268
4.603
4.591
4.587
4.576
4.572
4.566
4.560
4.550
4.547
4.535
3.614
3.602
3.587
3.575
3.508
3.491
3.481
3.464
2.670
2.642
2.617
2.602
2.587
2.571
1.937
1.920
1.915
1.703
1.320
1.289
1.283
1.271
0.900
0.883
0.865
-0.000
1.00
1.00
1.11
2.03
1.05
1.00
13.06
3.15

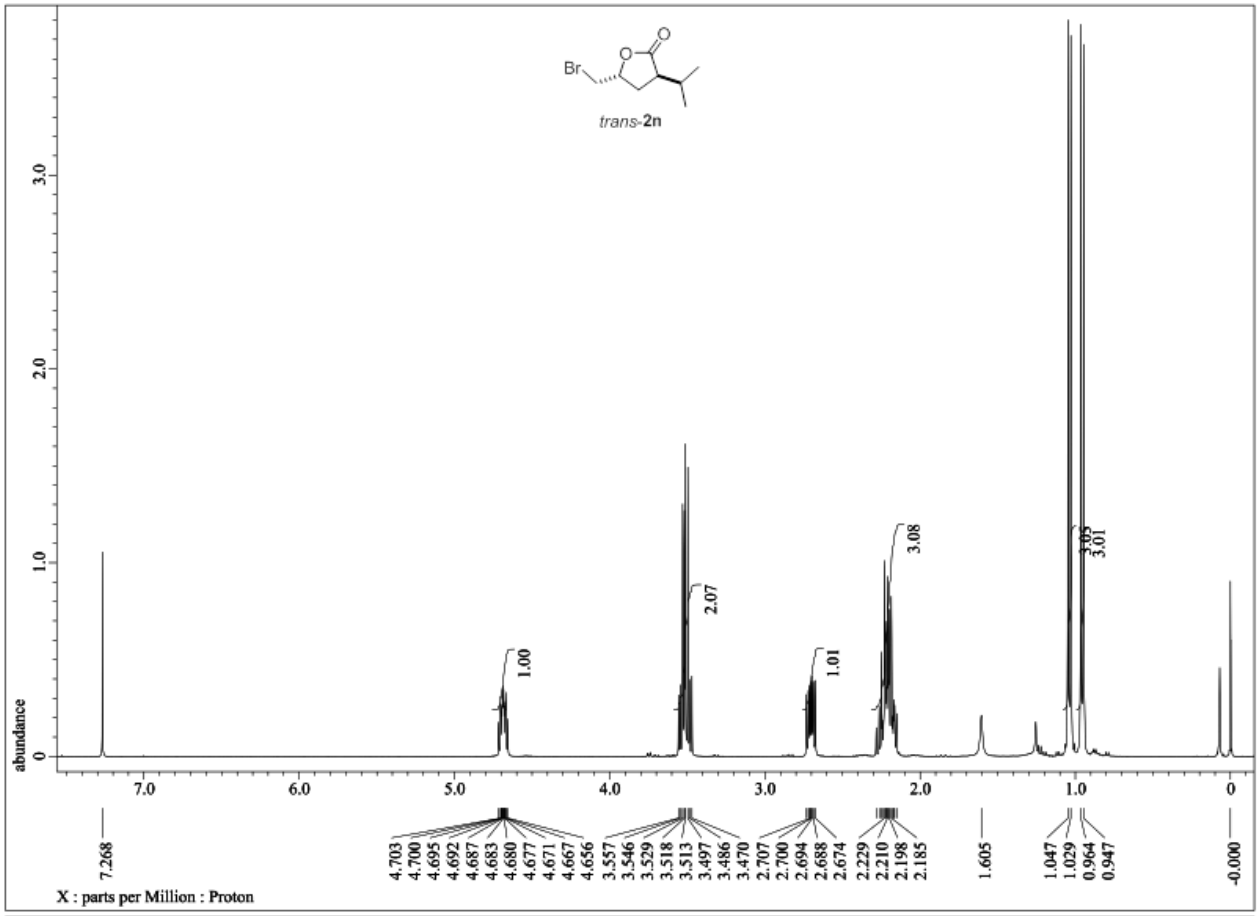

Br
O
O
cis-2m
abundance
X : parts per Million : Carbon13
77.881
77.326
77.201
77.000
76.684
76.080
40.729
33.639
33.400
31.800
30.258
29.338
29.290
29.194
27.269
22.622
14.086

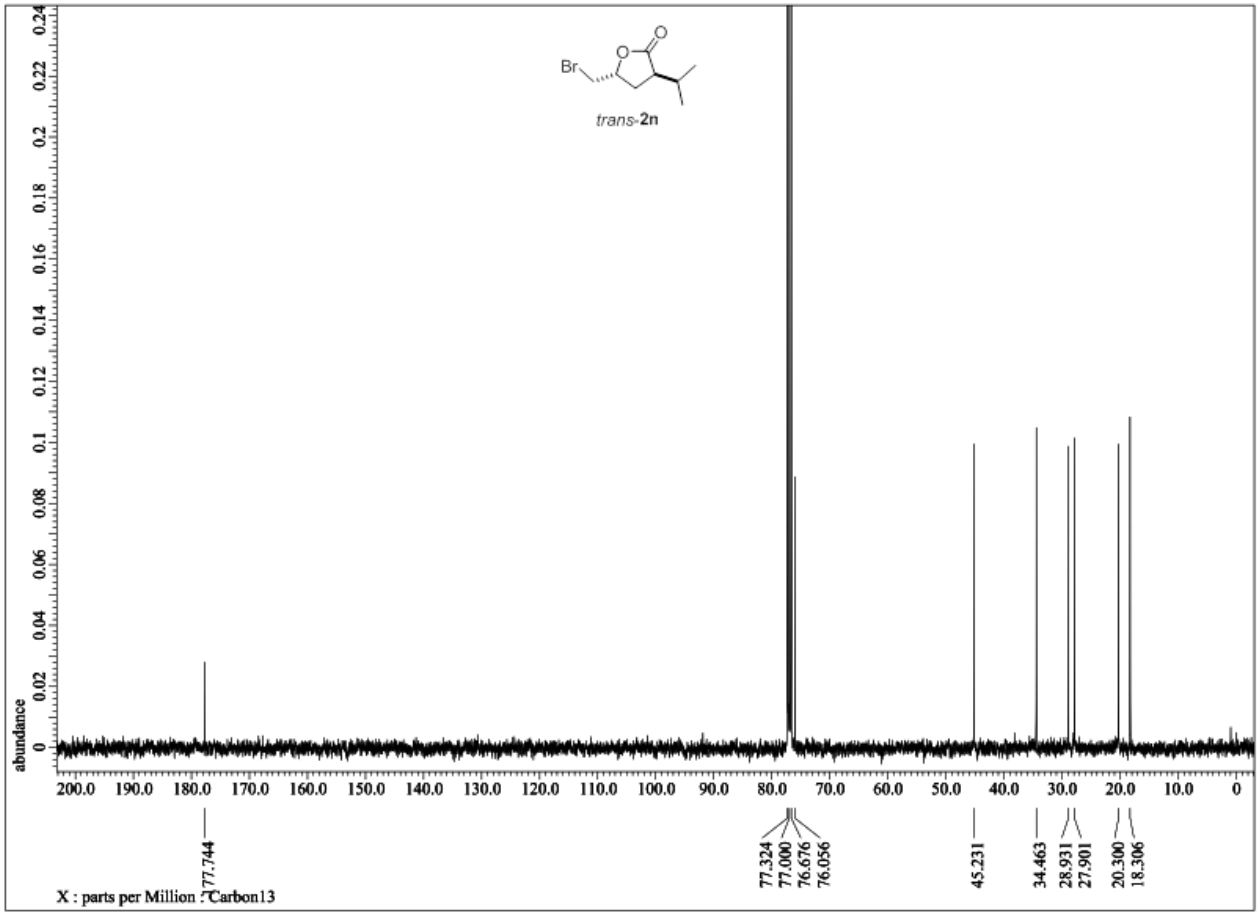

trans-2m
abundance
X : parts per Million : Proton
7.264
4.758
4.748
4.742
4.737
4.732
4.727
4.722
4.716
4.711
4.700
3.560
3.549
3.532
3.521
3.509
3.493
3.481
3.465
2.735
2.730
2.723
2.711
2.336
2.324
2.147
1.863
1.845
1.318
1.288
1.282
1.270
0.900
0.882
0.865
0.000
1.00
2.06
1.01
1.01
1.00
1.02
13.03
3.00

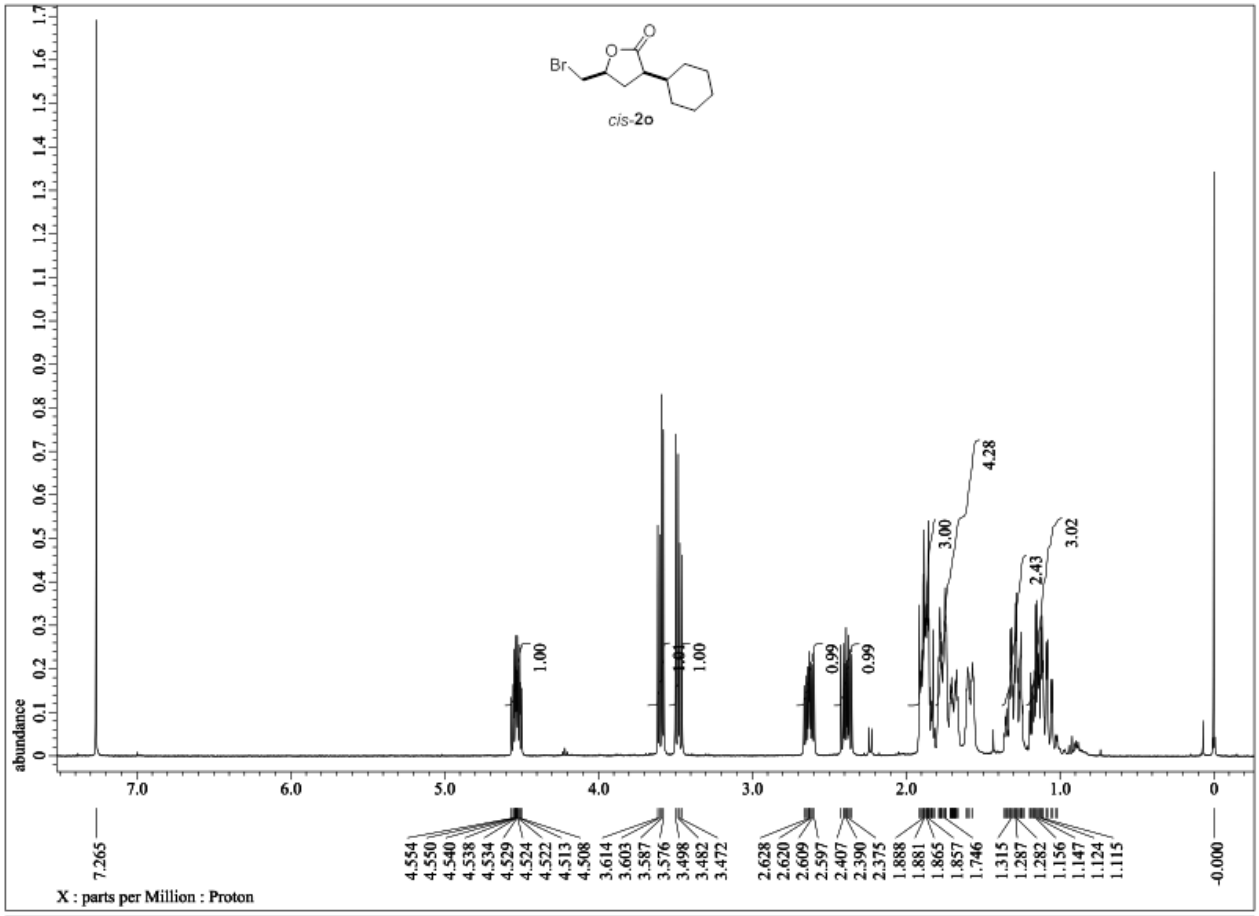

trans-2m
abundance
X : parts per Million : Carbon13
178.542
77.326
77.000
76.684
75.994
39.043
34.099
31.886
31.752
31.101
29.280
29.233
29.127
27.134
22.574
14.029

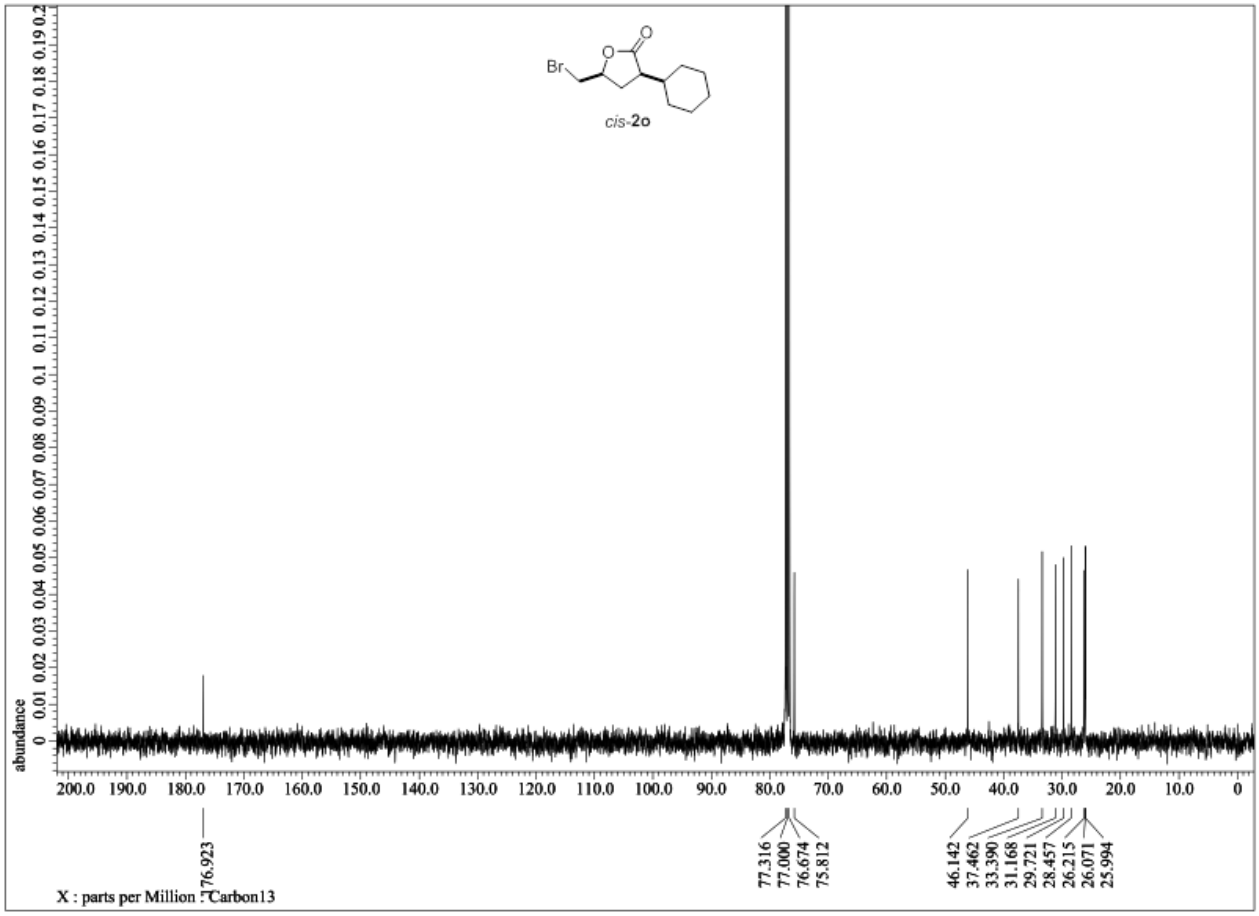

cis-2n
abundance
X : parts per Million : Proton
7.264
4.562
4.558
4.548
4.546
4.542
4.537
4.532
4.530
4.521
4.517
3.622
3.610
3.595
3.583
3.507
3.490
3.480
2.652
2.644
2.633
2.621
2.400
2.384
2.234
1.895
1.869
1.863
1.838
1.067
1.049
0.959
0.941
0.000
1.00
1.03
1.10
1.01
1.02
1.15
1.03
3.19
3.11

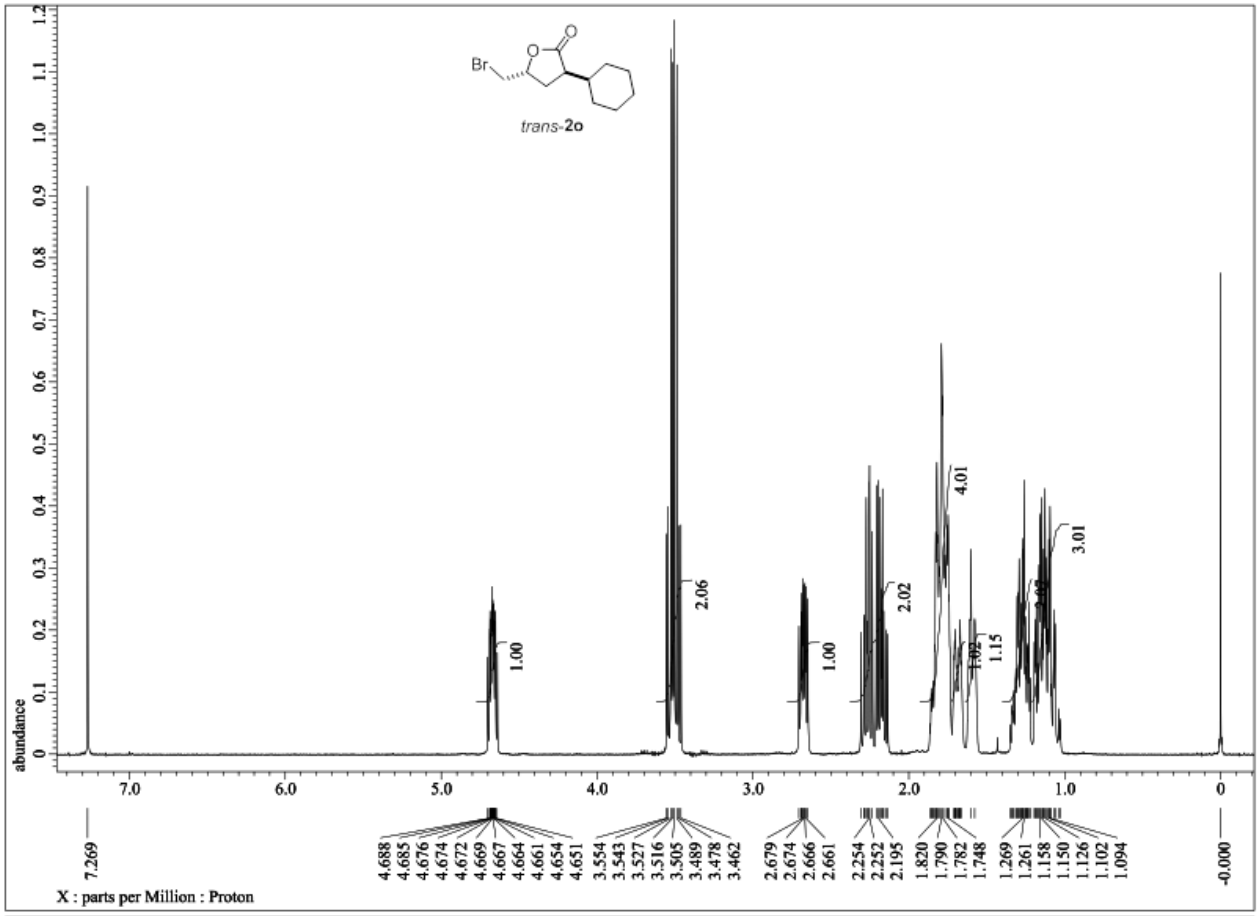

cis-2n
abundance
X : parts per Million : Carbon13
76.856
77.316
77.000
76.674
75.678
46.755
33.390
29.060
27.623
20.524
18.206

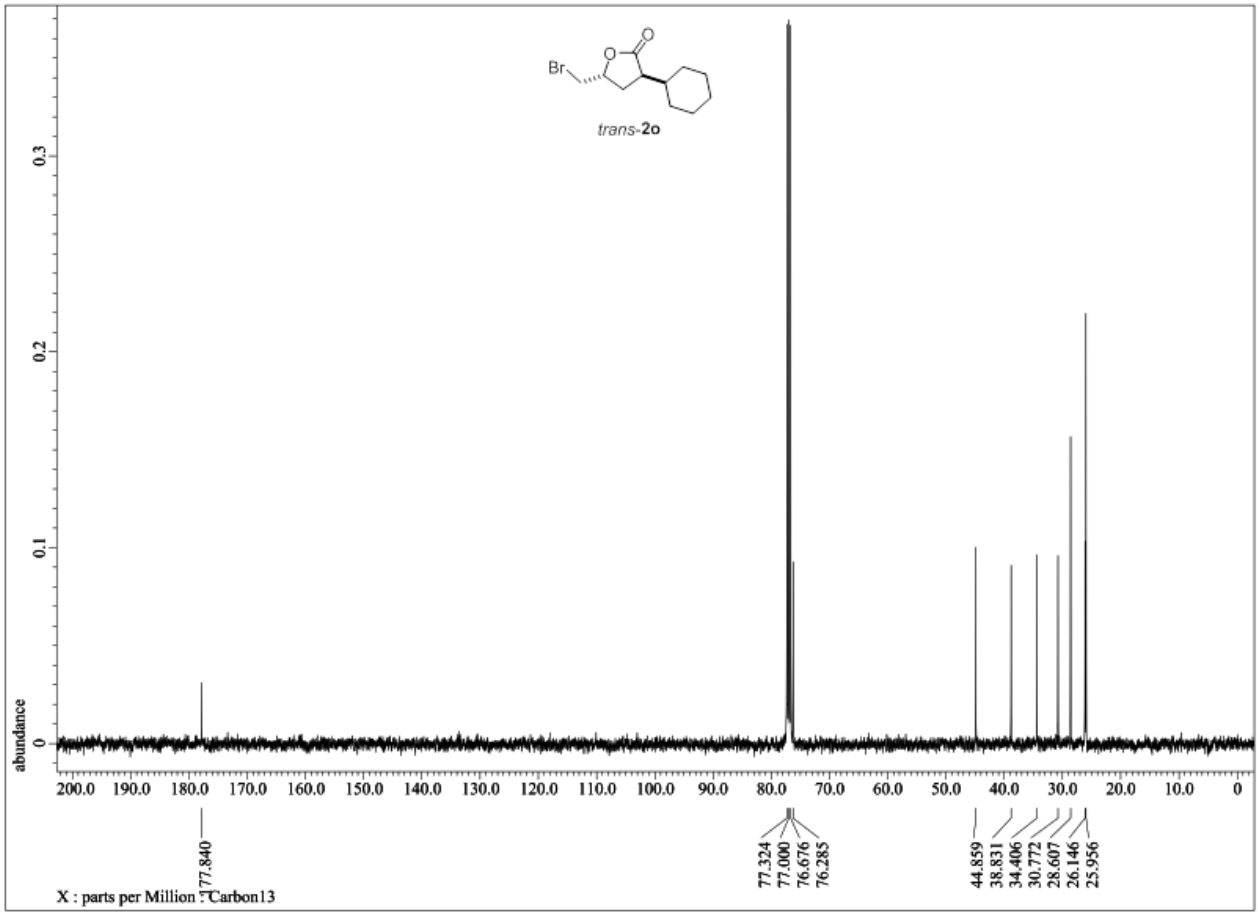

trans-2n
abundance
X : parts per Million : Proton
7.268
4.703
4.700
4.695
4.692
4.687
4.683
4.680
4.677
4.671
4.667
4.656
3.557
3.546
3.529
3.518
3.513
3.497
3.486
3.470
2.707
2.700
2.694
2.688
2.674
2.229
2.210
2.198
2.185
1.605
1.047
1.029
0.964
0.947
-0.000
1.00
2.07
1.01
3.08
3.05
3.01

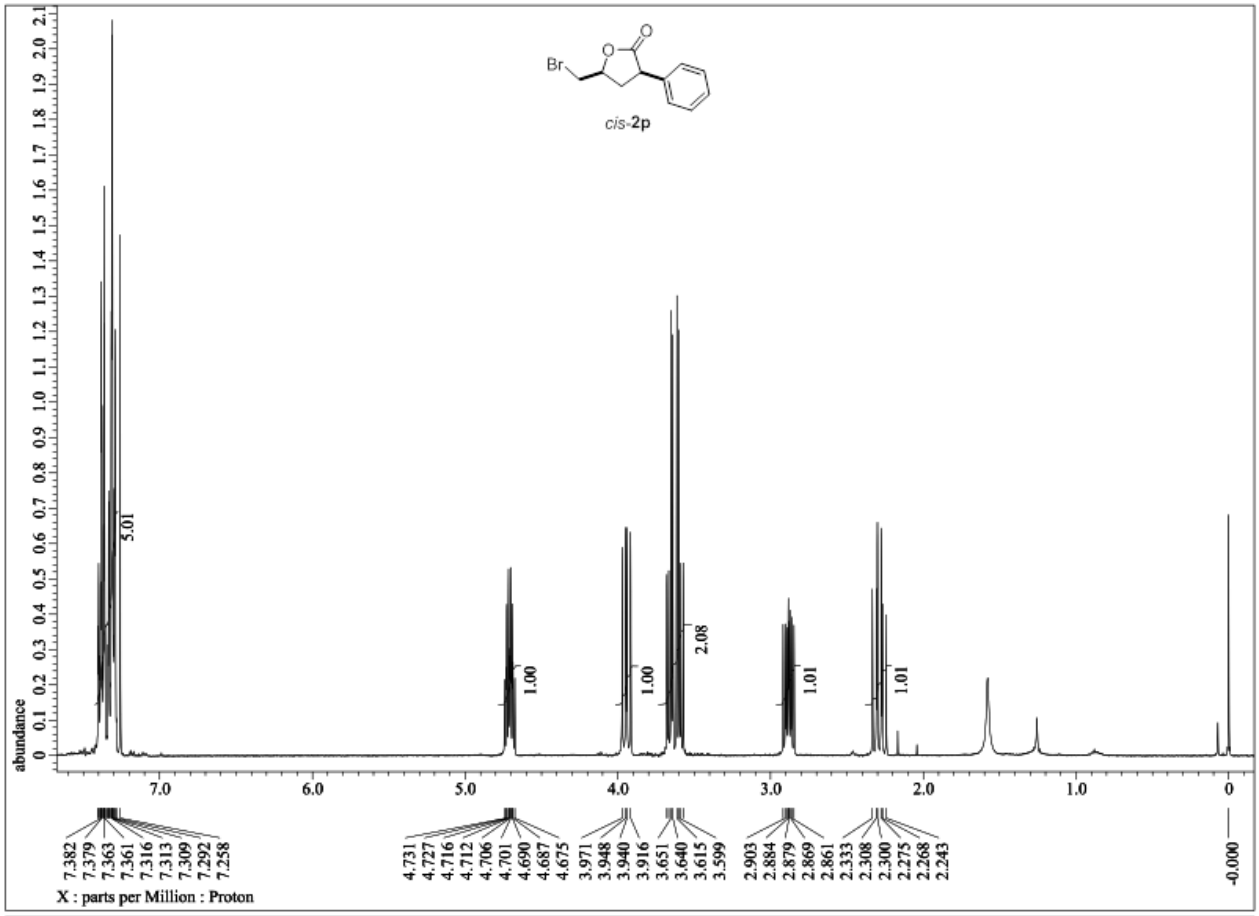

trans-2n
abundance
X : parts per Million : Carbon13
177.744
77.324
77.000
76.676
76.056
45.231
34.463
28.931
27.901
20.300
18.306

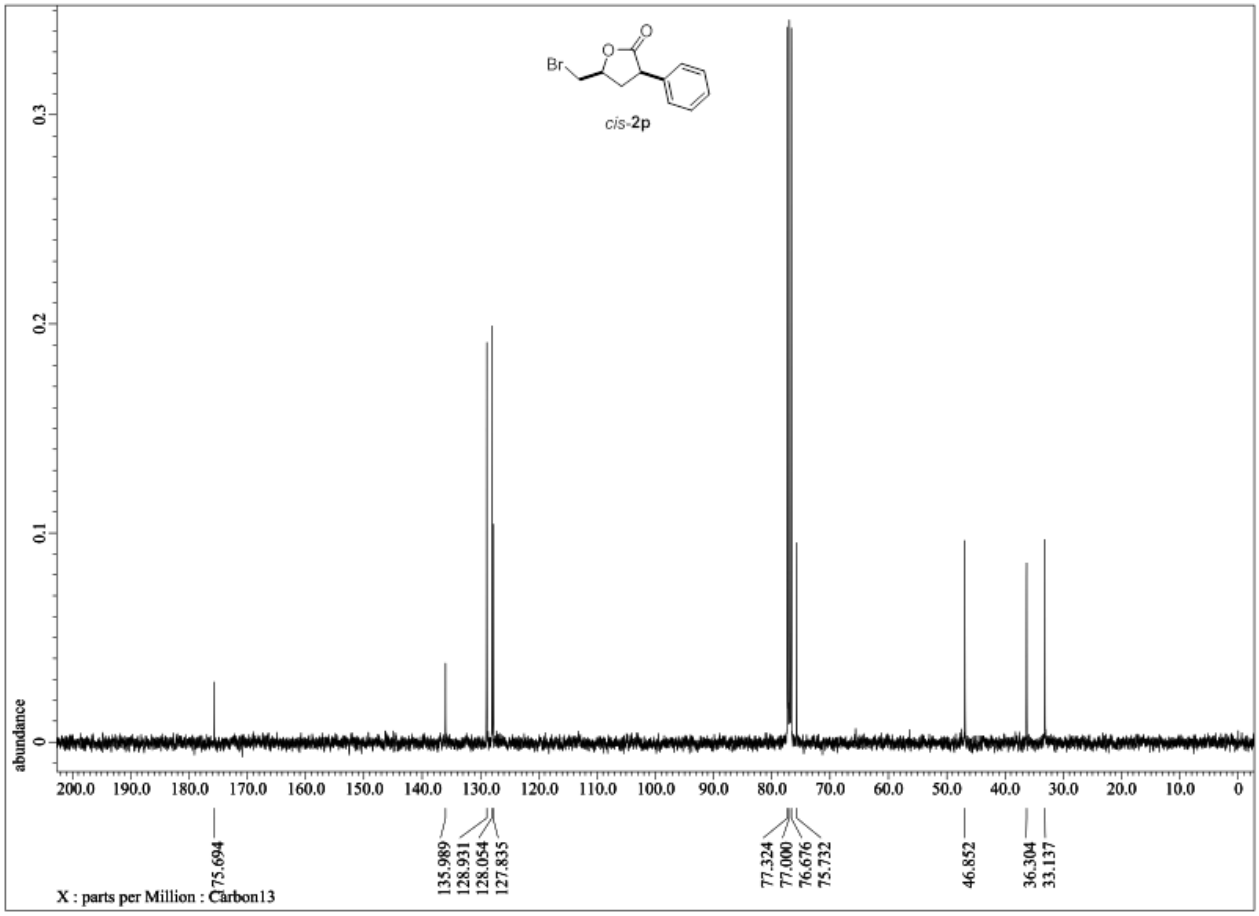

Br
O
O
cis-2o
abundance
1.00
1.01
1.00
0.99
0.99
3.00
4.28
2.43
3.02
7.265
4.554
4.550
4.540
4.538
4.534
4.529
4.524
4.522
4.513
4.508
3.614
3.603
3.587
3.576
3.498
3.482
3.472
2.628
2.620
2.609
2.597
2.407
2.390
2.375
1.888
1.881
1.865
1.857
1.746
1.315
1.287
1.282
1.156
1.147
1.124
1.115
-0.000
X : parts per Million : Proton

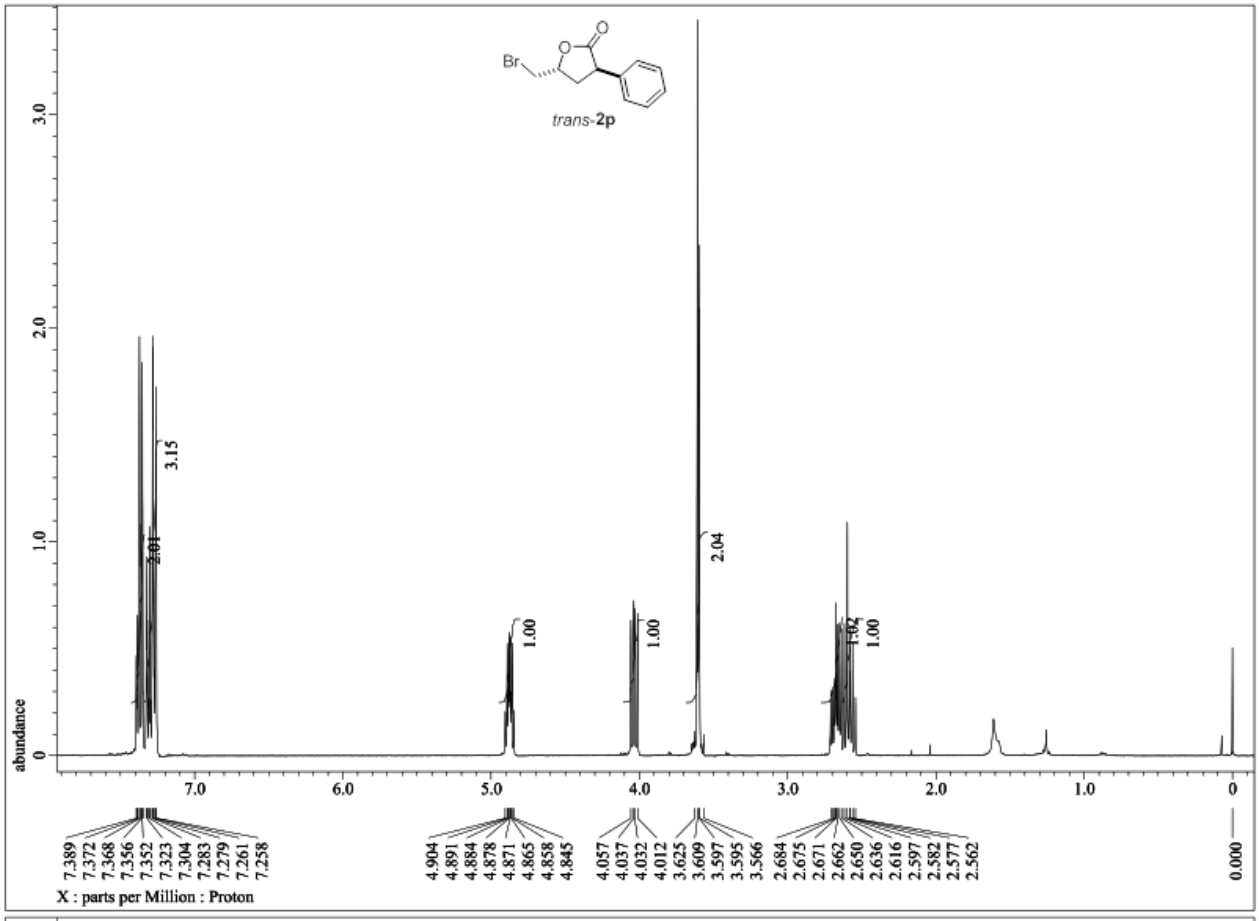

Br
O
O
cis-2o
abundance
76.923
77.316
77.000
76.674
75.812
46.142
37.462
33.390
31.168
29.721
28.457
26.215
26.071
25.994
X : parts per Million : Carbon13

