Supporting information

Synthesis of Benzothiazonine by Rhodium-Catalyzed Denitrogenative Transannulation of 1-Sulfonyl-1,2,3-Triazole and Thiochromone

Saygbechi T. Jablasone Jr, Zihang Ye, Shengguo Duan, Ze-Feng Xu* and Chuan-Ying Li*

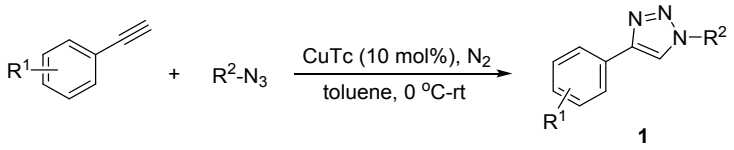
Department of Chemistry, Zhejiang Sci-Tech University, Xiasha West Higher Education District, Hangzhou, 310018, China

Contents

1. General Comments

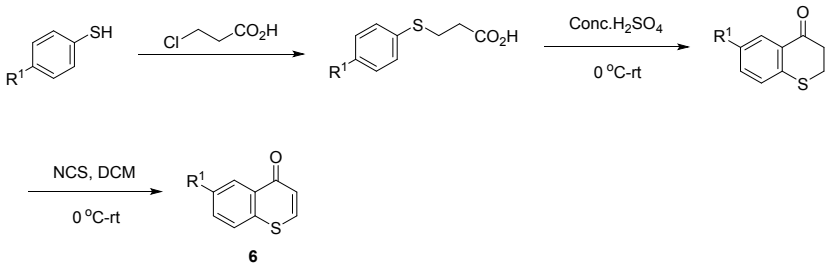
Analytical thin layer chromatography (TLC) was performed using Silica Gel HSGF254 pre-coated plates. Flash column chromatography was performed using 200 - 300 Mesh Silica Gel. Proton nuclear magnetic resonance (^{1}H-NMR) spectra were recorded using Brucker Avance IIDMX 400MHz spectrometers. Chemical shift (δ) is reported in parts per million (ppm) downfield relative to tetramethylsilane (TMS, 0.00 ppm) or $CDCl_3$ (7.26 ppm). Coupling constants (*J*) are reported in Hz. Multiplicities are reported using the following abbreviations: s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; br, broad; Carbon-13 nuclear magnetic resonance (^{13}C-NMR) spectra were recorded using a Brucker Avance II DMX 400 spectrometer at 100 MHz Chemical shift is reported in ppm relative to the carbon resonance of $CDCl_3$ (77.00 ppm). High resolution mass spectra (HRMS) were obtained using a Waters TOFMS GCT Premier instrument for HRMS by Center for Instrumental Analysis of Zhejiang Sci-Tech University. The results are reported as m/e (relative ratio); Accurate masses are reported for the molecular ion (M+) or a suitable fragment ion.

2. Procedure for the preparation of 1-sulfonyl-1,2,3-triazole



General procedure: [1] Under a nitrogen atmosphere, dry toluene (15 mL) was added to a flask charged with copper (I) thiophene-2-carboxylate (CuTC, 0.095 g, 0.5 mmol, 0.1 equiv in regards to alkyne) and the alkyne (5 mmol, 1 equiv). The reaction mixture was cooled in an ice-water bath. Subsequently, the sulfonyl azide (6 mmol, 1.2 equiv) was added slowly as the limiting reagent to avoid a run-away exotherm, and the reaction mixture was allowed to warm to room temperature and stirred until TLC analysis showed that alkyne was completely consumed. The reaction mixture was filtered through a short plug of silica gel. The filtrate was concentrated and then purified by flash chromatography with PE/EtOAc (2:1) as eluent to give the corresponding product **1**.

3. Procedure for the preparation of thiochromone



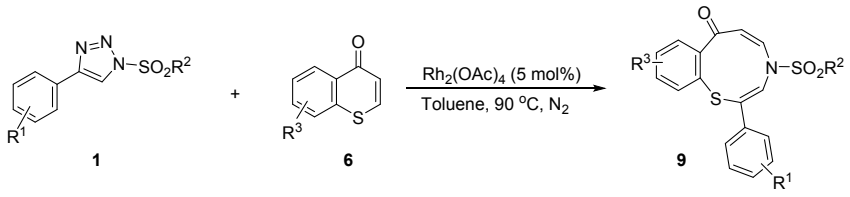
6

General procedure:[2] Thiochromone were prepared according to previously reported procedures. Thiophenols were purchased and used as received. A 250 mL flask was fitted with a stirrer bar and charged with 1M NaOH (50 mL) and 1M Na_2CO_3 (50 mL). A solution of thiophenols **1** (100 mmol) in 60 mL EtOH and 3-chloropropanoic acid (11 g, 102 mmol) in 40 mL H_2O were added respectively to the above solution. The reaction mixture was stirred at room temperature for 2 h, and then temperature increased to reflux. After the reaction was completed as determined by TLC and cooled down to room temperature, EtOH was evaporated and then the aqueous phase was acidified to pH 1~2 with conc HCl. The solution was extracted with CH_2Cl_2 for three times and the combined organic layers were dried over anhydrous Na_2SO_4, filtered, and concentrated. The residue was purified by flash column chromatography (hexane/EtOAc, 20/1 to 3/1) to produce 3-(phenylthio) propanoic acid in 85-95% yield.

A 250 mL flask was filled with 45 mL conc. H_2SO_4 and cooled down to 0 °C. 3-(phenylthio) propanoic acid was added slowly. Then the mixture was stirred at room temperature overnight. After the reaction was completed as determined by TLC, the reaction was quenched by pouring onto ice and extracted with CH_2Cl_2 for three times. The combined organic layers were dried over anhydrous Na_2SO_4, filtered, and concentrated. The residue was purified by flash column chromatography (hexane/EtOAc, 10/1) to afford thiochroman-4-one in 70-95% yield.

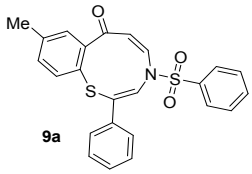
To a solution of thiochroman-4-one (30.5 mmol) in CH_2Cl_2 (100 mL) was added N-chlorosuccinimide (NCS) (30.5 mmol, 1.0 equiv) in one portion. This was stirred for 20 min at 5 °C, and then allowed to warm to room temperature overnight. Water (50 ml) was added and the organic layer was separated and dried (Na_2SO_4), and the product was purified by column chromatography (hexane/EtOAc, 5/1) to give thiochromone **6** in 40-80% yield.

4. Procedure for the preparation of 9



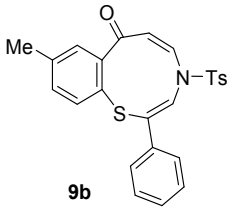
General procedure: Under a nitrogen atmosphere, dry toluene (1.0 mL) was added to reaction flask charged with $Rh_2(OAc)_4$ (5 mol%), 1-sulfonyl-1,2,3-triazoles **1** (0.28 mmol, 1.4 equiv) and thiochromone **6** (0.2 mmol) at room temperature. Then the reaction mixture was stirred at 90 °C for the indicated time in the manuscript. Upon completion of reaction by TLC, the reaction mixture was cooled to room temperature and filtered through a short plug of silica gel. The filtrate was concentrated and the residue was purified by flash chromatography with PE/EtOAc (15:1) as eluent to give the corresponding product **9**.

5. Analytical data for 9



9a

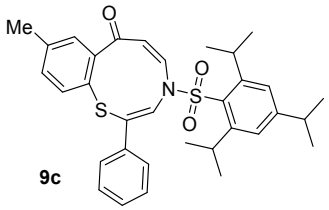
(2Z,5Z)-9-methyl-2-phenyl-4-(phenylsulfonyl)benzo[h][1,4]thiazonin-7(4H)-one (9a): yellow oil, 71.1 mg, yield: 82%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, *J* = 7.5 Hz, 2H), 7.74 (t, *J* = 7.4 Hz, 1H), 7.62 (t, *J* = 7.7 Hz, 2H), 7.49 – 7.42 (m, 2H), 7.28 (t, *J* = 6.7 Hz, 3H), 7.22 (d, *J* = 7.9 Hz, 1H), 7.10 (d, *J* = 7.9 Hz, 1H), 7.05 (s, 1H), 6.72 (s, 1H), 6.60 (d, *J* = 9.8 Hz, 1H), 5.72 (d, *J* = 9.8 Hz, 1H), 2.25 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.8, 141.2, 139.5, 139.1, 137.4, 136.3, 133.8, 133.3, 132.6, 130.0, 129.5, 129.4, 128.3, 127.9, 127.3, 126.4, 125.9, 21.0. HRMS (ESI) calcd for $C_{24}H_{20}NO_3S_2^+$ 434.0879, found 434.0877.



9b

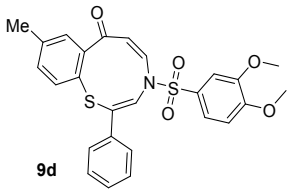
(2Z,5Z)-9-methyl-2-phenyl-4-tosylbenzo[h][1,4]thiazonin-7(4H)-one (9b): yellow oil, 88.1 mg, yield: 98%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 8.1 Hz, 2H), 7.55 – 7.50 (m, 2H), 7.46 (d, *J* = 8.0 Hz, 2H), 7.33 (d, *J* = 6.2 Hz, 3H), 7.27 (d, *J* = 7.9 Hz, 1H), 7.15 (d, *J* = 7.9 Hz, 1H), 7.10 (s, 1H), 6.76 (s, 1H), 6.63 (d, *J* = 9.8 Hz, 1H), 5.78

(d, J = 9.8 Hz, 1H), 2.58 (s, 3H), 2.29 (d, J = 17.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.8, 144.9, 139.1, 133.3, 132.7, 130.2, 130.0, 129.3, 128.4, 128.0, 127.6, 127.4, 126.0, 21.8, 21.0. HRMS (ESI) calcd for $C_{25}H_{22}NO_3S_2^+$ 448.1036, found 448.1034.



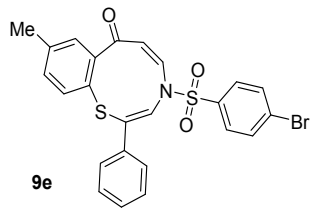
9c

(2Z,5Z)-9-methyl-2-phenyl-4-((2,4,6-triisopropylphenyl)sulfonyl)benzo[h][1,4]thiazonin-7(4H)-one (9c): brown oil, 105 mg, yield: 94%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 – 7.39 (m, 2H), 7.25 (s, 3H), 7.22 (s, 1H), 7.06 (d, J = 7.8 Hz, 1H), 6.98 (s, 1H), 6.83 (d, J = 10.3 Hz, 1H), 6.83 (d, J = 10.3 Hz, 1H), 6.77 (s, 1H), 5.49 (d, J = 10.2 Hz, 1H), 4.16 – 3.96 (m, 3H), 2.96 (dd, J = 13.8, 6.9 Hz, 1H), 2.23 (s, 3H), 1.33 – 1.27 (m, 18H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.0, 154.2, 151.7, 140.6, 138.6, 137.8, 136.3, 132.6, 132.3, 130.2, 129.8, 129.0, 128.3, 128.0, 127.8, 126.8, 125.7, 124.4, 111.2, 34.1, 24.9, 23.5, 20.9. HRMS (ESI) calcd for $C_{33}H_{38}NO_3S_2^+$ 560.2288, found 560.2286.



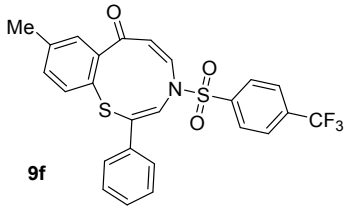
9d

(2Z,5Z)-4-((3,4-dimethoxyphenyl)sulfonyl)-9-methyl-2-phenylbenzo[h][1,4]thiazonin-7(4H)-one (9d): brown oil, 99.4 mg, yield: 99%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 – 7.42 (m, 3H), 7.27 (d, J = 4.9 Hz, 3H), 7.22 (d, J = 1.8 Hz, 2H), 7.08 (d, J = 7.8 Hz, 1H), 7.03 (d, J = 8.4 Hz, 2H), 6.75 (s, 1H), 6.63 (d, J = 9.9 Hz, 1H), 5.66 (d, J = 9.9 Hz, 1H), 4.03 (s, 3H), 3.93 (s, 3H), 2.24 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.1, 153.5, 149.4, 141.1, 139.0, 136.3, 133.15, 132.6, 132.6, 129.9, 129.3, 129.1, 128.4, 128.0, 127.9, 126.4, 126.3, 126.1, 121.6, 110.8, 109.5, 56.3, 20.9. HRMS (ESI) calcd for $C_{26}H_{24}NO_5S_2^+$ 494.1090, found 494.1090.



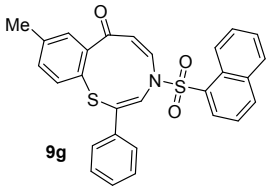
9e

(2Z,5Z)-4-((4-bromophenyl)sulfonyl)-9-methyl-2-phenylbenzo[h][1,4]thiazonin-7(4H)-one (9e): yellow oil, 83 mg, yield: 81%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8.7 Hz, 2H), 7.69 (d, *J* = 8.7 Hz, 2H), 7.54 – 7.43 (m, 2H), 7.29 – 7.30 ((m, 3H), 7.24 (s, 1H), 7.12 (d, *J* = 7.9 Hz, 1H), 7.06 (s, 1H), 6.70 (s, 1H), 6.57 (d, *J* = 9.8 Hz, 1H), 5.77 (d, *J* = 9.8 Hz, 1H), 2.27 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.5, 141.1, 139.9, 139.3, 136.5, 136.1, 133.4, 132.8, 132.8, 130.0, 129.5, 129.1, 128.8, 128.4, 128.0, 126.9, 126.3, 125.5, 21.0. HRMS (ESI) calcd for $C_{24}H_{19}BrNO_3S_2^+$ 511.9984, found 511.9982.



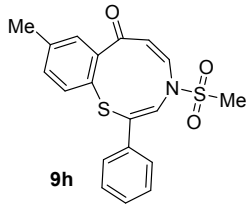
9f

(2Z,5Z)-9-methyl-2-phenyl-4-((4-(trifluoromethyl)phenyl)sulfonyl)benzo[h][1,4]thiazonin-7(4H)-one (9f): yellow oil, 92 mg, yield: 91%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.2 Hz, 2H), 7.89 (d, *J* = 8.3 Hz, 2H), 7.29 (d, *J* = 6.7 Hz, 2H), 7.25 (d, *J* = 7.9 Hz, 3H), 7.23 (d, *J* = 7.9 Hz, 1H), 7.12 (d, *J* = 7.9 Hz, 1H), 7.07 (s, 1H), 6.71 (s, 1H), 6.58 (d, *J* = 9.8 Hz, 1H), 5.79 (d, *J* = 9.8 Hz, 1H), 2.26 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.4, 141.0, 140.9, 140.4, 139.3, 136.0, 135.2 (q, *J* = 25 Hz), 133.4, 132.8, 130.07, 129.6, 128.4, 128.0, 126.7, 126.7, 126.5, 126.2, 125.2, 123.2 (q, *J* = 245 Hz), 20.9. HRMS (ESI) calcd for $C_{25}H_{19}F_3NO_3S_2^+$ 502.0753, found 502.0751.



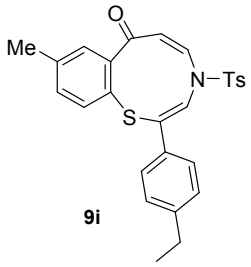
9g

(2Z,5Z)-9-methyl-4-(naphthalen-1-ylsulfonyl)-2-phenylbenzo[h][1,4]thiazonin-7(4H)-one (9g): yellow solid, m.p: 133.2-134.3 ^{o}C, 68 mg, yield:70%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42 (s, 1H), 8.08 (d, *J* = 8.7 Hz, 1H), 8.03 (d, *J* = 7.9 Hz, 3H), 8.02 – 7.58 (m, 4H), 7.47 (d, *J* = 7.5 Hz, 2H), 7.28 (d, *J* = 7.1 Hz, 2H), 7.20 (d, *J* = 7.8 Hz, 1H), 7.09 (d, *J* = 7.9 Hz, 1H), 7.05 (s, 1H), 6.79 (s, 1H), 6.65 (d, *J* = 9.7 Hz, 1H), 5.79 (d, *J* = 9.7 Hz, 1H), 2.23 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.6, 141.2, 139.4, 139.1, 136.4, 135.2, 134.4, 133.4, 132.6, 132.15, 130.0, 1230.0, 129.5, 129.4, 129.3, 129.1, 128.3, 128.1, 128.0, 127.9, 127.3, 126.5, 125.9, 122.0, 20.9. HRMS (ESI) calcd for $C_{28}H_{22}NO_3S_2^+$ 484.1036, found 484.1033.



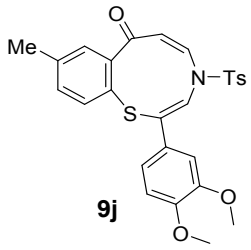
9h

(2Z,5Z)-9-methyl-4-(methylsulfonyl)-2-phenylbenzo[h][1,4]thiazonin-7(4H)-one (9h): yellow oil, 69.9 mg, yield: 90%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 7.8 Hz, 2H), 7.35 (d, *J* = 7.9 Hz, 1H), 7.31 (d, *J* = 7.8 Hz, 3H), 7.16 (d, *J* = 7.9 Hz, 1H), 7.12 (s, 1H), 6.83 (s, 1H), 6.57 (d, *J* = 9.7 Hz, 1H), 5.84 (d, *J* = 9.7 Hz, 1H), 2.93 (s, 3H), 2.29 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.4, 141.1, 139.4, 137.7, 136.3, 133.6, 132.8, 129.9, 129.4, 128.4, 128.0, 127.49, 125.6, 39.3, 20.9. HRMS (ESI) calcd for $C_{19}H_{18}NO_3S_2^+$ 372.0723, found 372.0722.



9i

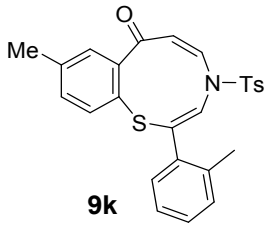
(2Z,5Z)-2-(4-ethylphenyl)-9-methyl-4-tosylbenzo[h][1,4]thiazonin-7(4H)-one (9i): brown oil, 77.1 mg, yield: 81%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.3 Hz, 2H), 7.42 – 7.37 (m, 4H), 7.25 (d, *J* = 7.8 Hz, 1H), 7.11 (d, *J* = 8.2 Hz, 3H), 7.06 (s, 1H), 6.68 (s, 1H), 6.56 (d, *J* = 9.8 Hz, 1H), 5.72 (d, *J* = 9.7 Hz, 1H), 2.61 (q, *J* = 7.6 Hz, 2H), 2.52 (s, 3H), 2.26 (s, 3H), 1.21 (t, *J* = 7.6 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.8, 145.7, 144.8, 141.3, 139.2, 139.0, 134.6, 133.7, 133.3, 132.6, 130.1, 129.9, 127.9, 127.4, 126.7, 126.0, 28.5, 21.7, 21.0, 15.2. HRMS (ESI) calcd for $C_{27}H_{26}NO_3S_2^+$ 476.1349, found 476.1347.



9j

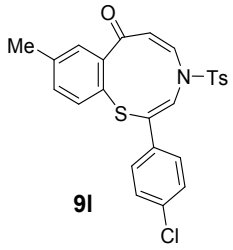
(2Z,5Z)-2-(3,4-dimethoxyphenyl)-9-methyl-4-tosylbenzo[h][1,4]thiazonin-7(4H)-one (9j): brown oil, 29.3 mg, yield: 29%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.3 Hz, 2H), 7.41 (d, *J* = 8.1 Hz, 2H), 7.20 (d, *J* = 7.9 Hz, 1H), 7.08 (d, *J* = 7.9 Hz, 1H), 7.00 (d, *J* = 6.1 Hz, 3H), 6.74 (d, *J* = 8.9 Hz, 1H), 6.69 – 6.65 (m, 2H), 5.59 (d, *J* = 12.7 Hz, 1H), 3.88 (s, 3H), 3.85 (s, 3H), 2.53 (s, 3H), 2.26 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.3, 150.0, 148.5, 144.8,

141.1, 139.1, 138.9, 134.7, 132.9, 132.4, 130.1, 129.9, 128.8, 127.4, 126.8, 126.1, 126.1, 120.8, 111.1, 110.7, 55.9, 55.8, 21.7, 20.9. HRMS (ESI) calcd for $C_{27}H_{26}NO_5S_2^+$ 508.1247, found 508.1246.



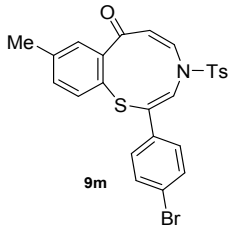
9k

(2Z,5Z)-9-methyl-2-(o-tolyl)-4-tosylbenzo[h][1,4]thiazonin-7(4H)-one (9k): yellow oil, yield: 69%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.3 Hz, 2H), 7.40 – 7.38 (m, 3H), 7.22 (s, 1H), 7.16 (t, *J* = 2.6 Hz, 1H), 7.12 – 7.13 (m, 3H), 7.01 (d, *J* = 2.3 Hz, 1H), 6.58 (d, *J* = 9.7 Hz, 1H), 6.45 (s, 1H), 5.85 (d, *J* = 9.6 Hz, 1H), 2.51 (s, 3H), 2.33 (s, 3H), 2.28 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.9, 144.8, 139.3, 138.3, 136.2, 133.8, 132.9, 130.3, 130.2, 130.0, 129.9, 129.8, 128.6, 127.5, 126.5, 126.2, 125.6, 21.7, 21.0, 20.1. HRMS (ESI) calcd for $C_{26}H_{24}NO_3S_2^+$ 462.1192, found 462.1190.



9l

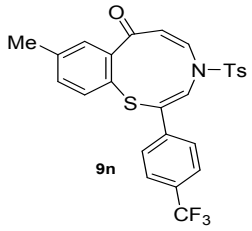
(2Z,5Z)-2-(4-chlorophenyl)-9-methyl-4-tosylbenzo[h][1,4]thiazonin-7(4H)-one (9l): yellow oil, 69.5 mg, yield: 73%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.3 Hz, 2H), 7.43 – 7.39 (m, 4H), 7.37 (s, 3H), 7.21 (d, *J* = 8.1 Hz, 3H), 7.10 (d, *J* = 8.1 Hz, 1H), 7.02 (s, 1H), 6.72 (s, 1H), 6.64 (d, *J* = 9.9 Hz, 1H), 5.67 (d, *J* = 9.9 Hz, 1H), 2.53 (s, 3H), 2.26 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.9, 145.0, 140.9, 139.2, 137.2, 135.2, 134.9, 134.5, 133.0, 132.6, 130.1, 129.9, 129.1, 128.5, 128.2, 127.3, 126.1, 126.0, 21.7, 20.9. HRMS (ESI) calcd for $C_{25}H_{21}ClNO_3S_2^+$ 482.0646, found 482.0644.