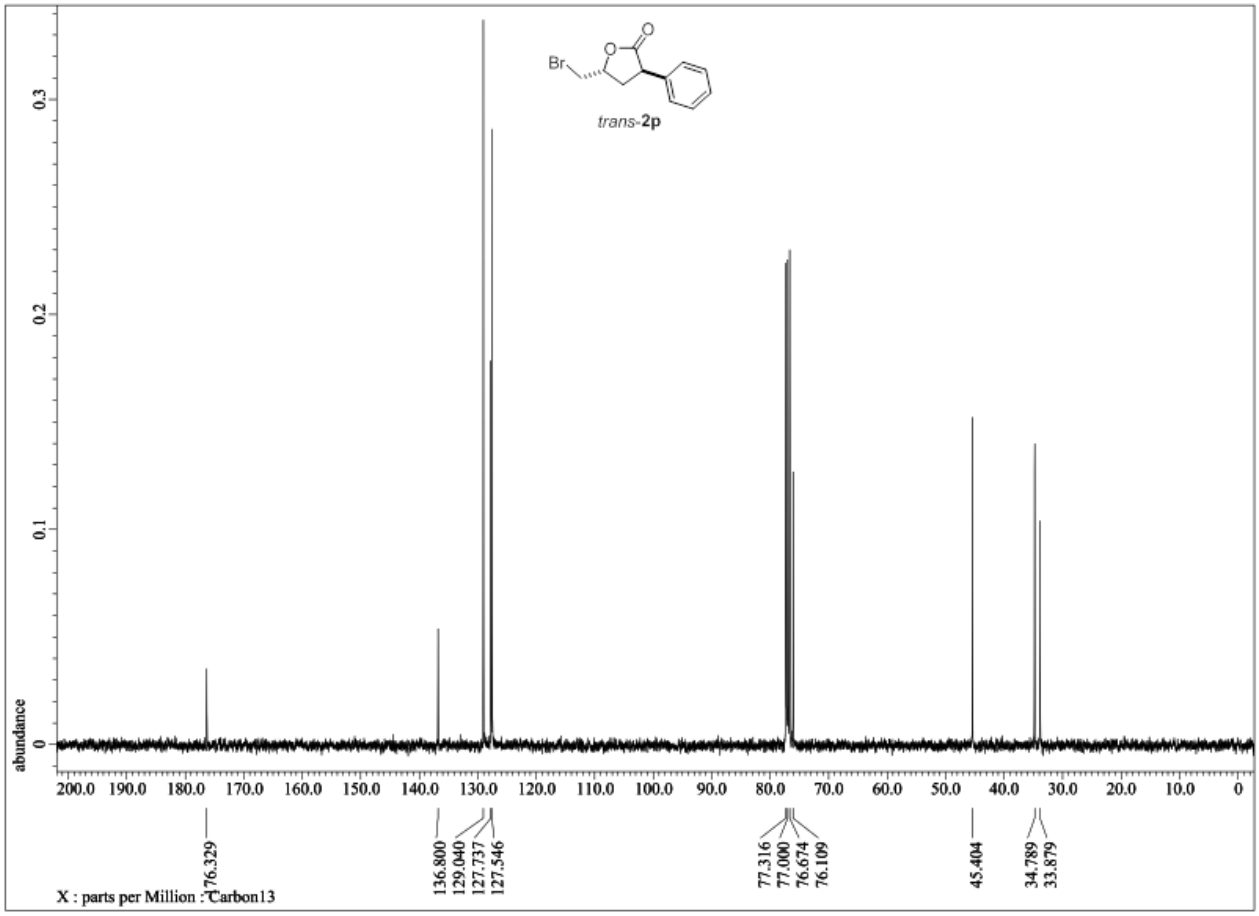

Br
O
O
trans-2o
abundance
1.00
2.06
1.00
2.02
4.01
1.02
1.15
3.01
7.269
4.688
4.685
4.676
4.674
4.672
4.669
4.667
4.664
4.661
4.654
4.651
3.554
3.543
3.527
3.516
3.505
3.489
3.478
3.462
2.679
2.674
2.666
2.661
2.254
2.252
2.195
1.820
1.790
1.782
1.748
1.269
1.261
1.158
1.150
1.126
1.102
1.094
-0.000
X : parts per Million : Proton

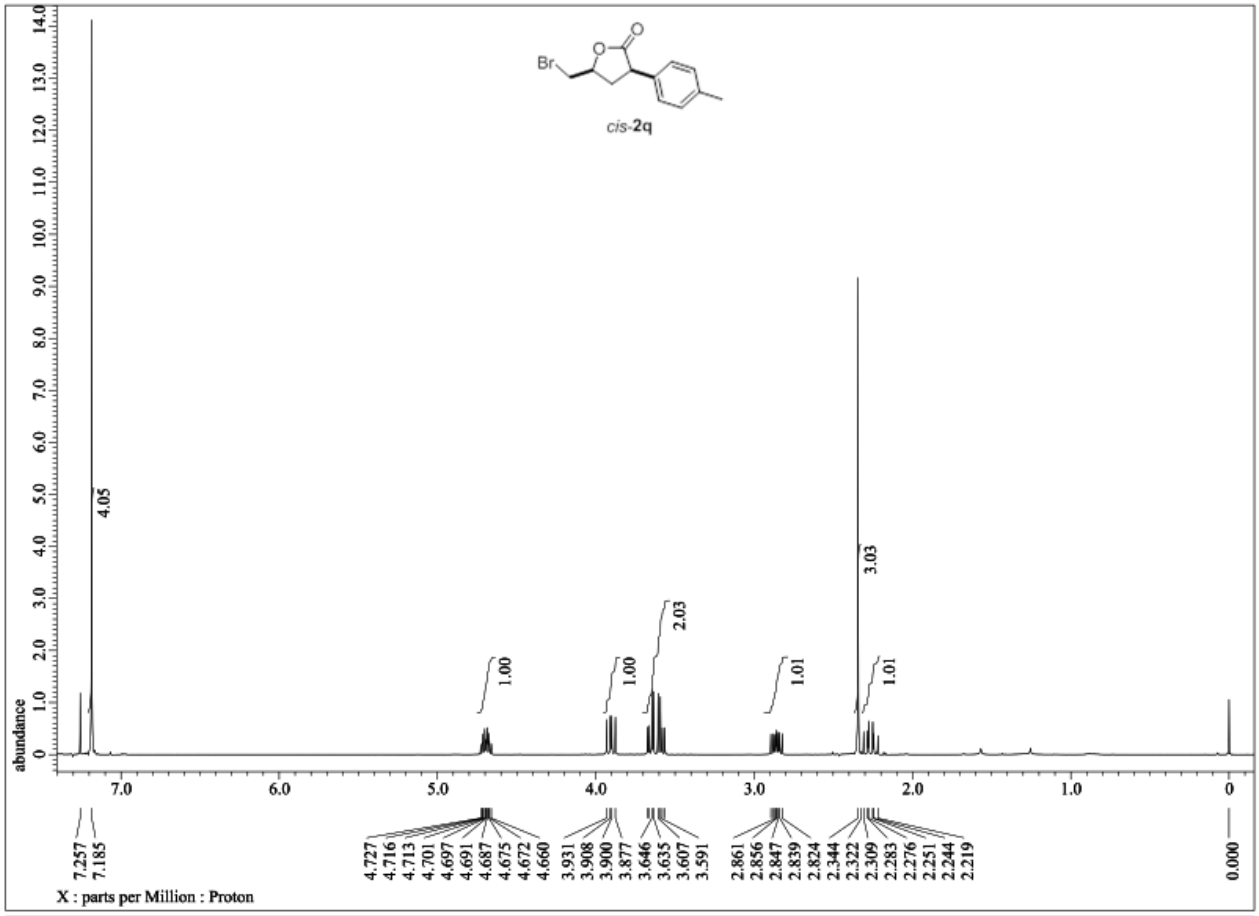

Br
O
O
trans-2o
abundance
177.840
77.324
77.000
76.676
76.285
44.859
38.831
34.406
30.772
28.607
26.146
25.956
X : parts per Million : Carbon13

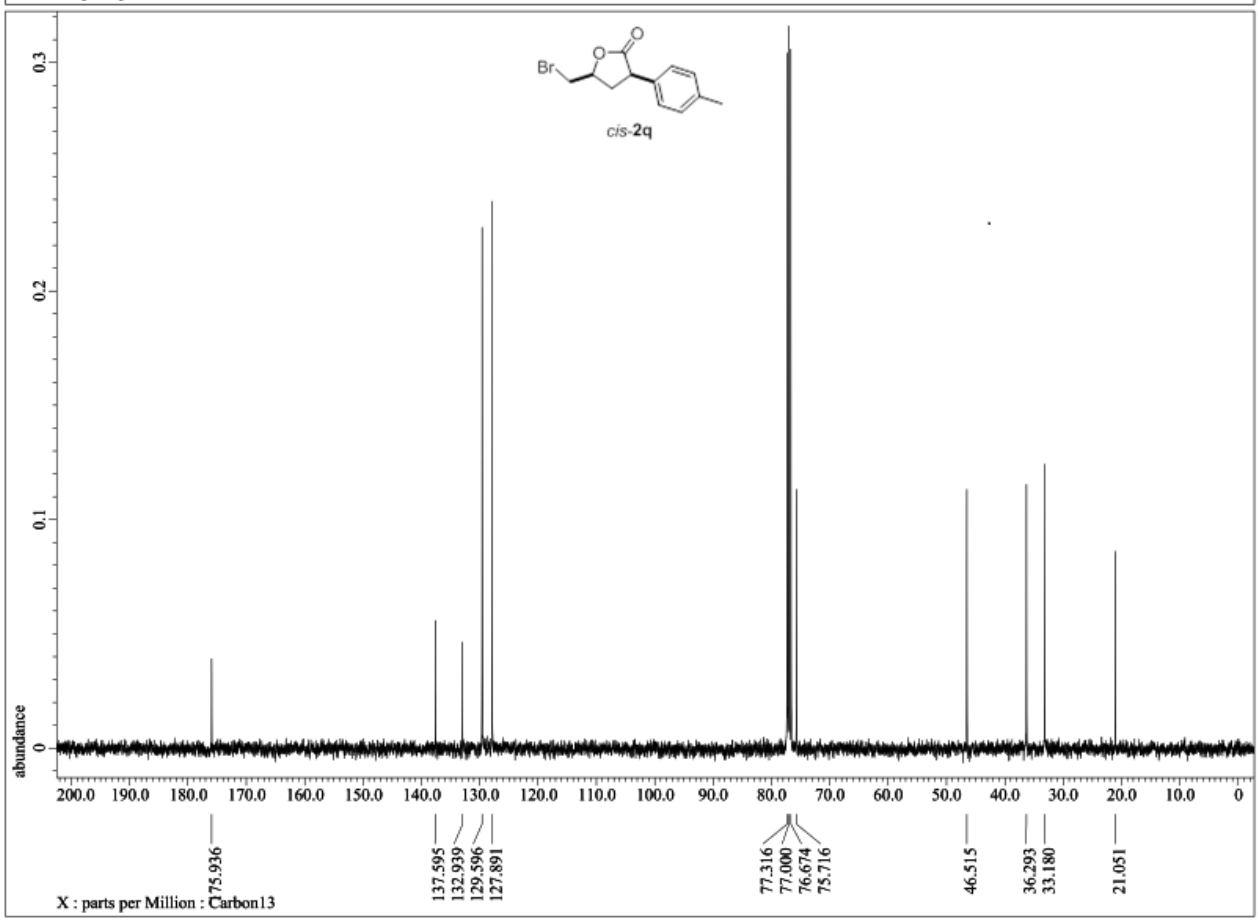

Br
O
O
cis-2p
abundance
5.01
1.00
1.00
2.08
1.01
1.01
7.382
7.379
7.363
7.361
7.316
7.313
7.309
7.292
7.258
4.731
4.727
4.716
4.712
4.706
4.701
4.690
4.687
4.675
3.971
3.948
3.940
3.916
3.651
3.640
3.615
3.599
2.903
2.884
2.879
2.869
2.861
2.333
2.308
2.300
2.275
2.268
2.243
-0.000
X : parts per Million : Proton

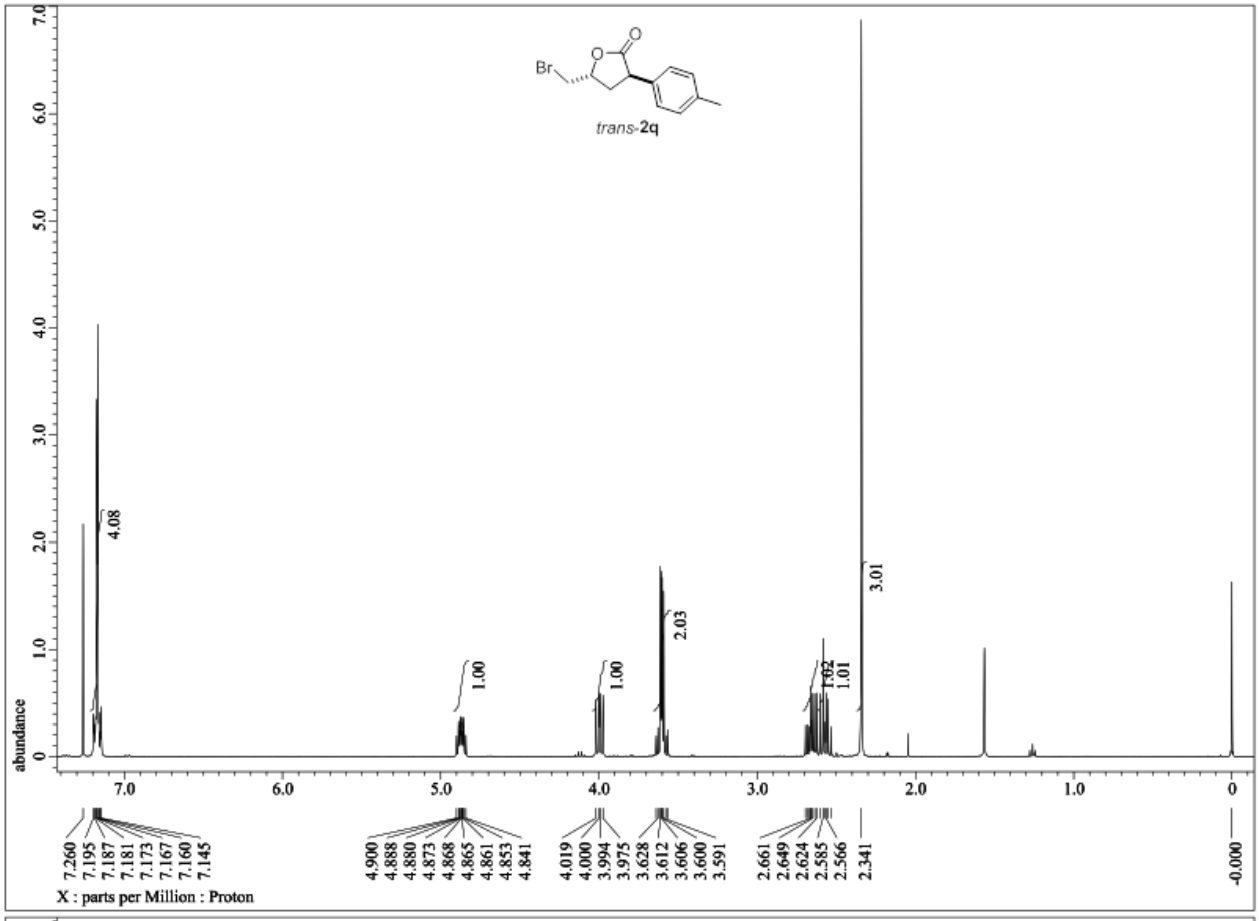

Br
O
O
cis-2p
abundance
75.694
135.989
128.931
128.054
127.835
77.324
77.000
76.676
75.732
46.852
36.304
33.137
X : parts per Million : Carbon13

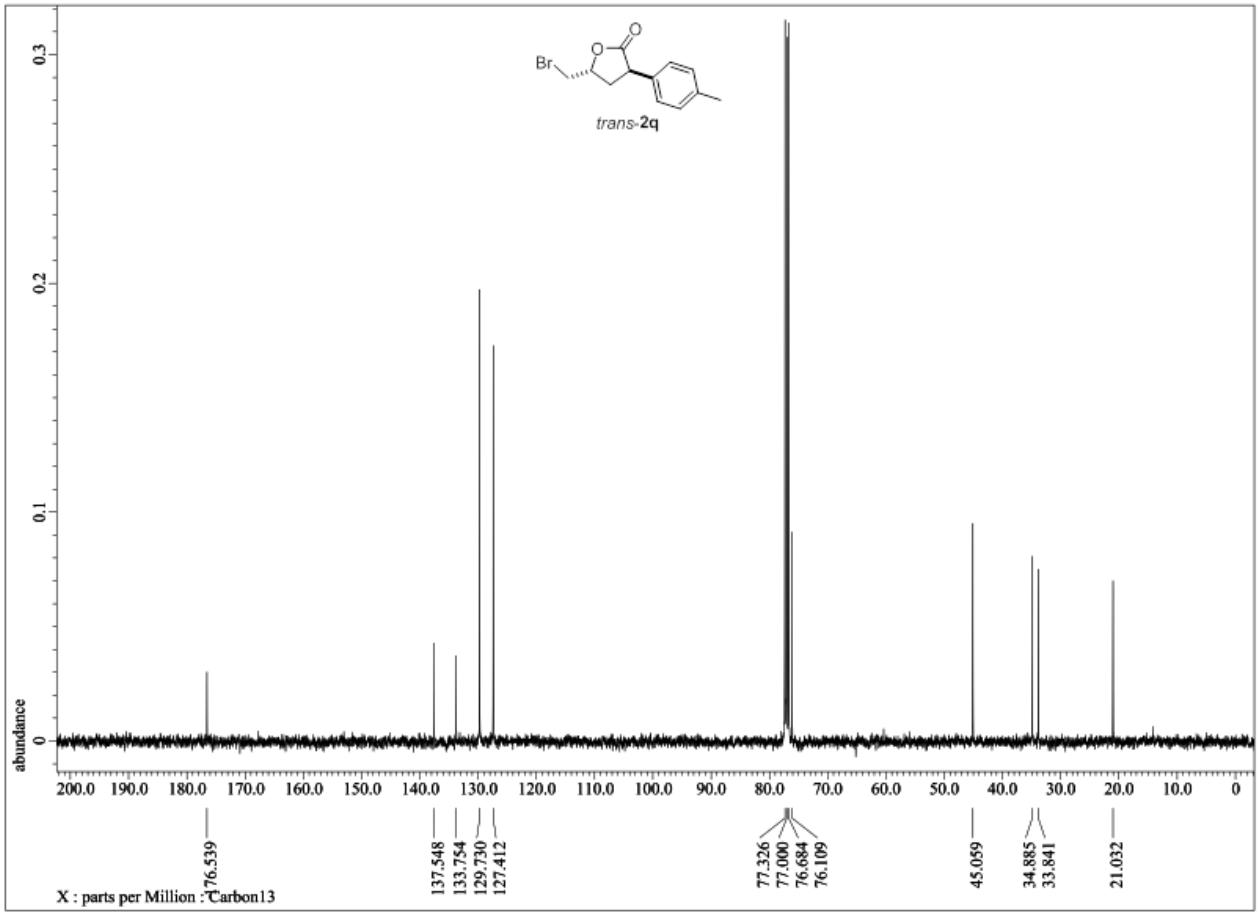

Br
O
O
trans-2p
abundance
3.0
2.0
1.0
0
3.15
3.01
1.00
1.00
2.04
1.02
1.00
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.389
7.372
7.368
7.356
7.352
7.323
7.304
7.283
7.279
7.261
7.258
4.904
4.891
4.884
4.878
4.871
4.865
4.858
4.845
4.057
4.037
4.032
4.012
3.625
3.609
3.597
3.595
3.566
2.684
2.675
2.671
2.662
2.650
2.636
2.616
2.597
2.582
2.577
2.562
0.000
X : parts per Million : Proton

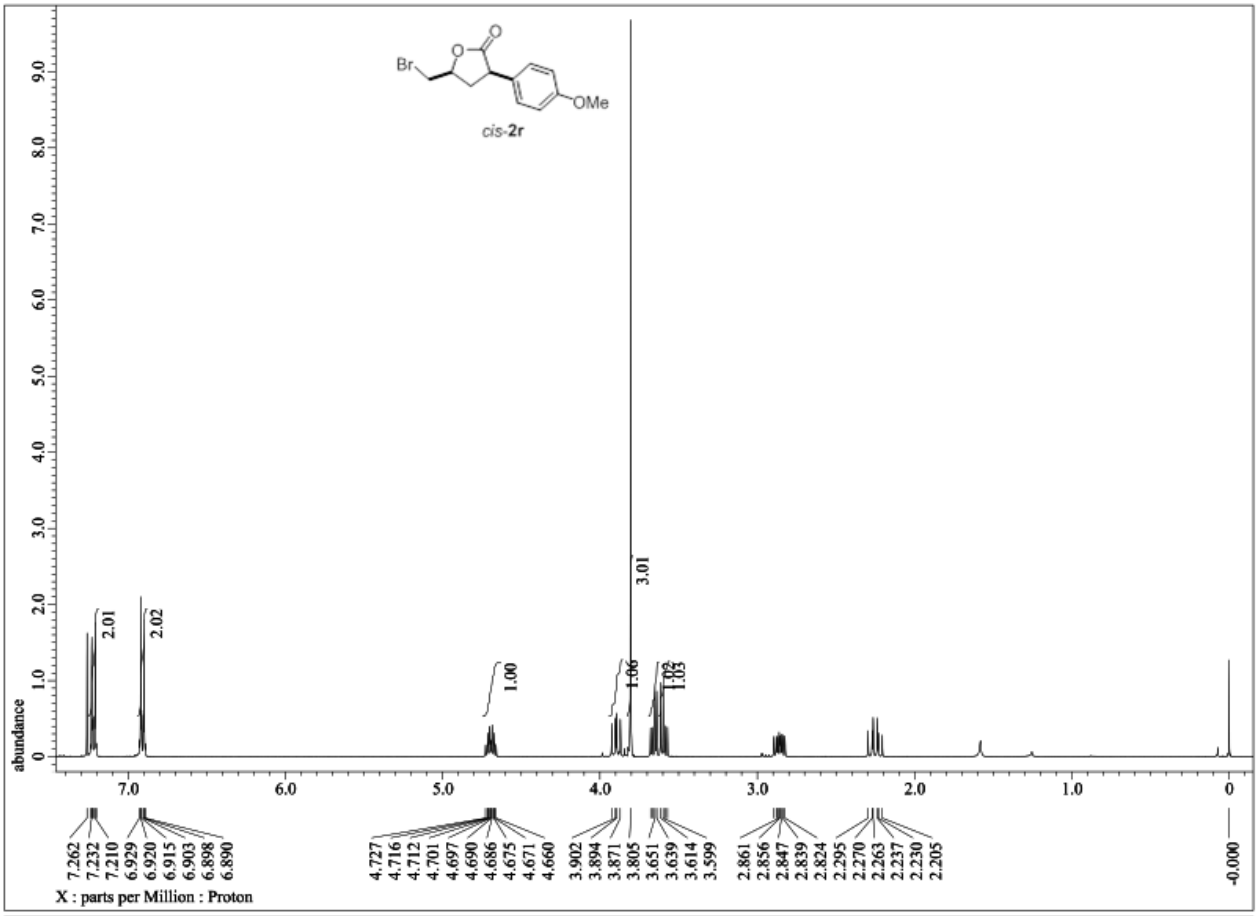

Br
O
O
trans-2p
abundance
0.3
0.2
0.1
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
76.329
136.800
129.040
127.737
127.546
77.316
77.000
76.674
76.109
45.404
34.789
33.879
X : parts per Million : Carbon13

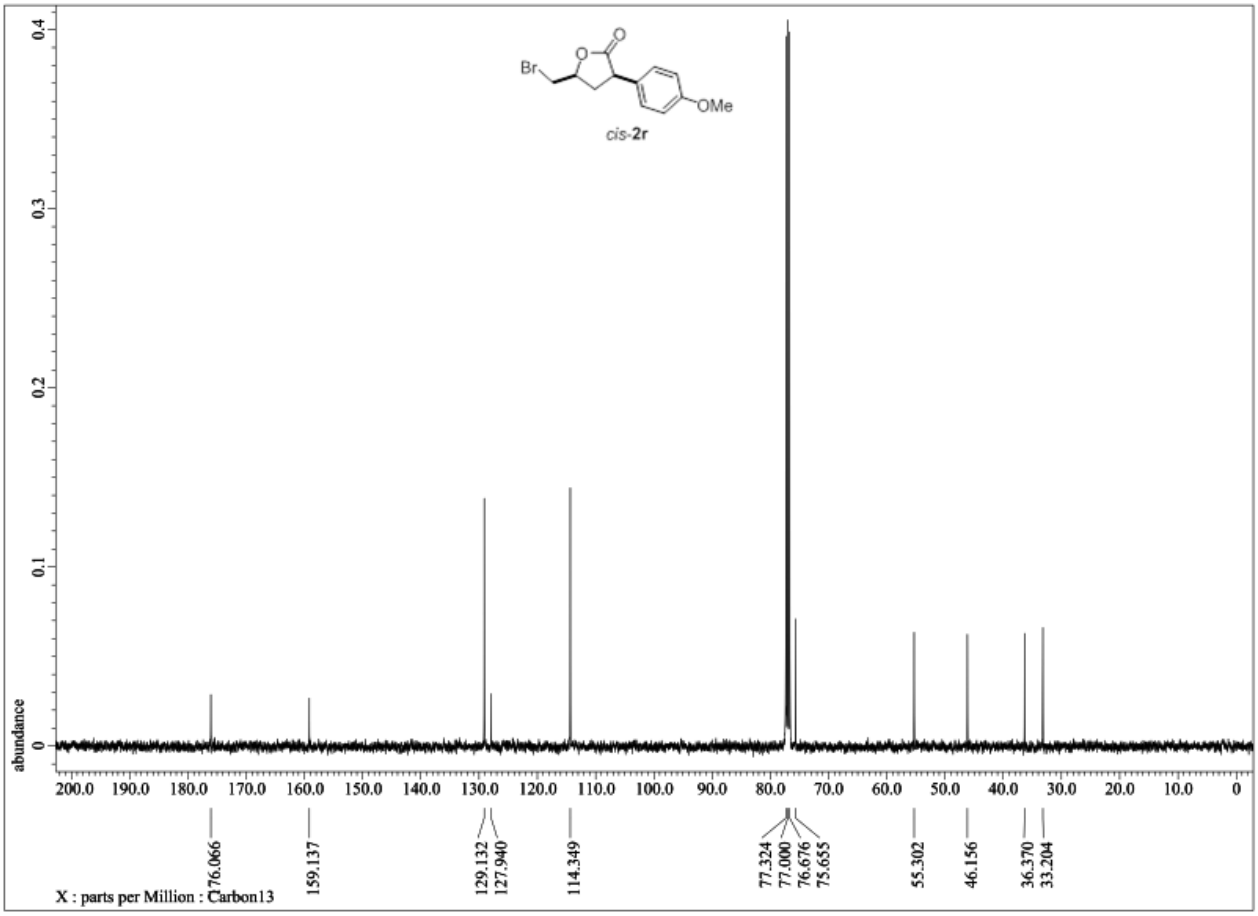

Br
O
O
cis-2q
abundance
4.05
1.00
1.00
2.03
1.01
3.03
1.01
7.257
7.185
4.727
4.716
4.713
4.701
4.697
4.691
4.687
4.675
4.672
4.660
3.931
3.908
3.900
3.877
3.646
3.635
3.607
3.591
2.861
2.856
2.847
2.839
2.824
2.344
2.322
2.309
2.283
2.276
2.251
2.244
2.219
0.000
X : parts per Million : Proton

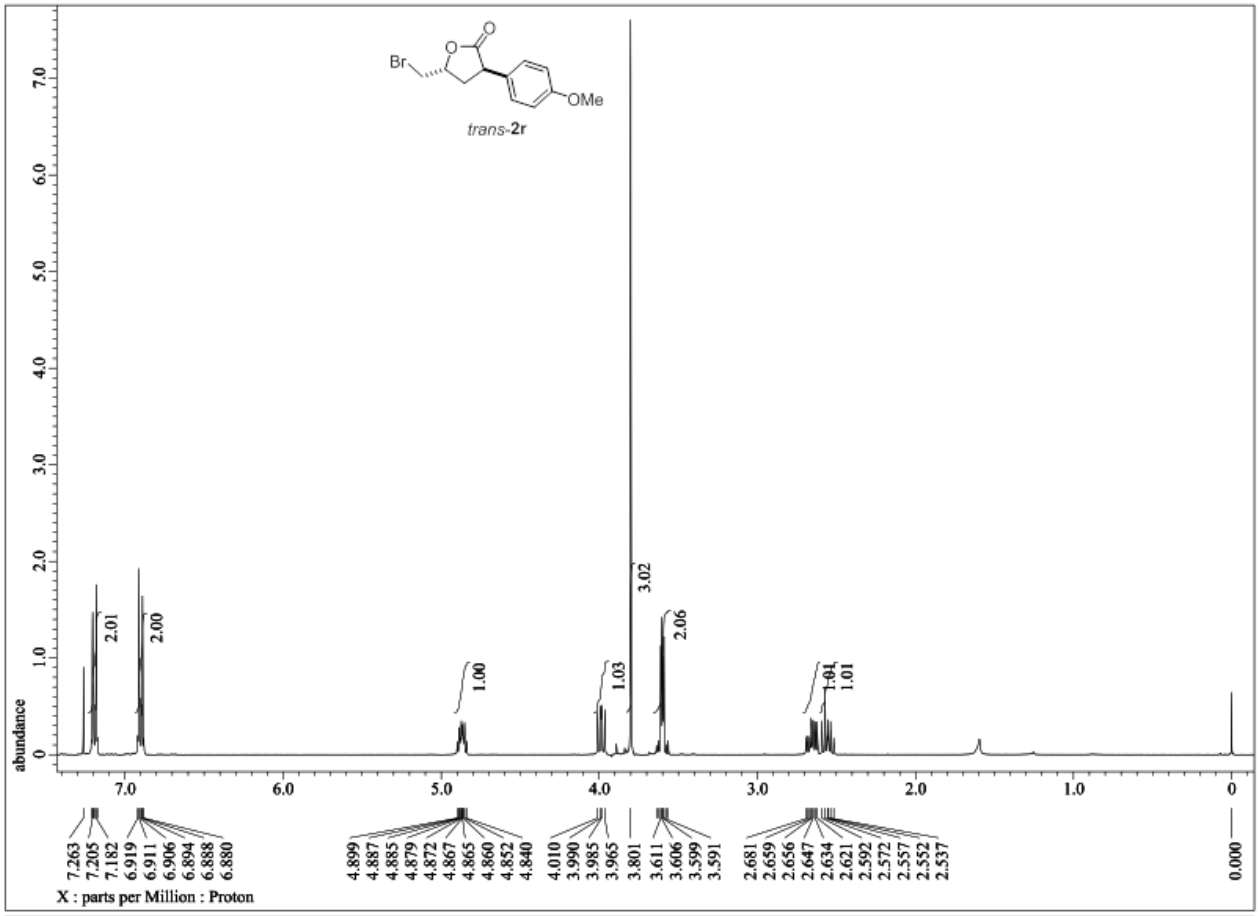

Br
O
O
cis-2q
abundance
175.936
137.595
132.939
129.596
127.891
77.316
77.000
76.674
75.716
46.515
36.293
33.180
21.051
X : parts per Million : Carbon13

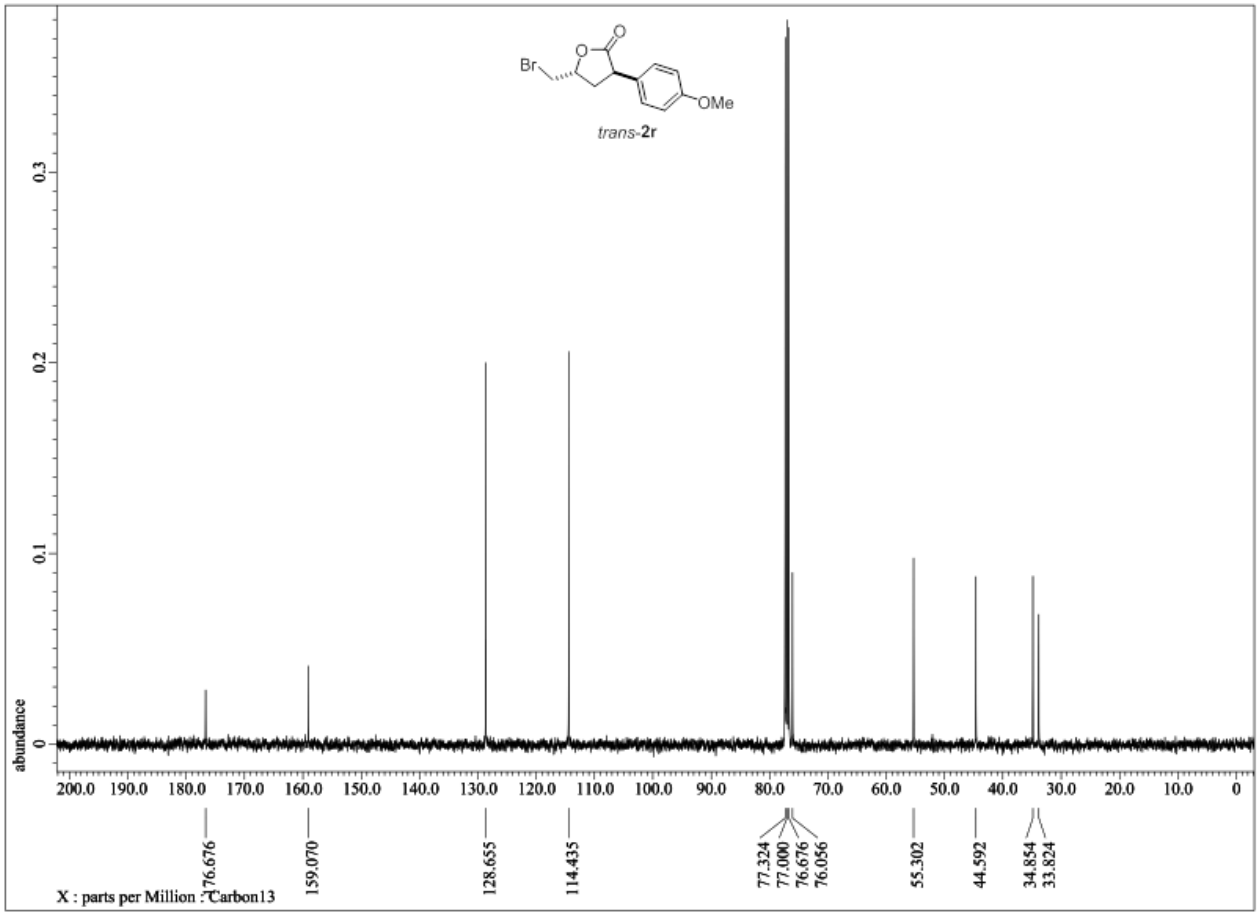

trans-2q
abundance
4.08
1.00
1.00
2.03
1.02
1.01
3.01
7.260
7.195
7.187
7.181
7.173
7.167
7.160
7.145
4.900
4.888
4.880
4.873
4.868
4.865
4.861
4.853
4.841
4.019
4.000
3.994
3.975
3.628
3.612
3.606
3.600
3.591
2.661
2.649
2.624
2.585
2.566
2.341
-0.000
X : parts per Million : Proton