9m

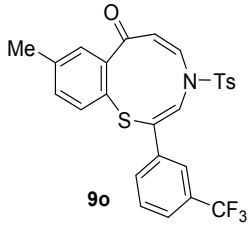
(2z,5z)-2-(4-bromophenyl)-9-methyl-4-tosylbenzo[h][1,4]thiazonin-7(4h)-one (9m): yellow oil, 75.1 mg, yield: 71% ; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.1 Hz, 2H), 7.44 – 7.37 (m, 4H), 7.32 (d, *J* = 8.7 Hz, 2H), 7.21 (d, *J* = 7.8 Hz, 1H), 7.11 (d, *J* = 7.5 Hz, 1H), 7.02 (s, 1H), 6.73 (s, 1H), 6.65 (d, *J* = 9.9 HZ, 1H), 5.67 (d, *J* = 9.9 HZ, 1H), 2.54 (s, 3H), 2.27 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.0, 145.0, 140.9, 139.2, 137.2, 135.4, 134.5, 133.0,

132.6, 131.5, 130.2, 129.95, 129.4, 128.2, 127.3, 126.0, 123.5, 21.8, 21.0. HRMS (ESI) calcd for $C_{25}H_{21}BrNO_3S_2^+$ 526.0141, found 526.0138.



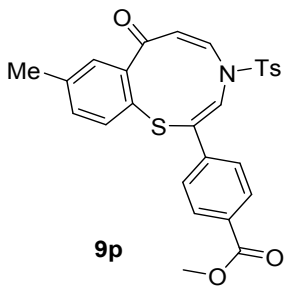
9n

(2Z,5Z)-9-methyl-4-tosyl-2-(4-(trifluoromethyl)phenyl)benzo[h][1,4]thiazonin-7(4H)-one (9n): yellow oil, 70.0 mg, yield: 68%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 8.1 Hz, 2H), 7.57 (d, *J* = 8.2 Hz, 2H), 7.51 (d, *J* = 8.3 Hz, 2H), 7.43 (d, *J* = 8.1 Hz, 2H), 7.23 (d, *J* = 7.9 Hz, 1H), 7.12 (d, *J* = 7.8 Hz, 1H), 7.02 (s, 1H), 6.81 (s, 1H), 6.67 (d, *J* = 9.9 Hz, 1H), 5.72 (d, *J* = 9.9 Hz, 1H), 2.54 (s, 3H), 2.27 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.00, 145.1, 140.8, 140.0, 139.4, 136.2, 134.4, 133.00, 132.8, 131.2 (q, *J* = 21 Hz), 130.2, 129.9 (q, *J* = 8 Hz), 129.8, 128.10, 127.3, 126.0, 125.7, 125.3, 125.3. 121.0 (q, *J* = 256 Hz), 21.8, 21.0. HRMS (ESI) calcd for $C_{26}H_{21}F_3NO_3S_2^+$ 516.0909, found 516.0907.



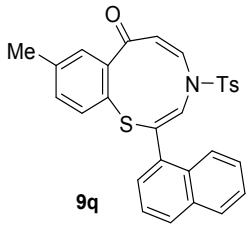
9o

(2Z,5Z)-9-methyl-4-tosyl-2-(3-(trifluoromethyl)phenyl)benzo[h][1,4]thiazonin-7(4H)-one (9o): yellow oil, 49.9 mg, yield: 48%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 – 7.71 (m, 3H), 7.62 (d, *J* = 7.8 Hz, 1H), 7.53 (d, *J* = 7.7 Hz, 1H), 7.60 – 7.20 (m, 3H), 7.24 (d, *J* = 7.9 Hz, 1H), 7.11 (d, *J* = 7.9 Hz, 1H), 7.04 (s, 1H), 6.80 (s, 1H), 6.60 (d, *J* = 9.8 Hz, 1H), 5.75 (d, *J* = 9.8 Hz, 1H), 2.54 (s, 3H), 2.26 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.6, 144.8, 141.7, 141.0, 140.2, 139.4, 137.4, 136.3, 135.4, 133.2, 132.8, 131.8 (q, *J* = 21 Hz), 130.9, 130.2, 130.0, 129.8 (q, *J* = 9 Hz), 128.9, 128.3, 127.3, 124.1, 120.9 (q, *J* = 255 Hz), 111.2, 21.7, 21.2. HRMS (ESI) calcd for $C_{26}H_{21}F_3NO_3S_2^+$ 516.0909, found 516.0907.



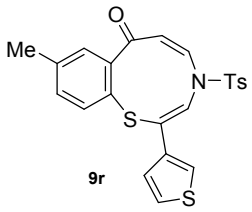
9p

Methyl 4-((2Z,5Z)-9-methyl-7-oxo-4-tosyl-4,7-dihydrobenzo[h][1,4]thiazonin-2-yl)benzoate(9p): yellow oil, 88.4 mg, yield: 87%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.3 Hz, 2H), 7.73 (d, *J* = 8.2 Hz, 2H), 7.52 (d, *J* = 8.4 Hz, 2H), 7.42 (d, *J* = 8.1 Hz, 2H), 7.22 (d, *J* = 7.9 Hz, 1H), 7.09 (d, *J* = 7.9 Hz, 1H), 7.01 (s, 1H), 6.82 (s, 1H), 6.63 (d, *J* = 9.9 Hz, 1H), 5.73 (d, *J* = 9.9 Hz, 1H), 3.90 (s, 3H), 2.53 (s, 3H), 2.24 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.7, 166.5, 145.1, 140.9, 140.9, 139.3, 136.8, 134.4, 133.1, 132.7, 130.6, 130.2, 128.0, 129.6, 129.4, 127.8, 127.3, 126.0, 52.2, 21.8, 21.0. HRMS (ESI) calcd for $C_{27}H_{24}NO_5S_2^+$ 506.1090, found 506.1090.



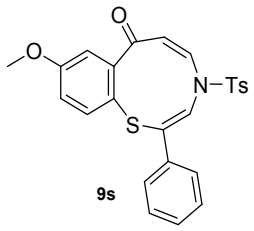
9q

(2Z,5Z)-9-methyl-2-(naphthalen-1-yl)-4-tosylbenzo[h][1,4]thiazonin-7(4H)-one (9q): yellow solid, 80.6 mg, yield: 81%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (s, 1H), 7.87 – 7.83 (m, 1H), 7.81 – 7.77 (m, 1H), 7.6 – 7.74 (m, 3H), 7.60 (d, *J* = 8.6 Hz, 1H), 7.51 – 7.47 (m, 2H), 7.43 (d, *J* = 8.1 Hz, 2H), 7.28 (d, *J* = 7.9 Hz, 1H), 7.07 (d, *J* = 7.9 Hz, 1H), 7.03 (s, 1H), 6.84 (s, 1H), 6.65 (d, *J* = 9.8 Hz, 1H), 5.74 (d, *J* = 9.8 Hz, 1H), 2.55 (s, 3H), 2.22 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.9, 144.9, 139.0, 133.8, 133.6, 133.2, 132.9, 132.6, 130.1, 130.0, 128.5, 128.0, 128.0, 127.6, 127.6, 127.5, 127.4, 126.6, 126.5, 126.4, 126.1, 125.4, 21.8, 20.9. HRMS (ESI) calcd for $C_{29}H_{24}NO_3S_2^+$ 498.1192, found 498.1190.



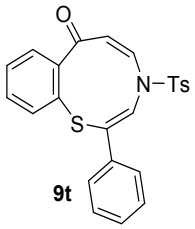
9r

(2Z,5Z)-9-methyl-2-(thiophen-3-yl)-4-tosylbenzo[h][1,4]thiazonin-7(4H)-one (9r): yellow oil, 60.4 mg, yield: 67%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.2 Hz, 2H), 7.41 – 7.39 (m, 3H), 7.27 (d, *J* = 7.9 Hz, 1H), 7.22 (dd, *J* = 5.0, 3.1 Hz, 1H), 7.16 (dd, *J* = 4.4, 3.3 Hz, 2H), 7.08 (s, 1H), 6.76 (s, 1H), 6.54 (d, *J* = 9.6 Hz, 1H), 5.75 (d, *J* = 9.6 Hz, 1H), 2.53 (s, 3H), 2.30 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.7, 144.8, 139.1, 138.1, 134.5, 133.3, 132.7, 130.1, 130.1, 130.0, 127.4, 127.3, 126.5, 126.3, 126.3, 126.2, 126.1, 124.6, 21.8, 21.0. HRMS (ESI) calcd for $C_{23}H_{20}NO_3S_3^+$ 454.0600, found 454.0599.



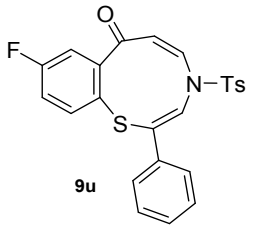
9s

(2Z,5Z)-9-methoxy-2-phenyl-4-tosylbenzo[h][1,4]thiazonin-7(4H)-one (9s): yellow oil, 66.6 mg, yield: 90%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.2 Hz, 2H), 7.51 (d, *J* = 7.7 Hz, 2H), 7.40 (d, *J* = 8.1 Hz, 2H), 7.35 – 7.25 (m, 4H), 6.90 – 6.81 (m, 2H), 6.67 (s, 1H), 6.44 (d, *J* = 9.4 Hz, 1H), 5.91 (d, *J* = 9.4 Hz, 1H), 3.76 (s, 3H), 2.52 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.6, 160.1, 144.8, 142.9, 139.4, 136.6, 135.2, 134.6, 130.1, 129.3, 128.36, 128.0, 127.3, 126.6, 125.9, 120.6, 118.5, 114.1, 55.5, 21.7. HRMS (ESI) calcd for $C_{25}H_{22}NO_4S_2^+$ 464.0985, found 464.0983.



9t

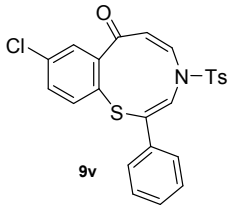
(2Z,5Z)-2-phenyl-4-tosylbenzo[h][1,4]thiazonin-7(4H)-one (9t): yellow oil, 72.8 mg, yield: 85%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.3 Hz, 2H), 7.47 (dd, *J* = 7.3, 2.2 Hz, 2H), 7.42 (d, *J* = 8.1 Hz, 2H), 7.37 (d, *J* = 7.6 Hz, 1H), 7.32 – 7.29 (m, 1H), 7.28 – 7.26 (m, 3H), 7.24 (d, *J* = 4.1 Hz, 2H), 6.73 (s, 1H), 6.61 (d, *J* = 9.8 Hz, 1H), 5.73 (d, *J* = 9.8 Hz, 1H), 2.53 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.5, 144.9, 141.4, 138.6, 136.3, 134.56, 133.3, 131.8, 130.2, 130.1, 129.4, 129.3, 128.8, 128.3, 128.0, 127.8, 127.4, 126.1, 21.7. HRMS (ESI) calcd for $C_{24}H_{20}NO_3S_2^+$ 434.0879, found 434.0879.



9u

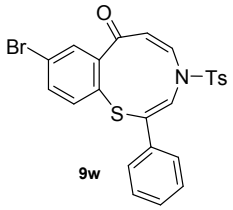
(2Z,5Z)-9-fluoro-2-phenyl-4-tosylbenzo[h][1,4]thiazonin-7(4H)-one (9u): brown oil, 83.2 mg, yield: 92%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.2 Hz, 2H), 7.50 (d, *J* = 7.7 Hz, 2H), 7.41 (d, *J* = 8.2 Hz, 3H), 7.36 – 7.28 (m, 3H), 7.07 – 6.95 (m, 2H), 6.69 (s, 1H), 6.48 (d, *J* = 9.4 Hz, 1H), 5.89 (d, *J* = 9.4 Hz, 1H), 2.53 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.3, 162.8 (q, *J* = 249 Hz), 145.0, 138.8, 136.2, 135.8 (q, *J* = 8 Hz), 134.4, 130.2, 129.5, 128.5,

128.0, 127.3, 127.1, 126.4, 125.2, 119.2, 118.9, 116.8 (q, J = 24 Hz), 21.7. HRMS (ESI) calcd for $C_{24}H_{19}FNO_3S_2^+$ 452.0785, found 452.0783.



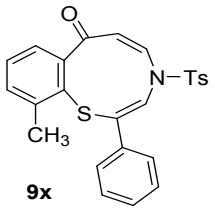
9v

(2Z,5Z)-9-chloro-2-phenyl-4-tosylbenzo[h][1,4]thiazonin-7(4H)-one (9v): yellow solid, 68.5 mg, yield: 73%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, J = 8.3 Hz, 2H), 7.47 (d, J = 7.9 Hz, 2H), 7.42 (d, J = 8.1 Hz, 2H), 7.29 – 7.27 (m, 5H), 7.19 (d, J = 2.2 Hz, 1H), 6.75 (s, 1H), 6.62 (d, J = 9.7 Hz, 1H), 5.74 (d, J = 9.7 Hz, 1H), 2.51 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.8, 145.1, 142.5, 138.2, 136.0, 135.0, 134.7, 134.4, 131.7, 130.2, 129.6, 129.5, 129.3, 128.5, 128.4, 127.9, 127.4, 126.7, 21.8. HRMS (ESI) calcd for $C_{24}H_{19}ClNO_3S_2^+$ 468.0489, found 468.0488.



9w

(2Z,5Z)-9-bromo-2-phenyl-4-tosylbenzo[h][1,4]thiazonin-7(4H)-one (9w): yellow oil, 72.2 mg, yield: 71%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, J = 8.1 Hz, 2H), 7.46 (d, J = 6.3 Hz, 2H), 7.41 – 7.39 (m, 4H), 7.31 – 7.32 (m, 3H), 7.22 (d, J = 8.2 Hz, 1H), 6.76 (s, 1H), 6.64 (d, J = 9.7 Hz, 1H), 5.70 (d, J = 9.7 Hz, 1H), 2.54 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.8, 145.1, 142.5, 138.0, 136.00, 134.7, 134.6, 134.4, 132.1, 130.2, 129.6, 129.1, 128.5, 128.2, 127.9, 127.4, 126.7, 122.8, 21.8. HRMS (ESI) calcd for $C_{24}H_{19}BrNO_3S_2^+$ 511.9984, found 511.9982.

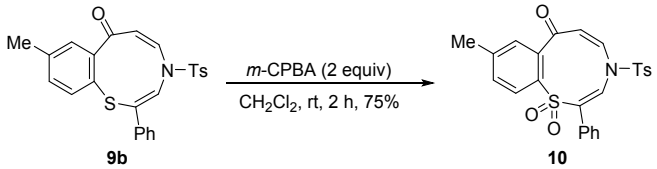


9x

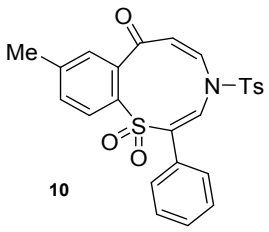
(2Z,5Z)-11-methyl-2-phenyl-4-tosylbenzo[h][1,4]thiazonin-7(4H)-one (9x): yellow oil, 14.6 mg, yield:16%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, J = 8.3 Hz, 2H), 7.44 – 7.42 (m, 4H) , 7.24 (d, J = 7.0 Hz, 3H), 7.17 (d, J = 7.3 Hz, 1H), 7.09 (t, J = 7.5 Hz, 1H), 7.00 (d, J = 7.4 Hz, 1H), 6.79 – 6.73 (m, 2H), 5.58 (d, J = 7.9 Hz, 1H) 2.54 (s, 3H), 2.42 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.2, 144.9, 141.4, 139.7, 137.8, 136.3, 134.6, 133.1, 130.1, 129.3,

129.3, 128.2, 127.9, 127.6, 127.4, 127.2, 126.2, 21.7, 20.3. HRMS (ESI) calcd for $C_{25}H_{22}NO_3S_2^+$ 448.1036, found 448.1034.

6. Synthesis of sulfone derivatives

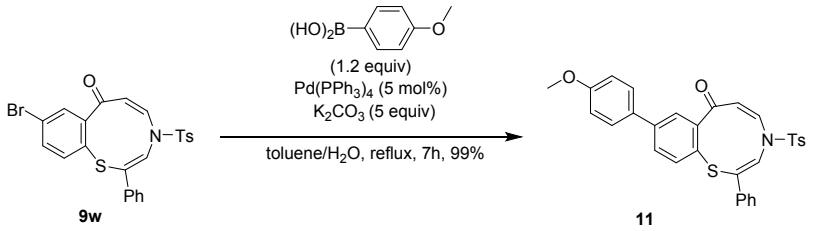


General procedure: [3] To a 25 mL round bottom flask equipped with stir bar, **9b** (0.1 mmol) was dissolved with dry CH_2Cl_2 (2 mL), transferred to a magnetic stir with ice-bath. Next, at 0 °C temperature *m*-CBPA (0.2 mmol, 2 equiv) was added via portion-wise and allowed to stir for 2 hours at room temperature. After completion of the reaction, by TLC, the reaction was neutralized with $NaHCO_3$ solution and workup with CH_2Cl_2, the organic layer was evaporated under reduced pressure. The crude product obtained was purified by column chromatography using hexane/ethyl acetate mixture as eluent to afford sulfone derivatives **10**

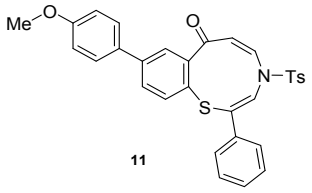


(2Z,5Z)-9-methyl-2-phenyl-4-tosylbenzo[h][1,4]thiazonin-7(4H)-one 1,1-dioxide (10): brown oil**,** 35.9 mg, yield: 75%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.2 Hz, 2H), 7.50 (d, *J* = 8.1 Hz, 2H), 7.42 (d, *J* = 8.0 Hz, 1H), 7.30 – 7.23 (m, 3H), 7.17 (t, *J* = 7.6 Hz, 2H), 7.11 (d, *J* = 10.1 Hz, 1H), 6.96 (d, *J* = 7.5 Hz, 2H), 6.59 (s, 1H), 5.59 (d, *J* = 10.1 Hz, 1H), 2.56 (s, 3H), 2.36 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.3, 145.8, 144.3, 141.4, 135.8, 135.5, 133.7, 133.6, 130.4, 129.6, 129.3, 128.8, 128.7, 127.8, 127.5, 124.9, 113.1, 21.8, 21.0. HRMS (ESI) calcd for $C_{25}H_{22}NO_5S_2^+$ 480.0934, found 480.0933.

7. Suzuki reaction of 9w



General procedure; To a 10 mL round bottom flask equipped with stir bar was added **9w** (0.1 mmol), boronic acid (1.2 equiv), $Pd(PPh_3)_4$ and K_2CO_3 under nitrogen atmosphere was dissolved in toluene/H_2O(5:1).The mixture was stirred at room temperature for 10 mins to dissolve the reacting species. The reaction was later heated at reflux. After completion of the reaction by TLC, the reaction was cooled to room temperature and neutralized with water and then extracted using EtOAc. The organic layer was dry using Na_2SO_4, filter and evaporated under reduced pressure. The crude product was purified by flash chromatography with PE/EtOAc (5:1) as eluent to give the corresponding product **11.**



(2Z,5Z)-9-(4-methoxyphenyl)-2-phenyl-4-tosylbenzo[h][1,4]thiazonin-7(4H)-one (11): brown oil, 89.8 mg, yield: 99%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, J = 8.3 Hz, 2H), 7.53 – 7.49 (m, 3H), 7.49 – 7.44 (m, 2H), 7.42 – 7.37 (m, 3H), 7.30 (d, J = 3.5 Hz, 4H), 6.95 (d, J = 8.8 Hz, 2H), 6.77 (s, 1H), 6.64 (d, J = 9.8 Hz, 1H), 5.77 (d, J = 9.8 Hz, 1H), 3.86 (s, 1H), 2.51 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.6, 197.7, 159.6, 144.9, 141.3, 141.2, 138.5, 136.4, 135.1, 135.1, 134.5, 133.7, 131.5, 130.1, 129.6, 129.4, 128.4, 128.0, 127.4, 126.2, 114.3, 55.4, 21.7. HRMS (ESI) calcd for $C_{31}H_{26}NO_4S_2^+$ 540.1298, found 540.1297.

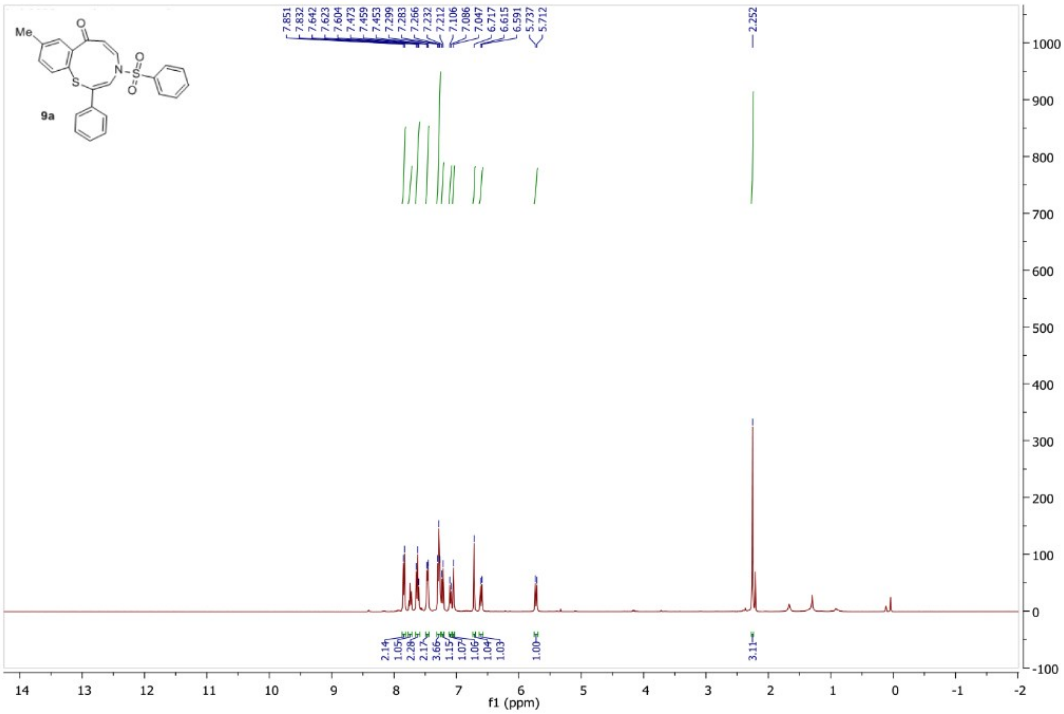
8. References.

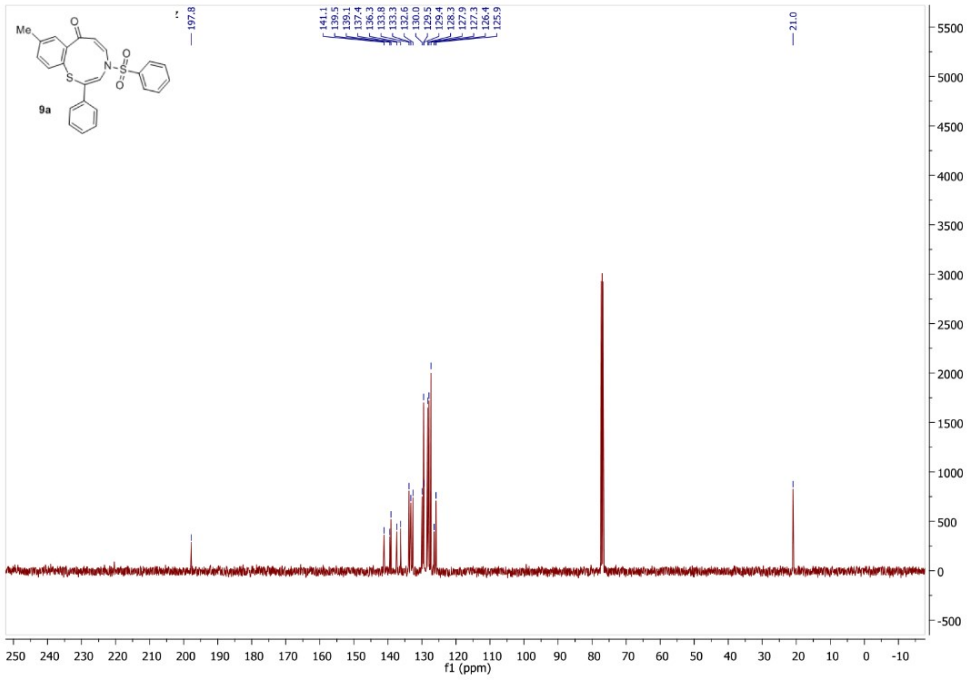
[1] J. Raushel and V. V. Fokin, *Org. Lett.*, 2010, **12**, 4952-4955.

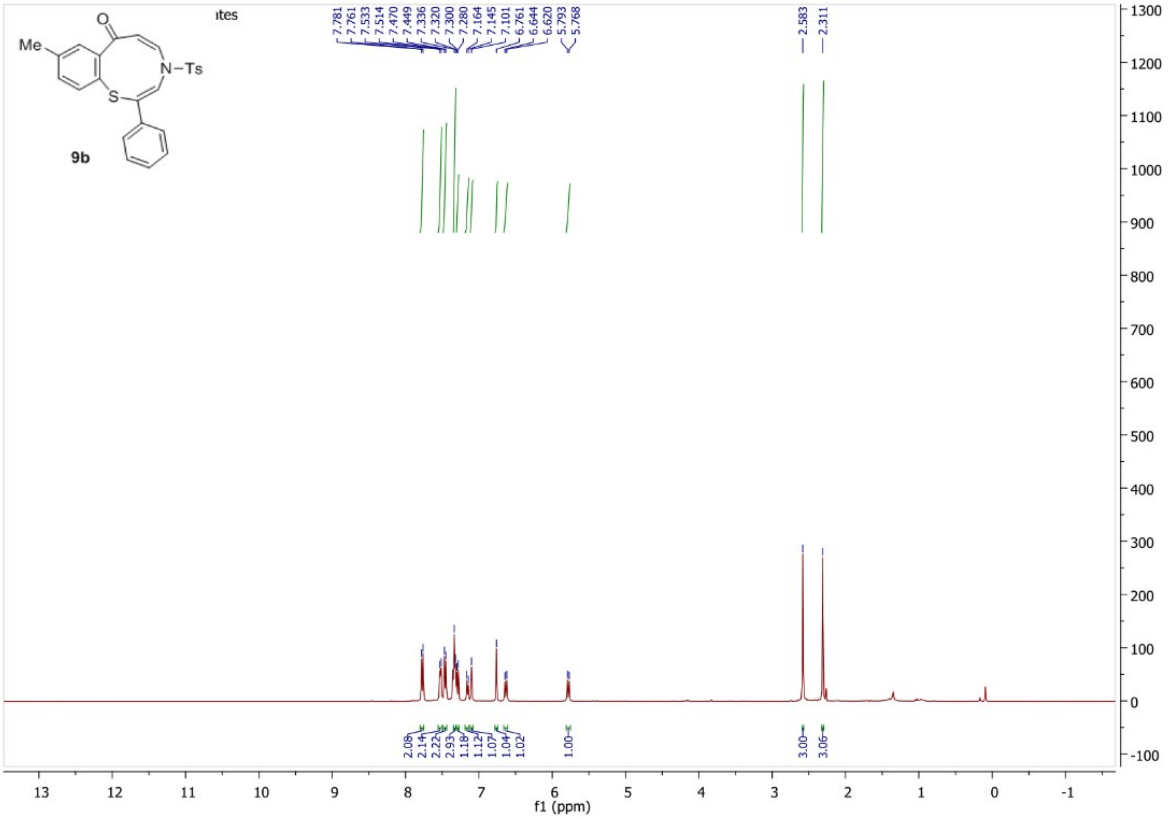
[2] L. Meng, Ka. Y. Ngai, X. Chang, Z. Lin, and J. Wang, *Org. Lett*., 2020, **22**, 1155-1159.

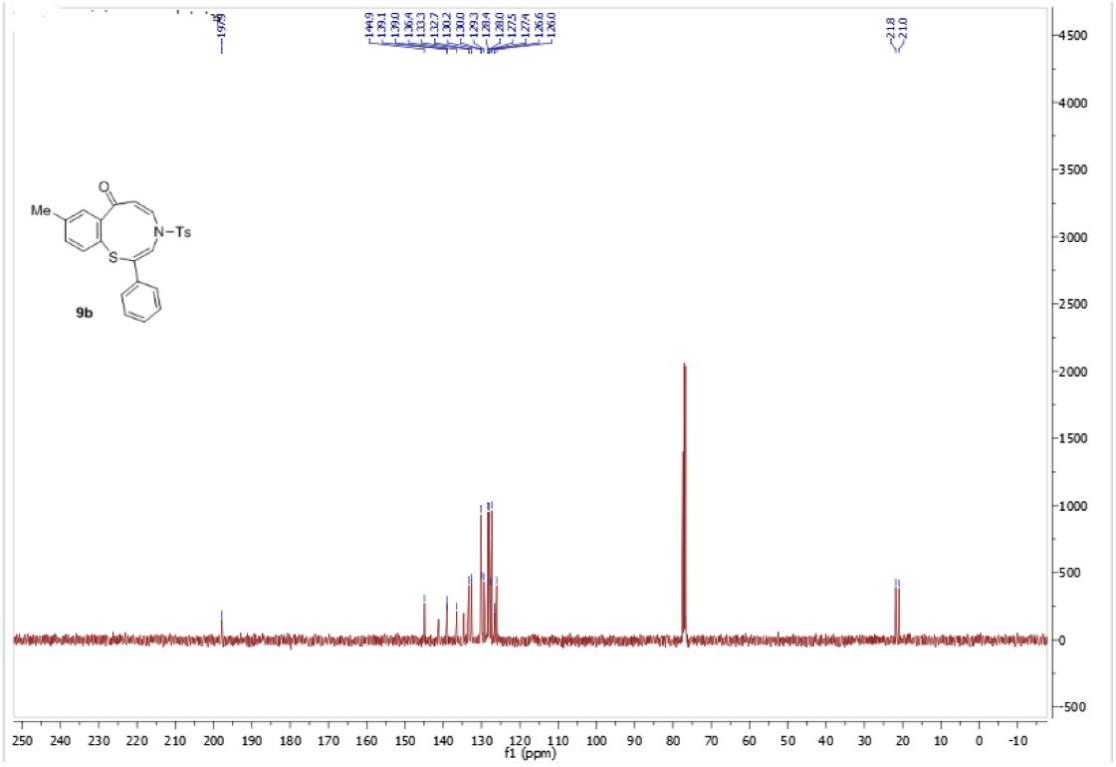
[3] A. C. S.Reddy, K. Ramachandran, P. M. Reddy and P. Anbarasan, *Chem. Commun.*, 2020, **56**, 5649-5652.

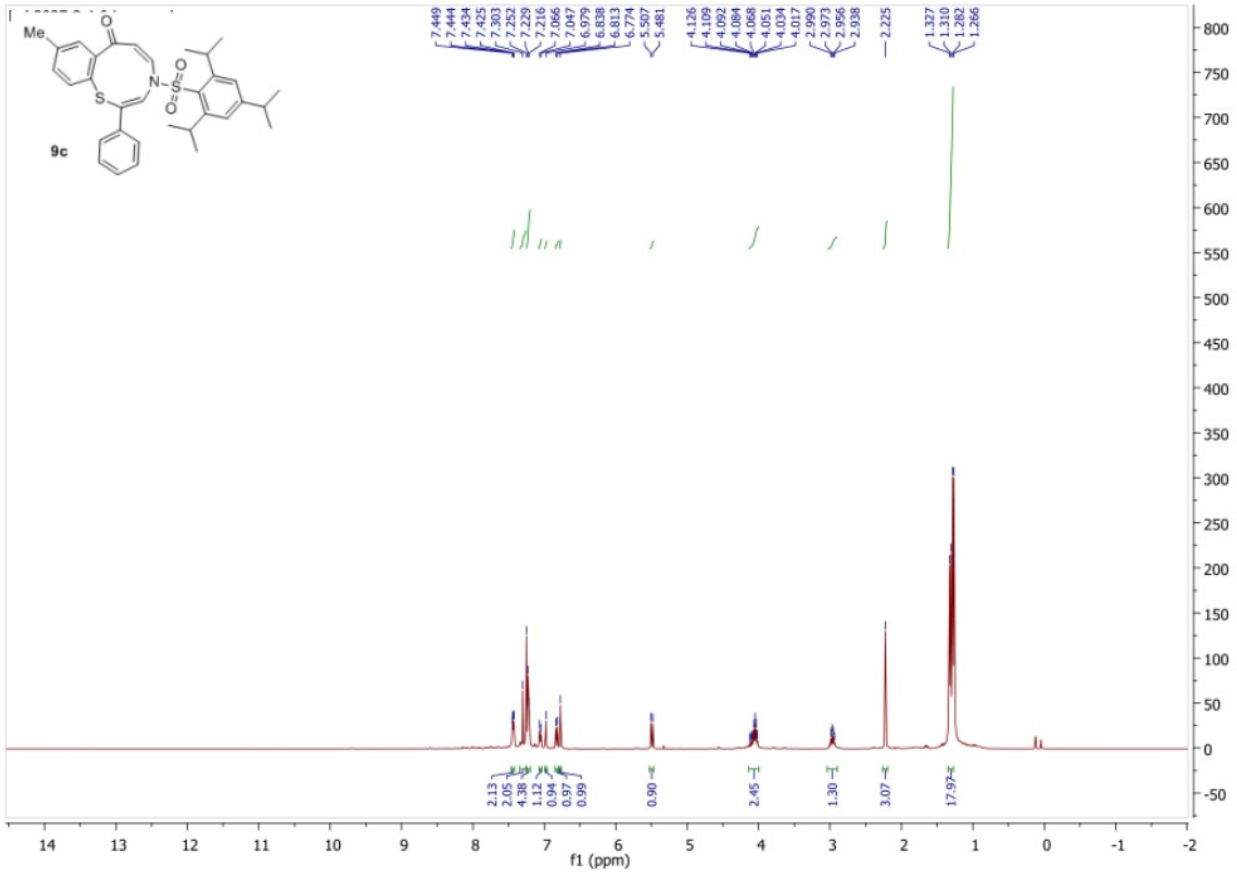
9. ^{1}H and ^{13}C NMR spectra for new compounds

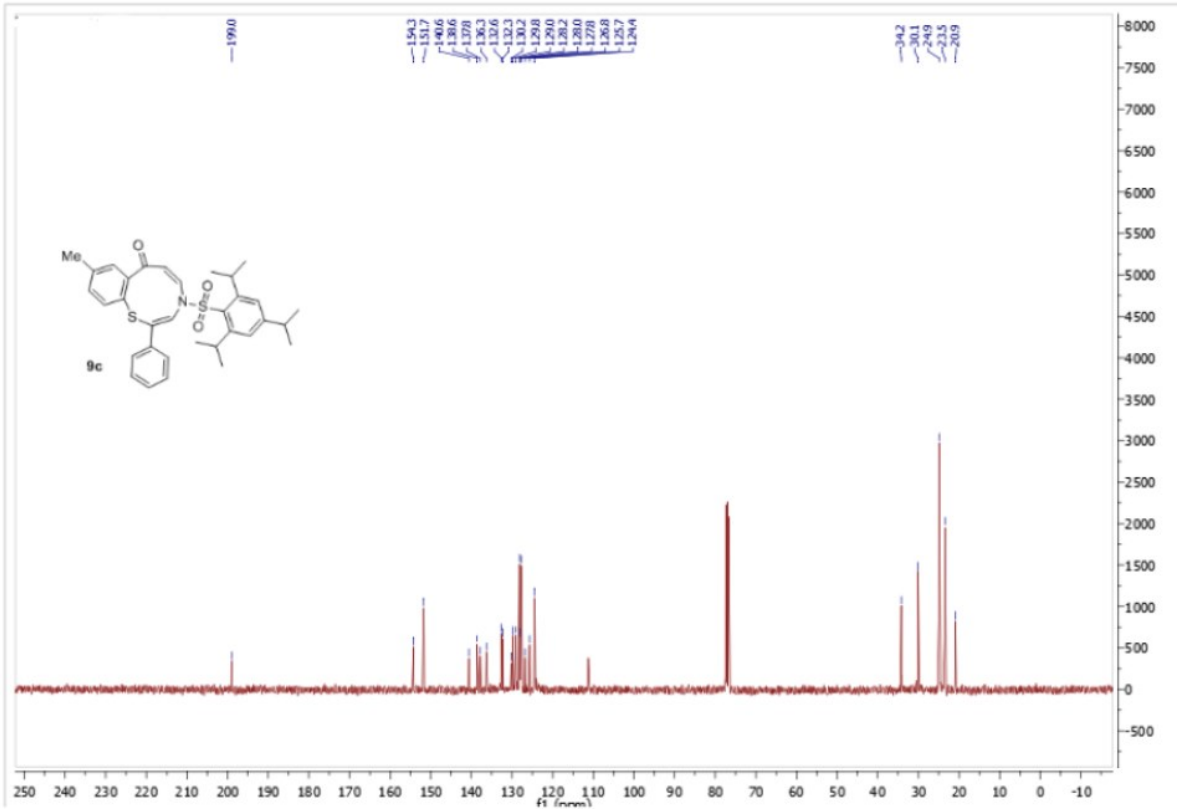


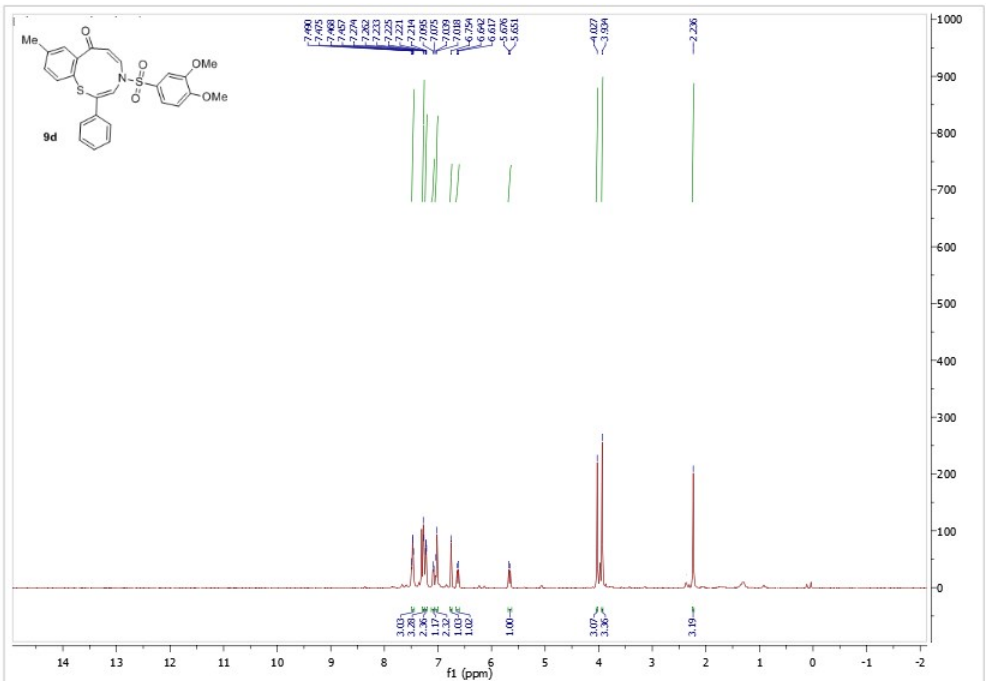


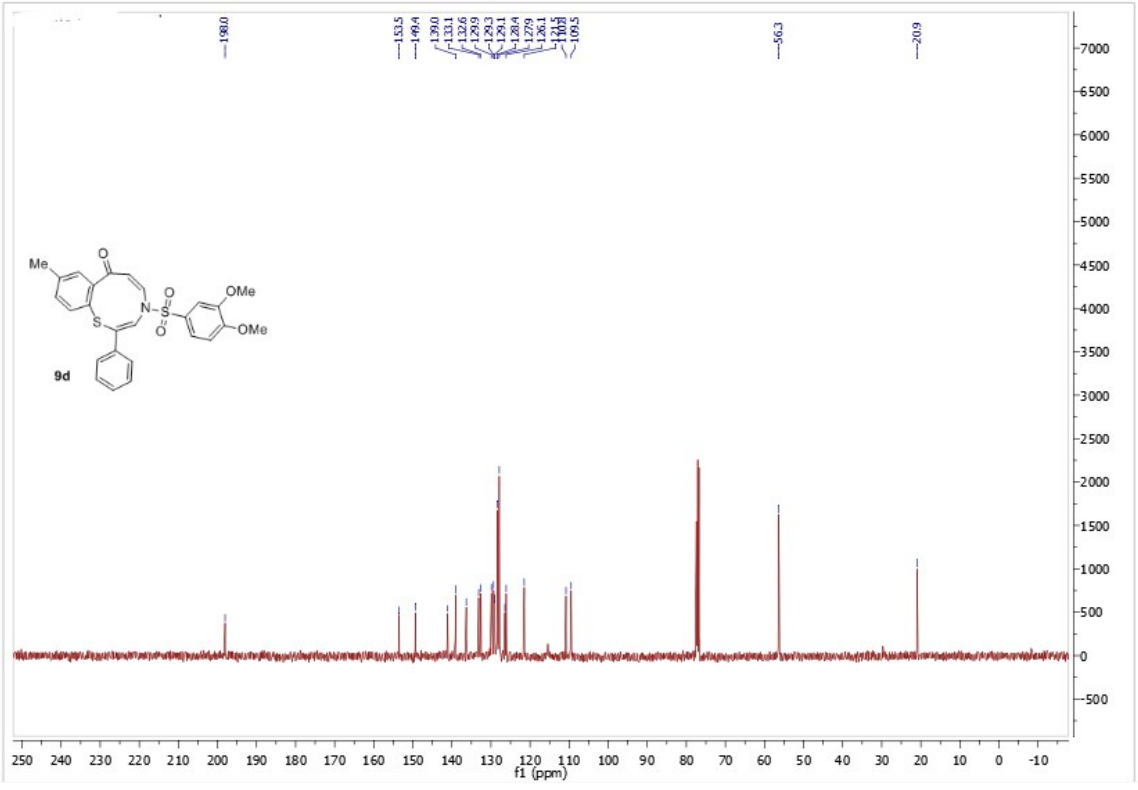

Me
O
N–Ts
S
9b
7.781
7.761
7.533
7.514
7.470
7.449
7.336
7.320
7.300
7.280
7.164
7.145
7.101
6.761
6.644
6.620
5.793
5.768
2.583
2.311
2.08
2.14
2.22
2.93
1.19
1.12
1.07
1.04
1.02
1.00
3.00
3.06
f1 (ppm)

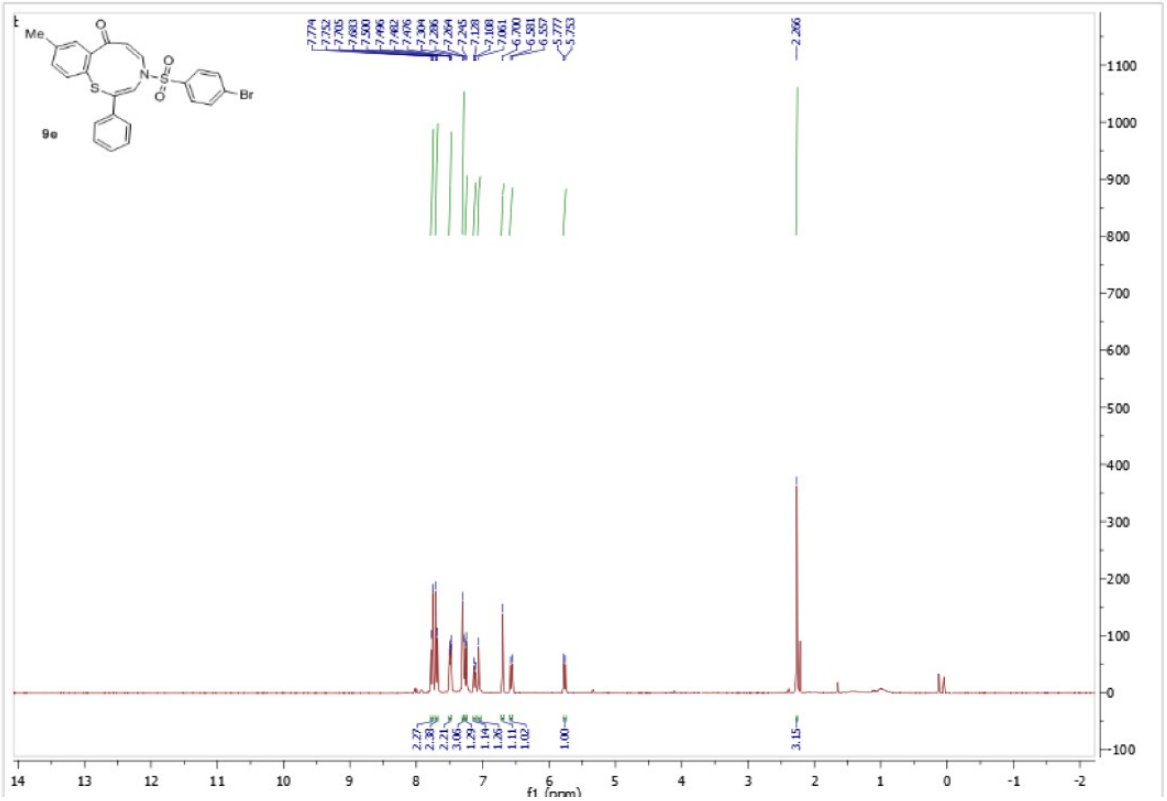

Me
O
N–Ts
S
9b
f1 (ppm)