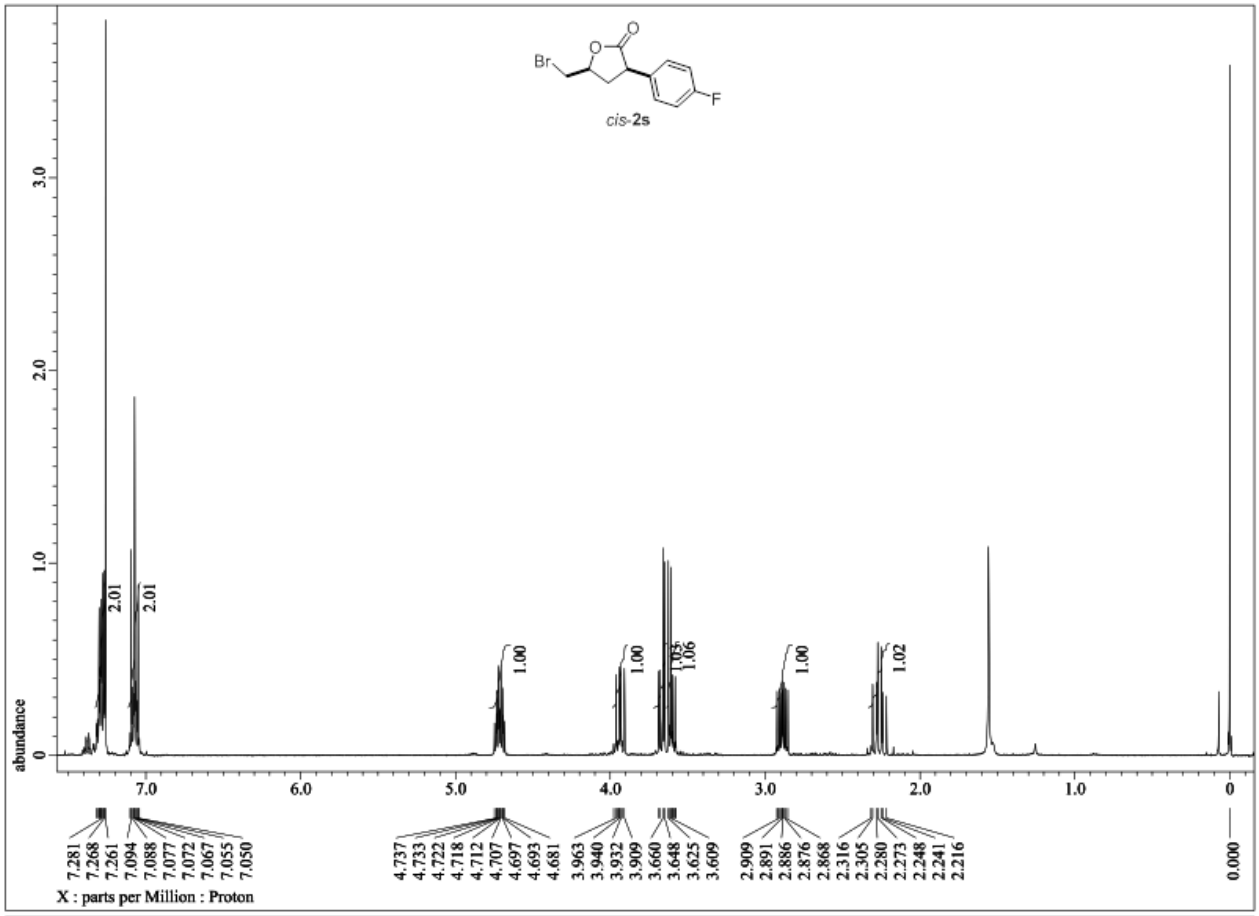

trans-2q
abundance
76.539
137.548
133.754
129.730
127.412
77.326
77.000
76.684
76.109
45.059
34.885
33.841
21.032
X : parts per Million : Carbon13

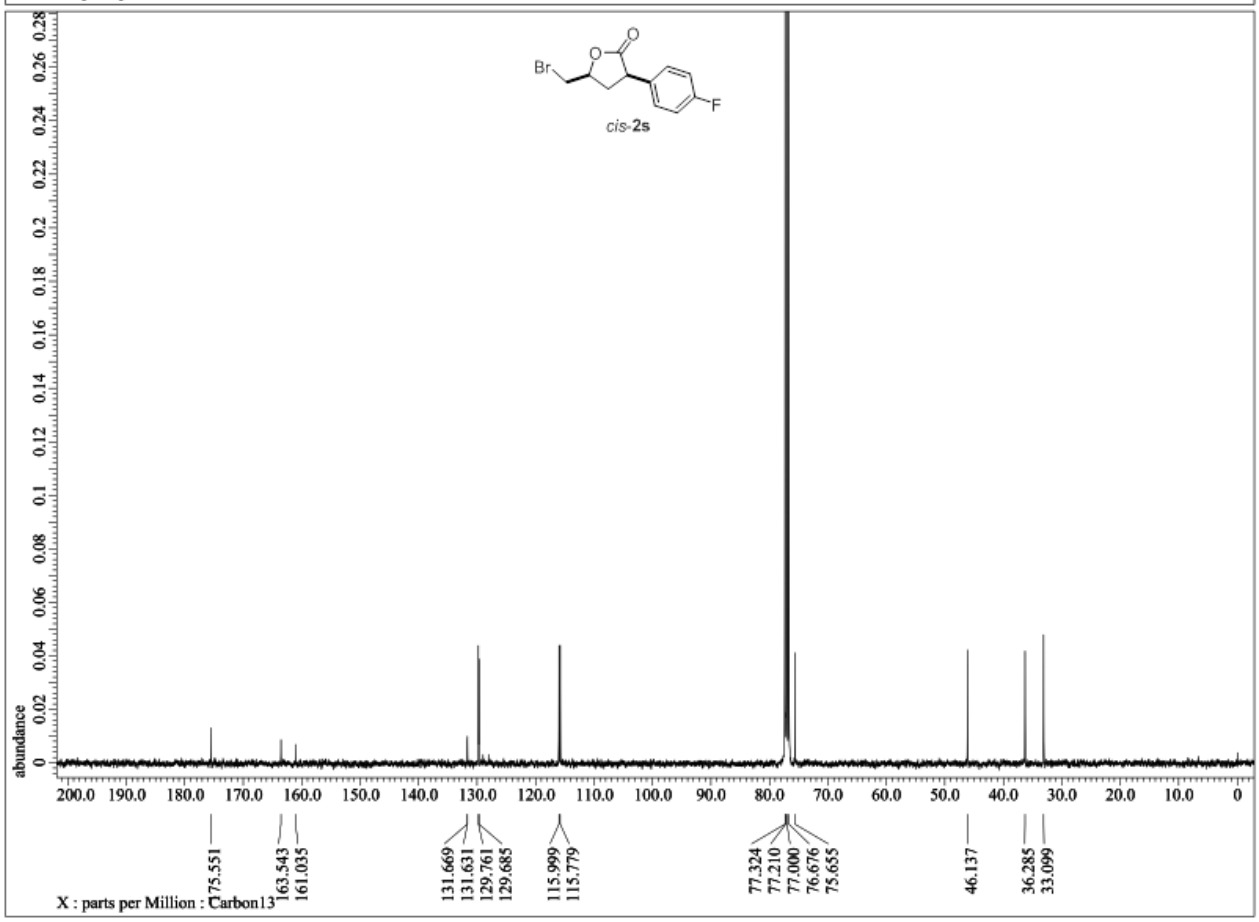

Br
O
O
OMe
cis-2r
abundance
X : parts per Million : Proton
2.01
2.02
1.00
3.01
7.262
7.232
7.210
6.929
6.920
6.915
6.903
6.898
6.890
4.727
4.716
4.712
4.701
4.697
4.690
4.686
4.675
4.671
4.660
3.902
3.894
3.871
3.805
3.651
3.639
3.614
3.599
2.861
2.856
2.847
2.839
2.824
2.295
2.270
2.263
2.237
2.230
2.205
-0.000

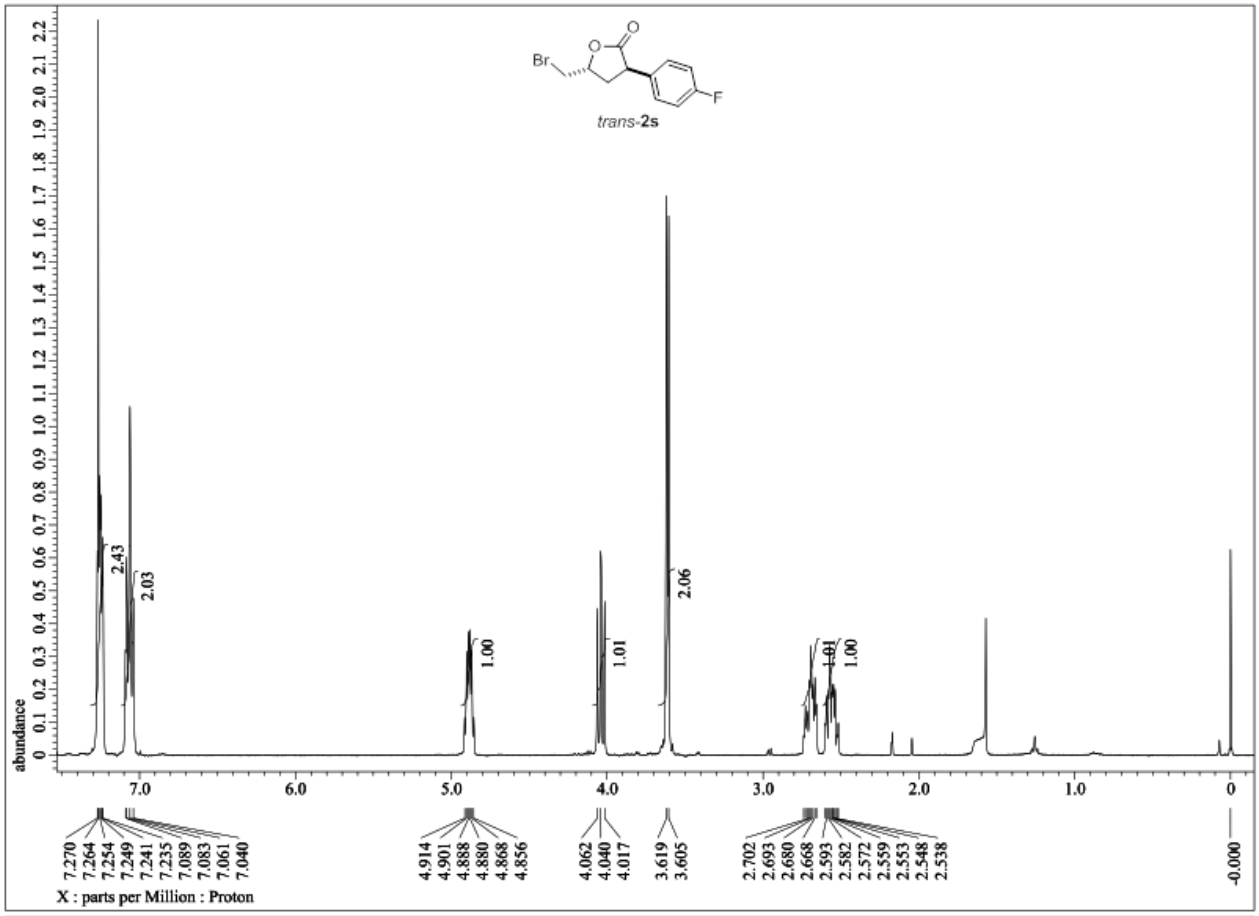

Br
O
O
OMe
cis-2r
abundance
X : parts per Million : Carbon13
76.066
159.137
129.132
127.940
114.349
77.324
77.000
76.676
75.655
55.302
46.156
36.370
33.204

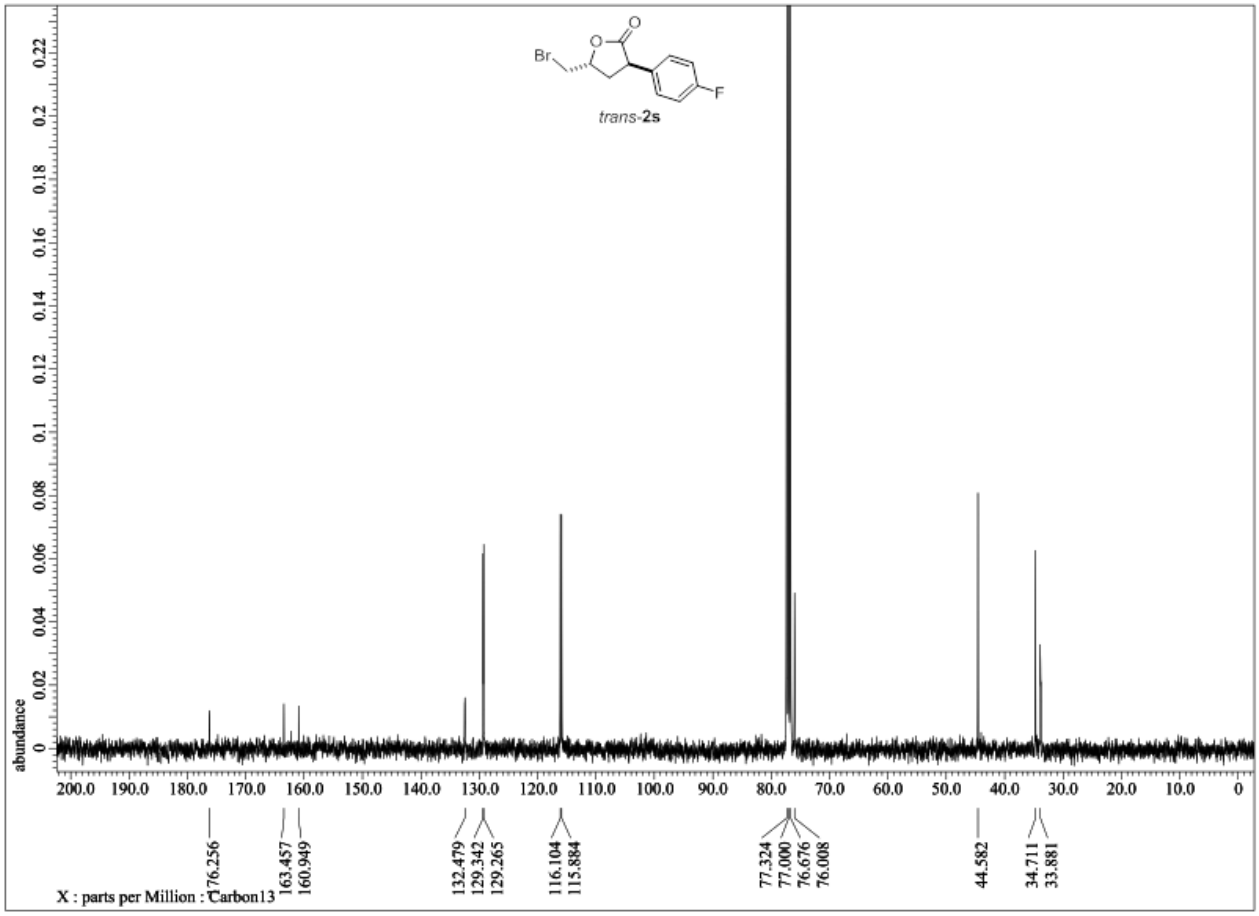

Br
O
O
OMe
trans-2r
abundance
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
2.01
2.00
1.00
1.03
3.02
2.06
1.01
7.263
7.205
7.182
6.919
6.911
6.906
6.894
6.888
6.880
4.899
4.887
4.885
4.879
4.872
4.867
4.865
4.860
4.852
4.840
4.010
3.990
3.985
3.965
3.801
3.611
3.606
3.599
3.591
2.681
2.659
2.656
2.647
2.634
2.621
2.592
2.572
2.557
2.552
2.537
0.000
X : parts per Million : Proton

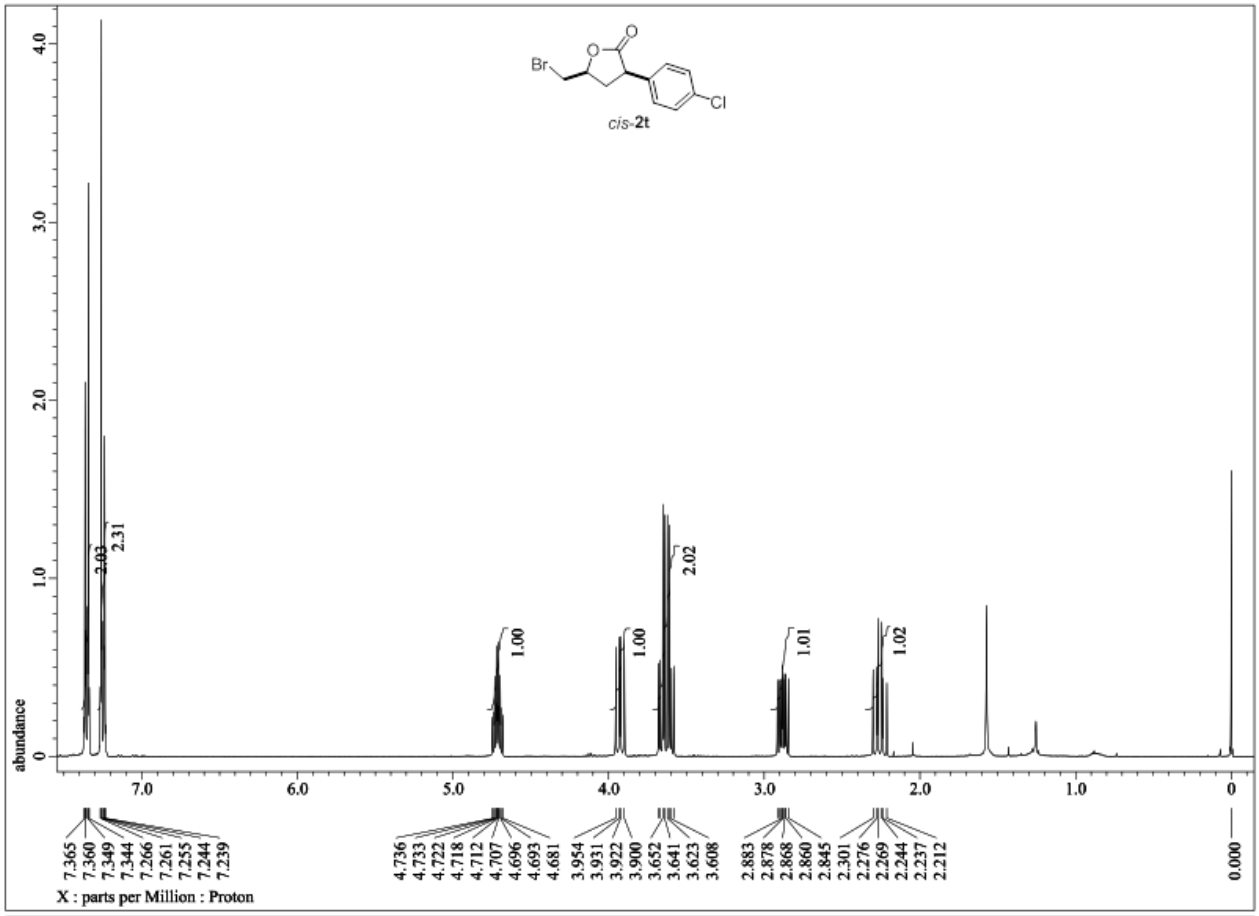

Br
O
O
OMe
trans-2r
abundance
0.3
0.2
0.1
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
76.676
159.070
128.655
114.435
77.324
77.000
76.676
76.056
55.302
44.592
34.854
33.824
X : parts per Million : Carbon13

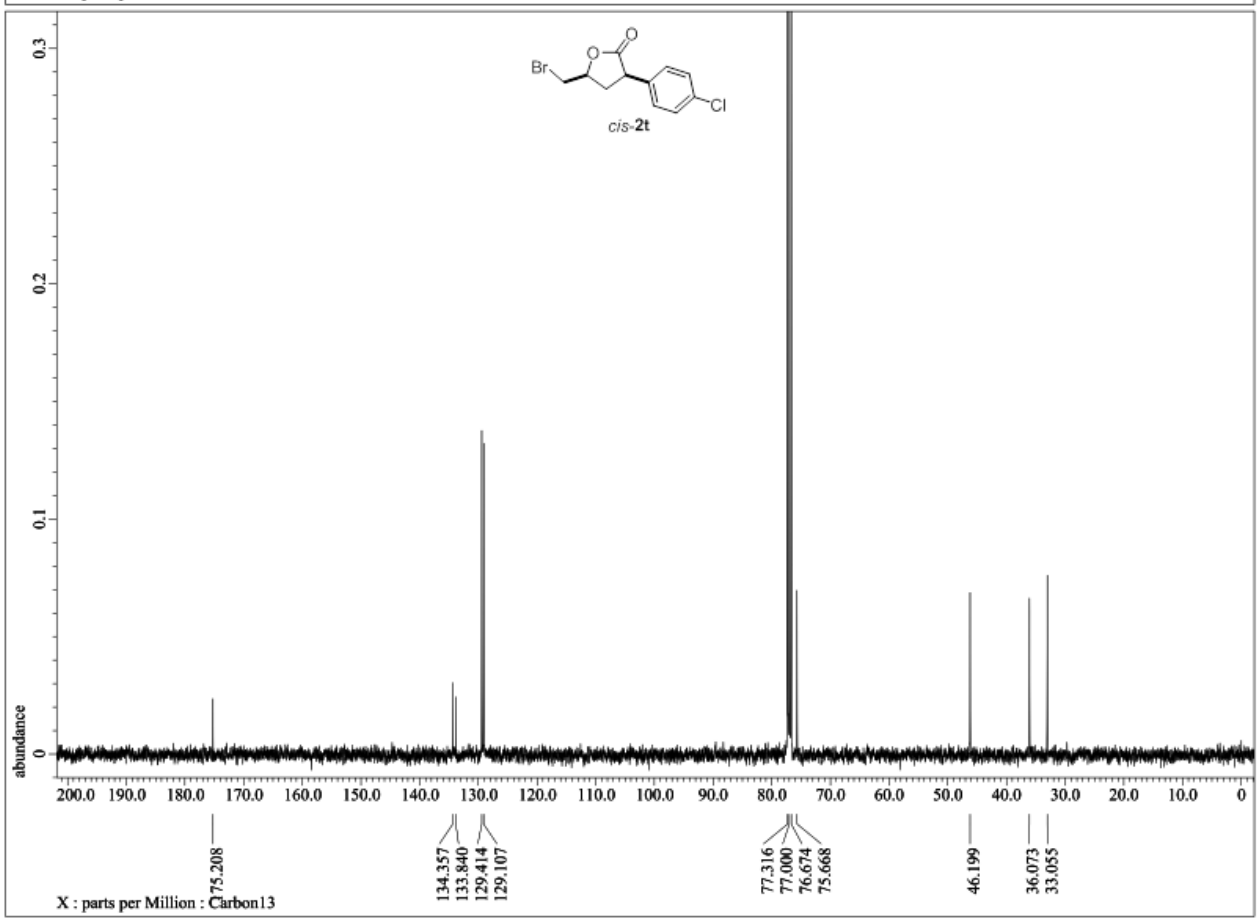

cis-2s
abundance
X : parts per Million : Proton
7.281
7.268
7.261
7.094
7.088
7.077
7.072
7.067
7.055
7.050
4.737
4.733
4.722
4.718
4.712
4.707
4.697
4.693
4.681
3.963
3.940
3.932
3.909
3.660
3.648
3.625
3.609
2.909
2.891
2.886
2.876
2.868
2.316
2.305
2.280
2.273
2.248
2.241
2.216
0.000

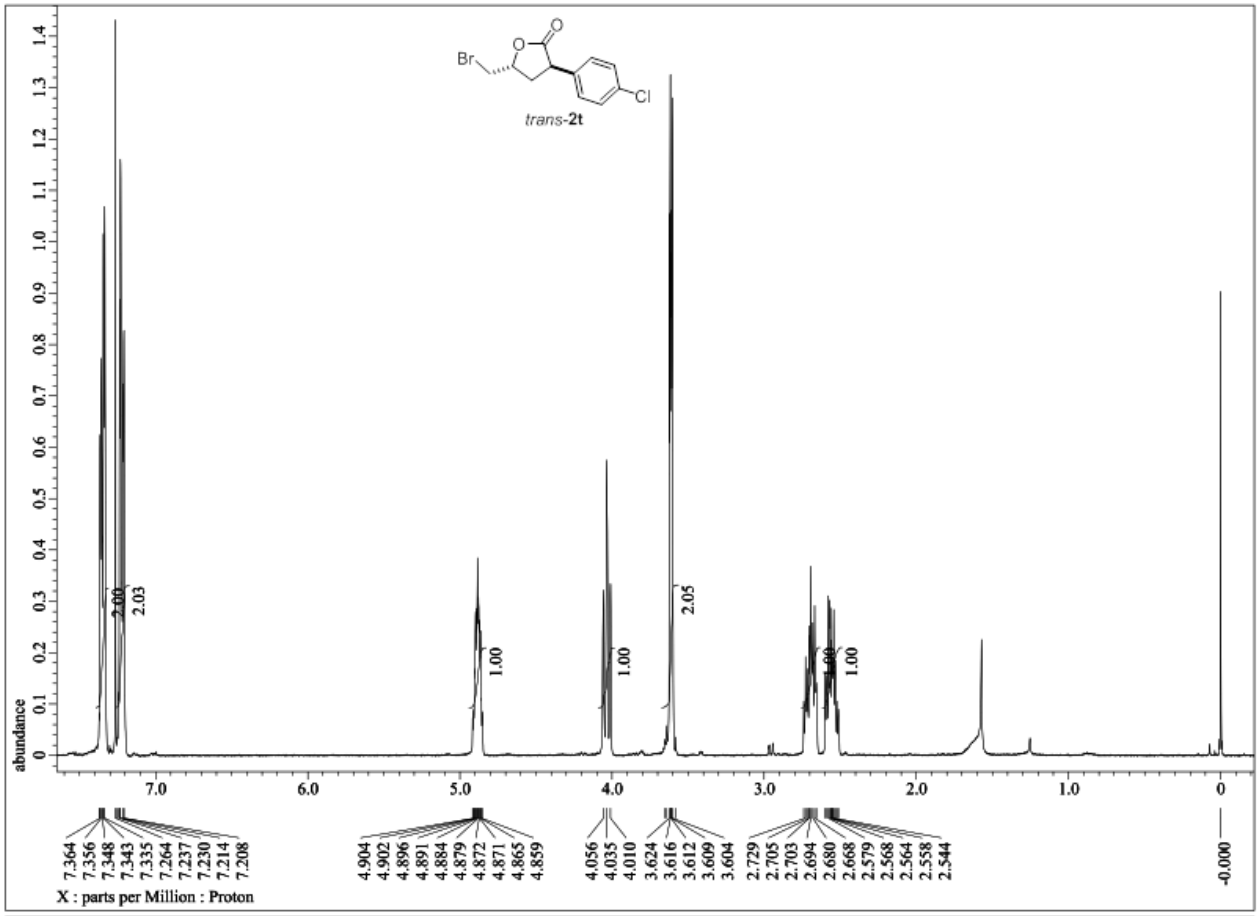

cis-2s
abundance
X : parts per Million : Carbon13
75.551
163.543
161.035
131.669
131.631
129.761
129.685
115.999
115.779
77.324
77.210
77.000
76.676
75.655
46.137
36.285
33.099

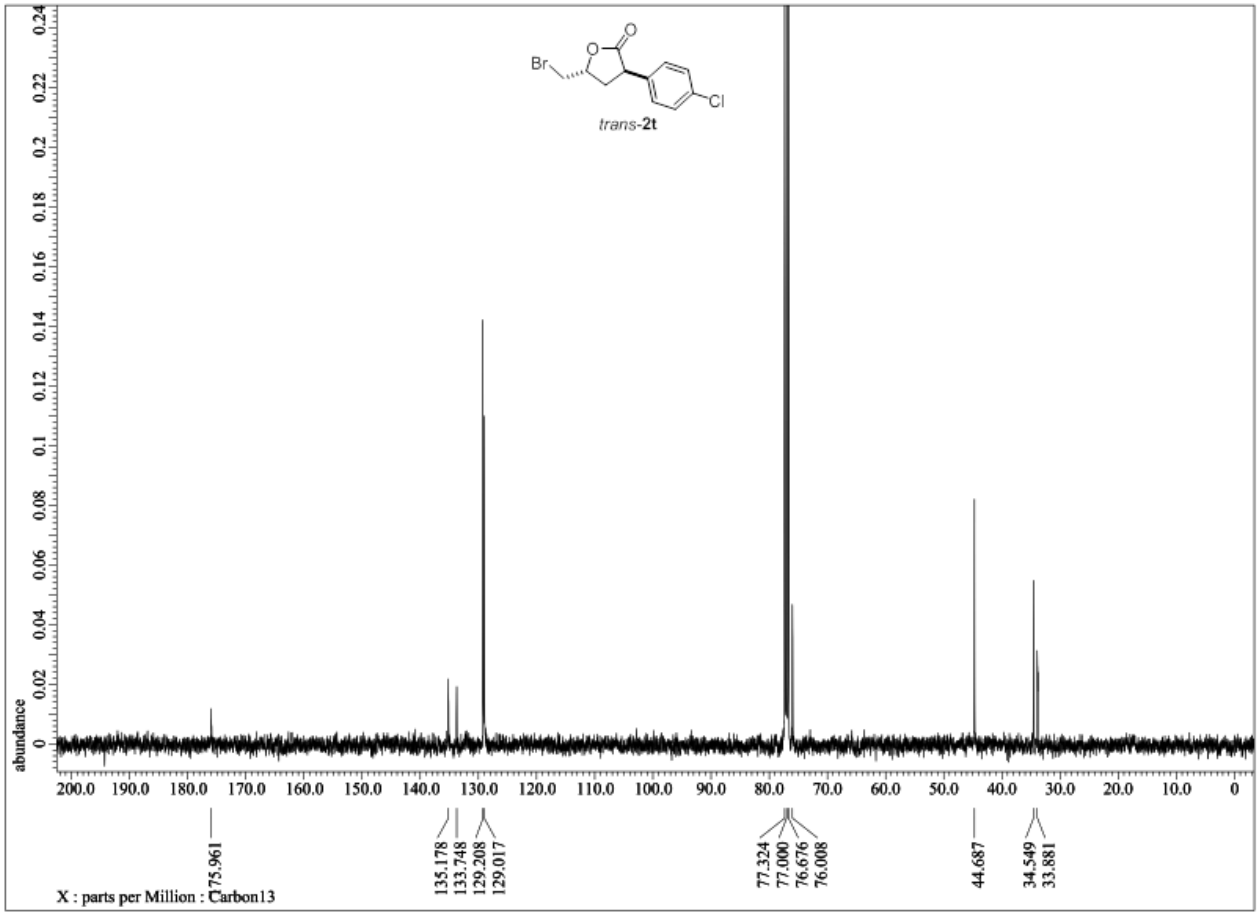

Br
O
O
F
trans-2s
abundance
2.43
2.03
1.00
1.01
2.06
1.01
1.00
7.270
7.264
7.254
7.249
7.241
7.235
7.089
7.083
7.061
7.040
4.914
4.901
4.888
4.880
4.868
4.856
4.062
4.040
4.017
3.619
3.605
2.702
2.693
2.680
2.668
2.593
2.582
2.572
2.559
2.553
2.548
2.538
-0.000
X : parts per Million : Proton

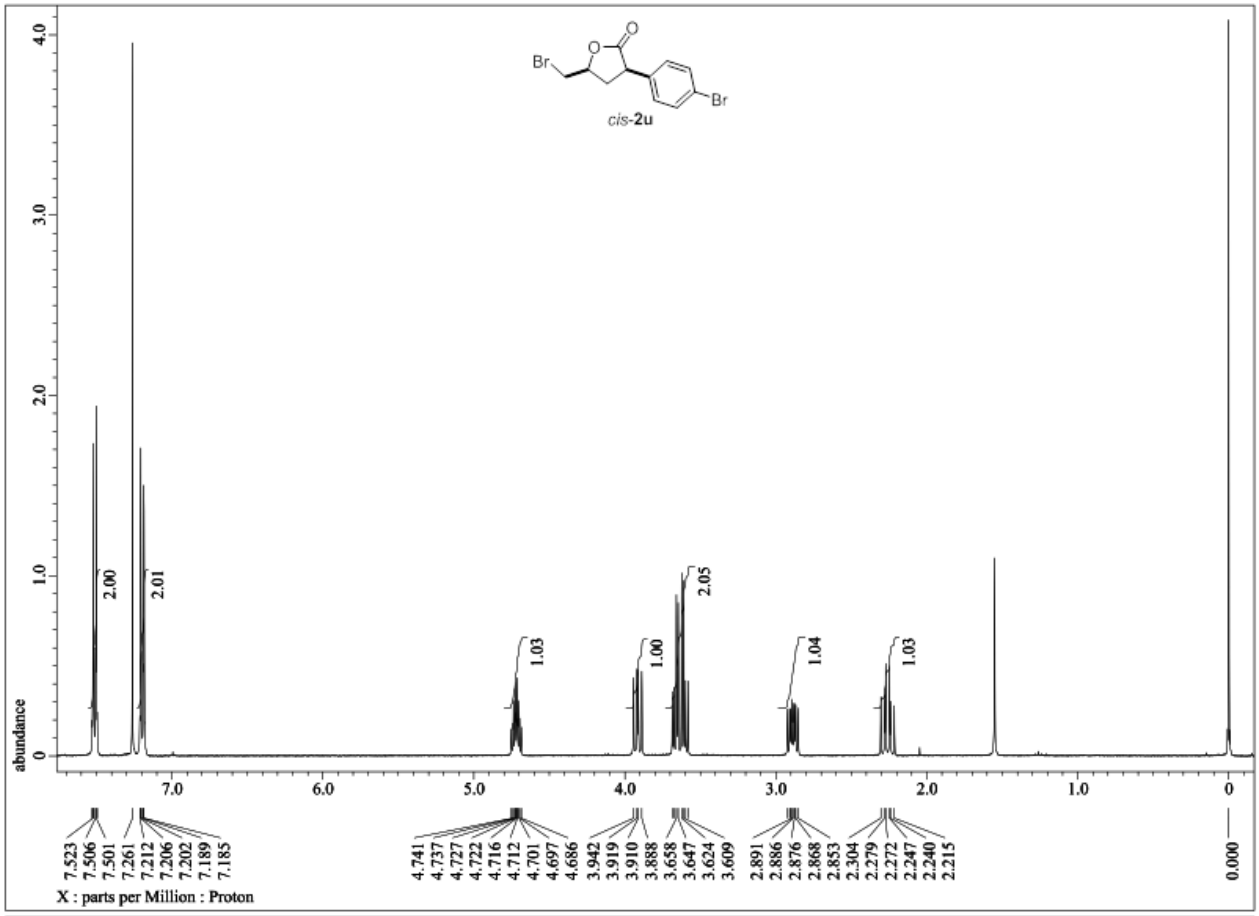

Br
O
O
F
trans-2s
abundance
76.256
163.457
160.949
132.479
129.342
129.265
116.104
115.884
77.324
77.000
76.676
76.008
44.582
34.711
33.881
X : parts per Million : Carbon13