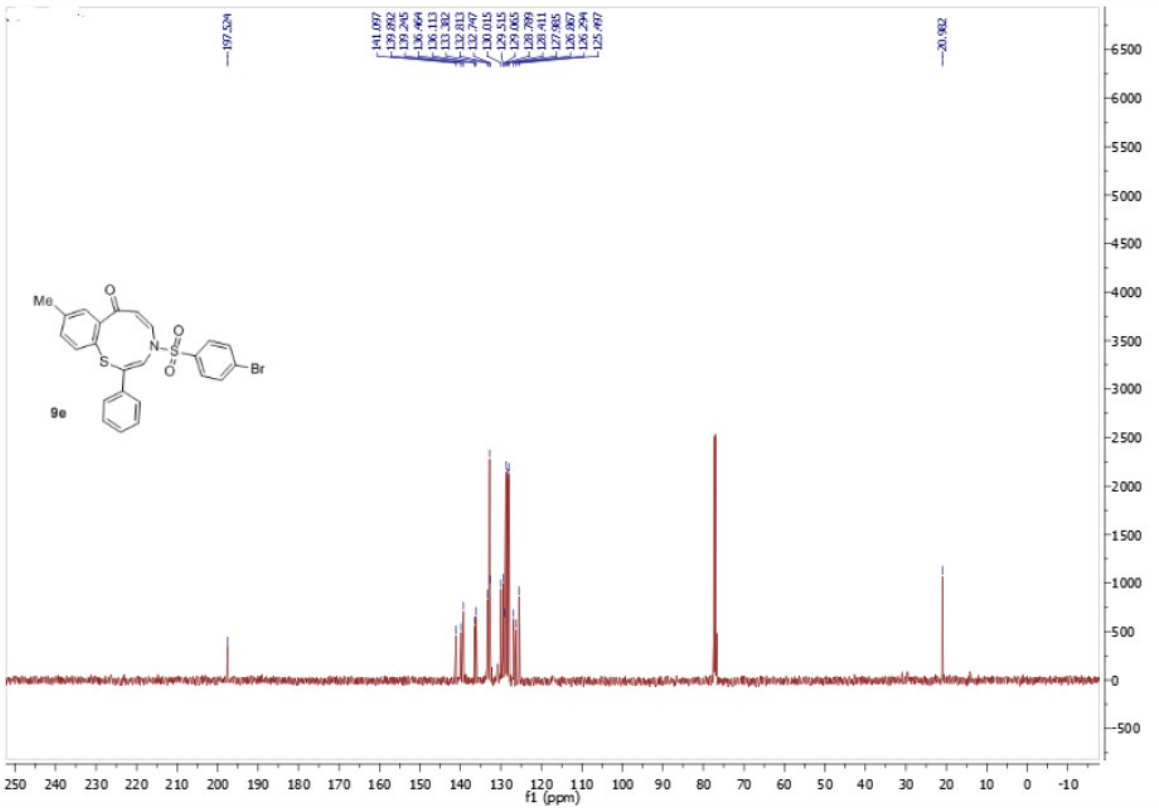

Me
9c
f1 (ppm)

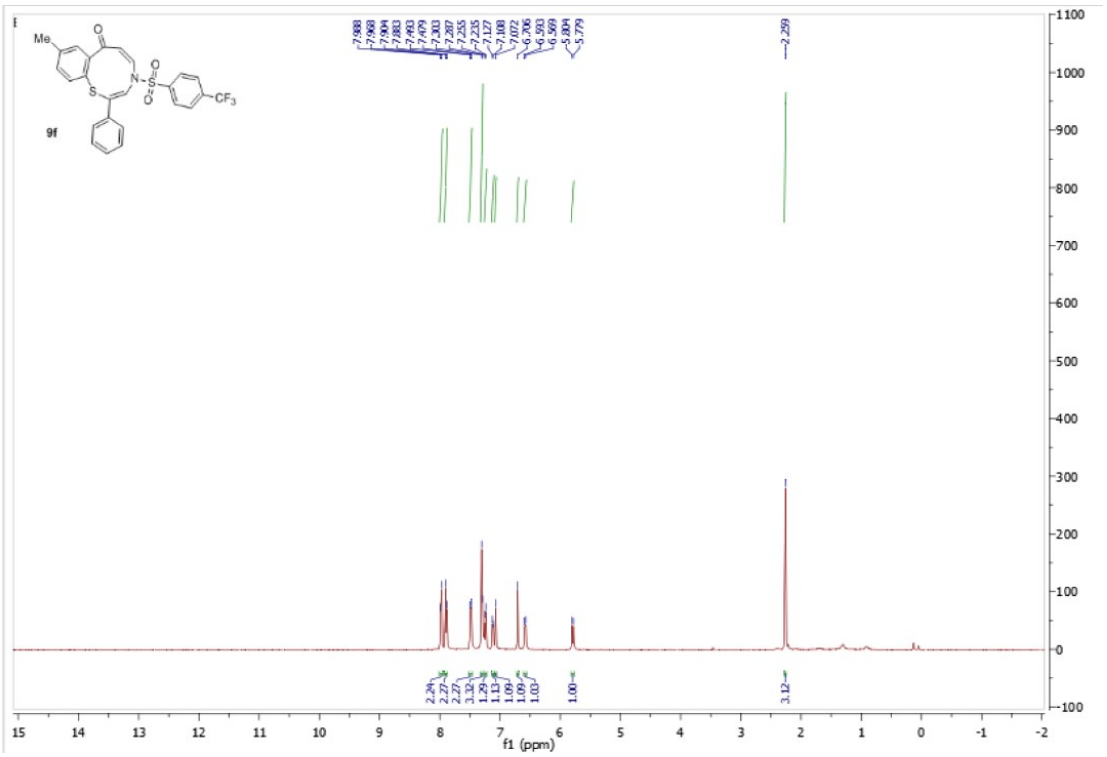

Me
9c
f1 (ppm)

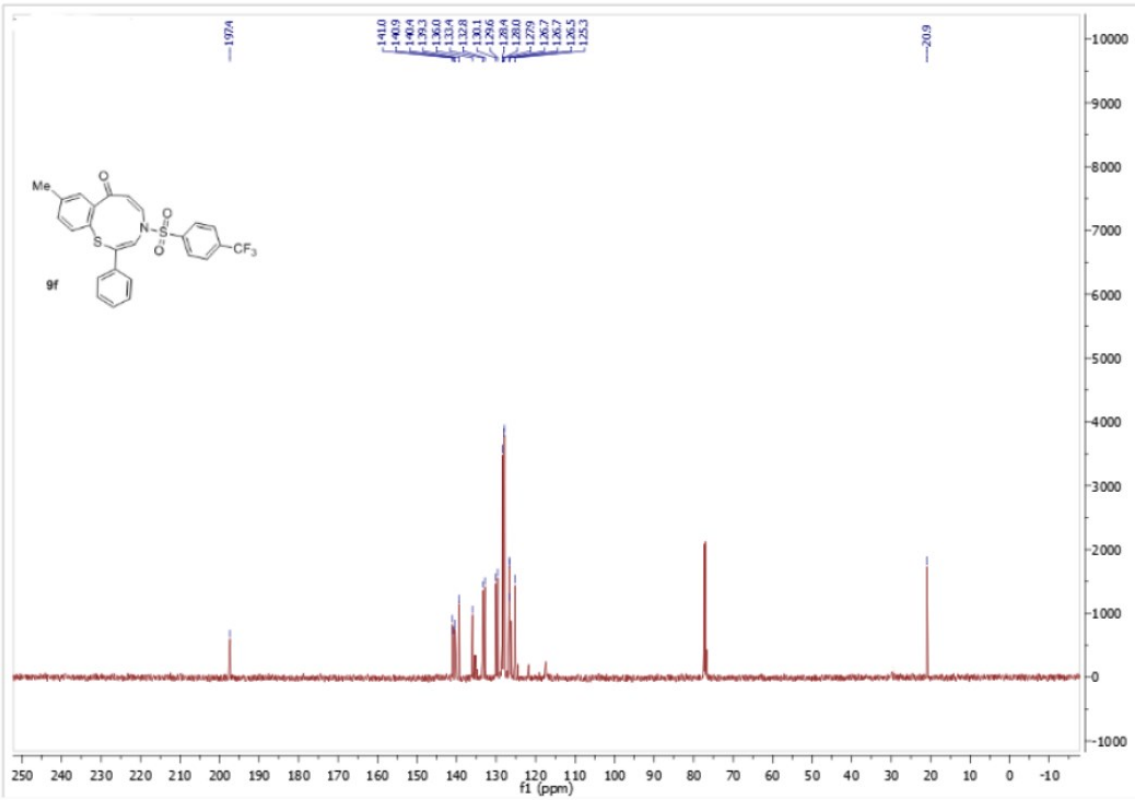

Me
OMe
OMe
9d
7.490
7.485
7.468
7.457
7.274
7.262
7.233
7.225
7.221
7.214
7.095
7.075
7.039
7.018
6.759
6.642
6.617
5.676
5.651
4.027
3.934
2.236
3.03
3.28
2.36
1.17
2.24
1.03
1.02
1.00
3.07
3.36
3.19
f1 (ppm)

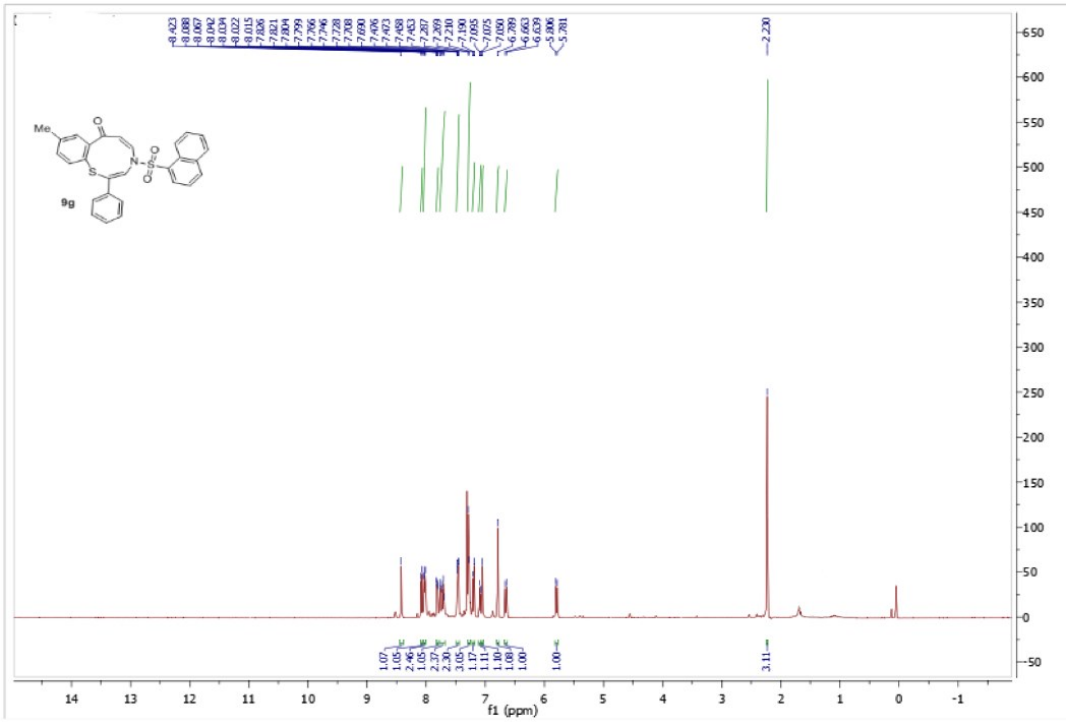

198.0
153.5
149.4
139.0
133.1
132.6
129.9
129.3
129.1
128.4
127.9
126.1
109.5
56.3
20.9
Me
OMe
OMe
9d
f1 (ppm)

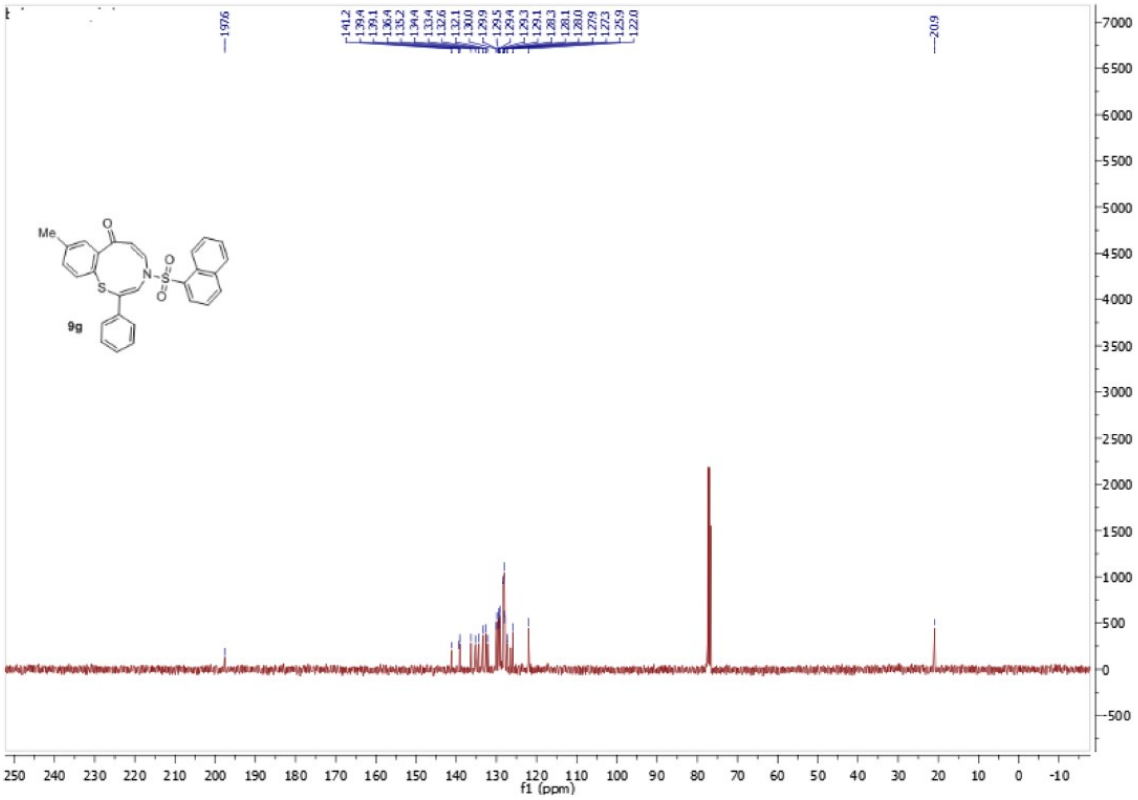

Me
Br
9e
7.774
7.732
7.705
7.693
7.500
7.496
7.482
7.476
7.309
7.286
7.264
7.245
7.128
7.108
7.061
6.700
6.581
6.557
5.777
5.753
2.266
2.27
2.38
2.21
3.06
1.29
1.14
1.26
1.11
1.02
1.00
3.15
f1 (ppm)

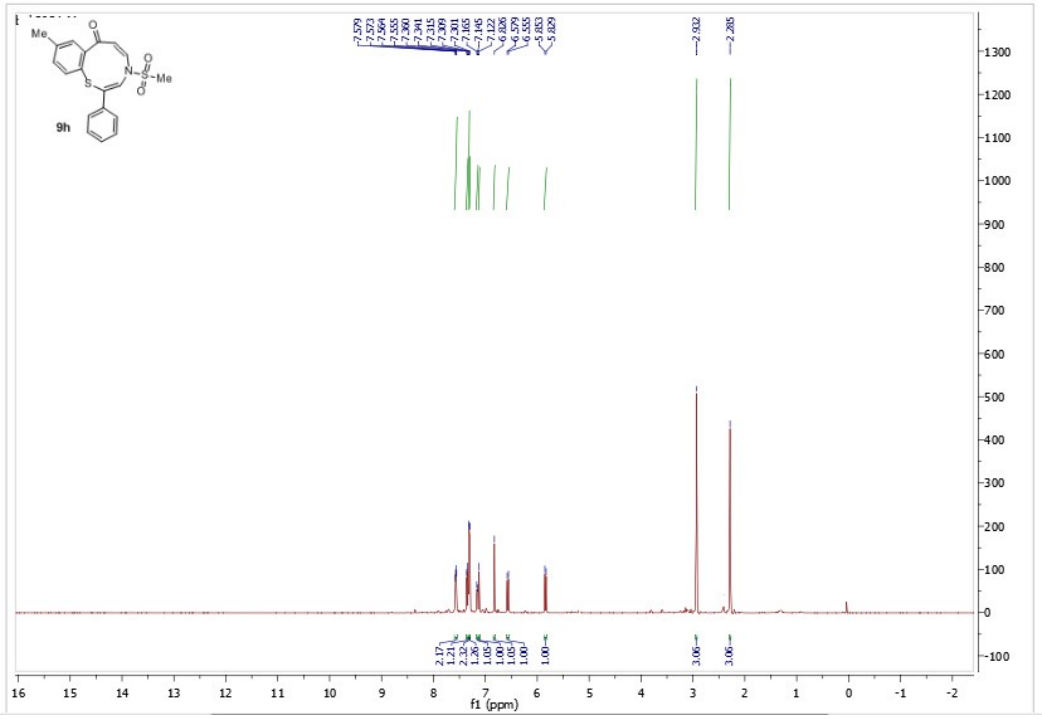

Me
Br
9e
197.524
141.097
139.892
139.245
136.464
136.113
133.302
132.813
132.747
130.015
129.515
129.065
128.789
128.411
127.985
126.867
126.294
125.497
20.982
f1 (ppm)

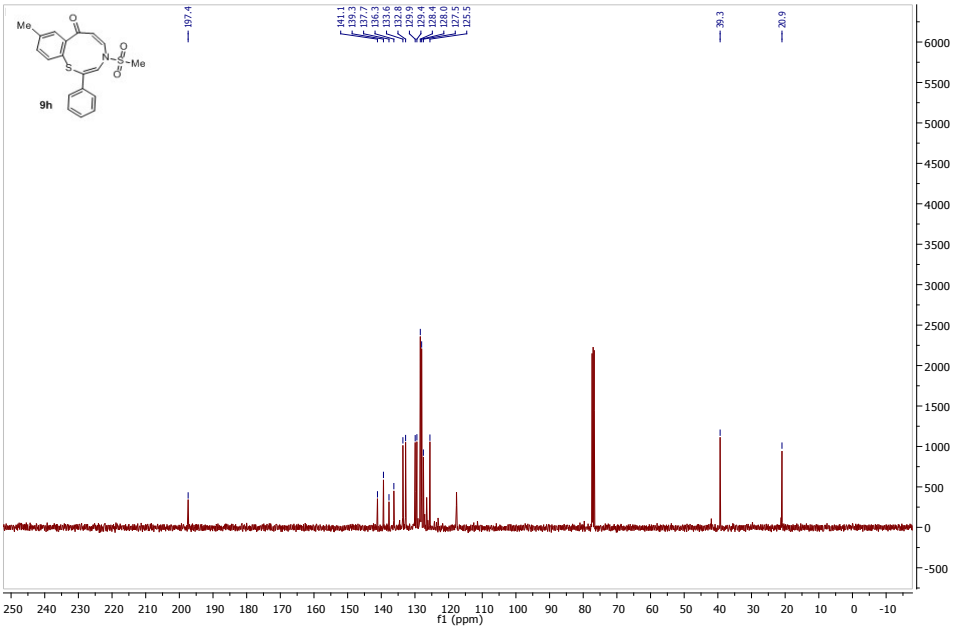

Me
O
N
S
O
O
S
CF3
9f
7.988
7.968
7.904
7.883
7.493
7.479
7.303
7.287
7.235
7.127
7.108
7.072
6.706
6.593
6.569
5.804
5.779
2.299
2.24
2.27
2.27
3.32
1.29
1.13
1.09
1.09
1.03
1.00
3.12
f1 (ppm)

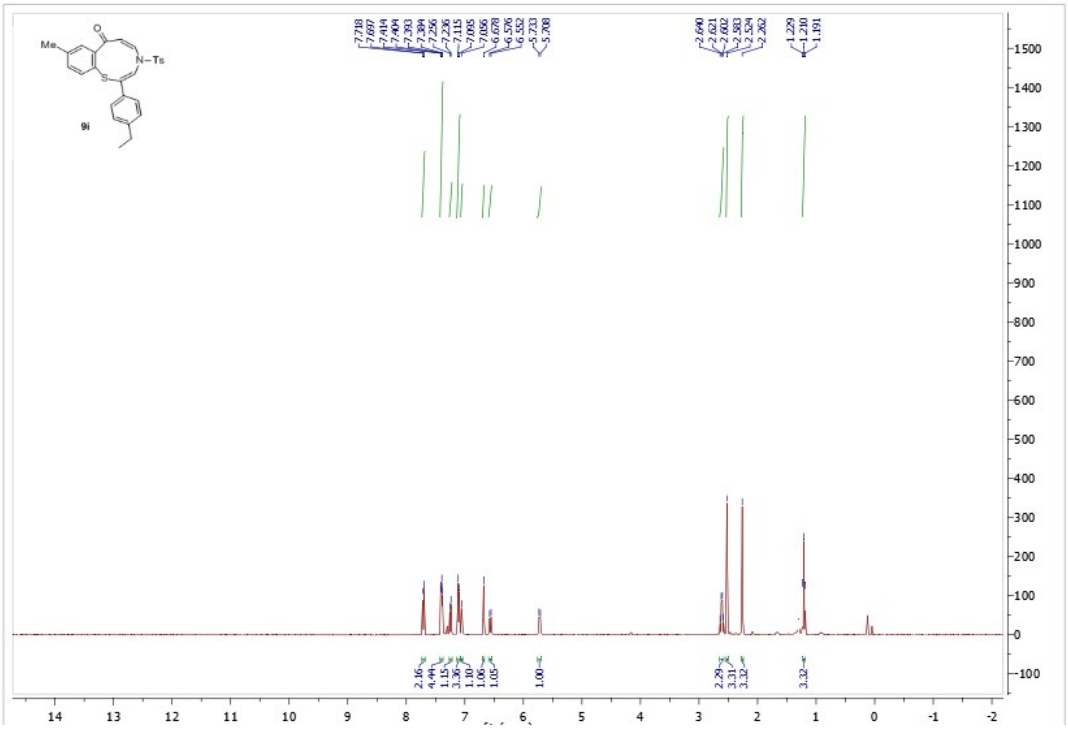

Me
O
N
S
O
O
S
CF3
9f
197.4
141.0
140.9
140.4
139.1
136.0
133.4
132.8
130.1
129.6
128.4
128.0
127.9
126.7
126.7
126.5
125.3
20.9
f1 (ppm)


9g
f1 (ppm)


9g
f1 (ppm)


9h
7.579
7.573
7.564
7.555
7.300
7.301
7.315
7.300
7.301
7.165
7.145
7.122
6.568
6.579
6.555
5.853
5.829
2.932
2.285
2.17
1.21
2.32
2.36
1.05
1.00
1.05
1.00
1.00
3.06
3.06
f1 (ppm)


9h
197.4
141.1
139.3
137.7
136.3
133.6
132.8
129.9
129.4
128.4
128.0
127.5
125.5
39.3
20.9
f1 (ppm)


9i
Me
N–Ts
7.718
7.697
7.414
7.404
7.393
7.384
7.236
7.226
7.115
7.095
7.056
6.678
6.576
6.552
5.733
5.708
2.690
2.631
2.602
2.583
2.524
2.262
1.229
1.210
1.191
2.46
4.44
1.15
3.06
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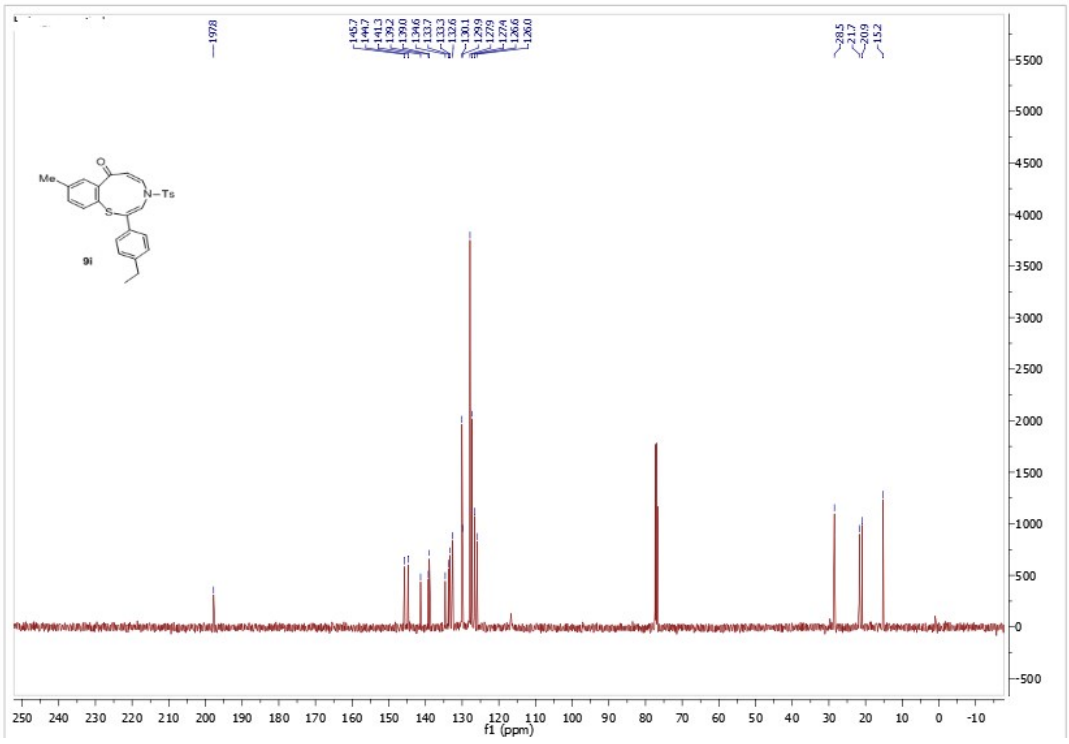
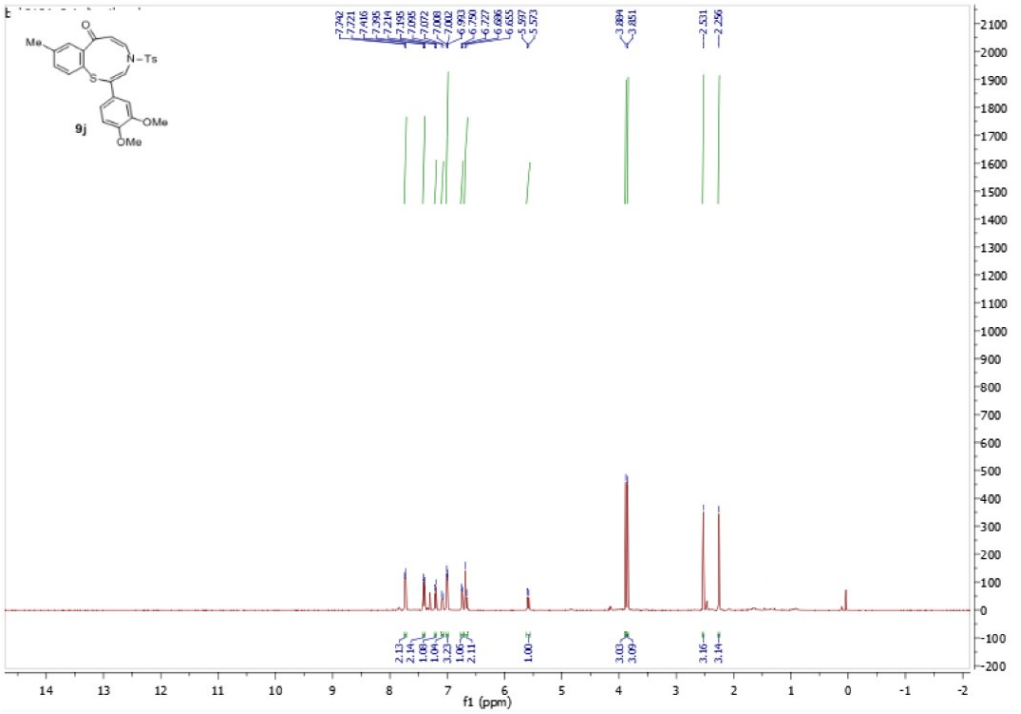
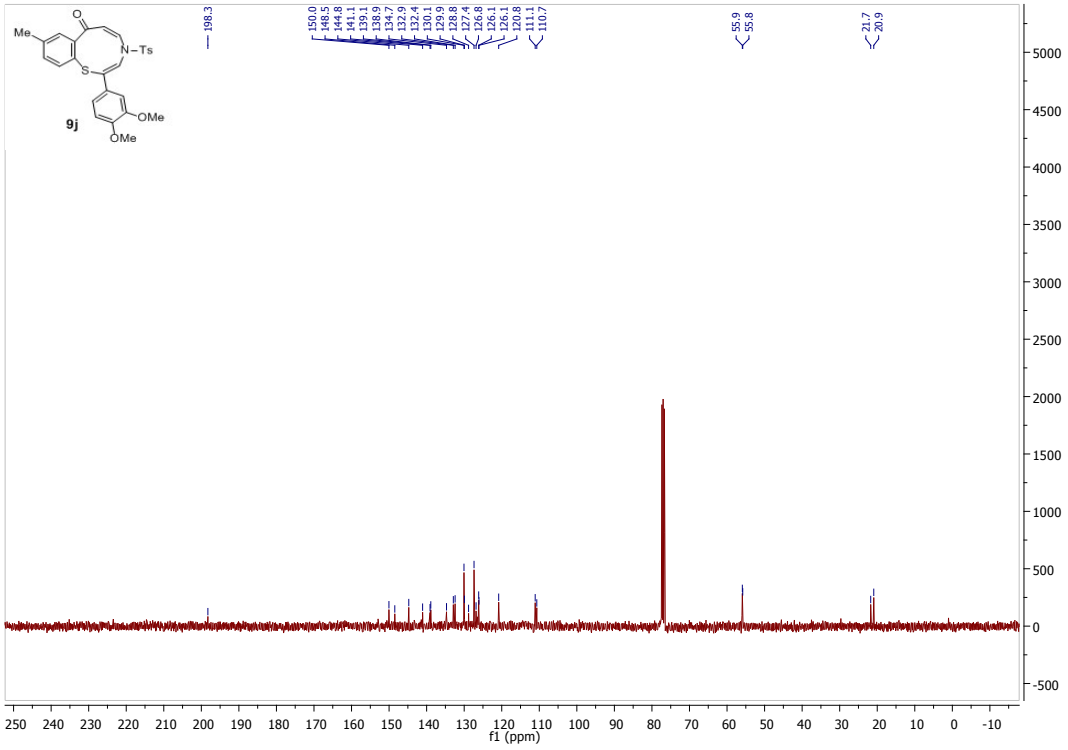
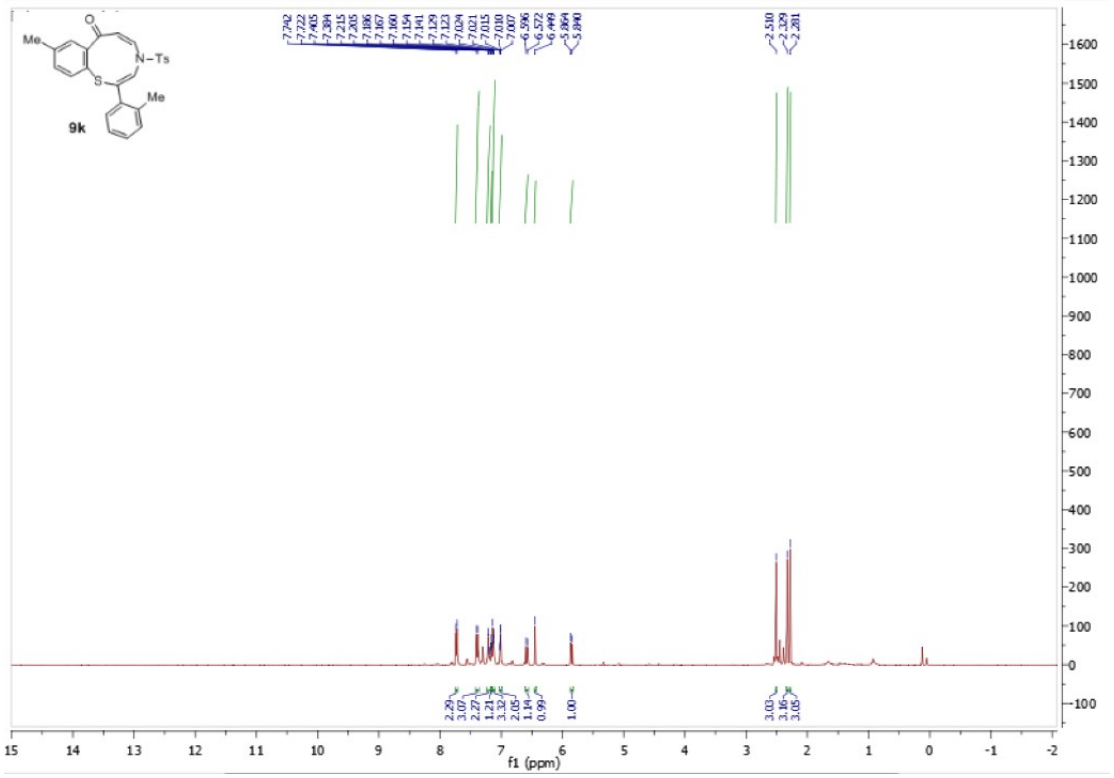
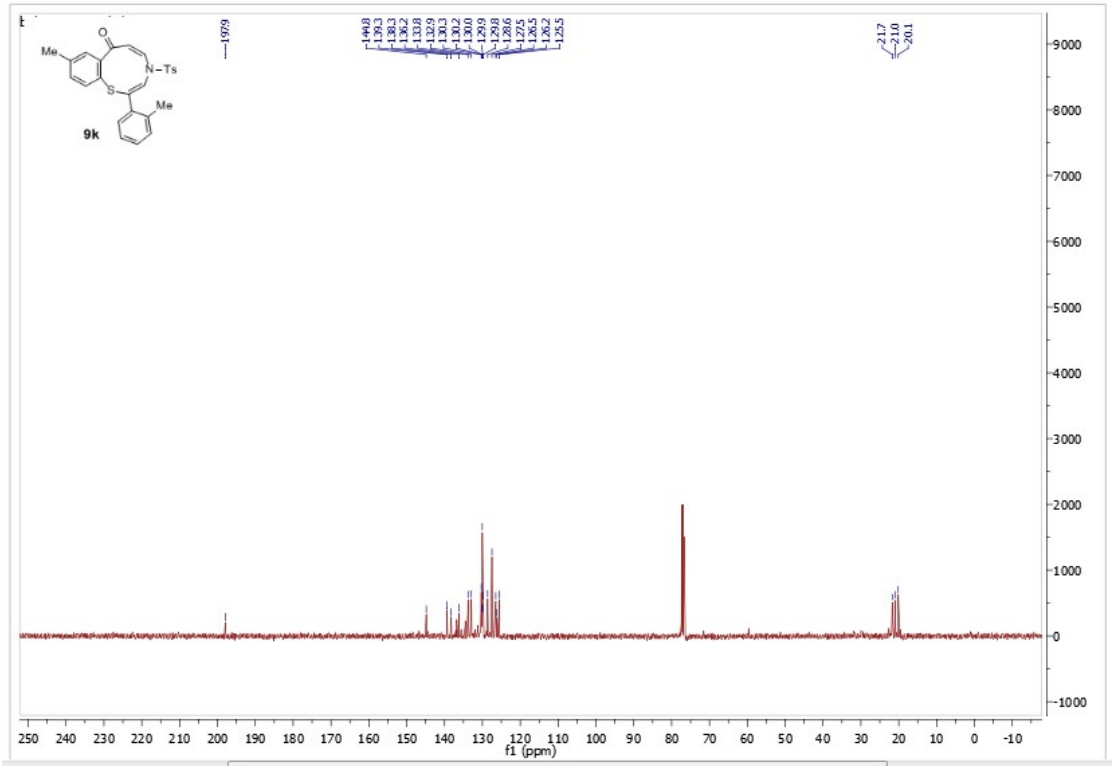
1.05
1.00
2.29
3.31
3.32
3.32

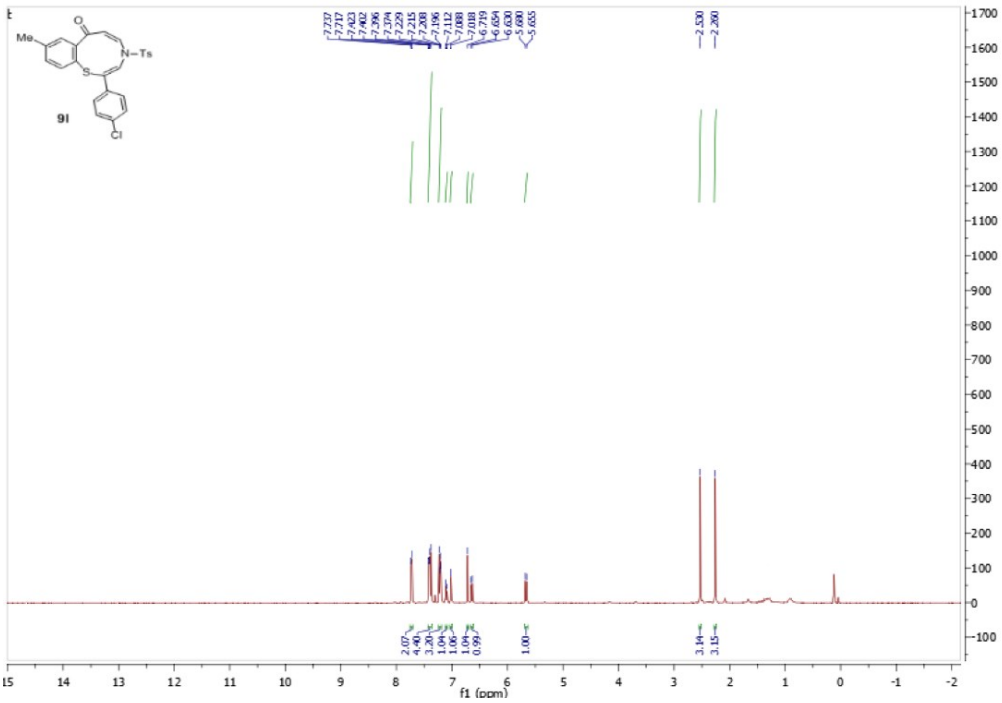

9i
Me
N–Ts
197.8
145.7
144.7
141.3
139.2
139.0
134.6
133.7
133.3
132.6
130.1
129.9
127.9
127.4
126.6
126.0
28.5
21.7
20.9
15.2
f1 (ppm)

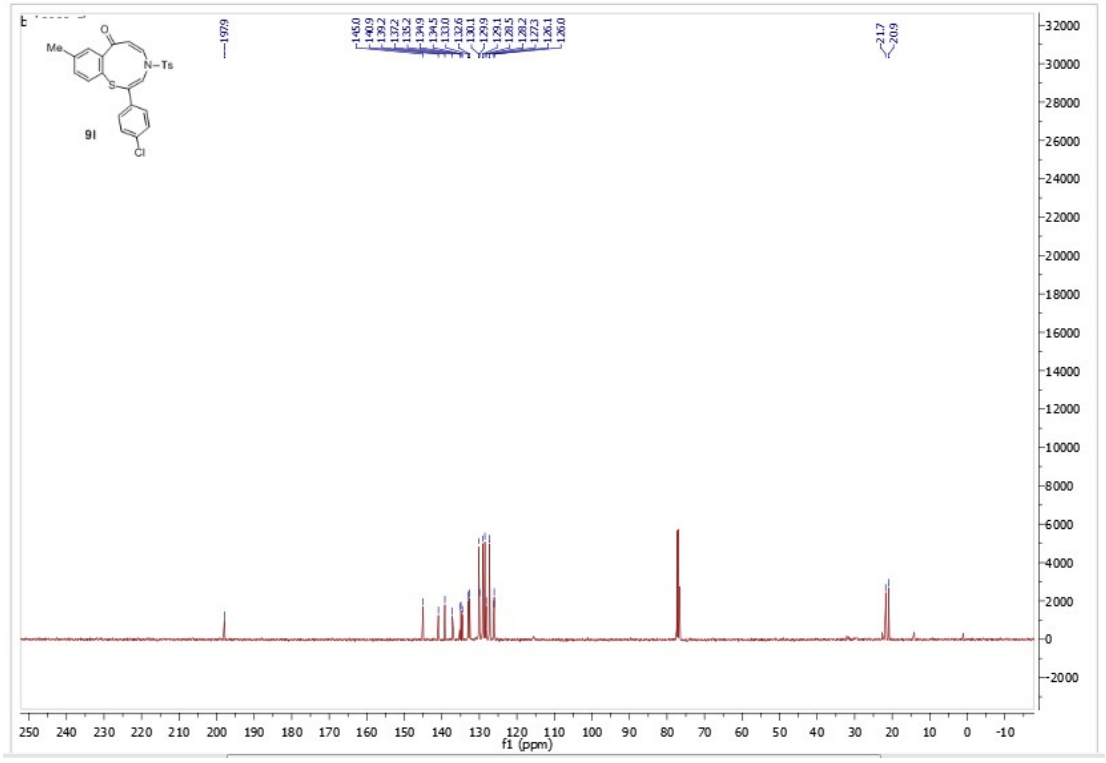

9j
Me
N–Ts
S
OMe
OMe
f1 (ppm)

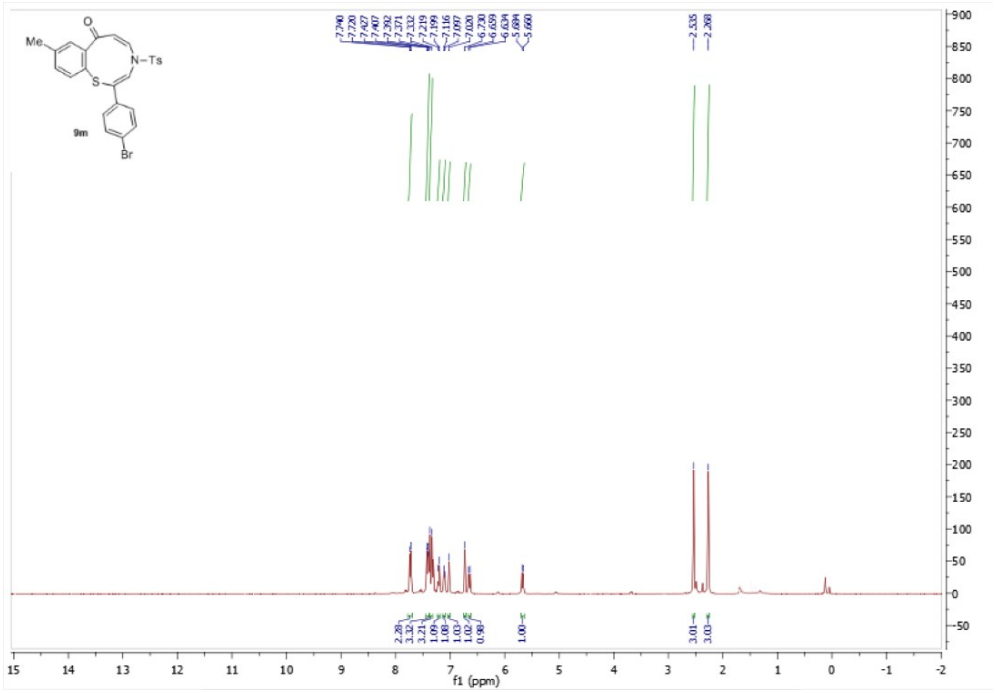

9j
Me
N–Ts
S
OMe
OMe
198.3
150.0
149.5
144.8
141.1
139.1
138.9
134.7
132.9
132.4
130.1
129.9
128.8
127.4
126.8
126.1
126.1
120.8
111.1
110.7
55.9
55.8
21.7
20.9
f1 (ppm)

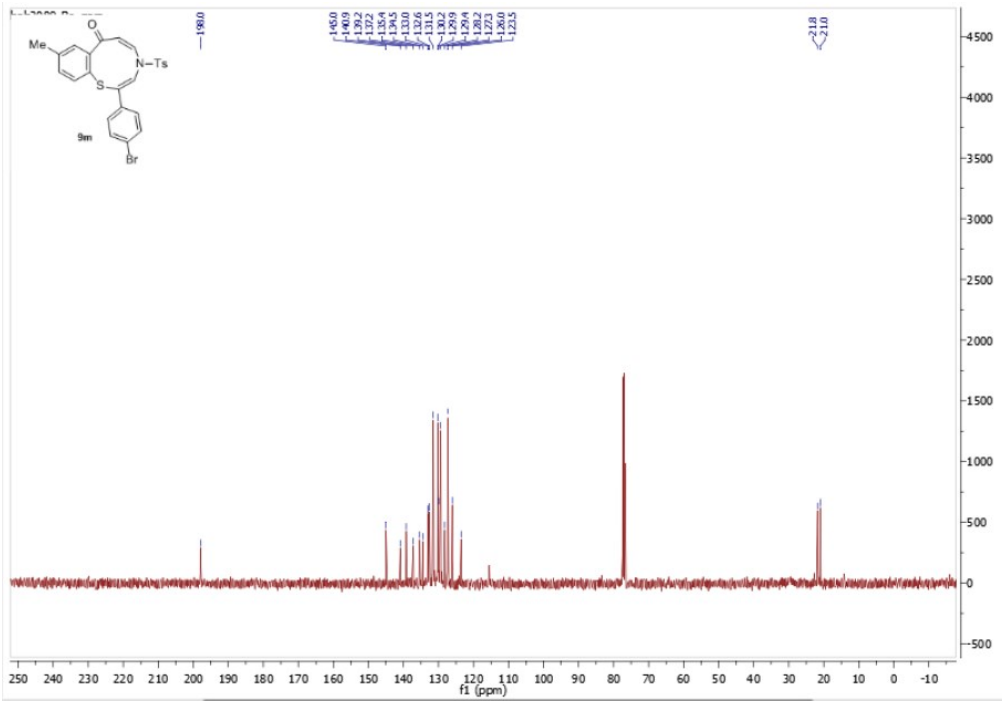

9k
Me
N–Ts
S
Me
7.742
7.722
7.402
7.394
7.215
7.205
7.186
7.167
7.160
7.154
7.141
7.129
7.123
7.024
7.021
7.015
7.010
7.007
6.396
6.372
6.449
5.869
5.840
2.510
2.329
2.281
2.29
3.07
2.27
1.21
3.32
2.05
1.14
0.99
1.00
3.03
3.16
3.05
f1 (ppm)