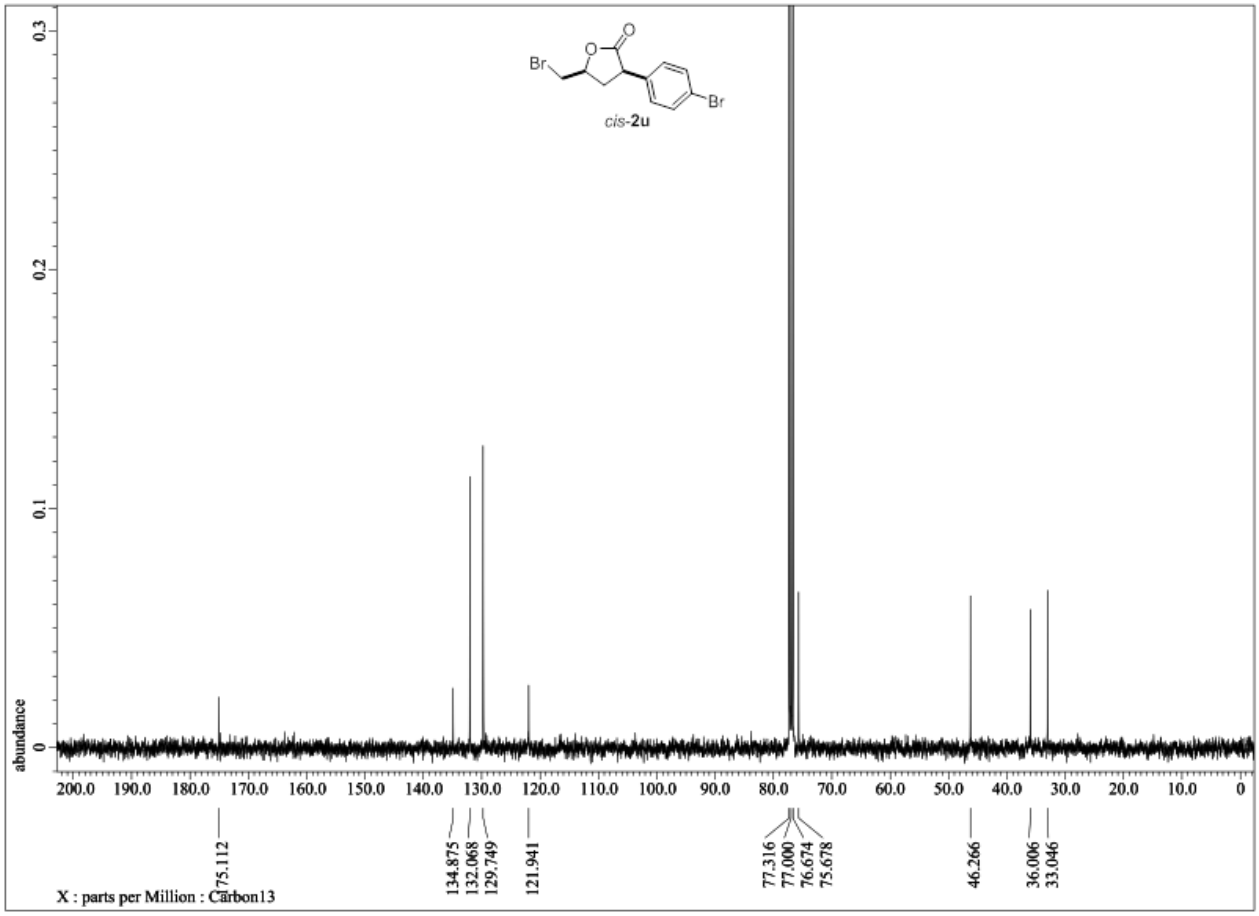

Br
O
O
Cl
cis-2t
abundance
4.0
3.0
2.0
1.0
0
3.03
2.31
1.00
1.00
2.02
1.01
1.02
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.365
7.360
7.349
7.344
7.266
7.261
7.255
7.244
7.239
4.736
4.733
4.722
4.718
4.712
4.707
4.696
4.693
4.681
3.954
3.931
3.922
3.900
3.652
3.641
3.623
3.608
2.883
2.878
2.868
2.860
2.845
2.301
2.276
2.269
2.244
2.237
2.212
0.000
X : parts per Million : Proton

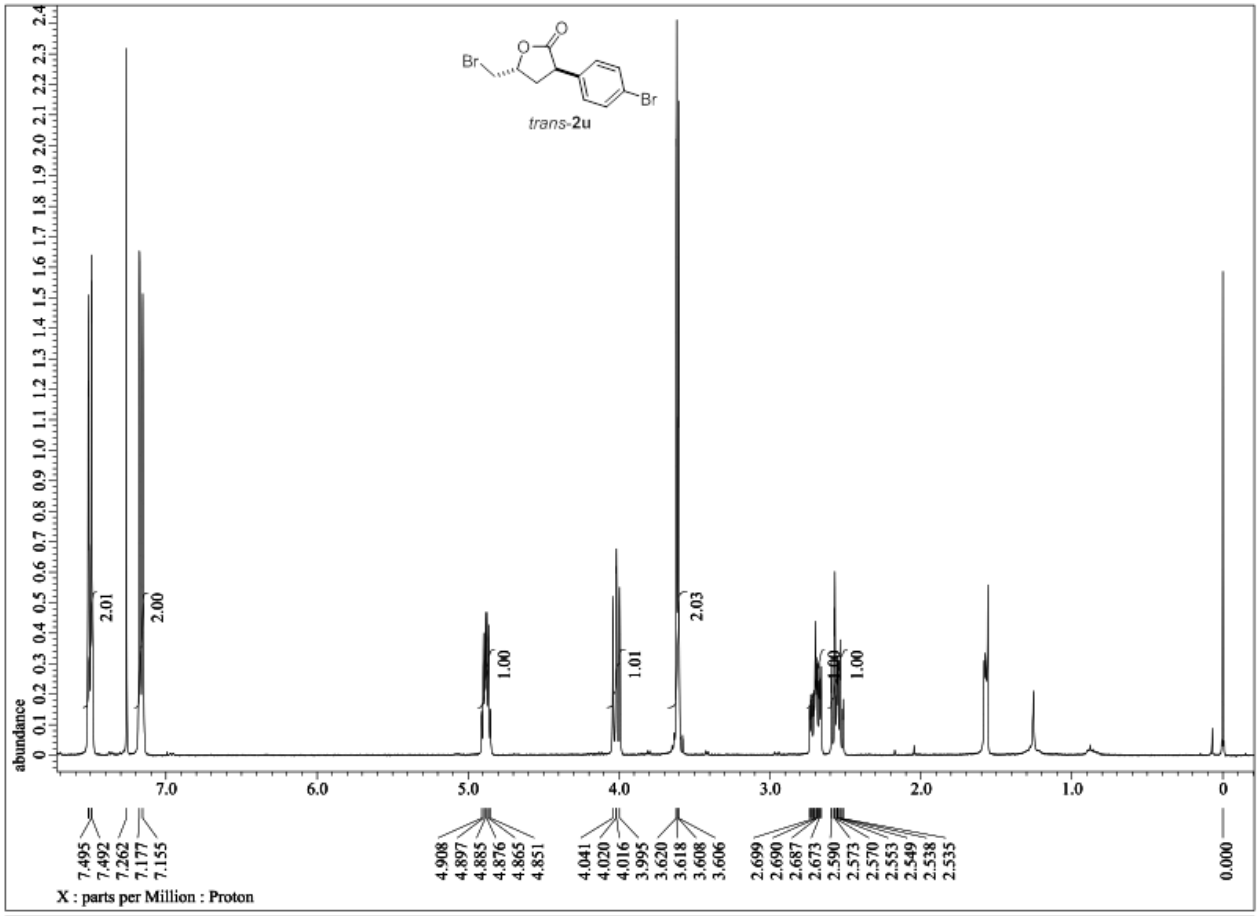

Br
O
O
Cl
cis-2t
abundance
0.3
0.2
0.1
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
75.208
134.357
133.840
129.414
129.107
77.316
77.000
76.674
75.668
46.199
36.073
33.055
X : parts per Million : Carbon13

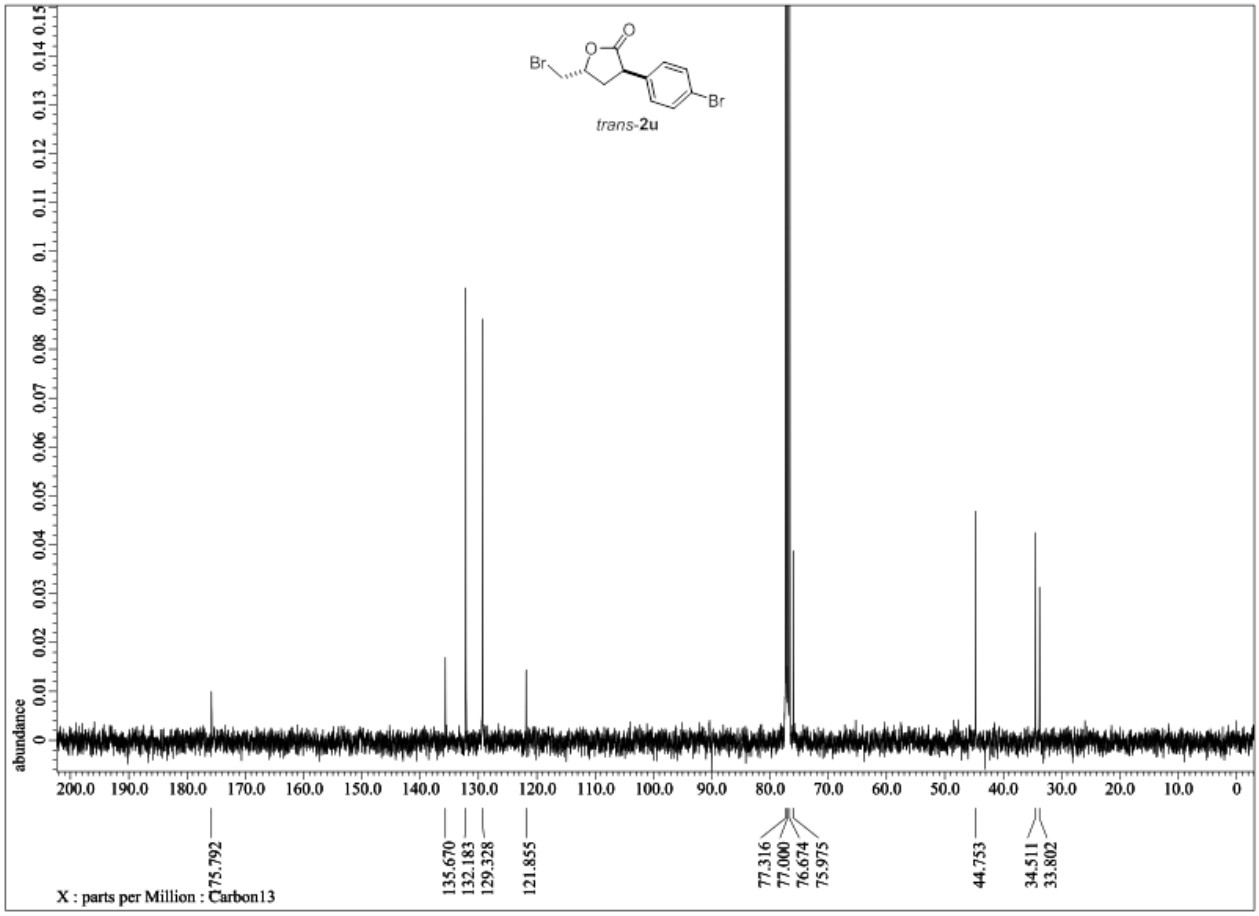

Br
O
O
Cl
trans-2t
abundance
X : parts per Million : Proton
7.364
7.356
7.348
7.343
7.335
7.264
7.237
7.230
7.214
7.208
4.904
4.902
4.896
4.891
4.884
4.879
4.872
4.871
4.865
4.859
4.056
4.035
4.010
3.624
3.616
3.612
3.609
3.604
2.729
2.705
2.703
2.694
2.680
2.668
2.579
2.568
2.564
2.558
2.544
-0.000
2.00
2.03
1.00
1.00
2.05
1.00
1.00

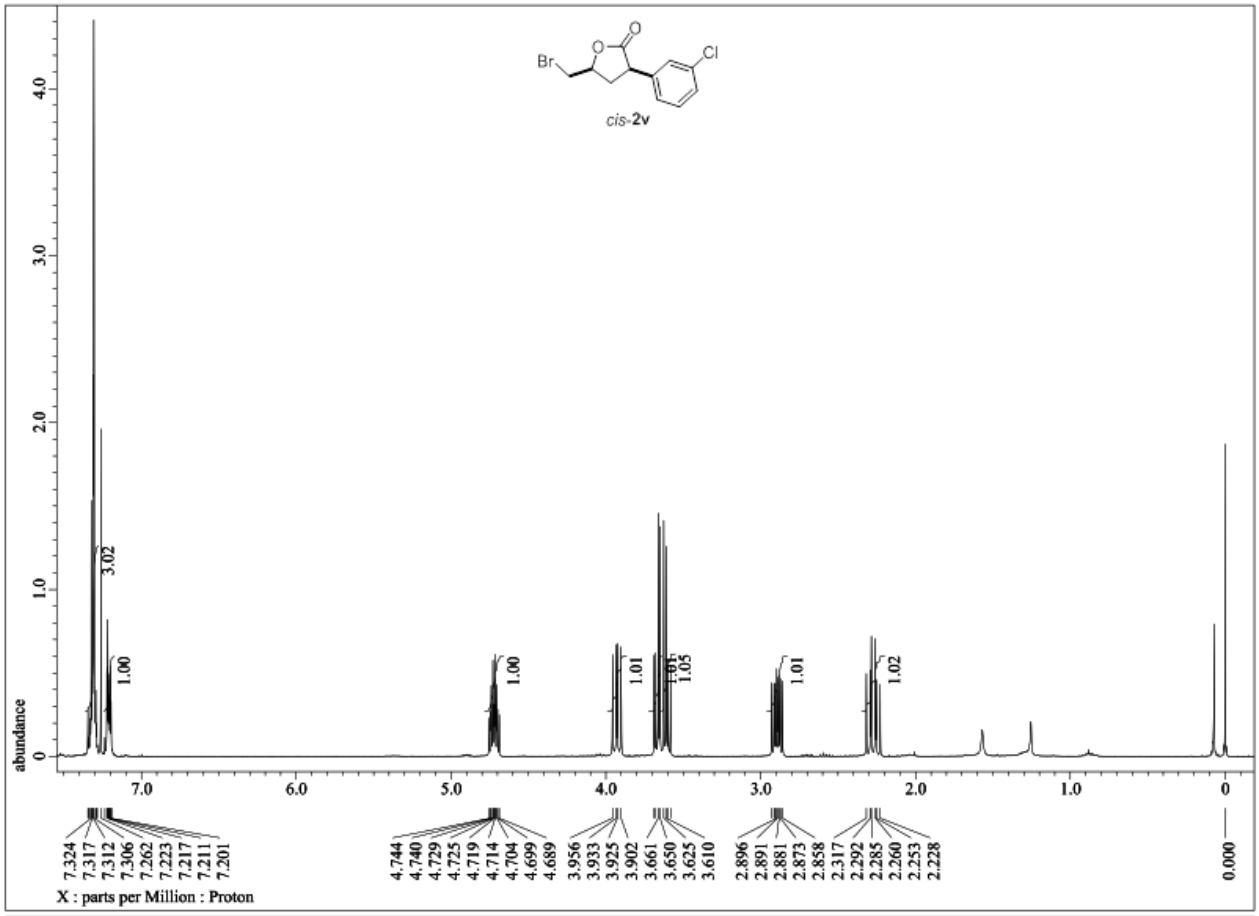

Br
O
O
Cl
trans-2t
abundance
X : parts per Million : Carbon13
175.961
135.178
133.748
129.208
129.017
77.324
77.000
76.676
76.008
44.687
34.549
33.881

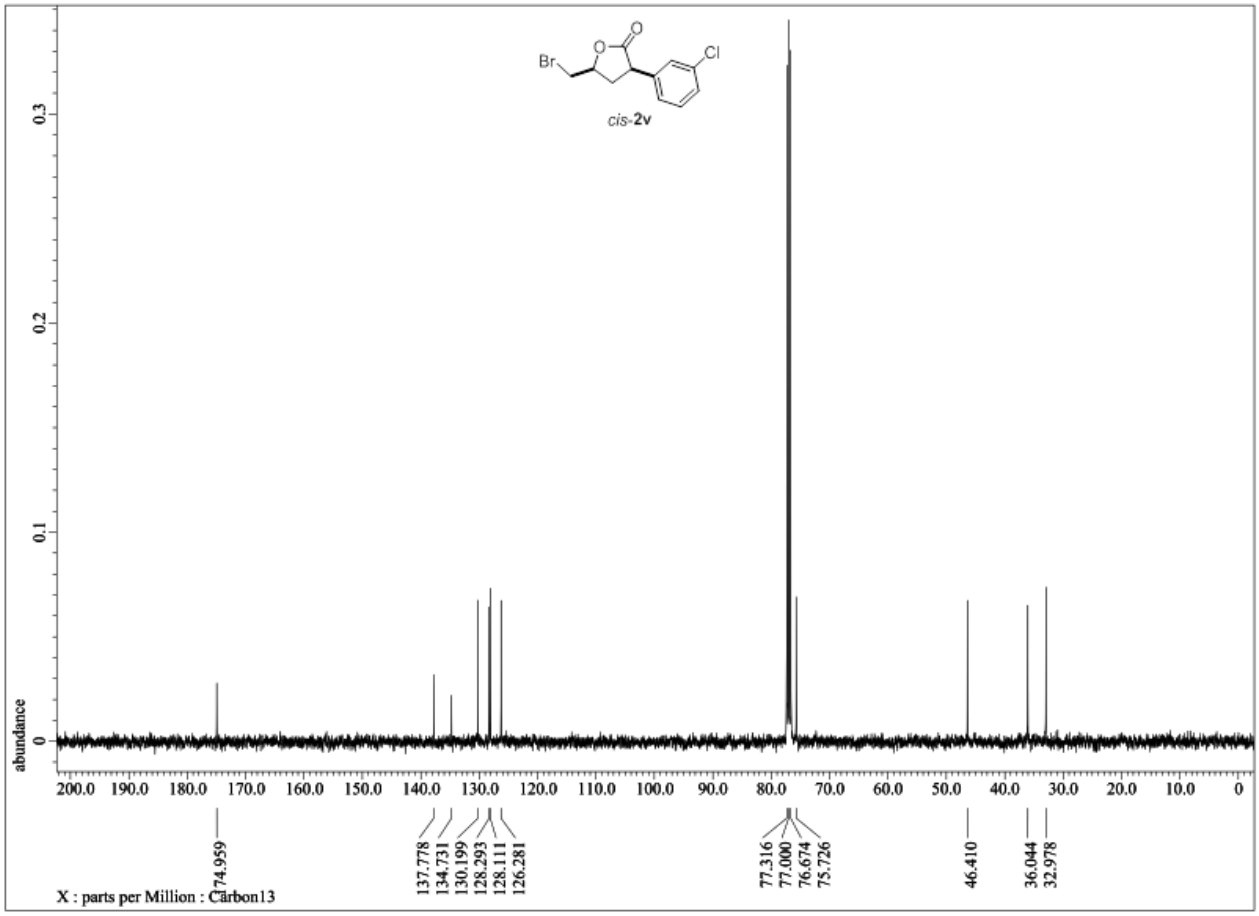

cis-2u
abundance
X : parts per Million : Proton
2.00
2.01
1.03
1.00
2.05
1.04
1.03
7.523
7.506
7.501
7.261
7.212
7.206
7.202
7.189
7.185
4.741
4.737
4.727
4.722
4.716
4.712
4.701
4.697
4.686
3.942
3.919
3.910
3.888
3.658
3.647
3.624
3.609
2.891
2.886
2.876
2.868
2.853
2.304
2.279
2.272
2.247
2.240
2.215
0.000

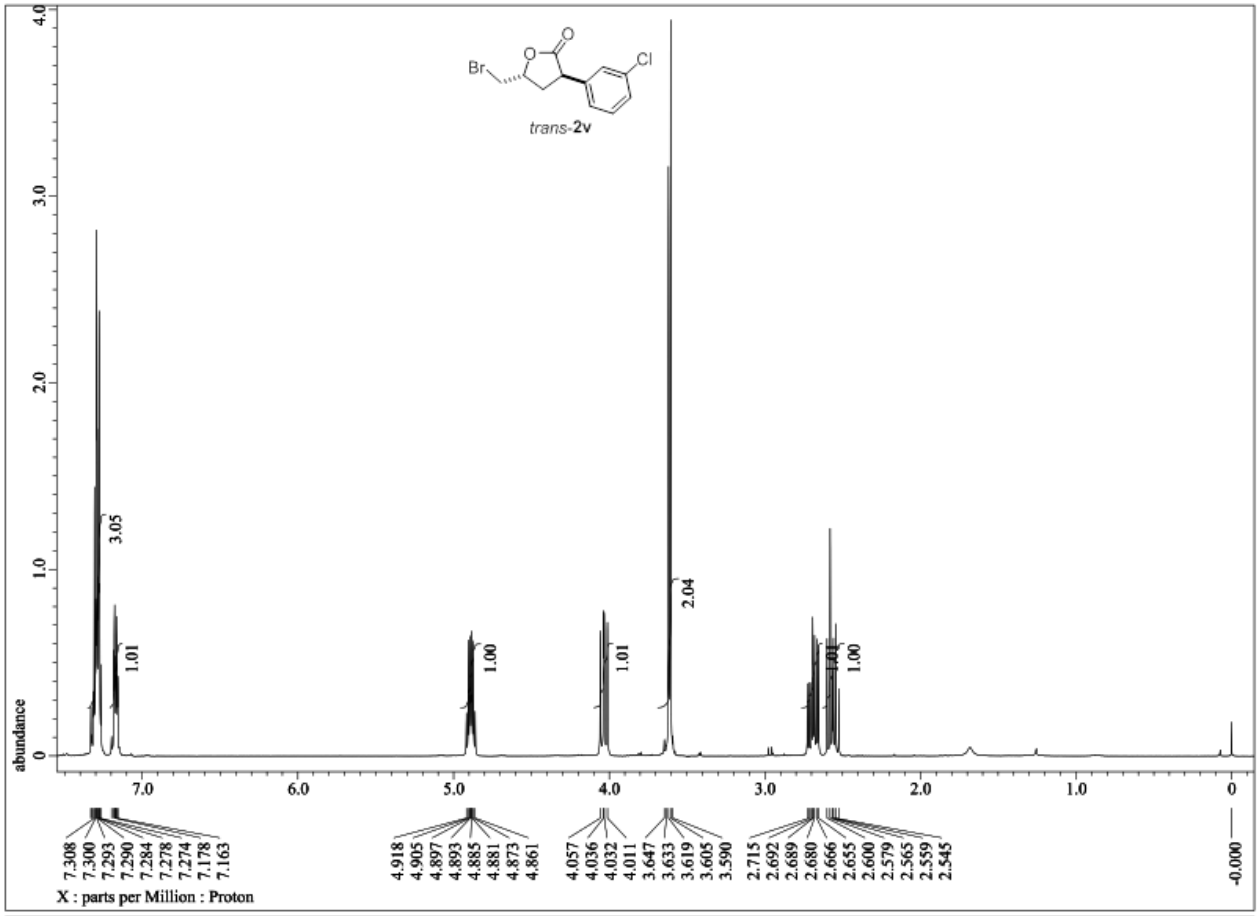

cis-2u
abundance
X : parts per Million : Carbon13
175.112
134.875
132.068
129.749
121.941
77.316
77.000
76.674
75.678
46.266
36.006
33.046

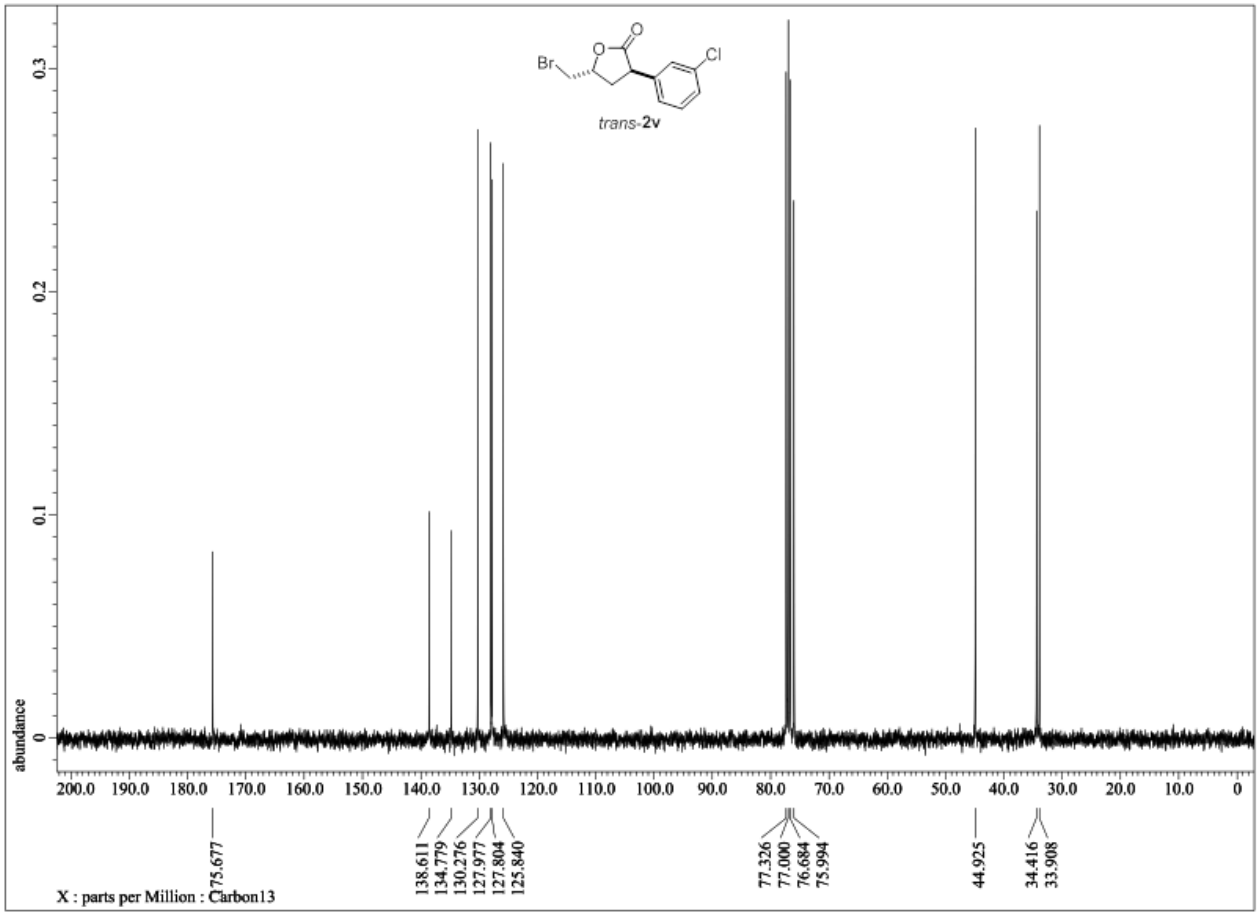

Br
O
O
Br
trans-2u
abundance
2.01
2.00
1.00
1.01
2.03
1.00
1.00
7.495
7.492
7.262
7.177
7.155
4.908
4.897
4.885
4.876
4.865
4.851
4.041
4.020
4.016
3.995
3.620
3.618
3.608
3.606
2.699
2.690
2.687
2.673
2.590
2.573
2.570
2.553
2.549
2.538
2.535
0.000
X : parts per Million : Proton

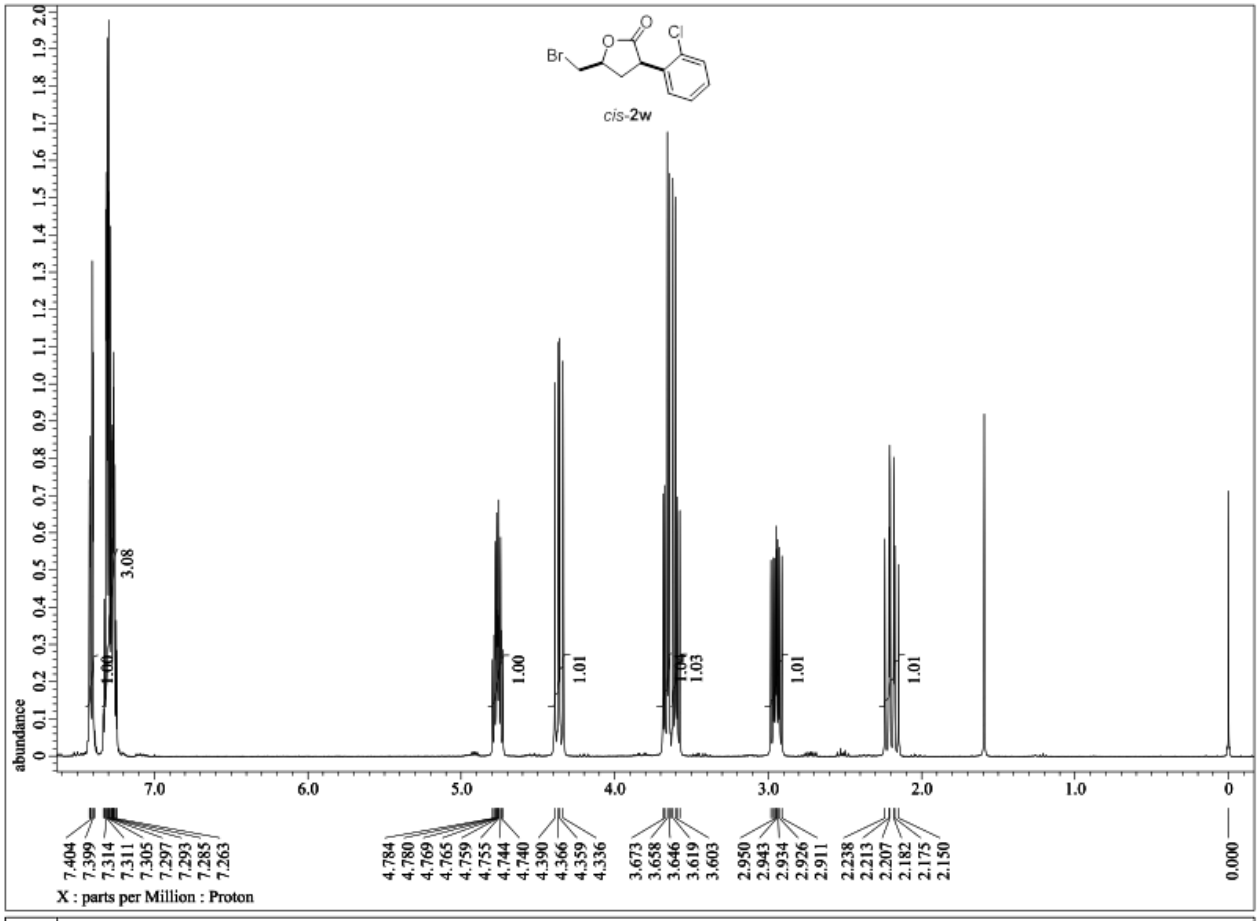

Br
O
O
Br
trans-2u
abundance
75.792
135.670
132.183
129.328
121.855
77.316
77.000
76.674
75.975
44.753
34.511
33.802
X : parts per Million : Carbon13

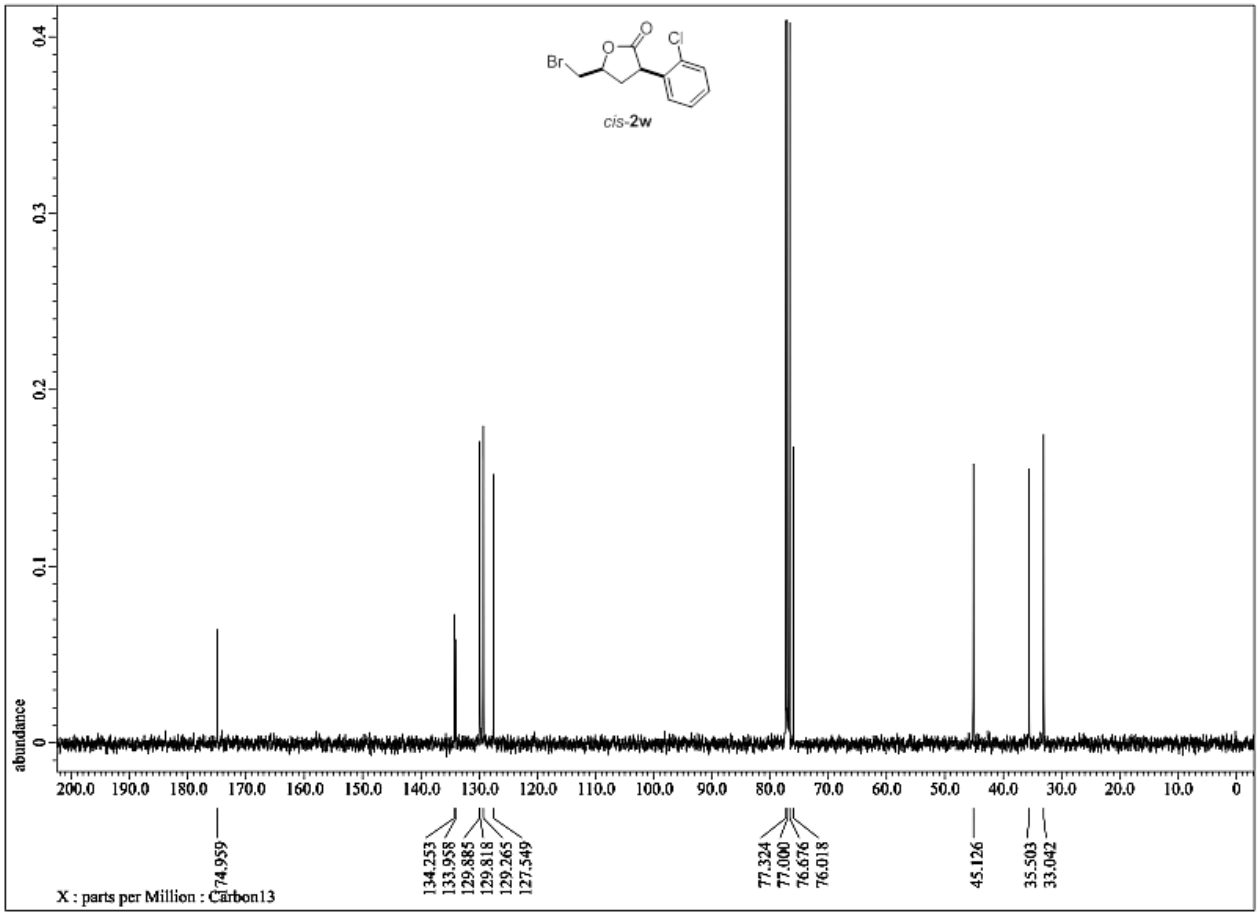

Br
O
O
Cl
cis-2v
abundance
4.0
3.0
2.0
1.0
0
3.02
1.00
1.00
1.01
1.05
1.01
1.02
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.324
7.317
7.312
7.306
7.262
7.223
7.217
7.211
7.201
4.744
4.740
4.729
4.725
4.719
4.714
4.704
4.699
4.689
3.956
3.933
3.925
3.902
3.661
3.650
3.625
3.610
2.896
2.891
2.881
2.873
2.858
2.317
2.292
2.285
2.260
2.253
2.228
0.000
X : parts per Million : Proton

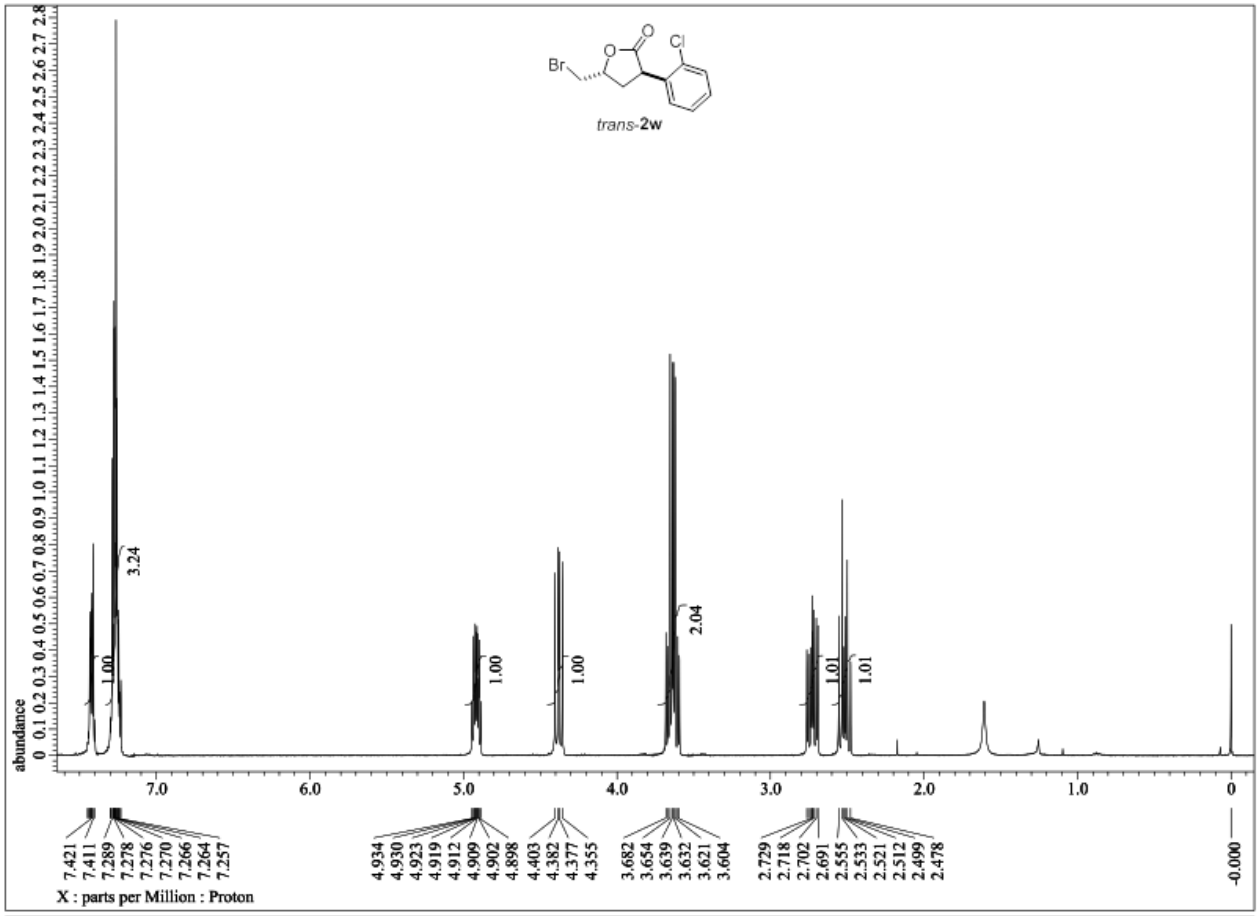

Br
O
O
Cl
cis-2v
abundance
0.3
0.2
0.1
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
174.959
137.778
134.731
130.199
128.293
128.111
126.281
77.316
77.000
76.674
75.726
46.410
36.044
32.978
X : parts per Million : Carbon13

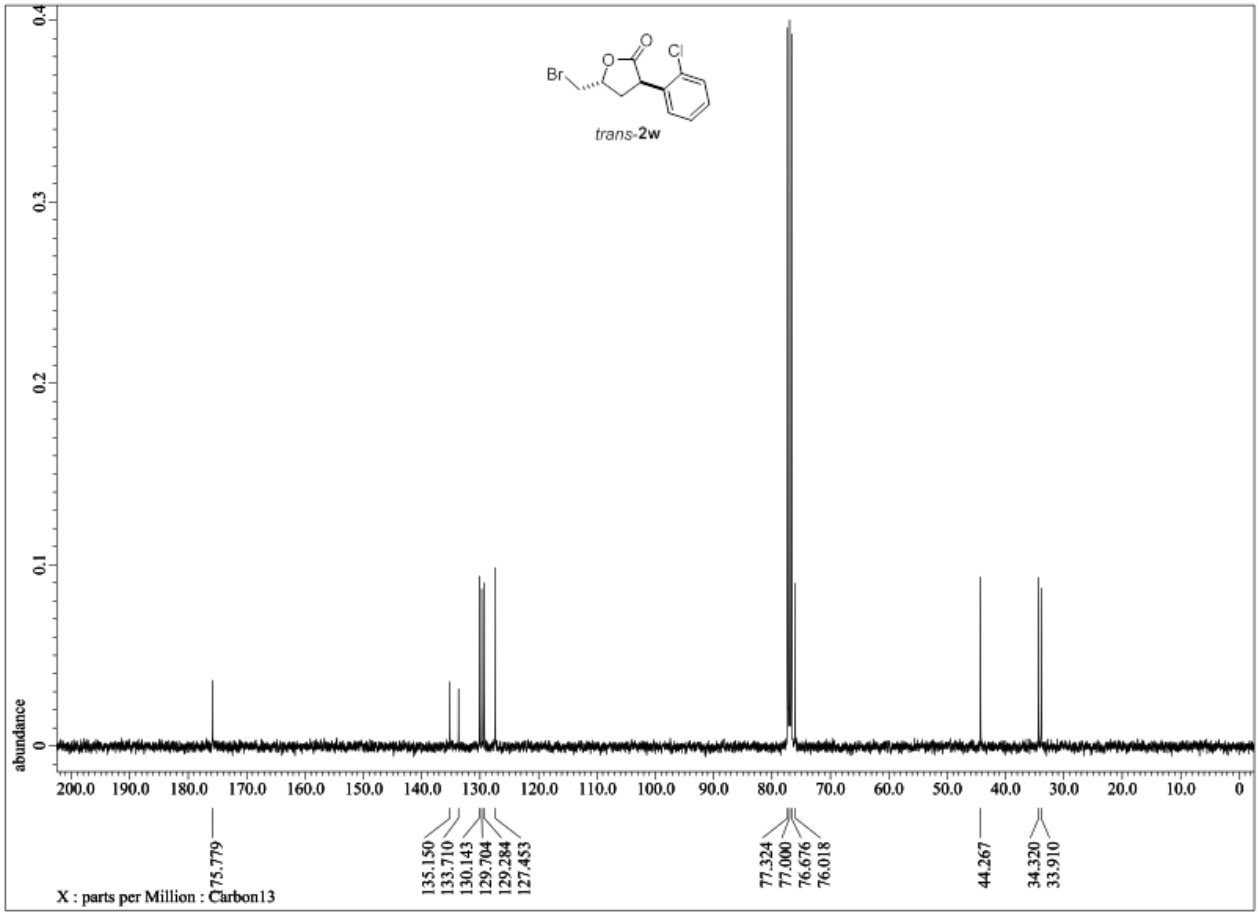

trans-2v
abundance
X : parts per Million : Proton

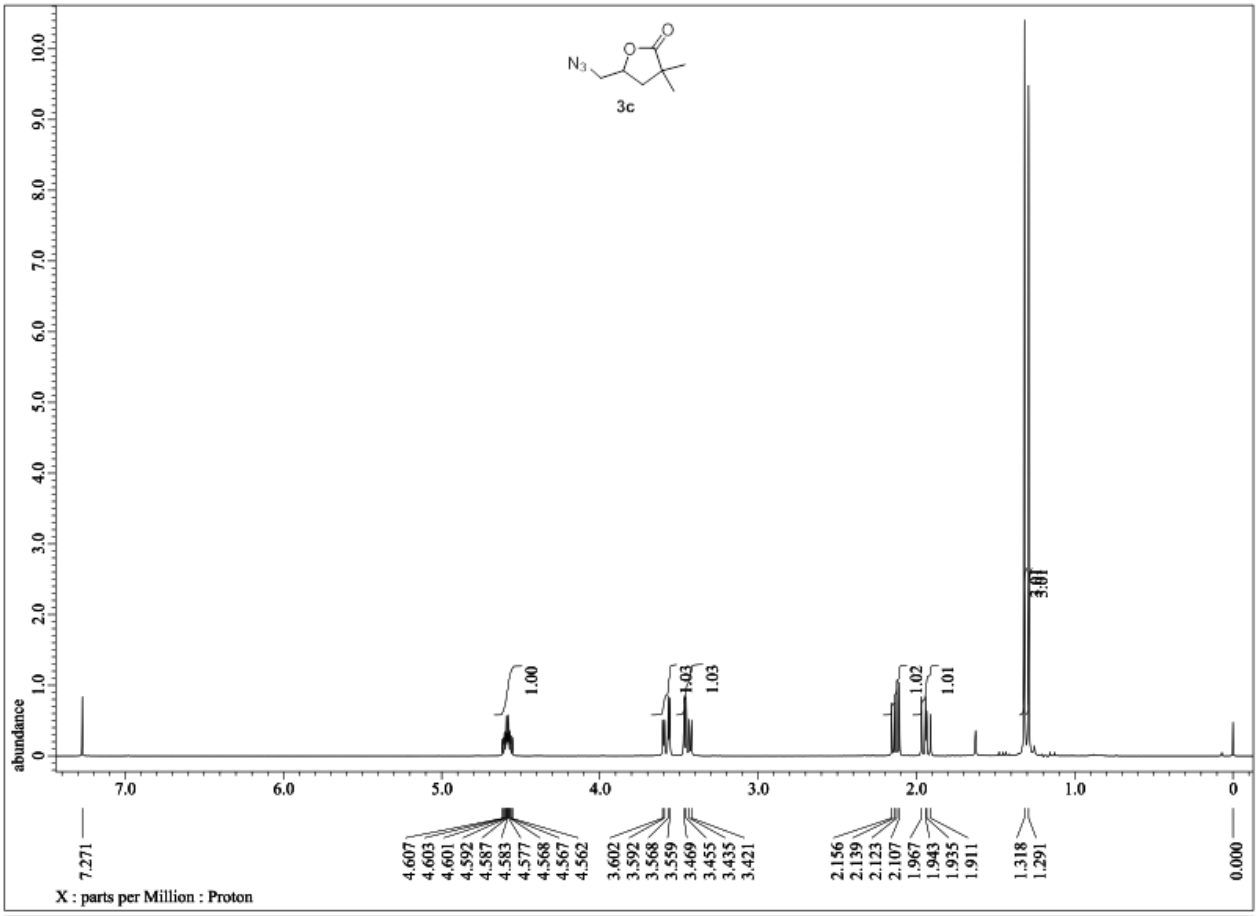

trans-2v
abundance
X : parts per Million : Carbon13

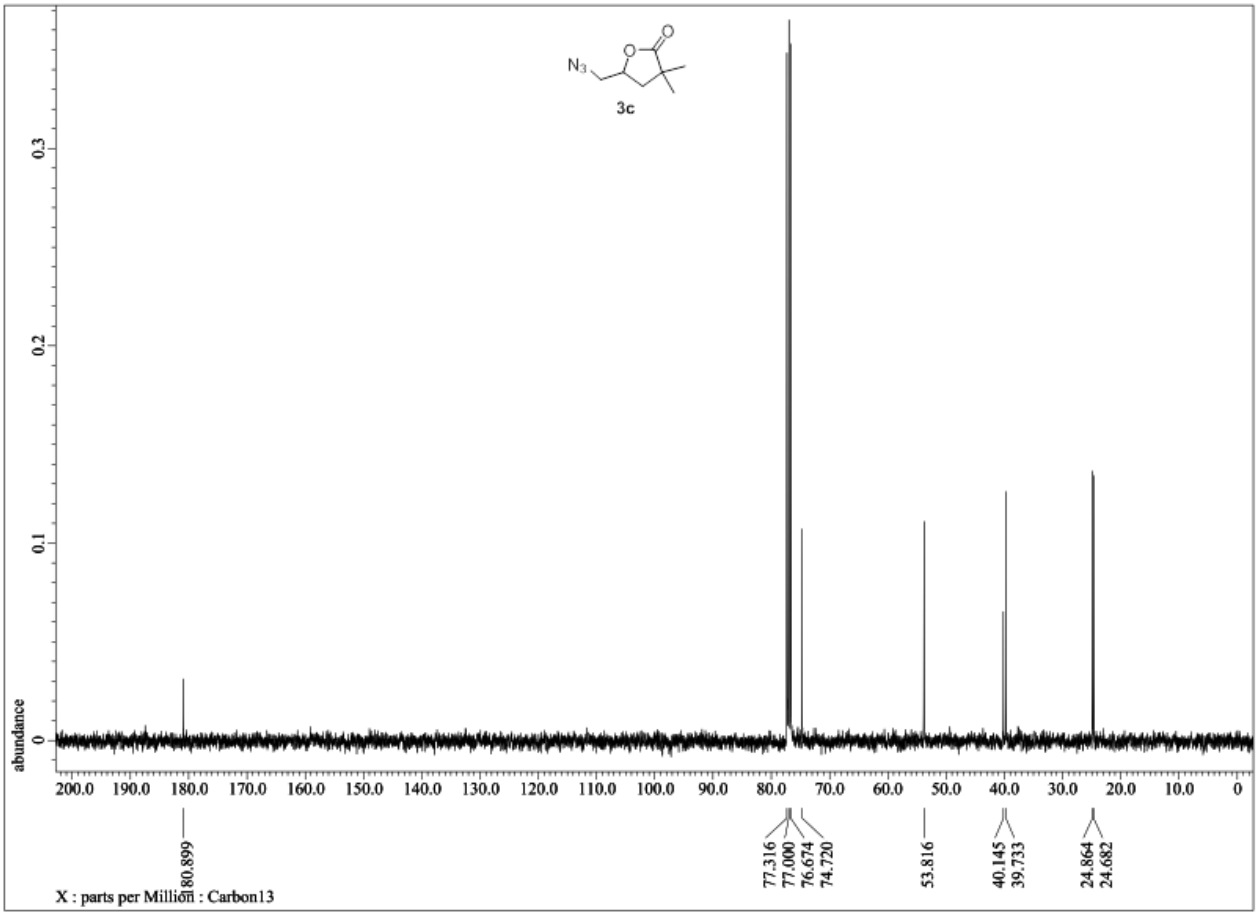

cis-2w
abundance
3.08
1.00
1.01
1.04
1.03
1.01
1.01
7.404
7.399
7.314
7.311
7.305
7.297
7.293
7.285
7.263
4.784
4.780
4.769
4.765
4.759
4.755
4.744
4.740
4.390
4.366
4.359
4.336
3.673
3.658
3.646
3.619
3.603
2.950
2.943
2.934
2.926
2.911
2.238
2.213
2.207
2.182
2.175
2.150
0.000
X : parts per Million : Proton

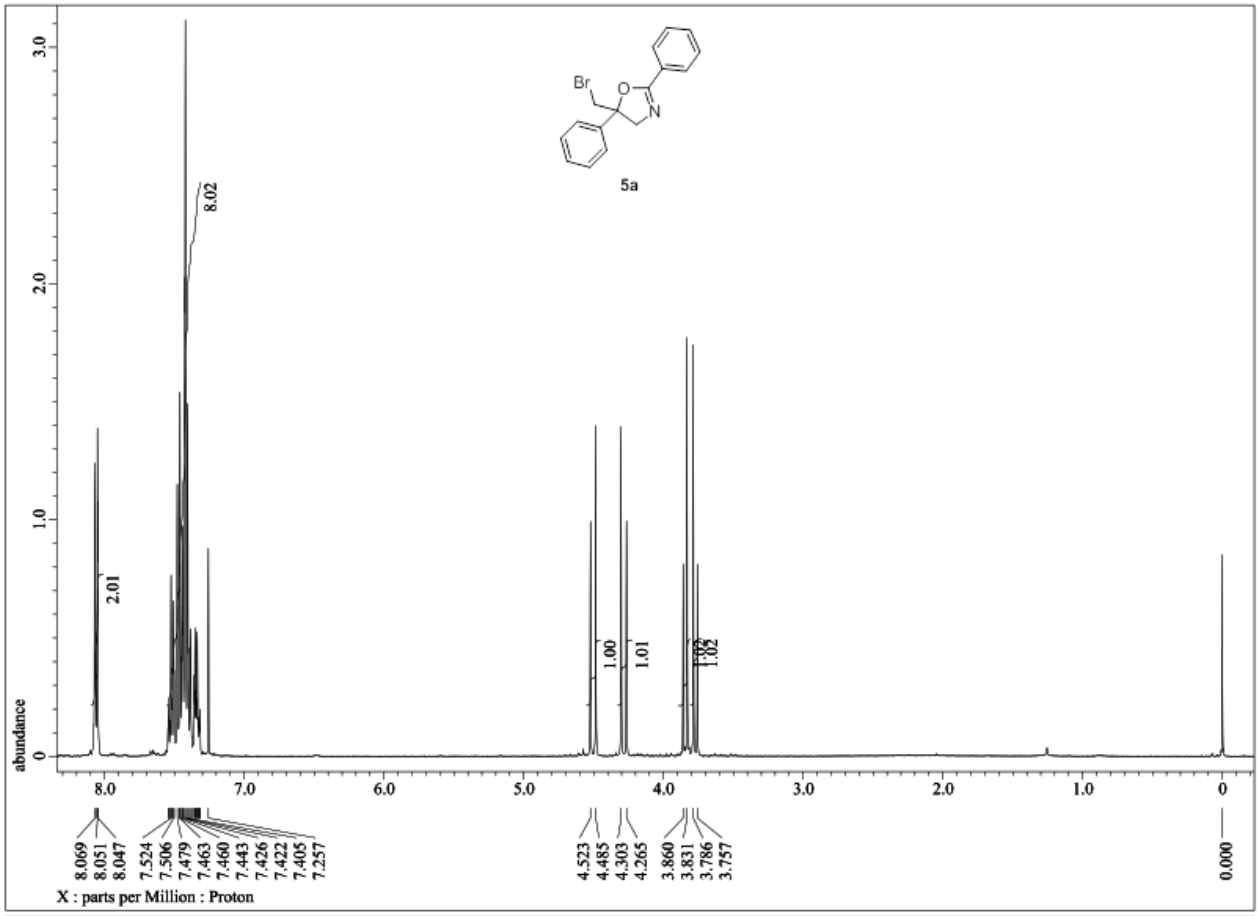

cis-2w
abundance
74.959
134.253
133.958
129.885
129.818
129.265
127.549
77.324
77.000
76.676
76.018
45.126
35.503
33.042
X : parts per Million : Carbon13

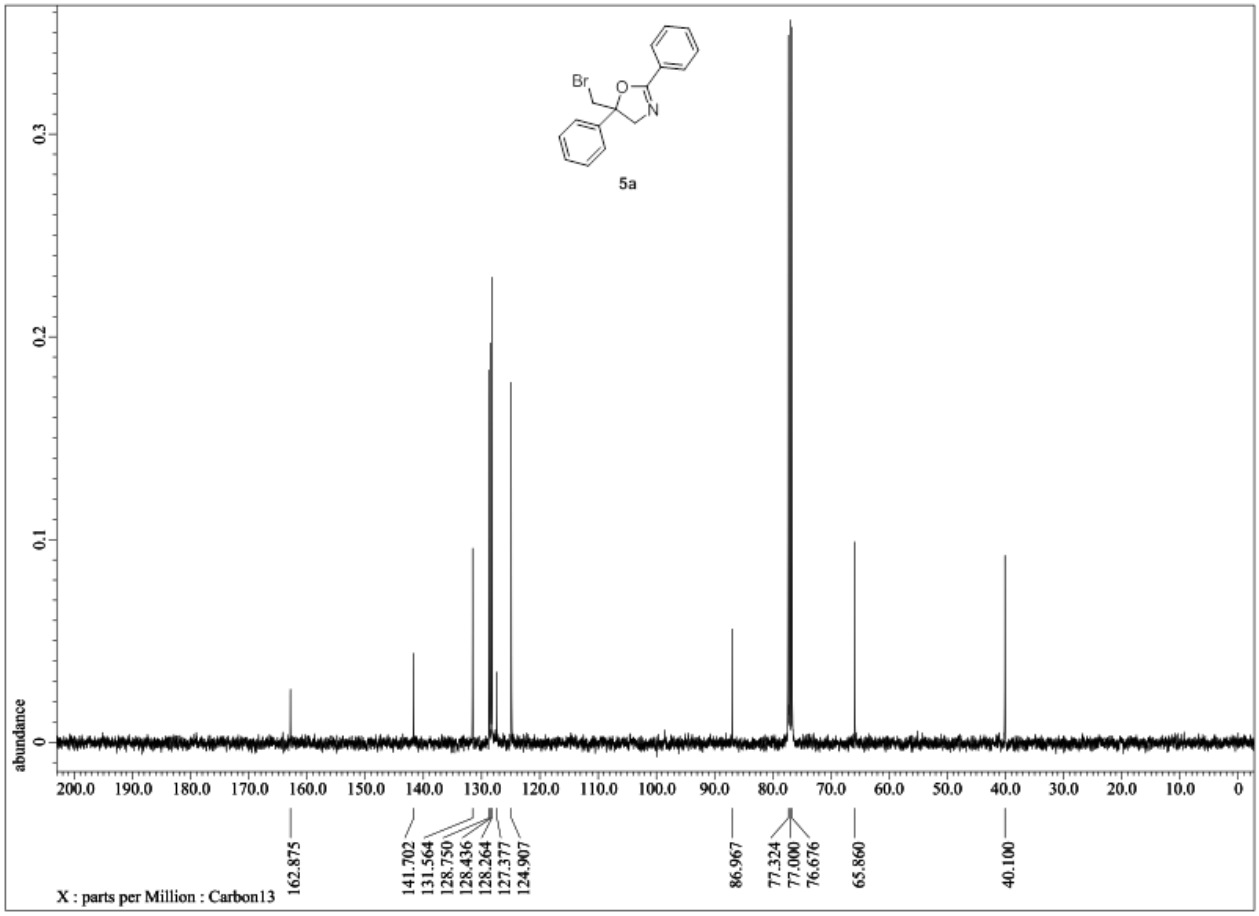

trans-2w
abundance
X : parts per Million : Proton

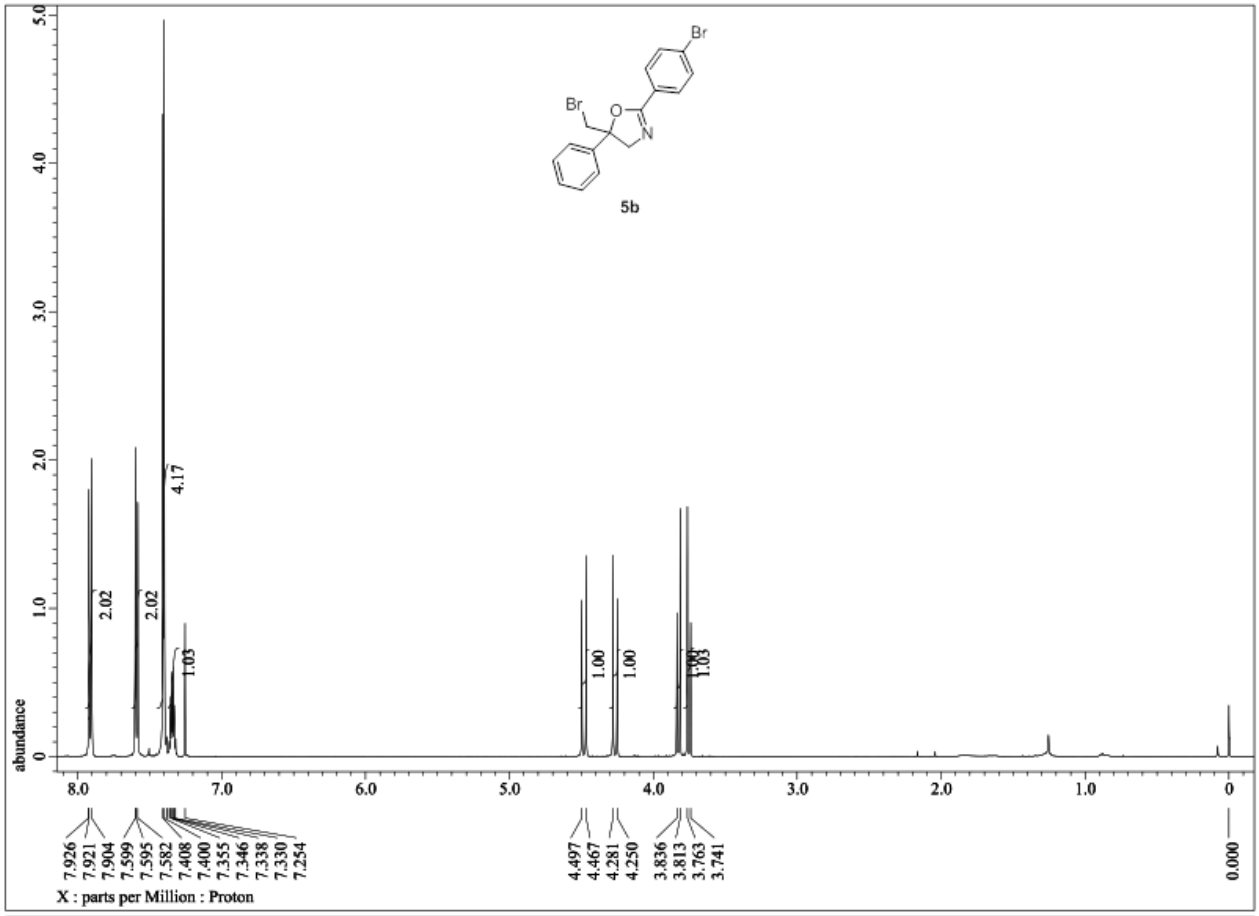

trans-2w
abundance
X : parts per Million : Carbon13

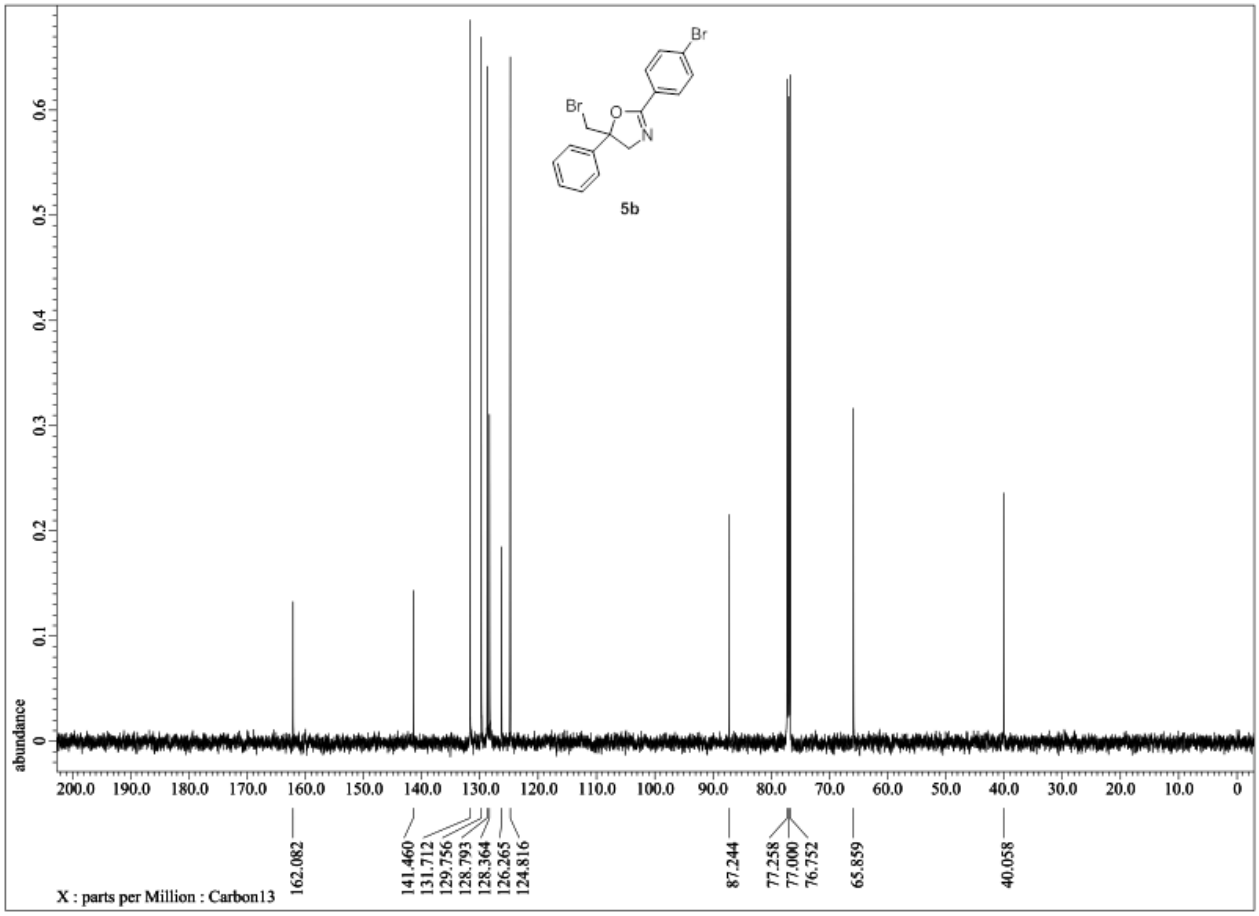

3c
abundance
7.271
4.607
4.603
4.601
4.592
4.587
4.583
4.577
4.568
4.567
4.562
3.602
3.592
3.568
3.559
3.469
3.455
3.435
3.421
2.156
2.139
2.123
2.107
1.967
1.943
1.935
1.911
1.318
1.291
0.000
1.00
1.03
1.02
1.01
X : parts per Million : Proton

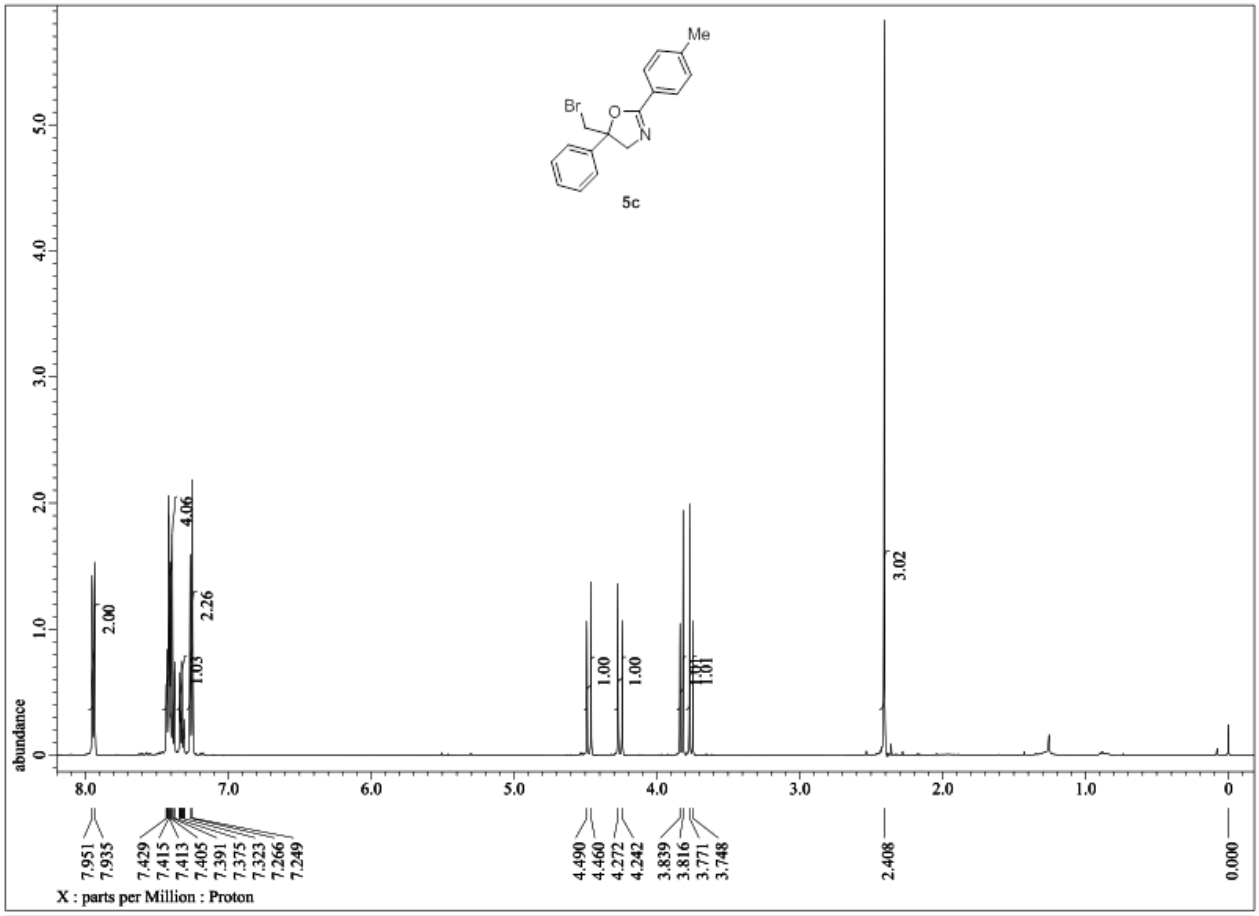

3c
abundance
80.899
77.316
77.000
76.674
74.720
53.816
40.145
39.733
24.864
24.682
X : parts per Million : Carbon13