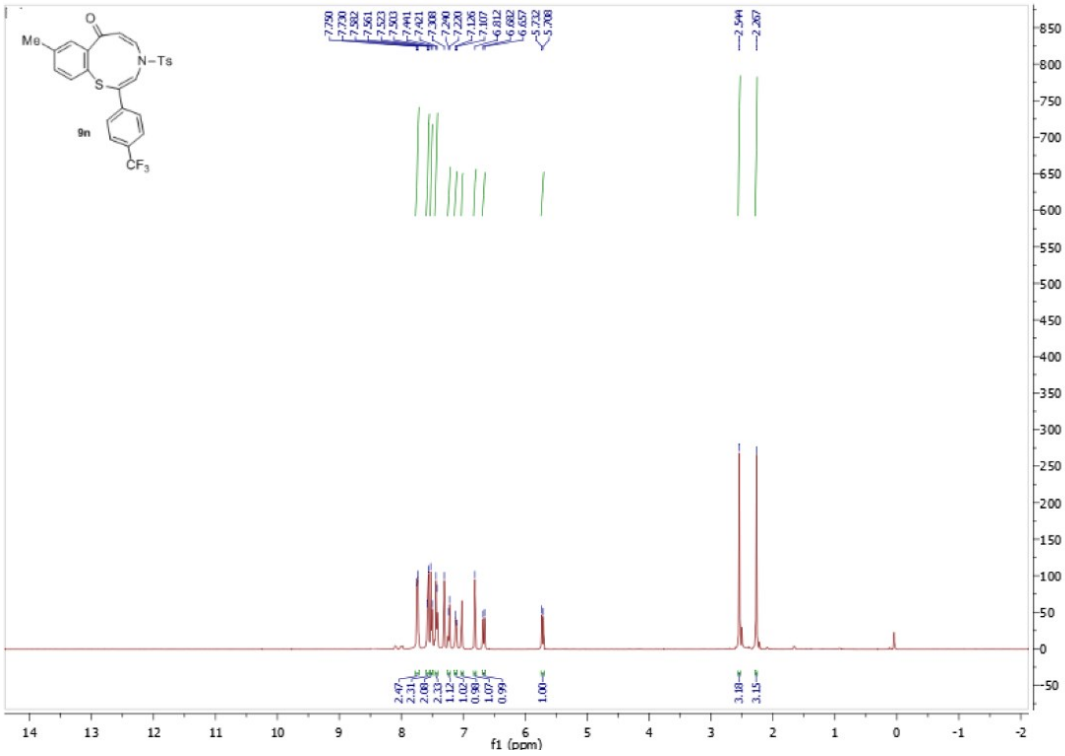

9k
Me
N–Ts
S
Me
197.9
144.8
139.3
138.3
136.2
133.8
132.9
130.3
130.2
130.1
129.9
129.8
128.6
127.5
126.5
126.2
125.5
21.7
21.0
20.1
f1 (ppm)

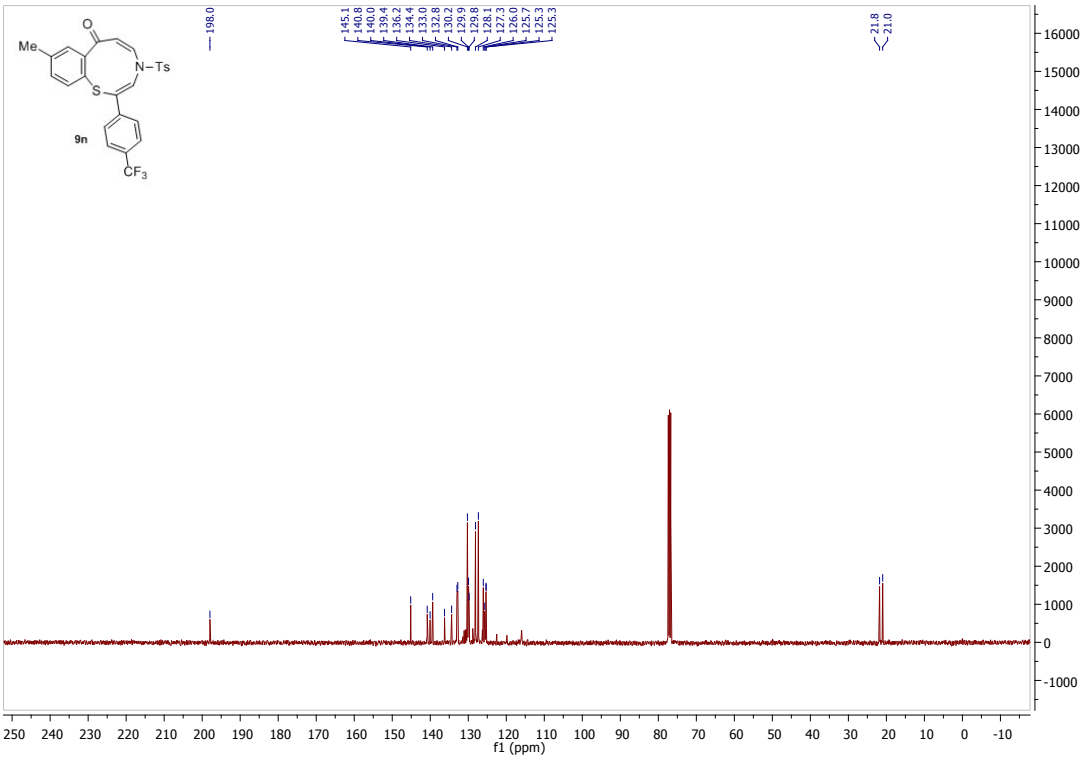

9l
Me
N–Ts
S
Cl
f1 (ppm)

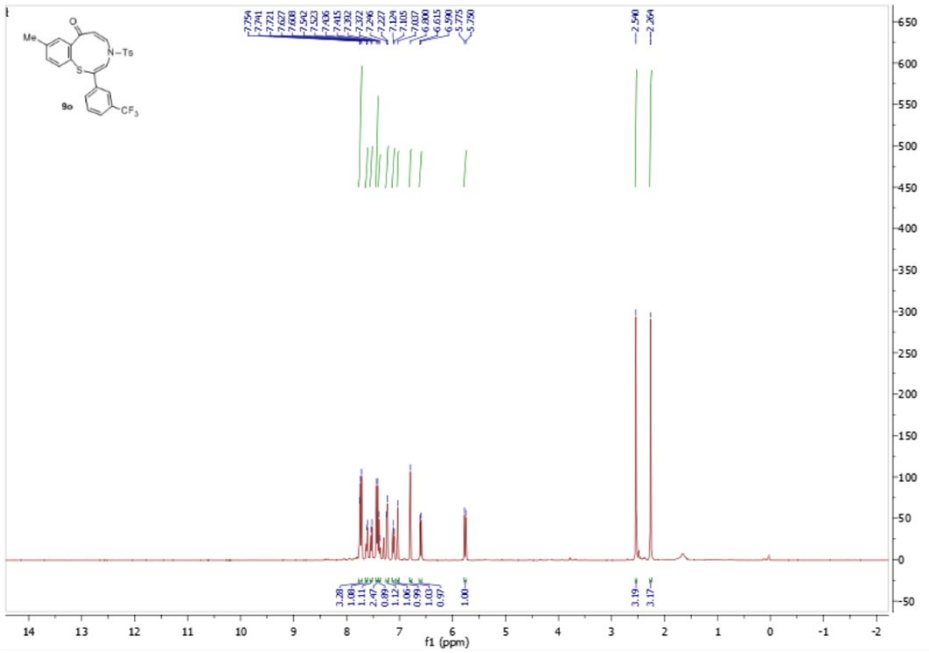

9l
Me
N–Ts
S
Cl
f1 (ppm)

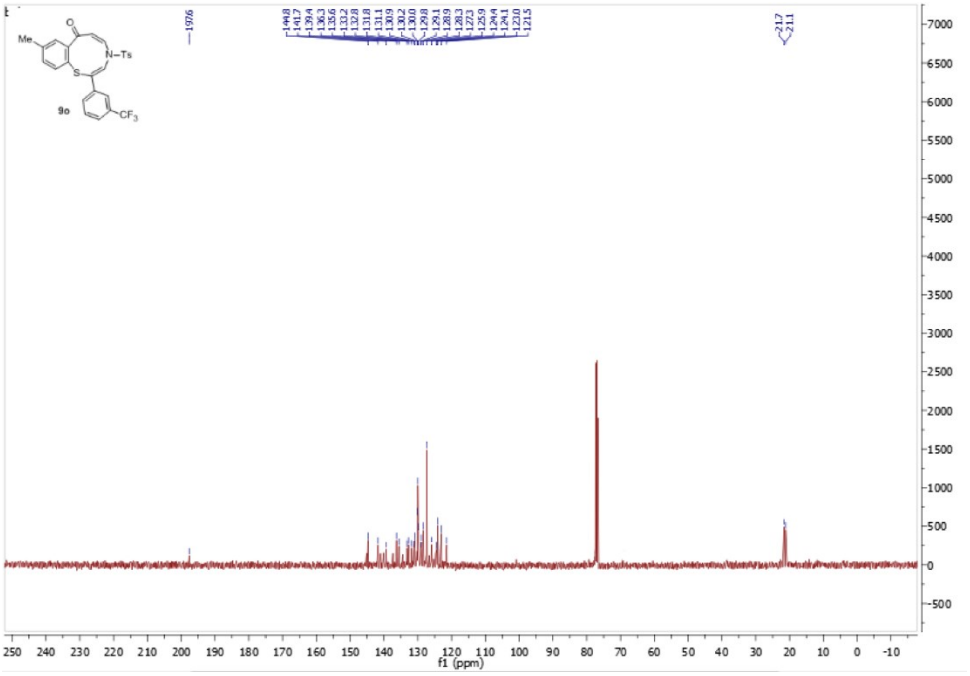

Me
N–Ts
S
O
9m
Br
f1 (ppm)

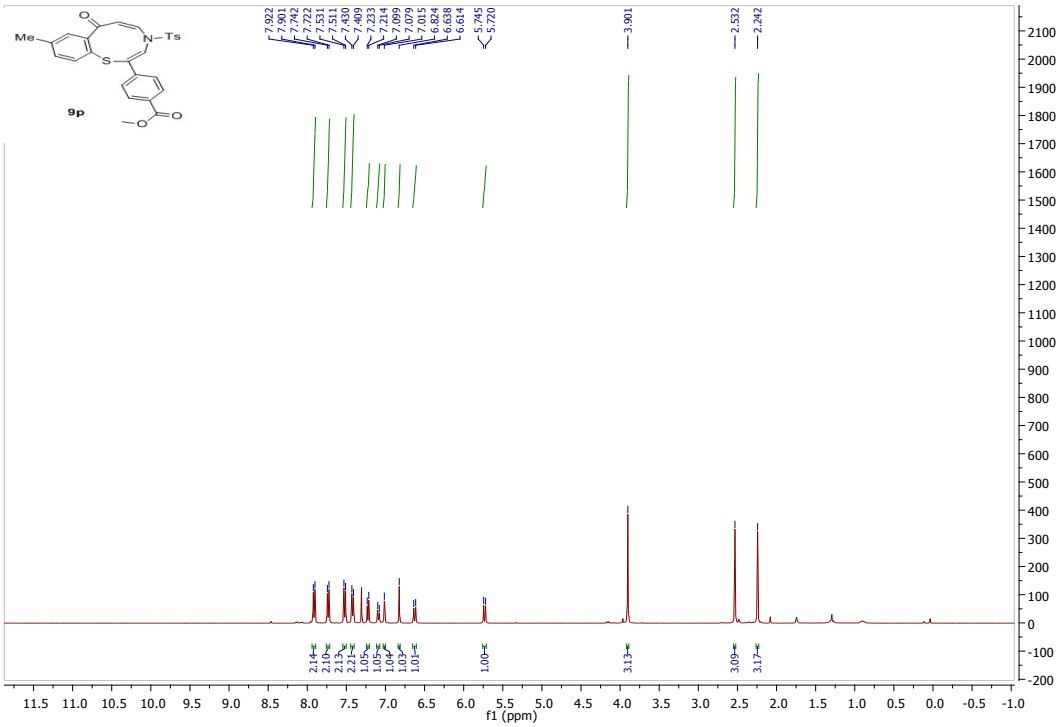

Me
N–Ts
S
O
9m
Br
f1 (ppm)

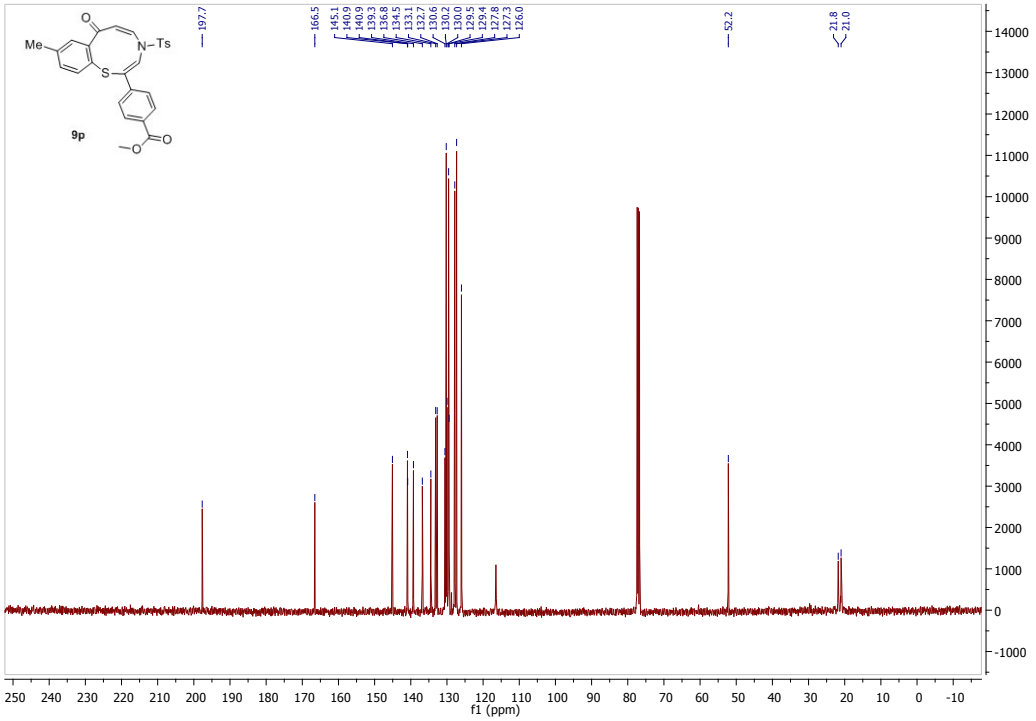

Me
O
N–Ts
S
9n
CF3
7.790
7.730
7.582
7.561
7.523
7.503
7.441
7.421
7.308
7.240
7.220
7.126
7.107
6.812
6.682
6.657
5.732
5.708
2.544
2.267
2.47
2.31
2.08
2.33
1.12
1.02
0.98
1.07
0.99
1.00
3.18
3.15
f1 (ppm)

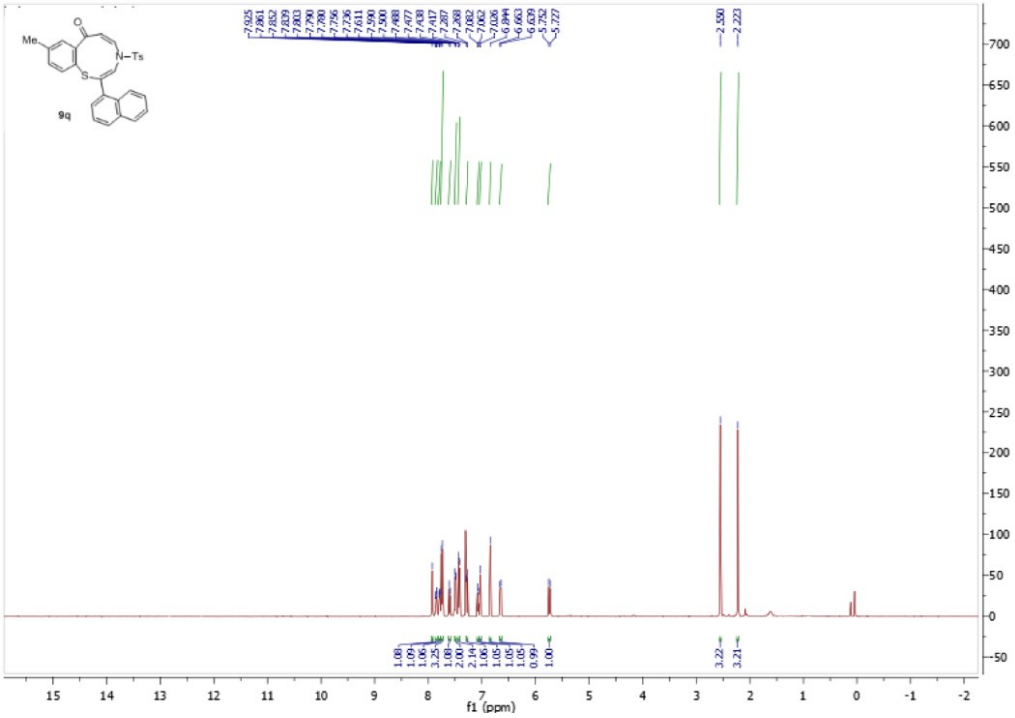

Me
O
N–Ts
S
9n
CF3
198.0
145.1
140.8
140.0
139.4
136.2
134.4
133.0
132.8
130.2
129.9
129.8
128.1
127.3
126.0
125.7
125.3
125.3
21.8
21.0
f1 (ppm)

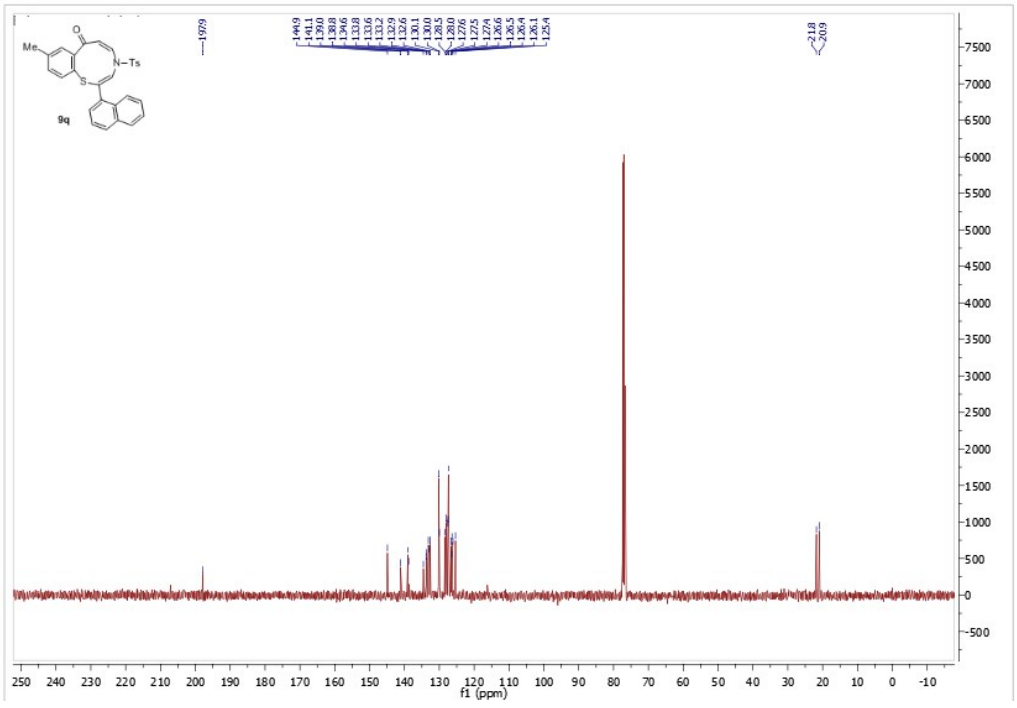

Me
N–Ts
S
9o
CF3
7.754
7.741
7.721
7.627
7.608
7.542
7.523
7.406
7.385
7.372
7.246
7.227
7.184
7.165
7.037
6.800
6.615
6.596
5.775
5.750
2.540
2.264
3.28
1.00
1.11
2.47
0.89
1.12
1.46
0.99
1.03
0.97
1.00
3.19
3.17
f1 (ppm)

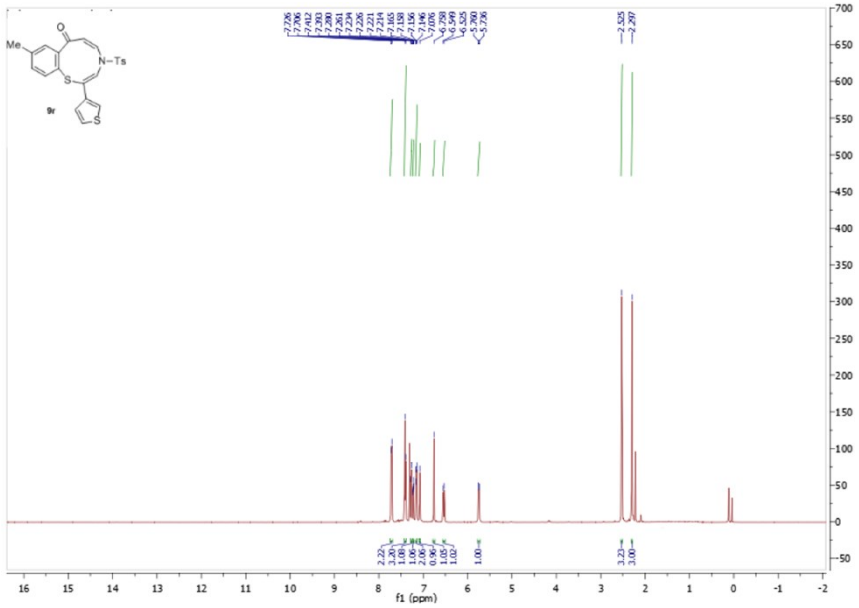

Me
N–Ts
S
9o
CF3
197.6
149.8
149.7
139.4
136.3
135.6
133.2
133.0
131.8
131.1
130.9
130.2
130.0
129.9
129.1
128.9
128.3
127.1
125.9
124.4
124.1
122.0
121.5
21.7
21.1
f1 (ppm)