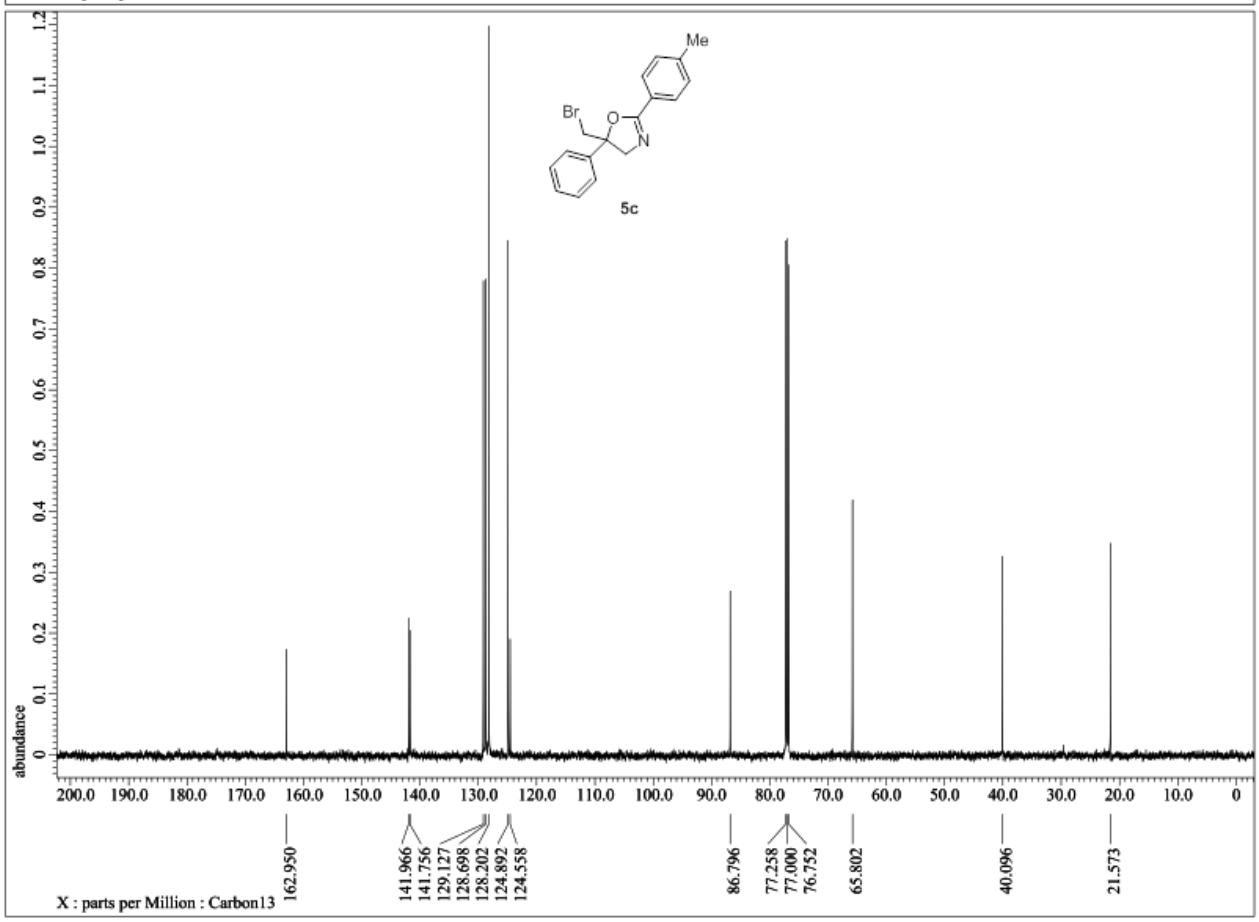

Br
O
N
5a
8.02
2.01
1.00
1.01
1.02
abundance
8.069
8.051
8.047
7.524
7.506
7.479
7.463
7.460
7.443
7.426
7.422
7.405
7.257
4.523
4.485
4.303
4.265
3.860
3.831
3.786
3.757
0.000
X : parts per Million : Proton

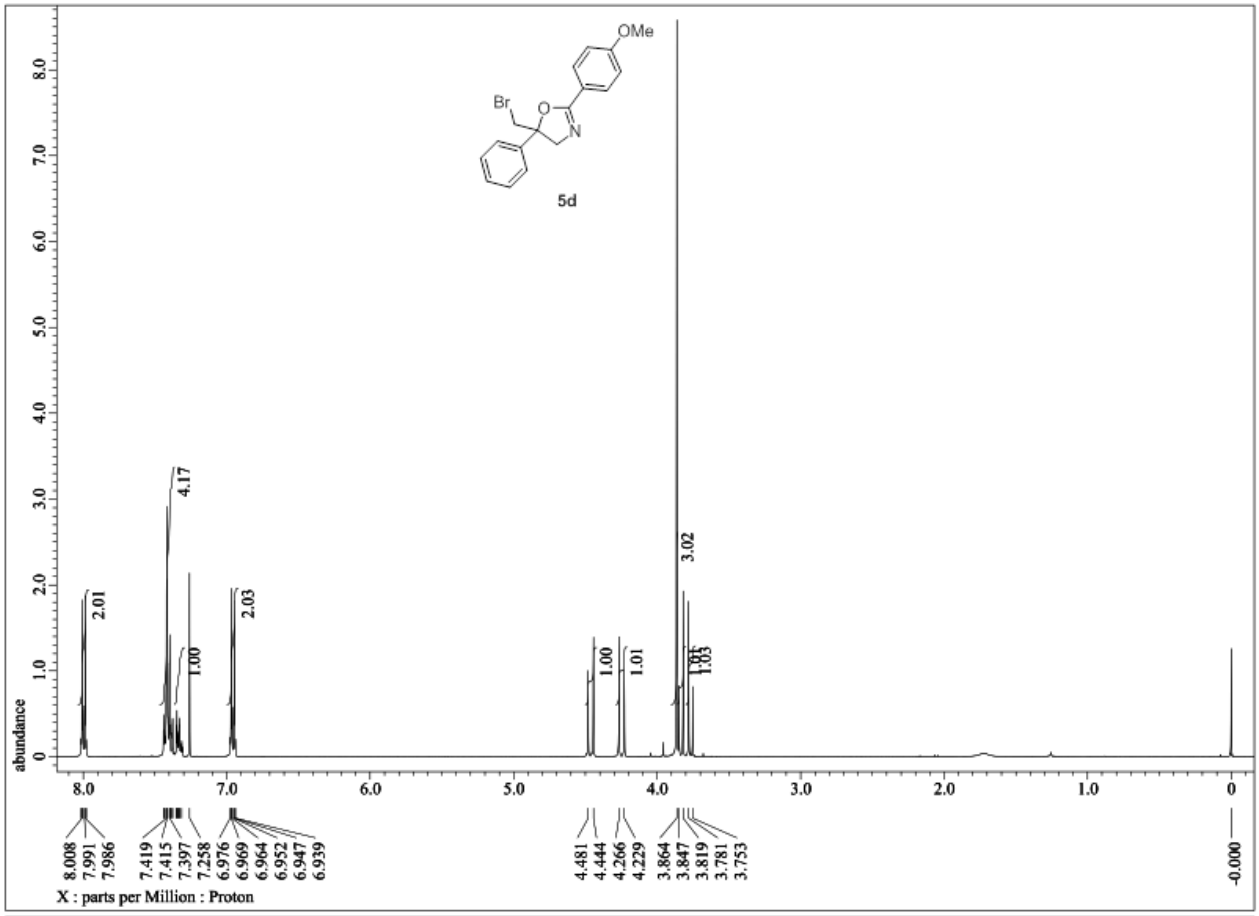

Br
O
N
5a
abundance
162.875
141.702
131.564
128.750
128.436
128.264
127.377
124.907
86.967
77.324
77.000
76.676
65.860
40.100
X : parts per Million : Carbon13

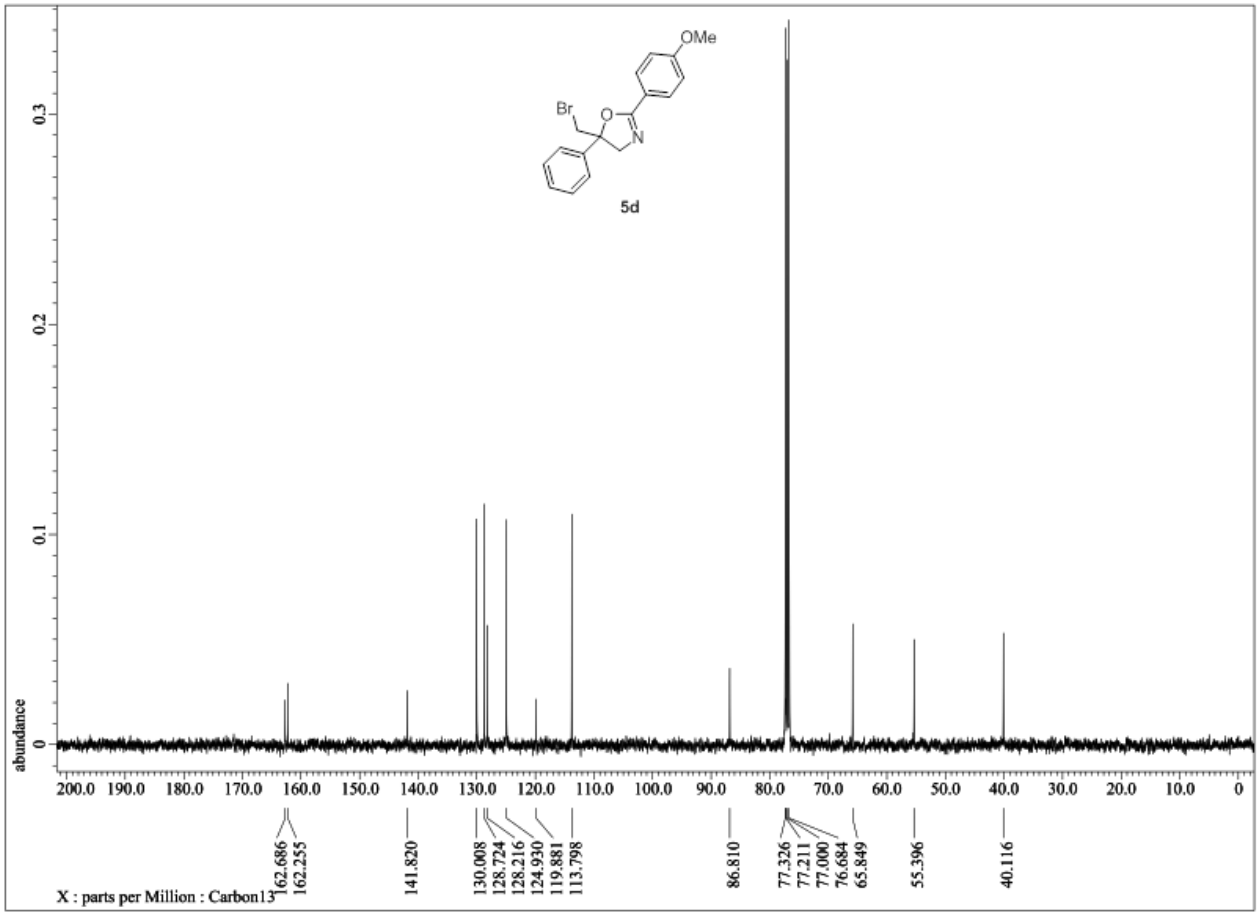

Br
Br
O
N
5b
abundance
5.0
4.0
3.0
2.0
1.0
0
2.02
2.02
4.17
1.03
1.00
1.00
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.926
7.921
7.904
7.599
7.595
7.582
7.408
7.400
7.355
7.346
7.338
7.330
7.254
4.497
4.467
4.281
4.250
3.836
3.813
3.763
3.741
0.000
X : parts per Million : Proton

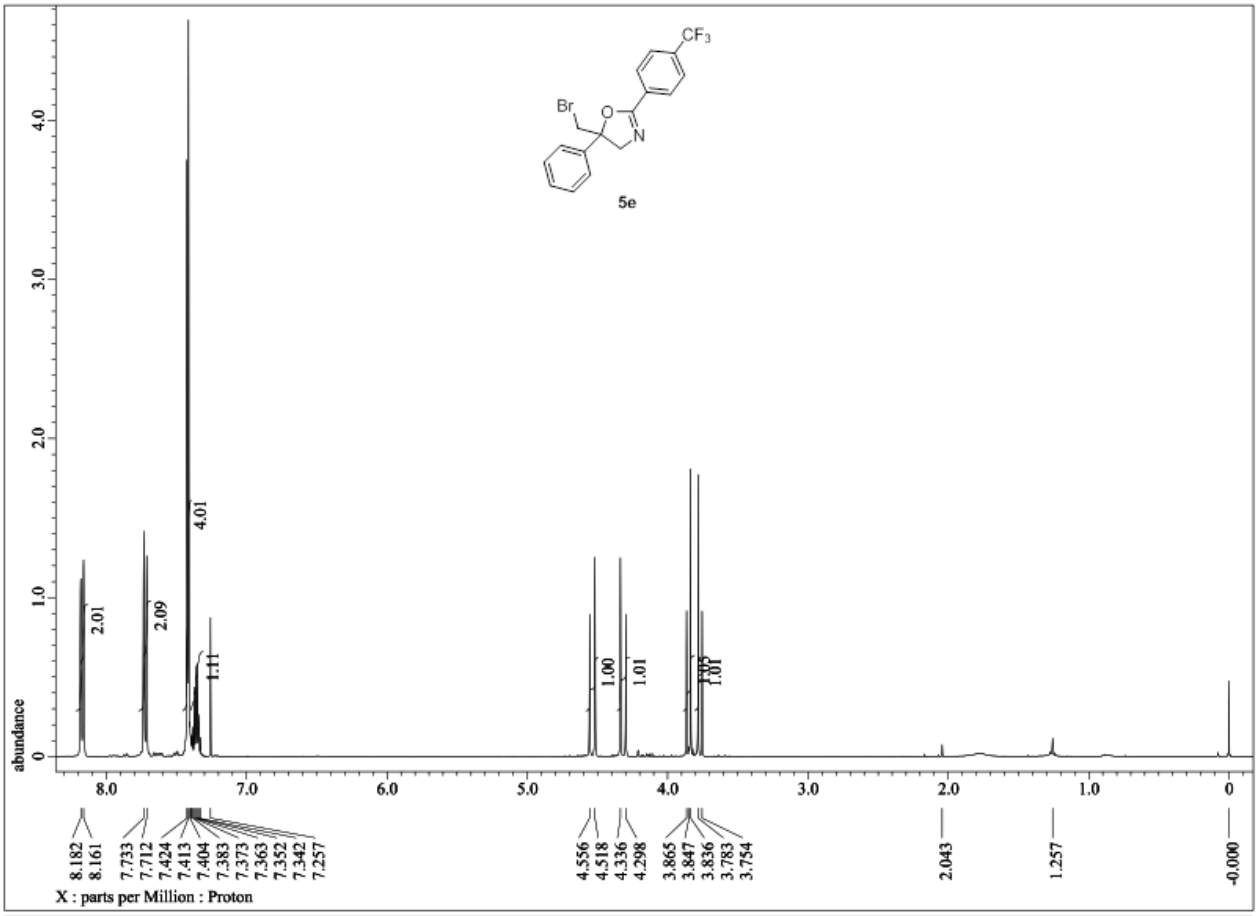

Br
Br
O
N
5b
abundance
0.6
0.5
0.4
0.3
0.2
0.1
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
162.082
141.460
131.712
129.756
128.793
128.364
126.265
124.816
87.244
77.258
77.000
76.752
65.859
40.058
X : parts per Million : Carbon13

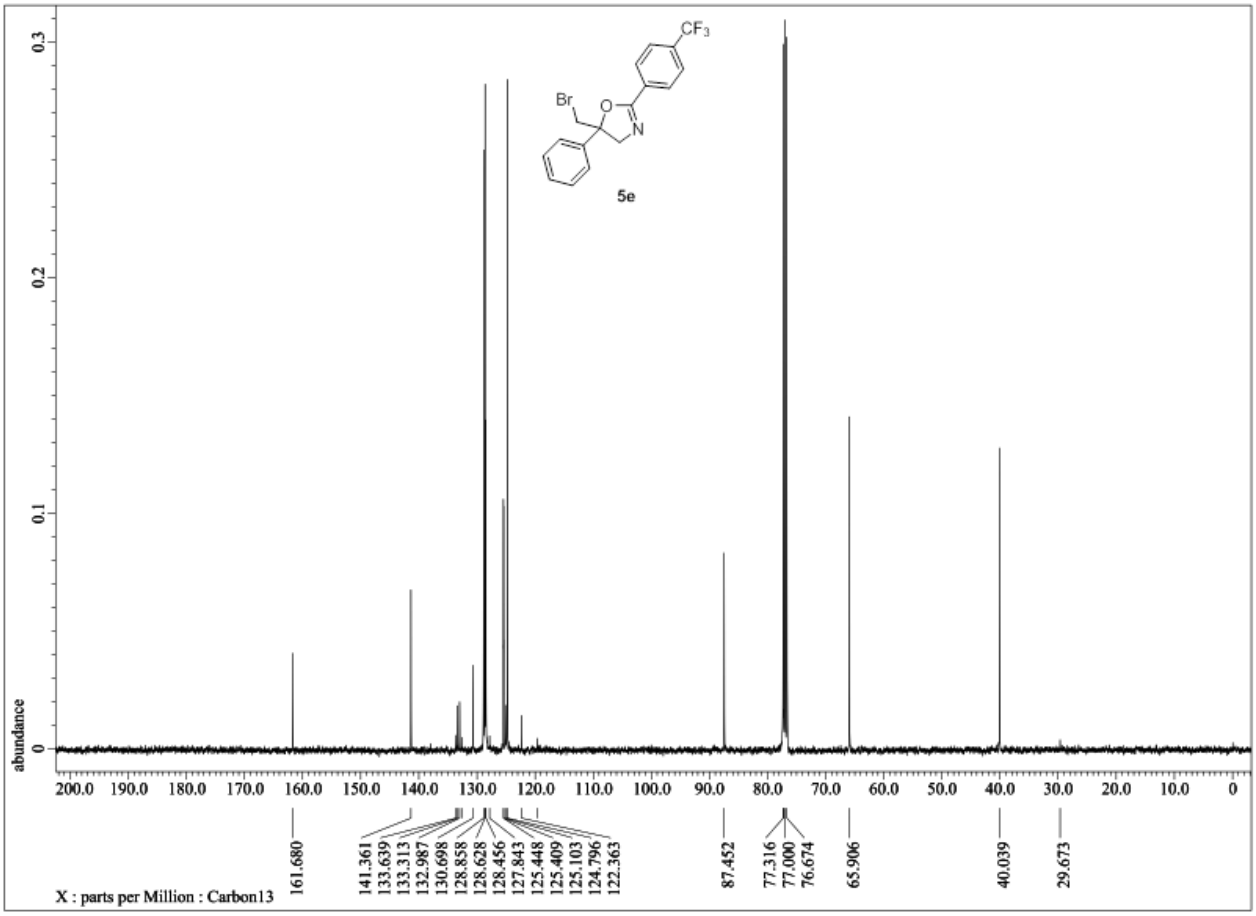

Me
Br
O
N
5c
abundance
X : parts per Million : Proton
2.00
4.06
2.26
1.03
1.00
1.00
1.01
1.01
3.02
7.951
7.935
7.429
7.415
7.413
7.405
7.391
7.375
7.323
7.266
7.249
4.490
4.460
4.272
4.242
3.839
3.816
3.771
3.748
2.408
0.000

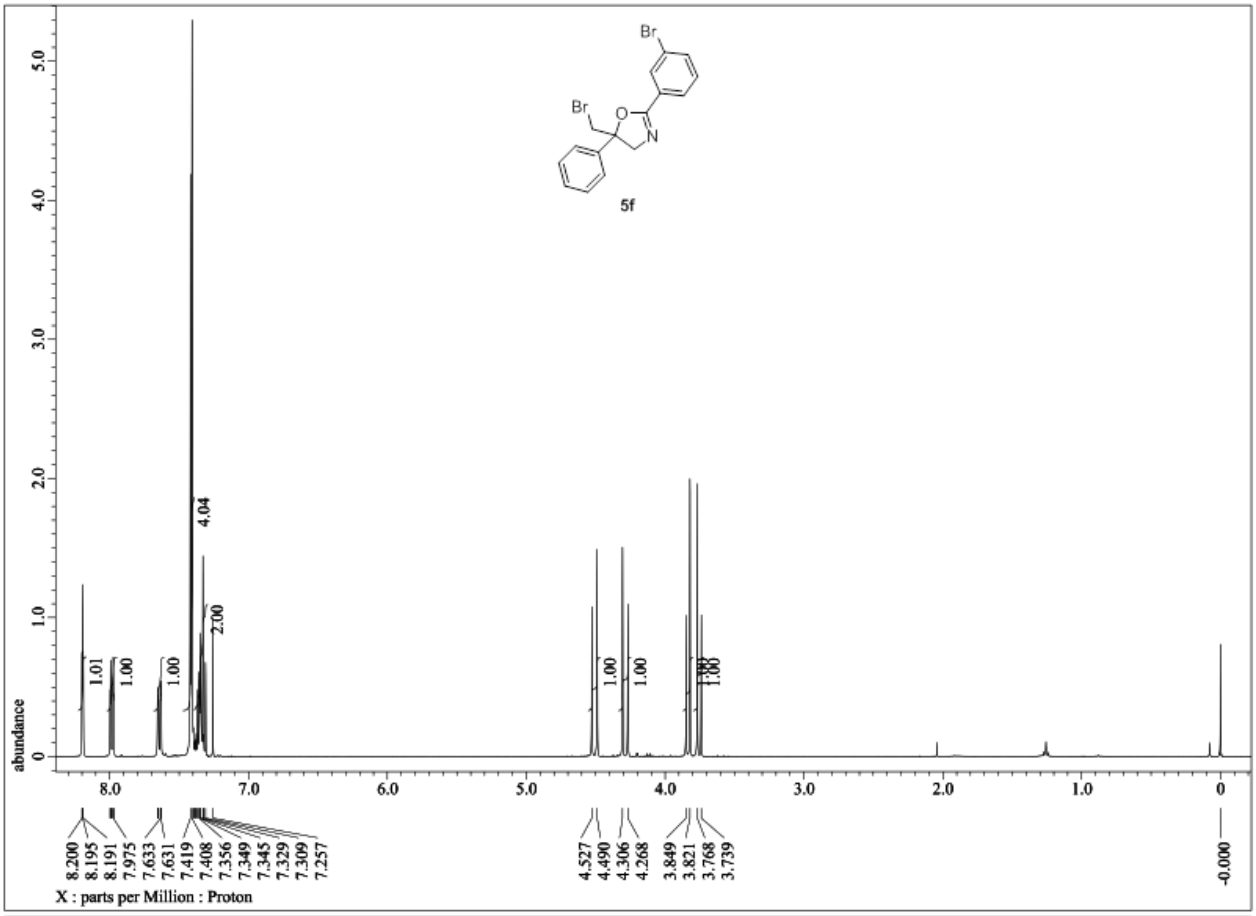

Me
Br
O
N
5c
abundance
X : parts per Million : Carbon13
162.950
141.966
141.756
129.127
128.698
128.202
124.892
124.558
86.796
77.258
77.000
76.752
65.802
40.096
21.573


OMe
Br
O
N
5d
abundance
2.01
4.17
1.00
2.03
1.00
1.01
3.02
8.008
7.991
7.986
7.419
7.415
7.397
7.258
6.976
6.969
6.964
6.952
6.947
6.939
4.481
4.444
4.266
4.229
3.864
3.847
3.819
3.781
3.753
-0.000
X : parts per Million : Proton


OMe
Br
O
N
5d
abundance
162.686
162.255
141.820
130.008
128.724
128.216
124.930
119.881
113.798
86.810
77.326
77.211
77.000
76.684
65.849
55.396
40.116
X : parts per Million : Carbon13


CF3
Br
O
N
5e
abundance
4.0
3.0
2.0
1.0
0
2.01
2.09
4.01
1.11
1.00
1.01
1.05
1.01
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.182
8.161
7.733
7.712
7.424
7.413
7.404
7.383
7.373
7.363
7.352
7.342
7.257
4.556
4.518
4.336
4.298
3.865
3.847
3.836
3.783
3.754
2.043
1.257
-0.000
X : parts per Million : Proton


CF3
Br
O
N
5e
abundance
0.3
0.2
0.1
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
161.680
141.361
133.639
133.313
132.987
130.698
128.858
128.628
128.456
127.843
125.448
125.409
125.103
124.796
122.363
87.452
77.316
77.000
76.674
65.906
40.039
29.673
X : parts per Million : Carbon13


Br
Br
O
N
5f
abundance
5.0
4.0
3.0
2.0
1.0
0
4.04
2.00
1.01
1.00
1.00
1.00
1.00
1.00
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.200
8.195
8.191
7.975
7.633
7.631
7.419
7.408
7.356
7.349
7.345
7.329
7.309
7.257
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4.306
4.268
3.849
3.821
3.768
3.739
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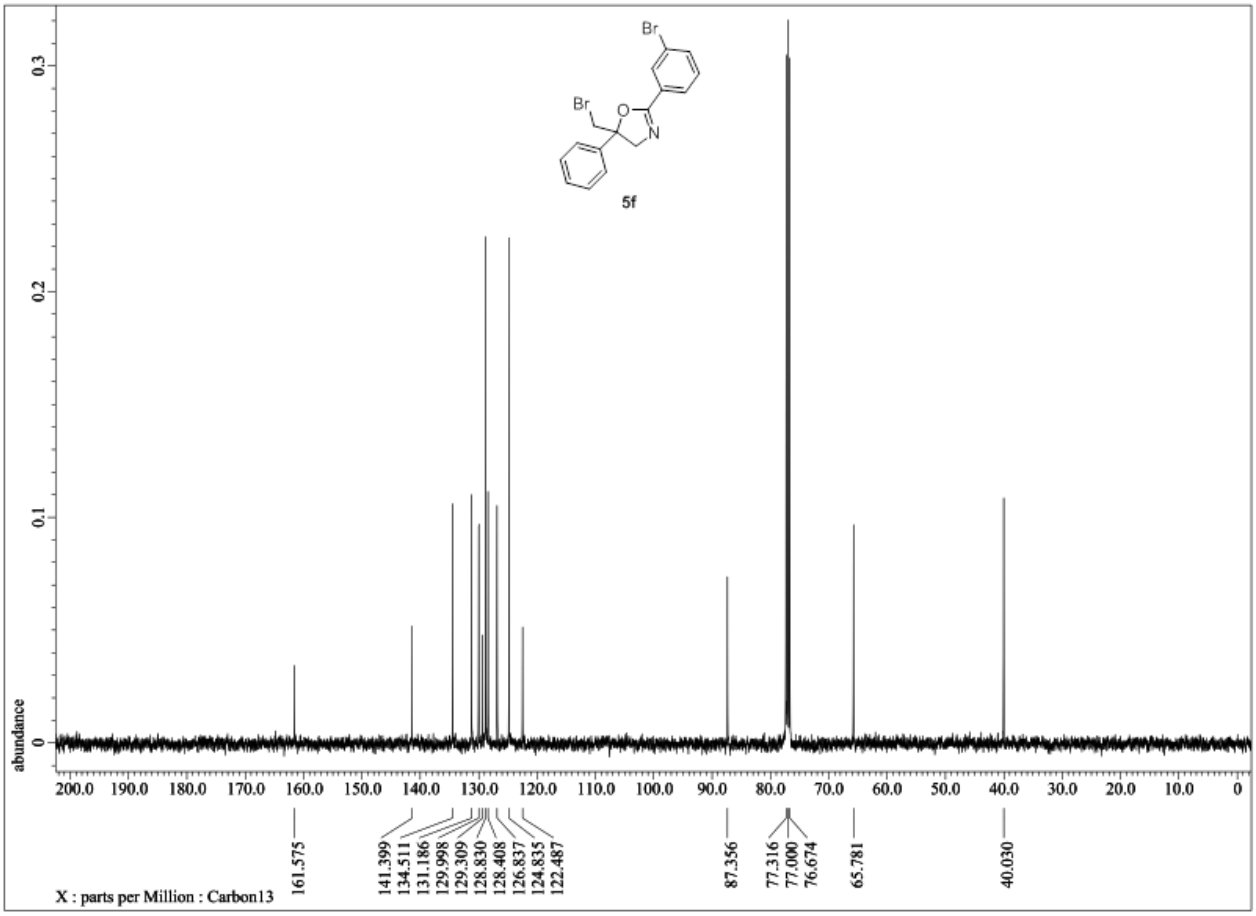
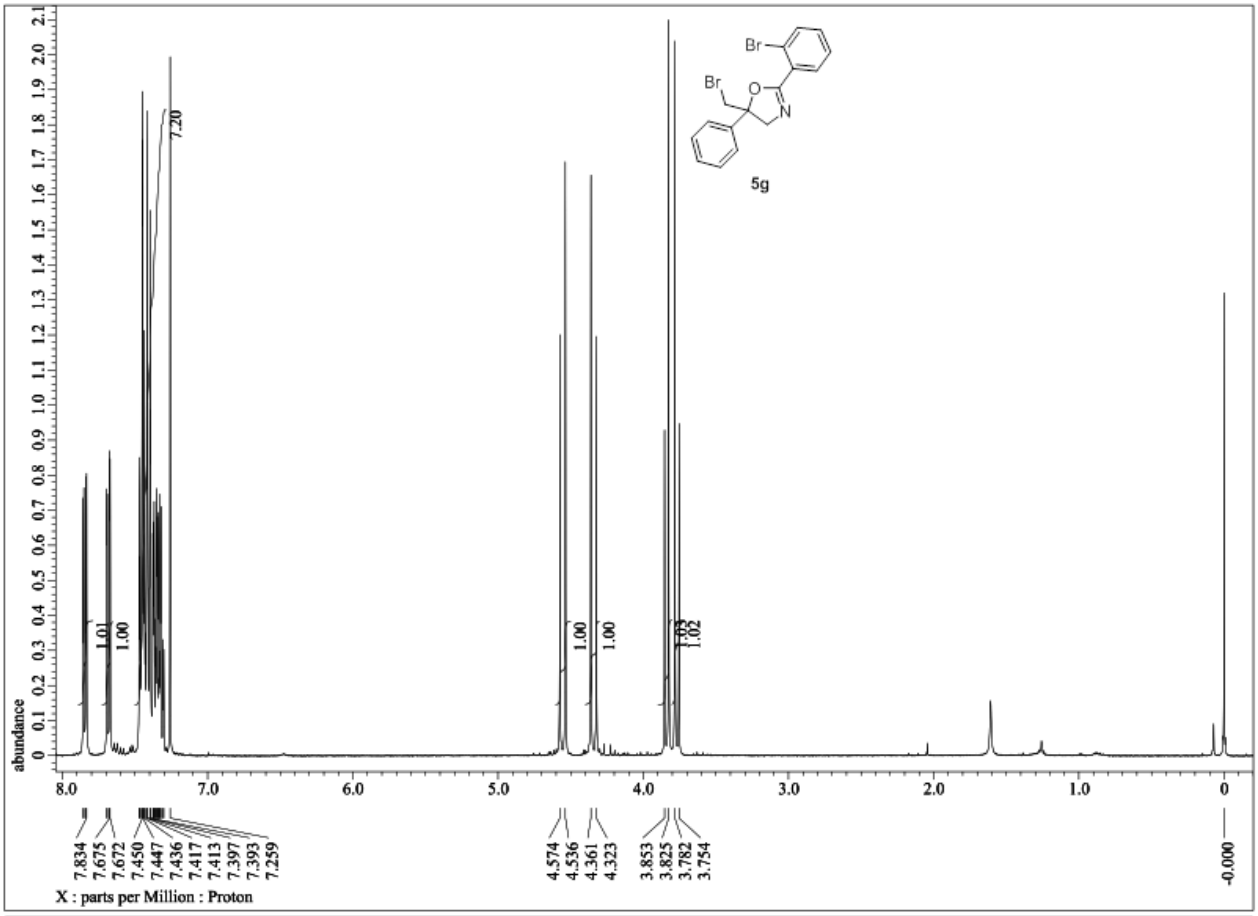
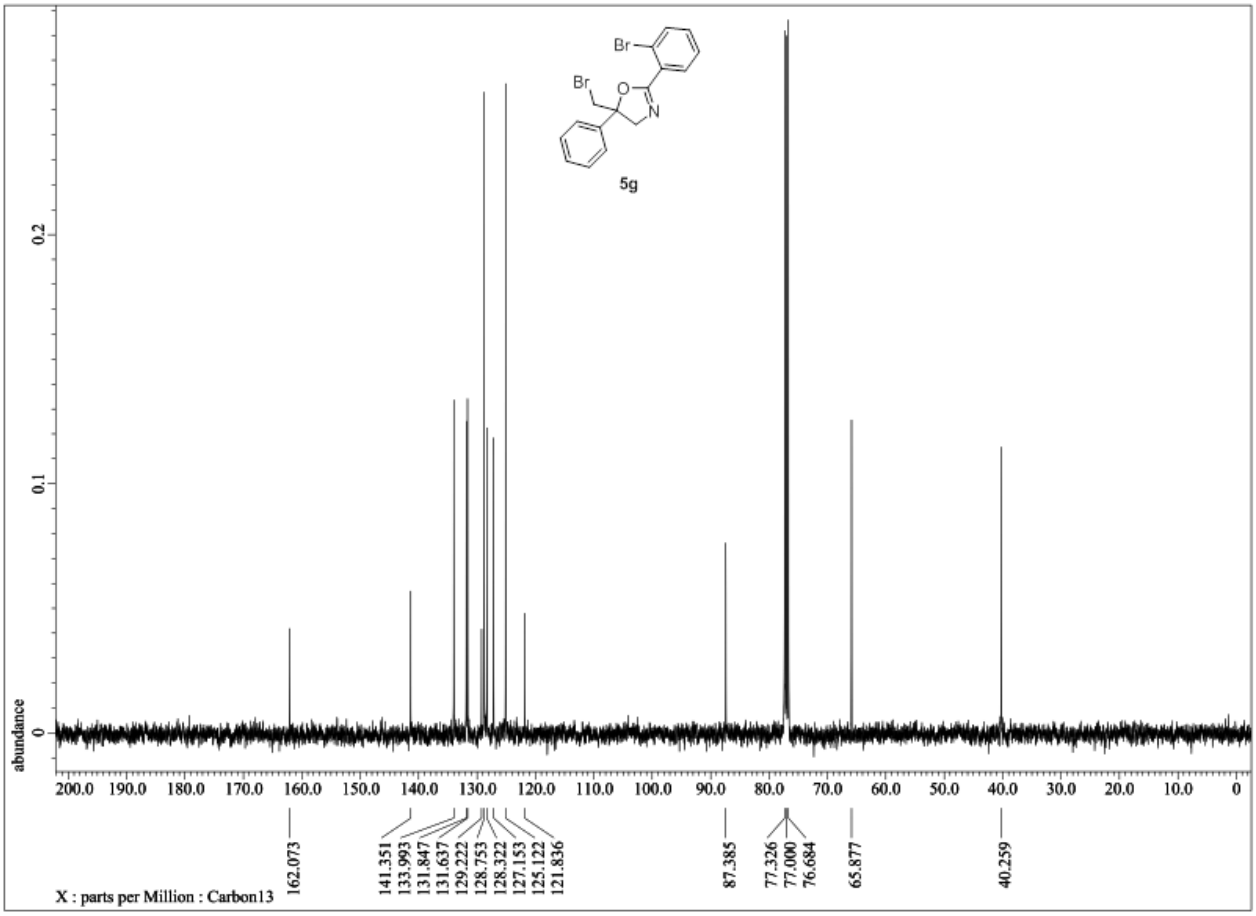
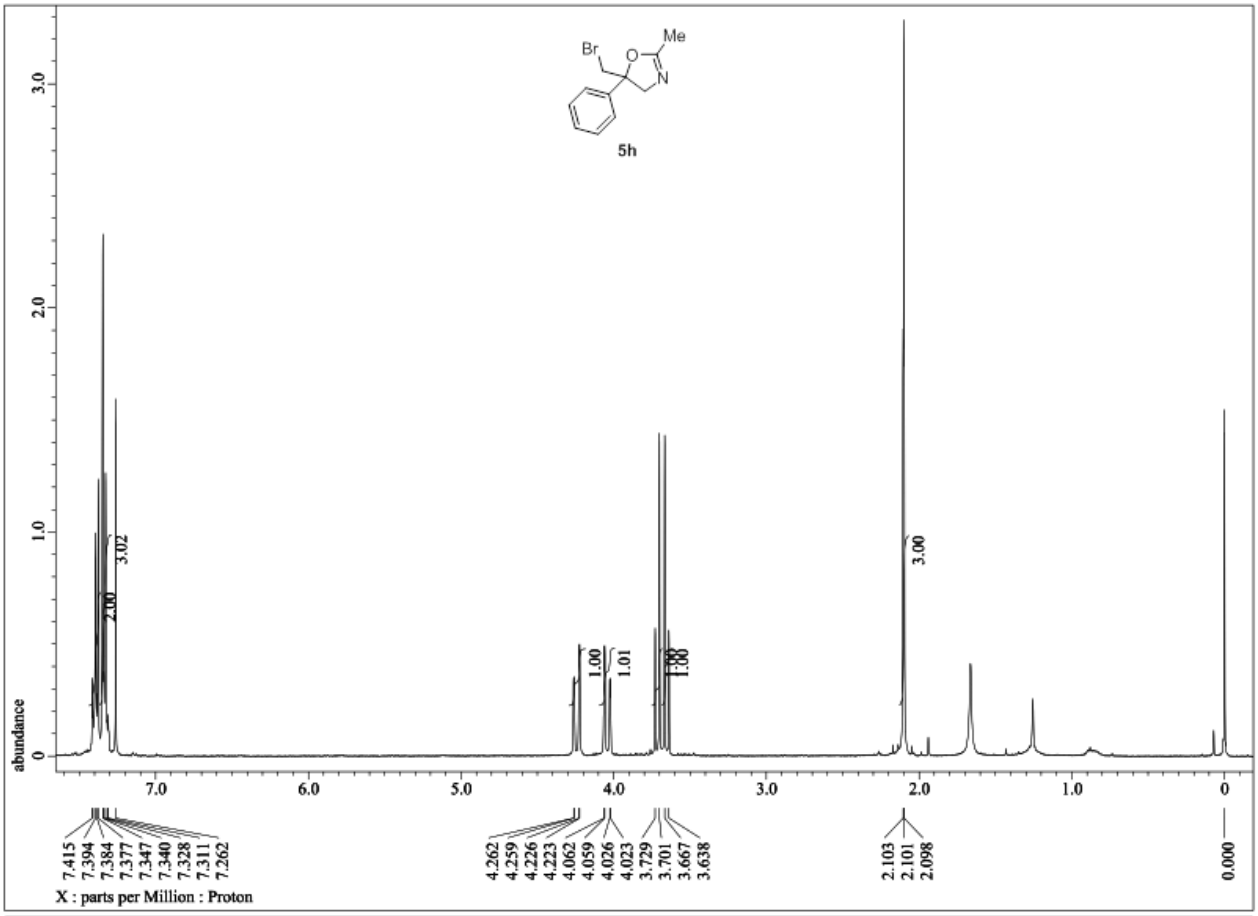
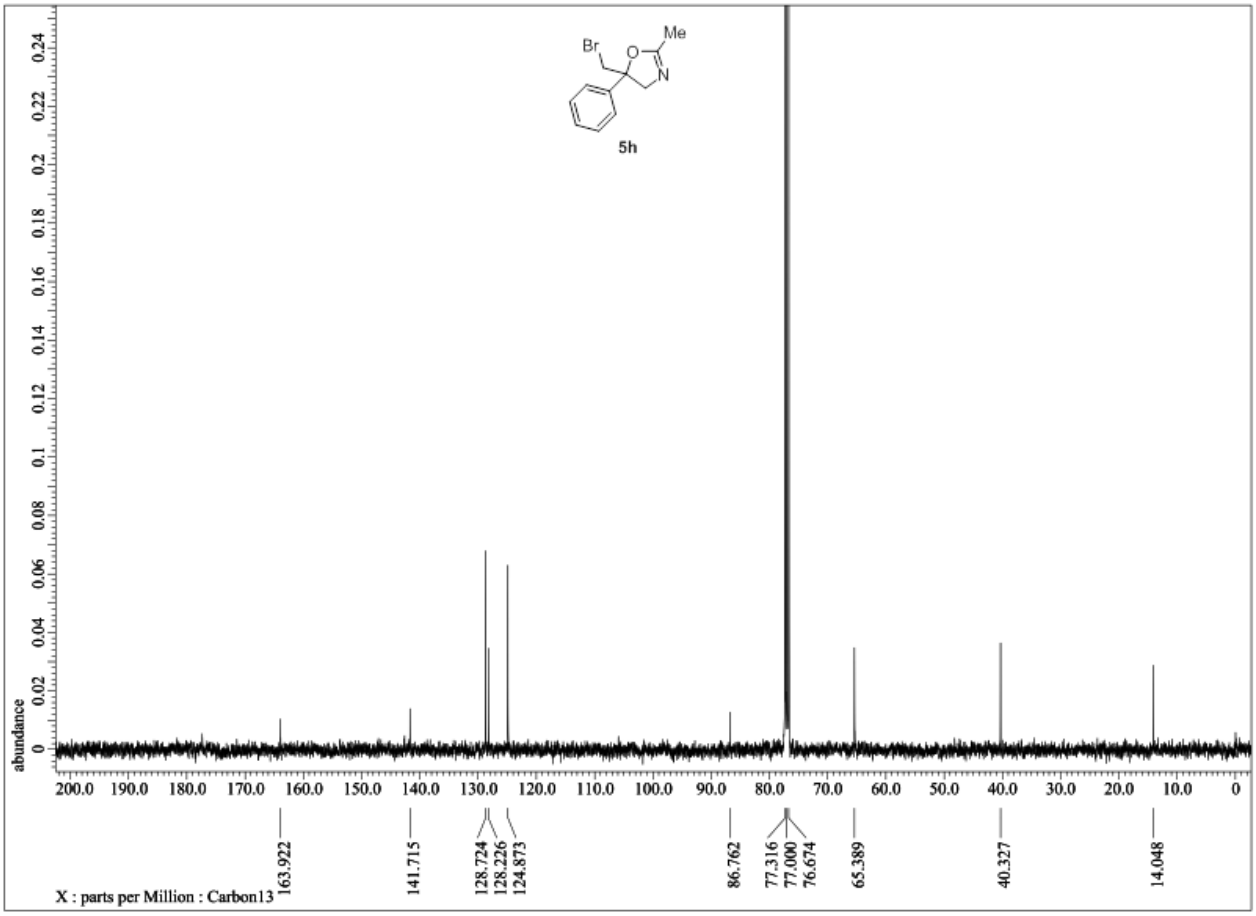
X : parts per Million : Proton

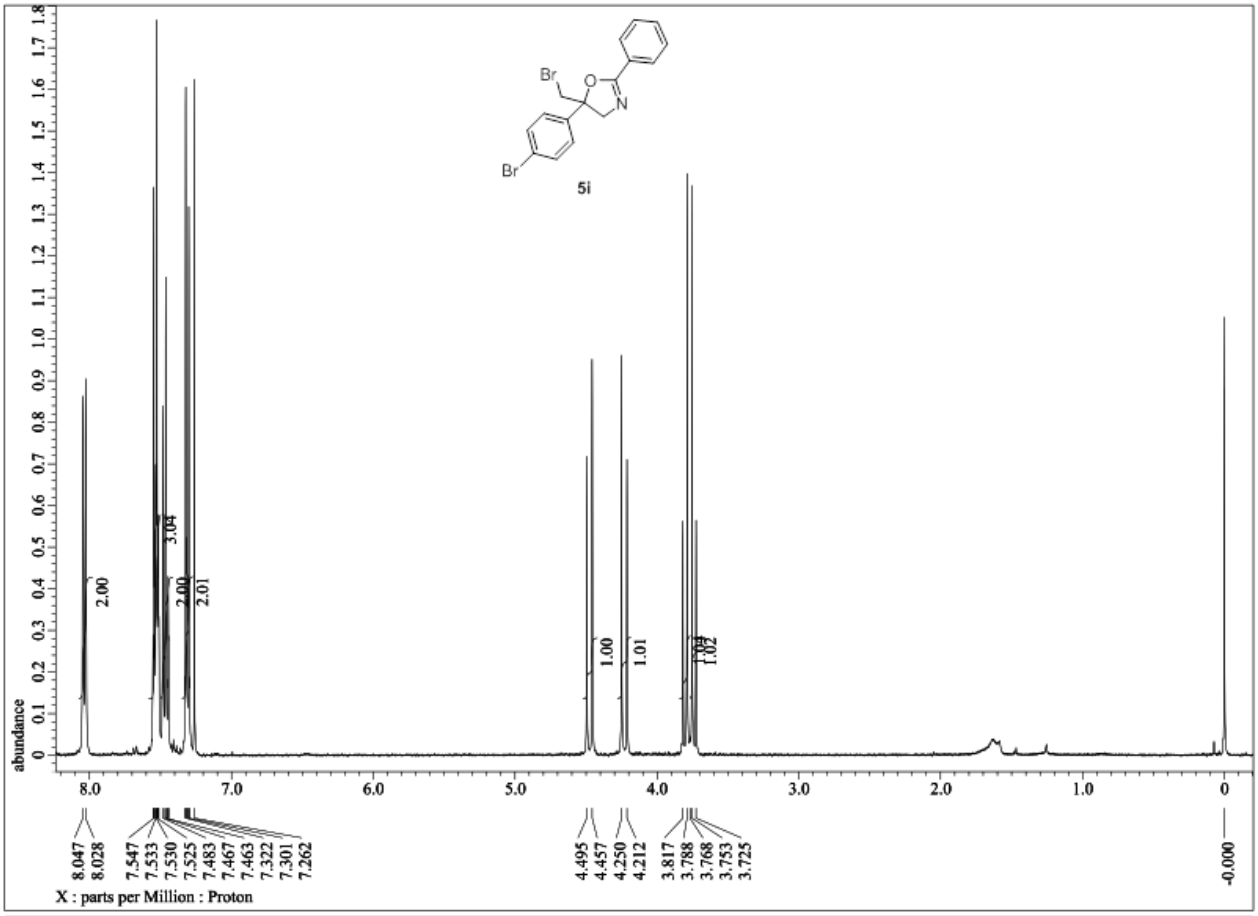

Br
Br
O
N
5f
abundance
0.3
0.2
0.1
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
161.575
141.399
134.511
131.186
129.998
129.309
128.830
128.408
126.837
124.835
122.487
87.356
77.316
77.000
76.674
65.781
40.030
X : parts per Million : Carbon13

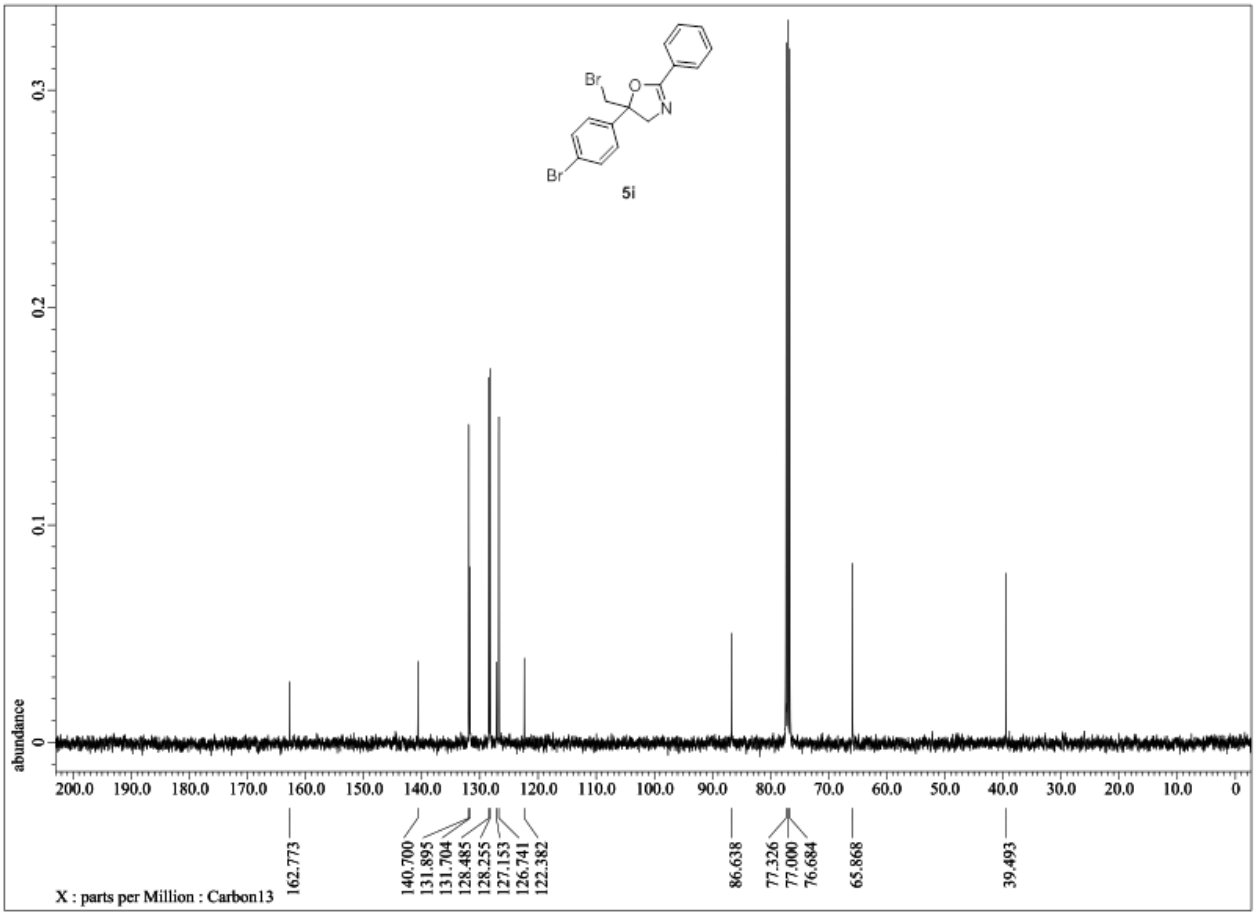

Br
Br
O
N
5g
abundance
7.20
1.01
1.00
1.00
1.00
1.03
1.02
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.834
7.675
7.672
7.450
7.447
7.436
7.417
7.413
7.397
7.393
7.259
4.574
4.536
4.361
4.323
3.853
3.825
3.782
3.754
-0.000
X : parts per Million : Proton


Br
Br
O
N
5g
abundance
0.2
0.1
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
162.073
141.351
133.993
131.847
131.637
129.222
128.753
128.322
127.153
125.122
121.836
87.385
77.326
77.000
76.684
65.877
40.259
X : parts per Million : Carbon13


Br
O
Me
N
5h
abundance
3.0
2.0
1.0
0
2.00
3.02
1.00
1.01
3.00
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.415
7.394
7.384
7.377
7.347
7.340
7.328
7.311
7.262
4.262
4.259
4.226
4.223
4.062
4.059
4.026
4.023
3.729
3.701
3.667
3.638
2.103
2.101
2.098
0.000
X : parts per Million : Proton


Br
O
Me
N
5h
abundance
0.24
0.22
0.2
0.18
0.16
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
163.922
141.715
128.724
128.226
124.873
86.762
77.316
77.000
76.674
65.389
40.327
14.048
X : parts per Million : Carbon13


Br
O
N
Br
5i
abundance
2.00
3.04
2.00
2.01
1.00
1.01
1.03
1.02
8.047
8.028
7.547
7.533
7.530
7.525
7.483
7.467
7.463
7.322
7.301
7.262
4.495
4.457
4.250
4.212
3.817
3.788
3.768
3.753
3.725
-0.000
X : parts per Million : Proton


Br
O
N
Br
5i
abundance
162.773
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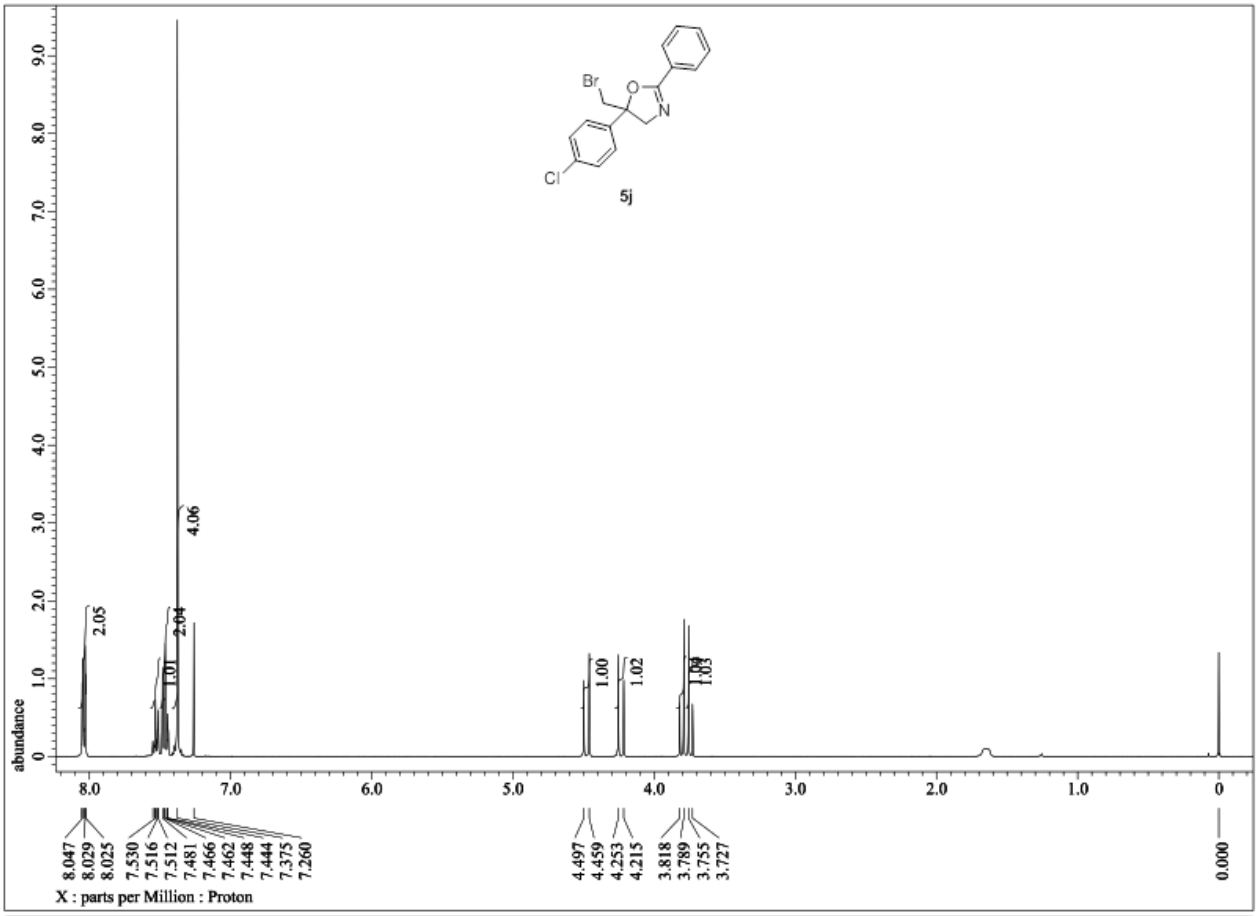
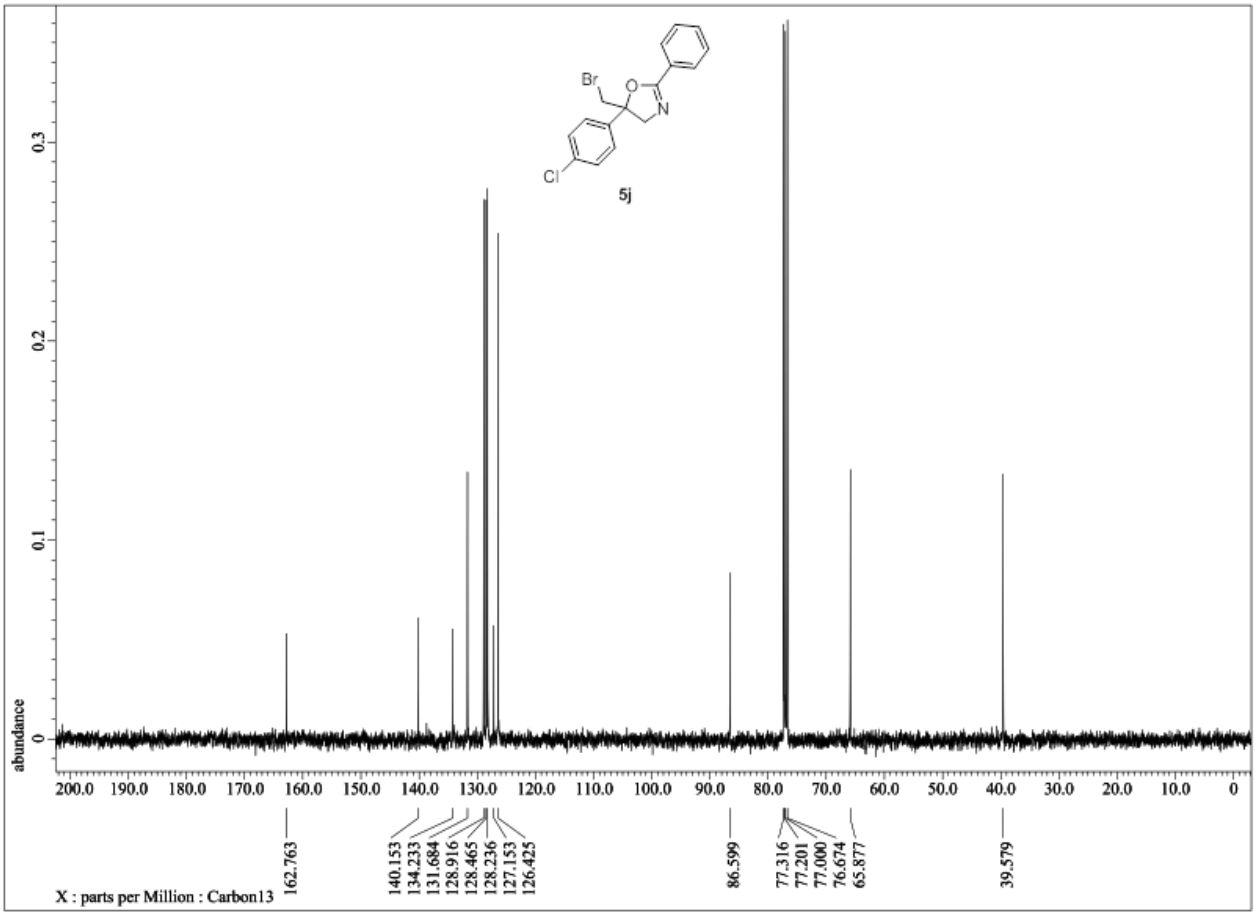
131.704
128.485
128.255
127.153
126.741
122.382
86.638
77.326
77.000
76.684
65.868
39.493
X : parts per Million : Carbon13


Br
O
N
Cl
5j
abundance
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
2.05
2.04
4.06
1.01
1.00
1.02
1.09
1.05
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.047
8.029
8.025
7.530
7.516
7.512
7.481
7.466
7.462
7.448
7.444
7.375
7.260
4.497
4.459
4.253
4.215
3.818
3.789
3.755
3.727
0.000
X : parts per Million : Proton


Br
O
N
Cl
5j
abundance
0.3
0.2
0.1
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
162.763
140.153
134.233
131.684
128.916
128.465
128.236
127.153
126.425
86.599
77.316
77.201
77.000
76.674
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39.579
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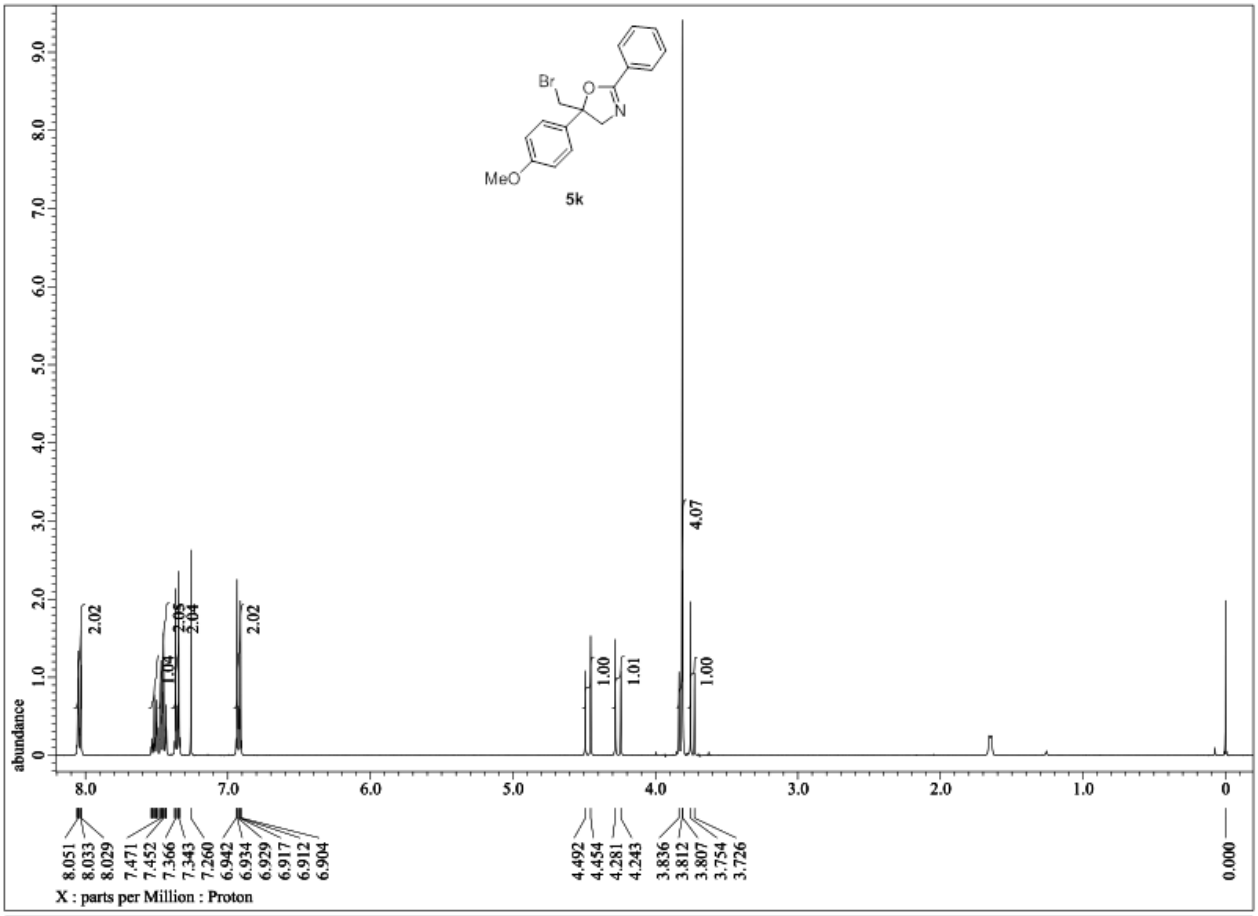
Br
O
N
MeO
5k
abundance
2.02
2.02
1.04
2.05
2.04
2.02
4.07
1.00
1.01
1.00
8.051
8.033
8.029
7.471
7.452
7.366
7.343
7.260
6.942
6.934
6.929
6.917
6.912
6.904
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4.454
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4.243
3.836
3.812
3.807
3.754
3.726
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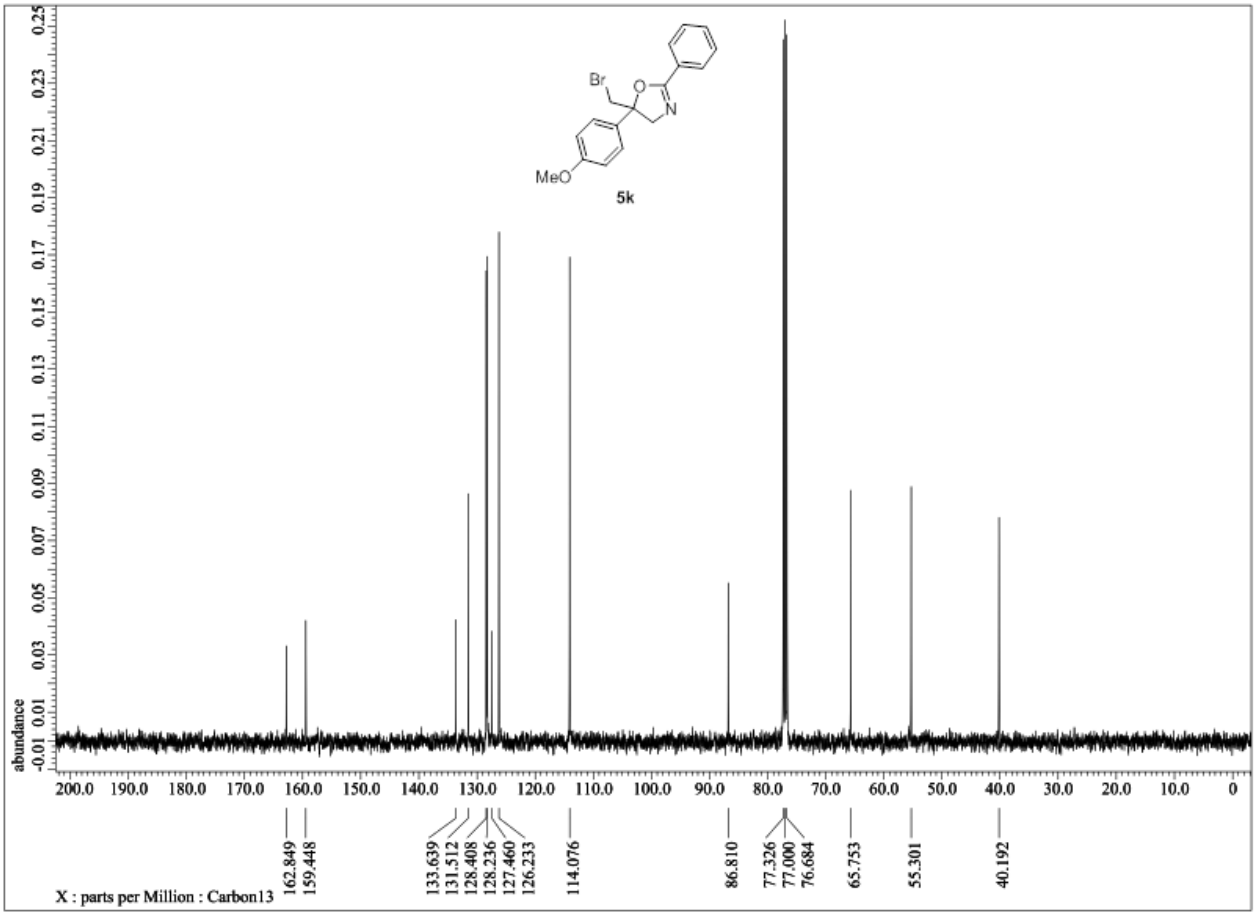
X : parts per Million : Proton