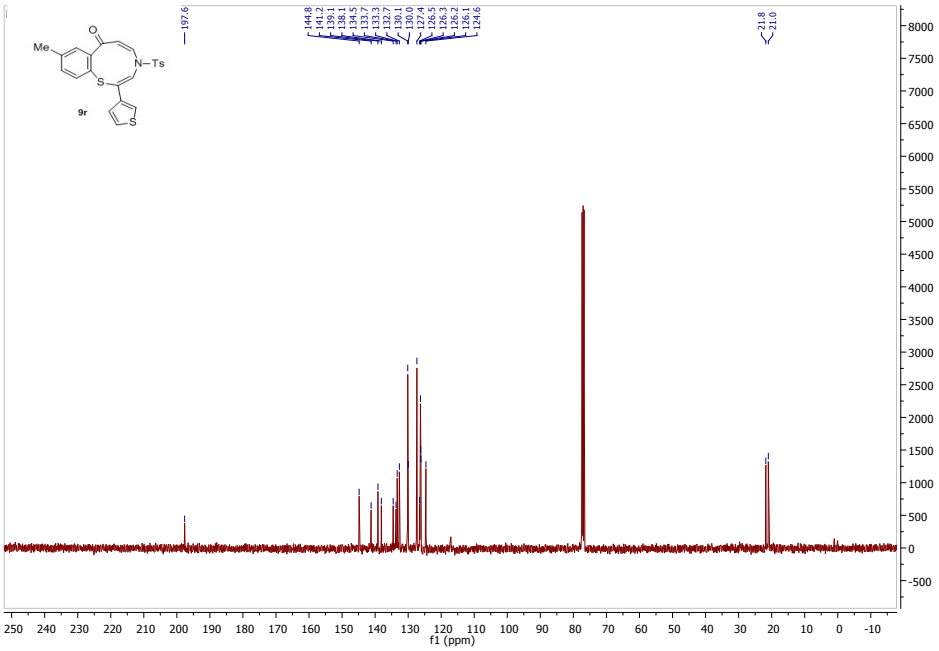

9p
7.922
7.901
7.742
7.722
7.531
7.511
7.430
7.409
7.233
7.214
7.099
7.079
7.015
6.824
6.638
6.614
5.745
5.720
3.901
2.532
2.242
f1 (ppm)

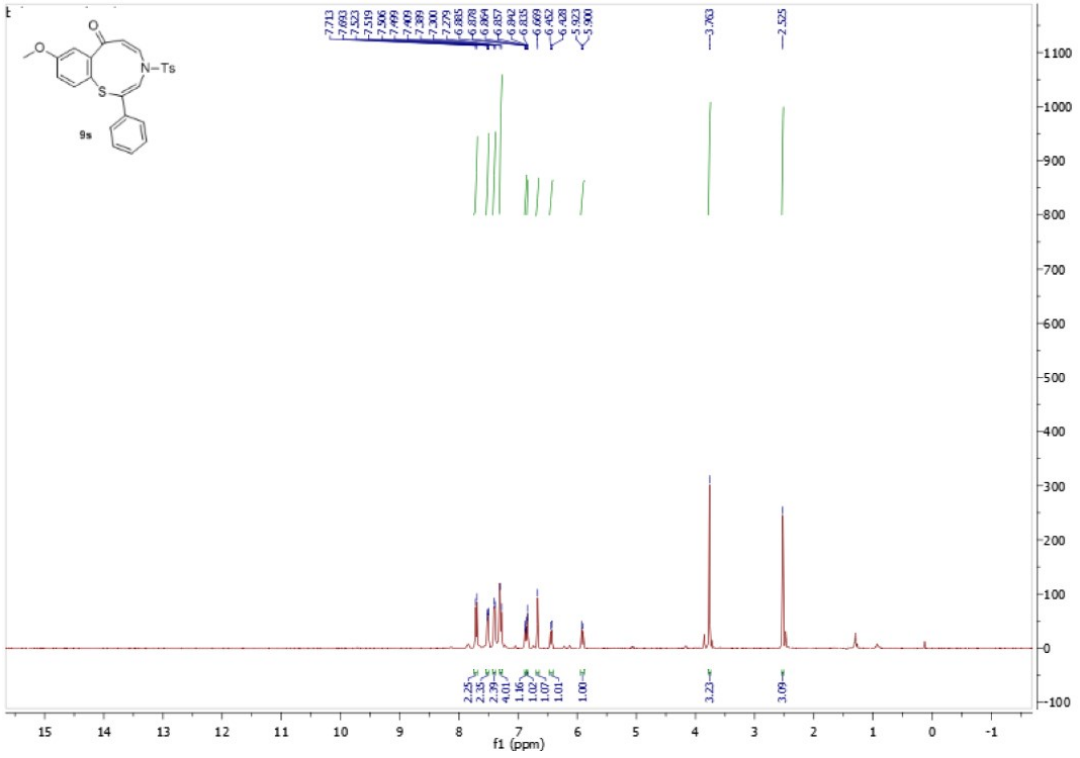

9p
197.7
166.5
145.1
140.9
140.0
139.3
136.8
134.5
133.1
132.7
130.6
130.2
130.0
129.5
129.4
127.8
127.3
126.0
52.2
21.8
21.0
f1 (ppm)

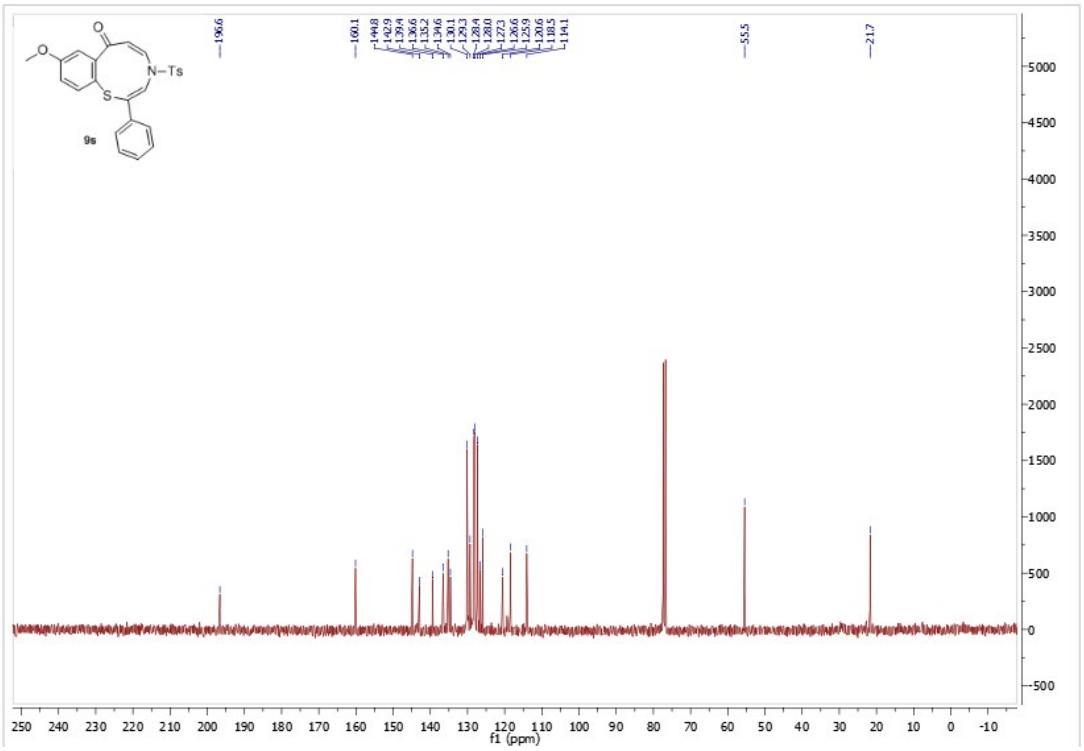

Me
N–Ts
9q
f1 (ppm)

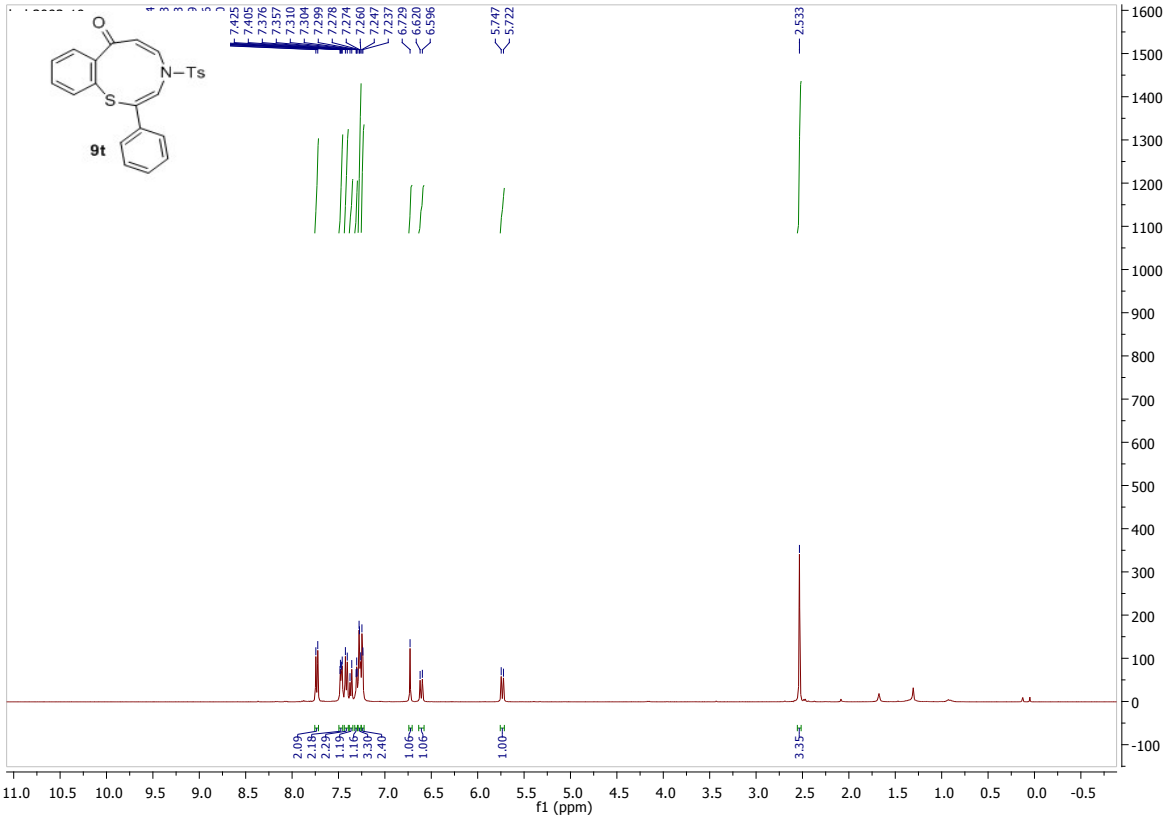

Me
N–Ts
9q
f1 (ppm)

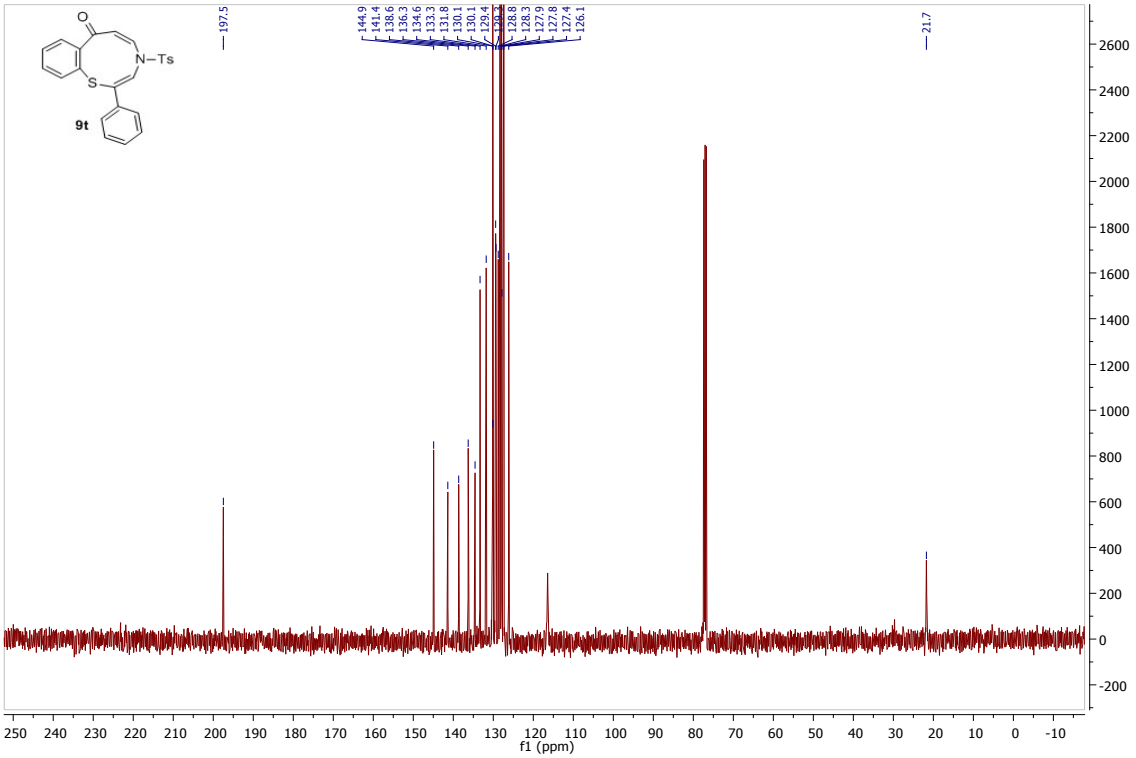

Me
N–Ts
S
9r
f1 (ppm)

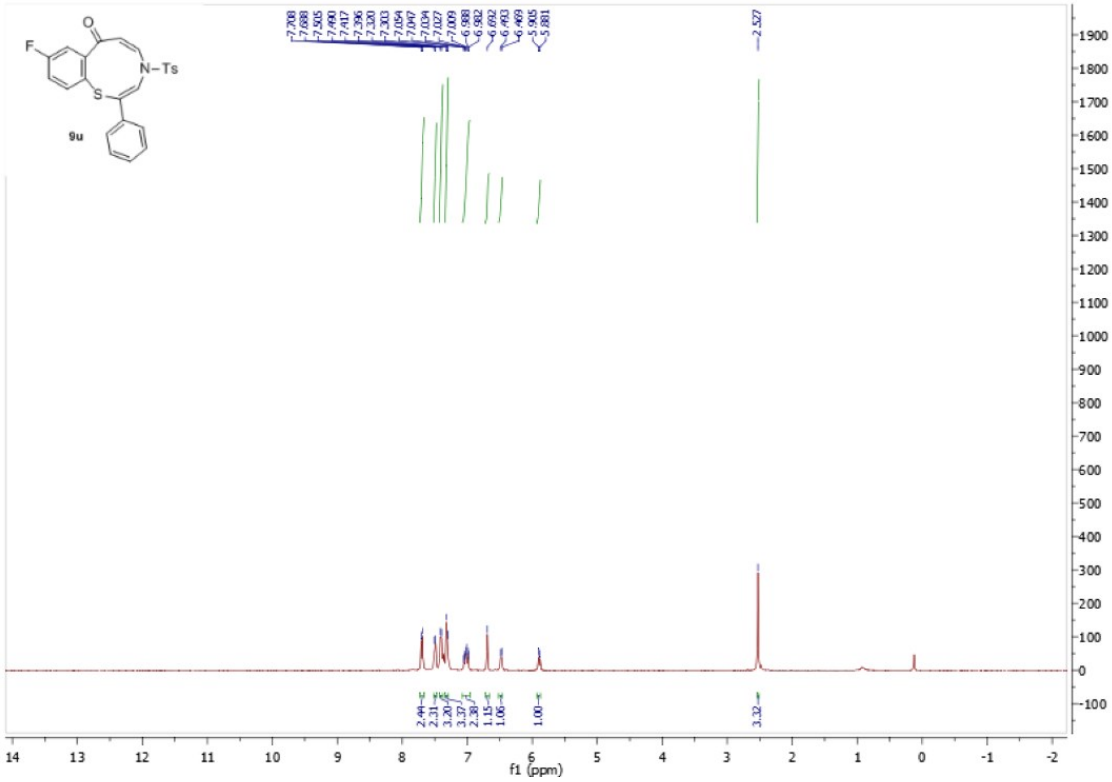

Me
N–Ts
S
9r
f1 (ppm)

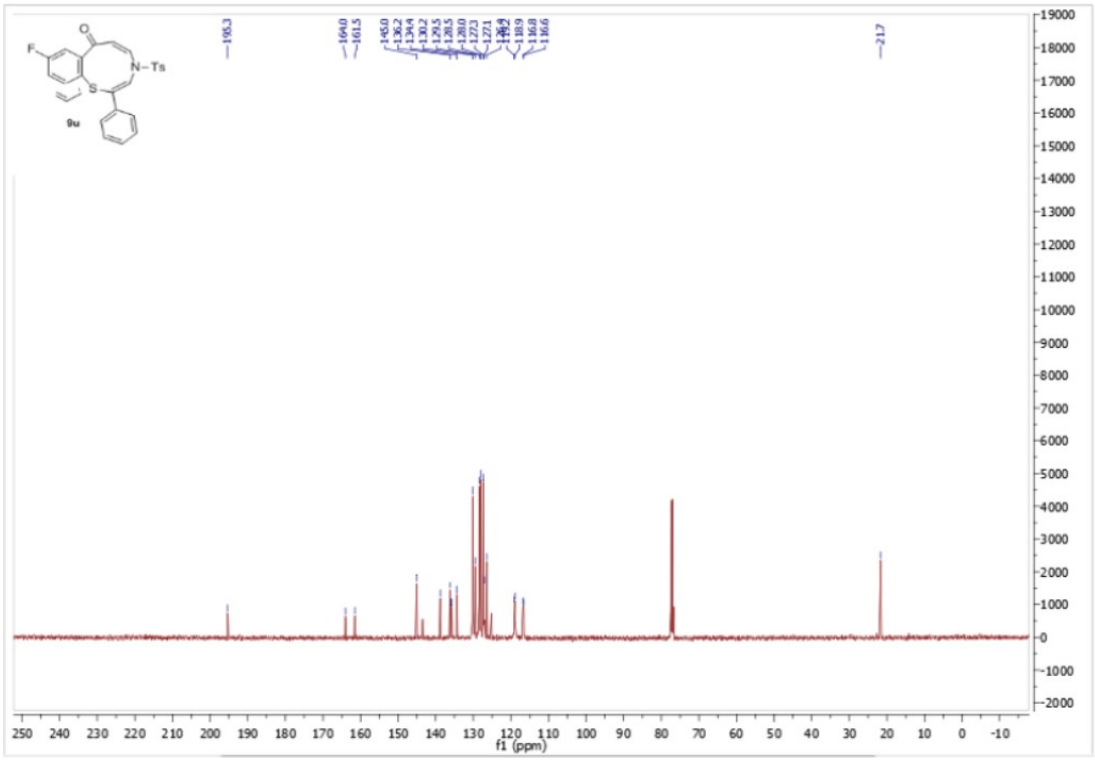

9s
N–Ts
7.713
7.693
7.553
7.536
7.506
7.499
7.409
7.389
7.300
7.279
6.885
6.878
6.864
6.857
6.842
6.635
6.469
6.452
6.428
5.923
5.900
3.763
2.525
f1 (ppm)

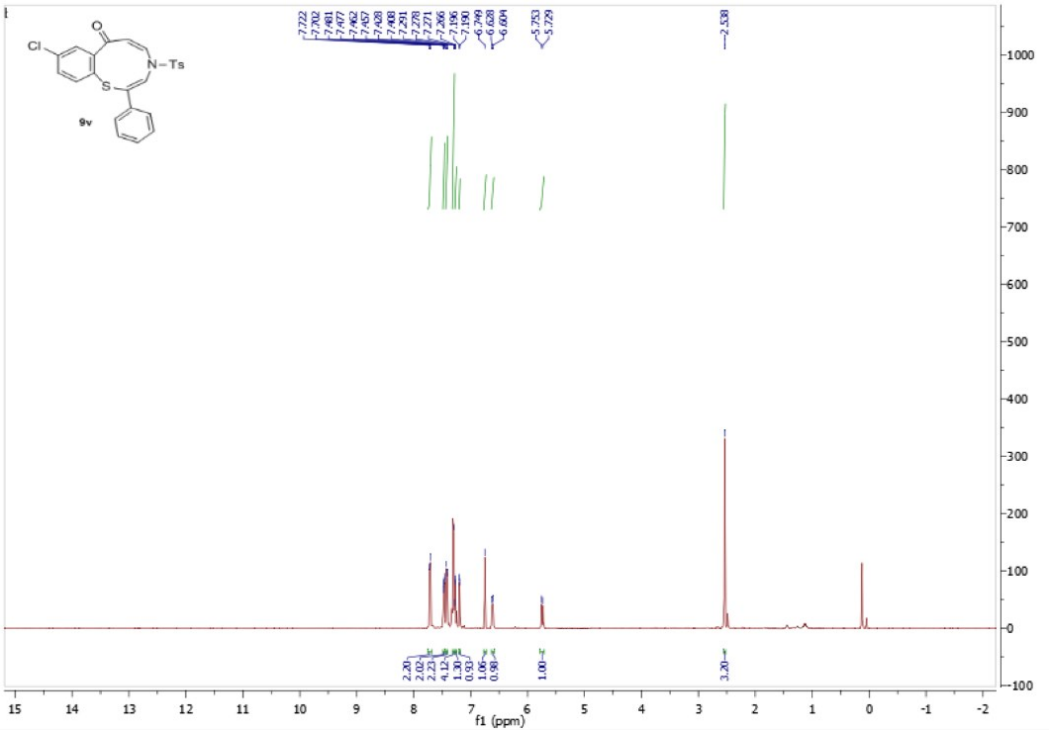

9s
N–Ts
196.6
160.1
144.8
142.9
139.4
136.6
135.2
134.6
130.1
129.3
128.4
128.0
127.3
126.6
125.9
120.6
118.5
114.1
55.5
21.7
f1 (ppm)

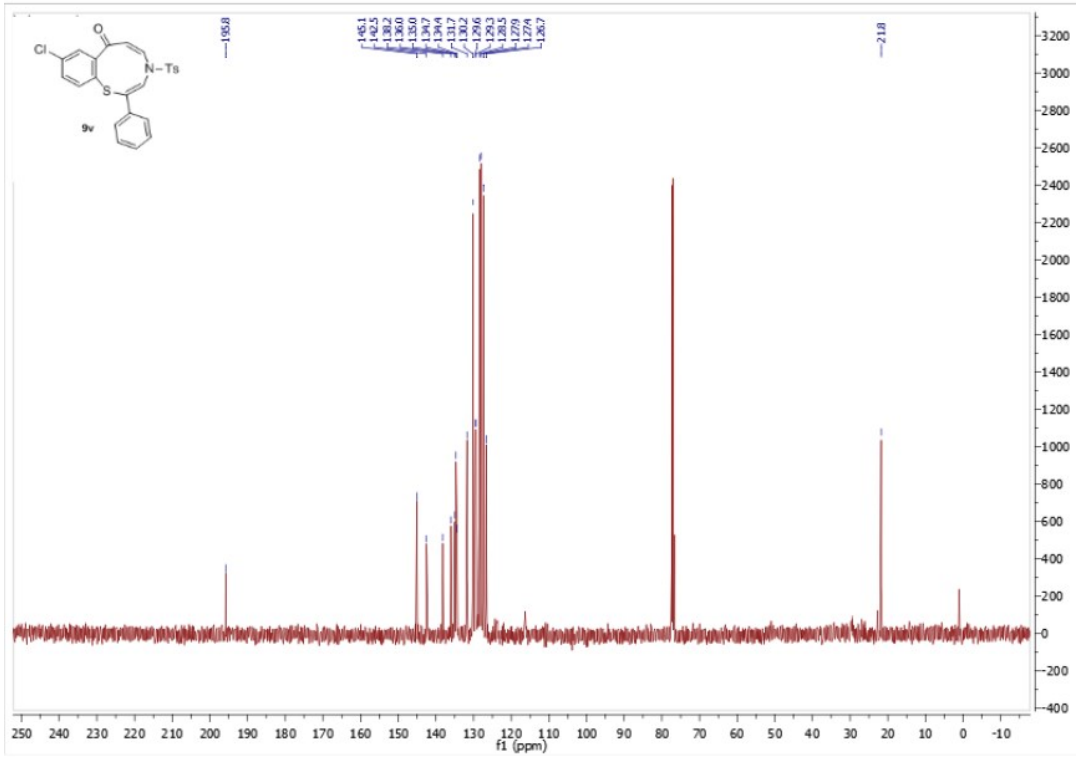

9t
N–Ts
7.425
7.405
7.376
7.357
7.310
7.304
7.299
7.278
7.274
7.260
7.247
7.237
6.729
6.620
6.596
5.747
5.722
2.533
2.09
2.18
2.29
1.19
1.16
3.30
2.40
1.06
1.06
1.00
3.35
f1 (ppm)