Br
O
N
MeO
5k
abundance
162.849
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131.512
128.408
128.236
127.460
126.233
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86.810
77.326
77.000
76.684
65.753
55.301
40.192
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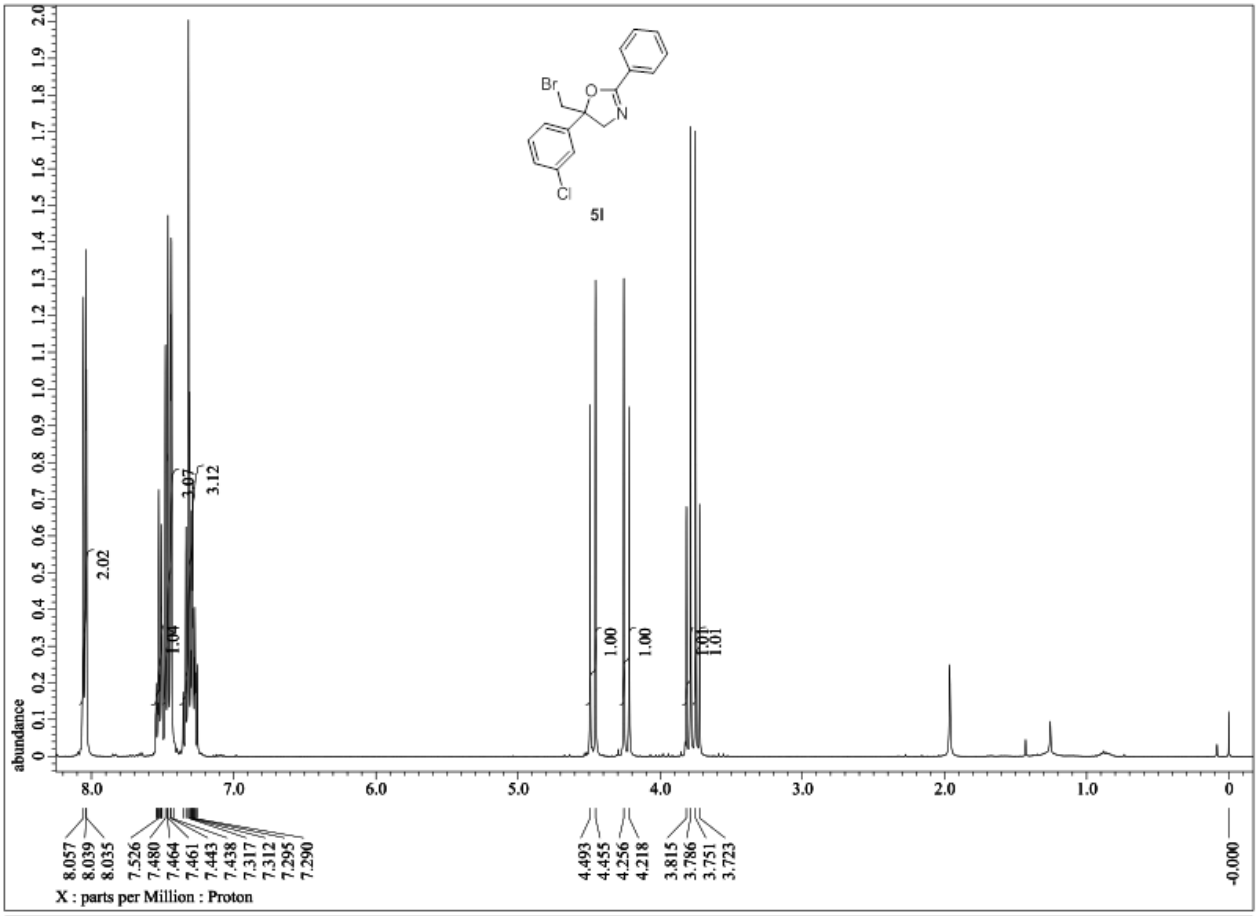
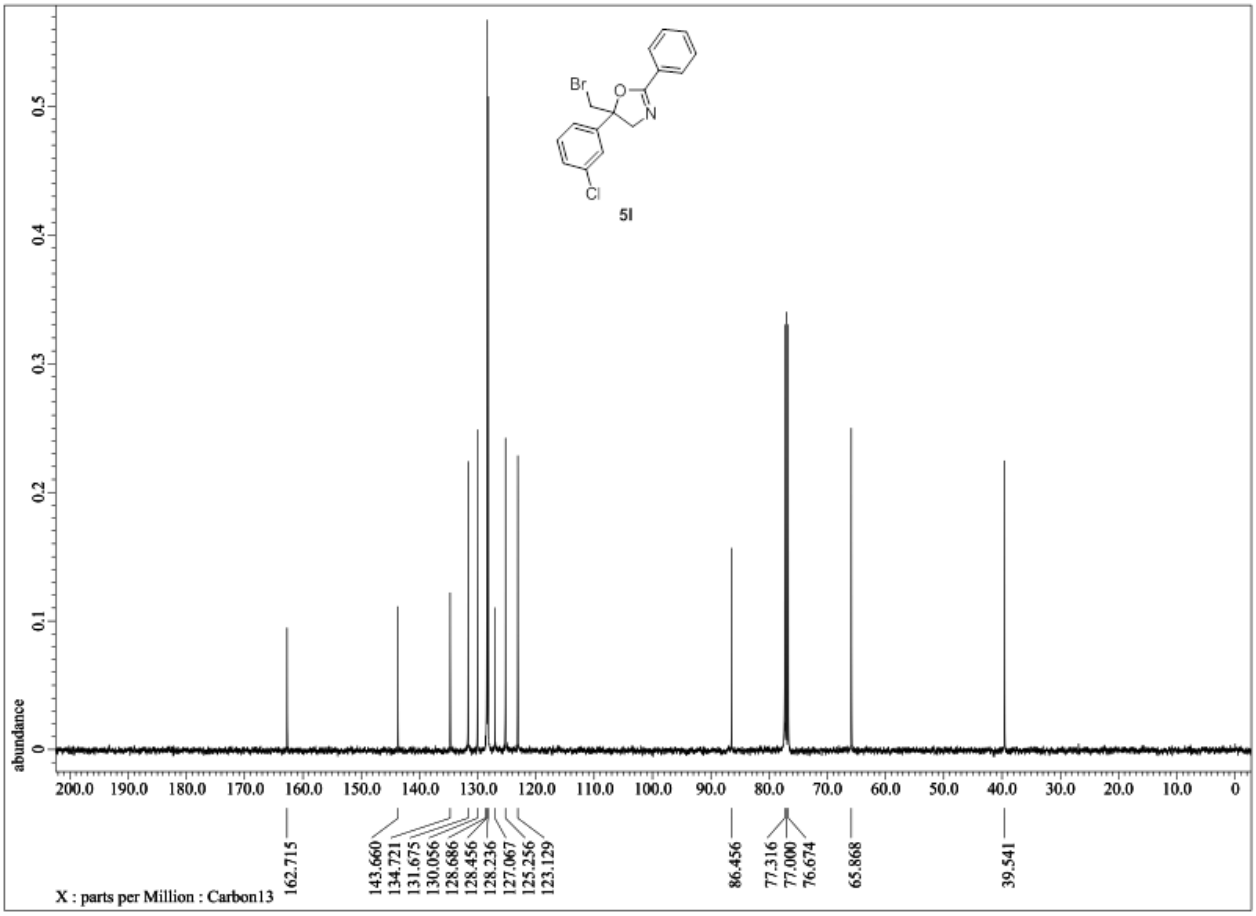

Br
O
N
Cl
5l
abundance
2.02
1.00
3.07
3.12
1.00
1.00
1.01
1.01
8.057
8.039
8.035
7.526
7.480
7.464
7.461
7.443
7.438
7.317
7.312
7.295
7.290
4.493
4.455
4.256
4.218
3.815
3.786
3.751
3.723
-0.000
X : parts per Million : Proton


Br
O
N
Cl
5l
abundance
162.715
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131.675
130.056
128.686
128.456
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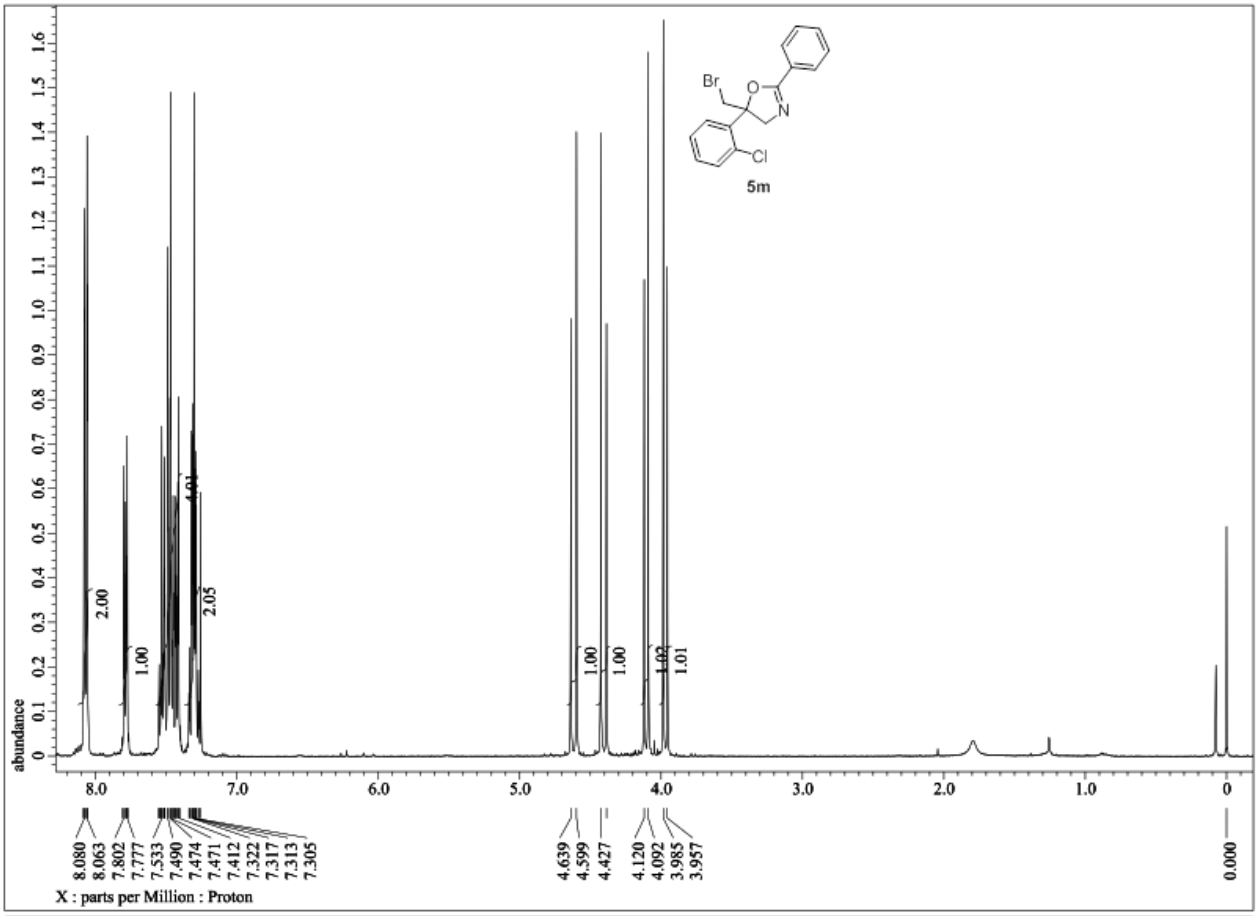
123.129
86.456
77.316
77.000
76.674
65.868
39.541
X : parts per Million : Carbon13


Br
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N
Cl
5m
abundance
2.00
1.00
4.01
2.05
1.00
1.00
1.00
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1.01
8.080
8.063
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7.777
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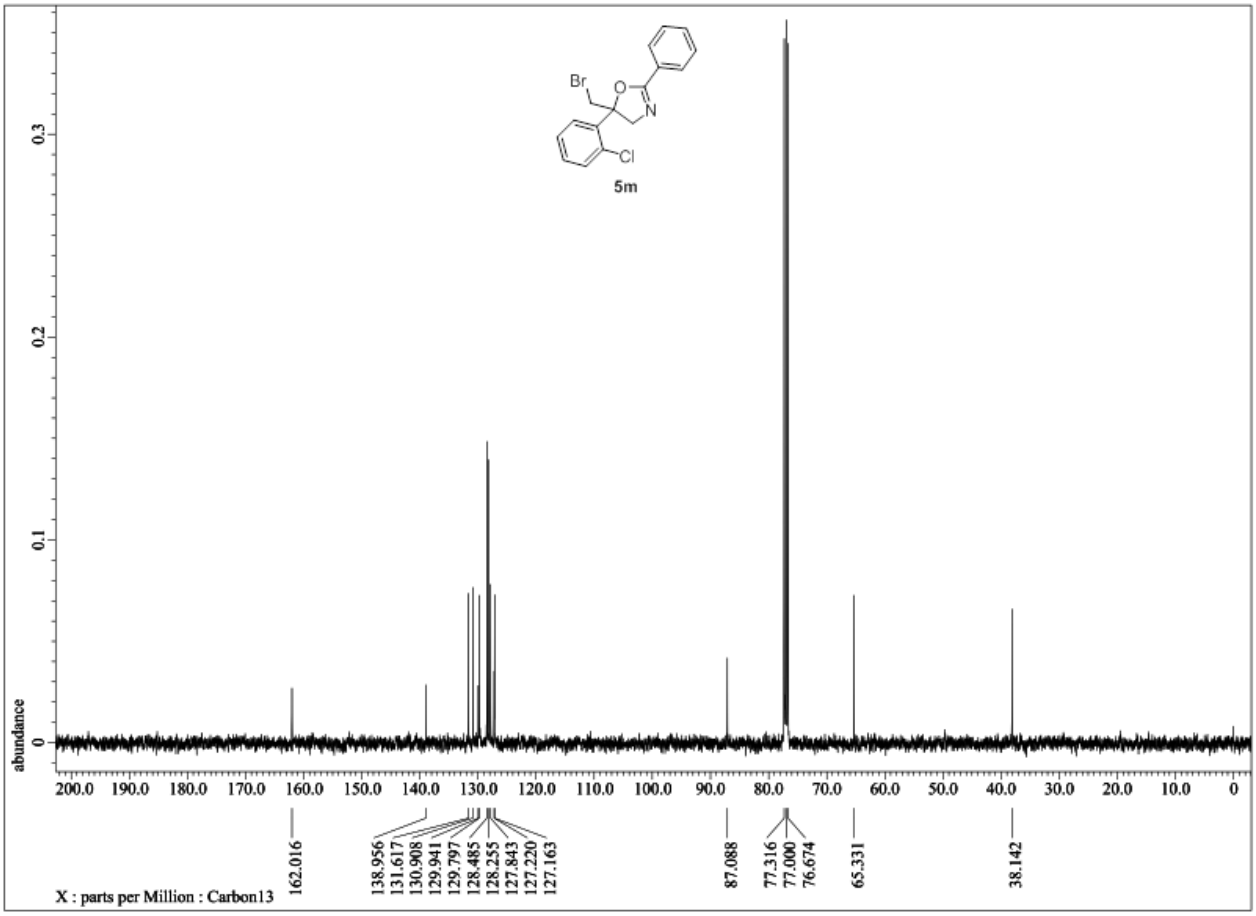
7.471
7.412
7.322
7.317
7.313
7.305
4.639
4.599
4.427
4.120
4.092
3.985
3.957
0.000
X : parts per Million : Proton


Br
O
N
Cl
5m
abundance
162.016
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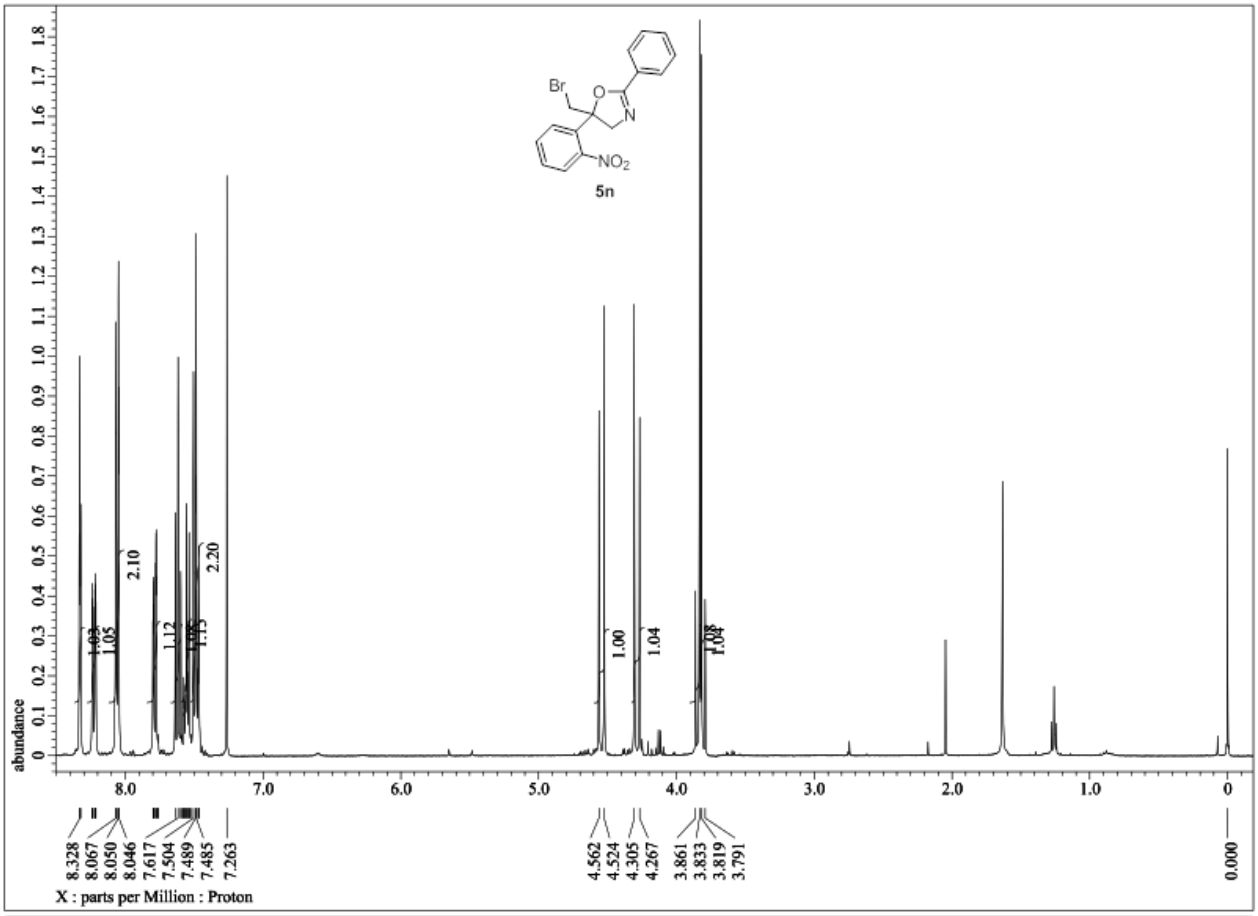
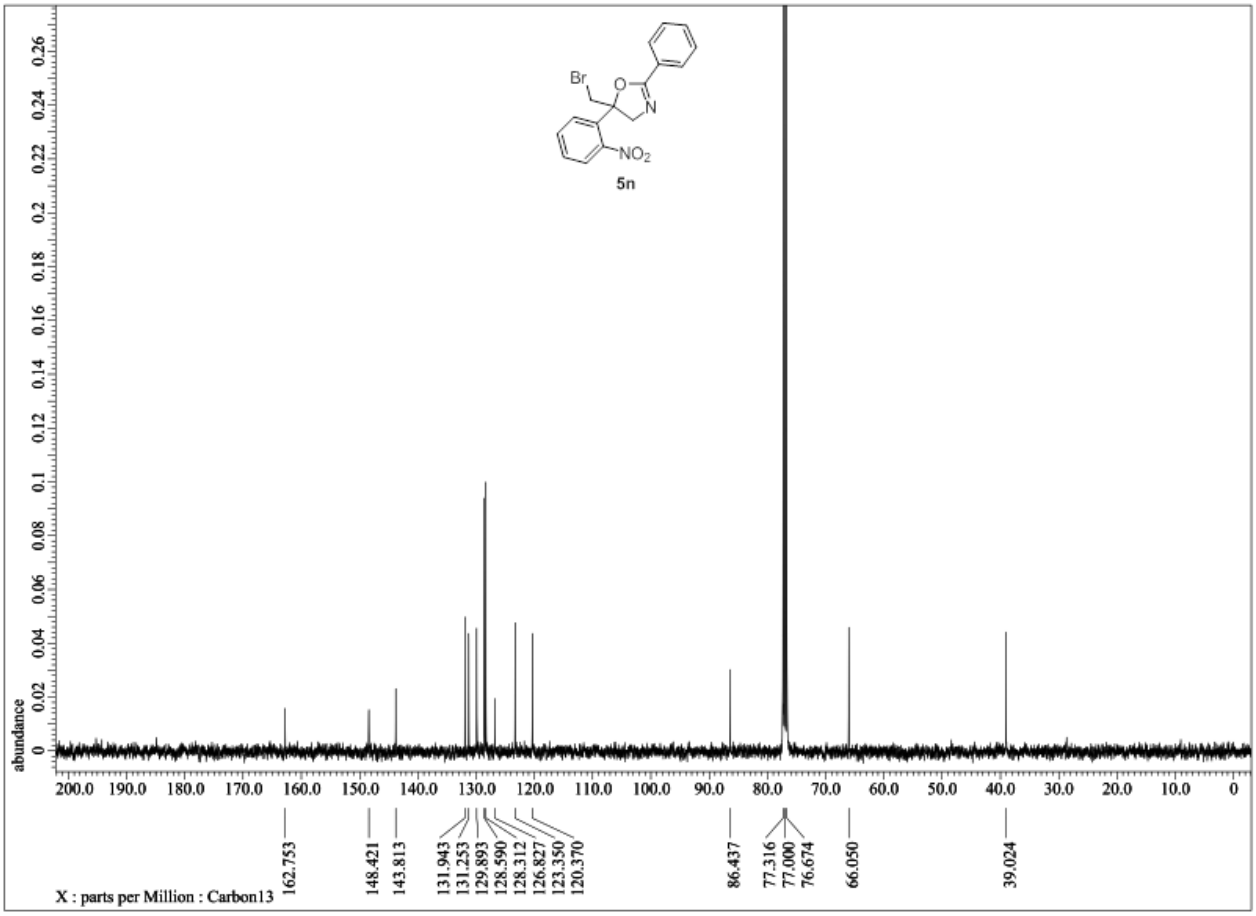
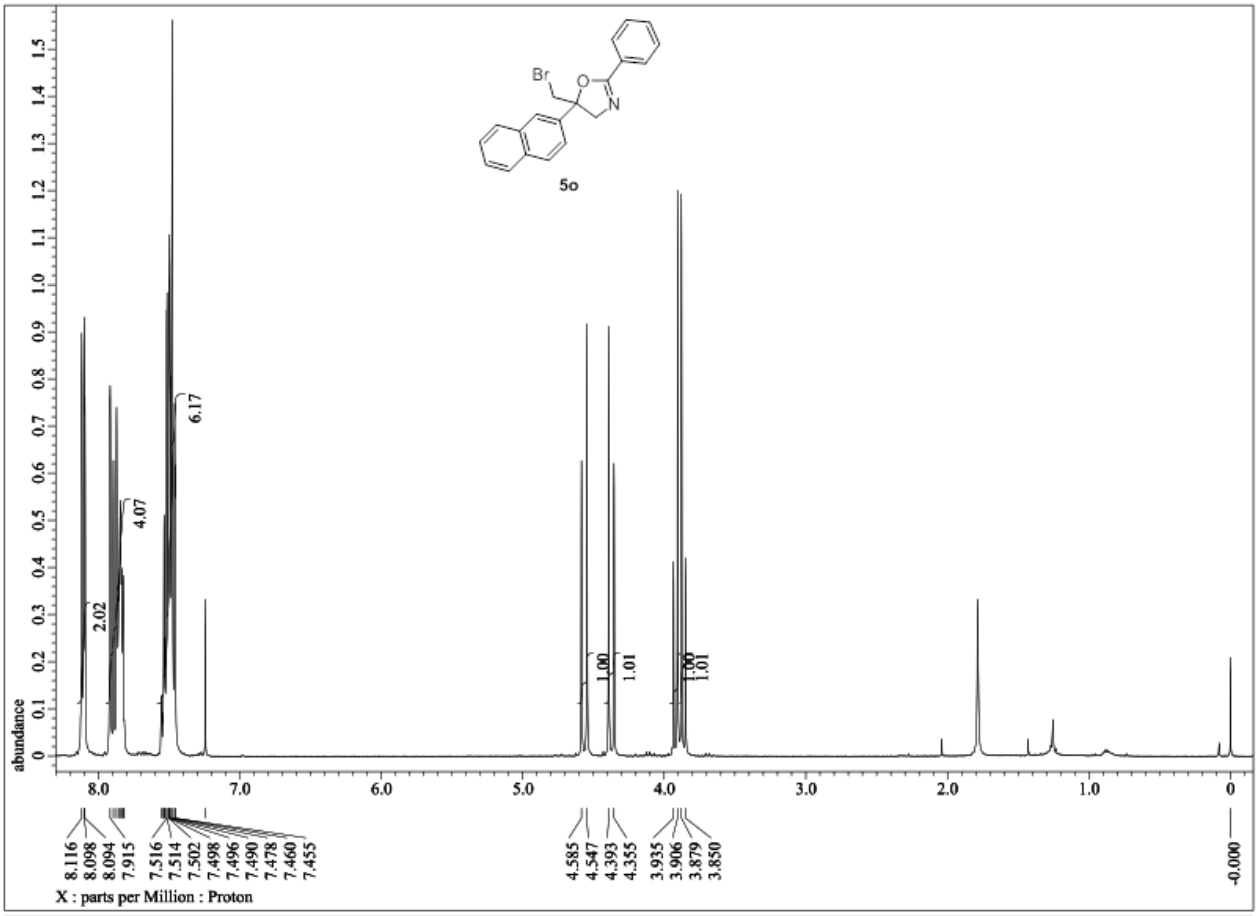
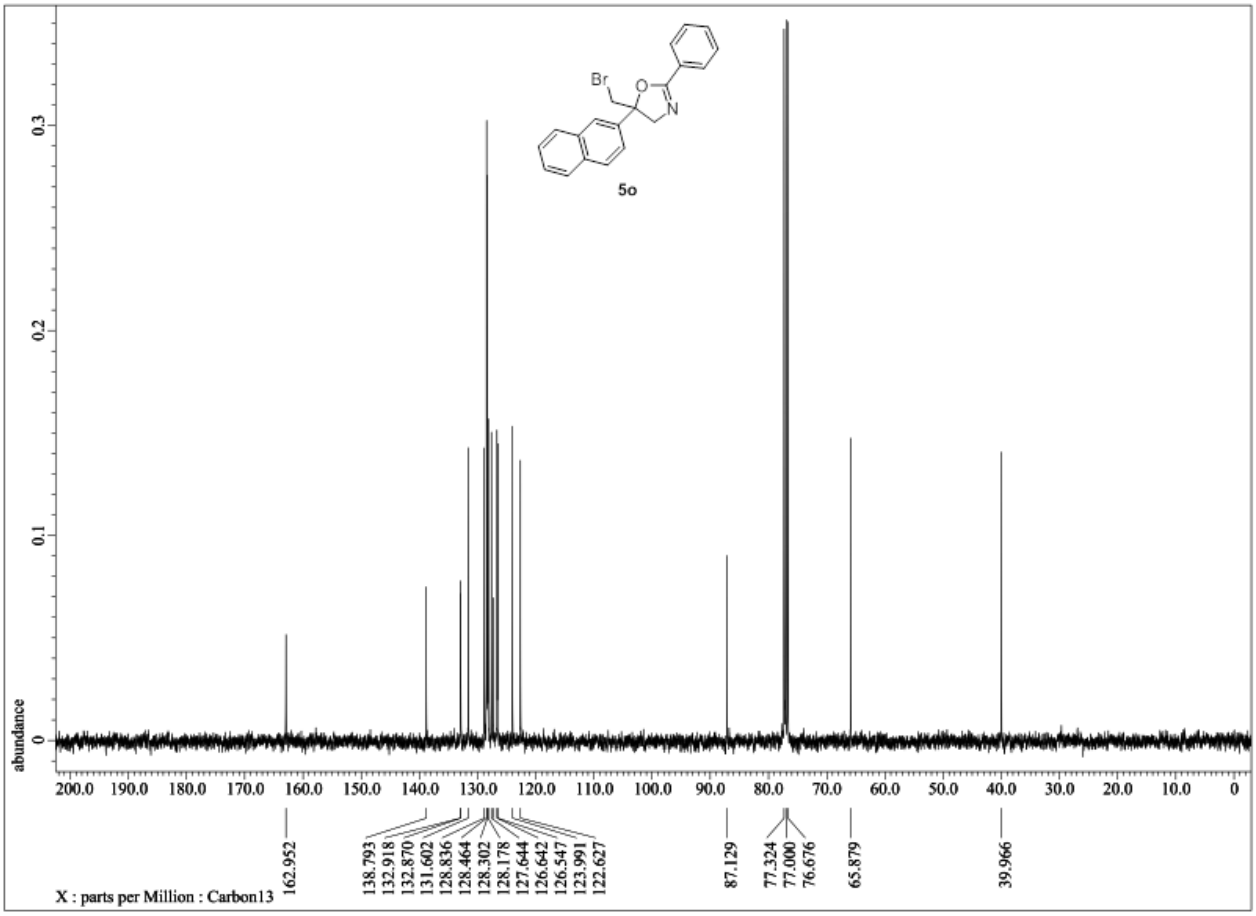
131.617
130.908
129.941
129.797
128.485
128.255
127.843
127.220
127.163
87.088
77.316
77.000
76.674
65.331
38.142
X : parts per Million : Carbon13


Br
O
N
NO2
5n
abundance
8.328
8.067
8.050
8.046
7.617
7.504
7.489
7.485
7.263
4.562
4.524
4.305
4.267
3.861
3.833
3.819
3.791
0.000
X : parts per Million : Proton


Br
O
N
NO2
5n
abundance
162.753
148.421
143.813
131.943
131.253
129.893
128.590
128.312
126.827
123.350
120.370
86.437
77.316
77.000
76.674
66.050
39.024
X : parts per Million : Carbon13


Br
O
N
5o
abundance
2.02
4.07
6.17
1.00
1.01
1.00
1.01
8.116
8.098
8.094
7.915
7.516
7.514
7.502
7.498
7.496
7.490
7.478
7.460
7.455
4.585
4.547
4.393
4.355
3.935
3.906
3.879
3.850
-0.000
X : parts per Million : Proton


Br
O
N
5o
abundance
162.952
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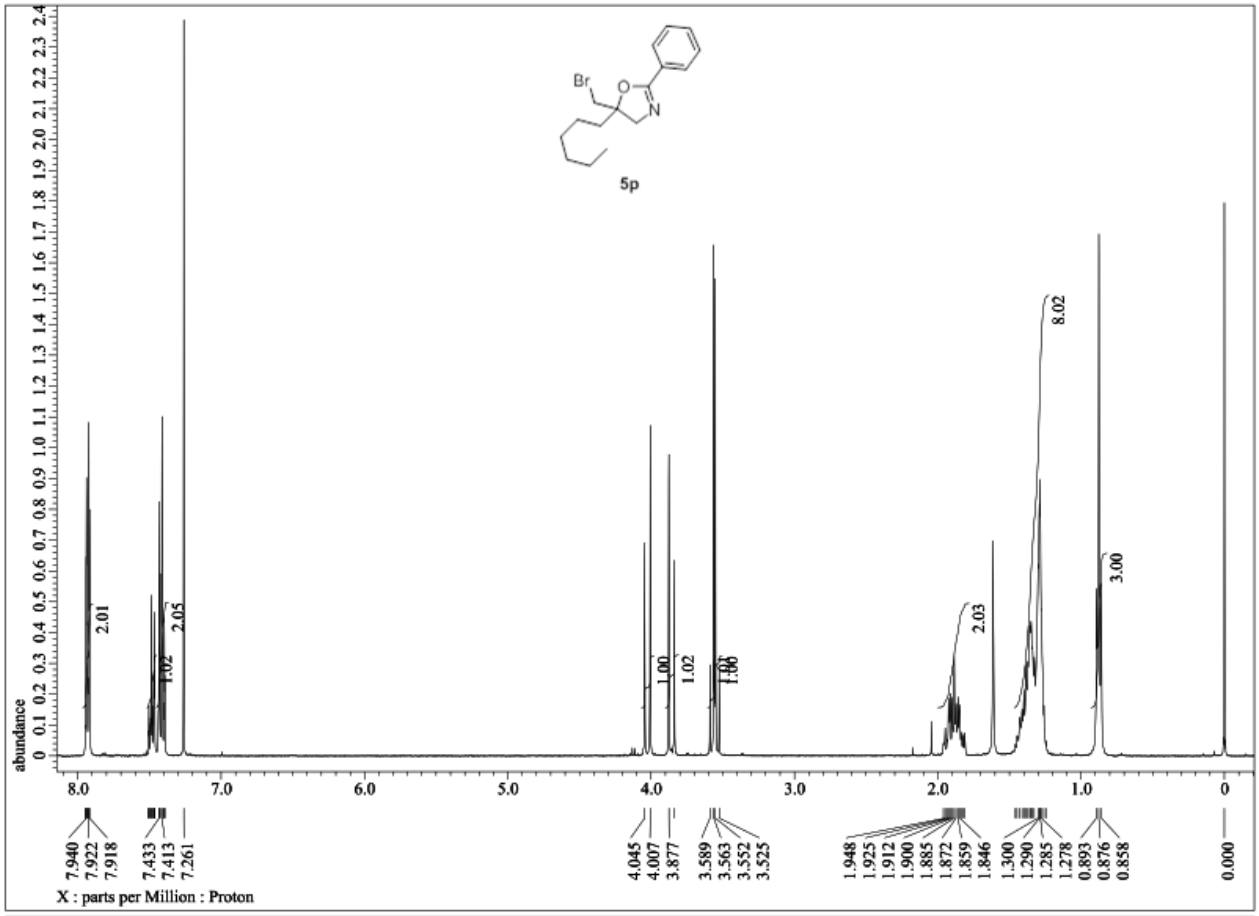
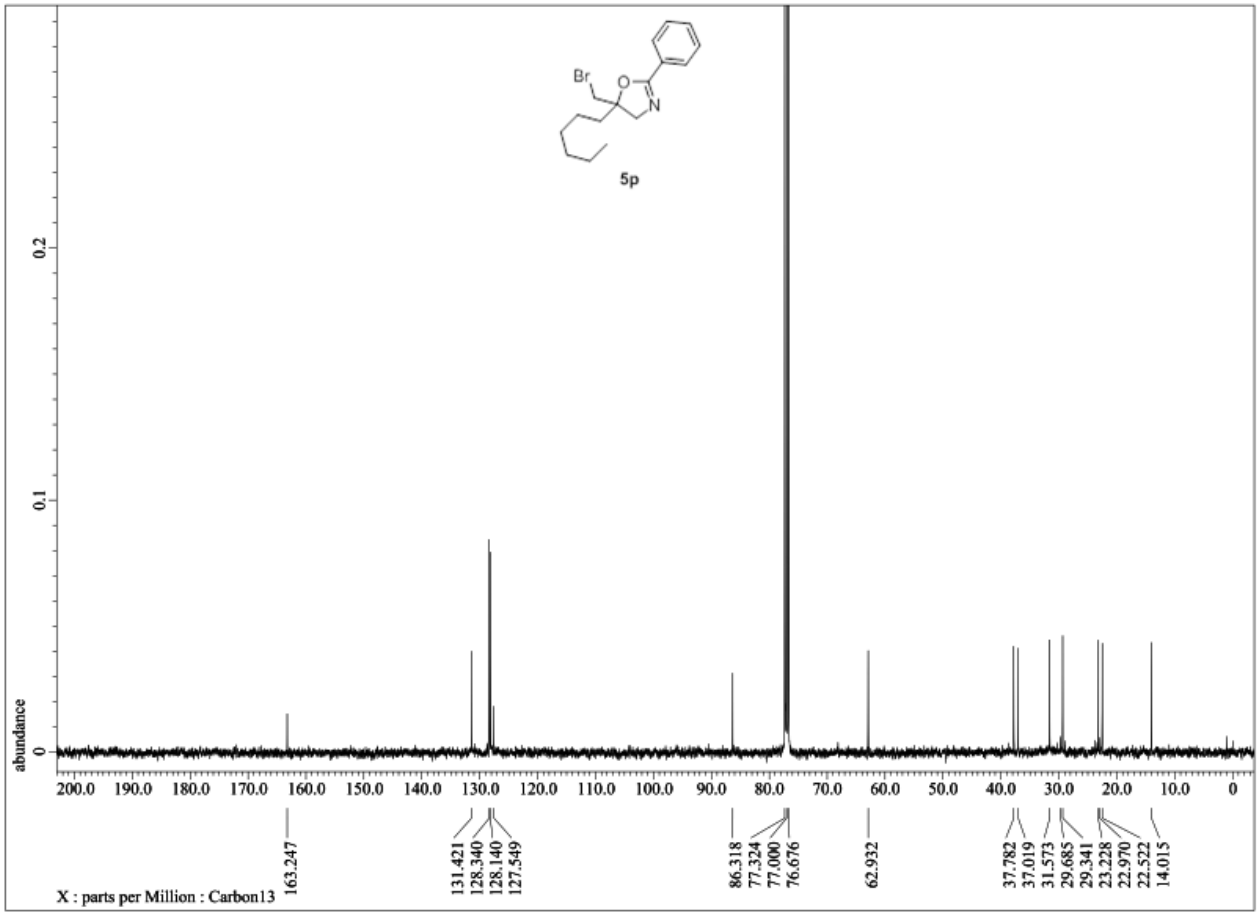
132.918
132.870
131.602
128.836
128.464
128.302
128.178
127.644
126.642
126.547
123.991
122.627
87.129
77.324
77.000
76.676
65.879
39.966
X : parts per Million : Carbon13


Br
O
N
5p
abundance
2.01
2.05
1.02
1.00
1.02
2.03
8.02
3.00
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.940
7.922
7.918
7.433
7.413
7.261
4.045
4.007
3.877
3.589
3.563
3.552
3.525
1.948
1.925
1.912
1.900
1.885
1.872
1.859
1.846
1.300
1.290
1.285
1.278
0.893
0.876
0.858
0.000
X : parts per Million : Proton


Br
O
N
5p
abundance
0.2
0.1
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
163.247
131.421
128.340
128.140
127.549
86.318
77.324
77.000
76.676
62.932
37.782
37.019
31.573
29.685
29.341
23.228
22.970
22.522
14.015
X : parts per Million : Carbon13