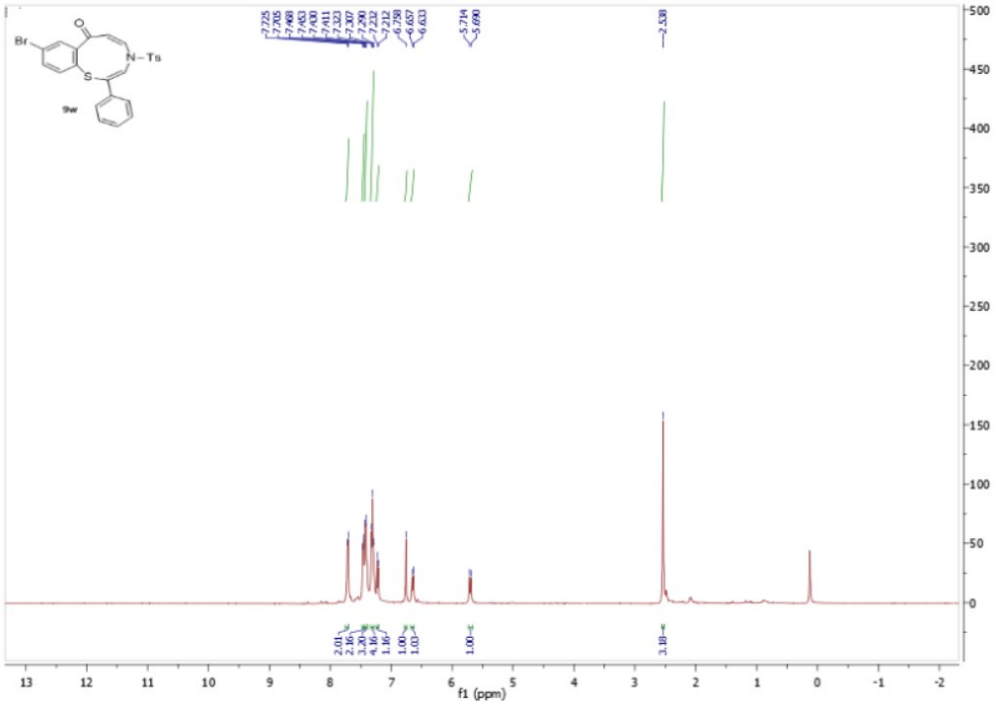

9t
N–Ts
197.5
144.9
141.4
138.6
136.3
134.6
133.3
131.8
130.1
130.1
129.4
128.8
128.3
127.9
127.8
127.4
126.1
21.7
f1 (ppm)

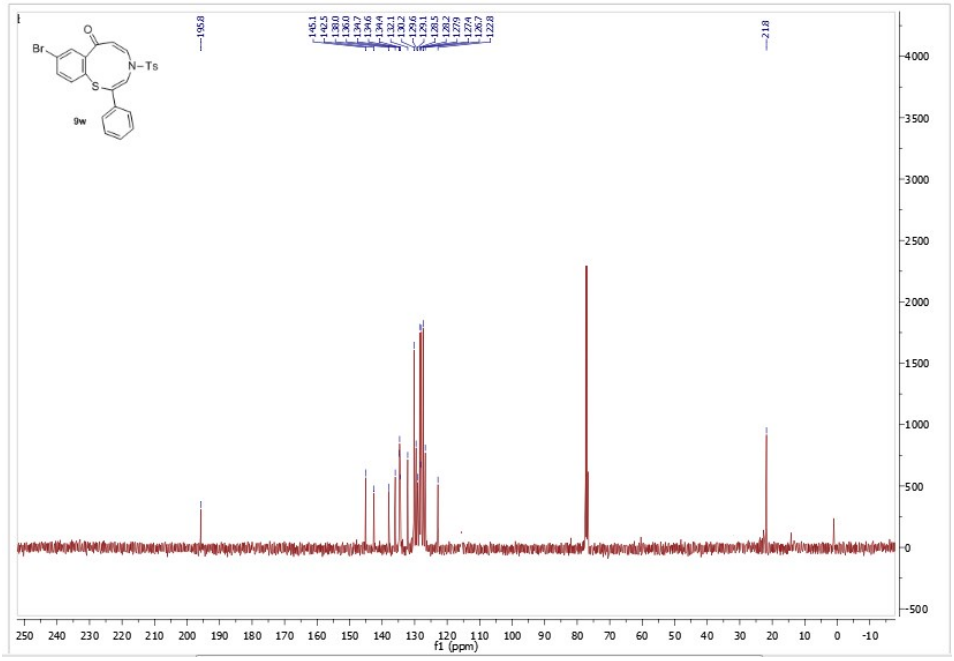

9u
f1 (ppm)

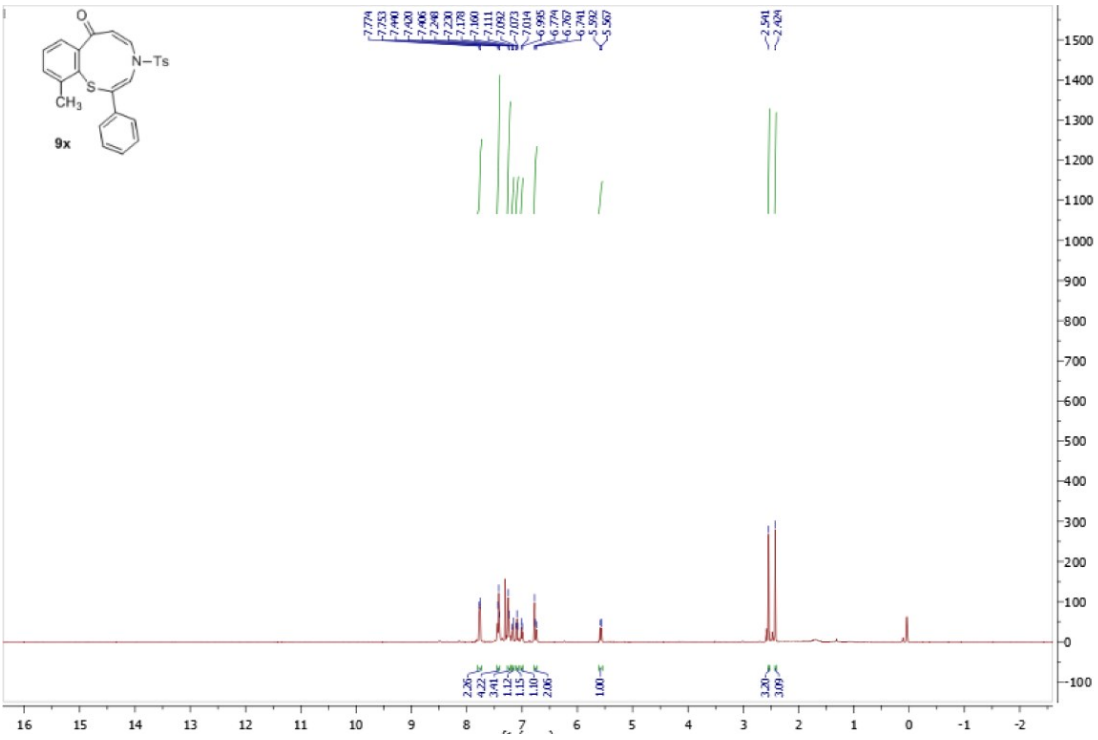

9u
f1 (ppm)

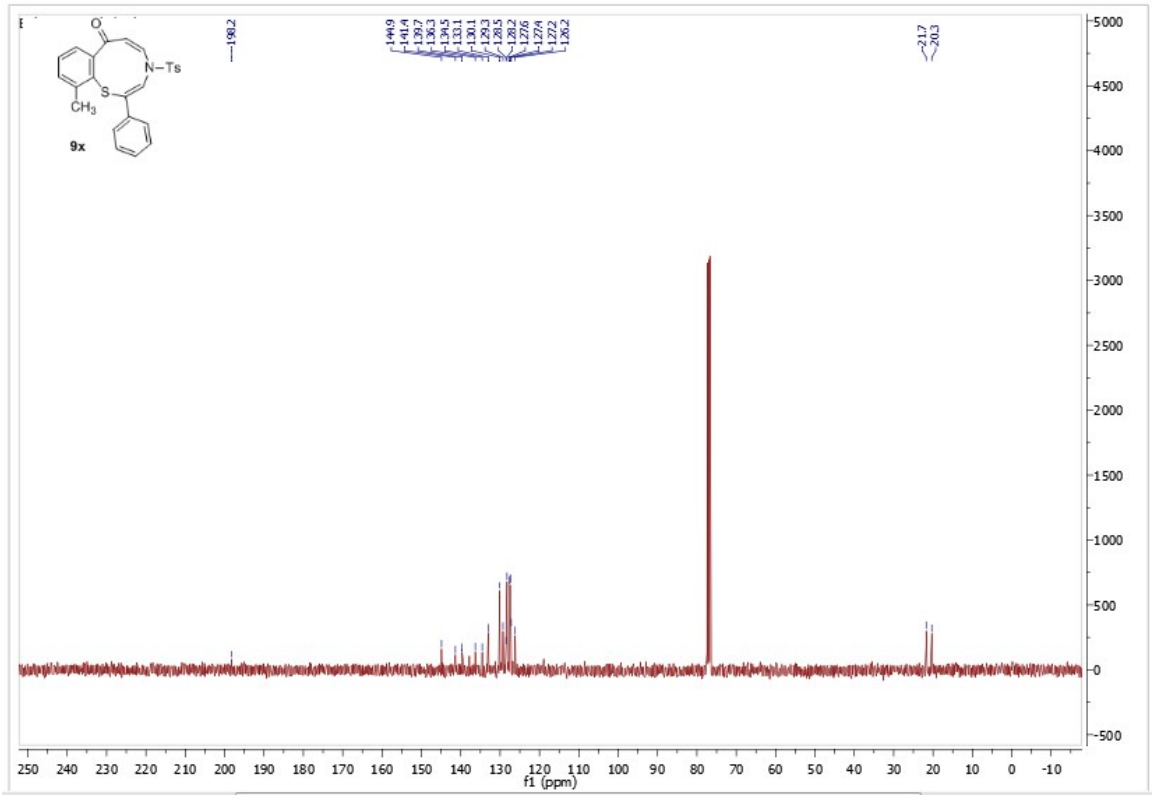

9v
7.722
7.702
7.481
7.477
7.462
7.457
7.408
7.291
7.278
7.271
7.266
7.196
7.190
6.629
6.628
6.604
5.753
5.729
2.538
2.20
2.02
2.23
4.12
1.30
0.93
1.06
0.98
1.00
3.20
f1 (ppm)

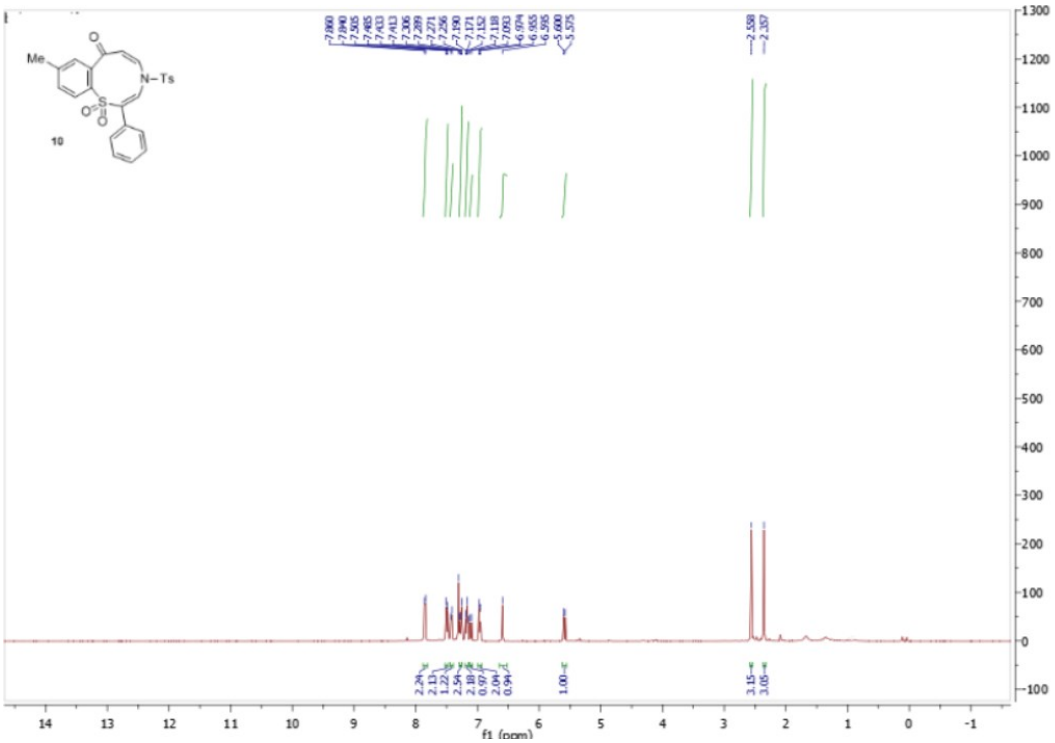

9v
195.8
145.1
142.5
138.2
136.0
135.0
134.7
134.4
131.7
130.2
129.6
129.3
128.5
127.9
127.4
126.7
21.8
f1 (ppm)

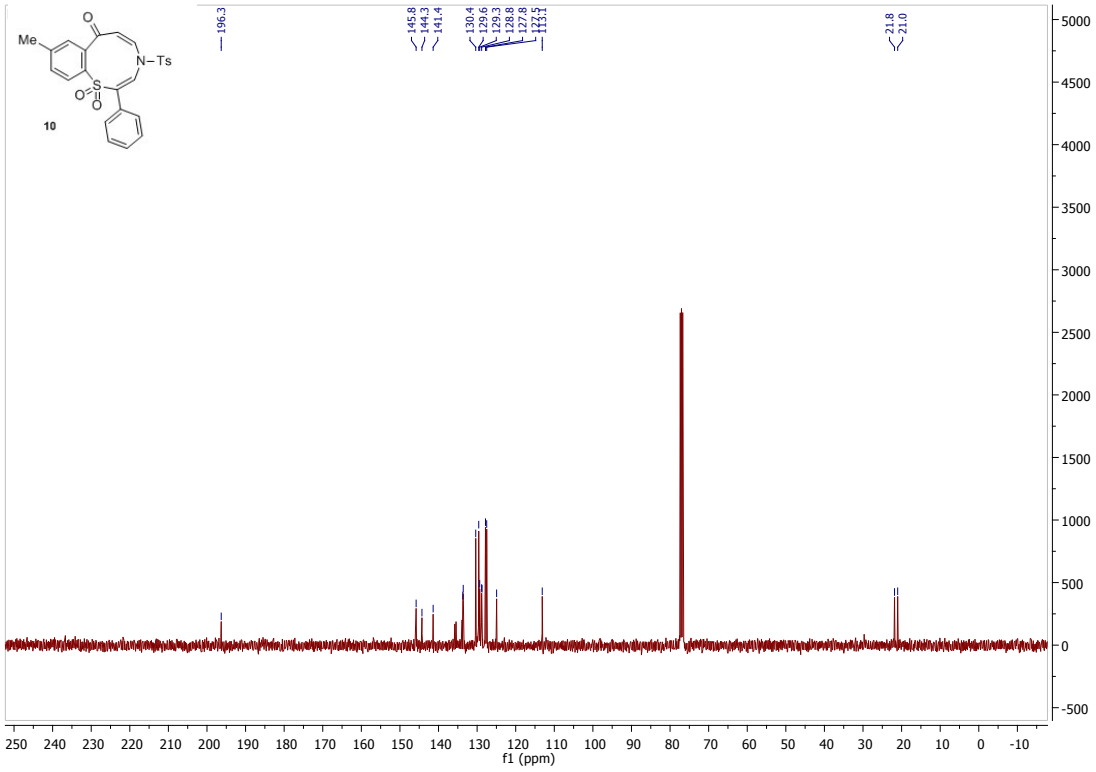

9w
f1 (ppm)

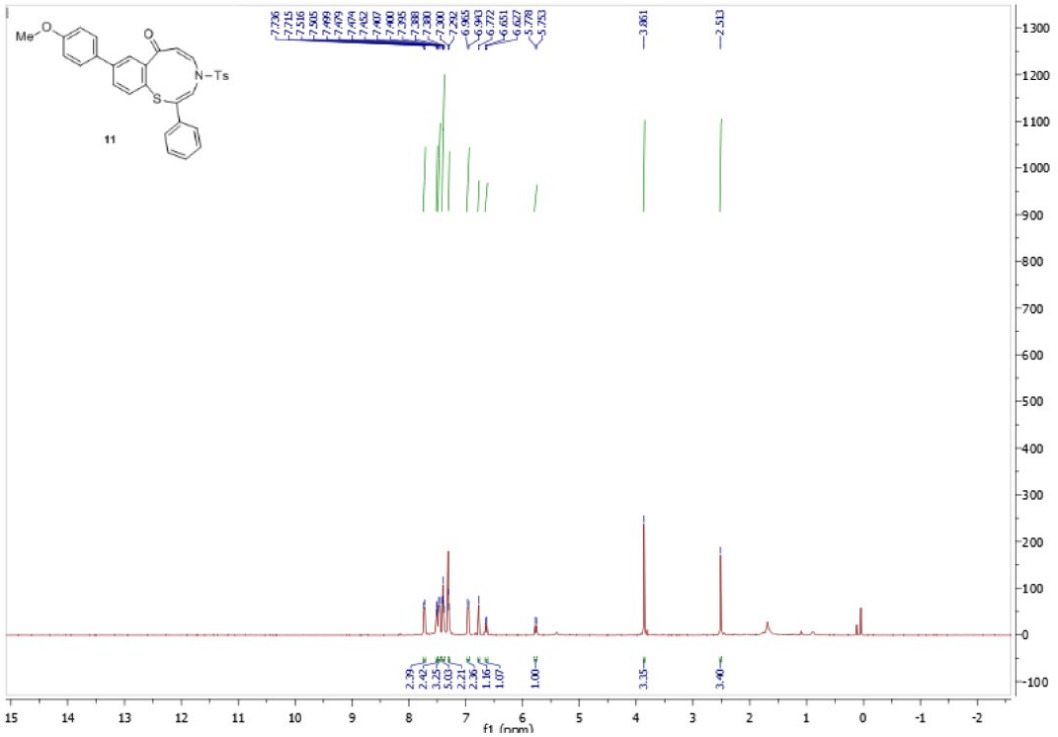

9w
f1 (ppm)

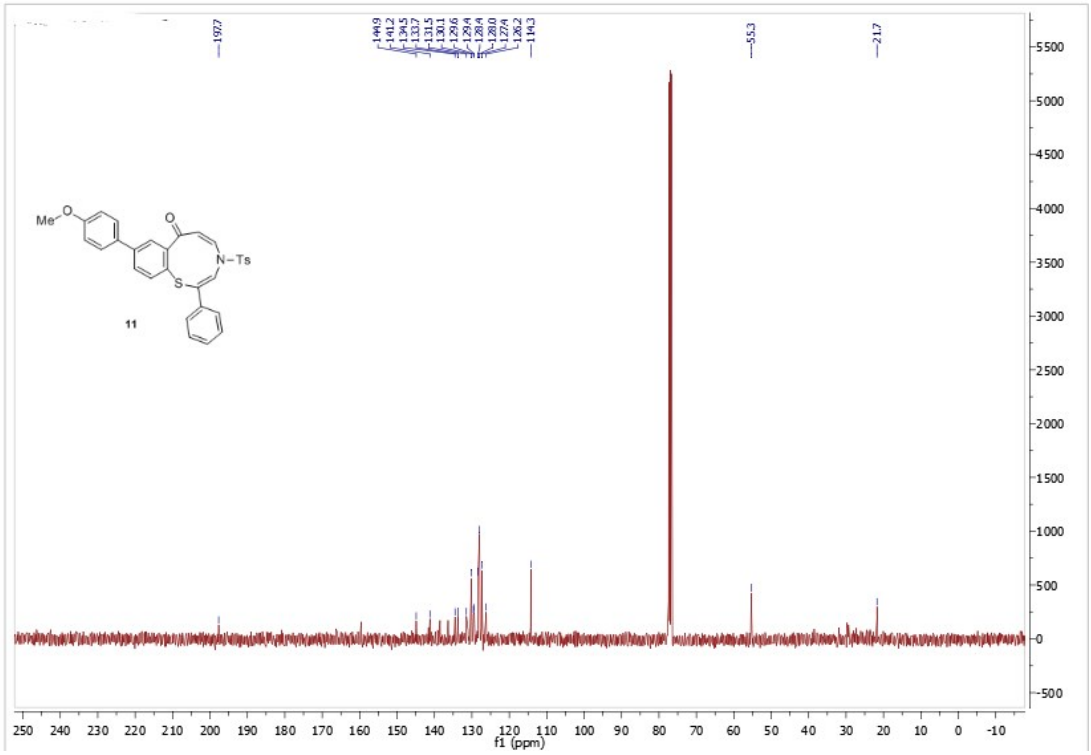

9x
N–Ts
CH3
S
O
7.774
7.753
7.440
7.400
7.406
7.248
7.230
7.178
7.160
7.111
7.092
7.073
7.014
6.998
6.779
6.767
6.741
5.592
5.567
2.541
2.424
2.26
4.21
3.41
1.12
1.15
1.10
2.06
1.00
3.20
3.09


9x
N–Ts
CH3
S
O
190.2
144.9
141.4
139.7
136.3
134.5
133.1
130.1
129.3
128.5
128.2
127.6
127.4
127.2
126.2
21.7
20.3
f1 (ppm)


Me
N–Ts
10
f1 (ppm)


Me
N–Ts
10
f1 (ppm)


Me
O
N–Ts
S
11
7.736
7.715
7.516
7.505
7.499
7.479
7.474
7.452
7.407
7.400
7.395
7.388
7.380
7.370
7.290
6.965
6.943
6.772
6.651
6.627
5.778
5.753
3.861
2.513
2.39
2.42
3.25
5.03
2.21
2.36
1.16
1.07
1.00
3.35
3.40
f1 (ppm)


Me
O
N–Ts
S
11
197.7
144.9
141.2
134.5
133.7
131.5
131.1
129.6
129.4
128.4
128.0
127.4
126.2
114.3
55.3
21.7
f1 (ppm)